

# Workflow Events and Specifications for RESULT Integration Software



The information in this publication is provided for reference only. All information contained in this publication is believed to be correct and complete. Thermo Fisher Scientific shall not be liable for errors contained herein nor for incidental or consequential damages in connection with the furnishing, performance or use of this material. All product specifications, as well as the information contained in this publication, are subject to change without notice.

This publication may contain or reference information and products protected by copyrights or patents and does not convey any license under our patent rights, nor the rights of others. We do not assume any liability arising out of any infringements of patents or other rights of third parties.

We make no warranty of any kind with regard to this material, including but not limited to the implied warranties of merchantability and fitness for a particular purpose. Customers are ultimately responsible for validation of their systems.

© 2004-2011 Thermo Fisher Scientific Inc. All rights reserved. No part of this publication may be stored in a retrieval system, transmitted, or reproduced in any way, including but not limited to photocopy, photograph, magnetic or other record, without our prior written permission.

For Technical Support, please contact:

Thermo Fisher Scientific

5225 Verona Road

Madison, WI 53711-4495 U.S.A.

Telephone: 1 800 532 4752

E-mail: [us.techsupport.analyze@thermofisher.com](mailto:us.techsupport.analyze@thermofisher.com)

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

For International Support, please contact:

Thermo Fisher Scientific

Telephone: +1 608 273 5017

E-mail: [support.madison@thermofisher.com](mailto:support.madison@thermofisher.com)

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

Microsoft, Windows, and Excel are trademarks or registered trademarks of Microsoft Corporation in the United States and/or other countries. Intel and Pentium are trademarks or registered trademarks of Intel Corporation in the United States and/or other countries. Adobe and Reader are trademarks or registered trademarks of Adobe Systems Incorporated in the United States and/or other countries. Spectralon is a trademark or registered trademark of Labsphere, Inc. in the United States and/or other countries. Viton and Tedlar are trademarks or registered trademarks of Du Pont in the United States and/or other countries. All other trademarks are the property of Thermo Fisher Scientific Inc. and its subsidiaries.

# Contents

<b>Chapter 1</b>	<b>Overview .....</b>	<b>1</b>
<b>Chapter 2</b>	<b>Simple Workflow Events .....</b>	<b>3</b>
	Adding simple events to workflows .....	4
	Archive events .....	7
	Calculate events .....	23
	Check events .....	32
	Clear events.....	38
	Collect events.....	43
	Collect Dual Tablet events .....	55
	Collect Multi- Channel events .....	64
	Compare events .....	75
	Delay events.....	82
	Load Spectrum events .....	84
	Measure events.....	86
	Process events.....	91
	Read from I/O events.....	99
	Read from Excel events .....	103
	Report events .....	106
	Report to OPC events.....	111
	Report To Spectrum events.....	116
	Report To Text File events.....	125
	Request events.....	131
	Run Exe events.....	138
	Store events.....	140
	Write To I/O events .....	145
	Write To Excel events .....	151
<b>Chapter 3</b>	<b>Structural Workflow Events .....</b>	<b>155</b>
	Adding structural events to workflows.....	157
	Perform events .....	158
	Repeat events .....	161
	Perform-If events .....	168
	Perform-While events .....	172
	StartStop events .....	177
<b>Chapter 4</b>	<b>Device-Specific Workflow Events.....</b>	<b>180</b>
	Position autosampler events .....	182
	Configure temperature/pressure events.....	189

<b>Chapter 5</b>	<b>Sequence Module Events .....</b>	<b>194</b>
	Adding sequence events to a workflow .....	196
	Run sequence events .....	197
	Collect sequence events .....	204
<b>Chapter 6</b>	<b>Workflow Specifications.....</b>	<b>216</b>
	Logic specifications .....	218
	Measurement specifications.....	235
	General specifications.....	263
	Report specifications .....	277
	Report format specifications.....	286
	Sample specifications.....	346
	Background specifications .....	392
	StartStop specifications .....	425
	Correction specifications .....	430
	<b>Index .....</b>	<b>444</b>

# Chapter 1 Overview

A functional workflow is comprised of workflow events and their associated specifications. Workflow events specify tasks that will be carried out when the workflow is run. The software carries out the events in the order in which they appear in the workflow navigation frame when you display the workflow in RESULT Integration.

Workflow specifications define how certain tasks will be carried out. The collect event, for example, instructs the system to collect a spectrum at a given point in the workflow, while the associated sample and background specifications allow you to configure data collection for a particular sampling technique.

RESULT Integration is a tool for creating and testing workflows. You may add and delete workflow events and their associated specifications, arrange events in any order and place them in groups. Grouped events can be performed one event at a time, repeated, or performed based on the results of a conditional test.

This section describes the events available for use in workflows created in RESULT Integration. It also details all the specifications that are available for use in workflows. The major chapters in this section are:

- **Simple Workflow Events.** This chapter describes the simple events available for use in workflows created in RESULT Integration. Simple workflow events carry out a single task, such as collecting a spectrum, measuring the spectrum, or using collected or measured data to create sample reports. They are the building blocks that define the overall task the workflow will perform.
- **Structural Workflow Events.** This chapter describes the structural workflow events available in RESULT Integration. Structural events operate on a string of events positioned in a group, allowing you to perform or repeat the events in the group or to perform them based on the results of a conditional test. Structural events allow you to control when and how certain workflow tasks will be performed.

- **Device-Specific Workflow Events.** This chapter details the device-specific workflow events available in RESULT Integration. Device-specific events allow the workflow to control a particular hardware device such as an autosampler or temperature controller.
- **Sequence Module Events.** This chapter describes the events included in the sequence module. The sequence module is an option for RESULT Integration. Sequence module events allow you to use RESULT software to collect and process a series of spectra at regular intervals over a specified period of time.
- **Workflow Specifications.** This chapter describes the workflow specifications available in RESULT Integration. Workflow specifications define how certain workflow events will be carried out. The collect event, for example, instructs the system to collect a spectrum at a given point in the workflow, while the associated sample and background specifications allow you to customize data collection for a given sampling technique.

Anyone who is responsible for developing workflows in RESULT Integration should read this section. If you want to learn how to add, delete and arrange events to create functional workflows, or how to link specifications to workflow events, see “Chapter 2 Creating and Editing Workflows” in your “RESULT Integration Software User Guide.” If you want to learn about the production application for RESULT, called RESULT Operation, or the application for viewing sequence data files, called RESULT Data View, see the document with that name.

## Chapter 2 Simple Workflow Events

Simple workflow events carry out a single task, such as collecting a spectrum, measuring the spectrum, or using collected or measured data to create sample reports. They are the building blocks that define the overall task the workflow is to perform. This section lists each simple workflow event and details its application and use.

For information about structural events, see “Chapter 2 Structural Workflow Events.” Events that can be used to control a hardware device are explained in “Chapter 3 Device-Specific Events.” To learn about events that can be used to collect and process spectral data continuously over a specified period, see “Chapter 4 Sequence Module Events.” To learn about adding specifications to workflows and linking specifications to workflow events, see “Chapter 5 Workflow Specifications.”

The following information may be provided for each workflow event:

- **Description**, which is a brief explanation of the event and how it works.
- **Event result**, which indicates the type of result, if any, the event produces. For example, collect events produce a spectrum and check events produce a pass or fail indicator. The result type will be important when adding items to report events and archive events in order to specify which workflow result you want to report or save.
- **Associated specifications**, which lists the required and optional specifications that can be linked to the described event.
- **Related events**, which lists other events that operate like the described event or perform a similar function, and events that may be tied to the described event. For example, if a measure event can be used to measure the result from the described event, then the measure event would be listed as a related event.

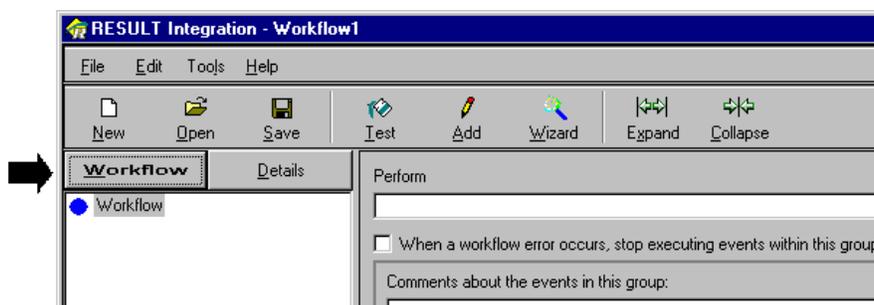
- **Related specifications**, which lists other specifications that can be tied to the described event. For example, if a table item specification might be used to add a result from the described event to a sample report, then the table item specification would be listed as a related specification.
- **Parameters**, which explains the parameters for the described event. Parameters are described in the order in which they appear in the software when the described event is selected in a workflow.
- **Usage**, which provides practical examples of how the described event is typically used in a workflow. It also lists any events that must appear before or after the described event in a workflow, and lists events that operate on results produced by the described event.

## Adding simple events to workflows

When a workflow is displayed in the workflow navigation frame, you can use the Add command in the Edit menu or the Add button on the toolbar to add simple events to the workflow. The new event is added immediately below the selected event or at the end of an event group.

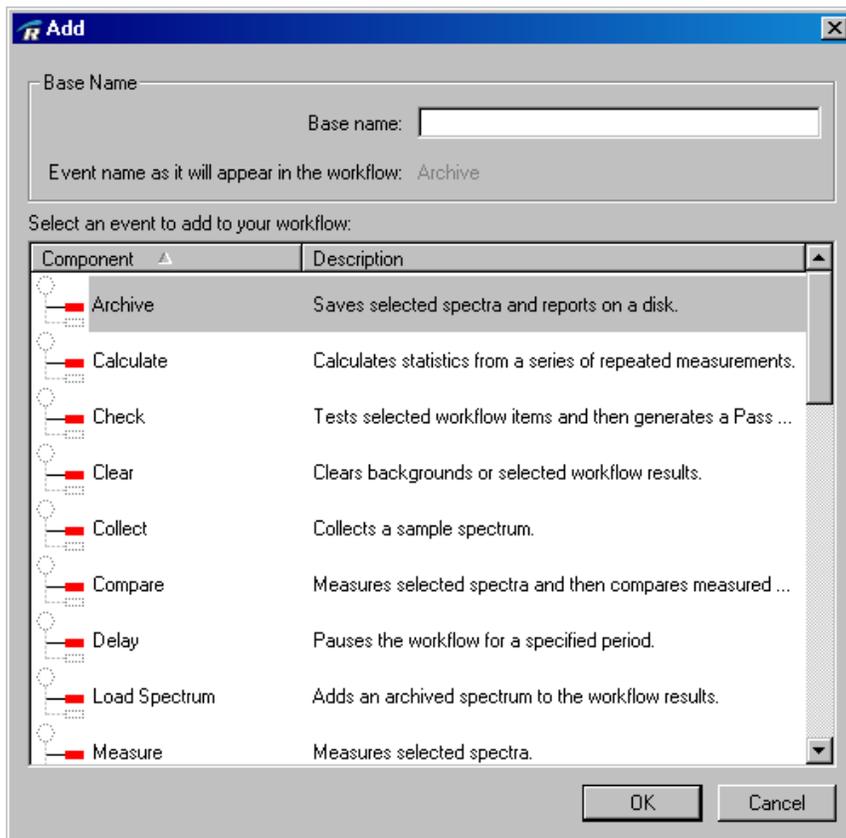
To add a simple event to a workflow:

1. **Create or open a workflow and make sure the Workflow tab is selected in the workflow navigation frame.**



2. **Choose the Add button on the toolbar or choose Add from the Edit menu.**

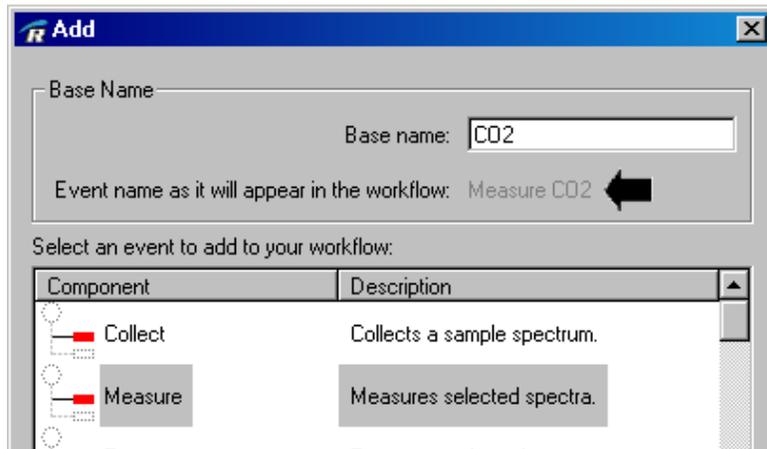
A list of available events displays.



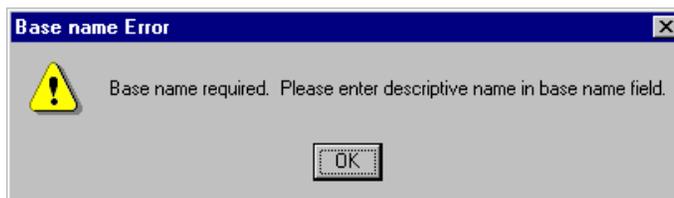
Notice that events are named with action words, such as “collect” and “measure.” The simple events, which perform a single task, are marked with a red rectangle. The Description column explains the task each event will perform when you run the workflow.

- 3. Select a simple event so that its name is highlighted in the list of available events.**
- 4. Select the Base Name For This Event text box and enter a descriptive name for the new event.**

The name you enter is appended to the event name. For example, if you select the Measure event and then enter the name “CO2,” then the event will be named “Measure CO2.” The software demonstrates how workflow events are named by showing the full name as you type, as shown below.



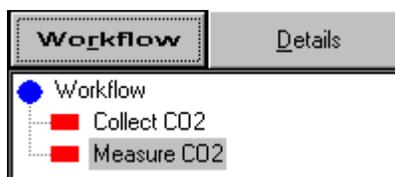
**Note** You must enter a base name before continuing. If you don't, the software displays an error message.



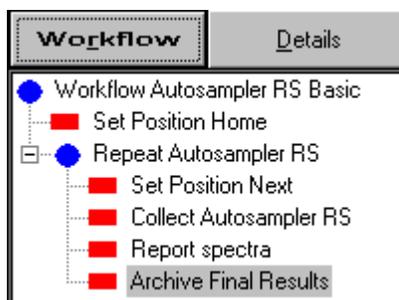
Choose OK to close the message and then enter a base name in the Add dialog box. ▲

**5. When you are finished, choose OK to close the dialog box.**

The new event is added immediately below the selected event in the workflow as shown in the example below.



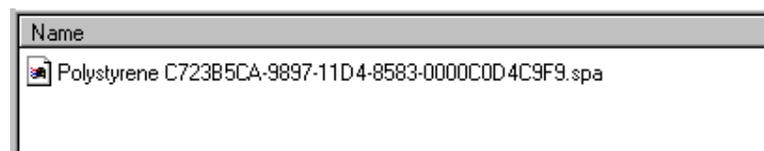
If an event group is selected, such as the Repeat event in the next example, the new event is placed at the end of the events in the group.



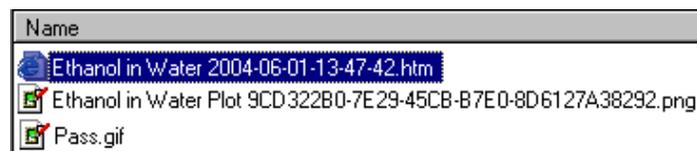
## Archive events

Archive events can be used to archive selected sample spectra and/or sample reports generated by a workflow, using the selected file format and the specified folder and path.

Each file can be saved with a unique user-specified file name or all the files can be saved automatically with either a user-specified base name or a base name selected by the software (typically the name of the corresponding collect or report event). The file name of an archived spectrum or report may include a globally unique identifier (GUID), a date and time stamp, an index number, the spectrum title, or any combination of these. The file name extension is determined by the current setting for Spectrum Format or Report Format in the archive event parameters. The following example shows a spectrum archived using a file name selected by the software plus a GUID, and the Nicolet Spectrum (\*.spa) file format.



RESULT Integration archives reports as hypertext markup language (HTML) documents (\*.htm file name extension), which are viewable by RESULT software, as well as web browsers and other applications that can open HTML files. If the report includes images, such as the pass or fail image provided with the software, or even a spectrum, a copy of those image files is archived with the report. The following example shows a report that includes a spectrum image (\*.png) and the “pass” image provided with RESULT software (pass.gif).



HTML documents can display embedded images only if the corresponding image files are present in the same directory as the document. So if you copy a report file to another directory, make sure you also copy its associated image files. If you don't copy the image files, when you open the report, the image fields will be blank.

**Tip** If you don't want to keep track of archived spectra and report files, select Save List Of Archived File Names in the archive event parameters. The software generates a comprehensive list of all spectra and report files archived by the workflow, including any image files associated with each report. ▲

The paths for archiving data produced in workflows are relative to the base path for archiving spectra and reports set in the Options dialog box in the application used to run the workflow. Spectral and report files can be archived with their Windows access privilege set to "read-only" and with a digital signature. You can configure the workflow to save a list of the file names of any spectra or reports that it archives and a separate list of workflow errors or to make the archived file names and paths available to an OPC client.

**Note** If you run the workflow in RESULT Operation, the software automatically stores a record of any archived spectra and/or reports in the audit log database. The record stored in the audit log includes the spectrum or report file name and path, and the date and time the file was created, along with information about the computer and operator running the workflow. See "Chapter 4 Working With the Audit Log" in the "RESULT Operation Software User Guide" for information about making queries of the audit log. ▲

**Event result:** Archived spectral or sequence data files, archived report file(s)

**Associated specifications:** None

**Related events:** Collect event, Report event, Run sequence event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the archive event. These parameters appear in the display area of RESULT Integration when an archive event is selected in a workflow.

Archive

New

Archive these results:

Result Type	Name

Add

Location

Base path: C:\RESULT Data\Archive

Folder: \

Browse

File Format

Report format: Standard HTML

Spectrum format: Nicolet spectrum (\*.SP)

Save report files as read-only

Save spectral files as read-only

Require digital signature

Save workflow error report

Save list of archived file names

Report archiving information to OPC

File Name

Prompt for file name

Name files automatically

Use base name: New

Add GUID

Add date and time

Add index

Add spectrum title

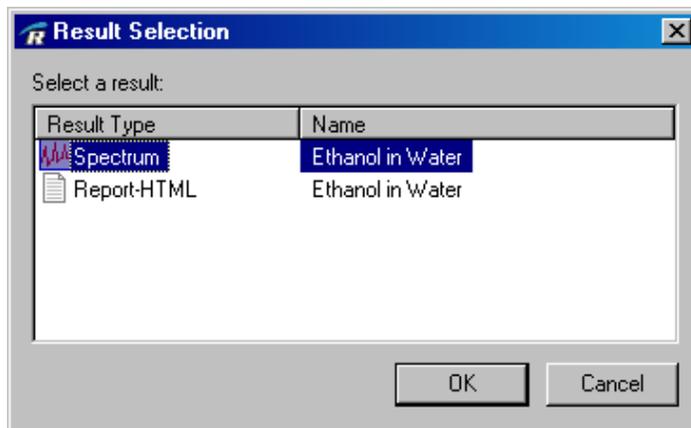
## Archive event parameters

The archive event parameters specify the workflow results to be archived, the file format and location for storing those results, any options for limiting access to the archived files, and whether a list of file names and workflow errors will also be archived. The following sections explain the archive event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Archive Results

The parameters in this group allow you to specify the workflow results to be archived. Archive events may be used to archive spectra and reports only. Measurement and other workflow results must be placed in a sample report if those results are to be archived.

- **Archive These Results.** Use this box to select the spectra, sequence data and/or reports that will be archived. To add a spectrum, sequence or report to the list, choose the Add button below the box. The following dialog box is displayed.



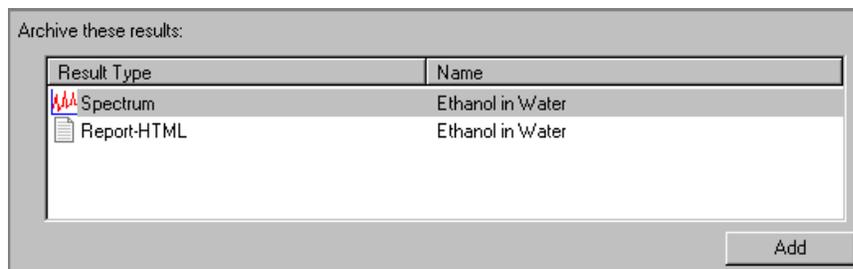
The list shows the spectrum, sequence, or report associated with each collect, sequence, and report event that is included in the workflow and the selected format for the spectra, sequence data, and reports.

**Note** If this dialog box is empty, then the workflow either does not contain a collect, run sequence, or report event or all of those events have already been added to the list. See “Collect events,” “Run sequence events,” and “Report events” in this chapter for instructions for adding collect, run sequence, and report events to a workflow. ▲

Select the spectrum, sequence, or report you want to add and then choose OK. Make sure the spectra, sequence, and reports you select are produced by collect, run sequence, and report events that appear before this archive event in the workflow.

After you choose OK, the dialog box closes and the selected items appear in the list of results to be archived.

To delete a spectrum, sequence, or report from the list, select the spectrum, sequence, or report name and then press the Delete key on the keyboard.



## Location

The parameters in this group allow you to specify the location where the files will be archived.



### Base path:

- **Base path.** This readout shows the current path for archiving spectra and reports in RESULT Integration (as defined in the Options dialog box available from the Edit menu in RESULT Integration). Any spectra and reports archived by this workflow will be placed in this location when the workflow is run in RESULT Integration.

If the workflow is transferred to RESULT Operation, the report event will archive the selected spectra and reports using the folder and path for archiving spectra and reports for that application (as defined in the RESULT Options dialog box available from the Administration menu in RESULT Operation). This allows you to separate data archived while developing or testing a workflow in RESULT Integration from data archived while running a workflow in production mode.

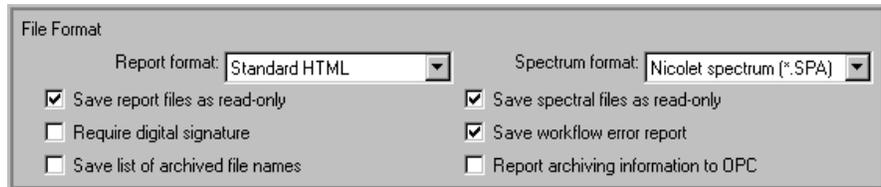


- **Folder.** Use this box to enter the folder that will be used to archive any spectra and reports that are generated by this workflow, or use the Browse button to locate or create and then select an appropriate folder. You can only select or create folders that are located in the base path for archiving spectra and reports in RESULT Integration (see above).

If you run the workflow in RESULT Operation, the spectra and reports will be archived in the specified folder, but the folder will be located in the base path for archiving spectra and reports in RESULT Operation. (If the folder doesn't exist, the software will create it.) See "Setting RESULT Integration Options" in the "RESULT Integration Software User Guide" and "Setting RESULT Operation Options" in the "RESULT Software Administration Guide" for information about setting the path for archiving spectra and reports in each of those applications.

## File Format

The parameters in this group allow you to specify the format for the archived data, whether a list of file names and workflow errors will be archived with the data, and whether the software will request a digital signature before archiving the data. You can also elect to make the archived file names and paths available to an OPC client.



The file format options include the following:



- **Report Format.** Use this list box to select a format for archiving HTML reports that are generated by this workflow. RESULT Integration provides two options for the format used to archive HTML reports: the standard hypertext markup language (HTML) format and the Unicode HTML format. Documents in the standard HTML format are viewable by RESULT software as well as web browsers and other applications that can open HTML files. You may prefer the Unicode HTML format if your report contains text from double-byte character sets such as Kanji. Both options create a text file that has an \*.htm file name extension.



- **Spectrum Format.** Use this list box to select a format for archiving any spectra that are generated by this workflow. The following options are available.
  - *Nicolet spectrum (\*.spa)*, which is the standard (and recommended) format for spectra for use with Thermo Scientific spectroscopy applications including TQ Analyst and RESULT software. Data that are stored in the Nicolet spectrum format contain complete information about the conditions used for data collection as well as the archived sample and background interferograms, and are compatible with the digital signature features of RESULT software.
  - *JCAMP-DX (\*.jdx)*, which is a file format that is compatible with other applications in the industry and includes only printable ASCII characters and some file heading information.

- *Galactic (\*.spe)*, which is 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 heading information.
- *Comma-Separated Values (\*.csv)*, which is a text 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.

**Note** If the workflow contains a run sequence event that is set up to retain all the sequence data, the data will be archived in two files: the \*.srs file contains all the spectra collected over the time of the data collection and the \*.sri file contains the interferogram data for all the spectra. If the run sequence group includes a measure event that is set up to measure the sequence data, the measurement results will be archived in a \*.cnc file. See “Sequence module events” in this chapter for more information. ▲

Save spectral files as read-only

- **Save Spectral Files As Read-Only.** Select this option to archive spectral data files with their Windows access privileges set to “read-only.” Spectral files which are saved (and maintained) as read-only may be opened and changed but the altered file cannot be resaved with the previous file name. File access privileges can also be set or changed from the Windows operating system. See your Windows workstation documentation for more information.

If this option is cleared, then the archived spectral files may be changed and then resaved with the previous file name.

Save report files as read-only

- **Save Report Files As Read-Only.** Select this option to archive report files with their Windows access privileges set to “read-only.” Report files which are saved (and maintained) as read-only may be opened and changed but the altered file cannot be resaved with the previous file name. File access privileges can also be set or changed from the Windows operating system. See your Windows documentation for more information.

If this option is cleared, then the archived report files may be changed and then resaved with the previous file name.

Require digital signature

- **Require Digital Signature.** Select this option to configure this archive event to request a digital signature before archiving these spectra and reports.

**Note** Using digital signatures for spectral and report files can help ensure the authenticity of the data. ▲

If this feature is selected, before the workflow archives the data specified in this archive event, the software opens a dialog box prompting the user to enter his or her Windows user name and password to sign the files. The software requests the digital signature when the workflow is run in RESULT Operation and RESULT Integration.

If you are unable to correctly enter your Windows password, the following error message appears:



You have three attempts to enter your password correctly when digitally signing a file. If you enter the wrong password three times, or if you cancel the Digital Signature dialog box, the workflow archives the unsigned files and reports the failed signature.

You can use the Check Signature feature in the File menu of RESULT Integration to determine whether a specific file has been signed. See “Checking File Signatures” in “Chapter 2 Creating and Editing Workflows” of the “RESULT Integration User Guide” for more information. To check for signatures in spectral and report files from RESULT Operation, use the query feature to display the archived spectra and/or reports in the report navigation frame. The status box will indicate the signed/unsigned status of the selected file. If a file has been signed, both applications show the name of the person who signed the file, the date and time the file was signed and the reason it was signed, if one was specified.

**Note** Files that have been signed and then altered will be reported as “unsigned” by both applications. ▲



- **Save List Of Archived File Names.** Select this option to create a document that lists the file names of the spectra and/or sample reports archived by this event. The software generates the file list document when you run the workflow in RESULT Integration or RESULT Operation. The file list allows someone who can't (or doesn't want to) access the audit log database to locate spectra and report files generated by a particular workflow, and to determine which image files are required to display a report outside of RESULT software.

For each spectrum and/or report the archive event is configured to archive, the list shows the name of the collection or report event that generated the data and the archived file name of the corresponding spectrum or report, as shown in the example below.

### Files Archived by Polystyrene Results

Date and time: 9/15/00 11:59:08 AM

Destination path: C:\RESULT Data\Archive

Type of File	Event Name	File Name
Spectrum	Polystyrene	Polystyrene 15447A87-8B29-11D4-94DD-0008C75B3D16.spa
Report	Polystyrene Results	Polystyrene Results 15447A88-8B29-11D4-94DD-0008C75B3D16.htm  Linked image files: <ul style="list-style-type: none"><li>• nicolet.jpg</li><li>• Pass.gif</li></ul>
Report	Another Test	Another Test 15447A89-8B29-11D4-94DD-0008C75B3D16.htm  Linked image files: <ul style="list-style-type: none"><li>• Another Test Report Plot 15447A85-8B29-11D4-94DD-0008C75B3D16.bmp</li></ul>

This file was digitally signed.  
By: Operator  
Date: 09-15-2000 11:59:08  
Reason: Authorship

If sample reports are archived, the list of file names includes the file names of any image files that are linked to each sample report. Both RESULT image files and user-generated image files are listed.

The date and time the files were archived and the location (directory and path) are provided at the top of the document.

If the archive event is set up to request digital signatures (see Request Digital Signature above) and the user enters a valid user name and password to archive the spectra and reports generated by the workflow, the software applies the same signature to the file list document and considers that document to be digitally signed. A record of the digital signature appears at the bottom of the report, as shown in the previous example.

The file list document is archived in the same directory as the spectra and reports (see Base Path and Folder above). The file name of the document starts with the prefix “List” followed by the naming convention specified in the File Name box on the archive event. The document is an HTML file (\*.htm extension), which is viewable by RESULT software as well as web browsers and other applications that can open HTML files.

Save workflow error report

- **Save Workflow Error Report.** Select this option to create a report of workflow errors. The software generates the error report when you run the workflow in RESULT Integration or RESULT Operation, but only if the workflow produces errors. The report can be useful for troubleshooting purposes.

The list includes the name of each workflow event that produced an error and a description of the error. The illustration below shows an example of a workflow error report.

### Errors While Running Workflow

Event Name	Error Description
Archive Ethanol in Water	The operator was requested to digitally sign files that were archived, but the operator was unable to authenticate in 3 attempts. None of the archived files were digitally signed.

If the archive event is set up to request digital signatures (see Request Digital Signature above) and the user enters a valid user name and password to archive the spectra and reports generated by the workflow, the software applies the same signature to the workflow error report and considers that file to be digitally signed. A record of the digital signature appears at the bottom of the error report.

The error report is archived in the same directory as the spectra and reports (see Base Path and Folder above) with the file name WORKFLOW ERRORS plus a globally unique identifier (GUID).

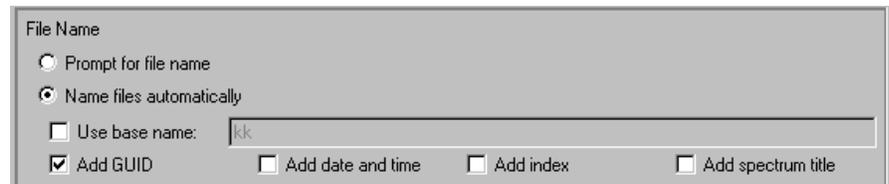
The document is an HTML file (\*.htm extension), which is viewable by RESULT software as well as web browsers and other applications that can open HTML files.

Report archiving information to OPC

- **Report archiving information to OPC.** Select this option to make the archived file names and paths available to an OPC client. OPC is a universal interface used to control process equipment and to monitor data results.

## File Name

The parameters in this group allow you to specify the file name that will be used to archive the data.



You can name the files with user-specified file names or a base name plus any combination of a globally unique identifier (GUID), date stamp, index number, or title.

**Note** When using digital signatures to archive files, we recommend that you add a GUID, a date stamp, or both to the file name to ensure the authenticity of the data. ▲

The file name options include the following:

- **Prompt for file name.** Before archiving each sample spectrum, the software displays a prompt asking for a file name for the spectrum. The user must enter a file name before the software will continue. Keeping this feature selected is helpful if your organization has specific naming conventions you want to use when archiving sample spectra.
- **Name files automatically.** Select this option if you want the software to name the files automatically. You can specify whether a base name will be used to archive the files, and select whether a globally unique identifier (GUID), a date stamp, an index number, the spectrum title or any combination of these will be added to the file name.

- *Use base name.* If you want to specify a base name for naming files automatically, select this check box and then enter a name in the associated text box or leave the default base name. The default base name matches the name of the archive event displayed in the workflow navigation frame in RESULT Integration. If you use a base name, the software will include that name at the beginning of the file name of each spectrum or report the archive event is set up to archive. This step is recommended because creating a base name for a set of sample spectra and reports can help you easily identify those spectra and reports after they are archived.

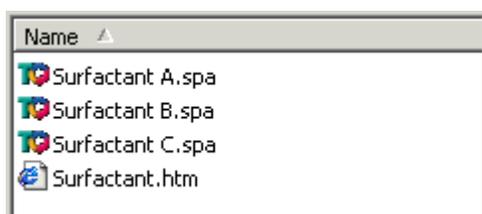
**Note** If you use only a base name to archive data and the archive event archives the data from multiple collect or report events, the software will only archive the spectrum or report that was created last. If you want to archive all of the files the workflow creates, add a GUID, date stamp, or index number to the base name (see below). ▲

If you clear the Use Base Name check box, the files will be named with the default file names assigned by the software. The default file names are copied from the associated collect and report events displayed in the workflow navigation frame in RESULT Integration. For example the following workflow collects three spectra, creates a report and then archives all three spectra and the report.

#### Workflow Fiber Optic Probe Collection

Collect Surfactant A  
Collect Surfactant B  
Collect Surfactant C  
Report Surfactant  
Archive spectra and report

If the archive event is set up to name the files automatically without a base name, the workflow produces four files using the default file names assigned by the software.



- *Add GUID.* If you want the software to use a globally unique identifier (GUID) to name the files, select Add GUID. A GUID is a string of characters generated by the software as an identifier for a particular file. Each GUID is unique and cannot be used for more than one file. If you leave this option selected, the software will never overwrite your files. The GUID appears immediately after the base name.

**Note** If a GUID, date stamp, and index are used, the file name includes the base name, followed by the GUID, followed by the date stamp, followed by the index. ▲

- *Add date and time.* If you want the software to use a date stamp to name the files, select Add Date And Time. The software adds the date stamp immediately after the base name.

The date stamp always reflects when the workflow implements the event that initiates the archiving of data. For linear workflows with one collect event, the workflow produces one set of files with the same date stamp. For example, if the archive event in the following workflow is set up to save the spectrum and the report using the default base name and a date stamp, the workflow will produce one set of files with the same date stamp.

#### Workflow Fiber Optic Probe Collection

Collect Sample

Report Sample

Archive spectrum and report

Name
 Ethanol in Water 2004-06-01-15-36-27.spa
 Ethanol in Water 2004-06-01-15-36-27.htm

If you add more collect events but archive them at the same time as in the next example,

#### Workflow Fiber Optic Probe Collection

Collect Sample a  
Collect Sample b  
Collect Sample c  
Report Samples  
Archive spectra and report

you still get one set of files with the same date stamp.

**Tip** If you want all the files produced by a workflow to be archived with the same date stamp but still need to differentiate the archived files, use a date stamp and an index number (see below). ▲

If the archive event occurs in a loop like the example below, the workflow produces a set of files each time it completes the loop.

#### Workflow Fiber Optic Probe Collection

Repeat sample collection (3)  
Collect Sample  
Report Sample  
Archive spectrum and report

For example, if the repeat event shown above is set up for three iterations and the archive event is configured to save the spectrum and the report, this workflow produces three sets of files. Each set of files will have a unique date stamp.

- *Add index.* If you want the software to use an index number to name the files, select Add Index. The index is a three-digit index number that increases by one each time it is applied (i.e., 001, 002, 003). The software adds the index immediately after the base name.

For linear workflows with one collect event, the workflow produces one set of files with the same index number. For example, if the archive event in the following workflow is set up to save the spectrum and the report using the default base name and a date stamp and index, the workflow will produce one set of files with the same date stamp and index.

Workflow Fiber Optic Probe Collection

- Collect Sample
- Report Sample
- Archive spectrum and report

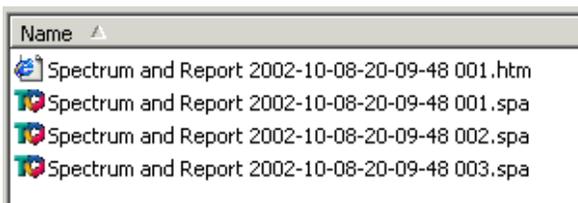


If you add more collect events but archive them at the same time as in the next example,

Workflow Fiber Optic Probe Collection

- Collect Sample a
- Collect Sample b
- Collect Sample c
- Report Samples
- Archive spectra and report

you still get one set of files with the same date stamp but the spectral files will have unique index numbers.



If the archive event occurs in a loop like the example below,

Workflow Fiber Optic Probe Collection

- Repeat sample collection (3)
- Collect Sample
- Report Sample
- Archive spectrum and report

the workflow will produce a set of files each time it completes the loop and all the files will have the same index number.

**Note** Use a date stamp or GUID instead of an index number in the above case. ▲

If the archive event occurs after a loop like the next example, the workflow produces one group of files after it completes the loop.

Workflow Fiber Optic Probe Collection

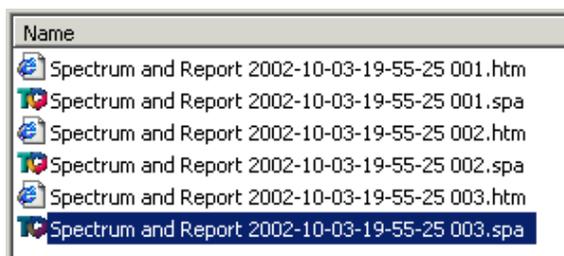
Repeat sample collection (3)

Collect Sample

Report Sample

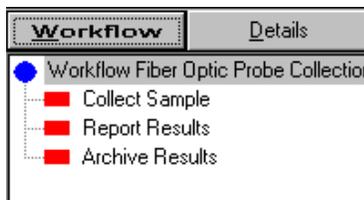
Archive spectrum and report

For example, if the repeat event shown above is set up for three iterations, the archive event is configured to save the spectrum and the report, and the collect and report events are configured to retain all the spectra and reports, this workflow produces three sets of files. All the spectral files will have the same date stamp but each set will have a unique index number.



- *Add spectrum title.* If you elect to use the spectrum titles for the file names, the software will archive the spectra using the titles the operator enters at run time or the titles specified in the sampling sequence. The titles will be appended to the base name and any other file name option selected in the File Name box.

**Usage:** Archive events are typically positioned after a collection or report event in a workflow, as shown in the example below.



**Note** Place the archive event after a loop if you want to archive all the spectra and reports with the same GUID or date and time stamp. ▲

See “Repeat event” and “Perform-While events” for more information.

## Calculate events

This event can be used to calculate statistics from a set of measurements. Calculation events are typically placed after a repeat or perform-while loop that includes a collect event and a measure event, so that multiple values are produced for each measurement.

You can calculate statistics from any event that produces numeric results. For each measurement, such as a spectral peak height or area, the calculated statistics can include:

- Minimum, maximum and average values
- Range (maximum minus minimum)
- Standard deviation and percent standard deviation
- Summation (simple sum)
- Count (number of measurements)
- First and second derivatives.

If the selected measurement produces only one value, the calculation result for standard deviation and percent standard deviation will be zero.

If the measure event measures more than one component or attribute, for example if it calculates concentration values for several compounds, a set of statistical values can be produced for each of those components or attributes. You can use a single calculate event to produce statistics from multiple measure events in the same workflow.

Each time a workflow performs a calculation event, the workflow produces a set of statistical data, referred to as the calculation result. The workflow automatically stores the latest result in the computer’s internal memory, so the result is available for use by subsequent events in the workflow, such as a report event.

**Note** If you want to include statistical data in a sample report and you don't need to access those data elsewhere in the workflow or store them in the audit log database, we recommend using a report event with an associated summary item specification to generate the statistical data instead of a calculation event. The report event allows you to easily create an elegant table of statistical data from one or more sets of measurement results in a single step, while the calculation event requires the user to add a table to the report and then add each calculation result to the table. ▲

**Event result:** Measurement statistics

**Associated specifications:** None

**Related events:** Check event, Measure event, Repeat event, Report event, Store event

**Related specifications:** Summary Item specification, Table Item specification, Logical Test Specification

**Parameters:** The illustration below shows the parameters for the calculation event. These parameters appear in the display area of RESULT Integration when a calculation event is selected in a workflow.

Calculate Result: measurement statistics

New

Calculate statistics from these events:

Name	Data Type	Attribute	Label
------	-----------	-----------	-------

Add Edit

Calculate these statistics

Minimum value  Range (max - min)  Summation  First derivative

Maximum value  Standard deviation  Count  Second derivative

Average  Percent standard deviation

Store raw values with calculated values

Delete source spectra after calculation

Multiple Event Results

Retain all event results

Retain most recent result

### Calculate event parameters

The calculate event parameters define statistical measurements for one or more measurement results and the storage of data from multiple calculation events that occur in a loop. The following sections explain the calculation event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Calculate Statistics from these Events

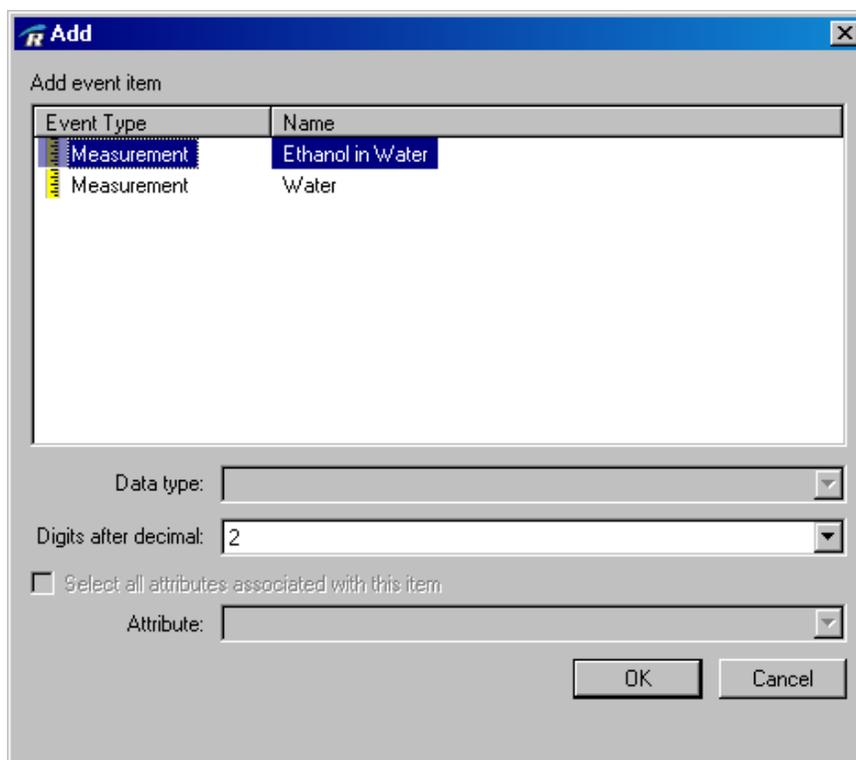
Use this features in this box to specify the measurement events to be used for statistical analysis. You can run calculations on the data produced by any combination of measure events in the workflow.

Name	Data type	Attribute	Label
------	-----------	-----------	-------

Add Edit



- **Add.** Choose this button to add a measure event to the list. The software displays the Add dialog box as shown below.



The dialog box lists all the measure events in the current workflow.

**Note** If this dialog box is empty, then the workflow either does not contain a measure event or all of those events have already been added. ▲

Select a measure event in the list. Make sure you select an event that is positioned before this calculate event in the workflow. Since a workflow implements events in sequence, only events positioned before the calculate event will have results that can be analyzed. If you select an event that occurs after the calculate event, it will be unable to find the corresponding data and the workflow will produce an error.

After you select a result, the following parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Examples are provided below.

- *Data Type.* Use this list box to select a result produced by the selected measure event, such as a value or an acceptance limit. The number and type of results produced depend on the event and the TQ Analyst or other method used for the measurement. For example, a measure event configured for quantitative analysis would always produce concentration values, but it may also include acceptance limits or known values, such as the expected concentration for a sample or standard. The Data Type drop-down list could include the following items for a quantitative measure event.

Data type: Value

- Value
- Acceptance limits
- Expected value

- *Digits After Decimal.* This box is available in the software only when the selected Data Type (see above) produces a numeric result.

Digits after decimal: 2

Use the box to select the number of digits the software will include after the decimal point in the numeric result. You can include up to six digits after the decimal point. The software rounds the number and retains only the specified digits after the decimal point.

- *Attribute.* Use this list box to select a specific component or other measured attribute or value for the selected data type and event. The number and type of items in the attribute drop-down list depend on the event and the TQ Analyst or other method used for the measurement. For example, a measure event configured for spectral measurements could include the following items in the Attributes drop-down list.

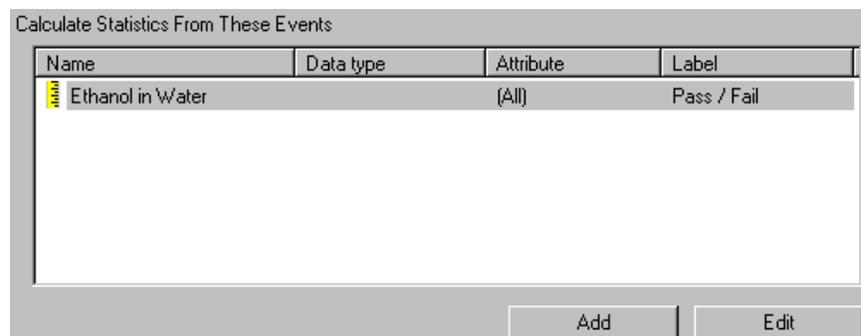
Attribute: Intensity at 4000 cm-1

- Intensity at 4000 cm-1
- Intensity at 6000 cm-1
- Intensity at 10000 cm-1

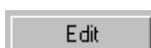
- *Select All Attributes Associated With This Item.* Select this option if you want to include all the measured components or other attributes or values for the selected data type and event.

Select all attributes associated with this item

When you are finished selecting a result, choose OK. The selected result is added to the list of items to include in the table, as shown in the example below.



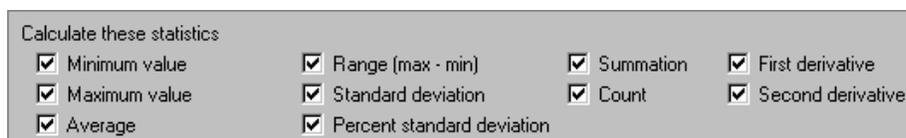
Repeat the steps described here for each measure event you want to include in the calculations.



- **Edit.** To edit the properties for a measure event shown in the table above, select the measure event and then choose the Edit button below the table. The new settings will be used the next time you run the workflow.

### Calculate These Statistics

Use the parameters in this group to specify the statistical values you want the workflow to calculate.



The following statistics are available:

- Minimum, maximum and average values
- Range (maximum minus minimum)
- Standard deviation and percent standard deviation
- Summation (simple sum)
- Count (number of measurements)

- First and second derivatives.

The values you specify will be calculated for each measured attribute listed in the calculate event.

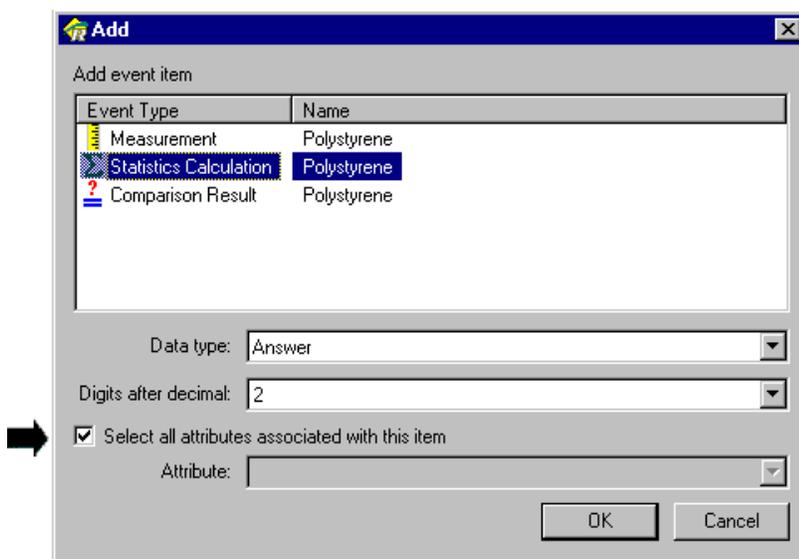
**Note** Using a calculate event to generate statistics makes them available for use by other events in a workflow. For example, if you want to calculate a statistical value, such as a standard deviation, and then use that standard deviation value in another event, such as a check event, use a calculate event to generate the standard deviation and then add the calculation result to the list of items to be checked. See “Check events” in this section for more information. If you simply want to report the statistical values, it is faster to use a report event with a table item specification to generate and report the statistical data instead of a calculate event and a subsequent report event. ▲

The parameters in this group allow you to specify the measurement result that will be used to calculate statistical data. The following parameters are included:

Store raw values with calculated values

- **Store Raw Values With Calculated Values.** Select this option to store the measurement results along with the calculation results in RESULT Integration. When this option is selected, the measured values from the associated measure event are added to the list of statistical values produced by the calculation event and stored in the computer’s internal memory.

Select Store Raw Values With Calculated Values if you want to access the measurement results as well as the calculation results for use in subsequent workflow events. This option is most useful when creating a sample report that includes a table of measurement data and statistical data. It allows you to use the Select All Attributes feature of the Add RESULT dialog box to add both sets of results to the table item specification at the same time.



If you clear the Store Raw Values With Calculated Values option in the Calculate event, you can still access the measurement results but only through the associated measure event.

Delete source spectra after calculation

- **Delete Source Spectra After Calculation.** Select this option if the spectral data associated with this calculate event are still in the computer's internal memory and the spectra are not used in subsequent workflow events. The spectra will be in computer memory unless they were deleted by an earlier event, such as a measure event.

If Delete Source Spectra After Calculation is selected, then the software will delete the stored sample and background spectra when the calculation is completed. Deleting the source spectra is recommended to release memory resources, especially when the workflow must handle multiple spectra produced in a loop.

Make sure this option is cleared if you need to archive the spectral data produced by the workflow and your archive event is positioned after the calculate event in the workflow, or if there are other subsequent workflow events that operate on the source spectra. If you want to delete the spectra later, use a clear event.

## Multiple Event Results

### Multiple Event Results

- Retain all event results
- Retain most recent result

If you place a calculate event in a repeat or perform-while loop, the event will produce one result (i.e., one set of statistical data) during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent results. The options for storing results include:

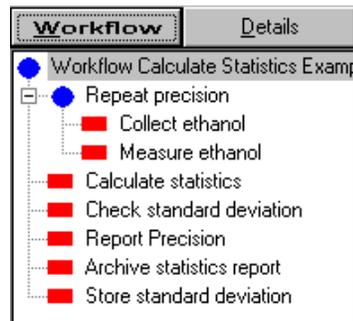
- **Retain All Event Results.** If the calculate event occurs in a loop, selecting this option causes the workflow to store all the statistical data. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the calculate event is not positioned in a loop or the loop includes all subsequent events that operate on the statistical data. This is the default setting and will maximize your computer processing speed.

See “Repeat events” and “Perform-While events” for more information about using stored data in a workflow.

**Usage:** A calculation event must specify a valid measurement result in order to produce a calculation result. Make sure you place the calculation event after its associated measure event in the workflow.

Calculation events are typically placed after a repeat or perform-while loop that contains a collect event and its associated measure event, as shown in the example below.

Configure the measure event to retain all the measurement results generated by the loop if the calculation event is located after the loop as in this example. See “Measure events” for more information.



This is the only way to produce many of the statistical values, such as range and standard deviation. See “Repeat Events” and “Perform-While events” for more information.

The following events can operate on the calculation result if those events are positioned after the calculation event in the workflow.

- **Check event**, which can be used to produce an overall pass or fail result based on a statistical value from a calculation event.
- **Store event**, which can be used to store calculation results in the audit log database so they can be accessed with the logs features of RESULT Operation and used to track trends in the data.
- **Report event**, which can be used to add the calculation result to a sample report.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Check events

This event can be used to test the status of other items in a workflow and then generate a pass/fail result. A logical test specification must specify at least one item to be tested and the conditions for passing or failing the test. The check event may also include a prompt specification, which defines a message displayed to the operator when the check result is “fail.” If the message dialog box is configured to allow the operator to respond by pressing the acknowledge button on the instrument, the red LED indicator will light when the dialog box is displayed on the screen.

Each time a workflow performs a check event, the workflow produces a pass or fail result. The workflow automatically stores the latest result in the computer’s internal memory, so the result is available for use by subsequent events in the workflow, such as a report event. You can configure a table or summary section in a sample report to include the pass or fail result, or the pass () or fail () image provided with the software.

The check event can also be configured to store the pass or fail result in the audit log database so it can be accessed with the logs features of RESULT Operation and used to track trends in your data. If you store pass/fail results in the audit log, you can set up a query of the pass/fail results of specific workflows, all workflows, or only passes or failures. The query creates a table of check events, including the pass or fail result of each event. See “Chapter 4 Working With The Audit Log” in the “RESULT Operation User Guide” for details on using logs.

**Note** A check event is your only mechanism for storing the pass or fail result in the audit log database. (Store events may only be used to store numeric results in the audit log.) ▲

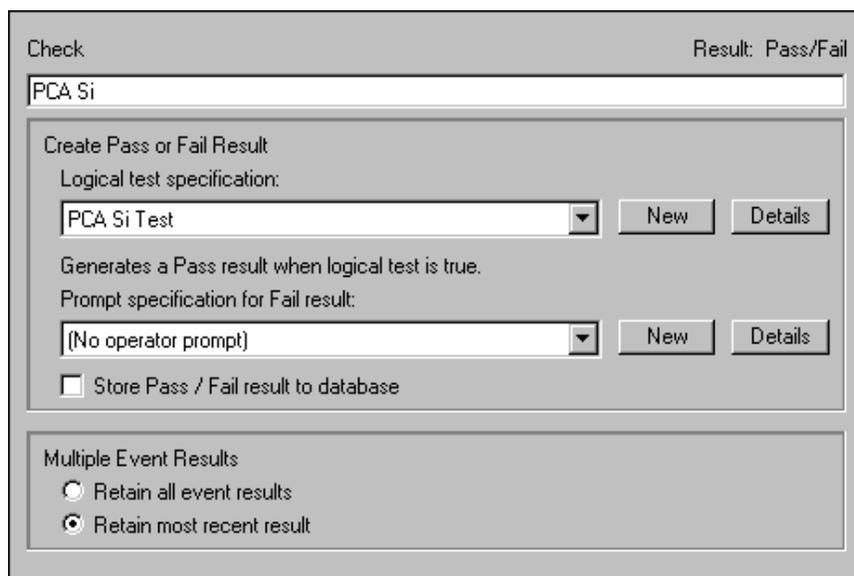
**Event result:** Pass or Fail string

**Associated specifications:** Logical test specification, Operator prompt specification

**Related events:** Perform-if event, Perform-while event, Store event

**Related specifications:** Table item specification, Summary item specification

**Parameters:** The illustration below shows the parameters for the check event. These parameters appear in the display area of RESULT Integration when a check event is selected in a workflow.



### Check event parameters

The check event parameters specify the workflow items to be tested, whether the pass or fail result will be stored in the audit log database, and the storage of data from multiple check events that occur in a loop. The following sections explain the check event parameters in detail. The parameters are explained in the order in which they appear in the software.

## Create Pass or Fail RESULT

These parameters allow you to select a logical test specification and an operator prompt specification to define the conditions and function of the test, and to specify whether the check results will be stored in the audit log database. The check parameters include the following:

- **Logical test specification.** Use this feature to link a logical test specification to this event. The logical test specification allows you to define the workflow result to be tested and how the test will function. If the workflow already contains an appropriate test specification, select its name in the drop down list (see below).



Use the Details button to the right of the list box to display the current settings, or the New button to create a logical test specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the check event. The new specification will be linked to the check event and its name will appear in the logical test specification list box. See “Logical Test Specifications” in “Chapter 5 Workflow Specifications” for more information.

- **Prompt Specification For Fail RESULT.** This operator prompt specification defines a dialog box that will be displayed to the operator when the check event produces a “fail” result. The operator must acknowledge the prompt before the workflow can continue. If the dialog box is configured to allow the operator to respond by pressing the acknowledge button on the instrument, the red LED indicator will light when the dialog box is displayed on the screen.

See “Prompt Specifications” in this chapter for information about setting up operator prompt specifications in a workflow. To link an operator prompt specification to a check event, select the specification name in the Prompt Specification For Fail RESULT drop-down list.



Use the New button at the right of the Prompt Specification list box to create an operator prompt specification and automatically link the new specification to this check event.

If this check event is already linked to an operator prompt specification, you can use the Details button to display that operator prompt specification.

Store Pass / Fail result to database

- **Store Pass/Fail RESULT To Database.** Select this option if you want to store all pass/fail results generated by this check event in the audit log database. The software stores the pass/fail results in the audit log only when the workflow is run in RESULT Operation. Storing pass/fail results in the audit log allows you to access them from queries set up in RESULT Operation. See “Chapter 4 Working With The Audit Log” in the “RESULT Operation User Guide” for information about setting up queries.

If you clear this option, pass/fail results generated by this check event may be stored in memory for use in other workflow events, but they will not be stored in the audit log.

The default setting for this check box is off (check box is cleared) because people typically want to store only global workflow pass/fail results in the audit log, rather than pass/fail results that are used for branching or other internal purposes within a workflow.

## Multiple Event Results

Multiple Event Results

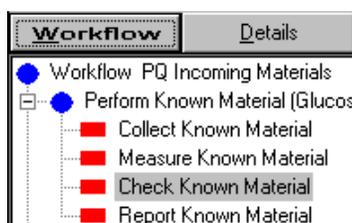
- Retain all event results  
 Retain most recent result

If you place a check event in a repeat or perform-while loop, the event will produce one pass or fail result during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent result. The options for storing results include:

- **Retain All Event Results.** If the check event occurs in a loop, selecting this option causes the workflow to store all the pass/fail results. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the check event is not positioned in a loop or the loop includes all subsequent events that operate on the pass/fail result. This is the default setting for Multiple Event Results and will maximize your computer processing speed.

See “Repeat Events” and “Perform-While events” for more information about using stored data in a workflow.

**Usage:** A check event must be linked to a valid logical test specification in order to produce a pass or fail result. When adding a check event to a workflow, make sure you place the check event after the event that produces the numerical result you want to check, as shown in the example below.

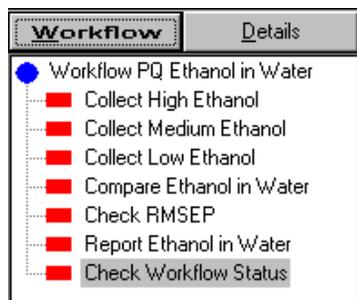


A check event can be set up to check the results of the following workflow events by adding those results to its associated logical test specification (see “Logical Test Specifications” in “Chapter 5 Workflow Specifications” for more information):

- **Measure event**, which can be used to analyze the collected spectra.
- **Calculate event**, which can be used to produce statistics from measurements that are part of a loop.
- **Compare event**, which can be used to chart actual versus expected values for a series of collections.
- **Request event**, which may produce up to ten numerical or yes/no answers from the operator in response to a message-response request.
- **Read From I/O event**, which passes values read from devices or signals to a workflow.
- **Check event**, which produces a pass or fail result. If one check event occurs in a loop and has Multiple Event Results set to Retain All Event Results, you can place a second check event after the loop and use it to generate one pass or fail result for the entire lot.

You can also use a check event to test for workflow errors by selecting Logical Test Is Always False If Workflow Errors Have Been Detected in the associated logic specification.

**Note** If you are setting up a qualification or verification workflow, make sure you place a check event called “workflow status” at the end of the workflow as shown in the example below.



The Check Workflow Status event must be configured to store the pass/fail result in the audit log database, and it should have the Logical Test Is Always False If Workflow Errors Have Been Detected option selected in the associated logical test specification. RESULT Operation is set up to check the (pass/fail) result of the “Check Workflow Status” event when the operator runs a qualification or verification workflow and use it to define the status of the associated production workflow. See “Chapter 2 Running Workflows” in the “RESULT Operation User Guide” for details. ▲

The check event can be used to compare the measurement or other result to predefined criteria and produce a pass or fail result based on the status of the comparison. For example, you can use a check event to test the result of a similarity match measurement that is set up to “find similarities” by adding the measurement result (match value) to the list of items to be tested and assigning “greater than 95” as the conditions for passing the test. The check event will produce a “pass” result only if the match value is 95 or above. Then you can add a perform-if group that contains a store event to store only those match values which passed the test in the audit log database. To set this up, simply add the check result (pass/fail rESULT) to the logical test specification that is linked to the perform-if event, and add the similarity match measurement to the list of results to be stored by the store event.

The following event can operate on the check result if that event is positioned after the check event in the workflow.

- **Report event**, which can be used to add the pass/fail result to a sample report.

For more information, see “Report events” in this chapter.

## Clear events

The clear event can help you ensure the workflow deletes all temporary workflow results, including any background spectra generated by the workflow, before the workflow finishes running. This feature is important, especially for workflows that generate lots of data such as one that uses a repeat or perform-while loop to collect data for over a long period. You can also use the clear event to force the software to prompt for a new background spectrum before the current background has expired.

The Clear event can be set up to delete the current background spectrum or spectra or to delete the results produced by the previous collect, measure, process, or report event, or any combination of those results. You can set up the Clear event to delete all the specified results or to keep the most recent results (you specify how many) and delete the rest. When the software encounters a clear event, it deletes the specified items before continuing.

After a workflow ends, the software automatically clears any spectra or data held in the computer’s internal memory. The clear event allows you to clear workflow results from memory without closing the workflow.

**Event results:** None

**Associated events:** None

**Associated specifications:** None

**Parameters:** The illustration below shows the parameters for the clear event. These parameters appear in the display area of RESULT Integration when a clear event is selected in a workflow.

Clear

New

Clear backgrounds  
 Clear workflow results  
 Clear all but most recent  results

Clear results by event type:

Clear all background spectra  
 Clear results from all Collect events  
 Clear results from all Measure events  
 Clear results from all Process events  
 Clear results from all Report events  
 Clear remaining workflow results

Clear results by event:

Result Type	Name

### Clear event parameters

The clear event parameters specify the type and number of workflow results and background spectra to be deleted. The following sections explain the clear event parameters in detail. The parameters are explained in the order in which they appear in the software.

- Clear All But Most Recent Results.** Select this option if you want the workflow to retain the most recent workflow results and delete the rest. When used with a Calculate event, this feature allows you to calculate running statistics such as a moving block average. Specify the number of workflow results you want to keep in the corresponding entry box.

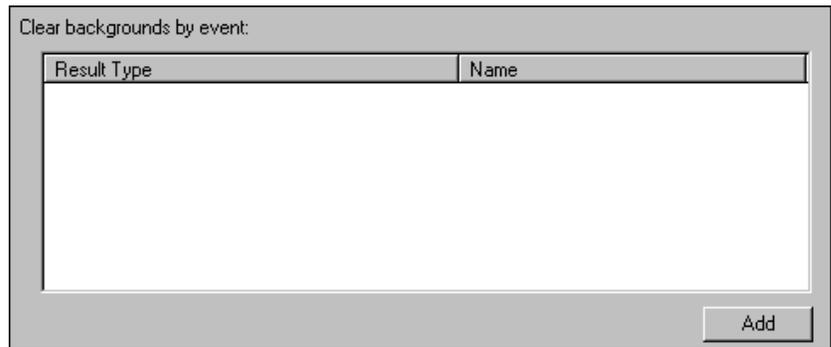
Clear all but most recent  results

If you clear this option, when the workflow implements the clear event, it will clear all the specified workflow results.

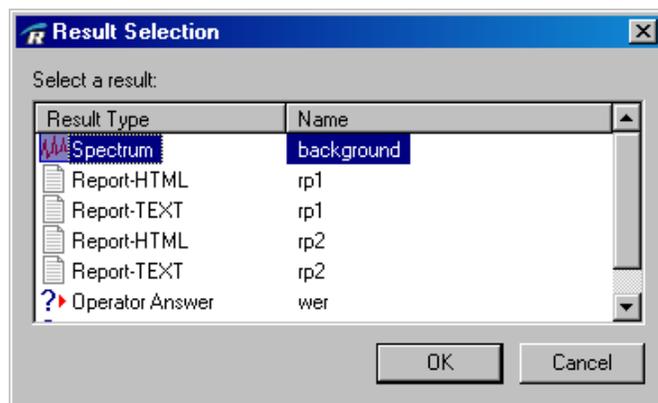
- **Clear Backgrounds.** Select this option to set up the clear event to delete background spectra. When you select this option, other background options become available in the software.
- *Clear Backgrounds By Type.* This option becomes available in the software only when Clear Background is selected (above). If you want to clear all the background spectra generated at this point in the workflow, then select Clear All Background Spectra.

Clear all background spectra

- *Clear Backgrounds By Event.* If you want to clear only the background spectra generated by specific workflow events, use the features in this group to specify the events.



Use the Add button to select an event. The software displays the following dialog box.



Select a background spectrum event result in the list and then choose OK. Repeat this step to add each background result to the clear event. If no background spectrum is listed, then the workflow does not generate a background spectrum.

- **Clear Workflow Results.** Select this option to set up the clear event to delete workflow results. When you select this option, the features for clearing specific types of workflow results become available in the software.
- *Clear Results By Event Type.* If you want to clear all the results from a specific type of workflow event, such as all the spectra generated by all the collect events in the workflow, then select the corresponding check box.

Clear results by event type:

- Clear all background spectra
- Clear results from all Collect events
- Clear results from all Measure events
- Clear results from all Process events
- Clear results from all Report events
- Clear remaining workflow results

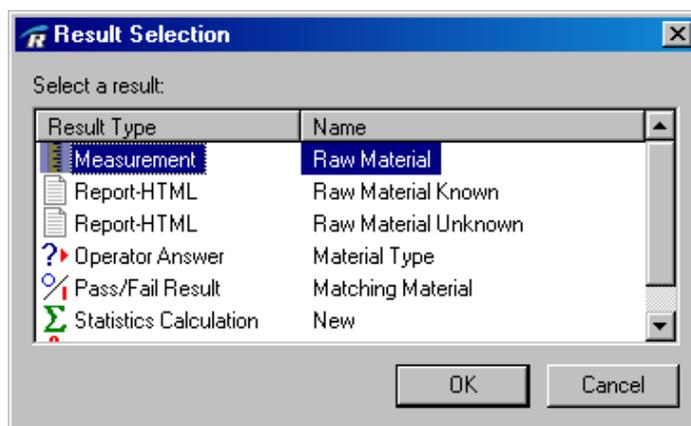
- *Clear Results By Event.* If you want to clear only the sample spectra generated by specific workflow events, use the features in this group to specify the events.

Clear results by event:

Result Type	Name

Add

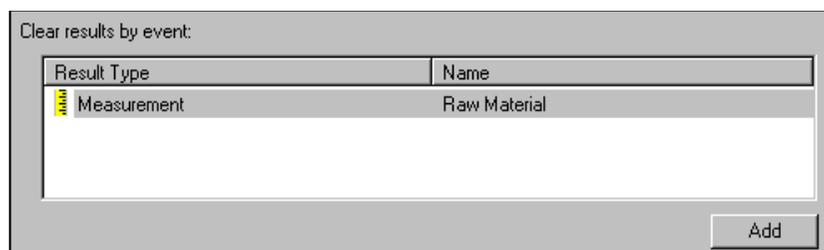
Use the Add button to select an event. The software displays the following dialog box.



Select a workflow result in the list and then choose OK. If no results are listed, then the workflow does not generate a workflow result or all those results have been added to the clear event.

The software closes the dialog box and returns to the clear event. The item you selected appears in the Clear Results By Event box.

To delete an item from this list, select the item and then press the Delete key on the keyboard.



Repeat this step to add each workflow result to the clear event.

**Usage:** Clear events may be placed anywhere in a workflow. If the Clear event occurs in a repeat loop, the software deletes the specified background or workflow result produced in each iteration of the loop. If the Clear event occurs after a loop, the software will delete the specified items produced in all iterations of the loop, even if the event that produced the results specified that those results be retained. There are no other requirements and no clear event results that can be accessed by other events in a workflow.

The following examples show possible uses for clear events in a workflow:

- **Process event.** Combine a clear event with a process event to calculate an average or variance spectrum on the most recent block of collected spectra by setting Clear All But Most Recent Results in the clear event.

- **Calculate event.** Combine a clear event with a calculate event to calculate statistics using the most recent block of collected spectra by setting Clear All But Most Recent Results in the clear event.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Collect events

Use a collect event to set up data collection from a workflow. The collect event parameters define the number of scans to collect of the sample material, the format of the collected data and the frequency of background collections.

A collect event must be linked to a valid sample and background specification, which define the instrument parameters used for data collection. The collect event may have an associated sample correction specification, which can be used to define a transfer or dark background correction for the collected data. The collect event may also include operator prompt specifications for the sample and background collections. Prompt specifications can be used to define message dialog boxes that will be displayed before the start of sample and background collection in the workflow. For example, a message might explain how to position the sample to collect the sample data and then wait until the operator responds to the prompt before collecting the sample scans.

Each time a workflow performs a collect event, the workflow produces a spectrum. The workflow automatically stores the latest spectrum in the computer's internal memory so the spectrum is available for use by subsequent events in the workflow such as a measure event or a report event. If you want to archive the spectrum, you must add an archive event to your workflow and then add the spectrum to the list of results to be archived. See "Archive Events" in this chapter for more information.

**Event result:** Spectrum

**Associated specifications:** Sample specification, Background specification, Before Background operator prompt specification, Before Sample operator prompt specification, sample correction specification

**Related events:** Measure event, Report event, Archive event, Compare event

**Related specifications:** Spectrum Item specification

**Parameters:** The illustration below shows the parameters for the collect event. These parameters appear in the display area of RESULT Integration when a collect event is selected in a workflow.

Collect Result: spectrum

New

Sample Parameters

Sample specification:  New Details

Number of sample scans: 16

Data format: Absorbance

Background frequency: Before every sample

Background folder: C:\RESULT Data\Backgrounds

Collect background only

Correct sample spectrum

Correction specification:  New Details

Operator Prompts

Before background: (No operator prompt) New Details

Before sample: (No operator prompt) New Details

Multiple Event Results

Retain all event results

Retain most recent result

### Collect event parameters

The collect event parameters define data collection in a workflow, including software and instrument settings, operator prompts, spectral corrections, and the storage of data from multiple collect events positioned in a repeat or perform-while loop. The following sections explain the collect event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Sample Parameters

The sample parameters define data collection for a given sample type or material. These parameter settings are independent of the sampling technique. The sample parameters include the following:

If you use the workflow wizard to add a collect event to a workflow, the wizard also creates and links appropriate sample and background specifications.

- **Sample Specification.** Use this feature to link a sample specification to this event. The sample specification contains advanced collection parameters that are optimized for a given sampling technique. If the workflow already contains an appropriate sample specification, select its name in the drop down list (see below).



Use the Details button to the right of the list box to display the selected sample specification, or the New button to create a sample specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the collect event. The new specification will be linked to the collect event and its name will appear in the sample specification list box. See “Sample specifications” in “Chapter 5 Workflow Specifications” for more information.

**Note** The sample specification must be linked a background specification, which defines background collection for the technique. ▲



- **Number Of Sample Scans.** This parameter determines how many scans are performed during a data collection. If you perform more than one scan, the system averages all of them.

Increasing the number of scans reduces the noise level of the data (increases the signal-to-noise ratio) and increases the sensitivity; that is, the ability to distinguish small peaks from noise. However, if you have already collected a large number of scans, it will take many more scans to achieve a significant increase in sensitivity.

Optimize the Number Of Sample Scans setting whenever you analyze a new type of sample or use a new sampling technique or accessory. If you're not sure how long to scan, start by collecting 16 scans and then measure the signal-to-noise ratio. This will give an indication of how many scans to collect for the desired results. See the section entitled “Antaris Sampling” in your main analyzer user guide for recommendations for setting Number of Sample Scans for each Antaris sampling module or system.

For a given resolution, increasing the number of scans increases the total collection time. When collecting data from many samples in a production environment, collection time may be a considerable factor when setting up workflows. The table below contains various collection times, along with the combinations of Resolution and Number Of Sample Scans parameter settings that will achieve those times. The Number Of Sample Scans settings and times are approximations.

Time (in seconds)	Resolution (cm-1)	Number of Scans
15	2	18
	4	19
	8	28
	16	35
	32	43
	64	46
30	2	36
	4	38
	8	56
	16	70
	32	86
	64	92
60	2	72
	4	76
	8	112
	16	140
	32	172
	64	184
120	2	144
	4	152
	8	224
	16	280
	32	344
	64	368

**Note** Because the standard tablet analyzer contains a highly sensitive detector and operates at a slower mirror velocity than other sampling accessories, the accessory’s collection times will differ from other sampling accessories. See “Tablet Analyzer Sampling Module” in your main analyzer user guide for a table of collection times for the standard tablet analyzer sampling module. ▲



- **Data Format.** This parameter determines the units used for the collected data. The following tables show the recommended format settings and corresponding units for diffuse-reflection and transmission

sampling. See “Antaris Sampling” in your main analyzer user guide for recommendations for setting Data Format for each Antaris sampling module or system.

For diffuse-reflection sampling (Antaris integrating sphere and fiber optic sampling module with SabIR probe), set Data Format to one of the following:

Setting	X-axis unit	Y-axis unit
% Reflectance	Wavenumber (cm-1)	% reflectance units
Log (1/R)*	Wavenumber (cm-1)	Log (1/R) units
Kubelka-Munk*	Wavenumber (cm-1)	Kubelka-Munk units
Single beam	Wavenumber (cm-1)	arbitrary units
Single beam (raw)	Wavenumber (cm-1)	arbitrary units
Interferogram	Data points	volt

\* Recommended format for spectra that will be used for quantitative measurements.

For transmission sampling (Antaris transmission module and tablet analyzers), set Data Format to one of the following:

Setting	X-axis unit	Y-axis unit
% Transmittance	Wavenumber (cm-1)	% transmittance
Absorbance*	Wavenumber (cm-1)	absorbance units
Single beam	Wavenumber (cm-1)	arbitrary units
Single beam (raw)	Wavenumber (cm-1)	arbitrary units
Interferogram	Data points	volt

\* Recommended format for spectra that will be used for quantitative measurements.

The Interferogram setting allows you to access the unprocessed data produced by the analyzer. The interferogram contains the encoded detector response at all frequencies in the spectral range.

A single-beam spectrum is produced by Fourier transforming an interferogram. A single-beam spectrum shows the measurable detector response at all frequencies in the spectral range.

A sample single-beam spectrum is ratioed against a background single-beam spectrum to produce a sample transmission or reflection spectrum with the background information removed. The other data formats are produced by mathematically converting the sample transmission or reflection spectrum to the selected Y-axis unit.

Select the Single Beam format, rather than Single Beam (raw), if you want to collect single-beam background and/or sample spectra in a workflow.

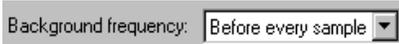
These single-beam spectra are normalized using the following equation:

$$\text{Single beam} = \text{single beam (raw)} \times \text{attenuation screen factor} \times \text{detector gain factor}$$

**Note** To view the current values for the screen factors, choose Instrument Status from the Maintenance menu in RESULT Operation, select Show Detailed Detector Information, and then choose OK. □▲

The normalized single-beam spectra have been adjusted to account for natural variations in the screens mounted in the attenuation wheel, and in the detector response. Using normalized single-beam spectra helps ensure that these differences do not affect the analytical results when workflows are transferred between systems. Using normalized single-beam spectra will also improve prediction accuracy when using different attenuation and detector gain settings for background and sample collection.

**Note** The Single Beam (raw) data format is used for diagnostic purposes only. ▲



- **Background Frequency.** This option lets you specify when to collect a background for ratioing sample spectra produced by a collect event. The Background Frequency parameter is available in the software, except when Data Format is set to Single Beam, Single Beam (Raw), or Interferogram.

Select Before Every Sample if you want to collect a background spectrum before each sample spectrum or Once For Each Workflow Run to collect one background and use it to process all of the sample spectra produced by a collect event in the workflow. (If the collect event is positioned in a repeat or perform-while loop, all of the spectra produced by the loop will be processed using the same background spectrum.)

The remaining options allow you to specify the maximum amount of time a background is valid before it expires. If you select one of these options, before the software collects a sample spectrum, it examines the current background to determine if it has expired. If the current background is still valid, then the software continues collecting the sample data. If the current background has expired, then the software either prompts the operator to collect a background (if a Before Background operator prompt is specified), or simply collects a background without prompting the operator if background measurements are taken using an internal background path or reference.

Set Background Frequency to No Expiration if you want the workflow to collect one background spectrum and use it to process all the spectral data from this collect event. The workflow will not initiate another background collection.

**Note** If you want the workflow to process the sample data using an archived background spectrum, use a Load Spectrum event to load the archive file into the workflow and then add a sample correction specification to the collect event (see “Correct Sample Spectrum” below). In the correction specification, set Spectrum CB to the background spectrum and set Correction Equation to S/CB. ▲

**Note** For demanding applications, you can obtain the best results by collecting the background just before each sample spectrum. ▲

Background folder: C:\RESULT\Backgrounds

- **Background Folder.** This readout shows the current folder and path for archiving backgrounds in RESULT Integration (as defined in the Options dialog box available from the Edit menu in RESULT Integration). Any background spectra collected by this workflow will be placed in this location when the workflow is run in RESULT Integration.

If the workflow is transferred to RESULT Operation, backgrounds will be archived using the folder and path for archiving backgrounds for that application (as defined in the RESULT Options dialog box available from the Administration menu in RESULT Operation). See “Chapter 4 Setting RESULT Operation Options” in the “RESULT Software Administration” manual for information about setting the path for archiving backgrounds in RESULT Operation.

**Note** Background files are archived except when Background Frequency is set to Before Every Sample. ▲

Collect background only

- **Collect Background Only.** Select this option if you want this collect event to collect and store only a background spectrum (no sample spectra will be collected). This feature is helpful for performing quality checks on a background spectrum before using it to process sample spectra in a workflow. When Collect Background Only is selected, the software automatically sets Data Format to Single Beam, which is the typical format for displaying and archiving background spectra, and Background Frequency is unavailable. The software uses the setting for Number Of Background Scans in the background specification to determine the number of scans to collect for the background spectrum.

Correct sample spectrum

- **Correct sample spectrum.** Select this option if you want to apply a spectral correction to the sample spectra produced by this collect event. Spectral corrections can improve accuracy for some NIR experiments. When this option is selected, the correction specification drop-down list box becomes available in the software.

Use the list box to link a correction specification to this event. If the workflow already includes an appropriate correction specification, select its name in the drop-down list.



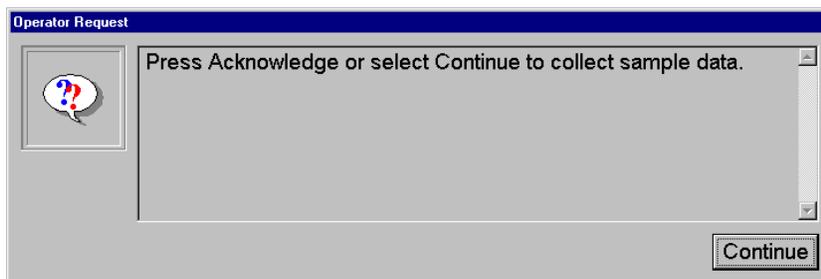
Use the Details button to the right of the list box to display the current settings for the correction specification parameters, or the New button to create a correction specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the collect event. The new specification will be linked to the collect event and its name will appear in the correction specification list box. See “Correction specifications” in “Chapter 5 Workflow Specifications” for more information.

## Operator Prompts

The operator prompts allow you to attach two operator prompt specifications to the collect event. Each operator prompt specification creates a dialog box that contains a user-defined message and one button for the operator response.

Each time a workflow performs a collect event, the workflow typically collects background and sample data to produce a spectrum. (If Collect Background Only is selected, then the collect event will produce a background spectrum only.) If a collect event includes a “before background” operator prompt, the prompt will be displayed immediately before the instrument collects a background spectrum. The “before sample” operator prompt (if included in the workflow) appears immediately before sample collection. The operator must acknowledge the prompt before data collection will begin by responding to the dialog box in the software or by pressing the Acknowledge button on the instrument front panel (available on Antaris Near-IR systems only).

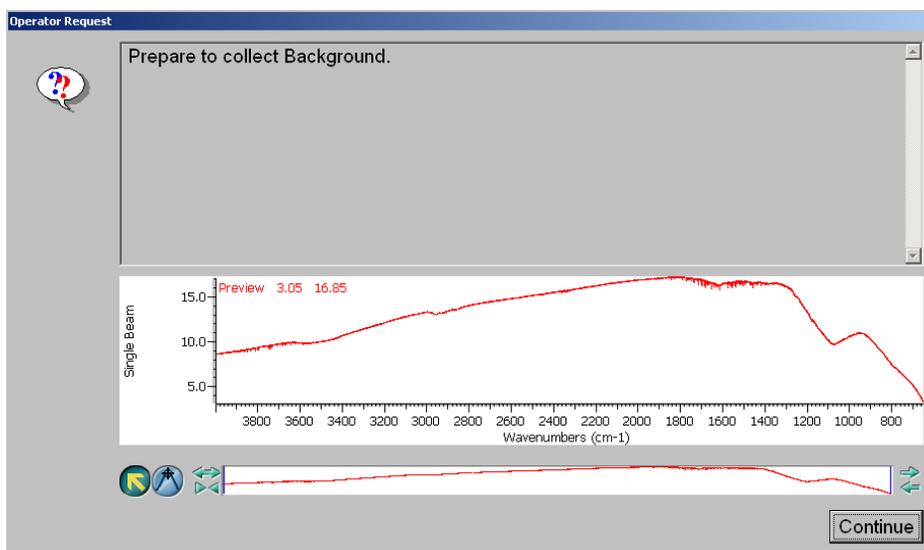
These prompts are typically used to provide instructions to the operator to prepare for background and sample collection in a workflow. An example operator prompt for sample collection is provided below.



If Preview Data Collection is selected on the prompt specification, the workflow displays the prompt at run time and begins collecting data. The dialog box is expanded to include a collection window, as shown in the example below. The sample data are displayed in the format specified in the workflow.

The workflow continues collecting (but not saving) the data until the operator chooses Continue in the prompt. After the operator chooses Continue, the workflow continues.

The background preview shows single scans of the background. If the workflow is designed to collect multiple background scans, the final background spectrum will be the average of all collected scans.



See “Prompt specifications” in “Chapter 5 Workflow Specifications” for more information about the Preview Data Collection feature.

- **Before Background.** Use this list box to link a Before Background prompt specification to this collect event by selecting the specification name in the Before Background drop-down list.



Use the New button next to the list box to create an operator prompt specification and automatically link the new specification to this collect event. If this collect event is already linked to a prompt specification, use the Details button to the right of the list box to display that specification.

**Note** Background prompts are often unnecessary, especially when background spectra are collected using an internal background path or reference. Workflows designed to collect spectra using an Antaris tablet analyzer, or to collect a background using an external reference may require a background prompt. ▲

- **Before Sample.** Use this list box to link a Before Sample prompt specification to this collect event by selecting the specification name in the Before Sample drop-down list.



Use the New button next to the list box to create an operator prompt specification and automatically link the new specification to this collect event. If this collect event is already linked to a prompt specification, use the Details button to the right of the list box to display that specification.

See “Prompt Specifications” in this chapter for information about setting up operator prompt specifications in a workflow. See “Antaris Sampling” in your main analyzer user guide for suggested operator prompt text for each Antaris sampling module or system.

### Multiple Event Results

#### Multiple Event Results

- Retain all event results
- Retain most recent result

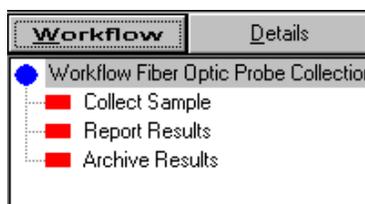
If you place a collect event in a repeat or perform-while loop, the event will produce one result (spectrum) during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent result. The options for storing results include:

- **Retain All Event Results.** If the collect event occurs in a loop, selecting this option causes the workflow to store all the collected data. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the collect event is not positioned in a loop or the loop includes all subsequent events that operate on the stored data. This is the default setting and will maximize your computer processing speed.

See “repeat events” and “perform-while events” for more information about using stored data in a workflow.

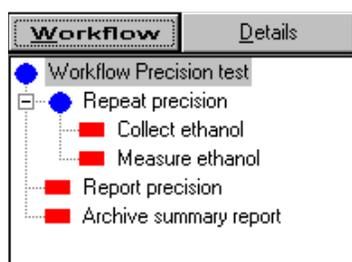
**Usage:** A collect event must be linked to a valid sample specification, and that sample specification must be linked to a valid background specification in order to produce a spectrum.

Collect events may be placed anywhere in a workflow. The example below shows a workflow that collects a spectrum, creates a sample report, and then archives the spectrum and the report.



Place the collect event in a repeat or perform-while loop to collect spectra from a series of similar samples as shown below. See “Repeat events” and “Perform-while events” for more information.

Set up the collect event to retain all the spectra generated by the loop if you want to add them to the sample report. See “Multiple Event Results” above for more information.



The following events can operate on the collection result (spectrum) if those events are positioned after the collect event in the workflow.

- **Measure event**, which can be used to analyze the collected spectra.
- **Compare event**, which can be used to compare a series of spectra and their measured values against expected values to produce correlation coefficients, root mean square error of prediction (RMSEP) values, and slope and y-intercept values for those measurements.
- **Process event**, which can be used to calculate an average spectrum, a variance spectrum or a series of difference spectra from the collected spectra when the collect event occurs in a loop. You can also calculate a difference spectrum from multiple spectra produced by a collect event.
- **Archive event**, which can be used to archive the collected spectra.
- **Report event**, which can be used to add the collected spectra to a sample report.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Collect Dual Tablet events

This event can be used to collect a transmission and reflection spectrum at the same time using a tablet analyzer with an Antaris II instrument. The event must be linked to valid sample and background specifications for the tablet analyzer and for the Antaris integrating sphere. Each spectrum can have an associated sample correction specification.

**Note** You can also use a normal Collect event to collect a sample and background specification with a tablet analyzer. See “Collect events” for details. ▲

The Collect Dual Tablet event may also include operator prompt specifications for the sample and background. Prompt specifications can be used to define message dialog boxes that will be displayed before the start of sample and background collection in the workflow. For example, a message might explain how to position the sample to collect the sample data and then wait until the operator responds to the dialog before collecting the sample scans.

Each time a workflow performs a Collect Dual Tablet event, the workflow produces two spectra, including a reflection spectrum taken with the integrating sphere module on the instrument and a transmission spectrum collected with the detector in the tablet analyzer module. The workflow automatically stores the latest set of spectra in the computer’s internal memory so the spectra are available for use by subsequent events in the workflow such as a measure event or report event. If you want to archive the spectra, you must add an archive event to your workflow and then add each spectrum to the list of results to be archived.

You can use a Collect Dual Tablet event with both types of tablet analyzer modules (standard tablet and softgel tablet).

**Event result:** One reflection spectrum and one transmission spectrum

**Associated specifications:** Standard Tablet Analyzer sample specification, SoftGel Tablet Analyzer sample specification, Standard Tablet Analyzer background specification, SoftGel Tablet Analyzer background specification, Sample Correction specification, Before Background operator prompt specification, Before Sample operator prompt specification

**Related events:** Measure event, Report event, Archive event, Compare event

**Related specifications:** Measurement specification, table item specification, spectrum item specification

**Parameters:** The illustration below shows the parameters for the Collect Dual Tablet event. These parameters appear in the display area of RESULT Integration when a Collect Dual Tablet event is selected in a workflow.

Collect Transmission/Reflection Result: spectra

New

Sample Parameters

Number of sample scans: 16 Data format: Absorbance

Pre-collection delay (sec): 0 Attenuator: Empty

Resolution: 8.0 cm-1

Background frequency: Before every sample

Background folder: C:\RESULT Data\Backgrounds

Collect background only

Transmission Sample specification: New Sample New Details

Correct transmission sample spectrum

Correction specification: New Details

Reflection Sample specification: New Details

Correct reflection sample spectrum

Correction specification: New Details

Operator Prompts

Before background: (No operator prompt) New Details

Before sample: (No operator prompt) New Details

Multiple Event Results

Retain all event results

Retain most recent result

### Collect Dual Tablet event parameters

The Collect Dual Tablet event parameters define software and instrument settings, operator prompts, spectral corrections and the storage of data from multiple events placed in a loop. The following sections explain the Collect Dual Tablet event parameters in detail. The parameters are explained in the order in which they appear in the software.

## Sample Parameters

The sample parameters define data collection for a given sample type or material. The parameter settings apply to both beam paths (transmission and reflection) and to the sample and background spectra. The sample parameters include the following:

Number of sample scans:

- **Number Of Sample Scans.** This parameter determines how many scans are performed during a data collection. Choose a setting that meets the signal-to-noise requirements of both spectra. If you perform more than one scan, the system averages all of them. See “Collect events” in this chapter for more information about setting this parameter in workflows.

Pre-collection delay (sec):

- **Pre-collection delay.** Use this box to specify a delay before sample collection begins. If you specify a pre-collection delay, when you run the workflow, the system will wait the specified number of seconds before it begins collecting the sample data. This is often useful for allowing a cooled or heated sample time to reach room temperature and stabilize before starting the analysis.

Leave Pre-collection Delay set to zero if you don't want to delay data collection.

Resolution:

- **Resolution.** Use this list box to specify the resolution of the collected spectra. Resolution is a measure of how well closely spaced peaks in a spectrum are differentiated. The higher the resolution, the more closely spaced peaks can be and still be differentiated.

The Resolution drop-down list includes all the resolution settings available for the instrument model configured in the RESULT Integration Options dialog box (see “Setting RESULT Integration options” in “Chapter 2 Getting Started” of the “RESULT Integration User Guide” for details). Although the highest ( $2\text{ cm}^{-1}$ ) resolution setting is available on all Antaris near-infrared systems, the optional two-position aperture is required to achieve maximum spectral resolution at that resolution setting across the full spectral range. The software automatically selects the smaller aperture (if available) when the  $2\text{ cm}^{-1}$  resolution setting is selected in the workflow. Antaris II systems that include the optional two-position aperture will use the small aperture setting automatically when Resolution is set to  $2\text{ cm}^{-1}$ . Other systems that only have the larger aperture or no aperture can produce the  $2\text{ cm}^{-1}$  resolution but the bands will not be as sharp.

For recommended resolution settings for a specific Antaris instrument, see the section titled “Antaris Sampling” in your *Antaris User Guide*.

**Note** A higher resolution is expressed by a lower numerical value. For example, a spectrum with 4 cm<sup>-1</sup> resolution has higher resolution than a spectrum with 8 cm<sup>-1</sup> resolution. Keep this in mind when you set the Resolution parameter. ▲

Background frequency: Before every sample ▼

- **Background Frequency.** This option lets you specify when to collect a background for ratioing sample spectra produced by a Collect Dual Tablet event. The Background Frequency parameter is relevant except when Data Format (see below) is set to Single Beam, Single Beam (Raw), or Interferogram. (None of these settings requires a background spectrum.) See “Collect events” in this section for more information about setting this parameter in workflows.

Background folder: C:\RESULT Data\Backgrounds

- **Background Folder.** This readout shows the current folder and path for archiving backgrounds in RESULT Integration (as defined in the Options dialog box available from the Edit menu in RESULT Integration). Any background spectra collected by this workflow will be placed in this location when the workflow is run in RESULT Integration.

If the workflow is transferred to RESULT Operation, backgrounds will be archived using the folder and path for archiving backgrounds for that application (as defined in the RESULT Options dialog box available from the Administration menu in RESULT Operation).

**Note** Background files are archived except when Background Frequency is set to Before Every Sample. ▲

Collect background only

- **Collect Background Only.** Select this option if you want this event to collect and store a background spectrum only (no sample spectra will be collected). This feature is helpful for performing quality checks on a background spectrum before using it to process sample spectra in a workflow. When Collect Background Only is selected, the software automatically sets Data Format to Single Beam, which is the typical format for displaying and archiving background spectra, and Background Frequency is unavailable. The software uses the setting for Number Of Background Scans in the background specification to determine the number of scans to collect for the background spectrum.

Data format: Absorbance

Attenuator: C Screen

- **Data Format.** This parameter determines the units used for the collected data. The Collect Dual Tablet event offers the same options for Data Format as the single Collect event. See “Data Format” in “Collect events” for information about selecting a data format for your spectra.
- **Attenuator.** The detectors installed in the Antaris Near-IR analyzers are highly sensitive and can become saturated or produce a distorted signal if too much light reaches the detector element. The attenuation wheel provides two calibrated, energy-limiting screens that can be used to lower the energy sent to a sample. The screens are software selectable and have the following effect on the incident infrared beam.

Screen	Percent of Incident Light Transmitted
None (Empty)	100
B	6 - 10 %
C	2.5 - 3.5%
C + polystyrene	2.5 - 3.5%

### Attenuation screens in the Antaris Near-IR analyzer

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

Tablet samples are typically measured without an attenuator screen (set Attenuator to Empty) and with a higher gain setting because they are often highly absorbing. If the sample peaks in the resulting spectrum are totally absorbing when measured without a screen, switch to the B screen. See the Tablet Analyzer chapter in your *Antaris User Guide* for more information.

**Note** See Optimize Gain on the Dual Tablet sample specifications for information about using the Optimize Gain feature on the sample specification to select the appropriate attenuation and gain settings for a particular sample. ▲

For most analyses, the software uses the selected Attenuator setting to collect both the background spectrum and the sample spectrum. The tablet analyzer sampling module is an exception because, in default

mode, it uses the C screen (with a gain setting of “1”) to collect background data for transmission analyses. The Attenuator setting selected in the software is used only for the samples. To override the default attenuation and gain settings for transmission backgrounds collected with a tablet analyzer, select Use Sample Position, Gain, And Attenuation Settings in the background specification that is linked to this sample specification. See “Dual Tablet Background Specifications” in this section for more information.

## Transmission Specifications

The features in this group can be used to link a sample and correction specification to the Collect Dual Tablet event to define transmission data collection with the Antaris tablet analyzer. The transmission specification parameters include the following:

- **Transmission Sample Specification.** Use this feature to link a tablet analyzer sample specification to this event. The sample specification contains advanced collection parameters that are optimized for a given sampling technique. If the workflow already contains an appropriate sample specification, select its name in the drop down list (see below).



