

RESULT Integration Software User Guide



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Chapter 1 Overview

Welcome to RESULT Integration software. RESULT Integration is the development portion of the Thermo Scientific RESULT software for routine sample analysis. You can use RESULT to set up a controlled operating environment for the Thermo Scientific Antaris analyzers.

Use RESULT Integration to create and test workflows, which contain software commands for collecting, measuring, reporting and archiving spectral data. Based on the overall task the workflow is to perform, you decide which commands you want to include and arrange them however you wish. Once the workflow has been completed, tested and saved, you can transfer the workflow to a production system where it can be systematically called up and run from RESULT Operation, which is the production application for RESULT.

This manual describes RESULT Integration software and explains how RESULT Integration interacts with other applications, such as RESULT Operation, RESULT Data View, and Thermo Scientific TQ Analyst method development software. The major chapters in this manual are:

- **Getting Started.** Read this chapter to learn how to start, quit and customize RESULT Integration and interact with the software's main features.
- **Creating and Editing Workflows.** This chapter describes how to use RESULT Integration software to create and edit workflows, test a workflow by running it in a simulated production mode, save a workflow, apply digital signatures to workflows and their associated files, add a sampling sequence to a workflow, create instruction files for workflows, and transfer a workflow to a production system for repeated use.

- **Tools for Building Methods and Viewing Spectra.** This chapter describes how to use the options in the Tools menu of RESULT Integration software and your TQ Analyst method development software to build an analytical method and assign the method to a workflow. The chapter also covers tools for collecting and viewing spectra using RESULT Integration software and information about using third-party method development applications with RESULT.
- **Troubleshooting Workflows in RESULT Integration Software.** This chapter discusses errors that may occur when running workflows in RESULT Integration software and explains how to resolve the errors.

Anyone who is responsible for setting up processes and instructions to run Thermo Scientific application-based analyzers should read this manual. To learn about the software commands that are available for use in workflows created in RESULT Integration software, see the manual titled “Workflow Events and Specifications.” 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 user guide with that name. If you want a quick overview of RESULT Integration, read *Getting Started using RESULT* and complete the steps in the software to develop and run a basic workflow.

Chapter 2 Getting Started

This chapter demonstrates how to start, quit and customize RESULT Integration and explains how to interact with the software's main features.

Starting RESULT Integration

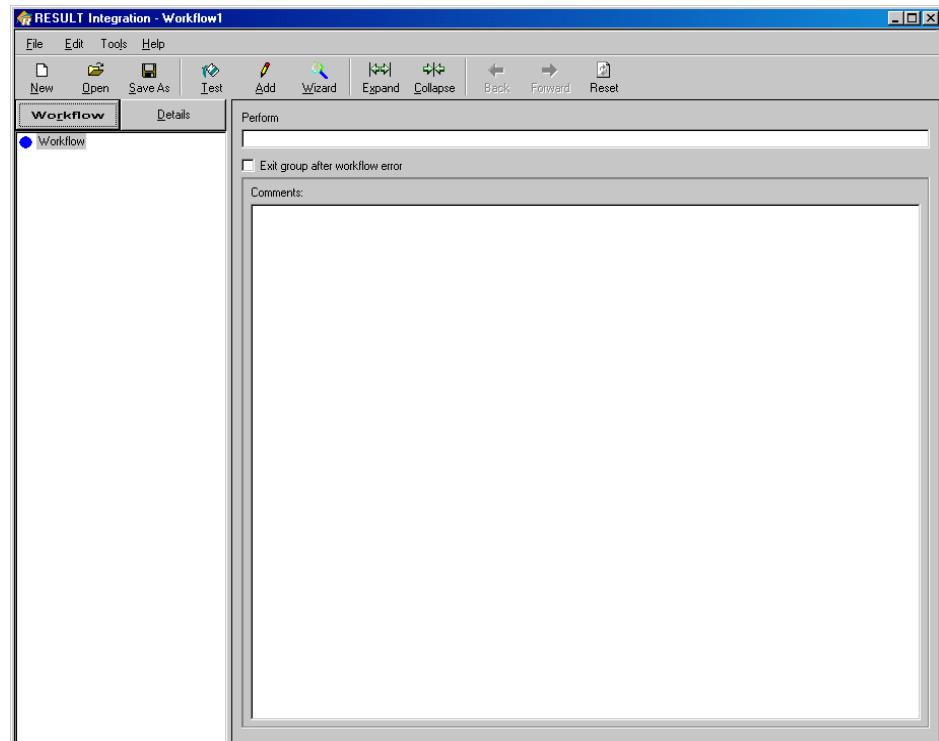
Before you can log on to the computer workstation, you must receive a Windows user name and password from your Windows administrator.

To start RESULT Integration software:



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

After you have successfully started RESULT Integration, the RESULT main window displays.



RESULT Integration software main window

Setting RESULT Integration options

You may customize the directory locations (paths) in RESULT Integration software. This allows you to quickly locate and store files in selected locations when creating and testing workflows. You can also select the instrument model that will be used to run your workflows and specify whether the system includes the ValPro System Qualification option. The selected instrument model defines the options available in RESULT Integration software for configuring instrument settings, such as sampling technique and instrument gain.

The directory paths and other options you can specify are listed below:

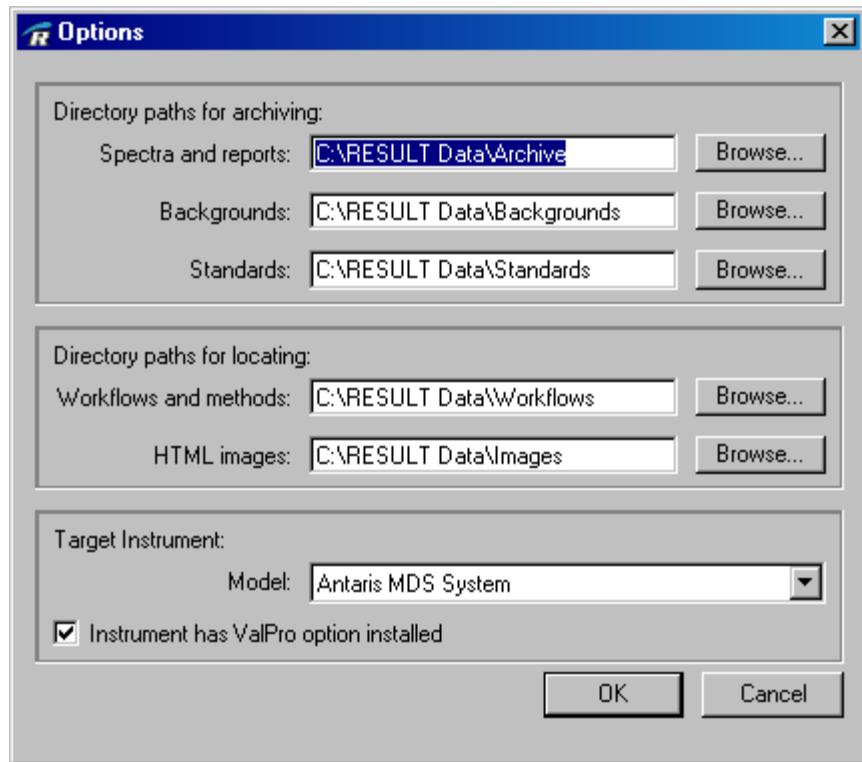
- **Paths for archiving data.** These options define the directory paths the software uses to archive spectral and report files created while setting up and testing workflows in RESULT Integration. Spectral data files of backgrounds, samples and standards may be archived using unique directory paths.
- **Paths for locating workflows and methods and HTML image files.** These options define the default directory paths the software uses for locating workflow and method files and image files when those files are accessed through RESULT Integration software.
- **Target Instrument.** These options specify the instrument model for your workflows and whether the system includes the optional ValPro System Qualification package. The selected instrument model defines the options available in RESULT Integration software for configuring data collection and other instrument settings.

Note These are the same types of options that can be specified in RESULT Operation software. Directory paths and other options that are specified in RESULT Integration do not affect those settings in RESULT Operation when workflows are transferred between the two applications. ▲

To configure RESULT options:

1. **Choose Options from the Edit menu in the RESULT Integration main window.**

The Options dialog box is displayed, as shown below.



Note You may create and select subfolders for archiving standards when setting up a method but you cannot select folders that are above the directory path specified here. See “Configuring Standards” in “Chapter 4 Tools for Building Methods and Viewing Spectra” for more information. The path for archiving backgrounds can only be specified in the RESULT Options dialog box. □

3. Select a path for locating workflow and method files and HTML image files by choosing the associated Browse button and then locating and selecting an appropriate directory.

These will be the default paths for opening and saving workflows and their associated TQ Analyst method files and image files in RESULT Integration software. When using RESULT Integration, you may browse to any directory to locate or save these items. For convenience, store these items in one directory and then specify the path in this dialog box.

Note Workflows and their associated TQ Analyst method files must be stored in the same directory. ▲

The original path for images points to the bitmap and other image files provided by the software, such as the pass (✓) and fail (✗) image files. These image files are available to users for placement in sample reports or other HTML documents created using RESULT Integration software. See “Report Item Specifications” in “Workflow Events And Specifications” for details on adding the pass or fail image to heading and table sections in a sample report.

You can add your own image files to a sample report by placing the files in the image folder specified here and setting up a heading section that calls the image. See “Heading Item Specification” in “Workflow Events And Specifications” for details on adding other images to reports created using RESULT Integration software.

If you reset the path for locating images, you must copy the images stored in the default image folder to the new image folder before those images can be used in subsequent reports. If you transfer a workflow that specifies one or more images in a sample report to RESULT Operation software, make sure you copy the image files along with the workflow. See “Transferring A Workflow To RESULT Operation” in “Chapter 2 Creating And Editing Workflows” for more information.

4. Specify the configuration of the instrument that will be used to run any workflows developed in RESULT Integration software by selecting the instrument model.



- **Model.** Your selection in this list box will determine the options available in RESULT Integration software for configuring instrument settings. For example, if you want to develop workflows for an Antaris or Antaris II Method Development Sampling (MDS) system, set Model to “Antaris MDS System” to ensure that all of the available options appear in the software. If you are working with another Antaris system, such as the Fiber Optic System or the Antaris IGS, select the option in the Model drop-down list that matches your system name. If you have a configurable Antaris II system, set Model to “Antaris MDS System” to see all the options in the software or select an option that matches your instrument configuration. For example, if you have an Antaris II that is configured for fiber optic sampling, set Model to “Antaris Fiber Optic System” to limit the software to features that apply to fiber optic sampling. The following table describes the available options:

Instrument Model	Description
Antaris II or Antaris MDS System	Includes transmission module, integrating sphere and fiber optic sampling station.
Antaris Liquid Analyzer System	Configurable Antaris or Antaris II system that includes only the transmission module.
Antaris Fiber Optic System	Configurable Antaris or Antaris II system that includes only the fiber optic sampling station.
Antaris Solid Sampling System	Configurable Antaris or Antaris II system that includes only the integrating sphere.
Antaris Tablet Analyzer System	Configurable Antaris or Antaris II system that includes only the standard and/or softgel tablet analyzer.

Instrument Model	Description
Antaris RTS System	Configurable Antaris or Antaris II system that includes the transmission module and integrating sphere.
Antaris MX or EX System	A compact fiber optic system with 2 or 4 channels for connecting fiber optic accessories.
Antaris Target Series System	A compact, near-infrared analyzer dedicated to real-time monitoring of pharmaceutical powder blending. Installs directly on the bin and can also be used for desktop sampling.

5. When you are finished configuring RESULT options, choose OK to save your changes and close the dialog box.

The new settings will apply to any new workflows created in RESULT Integration software or run using the Test Workflow feature in RESULT Integration.

Note Directory paths and other options that are specified in RESULT Integration do not affect those settings in RESULT Operation when workflows are transferred between the two applications. □

Software basics

Read this section to learn about the unique features of RESULT Integration and how to operate the software. The following features are introduced:

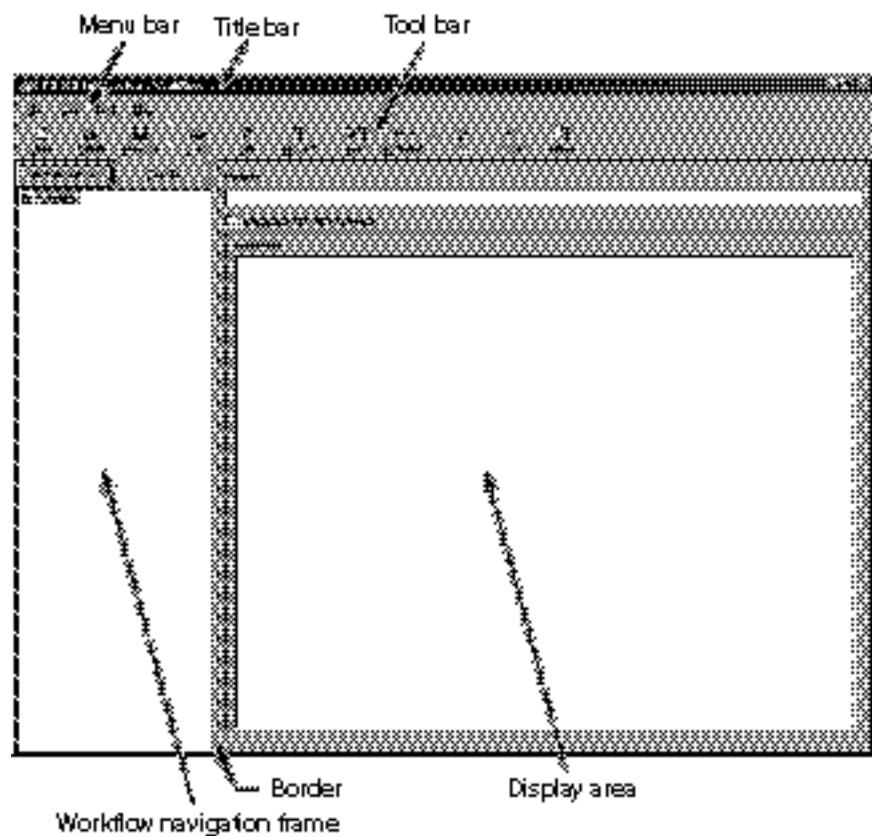
- RESULT Integration main window
- Menu bar
- Toolbar
- Workflow navigation frame
- Workflow tree
- Specification tree
- Display area

You should understand how to use these features before attempting to create or edit workflows using RESULT Integration software.

Main window components

You can change the relative sizes of the workflow navigation frame and the display area by dragging their common border right or left.

After you start RESULT Integration, the software's main window is displayed on the screen, as shown below.



RESULT Integration software main window

You can maximize, minimize and resize the RESULT Integration window just as you can other application windows that run with Windows software. See your Microsoft Windows documentation for information on these standard Windows features.

The RESULT Integration main window is divided into five parts: the title bar, the menu bar, the toolbar, the workflow navigation frame, and the display area. All of these features are described in the sections that follow.

Title bar

The title bar appears at the top of the RESULT Integration main window. When you create or open a workflow, the workflow's file name appears in the title bar. If no workflows are open, the default file name (Workflow1) appears in the title bar.

If you open and then change a workflow that has been previously saved on a disk, an asterisk appears after the workflow's file name in the title bar, as shown below.



Menu bar

The menu bar appears below the title bar in the RESULT Integration main window and contains the menu names. The menus provide useful commands for working with workflow files and spectral data.

You can choose commands in RESULT Integration menus just as in other Windows applications: by using the mouse or by typing key combinations on the keyboard. The key combinations are shown in the menus. See “Software Accessibility” for specific information on selecting menus and choosing commands using the keyboard.

The following menus appear in the RESULT Integration menu bar:



- **File.** Provides program and file management functions, such as creating, opening, saving, signing, and testing workflow files, and exiting the software.
- **Edit.** Provides commands for adding elements to a workflow, either individually or by using the Workflow wizard, and commands for standard editing functions, such as cutting, copying and pasting items in a workflow.
- **Tools.** Provides tools for building a TQ Analyst method, including configuring and collecting standards, and for collecting and viewing spectra using RESULT Integration software.
- **Help.** Gives the version number for RESULT Integration software.

See “Chapter 2 Creating And Editing Workflows” for details on each menu command or look up the command name in the index at the end of this document.

Toolbar

The toolbar appears below the menu bar at the top of the RESULT Integration main window. It provides a convenient way to initiate frequently used menu commands and other functions in a single step.



You can use the toolbar to perform the following operations with the open workflow:



New. Use the New tool to create a new workflow.



Open. The Open tool allows you to open an existing workflow that was saved on a computer disk or network location.



Save. Use Save As to save the open workflow. If the workflow was not previously saved, you must enter a file name before saving.



Test. The Test tool runs the open workflow so you can see how it will operate on a production system. The test feature of RESULT Integration mimics RESULT Operation, which is the production application for RESULT.



Add. Use this tool to add software commands, called “events,” and parameter groups, called “specifications,” to the open workflow. The selected event is added after the current cursor location in the workflow tree. Added specifications are placed in the selected group in the specification tree.



Wizard. Select this button to start the Workflow wizard. The wizard is a handy tool for quickly creating a functional workflow that contains the basic components to collect, measure, report, and archive spectral data, or for adding those components to a workflow.



Expand. Choose this tool to expand the workflow or specification tree that is currently displayed in the workflow navigation frame so that all of the items contained in the tree are visible.



Collapse. This tool collapses the displayed workflow or specification tree so that only the first level structures are visible.



Back. Use this tool to navigate between screens in the open workflow. The Back button returns to the previous screen. After you use the Back button, the Forward button becomes available in the software.



Forward. Use this tool to navigate between screens in the open workflow. Use the Next button to return to the screen that was displayed the last time you pressed the Back button.

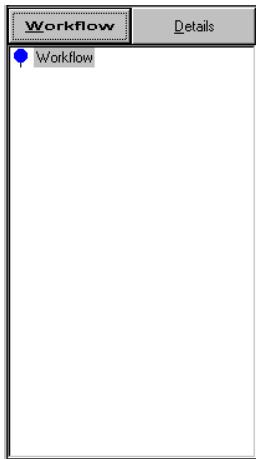


Reset. After editing the parameter settings for a displayed workflow event or specification, you can use the Reset button to restore those parameters to the settings displayed when you first selected that workflow event or specification.

To use a feature on the toolbar, use the mouse to choose the icon or hold down the Alt key on your keyboard while you type the underlined letter in the name that appears below the icon. To save the open workflow, for example, either choose the Save As icon or type Alt + S.

Workflow navigation frame

The workflow navigation frame appears at the left side of the RESULT Integration main window. You will use this frame to create, add to or simply display the contents of the open workflow.

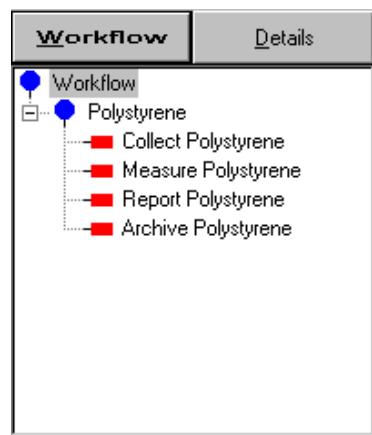


What is a workflow?

Workflows are the underlying concept behind RESULT software, which provides development and production tools for routine sample analysis. Each workflow may contain one or more software commands for collecting, measuring, reporting, or archiving spectral data. Based on the overall task the workflow is to perform, you decide which commands you want to include and arrange them however you wish. Once the workflow has been completed, tested and saved on a disk, you can transfer the workflow to a production system where it can be systematically called up and run. The software commands within a workflow will be carried out precisely as they appear in the workflow—with the same detail and in the same order.

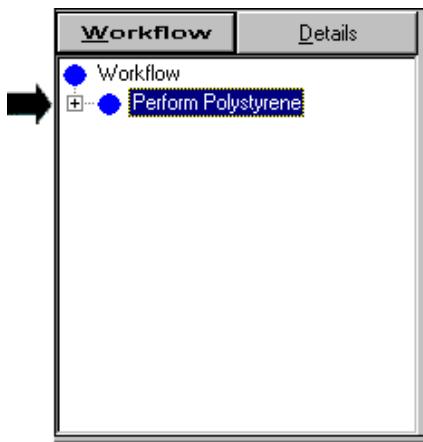
Workflow tree

The workflow navigation frame is your palette for creating and editing a workflow. If you use the Workflow wizard to get started, the basic components of a functional workflow (collect, measure, report, and archive) are added automatically, as shown below.



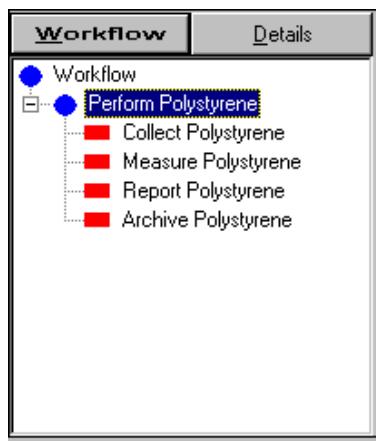
We call these commands “events” because they specify a task that will be carried out only when the workflow is run. You may add and delete events and arrange them in any order. The events may be linear or grouped. Grouped events can be performed, repeated, or performed based on the results of a conditional test.

As you build a workflow, we call the basic structure a workflow tree because it looks and operates similar to a computer directory tree. To display or hide the events within a group, click the plus (+) or minus (-) sign to the left of the group name or double-click the group symbol (●). For example, to see the events in the group called “Polystyrene” in the illustration below, click the plus sign to the left of the group name.



Collapsed workflow tree

The group is expanded to show the workflow events it contains, as shown below.



Expanded workflow tree



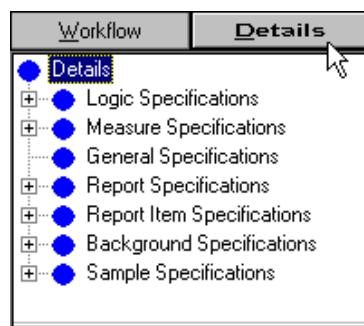
To quickly expand the entire workflow to show all of the events within every group, choose the Expand button on the toolbar.

Specification tree

Most of the workflow events have one or more associated specifications, which define how the event will be performed. The collect event, for example, has an associated sample specification, which defines sample collection for a given sample type or material.

A collect event may have other associated specifications as well. For example, if you want to display a dialog box that tells the operator how or where to insert the sample, you will need to add an operator prompt specification, which defines the prompt text and the action for the operator's response.

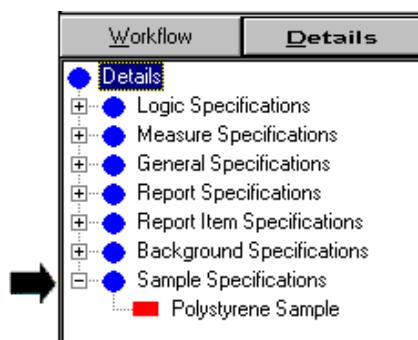
To see the names of the specifications that are contained in the open workflow, select the Details tab in the workflow navigation frame, as shown below.



Collapsed specification tree

We call this the “specification tree.” Specifications are automatically placed in functional groups. You can add and delete specifications but you cannot add, delete or change the group names.

To see the specifications within a group, click the plus (+) sign to the left of the group name or double-click the group symbol (●). To show the sample specifications, for example, open the Sample Specifications group, as shown below.



Expanded specifications group



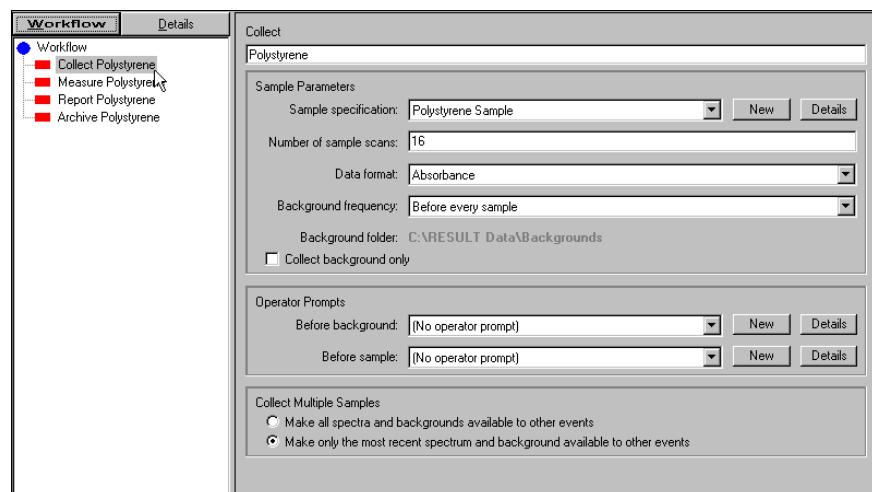
To quickly expand the entire specification tree to show all of the specifications within every group, choose the Expand button on the toolbar.

Display area

The display area is at the right side of the RESULT Integration main window.

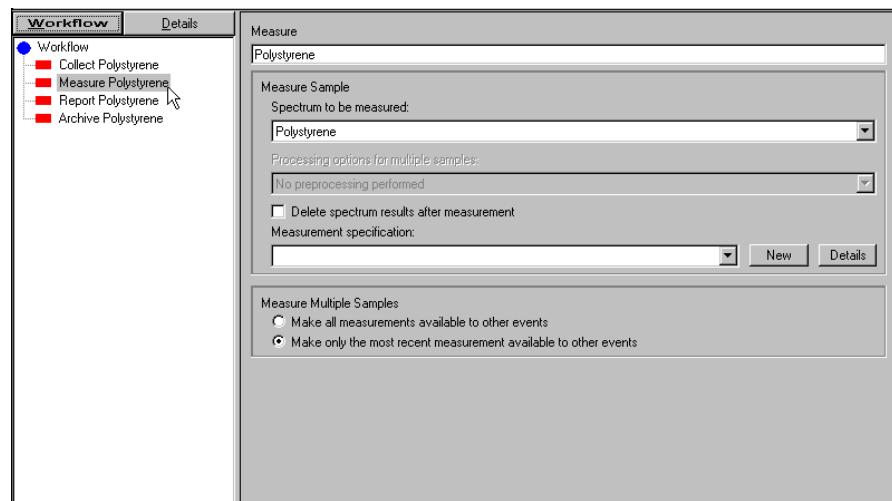


If the workflow tree is displayed in the workflow navigation frame, the display area shows the general options for the selected event, including the names of any associated specifications. When the collect event is selected, for example, the general collection options appear in the display area along with the names of the specifications for sample collection and any sample and background operator prompts, as shown in the next illustration.



Collect Polystyrene event

To see the general options for another event, choose the event name in the workflow tree. The event name is highlighted in the workflow tree and the general options for that event appear in the display area. The general options for the measure event are shown below.