Use the Details button to the right of the list box to display the current settings, or the New button to create a sample specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the collect event. The new specification will be linked to the collect event and its name will appear in the sample specification list box. See “Sample specifications” in “Chapter 5 Workflow Specifications” for more information.

Correct transmission spectrum

Clear this check box if you do not wish to apply a spectral correction to the transmission data.

- **Correct Transmission Spectrum.** Select this option if you want to apply a spectral correction to the transmission sample spectra produced by this event. Spectral corrections can improve accuracy for some NIR experiments. When this option is selected, the correction specification drop-down list box becomes available in the software.

Use the list box to link a correction specification to the transmission sample spectrum. If the workflow already contains an appropriate correction specification, select its name in the drop-down list.



Use the Details button to the right of the list box to display the current settings, or the New button to create a correction specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the collect event. The new specification will be linked to the collect event and its name will appear in the correction specification list box. See “Correction specifications” in “Chapter 5 Workflow Specifications” for more information.

## Reflection Specifications

The features in this group can be used to link a sample and correction specification to the Collect Dual Tablet event to define reflection data collection with the Antaris integrating sphere. The reflection specification parameters include the following:

- **Reflection Sample Specification.** Use this feature to link an integrating sphere sample specification to this event. If the workflow already contains an appropriate sample specification, select its name in the drop down list, as shown below.



Use the Details button to the right of the list box to display the current settings, or the New button to create a sample specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the collect event. The new specification will be linked to the collect event and its name will appear in the sample specification list box. See “Sample specifications” in “Chapter 5 Workflow Specifications” for more information.

Correct reflection spectrum

Clear this check box if you do not wish to apply a spectral correction to the reflection data.

- **Correct Reflection Spectrum.** Select this option if you want to apply a spectral correction to the reflection sample spectra produced by this event. Spectral corrections can improve accuracy for some NIR experiments. When this option is selected, the correction specification drop-down list box becomes available in the software.

Use the list box to link a correction specification to the reflection sample spectrum. If the workflow already contains an appropriate correction specification, select its name in the drop-down list.



Use the Details button to the right of the list box to display the current settings, or the New button to create a correction specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the collect event. The new specification will be linked to the collect event and its name will appear in the correction specification list box. See “Correction specifications” in “Chapter 5 Workflow Specifications” for more information.

## Operator Prompts

The operator prompts allow you to attach two operator prompt specifications to the Collect Dual Tablet event. Each operator prompt specification creates a dialog box that contains a user-defined message and one button for the operator response. If this event includes a “before background” operator prompt, the prompt will be displayed immediately before the instrument collects a background spectrum. The “before sample” operator prompt (if included) appears immediately before sample collection. The operator must acknowledge the prompt before data collection will begin. See “Operator Prompts” in “Collect events” for more information.

## Multiple Event Results

### Multiple Event Results

- Retain all event results
- Retain most recent result

If you place a Collect Dual Tablet event in a repeat or perform-while loop, the event will produce one set of results (spectra) during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent result or set of results. The options for storing results include:

- **Retain All Event Results.** If the Collect Dual Tablet event occurs in a loop, selecting this option causes the workflow to store all the collected data. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the Collect Dual Tablet event is not positioned in a loop or the loop includes all subsequent events that operate on the stored data. This is the default setting and will maximize your computer processing speed.

See “Repeat events” and “Perform-while events” for more information about using stored data in a workflow.

**Usage:** A Collect Dual Tablet event must be linked to a valid transmission and reflection sample specification in order to produce the two spectra. In many cases, background specifications must also be included.

If you want the workflow to archive the spectra from a Collect Dual Tablet event, you must add a subsequent archive event to the workflow and add each spectrum to the list of results to be archived.

The following events can operate on the collection results (spectra) if those events are positioned after the Collect Dual Tablet event in the workflow.

- **Measure event**, which can be used to analyze the collected spectra.
- **Compare event**, which can be used to compare a series of spectra and their measured values against expected values to produce correlation coefficients, root mean square error of prediction (RMSEP) values, and slope and y-intercept values for those measurements.

- **Process event**, which can be used to calculate an average spectrum, a variance spectrum or a series of difference spectra from the collected spectra when the Collect Dual Tablet event occurs in a loop. You can also calculate a difference spectrum from the two spectra produced by a Collect Dual Tablet event.
- **Archive event**, which can be used to archive the collected spectra.
- **Report event**, which can be used to add the collected spectra to a sample report.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Collect Multi-Channel events

This event works with the Antaris MX and Antaris EX systems only. You can use a collect multi-channel event to set up data collection from two or more *fiber optic sampling accessories* at the same time. Each instrument channel configured for data collection must have an associated multi-channel sample specification. Each spectrum can have an associated background specification and sample correction specification.

**Note** You can also use a normal Collect event to collect a sample and background specification with the Antaris MX and Antaris EX. See “Collect events” for details. ▲

The collect multi-channel event may also include operator prompt specifications for the sample and background. Prompt specifications can be used to define message dialog boxes that will be displayed before the start of sample and background collection in the workflow. For example, a message might explain how to position the sample and probe to collect the sample data and then wait until the operator responds to the prompt before collecting the sample scans.

Each time a workflow performs a collect multi-channel event, the workflow produces one spectrum from each configured fiber optic channel. The workflow automatically stores the latest spectrum or group of spectra in the computer’s internal memory so the spectra are available for use by subsequent events in the workflow such as a measure event or a report event. If you want to archive the spectra, you must add an archive event to your workflow and then add each spectrum to the list of results to be archived.

**Event result:** One spectrum for each fiber optic channel configured for data collection

**Associated specifications:** Multi-Channel sample specification, Multi-Channel background specification, sample correction specification, Before Background operator prompt specification, and Before Sample operator prompt specification

**Related events:** Measure event, Report event, Archive event, Compare event

**Related specifications:** Measurement specification, table item specification, spectrum item specification

**Parameters:** The illustration below shows the parameters for the collect multi-channel event. These parameters appear in the display area of RESULT Integration when a collect multi-channel event is selected in a workflow.

Multi-Channel Collect Result: spectra

kk

**Sample Parameters**

Number of sample scans: 16      Sample position: Empty

Pre-collection delay (sec): 0      Resolution: 8.0 cm-1

Background frequency: Before every sample

Background folder: C:\RESULT Data\Backgrounds

Use sample channel for background measurements       Correct sample spectrum

**Operator Prompts**

Before background: (No operator prompt)      New      Details

Before sample: (No operator prompt)      New      Details

**Channel Set Up**

Sample Channel	Final Format	Sample Specification	Background Chan...	Background Specificat...

Specification Type: Sample Specification      New      Details

**Multiple Event Results**

Retain all event results

Retain most recent result

### Collect multi-channel event parameters

The collect multi-channel event parameters define data collection for the Antaris MX and Antaris EX systems, including software and instrument settings, operator prompts, sample corrections, and the storage of data from

multiple collect multi-channel events positioned in a repeat or perform-while loop. The following sections detail the collect multi-channel event parameters. The parameters are explained in the order in which they appear in the software.

## Sample Parameters

The sample parameters define data collection for a given sample type or material. The parameter settings apply to all channels configured for data collection and to both the background and the sample spectra.

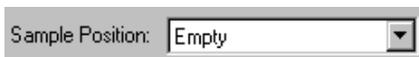
**Note** Multi-channel collection works best with similar types of samples and fiber optic probes that are the same or similar in design and operation. If the workflow will be used to collect data from materials or fiber optic accessories that have different sampling requirements, use sample parameter settings that meet the requirements of the most demanding sample, application or fiber optic accessory, or use a separate collect multi-channel event for each material, application or accessory. ▲

The sample parameters include the following:



Number of sample scans: 16

- **Number Of Sample Scans.** This parameter determines how many scans are performed during a data collection. Choose a setting that meets the signal-to-noise requirements of all channels. For example, if a sample measured from one channel requires 60 scans to achieve adequate signal-to-noise and a sample measured at a different channel requires only 32 scans, set Number Of Scans to 60. If you perform more than one scan, the system averages all of them. See “Collect events” in this section for more information about setting this parameter in workflows.



Sample Position: Empty



Background Position: Empty

See “Setting RESULT Integration options” in the “RESULT Integration User Guide” for instructions to configure the validation wheel.

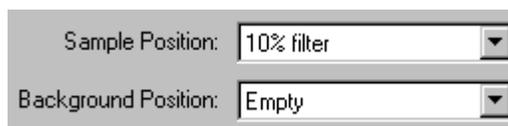
- **Sample Position/Background Position.** These options appear on the collect multi-channel event only when the optional internal validation wheel is installed in the instrument and properly configured in RESULT software. The validation wheel contains standard samples that can be used for diagnostic purposes and for running qualification tests with the Thermo Scientific optional ValPro System Qualification package. The wheel also has an opening that contains no sample. The empty position is used for sample and background measurements through the fiber optic channels on the instrument.

Use the Sample Position and Background Position drop down list boxes to define the validation wheel position for collecting sample and background data with the instrument.

- *To collect data through a fiber optic channel on the instrument, use the table in Channel Setup to define sample and background collection and set Sample Position and 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 validation wheel setting affects all channels. When collecting data from samples using fiber optic accessories connected to the instrument, be sure to set Sample Position and Background Position to Empty. ▲

- *To collect data from a sample in the validation wheel, set Sample Position to the appropriate sample and set Background Position to Empty.*



Sample Position: 10% filter

Background Position: Empty

The validation 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.

See the example workflows that came with ValPro System Qualification and your ValPro user manuals for information about the use of validation wheel samples for instrument qualification. To learn how to run instrument performance tests with the polystyrene sample, see “Instrument check spectra” in “Chapter 5 System Maintenance” of the “RESULT Operation Software User Guide.”

Pre-collection delay (sec):

- **Pre-collection delay.** Use this box to specify a delay before sample collection begins. If you specify a pre-collection delay, when you run the workflow, the workflow will wait the specified number of seconds before it begins collecting data from a fiber optic or validation wheel sample.

Leave Pre-collection Delay set to zero if you don't want to delay data collection.

Resolution:

- **Resolution.** Use this list box to specify the resolution of the collected spectra. Resolution is a measure of how well closely spaced peaks in a spectrum are differentiated. The higher the resolution, the more closely spaced peaks can be and still be differentiated.

The Resolution drop-down list includes all the resolution settings for the Antaris MX and Antaris EX.

**Note** The highest (2 cm<sup>-1</sup>) resolution setting is available for the Antaris MX and Antaris EX systems. However, since these analyzers do not include the smaller aperture, the band shape will not be optimized across the full spectral range. ▲

For recommended resolution settings for the MX, see the section titled “Antaris Sampling” in your *Antaris MX User Guide*.

**Note** A higher resolution is expressed by a lower numerical value. For example, a spectrum with 4 cm<sup>-1</sup> resolution has higher resolution than a spectrum with 8 cm<sup>-1</sup> resolution. Keep this in mind when you set the Resolution parameter. ▲

Background frequency:

- **Background Frequency.** This option lets you specify when to collect a background for ratioing sample spectra produced by a collect multi-channel event. The Background Frequency parameter is relevant except when Data Format (see below) is set to Single Beam, Single Beam (Raw), or Interferogram. (None of these settings requires a background spectrum.) See “Collect events” in this section for more information about setting this parameter in workflows.

Background folder: C:\RESULT Data\Backgrounds

- **Background Folder.** This readout shows the current folder and path for archiving backgrounds in RESULT Integration. Use the RESULT Options dialog box in the Edit menu to specify the location for archiving backgrounds produced by workflows run in RESULT Integration.

If the workflow is transferred to RESULT Operation, backgrounds will be archived using the folder and path for archiving backgrounds for that application. See “Chapter 4 Setting RESULT Operation Options” in the “RESULT Software Administration” guide for information about setting the path for archiving backgrounds in RESULT Operation.

**Note** Background files are archived except when Background Frequency is set to Before Every Sample or No Expiration. ▲

Use sample channel for background

- **Use Sample Channel For Background Measurements.** Select this option if you want to ensure that the background spectra are collected through exactly the same beam path as the sample spectra, typically when collecting backgrounds from an external reference. Using the sample beam path for the background measurement will help to minimize any differences between the sample and background beam paths on the final spectra because they cancel each other out when the sample is ratioed against the background. You can also use this feature to measure a 100% line spectrum (i.e., no sample or background material in the beam path). A 100% line spectrum can be useful for diagnostic purposes and is part of the Instrument Check feature of RESULT Operation (see “Instrument Check” in the “RESULT Operation User Guide” for more information). When the check box is selected, all background collections occur at the corresponding sample channel and the Background Channel column disappears from the Channel Setup group (see below).

Clear the check box if you want to select a specific location for taking background measurements for each channel. See “Background Channel” (below) for details.

Correct sample spectrum

- **Correct sample spectrum.** Select this option if you want to apply a spectral correction to the sample spectra produced by this collect multi-channel event. Spectral corrections can improve accuracy for some NIR experiments. When this option is selected, the correction specification drop-down list box becomes available in the software.

When Correct Sample Spectrum is selected on the collect multi-channel event, the software adds a Correction Specification column to the table in the Channel Setup group. See “Channel Setup” (below) to learn how to link a correction specification to a multi-channel sample collection. For information about how to define a correction equation, see “Correction specifications” in “Chapter 5 Workflow specifications” of this document.

Clear the check box if you do not wish to apply a spectral correction to your sample data.

### **Operator Prompts**

The operator prompts allow you to attach two operator prompt specifications to the collect multi-channel event. Each operator prompt specification creates a dialog box that contains a user-defined message and one button for the operator response. If a collect multi-channel event includes a “before background” operator prompt, the prompt will be displayed immediately before the instrument collects a background spectrum. The “before sample” operator prompt (if included) appears immediately before sample collection. The operator must acknowledge the prompt before data collection will begin. See “Operator Prompts” in “Collect Events” for more information.

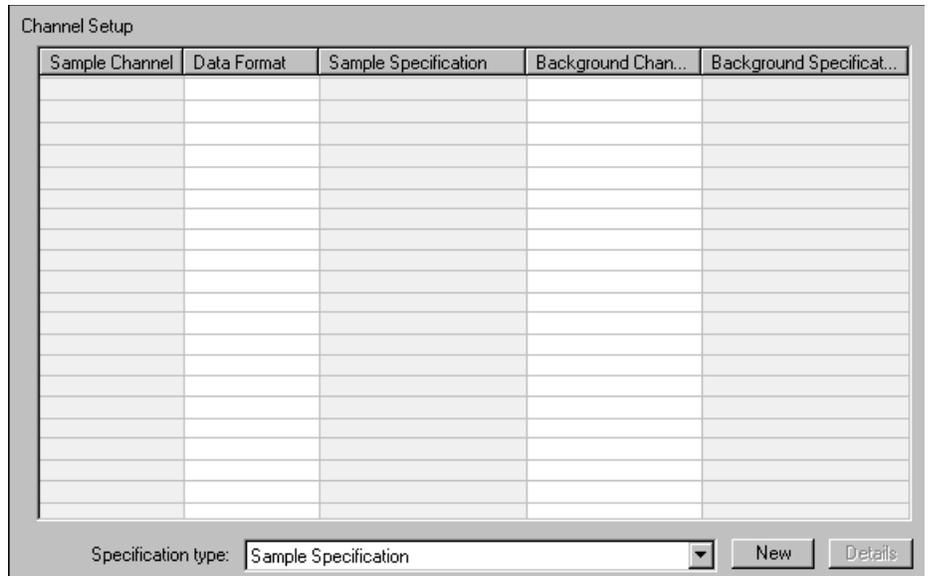
### **Channel Setup**

Use the features in this group to specify data collection for each active channel on the instrument. You can set up data collection from a single fiber optic channel or specify collections from multiple sample and background locations at the same time. Similar to collect events in a workflow, sample and background collections for the collect multi-channel event are based on associated sample and background specifications. If Correct Sample Spectrum is selected on the collect multi-channel event (see above), you can also apply a spectral correction to the sample data by using an associated sample correction specification.

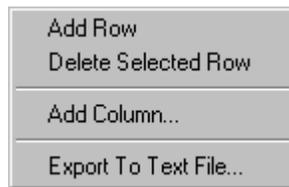
To delete a row in the table, right-click the row to display a shortcut menu and choose Delete Selected Row, or select the row and press Delete on the keyboard.

Use Export To Text File to write the device information displayed in the table to a text file with a file name and path you specify.

To change the order in which the workflow will collect the data, drag the corresponding row to a new location in the table. To sort a column of entries in numeric or alphabetic order, right-click the column heading to display a shortcut menu and then choose Sort Ascending or Sort Descending.



The table is interactive and easy to work with. Right click an empty row to display a shortcut menu and then choose Add Row. The software displays a shortcut menu with the following options.



The columns in the table are described below. To edit a cell in a specific row and column, double-click the cell.

For each column in the table, you can specify a location (channel) for the sample and background collection and up to three specifications including a sample specification, background specification, and sample correction specification.

Sample Channel
1

- Sample Channel.** To specify the fiber optic channel for a sample measurement, double-click the corresponding cell in the Sample Channel column. The software displays a drop-down list box with the following options: None selected, 0, 1, 2, 3 and 4. To assign sample collection to channels 1, 2, 3 or 4 on the instrument, select the corresponding channel number. Use 0 to collect sample data from the instrument’s internal reference sample. This is usually appropriate for diagnostic purposes or to monitor instrument performance (see “Instrument check spectra” in “Chapter 6 System Maintenance” of the “RESULT Operation User Guide” for details. Use the “None selected”

option to suspend data collection for a given channel without deleting the associated specifications.

Final Format
% Reflectance

- **Data Format.** This column specifies the unit used for the collected data. To specify the unit for a sample measurement, double-click the corresponding cell in the Final Format column. The software displays a drop-down list box with multiple options. The collect multi-channel event offers the same options for Data Format as the single collect event. See the “Data Format” in “Collect events” for information about selecting a data format for your spectra.

Sample Specification
Fiber Sample 1

Specification Type:  ▼

- **Sample Specification.** Use this column to associate a sample specification with the sample measurement. To select a sample specification from existing multi-channel sample specifications in the workflow, double-click the appropriate cell in the Sample Specification column. The software displays a drop-down list box with the names of all the multi-channel sample specifications in the current workflow. Select a name from the drop-down list.

Background Channel
1

- **Background Channel.** To specify the fiber optic channel for the background measurement, double-click the corresponding cell in the Background Channel column. The software displays a drop-down list box with the following options: None selected, 0, 1, 2, 3 and 4. To assign background collection to channels 1, 2, 3 or 4 on the instrument, select the corresponding channel number. Use 0 to collect a background using the instrument’s internal reference. See your instrument user guide for more information about collecting backgrounds for fiber optic experiments.

**Note** The Background Channel column appears in the Channel Setup table unless the Use Sample Channel For Background Measurement check box is selected on the Collect multi-channel event (see above). If the check box is selected, background measurements will occur at the specified sample channel and the Background Channel option is not needed. ▲

Background Specification
New Fiber Optic Background1

Specification Type:  ▾

Correction Specificat...
NewCorrection1

Specification Type:  ▾

- Background Specification.** Use this column to associate a background specification with a sample measurement. To select a background specification from existing multi-channel background specifications in the workflow, double-click the appropriate cell in the Background Specification column. The software displays a drop-down list box with the names of all the multi-channel background specifications in the current workflow. Select a name from the drop-down list.
- Correction Specification.** Use this column to associate a sample correction specification with a sample measurement. To select a correction specification from existing correction specifications in the workflow, double-click the appropriate cell in the Correction Specification column. The software displays a drop-down list box with the names of all the correction specifications in the current workflow. Select a name from the drop-down list.

To display the parameters for a sample specification, background specification or correction specification associated with this collect multi-channel event, make sure the Specification Type list box is set to the type of specification you want to display, click the corresponding cell in the table and then choose the Details button next to Specification Type. For example, to display the background specification for channel 1, set Specification Type to Background Specification, click the cell that corresponds with Background Specification/Row 1 and then choose Details. (Click the Back button on the toolbar when you are ready to return to the collect multi-channel parameters.) Use the New button to create a specification for the selected column and row.

For more information, see “Multi-Channel sample specifications,” “Multi-Channel Background Specifications” and “Correction Specifications” in “Chapter 5 Workflow Specifications” of this document.

### Multiple Event Results

Multiple Event Results

Retain all event results

Retain most recent result

If you place a Collect multi-channel event in a repeat or perform-while loop, the event will produce one result (spectrum) or a set of results (spectra) during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent result. The options for storing results include:

- **Retain All Event Results.** If the Collect multi-channel event occurs in a loop, selecting this option causes the workflow to store all the collected data. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the Collect multi-channel event is not positioned in a loop or the loop includes all subsequent events that operate on the stored data. This is the default setting and will maximize your computer processing speed.

See “Repeat events” and “Perform-while events” for more information about using stored data in a workflow.

**Usage:** A collect multi-channel event must be linked to a valid sample specification in order to produce a spectrum. In many cases, a background specification must also be included. If you want the workflow to archive the spectra from a collect multi-channel event, you must add a subsequent archive event to the workflow and add each spectrum to the list of results to be archived.

The following events can operate on the collection results (spectra) if those events are positioned after the collect multi-channel event in the workflow.

- **Measure event**, which can be used to analyze the collected spectra.
- **Compare event**, which can be used to compare a series of spectra and their measured values against expected values to produce correlation coefficients, root mean square error of prediction (RMSEP) values, and slope and y-intercept values for those measurements.
- **Process event**, which can be used to calculate an average spectrum, a variance spectrum or a series of difference spectra from the collected spectra when the Collect Dual Tablet event occurs in a loop and Multiple Event Results is set to Retain All Event Results. You can also calculate a difference spectrum from the two spectra produced by a Collect Dual Tablet event.
- **Archive event**, which can be used to archive the collected spectra.
- **Report event**, which can be used to add the collected spectra to a sample report.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Compare events

This event can be used to measure a series of spectra and then compare the measurement results (calculated values) to the expected values using standard statistical techniques. For each measurement, such as a spectral peak height or a component concentration value, the comparison event produces the following information:

- **Expected value**, which is the known concentration value or spectral measurement for each spectrum. You must specify an expected value for each collected spectrum when you add the comparison event to your workflow. The comparison event lets you access the expected values from other events in the workflow.
- **Measured value**, which is the concentration value or spectral measurement produced by the calibrated method for each spectrum.
- **Correlation coefficient**, which is the standard correlation coefficient for the measured and expected values. The closer this value is to one the more linear is the relationship between the measured and expected values for the specified component.
- **Slope and y-axis intercept for the plotted measured versus expected values**. If a method measures concentration values perfectly (i.e., the measured value for every check sample matches its expected value exactly), the slope will be “1” and the y-axis intercept will be zero.
- **RMSEP (Root Mean Square Error of Prediction)**, which refers to the uncertainty of prediction for the selected component. RMSEP is calculated by squaring the error values, calculating the average and then taking the square root of the result. The unit for RMSEP is the same as the sample measurement, making it a good indicator of measurement error. For example, if concentration values are calculated in grams/milliliter, the RMSEP value will also be in grams/milliliter.

If the calibrated method measures more than one component or attribute, if it calculates concentration values for several compounds, for example, a set of comparison values is produced for each of those components or attributes.

Each time a workflow performs a comparison event, the workflow produces a set of data, referred to as the comparison result. The workflow automatically stores the latest result in the computer's internal memory, so the result is available for use by subsequent events in the workflow, such as a report event or a store event.

The comparison event must be linked to a valid measurement specification that points to a calibrated TQ Analyst quantitative or spectral measurement method to produce a comparison result. You must specify an expected value for each collected spectrum when you add the comparison event to your workflow.

**Event result:** Comparison statistics

**Associated specifications:** Measurement specification

**Related events:** Check event, Collect event, Report event, Store event

**Related specifications:** Logical test specification, Summary Item specification, Table Item specification

**Parameters:** The illustration below shows the parameters for the comparison event. These parameters appear in the display area of RESULT Integration when a comparison event is selected in a workflow.

Compare Result: Comparison statistics

Ethanol in Water

Compare calculated to expected values

Measurement specification: Ethanol in Water Measurem... New Details

Store raw values with calculated values

Measure these spectra:

Add Delete

Expected Values

Component: % Ethanol Value:

Multiple Event Results

Retain all event results

Retain most recent result

## Compare event parameters

The compare event parameters specify the measurement and the expected values for a series of collection results (spectra) in a workflow and the storage of data from multiple comparison events that occur in a loop. The following sections explain the comparison event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Compare Calculated To Expected Values

The parameters in this group allow you to specify the spectra to be measured, the measurement specification (which points to a calibrated TQ Analyst method), and the expected value for each component or attribute that method is set up to measure.

Compare calculated to expected values

Measurement specification: Ethanol in Water Measurr New Details

Store raw values with calculated values

---

Measure these spectra:

Ethanol in Water  
Ethanol in Water

Add Delete

---

Expected Values

Component: % Ethanol Value: 0.0000

The following parameters are included:

- Measurement Specification.** A measurement specification contains advanced measurement parameters that are optimized for a given method development software package and measurement type. See Measurement Specification in this chapter for information about setting up measurement specifications in a workflow. To link a measurement specification to a comparison event, select the specification name in the Measurement Specification drop-down list, as shown below.

Measurement specification: Surfactant Measurement New Details

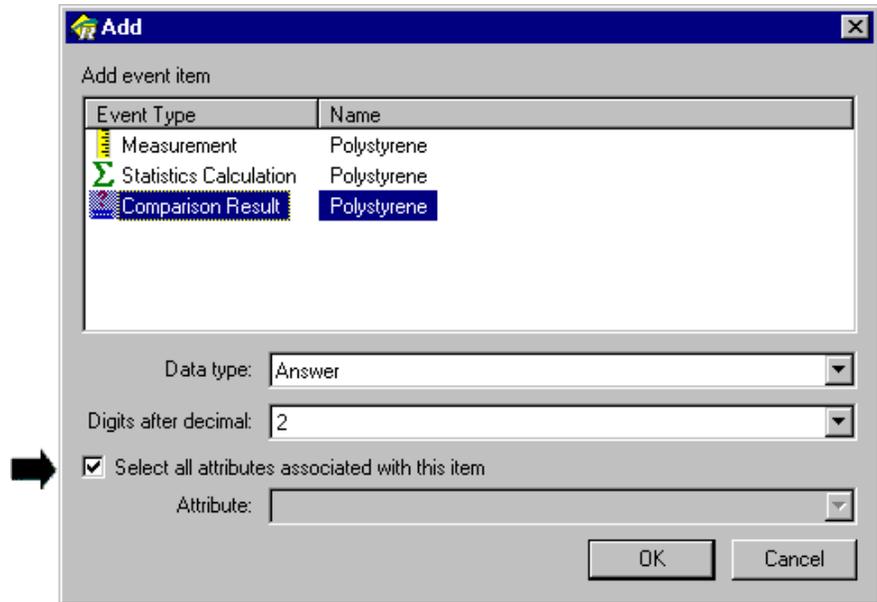
Use the New button at the right of the Measurement Specification list box to create a measurement specification and automatically link the new specification to this comparison event.

If this comparison event is already linked to a measurement specification, you can use the Details button to display that measurement specification.

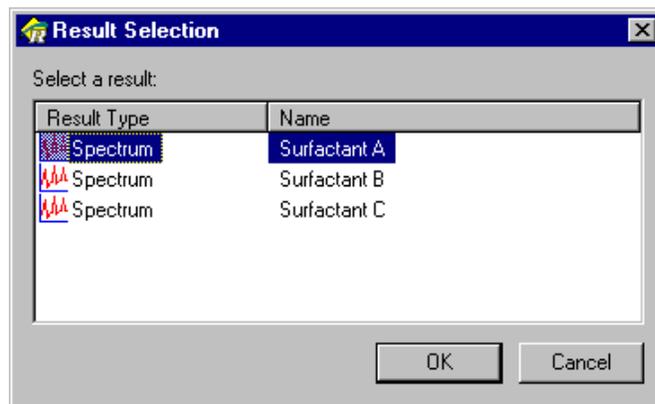
Store raw values with calculated values

- Store Raw Values With Calculated Values.** Select this option to store the measurement results along with the comparison results in RESULT Integration. When this option is selected, the measured values from the associated measurement specification are added to the list of values produced by the comparison event and stored in the computer's internal memory.

Select Store Raw Values With Calculated Values if you want to access the measurement results as well as the comparison result for use in subsequent workflow events. This option is most useful when creating a sample report that includes a table of measurement data and comparison data. It allows you to use the Select All Attributes feature of the Add RESULT dialog box (see example below) to add both sets of results to the table item specification at the same time.



- **Measure These Spectra.** Use this box to select the spectra that will be measured and their measurement values compared. To add a spectrum to the list, choose the Add button below the box. The following dialog box is displayed.

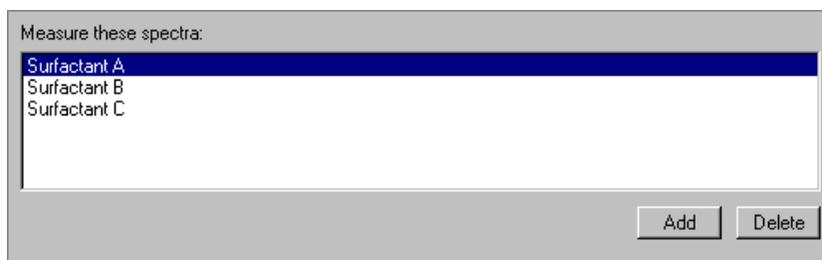


The list shows the collection result (spectrum) associated with each collect event in the current workflow.

**Note** If this dialog box is empty, then the workflow either does not contain a collect event or all the collect events have already been selected. See Collect Event in this chapter for instruction on adding collect events to a workflow. ▲

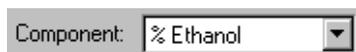
Select the spectrum you want to add and then choose OK. Make sure you select the spectrum from a collect event that appears before this comparison event in the workflow.

After you choose OK, the dialog box closes and the selected spectrum appears in the list of spectra to be measured in the comparison event, as shown below.

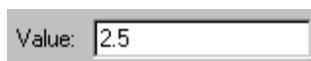


To delete a spectrum from the list, select the spectrum name and then choose the Delete button below the box.

- **Expected Values.** These parameters allow you to specify the expected concentration value or spectral measurement for each component or attribute the associated TQ Analyst method is set up to measure. To specify expected values, set the Component list box to the component or attribute name, as shown below.



Then select the Value box and enter the expected value for that component or attribute in the appropriate unit, as shown below:



Repeat the previous step for each component or attribute you want to include in the comparison result.

**Note** The expected values are known values or values that are measured using another analysis technique. If you don't know the expected values or those values can't be measured another way, use the measured values produced by the workflow the first time you run it. Subsequent workflow runs can then be used to track instrument change over time. ▲

### Multiple Event Results

#### Multiple Event Results

- Retain all event results
- Retain most recent result

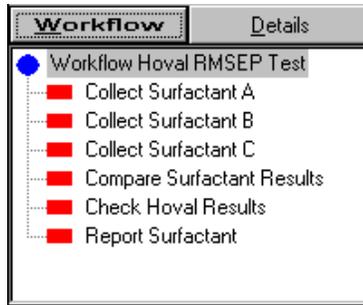
If you place a compare event in a repeat or perform-while loop, the event will produce one result (i.e., one set of comparison data) during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent result. The options for storing results include:

- **Retain All Event Results.** If the compare event occurs in a loop, selecting this option causes the workflow to store all the data. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the compare event is not positioned in a loop or the loop includes all subsequent events that operate on the stored data. This is the default setting and will maximize your computer processing speed.

See “Repeat events” and “Perform-While events” for more information about using stored data in a workflow.

**Usage:** A compare event must be linked to a valid measurement specification and set up to measure at least two spectra in order to produce a result. Make sure you place the comparison event after its associated collection events in the workflow.

Compare events are typically inserted after two or more collection events that are set up to collect data from check samples (samples for which the sample composition is known). If you run multiple check samples that contain different amounts of the components being measured (recommended), the results from the Compare event can show whether the calibrated method is appropriate for the samples you want to analyze. The example workflow shown below uses a comparison event to compare the measurement results from three collect events.



The following events can operate on the comparison result if those events are positioned after the compare event in the workflow.

- **Check event**, which can be used to produce an overall pass or fail result based on a comparison result. For example, a check event can be used to determine the pass/fail status of a check sample by comparing the calculated RMSEP value to an expected RMSEP value. If a calculated RMSEP value is greater than the expected RMSEP value, check the following:
  - The expected concentration value was entered correctly.
  - The quality of the check sample (it may be damaged or degraded) and obtain a fresh sample, if necessary.
  - Display the spectrum. If the quality of the spectrum is poor, rerun the check sample.
- **Store event**, which can be used to store comparison results in the audit log database so they can be accessed with the logs features of RESULT Operation and used to track trends in the data.
- **Report event**, which can be used to add the comparison result to a sample report.

## Delay events

This event can be used to pause the workflow for a specific time interval. The workflow will begin the pause immediately after it implements the delay event. The next workflow event will begin immediately after the specified delay interval has passed.

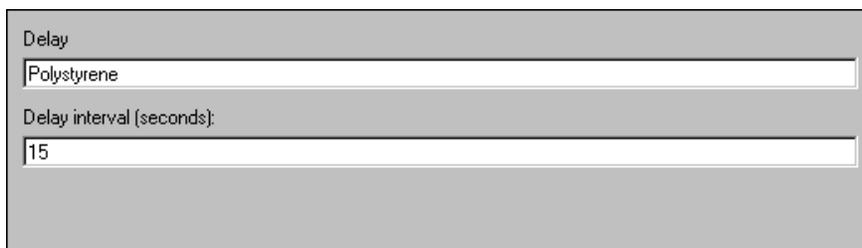
**Event result:** None

**Associated specifications:** None

**Related events:** None

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the delay event. These parameters appear in the display area of RESULT Integration when a delay event is selected in a workflow.



Delay

Polystyrene

Delay interval (seconds):

15

### Delay event parameters

The delay parameter allows you to specify the interval for the delay, as described below.

- **Delay Interval.** Use this box to specify the period of time (in seconds) to pause the workflow.



Delay interval (seconds):

15

**Usage:** Delay events may be positioned anywhere in a workflow, typically before an event that requires time for an operator or instrument activity or in workflows that do not require operator input. Some examples of this include:

- Pausing the instrument between periodic data collections.
- Waiting for the instrument to stabilize before starting data collection.
- Waiting for the temperature of a sample to stabilize.

You may place a delay event inside a repeat or perform-while loop or after a loop to pause the workflow before continuing to the next event.

## Load Spectrum events

Use this event to load an archived spectrum such as a background spectrum into a workflow. The spectrum can then be used by other events in the workflow.

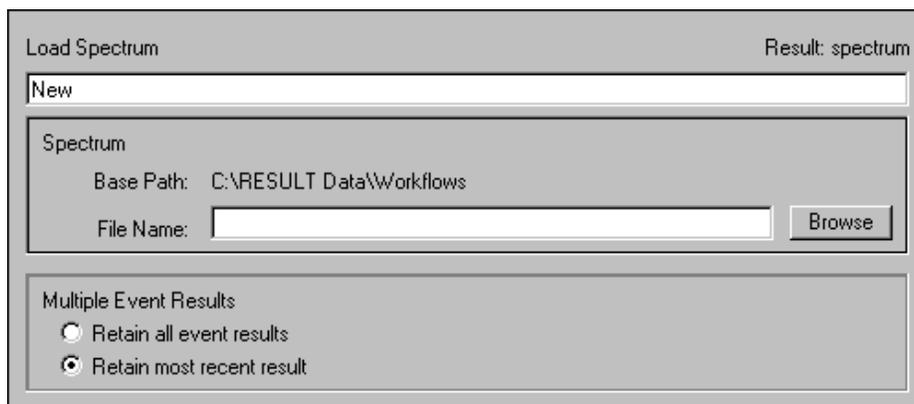
**Event result:** Spectrum

**Associated specifications:** None

**Related events:** None

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the Load Spectrum event. These parameters appear in the display area of RESULT Integration when a Load Spectrum event is selected in a workflow.



The screenshot shows a dialog box titled "Load Spectrum" with a "Result: spectrum" label in the top right corner. Below the title bar is a text input field containing the word "New". Underneath is a section titled "Spectrum" containing a "Base Path:" label followed by the text "C:\RESULT Data\Workflows". Below that is a "File Name:" label followed by an empty text input field and a "Browse" button. At the bottom of the dialog is a section titled "Multiple Event Results" with two radio button options: "Retain all event results" (which is unselected) and "Retain most recent result" (which is selected).

### Load Spectrum event parameters

The Load Spectrum event parameters allow you to specify the file name and path of the spectrum you want the workflow to load. A Load Spectrum event may only be used to load spectral files (\*.spa).

### Spectrum

These settings define the path and file name of the spectrum the workflow will load.

Base path:

- **Base path.** This readout shows the base path required for the archived spectrum. If you run the workflow in RESULT Integration, the spectral file must be located in the base path specified here, which is the current path for archiving workflows and methods in RESULT Integration. See “Setting RESULT Integration Options” in the “RESULT Integration User Guide” for information about setting this path.

**Note** If you transfer the workflow to RESULT Operation, this base path is not used. Instead, the software uses the base path for archiving workflows in RESULT Operation. You must be sure to copy the spectral data file along with the workflow and place the spectral and workflow files in the correct path. For details, see “Transferring Workflows to RESULT Operation” in “Chapter 6 Managing Workflows” of the “RESULT Software Administration” guide.” ▲

- **File Name.** Use this box to specify a specific folder and file name for the spectral file. You can use the Browse button to locate and select the file or enter a file name in the text box. The file can be in the same folder as your workflows and methods or you can create a folder for archiving spectral files. You can only select or create folders that are located in the base path for archiving workflows and methods in RESULT Integration.

If you transfer the workflow to RESULT Operation, take care to transfer the correct spectrum with the correct file name and folder along with the workflow. For details, see “Transferring Workflows to RESULT Operation” in “Chapter 6 Managing Workflows” of the “RESULT Software Administration” guide.

### Multiple Event Results

Multiple Event Results

- Retain all event results
- Retain most recent result

If you place a load spectrum event in a repeat or perform-while loop, the event will reload the spectrum during each iteration of the loop. This feature allows you to select whether the workflow will store all the spectra loaded by the loop or only the most recent spectrum. The options for storing results include:

- **Retain All Event Results.** If the Load Spectrum event occurs in a loop, selecting this option causes the workflow to store all the loaded spectra. This makes the individual spectra available for use in subsequent workflow events such as a report event that are placed after the loop.

- **Retain Most Recent Result.** Select this option if the load spectrum event is not positioned in a loop or the loop includes all subsequent events that operate on the stored spectrum. This is the default setting for Multiple Event Results and will maximize your computer processing speed.

See “Repeat events” and “Perform-while events” for more information about using stored data in a workflow.

**Usage:** Load spectrum events may be placed anywhere in a workflow. There are no other requirements. Load spectrum events are useful for spectral corrections because you can load a correction spectrum saved on your computer disk into a workflow and use it in the correction equation.

The following events can operate on a loaded spectrum if those events are positioned after the load spectrum event in the workflow.

- **Archive event**, which can be used to archive the spectra produced by the load spectrum event.
- **Process event**, allows you to use the loaded spectra to calculate an average spectrum, a variance spectrum or a series of difference spectra. You can also calculate a difference spectrum from the spectra generated by two different load spectrum events.
- **Measure event**, which can be used to analyze the spectra.
- **Compare event**, which can be used to chart actual versus expected values for a series of spectra.
- **Report event**, which can be used to add the spectra to a sample report.

## Measure events

This event can be used to measure the spectra generated from a workflow. The event must be linked to a valid measurement specification, which defines the measurement. A measurement specification can be used to define a composite measurement or it can be linked to a TQ Analyst or other compatible method that defines the measurement.

Each time a workflow performs a measure event, the workflow produces a measurement result such as a spectral peak height or area. If the measure event makes more than one measurement, for example, if it calculates concentration values for several components, the measurement result

contains a set of data rather than a single value. The workflow automatically stores the latest result, or result set, in the computer's internal memory, so the result is available for use by subsequent events in the workflow such as a calculation event or a report event.

**Event result:** Measured value(s)

**Associated specifications:** Measurement specification

**Related events:** Collect event, Calculate event, Compare event, Report event, Request event, Store event

**Related specifications:** Logic specification, Summary Item specification, Table Item specification

**Parameters:** The illustration below shows the parameters for the measure event. These parameters appear in the display area of RESULT Integration when a measure event is selected in a workflow.

The screenshot shows a dialog box titled "Measure" with a "Result: measured values" label in the top right corner. The main content area contains a text field with "Ethanol in Water". Below this is a section titled "Measure Sample" containing a dropdown menu for "Spectrum to be measured:" with "Ethanol in Water" selected, and another dropdown menu for "Processing options for multiple samples:" with "No preprocessing performed" selected. There is an unchecked checkbox labeled "Delete source spectra after measurement". Below that is a dropdown menu for "Measurement specification:" with "Ethanol in Water Measurement" selected, and two buttons labeled "New" and "Details". At the bottom is a section titled "Multiple Event Results" with two radio button options: "Retain all event results" (unselected) and "Retain most recent result" (selected).

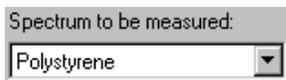
### Measure event parameters

The measure event parameters define sample measurement for a given collection result (spectrum), and the storage of data from multiple measure events that occur in a loop. The following sections explain the measure event parameters in detail. The parameters are explained in the order in which they appear in the software.

## Measure Sample

The parameters in this group allow you to specify the spectrum to be measured and any processing operations that will be applied to the spectrum before it is measured. These parameter settings are independent of the calibrated method that will be used to measure the spectrum.

The sample measurement parameters include the following:



- **Spectrum To Be Measured.** Use this list box to specify the spectrum to be measured by selecting a name in the drop-down list. The list includes the sample names from all the collect events that are included in the workflow.

Make sure you select a spectrum that is produced by a collect event that appears before this measure event in the workflow.

**Note** This drop down list box is grayed out for measure events that are associated with a composite measurement specification because no spectrum is needed. ▲



- **Processing Options For Multiple Samples.** If the collect event associated with the selected spectrum (see “Spectrum To Be Measured” above) is set up to store all samples and backgrounds (see “Collect Multiple Samples” in “Collect events”), you may specify processing operations for the collected spectra, such as averaging the spectra or calculating a variance spectrum. The processing options are described below.

**Note** The associated collect event must be part of a repeat or perform-while loop that specifies at least two repetitions in order to calculate an average or variance spectrum. If fewer than two repetitions are specified, the measure event will produce an error when you run the workflow. ▲

- *Create Average Spectrum From Multiple Source Spectra.* Select this option to calculate an average spectrum. The software will calculate the arithmetic mean of the Y values for each data point. (The Y values for a data point are added together, and then the total is divided by the number of spectra.)

By calculating the average of a group of spectra (of samples from a production run, for example), you can “average out” sample preparation and sampling variations.

- *Create Variance Spectrum From Multiple Source Spectra.* Select this option to create a variance spectrum. The software will calculate the standard deviation of the Y values at each X value over all of the spectra. (The mathematical formula for standard deviation is used.)

A variance spectrum can show you which parts of a repeated collection of sample spectra are different. You can also use the calculated variance of spectra collected from periodic measurements of a check sample to check the repeatability of the instrument's measurements.

**Note** If Processing Options For Multiple Samples is unavailable in a measure event, make sure the collect event associated with the selected spectrum to be measured has Multiple Event Results set to Retain All Event Results. See “Collect events” for more information. ▲

Delete source spectra after measurement

- **Delete source spectra after measurement.** Select this option if you don't need to archive the spectral data produced by the associated collect event, or if the archive event appears before this measure event in the workflow. If Delete Source Spectra After Measurement is selected, then the software will delete the sample and background spectra that are stored in the computer's internal memory when the measurement is completed. Deleting the source spectra is recommended to release memory resources, especially when the measure event handles multiple spectra produced in a loop.

Make sure this option is cleared if you need to archive the spectral data produced by the associated collect event and your archive event is located after the measure event in the workflow, or if there are other subsequent workflow events that operate on the source spectra. If you want to delete the spectra later, use a clear event.

- **Measurement Specification.** A measurement specification contains advanced measurement parameters that are optimized for a given method development software package and measurement type. See “Measurement specifications” in this chapter for information about setting up measurement specifications in a workflow.

To link a measurement specification to a measure event, select the specification name in the Measurement Specification drop-down list, as shown below.

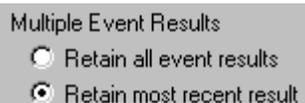


Use the New button at the right of the Measurement Specification list box to create a measurement specification and automatically link the new specification to the measure event.

If this measure event is already linked to a measurement specification, you can use the Details button to display that measurement specification.

**Note** If the workflow wizard is used to add a measure event to a workflow, the wizard also creates and links the measurement specification. ▲

### Multiple Event Results

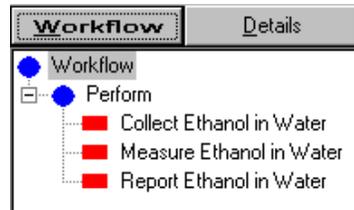


If you place a measure event in a repeat or perform-while loop, the event will produce one result or set of results during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent results. The options for storing results include:

- **Retain All Event Results.** If the measure event occurs in a loop, selecting this option causes the workflow to store all the measured data. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the measure event is not positioned in a loop or the loop includes all subsequent events that operate on the stored data. This is the default setting and will maximize your computer processing speed.

See “Repeat events” and “Perform-While events” for more information about using stored data in a workflow.

**Usage:** A measure event must be linked to a valid measurement specification and set up to measure at least one spectrum in order to produce a measurement result. The spectrum can be from a Collect event, a Collect Dual Tablet event or a Collect Multi-Channel event. Make sure you place the measure event after its associated collection event in the workflow, as shown in the example below.



The following events can operate on the measurement result if those events are positioned after the measure event in the workflow.

- **Calculate event**, which can be used to produce statistics from measurements that are part of a loop.
- **Check event**, which can be used to produce an overall pass or fail result based on a measurement result.
- **Compare event**, which can be used to chart actual versus expected values for a series of spectra.
- **Store event**, which can be used to store measurement or other results in the audit log database so they can be accessed with the logs features of RESULT Operation and used to track trends in the data.
- **Request event**, which can be used to request the operator to specify the type (class) of material to be analyzed. This type of operator prompt is appropriate only when placed after a measure event that has an associated qualitative (classification) method that specifies more than one class.
- **Report event**, which can be used to add the measurement results to a sample report.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Process events

In workflows that produce multiple spectra from a collect event, such as the spectra collected from an autosampler, a process event allows you to use the collection result to calculate an average spectrum, a variance spectrum, or a series of difference spectra. You can also calculate a difference spectrum from the spectra generated by two different collect events.

The process event instructs the workflow to perform the specified operation using all of the spectra generated by the selected collect event. When using the process event to calculate an average or variance spectrum, the result is a single “processed” spectrum, which can be added to subsequent events in the workflow such as an archive event. When using the process event to calculate a difference spectrum, the result depends on how the subtraction is defined. If you subtract one spectrum from another, the process event produces one difference spectrum. If you subtract one spectrum from multiple spectra generated in a repeat loop, the process event produces one difference spectrum during each iteration of the loop. In this case, you can configure the process event to retain the difference spectrum only until the next process event occurs in the workflow, or to record all the difference spectra generated by the loop.

**Notice** The process event automatically deletes the original spectra produced by the associated collection event after processing is completed. This happens even if the Collect Multiple Samples feature of the associated collect event is set to the “Retain All Event Results” option. If you want to save those spectra, place an archive event that archives the collected spectra before the process event in the workflow. ▲

**Event result:** Processed spectrum (average spectrum, variance spectrum or difference spectrum)

**Associated specifications:** None

**Related events:** Collect event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the process event. These parameters appear in the display area of RESULT Integration when a process event is selected in a workflow.

Process Result: processed spectrum

New

Process Samples

Spectra to be processed:  
Ethanol in Water

Processing options:  
Calculate variance spectrum

Subtraction Spectrum

Use workflow generated spectrum  
Subtraction spectrum: Ethanol in Water

Use spectral file  
Subtraction file name:

Subtraction Factor

Calculate factor  
Starting location:  Ending location:

Specify factor  
Subtraction factor:

Multiple Event Results

Retain all event results  
 Retain most recent

## Process event parameters

The process event parameters define the spectra to be processed, the processing operation, and the storage of results from multiple process events in a workflow. The following sections explain the process event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Spectra to be processed

Spectra to be processed:

Use this list box to link the process event to a collect event in your workflow. The names of all the collect events in the workflow appear in the drop-down list. Choose a collect event that appears before the process event in the workflow. If you choose a collect event that appears after the process event, the workflow will produce an error.

If you plan to use this process event to create an average spectrum or a variance spectrum from the data, make sure you choose a collect event that will produce at least two spectra when you run the workflow. This means

the collect event should appear in a repeat loop that is set up to perform at least two iterations. See “Repeat events” in this section for information about setting up repeat loops in a workflow.

If you want to use this process event to subtract one spectrum from another, use this list box to select the spectrum on which the software will perform the subtraction. You can perform the subtraction on a single spectrum or on a series of spectra collected in a repeat loop.

**Note** If you select a collect event that occurs in a repeat loop, make sure the collect event has Collect Multiple Samples set to the “Make All Spectra And Backgrounds Available To Other Events” option. See “Collect Events” for more information. ▲

### Processing options



Use this list box to select a processing operation. The following options are available.

- **Calculate variance spectrum.** Select this option to use all the spectra generated by the associated collect event to calculate a variance spectrum representing the square root of the variance present in all the processed spectra. To create the “variance spectrum,” the software calculates the standard deviation of the Y-values for each data point (X value).

The associated collect event must be part of a repeat or perform-while loop that specifies at least two iterations in order to calculate a variance spectrum. If fewer than two iterations are specified, the process event will produce an error when you run the workflow.

A variance spectrum can show you which parts of a repeated collection of sample spectra are different. You can also use the calculated variance of spectra collected from periodic measurements of a check sample to check the repeatability of the instrument’s measurements.

- **Calculate average spectrum.** Select this option to use all the spectra generated by the associated collect event to calculate an average spectrum. To create the average spectrum, the software calculates the arithmetic mean of the Y values for each data point. (The Y values for a data point are added together and the total is divided by the number of spectra.)

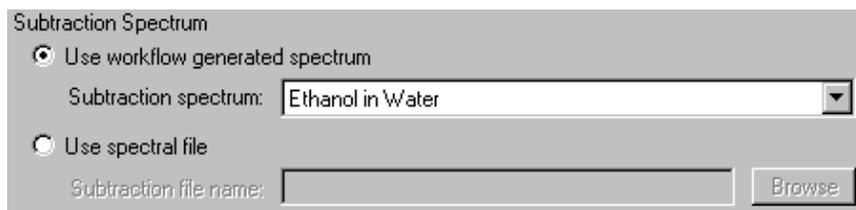
The associated collect event should be part of a repeat or perform-while loop that specifies at least two iterations in order to calculate an average spectrum. If fewer than two iterations are specified, the process event will still calculate an average spectrum but it will be the average of one spectrum.

By calculating the average of a group of spectra (of samples from a production run, for example), you can “average out” variations in the spectra that are due to differences in the techniques used to prepare and measure the samples.

- **Calculate difference spectrum.** Select this option to use the spectrum generated by the associated collect event and another spectrum (the subtraction spectrum) to calculate a difference spectrum. When you use a process event to subtract one spectrum from another, the software calculates data point by data point the difference between the two. Subtraction is commonly used to remove spectral features of solvent residues or pure components from the spectrum of a mixture of compounds.

The reference spectrum can be a spectrum produced by another collect event in the same workflow, or a spectrum saved in a file on a disk. The software can calculate the subtraction factor automatically or you can specify a value. If the software calculates the subtraction factor, you can set the X-axis limits of the region used for the calculation. The software will subtract the reference spectrum from each spectrum produced by the associated collect event. If the workflow is configured so the collect event collects one spectrum, the process event will produce one difference spectrum. If the process event and its associated collect event occur in a repeat loop, the process event will produce a difference spectrum during each iteration of the loop.

## Subtraction Spectrum



Subtraction Spectrum

Use workflow generated spectrum

Subtraction spectrum: Ethanol in Water

Use spectral file

Subtraction file name:

The features in this group allow you to specify the reference spectrum used for subtraction (subtraction spectrum). These features are available in the software only when the Processing Options list box (see above) is set to the “Calculate Difference Spectrum” option. RESULT Integration provides the following options for specifying the subtraction spectrum.

- **Use Workflow Generated Spectrum.** Select this option if you want to use the spectrum produced by another collect event in the workflow as the subtraction spectrum. Then select the collect event in the drop-down list as shown above. If the selected collect event produces multiple spectra, for example if it occurs in a repeat loop, the software calculates an average spectrum and used the average spectrum for the subtraction spectrum.
- **Use Spectral File.** Select this option if you want to use a spectrum saved in a file as the subtraction spectrum. Then use the Browse button to locate and select the file. Choose a spectrum that has the same spectral resolution and spectral range as the spectrum you want to process by subtraction.

The following file types are available:

- *Nicolet (\*.SPA)*, which is compatible with many Thermo Scientific spectroscopy applications including TQ Analyst and RESULT.
- *JCAMP-DX (\*.JDX)*, which uses printable ASCII characters and is compatible with other software applications used in the industry.
- *Galactic (\*.SPC)*, which is a binary format that is compatible with other applications and other types of data in the industry.
- *Comma-Separated Values (\*.CSV)*, which is a text file that specifies each data point in the spectrum as a set of X and Y values and can be read by any compatible spreadsheet or other program.

## Subtraction Factor

Subtraction Factor

Calculate factor

Starting location: 4,000.00 Ending location: 10,000.00

Specify factor

Subtraction factor: 1.00

Use the features in this group to specify the subtraction factor. The factor allows you to adjust the intensities of the peaks in the subtraction spectrum so they match those in the original spectrum in order to optimize the subtraction. Algebraically, the subtraction works like this:

$$\text{Spectrum} - \text{Factor} * \text{Subtraction spectrum} = \text{Difference spectrum}$$

You can specify a factor or let the software calculate the factor automatically. If the software calculates the factor, you can specify the spectral region from which the factor is calculated.

These features are available in the software only when the Processing Options list box (see above) is set to the “Calculate Difference Spectrum” option. RESULT Integration provides the following options for specifying the subtraction factor.

- **Calculate factor.** Select this option if you want the software to calculate the subtraction factor automatically. Then specify the starting and ending point of the X-axis region the software should use to calculate the factor.
- **Specify factor.** Select this option if you want to enter a value for the subtraction factor. Then type the value in the Subtraction Factor entry box. Use a subtraction factor that lets you subtract the unwanted absorptions without subtracting other important spectral information. When specifying the factor, users typically set the factor to “1” or the ratio of the pathlengths (thicknesses) of the two samples (the pathlength of the original sample is the numerator and the pathlength of the subtraction sample is the denominator).

For best results, display representative examples of the two spectra you want to subtract using your TQ Analyst method development software, adjust the factor interactively to determine the optimum value, and then enter the value in RESULT Integration. See your TQ Analyst on-line help for details.

## Multiple Event Results

### Multiple Event Results

- Retain all event results
- Retain most recent result

If you place a process event in a repeat or perform-while loop, the event will produce one result or set of results during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent results. The options for storing results include:

- **Retain All Event Results.** If the process event occurs in a loop, selecting this option causes the workflow to store all the processed data. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the process event is not positioned in a loop or the loop includes all subsequent events that use the processed spectra. This is the default setting and will maximize your computer processing speed.

See “Repeat events” and “Perform-While events” for more information about using stored data in a workflow.

**Usage:** A process event may be placed anywhere in a workflow but must occur after its associated collection event. A process event that is set up to generate a variance spectrum must be linked to a collection event that generates at least two spectra. A process event that is configured to calculate an average or difference spectrum may be linked to a collection event that produces a single spectrum or one that produces multiple spectra.

The following events can operate on the processed data if you place those events after the process event in the workflow.

- **Measure event**, which can be used to analyze the processed spectra.
- **Compare event**, which can be used to compare a series of spectra and their measured values against expected values to produce correlation coefficients, root mean square error of prediction (RMSEP) values, and slope and y-intercept values for those measurements.
- **Archive event**, which can be used to archive the processed spectra.
- **Report event**, which can be used to add the processed spectra to a sample report.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Read from I/O events

This event is one of a read/write pair that allows a workflow to communicate with a hardware device such as a simple alarm, a valve, or a control system.

You must have one of the optional input/output kits and an available Ethernet connection to output and receive external signals with RESULT. Each kit includes a controller and a mounting rack that holds standard I/O modules (digital and 4-20 milliamp analog modules are available from us). RESULT communicates with the controller via the Ethernet connection; the I/O lines can be connected to the specific equipment you need to monitor, control, or acquire data from such as a programmable logic controller (PLC), host computer or other device in your factory.

You can use a Read From I/O event to read from a hardware device connected to a specific I/O line, also called a point. For information about using RESULT to change the status of an I/O device, see the Write To I/O event described later in this chapter.

**Event result:** Data read from a hardware device

**Associated specifications:** None

**Related events:** None

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the Read From I/O event. These parameters appear in the display area of RESULT Integration when a Read From I/O event is selected in a workflow.



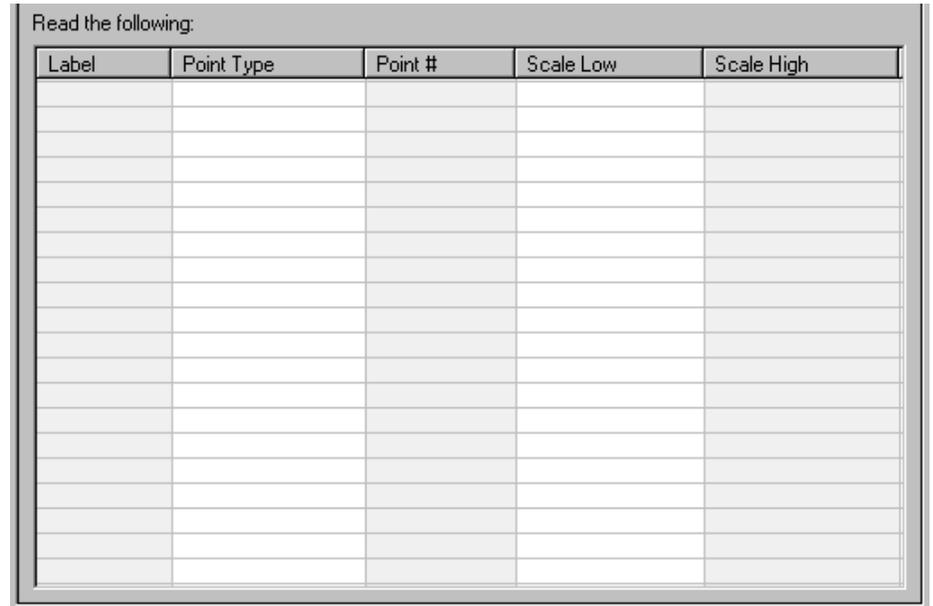
## Read Data

Use this table to specify which hardware devices the workflow needs to poll and, for devices that produce an analog signal, any limits for the input range.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete Selected Row, or select the row and press Delete on the keyboard.

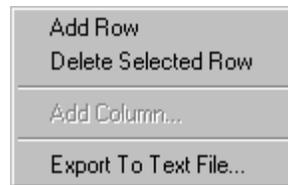
Use Export To Text File to write the device information displayed in the table to a text file with a file name and path you specify.

To specify a default value for Point #, Scale Low and Scale High, right click the column heading and choose Edit Column. In the Add/Edit Column dialog box, select Apply Default Setting, enter a default value and choose OK.



The screenshot shows a dialog box titled "Read the following:" containing a table. The table has five columns: "Label", "Point Type", "Point #", "Scale Low", and "Scale High". The table is currently empty, with only the header row visible. The dialog box has a standard Windows-style border and a title bar.

The table is interactive and easy to work with. To add a row to the table, right click an empty row to display a shortcut menu and then choose Add Row.



The columns in the table are described below. To edit a cell in a specific row and column, double-click the cell.

- **Label.** Double-click to activate the cell and then enter a description for the specific value the workflow will read.
- **Point Type.** Double-click the cell to activate a drop down list box with the available options for specifying the type of signal. Select an option from the list below.
  - *Digital Point.* Used to read a digital signal.

- *Analog Point*. Used to read an analog signal such as a 4-20 milliamp signal.
- *String Memory*. Used to read a text string from the controller.
- *Float Memory*. Used to read a floating point number (allows decimal points) from the controller.
- *Integer Memory*. Used to read an integer (whole number) from the controller.

**Note** For more information about mapping to memory points, see the user guide that came with your Opto 22 controller. ▲

- **Point #**. Double-click to activate the cell and then enter the point number on the I/O module that is associated with the signal.
- **Scale Low/High**. Scale low and high are useful only for analog signals. These settings allow RESULT to normalize a scale for the analog input. For example, you might want to normalize the scale when using RESULT to read a scale factor by setting Scale Low to the 0 and Scale High to 1.

### Multiple Event Results

#### Multiple Event Results

- Retain all event results
- Retain most recent result

If you place a Read From I/O event in a repeat or perform-while loop, the event will produce one result during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent result. The options for storing results include:

- **Retain All Event Results**. If the Read From I/O event occurs in a loop, selecting this option causes the workflow to store all the collected data. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result**. Select this option if the Read From I/O event is not positioned in a loop or the loop includes all subsequent events that operate on the stored data. This is the default setting and will maximize your computer processing speed.

See “Repeat events” and “Perform-while events” for more information about using stored data in a workflow.

**Usage:** Read From I/O events may be placed anywhere in a workflow. There are no other requirements.

The following events can operate on the Read From I/O result if those events are positioned after the Read From I/O event in the workflow.

- **Calculate event**, which may be used to produce statistics from measurement results or other results that are part of a loop.
- **Check event**, which may be used to produce a pass or fail result based on a value read from the controller.
- **Store event**, which may be used to store numeric values read from the controller in the audit log database so they can be accessed with the logs features of RESULT Operation and used to track trends in the data.
- **Report event**, which may be used to add values read from an I/O device to a table or summary section in a sample report.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Read from Excel events

Allow a workflow to import data from an Excel file (filename extension must be .xls). Must have Microsoft® Excel version 2003 or higher installed on the computer or network.

To learn how to set up a workflow to export data to an Excel file, see “Write To Excel events” in this chapter.

**Event result:** Data read from an Excel spreadsheet.

**Associated specifications:** None

**Related events:** None

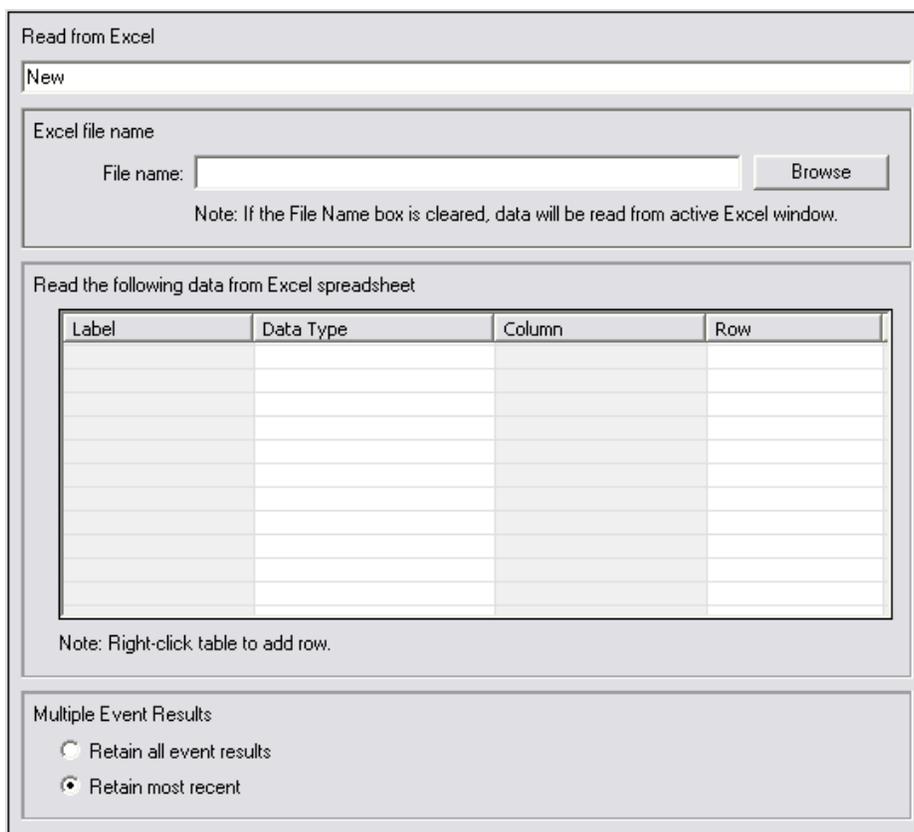
**Related specifications:** None

**Parameters:** Read From Excel event parameters specify a location for the Excel file and the data to be read.

Right-click table to display shortcut menu with options to add to, delete from and edit table.

Use Export To Text File in shortcut menu to write information in table to a text file with a file name and path you specify.

To specify default value for Column or Row, right-click column heading and choose Edit Column. In dialog box, select Apply Default Setting, enter default value and choose OK.



Read from Excel

New

Excel file name

File name:

Note: If the File Name box is cleared, data will be read from active Excel window.

Read the following data from Excel spreadsheet

Label	Data Type	Column	Row

Note: Right-click table to add row.

Multiple Event Results

Retain all event results

Retain most recent

### Excel File Name

Specify or open the Excel file to be read. To specify a file, enter a file name or browse to the file.

To read from the current Excel file, clear the File Name text box and use Excel (or a Write To Excel event) to open the file.

### Read Data

Use this table to specify the Excel data to be read. The columns and functions presented in the table are explained below.

Column	Description
Label	Double-click to activate cell and then enter a description for the value the workflow will read.
Data Type	Double-click cell to activate drop down list box. Data Type options include: <ul style="list-style-type: none"> <li>• Boolean - Accepts only true or false values.</li> <li>• Floating point number - Requires a numerical entry. Allows any number, including decimal fractions.</li> <li>• Integer - Requires a numerical entry. Allows only whole numbers (1, 2, 3, etc.). If workflow produces fractional value, it is rounded to the nearest integer.</li> <li>• String - Accepts text and/or numeric values. Commonly used to request input from bar code reader. However, correct data type setting depends on information embedded in bar code.</li> </ul>
Column/Row	Double-click to activate cell for specifying column and row where formula resides in Excel spreadsheet.

Function	Description
Add Row	Right-click table and choose Add Row.
Delete Row	Right-click row and choose Delete Selected Row or select row and press Delete key.

## Multiple Event Results

Select whether the workflow will store all results produced by a repeat or perform-while loop or only the most recent result. Options include:

- **Retain All Event Results.** If Read From Excel occurs in a loop, select this option to store all collected data for use by events located after the loop.
- **Retain Most Recent Result (default).** Select if Read From Excel is not in a loop or the loop includes all subsequent events that operate on the stored data.

See “Repeat events” and “Perform-while events” for more information about using stored data in a workflow.

**Usage:** Read From Excel events may be placed anywhere in a workflow. There are no other requirements.

These events can operate on the Read From Excel result if placed after the Read From Excel event in the workflow.

- **Calculate event.** Produces statistics from measurement results or other results that are part of a loop.
- **Check event.** Produces a pass or fail result based on a value read from Excel.
- **Store event.** Stores numeric values read from Excel in the audit log database so they can be accessed with the logs features of RESULT Operation and used to track trends in the data.
- **Report event.** Adds values read from Excel to a table or summary section in a sample report.
- **Report To Text File event.** Exports specific workflow results to a text file so they can be accessed, viewed or printed from other applications.
- **Report To OPC event.** Identifies workflow results that will be available to an OPC client.
- **Report To Spectrum event.** Adds information or workflow results to spectra generated in a workflow.
- **Write To Excel event.** Sends workflow results or statistical data to an Excel file.
- **Write To I/O Device event.** Sends workflow results to a hardware device.

## Report events

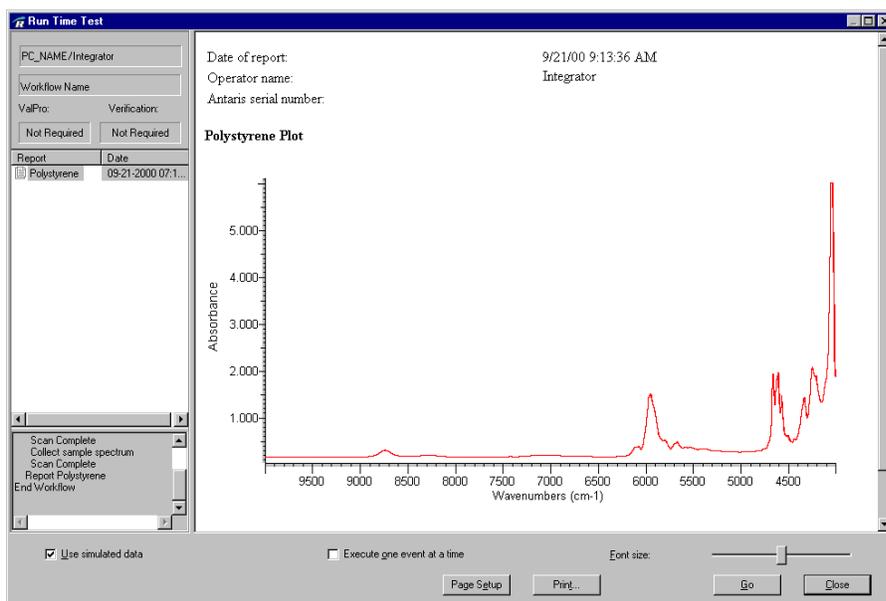
This event can be used to generate a sample report from a workflow. The event must be linked to a valid report specification, which defines the sections in the report. The report specification must be linked to at least one report item specification, which define the spectra, measurement or other results included in each section of the report.

A sample report can include any number and combination of the following items:

- Headings, such as Operator Name, Date, etc. or a corporate logo
- Spectral plots
- Tables of workflow results
- Tables of summarized workflow results
- Text.

See “Report Specifications” and “Report Item Specifications” in “Chapter 5 Workflow specifications” for more information.

Each time a workflow performs a report event, the workflow produces a sample report. The example below shows a report that includes a heading and a spectral plot.



### Displayed sample report

The workflow automatically stores the latest report in the computer’s internal memory, so the report is available for use by subsequent events in the workflow, such as an archive event.

**Note** If a workflow is configured to archive a report, each time the workflow is run in RESULT Operation, the software automatically stores a record of the archived report in the audit log database. See “Archive events” in this chapter for more information. ▲

**Event result:** HTML report, Text report

**Associated specifications:** Report specification

**Related events:** Archive event

**Related specifications:** Heading item specification, Memo Item specification, Spectrum Item specification, Summary Item specification, Table Item specification

**Parameters:** The illustration below shows the parameters for the report event. These parameters appear in the display area of RESULT Integration when a report event is selected in a workflow.

Report Result: report

New

Create Report

Report specification:

Ethanol in Water Report New Details

Print HTML report after report is displayed

Generate a text report

Multiple Event Results

Retain all event results

Retain most recent result

### Report event parameters

The report event parameters specify the name of a report specification, which defines the sections in the report, whether the report will print automatically and the storage of data from multiple report events that occur in a loop. The following sections detail the report event parameters. The parameters are explained in the order in which they appear in the software.

## Create Report

These parameters allow you to select or create a report specification and specify whether the report will be printed or exported to a text file. The report parameters include the following:

- **Report Specification.** Use this feature to link a report specification to this event. The report specification defines the sections in the report and any workflow results that will be included in each section. If the workflow already contains an appropriate report specification, select its name in the drop down list (see below).



Use the Details button to the right of the list box to display the current settings, or the New button to create a report specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the report event. The new specification will be linked to the report event and its name will appear in the report specification list box. See “Report specifications” in “Chapter 5 Workflow Specifications” for more information.

**Note** If the workflow wizard is used to add a report event to a workflow, the wizard also creates and links the report specification. ▲

Print HTML report after report is displayed

- **Print HTML Report After Report Is Displayed.** Select this option if you want the workflow to print the report automatically in HTML format. The report will be printed immediately after the software displays it. You can use any text editing application, such as the Windows Notepad program, to open, edit, and print an HTML file.

If you clear this option, the reports may still be stored in memory for use in other workflow events or printed manually from RESULT Operation or RESULT Integration.

Generate a text report

- **Generate a Text Report.** Select this option if you want the workflow to create a text report in addition to the HTML report. The text report is a simplified format that can be easily read by other workflow events, such as a request event, or by an external program. If the workflow includes an archive event to archive the reports, you will be able to add both the text report and the HTML report to the list of items to be archived.

### Multiple Event Results

Multiple Event Results

- Retain all event results  
 Retain most recent result

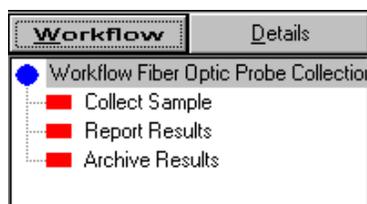
If you place a report event in a repeat or perform-while loop, the event will produce one report during each iteration of the loop. This feature allows you to select whether the workflow will store all the reports produced by the loop or only the most recent report. The options for storing reports include:

- **Retain All Event Results.** If the report event occurs in a loop, selecting this option causes the workflow to store all the reports. This makes them available for use in subsequent workflow events such as an archive event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the report event is not positioned in a loop or the loop includes all subsequent events that operate on the stored reports. This is the default setting and will maximize your computer processing speed.

See “Repeat Events” and “Perform-While events” for more information about using stored data in a workflow.

**Usage:** A report event must be linked to a report specification that includes at least one functional report item specification to create a sample report. The report specification specifies the sections in the report. The report item specifications define the spectra, measurement or other results included in each section of the report.

Report events can be placed anywhere in a workflow. Any workflow results that are included in a sample report must be generated before the report event in the workflow. For example, if a report is set up to include a spectrum, the collect event that produces the spectrum must be positioned before the report event in the workflow, as shown in the example below.



The following events produce results that can be added to a sample report:

- **Collect event**, which produces a spectrum.
- **Measure event**, which, depending on its associated method, can generate numerical concentration values, match values, class names, or spectral measurements such as a peak height or area.
- **Calculate event**, which produces statistical values from measurements that are part of a loop, including minimum, range, standard deviation, percent standard deviation, sum, and count.
- **Compare event**, which uses the actual and expected values for a series of measurements to produce correlation coefficients, root mean square error of prediction (RMSEP) values, and slope and y-intercept values for those measurements.
- **Check event**, which produces a pass or fail result.
- **Request event**, which produces either numerical values (from a message-response request) or a class name (from a class request).

## Report to OPC events

This event can be used to specify workflow results that will be available to an OPC client. OPC is a universal interface used to control process equipment and to monitor data results. RESULT software provides a basic interface to communicate with an OPC server.

You can select results from the following types of workflow events:

- Check events
- Measure events
- Calculate events
- Compare events

- Request events

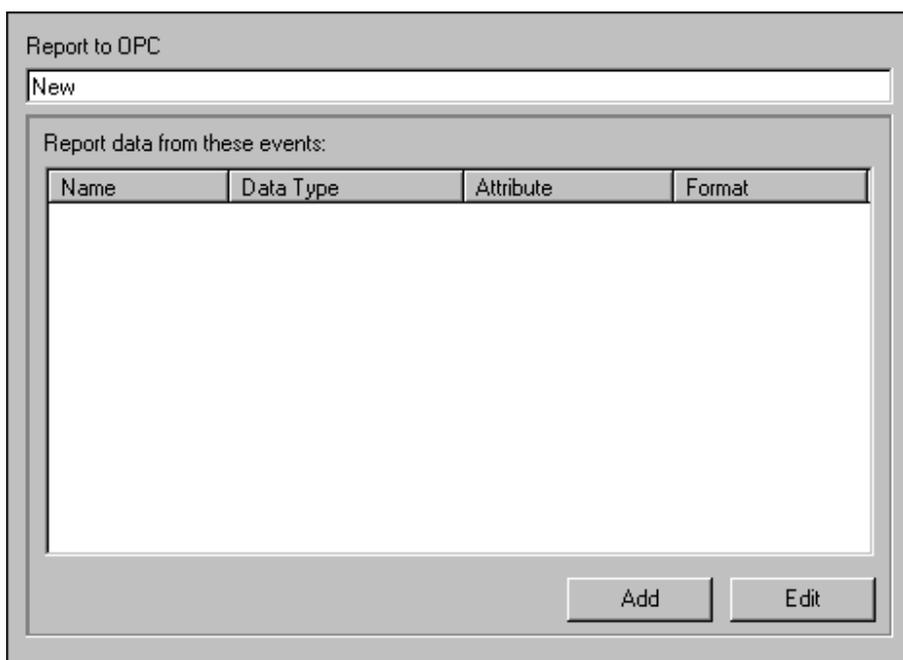
**Event result:** None

**Associated specifications:** None

**Related events:** Check events, Measure events, Calculate events, Compare events, Request events

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the report to OPC event. These parameters appear in the display area of RESULT Integration when a report to OPC event is selected in a workflow.

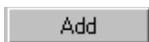


### Report to OPC event parameters

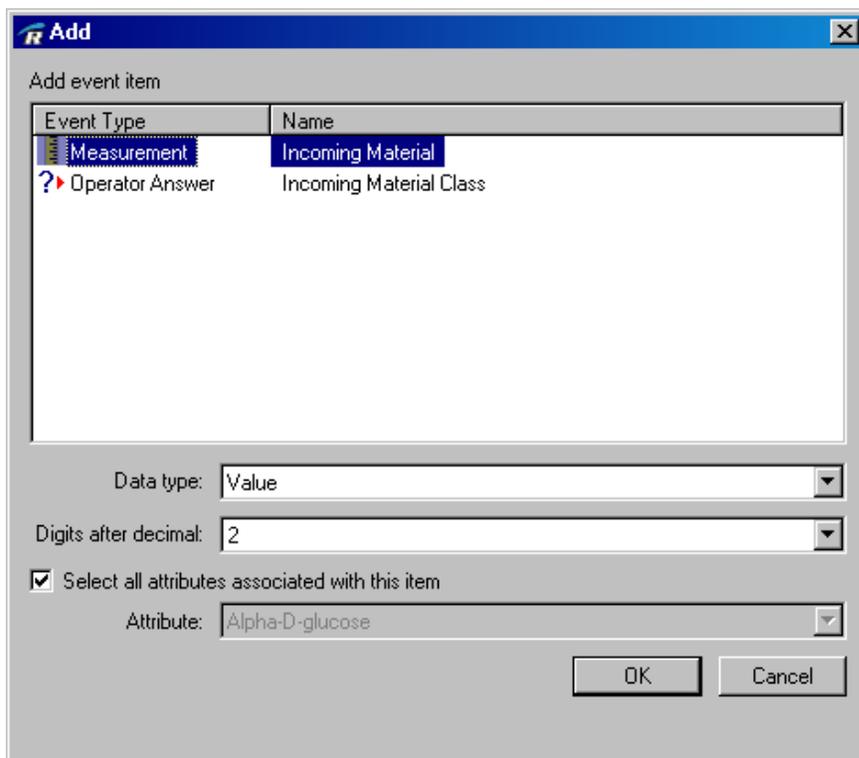
The report to OPC event parameters specify the workflow results that will be available to an OPC client. The following sections explain the report to OPC event parameters in detail. The parameters are explained in the order in which they appear in the software.

#### Report Data

Use this box to specify the workflow results you want to report to an OPC client.



- **Add.** Choose this button to add an event result to the list. The Add dialog box appears, as shown below.



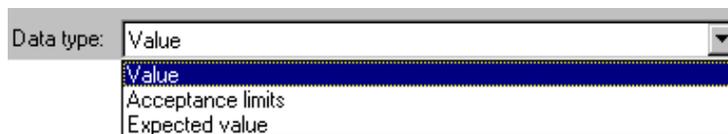
The list shows the events in the workflow that provide measurement or other results that can be released to an OPC client.

**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a result that can be released, or all of those events have already been added to the list. See the Usage heading below for a list of events that produce results that can be released to an OPC client. ▲

Select a result in the list. Make sure you select a result that exists at this point in the workflow. Since a workflow implements events in sequence, only results produced by events that occur before this report to OPC event will have results. If you select a result that is produced by an event that occurs after this report to OPC event, the report to OPC event will be unable to find the specified result and the workflow will produce an error.

After you select a result, the following parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Examples are provided below.

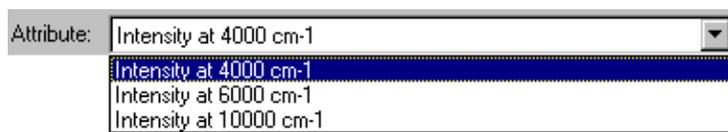
- *Data Type.* Use this list box to select a result produced by the selected event, such as a value or an acceptance limit. The number and type of results produced by an event depend on the event, and, for measure events, on the TQ Analyst or other method used for the measurement. For example, a measure event configured for quantitative analysis would always produce concentration values, but it may also include acceptance limits or known values, such as the expected concentration for a sample or standard. The Data Type drop-down list could include the following items for a quantitative measure event.



- *Digits After Decimal.* This box is available in the software only when the selected Data Type (see above) produces a numerical result.

Use the box to select the number of digits the software will include after the decimal point in the numeric result. You can include up to six digits after the decimal point. The software rounds the number and retains only the specified digits after the decimal point.

- *Attribute.* Use this list box to select a specific component or other measured attribute or value, or a pass or fail result (or the pass or fail image) for the selected data type and event. The number and type of items in the attribute drop-down list depend on the event, and, for measure events, on the TQ Analyst or other method used for the measurement. For example, a measure event configured for spectral measurements could include the following items in the Attributes drop-down list.



The Attributes drop-down list will include the following items for a compare event.



The pass or fail result is available only for a check event. If you select the check event result and turn off Select All Attributes (see below), you can add either the pass or fail result or the pass (✔) or fail (✘) image provided by the software.

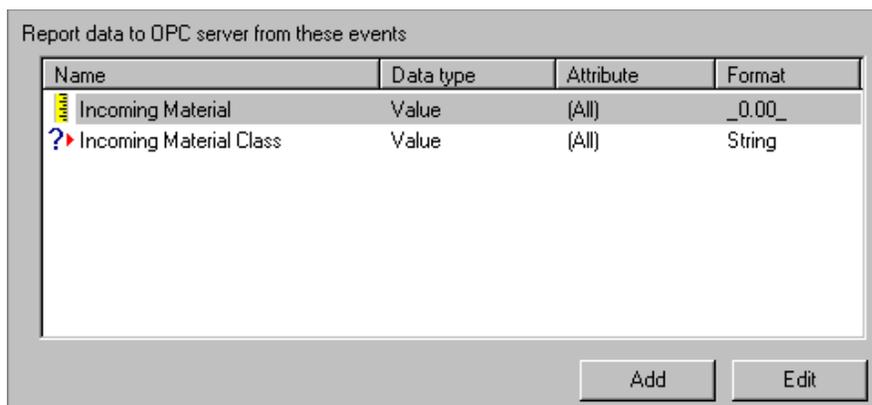


- *Select All Attributes Associated With This Item.* Select this option if you want to include all the measured components or other attributes or values for the selected data type and event.

When you have finished selecting a result, choose OK. The selected result is added to the list of items to include in the table, as shown in the example below.

The workflow will report the results in the order indicated in the table, starting with the result listed at the top. To change the reporting order, click an item in the table and drag it up or down.

To remove a workflow result from the list, select the result and then press the Delete key on the keyboard. The result will remain in the workflow but it will not be reported to the OPC client.



Repeat the steps described here for each workflow event that will generate results you want to report to an OPC client.



- **Edit.** To edit results that are included in the table, select the result and then choose the Edit button located below the table. You can edit the data type, digits after decimal, and attribute settings for the selected event. The new settings will be used for any subsequent reports produced by the workflow.

**Usage:** Report to OPC events may be placed anywhere in a workflow. There are no other requirements and no report to OPC event results that can be accessed by other events in a workflow.

A report to OPC event can report the result of any workflow event that produces a numerical value or pass/fail response, including:

- **Check event**, which produces a pass or fail result.
- **Measure event**, which can be used to analyze collected spectra to produce numerical concentration values, library index values, match values or spectral measurements such as a peak height or area.
- **Calculate event**, which can be used to produce statistics from measurements that are part of a loop.
- **Compare event**, which can be used to chart actual versus expected values for a series of spectra.
- **Request event**, which may produce up to ten numerical or yes/no answers from the operator in response to a message-response request.

## Report To Spectrum events

Use this event to add information or specific workflow results to the spectra generated by a specific collect event in a workflow. You can place text or results in three areas of a spectral data file including the spectrum title, spectrum comments and spectrum history. Information you place in the title and comments can replace or be appended to the existing title and comments.

Examples of information you might want to add to a spectral file are provided below.

- **Request event results.** You can set up a request event to query information from the operator and add the responses to your spectral data. Examples include the operator name, the sample material or bin number, and parameter settings that are important to the experiment.

The example below shows the operator name reported to the comments section of a spectral data file.

```
Comments: Operator name: Mary Doe
```

- **Check event results.** Pass/fail results from a check event can also be saved with the spectral data. Pass/fail results reported to the comments section of a spectral data file look like this:

```
Comments: Pass/Fail result: PASS
```

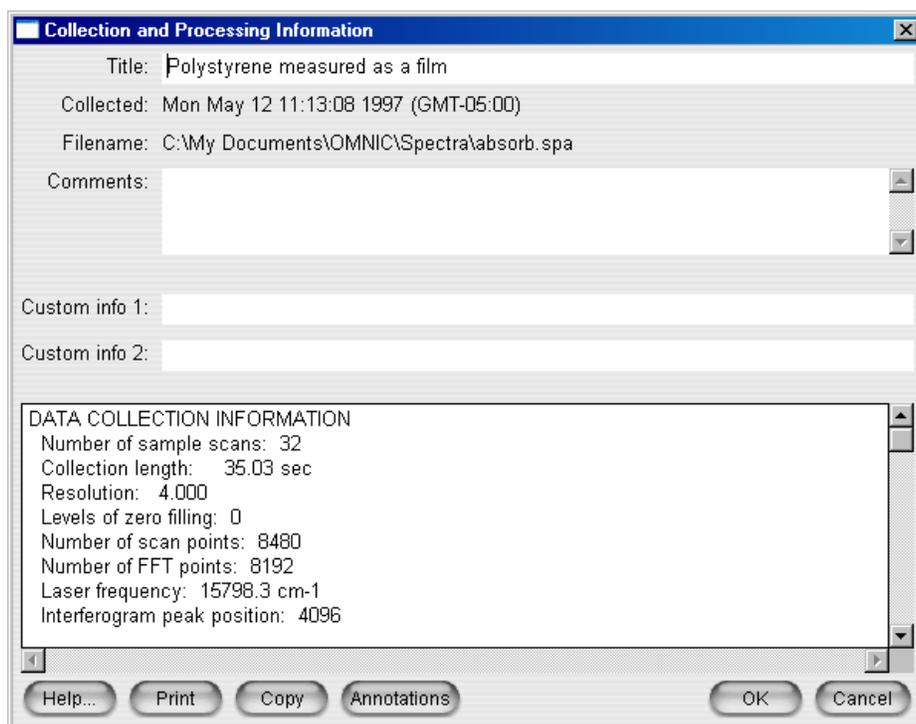
- **Sample position number.** When using an autosampler for data collection, it is useful for tracking purposes to report the carousel position and cycle number to the corresponding spectrum. This also applies to the channel and cycle number for the Antaris MX and Antaris EX systems. For autosamplers, the Report To Spectrum event retrieves the sample position and cycle numbers from the Position Autosampler event. For Antaris MX and Antaris EX analyzers, the information comes from a Collect multi-channel event.
- **Measure, calculate or compare event results.** You can select specific results produced by a measure event, a calculate event or a compare event in the workflow (by Data Type and Attribute). Examples include component concentrations and uncertainty limits from a measure event, the maximum or average value from a calculate event, and the correlation coefficient from a compare event. Each result is reported along with its associated description. The following example shows the concentration value and uncertainty limit for ethanol reported to the comments section of a spectral data file.

```
Comments: % Ethanol(Concentration): 49.41  
          % Ethanol(Uncertainty): 0.97
```

Each time a workflow archives a spectrum, RESULT saves information about how the spectrum was collected and processed along with the spectral data. You can view the collection and processing information using Thermo Scientific TQ Analyst method development and OMNIC spectroscopy software if those applications are available on your computer.



To display the collection and processing information for a spectrum that is open and selected in TQ Analyst or OMNIC, click the Information button (labeled “i”) above the spectral window. The software opens the Collection and Processing Information window, which looks like this:



Workflow results and other information reported to the spectrum title or comments will appear in the Title and Comments boxes respectively. results and information reported to the spectrum history will be appended to the Data Processing History section of the Data Collection Information. You will need to scroll the bottom portion of the window to display the Data Processing History. You can overwrite the existing title or comments or append the new information to what was already there. Information and results placed in the Data Processing History can only be appended.

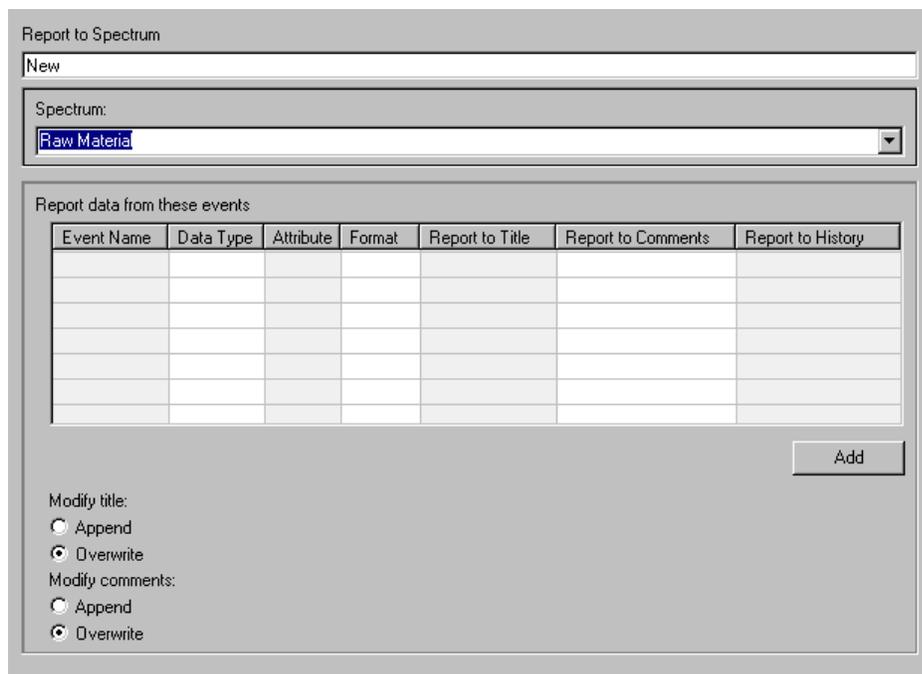
**Event result:** None

**Associated specifications:** None

**Related events:** Collect event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the report to spectrum event. These parameters appear in the display area of RESULT Integration when a report to spectrum event is selected in a workflow.



Event Name	Data Type	Attribute	Format	Report to Title	Report to Comments	Report to History

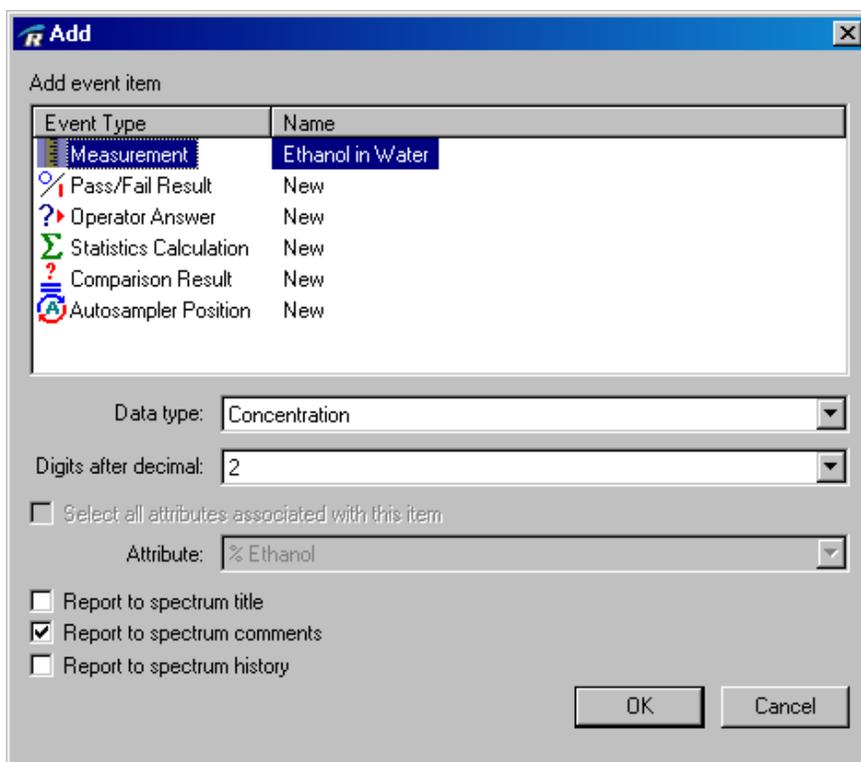
### Report To Spectrum event parameters

The Report To Spectrum event parameters specify the spectrum the information will report to, the workflow results to report, the format of the reported information and the destination within the collection and processing information window. The following sections explain the Report To Spectrum event parameters in detail. The parameters are explained in the order in which they appear in the software.

#### Spectrum

Use this list box to specify the spectrum the information will be reported to by selecting a name in the drop-down list. The list gives the names of all the collect events included in the workflow.





The dialog box lists all the results in the current workflow.

**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a text string or value or all of those events have already been added to the Report To Spectrum event. ▲

Select a workflow event in the list. Make sure you select an event that is positioned before this Report To Spectrum event in the workflow. Since a workflow implements events in sequence, only events positioned before the Report To Spectrum event will have results that can be reported. If you select an event that occurs after the Report To Spectrum event, the workflow will be unable to find the corresponding data and will produce an error.