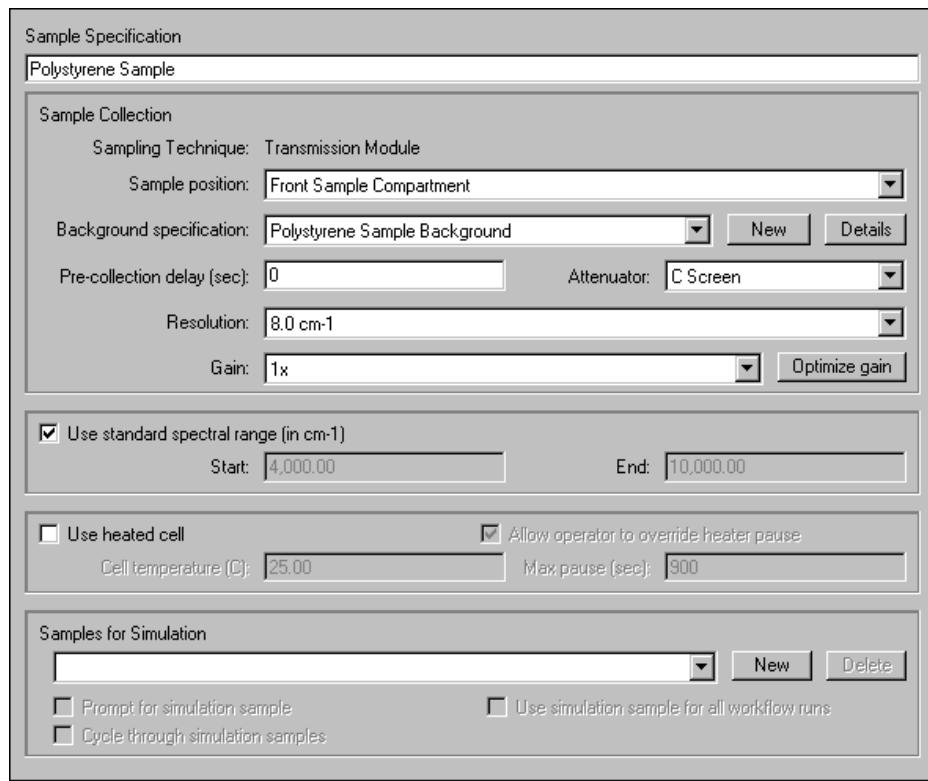


Measure Polystyrene event

To see a specification that is linked to the selected event, choose the Details button next to the specification name. For example, to see the sample specification for polystyrene, select the collect event by choosing its name in the workflow navigation frame and then choose the Details button next to "Sample Specification: Polystyrene Sample," as shown below

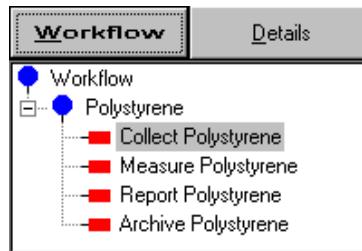


The selected specification appears in the display area, as shown below.



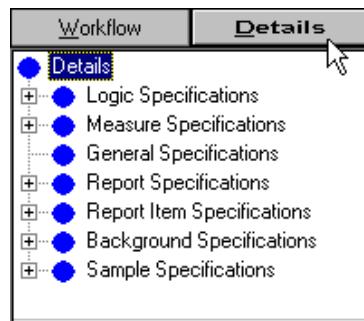
Polystyrene sample specification

To return to the previous screen, select the appropriate event in the workflow tree or click the Back button on the toolbar.



You can use the workflow tree to view the general options or an associated specification for any event in the open workflow.

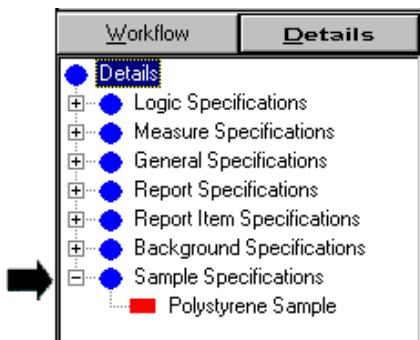
If you want to access all of the specifications for the open workflow, switch to the specification tree by choosing the Details tab in the workflow navigation frame.



Collapsed specification tree

To see the specifications within a group, click the plus (+) sign to the left of the group name or double-click the group symbol (●).

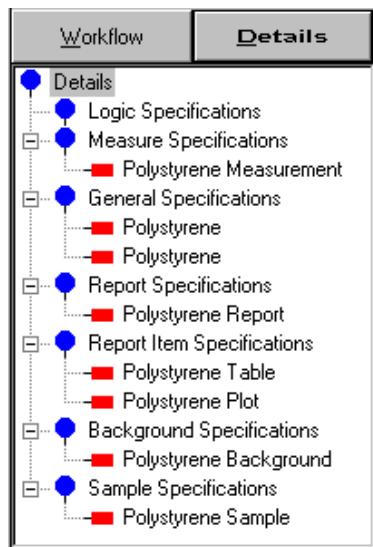
To show the sample specifications, for example, open the Sample Specifications group, as shown below.



Expanded specifications group



To quickly expand the entire specification tree to show all of the specifications within every group, choose the Expand button on the toolbar.



Expanded specification tree

To see the options in a particular specification, choose its name in the specification tree. The specification name is highlighted in the specification tree and the details for that specification appear in the display area. The next illustration shows the sample specification for polystyrene.

Sample specification for polystyrene

This is the same specification displayed from the workflow tree earlier in this lesson (after selecting the Details button next to the Sample Specification list box, as shown below).



You can display specifications from the workflow tree or the specification tree. However, only specifications that have been assigned to a workflow event can be accessed from the workflow tree, while the specification tree allows you to see all of the specifications that exist in the open workflow.

Note

You can use the specification tree to view the options for any specification in the open workflow. Options for workflow events may only be accessed from the workflow tree. □

Accessibility

RESULT Integration software has standard accessibility features, including hot keys and the ability to change display colors.

Hot keys

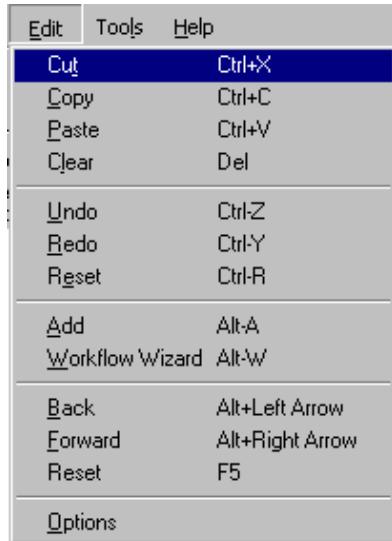
Each software feature can be accessed either by choosing a toolbar button or selecting a menu command or other item with the mouse, or by pressing a hot key or other key combination on the keyboard.

If a command or button has an associated hot key, the hot key is indicated by the underlined letter in the command name. Some examples are:

- The hot keys for starting the workflow wizard is Alt + W, as indicated by the underlined letter below.



- The hot keys to open the Edit menu and choose the Add command from the Edit menu are Alt + E, and then A, as shown below.



- or -

You can also choose Alt + E to open the menu, use the up and down arrow keys on the keyboard to select the command, and then press the Enter key to implement the command.

- or -

You can press Alt + A to choose the Add command without opening the Edit menu.

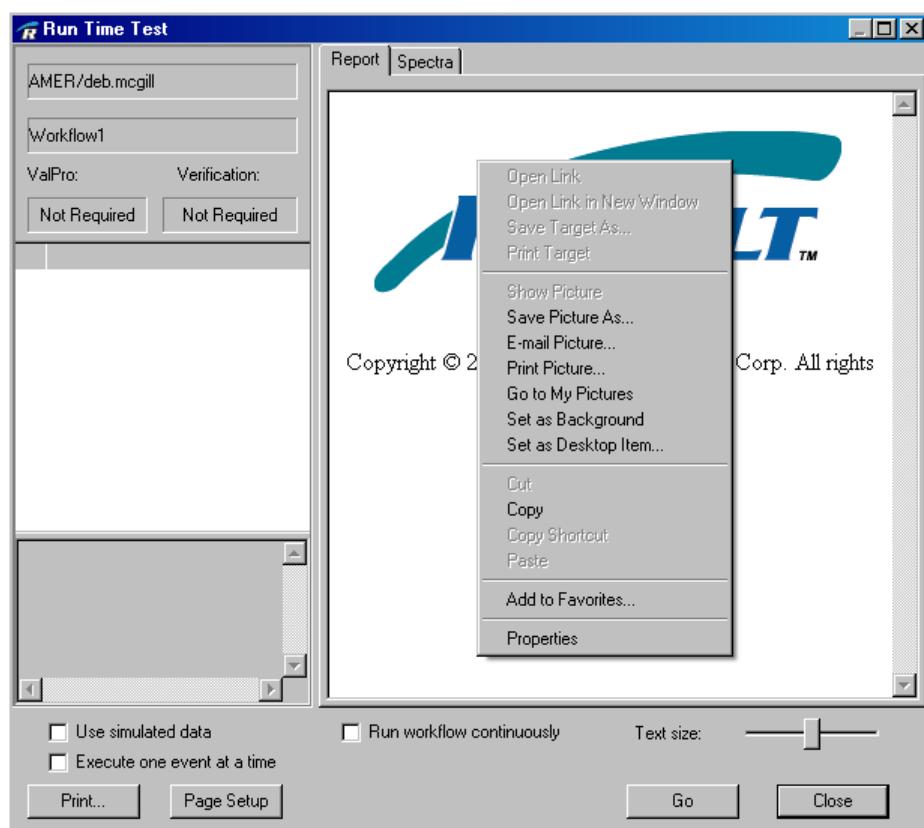
Use the Tab key to make the items in a window or dialog box active. As you “tab” through a window or dialog box, the features become highlighted or marked with a dotted rectangle (or both) as they become active. Once a feature is active, you can use the appropriate keys on the keyboard to interact with it. Some examples include:

- To select an item in a list, tab to the list and then use the up or down arrow key to move to the item.
- To turn a check box on or off, tab to the check box and then press the space bar.
- To select an option from a group of option buttons, tab to the option and then press the space bar.

- To choose a command button (such as OK) after tabbing to it, press Enter.

Shortcut menus

Use the right mouse button to display a menu of commands that apply to a selected item. For example, if you place the mouse cursor over the display area in the Run Time Test window and then hold down the right mouse button, the following shortcut menu appears:



Select an item in the menu to apply it to the selected window.

See your Windows documentation for complete information about using the keyboard to perform these and other standard Windows operations.

Display colors

Some of the display colors for RESULT can be modified by changing Windows system colors. See your Windows documentation or on-line help for information about changing display colors.

Note

If you are unable to change these settings or you are required to change the settings each time you log on to the workstation, then you have been assigned a mandatory profile or you do not have the Windows right to permanently change these settings. See your Windows administrator for more information. ▲

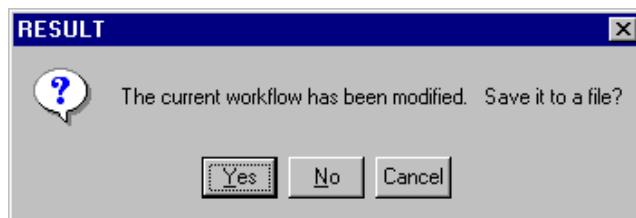
Quitting RESULT Integration

You should quit RESULT Integration software before shutting off your computer workstation.

To quit RESULT Integration:

1. Choose Exit from the RESULT Integration File menu.

Depending on whether you changed anything in the workflow without resaving the workflow, the following message may appear.



2. Choose Yes to save your changes before closing RESULT Integration.

Choosing No closes RESULT Integration without saving the open workflow. Any change made to the workflow since the workflow was last saved will be lost. Choosing Cancel will keep RESULT Integration open.

After closing RESULT Integration, you are returned to the workstation desktop and remain logged on to Windows.

Chapter 3 Creating and Editing Workflows

This chapter describes how to use RESULT Integration software to create and edit workflows, test a workflow by running it in a simulated production mode, save a workflow, apply digital signatures to workflows and their associated files, create instruction files for workflows, and transfer a workflow to a production system for repeated use.

Example workflows are provided with RESULT software to help you “get the feel” of RESULT Integration software before creating a workflow. The example workflows demonstrate a variety of operations, ranging from basic data collection using the various sampling modules to conditional executions and loops.

Look for the example workflows in the default directory for locating workflows after you install RESULT Integration software (C:\RESULT DATA\WORKFLOWS). All of the example workflows include simulated spectra (spectra stored with the workflow) that are appropriate for the workflow’s intended purpose.

To run an example workflow using simulated spectra, choose Open from the RESULT Integration File menu and select the example workflow you want to run. Then choose Test from the RESULT Integration toolbar to display the Run Time Test window. Select Use Simulated Data at the bottom of the Run Time Test window, and then choose Go.

The workflow simulates data collection by showing you any prompts or status information that will appear when the workflow is run normally. However, all workflow events that normally operate on the collected spectrum will use the simulated spectrum stored with the workflow instead. See “Testing a workflow” in this section for information about running workflows in RESULT Integration.

The software also includes the on-line document, EXAMPLE DESCRIPTIONS.PDF, which describes each example workflow. The document is stored in the default directory for locating instructions (C:\RESULT DATA\INSTRUCTIONS) as defined in the Options dialog box in RESULT Operation software. If you have a current version of Adobe® Reader® software, you can display the document from Windows Explorer by double-clicking the document name. You can also display the document in RESULT Operation software by selecting Example Descriptions from the Instructions list box in the RESULT Operation main window.

Starting a new workflow

There are three ways to start a new workflow in RESULT Integration software. You can start a new workflow by:

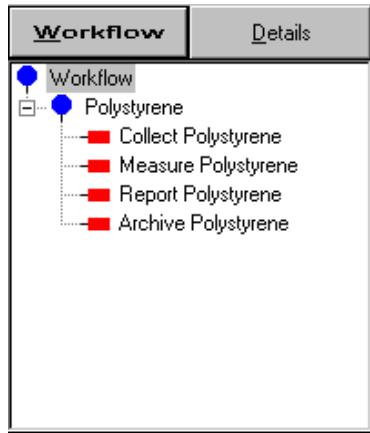
- Choosing the workflow wizard on the RESULT Integration toolbar.
- Choosing the New Workflow command in the RESULT Integration File menu.
- Using the Open Workflow command to open an existing workflow and then resaving the workflow with a different file name.

All three of these methods are discussed in the sections that follow.

Using the wizard to create or add to a workflow

RESULT Integration offers a handy tool to help you create a functional workflow that contains the basic components to collect, measure, report, and save spectral data. You choose which components you want to include from a single dialog box. When you close the dialog box, the new workflow appears in the workflow navigation frame. The new workflow contains all the events you selected and their associated specifications.

If you select all the options available from the workflow wizard, your workflow will contain the basic components to collect, measure, report, and archive spectral data, as shown below.