After you select a result, the following parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Examples are provided below.

- *Data Type.* Use this list box to select a result produced by the selected event, such as a concentration or uncertainty value. The number and type of results produced depends on the event and, for measure events, the TQ Analyst or other method used for the measurement.
- *Digits After Decimal.* This box is available in the software only when the selected Data Type (see above) produces a numeric result.

Use the box to select the number of digits the software will include after the decimal point in the numeric result. You can include up to six decimal places. The software rounds the number and retains only the specified decimal places.

- *Attribute.* Use this list box to select a specific component or other measured attribute or value for the selected data type and event. The number and type of items in the attribute drop-down list depend on the event and, for measure events, the TQ Analyst or other analytical method used for the measurement. For example, a measure event configured for spectral measurements could include the following items in the Attributes drop-down list.

- *Select All Attributes Associated With This Item.* Select this option if you want to include all the measured components or other attributes or values for the selected data type and event.

- *Report to Title/Comments/History.* Use these features to specify where the workflow results should be reported in the collection and processing information window. You can report the information to the spectrum title, the spectrum comments or the data processing history.

<input type="checkbox"/>	Report to spectrum title
<input checked="" type="checkbox"/>	Report to spectrum comments
<input type="checkbox"/>	Report to spectrum history

-- Report to spectrum title. The title of a spectral data file appears in the spectral display window of RESULT software if the Spectra tab is enabled and selected during data collection. The default title gives the date and approximate time the spectrum was collected and the name of the associated collect event in the workflow.

Select this option if you want to customize the title by adding text or values from the selected workflow result. The spectrum title is limited to approximately one line that fits the width of the spectral window.

If the spectrum is archived, the software saves the spectrum title with the spectrum. If Save Files Automatically and Add Spectrum Title are selected on the archive event, the software will use the spectrum title as the spectrum file name.

**Note** You may want to limit the number of characters in the spectrum title if you elect to use it to name the archived data file. ▲

-- Report to spectrum comments. Select this option if you want to add text or values from the selected workflow result to the comments section of the collection and processing information for the selected spectrum. The comments section is normally empty and the information cannot be displayed in RESULT software. However, any workflow results reported here will be archived with the spectral data file and can be displayed in TQ Analyst and OMNIC.

-- Report to spectrum history. Select this option if you want to add text or values from the selected workflow result to the data processing history for the selected spectrum. RESULT uses the data processing history to log information about how the spectrum has been modified. This information can be used as part of an audit trail for the spectrum. The information cannot be edited or deleted in any application but you can use a Report To Spectrum event to add to it. Workflow results reported here can only be displayed in TQ Analyst and OMNIC.

When you are finished selecting a workflow result, choose OK. The selected result is added to the list of items to be reported to the selected spectrum.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete Selected Row, or select the row and press Delete on the keyboard. To edit a property for a workflow result, double-click the corresponding cell in the table.

To change the order in which workflow results are reported to a spectrum, drag the corresponding row to a new location in the table. To sort a column of entries in numeric or alphabetic order, right-click the column heading to display a shortcut menu and then choose Sort Ascending or Sort Descending.

Event Name	Data Type	Attribute	Format	Report to Title	Report to Comments	Report to History
Ethanol...	Concent...	% Ethanol	_0.00_	No	Yes	No

Modify title:  
 Append  
 Overwrite

Modify comments:  
 Append  
 Overwrite

Add

Repeat these steps for each workflow event that will generate results you want to report to the spectrum.

Modify title:  
 Append  
 Overwrite

Modify comments:  
 Append  
 Overwrite

- **Modify Title/Modify Comments.** Use these features to specify whether the selected workflow results will replace any existing information in the spectrum title or comments or add to it. The settings for these features will affect all results reported to the spectrum title and comments.

**Note** Workflow results placed in the spectrum history are always appended. ▲

Edit

- **Edit.** To edit the properties for a workflow result shown in the table above, double click the appropriate column and row. If you double-click the Event Name, Data Type, Attribute or Format column, the software opens the Add Event Item dialog box. Edit the settings as desired and then choose OK to save your changes.

If you double-click the one of the Report To Title/Comments/History columns, the software activates a list box which allows you to turn the corresponding option on and off. The new settings will be used the next time you run the workflow.

**Usage:** A Report To Spectrum event must specify a valid collection result (spectrum) in order to report the selected workflow results.

Make sure you place the Report To Spectrum event after its associated collect event in the workflow. If the Report To Spectrum event appears before the associated collect event, the workflow will produce an error. If the collect event occurs in a loop, make sure the loop also includes the associated Report To Spectrum event.

If you want the workflow to archive the information placed in the spectrum title, comments or history, you must add a subsequent archive event to the workflow and add the spectrum to the list of items to be archived.

## Report To Text File events

Use this event to export specific workflow results to a text file so they can be accessed, viewed, and printed from other applications. The text file provides the data in a simple tabular format that is accepted by data management applications and LIMS systems for post processing.

You can export both numeric and text results. The results are placed in a tab-separated text (\*.txt) file with a file name you specify. You can append the new data to the file or overwrite the file's previous contents.

**Event result:** None

**Associated specifications:** None

**Related events:** None

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the Report To Text File event. These parameters appear in the display area of RESULT Integration when a Report To Text File event is selected in a workflow.

Report to Text File

New

Text File:

Base path: C:\RESULT Data\Workflows

File name:

Report data from these events:

Event Name	Data Type	Attribute	Format

Clear previous contents

Add header line

## Report To Text File event parameters

The Report To Text File event parameters specify the workflow results to report in text format and the path and file name of the text file. The following sections detail the Report To Text File event parameters. The parameters are explained in the order in which they appear in the software.

### Text File

Use these features to specify a destination for the selected workflow results.

Text File:

Base path: C:\RESULT Data\Workflows

File name:

- Base path.** This readout shows the base path for the text file. The file must be located in the current path for archiving workflows and methods in RESULT Integration. See “Setting RESULT Integration Options” in the “RESULT Integration User Guide” for information about setting this path.

**Note** If you transfer the workflow to RESULT Operation, this base path is not used. Instead, the software uses the base path for archiving workflows and methods in RESULT Operation. This allows you to separate data produced while developing or testing a workflow in RESULT Integration from data produced while running a workflow in production mode. ▲

- **File Name.** Use this box to specify the path and file name for the text file. You can use the Browse button to locate and select an existing text file or create a file by typing a name in the File Name box. If you add a file name extension that is recognized by your text processing application (for example .txt), you will be able to double-click the file to quickly open it. If not, Windows lets you select an application when you try to open the file.

The file can be in the same folder as your workflows and method or you can create a folder for archiving text files. You can only select or create folders that are located in the base path for archiving spectra and reports in RESULT Integration.

If you run the workflow in RESULT Operation, the workflow results will be exported to the specified text file and folder, but the folder will be located in the base path for archiving workflows and methods in RESULT Operation. (If the folder or file doesn't exist, the software will create it.) See "Setting RESULT Integration Options" in the "RESULT Integration User Guide" and "Setting RESULT Operation Options" in the "RESULT Software Administration" guide for information about setting the path for archiving workflows and methods in each of those applications.

## Report Data From These Events

Use these features to specify workflow results to export to a text file.

Report data from these events:

Event Name	Data Type	Attribute	Format
------------	-----------	-----------	--------

Clear previous contents  
 Add header line

Add Edit



- **Add.** Choose this button to add a workflow event to the Report To Text File event. The software displays the Add dialog box.

R Add

Add event item

Event Type	Name
Measurement	Ethanol in Water
Measurement	Water

Data type:

Digits after decimal:

Select all attributes associated with this item

Attribute:

OK Cancel

The dialog box lists all the events in the current workflow that produce results that can be exported to a text file (anything but a spectrum).

**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a text string or value or all of those events have already been added to the Report To Text File event. ▲

Select a workflow event in the list. Make sure you select an event that is positioned before this Report To Text File event in the workflow. Since a workflow implements events in sequence, only events positioned before the Report To Text File event will have results that can be exported. If you select an event that occurs after the Report To Text File event, the workflow will produce an error.

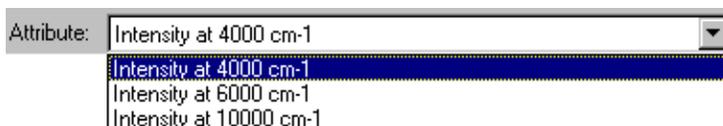
After you select a result, the following parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Examples are provided below.

- *Data Type*. Use this list box to select a result produced by the selected event, such as a concentration or uncertainty value. The number and type of results produced depends on the event and, for measure events, the TQ Analyst or other method used for the measurement.
- *Digits After Decimal*. This list box is available in the software only when the selected Data Type (see above) produces a numeric result.

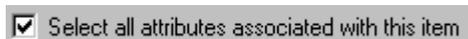
A screenshot of a software dialog box. It features a label 'Digits after decimal:' followed by a text input field containing the number '2'. To the right of the input field is a small downward-pointing arrow icon, indicating a dropdown menu.

Select the number of digits the software will include after the decimal point in the numeric result. You can include up to six digits after the decimal point. The software rounds the number and retains only the specified decimal places.

- *Attribute*. Use this list box to select a specific component or other measured attribute or value for the selected data type and event. The number and type of items in the attribute drop-down list depend on the event, and the TQ Analyst or other method used for the measurement. For example, a measure event configured for spectral measurements could include the following items in the Attributes drop-down list.



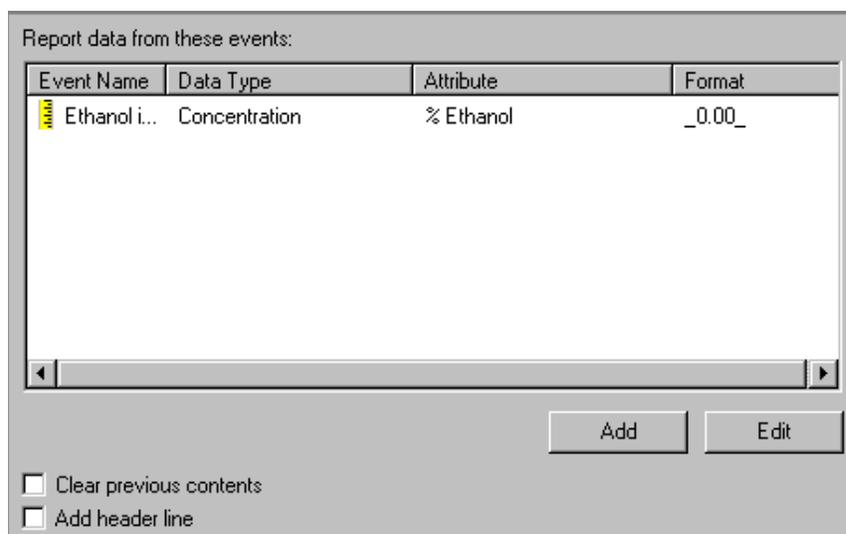
- *Select All Attributes Associated With This Item.* Select this option if you want to include all the measured components or other attributes or values for the selected data type and event.



When you are finished selecting a workflow result, choose OK. The selected result is added to the list of items to be exported to the specified text file.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete, or select the row and press Delete on the keyboard. Use Export To Text File to write the information displayed in the table to a text file with a file name and path you specify.

To change the order in which the workflow will write the data to the text file, drag the corresponding row to a new location in the table.



Repeat these steps for each workflow event that will generate results you want to export to the text file.



- **Edit.** To edit the properties for a workflow event shown in the table above, select the event and then choose the Edit button below the table. The new settings will be used the next time you run the workflow.
- **Clear previous contents.** Select this option if you want the workflow to overwrite any previous data in the specified text file each time the workflow is run. When this option is cleared, each time the workflow is run it will add a new line of data to the file.

- **Add header line.** Select this option if you want the workflow to write the title of each item that is reported to the first line of the text file. The titles will always reference the Attribute names. If an Attribute has multiple Data Types listed, the title will also contain the Data Type.

**Note** The workflow can only add a header line to a blank file. If Add Header Line is selected in the workflow but the header line does not appear in your text file, recreate the file (either type a new name in the File Name box or use Windows Explorer to delete the previous file) or select Clear Previous Contents in the Report To Text File event and run the workflow again. ▲

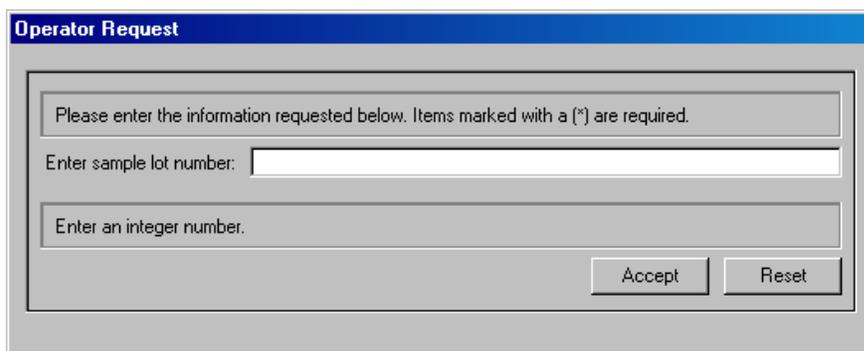
**Usage:** You can place a Report To Text File event anywhere in a workflow. A Report To Text File event must specify a valid workflow result in order to report those results to a text file. There are no other requirements for this event.

## Request events

This event can be used to create a dialog box that will request information from the operator at run time. You can configure the dialog box to require the operator to supply the requested information to continue running the workflow, or the information can be optional.

You can use a Request event to define two kinds of dialog boxes, a message-response dialog box and a class request dialog box.

- **Message-response dialog box.** This type of dialog box may contain up to ten messages, each requesting a specific response from the operator. An example of a message-response dialog box is shown below.

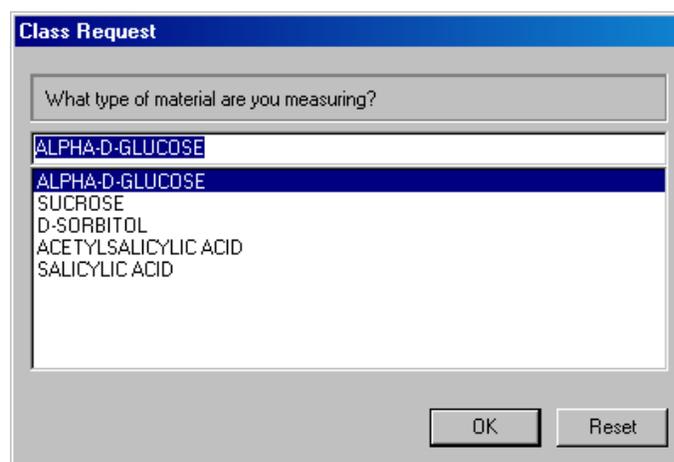


### Message-response dialog box

A request specification must define the message, the format for the operator response, and whether the operator is required to enter the requested information before the workflow can continue. A message-response dialog box generates a result containing all the messages and the corresponding responses.

- **Class-request dialog box.** This type of dialog box 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.

An example of a class request dialog box is shown below.



### Class request dialog box

This type of dialog box is appropriate only when placed after a measure event that has an associated TQ Analyst qualitative (classification) method that specifies more than one class.

**Note** This feature is not available for methods created using third-party method development software. ▲

A class request dialog box generates a result containing the selected class name (expected class), the index number for that class (as defined in the associated TQ Analyst method), and a pass or fail result. The workflow uses the associated measure event to compare the expected class to the measured (calculated) class. The request event generates a pass result when the expected class matches the calculated class, and a fail result when it does not.

Each time a workflow performs a request event, the workflow produces a result or set of results as described above. The workflow automatically stores the latest result, or result set, in the computer's internal memory so the result is available for use by subsequent events in the workflow.

**Event result:** Operator response or pass/fail string

**Associated specifications:** Request Specification

**Related events:** Check event, Measure event, Report event, Store event

**Related specifications:** Table Item specification, Summary item specification, Logical test specification

**Parameters:** The illustration below shows the parameters for the request event. These parameters appear in the display area of RESULT Integration when a request event is selected in a workflow.

The screenshot shows a dialog box titled "Request" with a subtitle "Result: operator response or Pass/Fail result". The dialog is divided into several sections:

- Request:** A text field containing "Known Class".
- Operator Request:**
  - A "Request specification:" dropdown menu with a "New" button and a "Details" button.
  - A checked checkbox labeled "Prompt for expected class".
  - A "Measure event:" dropdown menu containing "Known Class".
  - A "Test Dialog" button.
- Request input from:**
  - Three radio buttons: "Operator" (selected), "Text file", and "Text file (require operator confirmation)".
  - A "Base path:" field containing "C:\RESULT Data\Workflows".
  - A "File name:" field and a "Browse" button.
- Multiple Event Results:**
  - Two radio buttons: "Retain all event results" (selected) and "Retain most recent".

### Request event parameters

The request event parameters specify an operator request dialog box and the storage of data from multiple request events that occur in a loop. The following sections explain the request event parameters in detail. The parameters are explained in the order in which they appear in the software.

## Operator Request

The parameters in this group allow you to select a request specification, which defines the dialog box for a message-response request, or to create a special dialog box for entering the expected class for a particular sample. You can use the Test Dialog button to display either style dialog box, so you can see what it looks like without running the workflow.

- **Message-Response request dialog box.** Use these parameters to set up a message-response dialog box:
- **Request Specification.** A request specification defines up to ten messages to include in the dialog box and, for each message, the format for the operator response and whether the operator is required to enter the requested information before the workflow can continue. See “Request Specifications” in this chapter for information about setting up request specifications in a workflow. To link a request specification to a request event, select the specification name in the Request Specification drop-down list.

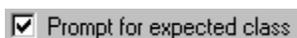


Use the New button at the right of the Request Specification list box to create a request specification and automatically link the new specification to the request event.

If the request event is already linked to a request specification, you can use the Details button to display that request specification.



- **Test Dialog.** Use this button to display the message-response dialog box so you can see what it looks like without running the workflow.
- **Class request dialog box.** Use these parameters to set up a class request dialog box:
- **Prompt For Expected Class.** This check box switches the dialog box from a message-response style to a class request style. When this option



is selected, the Request Specification list box becomes unavailable (it isn't required) and the Measure Event list box becomes available. Use the Measure Event list box (see below) to select a measure event in the workflow. (The request event must be positioned after the specified measure event in the workflow.) The specified measure event must be associated with a measurement specification for a valid TQ Analyst qualitative (classification) method. The software can use the operator's response to determine whether the expected material (expected class) matches the measurement result (measured class) and produce a pass or fail result for the measurement.



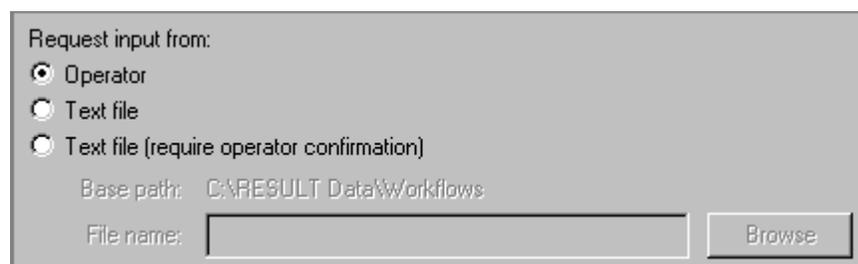
- **Measure Event.** This list box is available in the software only when Prompt For Expected Class (see above) is selected. Use the Measure Event list box to select a measure event in this workflow by selecting a name in the drop-down list. The list includes all the measure events that are included in the workflow.

Make sure you select a result that is produced by a measure event that appears before this request event in the workflow. The measure event must be associated with a measurement specification for a valid TQ Analyst qualitative (classification) method.

The software can use the operator's response to the class request dialog box defined above to determine whether the expected material (class) matches the measurement result and produce a pass or fail result for the measurement. The expected result (class name), the index number for that class, and the pass or fail result are included in the results for this type of request.

### Request Input From

The parameters in this group allow you to specify the source for the response.

A screenshot of a dialog box titled 'Request input from:'. It contains three radio button options: 'Operator' (which is selected), 'Text file', and 'Text file (require operator confirmation)'. Below the options, there is a 'Base path:' label followed by the text 'C:\RESULT Data\Workflows'. Below that is a 'File name:' label followed by an empty text input field. To the right of the text input field is a 'Browse' button.

You can require that the operator respond to the request directly, or that the requested response must be read from a text file with or without input from the operator. The available options are described below:

- **Operator.** Select this option if you want the software to prompt the operator to respond to the request at run time. The operator will have to provide a valid response before the workflow will continue.
- **Text File.** Select this option if you want the workflow to always use a specific text file that contains the requested information. When you select this option, the File Name box becomes available in the software. Use the File Name box to enter a valid file name for the requested information (must have a \*.txt file name extension), or choose Browse and then select an appropriate text file. The base path is the default path for storing workflows in RESULT Integration.
- **Text File (require operator confirmation).** Select this option if you want the workflow to provide the requested information but allow the operator to override the selection at run time. Then use the File Name box to enter a valid file name for the default response (must have a \*.txt file name extension), or choose Browse and then select an appropriate text file. When you run the workflow, the operator will have the option of confirming the default response, entering the requested information, or selecting another text file that contains the correct information.

### Multiple Event Results

#### Multiple Event Results

- Retain all event results
- Retain most recent result

If you place a request event in a repeat or perform-while loop, the event will produce one result or set of results during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent result. The options for storing results include:

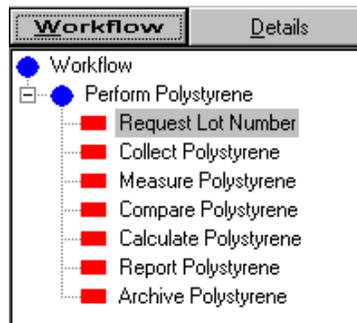
- **Retain All Event Results.** If the request event occurs in a loop, selecting this option causes the workflow to store all the results. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the request event is not positioned in a loop or the loop includes all subsequent events that operate on the result. This is the default setting for Multiple Event Results and will maximize your computer processing speed.

See “Repeat Events” and “Perform-while events” for more information about using stored data in a workflow.

**Usage:** A request event must be linked to a valid request specification to produce a message-response request dialog box, or it must specify a valid measurement result to produce a class request dialog box.

A request event that generates a message-response dialog box may be positioned anywhere in a workflow, typically before an event that requires input from the operator. Some examples of this include:

- Requesting the operator to enter the lot number for a sample or a group of samples (see example below).



- Requesting the operator to describe the environmental conditions (temperature, humidity, etc.) for the analysis.
- Requesting the operator to enter a sample weight or volume.

**Note** If you are using a request event to set up a class request dialog box and you want the software to generate a pass or fail result after comparing the operator’s response (expected class) to a measurement result (measured class), make sure you place the request event after the measure event that produces the measurement result. ▲

If you want the workflow to archive all of the operator responses from a message-response dialog box, or the selected class name (expected class) and index number from a class request dialog box, add a report event that includes a table or summary item specification to the workflow, add the request event result to the specification, and then use an archive event to archive the report. To archive the pass or fail result generated by a class request dialog box, either add the pass/fail result to a table item specification in a report as described above, or use a check event to store the pass/fail result in the audit log database.

The following events can operate on the operator response from a request event if those events are positioned after the request event in the workflow.

- **Check event**, which can be used to store the pass or fail result from a class request in the audit log database.
- **Report event**, which can be used to add the operator responses from a request event to a sample report.
- **Store event**, which can be used to store numeric responses from a request event in the audit log database so they can be accessed with the logs features of RESULT Operation and used to track trends in the data.

**Note** The store event may only be used to store floating point and integer responses in the audit log database. If you add an operator response that includes a text string, a calendar date, a yes/no response, or a class name, the store event will not store those items in the audit log. ▲

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Run Exe events

The run exe event allows you to run an executable program from a RESULT workflow. This feature is handy for embedding small tasks in a workflow that must be performed while the workflow is running. For example, you can set up a workflow to start a program that positions a customized sampling apparatus such as a robot before collecting data, or a program that accesses an archived spectrum or report, reformats the data and then sends it to your laboratory database software or LIMS.

The run exe event instructs the workflow to run the specified program. You must specify the file name of the executable program file. You may also specify a path name, any supporting information the program requires and a period of time the workflow must wait if the program fails to run.

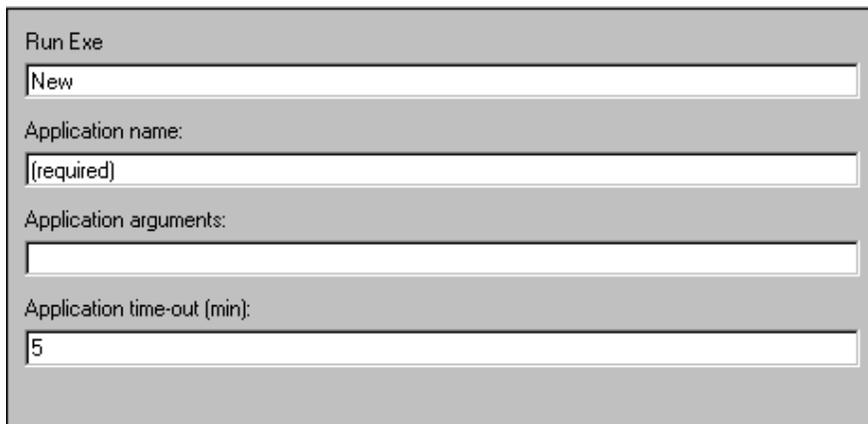
**Event result:** None

**Associated specifications:** None

**Related events:** None

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the run exe event. These parameters appear in the display area of RESULT Integration when a run exe event is selected in a workflow.



Run Exe

New

Application name:

(required)

Application arguments:

Application time-out (min):

5

### Run Exe event parameters

The run exe event parameters specify the executable program to be run, any supporting information the program requires and whether the workflow should wait for a specified period if the program fails. The following sections explain the run exe event parameters in detail. The parameters are explained in the order in which they appear in the software.

- **Application Name.** Use this text box to enter the file name of the executable program to be run. The program can be written in any programming language but the file must have an “.exe” file name extension.

If you enter a path name, the program must be located in that path when you run the workflow or the workflow will produce the following error when it implements the run exe event:

External application file not found

For example, if you enter the application name C:\RESULT Programs\robot.exe, the program must be located in a folder called RESULT Programs on a disk drive labeled “C” in order to run. This is true whether you run the workflow in RESULT Integration or RESULT Operation. If you don’t enter a path name, make sure you place the program in the same directory as the workflow.

- **Application Arguments.** Use this text box to specify any command line arguments the program requires. For example, an executable program that positions a robot might need the location coordinates of the next sample to complete the move.
- **Application Time-out.** Use this entry box to specify how long the workflow should wait before continuing if it starts the external program and the program fails. Enter the time in minutes in the Application Time-Out box. The default value is 5 minutes; entries of “zero” minutes are not accepted.

**Usage:** Run exe events may be placed anywhere in a workflow. There are no other requirements and no run exe event results that can be accessed by other events in a workflow.

## Store events

This event can be used to store selected workflow results in the *audit log database*. A store event may only be used to store numeric values in the audit log. The numeric results from the selected events will be stored in the audit log only when the workflow is run in RESULT Operation. The workflow stores the results in the audit log database that is currently configured for use with RESULT Operation (or a default database if a database has not been configured). See “Chapter 3 Configuring RESULT Operation” in the “RESULT Software Administration” manual for information about selecting and configuring the audit log database.

Results placed in the audit log by a store event can be used to track changes in the data over time. RESULT Operation provides two ways to access this type of data:

- **Measurement query.** You can access numerical data stored in the audit log by performing a measurement query using the Measurement option in the Logs menu of RESULT Operation. You can query the results of specific workflows, all workflows, specific events, or specific values, including components, attributes, and any requested values. You can also specify whether to report the data as a graph of measurement trends or to show results of your query in a table. See “Chapter 4 Working With The Audit Log” in the “RESULT Operation User Guide” for information about creating reports from data stored in the audit log.

- **Trend tab.** You can also access data stored in the audit log by using the features on the Trend tab in the RESULT Operation display window. The Trend tab displays selected workflow results in a graphically rich and interactive format. You can include historical data or data from a workflow that is currently running or a combination of these. See “Viewing trends in acquired data while running a workflow” in the “RESULT Operation User Guide” for more information.

**Note** A store event may not be used to store spectra, reports, the pass/fail result from a check event, or a text string, calendar date, or yes/no response from a request event in the audit log database. However, the archive event automatically stores a record of the selected spectrum or report (not the spectrum or report itself) in the audit log when a workflow is run in RESULT Operation (see “Archive events” in this chapter for more information). If you want to store a pass/fail result in the audit log, select Store Pass/Fail RESULT To Database in the check event parameters (see “Check events” in this chapter for details). If you want to store a text string, calendar date, or yes/no response from an operator request in the audit log, add those items to a sample report and then use an archive event to archive the report. ▲

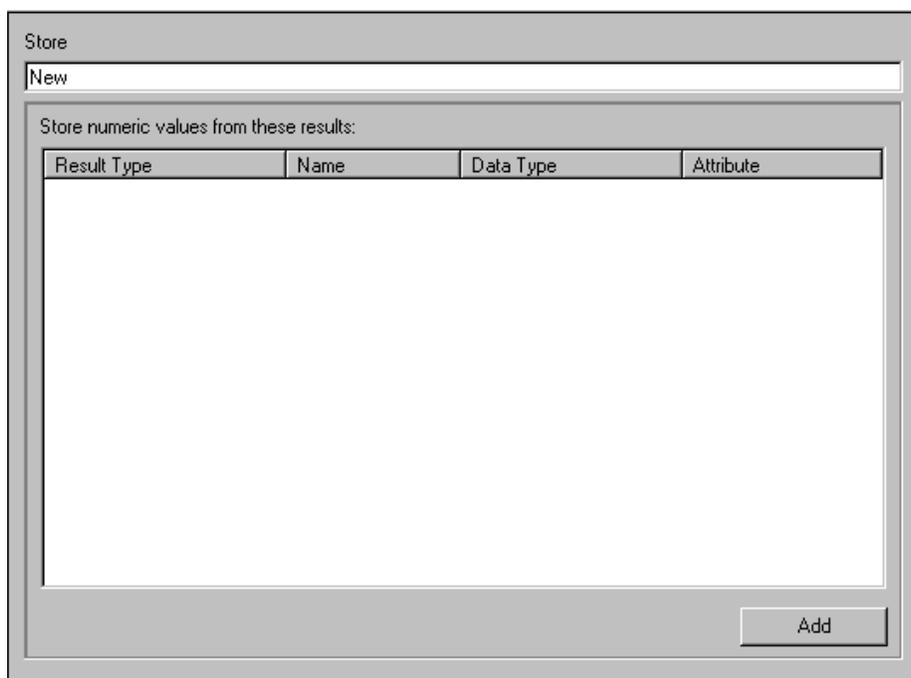
**Event result:** None

**Associated specifications:** None

**Related events:** Calculate event, Compare event, Measure event, Request event

**Related specifications:** None

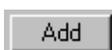
**Parameters:** The illustration below shows the parameters for the store event. These parameters appear in the display area of RESULT Integration when a store event is selected in a workflow.



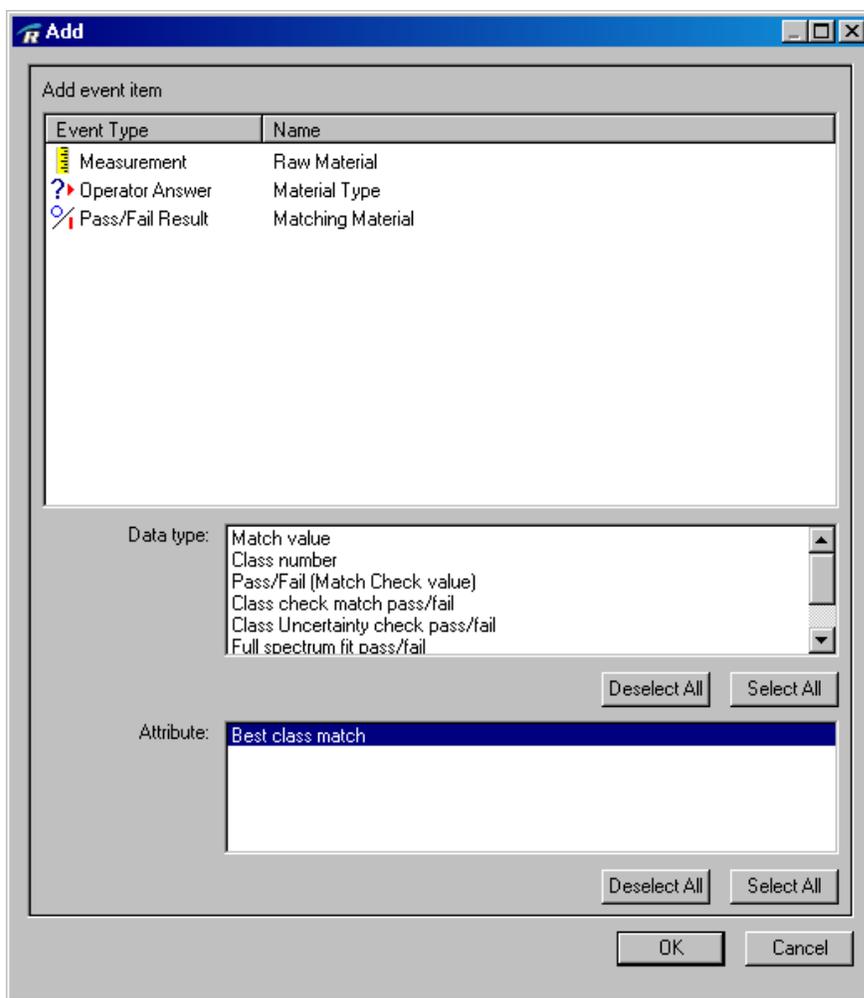
### Store event parameters

The store event parameters allow you to specify the workflow results that will be stored. A store event may only be used to store floating point (numbers that allow decimal points) and integer (whole numbers) values in the audit log.

- **Store Numeric Values From These Results.** Use this box to select the workflow results that will be stored in the audit log database.



- **Add.** Choose this button to add a workflow result to the list of items to be stored. The following dialog box is displayed.



The list shows all the workflow events that produce at least one result that is a floating point or integer value.

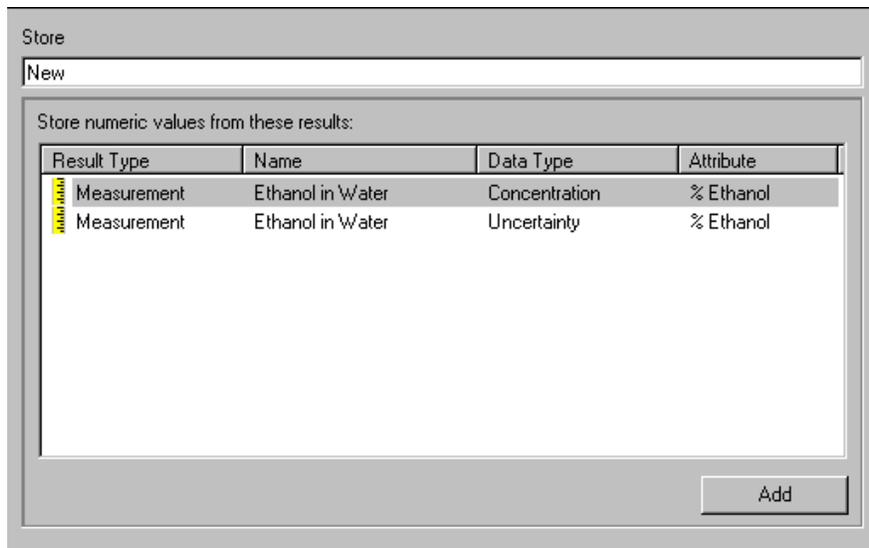
**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a numeric result or all of those events have already been added to the store event. See the Usage heading for this Store event for a list of events that can produce numeric results. ▲

For each event item, use the Data Type and Attribute selection boxes to identify specific workflow results you want to store. For example, to store only the concentration value for the %Ethanol component, select Concentration in the Data Type box and then select %Ethanol in the Attribute box. Make sure the results you select are produced by events that appear before this store event in the workflow.

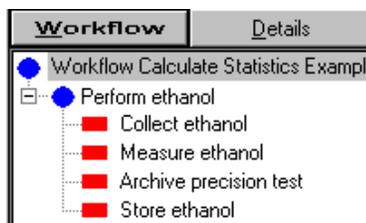
Use the Select All and Deselect buttons to select or Deselect all the listed Data Types or Attributes at once.

When you are finished selecting workflow results for the first event, choose OK to close the dialog box. The selected results appear in the list of results to be stored, as shown in the example below.

To delete a workflow result from the list, select the result name and then press the Delete key on the keyboard.



**Usage:** Store events must be placed after the event or events that produce the numeric values you want to store as in the example below.



You can use one store event to store values from all the results that are generated by a workflow, or insert multiple store events to store specific values. Only numeric results from the following events may be stored:

- **Request event**, which may produce up to ten numeric values from the operator in response to a message-response request.
- **Measure event**, which can be used to analyze collected spectra to produce numeric concentration values, library index values, match values, or spectral measurements such as a peak height or area.
- **Calculate event**, which can be used to produce statistics from measurements that are part of a loop including minimum, range, standard deviation, percent standard deviation, sum, and count.

- **Compare event**, which can be used to compare a series of spectra and their measured values against expected values to produce correlation coefficients, root mean square error of prediction (RMSEP) values, and slope and y-intercept values for those measurements.

For more information, refer to the descriptions of these events located elsewhere in this chapter.

## Write To I/O events

This event is one of a read/write pair that allows a workflow to communicate with a hardware device such as a valve or alarm or control system.

You must have one of the optional input/output kits and an available Ethernet connection to output and receive external signals with RESULT. Each kit includes a controller and a mounting rack that holds standard I/O modules (digital and 4-20 milliamp analog modules are available from us). RESULT communicates with the controller via the Ethernet connection; the I/O lines can be connected to the specific equipment you need to monitor, control, or acquire data from such as a programmable logic controller (PLC), host computer or other device in your factory.

You can use a Write To I/O event to send data or signals to a hardware device connected to a specific I/O line, also called a point. For information about using RESULT to read or acquire data from an I/O device, see the Read From I/O event described earlier in this chapter.

**Event results:** None (this event does not produce results)

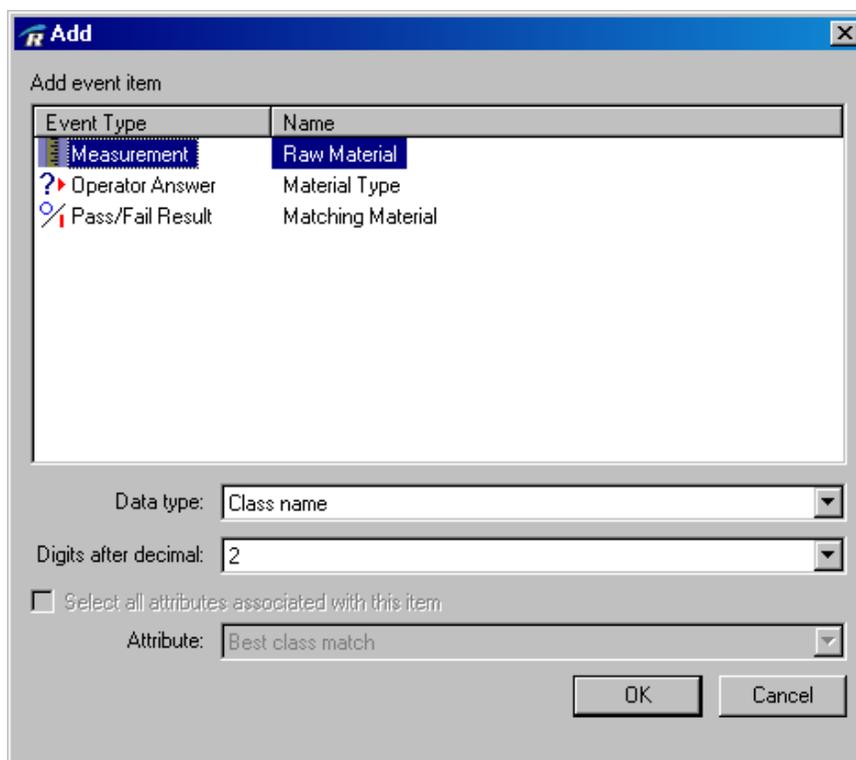
**Associated events:** None

**Associated specifications:** None

**Parameters:** The illustration below shows the parameters for the Write To I/O event. These parameters appear in the display area of RESULT Integration when a Write To I/O event is selected in a workflow.







The dialog box lists all the results in the current workflow that can be sent through an I/O line. This type of communication is limited to numeric and text results and excludes spectral data.

**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a text string or value or all of those events have already been added to the Write To I/O event. ▲

Select a workflow result in the list. Make sure you select a result from an event that is positioned before this Write To I/O event in the workflow or the workflow will produce an error. After you select a result, the following parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Examples are provided below.

- *Data Type.* Use this list box to select a result produced by the selected event, such as a concentration or uncertainty value. The number and type of results produced depends on the event and, for measure events, the TQ Analyst or other method used for the measurement. See “measure events” in this section for more information.

- *Digits After Decimal.* This list box is available in the software only when the selected Data Type (see above) produces a numeric result. Use the box to specify up to six decimal places for the numeric result. The software rounds the number and retains the specified decimal places.
- *Attribute.* Use this list box to select a specific component or other measured attribute or value for the selected data type and event. The number and type of items in the attribute drop-down list depend on the event and, for measure events, the TQ Analyst or other analytical method used for the measurement. For example, a measure event configured for spectral measurements could include the following items in the Attributes drop-down list.



- *Select All Attributes Associated With This Item.* Select this option if you want to include all the measured components or other attributes or values for the selected data type and event.

When you are finished selecting a workflow result, choose OK. The selected result is added to the list of items to be sent to through the I/O line.



-- Float Memory. Used to write a floating point (allows decimal point) number to the controller.

-- Integer Memory. Used to write an integer (whole number) to the controller.

**Note** For more information about mapping to memory points, see the user guide that came with your Opto 22 controller. ▲

- *Point #*. Double-click to activate the cell and then enter the point number on the I/O module that is associated with the signal.
- *Scale Low/High*. Scale low and high are useful only for analog signals. These settings allow RESULT to normalize a scale for the analog output. For example, you might want to normalize the scale when using RESULT to write the concentration of a component that ranges from 0% to 100% by setting Scale Low to 0 and Scale High to 100.

**Usage:** Write To I/O events may be placed anywhere in a workflow. There are no other requirements.

## Write To Excel events

Allow a workflow to send data and statistics to an Excel file (filename extension must be .xls). Must have Microsoft® Excel version 2003 or higher installed on the computer or network.

To learn how to set up a workflow to read data from an Excel file, see “Read From Excel events” in this chapter.

**Event results:** None (this event does not produce workflow results)

**Associated events:** None

**Associated specifications:** None

**Parameters:** Write To Excel event parameters specify a location for the Excel file, the RESULT event and data type to be reported, any statistical functions applied to the data and the locations to write to in the Excel spreadsheet.

Right-click table to display shortcut menu with options to add to, delete from and edit table.

Use Export To Text File in shortcut menu to write information in table to a text file with a file name and path you specify.

To specify default value for Initial Column, Initial Row or Excel Chart, right-click column heading and choose Edit Column. In dialog box, select Apply Default Setting, enter default value and choose OK.

### Excel file name

Specify or open an Excel file to be written to. To specify a file, enter a file name or browse to the file.

If you leave the file name box empty, RESULT software will create and use a new Excel window in the specified path.

### Report data from these events

Use this table to specify the data the workflow will send to Excel and the locations to write to in the Excel spreadsheet. The columns and features presented in the table are defined below.

Column	Description
Event Name	Filled automatically after you add a workflow result to the table. Event name comes from first editable field in the event parameters and also appears in the Add dialog box.
Data Type	Filled automatically after you add a workflow result to the table. Data Type comes from Data Type drop down list box in Add dialog box. Examples include a concentration or uncertainty value. See “Measure events” for details.

Attribute	Filled automatically after you add a workflow result to the table. Attribute comes from Attribute drop down list box in Add dialog box. Examples include a component or intensity value.
Format	Filled automatically after you add a workflow result to the table. Format comes from Digits After Decimal drop down list box in Add dialog box. Specify up to six decimal places for numeric result. Text results are reported as text string.
Initial Column/ Initial Row	Enter column and row where first reported data for corresponding event will appear in the Excel file.
Excel Chart	Select whether the data will also appear in a trend chart in the Excel file.

Function	Description
Add Row	Right-click table and choose Add Row. In Add dialog box, select a workflow event result (numeric and text only) to be sent to Excel and the corresponding Data Type, Attribute & Format. Make sure the event is positioned before this Write To Excel event or the workflow will produce an error. <b>Note:</b> If Add dialog box is empty, the workflow either does not contain an event that produces a text string or value or all of those events have already been added.
Edit Row	Double-clicking a row displays Add dialog box so you can edit Data Type, Digits After Decimal or Attribute settings for a workflow result.
Delete Row	Right-click the row and choose Delete Selected Row or select the row and press the Delete key.

## Use Excel Functions

Use this table to specify any statistical functions you want to apply to the data sent to Excel and the locations to write to in the spreadsheet. The columns and features presented in the table are defined below.

Column	Description
Excel Function	Double-click to select a statistical function to apply to a reported workflow result.
Attribute	Double-click to select a reported workflow result that will be used to calculate the statistic. All results listed in Attribute column of previous table will appear in this Attribute list box.
Column/Row	Enter column and row where the first reported statistic for the corresponding workflow result will appear in the Excel file.
Function	Description
Preview	Click to see a preview of the Excel file as defined in the table.

**Usage:** Write To Excel events may be placed anywhere in a workflow. There are no other requirements.

## Chapter 3 Structural Workflow Events

Structural workflow events help you organize your workflow by grouping related events and allow you to control when and how workflow tasks are performed. The structural events provided in RESULT Integration include:

- **Perform events**, which can be used to group related events that perform a similar or high-level task such as to collect, measure, and report a spectrum, and to stop a workflow or skip a group of events if the workflow reports an error. The workflow implements all the events in a perform group in sequence unless the perform event is set up to check for workflow errors and errors have occurred.
- **Repeat events**, which can be used to group related events that are repeated for a series of samples such as a collect, measure, and report event. The workflow performs all the events in a repeat group in sequence and then repeats the sequence a specific number of times.
- **Perform-if events**, which can be used to group related events that perform a specific task that should only be executed under certain conditions. One example is to set up a workflow that prints one report if the workflow encounters an error and a different report if it doesn't. The workflow executes all the events in a perform-if group when the condition is met.
- **Perform-while events**, which can be used to group related events that are repeated under certain conditions. One example is to design a workflow that requests the number of samples remaining and continues collecting data only when the operator responds with a number greater than zero. The workflow performs all the events in a perform-while group and repeats them when the condition is met.
- **StartStop event**, which can be used to allow the operator to control when the workflow will start and/or stop implementing a group of events.

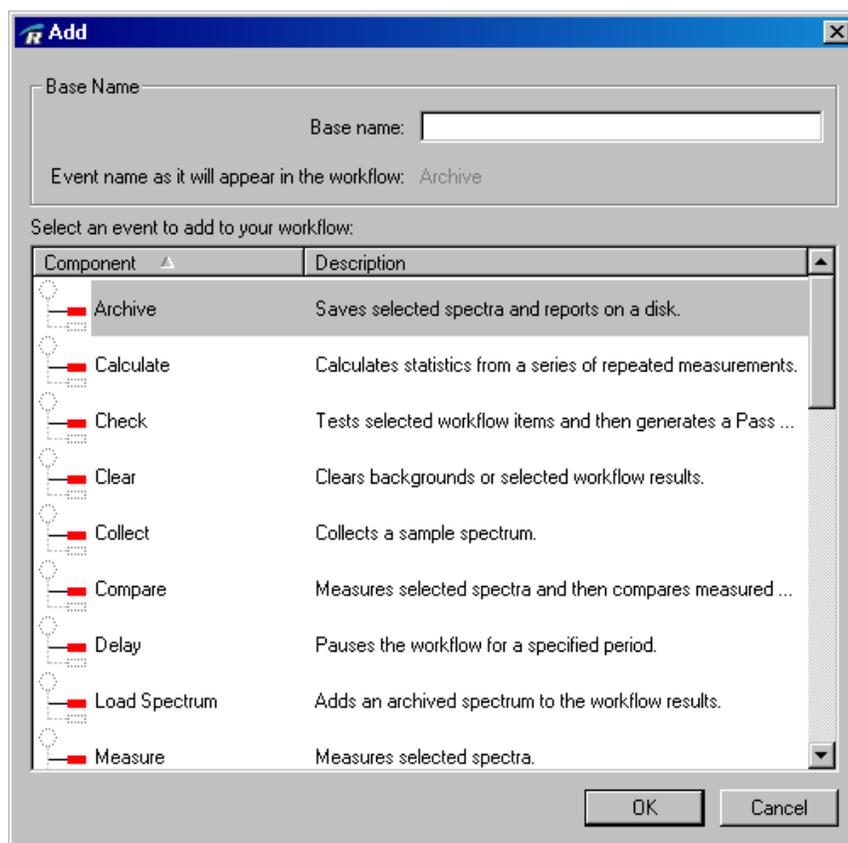
For information about other events that can be added to workflows, see “Chapter 1 Simple Workflow Events.” Events that can be used to control a specific hardware device are explained in “Chapter 3 Device-Specific Events.” To learn how to use RESULT software to collect and process spectral data continuously over a specified period, see “Chapter 4 Sequence Module Events.”

This section lists each structural workflow event and details its application and use. The following information is provided for each event:

- **Description**, which is a brief explanation of the event and how it works.
- **Associated specifications**, which lists the required and optional specifications that can be linked to the described event.
- **Related events**, which lists other events that operate like the described event or perform a similar function, and events that may be tied to the described event. For example, if a measure event can be used to measure the results from the described event, then the measure event would be listed as a related event.
- **Related specifications**, which lists other specifications that can be tied to the described event. For example, if a table item specification might be used to add a result from the described event to a sample report, then the table item specification would be listed as a related specification.
- **Parameters**, which explains the parameters for the described event. Parameters are described in the order that they appear in the software when the described event is selected in a workflow.
- **Usage**, which provides practical examples of how the described event is typically used in a workflow. It also lists any events that must appear before or after the described event in a workflow, and lists events that operate on results produced by the described event.

## Adding structural events to workflows

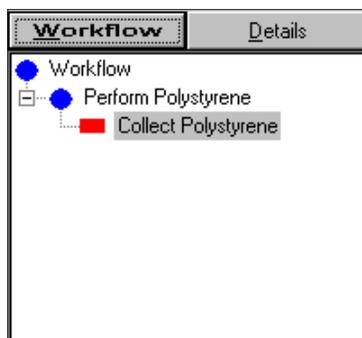
To create an event group using a structural workflow event, begin by adding the structural event to the workflow. For example, to create a perform group, select the main workflow group in the workflow navigation frame and then choose Add on the RESULT Integration toolbar. The following dialog box is displayed.



Select the perform event in the list of available events, enter a base name at the top of the dialog box, and then choose OK. The perform event is added to the workflow, as shown below.

To add events to an event group, select the structural event and then use the Add button to add events. Each new event is added to the end of the event group. For example, to add an event to the perform group shown above, select the perform event, choose Add, select the event you want to add and then choose OK. The added event appears indented under the perform event in the workflow navigation frame, as shown below.

Notice that the structural events are associated with a blue dot when displayed in the workflow navigation frame while simple events are associated with a red bar. These symbols are designed to help you differentiate between the two types of events and to reinforce the workflow's organization.



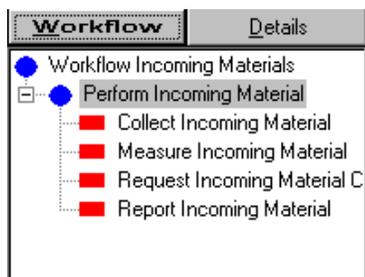
You can use the drag and drop and other editing features of RESULT Integration to arrange the events in an event group. See “Editing a workflow” in the “RESULT Integration User Guide” for more information.

**Note** When you are finished creating an event group and are ready to place the next event immediately after (but not in) that group, add the next event anywhere in the workflow and then hold down the Shift key on your keyboard while you drag the new event to the structural event at the head of the group. The dragged event will appear immediately below (but not in) the group. ▲

**Note** To learn about adding specifications to workflows and linking specifications to workflow events, see “Chapter 5 Workflow Specifications.” ▲

## Perform events

Perform events are used to set a series of events apart from the rest of the workflow as shown in the example below, and to stop a workflow or skip a group of events if the workflow reports an error.



Placing events in a group is often useful for convenience, for clarity, or for other purposes. The workflow implements all the events in a perform group in sequence unless the perform event is set up to check for workflow errors and errors have occurred.

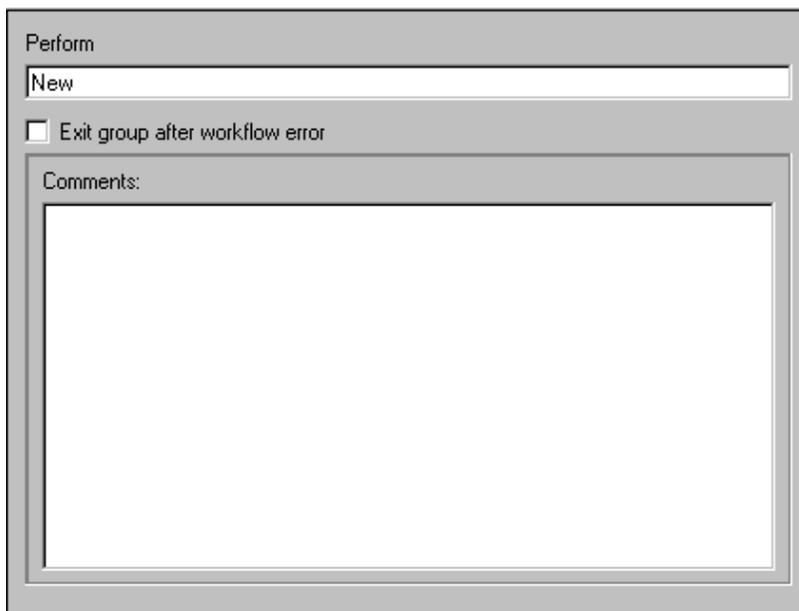
See “Adding structural events to a workflow” at the beginning of this manual for information about adding perform events to workflows and adding events to a perform group.

**Associated specifications:** None

**Related events:** Repeat event, Perform-If event, Perform-While event, StartStop event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the perform event. These parameters appear in the display area of RESULT Integration when a perform event is selected in a workflow.

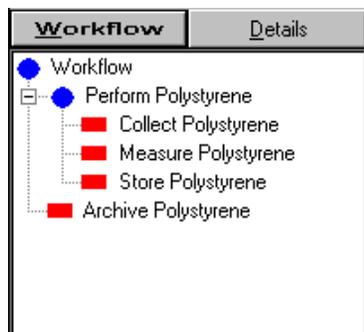


### Perform event parameters

The perform event parameters allow you to add comments to the group and to specify whether the workflow will check the group for errors. The perform event parameters include the following:

Exit group after workflow error

- **Exit Group After Workflow Error.** Select this option if you want the workflow to check the events in this group for errors.



If an error is found, the workflow skips to the next event, if any, that appears outside the group in the workflow tree. For example, if a workflow error was found in the Collect Polystyrene event shown in the illustration at the left, the workflow would skip to the Archive Polystyrene event and the Measure Polystyrene and Store Polystyrene events would not be implemented.

If this option is cleared and a workflow error occurs within the perform event group, the workflow will continue implementing the events in the group before continuing to the next event or event group. If you run a workflow in RESULT Integration by using Test Workflow in the

File menu and the workflow produces an error, the software will display an error message in the status box and continue running the workflow until it finishes implementing the last event. A report describing the workflow errors appears in the display area when the workflow is completed.

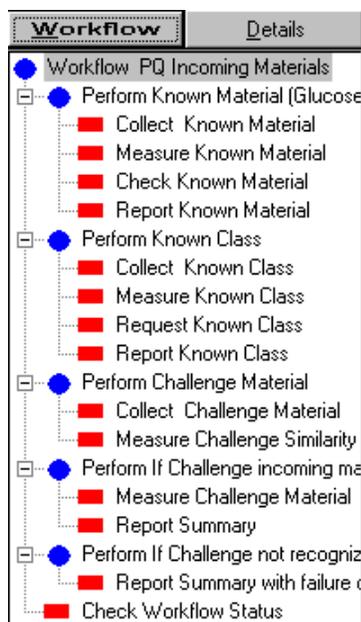
- **Comments.** Use this box to enter comments about the events that are included in a perform event group, typically describing the overall task the events are set up to perform. Grouping workflow events and adding comments to each group allows others to quickly understand how the workflow is configured and will help you troubleshoot any problems that occur when testing or running the workflow.

**Usage:** A perform event may be positioned anywhere in a workflow. These events are typically used to group related events that perform a similar or high-level task. Some examples of this include:

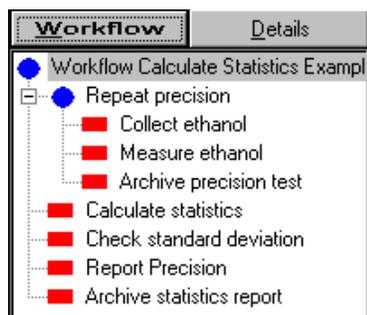
- Performing collection and analysis of a particular sample material.
- Requesting and then using data supplied by an operator.

A perform event may also be used to stop a workflow or skip a group of events if the workflow produces an error.

The workflow shown in the example below includes multiple perform groups, which are used to organize and identify high-level tasks.



## Repeat events



Repeat events may be used to set a series of events apart from the rest of the workflow in order to repeat those events, as shown in the example at the left. The workflow performs the events in a repeat group in sequence and then repeats the sequence a specified number of times. You may define the number of times the events are repeated, or set up an operator prompt or sampling sequence to define the number of repetitions. The repeat event can be set up to stop after the specified repetitions have completed or to exit if a condition is met.

See “Adding structural events to a workflow” at the beginning of this manual for information about adding repeat events to workflows and adding events to a repeat group.

**Associated specifications:** Logical test specification, Compare text specification

**Related events:** Perform event, Perform-If event, Perform-While event, StartStop event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the repeat event. These parameters appear in the display area of RESULT Integration when a repeat event is selected in a workflow.

Repeat

New

Number of Repetitions

Specify number of repetitions

Number of repetitions:

Prompt for number of repetitions

Default value:

Prompt text:

Use sampling sequence

Use sequence from text file  Require operator confirmation

Sampling Sequence

File name:

Early Exit

Allow early exit

Logic specification:

Condition for early exit:

Exit loop if test result is True

Exit loop if test result is False

## Repeat event parameters

The repeat event parameters allow you to specify the number of times the events in the repeat group will be repeated and whether to allow an early exit from the repeat loop. The following sections explain the repeat event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Number of Repetitions

Use this parameter to indicate whether the workflow will repeat the events a specific number of times or allow the operator or a sampling sequence to specify the number of repetitions at run time. The following options are available:

Specify number of repetitions

- **Specify Number Of Repetitions.** Select this option if you want the workflow to define the number of times the events in the repeat group will be executed. When this options is selected, the Number Of Repetitions box becomes available in the software. Select the Number Of Repetitions box and enter the total number of times you want to execute the repeat group, including the first time.

Prompt for number of repetitions

- **Prompt For Number Of Repetitions.** Select this option if you want to allow the person running this workflow to specify the number of times the events in the repeat group will be executed. When this option is selected, the next two entry boxes become available in the software.
  - *Default Value.* Use this entry box to specify a default value for the operator prompt. The default value will appear in the entry box below the operator message when the prompt is initially displayed.
  - *Prompt Text.* Use this text box to enter the message that will appear in the operator prompt. The message should request the operator to enter the number of repetitions for the events in the repeat group.

Use sampling sequence:

- **Use Sampling Sequence.** Select this option if you want to use a sampling sequence to define the number of times the events will be executed. This is useful for running an autosampler or for running a series of samples manually. You can define a sampling sequence in the workflow or import a sequence from a text file. The workflow can be set up to require a specific sampling sequence or allow the operator to create or import a sequence at run time.

When this option is selected, the software activates the table in the Sampling Sequence group. Use the table to set up a sampling sequence or, to import a sequence, select Use Sequence From Text File (below). The sampling sequence must specify a sample name and identification (ID) number, or position number if using an autosampler, for each sample. You can also add other kinds of information such as a descriptive title or comment. To add information to the table, right-click an empty row to display a shortcut menu and choose Add Row or right click a column and choose Add Column. Double-click to activate the cells. See “Using a sampling sequence with a workflow” in “Chapter 2 Creating and Editing Workflows” of the “RESULT Integration User Guide” for details.

Select one of the options below to specify whether the sampling information must be entered manually or imported from a text file with or without operator input.

- *Use Sequence From Text File.* Select this option if you want the workflow to always use a specific text file that contains the sequence information. When you select this option, the software activates the File Name box and Browse button in the Sampling Sequence group. Use the File Name box to enter a valid file name for the sampling sequence (must have a \*.txt file name extension), or choose Browse and then select an appropriate sequence file. The base path is the default path for storing workflows in RESULT Integration. See “Importing a sampling sequence” in “Chapter 2 Creating and Editing Workflows” of the “RESULT Integration User Guide” for more information.
- *Require Operator Confirmation.* Use this check box to specify whether the operator can view and edit the sampling sequence at run time. If the check box is selected, the software will prompt the operator to specify a sampling sequence. The operator will have the option of using the sampling sequence saved with the workflow or editing or re-entering the sequence information or selecting a text file that contains the sequence information. If this check box is cleared, the workflow will only run with the sampling sequence saved with or attached to the repeat event.

## Early Exit

The parameters in this group may be used to allow an early exit from the repeat event and to define the conditions for granting an early exit.

Early Exit

Allow early exit

Logic specification:

▼ New Details

Condition for early exit:

Exit loop if test result is True

Exit loop if test result is False

- **Allow Early Exit.** Select this option if you want to specify a condition for exiting the loop before the specified number of repetitions are completed. When this option is selected, the following two features become available in the software.
- **Logic Specification.** Use this feature to link a logic specification to this event. The logic specification allows you to define the workflow result to be tested and how the test will function. If the workflow already contains an appropriate logic specification, select its name in the drop down list (see below).



Use the Details button to the right of the list box to display the current settings, or the New button to create a logic specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the perform-if event. The new specification will be linked to the repeat event and its name will appear in the logic specification list box. See “Logic Specifications” in “Chapter 5 Workflow Specifications” for more information.

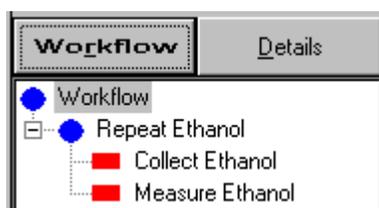
- **Condition For Early Exit.** Use these buttons to specify the action the workflow will take based on the true/false result of the logical test. The workflow will check the result of the compare text specification or the combined result of the logical test specification after implementing each event in the repeat group, and take the appropriate action based on the test result.



- *Exit Loop If Test RESULT Is True.* Select this option if you want the workflow to stop executing the events in the repeat group when the test result is true.
- *Exit Loop If Test RESULT Is False.* Select this option if you want the workflow to stop executing the events in the repeat group when the test result is false.

**Usage:** Repeat events may be positioned anywhere in a workflow. These events are typically used to group related events that you want to execute more than once, such as a series of events to collect, measure and report a spectrum collected from a group of similar samples. The repeat event may be linked to an optional logic specification to test for an early exit condition.

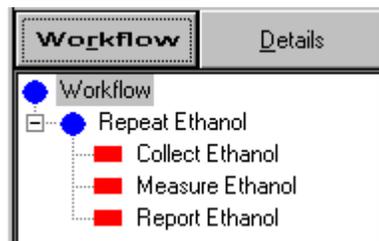
Each event that is part of a loop will produce one result from each loop iteration. For example, for each iteration of a loop that includes a collect event and a measure event (see the example below), the collect event will generate one spectrum and the measure event will produce one set of measured data.



### Repeat loop with two events

If you want the workflow to do something with the data, for example to store it in the audit log, archive it or add it to a sample report, you can set this up two ways. The simplest way is to include that task in the loop. The illustration below shows a report event added to the loop.

If you configure the loop this way and retain all the collect and measure event results, the workflow will report multiple copies of the data. See “Collect events” and “Measure events” for details.

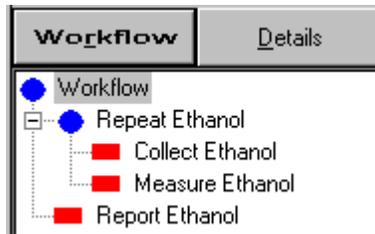


### Report event inside repeat loop

When a loop is configured this way, each event in the loop should have the Multiple Event Results option set to Retain Most Recent Result. For each iteration of the loop, the workflow will collect a spectrum, measure the spectrum, create a report that contains the measured data and the spectrum, and then clear the data from the computer’s internal memory.

An alternative option is to place the next task after the loop as in the next illustration. (This has certain benefits, which are explained below.)

If you configure the loop this way and retain only the most recent collect and measure event results, the workflow will only report the data generated the last time the workflow implements the loop.



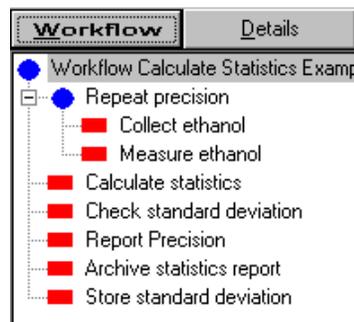
### Report event outside repeat loop

When a loop is configured this way, each event in the loop must have the Multiple Event Results option set to Retain All Event Results. For each iteration of the loop, the workflow will collect and measure a spectrum and keep the spectrum and the measured data in computer memory so the report event can add it to the sample report.

**Note** Use a clear event (positioned after the report event) to clear the data from the computer's internal memory. ▲

**Tip** Place an archive event after a loop if you want to archive all the spectra and/or reports with the same GUID or date and time stamp. ▲

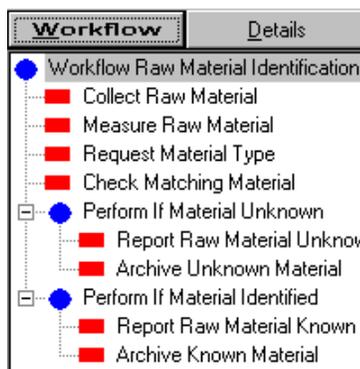
**Tip** Calculate events are typically placed after a repeat loop that contains a collect event and its associated measure event, as shown in the example below:



Make sure you configure the measure event to retain all the event results. This is the only way to produce many of the statistical values, such as range and standard deviation. ▲

## Perform-If events

Perform-if events may be used to set a series of events apart from the rest of the workflow so those events can be executed based on the results of a logical test. The perform-if event uses a logical test specification to define the test and specifies the condition for the test result. The picture below shows an example of a perform-if event used in a workflow.



See “Adding structural events to a workflow” at the beginning of this manual for information about adding perform-if events to workflows and adding events to a perform-if group.

**Associated specifications:** Logical test specification, Compare text specification

**Related events:** Perform event, Perform-While event, Repeat event, StartStop event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the perform-if event. These parameters appear in the display area of RESULT Integration when a perform-if event is selected in a workflow.

## Perform-if event parameters

The parameters for the perform-if event specify the conditional test and an optional early exit. The following sections detail the perform-if event parameters. The parameters are explained in the order in which they appear in the software.

### Conditional Test

The parameters in this group allow you to select a logic specification, which defines the test, and the condition for the test result.

- Logic Specification.** Use this feature to link a logic specification to this event. The logic specification allows you to define the workflow result to be tested and how the test will function. If the workflow already contains an appropriate logic specification, select its name in the drop down list (see below).

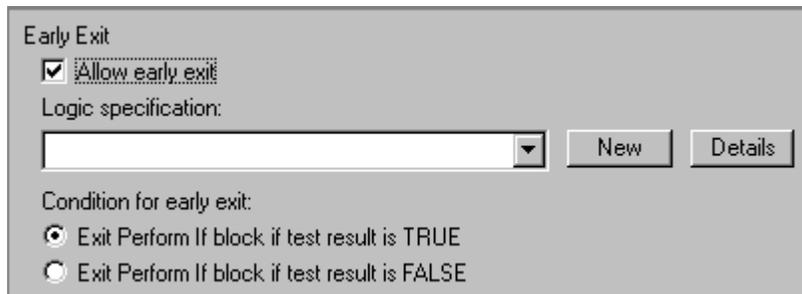
Use the Details button to the right of the list box to display the current settings, or the New button to create a logic specification. The workflow displays the parameters on the right side of the RESULT

Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the perform-if event. The new specification will be linked to the perform-if event and its name will appear in the logic specification list box. See “Logic Specifications” in “Chapter 5 Workflow Specifications” for more information.

- **Perform-If Condition.** Use these buttons to specify the action the workflow will take based on the true/false result of the logical test. The workflow will check the result of the test specification before executing the first event in the group and take the appropriate action based on the test result.
  - *Execute Events If Test RESULT Is True.* Select this option if you want the workflow to execute the events in the group when the test result is true.
  - *Execute Events If Test RESULT Is False.* Select this option if you want the workflow to execute the events in the group when the test result is false.

### Early Exit

The parameters in this group may be used to allow an early exit from the perform-if event and to define the conditions for granting an early exit.



- **Allow Early Exit.** Select this option if you want to specify a condition for exiting the perform-if event after the event has started running. When this option is selected, the next two features become available in the software.

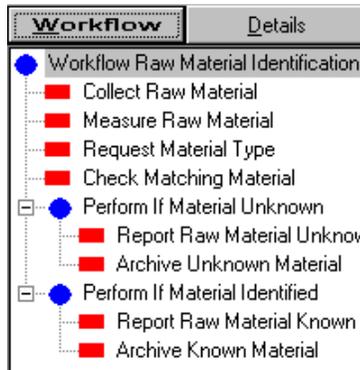
- **Logic Specification.** Use this option to create or select a logic specification, which defines the workflow results to be tested and how the test will function. See “Logic Specification” above for information about linking a test specification to this event. For information about setting up test specifications in workflows, see “Logic Specifications” in “Chapter 5 Workflow Specifications.”
- **Condition For Early Exit.** Use these buttons to specify the action the workflow will take based on the true/false result of the logical test. The workflow will check the result of the test specification after implementing each event in the perform-if group, and take the appropriate action based on the test result.
  - *Exit Perform If Block If Test RESULT Is True.* Select this option if you want the workflow to stop executing the events in the group when the test result is true.
  - *Exit Perform If Block If Test RESULT Is False.* Select this option if you want the workflow to stop executing the events in the group when the test result is false.

**Usage:** A perform-if event must be linked to a valid logic specification, such as a logical test specification or a compare text specification, in order to perform events based on a conditional test. The perform-if event may also be linked to an optional logic specification to test for early exit.

Perform-if events may be positioned anywhere in a workflow. These events are typically used to group related events that perform a similar or high-level task which should be executed only under certain conditions. Some examples of this include:

- Checking the status of measurement or other results and then storing those results only when they meet a defined standard.
- Printing one report if the workflow encounters an error, and a different report if it doesn't.

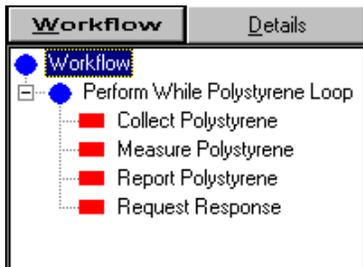
The workflow shown in the example below includes two perform-if groups. The first one (Perform If Material Unknown) creates and archives a report when the measurement results indicate that the sample material is unknown (no matching spectrum found in the method standards).



The second perform-if group (Perform If Material Identified) creates and archives a report when the measurement result indicates that the sample material is known (closely matched spectrum found in the method standards).

If the perform-if event is set up to test the result from a measurement or other event in the workflow, then the measurement or other event that produces that result must occur before the perform-if event in the workflow.

## Perform-While events



Perform-while events may be used to set a series of events apart from the rest of the workflow so those events can be executed or repeated based on the results of a logical test. The perform-while event uses a logical test specification to define the test and the condition for the test result. The picture at the left shows an example of a perform-if event used in a workflow.

See “Adding structural events to a workflow” at the beginning of this manual for information about adding perform-while events to workflows and adding events to a perform-while group.

**Associated specifications:** Logical test specification, Compare text specification

**Related events:** Perform event, Perform-If event, Repeat event, StartStop event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the perform-while event. These parameters appear in the display area of RESULT Integration when a perform-while event is selected in a workflow.

Perform While

New

Conditional Test

Logic specification:

Repeat events at least once

Perform While condition:

Repeat events if test result is TRUE

Repeat events if test result is FALSE

---

Early Exit

Allow early exit

Logic specification:

Condition for early exit:

Exit loop if test result is TRUE

Exit loop if test result is FALSE

## Perform-while event parameters

The parameters for the perform-while event specify the conditional test and an optional early exit. The following sections explain the perform-while event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Conditional Test

The parameters in this group allow you to select a logic specification, which defines the test, and to select the condition for the test result.

- Logic Specification.** Use this feature to link a logic specification to this event. The logic specification allows you to define the workflow result to be tested and how the test will function. If the workflow already contains an appropriate logic specification, select its name in the drop down list (see below).

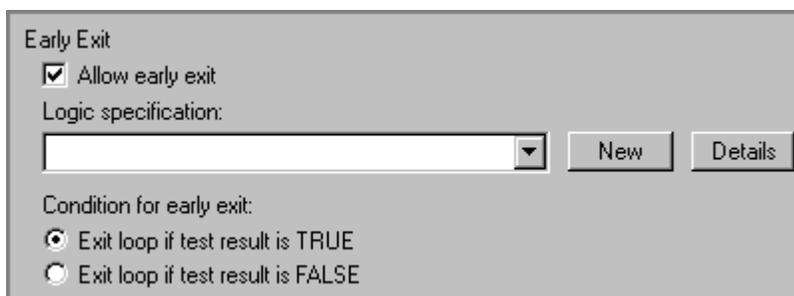
Logic specification:

Use the Details button to the right of the list box to display the current settings, or the New button to create a logic specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the perform-while event. The new specification will be linked to the perform-while event and its name will appear in the logic specification list box. See “Logic Specifications” in “Chapter 5 Workflow Specifications” for more information.

- **Repeat events at least once.** Selecting this check box causes the workflow to delay testing for the perform-while condition until it has completed the first pass through all the events in the Perform-While loop. Clear the check box if you want the workflow to test the perform-while condition before it begins executing the events in the perform-while loop.
- **Perform-While Condition.** Use these buttons to specify the action the workflow will take based on the true/false result of the logical test. If Repeat Events At Least Once (see above) is cleared, the workflow will check the result of the logic specification before executing the first event in the perform-while loop and take the appropriate action based on the test result. If Repeat Events At Least Once is selected, the workflow will complete one pass through all the events in the perform-while loop and then test the result of the logic specification before it repeats the loop.
  - *Repeat Events If Test RESULT Is True.* Select this option if you want the workflow to execute or repeat the events in the group when the test result is true.
  - *Repeat Events If Test RESULT Is False.* Select this option if you want the workflow to execute or repeat the events in the group when the test result is false.

### **Early Exit**

The parameters in this group may be used to allow an early exit from the perform-while event and to define the conditions for granting an early exit.

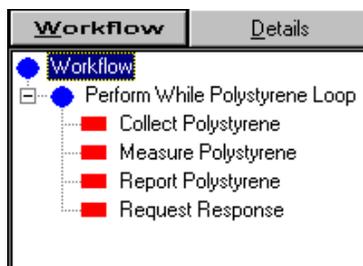


- **Allow Early Exit.** Select this option if you want to specify a condition for exiting the perform-while event after the event has started running. When this option is selected, the next two features become available in the software.
- **Logic Specification.** Use this option to create or select a logic specification, which defines the workflow results to be tested and how the test will function. See “Logic Specification” above for information about linking a logic specification to this event. For information about setting up logic specifications in workflows, see “Logic Specifications” in “Chapter 5 Workflow Specifications.”
- **Condition For Early Exit.** Use these buttons to specify the action the workflow will take based on the true/false result of the logical test. The workflow will check the result of the test specification after implementing each event in the perform-while group and take the appropriate action based on the test result.
  - *Exit Loop If Test RESULT Is True.* Select this option if you want the workflow to stop executing or repeating the events in the group when the test result is true.
  - *Exit Loop If Test Result Is False.* Select this option if you want the workflow to stop executing or repeating the events in the group when the test result is false.

**Usage:** A perform-while event must be linked to a valid logic specification such as a logical test specification or a compare text specification in order to repeat events based on a conditional test. The perform-while event may also be linked to an optional logic specification to test for early exit.

Perform-while events may be positioned anywhere in a workflow. These events are typically used to group related events that perform a similar or high-level task that should be executed and repeated only under certain

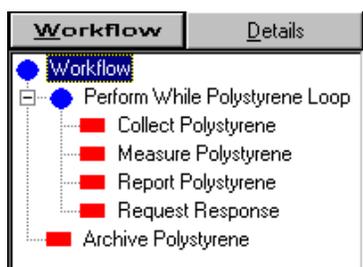
conditions. The example below shows a data collection series that ends by prompting the operator if there are any more samples to analyze in the current batch.



The data collection group is repeated only when the operator's response is "yes."

If the perform-while event is set up to test the result from a measurement or other event in the workflow, then the measurement or other event that produces that result must occur before the perform-while event in the workflow.

If you want the workflow to keep all the data produced by each iteration of a loop in the computer's internal memory (so the data can be used by subsequent events that are not part of the loop), make sure every event that is included in the loop is set up to retain all of its results. For example, if the loop includes a collect event whose results (spectra) are used by an archive event that is positioned after the loop (see example below), make sure the collect event has Multiple Event Results set to Retain All Event Results.

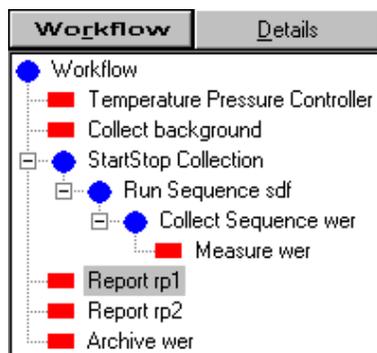


### **Archive event outside perform-while loop**

If you retain only the most recent result, the workflow will only archive the spectrum generated the last time the workflow implements the loop.

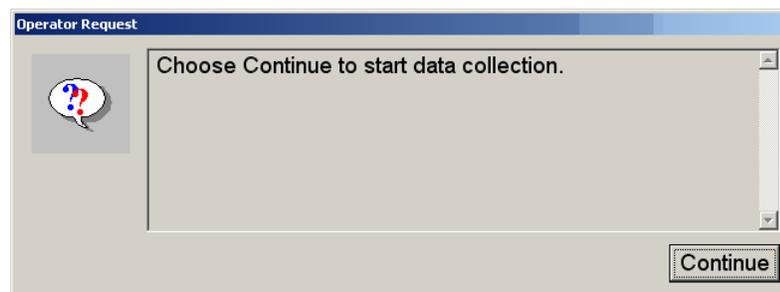
If the archive event is included in the loop, only the most recent spectrum needs to be stored in memory. If you configure the loop this way and retain all the collect event results, the workflow will archive multiple copies of the spectra. See “Archive Events” for more information.

## StartStop events

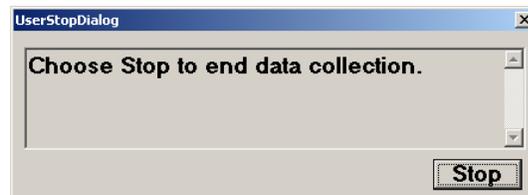


A StartStop event may be used to set a series of events apart from the rest of the workflow in order to allow the operator to control when those events start and end. In the example at the left, the workflow allows the operator to control the start and end of sequence data collection. See “Adding structural events to a workflow” at the beginning of this manual for information about adding StartStop events to workflows and adding events to a StartStop group.

The StartStop event can be linked to two prompt specifications, one to start the run and another to stop it. The start run specification defines an operator prompt that starts performing the events in the StartStop group. The start run prompt will look something like the example below.



The stop run specification defines an operator prompt that stops performing the events in the StartStop group. The StopRun prompt may look similar to the example below.



When you test or run a workflow that contains a StartStop group, the workflow displays the start run prompt after it encounters the group. The operator must respond to the prompt by choosing Continue before the workflow will continue.

After the operator responds to the prompt, the workflow displays the stop run prompt. If the operator chooses Stop in the prompt, the workflow stops executing the events in the StartStop group and skips to the first event after the group. The workflow may also generate an error.

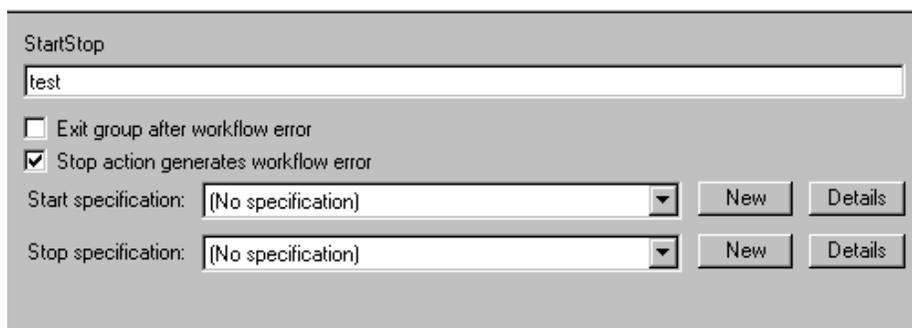
If the operator does not respond to the stop run prompt, the workflow performs all the events in the group in sequence and then continues with the first event after the group.

**Associated specifications:** Start run specification, Stop run specification

**Related events:** Perform event, Perform-If event, Repeat event, StartStop event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the StartStop event. These parameters appear in the display area of RESULT Integration when a StartStop event is selected in a workflow.



### StartStop event parameters

The StartStop event parameters allow you to define prompts to start and stop executing the events in the group and to specify whether the workflow will check the group for errors or generate an error. The following sections detail the StartStop event parameters. The parameters are explained in the order in which they appear in the software.

Exit group after workflow error

- **Exit Group After Workflow Error.** Select this option if you want the workflow to check the events in this group for errors. If an error is found, the workflow skips to the next event, if any, that appears outside the group in the workflow tree.

If this option is cleared and a workflow error occurs within the StartStop group, the workflow will display an error message in the

status box and implement the rest of the events in the group before continuing to the next event or event group. A report describing the workflow errors appears in the display area after the workflow is completed.

Stop action generates workflow error

- **Stop Action Generates Workflow Error.** Select this option if you want the workflow to generate an error if the operator stops the workflow by choosing Stop in the StopRun prompt.
- **Start Specification.** Use this feature to link a start run specification to this event. The start run specification allows you to define the contents and operation of the StartRun prompt displayed at run time. If the workflow already contains an appropriate start run specification, select its name in the drop down list (see below).



Start specification: Start prompt [v] [New] [Details]

Use the Details button to the right of the list box to display the current settings, or the New button to create a start run specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the start/stop event. The new specification will be linked to the StartStop event and its name will appear in the Start Specification list box. See “Start Run Specifications” in “Chapter 5 Workflow Specifications” for more information.

- **Stop Specification.** Use this option to create or select a stop run specification, which defines the contents and operation of the StopRun prompt displayed at run time. See “Start Run Specification” above for information about linking a specification to this event. For information about setting up stop run specifications in workflows, see “Stop Run Specifications” in “Chapter 5 workflow specifications.”

**Usage:** StartStop events may be placed anywhere in a workflow and must be linked to both a start run specification and a stop run specification. These events are typically used to group related events that require time or preparation at run time or events the operator may choose to skip.

There are no other requirements and no StartStop event results that can be accessed by other events in a workflow.

## Chapter 4 Device-Specific Workflow Events

Device-specific workflow events allow you to control a particular hardware device such as an autosampler or temperature controller. The device-specific events provided in RESULT Integration include:

- **Position autosampler events.** The position autosampler event instructs the workflow to rotate the carousel for the specified autosampler to another position or to prompt the operator to change the autosampler carousel. Depending upon the autosampler type and the number of positions in each carousel, you can configure a position autosampler event to move the autosampler to the next sequential position, the reference position, a specific position number, the position specified by the operator at run time, or the next position in a predefined sampling sequence.
- **Configure temperature/pressure events.** When you analyze gases quantitatively, the gas cell temperature and pressure must be controlled or known in order to achieve reliable, reproducible results. Use the configure temperature/pressure event to set up a workflow to save temperature and pressure information with the collected spectra.

For information about other events that can be added to workflows, see “Chapter 1 Simple Workflow Events” and “Chapter 2 Structural Workflow Events.” To learn how to use RESULT software to collect and process spectral data continuously over a specified period, see “Chapter 4 Sequence Module Events.”

This section lists each device-specific workflow event and details its application and use. The following information may be provided for each workflow event:

- **Description**, which is a brief explanation of the event and how it works.
- **Event Result**, which indicates the type of result, if any, the event produces. For example, position autosampler events produce a position

number or cycle number. The result type will be important when adding items to report events and archive events in order to specify which workflow results you want to report or save.

- **Associated specifications**, which lists the required and optional specifications that can be linked to the described event.
- **Related events**, which lists other events that operate like the described event or perform a similar function, and events that may be tied to the described event. For example, if a measure event can be used to measure the results from the described event, then the measure event would be listed as a related event.
- **Related specifications**, which lists other specifications that can be tied to the described event. For example, if a table item specification might be used to add a result from the described event to a sample report, then the table item specification would be listed as a related specification.
- **Parameters**, which explains the parameters for the described event. Parameters are described in the order in which they appear in the software when the described event is selected in a workflow.
- **Usage**, which provides practical examples of how the described event is typically used in a workflow. It also lists any events that must appear before or after the described event in a workflow, and lists events that operate on results produced by the described event.

For information about adding device-specific events to a workflow, see “Adding simple events to workflows” in “Chapter 1 Simple Workflow Events.” To learn about adding specifications to workflows and linking specifications to workflow events, see “Chapter 5 Workflow Specifications.”

## Position autosampler events

The position autosampler event instructs the workflow to rotate the carousel for the specified autosampler to another position or to prompt the operator to change the autosampler carousel. Depending upon the autosampler type and the number of positions in each carousel, you can configure a position autosampler event to move the autosampler to the next sequential position, the reference position, a specific position number, the position specified by the operator at run time, or the next position in a predefined sampling sequence.

Each time a workflow performs a position autosampler event, the software moves the carousel to the specified position or prompts the operator to change the carousel and then moves the new carousel to the specified position. The workflow automatically generates position autosampler event results containing the current carousel position number and the cycle number, if using multiple carousels. Those results can be added to subsequent events in the workflow such as a report event. You can configure the position autosampler event to retain the current position and cycle number only until the next position autosampler event occurs, or to record all the position and cycle numbers used in the workflow.

**Event result:** Sample location (carousel position number and cycle number, if using multiple carousels).

**Associated specifications:** Autosampler specifications, operator prompt specifications

**Related events:** Collect events, Repeat events

**Related specifications:** Autosampler Tablet Transmission Module sample specifications, Autosampler SoftGel Tablet Analyzer Module sample specifications, Autosampler Integrating Sphere sample specifications, Standard Tablet Analyzer background specifications, SoftGel Tablet Analyzer background specifications, Autosampler Integrating Sphere background specifications

**Parameters:** The illustration below shows the parameters for the position autosampler event. These parameters appear in the display area of RESULT Integration when a position autosampler event is selected in a workflow.

Position Autosampler Results: Position number, Cycle number

New

Autosampler specification:

New Details

Autosampler Position

Next position

Reference (zero) position

Position number:

Prompt for position number:

Prompt text:

Next position in sampling sequence

Multiple Sample Sets

Prompt for next set of samples

Prompt specification:  New Details

Multiple Event Results

Retain all event results

Retain current results only

## Position autosampler event parameters

The position autosampler event parameters define the associated autosampler specification, the autosampler movement, whether an operator prompt occurs when the autosampler finishes the last sample in the current carousel, and the storage of results from multiple position autosampler events in a workflow. The following sections explain the position autosampler event parameters in detail. The parameters are explained in the order in which they appear in the software.

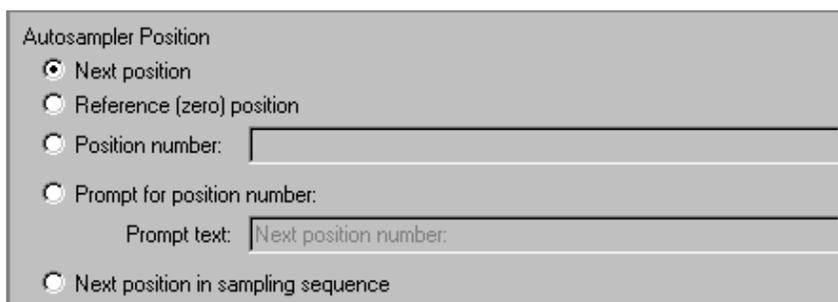
### Autosampler Specification

A position autosampler event must be linked to a valid autosampler specification in order to move the autosampler carousel. The autosampler specification contains parameters that define the autosampler type and the number of samples in each carousel. See “Autosampler Specifications” for information about setting up an autosampler specification in a workflow. To link an autosampler specification to a position autosampler event, select the specification name in the Autosampler Specification drop-down list, as shown below.



Use the New button at the right of the Autosampler Specification list box to create an autosampler specification and automatically link the new specification to the position autosampler event. If this position autosampler event is already linked to an autosampler specification, you can use the Details button to display that autosampler specification.

### Autosampler Position



The Autosampler Position parameter defines the autosampler movement. You can configure a position autosampler event to move the autosampler to the next sequential position, the reference position, or a specific position number. You can also make it prompt the operator for a position number at run time or use the position numbers specified in a sampling sequence. All of these options are explained below.

The number of positions available depends on the number of samples you plan to analyze. The direction of movement (clockwise or counterclockwise) is determined by the shortest distance between the previous carousel location and the new location.

- **Next Position.** Select this option to direct the current carousel to the next sequential position. The location of the next sequential position depends on the structure of the workflow. If the position autosampler event appears first in the workflow, the first time the workflow implements the position autosampler event, it moves the autosampler to the first available position in the first carousel. If the reference (zero) position is reserved for background collections, the first available position is position number 1. If the reference position contains a sample, the first available position is position 0. See “Autosampler Specifications” for more information.

- **Reference (Zero) Position.** Select this option to move the current carousel to the reference position (labeled “zero” on Thermo Scientific autosampler carousels). This is often the preferred starting point for the workflow or for a new carousel. Depending on the collection technique and material used for background and sample collections, the reference position may contain a sample, a background reference sample, or nothing. See “Collecting backgrounds” and “Autosampler specifications” in your autosampler user manual for more information.
- **Position Number.** Select this option to move the current carousel to a specific position number and then enter the position number in the corresponding entry box, as shown below.

A screenshot of a software interface. On the left, there is a radio button that is selected, followed by the text "Position number:". To the right of this text is a rectangular text input box containing the number "5".

**Note** If you specify the reference position (position zero), the software moves the carousel to that position even if it is reserved for background collections. See the “Autosampler Specifications” section in your autosampler user manual for details about reserving the reference position for background collections. ▲

- **Prompt For Position Number.** Use this option to set up a dialog box that will prompt the operator to enter a carousel position number at run time. Then enter the text for the operator prompt in the Prompt Text box, as shown below.

A screenshot of a software interface. On the left, there is a radio button that is selected, followed by the text "Prompt for position number:". Below this, there is a label "Prompt text:" followed by a text input box containing the text "Next position number:".

The workflow will display the prompt each time it implements this position autosampler event. The operator must respond to the prompt by entering a valid carousel position number before the workflow will continue.

- **Next Position In Sampling Sequence.** If the position autosampler event appears in a repeat loop, you can use a sampling sequence to determine the next carousel position. The corresponding repeat event must be set up to use a sampling sequence at run time. The sampling sequence must specify a sample name and carousel position number for each iteration of the loop.

When this option is selected and the corresponding repeat event is configured to use a sampling sequence at run time, the first time the workflow implements the position autosampler event, it moves the current carousel to the first position number and sample specified in the sampling sequence. The next iteration of the position autosampler event moves the carousel to the second position number in the sampling sequence. This process continues until all the samples specified in the sequence have completed the operations in the loop. See “Using a Sampling Sequence with RESULT Software” in this document for more information.

### Multiple Sample Sets

If you are analyzing more samples than will fit in one carousel, use the parameters in this group to define a prompt that will be displayed to the operator after the workflow finishes analyzing the last sample in each carousel.

To set up this type of prompt, first select the Prompt For Next Set Of Samples check box as shown below.



When the check box is selected, the Prompt Specification list box becomes available in the software. Use the Prompt Specification list box to link an operator prompt specification to this position autosampler event by selecting the specification name in the Prompt Specification list box as shown above.

Use the New button next to the list box to create an operator prompt specification and automatically link the new specification to this position autosampler event. If this position autosampler event is already linked to a prompt specification, use the Details button to the right of the list box to display that specification.

The prompt specification defines the contents and operation of the operator prompt. See “Prompt specifications” in this chapter for information about setting up prompt specifications in a workflow. If the prompt is configured to allow the operator to respond by pressing the green acknowledge button on the instrument (not available on the Antaris IGS),

the green LED indicator will light when the dialog box is displayed on the screen. Depending upon how the workflow is set up, after you install the new carousel, the autosampler either collects a background or positions the first sample for analysis.

## Multiple Event Results

### Multiple Event Results

- Retain all event results
- Retain most recent result

If you place a Position Autosampler event in a repeat or perform-while loop, the event will produce one result or set of results during each iteration of the loop. This feature allows you to select whether the workflow will store all the results produced by the loop or only the most recent results. The options for storing results include:

- **Retain All Event Results.** If the Position Autosampler event occurs in a loop, selecting this option causes the workflow to store the position and cycle number of every spectrum produced in every iteration of the loop. This makes the information available for use in subsequent workflow events such as a report event that are placed after the loop.
- **Retain Most Recent Result.** Select this option if the position autosampler event is not positioned in a loop or the loop includes all subsequent events that use the sample position and cycle number. This is the default setting and will maximize your computer processing speed.

**Usage:** Position autosampler events may be placed anywhere in a workflow. They are typically placed right before or after a collect event. A position autosampler event must be linked to a valid autosampler specification in order to move the autosampler carousel.

We recommend using one position autosampler event at the beginning of your workflow to initialize the autosampler. In order to initialize the autosampler, the Autosampler Position parameter must be set to the Reference (Zero) Position option.

If your workflow includes a repeat loop for collecting and measuring spectra using the autosampler, we recommend adding a second position autosampler event to the loop. If you are using the reference (zero) carousel position to collect backgrounds and your first sample is in position 1, place the position autosampler event at the beginning of the loop to move the carousel to the next sampling position before data collection begins.

If you are using the internal gold reference to collect backgrounds and the reference (zero) position contains your first sample, add a position autosampler event to the loop but place it after the collect event. This leaves the carousel in the reference position while it collects data from the first sample and then moves the carousel to the next specified position.

If running a transmission experiment or a diffuse reflection experiment using an external background reference and the background collection is set up correctly, the workflow will use the reference position for background collections and then skip to the specified position to collect a sample spectrum. See “Transmission Backgrounds” and “Diffuse reflection backgrounds using an external reference” in your *MultiPro Autosampler User Guide* to learn how to set up background collections for these applications.

If running a diffuse reflection experiment only using the Antaris internal gold background reference and the background collection is set up correctly, the workflow collects a background without moving the autosampler and regards any material located in position 0 as a sample. See “Diffuse reflection backgrounds using the internal reference” in your autosampler user manual to learn how to set up background collections using the internal gold background reference.

The following events can operate on the position autosampler results (carousel position number and cycle number) if you place those events after the position autosampler event in the workflow.

- **Report event.** If your workflow includes a position autosampler event followed by a collect event, use a report event that includes a table or summary item specification to add the carousel position and cycle number along with the measurement result to a sample report.
- **Check event.** A check event that is linked to a valid logical test specification may be used to produce an overall pass or fail result based on a position autosampler result.
- **Store event.** A store event may be used to store position autosampler results in the audit log database so they can be accessed with the logs features of RESULT Operation and used to track trends in your data.

## Configure temperature/pressure events

Use a configure temperature/pressure event to specify the gas cell temperature and pressure values that will be used for data collection. Temperature and pressure information is important to gas analysis experiments because the temperature and pressure of the gas cell affect the number of gas molecules in the path of infrared light. Pressure information is also important because the gas cell pressure affects the peak shapes in the resulting spectrum.

The configure temperature/pressure event allows the temperature and pressure values to be specified manually or recorded automatically from a compatible temperature and pressure controller system. Values specified manually can be entered in the workflow or entered by the operator at run time.

If your system includes the Antaris IGS temperature controller, you can also use the configure temperature/pressure event to set up or adjust the controller at run time, including the temperature set point value and any delay period while the gas cell adjusts to the new setting.

When you run the workflow, the configure temperature/pressure event saves the temperature and pressure information with the collected spectra.

**Event result:** None

**Associated specifications:** None

**Related events:** Collect events, run sequence events, collect sequence events

**Related specifications:** Gas cell sample specifications, Gas cell background specifications

**Parameters:** The illustration below shows the parameters for the configure temperature/pressure event. These parameters appear in the display area of RESULT Integration when a configure temperature/pressure event is selected in a workflow.

Configure Temperature/Pressure

New

Gas Cell Temperature for Data Collection

Read temperature  
 Control temperature

Setpoint (C): 165.00

Delay: None

Settle time (sec): 10

Use fixed temperature  
 Temperature(C): 0.00

Prompt for temperature

Gas Cell Pressure for Data Collection

Read pressure  
 Use fixed pressure

Pressure(torr): 650.00

Prompt for pressure

### Configure temperature/pressure event parameters

The configure temperature/pressure event parameters define the temperature and pressure values that will be stored with each collected spectrum or how those values will be specified at run time. The following sections explain the configure temperature/pressure event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Gas Cell Temperature

Gas Cell Temperature for Data Collection

Read temperature  
 Control temperature

Setpoint (C): 165.00

Delay: None

Settle time (sec): 10

Use fixed temperature  
 Temperature(C): 165.00

Prompt for temperature

The Gas Cell Temperature parameter allows you to define a fixed temperature that will be saved with every spectrum, or to specify that the software will prompt the operator for the gas cell temperature at run time. If your Antaris IGS includes the standard IGS temperature controller, you can also specify that the software will read the current temperature of the gas cell as each spectrum is collected. All of these options are explained below.

- **Read Temperature.** Select this option if you want the workflow to read the current temperature of the gas cell as it collects each spectrum and store the value with the collected data. This option is available only for Antaris IGS systems that include the optional Antaris IGS temperature controller. This setting ensures that each spectrum has an associated temperature reading.
- **Control Temperature.** Select this option if your Antaris IGS system includes the optional IGS temperature controller and you want the workflow to set up or adjust the controller at run time. Use the Setpoint and Delay parameters to specify the temperature setpoint value and any delay period while the gas cell adjusts to the new setting. The delay can be configured to continue until the controller reaches the setpoint temperature or until a specified period has elapsed (use Settle Time to specify the delay period). The software will also store the current temperature of the gas cell with the collected spectra.
  - *Setpoint (C).* Use this entry box to specify the gas cell temperature that should be used for data collection. Specify the temperature value in degrees centigrade.
  - *Delay.* Use this list box to specify how the software will determine when the gas cell has reached the setpoint temperature. If you select Wait For Setpoint, the software will wait until the controller verifies that the gas cell has reached the setpoint value before it starts collecting data. If you select Wait For Settle Time, the software will wait a specified length of time before collecting data. Use the Settle Time parameter (see below) to specify the waiting period.
  - *Settle Time(Sec).* This option is available in the software only when Delay (see above) is set to Wait For Settle Time. Use the Settle Time box to specify in seconds the length of time the software will wait for the gas cell to heat or cool before collecting data.

- **Use Fixed Temperature.** Select this option if you want to specify the gas cell temperature in the workflow. When this option is selected, the Temperature box becomes available in the software. Use the Temperature box to specify the gas cell temperature in degrees centigrade that will be used for this experiment. This option is recommended only for experiments that are always run at a fixed temperature and the temperature control system is accurate and very stable.
- **Prompt For Temperature.** Select this option if you want the software to prompt the operator to specify the gas cell temperature at run time. This option is recommended for experiments that may be run at various temperatures but the temperature control system must be accurate and very stable.

**Note** Keep in mind that temperature values that are specified manually, either by entering a fixed temperature or by having the operator enter the temperature at run time, will be saved with the entire data set. If the workflow is designed to collect data continuously over a significant length of time, the temperature may fluctuate during data collection and those changes will not be recorded with the spectra. To ensure accurate temperature readings for continuous data collection, we recommend using a temperature controller that is compatible with RESULT so the software can automatically read and store temperature values with the collected spectra. ▲

### Gas Cell Pressure for Data Collection

Gas Cell Pressure for Data Collection

Read pressure  
 Use fixed pressure  
 Prompt for pressure

Pressure(torr):

The Gas Cell Pressure parameter allows you to define a fixed pressure that will be saved with every spectrum, or to specify that the software will prompt the operator for the gas cell pressure at run time. If your Antaris IGS is configured with an Antaris IGS temperature controller that includes the optional pressure gauge and sensor, you can also specify that the software will read the current pressure of the gas cell as each spectrum is collected. All of these options are explained below.

- **Read Pressure.** Select this option if you want the workflow to read the current pressure of the gas cell as it collects each spectrum and store the value with the collected data. This option is available only for Antaris IGS systems configured with an Antaris IGS temperature controller that includes the optional pressure gauge and sensor. This setting ensures that each spectrum has an associated pressure reading.
- **Use Fixed Pressure.** Select this option if you want to specify the gas cell pressure in the workflow. When this option is selected, the Pressure box becomes available in the software. Use the Pressure box to specify the gas cell pressure in torr that will be used for this experiment. This option is recommended only for experiments that are always run at a fixed pressure and the pressure control system is accurate and very stable.
- **Prompt For Pressure.** Select this option if you want the software to prompt the operator to specify the gas cell pressure at run time. This option is recommended for experiments that may be run at various pressures but the pressure control system must be accurate and very stable.

**Note** Keep in mind that pressure values that are specified manually, either by entering a fixed pressure or by having the operator enter the pressure at run time, will be saved with the entire data set. If the workflow is designed to collect data continuously over a significant length of time, the pressure may fluctuate during data collection and those changes will not be recorded with the spectra. To ensure accurate pressure readings for continuous data collection, we recommend using a pressure gauge and sensor that are compatible with RESULT so the software can automatically read and store pressure values with the collected spectra. ▲

**Usage:** Configure temperature/pressure events may be placed anywhere in a workflow. They are typically needed only in gas analysis experiments where accurate temperature and pressure readings are critical to achieving reliable, reproducible results.

To set up a workflow to automatically save temperature and pressure information with data collected from gas samples, place a configure temperature/pressure event before the collect event in the workflow. The configure temperature/pressure event can be configured to set up the controller and then read and store the temperature and pressure values with the collected spectra, or to simply read and store the values at run time.

## Chapter 5 Sequence Module Events

RESULT includes an optional software module to allow sequence data collection. 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. The collection time is determined by the number of sample scans collected and the resolution (also mirror velocity and scan type if using an Antaris IGS analyzer). The results provide you with a series of closely related spectra; each spectrum represents a snapshot of the sample at a particular moment in time. The entire sequence data set can be used to determine the changes in component concentrations of the sample over the time of the data collection. This technique is typically used to monitor a sample as it flows through a chamber or evolves, so that any fluctuations in the concentrations of the sample components can be measured and recorded.

The sequence module includes the following workflow events:

- **Run Sequence events.** Use a run sequence event in a workflow to set up continuous data collection. The run sequence event allows you to specify the data to be displayed during sequence data collection and the sequence data you want to save. Each run sequence event must include at least once collect sequence event (see below) to define the collection parameters.
- **Collect Sequence events.** Use the collect sequence event to define the total collection time and the number of scans used to process each spectrum for each phase of data collection. You can also specify options to pause the workflow before collecting the data, to specify the format of the collected spectra and to define the frequency of background collection. A collect sequence event can include one or more measure events to measure the collected spectra.

This section lists each sequence module event and details its application and use. The following information is provided for each sequence module event:

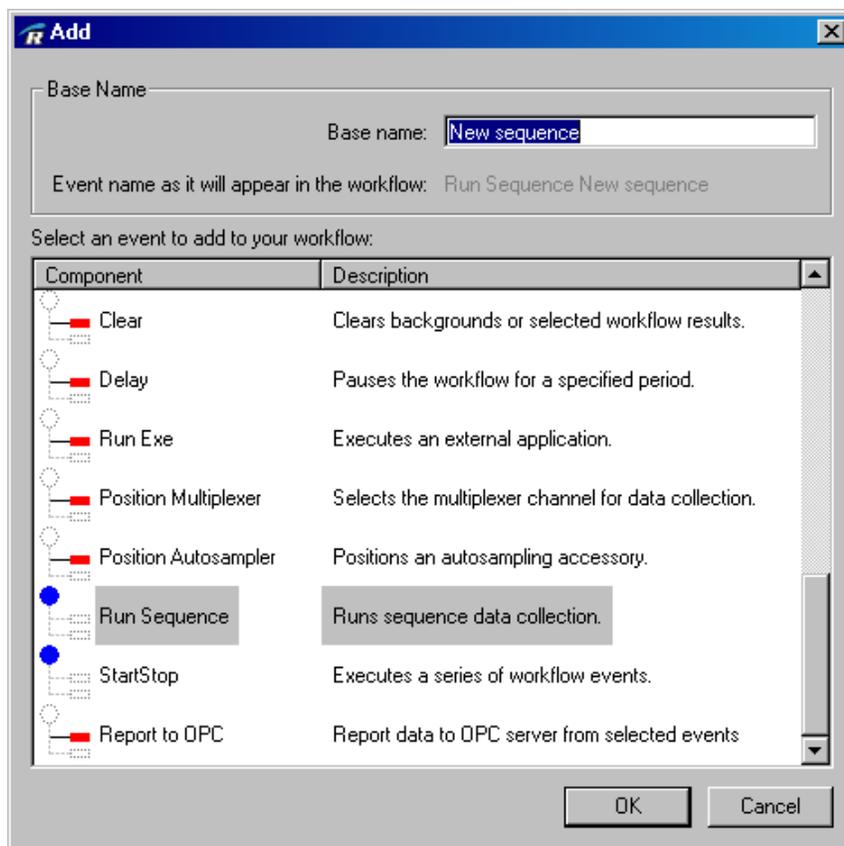
- **Description**, which is a brief explanation of the event and how it works.

- **Event result**, which indicates the type of result, if any, the event produces. For example, run sequence events produce a series of spectra and measure events produce a measurement result. The result type will be important when adding items to report events and archive events in order to specify which workflow results you want to report or save.
- **Associated specifications**, which lists the required and optional specifications that can be linked to the described event.
- **Related events**, which lists other events that operate like the described event or perform a similar function, and events that may be tied to the described event. For example, if a measure event can be used to measure the results from the described event, then the measure event would be listed as a related event.
- **Related specifications**, which lists other specifications that can be tied to the described event. For example, if a table item specification might be used to add a result from the described event to a sample report, then the table item specification would be listed as a related specification.
- **Parameters**, which explains the parameters for the described event. Parameters are described in the order that they appear in the software when the described event is selected in a workflow.
- **Usage**, which provides practical examples of how the described event is typically used in a workflow. It also lists any events that must appear before or after the described event in a workflow, and lists events that operate on results produced by the described event.

For information about adding simple events to a workflow, see “Chapter 1 Simple Workflow Events.” To learn about adding structural events to a workflow, see “Chapter 2 Structural Workflow Events.” For information about adding device-specific events to control a hardware device, see “Chapter 3 Device-Specific Events.” To learn about adding specifications to workflows and linking specifications to workflow events, see “Chapter 5 Workflow Specifications.”

## Adding sequence events to a workflow

To create a sequence event group, begin by adding the run sequence event to the workflow. To add a run sequence event, select the main workflow group in the workflow navigation frame and then choose Add on the RESULT Integration toolbar. The following dialog box is displayed.

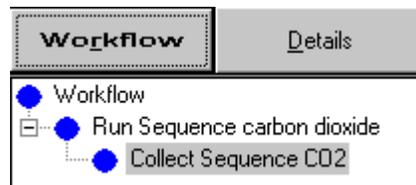


**Note** If the run sequence event does not appear in the Add dialog box, the sequence module is not installed. See your RESULT administrator for help. ▲

Select the Run Sequence event in the list, enter a base name at the top of the dialog box and then choose OK. The run sequence event appears as an event group in the workflow navigation frame as shown below.

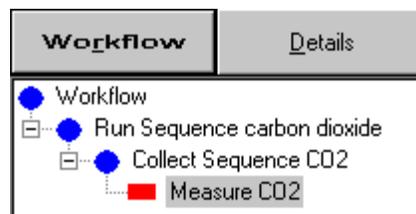


The run sequence event must specify at least one data collection phase. To add a collection phase, select the Run Sequence event group in the workflow and then use the Add button on the toolbar to add a collect sequence event. The workflow should look similar to the example below.



**Note** When you display the Add dialog box with a run sequence event selected, the dialog box includes a subset of the events available in RESULT Integration. These are the only events that can be added to a run sequence group. ▲

Similar to the traditional collect event, a collect sequence event requires a valid sample and background specification before data collection is possible. If you want the workflow to calculate the changes in component concentrations of the sample during data collection, the collect sequence event must also include a measure event, which allows you to specify the components to be measured and a quantitative method.



The measure event must be associated with a valid measurement specification and the measurement specification must specify a calibrated analytical method before the workflow will run. See “Measure events” and “Measurement specifications” in this chapter for information about setting up measure events and measurement specifications in workflows.

## Run sequence events

The run sequence event allows you to specify the data to be displayed during sequence data collection and the sequence data you want to save.

Each time a workflow performs a run sequence event, the workflow produces a series of spectra. The workflow automatically stores the spectra in a temporary location on the computer’s hard disk, so the spectra are available for use by subsequent events in the workflow, such as a measure

event or a report event. If you want to archive the spectra, you must add an archive event to your workflow and then add the spectra to the list of results to be archived.

**Event result:** Sequence data, which may include spectra (\*.srs), interferograms (\*.sri), and concentration values (\*.cnc)

**Associated specifications:** None

**Related events:** Collect sequence events, measure events, report events, archive events, compare events

**Related specifications:** Sample specifications, background specifications, measurement specifications, spectrum item specifications

**Parameters:** The illustration below shows the parameters for the run sequence event. These parameters appear in the display area of RESULT Integration when a run sequence event is selected in a workflow.

Run Sequence Result: sequence data

New Sequence

Component Display

Component Name	Measure Event	Report to DPC Server	Show Text Value	Show Run Chart	Minir

Edit

Spectral Display

Show spectral data

Minimum spectrum Y value: 0.00

Maximum spectrum Y

Starting spectrum X value: 4.000.00

Ending spectrum X

Sequence Event Results

Retain all spectral data (\*.srs)

Retain all interferogram data (\*.sri)

Retain all concentration data (\*.cnc)

Sequence Sample for Simulation

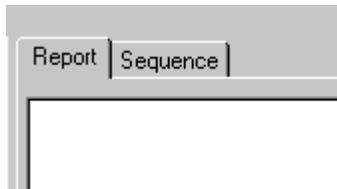
Use simulation sample for all workflow runs

Base path: C:\RESULT Data\Archive

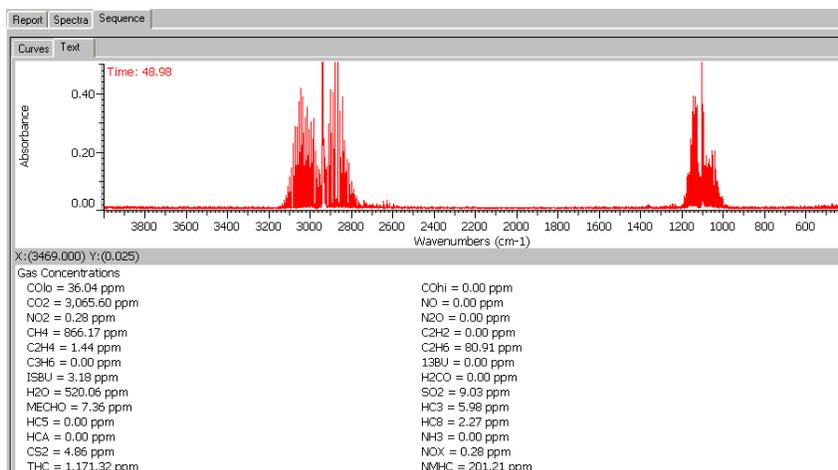
File name:

### Run sequence event parameters

The run sequence event parameters define the sequence collection display and the sequence data that will be available to other events in the workflow. If a workflow includes a valid run sequence event, the sequence tab appears in the display area during data collection.



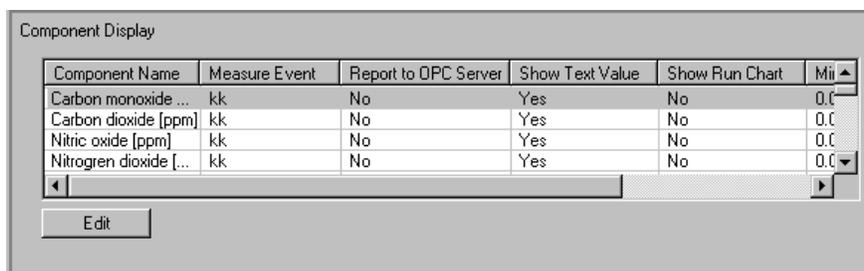
This is true whether you run the workflow from the RESULT Integration or RESULT Operation application. The sequence tab allows the operator to view the sequence data as the data are collected. The tab can include spectral data. If the run sequence group contains a measure event, the tab can also show the calculated measurement results as shown in the example below.



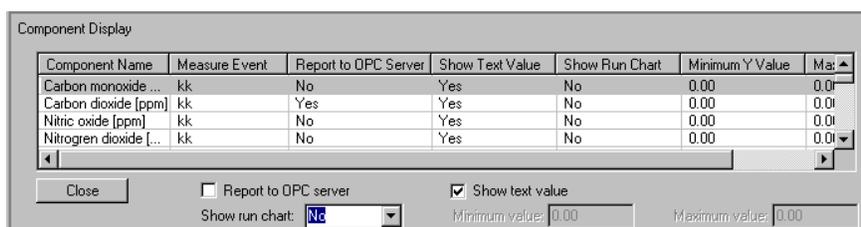
Use the controls in the run sequence event to set up the sequence display. The following sections explain the run sequence event parameters in detail. The parameters are explained in the order in which they appear in the software.

### Component Display

If the run sequence group contains a measure event and an associated measurement specification that points to a valid quantitative method, the table in the Component Display group will list the method components and show the default settings for the component display parameters as shown below.

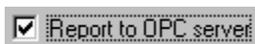


Use the Edit button to adjust the settings for the display parameters. When you choose Edit, the display parameters appear below the table and the Edit button changes to the Close button.



Each of the display parameters is described below:

- Component Name.** This column is filled in automatically and cannot be edited. The software retrieves the component list from the quantitative method associated with the measure event in this run sequence group. If the run sequence group includes multiple measure events that point to different quantitative methods, the Component Name column will list all the components in all the quantitative methods, starting with the method that appears first in the run sequence event and ending with the method that appears last (use the vertical scroll bar to review the entire list). If the methods contain duplicate component names, use the Measure Event column to determine which component came from which method.
- Measure Event.** This column indicates the measure event associated with each component listed in the Component Display table. The software fills in this column automatically.
- Report to OPC Server.** RESULT software provides a basic interface to communicate with an OPC client. OPC is a universal interface used to control process equipment and to monitor data results. Use this feature to indicate whether a copy of the concentration result for the selected component will be released to an OPC client.



The default setting is “No.” To edit the setting for a component, select the component name in the table and then select or clear the Report To OPC Server check box located below the table. When the check box is selected, the word “Yes” appears in the corresponding column in the table; when the check box is cleared, the setting in the table changes to “No.”

Show text value

- **Show Text Value.** Use this feature to indicate whether the concentration result for this component will be included in the text display of component concentration values. The default setting is “Yes.” To edit the setting for a component, select the component name in the table and then select or clear the Show Text Value option located below the table. When the check box is selected, the word “Yes” appears in the corresponding column in the table; when the check box is cleared, the setting in the table changes to “No.”

The text display includes only the component names and their associated concentration values. To display the list of concentration values for the selected components at run time, select the Text tab in the sequence display as shown in the example below.

Curves Text

The list appears in a separate pane below the spectral data.

```
A
CO = 52.27 ppm          CO2 = 5,602.06 ppm
NO = 11.92 ppm         NO2 = -6.42 ppm
N2O = -2.37 ppm       CH4 = -0.44 ppm
C2H2 = 13.16 ppm      C2H4 = -1.37 ppm
C2H6 = -28.07 ppm     C3H6 = 49.92 ppm
13BU = 39.69 ppm      ISBU = -36.48 ppm
H2CO = -9.75 ppm      H2O = -5,907.88 ppm
SO2 = 11.61 ppm       MECHO = 57.55 ppm
HC3 = 17.18 ppm       HC5 = -2.96 ppm
HC8 = -3.55 ppm       HCA = -48.62 ppm
NH3 = -1.02 ppm       CS2 = -0.95 ppm
NOX = 5.50 ppm        THC = -150.62 ppm
NMHC = -150.13 ppm
```

Show run chart:

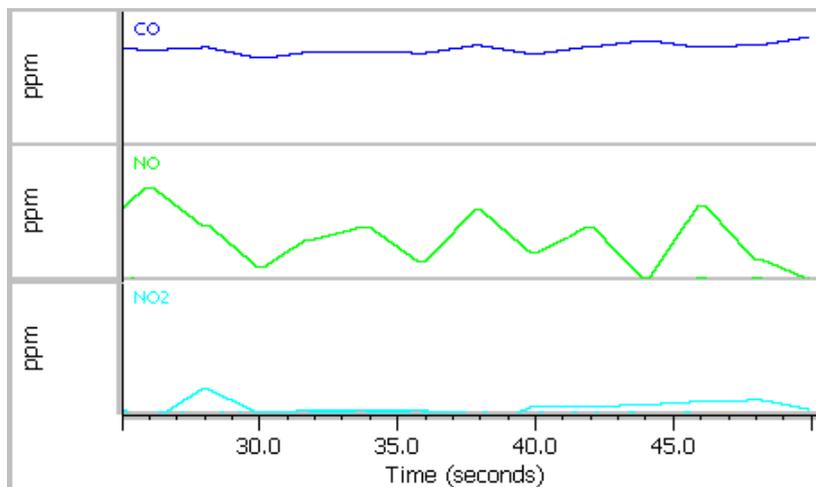
- **Show Run Chart.** Use this feature to indicate whether the concentration result for this component will be included in the graphic display of component concentration values. The default setting is “No.” To edit the setting for a component, select the component name in the table and then use the Show Run Chart list box located below the table to indicate the component’s priority. Set the list box to “1” to

display the concentration curve for the selected component in the first pane. Set the list box to “2” for the second pane and so on. You can also set the list box by simply clicking the Show Run Chart field for a particular component in the Component Display table. Each time you click the field, the setting increments.

The graphic display shows the changes in component concentration values over time for the selected components. To display the concentration curves for the selected components at run time, select the Curves tab in the sequence display as shown below.



Each component concentration curve appears in a separate pane. The component name is listed in the upper left corner of the pane.



Minimum value:

Maximum value:

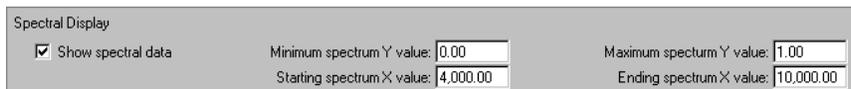
- **Min/max Y Value.** For components that are selected to be displayed in run charts (see above), use these features to indicate the minimum and maximum Y-axis values for the charts. For a given component, the Min/Max Y Value features are available in the software only when Show Run Chart is set to something other than “No.”

The default Min/Max Y Value settings are all zero. To edit the setting for a component, select the component name in the table and then use the Minimum Value and Maximum Value entry boxes located below the table to indicate the upper and lower Y values for the chart.

When you are finished editing the parameter settings, choose Close to hide the component display parameters.

## Spectral Display

If you want to view the spectra as they are collected at run time, select Show Spectral Data in the Spectral Display group. Then use the remaining parameters to configure the X and Y limits of the spectral display.



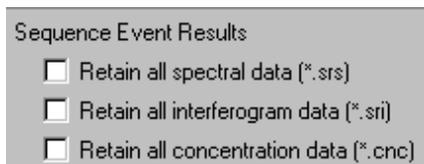
The screenshot shows a control panel titled "Spectral Display". It contains a checked checkbox labeled "Show spectral data". To the right of this checkbox are four input fields: "Minimum spectrum Y value" with a value of 0.00, "Maximum spectrum Y value" with a value of 1.00, "Starting spectrum X value" with a value of 4,000.00, and "Ending spectrum X value" with a value of 10,000.00.

The software displays new spectral data each time it collects a new spectrum. The collection times appear in the upper left corner of the spectral display. The Data Format parameter on the collect sequence event determines the format of the displayed spectra.

## Sequence Event Results

The sequence event can produce three kinds of data: spectral data, interferogram data, and calculated measurement results. The spectral data refer to the infrared sample spectra; they are saved in the format specified in the workflow. All sample spectra collected over the duration of the sequence are saved together. The interferogram data include the raw background and sample data used to create each sample spectrum. The measurement results include all the concentration or other values the associated analytical method is set up to produce.

You can instruct the workflow to keep the spectral data, the interferogram data, the measurement results, or any combination of the three by selecting the corresponding check boxes in the Sequence Event Results group.



The screenshot shows a control panel titled "Sequence Event Results". It contains three unchecked checkboxes: "Retain all spectral data (\*.srs)", "Retain all interferogram data (\*.sri)", and "Retain all concentration data (\*.cnc)".

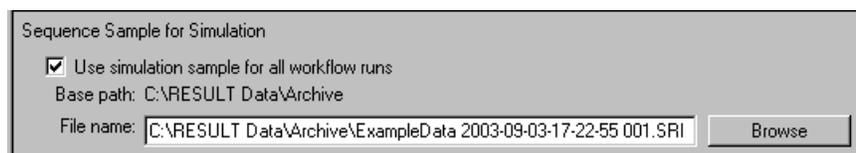
Due to the potentially large volume of data a sequence collection can produce over a short period of time, the workflow stores the data in a temporary location on the hard disk rather than trying to keep it in the computer's internal memory. This ensures that the data can be accessed by other events in the workflow such as a process event or an archive event.

If you store the spectral data and the concentration data, you will be able to view the individual spectra and the corresponding run charts using the RESULT Data View application included with RESULT software. Storing the spectra will also allow you to recalculate the measurement results using the Quantify Sequence Or Map feature of TQ Analyst software. The interferograms are needed to run the workflow in simulation mode. Running a workflow in simulation mode will allow you to reprocess the spectra using different settings for the processing parameters, such as apodization and zero filling, and to see how those changes affect the calculated results.

If the workflow doesn't include an archive event to save the data in permanent files on a computer disk, the data will be lost when the workflow finishes running. See "Archive events" in this chapter for more information.

### Sequence Sample for Simulation

Use the options in this group to specify simulated spectra that can substitute for the actual spectra collected by the workflow.



This technique can help you shorten workflow development time and facilitate testing and verifying the workflow when it is completed.

The simulated spectra must be in a sequence spectral file (\*.sri extension) saved on a disk. Use the File Name box to enter the file name or use the Browse button to locate and select an appropriate file.

To configure the workflow to always run with the simulated spectral file, select Use Simulation Sample For All Workflow Runs. If you leave this check box cleared, you can still elect to run the workflow with simulated data from RESULT Integration. See "Testing A Workflow" in the "RESULT Integration User Guide" for more information.

## Collect sequence events

Use the collect sequence event to define the total collection time and the number of scans used to process each spectrum for each phase of data collection. You can also specify options to pause the workflow before

collecting the data, to specify the format of the collected spectra and to define the frequency of background collections.

If you need to collect data over an extended period and the requirements for data collection vary, use multiple collect sequence events to define each phase of data collection. To extend the time between each collection phase, pause the workflow before starting the next phase.

Each collect sequence event must be linked to a valid sample specification before the workflow will collect data. See “Sample specifications” in the next section for more information.

Each time a workflow performs a collect sequence event, the workflow produces a block of spectra collected in series. The software passes the spectra to the run sequence event, which combines the spectra produced by all the collect sequence events into one set of files.

**Event Result:** None (passed to run sequence event)

**Associated specifications:** Sample specification

**Related events:** Run sequence events, measure events

**Related specifications:** Sample specification, background specification, measurement specification

**Parameters:** The illustration below shows the parameters for the collect sequence event. These parameters appear in the display area of RESULT Integration when a collect sequence event is selected in a workflow.

Collect Sequence

A

Collection Time

Total collection time (seconds): 120

Integration time (seconds): 1.66

Sampling Rate

Justify concentration data to time interval

Justified time interval (seconds): 0.00

Use specific sampling interval

Sampling interval (seconds): 0.00

Interval should be larger than single spectrum collection time.

Operator Prompt

Pause at start of sequence

Prompt text:

Action

Wait for operator response

Wait for specified time

Time (seconds): 0

Sample Parameters

Sample specification: werSample

Number of scans per spectrum: 1 Number of scans per standard: 16

Data format: Absorbance

Background frequency: Before every sample

Background folder:

Collect background only

## Collect sequence event parameters

The collect sequence event parameters define the total collection time and the number of scans used to process each spectrum for each phase of data collection. You can also specify options to pause the workflow before collecting the data, to specify the format of the collected spectra and to define the frequency of background collections.

### Collection Time

The parameters in this group define the total collection time for this phase of data collection and show the current rate of data collection.

Collection Time

Total collection time (seconds): 120

Integration time (seconds): 1.66

- **Total Collection Time (seconds).** Use this parameter to specify the length in seconds of the phase of data collection. The setting of this parameter is used along with the number of scans per spectrum to determine the total number of 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.
- **Integration Time (seconds).** This readout shows the current rate of data collection for this collect sequence event (i.e., the number of seconds between one collected spectrum or interferogram and the next). The current rate of data collection depends on the settings for number of scans per spectrum and the other parameters in the associated sample specification.

### Sampling Rate

The parameters in this group provide options for fine tuning the current rate of data collection for this phase. For example, you can justify the output of concentration values to a specific time interval or require that the spectra or interferograms are collected at specific intervals. In both cases, the specified sampling rate must be longer than the integration time (see above).

Sampling Rate

Justify concentration data to time interval

Justified time interval (seconds): 0.00

Use specific sampling interval

Sampling interval (seconds): 0.00

Interval should be larger than single spectrum collection time.

- **Justify Concentration Data To Time Interval.** Select this option only if you want to justify the output of concentration values to a specific time interval. Then use the Justified Time Interval entry box to specify the desired time interval in seconds. Make sure the number you enter is larger than the current value for Integration Time (see above).

When this option is selected, the software continues to collect and process the spectra or interferograms at the current rate of data collection (i.e., the integration time) but will report concentration values only at the specified time interval. For example, if the current integration time is 1.66 seconds and you select this option and set the justified time interval to 5 seconds, the software uses all the spectral information collected in that time interval (i.e., 5 seconds) to calculate a concentration value for each component. The reported concentration values that appear on the Text tab in the sequence data collection window and the values shown in the graphical display (Curves tab) will be updated every 5 seconds.

**Note** The Justify Concentration Data To Time Interval works only when the collect sequence event group contains at least one measure event. ▲

- **Use Specific Sampling Interval.** Select this option only if you want to require that the spectra or interferograms are collected at a specific time interval. Then use the Sampling Interval entry box to specify the desired time interval in seconds. Make sure the number you enter is larger than the current value for Integration Time (see above).

When this option is selected, the software collects and processes the spectra or interferograms at the specified sampling interval. The integration time shows the fastest possible rate of data collection but not the actual rate of data collection. If Justify Concentration Data To Time Interval is cleared, then the software will also report the calculated concentration values at the specified sampling interval. If Justify Concentration Data To Time Interval is selected and the justified time interval is longer than the sampling interval, then the software will collect the spectra and interferograms at the specified sampling interval and report them at the justified time interval.

### **Operator Prompt**

The parameters in this group provide options for pausing the workflow before the start of data collection for this phase. You can set up the workflow to wait until the operator responds to a prompt in the software or to wait for a specified length of time.

Operator Prompt

Pause at start of sequence

Prompt text:

Action

Wait for operator response

Wait for specified time

Time (seconds):

- **Pause At Start Of Sequence.** Select this option if you want to pause the workflow before collecting the sample data for this phase. Examples of situations that might require a pause include gas analysis experiments where the sample gas requires time to reach the gas cell or reaction experiments where a compound requires time to evolve or elute.

- *Prompt Text.* Use this box to enter the text for the operator prompt that will be displayed at run time. It is recommended that you include a detailed operator prompt to ensure that sample data are collected properly. An example prompt for sample collection could include the following:

Start the flow of sample gas through the gas cell to prepare for sample collection. Choose Continue when you are ready to begin collecting the sample data.

- **Action.** This feature defines how the operator prompt will function at run time.

Select Wait For Operator Response to specify that the prompt remain on the screen until the operator responds by choosing Continue.

Select Wait For Specified Time to require that the prompt remain on the screen for a specified period of time. Then use the Time box to specify the time period. After the period has elapsed, the workflow will continue.

You can specify that the prompt will remain on the display for a specified period of time or until the operator responds by choosing Continue.

## Sample Parameters

The sample parameters define data collection for a given sample type or material. These parameter settings are independent of the sampling technique.

Sample Parameters

Sample specification: Sample [v] [New] [Details]

Number of scans per spectrum: 1 Number of scans per standard: 16

Data format: Absorbance [v]

Background frequency: Before every sample [v]

Background folder:

Collect background only

The sample parameters include the following:

- **Sample Specification.** A sample specification contains advanced collection parameters that are optimized for a given sampling technique. Each sample specification includes a background specification, which defines background collection for the technique. See “Sample Specifications” in this chapter for information about setting up sample specifications in a workflow. To link a sample specification to a collect event, select the specification name in the Sample Specification drop-down list, as shown below.

Sample specification: Polystyrene Sample [v] [New] [Details]

Use the New button at the right of the Sample Specification list box to create a sample specification and automatically link the new specification to the collect event.

If this collect sequence event is already linked to a sample specification, you can use the Details button to display that sample specification.

Number of scans per spectrum: 1

- **Number Of Scans Per Spectrum.** This parameter determines how many scans are collected to produce each spectrum or interferogram. If you collect more than one scan, the system averages all of them.

Optimize the Number Of Scans Per Spectrum setting whenever you analyze a new type of sample or use a new sampling technique or accessory. For slow, intermittent sampling of a flowing sample, try collecting 16 scans per spectrum and then measure the signal-to-noise ratio. This will give an indication of how many scans to collect for the desired results. If the sample composition is changing rapidly, collect 1 or 2 scans per spectrum.

If collecting data that will be used for quantitative analysis, the appropriate number of scans will depend on the detection limits required for the analysis. For example, if you are looking for trace components in a gas sample that is flowing through the gas cell, you may need 16 or more scans per spectrum to achieve an adequate ratio of signal to noise.

Increasing the number of scans reduces the noise level of the data (increases the signal-to-noise ratio) and increases the sensitivity; that is, the ability to distinguish small peaks from noise. Keep in mind, however, that the more scans you collect, the longer is the analysis time. Also, as you increase the number scans, the improvements in sensitivity diminish. For example, if you have already collected a large number of scans, it will take many more scans to achieve a significant increase in sensitivity.

Number of scans per standard:

- **Number Of Scans Per Standard.** This parameter determines how many scans are collected to produce a spectrum or interferogram of each standard. Normally, RESULT Integration collects standards using the same parameter settings as are used to collect the sample data. However, when using the sequence module events to collect the sample data and collecting only a few scans per spectrum, it is recommended that you specify more scans for the standards to improve quantitative accuracy. See “Collecting Standards” in “Chapter 4 Tools For Building Methods and Viewing Spectra” of the “RESULT Integration User Guide” for more information.

If you collect more than one scan of the standards, the system averages all of them.



- Data Format.** This parameter determines the unit used for the collected data. The following tables show the recommended format settings and corresponding units for diffuse-reflection and transmission sampling. See “Antaris Sampling” in your main analyzer user guide for recommendations for setting Data Format for each Antaris sampling module or system.

For diffuse-reflection sampling (Antaris integrating sphere and fiber optic sampling module with SabIR probe), set Data Format to one of the following:

Setting	X-axis unit	Y-axis unit
% Reflectance	Wavenumber (cm-1)	% reflectance units
Log (1/R)*	Wavenumber (cm-1)	Log (1/R) units
Kubelka-Munk*	Wavenumber (cm-1)	Kubelka-Munk units
Single beam	Wavenumber (cm-1)	arbitrary units
Single beam (raw)	Wavenumber (cm-1)	arbitrary units
Interferogram	Data points	volt

\* Recommended format for spectra that will be used for quantitative measurements.

For transmission sampling (Antaris NIR transmission module and tablet analyzers and Antaris IGS systems), set Data Format to one of the following:

Setting	X-axis unit	Y-axis unit
% Transmittance	Wavenumber (cm-1)	% transmittance
Absorbance*	Wavenumber (cm-1)	absorbance units
Single beam	Wavenumber (cm-1)	arbitrary units
Single beam (raw)	Wavenumber (cm-1)	arbitrary units
Interferogram	Data points	volt

\* Recommended format for spectra that will be used for quantitative measurements.

The Interferogram setting allows you to access the unprocessed data produced by the analyzer. The interferogram contains the encoded detector response at all frequencies in the spectral range.

A single-beam spectrum is produced by Fourier transforming an interferogram. A single-beam spectrum shows the measurable detector response at all frequencies in the spectral range.

A sample single-beam spectrum is ratioed against a background single-beam spectrum to produce a sample transmission or reflection spectrum with the background information removed. The other data formats are produced by mathematically converting the sample transmission or reflection spectrum to the selected Y-axis unit.

Select the Single Beam format, rather than Single Beam (raw), if you want to collect single-beam background and/or sample spectra in a workflow. These single-beam spectra are normalized using the following equation:

$$\text{Single beam} = \text{single beam (raw)} \times \text{attenuation screen factor} \times \text{detector gain factor}$$

**Note** To view the current values for these factors, choose Instrument Status from the Maintenance menu in RESULT Operation, select Show Detailed Detector Information, and then choose OK. ▲

The normalized single-beam spectra have been adjusted to account for natural variations in the screens mounted in the attenuation wheel, and in the detector response. Using normalized single-beam spectra helps ensure that these differences do not affect the analytical results when workflows are transferred between systems. Using normalized single-beam spectra will also improve prediction accuracy when using different attenuation and detector gain settings for background and sample collection.

**Note** The Single Beam (raw) data format is used for diagnostic purposes only. ▲



- **Background Frequency.** This option lets you specify when to collect a background for ratioing sample spectra produced by a collect sequence event. The Background Frequency parameter is available in the software, except when Data Format is set to Single Beam, Single Beam (Raw), or Interferogram.

Set Background Frequency Select to Before Every Sample if you want to collect a background spectrum before each sample spectrum or Once For Each Workflow Run to collect one background and use it to process all of the sample spectra produced by a collect sequence event

in the workflow. (If the collect event is positioned in a repeat or perform-while loop, all the spectra produced by the loop will be processed using the same background spectrum.)

The remaining options allow you to specify the maximum amount of time a background is valid before it expires. If you select one of these options, before the software collects a sample spectrum, it examines the current background to determine if it has expired. If the current background is still valid, then the software continues collecting the sample data. If the current

background has expired, then the software either prompts the operator to collect a background (if a Before Background operator prompt is specified), or simply collects a background without prompting the operator if background measurements are taken using an internal background path or reference.

**Note** For demanding applications, you can obtain the best results by collecting the background just before each sample spectrum. ▲

**Tip** If collecting a small number of scans for the samples (i.e., Number Of Scans Per Spectrum is set to 1 or 2) and you need to collect significantly more scans for the background, set Background Frequency to Once Per Day (this essentially disables background collection from the collect sequence event) and add a collect event to the beginning of the workflow to collect a background spectrum. In the collect event, set Number of Sample Scans to 32 or higher, select Collect Background Only, and make sure the collect event links to the same sample and background specifications used by the collect sequence event. This approach to background collection allows you to specify more scans for the background spectrum, which will improve your results (see “Background specifications” in this chapter for more information). ▲

Background folder: C:\RESULT\Backgrounds

- **Background Folder.** This readout shows the current folder and path for archiving backgrounds in RESULT Integration. Use the RESULT Options dialog box in the Edit menu to specify the location for archiving backgrounds produced by workflows run in RESULT Integration.

If the workflow is transferred to RESULT Operation, backgrounds will be archived using the folder and path for archiving backgrounds for that application. See “Chapter 4 Setting RESULT Operation Options” in the “RESULT Software Administration Guide” for information about setting the path for archiving backgrounds in RESULT Operation.

**Note** Background files are archived except when Background Frequency is set to Before Every Sample. ▲

Collect background only

- **Collect Background Only.** Select this option if you want this collect sequence event to collect and store only a background spectrum (no sample spectra will be collected). This feature is helpful for performing quality checks on a background spectrum before using it to process sample spectra in a workflow. When Collect Background Only is selected, the software automatically sets Data Format to Single Beam, which is the typical format for displaying and archiving background spectra, and Background Frequency is unavailable. The software uses the setting for Number Of Background Scans in the background specification to determine the number of scans to collect for the background spectrum.

## Chapter 6 Workflow Specifications

Workflow specifications define how certain workflow events will be carried out. The collect event, for example, instructs the system to collect a spectrum at a given point in the workflow, while the associated sample and background specifications allow you to customize data collection for a given sampling technique.

RESULT Integration provides seven types of workflow specifications, including:

- **Logic specifications**, which define a test of numeric, yes/no or true/false results or compared text to produce a true or false workflow result. The true/false result may be used by other workflow events such as a Repeat or Perform-If event to define a conditional test.
- **Measurement specifications**, which specify a TQ Analyst or other method applied to spectra collected in a workflow to produce numeric or other results, or a mathematical function applied to the results of other events to produce a composite value.
- **General specifications**, which include request specifications to request information from the operator, prompt specifications to provide information to the operator, and specifications for hardware devices such as an autosampler.
- **Report specifications**, which list the sections to be included in a sample report and the order those sections will appear when the report is displayed or printed.
- **Report Item specifications**, which define the sections in a sample report, including headings, tables, statistical or other summarized data, and text, as well as the workflow results included in each section and how those results will be formatted.
- **Sample specifications**, which contain advanced collection parameters that are optimized for a given Antaris sampling module and analysis technique.

- **Background specifications**, which define data collection for background spectra generated by a workflow.
- **StartStop specifications**, which define operator prompts for StartStop events.
- **Correction specifications**, which define spectral corrections for spectra collected in a workflow.

For information about adding simple events to a workflow, see “Chapter 1 Simple Workflow Events.” To learn about adding structural events to a workflow, see “Chapter 2 Structural Workflow Events.” For information about adding device-specific events to control a hardware device, see “Chapter 3 Device-Specific Events.” To learn how to use RESULT software to collect and process spectral data continuously over a specified period, see “Chapter 4 Sequence Module Events.”

This chapter describes all the specifications that are available for use in workflows created in RESULT Integration. The following information is provided for each workflow specification:

- **Description**, which is a brief explanation of the specification and how it works.
- **Associated events**, which lists the required and optional events that can be linked to the described specification.
- **Associated specifications**, which lists the required and optional specifications that can be linked to the described event.
- **Related events**, which lists events that can be tied to the described specification.
- **Related specifications**, which lists other specifications that operate like the described specification or perform a similar function, and specifications that may be related to the described specification.
- **Parameters**, which explains the parameters for the described specification. Parameters are explained in the order in which they appear in the software when the described specification is selected in a workflow.

- **Usage**, which provides practical examples of how the described specification is typically used in a workflow.

## Logic specifications

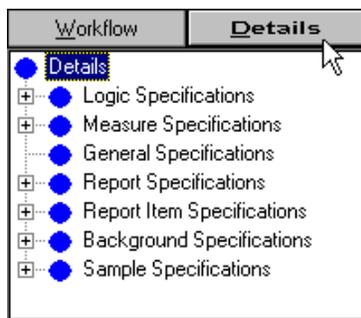
The Logic Specifications group provides two types of specifications for testing a workflow's status during operation, including:

- **Logical test specifications.** A logical test specification defines a logical test by specifying what to test and a true/false condition for the test result. You can use a logical test specification to test the results of workflow events and other logical test specifications, and to check the workflow for errors.
- **Compare text specifications.** A compare text specification defines a logical test of two text results by specifying what to test and the criteria for the comparison. You can use a compare text specification to test text results generated by other workflow events.

### Adding a logic specification to a workflow

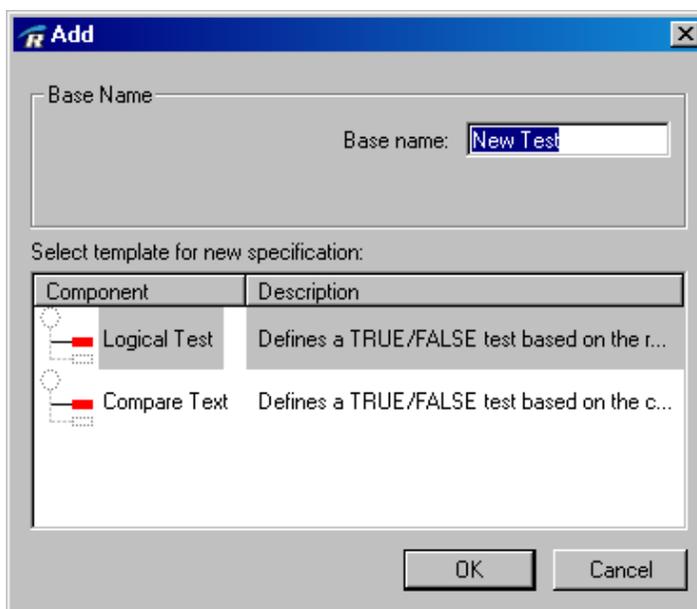
To add a logic specification to the open workflow:

1. **Select the Details tab.**



2. **Select Logic Specifications and then choose the Add button on the RESULT Integration toolbar.**

The software displays the following dialog box.



- 3. Select an appropriate specification, enter a base name for the new specification and then choose OK.**

The new specification appears in the display area of the RESULT Integration main window.

Read the next two sections to learn about the options available for setting up logical test specifications and compare text specifications in a workflow. For information about linking specifications to workflow events, see “Linking a specification to a workflow event” in “Chapter 2 Creating and Editing Workflows” of the “RESULT Integration User Guide.”

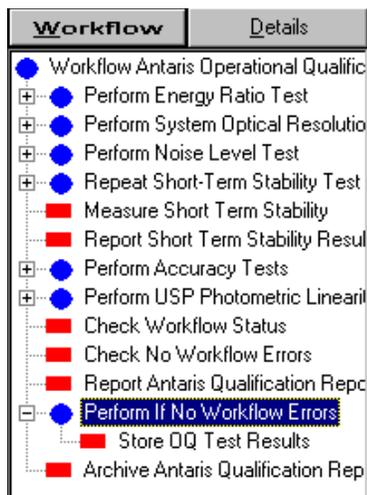
## Logical test specifications

A logical test specification can be used to test workflow results to determine if they pass or fail specific conditions. This is useful for defining multiple paths in workflows and conditions for starting and/or stopping activities such as the tasks in a repeated or conditional loop.

A logical test specification defines what to test and a true/false condition for the test result. You can set up a logical test specification to test the results of workflow events or the true or false result of another logical test specification. The logical test specification can also be used to check a workflow for errors.

The logical test specification produces a true/false result, which may be used by workflow events as the basis for a conditional test. Workflow events that may include a conditional test include check events, perform-if events, perform-while events, and repeat events. In the example below, the second check event tests for workflow errors and the Perform-If event executes (stores the OQ test results) if no errors are found.

Perform-if event set up to store workflow results if the workflow runs without errors



**Associated events:** Check event, Perform-If event, Perform-While event, Repeat event

**Associated specifications:** None

**Related events:** Check event, Calculate event, Compare event, Measure event, Request event, Read From I/O event

**Related specifications:** Compare text specification

**Parameters:** The illustration below shows the parameters for the logical test specification. These parameters appear in the display area of RESULT Integration when a logical test specification is selected in a workflow.

Logical Test Specification

New Test

Test the results of these items:

Measurement	Result	Component	Format

Add Event Item... Add Logical Test... Edit

Conditional Test

Selected test result item is true if:

< Less than

Low value:  Value

Event item

High value:  Value

Event item

Combination Logic

And: All test result items must be true to make this logical test TRUE

Or: Any test result item that is true will make this logical test TRUE

Logical test is always FALSE if workflow errors have been detected

Multiple Results

Use all logical test results for each test result item

Use only the most recent logical test result for each test result item

## Logical test specification parameters

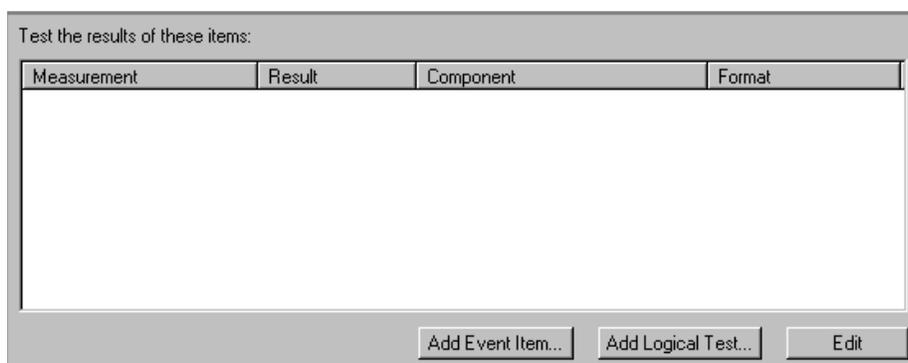
The logical test specification parameters specify what to test, a true/false condition for the test result, and how to handle multiple results from events that occur in a loop. The following sections explain the logical test specification parameters in detail. The parameters are explained in the order in which they appear in the software.

### Test The Results Of These Items

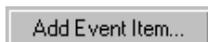
Use the features in this group to specify the workflow results to be tested.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete, or select the row and press Delete on the keyboard.

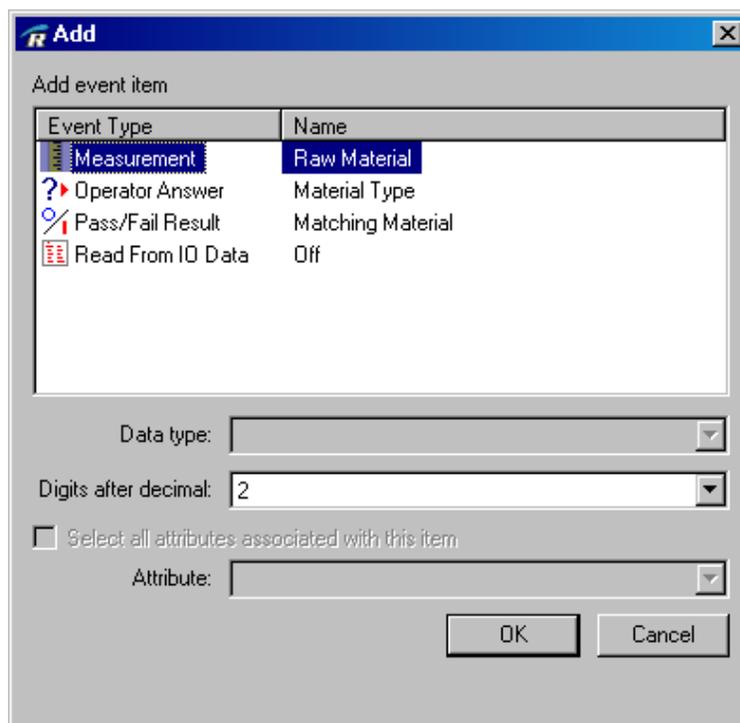
Use Export To Text File in the shortcut menu to write the information displayed in the table to a text file with a file name and path you specify.



You can configure a logical test specification to test the result of any workflow event that produces a numeric, pass/fail, or yes/no result, or the true/false result of another logical test specification. The selected results are listed in a table. The table is interactive and easy to work with. The features are described below.



- **Add Event Item.** Choose this button to add a workflow result to the list of results to be tested. After you choose Add Event Item, the following dialog box appears:



The list shows the events in the workflow that provide a numeric, pass/fail, or yes/no result that can be placed in a logical test specification.

**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a selectable result or all of those events have already been added. See the Usage heading for this logical test specification for a list of events that produce results that can be used in a logical test specification. ▲

Select a result in the list. Make sure you select a result that exists at this point in the workflow. Since a workflow implements events in the sequence, only results produced by events that occur before the event that calls this logical test specification will have testable results.

**Note** If this logical test specification is linked to a check event, don't add the check event's pass/fail result to the list of items to be tested or the workflow may produce unexpected results . ▲

After you select a result, the following parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Examples are provided below.

- *Data Type.* Use this list box to select a result produced by the selected event, such as a value or an acceptance limit. The number and type of results produced by an event depend on the event, and, for measure events, on the TQ Analyst method used for the measurement. For example, a measure event configured for quantitative analysis would always produce concentration values, but it may also include acceptance limits or known values, such as the expected concentration for a sample or standard. The Data Type drop-down list could include the following items for a quantitative measure event.



Many events produce only one type of result, including check events, calculation events, comparison events, and request events.

- *Digits After Decimal.* This box is available in the software only when the selected Data Type (see above) produces a numerical result.

Use the box to select the number of digits the software will include after the decimal point in the conditional test for this workflow result. You can include up to six digits after the decimal point for the conditional test (the software automatically includes 6 digits after the decimal point when calculating the workflow result). See High Value/Low Value in the Conditional Test parameter group for more information.

- *Attribute.* Use this list box to select a specific component or other measured attribute or value for the selected data type and event. The number and type of items in the Attribute drop-down list depend on the event, and, for measure events, on the TQ Analyst method used for the measurement. For example, a measure event configured for spectral measurements could include the following items in the Attributes drop-down list.



**Note** Workflow results must be added to a logical test specification one at a time. Creating individual entries allows you to specify a true/false condition for each result. The Select All Attributes Associated With This Item check box,

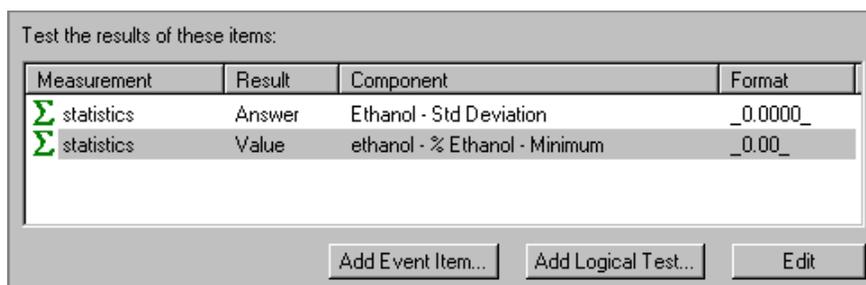


is not available in the Add RESULT dialog box when adding workflow results to a logical test specification. ▲

When you are finished selecting a result, choose OK. The selected result is added to the list of items to be tested.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete, or select the row and press Delete on the keyboard.

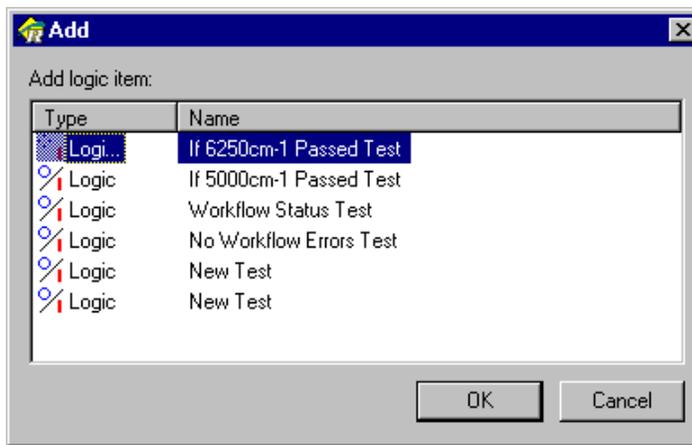
Use Export To Text File in the shortcut menu to write the information displayed in the table to a text file with a file name and path you specify.



Add Logical Test...

- **Add Logical Test.** Choose this button to add a logical test result to the list of results to be tested. After you choose Add Logical Test, the following dialog box appears:

This feature lets you use a logical test specification to test the result of another logical test specification in the same workflow.



The list includes all the logical test specifications in the current workflow except the current one, which cannot be added to itself.

- Note** If this dialog box is empty, then the workflow either has no other logical test specifications besides this one, or those logical test specifications have already been added. ▲

Select a name in the list and then choose OK. If the logical test specification you select is set up to test workflow results, make sure all of those results exist at this point in the workflow.

- Note** Don't select a logical test specification that is set up to test the result of this logical test specification, or you may send the workflow into a continuous loop □▲

The selected test specification is added to the list of items to be tested.

Edit

- **Edit.** To edit numeric or pass/fail results that are included in the list of results to be tested, select the result in the logical test specification and then choose Edit. You can edit the data type, digits after decimal, and attribute settings for the selected event. The new settings will be used for any subsequent tests performed using this logical test specification.

## Conditional Test

Use the parameters in this group to specify conditions for the logical test. You can specify a true/false condition for each tested result and a true/false condition for all the results combined.

The screenshot shows a dialog box titled "Conditional Test". It contains a section "Selected test result item is true if:" with a dropdown menu currently showing "Is PASS". Below this are two rows of input fields. The first row is for "Low value:" and the second for "High value:". Each row has two radio buttons: "Value" (selected) and "Event item". To the right of each row is a text input field and a "Select" button. Below these is a "Combination Logic" section with two radio buttons: "And: All test result items must be true to make this logical test TRUE" (selected) and "Or: Any test result item that is true will make this logical test TRUE". At the bottom, there is a checkbox labeled "Logical test is always FALSE if workflow errors have been detected".

The features are described below:

- **Selected Test Result Item Is True If.** Use this list box to specify a true/false condition of each workflow result you want to test. To specify the true/false condition of a workflow result, select the result in the Test The Results Of These Items box and then select a condition in the Selected Test Result Item Is True If drop-down list.

The screenshot shows a dropdown menu titled "Selected test result item is true if:". The menu is open, showing a list of comparison operators. The first item, "< Less than", is highlighted in blue. The other items in the list are: "<= Less than or equal to", "= Equal to", ">= Greater than or equal to", "> Greater than", ">< Between", ">=< Within", and "<> Outside".

The items in the drop-down list differ depending on the type of result that is selected. If a numeric workflow result (format equals 0 or 0.000) is selected, then the following settings are available:

- < Less than
- < = Less than or equal to
- = Equal to
- > = Greater than or equal to
- > Greater than

> < Between

> = < Within

< > Outside

**Note** If you are performing an equality test with results that contain floating point numbers (numbers that allow decimal points), then it is recommended that you do not use the Equal setting. Because computers can store only a fixed number of digits after a decimal place, they round numbers when performing calculations. When rounding occurs, you risk producing a false failure in your equality test. For example, if you select “= Equal to” as the operator and enter 1.22 as the comparison value, and the calculated value for the workflow result is 1.2219843, the test will be “is 1.2219843 equal to 1.22,” which will be false. ▲

**Note** To perform an equality test, we recommend that you use the Between setting, and specify a small range, for example, from 1.215 to 1.225 for the previous example. This will prevent your test from being affected by computer rounding. ▲

- **Low Value, High Value.** If a numeric result is selected, specify a low value and/or high value if desired. You can base the conditional test on a value you specify or the numeric result from another workflow event.
- *Value.* If the conditional test is based on a fixed low/high value, select the Value option and enter the number in the corresponding entry box.

**Note** The number of digits allowed for each workflow result is defined by the Digits After Decimal setting in the Add dialog box when you add each workflow result to the list of items to be tested. See Add Event Item in the description for this logical test specification for more information. ▲

- *Event Item.* If the conditional test is based on the numeric result from another workflow event, select the Event Item option and then choose Select. The software displays a dialog box showing the available workflow results. Select a result in the list and choose OK to close the dialog box. The event name appears next to the corresponding Event Item.



If a check event result (format equals pass/fail) is selected, the following settings are available:

- Is Pass
- Is Fail

The pass/fail settings may also show up for some measurement results, for example if an associated TQ Analyst method is set up to produce a pass/fail result.

If a yes/no response from an operator request is selected, the following settings are available:

- Is Yes
- Is No

If a logical test result is selected, the following options are available:

- Is True
- Is False

- **Combination Logic.** If the logical test specification is set up to test workflow results, use these buttons to specify the true/false condition of the combined result.

Combination Logic

- And: All test result items must be true to make this logical test TRUE
- Or: Any test result item that is true will make this logical test TRUE

You can elect to require that all test results must be true to make the combined test result true, or to allow any test result that is true to make the combined result true.

- **Logical Test Is Always False If Workflow Errors Have Been Detected.** Select this option if you want to use this logical test specification to test for workflow errors.

Logical test is always FALSE if workflow errors have been detected

When this option is selected, the combined result of the logical test will be false if the workflow produces an error before it encounters this logical test specification.

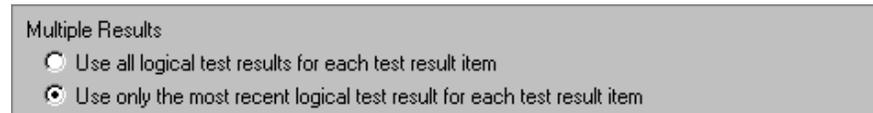
If the workflow runs with no errors and the logical test specification is set up to test for workflow errors only, the combined result of the logical test will be true. If the workflow runs with no errors and the logical test specification is set up to test workflow results and check for errors, the workflow results will determine the combined result of the logical test.

**Tip** If you want to test the entire workflow for errors, link this logical test specification to an event that is positioned at the end of the workflow. ▲

Clear this option if you don't want this logical test specification to test for workflow errors.

### Multiple Results

If the logical test specification is set up to test the result from one or more workflow events that occur in a loop, those events will produce a result during each loop iteration. This feature allows you to select whether this logical test specification will test all the results produced by the loop or only the most recent result. The options are described below:



- **Use All Logical Test Results For Each Test Result Item.** If the logical test specification will test workflow results produced in a repeat or perform-while loop, selecting this option causes the workflow to test all the results produced by the loop to determine the true/false result of each item and the Combination Logic setting to determine the overall true/false result.
- **Use Only The Most Recent Logical Test Result For Each Test Result Item.** Select this option if the logical test specification is not associated with a loop or you want the workflow to test only the most recent result to determine the true/false result of each item. This is the default setting and will maximize your computer processing speed.

See “repeat events” and “perform-while events” for more information about using stored data in a workflow.

**Usage:** A logical test specification may be linked to the following types of workflow events:

- **Check event**, which tests the combined true/false result of the associated logical test specification and produces a pass/fail result in the workflow.
- **Perform-if event**, which can execute or skip a group of sub-events based on the results of an associated logical test specification.
- **Perform-while event**, which can execute or repeat a group of sub-events, or skip the entire group, based on the results of an associated logical test specification.
- **Repeat event**, which can stop executing or repeating a group of sub-events based on the results of an associated logical test specification.

A logical test specification can test the result of any workflow event that produces a number or pass/fail response, including:

- **Check event**, which produces a pass or fail result.
- **Measure event**, which can be used to analyze the spectra to produce concentration values (quantitative methods), library index values and match values (classification methods), or spectral measurements, such as a peak height or area (spectral measurement methods).
- **Calculate event**, which can be used to produce statistics from measurements that are part of a loop.
- **Compare event**, which uses the actual and expected values for a series of measurements to produce correlation coefficient, root mean square error of prediction (RMSEP), and slope and y-intercept values for those measurements.
- **Request event**, which can be used to generate a message-response request dialog box. The request dialog box may produce up to ten numerical or yes/no responses from the operator.
- **Read From I/O event**, which can read values from other devices.

A logical test specification may also be set up to test the result of another logical test specification. The tested logical test specification may be linked to another event in the workflow, or it may be an orphan.

**Note** If you set up a logical test specification to test its own result, the workflow may enter a continuous loop □▲

You can also set up a logical test specification to test the workflow for errors.

## **Compare text specifications**

A compare text specification defines a logical test of two text results by specifying what to test and the criteria for the comparison. You can use a compare text specification to test text results generated by other workflow events.

The compare text specification produces a true/false result, which may be used by check events as the basis for a conditional test.

**Associated events:** Check event, Perform-If event, Perform-While event, Repeat event

**Associated specifications:** None

**Related events:** Check event, Measure event, Request event

**Related specifications:** Logical test specification, Measurement specification, Prompt specification, Request specification

**Parameters:** The illustration below shows the parameters for the compare text specification. These parameters appear in the display area of RESULT Integration when a compare text specification is selected in a workflow.

### Compare text specification parameters

The compare text specification parameters specify the text items to be compared and the criteria to be used for the comparison. The following sections explain the compare text specification parameters in detail. The parameters are explained in the order in which they appear in the software.

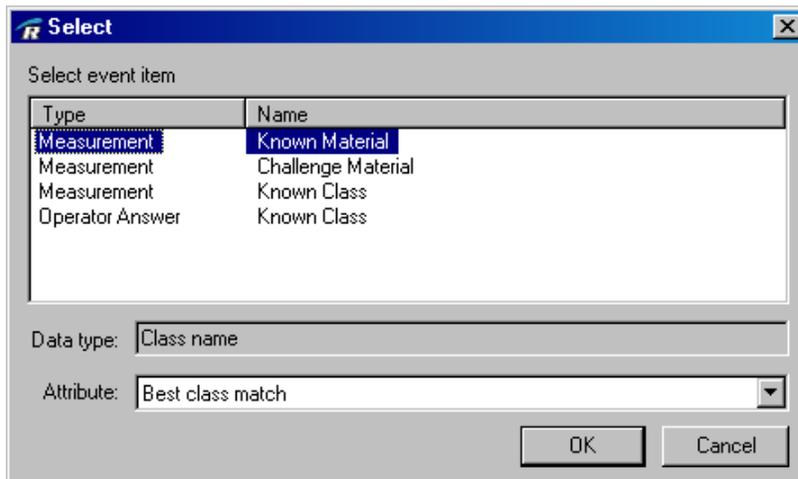
#### Compare The Text Results Of These Two Items

Use the parameters in this group to specify the two text results you want to compare. You can compare the text results from two workflow events or compare the text results from one event to a text string.

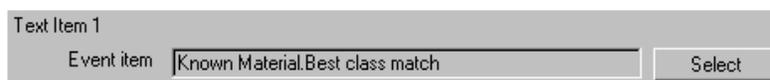
- **Text Item 1.** Use this option to specify the workflow event you want to test. Only events that produce a text result can be selected. Events that may produce a text result include the following:
  - Measure events that point to a classification method.
  - Request events that require a text response.

To select a workflow event, choose Select.

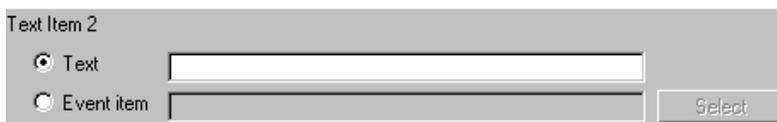
The software displays the following dialog box.



The dialog box lists the events that produce a text result in the current workflow. Select the event you want to test. If the event produces more than one text result, use the Attribute drop-down list box to select the text result you want to test. When you are finished, choose OK. The software shows the name of the selected event and its associated text result, as shown below:



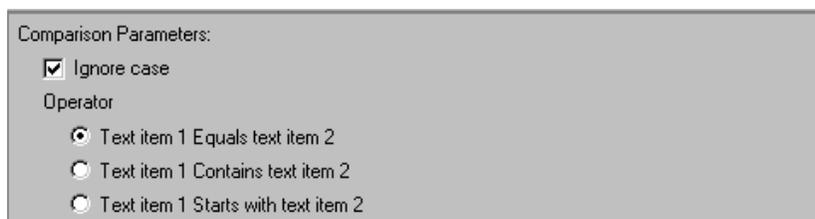
- **Text Item 2.** Use this option to specify what the workflow event (Text Item 1) should be compared to. You can compare the event to the text result from another event in the workflow, or to a text string.



- *Text.* Select this option if you want to compare the event to a text string. Then enter the string in the associated text box. The string can include any combination of letters, numbers, and other characters available from the computer keyboard or other input device.
- *Event Item.* Select this option if you want to compare the event to the text result from another workflow event. Then choose Select and select the workflow event. Only events that produce a text result can be selected.

## Comparison Parameters

Use the parameters in this group to specify the criteria to be used for the comparison.



Comparison Parameters:

Ignore case

Operator

Text item 1 Equals text item 2

Text item 1 Contains text item 2

Text item 1 Starts with text item 2

- **Operator.** Use this feature to specify the criteria for determining a match. The following options are available:
  - *Text Item 1 Equals Text Item 2.* Select this option to require that text item 1 match text item 2.
  - *Text Item 1 Contains Text Item 2.* Select this option to require that text item 2 is contained in text item 1.
  - *Text Item 1 Starts With Text Item 2.* Select this option to require that text item 1 starts with text item 2.
- **Ignore Case.** Use this feature to specify whether the match should be exact, including the letter case, or whether case should be ignored.

**Usage:** A compare text specification may be linked to the following types of workflow events:

- **Check event**, which uses the combined true/false result of the associated compare text specification to produce a pass/fail result.
- **Perform-if event**, which can execute or skip a group of sub-events based on the results of an associated compare text specification.
- **Perform-while event**, which can execute or repeat a group of sub-events, or skip the entire group, based on the results of an associated compare text specification.
- **Repeat event**, which can stop executing or repeating a group of sub-events based on the results of an associated compare text specification

A compare text specification can test the result of any workflow event that produces a text string, including:

- **Measure event**, which may produce text results such as a class name.
- **Request event**, which may produce up to ten text responses from a message-response dialog box.

## Measurement specifications

A measurement specification defines a TQ Analyst or other method applied to spectra collected in a workflow to produce specific workflow results, or a mathematical function applied to the results of other events in the workflow to produce a composite value. Measurement specifications may be linked to measure events and compare events in workflows.

RESULT provides three types of measurement specifications including:

- **Spectral measurement specifications.** These specifications can be used to set up a workflow that measures collected spectra using a compatible quantitative, classification, or spectral measurement method. RESULT Integration is designed to run with Thermo Scientific TQ Analyst method development software. RESULT is also compatible with several other method development applications created by Thermo Fisher Scientific and other manufacturers. The spectral measurement specifications include the following:
  - *TQ Analyst measurement specifications*, which can be linked to a method developed using TQ Analyst method development software.
  - *PLSplus/IQ measurement specifications*, which can be linked to a method created with Thermo Scientific PLSplus/IQ method development software for GRAMS/32® AI.
  - *Unscrambler measurement specifications*, which can be linked to a method developed with The Unscrambler® method development software from Camo AS.
  - *Pirouette measurement specifications*, which can be linked to a method produced with Pirouette method development software from InfoMetrix, Inc.

- **Classify Multiple measurement specifications**, which can be used to define a classification measurement using multiple TQ Analyst methods (must be based on the same classification analysis) or a TQ Analyst classification method requested by the operator.
- **Composite measurement specifications**, which can be used to set up a workflow that calculates a composite value based on numeric results produced by other events in a workflow.

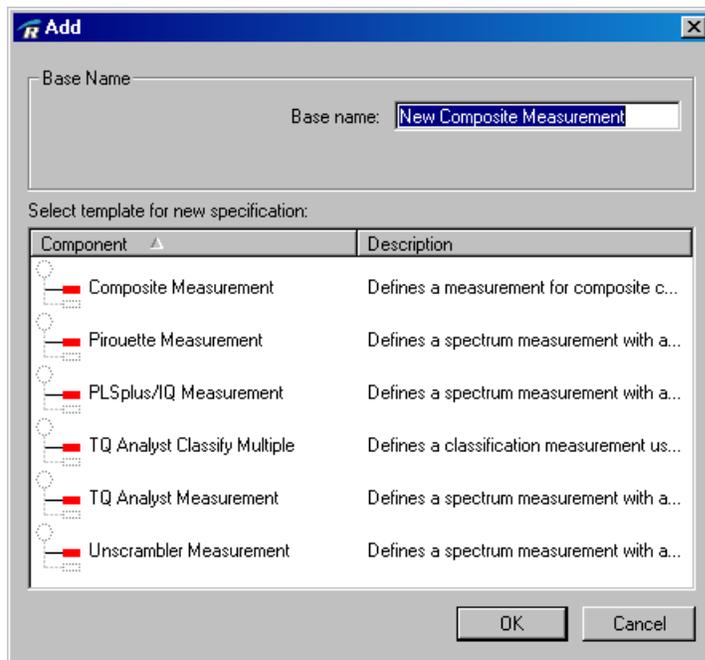
## Adding a measurement specification to a workflow

To add a measurement specification to a measure event or a compare event:

1. **Select the measure event or compare event in the workflow.**
2. **In the event parameters, choose the New button at the right of the Measurement Specification drop-down list box.**



The software displays the Add Specification dialog box.



### 3. Select a measurement specification.

See the previous section for brief descriptions or review the detailed descriptions in the sections that follow.

**Note** If a specification isn't listed for the application you want to use, make sure the application and any required run-time files are properly installed and configured on the computer you use to run RESULT. The RESULT add-in option for any third-party method development software must also be installed. See *Installing Your Software* in your RESULT software document set for more information. ▲

### 4. Enter a base name for the new specification at the top of the Add Specification dialog box and then choose OK.

The new specification appears in the display area of the RESULT Integration main window.

Read the next section to learn about the options available for setting up measurement specifications in workflows.

## Spectral measurement specifications

The specifications in this group can be used to attach a workflow to a specific analytical method developed using an application outside of RESULT. Spectral measurement specifications can also be linked to measure events and compare events, which can be linked to spectra produced by specific collect events in a workflow. Through this path, the workflow can collect and then analyze a spectrum using a specific analytical method to produce a set of measurement results such as component concentrations or class names.

RESULT provides four types of spectral measurement specifications including:

- *TQ Analyst measurement specifications*, which can be linked to methods developed using TQ Analyst method development software.
- *PLSplus/IQ measurement specifications*, which can be linked to methods created with Thermo Scientific PLSplus/IQ method development software for GRAMS/32® AI.

- *Unscrambler measurement specifications*, which can be linked to methods developed with The Unscrambler® method development software from Camo AS.
- *Pirouette measurement specifications*, which can be linked to methods produced with Pirouette method development software from InfoMetrix, Inc.

The user interfaces for all four types of spectral measurement specifications are basically the same (the TQ Analyst specification has a few additional features). However, each specification contains embedded instructions to recognize and extract information from method files created using a specific application.

**Associated events:** Measure event, Compare event

**Associated specifications:** none

**Related events:** Calculate event, Check event, Collect event, Request event, Store event, Report to OPC event

**Related specifications:** Logical test specification, Table Item specification, Summary Item specification

**Parameters:** The illustration below shows the parameters for the spectral measurement specification for TQ Analyst software. These parameters appear in the display area of RESULT Integration when a TQ Analyst measurement specification is selected in a workflow.

Measurement Specification

New

Measurements

Application name: TQ Analyst (tm)

Path: C:\RESULT Data\Workflows

File name: (None Selected)

Measurement type: Simple Beer's law

Measure these attributes:

New Delete

Test cases for selected measurement:

Name: Value: 0.000

New Delete

Prompt integrator to select test case during simulation

### TQ Analyst measurement specification parameters

The spectral measurement specification parameters allow you to specify the file name of a TQ Analyst or other compatible method that may be used to analyze sample spectra produced by a workflow. You can also use a measurement specification to create test-case criteria, which allow you to test certain elements in a workflow such as a check event without requiring a calibrated method or a spectrum.

**Note** When using TQ Analyst to develop methods, you can also use the measurement specification to specify certain components of a new method, such as the measurement type and the component or class names. If you then use the features on the Tools menu in RESULT Integration to create a new TQ Analyst method based on a measurement specification, the measurement type and other settings will be imported into TQ Analyst automatically. ▲

The following sections explain the parameters for all four types of spectral measurement specifications. The parameters are explained in the order in which they appear in the software.

Application Name: TQ Analyst (tm)

- **Application Name.** This readout shows the method development application that is compatible with this measurement specification. The application name is based on the selected specification. RESULT provides four spectral measurement specifications that can be used to link workflows to methods developed with TQ Analyst, Pirouette, Unscrambler, and PLSplus/IQ plus software. If the method developed for use with this workflow was not created with TQ Analyst software, use a different measurement specification. (To list the available specifications, select the Measure event and choose the New button at the right of the Measurement Specification drop down list box).

Path: C:\RESULT Data\Workflows

- **Path.** This readout indicates the current path for locating workflow and method files in RESULT Integration. RESULT will only allow the selection of methods that were created with the specified application (see above) and stored in this path.

See “Setting RESULT Integration Options” in the “RESULT Integration User Guide” for information about specifying the path for locating workflow and method files in RESULT Integration.

File name: (None Selected) ▼

- **File Name.** Use this list box to select the file name of a calibrated method to use for this measurement. The File Name drop-down list includes all the method files for the selected application which are located in the current directory for storing workflows and methods in RESULT Integration (see above). The selected method should be calibrated and thoroughly tested using materials that are representative of the samples the workflow will be used to analyze.

If the correct method file does not appear in the drop-down list, copy the file and any associated run-time files to the directory indicated for Path above. See “Building a TQ Analyst method” in “Chapter 4 Tools for Building Methods and Viewing Spectra” of the “RESULT Integration User Guide” for a list of the run-time files required for TQ Analyst methods. See *Installing Your Software* for a list of run-time files required for Pirouette, Unscrambler, and PLSplus/IQ methods.

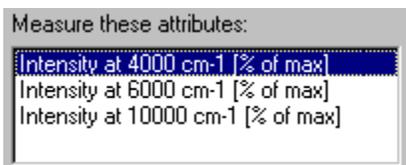
If you don't have an appropriate method for this measurement, leave File Name set to None Selected.



- **Measurement Type.** If you selected a valid method file above, the Measurement Type list box describes the kind of measurement the method is currently set up to run; the setting cannot be changed in RESULT Integration. To change the measurement type, you must open and resave the method using its native application.

**Note** After you change the measurement type or any other setting in a TQ Analyst or other method, make sure you check the settings for the other method parameters and calibrate and test the method before using it in a workflow. ▲

If File Name (above) is set to None Selected, the Measurement Type parameter is available in the software. If you plan to create a new method for this measurement, use the Measurement Type list box to select a measurement type for the new method. The drop-down list includes all the measurement types available in the selected application.

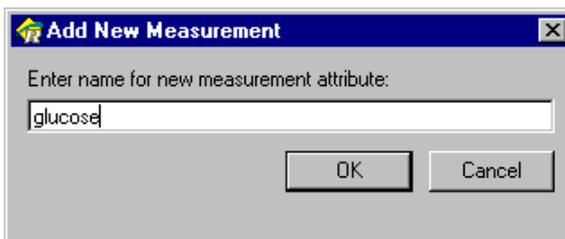


- **Measure These Attributes.** If you selected a valid method file above, this box shows the components or other attributes the method is currently set up to measure. In the example shown at the left, the selected method is set up to measure the intensity of the sample spectrum at several X-axis (frequency) locations.

If File Name (above) is set to None Selected, the Measure These Attributes box is available in the software and the box is empty. If you plan to create a new method for this workflow, use Measure These Attributes to specify what the method will measure. For example, use this box to enter names for the components that will be measured in a quantitative method.

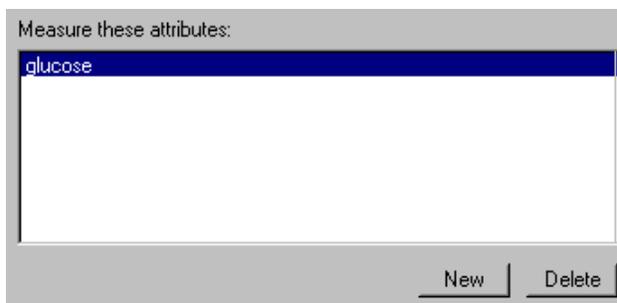
To add a component or other attribute to the list, choose the New button below the list. The following dialog box is displayed.

Choose Cancel to close the dialog box without adding a component or other name.



Type a descriptive name for the new measurement and then choose OK. The name you entered appears in the Measure These Attributes box on the measurement specification.

Use the Delete button to remove an item from the list.



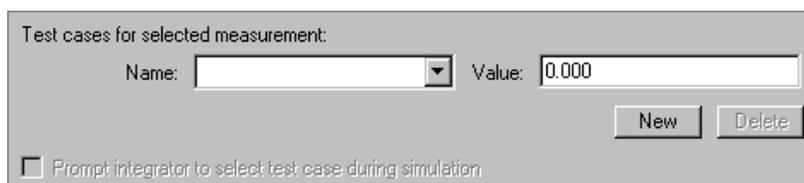
Repeat these steps for each additional component or attribute that will be measured.

When you have finished specifying the attributes to be measured, you are ready to create a new method. If using TQ Analyst, use the Configure Standards, Collect Standards, and Build TQ Analyst Method features on the Tools menu in RESULT Integration to create a method based on this measurement specification; RESULT Integration will set the measurement type and add the component or measurement names automatically. See “Chapter 4 Tools For Building Methods And Viewing Spectra” of the “RESULT Integration User Guide” for instructions.

If using a third-party application such as Unscrambler or Pirouette, see “Using third-party methods with RESULT” in the “RESULT Integration User Guide” for general information about creating third-party methods that are compatible with workflows developed in RESULT software.

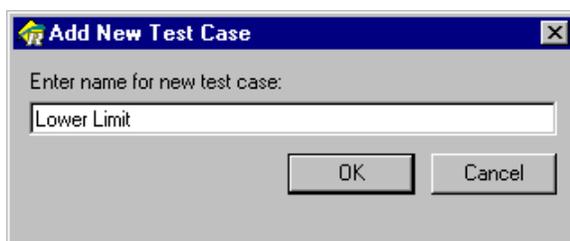
### Test Cases For Selected Measurement

The parameters in this group are available in the software only when File Name (see above) is set to None Selected. Use the parameter settings described below to define test-case criteria for your workflow. The test case features of RESULT Integration are designed to help you develop and test the measurements in a new workflow before you collect any spectra or create an associated method.



Use the parameters in this group to specify an acceptable result for each component or attribute this measurement specification is set up to measure. Supplying acceptable measurement results will allow you to test elements in your workflow that depend on the measurement results. For example, if you are using a check event to produce a pass or fail result for this measurement, you can use these test cases to define the pass/fail criteria, and then run the workflow using a test case that triggers a pass or fail result. You can also use test cases to “artificially” produce measured values that approach the method’s acceptance limits.

To specify the criteria for one or more test cases, choose New. The software displays the Add Test Case dialog box.



Enter a label for the new test case, such as Pass or Lower Limit and then choose OK.

- **Name, Value.** To associate a test case with a component or other attribute to be measured, select the attribute, select the test case in the Name drop-down list, and then select the Value box and enter a corresponding number. For example, to specify a minimum concentration value for glucose, select Glucose in the list of items to be measured, set the test case Name to Lower Limit, and then select the Value box and enter a number for the minimum concentration value.



Repeat these steps to specify test cases for any additional attributes to be measured.

If you want to delete the test case for an attribute, select the attribute and then choose Delete.

When you run a workflow that contains a measure event with a test case configured for one or more measured components, the workflow will produce the test case values as the measurement results. This allows you to continue developing the workflow without waiting for a completed method, and to test subsequent events that are triggered by certain measurement results.

- **Prompt Integrator To Select Test Case During Simulation.** If you specify one test case for each measured item, the workflow will use those test cases for all workflow runs. If a measured item has two or more test cases, you can set up the workflow to prompt the user to select an appropriate test case when running the workflow with simulated data by selecting Prompt Integrator To Select Test Case During Simulation.

Prompt integrator to select test case during simulation

**Usage:** A measurement specification may be linked to the following types of workflow events:

- **Measure event**, which measures the spectra produced by a collect event.
- **Compare event**, which measures the spectra produced by a collect event and compares the measurement results to the expected values using standard statistical techniques.

## Classify multiple specifications

A classify multiple specification can be used to analyze a spectrum collected in a workflow using multiple classification methods. This is the only way to analyze data using multiple classification methods to produce a single measurement result. The classify multiple specification can be configured to classify the sample spectra using all selected methods or only the method specified by the operator, a bar code, or another measure event at run time.

This feature is available only for methods developed using TQ Analyst application. Only classification methods can be used and all the methods must have the same classification type (e.g., Discriminant Analysis, Search Standards, QC Compare Search or Distance Match).

A classify multiple measurement specification can be linked to a measure event, which can be linked to spectra produced by a specific collect event in a workflow. Through this path, the workflow can collect and then classify a spectrum based on multiple TQ Analyst methods.

**Associated events:** Measure event, Request event

**Associated specifications:** none

**Related events:** Collect event, Report event, Store event, Report to OPC event

**Related specifications:** Request specification, Table Item specification, Summary Item specification

**Parameters:** The illustration below shows the parameters for the classify multiple specification. These parameters appear in the display area of RESULT Integration when a classify multiple specification is selected in a workflow.

Classify Multiple Specification

Classification

Classification Settings

Classify against all methods

Classify against matching method

Item

TQ Analyst Methods:

Method Name	Text Name	Comparison Type	Ignore Case

Selected Classification Type

Analysis Type: Discriminant analysis

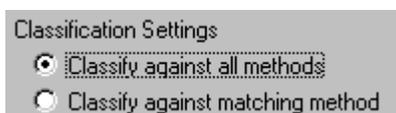
Attributes

Best class match

### Classify multiple specification parameters

The classify multiple specification parameters allow you to select the TQ Analyst classification methods that will be used to analyze the sample spectra produced by the workflow and whether the workflow will use all the specified methods to classify the sample spectra or only the method that matches certain criteria. The match can be based on the result from a request event or the result from another measure event in the workflow. If the specification is configured to use a matching method, then the specification parameters also define the criteria for the match.

The following sections explain the classify multiple specification parameters in detail. The parameters are explained in the order in which they appear in the software.

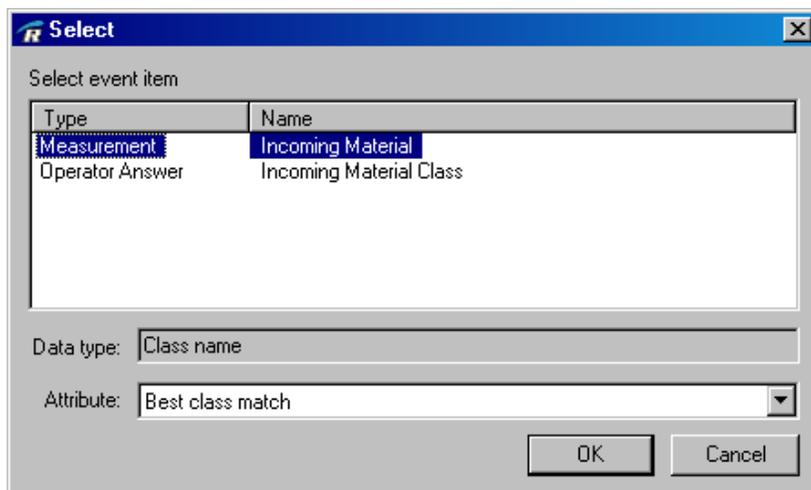


- **Classification Settings.** Use this feature to define the type of classification the associated measure event will perform.
  - *Classify against all methods.* Select this option if you want the workflow to classify each sample spectrum using all the TQ Analyst classification methods that are listed on the classify multiple specification.
  - *Classify against matching method.* Select this option if you want the workflow to classify each sample spectrum using a TQ Analyst classification method that is listed on the classify multiple specification and matches specific criteria. Use the Item box to specify the criteria that will be used to determine the appropriate method. The selection can be based on the result from a request event (such as an operator response or input from a bar code reader) or the result from another measure event in the workflow.

To select the criterion that will be used to determine the appropriate method, choose Select at the right of the Item box.



The Select dialog box is displayed listing the workflow results that can be used to determine the method for the classify multiple analysis. A typical example is shown below:



The following workflow results will show up in the list:

-- Results from measure events that are associated with a TQ Analyst spectral measurement specification that points to a classification method. See “Measure events” and “Spectral measurement specifications” in this chapter for more information. The measure event must appear before the measure event that is linked to this classify multiple specification and the associated TQ Analyst method must produce the various text strings listed on the classify multiple specification as the possible measurement results. See “Usage” below for more information.

-- Results from request events that are set up to produce a message-response type operator prompt that requests a method name or input from a bar code reader and allows a text response. See “Request events” and “Prompt specifications” in this chapter for more information. (The operator or bar code must be set up to select the correct method at run time. See “Text String Used For Comparison” below for details.)

Select the appropriate event result and then choose OK. After you choose OK, the event name and result type are listed in the text box as shown in the example below.



- **TQ Analyst Methods.** Use this table to specify the methods the associated measure event will use to classify the sample spectra (if “all methods” is selected for Classification Setting) or the available methods (if “matching method” is selected).

TQ Analyst Methods:

Method Name	Text Name	Comparison Type	Ignore Case

Add



- *Add.* Use this button to add methods to the list. The software displays the Add dialog box.

If Classify Against All Methods is selected for Classification Setting on the Classify Multiple specification, leave the Text String For Comparison and Comparison Type boxes blank in this dialog box.

**Add**

Path: C:\RESULT Data\Workflows\

TQ Analyst method file name: INCOMING MATERIALS.ONT

Analysis type: Discriminant analysis

Text string for comparison:

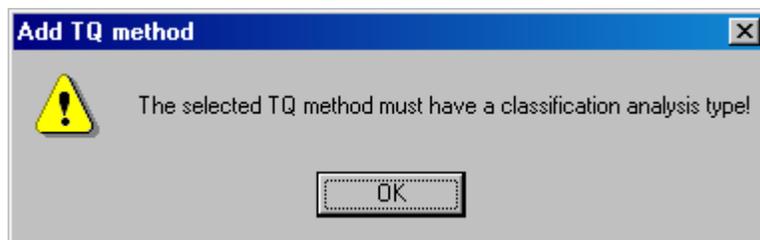
Comparison type: Equals

Ignore case

OK Cancel

Required Analysis Type: Classification

-- File Name. Use the File Name drop-down list box to select a TQ Analyst method. The list includes all the TQ Analyst methods that are stored in the default directory for workflows and methods in RESULT Integration. See “Configuring RESULT Integration Options” in the “RESULT Integration User Guide” for information about specifying this path. Only TQ Analyst classification methods will be accepted. If you select a quantitative or spectral measurement method, the software displays the following error message.



-- Analysis Type. This readout shows the analysis type setting for the selected method.

Text String For Comparison. If Classify Against Matching Method is selected for Classification Setting on the Classify Multiple specification, use this box to enter a text string that will be used to identify this method at run time. If the workflow uses a request event to select the matching method, the operator or bar code must include the text shown here to select this method at run time. If the workflow uses another measure event to select the matching method, that event result must include this text string to select this method at run time. This feature allows you to set up a tiered classification where the first measure event classifies the sample spectrum against classes that are dissimilar and the second measure event classifies the sample spectrum against one class that is highly similar. See “Usage” below for more information.

-- Comparison Type. If Classify Against Matching Method is selected for Classification Setting on the Classify Multiple specification, use this drop-down list box to specify the criteria for determining a match. The following options are available.

- Equals, which requires that the operator response, bar code or measure event result matches the text string exactly.
- Contains, which requires that the text string is included in the operator response, bar code, or measure event result.
- Starts With, which requires that the operator response, bar code, or measure event result starts with this text string.

Ignore Case. If Classify Against Matching Method is selected for Classification Setting on the Classify Multiple specification, use this feature to specify whether the match should be exact, including the letter case, or whether case should be ignored.