Example workflow created using the Workflow wizard

We call these components “events” because they specify a task that will be carried out only when the workflow is run. The tasks these events will perform are described briefly below:

Event Name	Description
Collect	Collects an infrared sample spectrum.
Measure	Can be linked to a custom TQ Analyst or other compatible method and used to make quantitative, qualitative or spectral measurements of the sample spectrum.
Report	Creates an HTML report that contains the sample spectrum and a table for organizing measurement or other results.
Archive	Saves the sample spectrum and/or the sample report in the specified location for archiving spectra and reports using unique file names.

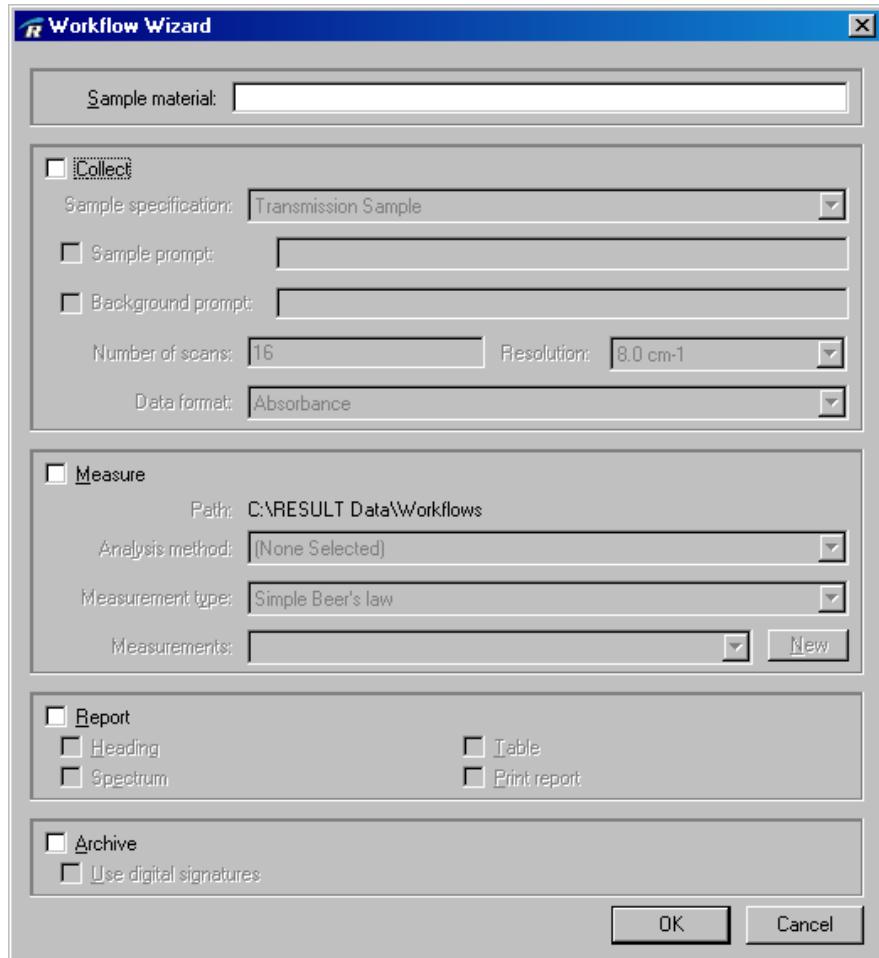
You can also use the workflow wizard to add these basic components to an existing workflow.

How to create or add to a workflow using the workflow wizard:



1. Start the RESULT Integration application and then choose the Wizard button on the RESULT Integration toolbar or choose Workflow Wizard from the Edit menu.

The following dialog box is displayed.



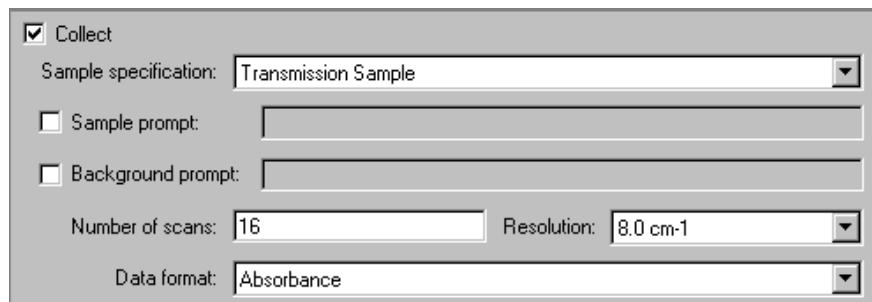
2. Select the **Sample Material** text box and type a descriptive name for the type of sample you want to analyze.

This is typically a specific name for the material the workflow will analyze, such as “polystyrene” or “aspirin.”

Sample Material:

3. If you want the workflow to collect a spectrum of your sample material, select the **Collect** option.

When the Collect check box is selected, the rest of the parameters in the Collect group become available, as shown below.



The parameters in the Collect group will define a data collect event for the workflow.

4. Specify the type of sample you want to analyze and the sampling module that will be used by selecting an option in the Sample Specification drop-down list.

One or more of the following selections should be available:

- **Transmission Sample.** Select this option if you want to analyze a liquid or film sample using the transmission sampling module of an Antaris FT-NIR analyzer.
- **Integrating Sphere Sample.** Select this option if you want to use the integrating sphere sampling module (or the integrating sphere portion of the tablet analyzer sampling module) of an Antaris FT-NIR analyzer to analyze a powder or solid sample.
- **Tablet Sample.** Select this option if you want to use the standard tablet module of an Antaris FT-NIR analyzer to run a transmission analysis of an opaque tablet sample.
- **SoftGel Tablet Sample.** Select this option if you want to use the softgel tablet module of an Antaris FT-NIR analyzer to run a transmission analysis of a softgel or gelcap tablet.
- **Fiber Optic Sample.** Select this option if you want to use the fiber optic module of an Antaris FT-NIR analyzer and attached probe to analyze a sample.
- **Gas Cell Sample.** Select this option if you want to collect data from a gas sample using the Antaris IGS (Industrial Gas System).

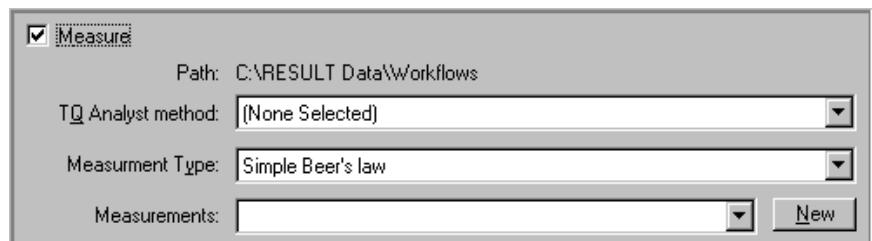
- **Blend Analyzer Sample.** Select this option if you want to collect data from a sample using the Antaris Target Blend Analyzer. The analyzer can be mounted on a blender bin or placed on a desk top.
 - **Validation Wheel Sample.** Select this option if you want to collect data from a sample on the optional validation wheel. The validation wheel is installed only in Antaris and Antaris IGS systems that include the ValPro System Qualification package.
- 5. Set the remaining collection parameters as desired using the table below as a general guide, or leave the default values displayed in the dialog box.**

For details on these and other options that define data collection, see “Collect events,” “Sample Specifications,” and “Background Specifications” in “Workflow Events and Specifications.”

Collection Option	Description
Sample Prompt	Defines an operator prompt that will appear before sample collection when the workflow is run.
Background Prompt	Defines an operator prompt that will appear before background collection when the workflow is run.
Number Of Scans	Defines the number of times the analyzer will scan the sample to produce a spectrum.
Resolution	Defines the resolution of the sample spectrum. Resolution is a measure of how well closely spaced peaks in a spectrum are differentiated.
Data Format	Defines the Y-axis unit that will be used to display or plot the sample spectrum in a sample report.

- 6. If you need the workflow to measure or extract data from the spectrum, select the Measure option.**

When the Measure check box is selected, the rest of the parameters in the Measure group become available, as shown below.



The parameters in the Measure group define how the sample spectrum will be measured in the new workflow.

7. Set the measurement parameters as desired or leave the default values displayed in the dialog box.

Use the descriptions provided below as a guide. For details on these and other parameters that define spectral measurements, see “Measure events” in “Workflow Events and Specifications.”

Measurement Option	Description
TQ Analyst Method	Allows you to select a TQ Analyst method (*.qnt) file that will be associated with this measure event. If an appropriate method does not exist, select None Selected in the drop-down list.
Measurement Type	Shows the Analysis Type setting in the selected TQ Analyst method. If no method is selected (see above), use this list box to specify the Analysis Type setting for a new TQ Analyst method.
Measurements	Lists the items the currently selected TQ Analyst method is set up to measure. If no method is selected (see above), use this text box to type the component names, class names, spectral measurements, or other attributes the new method will measure.

8. If you want the workflow to report the spectral data, select the Report option.

When the Report option is selected, the rest of the parameters in the Report group become available, as shown below.

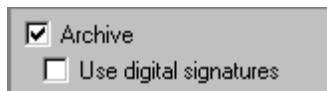


9. Choose the sections to include in the report (see the descriptions below) by selecting the appropriate check boxes.

For details on these and other options available for creating reports, see “Report Events” in “Workflow Events and Specifications.”

Report Option	Description
Heading	Defines a generic heading or title for the entire report, or a heading section in a report. A heading can contain text, images, and pertinent information, such as the instrument model or the current date and time (or any combination of these). A heading item specification defines each heading section in a report.
Spectrum	Defines a section in the report that will contain the spectrum of the sample collected by the workflow. If you select this option, the software adds the collection result (spectrum) to the spectrum item specification automatically. The spectrum item specification defines the spectrum or spectra to include in this section of the report.
Table	Defines a table of data that will be included in the report. A table can contain measurement, statistical, or other data, a pass or fail result, or the pass (✓) or fail (✗) image provided with the software. If you select this option, you must open the table item specification and add each measurement or other result to include in the table before running the workflow. See “Table Item Specifications” in “Workflow Events and Specifications” for more information.
Print Report	Specifies whether the report will be printed automatically after the workflow is run.

10. If you want the workflow to archive the sample spectra and/or the report, select the Archive check box.



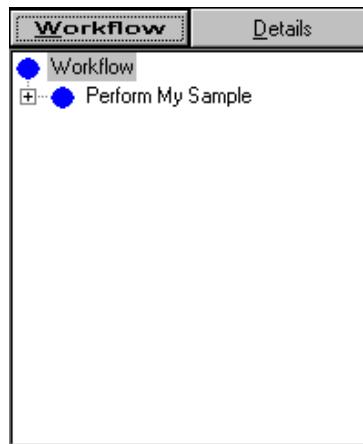
If you run the workflow in RESULT Integration software (using Test on the toolbar), the data will be archived using the base path for archiving spectra and reports as defined in the RESULT Options dialog box. See “Setting RESULT Integration Options” in “Chapter 1 Getting Started” for more information. Each spectral and report file is given a file name that includes a globally unique identifier (GUID).

If you elect to archive the data, you may also specify whether a user name and password will be required to archive the data by selecting Use Digital Signatures. When digital signatures are required, the workflow prompts the operator for a valid Windows user name and password before archiving the data.

Note Requiring digital signatures for spectra collected from production workflows can help ensure the authenticity of the data collected. ▲

11. When you are finished selecting items for the workflow and setting their associated options, choose OK.

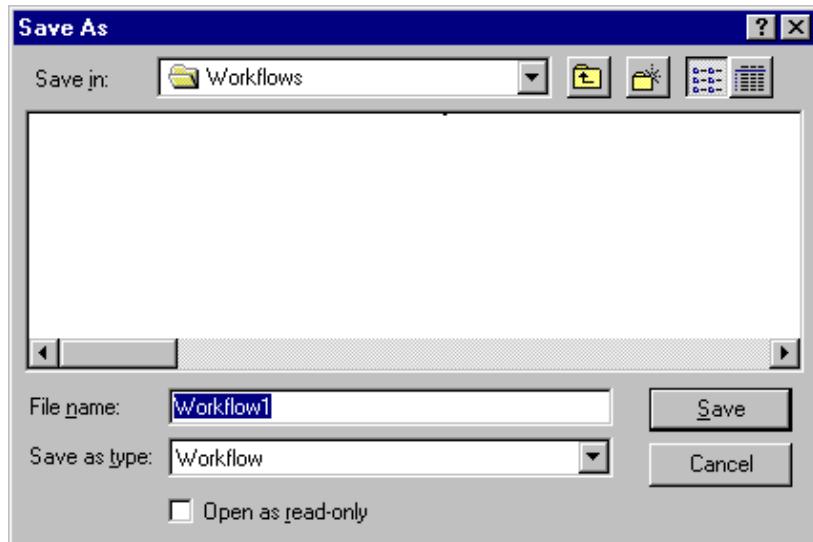
The wizard creates a workflow using the settings you specified. The workflow is displayed in the workflow navigation frame as shown in the example below.





12. Choose the Save button on the toolbar.

The Save As dialog box is displayed.



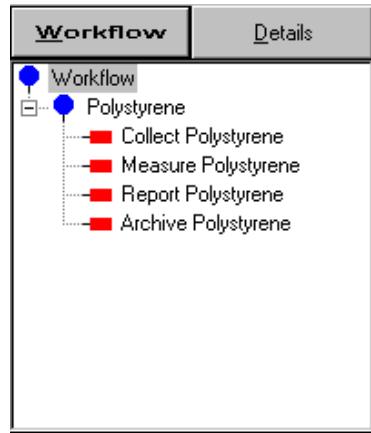
- 13. Select a folder for saving the new workflow or create and then select a new folder.**
- 14. Enter a descriptive name for the new workflow in the File Name box and then choose Save.**

The extension ".WFL" is automatically added to the file name.

After you choose Save, the file name for the new workflow appears in the title bar at the top of the RESULT Integration main window, as shown below.



Select the Expand button on the RESULT Integration toolbar to expand the workflow. The workflow contains the basic components to collect, measure, report, and archive spectral data, as shown below.



Use the Add button on the toolbar or the Add command in the Edit menu to add more events and specifications to the workflow. See “Adding Events And Specifications To A Workflow” in the next section for more information. You can also use the workflow wizard to add another collect, measure, report, and archive set to your workflow.