**Required Analysis Type.** This readout shows the type of method that can be selected. The first time this dialog box is displayed, the readout shows that a “Classification” method must be selected. After you have selected the first classification method, the readout shows the measurement type such as Discriminant Analysis or Search Standards for that method. Methods added to the list must have the same measurement type as the first method in the list or the software will display an error message.

After you add each method, the list shows the selection criteria. When you are finished selecting methods, the list should look something like the following:

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete Selected Row, or select the row and press Delete on the keyboard. To edit a property for a method, double-click the corresponding cell in the table.

To change the order in which the TQ Analyst methods will be searched, drag the corresponding row to a new location in the table. To sort a column of entries in numeric or alphabetic order, right-click the column heading to display a shortcut menu and then choose Sort Ascending or Sort Descending.

TQ Analyst Methods:

Method Name	Text Name	Comparison Type	Ignore Case
INCOMING MATERIALS.QNT	Canola	Equals	Yes
ALG_DA.qnt	Soy	Equals	Yes

Add

- **Selected Classification Type.** The features in this group are all readouts. They show the analysis type and attributes for all the methods the classify multiple specification is set up to measure.

Selected Classification Type

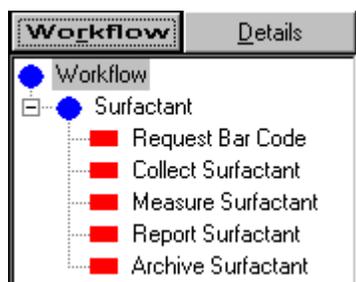
Analysis Type: Discriminant analysis

Attributes

Best class match

**Usage:** A classify multiple specification must be linked to a measure event in a workflow. The classify multiple specification can be configured to classify the sample spectra using all selected methods or only the method specified by the operator, a bar code, or another measure event at run time. Specific examples showing the use of a request event and a measure event to select the method used in a classify multiple experiment are provided below.

**Example 1:** Request event used to specify the method for a classify multiple experiment.



### **Request event used to specify method**

In this experiment, the workflow prompts the operator to scan a bar code that automatically selects an appropriate method to classify the sample material. The experiment uses multiple TQ Analyst methods; each method contains a group of similar spectra that are all in one class.

Follow the guidelines below to set up in a workflow to use a request event to specify the method for a classify multiple experiment.

Step 1: Add a Request event to the workflow. Make sure the Request event appears before the measure event in the workflow.

Step 2: Link the Request event to a Request specification. Set up the Request specification to request the text name for the method (as a text string) or to request input from a bar code reader. Here is an example:

Request Specification

New Request

Request these items:

Operator Prompt	Data Type	Required
Please scan the bar code for the next sample	String	Yes

Add

Barcode Options

Use field delimiter

Delimiter (in quotes): ""

Enter key handling

Enter same as press Accept

Enter advances field

Step 3: Add a Measure event to the workflow. Make sure the Measure event appears after the Request event in the workflow.

Step 4: Link the Measure event to a Classify Multiple measurement specification. In the Classify Multiple specification, set Classification Settings to Classify Against Matching Method and set Item to the Request event result as shown below:

Classification Settings

Classify against all methods

Classify against matching method

Item: Bar code.Please scan the bar code for the next sample

Select

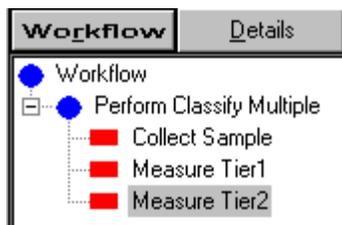
Add the TQ Analyst classification methods to the Classify Multiple specification. For each classification method, specify Text Name, Comparison Type and Ignore Case. Here is an example:

TQ Analyst Methods:

Method Name	Text Name	Comparison Type	Ignore Case
ALG_DA.qnt	Method A	Equals	Yes

Add

**Example 2:** Measure event used to specify the method for a classify multiple experiment.



### Measure event used to specify method

This experiment demonstrates how to set up a tiered classification analysis with a decision point. The experiment uses two measure events to differentiate a wide range of materials without operator decision making or input. The first (tier 1) measure event uses a single classification method to match each sample to a particular class. The second (tier 2) measure event is used to match the sample to a specific material within the selected class.

The tier 1 measure event is linked to a TQ Analyst measurement specification that points to a TQ Analyst classification method. The method typically contains multiple classes of materials that are very different.

The tier 2 measure event is linked to a classify multiple specification that points to multiple TQ Analyst classification methods. Each method typically contains a group of similar spectra that are all in one class. The class names used in the tier 1 measure event should match the method text names listed in the classify multiple specification.

Follow the guidelines below to set up in a workflow to use a measure event to specify the method for a classify multiple experiment.

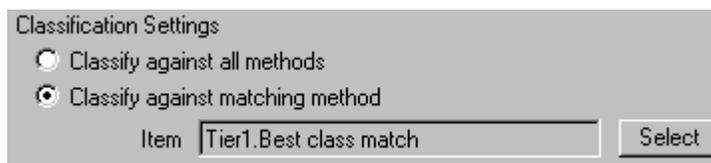
**Step 1:** Add the Tier 1 measure event to the workflow. Make sure the tier 1 measure event appears before the tier 2 measure event in the workflow.

**Step 2:** Link the Tier 1 Measure event to a TQ Analyst measurement specification.

**Step 3:** Link the measurement specification to a TQ Analyst classification method that has the same number of classes as the number of methods you plan to add to the Classify Multiple specification (see below). The class names should match the method text names you plan to use in the Classify Multiple specification (see below).

**Step 4:** Add the Tier 2 measure event to the workflow. Make sure the Tier 2 Measure event appears after the Tier 1 measure event in the workflow.

**Step 5:** Link the Tier 2 Measure event to a Classify Multiple measurement specification. In the Classify Multiple specification, set Classification Settings to Classify Against Matching Method and set Item to the Measure event result (Measurement: Tier 1: Best class match)



**Step 6:** Add the TQ Analyst classification methods to the Classify Multiple specification. For each classification method, specify Text Name, Comparison Type and Ignore Case.

## Composite Measurement specifications

A composite measurement specification can be used to produce calculated measurement results that are based on other workflow results or a combination of those results. Any workflow event that produces a numeric value can be used to define a composite component.

For each composite component, you may add, subtract, multiply, or divide numeric values provided by the workflow or perform these operations with a constant. Special functions are also available to calculate the sum, average or standard deviation of two or more workflow results or to determine the maximum or minimum values or range. You can also set up a composite component to report the total number of values used in a calculation (count). You can use all the component values in a composite measurement or specific values. The composite measurement specification can be linked to measure events and compare events in a workflow.

**Associated events:** Measure event, Compare event

**Associated specifications:** none

**Related events:** Collect event, Report event, Store event, Report to OPC event

**Related specifications:** Table Item specification, Summary Item specification

**Parameters:** The illustration below shows the parameters for the composite measurement specification. These parameters appear in the display area of RESULT Integration when a composite measurement specification is selected in a workflow.

Composite Measurement Specification

ethanol Composite Measurement

Formula Elements

Event Name	Component Name	Data Type	Label

Add

Decimal separator: .

Item separator: .

Operators:

+ Add

Functions:

AVG(A,B,...) Average of arguments

Compute these composite measurements:

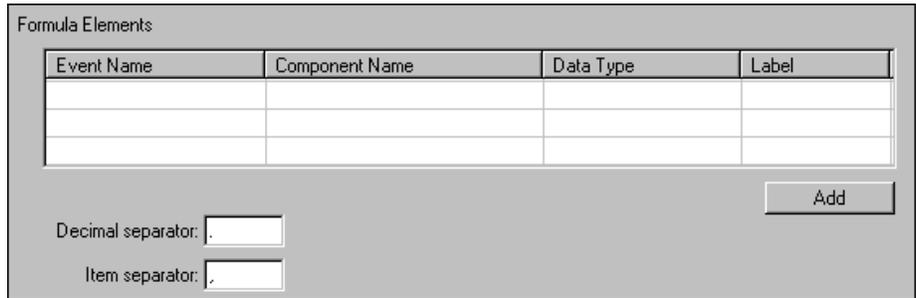
Composite Name	Abbreviation	Algebraic Formula	Unit

### Composite measurement specification parameters

The composite measurement specification parameters allow you to select the workflow results that will be used to define the component measurements and a mathematical equation that will be used to compute each composite measurement result. The following sections explain the composite measurement specification parameters in detail. The parameters are explained in the order in which they appear in the software.

## Formula Elements

Use the features in this group to specify the terms used in your equations for computing composite measurements including the workflow results and the designated characters for separating decimals and terms.



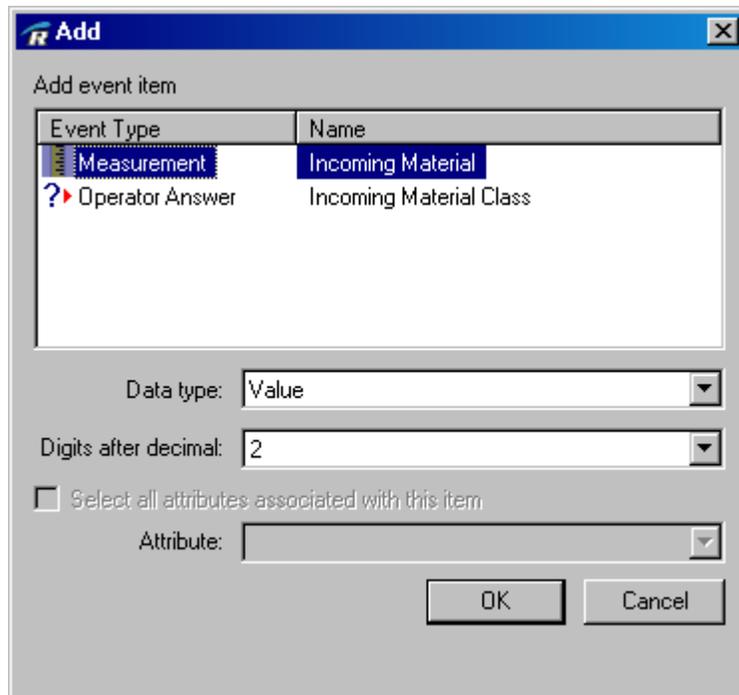
Event Name	Component Name	Data Type	Label

Decimal separator:

Item separator:

Add

- **Add.** Choose this button to add a workflow result to the table. (You can also add a row by right clicking the table to display a shortcut menu and then choosing Add). The following dialog box is displayed.



Event Type	Name
Measurement	Incoming Material
? Operator Answer	Incoming Material Class

Data type: Value

Digits after decimal: 2

Select all attributes associated with this item

Attribute:

OK Cancel

The list shows all the workflow events that produce numeric values.

**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a numeric result or all of those events have already been added to the composite specification. See the Usage heading for this Composite measurement specification for a list of events that can produce numeric results. ▲

Select a workflow event in the list. Make sure the results you select are produced by events that appear before this Composite Measurement Specification and it's associated Measure or Compare event in the workflow.

After you select a result, the following parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Examples are provided below.

- *Data Type.* Use this list box to select a result produced by the selected event such as a concentration or uncertainty value. The number and type of results produced depends on the event and, for measure events, the TQ Analyst or other method used for the measurement.
- *Digits After Decimal.* This box is available in the software only when the selected Data Type (see above) produces a numeric result. Use the box to select the number of digits the software will include after the decimal point in the numeric result. You can include up to six decimal places. The software rounds the number and retains only the specified decimal places.
- *Attribute.* Use this list box to select a specific component or other measured attribute or value for the selected data type and event. The number and type of items in the attribute drop-down list depend on the event and, for measure events, the TQ Analyst or other analytical method used for the measurement. For example, a measure event configured for spectral measurements could include the following items in the Attributes drop-down list.



- *Select All Attributes Associated With This Item.* Select this option if you want to include all the measured components or other attributes or values for the selected data type and event.

When you are finished selecting a workflow result, choose OK. The selected result is added to the table of equation elements and assigned a label. The labels are letters or combinations of letters from the English alphabet. Items 1 through 26 are given the labels A through Z. Items 27 through 52 will be BA through BZ. Items 53 through 78 will be CA through CZ and so on.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete, or select the row and press Delete on the keyboard. Use Export To Text File to write the formula elements displayed in the table to a text file with a file name and path you specify.

Event Name	Component Name	Data Type	Label
ethanol	Concentration	% Ethanol	A
ethanol	Concentration	% Ethanol	B

Decimal separator: .

Item separator: .

Add

Repeat these steps for each workflow event that will generate results you want to use in your equations for composite components.

- **Decimal Separator.** Use this entry box to specify the character that will be used to indicate the decimal point in any floating point numbers used in the equations for composite measurements (normally set to a period “.” (default) or comma “,”).

**Note** The decimal separator specified in a Composite Measurement specification is independent of the decimal separator specified in the Number feature of the Regional And Language Options dialog box in the Windows Control Panel. See your Windows documentation for details about the features in the Regional And Language Options dialog box. ▲

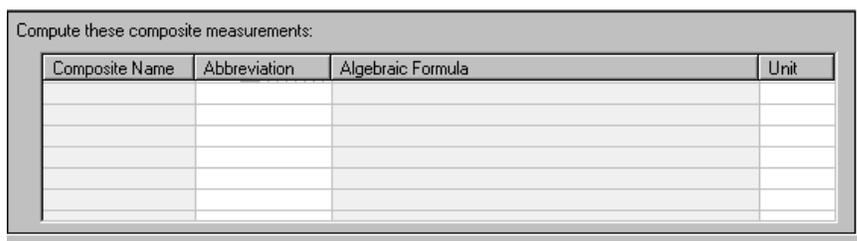
- **Item Separator.** Use this entry box to specify the character that will be used to indicate the end of one term and the start of another in the equations for composite measurements (normally set to a comma “,” (default) or semicolon “;”). The following examples show the use of an item separator to calculate the sum or average of two components using one of the special functions (see below):

SUM(A,B)  
AVG(BA,A)

**Note** Don't use the same character for the Decimal Separator and the Item Separator in a composite measurement specification. ▲

- **Compute These Composite Measurements.** Use this table to specify the algebraic formula used to compute each composite and the composite name and unit. The table is interactive and easy to work with.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete Selected Row, or select the row and press Delete on the keyboard. Use Export To Text File to write the formula elements displayed in the table to a text file with a file name and path you specify.



Composite Name	Abbreviation	Algebraic Formula	Unit

To add a row to the table, right click an empty row to display a shortcut menu and then choose Add Row.

The columns in the table are described below. To edit a cell in a specific row and column, double-click the cell.

- *Composite Name.* Enter a descriptive name for the component for identification purposes. If you add the composite result to a table item specification for a report event, this name will appear as the attribute name in the Add Event Item dialog box and in the sample report (if attribute names are included).
- *Abbreviation.* Enter an abbreviated name for the component. If you add the composite result to a table item specification for a report event and select the Composite Abbreviation Name in the Data Type list, this name will appear as a data type in the sample report (if data type names are included).
- *Algebraic Formula.* Use this text box to enter an equation for the composite component. The following table defines the proper format for the basic operators available for computing composite measurements. The available operators are also listed in the Operator drop down list box in the software.

Operator	Symbol	Examples
Add	+	A+B or BA+B
Subtract	-	A-B or BA-B
Multiply	*	A*B or B*BA
Divide	/	A/B or B/BA

**Note** Except for the Item Separator, which is used to define terms, do not use a space or any other character to separate other elements in the equation. You may use parentheses to define portions of the equation and the calculation order. For example, (A-B)/(C+D) or ((2.4\*A+3.7\*B)/C)+4/D. The software will accept an unlimited number of parentheses in an equation. ▲

RESULT also supports the following types of special functions for multiple components. If you don't specify the components, the software applies the function to all the components listed on the composite measurement specification. The available functions are also listed in the Function drop down list box in the software.

Function	Symbol	Examples*
Report the average	AVG	AVG or AVG(BA,A)
Report the sum	SUM	SUM or SUM(A,BA)
Report the standard deviation	STD	STD or STD(A,B,C)
Report the minimum	MIN	MIN or MIN(BA,BC,BD)
Report the maximum	MAX	MAX or MAX(BA,BC,BD)
Report the minimum of the absolute value	AMIN	AMIN or AMIN(BA,BC,BD)
Report the maximum of the absolute value	AMAX	AMAX or AMAX(BA,BC,BD)
Report the range (max-min)	RANGE	RANGE or RANGE(A,Z)
Report the number of values	COUNT	COUNT or COUNT(A,B,C)

\* Must specify two or more components or no components (will be applied to all components). When specifying components, use component labels and item separators and enclose in parentheses.

RESULT also supports the special functions for individual components described in the table below. These functions can be applied to individual components only; the component label must appear in parentheses as shown in the examples.

Function	Symbol	Examples*
Report the absolute value of the component value A	ABS	ABS(A)
Report e raised to the power of component value A	EXP	EXP(A)
Report e raised to the negative power of component value A	EXPNEG	EXPNEG(A)
Report 10 raised to the power of component value A	TEN	TEN(A)
Report 10 raised to the negative power of component value A	TENNEG	TENNEG(A)
Report the natural logarithm of component value A	LN	LN(A)
Report the negative of the natural logarithm of component value A	NEGLN	NEGLN(A)
Report the base 10 logarithm of component value A	LOG	LOG(A)
Report the negative of the base 10 logarithm of component value A	NEGLOG	NEGLOG(A)
Report the square root of component value A	SQRT	SQRT(A)
Report the inverse of the square root of component value A	INVSQRT	INVSQRT(A)

---

\* Must specify single component; component label must appear in parentheses

---

- *Unit.* Use this entry box to specify a unit, if applicable, for the composite component. If the composite does not have a defined unit, then leave this box blank.

**Usage:** A composite measurement specification may be linked to the following types of workflow events:

- **Measure event**, which measures spectra generated by a workflow using a calibrated analytical method. Depending on the method, measure events may produce numerical concentration values (quantitative methods), library index values and match values (classification methods), or spectral measurements, such as a peak height or area (spectral measurement methods).
- **Compare event**, which can be used to compare a series of spectra and their measured values against expected values to produce correlation coefficients, root mean square error of prediction (RMSEP) values, and slope and y-intercept values for those measurements.

A composite measurement specification can include the result of any workflow event that produces a number including:

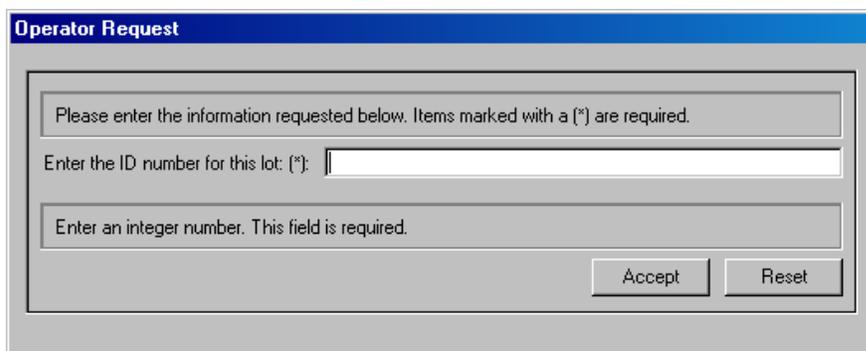
- **Measure event**, which, depending on its associated method, can generate numerical concentration values, match values, class names, or spectral measurements such as a peak height or area.
- **Calculate event**, which produces statistical values from measurements that are part of a loop, including minimum, maximum, average, range, standard deviation, percent standard deviation, sum, and count.
- **Compare event**, which uses the actual and expected values for a series of measurements to produce correlation coefficient, root mean square error of prediction (RMSEP), and slope and y-intercept values for those measurements.
- **Request event**, which may produce up to ten numerical or yes/no responses from the operator in response to a message-response request.
- **Read From I/O event**, which passes values read from devices or signals to a workflow.

A composite measurement specification may also include the result of another composite measurement.

## General specifications

The general specifications group provides two types of specifications for creating dialog boxes displayed to the operator running your workflow, including request specifications and prompt specifications. This group also includes specifications for configuring hardware devices such as an autosampler. The general specifications are described briefly below.

- **Request specifications**, which define a dialog box requesting information from the operator.



### Operator request dialog box

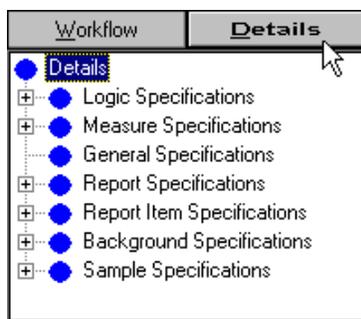
Request specifications may be linked to request events in a workflow.

- **Prompt specifications**, which define a message box providing information to the operator. The operator must acknowledge the prompt before the workflow can continue. Prompt specifications may be linked to collect events, check events, and StartStop events in a workflow. Here is an example of an operator prompt for a collect event:
- **Autosampler specifications**, which define the size of the carousels and specify whether the reference position is reserved for background measurements. Autosampler specifications may be linked to Position Autosampler events and autosampler sample specifications in a workflow.

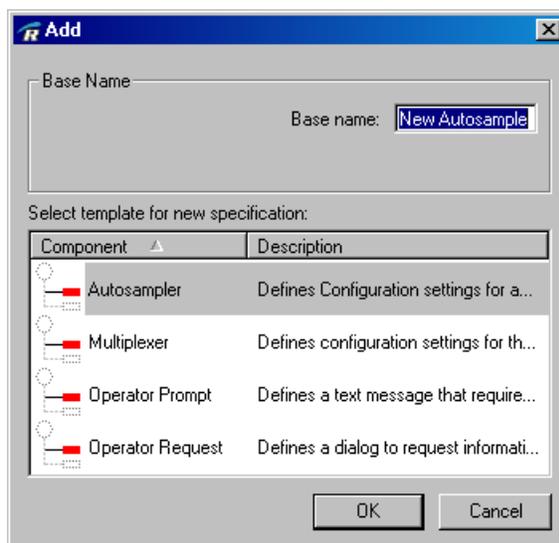
## Adding a general specification to a workflow

To add a general specification to the open workflow:

1. **Select the Details tab, select the General Specifications group and then choose the Add button on the RESULT Integration toolbar.**



The software displays a dialog box listing the general specifications available for your system.



**2. Select a specification, enter a base name for the new specification and choose OK.**

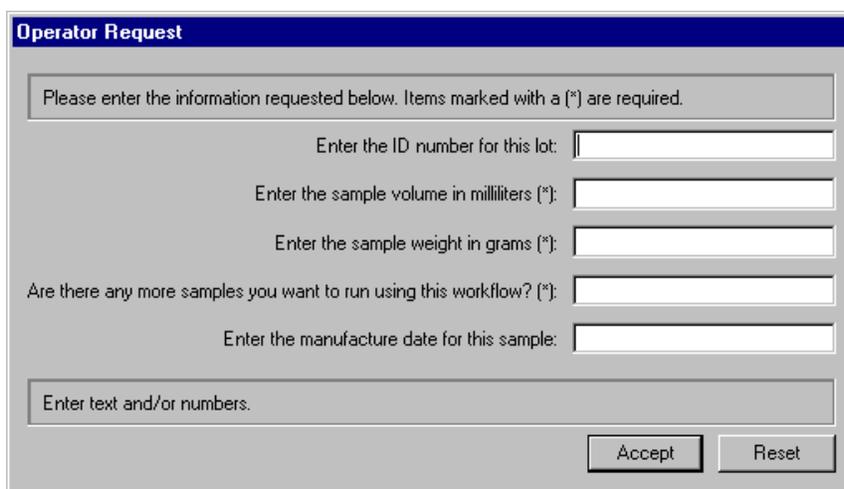
The new specification appears in the display area of the RESULT Integration main window.

Read the next two sections to learn about the options available for setting up request specifications, prompt specifications and autosampler specifications in a workflow. For information about linking a specification to a workflow event, see “Linking a specification to a workflow event” in “Chapter 2 Creating and Editing Workflows” of the “RESULT Integration User Guide.”

## Request specifications

A request specification defines a dialog box requesting information from the operator or input device such as a bar code reader. For each request included in the dialog box, you must specify the message to the operator, the format for the response, and whether the operator is required to enter the requested information before the workflow can continue.

Each request can be set up to request input from the operator. You can include multiple requests in the same dialog box (maximum of ten), as shown in the example below:



**Operator Request**

Please enter the information requested below. Items marked with a (\*) are required.

Enter the ID number for this lot:

Enter the sample volume in milliliters (\*):

Enter the sample weight in grams (\*):

Are there any more samples you want to run using this workflow? (\*):

Enter the manufacture date for this sample:

Enter text and/or numbers.

Accept Reset

### Operator request dialog box

The status box at the bottom of the dialog box indicates the kind of information that must be supplied to fulfill the request at the current cursor location. For example, the request for a lot ID shown in the example above requires a text and/or numeric response.

An asterisk is displayed at the end of the prompt message if a response is required before the workflow can continue. The dialog box shown above contains several examples of request entries that require a response.

When a workflow executes a request event, the instrument flashes its green LED light, indicating that the operator must respond to the request before continuing.

Request specifications may only be linked to a Request event in a workflow.

**Associated events:** Request event

**Associated specifications:** None

**Related events:** None

**Related specifications:** Prompt specification

**Parameters:** The illustration below shows the parameters for the request specification. These parameters appear in the display area of RESULT Integration when a request specification is selected in a workflow.

Request Specification

New Request

Request these items:

Operator Prompt	Data Type	Required

Add

Barcode Options

Use field delimiter

Delimiter (in quotes):

Enter key handling

Enter same as press Accept

Enter advances field

### Request specification parameters

The request specification parameters define the messages that appear in a message-response request dialog box. For each request included in the dialog box, you must specify the message to the operator, the format for the response, and whether the operator is required to enter the requested information before the workflow can continue.

The following sections explain the request specification parameters in detail. The parameters are explained in the order in which they appear in the software.

## Request These Items

Use this box and its associated buttons to specify the requests to include in message-response dialog box and the sequence of those requests.

Request these items:

Operator Prompt	Data Type	Required

Add



- **Add.** Choose this button to add a request to the dialog box. The Add/Edit Operator Request dialog box appears, as shown below.

**Add/Edit Operator Request**

Enter text for operator prompt:

Select data type:  
String

Operator must respond to this prompt

OK Cancel

- *Enter Text For Operator Prompt.* Type the message to request the desired information from the operator.

Enter text for operator prompt:

- *Select Data Type.* Select a format for the requested response.

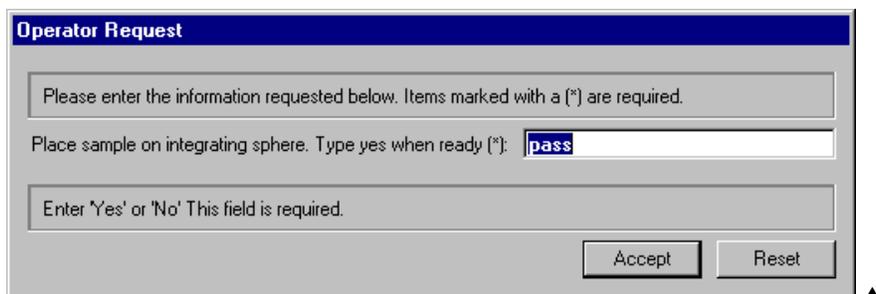
Select data type:  
String

- String
- Integer
- Floating point number
- Yes / No response
- Date

The options are described below.

- String, which allows text and/or numeric entries. The String option is commonly used when requesting input from a bar code reader. However, the correct data type setting will depend on the information embedded in the bar code.
- Integer, which requires a numerical entry but allows only integer values (whole numbers, such as 1, 2, 3, etc.). If the operator enters a fractional value, such as 5.4, the software rounds it to the nearest integer.
- Floating point number, which requires a numerical entry and allows any number, including decimal fractions.
- Yes/no response, which requires a text entry containing “Yes,” “No,” “Y,” or “N.” The characters can be upper or lower case.
- Date, which requires a typed calendar date. Acceptable date formats are based on regional settings in the Windows control panel. Most typical date formats are accepted.

**Note** If the operator makes an incorrect entry, for example, by typing something other than “yes” or “no” in an entry box that requires a yes or no response, the dialog box stays open and the incorrect entry is highlighted in bold, as shown below.



- *Operator Must Respond To This Prompt.* Select this option if you want to require the operator to respond to this request before the workflow can continue. If this option is selected and the operator tries to close the Operator Request dialog box without entering an appropriate response, the dialog box will not close and the word “required” will appear in bold type in the corresponding entry box, as shown below.

Enter the sample volume in milliliters (\*): **required**

The operator must replace the “required” response with an appropriate entry before choosing Accept and closing the dialog box.

If the Operator Must Respond To This Prompt option is cleared, the operator can close the Operator Request dialog box with this entry box filled or empty.

When you are finished specifying the request, choose OK. The new request entry is added to the list of items to include in the Operator Request dialog box, as shown in the example below.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete Selected Row, or select the row and press Delete on the keyboard. Use Export To Text File to write the information displayed in the table to a text file with a file name and path you specify. To edit a property for a request, double-click the corresponding cell in the table. To change the order in which specific requests are placed in the prompt, drag the corresponding row to a new location in the table. To sort a column of entries in numeric or alphabetic order, right-click the column heading to display a shortcut menu and then choose Sort Ascending or Sort Descending.

Operator Prompt	Data Type	Required
Are there any more samples in this lot?	Yes / No response	Yes

Add

Repeat these steps for each additional request. All the requests in a request specification are placed in one operator prompt.

### Bar code Options

If the operator will use a bar code reader to enter the information in the request dialog box, use the parameters in this group to define the bar code input and handling.

Barcode Options

Use field delimiter

Delimiter (in quotes):

Enter key handling

Enter same as press Accept

Enter advances field

- **Use Field Delimiter.** Select this option if the request specification is set up to request input from a bar code reader and the bar codes have multiple fields (for example, a single bar code may include the sample name, sample number, lot number or other identifying information). Then use the Delimiter box to specify the character that the bar code uses to separate the information in the bar code. When specifying the field delimiter, be sure to enclose the delimiter character in quotes. For example, if the field delimiter is a comma or a space, then enter “,” or “ ” in the Delimiter box.

If Use Field Delimiter is cleared, then the software will receive the entire bar code as the response to the first requested item in the request specification.

- **Enter Key Handling.** Use this feature to specify the operation of the Enter key in the bar code request dialog box by selecting one of the options below:
- **Enter Same As Press Accept.** Select this option if you want the software to interpret any Enter characters that may be included in a bar code as a carriage return. When the operator enters a bar code that contains an Enter character, the software reads the bar code and then closes the Request dialog box when it receives the Enter character. This option is useful when the request dialog box is set up to prompt only for the information contained in the bar code.
- **Enter Advances Field.** Select this option if you want the software to interpret any Enter characters that may be included in a bar code the same as pressing the Tab key on the keyboard. When the operator enters a bar code that contains an Enter character, the software reads the bar code and tabs to the next field in the request dialog box when it receives the Enter character. This option allows the operator to scan a bar code associated with each field in the request dialog box without having to use the mouse or keyboard to select the next field.

**Usage:** A request specification may be linked to the following workflow events:

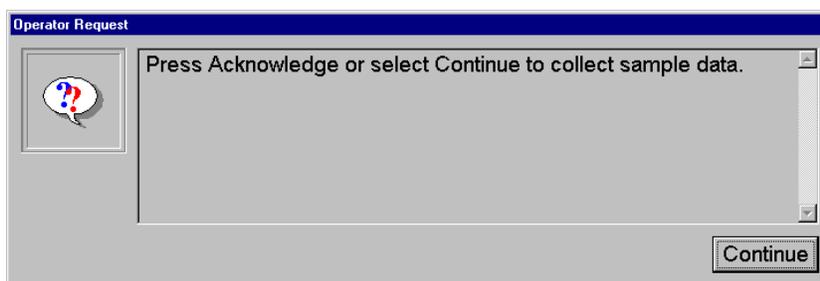
- **Request event**, which may produce up to ten numerical or yes/no answers from the operator in response to a message-response request.

**Note** You can use a request event to allow the operator to input a bar code and use the bar code to specify a classification method for the analysis. See Classify Multiple specifications in this section for details. ▲

## Prompt specifications

A prompt specification defines a dialog box providing information to the operator, including the message text and the button label. The operator must acknowledge the prompt before the workflow can continue.

You can set up the prompt so the operator can acknowledge it only by choosing the button displayed in the prompt, or you can allow the operator to acknowledge the prompt by choosing the button in the dialog box or by pressing the Acknowledge button on the instrument, as shown below.



### Operator prompt

Prompt specifications may be linked to collect events in a workflow to create operator prompts to initiate background and sample collection, and to check events to alert the operator when the workflow produces a “fail” result.

If you are defining a background or sample prompt for a collect event, the prompt can be set up to show the operator a preview of data collection. The preview allows the operator to verify that the spectrum contains no sample peaks or that it matches a previous background spectrum.

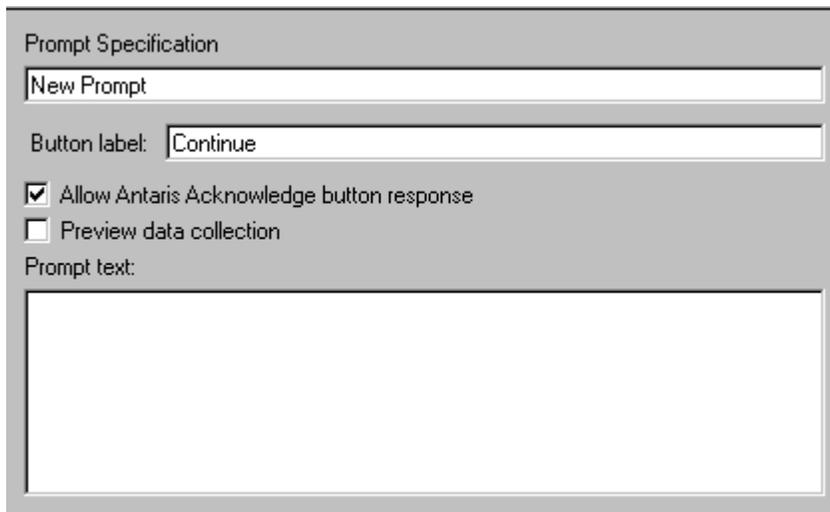
**Associated events:** Collect event, Check event, StartStop event

**Associated specifications:** None

**Related specifications:** Request specification

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the prompt specification. These parameters appear in the display area of RESULT Integration when a prompt specification is selected in a workflow.



The screenshot shows a dialog box titled "Prompt Specification". It contains the following elements:

- A text input field with the value "New Prompt".
- A "Button label:" label followed by a text input field containing "Continue".
- A checked checkbox labeled "Allow Antaris Acknowledge button response".
- An unchecked checkbox labeled "Preview data collection".
- A "Prompt text:" label followed by a large, empty text area.

### Prompt specification parameters

The prompt specification parameters define the message text and the button label for the operator prompt. The parameters also specify whether the prompt will include a preview of data collection and whether the operator can use the Acknowledge button on the instrument to acknowledge the prompt. The following sections explain the prompt specification parameters in detail. The parameters are explained in the order in which they appear in the software.

- **Button Label.** Use this box to enter a label for the button displayed in the operator prompt.

The label should indicate the intended action (to acknowledge that the operator read the message and is ready to continue with the workflow). The button appears in the lower right corner of the dialog box.

- **Allow Antaris Acknowledge Button Response.** Select this option if you want to allow the operator to acknowledge the prompt by pressing the Acknowledge button on the instrument.

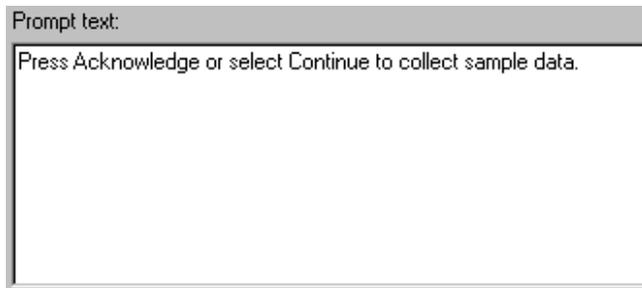
**Note** This feature is not available for the Antaris IGS analyzers. ▲

When this option is selected, the operator can choose whether to acknowledge the prompt from the instrument or from the software.

If the prompt was produced by a collect event, the green LED indicator on the instrument will be on steadily (not flashing). If the prompt was produced by a check event, the red LED will be on.

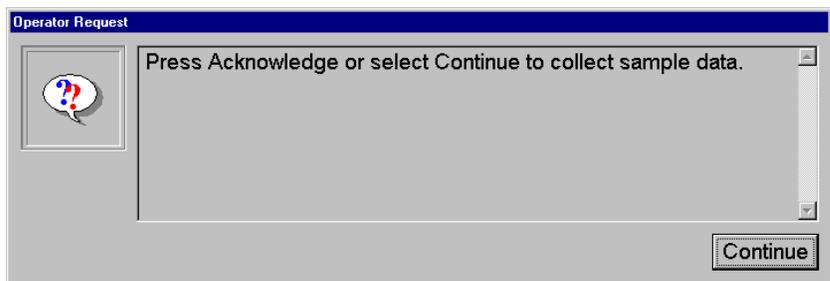
Clear this option if you want to require the operator to acknowledge the prompt only from the software (by choosing the button in the prompt). If the prompt was produced by a collect event, the green LED indicator on the instrument will flash. If the prompt was produced by a check event, the red LED will flash.

- **Prompt Text.** Use this box to enter a text message for the operator prompt. The following illustration shows an example prompt text to collect sample data.



A screenshot of a text input field. The label "Prompt text:" is at the top left. The text inside the field reads "Press Acknowledge or select Continue to collect sample data."

The message will appear in the center of the dialog box when it is displayed by the workflow, as shown in the example below.

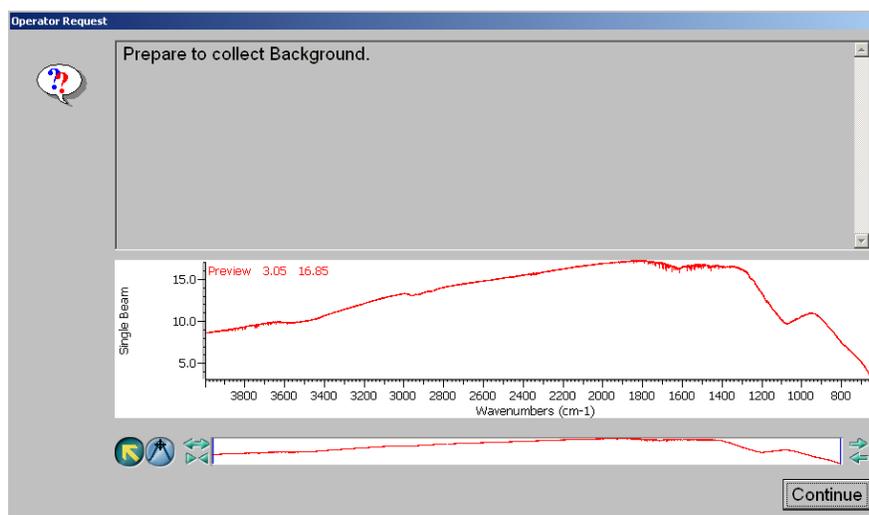


- **Preview Data Collection.** Select this feature if the prompt specification is linked to a collect event to initiate sample or background collection and you want the prompt to include a preview of data collection. See "Operator Prompts" in "Collect Events" for information about setting up prompts for sample and background collections in a workflow.

When Preview Data Collection is selected, the workflow displays the prompt at run time and begins collecting data. The dialog box is expanded to include a collection window, as shown in the example below. The sample data are displayed in the format specified in the workflow.

The workflow continues collecting (but not saving) the data until the operator chooses Continue in the prompt. After the operator chooses Continue, the workflow continues.

The background preview shows single scans of the background. If the workflow is designed to collect multiple background scans, the final background spectrum will be the average of all collected scans.



**Usage:** A prompt specification may be linked to the following workflow events:

- **Collect event**, which produces a spectrum.
- **Check event**, which tests the combined true/false result of the associated logical test specification and produces a pass/fail result in the workflow.
- **StartStop event**, which can be used to allow the operator to control when the workflow will start and/or stop implementing a group of events.

## Autosampler specifications

When the Autosampler RS or MultiPro Autosampler add-in option is installed, RESULT Integration includes the autosampler specification. The autosampler specification defines the maximum number of samples that fit in the autosampler carousels and specifies whether the reference position in each carousel is reserved for background measurements. You can specify the maximum number of samples when you set up the workflow, or configure the workflow to prompt the operator to enter the number of samples in each carousel at run time.

Autosampler specifications may be linked to Position Autosampler events and autosampler sample specifications in a workflow.

**Associated events:** Position Autosampler events

**Associated specifications:** Autosampler Tablet Transmission Module sample specification, Autosampler SoftGel Tablet Analyzer Module sample specification, Autosampler Integrating Sphere sample specification

**Related events:** None

**Related specifications:** Standard Tablet Analyzer background specifications, SoftGel Tablet Analyzer background specifications, Autosampler Integrating Sphere background specifications

**Parameters:** The illustration below shows the parameters for the autosampler specification. These parameters appear in the display area of RESULT Integration when an autosampler specification is selected in a workflow.

Autosampler Specification

New Autosample

Autosampler Carousels

Specify number of positions

Number of positions: 40

Prompt for number of positions:

Default value: 40

Prompt text: Enter the number of positions in the carousel:

Reference (zero) position reserved for background collections

### Autosampler specification parameters

The following sections explain the autosampler specification parameters in detail. The parameters are explained in the order in which they appear in the software.

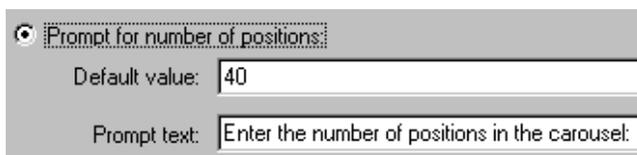
- **Autosampler Carousels.** Use this parameter to define whether the workflow or the operator will specify the number of positions in the autosampler carousels.
- *Specify Number Of Positions.* Select this option if you want to set up workflows that match a certain carousel type. Then enter the number of sampling positions in each carousel in the associated entry box as shown in the example below.



Specify number of positions  
Number of positions:

Workflows set up this way can accurately track sample position only when used with the specified carousel type.

- *Prompt For Number Of Positions.* Select this option if you want to allow the operator to specify the number of positions in the carousels at run time. Then enter a default value in the associated entry box and the text for the operator prompt in the Prompt Text box, as shown below.



Prompt for number of positions:  
Default value:   
Prompt text:

The workflow will display the prompt the first time it encounters this autosampler specification. Workflows set up this way can be used with any type of carousel.

- **Reference Position Reserved For Background Collections.** Use this check box to specify whether the reference (zero) position of each carousel will be reserved for background collections. Background collections that require the reference position include all transmission backgrounds and diffuse reflection backgrounds that require an external reference sample.



Reference (zero) position reserved for background collections

When this check box is selected, the software collects all background spectra from the reference position in the autosampler carousels.

Clear the check box if you are running diffuse reflection experiments only and using the internal gold reference for collecting backgrounds and you want to maximize the number of samples in each sample holder or carousel (you can use the reference position to analyze one additional sample).

**Usage:** An autosampler specification may be linked to the following workflow items:

- **Position autosampler event**, which instructs the workflow to rotate the specified autosampler to another position or to prompt the operator to change the autosampler carousel.
- **Autosampler tablet transmission module sample specification**, which defines transmission sample collection with the transmission detector for the standard tablet analyzer.
- **Autosampler SoftGel transmission module sample specification**, which defines transmission sample collection with the transmission detector for the softgel tablet analyzer.
- **Autosampler integrating sphere sample specification**, which defines diffuse reflection sample collection with the integrating sphere on the Antaris instrument.

## Report specifications

A report specification defines the title of a sample report, the sections in the report and the order those sections will appear when the report is displayed or printed. Each section has an associated report format specification, which defines the workflow results to include and the format. A report specification can only be linked to report events in workflows.

**Associated events:** Report event

**Associated specifications:** Heading item specification, Table Item specification, Summary Item specification, Memo Item specification, Spectrum Item specification, Sequence Heading Item specification, Sequence Summary Item Specification

**Related events:** None

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the report specification. These parameters appear in the display area of RESULT Integration when a report specification is selected in a workflow.

Report Specification

New Report

Report Format

Title of this report:

Items in this report:

Section Type	Section Name
--------------	--------------

New Details

Preview Report

Add

### Report specification parameters

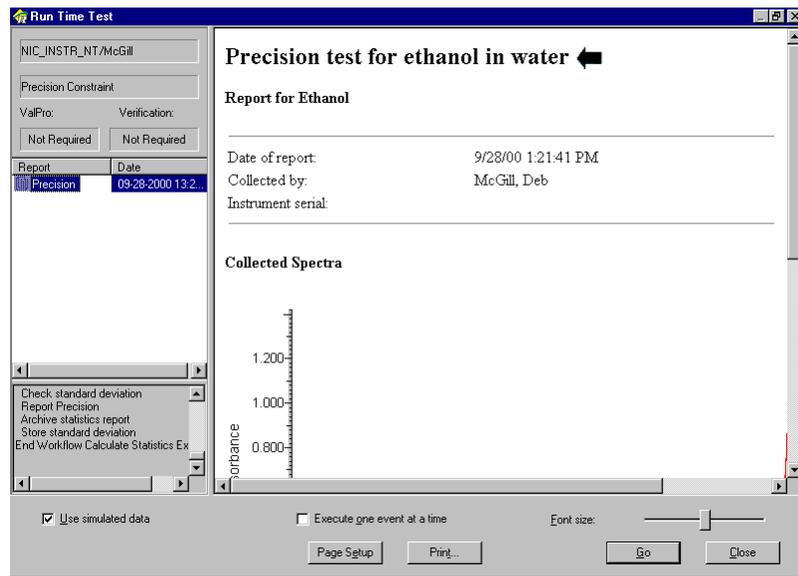
The report specification parameters define a title or heading for the entire report and specify the sections the report will include and the order those section will appear when the report is displayed or printed. The following sections explain the report specification parameters in detail. The parameters are explained in the order in which they appear in the software.

## Title Of This Report

Use this box to enter a title for your report.

Title of this report:

When you display the report, either by opening the report file or running the workflow, the title will appear at the top of the report, as shown below.



## Items In This Report

Use this box and its associated buttons to specify the sections to include in your report.

Items in this report:

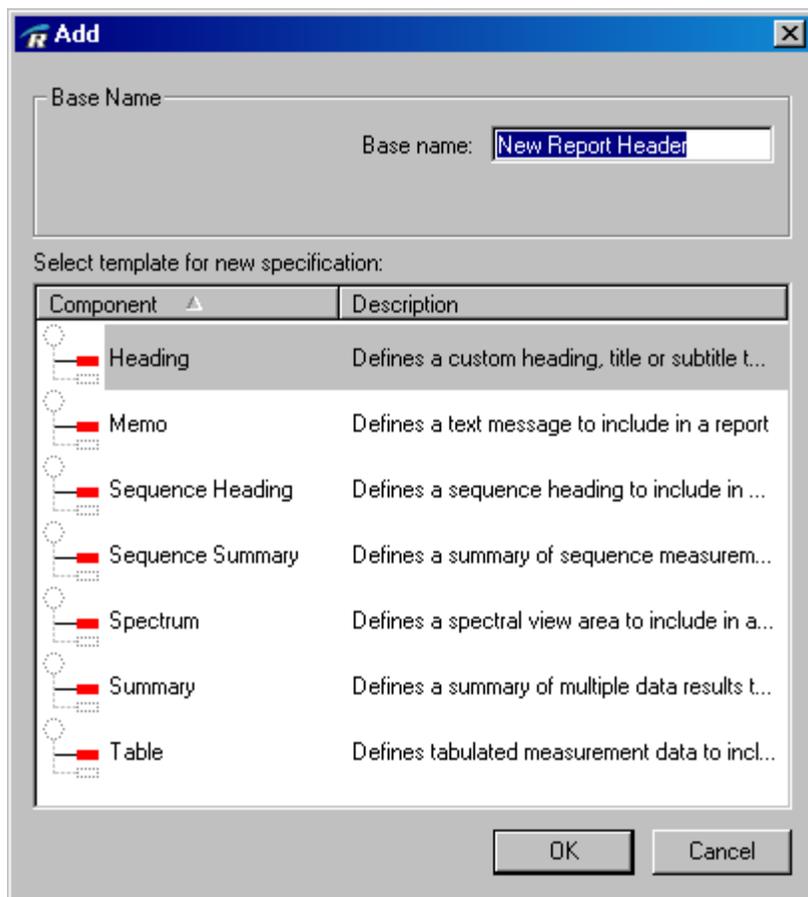
Section Type	Section Name	New	Details

Preview Report

Add



- **New.** Use this button to add a new section to a report. A dialog box appears listing the sections that can be added to a report.



Select a section, select Base Name For The New Item and enter a descriptive name for the new section and then choose OK. The format specification for the new section appears in the display area. Here is an example of a heading format specification:

Heading Item Specification

New heading

Heading Format

Title:

Border:

Items in this heading:

Label	Information to Print

Add Edit

### Heading Format Specification for defining a heading section in a report

Each report section has an associated format specification, called a report item specification. The report format specifications define the workflow results that are included in each section and how those results are formatted. See “Report format specifications” in this chapter for information about formatting headings and other sections in a sample report.

To return to the report specification, choose the Back button on the RESULT Integration toolbar. The new heading section is added to the list of items included in the report, as shown below.

Items in this report:

Section Type	Section Name	New	Details
Header Table	New heading		

The Section Name column shows the name of the report format specification associated with the new report section.

Repeat this step to add each new section to the report. You can include as many sections as you wish.



- **Details.** Use this button to display the format specification associated with a section in a report. For example, to display the format specification for the heading section, select the heading section and then choose Details.



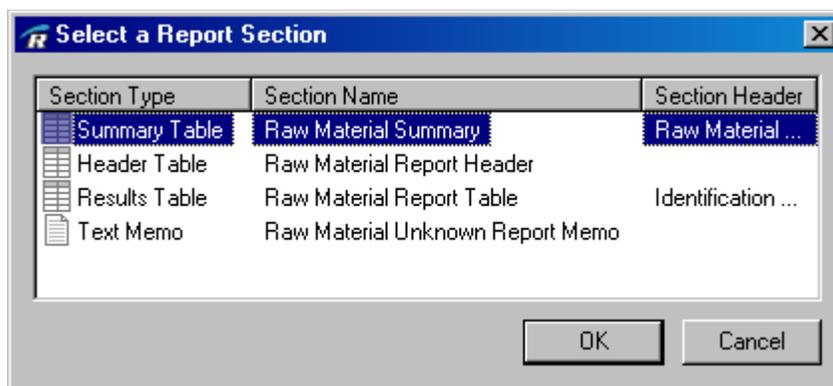
Use the Back button on the toolbar to return to the report specification.



- **Add.** Use this button to add a section from another report in the current workflow, or a report format specification that is not linked to a report. The software displays a dialog box listing all the report format specifications in the current workflow. Here is an example of the dialog box:

The column labeled Section Name shows the name of the corresponding report format specification.

The Section Heading column gives the title of the section, if a title was entered.

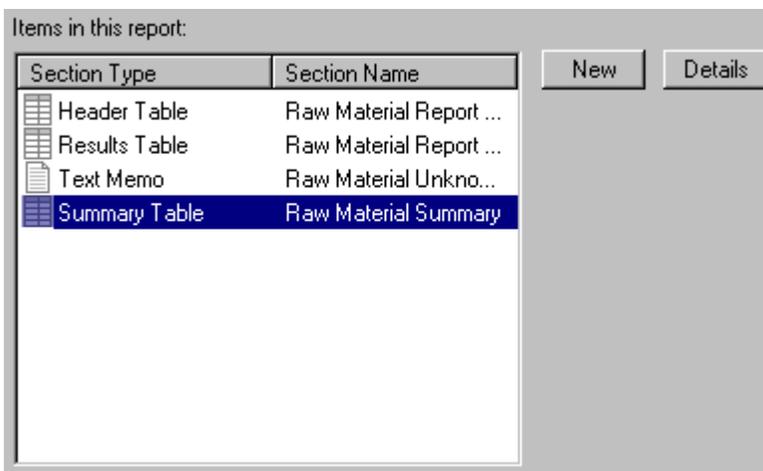


Select the section you want to add and then choose OK. The selected section will appear in the Items In This Report box on the report specification. Here is an example showing the Summary Table added to the report.

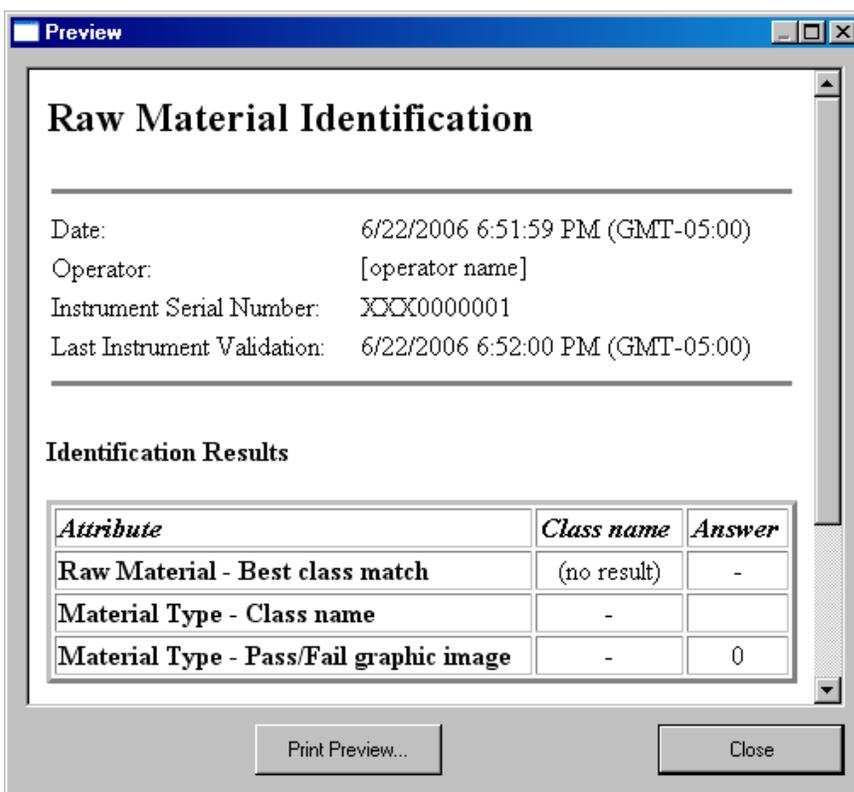
To delete a row in the table, right-click the row to display a shortcut menu and choose Delete, or select the row and press Delete on the keyboard.

Use Export To Text File in the shortcut menu to write the information displayed in the table to a text file with a file name and path you specify.

To change the order in which the sections will appear in the sample report, drag the corresponding row to a new location in the table.



- **Preview Report.** Use this button to see a preview of the sample report. The software displays the Preview window. Here is an example:



Use Print Preview to see how the report will look before you print it.

The preview shows the sections in the report in the specified order. Placeholders are used to represent the information that will be added when you run the workflow. When you are finished viewing the preview, choose Close to close the preview window.

**Usage:** A report specification may be linked to the following workflow event:

- **Report event**, which creates a sample report.

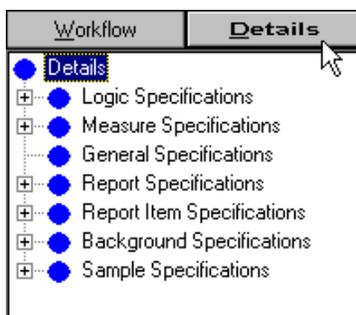
A report specification must be linked to at least one of the following report format specifications.

- **Heading format specification**, which defines a heading section in a sample report and the text, information, images, or other elements that will be included in the heading.
- **Spectrum format specification**, which defines a spectral plot section in a sample report and the workflow results (spectra) that will be included in the plot.
- **Table format specification**, which defines a table section in a sample report and the measurement results, spectral information, images, or other elements that will be included in the table.
- **Summary format specification**, which defines a table of summarized results in a sample report and the measurement results, summarized results, images, or other elements that will be included in the summary table.
- **Memo format specification**, which defines section that contains a line or lines of text in a sample report and the specific text that will be included.
- **Sequence heading format specification**, which adds a general summary of a sequence collection to a sample report. The sequence heading includes the sequence title, date and time the sequence collection started and ended and the file names of any archived data followed by details of each collection phase.
- **Sequence summary format specification**, which adds a summary of the sample component data produced by a run sequence event to a sample report. The summary can include the following for each selected component: count, minimum, maximum and average values, range, standard deviation and percent standard deviation, number of failures, and total area.

## Adding a report specification to a workflow

To add a report specification to the open workflow:

1. **Select the Details tab, select the Report Specifications group and then choose the Add button on the RESULT Integration toolbar.**



-- or --

select the Workflow tab, select the report event that requires a report specification and then choose the New button at the right of the Report Specification drop-down list box.



The new specification appears in the display area of the RESULT Integration main window.

2. **If you added the report specification from the Details tab, link the new specification to a report event.**

See “Linking a specification to a workflow event” in “Chapter 2 Creating and Editing Workflows” of the “RESULT Integration User Guide” for instructions.

## Report format specifications

A report format specification defines a section in a sample report. RESULT provides seven kinds of report format specifications for selecting and formatting data in a sample report, including:

- **Heading format specification**, which defines a heading section in a sample report and the text, information, images, or other elements in the heading. Heading format specifications are typically used to present information about the operator, the instrument, and the analysis at the top of a sample report. Here is an example:

### ➡ Operator Information

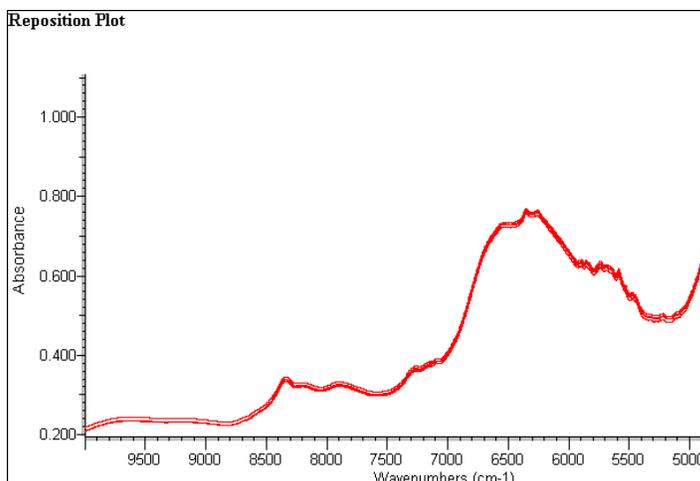
Operator:	Integrator
Date:	9/26/00 1:22:15 PM
Company Name:	Company A

- **Memo format specification**, which defines a section that contains a line or lines of text in a sample report and the specific text that will be included. You can use a memo format specification to add comments, descriptions, or other information to your report. The following example shows a memo section containing information about the workflow used to run the data.

### Workflow

Repeatability Verification

- **Spectrum format specification**, which defines a spectral plot section in a sample report and the workflow results (spectra) that will be presented in the plot. The plot can include one spectrum from each collection event, multiple spectra from a collect event that occurs in a repeat or perform-while loop, or multiple spectra from multiple collection events. The following example shows a plot section that includes multiple spectra produced by a collect event that occurs in a loop.



- Table format specification**, which defines a table section in a sample report and the workflow results or other information presented in the table. You can add any type of numerical or other result to a table, including a numerical result from a measurement, comparison, or calculation event, a pass or fail result from a check event, the pass (✔) or fail (✘) image, and an operator response from a request event. Here is an example of a simple table showing the measurement result from a quantitative analysis of ethanol:

<i>Attribute</i>	<i>% Ethanol - Std Deviation</i>	<i>Pass/Fail result</i>	<i>Pass/Fail graphic image</i>
<i>Answer</i>	0.0703	PASS	

- Summary format specification**, which defines a table of summarized results (minimum, maximum, average, etc.) in a sample report and the workflow results presented in the summary table. You can use a summary format specification to produce a useful summary of results from a variety of operations. A summary format specification works well for organizing data produced by events that are positioned in a repeat or perform-while loop. The summary table shown below presents measurement and statistical data from an experiment designed to demonstrate whether the operator's technique positioning the sample has a significant impact on the analytical results.

<i>Data Type</i>	<i>Reposition Maximum height [milli-A.U.]</i>	<i>Reposition Average Height [milli-A.U.]</i>
<i>Value (1)</i>	759.47	452.88
<i>Value (2)</i>	756.51	454.38
<i>Value (3)</i>	785.84	469.49
<i>Value (4)</i>	753.59	448.30
<i>Value (5)</i>	750.81	447.21
<i>Minimum</i>	750.81	447.21
<i>Maximum</i>	785.84	469.49
<i>Range</i>	35.04	22.28
<i>Sum</i>	3,806.22	2,272.27
<i>Average</i>	761.24	454.45
<i>Standard Deviation</i>	14.13	8.93
<i>% Standard Deviation</i>	1.86	1.96

- **Sequence heading format specification**, which adds a general summary of a sequence collection to a sample report. The sequence heading includes the sequence title, date and time the sequence collection started and ended and the file names of any archived data followed by details of each collection phase.

<b>Run Sequence title</b>	collection
<b>Run Sequence start time</b>	6/21/2004 8:33:31 AM (GMT-05:00)
<b>Run Sequence end time</b>	6/21/2004 8:33:55 AM (GMT-05:00)
<b>Archived base name</b>	No result files archived
<b>Run Sequence aborted</b>	False

<b>Collect Sequence title</b>	Sample
<b>Collect Sequence start</b>	6/21/2004 8:33:31 AM (GMT-05:00)
<b>Total collection time (seconds)</b>	20.029
<b>Number of spectra collected</b>	11
<b>Number of Fail results in Collect Sequence</b>	0
<b>Number of Pass results in Collect Sequence</b>	11
<b>Number of spectra archived</b>	0
<b>Requested temperature</b>	165
<b>Requested pressure</b>	650

- **Sequence summary format specification**, which adds a summary of the sample component data produced by a run sequence event to a sample report.

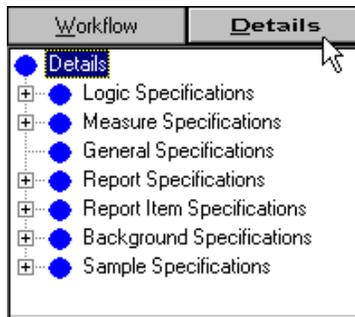
<i>Data type</i>	<i>Sample Methane [ppm]</i>	<i>Sample Carbon monoxide high [ppm]</i>	<i>Sample Carbon dioxide [ppm]</i>	<i>Sample Nitric oxide [ppm]</i>	<i>Sample Nitrogen dioxide [ppm]</i>	<i>Sample Nitrous oxide [ppm]</i>	<i>Sample Ethylene [ppm]</i>
<i>Count</i>	12	12	12	12	12	12	12
<i>Minimum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Maximum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Range</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>Average</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Standard deviation</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>% Standard deviation</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>Total area</i>	0.00	1,010.24	-1,101.86	333.87	34.05	28.01	182.86
<i>Fail results</i>	0	0	0	0	0	0	0

Report format specifications may only be linked to report specifications in a workflow.

## Adding a report format specification to a workflow

To add a report format specification to the open workflow:

1. **Select the Details tab, select the Report Item Specifications group and then choose the Add button on the RESULT Integration toolbar.**

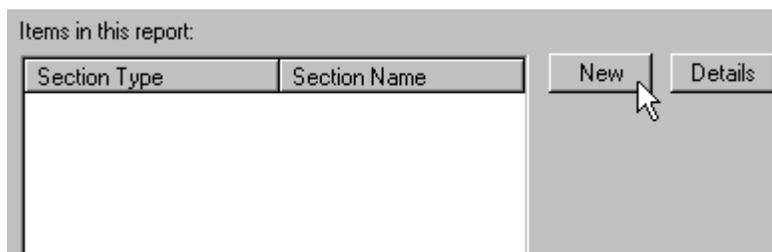


-- or --

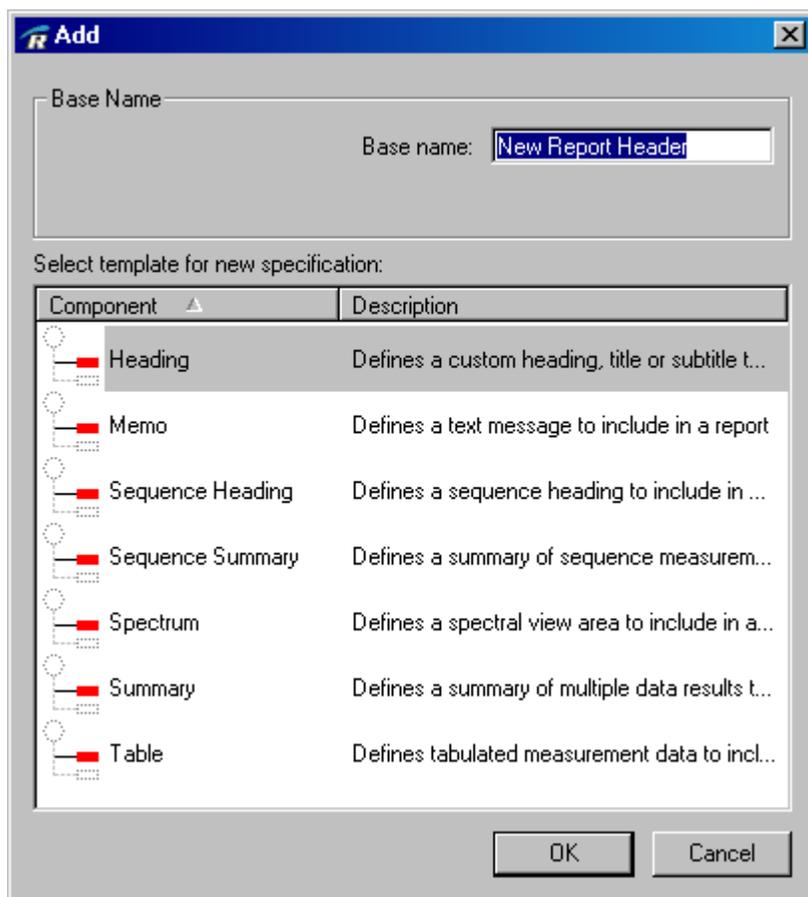
**select the Workflow tab, select a Report event and then choose the Details button to the right of the Report Specification drop-down list box.**



2. In the Report Specification, choose the New button at the right of the Items In This Report box.



The software displays the following dialog box.



**3. Select a report item specification, enter a base name for the new specification, and then choose OK.**

The new specification appears in the display area of the RESULT Integration main window.

Read the following sections to learn about the options available for formatting the sections in a sample report. For information about linking a report item specification to a workflow event, see “Linking a specification to a workflow event” in “Chapter 2 Creating and Editing Workflows” of the “RESULT Integration User Guide.”

## Heading format specifications

A heading format specification defines a heading section in a sample report and the text, information, images, or other elements that will be included in the heading. Heading format specifications are typically used to present information about the operator, the instrument, and the analysis at the top of a sample report, as shown in the example below.

### Operator Information

Operator:	Operator
Date:	9/26/00 1:22:15 PM
Company Name:	Company A

### Heading section in a sample report

A heading or subheading created using a heading format specification can include the following:

- Text that you enter when setting up the workflow.
- The date and time the workflow was run.
- The name of the person who signed the workflow, if the workflow is signed.
- The date and time the workflow was validated, if the workflow is validated.
- Information about the method used to measure the spectra.
- Information about the instrument, such as the serial number or status.

- The date and time the instrument was validated, if the instrument is validated.
- Serial numbers for qualification standards.
- Graphical images, such as the pass or fail image provided with RESULT software or another bitmap image.
- HTML formatting elements, such as a horizontal rule or a blank line.

Heading format specifications may only be linked to report specifications in a workflow, and must include at least one entry to create a heading section in a sample report.

**Associated events:** Report event

**Associated specifications:** Report specification

**Related events:** None

**Related specifications:** Memo Item Specification, Report specification, Spectrum Item specification, Summary Item specification, Table Item specification

**Parameters:** The illustration below shows the parameters for the heading format specification. These parameters appear in the display area of RESULT Integration when a heading format specification is selected in a workflow.

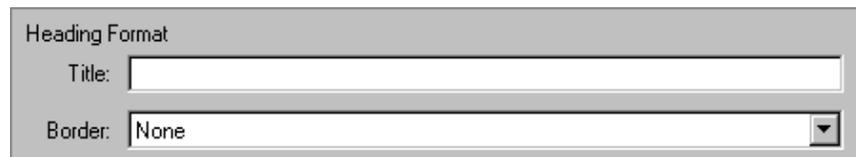
The screenshot shows a dialog box titled "Heading Item Specification". At the top is a text input field containing "New Header". Below this is a section titled "Heading Format" which contains two fields: "Title:" followed by an empty text box, and "Border:" followed by a dropdown menu currently set to "None". Underneath is a section titled "Items in this heading:" which contains a table with two columns: "Label" and "Information to Print". The table is currently empty. At the bottom of the dialog are five buttons: "Move Up", "Move Down", "Add", "Edit", and "Remove".

## Heading format specification parameters

The parameters for the heading format specification define the information included in the heading and the heading format. The following sections explain the heading format specification parameters in detail. The parameters are explained in the order in which they appear in the software.

### Heading Format

The parameters in this group allow you to enter a title and specify the format of a heading section in a sample report.



Heading Format

Title:

Border:

- **Title.** Use the title box to enter a descriptive title for the heading section. The title appears directly above the body of the heading, as shown in the example below.

#### ➡ Operator Information

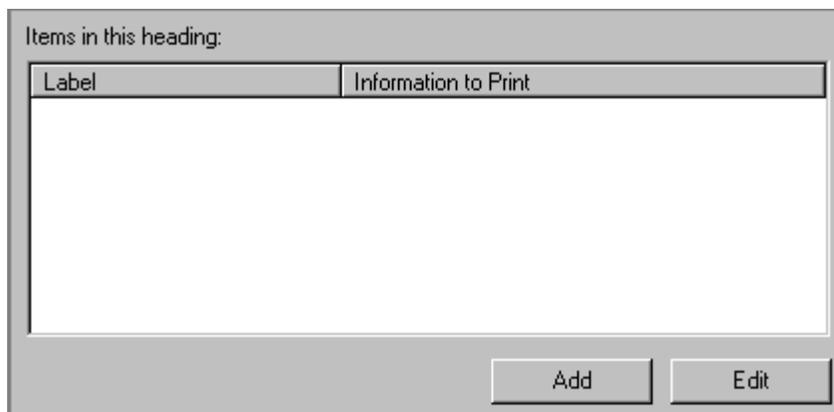
Operator:	Integrator
Date:	9/26/00 1:22:15 PM
Company Name:	Company A

- **Border.** Use this list box to specify a border style for the heading section. You can select a thin, medium, or thick border or include the heading with no border.

The selected setting is applied to the overall border around the heading, as well as the borders dividing the entries if the heading includes more than one entry. The example above has a medium border.

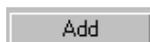
## Items In This Heading

The parameters in this group specify the text or data entries that will be included in the heading and the sequence of those entries.

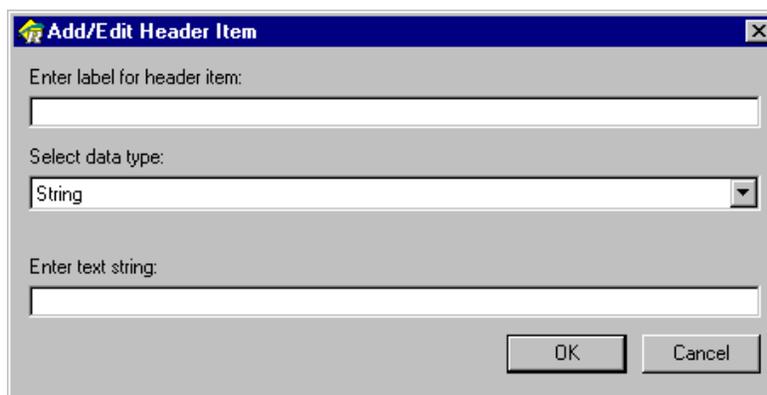


Label	Information to Print
-------	----------------------

Buttons: Add, Edit



- **Add/Edit.** Use these buttons to add an entry to the heading or to edit an existing entry. The Add/Edit Header dialog box appears:



Enter label for header item:

Select data type:

String

Enter text string:

Buttons: OK, Cancel

Use the features in the dialog box to specify the label and content of an entry to include in the heading. The options are described below:

- *Enter label for heading item.* Use this box to type a label for the heading entry. The label will appear to the left of the text, data, or image associated with this entry (see below) in the sample report. If you don't specify a label, then the text, data, or other element will span both columns in the table.
- *Select Data Type.* Use this list box to select the content of the heading entry. You can elect to enter a string of text or to request information, values or other items from the system. The options are listed in the following table:

## Heading options

Current date and time

Operator name

Workflow signature<sup>+</sup>

Measure method summary

Instrument serial number

Validation wheel serial number\*

Serial numbers for various external standards<sup>@</sup>

Instrument validation date\*

Workflow validation date\*

Instrument status information

Horizontal rules (in several formats)

Blank line (for vertical spacing)

Pass (  ) or fail (  ) image provided with the software

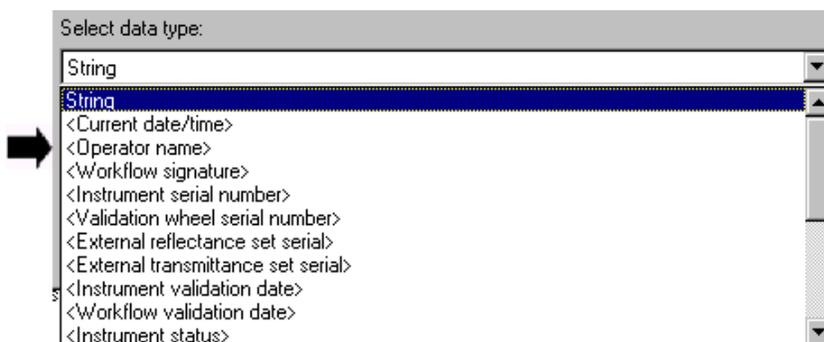
Custom bitmap image (centered or left/right justified)

\* Available only if you purchased the optional ValPro Qualification package.

@ Available only if you purchased the optional standards kit.

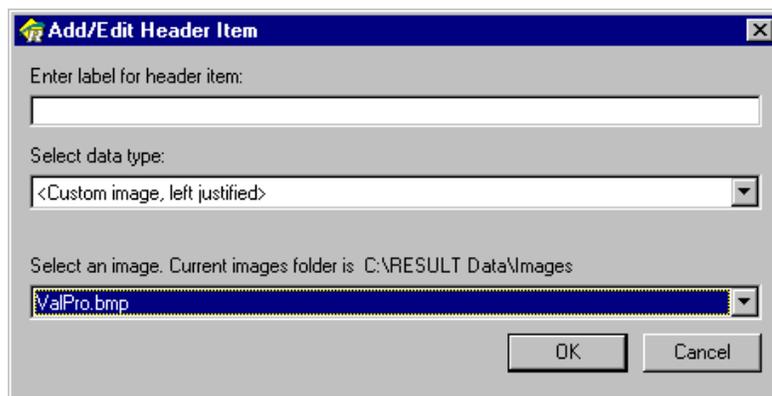
+ If you add a workflow signature to a sample report, RESULT Integration adds the following disclaimer below the signature: “Signature verification is performed on the workflow saved to disk and does not reflect any unsaved changes.”

Information, values or other items that can be requested are shown enclosed in < > in the drop-down list. Here are some examples:



- *Enter Text String.* This option is available in the software only when Data Type (see above) is set to Text String. Use the text box to type a string of text for a text label.

- *Select An Image.* This option is available in the software only when Data Type (see above) is set to Custom Image. To add a custom image to your heading, set Data Type to one of the Custom Image options (centered, or left/right justified). The Add Heading item dialog box changes to the following:



Use the Select An Image list box to select the image you want to add. RESULT allows you to add bitmap images in a range of formats that are compatible with most web browser applications, including \*.bmp, \*.gif, \*.jpeg, and \*.png.

If the image file doesn't appear in the drop-down list, copy it to the directory configured for HTML image files in RESULT Integration. The name of current directory for storing HTML image files in RESULT Integration is displayed above the list box, as shown in the above illustration. See "Setting RESULT Integration Options" in "Chapter 1 Getting Started" of the "RESULT Integration User Guide" for information about changing the directory for storing HTML image files in RESULT Integration.

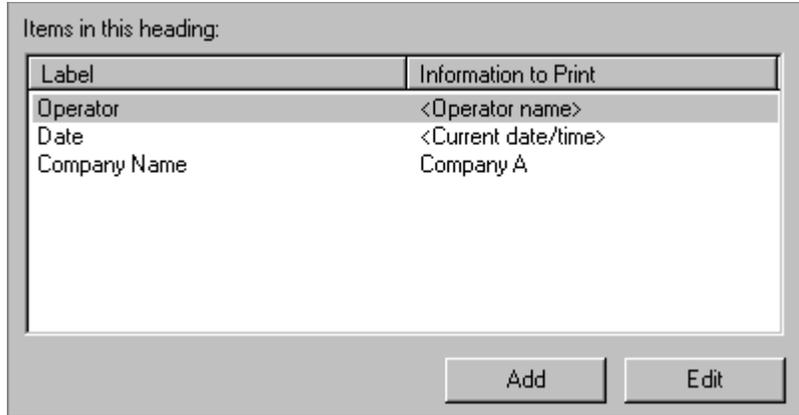
If the image file is located in the proper directory but still doesn't appear in the drop-down list, convert the file to one of the formats listed above.

**Note** If you add an image to a heading section in a sample report, make sure you copy the image file along with the workflow file when transferring the workflow. ▲

When you are finished specifying the heading entry, choose OK. The new entry is added to the list of items included in this heading section of the sample report. The illustration below shows an example.

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete, or select the row and press Delete on the keyboard. Use Export To Text File in the shortcut menu to write the information displayed in the table to a text file with a file name and path you specify.

To change the order in which the sections will appear in the heading section of your sample, drag the corresponding row to a new location in this list.



When you run the workflow and display the report, each label and its associated text or requested information or image will appear in the appropriate heading, as shown in the examples below. The first example has a medium border with three entries: an “Operator” label and the current operator name, a “Date” label and the current date and time, and a “Company Name” label with a text field.

➔ **Operator Information**

Operator:	Integrator
Date:	9/26/00 1:22:15 PM
Company Name:	Company A

The next example is set up as a centered custom image with the label “Measurement rESULT” and no border. (The standard pass and fail images are always left justified).



The last example includes only the ValPro image provided with the software. The image is set up as a left justified custom image with no border. The ValPro image indicates that the report was produced using the Thermo Scientific ValPro System Qualification package.



**Usage:** A heading format specification may be linked to the following workflow specification:

- **Report specification**, which defines the sections in a sample report and the order in which those sections appear when the report is displayed or printed.

## Memo format specifications

A memo format specification defines a simple line or lines of text in a sample report and the specific text that will be included. You can use a memo format specification to add comments, descriptions, or other information to your report. The following example shows a memo section containing information about the workflow used to run the data.

### Workflow

Repeatability Verification

### Memo section in a sample report

Memo format specifications may only be linked to report specifications in a workflow.

**Associated events:** Report event

**Associated specifications:** Report specification

**Related events:** None

**Related specifications:** Heading item specification, Report specification, Spectrum Item specification, Summary Item specification, Table Item specification

**Parameters:** The illustration below shows the parameters for the memo format specification. These parameters appear in the display area of RESULT Integration when a memo format specification is selected in a workflow.

### Memo format specification parameters

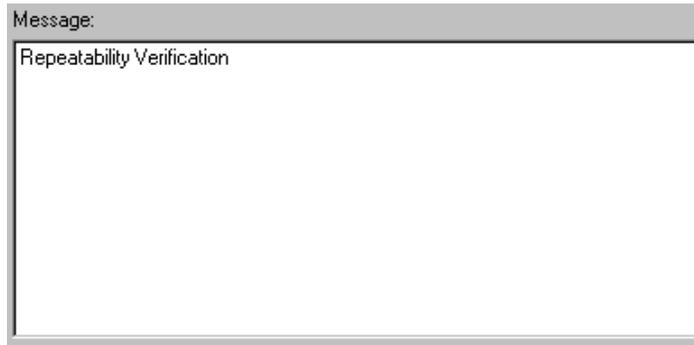
The memo format specification parameters define a label and associated text that may be included in a sample report.

- **Title of this memo.** Use the title box to enter a label for the text or memo.

The title appears directly above the memo section in the sample report. Here is an example:

➡ **Workflow**

- **Message.** Use the Message box to enter the text.



The text appears directly below the memo section title in the sample report (see the example above).

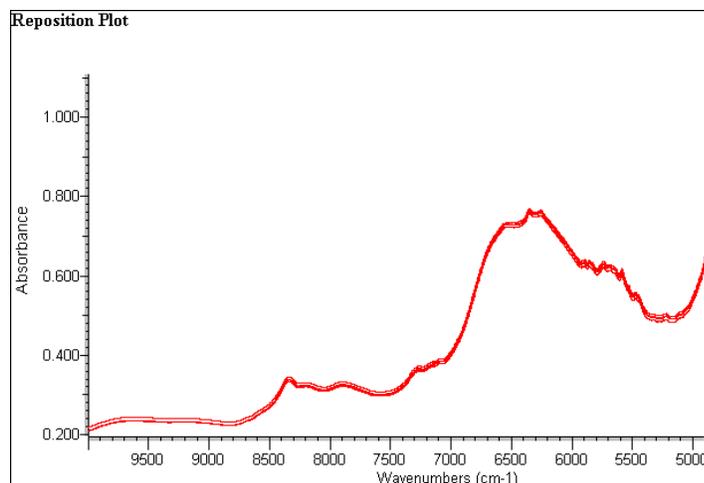
Memo sections always have a border. If you want to produce a message without a border, use a heading section rather than a memo section. See “Heading format specifications” in this chapter for more information.

**Usage:** A memo format specification may be linked to the following workflow specification:

- **Report specification**, which defines the sections in a sample report and the order in which those sections appear when the report is displayed or printed.

## **Spectrum format specifications**

A spectrum format specification defines a spectral plot section in a sample report and the workflow results (spectra) that will be included in the plot. The plot can include one spectrum from each collect event, multiple spectra from a collect event that occurs in a loop, or multiple spectra from multiple collect events. The following example shows a plot of multiple spectra collected from a collect event that occurs in a loop.



### Spectral plot section in a sample report

Spectrum format specifications may only be linked to report specifications in a workflow and must include at least one workflow result (spectrum) to create a spectral plot in a sample report.

**Associated events:** Report event

**Associated specifications:** Report specification

**Related events:** Collect event

**Related specifications:** Heading item specification, Memo Item specification, Report specification, Summary Item specification, Table Item specification

**Parameters:** The illustration below shows the parameters for the spectrum format specification. These parameters appear in the display area of RESULT Integration when a spectrum format specification is selected in a workflow.

Spectrum Item Specification

New Plot

Spectrum Item Format

Title:

Spectral Range

Use custom x-range

Begin:  End:

Use custom y-range

Begin:  End:

Spectra to include:

Add Delete

## Spectrum format specification parameters

The parameters in the spectrum format specification define the axes for the spectral plot and the workflow results (spectra) that will be plotted. The following sections explain the spectrum format specification parameters in detail. The parameters are explained in the order in which they appear in the software.

### Spectrum Item Format

The parameters in this group allow you to enter a title for the plot section and define limits for the X- and Y-axis of the spectral plot.

Spectrum Item Format

Title:

Spectral Range

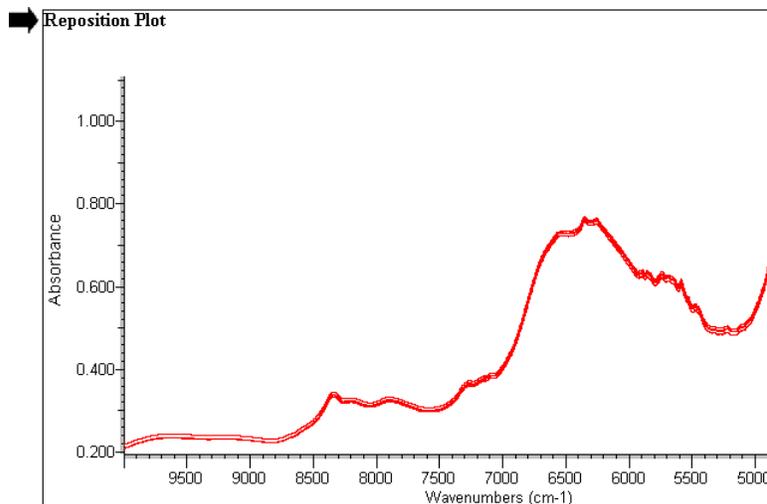
Use custom x-range

Begin:  End:

Use custom y-range

Begin:  End:

- **Title.** Use the title box to enter a descriptive title for the plot section. The title appears directly above the plot in the sample report. Here is an example:

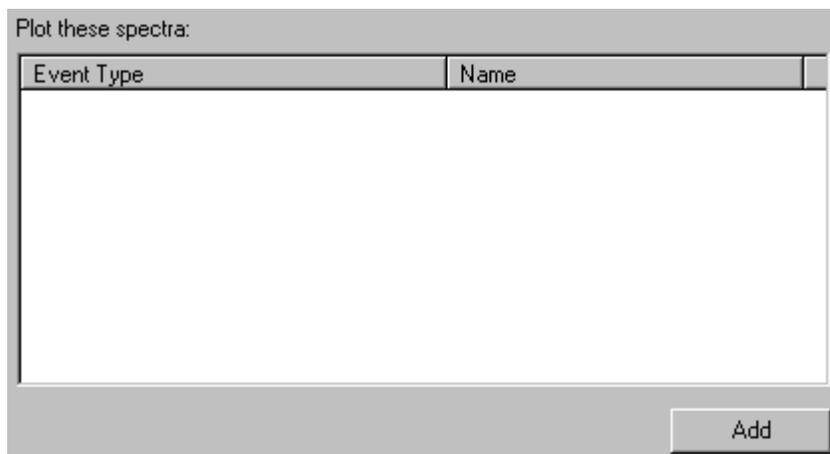


- **Spectral Range.** Use the parameters in this group to define custom X- and/or Y-axis limits for the spectral plot.
  - *Use Custom X-range.* Select this option if you want to specify limits for the X-axis. Use Begin and End to enter the starting and ending X-axis limit in wavenumbers. If you clear this option, the software will use the default spectral range for the selected sampling module.
  - *Use Custom Y-range.* Select this option if you want to specify Y-axis limits for the spectral plot. Use Begin and End to enter the starting and ending values for the Y-axis.

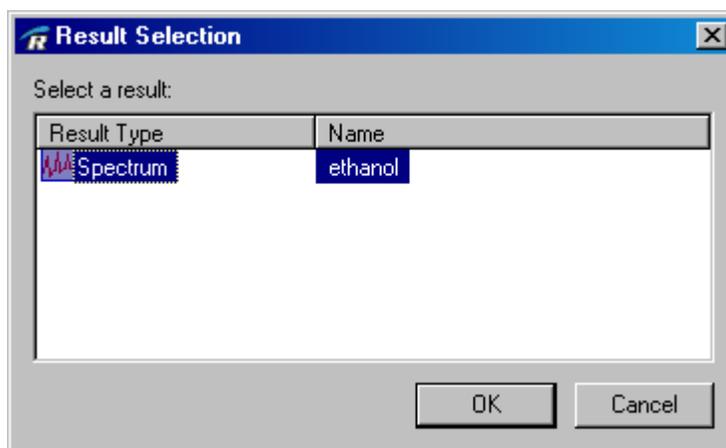
If you specify Y-axis limits, all of the spectra that appear in the plot will be displayed or printed using those limits, so that the spectra are on a common scale. If you clear this option, the limits stored with the spectrum will be used and each spectrum will be displayed or printed at full scale.

## Spectra To Include

Use this box and its associated buttons to specify the workflow results (spectra) to include in the plot.



- **Add.** Choose this button to add a workflow result to the plot. A dialog box appears listing the collection event results in the current workflow. Here is an example:



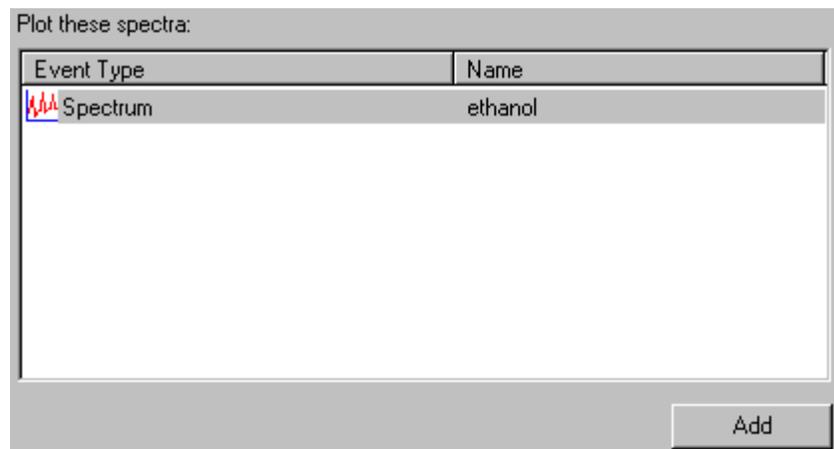
Select a collection result and choose OK.

**Note** If this dialog box is empty, then the workflow either does not contain a collection event or all of the collection event results have already been added. See “Collect events,” “Collect Dual Tablet events” and “Collect Multi-Channel events” in this chapter for instructions for adding collection events to a workflow. ▲

The selected result is added to the list of items to include in the spectral plot.

To delete a row in the list, right-click the row to display a shortcut menu and choose Delete, or select the row and press Delete on the keyboard. Use Export To Text File in the shortcut menu to write the information displayed in the list to a text file with a file name and path you specify.

To change the order in which the spectra will appear in the sample report, drag the corresponding row to a new location in the list.



When you run the workflow, the spectrum produced by the associated collection event will appear in the plot. If the collection event occurs in a loop, the plot will include the spectra produced from all iterations of the loop.

Repeat this step to add another collection result to the plot.

**Note** If you add the spectral result from two different collection events to the same spectrum format specification, all the spectra will appear in the same plot when you display or print the report. If you want the spectra from two different collection events to appear in separate plots in the same report, you must add two spectrum format specifications to the report and add one collection result to each specification. ▲

**Usage:** A spectrum format specification may be linked to the following workflow specification:

- **Report specification**, which defines the sections in a sample report and the order in which those sections appear when the report is displayed or printed.

## Table format specifications

A table format specification defines a table section in a sample report including the workflow results presented in the table and the table format. You can add any type of numeric or other result to a table, including a numeric result from a measurement, comparison, or calculation event. You can also add other items to a table. Here are some examples:

- The pass or fail result from a check event.
- The pass (✓) or fail (✗) image.
- An operator response from a request event.
- Information stored in the history of a spectral file.

Here is an example of a table that contains statistical and pass/fail results from a quantitative analysis of ethanol:

If you want the workflow to report the values from the five repeated measurements used to generate this statistical result, use a summary format specification described in the next section instead of a table format specification.

<i>Attribute</i>	<i>% Ethanol - Std Deviation</i>	<i>Pass/Fail result</i>	<i>Pass/Fail graphic image</i>
<i>Answer</i>	0.0703	PASS	

### Table of measurement results

This workflow makes five measurements of ethanol and reports the standard deviation of those measurements. The pass result is generated when the standard deviation is less than 0.5. The report includes the graphical pass or fail image so the operator can quickly confirm the analysis result.

Table format specifications may only be linked to report specifications in a workflow and must include at least one workflow result to create a table in a sample report.

**Associated events:** Report event

**Associated specifications:** Report specification

**Related events:** Calculate event, Check event, Compare event, Measure event, Request event



## Table Format

Use the parameters in this group to enter a title for the table section and specify the table format.

Table Format	
Title:	Measurement result
Layout:	Display data types in rows, attributes in columns
Border:	None
<input checked="" type="checkbox"/> Show column headers	<input checked="" type="checkbox"/> Show row headers
<input checked="" type="checkbox"/> Show event names with attribute names	<input type="checkbox"/> Place all data types in one row/column

- **Title.** Use the title box to enter a descriptive title for the table. The title appears directly above the table in the sample report, Here is an example:

### ➔ Measurement Result

<i>Attribute</i>	<i>% Ethanol - Std Deviation</i>	<i>Pass/Fail result</i>	<i>Pass/Fail graphic image</i>
<i>Answer</i>	0.0703	PASS	

- **Layout.** Each workflow result you select to include in the table has a corresponding Data Type and Attribute (see Add Item below for examples). Use the Layout list box to specify the information that will be placed in the table columns and rows. Select Display Data Types In Rows, Attributes In Columns to configure the table to place the reported value, text or image in the table rows with the descriptive names above. This setting works well for reporting values from a measure event where Data Type can include things like concentration and uncertainty values for each component. Here is a simple table with concentration and uncertainty values for Ethanol in water:

### Measurement of Ethanol in Water

<i>Attribute</i>	<b>Ethanol in Water - Concentration</b>	<b>Ethanol in Water - Uncertainty</b>
<i>Result</i>	49.41	0.97

### Table formatted with Data Types in rows, Attributes in columns

**Note** To create the table shown above, we used the Add Item button on the table format specification to select the Concentration and Uncertainty data types for the Ethanol In Water measurement in the workflow. These workflow results now appear in the list of events we want to include in the table section of our sample report as shown below.

Report these events:

Event Name	Data Type	Attribute	Label	Decimal...	Alig
Ethanol in Wa...	Value	Ethanol	Concentration	2	Cer
Ethanol in Wa...	Uncertainty	% Ethanol	Uncertainty	2	Cer

Preview Section      Add Break      Add Item

Then we used the Label entry boxes in the table (see above) to enter descriptive names (e.g., “Concentration” and “Uncertainty”) for each workflow result. In the Table Format group, we set Layout to Display Data Types In Rows, Attributes In Columns, set Border to Thin, selected Show Column Headers, selected Show Event Names With Attribute Names, cleared Show Row Headers, and selected Place All Data Types In One Row/Column. ▲

Select the other option to flip the rows and columns in the table. The next illustration shows the same table formatted with the reported values in the table columns with the descriptive names at the left.

To create this table, we set Layout to Display Attributes In Rows, Data Types In Columns, set Border to Medium and selected all of the following: Show Column Headers, Show Event Names With Attribute Names, Show Row Headers, and Place All Data Types In One Row/Column.

### Measurement of Ethanol in Water

<i>Attribute</i>	<i>Result</i>
<b>Ethanol in Water - Concentration</b>	49.41
<b>Ethanol in Water - Uncertainty</b>	0.97

### Table formatted with Attributes in rows, Data Types in columns

Border:

- **Border.** Use this list box to specify a border style for the table. You can select a thin, medium, or thick border or include the table with no border. The thin and medium border styles are shown in the two examples above.

The selected setting is applied to the overall border around the table as well as the borders around the individual cells.

Show column headers

- **Show Column Headers.** Use this option to specify whether the table will include column headings or be shown with no column headings in the sample report. The table shown in the previous illustration (Attributes in rows, Data Types in columns) looks like this with the column headings hidden:

#### Measurement of Ethanol in Water

<b>Ethanol in Water - Concentration</b>	49.41
<b>Ethanol in Water - Uncertainty</b>	0.97

Show row headers

- **Show Row Headers.** Use this option to specify whether the table will include row headings or be shown with no row headings in the sample report. The table shown in the previous illustration (Data Types in rows, Attributes in columns) looks like this with the row headings hidden.

#### Measurement of Ethanol in Water

<b>Ethanol in Water - Concentration</b>	<b>Ethanol in Water - Uncertainty</b>
49.41	0.97

Show event names with attribute names

- **Show Event Names With Attribute Names.** Use this option to specify whether the table will include the event name along with the descriptive name for each table entry. The event name refers to the name you entered for the event when you added it to the workflow. It appears at the top of the display area when the event is selected in the workflow. The table shown in the above illustration looks like this with the event name removed.

#### Measurement of Ethanol in Water

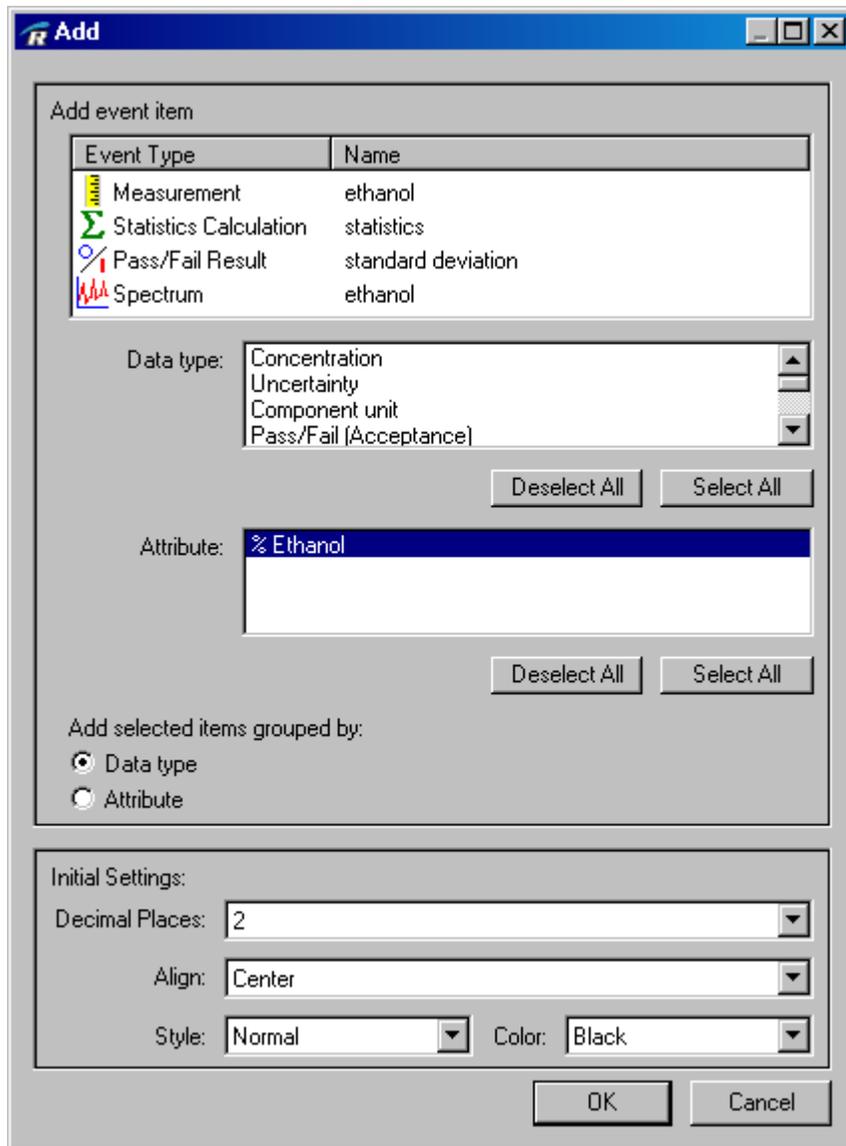
<b>Concentration</b>	<b>Uncertainty</b>
49.41	0.97



The features are described below:



- **Add Item.** Use this button to add a workflow result, image or text to the table. The software displays the following dialog box:



The list at the top of the dialog box shows the events in the workflow that provide measurement or other results that can be placed in a table.

**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a result that can be tabulated, or all of those events have already been added. See the Usage heading for this table format specification for a list of events that produce results that can be used in a table. ▲

Select a result in the list. Make sure you select a result that occurs before this table specification and its associated report event in the workflow.

After you select a result, the following parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Descriptions are provided below:

- *Data Type.* Use this list box to select a result produced by the selected event, such as a concentration value or acceptance limit from a measurement event. You may need to scroll the list to see all the available items. The number and type of results produced by an event depend on the event, and, for measure events, on the TQ Analyst method used for the measurement. For example, a measure event configured for quantitative analysis would always produce concentration values, but it may also include acceptance limits or known values, such as the expected concentration for a sample or standard. Many events produce only one type of data. Use the Select All and Deselect All buttons to help you select or deselect all the listed items at once.
- *Attribute.* For data types that produce multiple results, use this list box to select which results you want to include. You may need to scroll the list to see all the available items. Select a result in the list such as a component name from a measure event, the maximum value from a calculate event, the pass or fail text result from a check event, or an item from the history of a spectrum. Use the Select All and Deselect All buttons to help you select or deselect all the listed items at once. Use the Shift key on the keyboard to select multiple items listed sequentially or the Ctrl key to select multiple items that are not sequential.
- *Add Selected Items Grouped By.* Use this option to specify how your selections will be grouped (by data type or attribute) in the list displayed on the table format specification. This makes a difference only when you want to include a data type or attribute entry from multiple events in the workflow.

- *Decimal Places.* Use this list box to select the number of decimal places to include in any numeric results that are selected for the table. You can include up to six decimal places. The software rounds the number and retains only the specified number of decimal places.
- *Align.* Use this list box to specify the default alignment of the items in the table (left, center or right).
- *Style.* Use this list box to specify the default font style for any text results that are selected for the table. You can display text normally or in a bold, italic, or bold italic style.
- *Color.* Use this list box to specify the default font color for any text results that are selected for the table. The software includes the standard colors defined by the Windows operating system.

**Note** The Decimal Places, Align, Style, and Color list boxes in this dialog box allow you to specify an initial setting for each of these options. The initial settings will be applied to the selected Data Types and Attributes and will appear in their corresponding columns in the table format specification (see the next illustration). These items can also be defined for a specific workflow result by double-clicking the column and corresponding cell in the table. ▲

When you are finished selecting results for a workflow event, choose OK. The selected results are added to the list of items to include in the table. Here is an example:



rows appear at the top of the list of results you want to report. Select the last row of the heading and then choose Add Break. In the Add Break dialog box, select Heading and choose OK. The software will add a heading break immediately below the row you selected. Here is an example with the Spectrum Title selected as the heading:

Report these events:

Event Name	Data Type	Attribute
Surfactant	Value	Spectrum title
Heading (repeat for all tables)		
Surfactant	Value	Data collection date & time
Surfactant	Value	Spectrum file name
Table (next table)		
Surfactant	Value	Resolution
Surfactant	Value	Data point spacing

The corresponding report shows the spectrum title repeated in the first cell of both tables, as shown below:

Spectrum title	Data collection date & time	Spectrum file name
Surfactant 06-27-2006 16:32:27	06-27-2006 16:32:27	Spectrum has not been archived

Spectrum title	Resolution	Data point spacing
Surfactant 06-27-2006 16:32:27	8.000	3.857

- Table.* Use this option to separate the data into multiple tables. To specify a new table, select the last result you want to include in the previous table and then choose Add Break. In the Add Break dialog box, select Table and choose OK. The software will start a new table with the next workflow result in the list of results you want to report. The example above shows the data presented in two tables.
- Line.* Use this option to separate the data by starting a new line in the table. To add a line break, select the last result you want to include in the previous line and then choose Add Break. In the Add Break dialog box, select Line and choose OK. Here is a table specification with a line break:

Report these events:

Event Name	Data Type	Attribute
Surfactant	Value	Spectrum title
Surfactant	Value	Data collection date & time
Line (next line)		
Surfactant	Value	Spectrum file name
Surfactant	Value	Resolution

The corresponding table looks like this in the sample report:

Spectrum title	Data collection date & time
Spectrum file name	Resolution
Surfactant 06-27-2006 16:29:09	06-27-2006 16:29:09
Spectrum has not been archived	8.000

- Cell.** Use this option to separate the data by starting a new cell. To add a cell break, select the result you want to include before the cell break and then choose Add Break. In the Add Break dialog box, select Cell and choose OK. Here is a table specification with a cell break:

Report these events:

Event Name	Data Type	Attribute
Surfactant	Value	Spectrum title
Surfactant	Value	Data collection date & time
Cell (next cell)		
Surfactant	Value	Spectrum file name
Surfactant	Value	Resolution

The software will skip a cell at the specified location and place the next workflow result in the following cell. The skipped cell has a dash (“-”) placeholder. Here is the corresponding table in the sample report:

Spectrum title	Data collection date & time	-	Spectrum file name	Resolution
Surfactant 06-27-2006 16:24:24	06-27-2006 16:24:24	-	Spectrum has not been archived	8.000

Preview Section

- **Preview Section.** As you make selections in the table format specification to define the layout for your table, use the Preview Section button to view the effect on the final table. In preview mode, only the table headings are shown. Dashes (“-“) are used to represent cells that will be blank in the table as it appears in the sample report. The software uses the phrase (“no rESULT”) to indicate cells where data will appear.

**Usage:** A table format specification may be linked to the following workflow specification:

- **Report specification,** which defines the sections in a sample report and the order in which those sections appear when the report is displayed or printed.

## Summary format specifications

A summary format specification defines a table of summarized results in a sample report including the workflow results that will be included in the table and the table format. A summary table can be designed to serve a variety of needs, ranging from a simple compilation of data produced by multiple iterations of a loop (i.e., value 1, value 2, value 3, pass/fail 1, pass/fail 2, pass/fail 3), to an elegant presentation of statistical results from a multi-component analysis.

You can add any type of numerical or other result to a summary table, including a numerical result from a measurement, comparison, or calculation event, the pass or fail result from a check event, the pass (✔) or fail (✘) image, and an operator response from a request event, information stored in the history of a spectral file, plus a range of statistical values, including:

- Minimum, maximum and average values
- Range (maximum minus minimum)
- Standard deviation and percent standard deviation
- Summation (simple sum)
- Count (number of measurements)

You can set up the table to include only the source values from the measurements, to include only the statistical values, or it can include the source values and the statistical values. Here is an example of a table of summarized measurement results:

**Ethanol**

<i>Attribute</i>	<i>Measured Value</i>	<i>Unit</i>	<i>Concentration</i>	<i>Uncertainty</i>
<i>Result (1)</i>	49.47	%	49.47	0.90
<i>Result (2)</i>	49.41	%	49.41	0.97
<i>Result (3)</i>	49.37	%	49.37	0.99
<i>Result (4)</i>	49.39	%	49.39	1.03
<i>Result (5)</i>	49.28	%	49.28	1.04
<i>Count</i>	5	-	5	5
<i>Minimum</i>	49.28	-	49.28	0.90
<i>Maximum</i>	49.47	-	49.47	1.04
<i>Range</i>	0.19	-	0.19	0.14
<i>Sum</i>	246.92	-	246.92	4.93
<i>Average</i>	49.38	-	49.38	0.99
<i>Standard deviation</i>	0.07	-	0.07	0.06
<i>% Standard deviation</i>	0.14	-	0.14	5.67

**Table of summarized measurement results**

Summary format specifications may only be linked to report specifications in a workflow and must include at least one workflow result to create a summary table in a sample report.

**Associated events:** Report event

**Associated specifications:** Report specification

**Related events:** Calculate event, Check event, Compare event, Measure event, Request event

**Related specifications:** Report specification, Heading item specification, Table Item specification, Memo Item specification, Spectrum Item specification

**Parameters:** The illustration below shows the parameters for the summary item specification. These parameters appear in the display area of RESULT Integration when a summary item specification is selected in a workflow.

Summary Item Specification

New Report Summary

Table Format

Title:

Layout:

Border:

Show column headers
  Show row headers  
 Show event names with attribute names
  Place all data types in one row/column  
 Show raw source values
  Delete source spectra after reporting

Summarize these events:

Event Name	Data Type	Attribute	Label	Decimal...	Align	Col

Adding an event to this list will set its option to store all results.

## Summary format specification parameters

The summary format specification parameters define the workflow results presented in the summary table, any statistical data that will be included, and the table format. The following sections explain the summary format specification parameters in detail. The parameters are explained in the order in which they appear in the software.

### Table Format

Use the features in this group to define the format of your summary table.

Table Format

Title:

Layout:

Border:

Show column headers
  Show row headers  
 Show event names with attribute names
  Place all data types in one row/column  
 Show raw source values
  Delete source spectra after reporting

- **Title.** Use the title box to enter a descriptive title for the summary table. The title appears directly above the table in the sample report. Here is an example:

## ➔ Summarized Results

Fixed Position - Value	Fixed Position - Unit	Reposition - Value	Reposition - Unit
0.00	micro-A.U.	14,229.85	micro-A.U.

- Layout.** Each workflow result you select to include in the table has a corresponding Data Type and Attribute (see Add Item below for examples). Use the Layout list box to specify the information that will be placed in the table columns and rows. Select Display Data Types In Rows, Attributes In Columns to configure the table to place the reported value, text or image in the table rows with the descriptive names above. This setting works well for reporting values from a measure event where Data Type can include things like concentration and uncertainty values for each component. Here is a simple summary table set up this way:

### Ethanol

<i>Attribute</i>	ethanol - Measured Value	ethanol - Unit	ethanol - Concentration	ethanol - Uncertainty
<i>Result (1)</i>	49.37	%	49.37	0.99
<i>Result (2)</i>	49.39	%	49.39	1.03
<i>Count</i>	2	-	2	2
<i>Standard deviation</i>	0.01	-	0.01	0.03
<i>% Standard deviation</i>	0.03	-	0.03	2.80

### Table formatted with data types in rows, attributes in columns

Select the other option to flip the rows and columns in the table. The next example shows the same table formatted with the reported values in the table columns with the descriptive names at the left.

## Ethanol

<i>Attribute</i>	<i>Result (1)</i>	<i>Result (2)</i>	<i>Count</i>	<i>Standard deviation</i>	<i>% Standard deviation</i>
ethanol - Measured Value	49.47	49.41	2	0.04	0.09
ethanol - Unit	%	%	-	-	-
ethanol - Concentration	49.47	49.41	2	0.04	0.09
ethanol - Uncertainty	0.90	0.97	2	0.05	5.29

### Table formatted with attributes in rows, data types in columns

- **Border.** Use this list box to specify a border style for the table. You can select a thin, medium, or thick border or include the table with no border.

The selected setting is applied to the overall border around the table, as well as the borders around the individual cells. The table shown in the previous example has a medium border.

Show column headers

- **Show Column Headers.** Use this option to specify whether the table will include column headings or be shown with no column headings in the sample report. The table shown in the previous illustration (Attributes in rows, Data Types in columns) looks like this with the column headings hidden:

## Ethanol

<b>ethanol - Measured Value</b>	49.41	49.37	2	0.03	0.06
<b>ethanol - Unit</b>	%	%	-	-	-
<b>ethanol - Concentration</b>	49.41	49.37	2	0.03	0.06
<b>ethanol - Uncertainty</b>	0.97	0.99	2	0.01	1.44

If you include summary properties in your table (see Summary Properties below), you probably want to show the column headings so you can identify the reported values. The columns highlighted in grey in the table above contain values for Count, Standard Deviation, and % Standard Deviation.

Show row headers

- **Show Row Headers.** Use this option to specify whether the table will include row headings or be shown with no row headings in the report. The table shown in the previous illustration (Data Types in rows, Attributes in columns) looks like this with the row headings hidden.

## Ethanol

ethanol - Measured Value	ethanol - Unit	ethanol - Concentration	ethanol - Uncertainty
49.28	%	49.28	1.04
49.47	%	49.47	0.90
2	-	2	2
0.13	-	0.13	0.10
0.27	-	0.27	10.21

If you include summary properties in your table (see Summary Properties below), you probably want to show the row headings so you can identify the reported values. The rows highlighted in grey in the table above contain values for Count, Standard Deviation, and % Standard Deviation.

Show event names with attribute names

- **Show Event Names With Attribute Names.** Use this option to specify whether the table will include the event name along with the descriptive name for each table entry. The event name refers to the name you entered for the event when you added it to the workflow. It appears at the top of the display area when the event is selected in the workflow. It is helpful to show the event names when the table includes results from more than one event. Here is an example:

### Summarized Results

Fixed Position - Value	Fixed Position - Unit	Reposition - Value	Reposition - Unit
0.00	micro-A.U.	14,229.85	micro-A.U.

The workflow that produced this report contains two measure events which are titled “Measure Fixed Position” and “Measure Reposition.”

Place all data types in one row/column

- **Place All Data Types In One Row/Column.** Use this option to specify that all data types selected for display in the table are placed in one row or column. Selecting this option condenses the data and makes the table easier to read. Here is the same table with and without this option:

## Ethanol

<i>Attribute</i>	<b>Measured Value</b>	<b>Unit</b>	<b>Concentration</b>	<b>Uncertainty</b>
<i>Value (1)</i>	49.28	-	-	-
<i>Value (2)</i>	49.47	-	-	-
<i>Component unit (1)</i>	-	%	-	-
<i>Component unit (2)</i>	-	%	-	-
<i>Concentration (1)</i>	-	-	49.28	-
<i>Concentration (2)</i>	-	-	49.47	-
<i>Uncertainty (1)</i>	-	-	-	1.04
<i>Uncertainty (2)</i>	-	-	-	0.90

### Summary table formatted with Data Types in multiple rows

## Ethanol

<i>Attribute</i>	<b>Measured Value</b>	<b>Unit</b>	<b>Concentration</b>	<b>Uncertainty</b>
<i>Result (1)</i>	49.41	%	49.41	0.97
<i>Result (2)</i>	49.37	%	49.37	0.99

### Summary table formatted with Data Types in one row

Show raw source values

- **Show Raw Source Values.** Select this option if you want to include the source values for the summarized items in the table of results. For example, if you are summarizing the results from repeated measurements and Show Raw Source Values is selected, the table will have entries for the measured values along with the summarized results. The example below shows measured values produced in a repeat loop (RESULT 1, RESULT 2, etc.), followed by the summarized results (Count, Minimum, etc.).

Measured values

Summarized values

## Ethanol

<i>Attribute</i>	<i>Measured Value</i>	<i>Unit</i>	<i>Concentration</i>	<i>Uncertainty</i>
<i>Result (1)</i>	49.47	%	49.47	0.90
<i>Result (2)</i>	49.41	%	49.41	0.97
<i>Result (3)</i>	49.37	%	49.37	0.99
<i>Result (4)</i>	49.39	%	49.39	1.03
<i>Result (5)</i>	49.28	%	49.28	1.04
<i>Count</i>	5	-	5	5
<i>Minimum</i>	49.28	-	49.28	0.90
<i>Maximum</i>	49.47	-	49.47	1.04
<i>Range</i>	0.19	-	0.19	0.14
<i>Sum</i>	246.92	-	246.92	4.93
<i>Average</i>	49.38	-	49.38	0.99
<i>Standard deviation</i>	0.07	-	0.07	0.06
<i>% Standard deviation</i>	0.14	-	0.14	5.67

If Show Raw Source Values is cleared, only the summarized values will appear in the table.

Delete source spectra after reporting

- **Delete Source Spectra After Reporting.** Select this option if you don't need to archive the spectral data or if the archive event appears before the report event in the workflow. If Delete Source Spectra After Reporting is selected, then the software will delete the source sample and background spectra that are stored in the computer's internal memory after reporting the summarized results. Deleting the source spectra is recommended to release memory resources, especially when the report specification handles multiple spectra produced in a loop.

Make sure this option is cleared if you need to archive the spectral data and your archive event is located after the report event in the workflow, or if there are other subsequent workflow events that operate on the source spectra. If you want to delete the spectra later, use a clear event.

**Note** It is a violation of current good manufacturing practices (cGMP) and other federal regulations for a pharmaceutical company to refrain from archiving spectral data. ▲

### Summarize these events

Use the features in this group to select the workflow results you want to include in the summary table and the sequence of those results.

Summarize these events:

Event Name	Data Type	Attribute	Label	Decimal...	Align
? Lot Number	Value	Please Enter the Lot Numb...	Please Enter the...	2	Center

◀

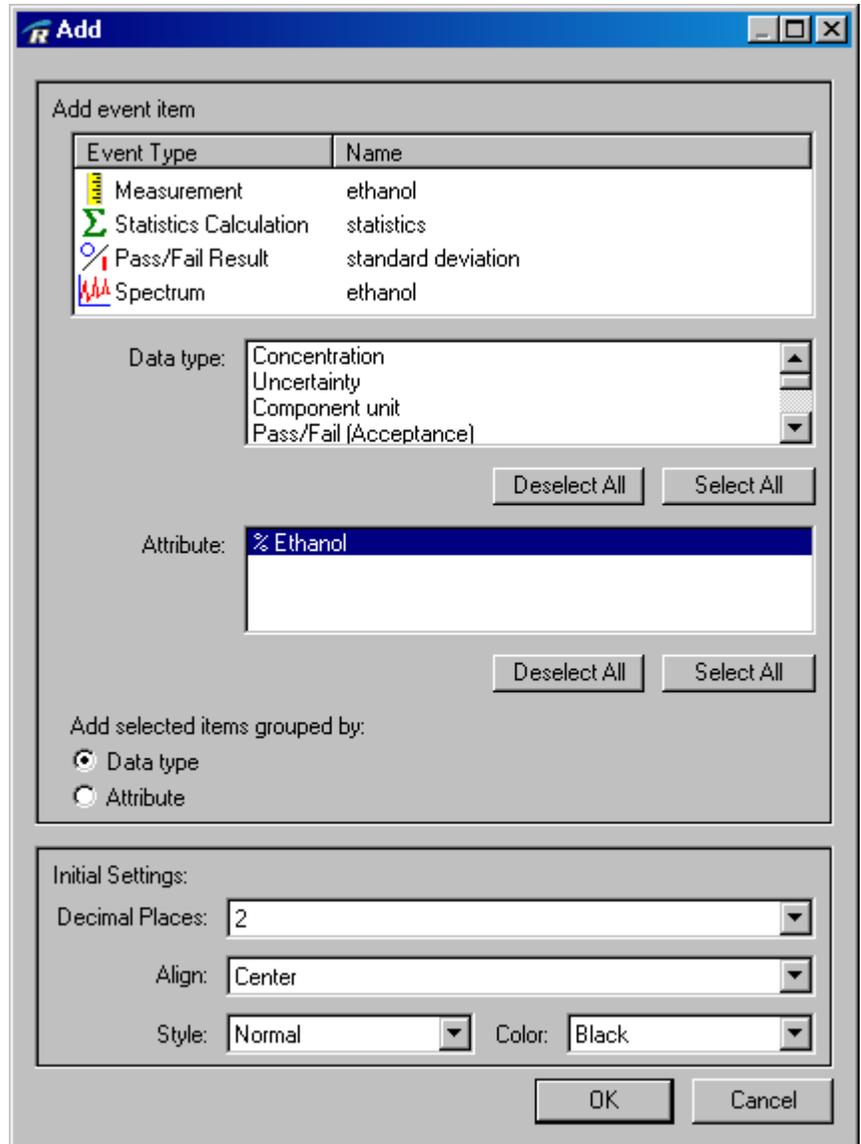
Preview Section   Summary Properties   Add Break   Add Item

Adding an event to this list will set its option to store all results.

The features are described below:



- **Add Item.** Use this button to add a workflow result, image or text to the table. The software displays the following dialog box:



The list at the top of the dialog box shows the events in the workflow that provide measurement or other results that can be placed in a table.

**Note** If this dialog box is empty, then the workflow either does not contain an event that produces a result that can be summarized, or all of those results have already been added. See the Usage heading for this summary format specification for a list of events that produce results that can be summarized. ▲

Select a result in the list. Make sure you select a result that exists at this point in the workflow.

After you select a result, the Data Type, Attribute, Add Selected Items Grouped By, Decimal Places, Align, Style, and Color parameters may become available in the software, allowing you to select a data type for the event, the components or other attributes or values to include for each data type, and the format for each component, attribute or value. Examples are provided below.

- *Data Type*. Use this list box to select a result produced by the selected event, such as a concentration value or acceptance limit from a measurement event. You may need to scroll the list to see all the available items.
- *Attribute*. For data types that produce multiple results, use this list box to select which results you want to include.
- *Add Selected Items Grouped By*. Use this option to specify how your selections will be grouped (by data type or attribute) in the list displayed on the table format specification. This makes a difference only when you want to include a data type or attribute entry from multiple events in the workflow.
- *Decimal Places*. Use this list box to select the number of decimal places to include in any numeric results that are selected for the table (up to 6). The software rounds the number and retains only the specified number of decimal places.
- *Align*. Use this list box to specify the default alignment of the items in the table (left, center or right).
- *Style*. Use this list box to specify the default font style for any text results that are selected for the table. You can display text normally or in a bold, italic, or bold italic style.
- *Color*. Use this list box to specify the default font color for any text results that are selected for the table. The software includes the standard colors defined by the Windows operating system.

**Note** The Decimal Places, Align, Style, and Color list boxes in this dialog box allow you to specify an initial setting for each of these options. The initial settings will be applied to the selected Data Types and Attributes and will appear in their corresponding columns in the table format specification (see the next illustration). These items can also be defined for a specific workflow result by double-clicking the column and corresponding cell in the table. ▲

When you are finished selecting results, choose OK. The selected results are added to the list of items to include in the table. Here is an example:

To delete a row in the table, right-click the row to display a shortcut menu and choose Delete Selected Row, or select the row and press Delete on the keyboard. Use Export To Text File to write the information displayed in the table to a text file with a file name and path you specify. To edit a property for an item in the table, double-click the corresponding cell. To change the order in which items are placed in the table, drag the corresponding row to a new location in this list. To sort a column of entries in numeric or alphabetic order, right-click the column heading and then choose Sort Ascending or Sort Descending.

Summarize these events:

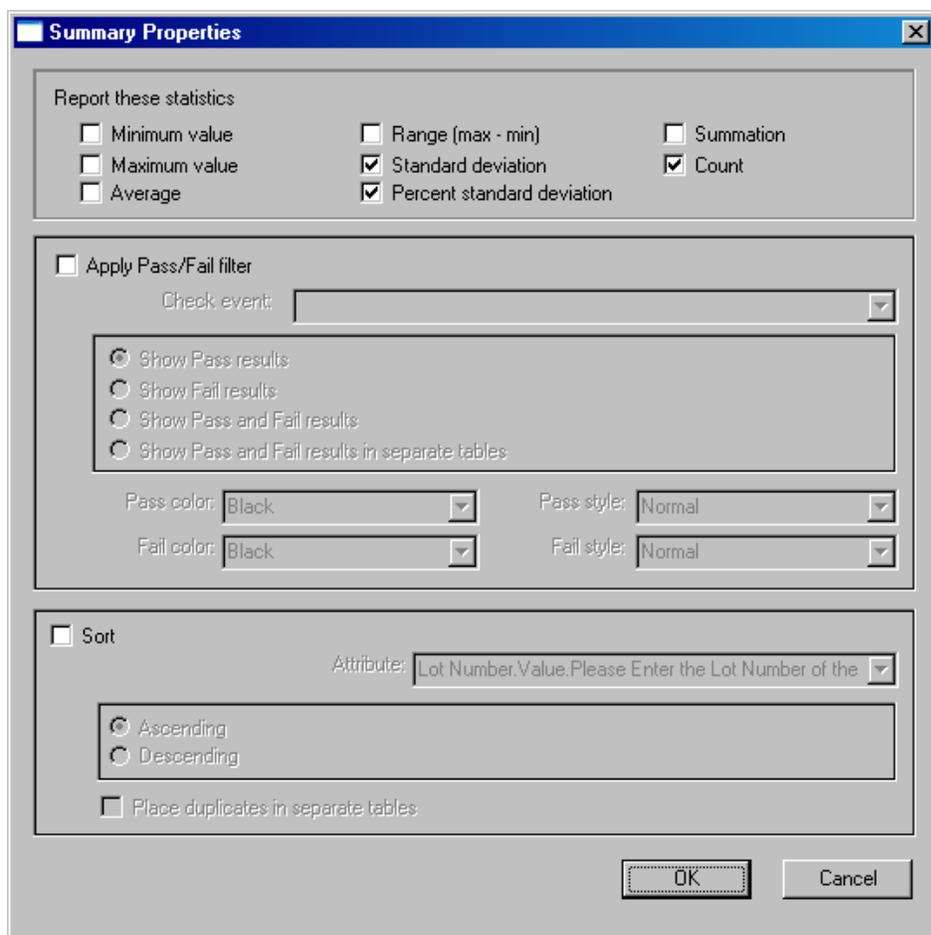
Event Name	Data Type	Attribute	Label	Decimal...	Align
Lot Number	Value	Please Enter the Lot Numb...	Please Enter the...	2	Center
Surfactant	Concentration	Hydroxyl Value	Hydroxyl Value	2	Center
Surfactant	Uncertainty	Hydroxyl Value	Hydroxyl Value	2	Center
Surfactant	Component ...	Hydroxyl Value	Hydroxyl Value	2	Center
Surfactant	Pass/Fail (A...	Hydroxyl Value	Hydroxyl Value	2	Center
Surfactant	Full spectru...	Hydroxyl Value	Hydroxyl Value	2	Center
Surfactant	Full spectru...	Hydroxyl Value	Hydroxyl Value	2	Center

Preview Section   Summary Properties   Add Break   Add Item

Adding an event to this list will set its option to store all results.

- **Label.** This column of editable entry boxes in the table format specification allows you to assign a unique name to each workflow result you want to include in the table section of your sample report. This feature provides a handy way to format the table exactly as you want it. The Label feature was used extensively to create the examples shown in this user guide.
- **Summary Properties.** Use this button to define any statistical values you want to include in the summary table and any options to filter or sort the data. The software displays the following dialog box.





The features are described below:

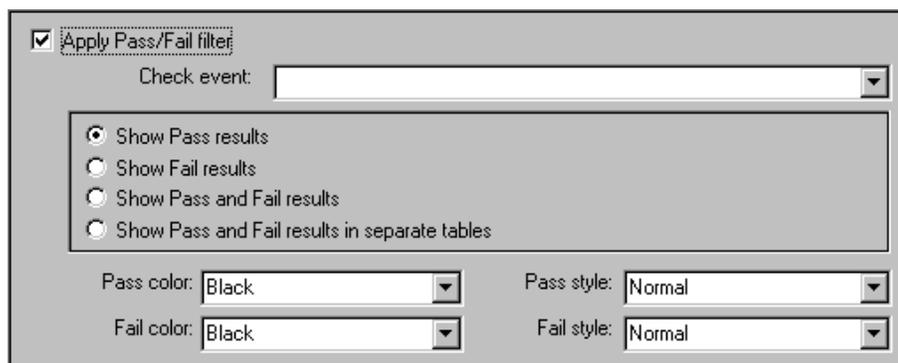
- *Report These Statistics.* The following statistics may be reported:
  - Minimum, maximum and average values
  - Range (maximum minus minimum)
  - Standard deviation and percent standard deviation
  - Summation (simple sum)
  - Count (number of measurements)

The selected statistical values will be reported for each measured attribute listed in the summary format specification. Here are statistical results for two measured values:

## Summarized Results

<i>Attribute</i>	<b>Reposition - Max Hgt</b>	<b>Reposition - Ave Hgt</b>
<i>Result (1)</i>	750,806.00	447,212.20
<i>Count</i>	1	1
<i>Minimum</i>	750,806.00	447,212.20
<i>Maximum</i>	750,806.00	447,212.20
<i>Range</i>	0.00	0.00
<i>Sum</i>	750,806.00	447,212.20
<i>Average</i>	750,806.00	447,212.20
<i>Standard deviation</i>	0.00	0.00
<i>% Standard deviation</i>	0.00	0.00

- *Apply Pass/Fail Filter.* If your workflow contains a check event, you can use the features in this group to define special formatting for the check event result in your summary table.



The options are explained below:

-- Check event. Use this drop down list box to select the check event that will produce the pass or fail result you want to format. Then use the associated radio buttons to indicate which pass/fail results you want to include in the summary report.

-- Pass/Fail color. Use these drop down list boxes to select a color for reporting the pass or fail text result.

-- Pass/Fail Style. Use these drop down list boxes to select a style for reporting the pass or fail text result. You can display the text normally or in a bold, italic, or bold italic style.

The example in the next section shows the pass results reported in green text and the fail results in red.

- *Sort*. You can use the features in this group to sort specific workflow results in ascending or descending order. This feature provides an easy way to sort numeric results (from low to high or the reverse) and items reported from a spectral history such as a spectrum title or file name in alphabetical order.

The options are explained below:

-- Attribute. Use this drop down list box to select the workflow result that will produce the numeric, text or other answer you want to sort. The drop down list includes all the summary results listed on the summary format specification. Then use the associated radio buttons to indicate whether you want to sort the results in ascending or descending order. The illustration above shows the Expected Conc value selected for sorting in ascending order. Here is the corresponding sample report showing the expected concentration values sorted from low to high.

Ethanol Report - Sorted Ascending Highlight Pass Fail

↓

Attribute	Range	Expected Conc	% Ethanol	% Ethanol	Pass/Fail result
Result (5)	Low	5.18	49.39	1.03	FAIL
Result (4)	Low	10.22	49.37	0.99	FAIL
Result (3)	Mid	33.45	49.41	0.97	FAIL
Result (2)	High	50.25	49.47	0.90	PASS
Result (1)	High	55.67	49.28	1.04	PASS
Count	-	5	5	5	-
Sum	-	154.77	246.92	4.93	-

-- Place Duplicates In Separate Tables. Use this check box to quickly separate results that have the same answer in separate tables. A good use of this option would be to sort the data from a range measurement (e.g., low, mid, high). The software will place all the results that fall in the low range in the first table, mid-range results in a second table, and high-range results in a third table.

**Note** Adding statistical results to a summary format specification does not make them available for use by other events in a workflow. If you want to calculate a statistical value, such as a standard deviation, and then use that standard deviation value in another event, such as a check event, use a calculate event to generate the standard deviation and then add the calculation result to the list of items to be checked. See “Check events” and “Calculate events” for more information. ▲



- **Add Break.** Use this button to add a break to the table. The software displays the following dialog box.



The options for adding breaks to the table section are described below:

- *Heading.* This option allows you to specify data that will become the first cell(s) of every table generated by this table format specification. To specify a heading, make sure the heading row or rows appear at the top of the list of results you want to report. Select the last row of the heading and then choose Add Break. In the Add Break dialog box, select Heading and choose OK. The software will add a heading break immediately below the row you selected.

- *Table.* Use this option to separate the data into multiple tables. To specify a new table, select the last result you want to include in the previous table and then choose Add Break. In the Add Break dialog box, select Table and choose OK. The software will start a new table with the next workflow result in the list of results you want to report.
- *Line.* Use this option to separate the data by starting a new line in the table. To add a line break, select the last result you want to include in the previous line and then choose Add Break. In the Add Break dialog box, select Line and choose OK. The software will skip a line and place the next workflow result on the following line. The skipped line has dashes (“-“) for placeholders.
- *Cell.* Use this option to separate the data by starting a new cell. To add a cell break, select the result you want to include before the cell break and then choose Add Break. In the Add Break dialog box, select Cell and choose OK. The software will skip a cell and place the next workflow result in the following cell. The skipped cell has a dash (“-“) placeholder.

To see how these settings affect the formatting of your summary table, review the examples in the “Table format specifications” section.


 A rectangular button with a grey gradient background and a thin black border. The text "Preview Section" is centered in a dark grey font.

- **Preview Section.** As you make selections in the table format specification to define the layout for your table, use the Preview Section button to view the effect on the final table. In preview mode, only the table headings are shown. Dashes (“-“) are used to represent cells that will be blank in the table as it appears in the sample report. The software uses the phrase (“no rESULT”) to indicate cells where data will appear.

**Usage:** A summary item specification may be linked to the following workflow specification:

- **Report specification.** This specification defines the sections in a sample report and the order in which those sections appear when the report is displayed or printed.

## Sequence heading format specifications

A sequence heading format specification adds a general summary of a sequence collection to a sample report. This is relevant only when the workflow contains a Run Sequence event that is configured properly. See “Chapter 4 Sequence Module Events” in this section for more information.

The sequence heading section 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 collection phase. Sequence heading format specifications allow you to quickly add information about a sequence collection at the top of a sample report. Here is an example:

Run Sequence title	collection
Run Sequence start time	6/21/2004 8:33:31 AM (GMT-05:00)
Run Sequence end time	6/21/2004 8:33:55 AM (GMT-05:00)
Archived base name	No result files archived
Run Sequence aborted	False

Collect Sequence title	Sample
Collect Sequence start	6/21/2004 8:33:31 AM (GMT-05:00)
Total collection time (seconds)	20.029
Number of spectra collected	11
Number of Fail results in Collect Sequence	0
Number of Pass results in Collect Sequence	11
Number of spectra archived	0
Requested temperature	165
Requested pressure	650

### Sequence heading section in a sample report

Sequence heading format specifications may only be linked to report specifications in a workflow.

**Associated events:** Report event

**Associated specifications:** Report specification

**Related events:** None

**Related specifications:** Sequence summary item specification, memo item specification, spectrum item specification, summary item specification, table item specification

**Parameters:** The illustration below shows the parameters for the sequence heading format specification. These parameters appear in the display area of RESULT Integration when a sequence heading format specification is selected in a workflow.

The screenshot shows a dialog box titled "Sequence Heading Item Specification". It contains the following elements:

- A text input field containing "New Sequence Heading".
- A section titled "Heading Format" containing:
  - A text input field for "Title".
  - A dropdown menu for "Border" with "None" selected.
- A section titled "Run Sequence event:" with a dropdown menu.

### Sequence heading format specification parameters

The parameters for the sequence heading format specification define the Run Sequence event that will provide the data and the format. The following sections explain the sequence heading format specification parameters in detail. The parameters are explained in the order in which they appear in the software.

#### Heading Format

The parameters in this group allow you to enter a title and specify the format of a sequence heading section in a sample report.

This close-up shows the "Heading Format" section with the "Title" text field and the "Border" dropdown menu set to "None".

- **Title.** Use the title box to enter a descriptive title for the sequence heading section. The title appears directly above the body of the heading, as shown in the example below.

#### ➔ Sequence Information

<b>Run Sequence title</b>	collection
<b>Run Sequence start time</b>	6/21/2004 9:02:45 AM (GMT-05:00)
<b>Run Sequence end time</b>	6/21/2004 9:03:11 AM (GMT-05:00)

- **Border.** Use this list box to specify a border style for the sequence heading section. You can select a thin, medium, or thick border.

The selected setting is applied to the overall border around the heading as well as to the cells within the heading. The table shown in the previous example has a medium border.

### Run Sequence event

This parameter defines the Run Sequence event that will supply the data to the summary heading.



Use the list box to link the sequence heading format specification to a run sequence event in your workflow. The names of all the run sequence events in the workflow appear in the drop-down list. Choose a run sequence event that appears before the report event associated with this sequence heading format specification in the workflow.

**Usage:** A sequence heading format specification may be linked to the following workflow specification:

- **Report specification,** which defines the sections in a sample report and the order in which those sections appear when the report is displayed or printed.

## Sequence summary format specifications

A sequence summary format specification defines a table of summarized results from a sequence collection in a sample report. This is relevant only when the workflow contains a Run Sequence event that is configured properly. See “Chapter 4 Sequence Module Events” in this section for more information.

You can use a sequence summary format specification to add the numeric results from a sequence measurement to sample report plus a range of statistical values including:

- Count, which tells you the number of measurements that were made.
- Minimum, maximum, and average values.

- Range (maximum value minus minimum value).
- Standard deviation and percent standard deviation.
- Number of failures, which indicates the number of measurements that fell outside any analysis limits specified in the corresponding method. (If no limits were specified, the software will report zero failures.)
- Total area, which provides the sum of the component concentration values over the time of the data collection.

You can set up the summary table to include only the source values from the measurements, to include only the statistical values, or it can include both. The software automatically adds the unit for each measurement to the table, if that information is available.

Here is an example of a simple table of summarized results from a Run Sequence event:

<i>Data type</i>	<i>Sample Methane</i> [ppm]	<i>Sample Carbon monoxide</i> <i>high</i> [ppm]	<i>Sample Carbon dioxide</i> [ppm]	<i>Sample Nitric oxide</i> [ppm]	<i>Sample Nitrogen dioxide</i> [ppm]	<i>Sample Nitrous oxide</i> [ppm]	<i>Sample Ethylene</i> [ppm]
<i>Count</i>	12	12	12	12	12	12	12
<i>Minimum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Maximum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Range</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>Average</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Standard deviation</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>% Standard deviation</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>Total area</i>	0.00	1,010.24	-1,101.86	333.87	34.05	28.01	182.86
<i>Fail results</i>	0	0	0	0	0	0	0

### Table of summarized sequence measurement results

Sequence summary format specifications may only be linked to report specifications in a workflow and must include at least one workflow result to create a sequence summary table in a sample report.

**Associated events:** Report event

**Associated specifications:** Report specification

**Related events:** None

**Related specifications:** Sequence heading item specification, memo item specification, spectrum item specification, summary item specification, table item specification

**Parameters:** The illustration below shows the parameters for the sequence summary format specification. These parameters appear in the display area of RESULT Integration when a sequence summary format specification is selected in a workflow.

Sequence Summary Item Specification

New Sequence Summary

Table Format

Title:

Layout:

Border:

Show acceptance limits  Show event names with attribute names

Table Elements

Run Sequence event:

Summarize these events

Measure event	Component	Format

Report these statistics

Minimum value  Range (max - min)  Total area

Maximum value  Standard deviation  Count

Average  Percent standard deviation  Number of failures

### Sequence summary format specification parameters

The sequence summary format specification parameters define the workflow results presented in the table, any statistical data that will be included, and the table format. The following sections explain the sequence summary format specification parameters in detail. The parameters are explained in the order in which they appear in the software.

## Table Format

The parameters in this group allow you to enter a title for the sequence summary section and specify the format of the summary table.

Table Format

Title:

Layout:

Border:

Show acceptance limits  Show event names with attribute names

- **Title.** Use the title box to enter a descriptive title for the summary table. The title appears directly above the table in the sample report. Here is an example:

### ➔ Summarized Results

<i>Data type</i>	<i>Sample Methane [ppm]</i>	<i>Sample Carbon monoxide high [ppm]</i>	<i>Sample Carbon dioxide [ppm]</i>	<i>Sample Nitric oxide [ppm]</i>	<i>Sample Nitrogen dioxide [ppm]</i>	<i>Sample Nitrous oxide [ppm]</i>	<i>Sample Ethyne [ppm]</i>
<i>Count</i>	12	12	12	12	12	12	12
<i>Minimum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96

- **Layout.** Use this list box to specify the information that will be placed in the table columns and rows. Select Display Data Types In Rows, Attributes In Columns to configure the table to place a descriptive name for each summarized item in each row and the corresponding value in each column. Here is an example of a summary table set up this way.

<i>Data type</i>	<i>Sample Methane [ppm]</i>	<i>Sample Carbon monoxide high [ppm]</i>	<i>Sample Carbon dioxide [ppm]</i>	<i>Sample Nitric oxide [ppm]</i>	<i>Sample Nitrogen dioxide [ppm]</i>	<i>Sample Nitrous oxide [ppm]</i>	<i>Sample Ethyne [ppm]</i>
<i>Count</i>	12	12	12	12	12	12	12
<i>Minimum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Maximum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Range</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>Average</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Standard deviation</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>% Standard deviation</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>Total area</i>	0.00	1,010.24	1,101.86	333.87	34.05	28.01	182.86
<i>Fail results</i>	0	0	0	0	0	0	0

### Table formatted with Data Types in rows, Attributes in columns

Select the other option to flip the rows and columns in the table. The next illustration shows an example of a table formatted this way.

<i>Data type</i>	<i>Count</i>	<i>Minimum</i>	<i>Maximum</i>	<i>Range</i>	<i>Average</i>
<i>Sample - Methane [ppm]</i>	13	0.00	0.00	0.00	0.00
<i>Sample - Carbon monoxide high [ppm]</i>	13	49.50	49.50	0.00	49.50
<i>Sample - Carbon dioxide [ppm]</i>	13	-53.99	-53.99	0.00	-53.99
<i>Sample - Nitric oxide [ppm]</i>	13	16.36	16.36	0.00	16.36
<i>Sample - Nitrogen dioxide [ppm]</i>	13	1.67	1.67	0.00	1.67
<i>Sample - Nitrous oxide [ppm]</i>	13	1.37	1.37	0.00	1.37
<i>Sample - Ethyne [ppm]</i>	13	8.96	8.96	0.00	8.96
<i>Sample - Ethene [ppm]</i>	13	-2.27	-2.27	0.00	-2.27

### Table formatted with Attributes in rows, Data Types in columns

- **Border.** Use this list box to specify a border style for the table. You can select a thin, medium, or thick border or include the table with no border.

The selected setting is applied to the overall border around the table as well as the borders around the individual cells. The table shown in the previous example has a medium border.

Show event names with attribute names

- **Show Event Names With Attribute Names.** Use this option to specify whether the table will include the event name along with the descriptive name for each measured component or attribute. The event name refers to the name you entered for the Run Sequence event when you added the event to the workflow. It appears at the top of the display area when the Run Sequence event is selected in the workflow. The table shown in the first illustration above (Data Types in rows, Attributes in columns) looks like this with the event names hidden.

<i>Data type</i>	<i>Methane [ppm]</i>	<i>Carbon monoxide high [ppm]</i>	<i>Carbon dioxide [ppm]</i>	<i>Nitric oxide [ppm]</i>	<i>Nitrogen dioxide [ppm]</i>	<i>Nitrous oxide [ppm]</i>	<i>Ethyme [ppm]</i>
<i>Count</i>	13	13	13	13	13	13	13
<i>Minimum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Maximum</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Range</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>Average</i>	0.00	49.50	-53.99	16.36	1.67	1.37	8.96
<i>Standard deviation</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>% Standard deviation</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>Total area</i>	0.00	1,083.65	-1,181.94	358.13	36.53	30.05	196.15
<i>Fail results</i>	0	0	0	0	0	0	0

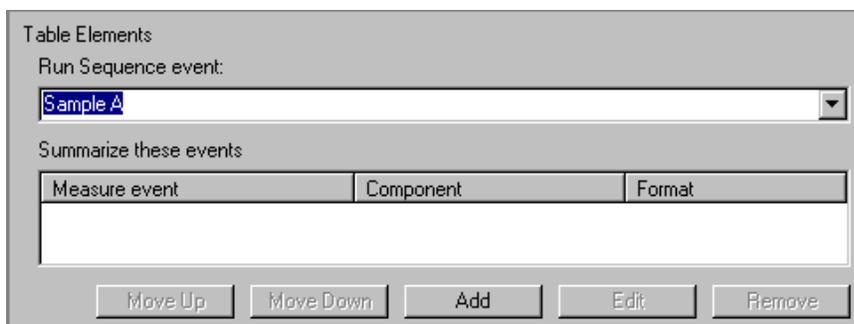
Event names are typically included when the report is set up to summarize the data from multiple Run Sequence events.

Show acceptance limits

- **Show Acceptance Limits.** Select this option if you want the table to include acceptance limits for the summarized components. The workflow extracts the corresponding acceptance limits from the method associated with the run sequence event that is linked to this sequence summary format specification. See your TQ Analyst or other user guide for your method development application to learn how to specify acceptance limits for an analytical method.

### Table Elements

The parameters in this group specify the Run Sequence event that will produce the summarized data, the workflow results that will be included in the table and the sequence of those results.

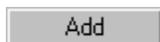


- **Run Sequence Event.** Use this list box to link the sequence summary format specification to a Run Sequence event in your workflow. See “Chapter 4 Sequence Module events” for information about adding Run Sequence events to workflows.

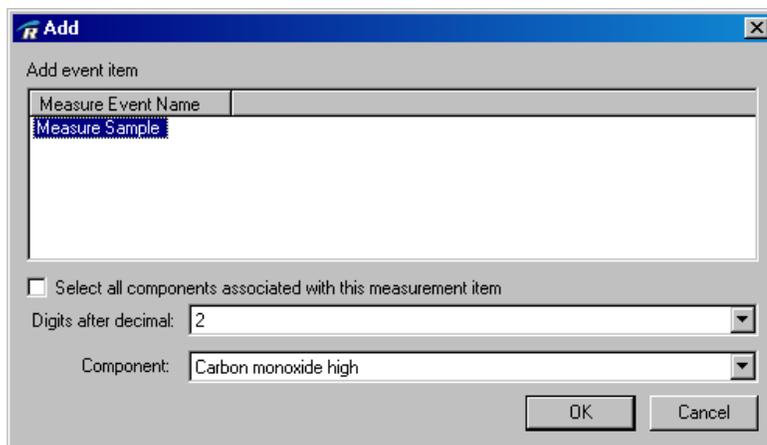


The names of all the run sequence events in the current workflow appear in the drop-down list. Choose a run sequence event that appears before the report event that is associated with this sequence summary format specification in the workflow.

- **Summarize These Events.** Use this feature to specify the workflow results that will be included in the table and the sequence of those results. The following options are available:



- *Add.* To add a workflow result to the table, choose the Add button at the bottom of the sequence summary format specification. The software displays the following dialog box:



The list shows the events in the workflow that provide, measurement results that can be placed in the table.

**Note** If this dialog box is empty, then the workflow either does not contain a Run Sequence event or all of the sequence event results have already been added. ▲

Select a result in the list. Make sure you select a result that exists at this point in the workflow. After you select a result, the following parameters may become available in the software, allowing you to select a component for the event and the format for each component. Examples are provided below.

-- Component. Use this list box to select a component measured by the selected event. The number of components produced by an event depends on the TQ Analyst or other method used for the measurement.

-- Digits After Decimal. Use this list box to select the number of digits the software will include after the decimal point in the numeric result.

A screenshot of a software dialog box. It features a label 'Digits after decimal:' followed by a text input field containing the number '2'. To the right of the input field is a small downward-pointing arrow icon, indicating a dropdown menu.

You can include up to six digits after the decimal point. The software rounds the number and retains only the specified digits after the decimal point.

-- Select All Components Associated With This Measurement Item. Select this option if you want to include all the measured components for the selected measurement event. This option is provided for convenience.

A screenshot of a software dialog box. It shows a single checkbox that is currently unchecked, followed by the text 'Select all components associated with this measurement item'.

When you are finished selecting a result, choose OK. The selected result is added to the list of items to include in the summary table. Here is an example:

Summarize these events

Measure event	Component	Format
Measure New	Hydroxyl Value	_.00_
Measure New	(All)	_.00_

- **Edit.** To edit workflow results that are included in the summary table, select the result in the list and then choose Edit. You can edit the data type, digits after decimal, and attribute settings for the selected event.

- **Remove.** To remove a workflow result from the summary table, select the result and choose Remove. The result will no longer be included in the list of items to be summarized but will remain part of the workflow.

- **Move Up, Move Down.** Use these buttons to move the selected result up or down in the list. The corresponding result will also be moved in any subsequent summary tables created from this workflow.

### Report These Statistics

Use the parameters in this group to specify any statistical values to include in the summary table.

Report these statistics

<input type="checkbox"/> Minimum value	<input type="checkbox"/> Range (max - min)	<input type="checkbox"/> Total area
<input type="checkbox"/> Maximum value	<input type="checkbox"/> Standard deviation	<input type="checkbox"/> Count
<input type="checkbox"/> Average	<input type="checkbox"/> Percent standard deviation	<input type="checkbox"/> Number of failures

The following statistics may be reported.

- Minimum, maximum and average values.
- Range (maximum minus minimum).
- Standard deviation and percent standard deviation.
- Total area (sum of component concentration values over the time of the data collection).
- Count (number of measurements).

- Number of failures (number of measurements that fell outside any analysis limits specified in the corresponding method. (If no limits were specified, the software will report zero failures.).

The selected statistical values will be reported for each measured attribute listed in the sequence summary item specification.

**Note** Adding statistical results to a sequence summary format specification does not make them available for use by other events in a workflow. If you want to calculate a statistical value such as a standard deviation and then use that standard deviation value in another event such as a check event, use a calculate event to generate the standard deviation and then add the calculation result to the list of items to be checked. See “Check events” and “Calculate events” for more information. ▲

**Usage:** A sequence summary item specification may be linked to the following workflow specification:

- **Report specification**, which defines the sections in a sample report and the order in which those sections appear when the report is displayed or printed.

## Sample specifications

A sample specification defines data collection for sample spectra generated by a workflow. Sample specifications may be linked to collection events in a workflow and must include a background specification.

RESULT provides a unique sample specification for each sampling configuration and for the optional validation wheel. The available sample specifications include the following:

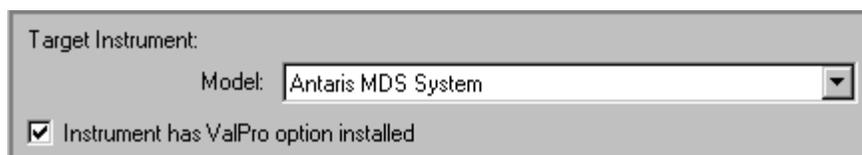
- **Standard Tablet Analyzer sample specification**, which is designed to collect transmission sample data from standard tablets using the Antaris standard tablet analyzer.
- **SoftGel Tablet Analyzer sample specification**, which is optimized for collecting transmission sample data from gel-cap and softgel tablets using the Antaris softgel tablet analyzer.
- **Integrating Sphere sample specification**, which can be used to collect diffuse-reflection sample data from powders and solids using the Antaris integrating sphere.

- **Transmission Module sample specification**, which is set up to collect transmission sample data from liquid and film samples using the Antaris transmission module.
- **Fiber Optic sample specification**, which can be used to analyze samples using a fiber optic accessory connected to any fiber optic module. The Fiber Optic sample specification can only be linked to collect events in a workflow.
- **Multi-Channel Fiber Optic sample specification**, which can be used to analyze samples using fiber optic accessories connected to the Antaris MX and Antaris EX Process analyzer. The Multi-Channel Fiber Optic sample specification can only be linked to Collect Multi-Channel events in workflows.
- **Autosampler Integrating Sphere sample specification**, which is optimized for collecting diffuse-reflection sample data from powders and solids using an autosampler mounted on the Antaris integrating sphere.
- **Autosampler Tablet Transmission Module sample specification**, which is designed for collecting transmission data using an autosampler with a standard tablet analyzer.
- **Autosampler SoftGel Transmission Module sample specification**, which is designed for collecting transmission data using an autosampler with a softgel tablet analyzer.
- **Gas Cell sample specification**, which is designed to collect data from gas samples that are captured in or flowing through a gas cell mounted on an Antaris IGS analyzer.
- **Blend Analyzer sample specification**, which can be used to collect data with the Antaris Target Blend analyzer.
- **Dual Tablet Standard Tablet Analyzer sample specification**, which can be used to collect transmission data from tablet samples that are mounted in the standard tablet analyzer along with the reflection data from the integrating sphere. The Dual Tablet Standard Tablet Analyzer sample specification can only be linked to Collect Dual Tablet events in workflows.

- **Dual Tablet SoftGel Tablet Analyzer sample specification**, which can be used to collect transmission data from tablet samples that are mounted in the softgel tablet analyzer along with the reflection data from the integrating sphere. The Dual Tablet SoftGel Tablet Analyzer sample specification can only be linked to Collect Dual Tablet events in workflows.
- **Dual Tablet Integrating Sphere sample specification**, which can be used to collect reflection data from tablet samples using the Antaris integrating sphere along with the transmission data from a tablet analyzer. The Dual Tablet Integrating Sphere sample specification can only be linked to Collect Dual Tablet events in workflows.
- **Validation Wheel sample specification**, which is designed for analyzing samples mounted on the optional validation wheel.

**Note** Each sample specification has a companion background specification, which defines background collection for the corresponding sampling configuration. See “Background Specifications” in this chapter for more information. ▲

The sample specifications available in RESULT at a given time are dependent on the Target Instrument settings in the Options dialog box (available from the Edit menu in RESULT Integration).



Model defines the possible sampling configurations on the instrument and the corresponding sample specifications available in the software. The check box determines whether the validation wheel sample specification will be available in the software. The validation wheel sample specification works properly only when the optional validation wheel is installed in the instrument.

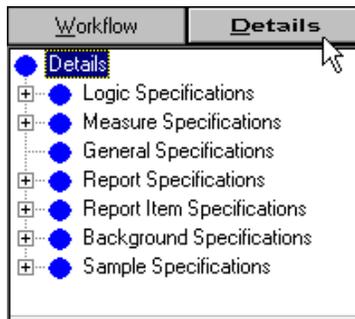
Some parameters are common to all the sample specifications. However, the specifications may have different default settings for those parameters. Other parameters are unique to a particular sample specification or they may appear on several sample specifications but not on others.

This section provides a complete discussion of the characteristics and content of all the sample specifications. Read the section titled “Features common to sample specifications” to learn about the common sample specification parameters. To learn about any additional features that are unique to a specific sampling module, skip to the section with that title.

## **Adding a sample specification to a workflow**

To add a sample specification to the open workflow:

- 1. Select the Details tab, select the Sample Specifications group and then choose the Add button on the RESULT Integration toolbar.**

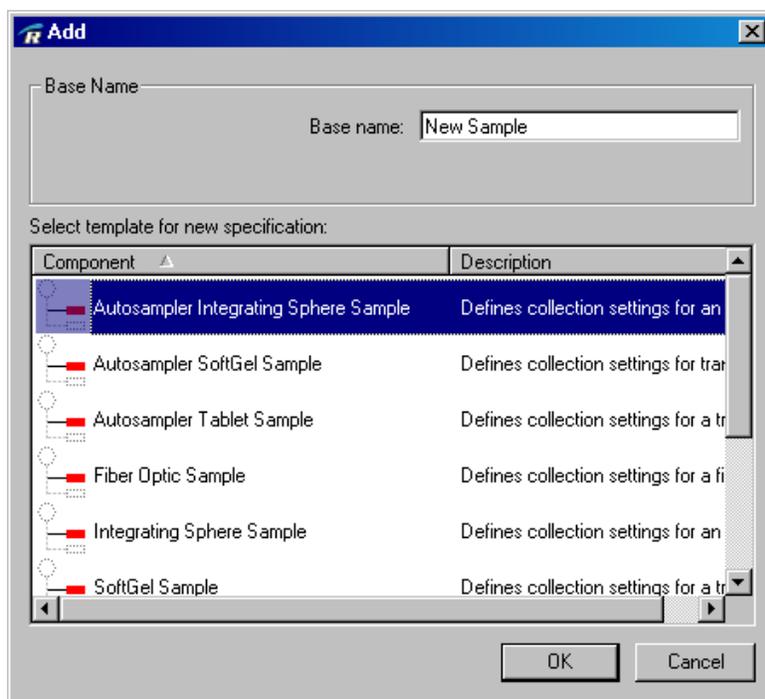


-- or --

**Select the Workflow tab, select the collection event that requires a sample specification and then choose the New button at the right of the Sample Specification drop-down list box.**



The software displays a dialog box listing the sample specifications available for your system. Here is an example:



2. **Select a sample specification, enter a base name for the new specification and then choose OK.**

The new specification appears in the display area of the RESULT Integration main window.

**Note** If a sample specification isn't listed for the sampling module or accessory you want to use, make sure the RESULT add-in option for that module or accessory is properly installed on the computer you use to run RESULT. See *Installing Your Software* in your RESULT document set for more information. You should also check that Model is set correctly in the Options dialog available from the Edit menu in RESULT Integration. ▲

3. **If you added the sample specification from the Details tab, link the new specification to a collection event.**

See "Linking a specification to a workflow event" in "Chapter 2 Creating and Editing Workflows" of the "RESULT Integration User Guide" for instructions.

## Features common to sample specifications

This section describes the features that are common to sample specifications. For information about a specific sample specification, such as the Antaris Standard Tablet Analyzer sample specification, refer to the section with that name later in this chapter.

**Associated events:** Collect event, Collect Dual Tablet event, Collect Multi-Channel event

**Associated specifications:** Background specification

**Related events:** None

**Related specifications:** Prompt specifications

**Parameters:** The illustration below shows the parameters that appear on all the sample specifications. These parameters appear in the display area of RESULT Integration when a sample specification is selected in a workflow.

The screenshot shows a dialog box titled "Sample Specification". At the top, there is a text field containing "New Sample". Below this, the "Sample Collection" section includes a "Sampling technique" dropdown set to "Standard Tablet Analyzer". It features a "Background specification" dropdown set to "New Background" with "New" and "Details" buttons. The "Pre-collection delay (sec)" is a text field with "0", and the "Attenuator" is a dropdown set to "Empty". The "Resolution" is a dropdown set to "8.0 cm-1", and the "Gain" is a dropdown set to "1x" with an "Optimize Gain" button. The "Spectral Range" section has a checked checkbox for "Use standard range in cm-1", with "Start" and "End" text fields containing "6,000.00" and "10,000.00" respectively. The "Samples for Simulation" section has a dropdown menu, "New" and "Delete" buttons, and three unchecked checkboxes: "Prompt for simulation sample", "Use simulation sample for all workflow runs", and "Cycle through simulation samples".

## Features common to sample specifications

The common sample specification parameters define sample data collection, the spectral range for the collected data and any sample spectra that can be used to run the workflow in simulation mode. These

parameters are independent of the sample type or material to be analyzed. (Parameters that are sample specific appear on the associated collection event.) The following sections detail the common sample specification parameters. The parameters are explained in the order in which they appear in the software.

## Sample Collection

Use the parameters in this group to specify sample data collection using a specific sampling module such as the Standard Tablet Analyzer module.

Sampling technique: Standard Tablet Analyzer

Background specification: New Background

- **Sampling Technique.** This readout gives the name of the sampling module and technique that will be used for data collection, such as the Antaris Tablet Analyzer, Integrating Sphere, or Transmission Module.
- **Background Specification.** Use this feature to link a background specification to this sample specification. The background specification defines background collection for the current sampling module and technique. If the workflow already contains an appropriate background specification, select its name in the drop down list (see below).

Background specification: Polystyrene Background

Only background specifications that correspond with the current sample specification appear in the drop-down list. For example, if you are setting up a sample specification that is based on the Standard Tablet Analyzer module, only background specifications that are based on the standard tablet analyzer will appear in the list.

Use the Details button to the right of the list box to display the selected background specification, or the New button to create a background specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the

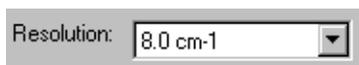
toolbar to return to the sample specification. The new background specification will be linked to the sample specification and its name will appear in the Background Specification list box. See “Background specifications” in this section for more information.

**Note** If you use the workflow wizard to add a collect event to a workflow, the wizard also creates and links appropriate sample and background specifications. ▲

A screenshot of a software interface showing a text input field labeled "Pre-collection delay (sec):" with the value "0" entered.

- **Pre-collection delay.** Use this box to specify a delay before sample collection begins. If you specify a pre-collection delay, when you run the workflow, the workflow will pause the specified number of seconds before it begins collecting the sample data. This is often useful for allowing a cooled or heated sample time to reach room temperature and stabilize before starting the analysis.

Leave Pre-collection Delay set to zero if you don't want to delay data collection.

A screenshot of a software interface showing a drop-down list labeled "Resolution:" with "8.0 cm-1" selected.

- **Resolution.** Use this list box to specify the resolution of the collected spectrum. Resolution is a measure of how well closely spaced peaks in a spectrum are differentiated. The higher the resolution, the more closely spaced peaks can be and still be differentiated.

The Resolution drop-down list includes all the resolution settings for the current sampling module, system, and technique. Although the highest ( $2\text{ cm}^{-1}$ ) resolution setting is available on all Antaris near-infrared systems, the optional two-position aperture is required to achieve maximum spectral resolution at that resolution setting across the full spectral range. The software automatically selects the smaller aperture (if available) when the  $2\text{ cm}^{-1}$  resolution setting is selected in the workflow. (If the two-position aperture is not available, the spectrum will be collected at the  $2\text{ cm}^{-1}$  resolution but the bands will not be as sharp.)

Collect your sample and background spectra using the same resolution. For recommended resolution settings for a particular Antaris sampling module, see the chapter with that title in your *Antaris User Guide*.

**Note** A higher resolution is expressed by a lower numerical value. For example, a spectrum with  $4\text{ cm}^{-1}$  resolution has higher resolution than a spectrum with  $8\text{ cm}^{-1}$  resolution. Keep this in mind when you set the Resolution parameter. ▲



- **Attenuator.** The detectors installed in the Antaris Near-IR analyzers are highly sensitive and can become saturated or produce a distorted signal if too much light reaches the detector element. The attenuation wheel provides two calibrated, energy-limiting screens that can be used to lower the energy sent to a sample. The screens are software selectable and have the following effect on the incident infrared beam.

Screen	Percent of Incident Light Transmitted
None	100
B	6 - 10 %
C	2.5 - 3.5%
C + polystyrene	2.5 - 3.5%

### Attenuation screens in the Antaris Near-IR analyzers

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

The C screen is required for most transmission analyses because the transmitted signal is often intense. If you are using the transmission module to run samples, we recommend starting with the C screen to avoid saturating the detector with excess light. If the sample peaks in the resulting spectrum are small, switch to the B screen, or try using the open position on the attenuation wheel.

The Antaris integrating sphere doesn't usually require screens for sample data collection because the infrared energy is distributed over the entire sphere and, thus, is less intense.

The recommended Attenuator settings for the remaining sampling modules and collection techniques are highly sample dependant. See the individual chapters on the sampling modules available for your system in your *Antaris User Guide* for more information.

**Note** See Optimize Gain (below) for information about using the Optimize Gain button on the sample specification to select the appropriate attenuation and gain settings for a specific sample. ▲

Backgrounds can be collected with the same Attenuator setting that is used for the samples or with the software default setting. The Use Sample Position, Gain, And Attenuation Settings check box on the background specification defines the Attenuator setting used for background collection. When the check box is selected, the software uses the Attenuator setting that is shown on the sample specification. When the check box is cleared, the software uses the default Attenuator setting. The default setting depends on the sampling module used for background collection and, in some cases, the type of background specification. See “Features common to background specifications” in this section for details.



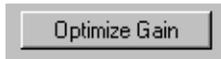
- **Gain.** Use the Gain list box to select the electronic gain for the spectrum. Gain determines how much the detector signal is amplified electronically, making it larger relative to the level of electronic noise. Amplifying the signal is helpful when the signal is weak. For example, the standard tablet analyzer may require a gain setting greater than 1 to achieve adequate signal-to-noise levels in transmission spectra collected from an opaque tablet sample, especially if the sample is thick.

The Gain drop-down list includes all the gain settings for the current sampling module and technique. For recommended gain settings for a particular Antaris sampling module, see the chapter with that name in your *Antaris User Guide*.

You can let the software automatically adjust the gain to maximize the signal by using Optimize Gain on the sample specification (see below). We recommend using Optimize Gain to ensure the best spectral quality.

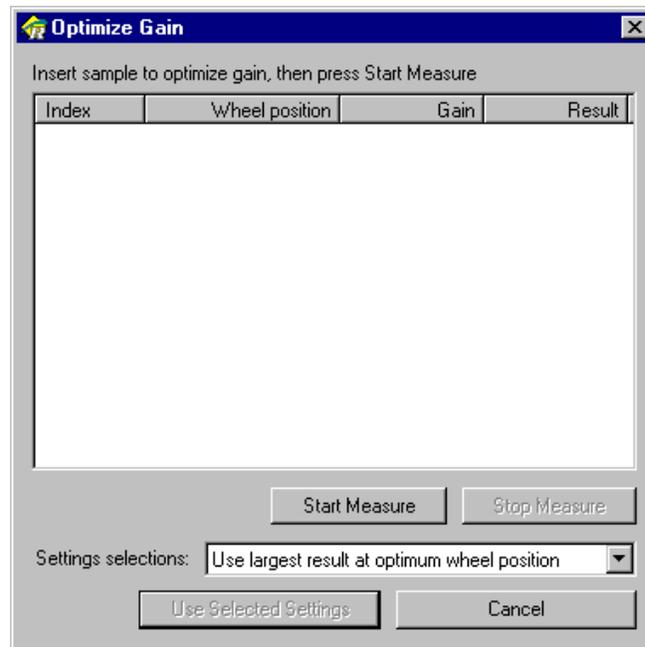
Backgrounds can be collected with the same Gain setting that is used for the samples or with the software default setting. The Use Sample Position, Gain, And Attenuation Settings check box on the background specification defines the gain setting used for background collections. When the check box is selected, the software uses the Gain setting that is shown on the sample specification.

When the check box is cleared, the software uses the default Gain setting. The default setting depends on the sampling module used for background collection and, in some cases, the type of background specification. See “Features common to background specifications” in this section for details.



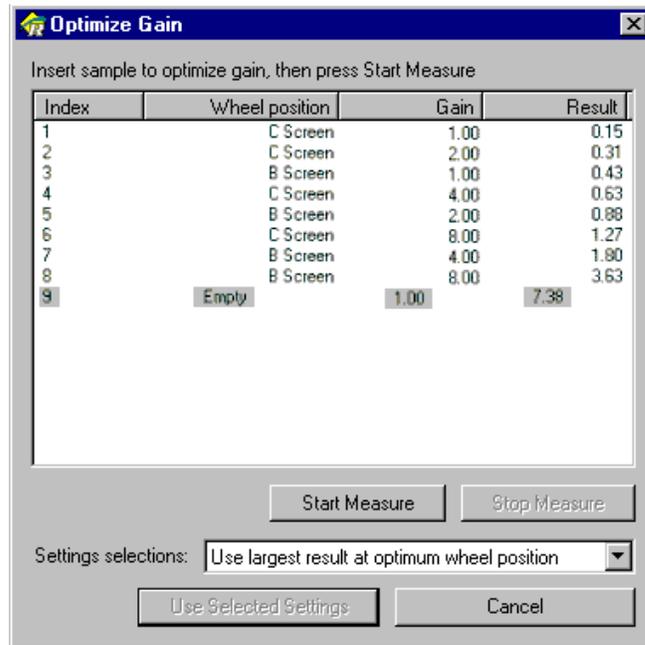
- **Optimize Gain.** This option is included on all the sample specifications except the validation wheel sample specification. The Optimize Gain button may be used to determine the appropriate gain and attenuation settings for a specific sample.

When you choose Optimize Gain on the sample specification, the following dialog box appears:



To determine the recommended gain and attenuation wheel settings for a sample material, prepare a representative sample for data collection, place the sample in the appropriate sampling module, and then choose Start Measure in the Optimize Gain dialog box. The software collects sample data using each possible combination of gain and attenuation settings to find the settings that produce the best results. This may take only a moment or it may take a minute or two, depending on the sample material and the detector used for data collection.

When the measurements are completed, the results appear in a table in the Optimize Gain dialog box, as shown below.



Use Stop Measure to end data collection before the software has finished measuring all the gain and attenuator combinations for the current sample.

The table shows the amplitude of the interferogram peak in volts measured at each attenuation wheel position and gain setting combination. The final (highlighted) values are the recommended settings. In the example shown above, the software recommends setting Attenuator to Empty and setting Gain to 1x.

If you want to use the Attenuator and Gain settings the software recommends, set Settings Selection to Use Largest RESULT At Optimum Wheel Position. If you want to use the gain and attenuation settings that produce the highest voltage value, set Settings Selection to Use Largest RESULT. If you want the software to automatically reset the Attenuator and Gain parameters in this sample specification with the settings your specified above, choose Use Selected Settings. The dialog box closes and the new Attenuator and Gain settings appear on the sample specification.

Choose Cancel to leave the previous settings for Attenuator and Gain parameters on the sample specification.

**Note** If you want to close the Optimize Gain dialog box before the software has completed all the measurements, choose Stop Measure and then wait for data collection to end before choosing Cancel. ▲

## Spectral Range

The parameters in this group define the spectral range of the collected data.



- **Use Standard Spectral Range.** Select this option if you want the software to collect data in the standard frequency range for the selected sampling module, typically between 10,000  $\text{cm}^{-1}$  and 4,000  $\text{cm}^{-1}$  for near-IR systems and between 650  $\text{cm}^{-1}$  and 4,000  $\text{cm}^{-1}$  for mid-IR systems (Antaris IGS only).

If you clear this option, the Start and End boxes become available in the software and may be used to specify a different X-axis range. If you specify custom X-axis limits, the software will only process the collected data between those limits.

**Note** If you are working with the gas cell sample specification for the Antaris IGS analyzer, each combination of detector, beamsplitter and window material installed in the analyzer has a recommended spectral range. See “Sample specifications” in “Chapter 3 Antaris Sampling” of your *Antaris IGS User Guide* for details. ▲

## Samples For Simulation

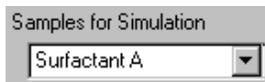
Use the options in this group to specify simulated sample spectra that can substitute for the actual sample spectra collected by the workflow.



This technique can help you shorten workflow development time and facilitate testing and verifying the workflow when it is completed.

The parameters for collecting simulated sample and background spectra, and for selecting the sample spectrum or spectra that will be used for simulated runs of the workflow are described below. You can also use the features in this group to configure the workflow to always run with simulated sample data.

**Note** For information about running workflows in RESULT Integration using simulated data, see “Testing a workflow” in the “RESULT Integration User Guide.” ▲



- **Samples For Simulation.** Use this list box to select a sample spectrum that will be used when this workflow is run with simulated data. If the sample specification contains more than one simulation spectrum, you may set up the workflow to use only the selected spectrum, to prompt the user to select a spectrum, or to use all the simulation spectra stored with this sample specification.

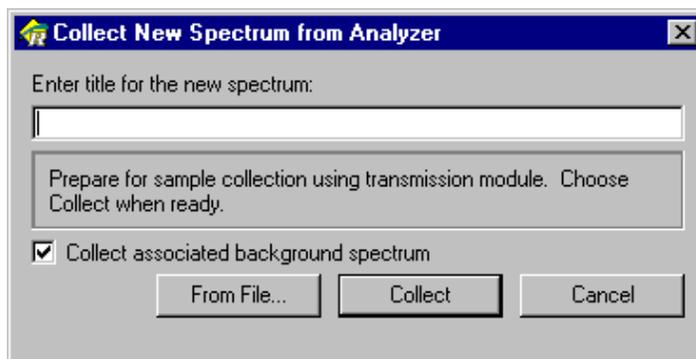
**Note** If you want the workflow to run with simulated sample data and simulated background data (recommended), make sure an appropriate background spectrum is selected in the Backgrounds For Simulation box on the associated background specification. ▲

Use the features described below to add and delete spectra from the list and to specify which spectra should be used for simulated runs of the workflow:



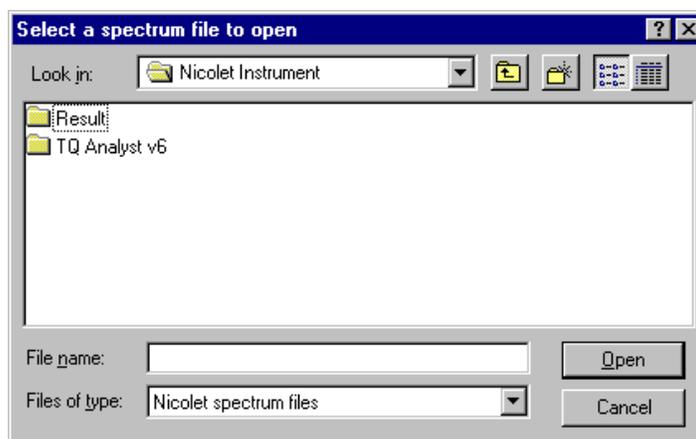
- **New.** Use this button to add a sample to the list of samples for simulation.

The software displays the following dialog box.



You may collect the spectra that will be used for simulated runs of the workflow using the parameter settings in the current workflow (recommended), or select spectral files that are saved on a disk.

- *From File.* If you want to select a spectrum to use for simulated runs of this workflow, choose From File. The following dialog box is displayed.



Locate and select a spectral (\*.spa) file and then choose Open. The software extracts the sample interferogram data and stores it as a simulation sample for this sample specification. If the spectrum has a title, then the title appears in the Samples For Simulation drop-down list on the current sample specification. If the spectrum does not have a title, then the software lists it as “unnamed.”

If Collect Associated Background Spectrum is selected in the Collect New Spectrum From Analyzer dialog box and the file includes background data, then the software also stores the background interferogram data from the selected file as a simulation background. If the background interferogram has a title, then the title appears in the Backgrounds For Simulation box on the associated background specification. If the background interferogram does not have a title, then the software uses the title for the associated sample interferogram, if one exists, or the default title that was used for the sample interferogram.

**Note** If the selected file contains an interferogram or single-beam spectrum, which do not include background data, the software reports an error and redisplay the Select A Spectrum File To Open dialog box allowing you to select a different file. You cannot use a stored interferogram or single-beam spectrum as a simulated sample spectrum. ▲

If Collect Associated Background Spectrum is cleared in the Collect New Spectrum From Analyzer dialog box, then the selected sample will not have an associated background for use in simulated runs of this workflow, and the workflow may produce an error when you run it in simulation mode.

Repeat these steps for each additional spectrum you want to add to the Samples For Simulation drop-down list.

- *Collect.* If you want to collect a spectrum and background to use for simulated runs of this workflow, make sure you first finalize the parameters in the sample and background specifications and in the associated collect event. Then prepare a representative sample for data collection and enter a descriptive title for the new spectrum in the appropriate entry box, as shown below.



Enter title for the new spectrum:  
Polystyrene sample

**Note** Make sure you title the new spectrum by filling in the Enter Title For New Spectrum box. You won't be able to edit or enter a title after the spectrum has been collected. ▲

- *Collect Associated Background Spectrum.* If you want to collect a background spectrum that will be used to process the sample data (recommended), make sure Collect Associated Background Spectrum is selected in the Collect New Spectrum From Analyzer dialog box, as shown below.



Collect associated background spectrum

We recommend that you collect an associated background spectrum for each simulation sample unless the workflow is set up to save only the interferogram or single-beam spectra. (See Data Format on the collect event that is associated with this sample specification in the workflow.) If you don't collect an associated background spectrum, the workflow may produce an error when you run it in simulation mode.

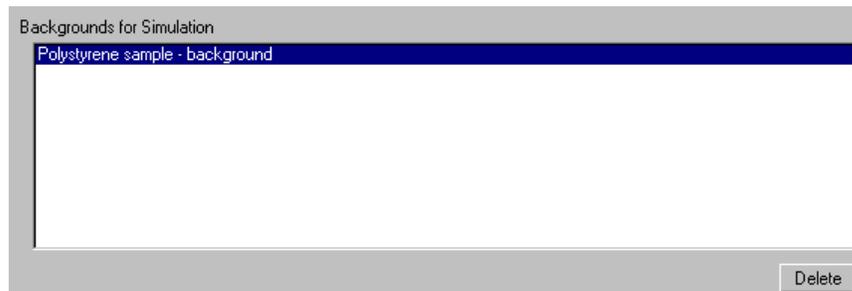
If you clear this option, then the software will use the background spectrum that is stored in the computer's internal memory to process your sample spectrum, if that background is appropriate for the current workflow and the background is still valid.

- *Collect Sample and background.* When the sample is ready, choose Collect. The software displays the status of the collection in the dialog box. If Collect Associated Background Spectrum is selected, the software collects one scan of the background, and then collects one scan of the sample. When data collection is completed, the

dialog box closes and the title of the new spectrum appears in the Samples For Simulation drop-down list, as shown below. (If the sample specification already contains a sample for simulation, the new sample will appear at the end of the drop-down list and not in the list box.)



If you collected an associated background spectrum for this sample, a corresponding background spectrum is added to the list of backgrounds for simulation on the background specification that is linked to this sample specification in the workflow. The new background for simulation has the same base title as its associated sample spectrum, as shown in the example below.



Repeat these steps for each additional simulated sample spectrum and associated background that you want to store with this sample specification in the workflow.

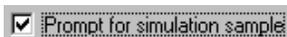
**Note** You can store up to 500 simulation spectra (backgrounds and samples) in a single workflow. ▲

Storing simulated spectra with a workflow can facilitate workflow development and testing. You can also use simulated spectra to verify pass/fail results or other elements in your workflow which are based on the results of a logical test by collecting one sample that produces each logical test result. For example, if you are using a check event to generate a pass/fail result from a measure event, collect one spectrum that will generate the pass result and another that will produce the fail result. If you allow the user to select a sample for simulation (see Prompt For Simulation Sample below), you can use the two samples to verify the check event when you run the workflow.



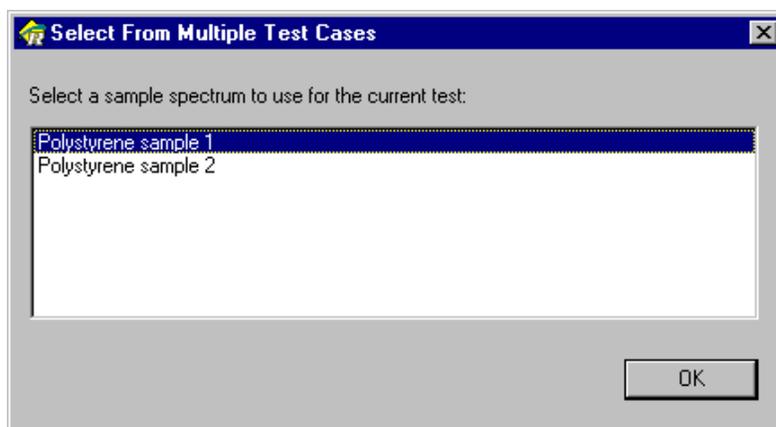
- **Delete.** To remove a sample spectrum so that it is no longer available for use in simulated runs of the workflow, select the spectrum listed in the Samples For Simulation drop-down list and then choose the Delete button at the right of the list box.

**Note** After you delete a spectrum from the list of samples for simulation, the operation cannot be reversed (for example with Undo). ▲

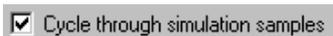


- **Prompt For Simulation Sample.** This option is available in the software only when the Samples For Simulation drop-down list contains at least two entries and the Cycle Through Simulation Samples check box is cleared. .

Select Prompt For Simulation Sample if you want the workflow to prompt the user to select a sample spectrum when the workflow is run using simulated data. The illustration below shows an example of this type of prompt.



If this option is cleared and the workflow is run using simulated data, then the workflow will run using the spectrum whose title appears in the Samples For Simulation list box.



- **Cycle Through Simulation Samples.** This option is available in the software only when the Samples For Simulation drop-down list contains at least two entries.

Select Cycle Through Simulation Samples if you want the workflow to cycle through all the simulation samples stored with this sample specification when the workflow is run using simulated data. The first time you run the workflow, the software will use the spectrum shown in the Samples For Simulation list box, as shown below.



The next time you run the workflow, the workflow will use the spectrum that appears below the first spectrum in the drop-down list, and so on until all the simulation samples have been used. Then the workflow starts again with the sample shown in the list box.

The feature is useful for running a workflow that contains a collection event positioned in a loop with simulated data by allowing the collect event to call a different simulated spectrum each time the loop is repeated.

If Cycle Through Simulation Samples is cleared and the workflow is run using simulated data, the workflow will run using the spectrum whose title appears in the Samples For Simulation list box.

Use simulation sample for all workflow runs

- **Use Simulation Sample For All Workflow Runs.** Select this option to configure the workflow to run only with simulated sample data. This feature applies when the workflow is run in RESULT Integration or RESULT Operation, and is the only way to run workflows with simulated sample data in RESULT Operation.

If the Prompt For Simulation Sample and Cycle Through Simulation Samples check boxes (see above) are both cleared, the workflow will run using the spectrum that is currently selected in the Samples For Simulation list box. If Prompt For Simulation Sample is selected (the workflow must contain at least two samples for simulation), the workflow will prompt the user to select a simulation sample. If Cycle Through Simulation Samples is selected, the first time you run the workflow, it will run with the first sample that appears in the Samples For Simulation list box. The next time you run the workflow, the workflow will use the sample that appears below the first sample in the Samples For Simulation drop-down list and so on until all of the simulation samples have been used. Then the workflow starts again with the sample shown in the list box.

**Note** If you want the workflow to run with simulated sample data and simulated background data (recommended), make sure Use Simulation Sample For All Workflow Runs is also selected on the associated background specification. See Backgrounds For Simulation in General Background Specification features for more information. ▲

When Use Simulation Sample For All Workflow Runs is cleared, the user may select whether to run the workflow normally or with simulated data when running the workflow in RESULT Integration.

**Usage:** A sample specification may be linked to the following workflow events:

- **Collect event**, which typically collects a sample and associated background spectrum in a workflow.
- **Collect Dual Tablet event**, which can be used to collect a transmission and reflection spectrum at the same time with an Antaris tablet analyzer.
- **Collect Multi-Channel event**, which can be used to collect data from two or more fiber optic sampling accessories at the same time.

A sample specification must be linked to a corresponding background specification in a workflow.

## **Standard Tablet Analyzer sample specifications**

This specification contains parameters that are optimized for collecting transmission sample data using the Antaris standard tablet analyzer. The Standard tablet analyzer sample specification may be linked to collect events in a workflow and must include a standard tablet analyzer background specification.

The illustration below shows the parameters for the Antaris standard tablet analyzer sample specification. These parameters appear in the display area of RESULT Integration when a standard tablet analyzer sample specification is selected in a workflow.

Sample Specification

New Sample

Sample Collection

Sampling technique: Standard Tablet Analyzer

Background specification: New Background

Pre-collection delay (sec): 0 Attenuator: Empty

Resolution: 8.0 cm<sup>-1</sup>

Gain: 1x

Spectral Range

Use standard range in cm<sup>-1</sup>

Start: 6,000.00 End: 10,000.00

Samples for Simulation

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

### Sample specification for standard tablet analyzer

There are no parameters that are unique to the sample specification for the Antaris standard tablet analyzer. The sample specification differs only in the default settings for those parameters. For descriptions of the parameters that are common to all the sample specifications, see “Features common to sample specifications” in this chapter. For information about recommended settings for the standard tablet analyzer, see “Developing workflows for a tablet analyzer” in your *Antaris User Guide*.

### SoftGel Tablet Analyzer sample specifications

This specification contains parameters that are optimized for collecting transmission sample data from gel-cap and softgel tablets using the Antaris SoftGel tablet analyzer. The softgel tablet analyzer sample specification may be linked to collect events in a workflow and must include a softgel tablet analyzer background specification.

The illustration below shows the parameters for the Antaris SoftGel Tablet Analyzer sample specification. These parameters appear in the display area of RESULT Integration when a softgel tablet analyzer sample specification is selected in a workflow.

Sample Specification

New Sample

Sample Collection

Sampling technique: SoftGel Tablet Analyzer

Sample position:

Background specification:

Pre-collection delay (sec):  Attenuator:

Resolution:

Gain:

Spectral Range

Use standard range in cm-1

Start:  End:

Samples for Simulation

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

### Sample specification for softgel tablet analyzer

There are no parameters that are unique to the sample specification for the Antaris SoftGel tablet analyzer. The sample specification differs only in the default settings for those parameters. For descriptions of the parameters that are common to all the sample specifications, see “Features common to sample specifications” in this chapter. For information about recommended settings for the SoftGel tablet analyzer, see “Developing workflows for a tablet analyzer” in your *Antaris User Guide*.

## Integrating Sphere sample specifications

This sample specification contains parameters that are optimized for collecting diffuse-reflection data from powders and solids using the Antaris integrating sphere module (or the integrating sphere portion of a tablet analyzer). The integrating sphere sample specification may be linked to collect events in a workflow and must include an integrating sphere background specification.

The illustration below shows the parameters for the integrating sphere sample specification. These parameters appear in the display area of RESULT Integration when an integrating sphere sample specification is selected in a workflow.

Sample Specification

New Sample

Sample Collection

Sampling technique: Integrating Sphere

Sample Cup Spinner: None

Background specification: [ ] New Details

Pre-collection delay (sec): 0 Attenuator: Empty

Resolution: 8.0 cm-1

Gain: 1x Optimize Gain

Spectral Range

Use standard range in cm-1

Start: 4,000.00 End: 10,000.00

Samples for Simulation

[ ] New Delete

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

### Sample specification for integrating sphere

The following parameter is unique to the integrating sphere sample specification.

- **Sample Cup Spinner.** This option is available in the software only when an integrating sphere sample specification is displayed in a workflow. The list box allows you to control the Sample Cup Spinner,

which is a sampling accessory that allows multi-point reflection measurements of heterogeneous solids such as powders, granules and pellets. Use the list box to specify whether the Sample Cup Spinner will be used for data collection and whether collection should occur with or without verifying sample cup rotation.

The options that appear in the Sample Cup Spinner drop down list are described below:

- *None.* Use this option to set up data collection using the integrating sphere and Sample Cup Spinner with no rotation of the sample cup. This is the default setting for the Sample Cup Spinner parameter and the recommended setting when no Sample Cup Spinner accessory is installed.
- *Spin Sample Cup.* Select this option if you want the software to spin the sample cup during sample collection without performing any error checking. This setting completes data collection slightly faster but does not produce an error if the cup fails to rotate or if no cup is installed.
- *Spin Sample And Verify Cup Rotation.* Select this option if you want the software to spin the sample cup during sample collection and perform error checking. If the cup fails to rotate during data collection or if no cup is installed, the software stops the workflow and displays the following workflow error:

### Errors While Running Workflow

Event Name	Error Description
Collect Test Sample Cup Spinner	Could not collect data using Antaris integrating sphere. Unable to verify Antaris sample cup rotation.

The remaining parameters on the integrating sphere sample specification are described in the section titled “Features common to sample specifications” in this chapter except the default settings may vary. For information about recommended settings for the integrating sphere, see “Developing workflows for the integrating sphere” in your *Antaris User Guide*.

## Transmission Module sample specifications

This sample specification contains parameters that are optimized for collecting transmission sample data from liquid and film samples using the Antaris transmission module.

The illustration below shows the parameters for the transmission module sample specification. These parameters appear in the display area of RESULT Integration when a transmission module sample specification is selected in a workflow.

Sample Specification

New Sample

Sample Collection

Sampling Technique: Transmission Module

Sample position: Front Sample Compartment

Background specification: New Background [New] [Details]

Pre-collection delay (sec): 0 Attenuator: C Screen

Resolution: 8.0 cm-1

Gain: 1x [Optimize Gain]

Use standard spectral range (in cm-1)

Start: 4,000.00 End: 10,000.00

Use heated cell  Allow operator to override heater pause

Cell temperature (C): 25.00 Max pause (sec): 900

Samples for Simulation

[New] [Delete]

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

### Sample specification for transmission module

The following parameters are unique to the transmission module sample specification.

- **Sample Position.** Use this list box to specify the location for sample data collection with the transmission module. The sample compartment for the transmission module accommodates a variety of three-position sample holders for analyzing liquids, transparent solids and thin films. The sample holders are referred to as having three

positions because they have both a front and a rear position where samples can be collected, and there is an opening in the center through which backgrounds can be collected.

If you plan to use the front position of the sample holder for collecting sample data, set Sample Position to Front Sample Compartment, as shown below.



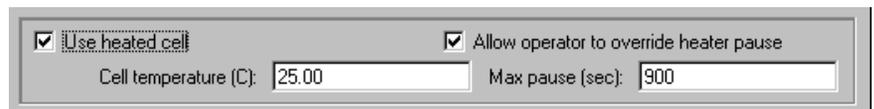
Sample position: Front Sample Compartment

If the samples will be located in the sample holder's back position, set Sample Position to Rear Sample Compartment.

- **Use Heated Cell.** Select this option if you want to use the heated version of the three-position sample tube holder for transmission analysis of liquid samples at elevated temperatures.

**Note** Pre-heating the samples using an external block heater is recommended because it eliminates having to wait for the sample holder to heat each sample. ▲

When this option is selected, additional features become available in the software allowing you to set the temperature of the sample holder and a time period for the sample to reach the target temperature.



Use heated cell  Allow operator to override heater pause  
Cell temperature (C): 25.00 Max pause (sec): 900

When Use Heated Cell is selected, the following options are available in the software.

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

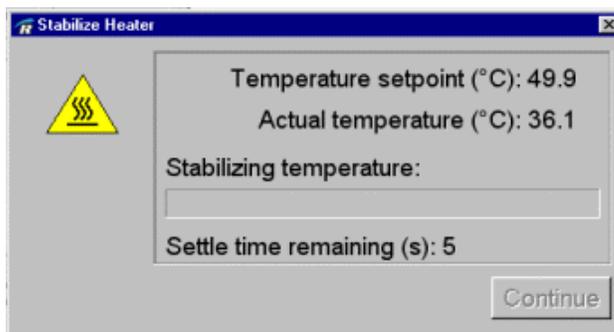
For practical purposes, do not heat the sample holder higher than 100 °C. Samples heated above that limit take a long time to stabilize. Also, remember that you cannot set the temperature below the internal temperature of the instrument. The heated sample holder cannot maintain a temperature lower than that of the surroundings.