To run the workflow, use the Test button on the toolbar or choose Test Workflow from the File menu. See “Testing a workflow”

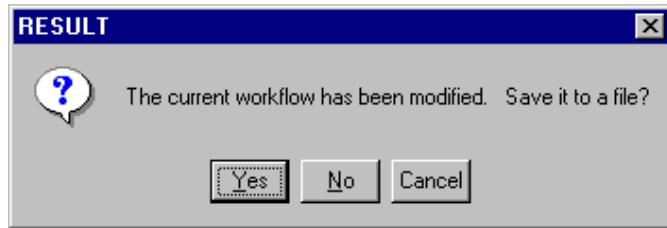
Using New Workflow to create a workflow

Use the New Workflow command to start a new workflow when you want to use the system’s default settings for the workflow events and their associated specifications. The New Workflow command clears the workflow navigation frame of workflow events and specifications. Events and specifications may be added to the workflow one item at a time or you may use the workflow wizard to add the basic components of a functional workflow (collect, measure, report and archive) in a single step.

To start a new workflow using the New Workflow command:

- 1. Start the RESULT Integration application and then choose New Workflow from the File menu.**

If the following message appears, choose Yes to save the open workflow before closing it.

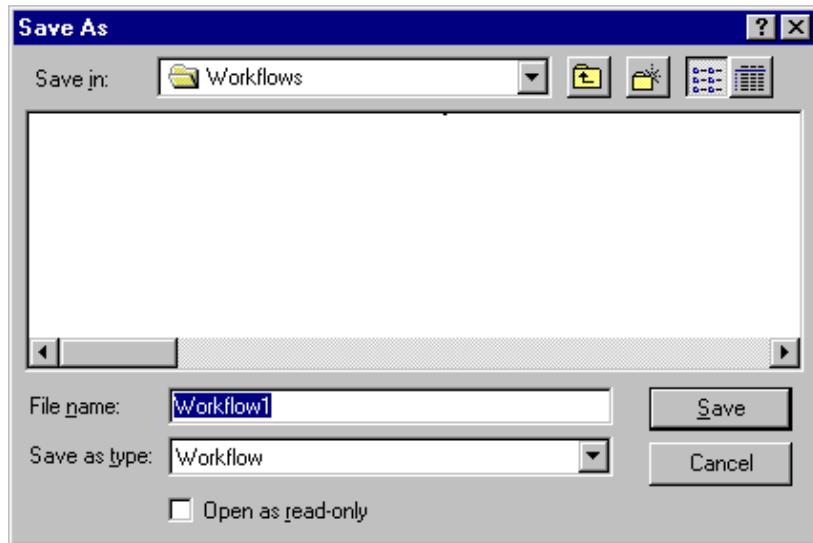


RESULT assigns the new workflow a default file name (Workflow1), which appears in the program's title bar, as shown below.



2. Choose the Save button on the toolbar.

The Save As dialog box is displayed.



Select a folder for storing the new workflow or create and then select a new folder.

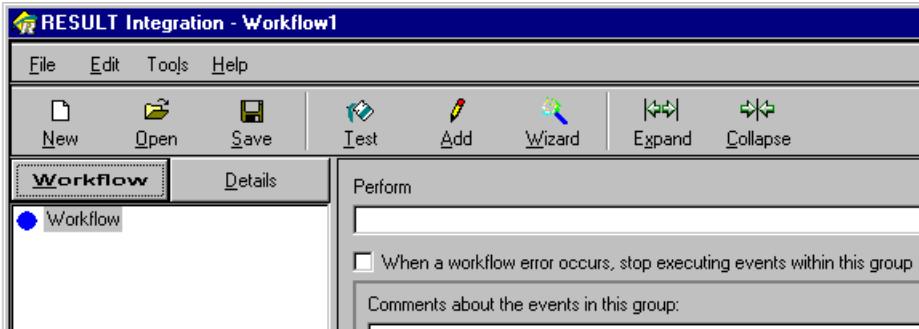
3. Enter a descriptive name for the new workflow in the File Name box and then choose Save.

The extension ".WFL" is automatically added to the file name.

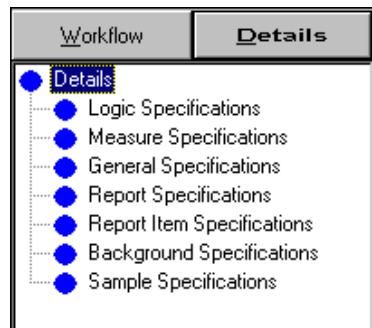
After you choose Save, the file name for the new workflow appears in the title bar at the top of the RESULT Integration main window, as shown below.



The workflow, displayed in the workflow navigation frame, consists of a single workflow group that contains no other items.



All of the groups in the specification tree are also empty.



Use the Add button on the toolbar or the Add command in the Edit menu to add events and specifications to the workflow. See “Adding events and specifications to a workflow” in the next section for more information.

You can also use the workflow wizard to add the basic components of a functional workflow (collect, measure, report and archive) in a single step. See “Using The Workflow Wizard To Create Or Add To A Workflow” in the previous section for more information.

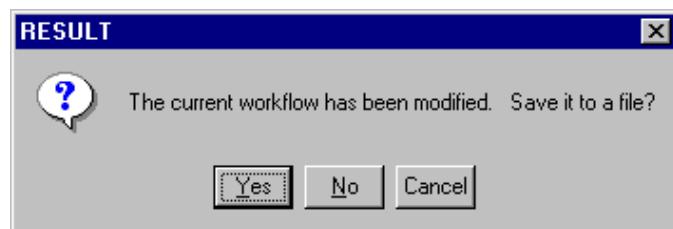
Using Open Workflow to create a workflow

Use the Open Workflow command to start a new workflow that will be similar to a workflow that already exists. Events and specifications may be added to the workflow one item at a time or you may use the workflow wizard to add the basic components of a functional workflow (collect, measure, report and archive) in a single step.

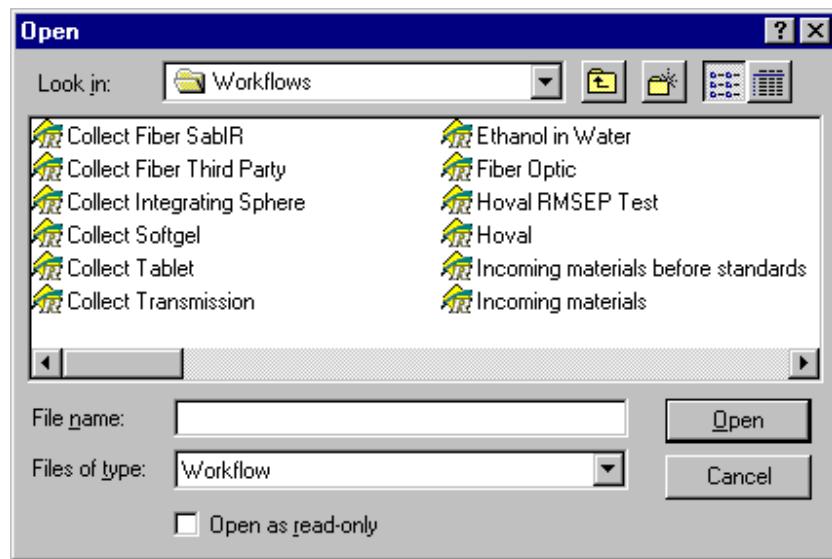
To create a workflow using the Open Workflow command:

- 1. Start the RESULT Integration application and then choose Open Workflow from the File menu.**

If the following message appears, choose Yes to save the open workflow before closing it.



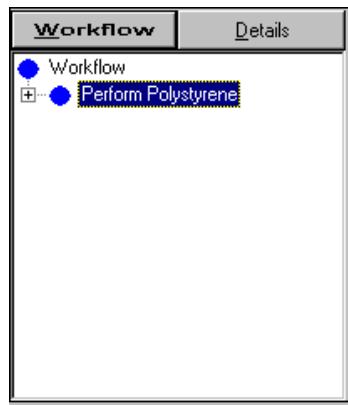
The Open dialog box is displayed listing the files in the default location for storing workflows.



See “Setting RESULT Integration Options” in “Chapter 1 Getting Started” for information about setting this and other directory paths in RESULT Integration software.

2. Select the workflow file and then choose Open.

You may need to change directories or disks to locate the file you want to open. When you choose Open, the software displays the contents of the selected workflow in the workflow navigation frame, as shown below.



3. Select the Save button on the toolbar.



The Save As dialog box is displayed.



4. Select a folder for storing the new workflow or create and then select a new folder.

5. Enter a descriptive name for the new workflow in the File Name box and then choose Save.

The extension “.WFL” is automatically added to the file name.

After you choose Save, the file name for the new workflow appears in the title bar at the top of the RESULT Integration main window, as shown below.



Use the Add button on the toolbar or the Add command in the Edit menu to add events and specifications to the workflow. See “Adding Events And Specifications To A Workflow” in the next section for more information.

You can also use the workflow wizard to add the basic components of a functional workflow (collect, measure, report and archive) in a single step. See “Using The Workflow Wizard To Create Or Add To A Workflow” in the previous section for more information.

Adding events and specifications to a workflow

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

Workflow specifications define how certain tasks will be carried out. The collect event, for example, has an associated sample and background specification, which define sample and background collection for a given sample type or material.

There are two ways to add events and specifications to a workflow. You can use the Add button on the RESULT Integration toolbar to add a specific event or specification, or you can use the workflow wizard to add the basic components of a functional workflow (collect, measure, report, and archive events and their associated specifications) in a single step.

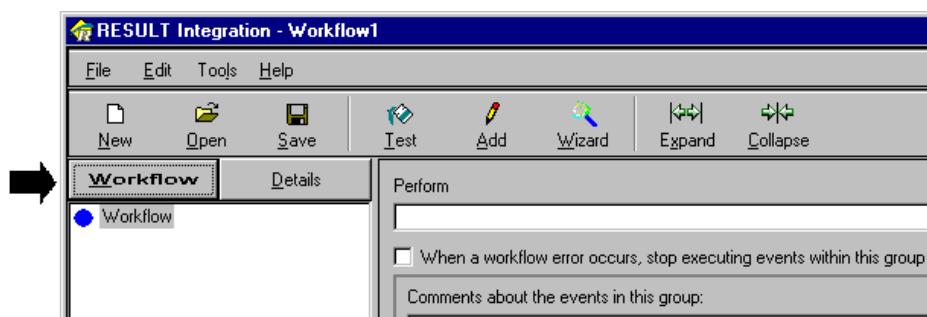
This section describes how to add events and specifications using the Add button on the RESULT Integration toolbar. See “Using the workflow wizard to create or add to a workflow” in the previous section to learn how to use the workflow wizard to add events and specifications to a workflow.

Adding 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 events to the workflow. The new event is added immediately below the selected event in the open workflow.

To add an event to a workflow:

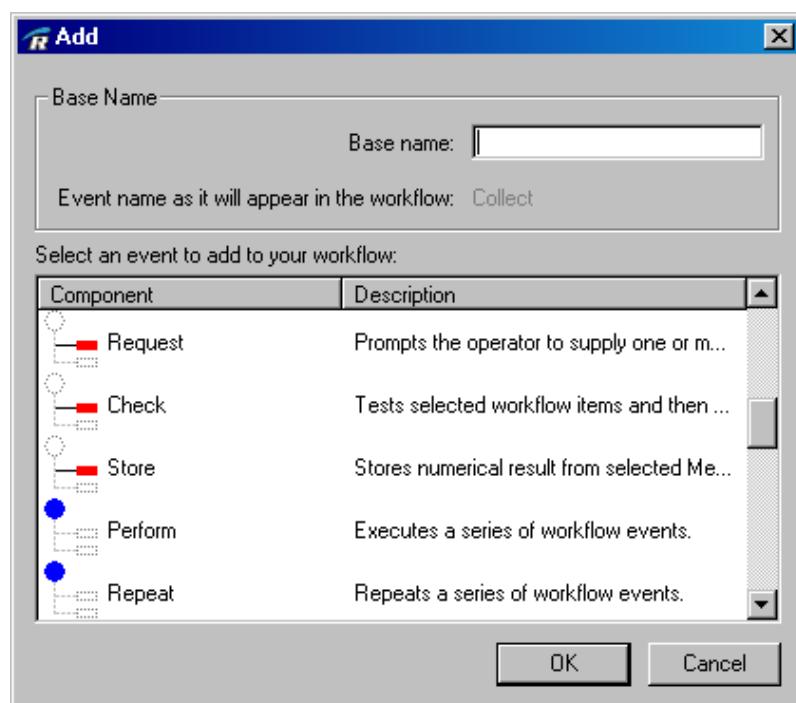
- 1. Create or open a workflow and make sure the Workflow tab is selected in the workflow navigation frame.**



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



A list of available events is displayed, as shown below.

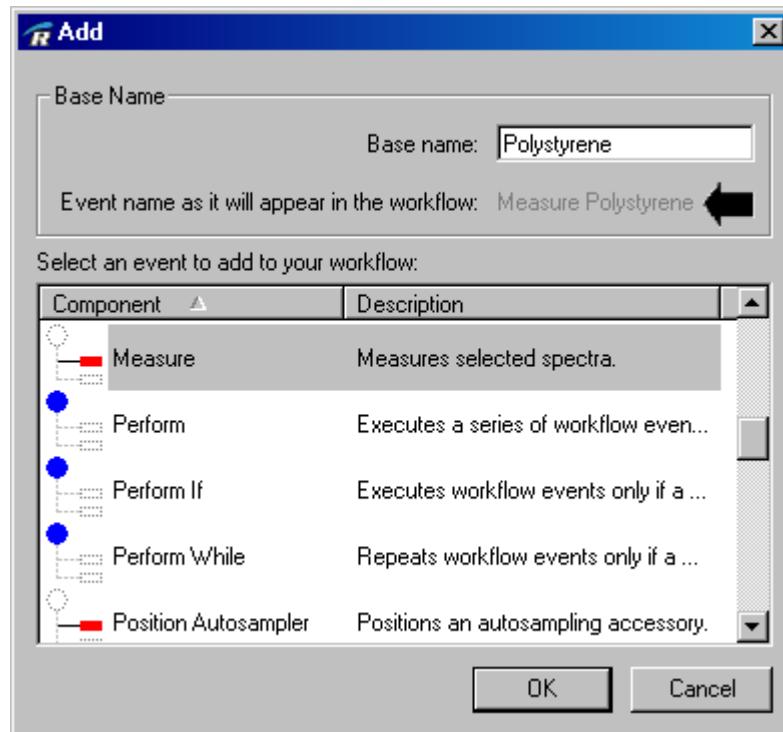


Notice that events are named with action words, such as “store” and “repeat.” The Description column explains the task the event will perform when you run the workflow.

Simple events, which carry out a specific task, are marked with a red rectangle. Structural events are marked with a blue circle. They allow you to group events in order to control how they will be implemented in the workflow.

3. Select an 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 will be appended to the event name. For example, if you select the Measure event and then enter the name “Polystyrene,” then the event will be named “Measure Polystyrene.” The software demonstrates how workflow events are named by showing the full name as you type. Here is an example:



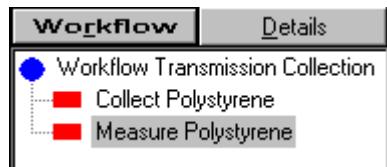
Note You must enter a base name before continuing. If you don't, the software displays an error message.



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.

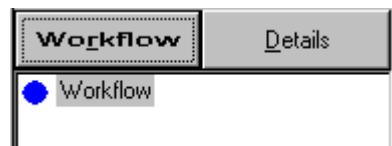
The new event is added immediately below the selected event in the open workflow. Here is an example showing a simple measure event added to a workflow:



Simple workflow events are marked with a red rectangle. Structural events have a blue circle because they create an event group. See “Chapter 1 Simple Workflow Events” and “Chapter 2 Structural Workflow Events” in “Workflow Events and Specifications” for more information.

Adding specifications to workflows

You may add a specification to a workflow from both the Workflow tab and the Details tab in the workflow navigation frame.



Workflow tab, Details tab

When you add a specification from the Workflow tab, the specification is automatically linked to the selected event. A workflow specification that is added from the Details tab is available for use in the workflow, but it will not be used by the workflow until the specification is linked to at least one workflow event.

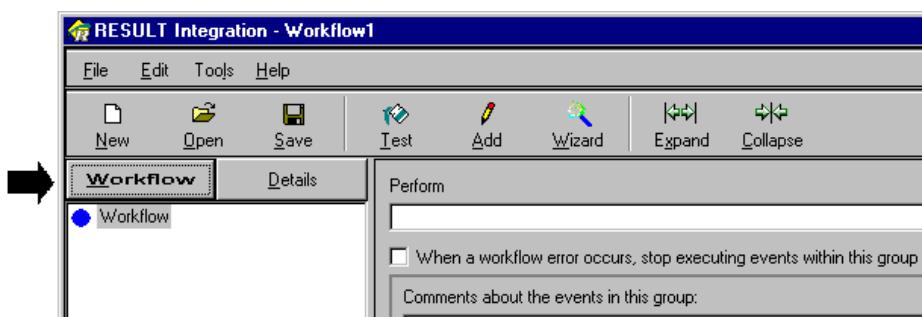
This section describes both methods for adding specifications to workflows. It also explains how to link a new or existing specification to a workflow event.

Adding a linked specification

If a workflow event requires a specification, use the New button next to the specification list box to create a new specification for that event. Specifications that are created this way are automatically linked to the workflow event.

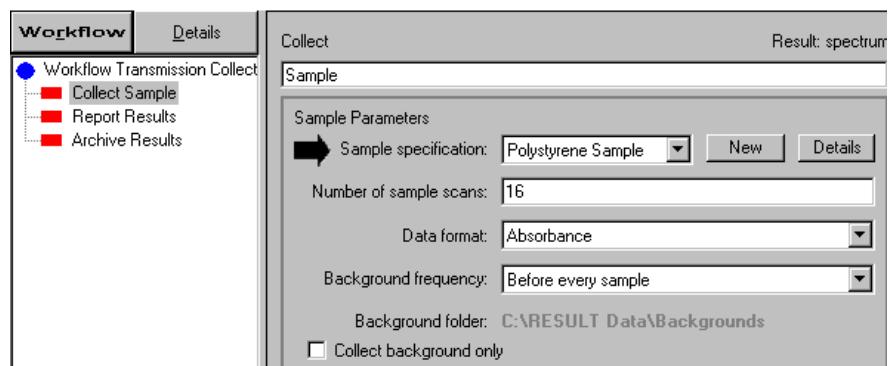
To add a specification that is linked to a workflow event:

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



- 2. Select the event that requires a specification in the workflow navigation frame.**

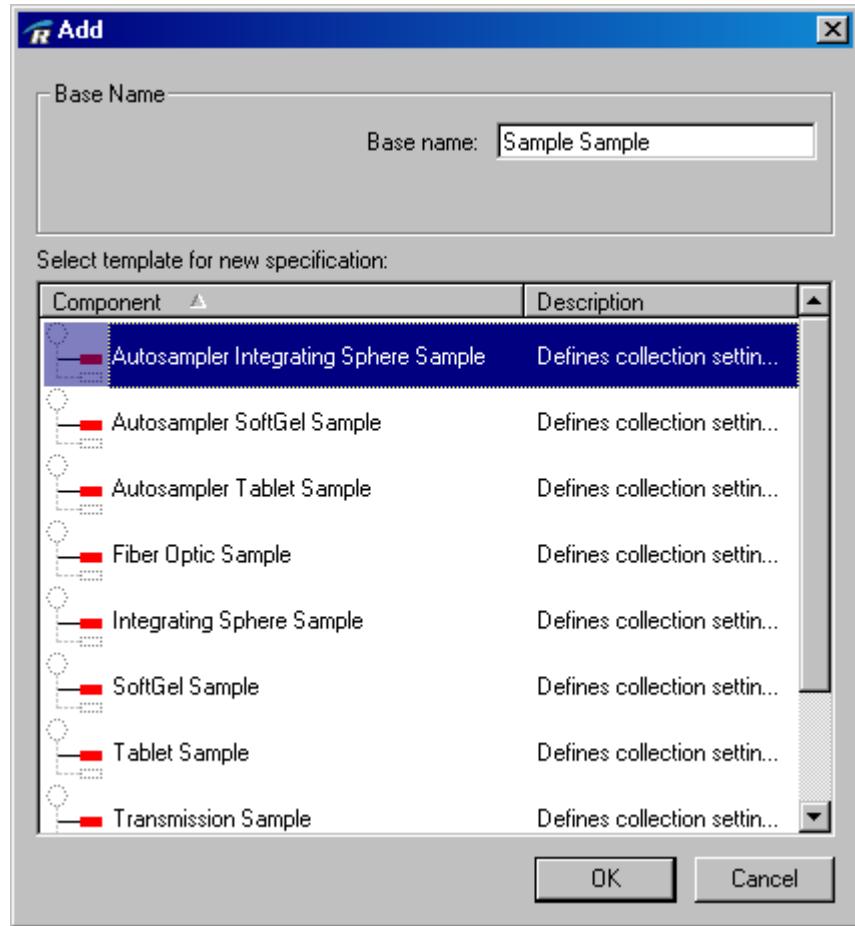
Here is a collect event that requires a sample specification:



3. Click the New button to the right of the specification list box.



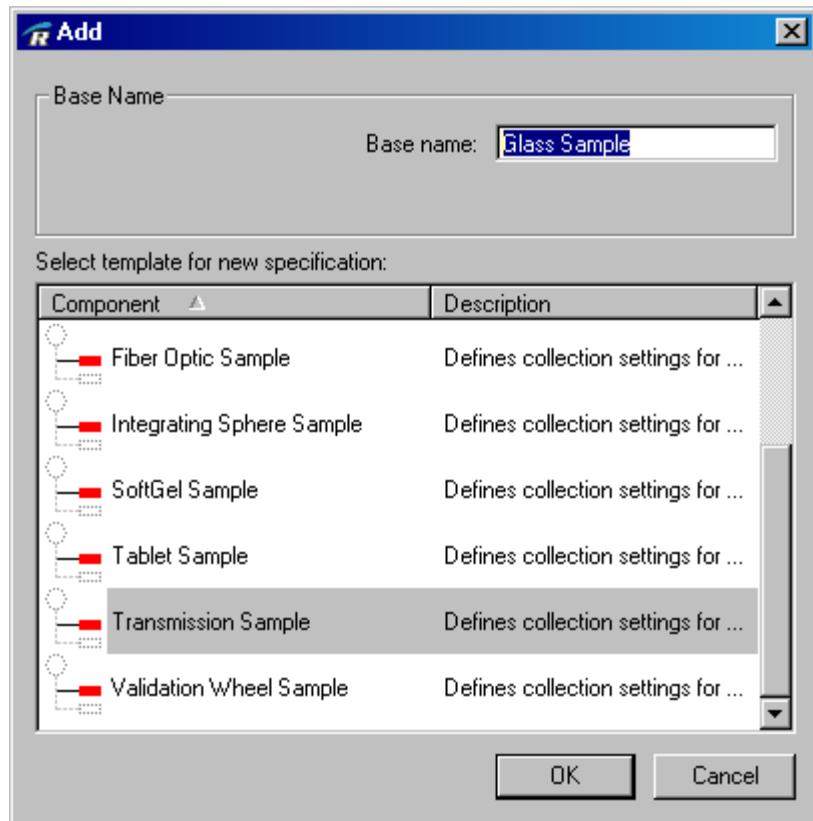
Depending on the specification type, a dialog box may appear showing the available options. Here are some of the sample specifications for the Antaris II systems:



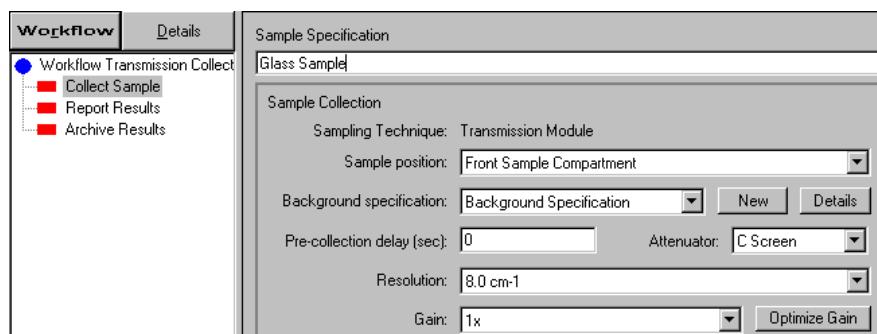
4. If a dialog box appeared in the previous step, select an appropriate specification for the current task, enter a base name for the new specification and then choose OK.

Here we've selected a transmission sample specification and entered the base name "Glass Sample."

If only one specification is available for the selected event, the software adds the appropriate specification automatically and gives it a default base name.



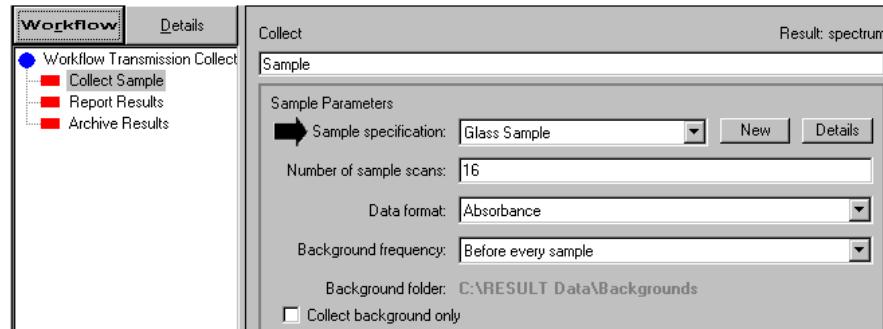
After you choose OK, the new specification appears in the display area. Here is the transmission sample specification:



The name "Glass Sample" appears in the text box at the top of the display area as shown in the above illustration. The default settings will be selected for all of the specification options. See "Workflow Events and Specifications" for information about customizing these settings for a particular sample.

5. Choose the Back button on the toolbar to return to the event.

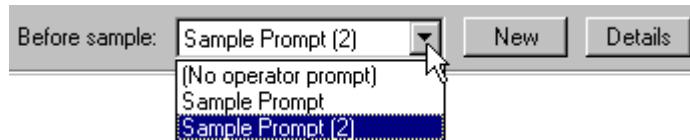
The specification name will appear in the list box. Here is the collect event with the sample specification named “Glass Sample” selected:



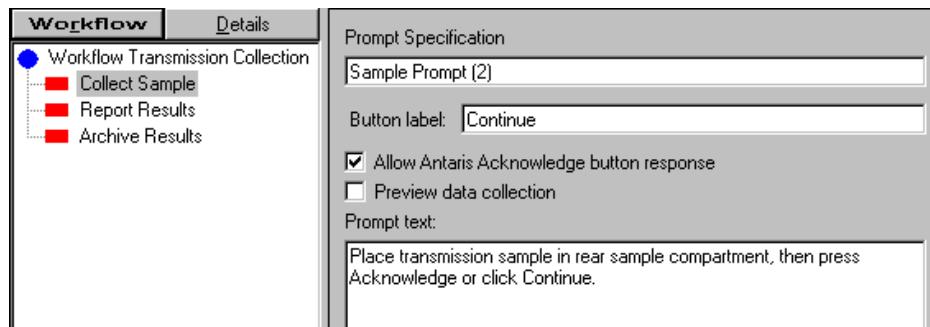
Use the Details button next to the sample specification list box to display the sample specification named “Glass Sample.” When the sample specification is displayed, use the Back button to return to the collect event.

Linking a specification to a workflow event

If your workflow already contains specifications that are appropriate for your task, use the specification drop down list box to select a specification. Here is an example showing several options for a Before Sample operator prompt for a collect event:



When the correct specification is selected, use the Details button next to the specification list box to show the selected specification in the display area. Here is the Before Sample prompt specification named “Sample Prompt (2)” shown in the display area:



When a specification is displayed, use the Back button to return to the associated event.