- *Maximum Pause.* The transmission module can be set to allow a specified amount of time for the temperature of the heated sample holder to stabilize before collecting data. The amount of time that is appropriate depends on the nature of your sample and the temperature you want to maintain.

If you want to require the workflow to pause with the sample holder positioned in the transmission module and the heating element activated, enter the number of seconds for the workflow to pause. The workflow will wait the specified interval unless the sample stabilizes before that time has elapsed. If the sample stabilizes sooner, the software will begin collecting data at that time.

- *Allow operator to override heater pause.* Select this option if you want to allow the operator to choose whether to wait until the specified pause interval has passed before starting data collection, or to begin collecting sample data earlier.

When this option is selected, the workflow displays a dialog box that contains a message indicating that the system is waiting for the sample to reach its set point and a Continue button. If the operator chooses Continue, the workflow stops waiting, even if the specified pause interval is not completed or the temperature is not stable, and proceeds with data collection.



**Notice** If temperature is critical to the analysis, the quality of your data may be affected by using this option. ▲

When this option is cleared, the workflow displays the same dialog box but the Continue button is unavailable in the dialog box and the operator is forced to wait until the specified pause interval has elapsed.

The remaining parameters on the transmission module sample specification are described in the section titled “Features common to sample specifications” in this chapter except the default settings may vary. For information about recommended settings for the transmission module, including a table of time and temperature values for heating the sample holder, see “Developing workflows for the transmission module” in your *Antaris User Guide*.

## Fiber Optic sample specifications

This sample specification contains parameters that are optimized for analyzing samples using the Antaris fiber optic module. You can use this fiber optic sample specification to collect sample data with an Antaris or Antaris II system that includes a fiber optic sampling station or to collect a sample spectrum using one channel of an Antaris MX or EX analyzer.

The illustration below shows the parameters for the fiber optic module sample specification. These parameters appear in the display area of RESULT Integration when a fiber optic module sample specification is selected in a workflow.

The screenshot shows a software interface titled "Sample Specification". At the top, there is a text field containing "New Sample". Below this, the "Sample Collection" section includes several parameters: "Sampling technique" is set to "Fiber Optic Probe", "Channel number" is "1", "Probe type" is "Third party", "Background specification" is "New Background" with "New" and "Details" buttons, "Pre-collection delay (sec)" is "0", "Attenuator" is "C Screen", "Resolution" is "8.0 cm-1", and "Gain" is "1x" with an "Optimize Gain" button. The "Spectral Range" section has a checked box for "Use standard range in cm-1", with "Start" at "4,000.00" and "End" at "10,000.00". The "Samples for Simulation" section features a dropdown menu, "New" and "Delete" buttons, and three unchecked checkboxes: "Prompt for simulation sample", "Use simulation sample for all workflow runs", and "Cycle through simulation samples".

### Sample specification for fiber optic module

The following parameters are unique to the fiber optic sample specification:

- **Channel Number.** Use this entry box to specify a fiber optic channel for collecting data with the Antaris MX analyzer. The number of channels available (typically, two or four) is dependent on how the Antaris MX is configured. See your *Antaris MX User Guide* for details.

The Channel Number setting has no effect for the other Antaris instrument models. It is available on the fiber optic sample specification so that users can use an Antaris or Antaris II analyzer to develop workflows for the Antaris MX.

- **Probe Type.** Use the Probe Type list box to specify the fiber optic probe that will be used for data collection. The following options are available:
  - *Antaris SabIR.* If you are using the Antaris SabIR probe, set Probe Type to Antaris SabIR. Selecting this option will enable the software to detect when the probe is properly inserted into the holster on the instrument. The probe must be properly inserted into the holster to collect backgrounds using the internal reference. This setting also allows the operator to use the probe trigger as the Acknowledge button on the instrument.
  - *Third Party.* All other fiber optic probes require the Third Party setting for Probe Type, as shown below.

The remaining parameters on the fiber optic sample specification are described in the section titled “Features common to sample specifications” in this chapter except the default settings may vary. For information about recommended settings for the fiber optic module and SabIR probe, see “Developing workflows for the fiber optic module” in your *Antaris User Guide*.

## **Multi-Channel Fiber Optic sample specifications**

This sample specification contains parameters that are optimized for analyzing samples with fiber optic accessories that are connected to an Antaris MX or Antaris EX Process analyzer. Multi-channel sample specifications can only be linked to Collect Multi-Channel events in a workflow.

The illustration below shows the parameters for the multi-channel sample specification. These parameters appear in the display area of RESULT Integration when a multi-channel sample specification is selected in a workflow.

Sample Specification

New Sample

Multi-Channel Sample Collection

Sampling technique: Fiber Optic Probe

Probe type: Antaris SabIR

Gain: 1x Optimize Gain

Spectral Range

Use standard range in cm-1

Start: 4,000.00 End: 10,000.00

Samples for Simulation

New Delete

Use simulation sample for all workflow runs

Cycle through simulation samples

### Sample specification for multi-channel fiber optic module

The following parameter is unique to the multi-channel sample specification:

- **Probe Type.** Use this list box to specify the fiber optic accessory that will be used for sample data collection from a specific fiber optic channel on the instrument. The following options are available:
  - *Antaris SabIR.* If you are using the Antaris SabIR probe, set Probe Type to Antaris SabIR. Selecting this option will enable the software to detect when the probe is properly inserted into the holster on the instrument. The probe must be properly inserted into the holster to collect backgrounds using the internal reference. This setting also allows the operator to use the probe trigger as the Acknowledge button on the instrument.
  - *Third Party.* Use this setting for all other fiber optic accessories purchased from us or elsewhere.

The remaining parameters on the multi-channel sample specification are described in the section titled “Features common to sample specifications” in this chapter except the default settings may vary. For information about recommended settings for fiber optic accessories, including the SabIR probe, see “Developing workflows for the Antaris MX” in your *Antaris MX User Guide*.

## Autosampler sample specifications

There are three autosampler sample specifications for the autosampler integrating sphere, autosampler tablet transmission module, and autosampler SoftGel transmission module. The autosampler integrating sphere sample specification contains parameters that are optimized for collecting diffuse-reflection data from powders and solids using an autosampler mounted on the Antaris integrating sphere sampling module. The autosampler standard and SoftGel transmission module sample specifications contain parameters that are optimized for collecting transmission data using an autosampler with a standard or SoftGel tablet analyzer.

The next illustration shows the parameters for the autosampler integrating sphere sample specification.

These parameters appear in the display area of RESULT Integration when an autosampler integrating sphere sample specification is selected in a workflow.

The screenshot shows a dialog box titled "Sample Specification" with a "New Sample" input field at the top. Below this, the "Sample Collection" section includes a "Sampling technique" dropdown set to "Autosampler - Integrating Sphere". It features two dropdown menus for "Background specification" and "Autosampler specification", each with "New" and "Details" buttons. The "Pre-collection delay (sec)" is set to 0, and the "Attenuator" is set to "Empty". The "Resolution" is set to "8.0 cm-1" and the "Gain" is set to "1x", with an "Optimize Gain" button. The "Spectral Range" section has a checked "Use standard range in cm-1" checkbox, with "Start" at 4,000.00 and "End" at 10,000.00. The "Samples for Simulation" section has a dropdown menu, "New", and "Delete" buttons, and three unchecked checkboxes: "Prompt for simulation sample", "Use simulation sample for all workflow runs", and "Cycle through simulation samples".

**Sample specification for autosampler integrating sphere**

The following parameter is unique to all three autosampler sample specifications (integrating sphere, standard tablet analyzer, and SoftGel tablet analyzer).

- **Autosampler Specification.** Use this feature to link an autosampler specification to this sample specification. The autosampler specification defines the autosampler configuration. If the workflow already contains an appropriate autosampler specification, select its name in the drop down list (see below).



Use the Details button at the right of the list box to display the selected autosampler specification, or the New button to create an autosampler specification. The workflow displays the parameters on the right side of the RESULT Integration main window. When you have finished reviewing or editing the parameters, choose the Back button on the toolbar to return to the sample specification. The new autosampler specification will be linked to the sample specification and its name will appear in the Autosampler Specification list box. See “Autosampler specifications” in this chapter for more information.

The remaining parameters on the autosampler sample specification are described in the section titled “Features common to sample specifications” in this chapter except the default settings may vary. For information about recommended settings for autosamplers, see the autosampler user guide.

## Gas Cell sample specifications

This sample specification contains parameters that are optimized for collecting transmission data from samples captured in or flowing through a gas cell. Gas cell sample specifications can only be used with the Antaris IGS (Industrial Gas Sampling) analyzer.

The illustration below shows the parameters for the gas cell sample specification. These parameters appear in the display area of RESULT Integration when a gas cell sample specification is selected in a workflow.

Sample Specification

NewSample

Sample Collection

Sampling technique: Gas Cell

Beam path: Gas Cell

Background specification:  New Details

Pre-collection delay (sec): 0

Resolution: 8.0 cm<sup>-1</sup>

Gain: 1x Optimize Gain

Apodization: Happ-Genzel

Zero filling: None

Velocity: 1.8988

Scan: Normal (full stroke)

Use standard spectral range (in cm<sup>-1</sup>)

Start: 650.00 End: 4,000.00

Samples for Simulation

New Delete

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

### Sample specification for gas cell sample

The following parameters are unique to the gas cell sample specification.

- **Beam Path.** Use the Beam Path list box to specify the path of the infrared beam when collecting data with the Antaris IGS analyzer.

Beam path: Gas Cell

The following Beam Path options are available:

- *Gas Cell.* Select this option to direct the beam through the *sample beam path compartment* and gas cell and back to the *detector*. This is the “upper” beam path referenced in the *Antaris IGS User Guide*. The Gas Cell beam path setting should be used to collect data from samples that are captured in or flowing through the gas cell.

- *Instrument.* Select this option to direct the beam through the *spectrometer compartment* and then directly to the detector. This is the “lower” beam path referenced in the *Antaris IGS User Guide*. The Instrument beam path setting is typically used only to check instrument operation or status.
- **Apodization.** The Apodization parameter determines the type of apodization that is used before the *interferogram* is *Fourier transformed*. Apodization removes peak side lobes that can occur because the interferogram is not an infinite set of data. The apodization types described in the following table are available. Collect your sample and background spectra using the same apodization type.

Setting	Description
Happ-Genzel	It suppresses side lobes more effectively than the triangular type and with less reduction in resolution than that type. (It results in more reduction in resolution than the boxcar type.) If you are measuring condensed-phase samples, use Happ-Genzel apodization.
Triangular	Mathematically weights interferogram data to reduce ringing effects (side lobes), resulting in lower resolution than that obtained with the boxcar and Happ-Genzel types. Some ringing will usually be present with this type. This setting is normally used only to reproduce the results of other experiments that used it.
Boxcar	The interferogram is unweighted; that is, the data are simply truncated at the beginning and end. Use this type when you are measuring a gas sample, want maximum resolution and are not concerned about ringing effects (side lobes). The greatest amount of ringing will be present with this type.
N-B* Weak	<p>This setting has a less pronounced smoothing effect on data than do the N-B medium and N-B strong types and degrades the resolution less than those types. Side lobes appear on both sides of peaks and are more pronounced for sharper peaks.</p> <p>Use this setting only when the best possible resolution is required. This setting is generally not recommended and is normally used only to reproduce the results of other experiments that used it.</p>

Setting	Description
N-B* Medium	This type has a smoothing effect on data which is between that of the N-B weak and N-B strong types. It suppresses side lobes as much as possible given that it only moderately degrades the resolution of the spectrum. The side lobe suppression is more significant than for N-B weak apodization. This setting is suitable for most normal samples; it gives results virtually identical to those obtained with Happ-Genzel.
N-B* Strong	This setting has a greater smoothing effect on data than do the N-B weak and N-B medium types and degrades the resolution of the spectrum more. The side-lobe suppression is more significant than for N-B medium apodization.
Cosine	This apodization lies between Boxcar and Triangular apodization. There is some reduction in the amplitude of the side lobes, but only a small loss of resolution. This setting is normally used only to reproduce the results of gas measurement experiments taken using cosine apodization.
Blackman-Harris	The 4-term Blackman-Harris function is a strong apodization function that is better than any of the others at suppressing side lobes. However, it results in greater line broadening than any of the others. In practice this has the effect of reducing random noise in a spectrum while causing band broadening.

---

\* "N-B" stands for Norton-Beer.

---

The N-B Medium apodization setting is recommended for collecting data from most types of gases. For higher resolution experiments, you may get better results with the N-B Strong or Happ-Genzel apodization setting. See “Tips for Developing Workflows” in your *Antaris IGS User Guide* for additional recommendations for optimizing the apodization setting for gas analysis experiments.

- **Zero Filling.** Zero Filling determines the number of levels of zero filling used when the data are Fourier transformed. Zero filling improves the line shape of a spectrum by adding data points between collected data points. Sharp features become smoother and more like typical peaks when zero filling is used.

Because data points are added, the transform takes longer. Zero filling does not increase the "true" resolution of the data, however, since that is determined by the number of data points collected. The available settings of Zero Filling are described in the following table.

Setting	Description
None	No zero filling is done.
1 Level	One data point is added between each data point.
2 Levels	This setting adds three points between each data point to better define band shapes.

Set Zero Filling to None for normal work. If the spectrum contains very sharp peaks, try setting Zero Filling to 1 Level or 2 Levels instead of None.

Collect your sample and background spectra using the same number of levels of zero filling.

- **Velocity.** Velocity determines the speed of the moving mirror in the interferometer. Depending on the type of detector installed in the Antaris IGS, start with the default velocity values given in the table below.

Detector	Velocity Setting
DTGS	0.6329 cm <sup>-1</sup>
MCT-A	3.1647 cm <sup>-1</sup>

The default velocity settings are recommended for most gas analysis experiments. If sample throughput is low, you may find that you can increase the signal intensity to an adequate level by using a slower velocity. The results will depend on the detector you are using.

Using a faster velocity will decrease the amount of time required to collect each scan; however, using a velocity that is faster than the recommended setting may produce a noisier signal. See "Collection times" in your *Antaris IGS User Guide* for information about optimizing velocity values for gas analysis experiments.

Collect your sample and background spectra using the same velocity.

**Note** If your Antaris IGS system is equipped with the closed-cycle MCT-A detector, do not use velocities that are slower than the default velocity setting ( $3.1647 \text{ cm}^{-1}$ ). That detector operates properly only when Velocity is set to  $3.1647 \text{ cm}^{-1}$  or higher. ▲

- **Scan.** Use this option to specify 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. The available Scan settings are described in the following table.

Setting	Description
Normal (full stroke)	Collects data over the entire length of the mirror path during the forward stroke. The mirror speed is constant throughout the forward and return strokes. Optimizes both resolution and stability.
Fast (full stroke, quick turnaround)	Collects data over the entire length of the mirror path during the forward stroke. The mirror speeds up while changing direction. Results in faster collection time than the Normal option but with very slight decrease in stability.
Faster (shorter stroke, quick turnaround)	Omits some data points at the end of each stroke of the mirror and employs the same quick turnaround technique described above. Results in faster collection time than the previous option but with slight decrease in resolution.
Faster (full bi-directional stroke)*	Collects data over the entire length of the mirror path during both forward and reverse travel of the moving mirror. Collects data at the same speed as the previous option but with slight decrease in stability.

---

\* Appropriate Scan setting only when collecting one scan per spectrum.

---

The Normal option is recommended for all gas analysis applications except when using flow-through sampling to monitor combustion or other reactions that require a very fast time response. To increase the speed of data collection with minimal compromise to spectral quality, select the Fast option for scanning the sample.

If you need to use the fastest possible collection speed but can't tolerate increased spectral noise, select the first "Faster" option in the Scan drop-down list box (shorter stroke, quick turnaround). If you need the fastest possible collection speed but can't compromise the resolution, select the second "Faster" option in the list box (full bi-directional stroke).

**Note** Because the forward and reverse scans of an FT-IR spectrometer are inherently different, bi-directional scans should not be co-added. Therefore, the Faster (Full Bi-directional Stroke) Scan option is appropriate only when collecting one scan per spectrum. ▲

See "Chapter 3 Antaris Sampling" in your *Antaris IGS User Guide* for recommended settings for the sample specification parameters for gas analysis experiments.

## **Blend Analyzer sample specifications**

This sample specification contains parameters that are optimized for analyzing samples with the Antaris Target Blend analyzers.

The illustration below shows the parameters for the blend analyzer sample specification. These parameters appear in the display area of RESULT Integration when a blend analyzer sample specification is selected in a workflow.

Sample Specification

New Sample

Sample Collection

Sampling technique: Blend Analyzer

Sample position: Empty

Background specification: [ ] New Details

Pre-collection delay (sec): 0

Resolution: 8.0 cm-1

Gain: 15x Optimize Gain

Buffer size (scans): Single scan

Data Collection Trigger

None

Rotation (degrees): 180

Spectral Range

Use standard range in cm-1

Start: 4,000.00 End: 10,000.00

Samples for Simulation

[ ] New Delete

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

### Sample specification for blend analyzer sample

The following parameters are unique to the blend analyzer sample specification:

- **Sample Position.** Use this list box to specify the location for sample data collection with the blend analyzer. The Location parameter controls the position of the instrument's internal reference wand. The wand contains a diffuse gold reference sample and it may also contain a polystyrene sample. The software provides the following options for sample collections with the Target Blend analyzer:

- *Internal gold reference.* Select this option to collect sample data using the blend analyzer's internal diffuse gold reference. The internal reference is an uncoated, highly reflective surface that is moved in front of the near-infrared light source so that it fully covers the sample window (from the inside) for sample collections.
- *Empty.* Select this option to collect a sample spectrum from an external sample. This setting is appropriate for sample collections with a Target Blend analyzer that is mounted on a blender or one that is configured for bench top sampling. The Empty setting moves the reference wand out of the light source, which allows the beam to exit the sample window to interact with an external sample. You can also use this setting to collect a single beam spectrum, which shows how the energy of the source is distributed over the measured frequency range. The spectrum can be compared to previous single beam spectra to help determine whether a problem exists with your instrument.
- *Polystyrene.* Select this option to collect a sample spectrum from the internal polystyrene sample (if one is included) mounted on the reference wand. The polystyrene spectrum can be used for diagnostic purposes. For example, the spectrum can be compared to previous polystyrene spectra to help determine whether a problem exists with your instrument.

**Note** The Instrument Check feature of RESULT Operation uses the internal reference wand to produce a single beam and polystyrene spectrum for diagnostic purposes. See “Instrument Check” in the “RESULT Operation User Guide” for details. ▲

- **Buffer Size (scans).** Use this feature to specify the number of scans you want the analyzer to store in its internal buffer before it sends the data to the computer for processing. The setting affects how the spectral data are displayed and, to some degree, the processing speed. To minimize the time required to send collected scans to the computer, set Buffer Size to the Total Scans Specified In Collect option. The system will collect the number of scans specified on the associated collection event and then send the entire set to the computer, which will average all the scans and display the resulting spectrum in the specified format (see Data Format on the associated collection event). The spectrum will not be updated until the blender completes another rotation and the

specified number of sample scans have been collected and sent to the computer.

If you want to see the individual scans before they are averaged, set Buffer Size to Single Scan. When Buffer Size is set to Single Scan, the system collects one scan and sends it to the computer, collects another scan and sends it to the computer and so on until the specified number of sample scans have been collected and sent to the computer. The computer displays the individual spectra in the specified format and updates the display each time a new scan arrives from the analyzer. This is the default setting for Buffer Size and the correct setting if you prefer to monitor the data collected during each blender rotation.

- **Data Collection Trigger.** Use this feature to specify whether data collection will be initiated manually or controlled by the position of the blender. The following options are available:
  - *None.* Select this option if you want the workflow to define when the instrument will begin collecting data with the blend analyzer. When this option is selected, data collection starts when the workflow encounters a collection event and stops when the specified number of scans have been collected. If the collection event occurs in a repeat loop, the analyzer will collect data continuously until the workflow directs it to stop or the user stops the analyzer. This is the only available option when collecting data in bench top mode.
  - *Rotation.* Select this option if you want the workflow to time the start of data collection according to the rotation angle of the blender. This option is available only when the analyzer is properly mounted on a blender. Enter a number from 0 to 360 degrees that corresponds with the rotation angle of the blender when data collection will start (where 0 is “up” and 180 is “down”). The software senses the direction of rotation and considers the current direction to be positive rotation when applying the specified angle for the start of data collection. For example, whether the blender is rotating clockwise or counterclockwise (or alternating between the two), if a rotation angle of 160 degrees is specified, data collection starts when the blender reaches 160 degrees from the 0 degree (up) position. For most applications, you will want to test collection with the analyzer to ensure that the sample completely covers the blender’s sampling window at the selected angle.

The remaining parameters on the blend analyzer sample specification are described in the section titled “Features common to sample specifications” in this chapter except the default settings may vary. For information about recommended settings for blend analyzers, see “Developing workflows for the blend analyzer” in your *Antaris Target Blend Analyzer User Guide*.

**Note** The default spectral range for the Antaris Target Blend analyzer is 4,000  $\text{cm}^{-1}$  to 10,000  $\text{cm}^{-1}$  although the blend analyzer actually uses a smaller range. This is intended to make the blend analyzer compatible with workflows and methods designed for use with other Antaris analyzers. If you leave the default settings, the software will automatically blank spectral regions that are outside the physical limitations of the Target Blend analyzer. If you want to collect and display data in the actual range for the Target Blend analyzer, specific start and end limits are provided in the *Antaris Target Blend Analyzer User Guide*. ▲

## **Dual Tablet Tablet Analyzer sample specifications**

This sample specification contains parameters that are optimized for collecting transmission data from tablet samples using an Antaris Tablet Analyzer (standard or softgel). Dual-Tablet Tablet Analyzer sample specifications can only be linked to Collect Dual Tablet events in workflows.

The illustration below shows the parameters for the dual tablet transmission sample specification for the standard tablet analyzer. These parameters appear in the display area of RESULT Integration when a Dual Tablet Standard Tablet Analyzer sample specification is selected in a workflow.

Sample Specification

New Sample

Sample Collection

Sampling technique: Dual Tablet Standard Tablet Analyzer

Background specification: New Background

Gain: 1x

Spectral Range

Use standard range in cm-1

Start: 6,000.00 End: 10,000.00

Samples for Simulation

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

### Dual Tablet Standard Tablet Analyzer sample specification

There are no parameters that are unique to the dual tablet transmission sample specifications (standard or softgel). The sample specifications differ only in the default settings for those parameters. For descriptions of the parameters, see “Features common to sample specifications” in this chapter. For information about recommended settings for dual tablet sampling, see “Developing workflows for a tablet analyzer” in your *Antaris User Guide*.

### Dual Tablet Integrating Sphere sample specifications

This sample specification contains parameters that are optimized for collecting reflection data from tablet samples that are mounted in a tablet analyzer using the Antaris integrating sphere. Dual tablet reflection sample specifications can only be linked to Collect Dual Tablet events in workflows.

The illustration below shows the parameters for the dual tablet integrating sphere sample specification. These parameters appear in the display area of RESULT Integration when a dual tablet integrating sphere sample specification is selected in a workflow.

Sample Specification

New Sample

Sample Collection

Sampling technique: Dual Tablet Integrating Sphere

Sample Cup Spinner: None

Background specification: New Sample Background

Gain: 1x

Spectral Range

Use standard range in cm-1

Start: 4,000.00 End: 10,000.00

Samples for Simulation

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

### Dual tablet integrating sphere sample specification

There are no parameters that are unique to the dual tablet integrating sphere sample specification. The sample specification differs only in the default settings for those parameters. For descriptions of the parameters, see “Features common to sample specifications” and “Integrating sphere sample specifications” in this chapter. For information about recommended settings for the dual tablet sampling, see “Developing workflows for a tablet analyzer” in your *Antaris User Guide*.

### Validation Wheel sample specifications

This sample specification contains parameters that are optimized for analyzing samples mounted on the optional validation wheel. The validation wheel sample specification is available in the software only when the instrument includes the optional ValPro System Qualification package and the validation wheel is installed and properly configured in RESULT Integration. See “Setting RESULT Integration Options” in the “RESULT Integration User Guide” for information about configuring RESULT Integration for ValPro.

The illustration below shows the parameters for the validation wheel sample specification. These parameters appear in the display area of RESULT Integration when a validation wheel sample specification is selected in a workflow.

Sample Specification

New Sample

Sample Collection

Sampling technique: Validation Wheel

Sample position: Empty Beam Path: Transmission Module

Background specification: [ ] New Details

Pre-collection delay (sec): 0 Attenuator: C Screen

Resolution: 8.0 cm-1

Gain: 1x

Spectral Range

Use standard range in cm-1

Start: 4,000.00 End: 10,000.00

Samples for Simulation

[ ] New Delete

Prompt for simulation sample

Use simulation sample for all workflow runs

Cycle through simulation samples

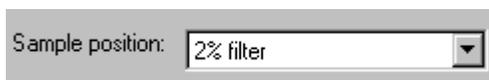
### Sample specification for validation wheel

The following parameters are unique to the validation wheel sample specification.

- **Sample Position.** Use this list box to specify the location for data collection with the validation wheel. The validation 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 may be used for instrument qualification using the optional ValPro System Qualification package. The polystyrene sample is calibrated to a thickness of 0.0325 inch, and can be used to validate instrument performance.

The seventh position in the wheel is empty. RESULT uses the empty position to collect the background spectra that are used to process sample spectra collected from samples mounted in the validation wheel.

To configure the workflow to collect data from a sample mounted in the validation wheel, set Sample Position to the appropriate sample, as shown in the example below. •



- **Beam Path.** Use the Beam Path list box to specify the detector that will be used to collect data from the validation wheel. This allows you to set up workflows that test instrument performance using a specific sampling module.

The following Beam Path options are available:

- *Transmission Module.* Collects data from the validation wheel with the detector for the Antaris transmission module.
- *Fiber Optic Probe.* Collects data from the validation wheel using the detector for the fiber optic sampling module of an Antaris or Antaris II analyzer or the currently selected channel of an Antaris MX.
- *Integrating Sphere.* Collects data from the validation wheel using the reflection detector for the Antaris integrating sphere.
- *Tablet/SoftGel Analyzer.* Collects data from the validation wheel using the transmission detector in the Antaris tablet analyzer (standard or softgel) installed on the instrument.

The remaining parameters on the validation wheel sample specification are described in the section titled “Features common to sample specifications” in this chapter except the default settings may vary. We recommend using the default settings in the validation wheel sample specification to collect data with the validation wheel samples.

## Background specifications

A background specification defines data collection for background spectra generated by a workflow. Background specifications may be linked to sample specifications in a workflow.

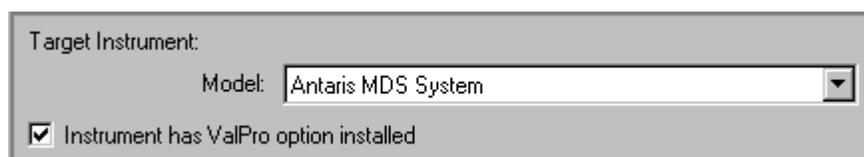
RESULT provides a unique background specification for each sampling configuration and for the optional validation wheel. The available background specification include the following:

- **Standard Tablet Analyzer background specification**, which is designed to collect transmission background data using the Antaris standard tablet analyzer. The Standard Tablet Analyzer background specification can be linked to Standard Tablet Analyzer sample specifications and Dual Tablet Standard Tablet Analyzer sample specifications in workflows.
- **SoftGel Tablet Analyzer background specification**, which is optimized for collecting transmission background data from gel-cap and softgel tablets using the Antaris softgel tablet analyzer. The SoftGel Tablet Analyzer background specification can be linked to SoftGel Tablet Analyzer sample specifications and Dual Tablet SoftGel Tablet Analyzer sample specifications in workflows.
- **Integrating Sphere background specification**, which can be used to collect diffuse-reflection background data from powders and solids using the Antaris integrating sphere. The integrating Sphere background specification can be linked to Integrating Sphere sample specifications and Dual Tablet Integrating Sphere sample specifications in workflows.
- **Transmission Module background specification**, which is optimized for collecting transmission background data from liquid and film samples using the Antaris transmission module.
- **Fiber Optic background specification**, which can be used to analyze samples using a fiber optic accessory connected to any fiber optic module.
- **Multi-Channel Fiber Optic background specification**, which can be used to analyze samples using fiber optic accessories connected to the Antaris MX and Antaris EX systems. The Multi-Channel Fiber Optic background specification can only be linked to Collect Multi-Channel events in workflows.

- **Autosampler Integrating Sphere background specification**, which is optimized for collecting diffuse-reflection background data from powders and solids using an autosampler mounted on the Antaris integrating sphere.
- **Gas Cell background specification**, which is designed to collect data from gas samples that are captured in or flowing through a gas cell mounted on an Antaris IGS analyzer.
- **Instrument background specification**, which is optimized for collecting transmission background data using the spectrometer beam path of an Antaris IGS analyzer (bypasses the gas cell).
- **Blend Analyzer background specification**, which can be used to collect data with the Antaris Target Blend analyzer.
- **Validation Wheel background specification**, which is designed for analyzing samples mounted on the optional validation wheel.

**Note** Each background specification has a companion sample specification, which defines sample collection for the corresponding sampling configuration. See “Sample Specifications” in this chapter for more information. ▲

The background specifications available in RESULT at a given time are dependent on the Target Instrument settings in the Options dialog box (available from the Edit menu in RESULT Integration).



Model defines the possible sampling configurations on the instrument and the corresponding background specifications available in the software. The check box determines whether the validation wheel background specification will be available in the software. The validation wheel background specification works properly only when the optional validation wheel is installed in the instrument.

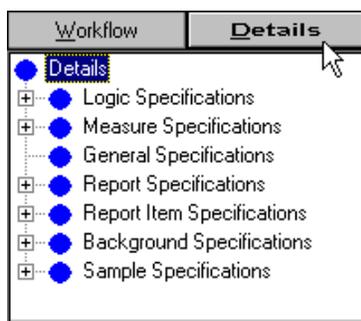
Some parameters are common to all the background specifications. However, the specifications may have different default settings for those parameters. Other parameters are unique to a particular background specification or they may appear on several background specifications but not on others.

This section provides a complete discussion of the characteristics and content of all the background specifications. Read the section titled “Features common to background specifications” to learn about the common background specification parameters. To learn about any additional features that are unique to a specific sampling module, skip to the section with that title.

## Adding a background specification to a workflow

To add a background specification to the open workflow:

1. **Select the Details tab, select the Background Specifications group and then choose the Add button on the RESULT Integration toolbar.**

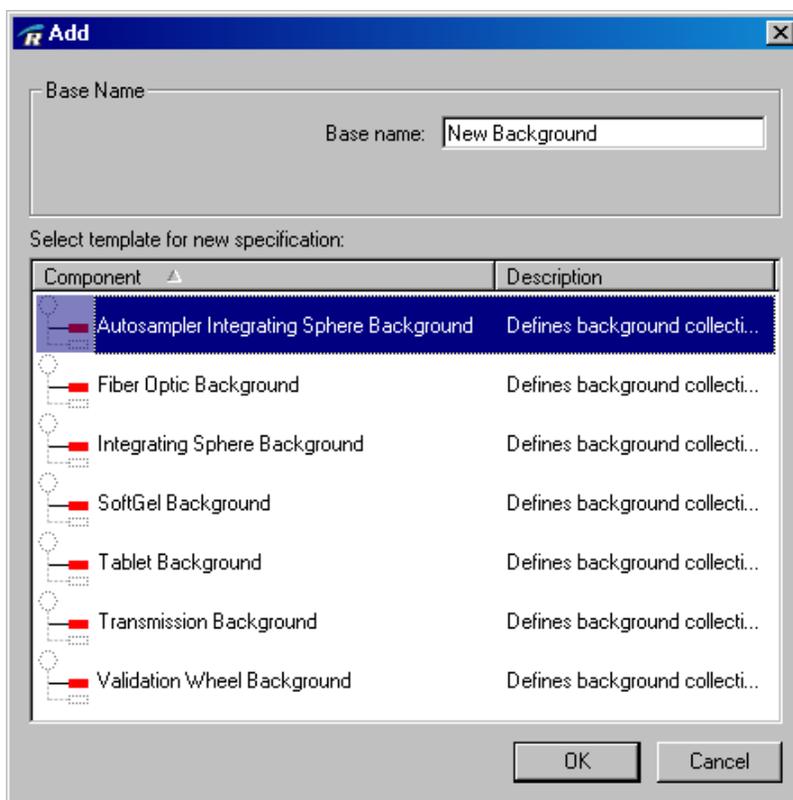


-- or --

**Select the Workflow tab, select the sample specification that requires a background specification and then choose the New button at the right of the Background Specification drop-down list box.**



The software displays a dialog box listing the background specifications available for your system. Here is an example:



- 2. Select a background specification, enter a base name for the new specification and then choose OK.**

The new specification appears in the display area of the RESULT Integration main window.

**Note** If a background specification isn't listed for the sampling module or accessory you want to use, make sure the RESULT add-in option for that module or accessory is properly installed on the computer you use to run RESULT. See *Installing Your Software* in your RESULT document set for more information. You should also check that Model is set correctly in the Options dialog available from the Edit menu in RESULT Integration. ▲

- 3. If you added the background specification from the Details tab, link the new specification to a sample specification.**

See "Linking a specification to a workflow event" in the "RESULT Integration User Guide" for instructions.

## Features common to background specifications

This section describes the features that are common to background specifications. For information about a specific background specification, such as the Antaris Standard Tablet Analyzer background specification, refer to the section with that name later in this chapter.

**Associated events:** None

**Associated specifications:** Sample specification

**Related events:** Collect event, Collect Dual Tablet event, Collect Multi-Channel event

**Related specifications:** None

**Parameters:** The illustration below shows the parameters that appear on background specifications. These parameters appear in the display area of RESULT Integration when a background specification is selected in a workflow.

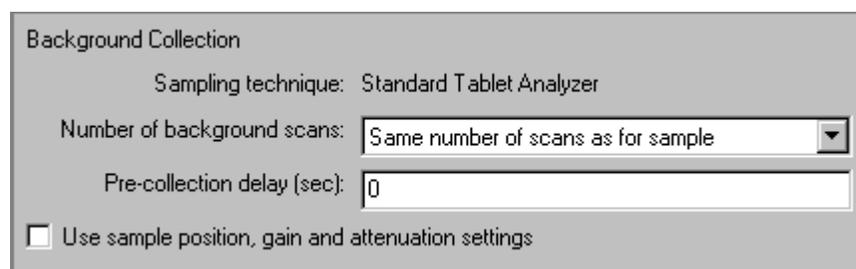
The screenshot shows a dialog box titled "Background Specification". At the top, there is a text input field containing "New Background". Below this is a section titled "Background Collection" which includes a "Sampling technique" dropdown menu set to "Standard Tablet Analyzer", a "Number of background scans" dropdown menu set to "Same number of scans as for sample", and a "Pre-collection delay (sec)" input field with the value "0". There is also a checkbox labeled "Use sample position, gain and attenuation settings" which is currently unchecked. Below the "Background Collection" section is a section titled "Backgrounds for Simulation" which contains an empty list box. At the bottom right of this section is a "Delete" button. At the bottom of the dialog box, there are three unchecked checkboxes: "Prompt for simulation background", "Use simulation background for all workflow runs", and "Cycle through simulation backgrounds".

## Features common to background specifications

The common background specification parameters define background data collection and any background spectra that can be used to run the workflow in simulation mode. These parameters are independent of the sample type or material to be analyzed. (Parameters that are sample specific appear on the associated collection event.) The following sections detail the common background specification parameters. The parameters are explained in the order in which they appear in the software.

## Background Collection

Use the parameters in this group to specify background data collection using a specific sampling module such as the *Standard Tablet Analyzer module*.



Sampling technique:

- **Sampling Technique.** This readout gives the name of the sampling module and technique that will be used for data collection, such as the Antaris tablet analyzer, integrating sphere or transmission module.

Number of background scans:

- **Number Of Background Scans.** This parameter determines how many scans are performed during a background data collection. If you perform more than one scan, the system averages all of them.

There are two settings for Number Of Background Scans. You can collect the same number of scans as you collect from the sample, or you can collect twice as many scans as you collect from the sample. The default setting collects the same number of background scans as are collected from the samples. Double the background scans if you need to increase the sensitivity; that is, the ability to distinguish small peaks from noise (recommended for collecting data with some fiber optic accessories). See the guide that came with your accessory for more information.

**Note** For a given resolution, increasing the number of background scans increases the total collection time. ▲

Pre-collection delay (sec):

- **Pre-collection delay.** Use this box to specify a delay before background collection begins. If you specify a pre-collection delay, when you run the workflow, the system will pause the specified number of seconds before it begins collecting the background data. This is often useful for allowing the instrument time to stabilize before starting the analysis.

Leave Pre-collection Delay set to zero if you don't want to delay data collection.

Use sample position, gain and attenuation

- **Use Sample Position, Gain And Attenuation Settings.** Use this option to specify the gain and attenuation for background measurements. The appropriate gain and attenuation settings for backgrounds depend on the background material and the instrument location used for data collection.

When the check box is selected, the software collects backgrounds using the same Gain and Attenuator settings used to collect the sample data (i.e., with the Gain and Attenuator settings shown on the sample specification). This setting is recommended when collecting a background from an external reference at the same location that is used for the sample collection.

If Use Sample Position, Gain And Attenuation Settings is unavailable in the software, use the Position or Location parameter to specify a location for collecting backgrounds. In these cases, the software will use the corresponding Attenuator and Gain settings from the table below.

When the check box is cleared, the software uses default position, gain and attenuation settings which will optimize the signal passed to the detector. The default settings depend on the sampling module used for background collection and, in some cases, the type of background specification. The following table gives the Attenuator and Gain settings used when Use Sample Position, Gain And Attenuation Settings is cleared on the background specification.

Sampling Technique	Background Position	Default Gain Setting	Default Attenuator Setting
Integrating Sphere	Integrating sphere measured with the internal gold reference (reference flag in closed position)	1x	Uses sample Attenuator setting
Standard Tablet Analyzer	Standard tablet analyzer measured with tablet transmission detector using no background material	1x	C screen
SoftGel Tablet Analyzer	Softgel tablet analyzer measured with softgel transmission detector using no background material	1x	C screen

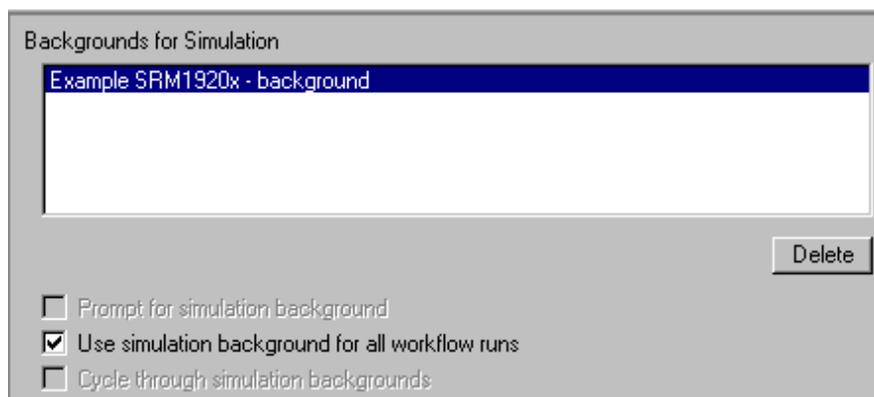
Sampling Technique	Background Position	Default Gain Setting	Default Attenuator Setting
Transmission Module	Transmission module, measured from center position of sample holder (no background material)	1x	C screen
Transmission Module	Transmission module using external reference measured in front or rear sample holder position	1x	C screen
Fiber Optic Module using third party probe	Fiber optic module measured with third party probe using external reference	1x	Uses sample Attenuator setting
Fiber Optic Module using SabIR probe	Fiber optic module measured with SabIR probe using internal Spectralon reference	1x	Uses sample Attenuator setting
Fiber Optic Module	Transmission module measured from center position of sample holder (no background material)	1x	C screen
Fiber Optic Module	Transmission module using external reference in rear position of sample holder	1x	C screen
Fiber Optic Module	Integrating sphere using the internal gold reference (reference flag in closed position)	1x	C screen
Fiber Optic Module	Integrating sphere using external reference (reference flag in open position)	1x	C screen
Target Blend analyzer	Measured using external reference sample	20	N/A
Target Blend analyzer	Measured using internal diffuse gold reference	20	N/A

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

## Default Attenuator and Gain settings for background collection

### Backgrounds For Simulation

Use the options in this group to specify simulated background spectra that can substitute for the actual background spectra collected by the workflow.

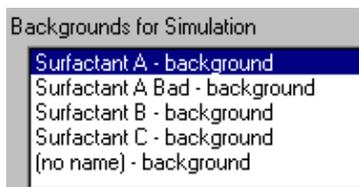


This technique can help you shorten workflow development time and facilitate testing and verifying the workflow when it is completed.

The parameters for specifying background spectra for simulated runs of the workflow are described below:

**Note** For information about collecting background spectra to use for simulated runs of a workflow, see “Sample for Simulation” in “Features common to sample specifications” in this section. ▲

**Note** For information about running workflows in RESULT Integration using simulated data, see “Testing a workflow” in the “RESULT Integration User Guide.” ▲



- **Backgrounds For Simulation.** Use this box to select a background spectrum or spectra that will be used when this workflow is run with simulated data. If the background specification contains more than one simulation spectrum, you may set up the workflow to use only the selected background, to prompt the user to select a background, or to use all the simulation backgrounds stored with this background specification.

**Note** If you want the workflow to run with simulated background data and simulated sample data (recommended), make sure an appropriate sample spectrum is selected in the Samples For Simulation box on the associated sample specification. ▲

Use the features described below to delete spectra from the list and to specify which spectra should be used for simulated runs of the workflow:



- **Delete.** To remove a background spectrum so that it is no longer available for use in simulated runs of the workflow, select the spectrum listed in the Backgrounds For Simulation box and then choose the Delete button below the box.

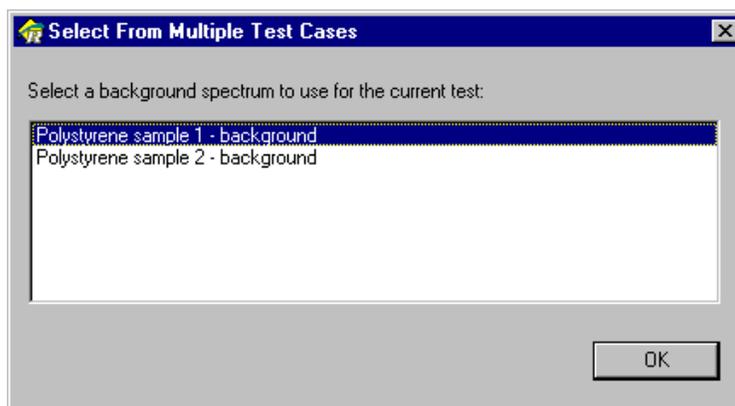
**Note** After you delete a spectrum from the list of backgrounds for simulation, the operation cannot be reversed (for example with Undo). ▲



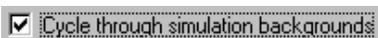
- **Prompt For Simulation Background.** This option is available in the software only when the Backgrounds For Simulation box on the background specification contains at least two entries and the Cycle

Through Simulation Backgrounds check box is cleared.

Select Prompt For Simulation Background if you want the workflow to prompt the user to select a background spectrum when the workflow is run using simulated data. The illustration below shows an example of this type of prompt.

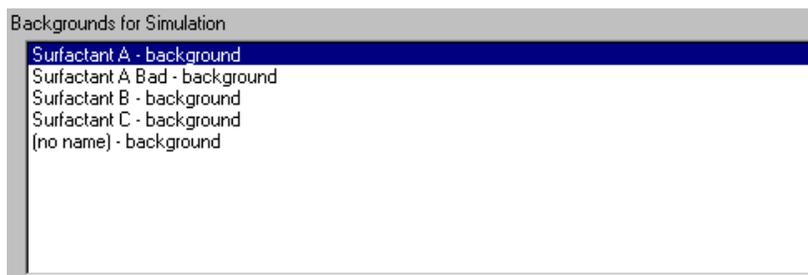


If this option is cleared and the workflow is run using simulated data, then the workflow will run using the background spectrum that is currently selected in the Backgrounds For Simulation box.



- **Cycle Through Simulation Backgrounds.** This option is available in the software only when the Backgrounds For Simulation box contains at least two entries.

Select Cycle Through Simulation Backgrounds if you want the workflow to cycle through all the background spectra stored with this background specification when the workflow is run using simulated data. The first time you run the workflow, the software will use the background spectrum that is currently selected in the Backgrounds For Simulation box, as shown in the following example.



The next time you run the workflow, the software will use the next background spectrum in the list, and so on until all the simulation

backgrounds have been used. Then the workflow starts again with the selected background. The feature is useful for running a workflow that contains a collection event positioned in a loop with simulated data by allowing the collect event to call a different simulated spectrum each time the loop is repeated.

If Cycle Through Simulation Backgrounds is cleared and the workflow is run using simulated data, the workflow will run using the spectrum that is currently selected in the Backgrounds For Simulation box.

Use simulation background for all workflow

- **Use Simulation Background For All Workflow Runs.** Select this option to configure the workflow to run only with simulated background data. This feature applies when the workflow is run in RESULT Integration and RESULT Operation, and is the only way to run workflows with simulated background data in RESULT Operation.

If Prompt For Simulation Background and Cycle Through Simulation Backgrounds (see above) are both cleared, the workflow will run using the background spectrum that is currently selected in the Backgrounds For Simulation box. If Prompt For Simulation Background is selected (the workflow must contain at least two background spectra for simulation), the workflow will prompt the user to select a simulation background. If Cycle Through Simulation Backgrounds is selected, the first time you run the workflow, it will run with the selected background spectrum. The next time you run the workflow, the workflow will use the next background spectrum in the list and so on until all the simulation background spectra have been used. Then the workflow starts again with the selected background.

**Note** If you want the workflow to run with simulated sample data and simulated background data (recommended), make sure Use Simulation Sample For All Workflow Runs is also selected on the associated sample specification. See Samples For Simulation in “Features common to sample specifications” for more information. ▲

When Use Simulation Background For All Workflow Runs is cleared, the user may select whether to run the workflow normally or with simulated data when running the workflow in RESULT Integration.

**Usage:** A background specification may be linked to a sample specification or one of the following events in a workflow:

- **Collect Dual Tablet event**, which can be used to collect a transmission and reflection spectrum at the same time with an Antaris tablet analyzer.
- **Collect Multi-Channel event**, which can be used to collect data from two or more fiber optic sampling accessories at the same time.

## Standard Tablet Analyzer background specifications

This specification contains parameters that are optimized for collecting transmission background data from standard tablets using the Antaris Standard Tablet Analyzer. The Standard Tablet Analyzer background specification may be linked to Standard Tablet Analyzer sample specifications, Autosampler Standard Tablet Analyzer sample specifications, and Collect Dual Tablet events in a workflow.

The illustration below shows the parameters for the Antaris standard tablet analyzer background specification. These parameters appear in the display area of RESULT Integration when a standard tablet analyzer background specification is selected in a workflow.

Background Specification

New Background

Background Collection

Sampling technique: Standard Tablet Analyzer

Number of background scans: Same number of scans as for sample

Pre-collection delay (sec): 0

Use sample position, gain and attenuation settings

Backgrounds for Simulation

Delete

Prompt for simulation background

Use simulation background for all workflow runs

Cycle through simulation backgrounds

## Background specification for standard tablet analyzer

There are no parameters that are unique to the background specification for the standard tablet analyzer. The background specification differs only in the default settings for those parameters. For descriptions of the parameters that are common to background specifications, see “Features common to background specifications” in this chapter. For information about recommended settings for the standard tablet analyzer, see “Developing workflows for a tablet analyzer” in your *Antaris User Guide*.

**Note** The Use Sample Position, Gain And Attenuation Settings check box defines the location and the Gain and Attenuator settings for background collections. To collect background data from an external reference, make sure this check box is selected. The software will collect the background data using the same Gain and Attenuator settings used for the sample collection (i.e., with the Gain and Attenuator settings shown on the sample specification). To collect background data without a reference (typical for transmission analyses), make sure this check box is cleared. The software will collect the background data with the default Gain and Attenuator settings. See “Features common to background specifications” for details. ▲

## SoftGel Tablet Analyzer background specifications

This specification contains parameters that are optimized for collecting transmission background data from gel-cap and softgel tablets using the Antaris SoftGel Tablet Analyzer. The SoftGel Tablet Analyzer background specification may be linked to SoftGel Tablet Analyzer sample specifications, Autosampler SoftGel Tablet Analyzer sample specifications, and Collect Dual Tablet events in a workflow.

The illustration below shows the parameters for the Antaris softgel tablet analyzer background specification. These parameters appear in the display area of RESULT Integration when a softgel tablet analyzer background specification is selected in a workflow.

Background Specification

New Sample Background

Background Collection

Sampling technique: SoftGel Tablet Analyzer

Number of background scans: Same number of scans as for sample

Pre-collection delay (sec): 0

Use sample position, gain and attenuation settings

Backgrounds for Simulation

Delete

Prompt for simulation background

Use simulation background for all workflow runs

Cycle through simulation backgrounds

### Background specification for softgel tablet analyzer

There are no parameters that are unique to the background specification for the softgel tablet analyzer. The background specification differs only in the default settings for those parameters. For descriptions of the parameters that are common to background specifications, see “Features common to background specifications” in this chapter. For information about recommended settings for the softgel tablet analyzer, see “Developing workflows for a tablet analyzer” in your *Antaris User Guide*.

**Note** The Use Sample Position, Gain And Attenuation Settings check box defines the location and the Gain and Attenuator settings for background collections. To collect background data from an external reference, make sure this check box is selected. The software will collect the background data using the same Gain and Attenuator settings used for the sample collection (i.e., with the Gain and Attenuator settings shown on the sample specification). To collect background data without a reference (typical for transmission analyses), make sure this check box is cleared. The software will collect the background data with the default Gain and Attenuator settings. See “Features common to background specifications” for details. ▲

## Integrating Sphere background specifications

This background specification contains parameters that are optimized for collecting diffuse-reflection data from powders and solids using the integrating sphere module (or the integrating sphere portion of a tablet analyzer). The integrating sphere background specification may be linked to integrating sphere sample specifications in workflows.

The illustration below shows the parameters for the integrating sphere background specification. These parameters appear in the display area of RESULT Integration when an integrating sphere background specification is selected in a workflow.

The screenshot shows a dialog box titled "Background Specification" with a text field containing "New Sample Background". Below this is a section titled "Background Collection" containing the following parameters:

- Sampling technique: Integrating Sphere
- Number of background scans: Same number of scans as for sample (dropdown menu)
- Pre-collection delay (sec): 0 (text input field)
- Use sample position, gain and attenuation settings

Below the "Background Collection" section is a section titled "Backgrounds for Simulation" which contains an empty list box and a "Delete" button. At the bottom of the dialog are three checkboxes:

- Prompt for simulation background
- Use simulation background for all workflow runs
- Cycle through simulation backgrounds

### Background specification for integrating sphere

There are no parameters that are unique to the background specification for the integrating sphere. The background specification differs only in the default settings for those parameters. For descriptions of the parameters that are common to background specifications, see “Features common to background specifications” in this chapter. For information about recommended settings for the integrating sphere, see “Developing workflows for the integrating sphere” in your *Antaris User Guide*.

**Note** The Use Sample Position, Gain And Attenuation Settings check box defines the location and the Gain and Attenuator settings for background collections. To collect background data from an external reference, make sure this check box is selected. The software will move the internal reference flag out of the near-infrared beam and collect the background data using the same Gain and Attenuator settings used for the sample collection (i.e., with the Gain and Attenuator settings shown on the sample specification). To collect background data from the integrating sphere’s internal diffuse gold reference, make sure this check box is cleared. The software will move the reference flag into the beam and collect the background data with the default Gain and Attenuator settings. See “Features common to background specifications” for details. ▲

## **Transmission Module background specifications**

This background specification contains parameters that are optimized for collecting transmission background data using the Antaris transmission module.

The illustration below shows the parameters for the transmission module background specification. These parameters appear in the display area of RESULT Integration when a transmission module background specification is selected in a workflow.

Background Specification

New Sample Background

Background Collection

Sampling technique: Transmission Module

Position: Background Position

Number of background scans: Same number of scans as for sample

Pre-collection delay (sec): 0

Use sample gain and attenuation settings

Backgrounds for Simulation

Delete

Prompt for simulation background

Use simulation background for all workflow runs

Cycle through simulation backgrounds

### Background specification for transmission module

The following parameters are unique to the transmission module background specification.

- Position.** Use this list box to specify the location for background data collection with the transmission module. The sample compartment for the transmission module accommodates a variety of three-position sample holders for analyzing liquids, transparent solids and thin films. The sample holders are referred to as having three positions because they have both a front and a rear position where samples can be collected, and there is an opening in the center through which backgrounds can be collected.

If you plan to collect a background that measures the response of the instrument with no sample in place, set Position to Background Position, as shown below.

When Position is set to “Background Position,” the software automatically uses the default Gain and Attenuator settings (Gain = 1x, Attenuator = C screen) for the background collection.



If a sample holder is installed in the transmission module sample compartment, the background spectrum will be taken through the opening in the center of the sample holder. If no sample holder is installed, the background will be collected through the empty sample compartment.

To collect a background spectrum using a background reference sample, place the sample in either the front or rear position of the sample holder and set Position to match the location of the reference sample.



To collect a background spectrum using an aperture, install the aperture in the front or rear position of the sample holder and then set Position to match the location of the aperture.

**Note** The Use Sample Gain And Attenuation Settings check box defines the Gain and Attenuator settings for background collections through the front and rear positions of the sample holder. To collect background data from an external reference with the same Gain and Attenuator settings used for the sample collection (i.e., with the Gain and Attenuator settings shown on the sample specification), make sure this check box is selected. Clear the check box if you want to collect background data from an external reference with the default Gain and Attenuator settings. See “Features common to background specifications” for details. ▲

The remaining parameters on the transmission module background specification are described in the section titled “Features common to background specifications” in this chapter except the default settings may vary. For information about recommended settings for the transmission module, see “Developing workflows for the transmission module” in your *Antaris User Guide*.

## Fiber Optic background specifications

This background specification contains parameters that are optimized for collecting background data using an Antaris fiber optic module. You can use this fiber optic background specification to collect backgrounds with an Antaris or Antaris II system that includes a fiber optic sampling station or to collect a background using one channel of an Antaris MX or EX analyzer.

The illustration below shows the parameters for the fiber optic module background specification. These parameters appear in the display area of RESULT Integration when a fiber optic background specification is selected in a workflow.

The screenshot shows a dialog box titled "Background Specification". At the top, there is a text field containing "New Sample Background". Below this is a section titled "Background Collection" which includes the following settings: "Sampling technique: Fiber Optic Probe", "Position: Fiber Optic Probe" (with a dropdown arrow), "Number of background scans: Same number of scans as for sample" (with a dropdown arrow), and "Pre-collection delay (sec): 0" (with a text input field). There is a checkbox labeled "Use sample position, gain and attenuation settings" which is currently unchecked. Below the "Background Collection" section is a section titled "Backgrounds for Simulation" which contains an empty list box. To the right of the list box is a "Delete" button. At the bottom of the dialog, there are three checkboxes: "Prompt for simulation background", "Use simulation background for all workflow runs", and "Cycle through simulation backgrounds", all of which are currently unchecked.

**Background specification for fiber optic module**

The following parameters are unique to the fiber optic background specification:

- **Position.** Use this list box to specify the location for background data collection for the fiber optic module. The following options are available:
  - *Fiber optic probe*, which collects a background spectrum from an external reference using a third-party fiber optic probe or from the internal Spectralon reference of the SabIR probe. The Probe Type parameter on the fiber optic sample specification defines the type of probe installed on the selected channel.

**Note** The Use Sample Position, Gain and Attenuation Settings check box is available only when Position is set to Fiber Optic probe. When collecting background data with an external reference, selecting this check box allows you to override the default gain and attenuator settings for background collections with the fiber optic module and use the same gain and attenuator settings that are used to collect the sample data (i.e., using the Gain and Attenuator settings shown on the sample specification). Clear this check box to collect background data with the default Position, Gain and Attenuator settings. The default settings used depend on the probe type. See “Features common to background specifications” for details. ▲

- *Transmission module (center position)*, which collects a background spectrum through the center (empty) position of the sample holder or through the empty transmission module if no sample holder is installed. This option is available only for Antaris and Antaris II systems that include the transmission module. This setting uses the default Gain setting (1x) and the default Attenuator setting (C screen).
- *Transmission module (rear position)*, which collects a background spectrum from an external reference located in the rear position of a sample holder installed in the Antaris transmission module. This option is available only for Antaris and Antaris II systems that include the transmission module. This setting uses the default Gain setting (1x) and the default Attenuator setting (C screen).

- *Integrating sphere (flag closed)*, which collects a background spectrum from the internal diffuse gold reference in the integrating sphere. This option is available for Antaris and Antaris II systems that include the integrating sphere. This setting uses the default Gain setting (1x) and the default Attenuator setting (C screen).
- *Integrating sphere (flag open)*, which collects a background spectrum from an external reference mounted on the Antaris integrating sphere. This option is available for Antaris and Antaris II systems that include the integrating sphere. This setting uses the default Gain setting (1x) and the default Attenuator setting (C screen).

The remaining parameters on the fiber optic background specification are described in the section titled “Features common to background specifications” in this chapter except the default settings may vary. For information about recommended settings for the fiber optic module and SabIR probe, see “Developing workflows for the fiber optic module” in your *Antaris User Guide*.

## **Multi-Channel Fiber Optic background specifications**

This background specification contains parameters that are optimized for collecting background data with fiber optic accessories that are connected to an Antaris MX or Antaris EX Process analyzer. Multi-channel background specifications can only be linked to Collect Multi-Channel events in a workflow.

The illustration below shows the parameters for the multi-channel background specification. These parameters appear in the display area of RESULT Integration when a multi-channel background specification is selected in a workflow.

### Background specification for multi-channel fiber optic module

The following parameter is unique to the multi-channel background specification:

- **Probe Type.** Use this list box to specify the fiber optic accessory that will be used for data collection from a specific fiber optic channel on the instrument. The following options are available:
  - *Antaris SabIR.* If you are using the Antaris SabIR probe, set Probe Type to Antaris SabIR. Selecting this option will enable the software to detect when the probe is properly inserted into the holster on the instrument. The probe must be properly inserted into the holster to collect backgrounds using the internal reference. This setting also allows the operator to use the probe trigger as the Acknowledge button on the instrument.
  - *Third Party.* Use this setting for all other fiber optic accessories purchased from us or elsewhere.
- **Gain.** Use the Gain list box to select the electronic gain for the spectrum. Gain determines how much the detector signal is amplified electronically, making it larger relative to the level of electronic noise. Amplifying the signal is helpful when the signal is weak. For example, the standard tablet analyzer may require a gain setting greater than 1 to achieve adequate signal-to-noise levels in transmission spectra collected from an opaque tablet sample, especially if the sample is thick.

The Gain drop-down list includes all the gain settings for the current sampling module and technique. For recommended gain settings for a particular Antaris sampling module, see the chapter with that name in your *Antaris User Guide*.

You can let the software automatically adjust the gain to maximize the signal by using Optimize Gain on the sample specification (see below). We recommend using Optimize Gain to ensure the best spectral quality.

- **Optimize Gain.** The Optimize Gain button may be used to determine the appropriate gain and attenuation settings for a specific background reference. See “Features common to sample specifications” for details.

The remaining parameters on the multi-channel background specification are described in the section titled “Features common to background specifications” in this chapter except the default settings may vary. For information about recommended settings for fiber optic accessories, including the SabIR probe, see “Developing workflows for the Antaris MX” in your *Antaris MX User Guide*.

## **Autosampler Integrating Sphere background specifications**

The autosampler integrating sphere background specification contains parameters that are optimized for collecting diffuse-reflection data from powders and solids using an autosampler mounted on the Antaris integrating sphere sampling module.

The illustration below shows the parameters for the autosampler integrating sphere background specification. These parameters appear in the display area of RESULT Integration when an autosampler integrating sphere background specification is selected in a workflow.

Background Specification

New Sample Background

Background Collection

Sampling technique: Autosampler - Integrating Sphere

Number of background scans: Same number of scans as for sample

Pre-collection delay (sec): 0

Location

Internal gold reference

Reference (zero) position

Same position as sample

Backgrounds for Simulation

Delete

Prompt for simulation background

Use simulation background for all workflow runs

Cycle through simulation backgrounds

### Background specification for autosampler integrating sphere

The following parameter is unique to the autosampler integrating sphere background specification:

- Location.** Use this parameter to specify a location for collecting diffuse reflection background data with the autosampler. Background collections can occur at the integrating sphere's internal reference, the reference (zero) position of the autosampler carousel, or the carousel position used to collect the sample data. The appropriate setting depends on the background material and any requirements for background collections at your facility. The workflow automatically moves the light beam to the correct location before background collection starts.

To specify the background location, one of the options described below:

- *Internal Gold Reference.* Select this option to collect background data using the integrating sphere's internal diffuse gold reference. Using this technique for background collections will optimize sample throughput and may reduce operator errors. If collecting a background using the internal gold reference, it is not necessary to add a background reference sample to the autosampler carousels.

The internal gold reference is mounted on a software-controlled arm that swings the reference into and out of the near-infrared beam. Normally, the reference is located in the beam except when the system is collecting sample data or data from an external background reference. When collecting a background from the gold reference, the reference stays in the beam and background collection begins automatically.

- *Reference (Zero) Position.* Select this option to collect a background using an external reference. If collecting a background using an external reference, place the background sample in the reference (zero) position of the autosampler carousel. If the workflow must analyze samples contained in multiple carousels, place a duplicate background sample in the reference position of each carousel. The background sample should fit the carousel openings snugly. See “Collecting backgrounds using an external reference” in your autosampler user guide for examples of materials that can be used as an external background sample.

**Note** If collecting a background using an external reference, make sure the associated autosampler specification has Reference (Zero) Position Reserved For Background Collections selected. See “Autosampler specifications” in this chapter and “Collecting backgrounds using an external reference” in your autosampler user guide for more information. ▲

- *Same Position As Sample.* Select this option to collect a background from the same autosampler position as the previous sample. The resulting spectrum will have no sample peaks (they ratio out) and may be used to evaluate instrument noise or to determine whether a given carousel position actually contains a sample.

The remaining parameters on the autosampler integrating sphere background specification are described in the section titled “Features common to background specifications” in this chapter except the default settings may vary. For information about recommended settings for the autosampler, see your autosampler user guide.

## Gas Cell background specifications

The gas cell background specifications contains parameters that are optimized for collecting transmission backgrounds using a gas cell mounted on the Antaris IGS analyzer.

The illustration below shows the parameters for the gas cell background specification. These parameters appear in the display area of RESULT Integration when a gas cell background specification is selected in a workflow.

The screenshot shows a dialog box titled "Background Specification". At the top, there is a text field containing "New". Below this, the "Background Collection" section contains the following parameters: "Sampling technique: Gas Cell", "Beam path: Gas Cell" (with a dropdown arrow), "Number of background scans: Same number of scans as for sample" (with a dropdown arrow), and "Pre-collection delay (sec): 0". There is an unchecked checkbox labeled "Use sample gain and attenuation settings". The "Backgrounds for Simulation" section features a large empty text area and a "Delete" button. At the bottom, there are three unchecked checkboxes: "Prompt for simulation background", "Use simulation background for all workflow runs", and "Cycle through simulation backgrounds".

**Background specification for Antaris IGS gas cell**

The following parameters are unique to the gas cell background specification:

- **Beam Path.** Use the Beam Path list box to specify the path of the infrared beam when collecting backgrounds with the Antaris IGS analyzer.



To select the beam path, select an option in the drop-down list. The following options are available:

- *Gas Cell.* Select this option to direct the beam through the sample beam path compartment and gas cell and then back to the detector. This is the “upper” beam path referenced in the *Antaris IGS User Guide*. The Gas Cell beam path setting should be used to collect background data through the gas cell.
- *Instrument.* Select this option to direct the beam through the spectrometer compartment and then directly to the detector. This is the “lower” beam path referenced in the *Antaris IGS User Guide*. The Instrument beam path setting is typically used only to check instrument operation or status.

**Note** The Use Sample Position, Gain And Attenuation Settings check box defines the location and the Gain and Attenuator settings for background collections. To collect background data from an external reference, make sure this check box is selected. The software will collect the background data using the same Gain and Attenuator settings used for the sample collection (i.e., with the Gain and Attenuator settings shown on the sample specification). To collect background data without a reference, make sure this check box is cleared. The software will collect the background data with the default Gain and Attenuator settings. See “Features common to background specifications” for details. ▲

The remaining parameters on the gas cell background specification are described in the section titled “Features common to background specifications” in this chapter except the default settings may vary. For information about recommended settings for the gas cell, see your *Antaris IGS User Guide*.

## Instrument background specifications

The Instrument background specification contains parameters that are optimized for collecting transmission backgrounds using the instrument beam path of the Antaris IGS analyzer (bypasses the gas cell).

The illustration below shows the parameters for the instrument background specification. These parameters appear in the display area of RESULT Integration when an instrument background specification is selected in a workflow.

The screenshot shows a dialog box titled "Background Specification". At the top, there is a text field containing the word "New". Below this, the dialog is divided into two main sections. The first section, "Background Collection", contains the following controls: "Sampling technique:" set to "Instrument"; "Beam path:" a dropdown menu currently showing "Instrument"; "Number of background scans:" a dropdown menu currently showing "Same number of scans as for sample"; "Pre-collection delay (sec):" a text input field containing "0"; and an unchecked checkbox labeled "Use sample gain and attenuation settings". The second section, "Backgrounds for Simulation", contains a large empty text area, a "Delete" button, and three unchecked checkboxes: "Prompt for simulation background", "Use simulation background for all workflow runs", and "Cycle through simulation backgrounds".

### Background specification for Antaris IGS instrument backgrounds

The following parameters are unique to the background specification for collecting instrument backgrounds with the Antaris IGS system:

- **Beam Path.** Use the Beam Path list box to specify the path of the infrared beam when collecting backgrounds with the Antaris IGS analyzer.

A close-up of the "Beam path:" dropdown menu, showing the word "Instrument" selected in the list box.

To select the beam path, select an option in the drop-down list. The following options are available:

- *Instrument.* Select this option to direct the beam through the spectrometer compartment and then directly to the detector. This is the “lower” beam path referenced in the *Antaris IGS User Guide*. The Instrument beam path setting is typically used only to check instrument operation or status.
- *Gas Cell.* Select this option to direct the beam through the sample beam path compartment and gas cell and then back to the detector. This is the “upper” beam path referenced in the *Antaris IGS User Guide*. The Gas Cell beam path setting should be used to collect background data through the gas cell.

**Note** The Use Sample Position, Gain And Attenuation Settings check box defines the location and the Gain and Attenuator settings for background collections. To collect background data from an external reference, make sure this check box is selected. The software will collect the background data using the same Gain and Attenuator settings used for the sample collection (i.e., with the Gain and Attenuator settings shown on the sample specification). To collect background data without a reference, make sure this check box is cleared. The software will collect the background data with the default Gain and Attenuator settings. See “Features common to background specifications” for details. ▲

The remaining parameters on the gas cell background specification are described in the section titled “Features common to background specifications” in this chapter except the default settings may vary. For information about recommended settings for collecting instrument backgrounds, see your *Antaris IGS User Guide*.

## **Blend Analyzer background specifications**

This background specification contains parameters that are designed for collecting background data with the Antaris Target Blend analyzer.

The illustration below shows the parameters for the blend analyzer background specification. These parameters appear in the display area of RESULT Integration when a blend analyzer background specification is selected in a workflow.

Background Specification

New Background

Background Collection

Sampling technique: Blend Analyzer

Location: Internal gold reference

Number of background scans: Same number of scans as for sample

Pre-collection delay (sec): 0

Use sample position, gain and attenuation settings

Backgrounds for Simulation

Delete

Prompt for simulation background

Use simulation background for all workflow runs

Cycle through simulation backgrounds

### Background specification for blend analyzer sample

The following parameters are unique to the blend analyzer background specification:

- Location.** Use this list box to specify the location for background data collection with the blend analyzer. The Location parameter controls the position of the instrument's internal reference wand. The wand contains a diffuse gold reference sample and it may also contain a polystyrene sample. The software provides the following options for background collections with the blend analyzer:

  - Internal gold reference.* Select this option to collect background data using the blend analyzer's internal diffuse gold reference. The internal reference is an uncoated, highly reflective surface that is moved in front of the near-infrared light source so that it fully covers the sample window (from the inside) for background collections. You can collect a background at the same time as a sample spectrum.

**Note** When collecting background data from the blend analyzer's internal diffuse gold reference, the software automatically uses the default Gain and Attenuator settings (Gain = 1x, Attenuator = C screen). ▲

- *Empty*. Select this option to collect a background from an external reference sample mounted on a Target Blend analyzer that is configured for bench top sampling. The Empty setting moves the reference wand out of the light source, which allows the beam to exit the sample window to interact with an external reference. You can also use this setting to collect a single beam spectrum, which shows how the energy of the source is distributed over the measured frequency range. The spectrum can be compared to previous single beam spectra to help determine whether a problem exists with your instrument.
- *Polystyrene*. Select this option to collect a background spectrum from the internal polystyrene sample (if one is included) mounted on the reference wand. The polystyrene spectrum can be useful for diagnostic purposes. For example, you can collect a sample and background spectrum of polystyrene to produce a 100% line spectrum, which shows the noise level in the sampling environment and the instrument. The spectrum can be compared to previous 100% line spectra to help determine whether a problem exists with your instrument.

**Note** The Instrument Check feature of RESULT Operation uses the internal reference wand to produce a single beam and 100% line spectrum for diagnostic purposes. See “Instrument Check” in the “RESULT Operation User Guide” for details. ▲

The remaining parameters on the blend analyzer background specification are described in the section titled “Features common to background specifications” in this chapter except the default settings may vary. For information about recommended settings for collecting blend analyzer backgrounds, see your *Antaris Target Blend Analyzer User Guide*.

**Note** The Use Sample Gain And Attenuation Settings check box defines the Gain and Attenuator settings for background collections with the blend analyzer. To collect background data from an external reference or the polystyrene sample using the same Gain and Attenuator settings used for the sample collection (i.e., with the Gain and Attenuator settings shown on the sample specification), make sure this check box is selected. Clear the check box to collect background data from an external reference or polystyrene using the default Gain setting and Attenuator settings. See “Features common to background specifications” for details. ▲

## **Validation Wheel background specifications**

This background specification contains parameters that are optimized for collecting transmission backgrounds using the optional validation wheel. The validation wheel background specification is available in the software only when the instrument includes the optional ValPro System Qualification package and the validation wheel is installed and properly configured in RESULT Integration. See “Setting RESULT Integration Options” in the “RESULT Integration User Guide” for information about configuring RESULT Integration for ValPro.

The illustration below shows the parameters for the validation wheel background specification. These parameters appear in the display area of RESULT Integration when a validation wheel background specification is selected in a workflow.

Background Specification

New Background

Background Collection

Sampling technique: Validation Wheel

Number of background scans: Same number of scans as for sample

Pre-collection delay (sec): 0

Use sample position, gain and attenuation settings

Backgrounds for Simulation

Delete

Prompt for simulation background

Use simulation background for all workflow runs

Cycle through simulation backgrounds

### Background specification for validation wheel

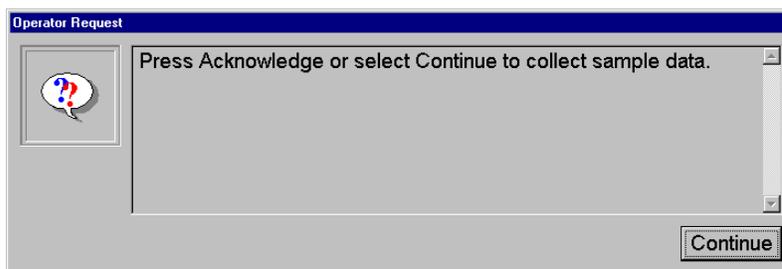
There are no parameters that are unique to the sample specification for the validation wheel. The background specification differs only in the default settings for those parameters. For descriptions of the parameters that are common to all the background specifications, see “Features common to background specifications” in this chapter. For information about recommended settings for collecting backgrounds with the validation wheel, see your *ValPro System Qualification manual*.

**Note** The Use Sample Position, Gain And Attenuation Settings check box defines the Position, Gain and Attenuator settings for background collections with the validation wheel. To collect background data using the same Position, Gain and Attenuator settings used for the sample collection (i.e., with the Sample Position, Gain and Attenuator settings shown on the sample specification), make sure this check box is selected. This setting allows you to collect a 100% line spectrum with the validation wheel samples. Clear the check box to collect background data through the empty position on the validation wheel using the default Gain and Attenuator settings. See “Features common to background specifications” for details. ▲

## StartStop specifications

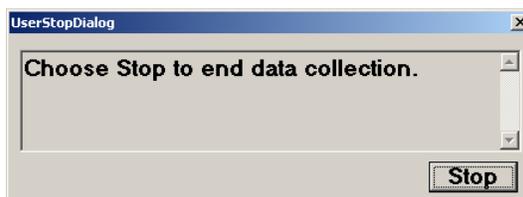
The StartStop Specifications group provides two types of prompt specifications that define the operator prompts for a StartStop event in a workflow, including:

- **StartRun specifications.** A StartRun specification defines a prompt to start implementing the events in a StartStop event group. The operator must acknowledge the prompt before the workflow can continue. StartRun specifications may be linked to StartStop events in a workflow to initiate background or sample collection, as shown in the example below.



### StartRun prompt

- **StopRun specifications.** The StopRun specification defines an operator prompt that stops performing the events in the StartStop group. The StopRun prompt will be similar to the example below.



When you test or run a workflow that contains a StartStop group, the workflow displays the StartRun prompt after it encounters the StartStop group. The operator must respond to the prompt by choosing Continue in the prompt before the workflow will continue.

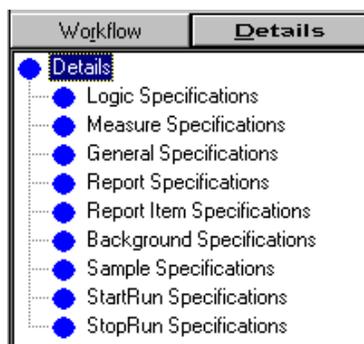
After the operator responds to the prompt, the workflow displays the StopRun prompt. If the operator chooses Stop in the prompt, the workflow stops executing the events in the StartStop group and skips to the first event after that group.

If the operator does not respond to the StopRun prompt, the workflow performs all the events in the StartStop group in sequence, starting with the first event in the group and ending with the last one, and then continues with the first event after that group.

## Adding a StartStop specification to a workflow

To add a StartStop specification to the open workflow:

### 1. Select the Details tab.



### 2. Select StartRun specifications or StopRun specifications and then choose the Add button on the RESULT Integration toolbar.

The software displays the Add Specification dialog box.

### 3. Select the StartRun specification or the StopRun specification, enter a base name for the new specification, and then choose OK.

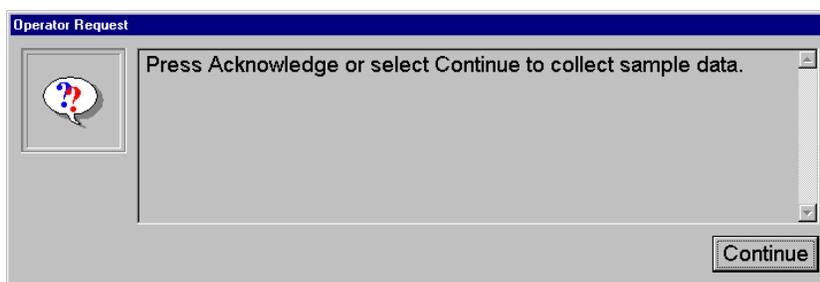
The new specification appears in the display area of the RESULT Integration main window.

Read the next two sections to learn about the options available for setting up StartRun specifications and StopRun specifications in a workflow. For information about linking specifications to workflow events, see “Linking a specification to a workflow event” in the “RESULT Integration User Guide.”

## StartRun prompt specifications

A StartRun specification defines a prompt to start implementing the events in a StartStop event group, including the message text and the button label. The operator must acknowledge the prompt before the workflow can continue.

StartRun specifications may be linked to StartStop events in a workflow to initiate background or sample collection, as shown in the example below.



### StartRun prompt

You can set up the prompt so the operator can acknowledge it only by choosing the button displayed in the prompt, or you can allow the operator to acknowledge the prompt by either choosing the button in the dialog box or by pressing an Acknowledge button on the instrument, as shown above.

If the dialog box is configured to allow the operator to respond by pressing the acknowledge button on the instrument (not available for Antaris IGS systems), the green LED indicator will light when the dialog box is displayed on the screen.

**Associated events:** StartStop event

**Associated specifications:** None

**Related events:** None

**Related specifications:** StopRun specification, Prompt specification

**Parameters:** The illustration below shows the parameters for the StartRun specification. These parameters appear in the display area of RESULT Integration when a StartRun specification is selected in a workflow.

Prompt Specification

New Prompt

Button label: Continue

Allow Antaris Acknowledge button response

Preview data collection

Prompt text:

### StartRun prompt specification parameters

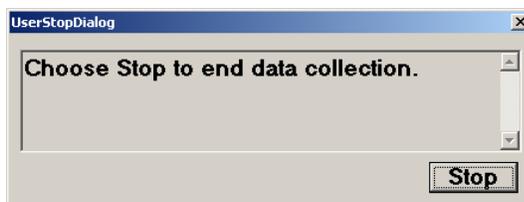
The StartRun specification parameters define the message text and the button label for the StartRun prompt.

There are no parameters that are unique to the StartRun specification. The StartRun specification differs from the prompt specification only in the default settings for those parameters. For descriptions of the parameters that are common to the StartRun specification and prompt specification, see “Prompt specifications” in this chapter.

### StopRun prompt specifications

A StopRun specification defines a prompt that allows the operator to stop executing the events in a StartStop event group. The stop run specification defines the message text. The button is always labeled Stop.

StopRun specifications may be linked to StartStop events in a workflow to allow the operator to control workflow operation. For example, a stop run specification can be set up to allow the operator to stop background or sample collection, as shown in the example below.



### StopRun prompt

If the operator chooses Stop in the prompt, the workflow stops executing the events in the StartStop group and skips to the first event after that group. If the operator does not respond to the StopRun prompt, the workflow performs all the events in the StartStop group in sequence, starting with the first event in the group and ending with the last one, and then continues with the first event after that group.

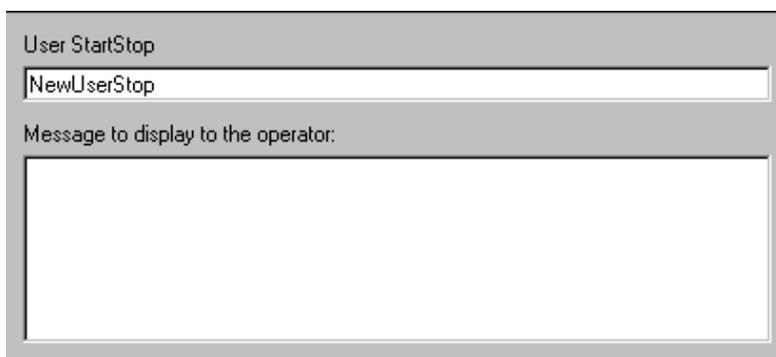
**Associated events:** StartStop event

**Associated specifications:** None

**Related events:** None

**Related specifications:** StartRun specification, Prompt specification

**Parameters:** The illustration below shows the parameters for the StopRun specification. These parameters appear in the display area of RESULT Integration when a StopRun specification is selected in a workflow.



### StopRun specification parameter

The StopRun specification parameters define the message for the StopRun prompt. Enter the text in the Message To Display To The Operator box. The message will be displayed in the center of the dialog box at run time.

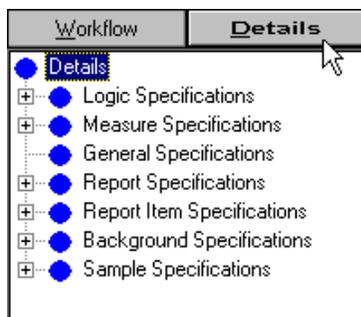
## Correction specifications

The Correction Specifications group provides specifications for correcting the spectral data produced by a workflow. Correction specifications can be linked to collection events in workflows.

### Adding a correction specification to a workflow

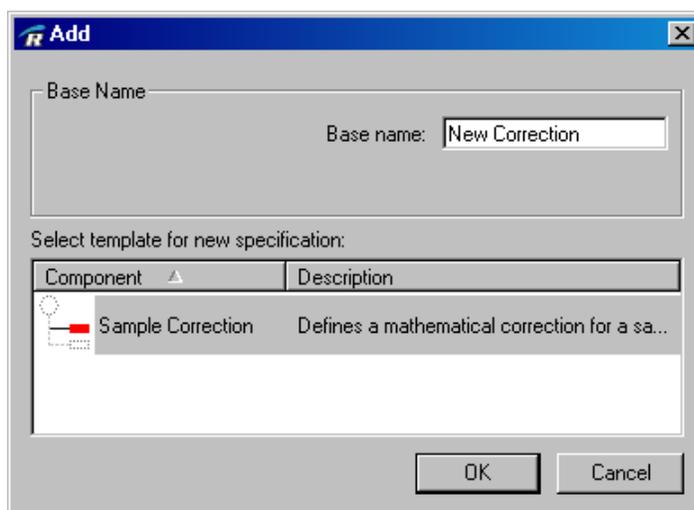
To add a correction specification to the open workflow:

1. Select the Details tab.



2. Select Correction Specifications and then choose the Add button on the RESULT Integration toolbar.

The software displays the following dialog box.



3. Select a correction specification, enter a base name for the new specification and choose OK.

The new specification appears in the display area of the RESULT Integration main window.

You can also create a correction specification from specific events such as Collect events and Collect multi-channel events. Read the next two sections to learn about the options available for setting up correction specifications in a workflow. For information about linking specifications to workflow events, see “Linking a specification to a workflow event” in the “RESULT Integration User Guide.”

## Sample correction specifications

A sample correction specification defines a dark background or transfer correction for spectra collected from a workflow. Dark background and transfer corrections can improve accuracy for some NIR experiments. The correction specification is used to select a correction function and identify the spectra used in the correction.

*Dark background corrections* can be useful for reflection measurements such as measurements taken with the Antaris integrating sphere module or a fiber optic reflection accessory when the experiment requires a high degree of photometric accuracy. A dark background correction removes undesirable back reflections from the sample spectra. Undesirable back reflections can be from the face of a glass vial or other container or from unwanted material clinging to the surface of the sample window or even 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 material are nonreflective, back reflections are not important to the analysis and a dark background correction is not needed. However, if back reflections are present in the sample and, perhaps, the background measurement, a dark background correction may be used to improve the photometric accuracy of the data. A dark background correction will be more useful for samples that are less reflective because the back reflections account for a higher percentage 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 reaches the reflection detector when there is no reflective sample in the beam path. The dark background spectrum can be subtracted from the single beam spectrum of the sample before the spectrum is ratioed to the background spectrum to produce a ratioed spectrum that is due solely to the sample. 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.

*Transfer corrections* can be used to correct the sample spectra for backgrounds taken with a sampling module, accessory or location that is different from the module, accessory or location used to measure the samples. 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 alternative background location can be the Antaris transmission module, the integrating sphere, or another fiber optic channel.

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. Several options are available for implementing a transfer correction depending on the format (single beam or ratioed) of the transfer spectrum. Options are also available for applying dark background and transfer corrections at the same time and for substituting an archived background spectrum for the background collected by the workflow.

Sample correction specifications can be linked to collection events in workflows. You can only apply a correction to individual spectra; the sample correction feature is not available for spectra produced by a collect sequence event.

**Associated events:** Collect event, Collect multi-channel event, Collect Dual Tablet event

**Associated specifications:** None

**Related events:** None

**Related specifications:** None

**Parameters:** The illustration below shows the parameters for the sample correction specification. These parameters appear in the display area of RESULT Integration when a sample correction specification is selected in a workflow.

### Sample correction specification parameters

The sample correction specification parameters define the correction equation and identify the spectra used in the correction. The following sections explain the parameters in detail. The parameters are explained in the order in which they appear in the software.

## Terms

Use the features in this group to define the spectra that will be used in the correction. The spectra required for a specific correction are defined by the correction equation (see “Correction Equation” below). These spectra must be collected by (use a collection event) or loaded into (use a Load Spectrum event) the workflow before the workflow encounters the sample correction specification and its associated collection event.

- **Sample Spectrum (S)**. The single beam spectrum of the **sample produced by the collection event** that is linked to this sample correction specification.
- **Background Spectrum (B)**. The single beam spectrum of an appropriate **background produced by the collection event** that is linked to this sample correction specification.
- **Spectrum 1 (X)**. Single beam spectrum defined by the selected correction equation. Can be **collected by** the workflow **or archived and loaded** into the workflow using a Load Spectrum event.
- **Spectrum 2 (Y)**. Single beam spectrum defined by the selected correction equation. Can be **collected by** the workflow **or archived and loaded** into the workflow using a Load Spectrum event.
- **Correction Background (CB)**. Single beam spectrum of an appropriate **background** (but not the one produced by the collection event). Can be **collected by** the workflow **or archived and loaded** into the workflow using a Load Spectrum event.
- **Transfer Background (TB)**. Single beam spectrum of an appropriate **background** reference measured at the same location as the normal **background** (spectrum B). Can be collected by the workflow or archived and loaded into the workflow using a Load Spectrum event. The spectrum should be collected at the same time as spectrum TS. Spectrum TB does not need to be updated unless a component in the beam path is changed.
- **Transfer Sample (TS)**. Single beam spectrum of a **background** reference measured at the same location as the **sample** (spectrum S) and the same material used for spectrum TB. For example, if an external sample such as Spectralon is measured for spectrum B, then spectrum TB should be collected with the same Spectralon sample. Can

be collected by the workflow or archived and loaded into the workflow using a Load Spectrum event. The spectrum should be collected at the same time as spectrum TB. Spectrum TS does not need to be updated unless a component in the beam path is changed.



## Correction Equation

Use this drop-down list box to select an equation for the correction. RESULT provides a range of functions for dark background and transfer corrections using a normal or archived background spectrum and options for applying dark background and transfer corrections at the same time. Brief descriptions of the available corrections and their associated spectra are provided in the software. Detailed descriptions are provided below. The workflow applies the correction to the single beam spectra. The corrected spectrum becomes the collection event result and is stored in the data format specified on the collection event.

- **(S-X)/(B-X) or (S-X)/(CB-X)**  
**Dark background correction for sample and background.**  
Removes undesirable back reflections from the sample and background. Appropriate for reflection experiments when the sample and background measurements have additional reflective components and they are collected at the same location and with the same conditions and the experiment requires a high degree of photometric accuracy. This correction is useful for samples that are not highly reflective especially when a highly reflective material such as Spectralon is used for the background measurement. For each sample spectrum collected by the workflow, this correction subtracts the same dark background (spectrum X) from the sample and background single beam spectra and then ratios the sample to the background to produce the final spectrum. The background can be from the associated collection event (spectrum B) or it can be from another event or file (spectrum CB).
- *Spectrum S.* Single beam spectrum of the sample and its container or other reflective surface collected with an integrating sphere module or fiber optic reflection accessory.
- *Spectrum B or CB.* Single beam spectrum of an appropriate background reference collected at the same location and with the same container or reflective surface used for the sample measurement.

- *Spectrum X*. Single beam spectrum that was collected at the same location and with the same container or reflective surface used for the sample and background measurements but without the sample or background material. This “dark background” spectrum represents the sum of any back reflections in the sample and background beam paths that cannot be attributed to the sample or background material.
- **(S-X)/B or (S-X)/CB**  
**Dark background correction for sample only.** Removes unwanted back reflections from the sample measurement. Appropriate for reflection measurements when unwanted back reflections may be present for the sample measurement but not for the background and the experiment requires a high degree of photometric accuracy. A common example is when samples are measured with an integrating sphere and the background is taken with a non-reflective background sample or the integrating sphere’s internal gold reference (the gold reference is considered to be non-reflective because it is positioned below the sample window on the instrument). This correction is also useful for samples collected with a fiber optic accessory when the background is collected with an internal reference. For each sample spectrum collected by the workflow, this correction subtracts a dark background (spectrum X) from the sample single beam spectrum and then ratios the sample to the background to produce the final spectrum. The background can be from the associated collection event (spectrum B) or it can be from another event or file (spectrum CB).
- *Spectrum S*. Single beam spectrum of the sample and its container or other reflective surface collected with an integrating sphere module or fiber optic reflection accessory.
- *Spectrum B or CB*. Single beam spectrum of an appropriate but non-reflective external background reference or the internal gold reference for the integrating sphere.
- *Spectrum X*. Single beam spectrum that was collected at the same location and with the same container or reflective surface used for the sample measurement but without the sample material. This “dark background” spectrum represents the sum of any back reflections in the sample beam path that cannot be attributed to the sample material.

- $(S/B) \cdot (TB/TS)$  or  $(S/CB) \cdot (TB/TS)$

**Transfer correction using single beam spectra.**

Corrects for backgrounds measured at a different fiber optic channel than the samples or at another location on the instrument such as an integrating sphere or transmission module or an internal reference. Can also be used to enhance performance for methods transferred between instruments. Allows frequent background collections using an alternative beam path without significantly compromising data quality. For each sample spectrum collected by the workflow, this correction ratios the single beam sample spectrum against a single beam background spectrum measured at an alternative location and then multiplies the data by a “transfer spectrum” to produce the final spectrum. The transfer spectrum is the ratio of two single beam background measurements taken at the alternative location (numerator) and at the sample location (denominator). The transfer spectrum represents the differences between the two beam paths. The background collected by the workflow at the alternative location (spectrum B) and the specified frequency should account for any changes in the instrument response over time. This correction is based on the assumption that the differences between the two beam paths are relatively constant. The background can be from the associated collection event (spectrum B) or from another event or file (spectrum CB).

- *Spectrum S*. Single beam spectrum of the sample collected on the Antaris instrument.
- *Spectrum B or CB*. Single beam spectrum of an appropriate background reference measured at an alternative location such as the Antaris integrating sphere or transmission module or a different fiber optic channel. This spectrum should be updated periodically to account for any changes in the instrument response over time.
- *Spectrum TB*. Single beam spectrum of a **background** reference measured at the **alternative** location, ideally using the same instrument and sampling module or fiber optic accessory as spectrum B. This “transfer background” spectrum should be collected at the same time as spectrum TS with a resolution that is the same or higher than the resolution used for the samples. Spectrum TB does not need to be updated unless a component in the beam path is changed.

- *Spectrum TS*. Single beam spectrum of a **background** reference measured at the **sample** location, ideally using the same instrument and sampling module or fiber optic accessory used for spectrum S and the same material used for Spectrum TB. This “transfer sample” spectrum should be collected at the same time and at the same resolution as spectrum TB. Spectrum TS does not need to be updated unless a component in the beam path is changed.
- **(S/B)\*X**  
**Transfer correction using scalar spectrum.**  
Open transfer correction that can be used to normalize or scale a collected spectrum, where spectrum X is the scalar spectrum. Spectrum X can also represent a ratioed transfer spectrum similar to (TB/TS) above. For each sample spectrum collected by the workflow, this correction ratios the single beam sample spectrum against the single beam background spectrum and then multiplies the data by spectrum X to produce the final spectrum. The Y-axis units of spectrum X are ignored.
  - *Spectrum S*. Single beam spectrum of the sample collected on the Antaris instrument.
  - *Spectrum B*. Single beam spectrum of an appropriate background reference.
  - *Spectrum X*. Scalar spectrum with any Y-axis unit. This spectrum will be multiplied data point by data point to spectrum S.

A representative background spectrum would be measured at the same location as the sample using the same instrument and sampling module or fiber optic accessory and updated frequently enough to capture any changes in the instrument response over time. However, depending on your samples and experimental requirements, you may be able to substitute an archived background spectrum that meets some of all of these requirements but is updated infrequently or not at all. The S/CB correction is designed for that purpose.

- **S/CB**  
**Transfer correction using stored spectrum.** This is the simplest form of a transfer correction where the sample spectra are ratioed against a static but representative background spectrum. The background spectrum can be collected by the current workflow, or collected and archived by a previous workflow and loaded into the current workflow with a Load Spectrum event. For each sample spectrum, this correction ratios the single beam sample spectrum against the archived single beam background spectrum to produce the final spectrum.
  - *Spectrum S*. Single beam spectrum of the sample collected with any Antaris sampling module or fiber optic accessory.
  - *Spectrum CB*. Single beam spectrum of an appropriate background reference.

- $(S-X)/(B-Y)$   
**Dark background correction with unique correction for sample and background.** Removes unique back reflections from the sample and background. Appropriate for fiber optic reflection experiments when unique, unwanted back reflections may be present for the sample and background measurements. A typical example is when the background is measured through a different channel using the same type of fiber optic cable and fiber optic sampling accessory. The correction is useful for experiments that require a high degree of photometric accuracy. For each sample spectrum collected by the workflow, this correction subtracts a dark background (spectrum X) from the sample single beam spectrum and a dark background (spectrum Y) from the background single beam spectrum and then ratios the sample to the background to produce the final spectrum. The correction is based on the assumption that the back reflections are more significant than any inherent differences between the two fiber optic accessories (a reasonable assumption if the two fiber optic accessories are the same brand and model and the fiber optic cables are the same type and approximately the same length).
  - *Spectrum S.* Single beam spectrum of the sample and its container or other reflective surface collected with a fiber optic reflection accessory.
  - *Spectrum B.* Single beam spectrum of an appropriate background reference and its container or other reflective surface collected with the same type of fiber optic reflection accessory attached to a different fiber optic channel on the instrument.
  - *Spectrum X.* Single beam spectrum measured at the same location and with the same container or reflective surface used for the **sample** measurement but without the sample material. This “dark background” spectrum represents the sum of any back reflections in the sample beam path that cannot be attributed to the sample material.
  - *Spectrum Y.* Single beam spectrum measured at the same location and with the same container or reflective surface used for the **background** measurement but without the background material. This “dark background” spectrum represents the sum of any back reflections in the background beam path that cannot be attributed to the background material.