Adding an unlinked specification

When the Details tab is selected in the workflow navigation frame, you can use the Add button on the toolbar or the Add command in the Edit menu to add specifications to the workflow. You might want to add specifications this way because the new specification is similar to an existing one. You can easily make a copy of the existing specification and customize it for the new application.

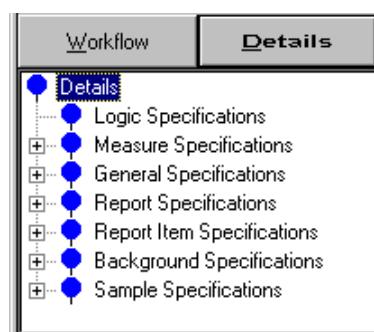
When you add specifications from the Details tab, those specifications are not automatically linked to a workflow event. See “Linking a specification to a workflow event” in the previous section for instructions to link an existing specification to a workflow event.

To add a specification to a workflow:

- 1. Create or open a workflow.**

- 2. Select the Details tab in the workflow navigation frame.**

The specification tree appears in the workflow navigation frame, as shown below.



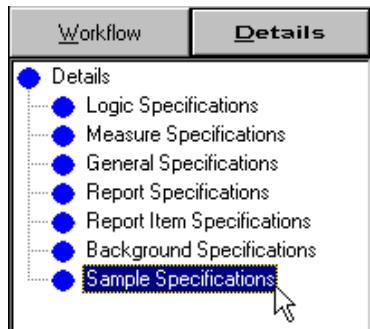
The specification tree shows the types of specifications that can be added to a workflow. The specifications are grouped by function.



Use the Expand and Collapse buttons on the toolbar to show or hide the specifications in all of the groups.

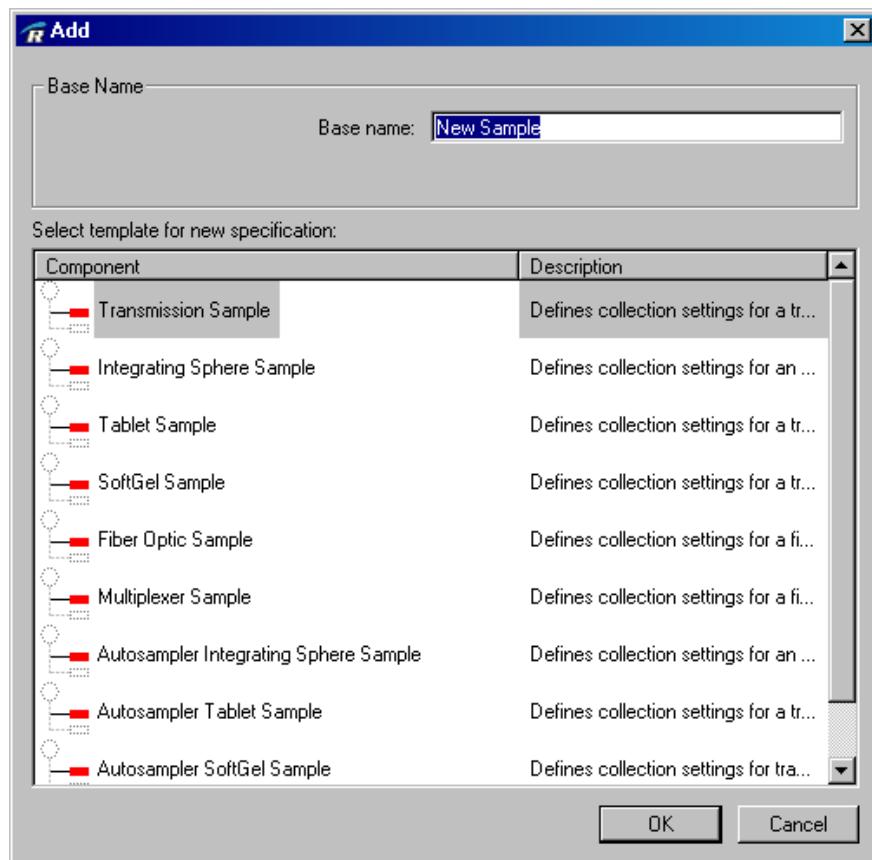
3. Select the specification group that corresponds with the type of specification you want to add to the workflow.

To add a sample specification, for example, select the Sample Specifications group on the Details tab, as shown below:



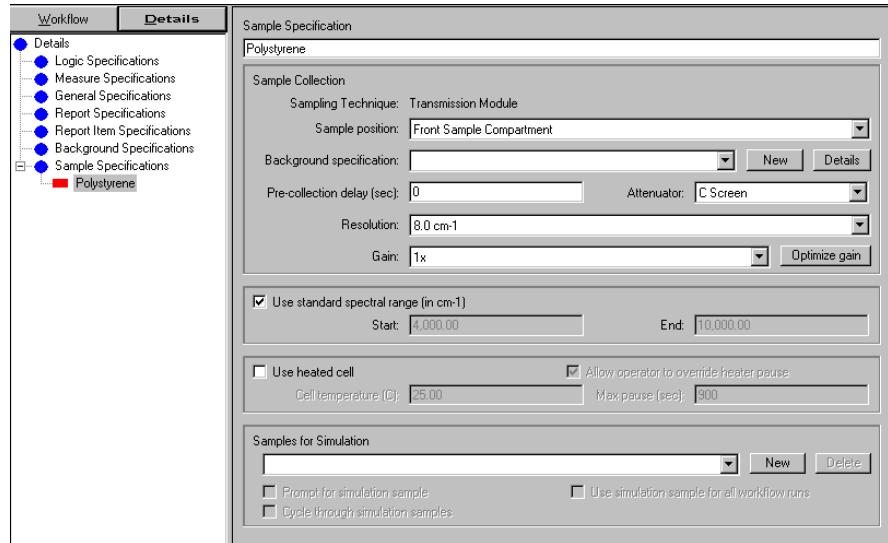
4. Choose Add from the Edit menu or choose the Add button on the toolbar.

Depending on which specification group is selected, a dialog box may appear showing the specifications available in the selected group. Here is an example of the Add dialog box showing the available sample specifications:



5. If a dialog box appeared in step 4 above, select a specification and then choose OK to close the dialog box.

The specification group is automatically expanded to show the name of the new specification. The options for the new specification appear in the display area. Here is the Transmission Sample Specification shown in the display area:



The new specification is given a generic name, which appears in the text box at the top of the display area. The default settings are selected for all of the specification options. See “Workflow Events and Specifications” for information about setting the options for a sample specification, or another specification in RESULT Integration.

Note The new specification is available for use only in the open workflow. However, it will not be used by the workflow until the specification is linked to at least one workflow event. See the next section to learn how to link workflow specifications to workflow events. ▲

Using a sampling sequence with a workflow

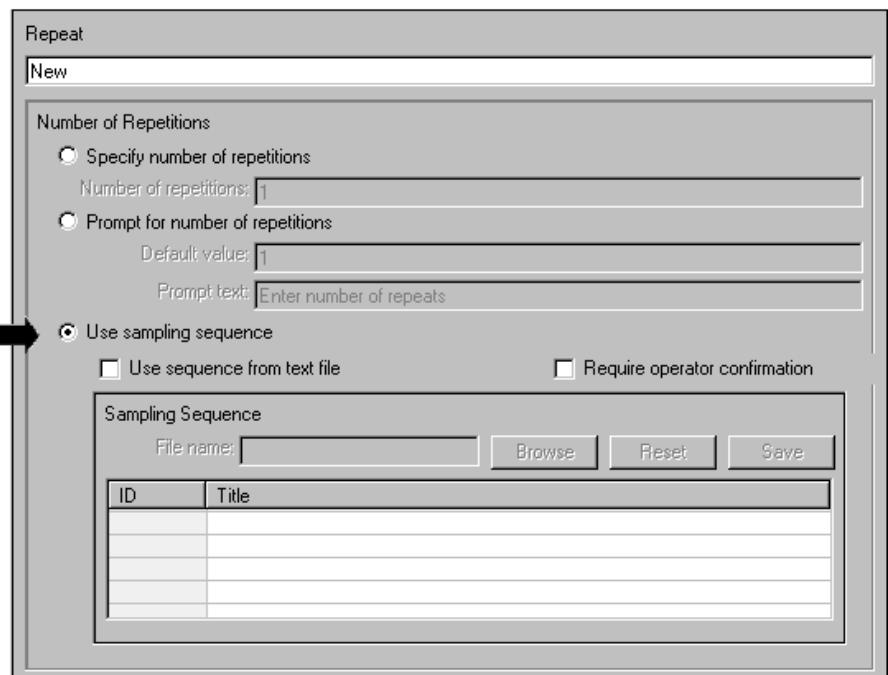
RESULT workflows can be configured to require a sampling sequence to define the order, title and any other information required for a set of samples. This is useful for running an autosampler or for running a series of samples manually without requiring the operator to enter information about each sample at run time.

The sampling sequence must specify a sample name and identification (ID) number, or position number if using an autosampler, for each sample. The sampling sequence can include other information in text or numeric format as needed.

The workflow can specify that the sampling information must be entered manually or imported from a text file with or without operator input. You can create a sampling sequence and save it in the workflow, or create or specify a sampling sequence text file. The workflow controls whether the operator can view, select, create or edit the sampling sequence at run time.

To set up a workflow to use a sampling sequence:

- 1. Add a repeat event to the workflow.**
- 2. In the repeat event, set Number of Repetitions to Use Sampling Sequence, as shown below.**



- 3. Specify the following options for defining the sampling sequence.**

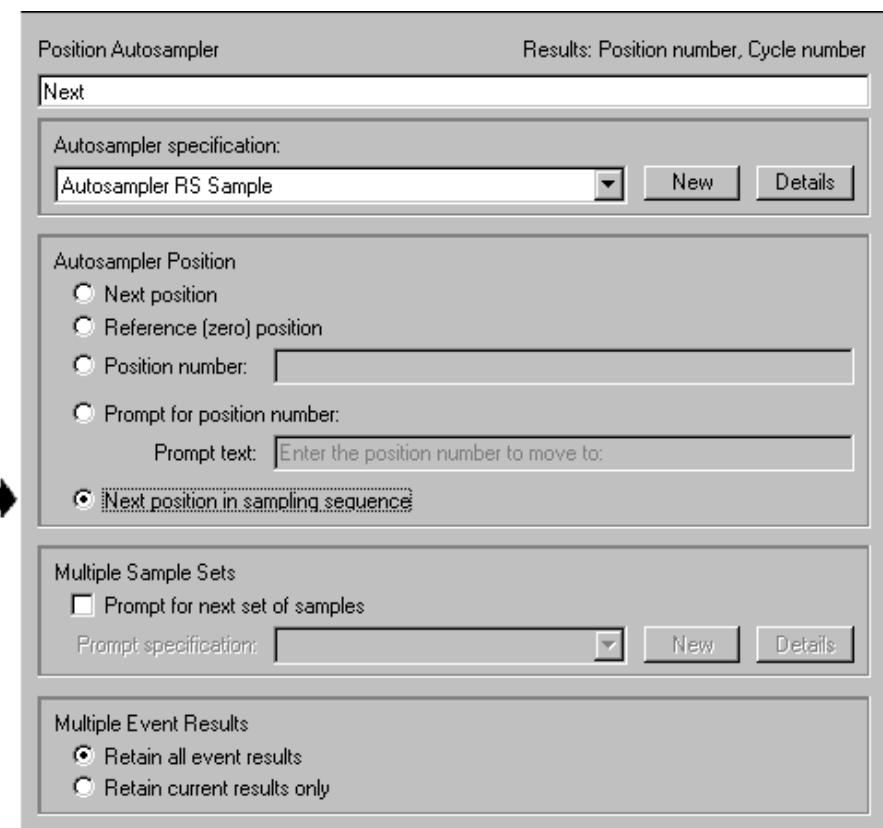
- Use Sequence From Text File.** Use this checkbox to specify a location for storing the sampling sequence.

To use a sampling sequence stored in a text file on the computer disk, select Use Sequence From Text File. 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 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 software. If the specified file does not exist or contains an error, the workflow will prompt the operator to enter a sampling sequence or select a sequence file at run time. Using a text file to store the sampling information allows you to create the file at another computer and

easily copy and reuse the sequence in multiple workflows, or quickly switch the sampling sequence in the current workflow.

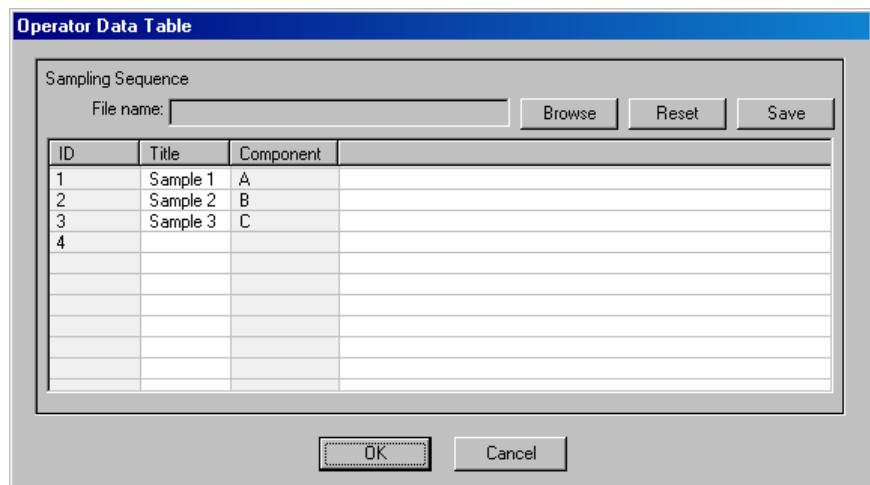
To store the sampling sequence in the workflow, clear Use Sequence From Text File. You must use the Sampling Sequence group in the Repeat event to create the sampling sequence (see “Creating a sampling sequence” in the next section for details. The sampling information will appear and be saved in the workflow.