- **(S-X)/B\*(TB/TS)**  
**Dark background correction for sample with transfer correction.**  
 Applies a dark background correction to the single beam sample spectrum and a transfer correction to the ratioed spectrum. Appropriate for fiber optic reflection measurements when interfering back reflections are present for the sample measurement but not for the background and the background is measured at another location on the instrument such the transmission module or an internal reference. The correction is useful only when the experiment requires a high degree of photometric accuracy. For each sample spectrum collected by the workflow, this correction subtracts a dark background (spectrum X) from the sample single beam spectrum, ratios the single beam sample spectrum against a single beam background spectrum measured at an alternative location and then multiplies the data by a “transfer spectrum” to produce the final spectrum. The transfer spectrum is the ratio of two single beam background measurements taken at the alternative location (numerator) and at the sample location (denominator).
  - *Spectrum S.* Single beam spectrum of the sample and its container or other reflective surface collected with a fiber optic reflection accessory.
  - *Spectrum B.* Single beam spectrum of an appropriate background reference measured at an alternative location such as an integrating sphere or transmission module or a different fiber optic channel or with the internal transmission reference for the Antaris MX or the internal diffuse-gold reference for the Antaris integrating sphere. This spectrum should be updated periodically to account for any changes in the instrument response over time.
  - *Spectrum X.* Single beam spectrum that was collected at the same location and with the same container or reflective surface used for the sample measurement but without the sample material. This “dark background” spectrum represents the sum of any back reflections in the sample beam path that cannot be attributed to the sample material.
  - *Spectrum TB.* Single beam spectrum of a **background reference** measured at the **alternative** location, ideally using the same instrument and sampling module or fiber optic accessory as spectrum B. This “transfer background” spectrum should be

collected at the same time as spectrum TS with a resolution that is the same or higher than the resolution used for the samples. Spectrum TB does not need to be updated unless a component in the beam path is changed.

- *Spectrum TS*. Single beam spectrum of a **background** reference measured at the **sample** location, ideally using the same instrument and sampling module or fiber optic accessory as spectrum S and the same material as spectrum TB. This “transfer sample” spectrum should be collected at the same time and at the same resolution as spectrum TB. Spectrum TS does not need to be updated unless a component in the beam path is changed.
- $(S-X)/(B-Y)*(TB/TS)$   
**Dark background correction with unique correction for sample and background and transfer correction.** Applies unique dark background corrections to the sample and background and a transfer correction to the resulting data. Appropriate for fiber optic reflection measurements when unique, undesirable back reflections may be present for the sample and background measurements and the background is measured at an alternative location. A typical example is when the background is measured through a different channel using a different type or length of fiber optic cable and/or fiber optic accessory. The correction is useful for experiments that require a high degree of photometric accuracy. For each sample spectrum collected by the workflow, this correction subtracts a dark background (spectrum X) from the sample single beam spectrum and a different dark background (spectrum Y) from a background single beam spectrum that is measured at an alternative location and then multiplies the data by a “transfer spectrum” to produce the final spectrum. The transfer spectrum is the ratio of two single beam background measurements taken at the alternative location (numerator) and at the sample location (denominator).
- *Spectrum S*. Single beam spectrum of the sample and its container or other reflective surface collected with a fiber optic reflection accessory.

- *Spectrum B*. Single beam spectrum of an appropriate background reference and its container or other reflective surface measured at a different fiber optic channel. This spectrum should be updated periodically to account for any changes in the instrument response over time.
- *Spectrum X*. Single beam spectrum that was collected at the same location and with the same container or reflective surface used for the sample measurement but without the sample material. This “dark background” spectrum represents the sum of any back reflections in the sample beam path that cannot be attributed to the sample material.
- *Spectrum Y*. Single beam spectrum that was collected at the same location and with the same container or reflective surface used for the background measurement but without the background material. This “dark background” spectrum represents the sum of any back reflections in the background beam path that cannot be attributed to the background material.

**Note** If the interfering back reflections present at the sample and background locations are essentially the same, use the same spectrum for spectrum X and spectrum Y. ▲

- *Spectrum TB*. Single beam spectrum of a **background** reference measured at the **alternative** location, ideally using the same instrument and sampling module or fiber optic accessory as spectrum B. This “transfer background” spectrum should be collected at the same time as spectrum TS with a resolution setting that is the same or higher than the resolution setting used for the samples. Spectrum TB does not need to be updated unless a component in the beam path is changed.
- *Spectrum TS*. Single beam of a **background** reference measured at the **sample** location, ideally using the same instrument and sampling module or fiber optic accessory as spectrum S and the same material as spectrum TB. This “transfer sample” spectrum should be collected at the same time and at the same resolution as spectrum TB. Spectrum TS does not need to be updated unless a component in the beam path is changed.

**Usage:** A sample correction specification may be linked to the following types of workflow events:

- **Collect event**, which can be used to collect a single beam sample and/or background spectrum and produce a ratioed spectrum in the selected format.
- **Collect multi-channel event**, which can be used to collect single beam sample and background spectra from two or more fiber optic sampling accessories at the same time. The single beam spectra can be used to produce ratioed spectra in a selected format.
- **Collect reflection/transmission event**, which can be used to collect a transmission spectrum using the detector located in the tablet analyzer cover and a reflection spectrum using the detector located in the Antaris integrating sphere at the same time.

The correction is applied only when a ratioed data format (e.g., Absorbance, %Transmission, etc.) is selected on the associated collection event. (If Data Format is set to “Single Beam,” the collection result will be the uncorrected single beam data.

# Index

- % standard deviation
  - adding to sequence reports, 338
  - calculating in workflows, 23
- 100% line spectrum
  - collecting with an autosampler, 416
  - collecting with blend analyzer, 422
  - collecting with validation wheel, 424
  - sample specification setting for blend analyzer, 385
- 4-20 milliamp signals
  - reading from devices into workflows, 99
  - writing to devices from workflows, 145
- A**
  - absolute maximum, minimum, or value
    - reporting as composite component, 260
  - absorbance
    - format for spectra collected from workflows, 47
  - Acknowledge button, 272
    - and operator prompts, 271
    - and startrun prompts, 427
  - Action parameter (for sequence collection prompt), 209
  - Add Break dialog box, 315, 333
  - Add Event dialog box, 5, 196, 222
  - Add Logical test dialog box, 225
  - Add New Measurement dialog box, 241
  - Add New Test Case dialog box, 243
  - Add Workflow Result To Summary Section dialog box, 327, 343
  - Add Workflow Result To Table Section dialog box, 312
  - Add/Edit Heading item dialog box, 294
  - Add/Edit Operator Request dialog box, 267
  - adding
    - components to create a composite component, 260
  - address
    - IP address for Opto 22 Controller, 100, 112, 146
  - Align parameter
    - setting for summary sections in reports, 328
    - setting for table sections in reports, 314
  - Allow Acknowledge Button parameter, 272
  - Allow Early Exit parameter, 165, 170, 175
  - Allow Operator To Override Heater Pause parameter, 372
  - amplifying, instrument signal, 355
  - analog signals
    - reading into workflows, 102
    - writing from workflows, 150
  - Analysis Type parameter, 249
  - angle, of rotation
    - for blend analyzer sampling, 386
  - Antaris autosampler
    - collecting 100% line spectrum, 416
    - external reference collections, 276
  - Antaris MX
    - collecting data from multiple channels at the same time, 64
    - validation wheel samples, 67
  - Antaris SabIR probe
    - configuring for fiber optic sampling module, 374
    - configuring for multi-channel sampling, 375, 413
  - aperture
    - limitations for high resolution spectra, 57
    - limitations for high resolution spectra with Antaris MX, 68
  - Apodization parameter, 379
  - Application Argument parameter, 140
  - Application Name parameter
    - for measurement specifications, 240
    - for run exe events, 139
  - Application Time-out parameter, 140
  - applications
    - adding to workflows, 138
  - archive events
    - and repeat loops, 23, 167
    - assigning file names to archived spectra and reports, 17
    - described, 7
    - parameters, 8
      - Base Path, 11
      - Report Archiving Information To OPC, 17
      - Report Format, 12
      - Save List Of Archived File Names, 15
      - Save Report Files As Read-Only, 13
      - Save Spectral Files As Read-Only, 13
      - Save Workflow Error Report, 16
      - Spectral Data Format, 12
      - Use Digital Signatures, 14
    - selecting a folder for archiving spectra and reports from a workflow, 11
    - specifying spectra and reports to be archived, 10
    - suggested uses in workflows, 22
    - using archived background spectrum to process sample data collected in workflows, 49

- archived files
  - configuring workflows to report to OPC client, 17
- archived spectra
  - loading archived spectra into workflows, 84
- archiving
  - background spectra, 50, 69, 215
  - backgrounds, 215
  - backgrounds from collect dual tablet events, 58
  - backgrounds from collect events, 49
  - backgrounds from collect multi-channel events, 69
  - pass/fail images, 7
  - pass/fail results, 7
  - RESULT Integration and RESULT Operation compared, 11
  - selecting a folder for an archive event, 11
  - spectra and reports, 11
- area, total
  - adding to sequence reports, 338
- attenuation
  - setting for sample collection, 354
- attenuation screen factors, 48, 213
- Attenuator parameter, 354
  - default settings for background collections, 398
  - for collect dual tablet events, 59
  - using the Optimize Gain feature, 356
- Attribute parameter
  - setting for a workflow result, 224, 313, 328
- attributes
  - for analytical method, 241
- audit log
  - storing workflow results in the database for measurement queries, 140
- automatically naming files saved by archive events in workflows, 17
- autosampler
  - adding autosampler position numbers to spectra from workflows, 117
  - collecting 100% line spectrum, 416
  - external reference collections, 276
  - location for external reference, 185
  - positioning from a workflow, 182
  - prompting for next carousel, 186
  - prompting for position number, 185
  - using a sampling sequence to specify position number, 185
- Autosampler Carousels parameter, 276
- autosampler integrating sphere
  - background specification parameters, 414
  - sample specification parameters, 376
- Autosampler Position parameter, 184
- Autosampler RS
  - configuring in a workflow, 377
- autosampler softgel tablet analyzer
  - background specification parameters in workflows, 404
  - sample specification parameters, 376
- Autosampler Specification parameter, 183
- autosampler specifications
  - described, 275
  - linking to sample specifications, 377
  - parameters, 275
    - Reference Position Reserved For Background Collections, 276
  - prompting for number of positions in carousels, 276
  - specifying number of positions in carousels, 276
  - suggested uses in workflows, 277
- autosampler standard tablet analyzer
  - background specification parameters in workflows, 403
- autosampler std tablet analyzer
  - sample specification parameters, 376
- average spectrum
  - calculating in workflows, 88, 91, 95
  - restrictions for generating, 88
- average values
  - adding to sequence summary sections in reports, 337
  - adding to summary sections in reports, 330
  - calculating in workflows, 23
- averaging
  - components to create a composite component, 260

**B**

- B screens, 354
- background
  - using archived background spectrum to process sample data collected in workflows, 49
- Background Channel parameter, 72
- background corrections, dark
  - defined, 431
- background corrections, transfer
  - defined, 432
- background data preview
  - and collection prompts, 274
- Background Frequency parameter, 213
- Background Frequency parameter for collect dual tablet events, 58
- Background Frequency parameter for collect events, 48
- Background Frequency parameter for collect multi-channel events, 68
- background position
  - setting for autosampler integrating sphere, 415
  - setting for blend analyzer sampling, 421
  - setting for gas cell sampling, 418
  - setting for transmission module, 408

- Background Position parameter
  - for collect multi-channel events, 66
- background prompts
  - and external background reference, 52
  - and internal reference collections, 214
  - and internal reference collectons, 49
- Background Specification parameter, 352
- background specifications
  - configuring simulated background spectra, 400
  - defining collection parameters, 397
  - described, 392
  - features common to background specifications, 396
  - linking to collect multi-channel events in workflows, 73
  - linking to sample specifications, 352
  - parameters
    - Backgrounds For Simulation, 400
    - Beam Path, 418
    - Cycle Through Simulation Backgrounds, 401
    - for autosampler integrating sphere sampling, 414
    - for autosampler softgel tablet sampling, 404
    - for autosampler standard tablet sampling, 403
    - for blend analyzer sampling, 420
    - for fiber optic sampling, 410
    - for gas cell sampling, 417
    - for integrating sphere sampling, 406
    - for multi-channel sampling, 412
    - for SabIR probe sampling, 410
    - for softgel tablet sampling, 404
    - for standard tablet sampling, 403
    - for transmission module sampling, 407
    - for validation wheel sampling, 423
    - Gain, 413
    - Location for blend analyzer backgrounds, 421
    - Location, for autosampler backgrounds, 415
    - Number Of Background Scans, 397
    - Optimize Gain, 414
    - Pre-collection Delay, 398
    - Probe Type, 413
    - Prompt For Simulation Background, 401
    - Sampling Technique, 397
    - Use Sample Position, Gain And Attenuation Settings, 398
    - Use Simulation Backgrounds For All Runs, 402
  - suggested uses in workflows, 402
- backgrounds
  - and Number Of Scans Per Spectrum, 214
  - clearing background spectra from a workflow, 40
  - collecting and storing as simulated spectra with a workflow, 361
  - collecting from a workflow, 43
  - for sequence collection, 214
  - restrictions for archiving, 50, 69, 215
  - using archived background spectrum to process sample data collected in workflows, 49
  - when to use prompts for collecting, 52
- Backgrounds For Simulation parameter, 400
- bar code options
  - setting Data Type in request specification, 268
  - setting Enter key handling, 270
  - setting field delimiter, 270
- base name error, 6
- base names
  - for files saved by archive events in workflows, 18
  - for workflow events, 5
- base path
  - for archived spectra, 85
  - for archived spectra and reports, 11
  - for text files, 126
  - RESULT Integration and RESULT Operation compared, 11
- Base Path parameter, 11, 85, 126
- Beam Path parameter, 378, 391, 418
- Before Background operator prompts, 52
- Before Sample operator prompts, 53
- bi-directional scanning, 382
- bitmap files
  - compatible formats, 296
- bitmap images
  - adding to sample reports, 296
- Blackman-Harris apodization, 380
- blank lines, adding to sample reports, 292
- blend analyzer
  - collecting 100% line spectrum, 422
  - default gain and attenuation settings for background collections, 399
  - setting Number Of Scans Per Batch, 386
  - setting Trigger, 386
  - specifying spectral range, 387
- blend analyzer sampling
  - background specification parameters in workflows, 420
  - sample specification parameters in workflows, 383
- Boxcar apodization, 379
- Button Label parameter, 272
  - for startrun prompts, 428
- buttons
  - for RESULT Integration software
    - Acknowledge, 272
    - Add Event Item, 222
    - Add Logical Test, 225
    - Optimize Gain, 356, 414
    - Preview Report, 283

- Preview Section, 318, 334
- Summary Properties, 329
- Test Dialog, 134

## C

- C screens, 354

- calculate events

  - and repeat loops, 31, 167

  - compared with sequence summary item specifications, 346

  - compared with summary item specifications, 24

  - described, 23

  - parameters, 24

    - Delete Source Spectra, 30

    - Multiple Event Results, 31

    - Store Raw Values, 29

  - selecting the data to be calculated, 25

  - suggested uses in workflows, 31

- calculating statistical values from workflows, 23

- calculation parameters, specifying, 24

- cell break

  - adding to sample reports, 317, 334

- Cell Temperature parameter, 371

- cells

  - heated, for transmission module sampling, 371

  - skipping cells in table sections of sample reports, 317, 334

  - specifying beam path for gas cell background collections, 418

  - specifying beam path for gas cell sample collections, 378

  - specifying delay for heated gas cells, 191

  - specifying delay for heated transmission cells, 372

  - specifying delay override for heated transmission cells, 372

  - specifying run-time pressure for gas cells, 192

  - specifying run-time temperature for gas cells, 191

  - specifying settle time for heated gas cells, 191

  - specifying temperature for heated transmission cells, 371

  - specifying temperature setpoint for heated gas cells, 191

- channel

  - workflow setting for fiber optic backgrounds with collect multi-channel events, 72

  - workflow setting for fiber optic sampling with collect events, 374

  - workflow setting for fiber optic sampling with collect multi-channel events, 72

- Channel Number parameter, 374

- check events

  - and repeat loops, 35

  - described, 32

  - generating operator prompt after fail rESULT, 34

  - parameters, 33

    - Multiple Event Results, 35

    - Prompt Specification For Fail Result, 34

    - Store Pass/Fail Result To Database, 35

  - restrictions for linked logical test specifications, 223

  - storing pass/fail result in RESULT database, 35

  - suggested uses in workflows, 36

  - using to add pass/fail results to spectra from workflows, 117

- class names

  - entering for analytical method, 241

- Classification Settings parameter, 246

- classify multiple specifications

  - described, 244

  - parameters, 245

    - Analysis Type, 249

    - Classification Setting, 246

    - Comparison Type, 249

    - Ignore Case, 249

    - Method File Name, 248

    - Required Analysis Type, 250

    - Text String For Comparison, 249

  - suggested uses in workflows, 251

- class-request dialog boxes, 132

- class-selection dialog boxes

  - specifying a measurement result, 135

- Clear All But Most Recent Results parameter, 39

- Clear Backgrounds parameter, 40

- clear events

  - and repeat loops, 167

  - described, 38

  - parameters, 38

    - Clear All But Most Recent Results, 39

    - Clear Backgrounds, 40

    - Clear Workflow Results, 41

  - specifying the background data to clear, 40

  - specifying the workflow results to clear, 41

  - suggested uses in workflows, 42

- Clear Workflow Results parameter, 41

- clearing

  - workflow data, 38

- closed-cycle MCT detector

  - recommended velocity, 382

- Collect Background Only parameter

  - for collect dual tablet events, 58

  - for collect events, 50

  - for collect sequence events, 215

- collect dual tablet events

  - and repeat loops, 63

  - Background Folder parameter, 58

  - described, 55

  - operator prompts, 62

  - parameters, 56

- Attenuator, 59
- Background Frequency, 58
- Collect Background Only, 58
- Correct Reflection Spectrum, 62
- Correct Transmission Spectrum, 60
- Data Format, 59
- Multiple Event Results, 63
- Number Of Sample Scans, 57
- Pre-collection Delay, 57
- Resolution, 57
- suggested uses in workflows, 63
- collect events
  - and repeat loops, 53
  - Background Folder parameter, 49, 215
  - clearing collect event results from a workflow, 41
  - described, 43
  - operator prompts, 50
  - parameters, 44
    - Background Frequency, 48
    - Collect Background Only, 50
    - Correct Sample Spectrum, 50
    - Data Format, 47
    - Multiple Event Results, 53
    - Number Of Sample Scans, 45
  - suggested uses in workflows, 53
- collect multi-channel events
  - and repeat loops, 74
  - Background Folder parameter, 69
  - described, 64
  - operator prompts, 70
  - parameters, 65
    - Background Channel, 72
    - Background Frequency, 68
    - Correct Sample Spectrum, 69
    - Data Format, 72
    - Multiple Event Results, 73
    - Number Of Sample Scans, 66
    - Pre-collection Delay, 68
    - Resolution, 68
    - Sample Channel, 72
    - Sample/Background Position, 66
  - parameters for validation wheel sampling
    - Sample Position, 67
  - suggested uses in workflows, 74
  - Use Sample Channel For Background Measurements
    - parameter, 69
- collect sequence events
  - adding measure events to, 197
  - adding to a workflow, 197
  - described, 205
  - integration time, 207
  - justifying the time interval, 207
  - parameters, 205
    - Action, 209
    - Background Frequency, 213
    - Collect Background Only, 215
    - Data Format, 212
    - Justified Time Interval, 207
    - Justify Concentration Data To Time Interval, 207
    - Number Of Scans Per Spectrum, 210
    - Number Of Scans Per Standard, 211
    - Pause At Start Of Sequence, 209
    - Prompt Text, 209
    - Sample specification, 210
    - Sampling Interval, 208
    - Total Collection Time, 207
    - Use Specific Sampling Interval, 208
  - sampling rate, 207
  - specifying the total collection time, 207
- collecting
  - samples and backgrounds in workflows, 43
  - sequence data from a workflow, 197
- collection
  - specifying in a workflow, 43
- collection and processing information
  - displaying in TQ Analyst or OMNIC, 118
- collection parameters
  - in background specifications, 397
  - in collect sequence events, 205
  - in sample specifications, 352
- collection phases
  - specifying duration, 207
  - using a workflow to define, 197, 205
- collection prompts
  - and data preview, 274
  - for background collection, 52
  - for sample collection, 53
- collection time
  - and mirror velocity, 381
  - and number of scans, 397
  - effect on number of sequence spectra collected, 207
- collection times, 46
- Color parameter
  - setting for table sections in reports, 314, 328
- combination logic
  - for logical test specifications, 228
- comma-separated values (CSV) file format, 96
- comments
  - adding to sample reports, 298
  - adding to workflows, 160

- reporting information to spectral comments from workflows, 123
- Comments parameter, 160
- compare events
  - and repeat loops, 81
  - described, 75
  - parameters, 76
    - Expected Values, 80
    - Multiple Event Results, 81
    - Store Raw Values, 78
  - selecting the spectra to be measured, 79
  - suggested uses in workflows, 81
- compare text specifications
  - described, 231
  - parameters, 231
    - Ignore Case, 234
    - Operator, 234
    - Text Item 1, 232
    - Text Item 2, 233
  - specifying criteria for tested items, 234
  - specifying results to test, 232
  - suggested uses in workflows, 234
- comparing actual versus expected values in workflows, 75
- Comparison Type parameter, 249
- component concentrations
  - specifying in workflows, 80
- Component Name parameter, 200
- component names
  - entering for analytical method, 241
- Component parameter
  - setting for a workflow result, 344
- components
  - validation wheel, 390
  - validation wheel for Antaris MX, 67
- composite components
  - adding to workflows, 254
  - specifying unit, 261
- composite measurement specifications
  - described, 254
  - parameters, 255
    - Algebraic Formula, 259
    - Composite Name, 259
    - Decimal Separator, 258
    - Formula Elements, 256
    - Item Separator, 258
  - suggested uses in workflows, 262
- concentration data
  - adding to sample reports, 312
  - displaying sequence concentrations in a workflow, 199
  - storing sequence concentrations in a workflow, 203
- concentration values
  - expected, specifying in workflows, 80
- condition
  - for exiting a conditional event, 171
  - for exiting a conditional repeat loop, 175
  - for exiting a repeat loop, 165
- conditional events
  - adding to workflows, 168, 172
  - exiting conditional events early, 170
  - exiting conditional repeat loops early, 174
- conditional test, adding to a workflow, 226
- configure temperature/pressure events
  - described, 189
  - parameters, 189
    - Control Temperature, 191
    - Delay, 191
    - Prompt For Pressure, 193
    - Prompt For Temperature, 192
    - Read Pressure, 193
    - Read Temperature, 191
    - Setpoint, 191
    - Settle Time, 191
    - Use Fixed Pressure, 193
    - Use Fixed Temperature, 192
  - suggested uses in workflows, 193
- Control Temperature parameter, 191
- controller
  - IP address for Opto 22 Controller, 100, 112, 146
- copying
  - component information by OPC client, 200
  - image files to the proper directory for inclusion in a sample report, 296
  - method files to the proper directory, 240
- Correct Reflection Spectrum parameter, 62
- Correct Sample Spectrum parameter, 50, 69
- Correct Transmission Spectrum parameter, 60
- Correction Background Spectrum
  - defined, 434
- Correction Equation parameter, 435
- correction specifications. *See also* sample correction specifications
  - described, 430
  - linking to collect dual tablet events in workflows, 61, 62
  - linking to collect events in workflows, 50
  - linking to collect multi-channel events in workflows, 73
- corrections, dark background
  - defined, 431
- corrections, transfer
  - defined, 432
- correlation coefficients

- calculating in workflows, 75
- Cosine apodization, 380
- count
  - reporting as composite component, 260
- count values
  - adding to sample reports, 318, 330
  - adding to sequence reports, 337
- CSV file format, 96
- custom images
  - adding to sample reports, 296
- Cycle Through Simulation Backgrounds parameter, 401
- Cycle Through Simulation Samples parameter, 363

## D

- dark background corrections
  - defined, 431
- data
  - adding summarized data to sample reports, 318
  - adding summarized sequence data to sample reports, 337
  - adding to sample reports, 306
  - archiving from workflows, 7
  - calculating statistical values in workflows, 23, 318, 337
  - checking in workflows, 32
  - collecting from multiple channels at the same time, 64
  - collecting transmission/reflection data simultaneously with tablet analyzers, 55
  - comparing actual vs. expected values in workflows, 75
  - processing spectra in workflows, 91
  - reading device data into workflows, 101
  - reading from devices into workflows, 99, 103
  - reporting from workflows, 106
  - reporting workflow results to OPC clients from workflows, 111
  - specifying collection from a workflow, 43
  - specifying sequence collection from a workflow, 197
  - storing from workflows, 140
  - storing with temperature/pressure values, 189
  - writing device data from workflows, 147
  - writing to devices from workflows, 145, 151
- data collection
  - collecting multiple phases, 205
  - setting Trigger for blend analyzer sampling, 386
  - specifying in a workflow, 43
- Data Format parameter, 212
  - for collect dual tablet events, 59
  - for collect events, 47
  - for collect multi-channel events, 72
- data points
  - optimizing, 382
- data simulation

- background data, 400
- coordinating samples and backgrounds, 365, 402
- sample data, 358
- sequence data, 204
- Data Type parameter
  - setting for a workflow result, 223, 313, 328
  - setting for operator response, 267
  - setting for picture headings in sample reports, 296
- data, spectral
  - adding to sample reports, 300
- database
  - storing check event pass/fail results, 35
  - storing numerical results from workflows, 140
  - storing pass/fail results from workflows, 32
  - storing records of archived sample reports, 108
  - storing records of archived spectra, 8
- date and time
  - used to name files saved by archive events in workflows, 19
- dates
  - adding to sample reports, 291
- Decimal Places parameter
  - setting for a workflow result, 328
- Decimal Separator parameter, 258
- default file names
  - for files saved by archive events in workflows, 18
- delay
  - setting for sample collection, 353
  - specifying for background collection, 398
  - specifying for heated cells, 372
  - specifying for heated gas cells, 191
  - specifying for sample collection with collect dual tablet events, 57
  - specifying for sample collection with collect multi-channel events, 68
  - specifying for sequence collection, 209
  - specifying for workflows, 82
- delay events
  - described, 82
  - parameters, 83
    - Delay Interval, 83
  - specifying the delay interval, 83
  - suggested uses in workflows, 83
- Delay Interval parameter, 83
- delay override
  - for heated sample holder, 372
- Delay parameter, 191, 398
- delaying
  - background collection, 398
  - sample collection for Antaris MX, 68
  - sample collection with collect dual tablet events, 57

- sequence collection, 209
- workflows, 82
- workflows while cell is heating, 372
- Delete Source Spectra After Calculation parameter, 30
- Delete Source Spectra After Measurement parameter, 89
- Delete Source Spectra After Reporting parameter, 325
- deleting
  - simulated sample spectra from a workflow, 363
  - workflow data, 38
- derivatives
  - calculating in workflows, 23
- detector
  - amplifying, 355
  - defining spectral range, 358
  - for gas cell background collections, 418
  - for gas cell sample collections, 378
  - gain factors used to normalize, 48
  - optimizing gain, 356
  - optimizing gain for multi-channel background collections, 414
  - recommended velocity, 381
  - used for validation wheel collection, 391
- detector gain factors, 213
- devices
  - reading data from devices into workflows, 99, 103
  - writing data to devices from workflows, 145, 151
- device-specific workflow events, 180
- difference spectrum
  - calculating in workflows, 91, 95
- digital signals
  - reading into workflows, 101
  - writing from workflows, 150
- digital signatures
  - requiring for spectral data and report files generated in a workflow, 14
- Digits After Decimal parameter
  - setting for a workflow result, 223, 314, 344
  - specifying for logical test results, 227
- dividing
  - components to create a composite component, 260
- DTGS detector
  - recommended velocity, 381
- Dual Tablet Integrating Sphere sampling
  - sample specification parameters in workflows, 388
- Dual Tablet Tablet Analyzer sampling
  - sample specification parameters in workflows, 387

## E

- Enter Key Handling parameter, 270

- equality tests
  - configuring logical test specifications for, 227
- error
  - Application Not Found, 139
  - root mean square error of prediction (RMSEP), 75
- error messages
  - Application Not Found, 139
  - Authenticate Operator, 14
  - Base Name Error, 6
  - incorrect TQ Analyst method, 248
  - reported as workflow error, 16
- error values
  - calculating in workflows, 75
- errors
  - configuring workflows to exit perform group after error, 159
  - configuring workflows to exit StartStop group after error, 178
  - configuring workflows to report errors, 16
  - using logical test specifications to test for workflow errors, 229
- events
  - adding sequence events to workflows, 196
  - adding simple events to workflows, 4
  - adding structural events to workflows, 157
  - adding to logical test specifications, 222
  - base names, 5
  - conditional, 168, 172
  - defined, 1
  - grouping, 158, 168, 172
  - repeating, 161, 172
- examples
  - for using classify multiple specifications in workflows, 251, 253
- executable programs
  - adding to workflows, 138
- Exit Group After Workflow Error parameter, 159, 178
- exiting
  - conditional events in workflows, 170
  - conditional loops in workflows, 174
  - repeat loops in workflows, 164
- expected values
  - defined, 81
  - reporting in workflows, 75
  - specifying in workflows, 80
- Expected Values parameter, 80
- exponent value
  - reporting as composite component, 261
- external reference
  - and background prompts, 52

- autosampler background specification parameters in workflows, 416
- for autosampler collections, 276
- location for autosampler carousels, 185
- setting background specifications
  - Use Sample Position, Gain And Attenuation Settings parameter, 398
- transmission module background specification parameters in workflows, 409

## F

- factors, for attenuation screens and detector gain, 48, 213

- fiber optic module

- background specification parameters in workflows, 410
- default gain and attenuation settings for background collections, 399
- sample specification parameters in workflows, 373
- setting background position, 411

- fiber optic probes

- configuring for background collections, 411
- setting channel number, 374
- setting Probe Type, 374, 375, 413

- file formats

- for bitmap images, 296
- for sample reports archived by workflows, 12
- for sequence data archived by workflows, 13
- for spectra archived by workflows, 12
- for spectrum image files archived by workflows, 7
- for subtraction reference spectra, 96
- Galactic (\*.SPC), 13
- JCAMP-DX (\*.JDX), 12
- Nicolet (\*.SPA), 12
- standard HTML (\*.htm), 12
- unicode HTML (\*.htm), 12

- file lists

- archiving, 15

- File Name parameter, 85, 127

- for simulation sample, 204

- file names

- for analytical methods, 240
- for archived spectra, 7
- for archived spectra to load into workflows, 85
- for list of archived files, 15
- for text files created with report to text file events in workflows, 127
- for TQ Analyst methods, 248
- of spectra and reports archived by a workflow, 15

- files

- configuring workflows to report archived files to OPC client, 17

- naming automatically by archive events in workflows, 17
- reporting workflow results to text files from workflows, 125

- first derivatives

- calculating in workflows, 23

- float memory

- reading into workflows, 102
- writing from workflows, 151

- format specifications

- for heading sections in sample reports, 291
- for memo sections in sample reports, 298
- for spectrum sections in sample reports, 300
- for table sections in sample reports, 306

- formats

- adding formatting elements to sample reports, 292
- for bitmap image files, 296
- for headings in sample reports, 293
- for sample reports, 12
- for sequence headings in sample reports, 336
- for simulated data, 360
- for spectral data in sample reports, 12
- for spectral plots in sample reports, 302
- for subtraction reference spectra, 96
- for tables of data in sample reports, 308
- for tables of summarized data in sample reports, 320
- for tables of summarized sequence data in sample reports, 340
- restrictions for Single Beam data format, 48, 213

- Formula Elements parameter, 256

## G

- Gain parameter

- default settings for background collections, 398
- in RESULT Integration, 355, 413
- using the Optimize Gain feature, 356

- Galactic file format, 13, 96

- gas cell

- background specification parameters in workflows, 417
- sample specification parameters in workflows, 377
- selecting beam path for background collections, 418
- selecting beam path for sample collections, 378
- storing temperature/pressure values with collected data, 189

- general specifications

- described, 263

- Generate Text Report parameter, 110

- glass standards

- placing in the beam path, 390
- placing in the beam path for Antaris MX, 67

- globally unique identifiers (GUIDs), 7

- gold reference

- positioning for blend analyzer backgrounds, 421

- positioning for blend analyzer sampling, 384
- graphics
  - adding to sample reports, 292
  - file formats, 296
- grouping events in workflows, 158
- groups
  - for sequence events in workflows, 196
  - for structural events in workflows, 157
- GUID
  - used to name files saved by archive events in workflows, 19
- GUIDs. See also globally unique identifiers

## H

- Happ-Genzel apodization, 379
- heading break
  - adding to sample reports, 316, 333
- heading format specifications. See heading item specifications
- heading item specifications
  - defining the heading layout, 293
  - described, 291
  - parameters, 292
    - Add/Edit Heading item, 294
    - Heading Label, 294
    - Heading Section Border, 293
    - Heading Section Title, 293
    - Heading Text, 295
    - Select Image File, 296
  - specifying information to include, 294
  - suggested uses in workflows, 298
  - titling the heading, 293
- Heading Label parameter, 294
- Heading Section Border parameter, 293, 337
- Heading Section Title parameter, 293, 336
- Heading Text parameter, 295
- headings
  - adding sequence headings to sample reports, 335
  - adding to sample reports, 291
  - formatting report headings, 293
  - formatting sequence report headings, 336
  - repeating table headings in sample reports, 316, 333
- heated sample holder
  - setting delay, 372
  - setting delay override, 372
  - setting sample specifications, 371
  - setting temperature, 371
- history
  - displaying spectral history information in TQ Analyst and OMNIC, 118
  - reporting information to spectral history from workflows, 123

- HTML (\*.htm) file formats, 12
- HTML image files
  - adding to sample reports, 296
- HTML report files
  - generating from workflows, 12

## I

- Ignore Case parameter, 234, 249
- image files
  - adding to sample reports, 296
- images
  - adding to a report summary, 328
  - adding to a table of reported data, 313
  - adding to reports, 32
  - adding to sample reports, 292, 296
  - archiving with a report, 7
  - file formats, 296
- index
  - used to name files saved by archive events in workflows, 20
- inputs
  - reading from devices into workflows, 99, 103
  - writing to devices from workflows, 145, 151
- instrument
  - selecting instrument beam path for gas cell backgrounds, 418
  - selecting instrument beam path for gas cell sampling, 378
- instrument gain
  - setting, 355
  - setting for multi-channel background collections, 413
- instrument serial numbers, adding to sample reports, 291
- integer memory
  - reading into workflows, 102
  - writing from workflows, 151
- integrating sphere
  - configuring for fiber optic background collections, 412
  - default gain and attenuation settings for background collections, 398
  - for dual tablet sampling
    - sample specification parameters, 388
- integrating sphere module
  - background specification parameters in workflows, 406
  - sample specification parameters in workflows, 368
- Integration Time parameter, 207
- intercept
  - of plotted expected vs measured values, 75
- interferogram, 212
- Interferogram
  - format for data collected from workflows, 47
- interferograms
  - from sequence collections

- setting up a workflow to store, 203
- interferometer
  - specifying mirror velocity, 381
- internal reference
  - and background prompts, 49, 214
  - and SabIR probe collections, 374, 375, 413
  - autosampler background specification parameters in workflows, 416
  - positioning for blend analyzer backgrounds, 421
  - positioning for blend analyzer sampling, 384
- IP address
  - for Opto 22 Controller, 100, 112, 146
- Item Separator parameter, 258

## J

- JCAMP-DX file format, 12, 96
- Justified Time Interval parameter, 207
- Justify Concentration Data To Time Interval parameter, 207

## K

- known values
  - defined, 81
  - specifying in workflows, 80
- Kubelka-Munk
  - format for spectra collected from workflows, 47

## L

- Label parameter, 101
- labels
  - entering for workflow results displayed in reports, 315, 329
- LED indicators
  - and collection prompts, 273, See also prompts
  - and operator requests, 265
  - and startrun prompts, 427
- line break
  - adding to sample reports, 316, 334
- lines
  - adding to sample reports, 292
  - skipping lines in table sections of sample reports, 316, 334
- load spectrum events
  - and repeat loops, 85
  - described, 84
  - parameters, 84
    - Base Path, 85
    - File Name, 85
    - Multiple Event Results, 85
  - suggested uses in workflows, 86

- loading
  - archived spectra into workflows, 84
- location
  - setting for autosampler module backgrounds, 415
  - setting for fiber optic module backgrounds, 411
  - setting for transmission module samples, 371, 408
- Location parameter
  - for autosampler backgrounds, 415
- Log (1/R)
  - format for spectra collected from workflows, 47
- log value
  - reporting as composite component, 261
- logic
  - configuring combination logic for logical test specifications, 228
- logic specifications
  - described, 218
  - linking to perform-if events, 169
  - linking to perform-if events in workflows, 171
  - linking to perform-while events in workflows, 173
  - linking to repeat events in workflows, 165
- Logical Test Is False After Workflow Error parameter, 228
- logical test specifications
  - adding to other logical test specifications, 225
  - configuring combination logic, 228
  - configuring digits for tested results, 227
  - configuring to check for workflow errors, 228
  - described, 219
  - linking to check events in workflows, 34
  - parameters, 220
    - Add Event Item, 222
    - Add Logic Item, 225
    - Attribute, 224
    - Combination Logic, 228
    - Data Type, 223
    - Digits After Decimal, 223
    - Logical Test Is False After Workflow Error, 228
    - Multiple Results, 229
  - restrictions for configuring, 225
  - restrictions for performing equality tests, 227
  - restrictions for using, 231
  - restrictions when linked to check events, 223
  - specifying results to test, 222
  - specifying test condition, 226
  - specifying true/false conditions for tested items, 226
  - storing multiple test results, 229
  - suggested uses in workflows, 230
- logos
  - adding to sample reports, 297

loops  
and archive events, 23  
creating conditional repeat loops in workflows, 172  
creating repeat loops in workflows, 161

## M

Max Pause (Sec) parameter, 372

maximum

reporting as composite component, 260

maximum value

adding to sample reports, 330

maximum values

adding to sample reports, 318

calculating in workflows, 23

maximum values, adding to sequence reports, 337

MCT detector

recommended velocity, 381

Measure Event parameter, 200

measure events

adding measurement results to spectra from workflows, 117

adding to a collect sequence group, 197

and repeat loops, 90

clearing measure event results from a workflow, 41

described, 86

parameters, 87

Delete Source Spectra After Measurement, 89

Multiple Event Results, 90

Processing Options For Multiple Samples, 88

selecting the spectrum to be measured, 88

spectral processing, 88

storing in the database for queries, 140

suggested uses in workflows, 90

using test cases to test, 242

measurement data

from sequence collections

setting up a workflow to store, 203

measurement error

calculating in workflows, 75

measurement parameters, specifying, 87

measurement specifications

described, 235

linking to compare events in workflows, 78

linking to measure events in workflows, 90

parameters

Application Name, 240

Measurement Type, 241

Method File Name, 240

Path, 240

Prompt Integrator To Select Test Case, 244

Select Attributes To Measure, 241

Test Case Name, 243

Test Case Value, 243

suggested uses in workflows, 244

Measurement Type parameter, 241

measuring spectra in workflows, 86

memo format specifications. See memo item specifications

memo item specifications

described, 298

entering comment text, 300

parameters, 298

Memo Section Text, 300

Memo Section Title, 299

suggested uses in workflows, 300

titling the comment section, 299

Memo Section Text parameter, 300

Memo Section Title parameter, 299

memory

reading float, integer or string memory into workflows, 102

writing float, integer or string memory from workflows, 151

memory, integer

reading into workflows, 102

writing from workflows, 151

memory, string

reading into workflows, 102

writing from workflows, 150

message-response dialog boxes, 131

method development software

application name, 240

measured attributes, 241

measurement type, 241

selecting method file name, 240

Method File Name parameter, 240, 248

Min/Max Spectrum Y Value parameter, 203

Min/Max Y Value parameter, 202

minimum

reporting as composite component, 260

minimum value

adding to sample reports, 330

minimum values

adding to sample reports, 318

adding to sequence reports, 337

calculating in workflows, 23

mirror

optimizing turnaround, 382

scanning during forward and reverse travel, 382

specifying velocity, 381

multi-channel background specifications

parameters for SabIR probe sampling, 412

multi-channel collections

setting Gain, 413

- multi-channel sample specifications
  - parameters for SabIR probe sampling, 374
- multi-channel sampling
  - background specification parameters in workflows, 412
  - sample specification parameters in workflows, 374
- Multiple Event Results
  - and Processing Options For Multiple Samples parameter, 89
  - and repeat loops, 166
- Multiple Event Results parameter, 31, 35, 53, 63, 73, 81, 85, 90, 98, 102, 110, 136, 187
- Multiple Results parameter, 229
- multiplying
  - components to create a composite component, 260
- MultiPro Autosampler
  - configuring in a workflow, 377

## N

- names, adding to sample reports, 291
- naming files automatically by archive events in workflows, 17
- N-B Medium apodization, 380
- N-B Strong apodization, 380
- N-B Weak apodization, 379
- New Simulation Spectrum dialog box, 359
- Nicolet file format, 12, 96
- noise, 45, 211
  - and mirror velocity, 381
  - and number of scans per spectrum, 211
- Number Of Background Scans parameter, 397
  - and collection times, 397
- number of failures
  - adding to sequence reports, 338
- Number Of Repetitions parameter, 163
- Number Of Sample Scans parameter
  - and collection times, 46
  - for collect dual tablet events, 57
  - for collect events, 45
  - for collect multi-channel events, 66
- number of scans per spectrum
  - and background frequency, 214
- Number Of Scans Per Spectrum parameter, 210
- Number Of Scans Per Standard parameter, 211

## O

- OPC client
  - configuring workflows to report archived files to OPC client, 17
- OPC clients
  - reporting workflow results to OPC clients, 111
- Operator Must Respond To Prompt parameter, 268

- Operator parameter, 234
- Operator Prompt parameter (for number of repetitions), 163
- operator prompt specifications, 271, See also prompt specifications
  - for startstop events (start run), 427
  - for startstop events (stop run), 428
- operator prompts. See also prompts and data preview, 274
  - configuring logical test specifications for yes/no responses, 228
- Operator Request dialog box, 51, 131, 265
- operator request specifications, 265
- Optimize Gain dialog box, 356
- Opto 22 Controller IP Address parameter, 100, 112, 146
- outputs
  - reading from devices into workflows, 99, 103
- overlapping peaks
  - resolving, 380

## P

- parameters
  - common to sample specifications, 351
  - for archive events, 8
  - for autosampler specifications, 275
  - for calculate events, 24
  - for check events, 33
  - for classify multiple specifications, 245
  - for clear events, 38
  - for collect dual tablet events, 56
  - for collect events, 44
  - for collect multi-channel events, 65
  - for collect sequence events, 205
  - for compare events, 76
  - for compare text specifications, 231
  - for composite measurement specifications, 255
  - for configure temperature/pressure events, 189
  - for delay events, 83
  - for heading item specifications, 292
  - for load spectrum events, 84
  - for logical test specifications, 220
  - for measure events, 87
  - for memo item specifications, 298
  - for perform events, 159
  - for perform-if events, 168
  - for perform-while events, 172
    - Repeat Events At Least Once, 174
  - for position autosampler events, 182
  - for process events, 92
  - for prompt specifications, 272
  - for read from I/O events, 99, 103

- for repeat events, 161
- for report events, 108
- for report specifications, 278
- for report to OPC events, 112
- for report to spectrum events, 119
- for report to text file events, 125
- for request events, 133
- for request specifications, 266
- for run exe events, 139
- for run sequence events, 198
- for sample correction specifications, 433
- for sequence heading item specifications, 336
- for sequence summary item specifications, 339
- for spectral specifications, 238
- for spectrum item specifications, 301
- for startrun specifications, 427
- for startstop events, 178
- for stoprun specifications, 429
- for store events, 141
- for summary item specifications, 319
- for table item specifications, 307
- for write to I/O events, 145
- in RESULT Integration software
  - Action (for sequence collection prompt), 209
  - Add Break, 315, 333
  - Add Event Item, 222
  - Add Logic Item, 225
  - Add Workflow Result To Table Section, 312
  - Add/Edit Heading item, 294
  - Add/Edit Operator Request, 267
  - Algebraic Formula, 259
  - Align, 314, 328
  - Allow Acknowledge Button, 272
  - Allow Early Exit, 165, 170, 175
  - Allow Operator To Override Heater Pause, 372
  - Analysis Type, 249
  - Apodization, 379
  - Application Argument, 140
  - Application Name, 240
  - Application Name (for run exe events), 139
  - Application Time-out, 140
  - Attenuator, 59, 354
  - Attribute, 224, 313, 328
  - Autosampler Carousels, 276
  - Autosampler Position, 184
  - Autosampler Specification, 183
  - Background Channel, 72
  - Background Frequency, 213
  - Background Frequency for collect dual tablet events, 58
  - Background Frequency for collect events, 48

- Background Frequency for collect multi-channel events, 68
- Background Specification, 352
- Backgrounds For Simulation, 400
- Base Path, 11, 85, 126
- Beam Path, 391
- Beam Path for background collections, 418
- Beam Path for sample collections, 378
- Button Label, 272
- Cell Temperature, 371
- Channel Number, 374
- Classification Settings, 246
- Clear All But Most Recent Results, 39
- Clear Backgrounds, 40
- Clear Workflow Results, 41
- Collect Background Only, 50, 58, 215
- Color, 314, 328
- Combination Logic, 228
- Comments, 160
- Comparison Type, 249
- Component, 344
- Component Name, 200
- Composite Name, 259
- Control Temperature, 191
- Correct Reflection Spectrum, 62
- Correct Sample Spectrum, 50, 69
- Correct Transmission Spectrum, 60
- Correction Equation, 435
- Cycle Through Simulation Backgrounds, 401
- Cycle Through Simulation Samples, 363
- Data Format, 47, 59, 72, 212
- Data Type, 223, 267, 313, 328
- Decimal Places, 328
- Decimal Separator, 258
- Delay, 191
- Delay Interval, 83
- Delete Source Spectra After Calculation, 30
- Delete Source Spectra After Measurement, 89
- Delete Source Spectra After Reporting, 325
- Digits After Decimal, 223, 314, 344
- Enter Key Handling, 270
- Exit Group After Workflow Error, 159, 178
- Expected Values, 80
- File Name, 85, 127
- File Name for simulation sample, 204
- Formula Elements, 256
- Gain, 355, 413
- Generate Text Report, 110
- Heading Label, 294
- Heading Section Border, 293, 337

Heading Section Title, 293, 336  
 Heading Text, 295  
 Ignore Case, 234, 249  
 Integration Time, 207  
 Item Separator, 258  
 Justified Time Interval, 207  
 Justify Concentration Data To Time Interval, 207  
 Label, 101, 315, 329  
 Location (for autosampler backgrounds), 415  
 Location for blend analyzer backgrounds, 421  
 Logical Test Is False After Workflow Error, 228  
 Max Pause, 372  
 Measure Event, 200  
 Measurement Type, 241  
 Memo Section Text, 300  
 Memo Section Title, 299  
 Method File Name, 240, 248  
 Min/Max Spectrum Y Value, 203  
 Min/Max Y Value, 202  
 Multiple Event Results, 31, 53, 63, 73, 81, 85, 90, 98,  
 102, 110, 136, 187  
 Multiple Event Results, 35  
 Multiple Results, 229  
 Number Of Background Scans, 397  
 Number Of Repetitions), 163  
 Number Of Sample Scans for collect dual tablet events,  
 57  
 Number Of Sample Scans for collect events, 45  
 Number Of Sample Scans for collect multi-channel  
 events, 66  
 Number Of Scans Per Spectrum, 210  
 Number Of Scans Per Standard, 211  
 Operator, 234  
 Operator Must Respond To Prompt, 268  
 Operator Prompt (for number of repetitions), 163  
 Optimize Gain, 356, 414  
 Opto 22 Controller IP Address, 100, 112, 146  
 Path, 240  
 Pause At Start Of Sequence, 209  
 Place All Data Types In One Row/Column, 311, 323  
 Point #, 102, 105, 151  
 Point Type, 101, 150  
 Position, 408, 411  
 Pre-collection Delay, 57, 68, 353, 398  
 Preview Data Collection, 273  
 Preview Section, 318, 334  
 Print HTML Report, 109  
 Probe Type, 374, 375, 413  
 Processing Options, 94  
 Processing Options For Multiple Samples, 88  
 Prompt For Expected, 135  
 Prompt For Next Set Of Samples, 186  
 Prompt For Pressure, 193  
 Prompt For Simulation Background, 401  
 Prompt For Simulation Sample, 363  
 Prompt For Temperature, 192  
 Prompt Integrator To Select Test Case, 244  
 Prompt Specification, 186  
 Prompt Specification For Fail Result), 34  
 Prompt Text, 267, 273, 429  
 Prompt Text (for sequence collection), 209  
 Read Data, 101  
 Read Pressure, 193  
 Read Temperature, 191  
 Reference Position Reserved For Background Collections,  
 276  
 Report Archiving Information To OPC, 17  
 Report Data From These Events, 112  
 Report Format, 12  
 Report These Statistics, 28, 345  
 Report Title, 279  
 Report To OPC Server, 200  
 Required Analysis Type, 250  
 Resolution, 57, 353  
 Resolution for collect multi-channel events, 68  
 Retain All Concentration Data, 203  
 Retain All Interferogram Data, 203  
 Retain All Spectral Data, 203  
 Sample Channel, 72  
 Sample Cup Spinner, 369  
 Sample Position, 371  
 Sample Position for blend analyzer sampling, 384  
 Sample Position for collect multi-channel events, 66  
 Sample Specification, 210  
 Samples For Simulation, 359  
 Sampling Interval, 208  
 Sampling Technique, 352, 397  
 Save List Of Archived File Names, 15  
 Save Report Files As Read-Only, 13  
 Save Spectral Files As Read-Only, 13  
 Save Workflow Error Report, 16  
 Scale Low/High, 102, 151  
 Scan, 382  
 Select All Components, 344  
 Select Attributes To Measure, 241  
 Select Image File, 296  
 Setpoint, 191  
 Settle Time, 191  
 Show Acceptance Limits, 342  
 Show Column Headings In Table Section, 310, 322

- Show Event Names In Summary Section, 323, 342
- Show Event Names In Table Section, 310
- Show Raw Source Values In Summary Table, 324
- Show Row Headings In Table Section, 310, 322
- Show Run Chart, 202
- Show Spectral Data, 203
- Show Text Value, 201
- Specify Number Of Scans Per Batch, 386
- Spectra To Be Processed, 93
- Spectral Data Format, 12
- Spectral Range, 303
- Spectrum Section Title, 303
- Start Specification, 179
- Start/End Spectrum X Value, 203
- Stop Action Generates Workflow Error, 179
- Stop Specification, 179
- Store Pass/Fail Result To Database, 35
- Store Raw Values With Calculated, 29
- Store Raw Values With Calculated Values, 78
- Style, 314, 328
- Subtraction Factor, 97
- Subtraction Spectrum, 96
- Summary Section Border, 322, 341
- Summary Section Layout, 321, 340
- Summary Section Title, 320, 340
- Table Section Border, 309
- Table Section Layout, 308
- Table Section Title, 308
- Test Case Name, 243
- Test Case Value, 243
- Text Item 1, 232
- Text Item 2, 233
- Text String For Comparison, 249
- Total Collection Time, 207
- Trigger for blend analyzer sampling, 386
- Use Digital Signatures, 14
- Use Field Delimiter, 270
- Use Fixed Pressure, 193
- Use Fixed Temperature, 192
- Use Heated Cell, 371
- Use Sample Channel For Background Measurements, 69
- Use Sample Position, Gain And Attenuation Settings, 398
- Use Sampling Sequence (for number of repetitions), 163
- Use Simulation Backgrounds For All Workflow Runs, 402
- Use Simulation Sample For All Workflow Runs, 204
- Use Simulation Samples For All Workflow Runs, 364
- Use Specific Sampling Interval, 208
- Use Standard Spectral Range, 358
- Velocity, 381
- Write Data, 147
- Zero Filling, 380
- specifying for spectral measurement, 87
- Total Collection Time, 207
- pass/fail filters
  - applied to sample reports, 331
- pass/fail images
  - adding to a table of data, 313
  - adding to a table of summarized data, 328
  - adding to reports, 32
  - archiving with a report, 7
  - storing, 32
- pass/fail results
  - adding to reports, 32
  - adding to spectra from workflows, 117
  - archiving with a report, 7
  - configuring logical test specifications for, 228
  - restrictions for storing in the RESULT database, 33
  - storing, 32
- Path parameter, 240
- paths
  - for archiving backgrounds collected in a workflow, 215
  - for archiving backgrounds collected with collect dual tablet events, 58
  - for archiving backgrounds collected with collect events, 49
  - for archiving backgrounds collected with collect multi-channel events, 69
  - for locating workflows and methods in RESULT Integration, 240
- Pause At Start Of Sequence parameter, 209
- pausing
  - before background collection, 398
  - before sample collection, 57
  - before sample collection with collect multi-channel events, 68
  - workflows, 82
  - workflows while cell is heating, 372
- peaks
  - resolving overlapping, 380
- percent standard deviation
  - adding to sample reports, 318, 330
  - adding to sequence reports, 338
  - calculating in workflows, 23
- perform events
  - parameters, 159
    - Comments, 160
    - Exit Group After Workflow Error, 159
    - suggested uses in workflows, 160

- perform-if events
  - described, 168
  - exiting perform-if events early, 170
  - parameters, 168
    - Allow Early Exit, 170
    - Condition For Early Exit, 171
    - Logic Specification, 169, 171
    - Perform-If Condition, 170
  - specifying condition for executing, 170
  - suggested uses in workflows, 171
- perform-while events
  - described, 172
  - exiting perform-while events early, 174
  - parameters, 172
    - Allow Early Exit, 175
    - Condition For Early Exit, 175
    - Logic Specification, 173, 175
    - Perform-While Condition, 174
    - Repeat Events At Least Once parameter, 174
  - specifying condition for executing, 174
  - suggested uses in workflows, 175
- phases
  - for data collection, 197, 205
- pictures
  - adding to sample reports, 296
  - file formats, 296
- Pirouette measurement specifications
  - adding to workflows, 238
- Place All Data Types In One Row/Column parameter, 311, 323
- PLC
  - reading data from PLCs into workflows, 99
  - writing data to PLCs from workflows, 145
- plots, of spectra
  - adding to sample reports, 300
  - and collection events, 305
  - formatting, 302
- PLSplus/IQ measurement specifications
  - adding to workflows, 237
- Point # parameter, 102, 105, 151
- Point Type parameter, 101, 150
- polystyrene sample
  - in attenuation wheel, 59, 354
  - in validation wheel, 390
  - in validation wheel for Antaris MX, 67
  - positioning for blend analyzer backgrounds, 421
  - positioning for blend analyzer sampling, 384
- position
  - adding autosampler position numbers to spectra from workflows, 117
    - setting for sample and background collections with collect multi-channel events, 66
- position autosampler events
  - and repeat loops, 187
  - described, 182
  - parameters, 182
    - Autosampler Position, 184
    - Autosampler Specification, 183
    - Multiple Event Results, 187
    - Prompt For Next Set Of Samples, 186
  - prompting for next carousel, 186
  - specifying position for multiple carousels, 186
  - specifying the autosampler position, 184
  - specifying the autosampler specification, 183
  - suggested uses in workflows, 187
- Position parameter
  - for transmission module sampling, 408
- positioning
  - an autosampler from a workflow, 182
  - backgrounds for blend analyzer, 421
  - backgrounds for gas cell module, 418
  - samples for blend analyzer, 384
  - samples for gas cell module, 378
- positioning backgrounds
  - for fiber optic module, 411
  - for transmission module, 408
- positioning samples
  - for transmission module, 371
  - for validation wheel, 390
  - for validation wheelwith Antaris MX, 67
- Pre-collection Delay parameter, 57, 68, 353, 398
- pressure
  - storing with collected data, 189
- Preview Data Collection parameter, 273
- Preview Report button, 283
- Preview Section button, 318, 334
- Print HTML Report parameter, 109
- printing
  - sample reports automatically from workflows, 109
- probe
  - configuring third-party probes for multi-channel sampling, 375
- Probe Type parameter, 374, 375, 413
- probes
  - configuring for background collections, 411
- probes, setting channel number, 374
- probes, setting Probe Type, 374, 375, 413
- process event parameters, 92
- process events
  - and repeat loops, 98

- clearing process event results from a workflow, 41
- described, 91
- parameters
  - Multiple Event Results, 98
  - Processing Options, 94
  - Spectra To Be Processed, 93
  - Subtraction Factor, 97
  - Subtraction Spectrum, 96
- suggested uses in workflows, 98
- Processing Options For Multiple Samples parameter, 88
  - and Multiple Event Results, 89
- Processing Options parameter, 94
- processing spectra from workflows, 91
- processing, spectral data, 88
- programs
  - adding to workflows, 138
- Prompt dialog box, 271
- Prompt For Expected Class parameter, 135
- Prompt For Next Set Of Samples parameter, 186
- Prompt For Pressure parameter, 193
- Prompt For Simulation Background parameter, 401
- Prompt For Simulation Sample parameter, 363
- Prompt For Temperature parameter, 192
- Prompt Integrator To Select Test Case parameter, 244
- Prompt Specification For Fail Result parameter, 34
- Prompt Specification parameter, 186
- prompt specifications
  - described, 271
  - for startstop events (start run), 427
  - for startstop events (stop run), 428
  - LED indicators for collection prompts, 273
  - linking to check events in workflows, 35
  - linking to collect events in workflows, 52
  - linking to Position Autosampler events, 186
  - parameters, 272
    - Allow Acknowledge Button, 272
    - Button Label, 272
    - Preview Data Collection, 273
    - Prompt Text, 273
  - suggested uses in workflows, 274
- Prompt Text parameter
  - for operator prompt dialog boxes, 273
  - for operator request dialog boxes, 267
  - for sequence collection, 209
  - for startrun prompts, 428
  - for stoprun prompts, 429
- prompts
  - creating custom, 131
    - allowing Acknowledge button response, 272
    - defining button label, 272

- defining message text, 273
  - including data collection preview, 273
- for autosampler position number, 185
- for background collection, 52
- for class names, 132
- for file names to archive files, 17
- for sample collection, 53
- for simulation backgrounds, 401
- for simulation samples, 363
- for test cases, 244
- generating after check event fail rESULT, 34
- LED indicators for collection prompts, 273
- operator requests, 131
- StartRun, 177
- StopRun, 177

## Q

- qualification workflows
  - requirements for creating, 37
- qualitative analysis, 240, 246
- quantitative analysis, 240
  - specifying concentration values in workflows, 80

## R

- range
  - calculating range values in workflows, 23
  - for X axis of collected spectra, 358
  - for X or Y axis of plotted spectra, 303
  - reporting as composite component, 260
- range values
  - adding to sample reports, 318, 330
  - adding to sequence reports, 338
- range, spectral
  - for blend analyzer sampling, 387
- ratio
  - of signal to noise, 45, 211
- Read Data parameter, 101
- read from I/O events
  - and repeat loops, 102, 105
  - described, 99, 103
  - parameters, 99, 103
    - Label, 101
    - Multiple Event Results, 102
    - Opto 22 Controller IP Address, 100, 112
    - Point #, 102, 105
    - Point Type, 101
    - Read Data, 101
    - Scale Low/High, 102
  - suggested uses in workflows, 103, 106

- Read Pressure parameter, 193
- Read Temperature parameter, 191
- reference
  - external, for autosampler background collections, 416
  - external, for autosampler collections, 276
  - internal, for autosampler background collections, 416
  - internal, for SabIR probe collections, 374, 375, 413
- Reference Position Reserved For Background Collections parameter, 276
- references
  - setting autosampler background specifications
    - Location parameter, 415
- Reflectance
  - format for spectra collected from workflows, 47
- repeat events
  - and Multiple Event Results, 166
  - described, 161
  - exiting repeat events early, 164
  - parameters, 161
    - Allow Early Exit, 165
    - Number Of Repetitions), 163
    - Operator Prompt (for number of repetitions), 163
    - Use Sampling Sequence (for number of repetitions), 163
  - suggested uses in workflows, 166
- repeat loops
  - and archive events, 23
  - creating, 161, 172
- repeating
  - table headings in sample reports, 316, 333
- Report Archiving Information To OPC parameter, 17
- Report Data From These Events parameter, 112
- report events
  - and repeat loops, 110
  - clearing report event results from a workflow, 41
  - described, 106
  - parameters, 108
    - Generate Text Report, 110
    - Multiple Event Results, 110
    - Print HTML Report, 109
  - suggested uses in workflows, 110
- Report Format parameter, 12
- report format specifications. See report item specifications
- report item specifications
  - described, 286
  - spectral plot format parameters, 302
- report specifications
  - adding comment sections to, 298
  - adding data sections to, 306
  - adding heading sections to, 291
  - adding sequence heading information to, 335
  - adding sequence summary data sections to, 337
  - adding spectral plot sections to, 300
  - adding summary data to, 318
  - described, 277
  - entering report title, 279
  - linking to report events in workflows, 109
  - parameters, 278
    - Preview Report, 283
    - Report Title, 279
  - previewing the report, 283
  - specifying report sections, 279
  - suggested uses in workflows, 284
- Report These Statistics parameter, 28, 345
- Report Title parameter, 279
- report title, example, 279
- report to OPC events
  - described, 111
  - parameters, 112
    - Report Data From These Events, 112
  - suggested uses in workflows, 116
- Report To OPC Server parameter, 200
- report to spectrum events
  - described, 116
  - parameters, 119
  - suggested uses in workflows, 125
- report to text file events
  - described, 125
  - parameters, 125
    - Base Path, 126
    - File Name, 127
  - suggested uses in workflows, 131
- reports
  - adding statistical values to sample reports, 28, 330
  - adding statistical values to sequence reports, 345
  - applying pass/fail filters to reported results, 331
  - archiving sample reports in workflows, 7
  - creating sample reports in workflows, 106
  - defining comment sections, 298
  - defining heading sections, 291
  - defining sections in, 286
  - defining sequence heading sections, 335
  - defining spectrum sections, 300
  - defining table of summarized sequence results, 337
  - defining table of summarized workflow results, 318
  - defining table of workflow results, 306
  - entering report title, 279
  - example, 107
  - format for reports generated by workflows, 12
  - previewing, 283
  - printing automatically from workflows, 109

- sorting reported workflow results, 332
  - specifying sections to include, 279
- request events
  - and repeat loops, 136
  - described, 131
  - parameters, 133
    - Multiple Event Results, 136
    - Prompt For Expected Class, 135
    - Test Dialog, 134
  - suggested uses in workflows, 137
  - using to add information to spectra from workflows, 117
- request specifications
  - described, 265
  - entering prompt text, 267
  - linking to request events, 134
  - parameters, 266
    - Add/Edit Operator Request, 267
    - Autosampler Carousels, 276
    - Data Type, 267
    - Enter Key Handling, 270
    - Operator Must Respond To Prompt, 268
    - Prompt Text, 267
    - Use Field Delimiter, 270
  - selecting items to request, 267
  - setting bar code options, 269
  - setting Data Type for operator response, 267
  - setting Enter key handling, 270
  - setting field delimiter, 270
  - setting required response, 268
  - suggested uses in workflows, 270
- Required Analysis Type parameter, 250
- Resolution parameter, 353
  - for collect dual tablet events, 57
  - for collect multi-channel events, 68
- RESULT Data View software
  - described, 204
- RESULT database
  - storing check event pass or fail results, 35
  - storing numerical results from workflows, 140
  - storing records of archived sample reports, 108
  - storing records of archived spectra, 8
- RESULT Integration
  - adding correction specifications to workflows, 430
  - adding general specifications to workflows, 263
  - adding logic specifications to workflows, 218
  - adding measurement specifications to workflows, 236
  - adding report item specifications to workflows, 289
  - adding report specifications to workflows, 285
  - adding sample specifications to workflows, 349
  - adding simple events to workflows, 4
- adding startstop specifications to workflows, 426
- checking for workflow errors, 178, 228
- common sample specification parameters, 351
- for autosampler integrating sphere sampling
  - background specification parameters, 414
  - sample specification parameters, 376
- for autosampler softgel tablet analyzer sampling
  - background specification parameters, 404
  - sample specification parameters, 376
- for autosampler standard tablet analyzer sampling
  - background specification parameters, 403
- for autosampler std tablet analyzer sampling
  - sample specification parameters, 376
- for blend analyzer sampling
  - background specification parameters, 420
  - sample specification parameters, 383
- for fiber optic sampling
  - background specification parameters, 410
  - sample specification parameters, 373
- for gas cell sampling
  - background specification parameters, 417
  - sample specification parameters, 377
- for integrating sphere sampling
  - background specification parameters, 406
  - sample specification parameters, 368
- for multi-channel sampling
  - background specification parameters, 412
  - sample specification parameters, 374
- for SabIR probe sampling
  - background specification parameters, 410
  - multi-channel background specification parameters, 412
  - multi-channel sample specification parameters, 374
  - sample specification parameters, 373
- for softgel tablet analyzer sampling
  - background specification parameters, 404
  - sample specification parameters, 366
- for standard tablet analyzer sampling
  - background specification parameters, 403
  - sample specification parameters, 365
- for transmission module sampling
  - background specification parameters, 407
  - sample specification parameters, 370
- for validation wheel sampling
  - background specification parameters, 423
- Optimize Gain feature, 356
- using simulated background data, 400
- using simulated sample data, 358
- using simulated sequence data, 204
- workflow errors
  - configuring a workflow to check for errors, 228

- configuring startstop events to check for errors, 178
- RESULT Integration
  - adding background specifications to workflows, 394
  - adding structural events to workflows, 157
  - archived files
    - configuring workflows to report to OPC client, 17
  - archived files, logging, 15
  - checking for workflow errors, 159
  - common background specification parameters, 396
  - for dual tablet reflection sampling
    - sample specification parameters, 388
  - for dual tablet transmission sampling
    - sample specification parameters, 387
  - for validation wheel sampling
    - sample specification parameters, 389
  - logging archived files, 15
  - logging workflow errors, 16
  - workflow errors
    - configuring perform events to check for errors, 159
    - logging workflow errors, 16
- Retain All Concentration Data parameter, 203
- Retain All Interferogram Data parameter, 203
- Retain All Spectral Data parameter, 203
- reverse scanning, 382
- RMSEP. See root mean square error of prediction
- root mean square error of prediction
  - calculating in workflows, 75
- rotation
  - setting for blend analyzer sampling, 386
- rotation, for Sample Cup Spinner, 369
- run exe events
  - described, 138
  - parameters, 139
    - Application Argument, 140
    - Application Name, 139
    - Application Time-out, 140
  - suggested uses in workflows, 140
- run sequence events
  - adding to a workflow, 196
  - described, 197
  - parameters, 198
    - Component Name, 200
    - File Name (for simulation sample), 204
    - Integration Time, 207
    - Measure Event, 200
    - Min/Max Spectrum Y Value, 203
    - Min/Max Y Value, 202
    - Report To OPC Server, 200
    - Retain All Concentration Data, 203
    - Retain All Interferogram Data, 203

- Retain All Spectral Data, 203
- Show Run Chart, 202
- Show Spectral Data, 203
- Show Text Value, 201
- Start/End Spectrum X Value, 203
- Use Simulation Sample For All Workflow Runs, 204
- specifying the component names for display, 200
- specifying the spectral display, 203

## S

- SabIR probe
  - background specification parameters in workflows, 410
  - configuring for background collections, 411
  - configuring for fiber optic sampling module, 374
  - configuring for multi-channel sampling, 375, 413
  - multi-channel background specification parameters in workflows, 412
  - multi-channel sample specification parameters in workflows, 374
  - sample specification parameters in workflows, 373
- Sample Channel parameter, 72
- sample correction specifications
  - described, 431
  - parameters, 433
  - suggested uses in workflows, 443
- Sample Cup Spinner parameter, 369
- sample data preview
  - and collection prompts, 274
- sample holder
  - for transmission sampling module
    - setting background position, 408
    - setting sample position, 371
- sample position
  - setting for Antaris fiber optic sampling module, 374
  - setting for blend analyzer sampling, 384
  - setting for fiber optic module, 411
  - setting for gas cell sampling, 378
  - setting for multi-channel sampling, 375, 413
  - setting for transmission module, 371
  - setting for validation wheel, 390
  - setting for validation wheel with Antaris MX, 67
- Sample Position parameter
  - for collect multi-channel events, 66
  - for fiber optic module backgrounds, 411
  - for transmission module sampling, 371
- sample reports. See also reports
  - defining comment sections, 298
  - defining data sections, 306
  - defining heading sections, 291
  - defining sequence heading sections, 335

- defining sequence summary data sections, 337
- defining spectral plot sections, 300
- defining summary data sections, 318
- printing automatically from workflows, 109
- sample specifications
  - defining collection parameters, 352
  - features common to sample specifications, 351
  - linking to autosampler specifications, 377
  - linking to collect dual tablet events in workflows, 60, 61
  - linking to collect events in workflows, 45
  - linking to collect multi-channel events in workflows, 72
  - linking to collect sequence events, 210
  - parameters
    - Apodization, 379
    - Attenuator, 354
    - Autosampler Specification, 377
    - Background Specification, 352
    - Beam Path, 378, 391
    - Channel Number, 374
    - Cycle Through Simulation Samples, 363
    - Gain, 355
    - Number Of Scans Per Batch, 386
    - Optimize Gain, 356
    - Pre-collection Delay, 353
    - Probe Type, 374, 375
    - Prompt For Simulation Sample, 363
    - Resolution, 353
    - Sample Cup Spinner, 369
    - Sample Position for blend analyzer sampling, 384
    - Samples For Simulation, 359
    - Sampling Technique, 352
    - Scan, 382
    - Trigger, 386
    - Use Simulation Sample, 364
    - Use Standard Spectral Range, 358
    - Velocity, 381
    - Zero Filling, 380
  - parameters for autosampler integrating sphere sampling, 376
  - parameters for autosampler softgel tablet analyzer sampling, 376
  - parameters for autosampler std tablet analyzer sampling, 376
  - parameters for blend analyzer sampling, 383
  - parameters for dual tablet reflection sampling, 388
  - parameters for dual tablet transmission sampling, 387
  - parameters for fiber optic sampling, 373
  - parameters for gas cell sampling, 377
  - parameters for integrating sphere sampling, 368
  - parameters for multi-channel sampling, 374
  - parameters for SabIR probe sampling, 373
  - parameters for softgel tablet sampling, 366
  - parameters for standard tablet sampling, 365
  - parameters for transmission module sampling, 370
  - parameters for transmission sampling
    - Sample Position, 371
  - parameters for validation wheel sampling, 389
    - Sample Position, 390
  - setting simulated sample spectra specifications, 358
  - suggested uses in workflows, 365
- sample spectrum
  - collecting from a workflow, 43
- Samples For Simulation parameter, 359
- Sampling Interval parameter, 208
- sampling rate
  - for collect sequence events, 207
- sampling sequence
  - with autosampler position number, 185
- Sampling Technique parameter, 352, 397
- Save List Of Archived File Names parameter, 15
- Save Report Files As Read-Only parameter, 13
- Save Spectral Files As Read-Only parameter, 13
- Save Workflow Error Report parameter, 16
- Scale Low/High parameter, 102, 151
- scan length, optimizing, 382
- Scan parameter, 382
- scanning
  - during forward and reverse mirror travel, 382
- scans
  - and collection time, 397
  - setting for background collection, 397
  - setting for sample collection with collect dual tablet events, 57
  - setting for sample collection with collect events, 45
  - setting for sample collection with collect multi-channel events, 66
- scans per spectrum
  - setting for sequence collection, 210
- scans per standard
  - setting for sequence collection, 211
- screens, for reducing light intensity, 354
- second derivatives
  - calculating in workflows, 23
- Select All Attributes parameter
  - restrictions for using, 224
- Select All Components parameter
  - setting for a workflow result, 344
- Select Attributes To Measure parameter, 241
- Select Image File parameter, 296
- Select Workflow Results To Archive dialog box, 10
- Select Workflow Results To Measure dialog box, 79
- Select Workflow Results To Store dialog box, 142

- sequence collection
  - number of spectra in sequence and total collection time, 207
  - setting up background collection, 214
- sequence concentrations
  - setting up a workflow to display, 199
- sequence data
  - reporting from a workflow, 335, 337
  - setting up a workflow to store, 203
- sequence data collection
  - setting up in a workflow, 196
- sequence display
  - setting up in a workflow, 199
- sequence event groups
  - creating, 196
- sequence heading item specifications
  - defining the heading layout, 336
  - described, 335
  - parameters, 336
    - Heading Section Border, 337
    - Heading Section Title, 336
  - specifying the run sequence event, 337
  - suggested uses in workflows, 337
  - titling the heading, 336
- sequence module events, 194
- sequence spectra
  - setting up a workflow to display, 199
- sequence summary item specifications
  - defining the table layout, 340
  - described, 337
  - parameters, 339
    - Add Workflow Result, 343
    - Component, 344
    - Digits After Decimal, 344
    - Select All Components, 344
    - Show Acceptance Limits, 342
    - Show Event Names, 342
    - Summary Section Border, 341
    - Summary Section Layout, 340
    - Summary Section Title, 340
  - restrictions for using, 346
  - specifying statistical values to include, 345
  - specifying the run sequence event, 343
  - specifying workflow results to be summarized, 343
  - suggested uses in workflows, 346
  - titling the table of summarized data, 340
- serial numbers
  - adding serial numbers for standards to sample reports, 292
  - adding to sample reports, 291
- Setpoint parameter, 191
- Settle Time parameter, 191
- Show Acceptance Limits (in sequence summary section)
  - parameter, 342
- Show Column Headings In Table Section parameter, 310, 322
- Show Event Names In Summary Section parameter, 323, 342
- Show Event Names In Table Section parameter, 310
- Show Raw Source Values In Summary Table parameter, 324
- Show Row Headings In Table Section parameter, 310, 322
- Show Run Chart parameter, 202
- Show Spectral Data parameter, 203
- Show Text Value parameter, 201
- signals
  - optimizing, 355
  - reading analog and digital signals into workflows, 102
  - writing analog and digital signals from workflows, 150
- signal-to-noise, 45, 211
  - and mirror velocity, 381
  - and number of scans per spectrum, 211
  - optimizing, 355
- simple workflow events, 3
- simulating data
  - background data, 400
  - coordinating samples and backgrounds, 365, 400, 402
  - maximum number of spectral files, 362
  - restrictions for selecting spectral files, 360
  - sample data, 358
  - sequence data, 204
- Single Beam
  - format for spectra collected from workflows, 47
- Single Beam data format, restrictions for using, 48, 213
- single-beam (raw), 213
- single-beam spectrum, 213
- slope
  - of plotted expected vs measured values, 75
- sofigel tablet analyzer
  - background specification parameters in workflows, 404
  - default gain and attenuation settings for background collections, 398
  - sample specification parameters in workflows, 366
- sorting
  - reported workflow results, 332
- specifications
  - autosampler specifications, 275
  - background specifications, 392
  - classify multiple specifications, 244
  - compare text specifications, 231
  - composite measurement specifications, 254
  - correction specifications, 430
  - defined, 1
  - for workflows, 216
  - general specifications, 263

- heading item specifications, 291
- logic specifications, 218
- logical test specifications, 219
- measurement specifications, 235
- memo item specifications, 298
- prompt specifications, 271
- report item specifications, 286
- report specifications, 277
- request specifications, 265
- sample correction specifications, 431
- sequence heading item specifications, 335
- sequence summary item specifications, 337
- spectral measurement specifications, 237
- spectrum item specifications, 300
- startrun specifications, 427
- startstop specifications, 425
- stoprun specifications, 428
- summary item specifications, 318
- table item specifications, 306
- Specify Number Of Scans Per Batch parameter, 386
- spectra
  - adding to sample reports, 300
  - archiving with same date and time stamp, 23
  - from sequence collections
    - setting up a workflow to display, 199
    - setting up a workflow to store, 203
  - loading archived spectra into workflows, 84
  - measuring in workflows, 86
  - reporting workflow results to, 116
- Spectra To Be Processed parameter, 93
- spectral data
  - adding to sample reports, 300
  - advanced processing options in workflows, 91
  - archiving from workflows, 7
  - archiving with same date and time stamp, 23
  - basic processing options in workflows, 88
  - calculating average spectrum, 88
  - calculating statistical values in workflows, 23, 318, 337
  - calculating variance spectrum, 89
  - checking in workflows, 32
  - collecting from multiple channels at the same time, 64
  - collecting transmission/reflection data simultaneously with tablet analyzers, 55
  - comparing actual vs. expected values in workflows, 75
  - format for spectra generated by workflows, 12
  - measuring in workflows, 86
  - reporting from workflows, 106
  - setting X and Y range for plots, 303
  - setting X-axis range of collected spectra, 358
  - storing from workflows, 140
- Spectral Data Format parameter, 12
- spectral files
  - generating from workflows, 12
- spectral measurement specifications
  - described, 237
  - parameters, 238
- spectral range
  - for blend analyzer sampling, 387
  - for X axis of collected spectra, 358
  - for X or Y axis of plotted spectra, 303
- Spectral Range parameter
  - setting for collected spectra, 358
  - setting for plotted spectra, 303
- spectral resolution
  - setting for sample collection, 353
  - setting for sample collection with collect dual tablet events, 57
  - setting for sample collection with collect multi-channel events, 68
- Spectralon reference
  - fiber optic sample specification parameters in workflows, 374
  - multi-channel background specification parameters in workflows, 413
  - multi-channel sample specification parameters in workflows, 375
- spectrum
  - storing with temperature/pressure values, 189
- spectrum format specifications. See spectrum item specifications
- spectrum information
  - displaying in TQ Analyst and OMNIC, 118
- spectrum item specifications
  - and collection events, 305
  - defining the plot layout, 302
  - described, 300
  - parameters, 301
    - Spectral Range, 303
    - Spectrum Section Title, 303
  - specifying collection results (spectra) to include, 304
  - suggested uses in workflows, 305
  - titling the spectral plot, 303
- Spectrum Section Title parameter, 303
- spectrum titles
  - used to name files saved by archive events in workflows, 22
- spectrum, average
  - calculating in workflows, 95
- spectrum, difference
  - calculating in workflows, 95
- spectrum, subtraction

- used in workflows, 96
- spectrum, variance
  - calculating in workflows, 94
- spin and rotation, for Sample Cup Spinner, 369
- spinner, setting spin and rotation, 369
- splitting
  - table sections in sample reports, 316, 334
- square root value
  - reporting as composite component, 261
- standard deviation
  - adding to sample reports, 318
  - adding to sequence reports, 338
  - calculating in workflows, 23
  - reporting as composite component, 260
- standard deviation of two or more spectra, 89
- standard deviation value
  - adding to sample reports, 330
- standard tablet analyzer
  - background specification parameters in workflows, 403
  - default gain and attenuation settings for background collections, 398
  - sample specification parameters in workflows, 365
- standards
  - placing in the beam path, 390
  - placing in the beam path for Antaris MX, 67
- Start Specification parameter, 179
- start specifications
  - linking to StartStop events, 179
- Start/End Spectrum X Value parameter, 203
- starting
  - workflow events interactively, 177
- StartRun prompt dialog box, 177, 427
- startrun specifications
  - described, 427
  - parameters, 427
- startstop events
  - described, 177
  - parameters, 178
    - Exit Group After Workflow Error, 178
    - Start Specification, 179
    - Stop Action Generates Workflow Error, 179
    - Stop Specification, 179
  - specifying the startrun specification, 179
  - specifying the stoprun specification, 179
  - suggested uses in workflows, 179
- startstop specifications
  - described, 425
- statistics
  - adding to sample reports, 28, 330
  - adding to sequence reports, 345
  - calculating in workflows, 23
- status information
  - adding to sample reports, 291
- Stop Action Generates Workflow Error parameter, 179
- Stop Specification parameter, 179
- stopping
  - workflows events interactively, 177
- StopRun prompt dialog box, 177, 428
- stoprun specifications
  - described, 428
  - parameters, 429
    - Prompt Text, 429
- store events
  - described, 140
  - parameters, 141
    - Store Numeric Values From These Results, 142
  - restrictions for using, 141
  - suggested uses in workflows, 144
- Store Pass/Fail RESULT To Database parameter, 35
- Store Raw Values With Calculated parameter, 29
- Store Raw Values With Calculated Values parameter, 78
- storing
  - archived spectra for use in a workflow, 85
  - autosampler position numbers for use in a workflow, 187
  - calculation results for use in a workflow, 31
  - check event pass/fail results for use in a workflow, 35
  - check event pass/fail results in RESULT database, 35
  - data read from devices for use in a workflow, 102, 105
  - logical test results for use in a workflow, 229
  - numerical results from workflows in RESULT database, 140
  - pass/fail images in RESULT database, 32
  - pass/fail results in RESULT database, 32
  - processed spectra for use in a workflow, 98
  - records of archived sample reports in RESULT database, 108
  - records of archived spectra in RESULT database, 8
  - reports for use in a workflow, 110
  - request event results for use in a workflow, 136
  - results for use in a workflow, 90
  - simulated background spectra with a workflow, 361
  - simulated sample spectra with a workflow, 359
  - spectra for use in a workflow, 53, 63, 74
  - workflow results for use in a workflow, 81
- string memory
  - reading into workflows, 102
- structural workflow events, 155
- Style parameter
  - setting for table sections in reports, 314, 328
- subtracting
  - components to create a composite component, 260
- Subtraction Factor parameter, 97

- subtraction reference spectrum
  - compatible file formats, 96
- subtraction spectrum
  - used in workflows, 96
- Subtraction Spectrum parameter, 96
- sum value
  - adding to sample reports, 330
- summary item specifications
  - compared with calculate events, 24
  - defining the table layout, 320
  - described, 318
  - parameters, 319
    - Add Workflow Result, 327
    - Attribute, 328
    - Data Type, 328
    - Decimal Places, 328
    - Delete Source Spectra, 325
    - Show Event Names, 323
    - Show Raw Source Values, 324
    - Summary Section Border, 322
    - Summary Section Layout, 321
    - Summary Section Title, 320
  - sorting reported results, 332
  - specifying pass/fail filter, 331
  - specifying results to include, 326
  - specifying statistical values to include, 28, 330
  - suggested uses in workflows, 334
  - titling the table of summarized data, 320
- Summary Properties button, 329
- Summary Section Border parameter, 322, 341
- Summary Section Layout parameter, 321, 340
- Summary Section Title parameter, 320, 340
- sums
  - adding to sample reports, 318
  - calculating in workflows, 23

## T

- table break
  - adding to sample reports, 316, 334
- table format specifications. See table item specifications
- table item specifications
  - defining the table layout, 308
  - described, 306
  - parameters, 307
    - Add Break, 315, 333
    - Add Workflow Result, 312
    - Align, 314, 328
    - Attribute, 313
    - Color, 314, 328
    - Data Type, 313

- Digits After Decimal, 314
- Label, 315, 329
- Place All Data Types In One Row/Column, 311, 323
- Preview Section, 318, 334
- Show Column Headings, 310, 322
- Show Event Names, 310
- Show Row Headings, 310, 322
- Style, 314, 328
- Table Section Border, 309
- Table Section Layout, 308
- Table Section Title, 308
  - specifying results to include, 311
  - suggested uses in workflows, 318
  - titling the table of data, 308
- Table Section Border parameter, 309
- Table Section Layout parameter, 308
- Table Section Title parameter, 308
- tables
  - adding summarized data to sample reports, 318
  - adding summarized sequence data to sample reports, 337
  - adding tables of data to sample reports, 306
  - formatting tables of data in sample reports, 308
  - formatting tables of summarized data in sample reports, 320
  - formatting tables of summarized sequence data in sample reports, 340
  - splitting tables in sample reports, 316, 334
- tablet analyzer
  - background specification parameters in workflows, 403, 404
  - collecting transmission/reflection data simultaneously, 55
  - sample specification parameters in workflows, 365, 366
- Target blend analyzer
  - default gain and attenuation settings for background collections, 399
- Target blend analyzer sampling
  - background specification parameters in workflows, 420
  - sample specification parameters in workflows, 383
- temperature
  - setting for heated gas cell, 191
  - setting for heated sample holder, 371
  - storing with collected gas cell spectra, 189
- temperature controller
  - setting from a workflow, 189
- Test Case Name parameter, 243
- Test Case Value parameter, 243
- Test Dialog button, 134
- testing
  - message-response dialog boxes in workflows, 134
  - workflows in RESULT Integration, 242
- text
  - adding to sample reports, 291

- reporting to spectra from workflows, 116
- text files
  - reporting workflow results to, 125
  - using as response to request events in workflows, 136
- Text Item 1 parameter, 232
- Text Item 2 parameter, 233
- text reports
  - generating in workflows, 110
- Text String For Comparison parameter, 249
- third-party probe
  - configuring for multi-channel sampling, 375
- throughput
  - and mirror velocity, 381
- time, adding to sample reports, 291
- titles
  - adding sequence titles to sample reports, 335
  - adding to sample reports, 291
  - reporting information to spectral titles from workflows, 123
  - using spectrum titles to name files saved by archive events in workflows, 22
- total area, for sequence data reporting, 338
- Total Collection Time parameter, 207
- TQ Analyst measurement specifications
  - adding to workflows, 237
- TQ Analyst software
  - analysis type, 249
  - application name, 240
  - classification settings for multiple methods, 246
  - measured attributes, 241
  - measurement type, 241
  - method file name, 240, 248
- Transfer Background Spectrum
  - defined, 434
- transfer corrections
  - defined, 432
- Transfer Sample Spectrum
  - defined, 435
- transmission module
  - background specification parameters in workflows, 407
  - configuring for fiber optic background collections, 411
  - configuring heated sample holder, 371
  - default gain and attenuation settings for background collections, 399
  - sample specification parameters in workflows, 370
  - setting background position, 408
  - setting delay for heated sample holder, 372
  - setting delay override for heated sample holder, 372
  - setting sample position, 371
  - setting temperature for heated sample holder, 371
- Transmittance

- format for spectra collected from workflows, 47
- Trend tab
  - storing workflow results in the database for use in trend charts, 141
- Triangular apodization, 379
- Trigger parameter, 386
- turnaround
  - optimizing for moving mirror, 382

## U

- uncertainty values
  - calculating in workflows, 75
- Unicode HTML (\*.htm) file format, 12
- unit
  - for composite component, 261
- Unscrambler measurement specifications
  - adding to workflows, 238
- Use Digital Signatures parameter, 14
- Use Field Delimiter parameter, 270
- Use Fixed Pressure parameter, 193
- Use Fixed Temperature parameter, 192
- Use Heated Cell parameter, 371
- Use Sample Gain And Attenuation Settings parameter, 398
- Use Sampling Sequence parameter
  - for repeat events, 163
- Use Simulation Backgrounds For All Workflow Runs
  - parameter, 402
- Use Simulation Sample For All Workflow Runs parameter, 204
- Use Simulation Samples For All Workflow Runs parameter, 364
- Use Specific Sampling Interval parameter, 208
- Use Standard Spectral Range parameter, 358

## V

- validation dates
  - adding instrument validation date to sample reports, 292
  - adding workflow validation date to sample reports, 291
- validation samples and standards
  - placing in the beam path, 390
  - placing in the beam path for Antaris MX, 67
- validation wheel
  - background specification parameters, 423
  - collecting 100% line spectrum, 424
  - described, 390
  - described for Antaris MX, 67
  - sample specification parameters, 389
  - selecting a detector, 391
  - setting sample position, 390
    - for Antaris MX with collect multi-channel events, 67

- ValPro logo
  - adding to sample reports, 297
- variance spectrum
  - calculating in workflows, 89, 91, 94
  - restrictions for generating, 88
- velocity
  - and collection time, 381
  - and detector type, 381
  - and signal throughput, 381
  - and signal-to-noise, 381
- Velocity parameter, 381
- verification workflows
  - requirements for creating, 37

## W

- wheels
  - validation, 390
  - validation for Antairs MX, 67
- workflow errors
  - configuring perform events to check for errors, 159
  - configuring startstop events to check for errors, 178
  - configuring startstop events to generate errors after stop action, 179
  - configuring workflows to check for errors, 228
  - configuring workflows to report errors, 16
  - using logical test specifications to error test, 229
- workflow events
  - adding comments to, 160
  - adding sequence events to workflows, 196
  - adding simple events to workflows, 4
  - adding structural events to workflows, 157
  - adding to logical test specifications, 222
  - base names, 5
  - creating event groups, 157
  - defined, 1
  - device-specific workflow events, 180
    - configure temperature/pressure, 189
    - position autosampler events, 182
  - sequence module workflow events, 194
    - collect sequence events, 205
    - run sequence events, 197
  - simple workflow events, 3
    - archive events, 7
    - calculate events, 23
    - check events, 32
    - clear events, 38
    - collect dual tablet events, 55
    - collect events, 43
    - collect multi-channel events, 64
    - compare events, 75
    - delay events, 82
    - load spectrum events, 84
    - measure events, 86
    - process events, 91
    - read from I/O events, 99, 103
    - report events, 106
    - report to OPC events, 111
    - report to spectrum events, 116
    - report to text file events, 125
    - request events, 131
    - run exe events, 138
    - store events, 140
    - write to I/O events, 145, 151
  - structural workflow events, 155
    - perform events, 158
    - perform-if events, 168
    - perform-while events, 172
    - repeat events, 161
    - startstop events, 177
- workflow results. See also results
  - entering labels for workflow results displayed in reports, 315, 329
  - specifying digits for use in logical test specifications, 227
  - storing in the database for queries, 140
- workflow specifications, 216
  - adding background specifications to workflows, 394
  - adding correction specifications to workflows, 430
  - adding general specifications to workflows, 263
  - adding logic specifications to workflows, 218
  - adding measurement specifications to workflows, 236
  - adding report item specifications to workflows, 289
  - adding report specifications to workflows, 285
  - adding sample specifications to workflows, 349
  - adding startstop specifications to workflows, 426
  - autosampler specifications, 275
  - background specifications, 392
  - classify multiple specifications, 244
  - compare text specifications, 231
  - composite measurement specifications, 254
  - correction specifications, 430
  - defined, 1
  - general specifications, 263
  - heading item specifications, 291
  - logic specifications, 218
  - logical test specifications, 219
  - measurement specifications, 235
  - memo item specifications, 298
  - prompt specifications, 271
  - report item specifications, 286
  - report specifications, 277

- request specifications, 265
- sample correction specifications, 431
- sequence heading item specifications, 335
- sequence summary item specifications, 337
- spectral measurement specifications, 237
- spectrum item specifications, 300
- startrun specifications, 427
- startstop specifications, 425
- stoprun specifications, 428
- summary item specifications, 318
- table item specifications, 306
- workflow status check event
  - and qualification/verification workflows, 37
- workflows
  - for RESULT Integration software
    - adding background specifications to workflows, 394
    - adding collect sequence events, 197
    - adding comments to a workflow, 160
    - adding conditional events in workflows, 168
    - adding correction specifications to workflows, 430
    - adding device-specific workflow events, 180
    - adding executable programs, 138
    - adding general specifications to workflows, 263
    - adding logic specifications to workflows, 218
    - adding measure events to a collect sequence group, 197
    - adding measurement specifications to workflows, 236
    - adding report item specifications to workflows, 289
    - adding report specifications to workflows, 285
    - adding run sequence events, 196
    - adding sample specifications to workflows, 349
    - adding simple events to workflows, 4
    - adding startstop specifications to workflows, 426
    - adding structural events to workflows, 157
    - calculating statistical values in workflows, 23
    - clearing data to improve performance, 38
    - collecting data continuously, 197
    - configuring early exits for conditional events, 170
    - configuring early exits for conditional repeat loops, 174
    - configuring early exits for repeat loops, 164
    - configuring perform events to check for errors, 159
    - configuring startstop events to check for errors, 178
    - configuring temperature/pressure for gas cell sampling, 189
    - creating conditional repeat loops in workflows, 172
    - creating loops in workflows, 161
    - grouping events, 158
    - loading archived spectra, 84
    - pausing a workflow, 82
    - pausing before background collection, 398
    - pausing before sample collection, 57, 68
    - positioning an autosampler, 182
    - processing spectra in workflows, 91
    - reading data from devices, 99, 103
    - repeating events in workflows, 161, 172
    - reporting workflow results to OPC clients, 111
    - reporting workflow results to spectra, 116
    - reporting workflow results to text files, 125
    - requirements for qualification and verification workflows, 37
    - saving a list of archived files, 15
    - sequence module workflow events, 194
    - simple workflow events defined, 3
    - specifying data collection for a workflow, 43
    - starting and stopping events interactively, 177
    - storing simulated background data with a workflow, 400
    - storing simulated sample data with a workflow, 358
    - storing simulated sequence data with a workflow, 204
    - structural workflow events defined, 155
    - using logical test specifications to error test, 229
    - using test cases to test new measurements, 242
    - workflow events defined, 1
    - workflow specifications defined, 1, 216
    - writing data to devices, 145, 151
  - heading item specifications, 291
  - in RESULT Integration software
    - pausing before sequence collection, 209
  - memo item specifications, 298
  - sequence heading item specifications, 335
  - sequence summary item specifications, 337
  - setting up collection phases, 205
  - setting up the sequence display, 199
  - setting up to display sequence concentrations, 199
  - setting up to display sequence spectra, 199
  - setting up to store sequence data, 203
  - spectrum item specifications, 300
  - summary item specifications, 318
  - table item specifications, 306
  - write to I/O events
    - described, 145, 151
    - parameters, 145
      - Opto 22 Controller IP Address, 146
      - Point #, 151
      - Point Type, 150
      - Scale Low/High, 151
      - Write Data, 147
    - suggested uses in workflows, 155

## X

- X-axis range
  - of collected spectra, 358

of plotted spectra, 303

## **Y**

y-axis intercept

of plotted expected vs measured values, 75

Y-axis range

of plotted spectra, 303

yes/no responses, configuring logical test specifications for, 228

## **Z**

Zero Filling parameter, 380