- **Require Operator Confirmation.** Use this check box to specify whether the operator can view and edit the sampling sequence at run time or select another text file that contains the correct sampling sequence.
4. If you are using an autosampler, add a position autosampler event to the repeat loop and set Autosampler Position to Next Position In Sampling Sequence.



When you run the workflow, if the repeat event is set up to use a sampling sequence with operator interaction (i.e., Require Operator

Confirmation is selected), the first pass through the repeat loop will display the following dialog box:



If Use Sequence From Text File is cleared, the dialog box contains the sampling information saved with the workflow. If Use Sequence From Text File is selected, the dialog box contains the sampling information in the specified text file.

If the sequence displayed in the dialog box is correct, the operator simply chooses OK and the workflow continues. If the displayed sequence is incorrect, the operator can either edit the displayed information or create or import a new sampling sequence (see the next section). When the operator is satisfied with the sampling sequence, he or she chooses OK and the workflow continues.

At a minimum, the sampling sequence should specify a sample name and ID, or position number if using an autosampler, for each sample. The workflow will implement the events in the repeat loop once for each line in the sampling sequence. See “Creating a sampling sequence” and “Importing a sampling sequence” in the sections that follow for more information.

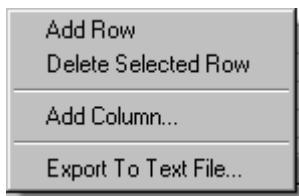
Creating a sampling sequence

Read this section to learn how to create and save a sampling sequence with a workflow. The workflow must contain a repeat event that is set up to use a sampling sequence (see the previous section).

Follow the instructions below to use the Repeat event to create a sampling sequence. If you want to learn how to import a sampling sequence to a workflow, skip to the next section.

To create and save a sampling sequence in a workflow:

1. **Display the Repeat event that will be used to initiate the sampling sequence.**
2. **Add a row to the table and enter a sequence number for the corresponding sample.**



To add a row, right click any row in the table to display a shortcut menu. Then choose Add Row. The software automatically assigns the new row the next available ID number (or Position number, if using an autosampler). You can edit the ID or Position number by double-clicking the field. Only integer values are accepted.

You can enter the position and ID numbers in any order. However, each row must contain an entry for this field. The ID or Position number will be saved along with the spectral data at run time.

If using an autosampler, the carousels typically start with position 0. However, depending on the workflow, position 0 may be reserved for background collections (see “Autosampler specifications” in your autosampler user’s guide for more information). If the workflow is configured to reserve position 0 for background collections, your first sample is probably located in position 1 or greater.

Notice If you are defining a sampling sequence for an autosampler, make sure the position number you enter in this dialog box matches the location of this sample in the autosampler carousel. ▲

3. **Enter a title for the sample in the Title text box.**

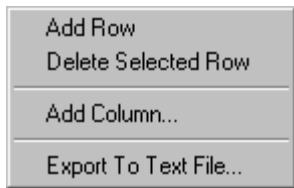
To enter a title for a sample, double click the Title field for the corresponding sample ID number (or position number if using an autosampler).

Each row must contain an entry for this field. The titles will be saved along with the spectral data at run time.

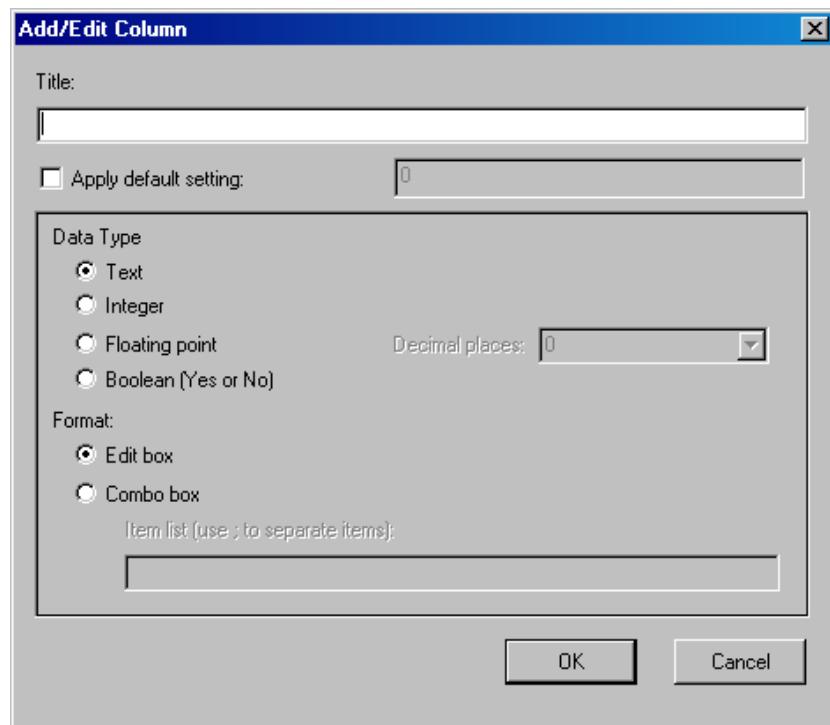
Note The title is a descriptive name saved within a spectral file; it is not the file name. ▲

4. If you have additional information you want to include for each sample such as a special code or comment, add a customized column to the table and enter the corresponding information in the specified format.

Information you add to a sampling sequence can be used in other places in the workflow such as a Report event or Report To Spectrum event.



To add a column, right click a row in the table to display a shortcut menu. Then choose Add Column. The software displays the following dialog box.



The following options are available:

- **Title.** Enter a descriptive heading for the information you want to add to the table. You cannot leave the Title field blank. When you close the dialog box, the title will appear as the heading for the new column in the sampling sequence table.

- **Apply Default Setting.** Select this check box if you want to apply a default value or setting for all the cells in the column. Then enter the default value or setting in the corresponding entry box. For example, you can set the initial value for integer or floating point cells to 0 or the initial setting for a Boolean toggle to “No.”
- **Data Type.** Use these radio buttons to indicate the type of data you want to enter for the fields in this column of the table. Text refers to a text string. The string can include any combination of letters, numbers, and other characters available from the computer keyboard or other input device. The Integer setting allows only positive whole numbers. If you want to enter fractions, use the Floating Point setting and then enter the number of digits you want to include to the right of the decimal point. Use the Boolean setting to define cells that toggle between Yes and No.
- **Format.** Use these radio buttons to specify a format for the column cells. The Edit Box setting defines an editable field. The Combo Box setting defines a drop-down list box.

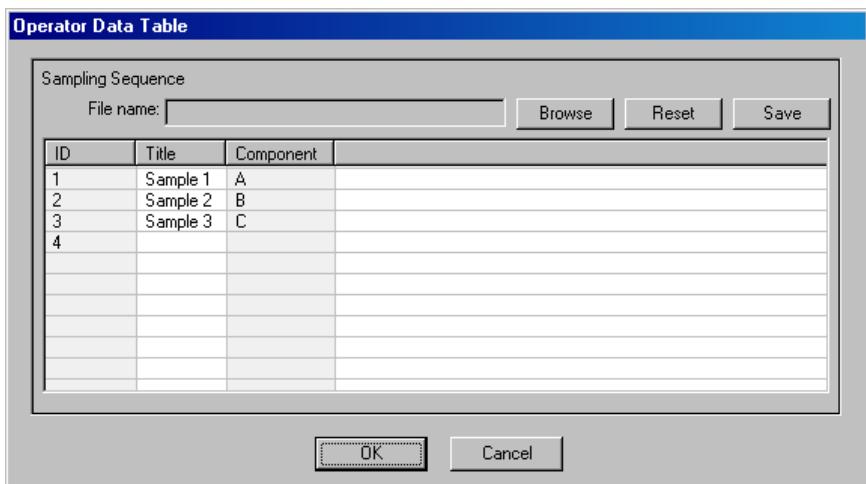
Use the Item List entry box to specify the items in the drop-down list for the combo box and separate your entries with a semi-colon character. For example, to define a drop-down list box with three items in the list (e.g., Yes, No, and Maybe), the Item List should look like this:

Item list (use ; to separate items):
Yes;No;Maybe

You can edit these settings at any time by double clicking a field in the custom column. The custom column fields are optional. The information in a custom field will be available for use by other events in the workflow such as a Report event, Report To Spectrum event, or Report To Text event.

5. Repeat steps 2 through 4 for each sample in the sequence.

The number of entries in your sampling sequence should match the number of samples you want to analyze.



The following additional options are available for editing the information displayed in the table.

- To delete a row from the table, select the row, right click to display a shortcut menu and choose Delete Selected Row or press Delete on the keyboard. To delete several rows at once, hold down the Shift key while you click sequential rows (or the Control key for split rows) and then choose Delete. To delete a column, select the column, right click and choose Delete Selected Column or press Delete on the keyboard.
 - To change the order of the entries in your sampling sequence, click a row in the table and drag it to the new location. To move several rows at once, hold down the Shift key while you click sequential rows (or the Control key for split rows) and then drag the selected rows to the new location.
 - You can sort numeric and alphabetic data displayed in the table in ascending or descending order. To sort the table based on a specific column, select the column, right click to display a shortcut menu and choose Sort Descending or Sort Ascending.
 - You can export the sampling information displayed in the table to a text file. This can be helpful if you have a specific format you like to use for sampling sequences. You can then import a pre-formatted sampling sequence when creating workflows for other experiments. See “Exporting a Sampling Sequence” in the next section for details.

6. Save the sampling sequence with the workflow.

To save the new sampling sequence in the workflow, choose Save from the File menu in RESULT Integration software.

Importing a sampling sequence

Creating a text file that contains a sampling sequence

Read this section to learn how to create a text file that contains a sampling sequence you can import to a RESULT workflow, and how to import the sampling information from your text file.

This section explains how to use a text editor application to create a sampling sequence you can use with RESULT software. This gives you the option to create the sampling sequence on any computer and easily import the sequence to a RESULT workflow.

You can also create a sampling sequence in RESULT software and save or export the sampling information to a text file. See “Creating a sampling sequence” in the previous section and “Exporting a sampling sequence” in the next section for more information.

Text files can be created in any word processing, spreadsheet, or text editor application such as Microsoft® Word, Microsoft Excel® or NotePad. Make sure you use tabs rather than spaces to separate the columns and save the file using the *.txt file name extension. (If you use Excel, export the file as tab-delimited text and it will add the tabs for you.)

The text file must contain at least two columns separated by tabs. The first column should contain the sample identification (ID) number or carousel position number if you plan to use an autosampler. The second column should contain the corresponding sample name. Additional columns of data can be included.

Additional information and an example text file are provided below.

- **Sample ID or Position Number.** The sample ID can be a number, letter or any other character representing sample index numbers, sequence numbers, bar code numbers, etc. and they can be in any order.
- If you are using an autosampler, the position number is required and must be an integer. Thermo Scientific carousels typically start with position 0. However, depending on the workflow, position 0 may be

reserved for background collections (see “Autosampler specifications” in your autosampler user’s guide for more information). If the workflow is configured to reserve position 0 for background collections, your first sample is probably located in position 1 or greater.

Notice If you are defining a sampling sequence for an autosampler, make sure the position numbers you enter in the text file match the locations of the samples in the autosampler carousels. ▲

- **Sample Title.** The second column should contain a descriptive title for each sample. The titles are saved along with the spectral data.

The following text file could be used to import a sampling sequence for manual operation:

001681	{tab}	Sample a
001749	{tab}	Sample f
001853	{tab}	Sample i
001992	{tab}	Sample l
002501	{tab}	Sample o
003695	{tab}	Sample x

This one could be used for an autosampler:

1	{tab}	Sample a	Rep1
1	{tab}	Sample a	Rep2
2	{tab}	Sample b	Rep1
2	{tab}	Sample b	Rep2
3	{tab}	Sample c	Rep1
6	{tab}	Sample d	Rep1
8	{tab}	Sample h	Rep1
10	{tab}	Sample j	Rep1

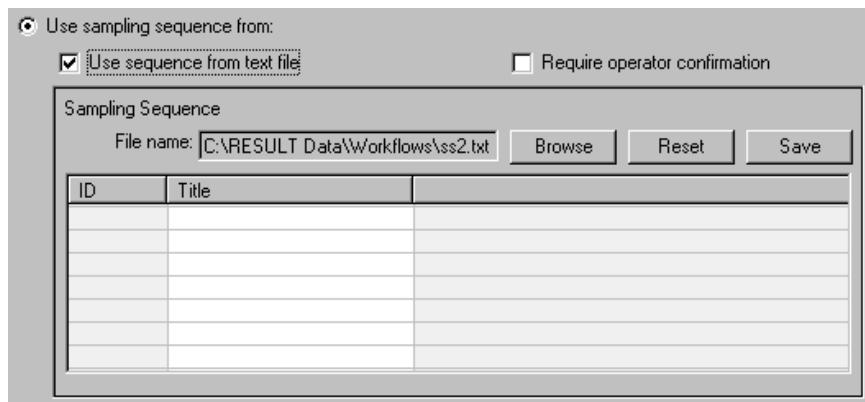
Importing a sampling sequence from a text file

Follow the steps below to import a sampling sequence from a tab-separated text file. For information about creating the text file, see the previous section.

Before you can import a sampling sequence to a workflow, you must add a Repeat event to the workflow, set Number of Repetitions to Use Sampling Sequence, and select Use Sequence From Text File.

To import a sampling sequence from a text file:

1. In the Repeat event Sampling Sequence group, select Use Sequence From Test File and then choose Browse.



The Open dialog box is displayed.

2. Locate the folder and file you want to import.

You can only import text files (*.txt file name extension). Text files can be created in any word processing, spreadsheet or text editor application such as Microsoft Word, Microsoft Excel or NotePad. The file must be formatted with tab-separated text like the examples shown in the previous section.

3. Choose Open.

The file name appears at the top of the Sampling Sequence group and the sampling information contained in the file appears in the table below the file name.

Sampling Sequence	
File name: C:\RESULT Data\Workflows\ss2.txt	
ID	Title
1	Sample C
2	Sample D
3	Sample E
4	

You can edit the sampling sequence you just opened and easily resave it. Use the features below:

- **Add/delete row.** Select any row in the table and then right click to display a shortcut menu that contains options to add and delete rows in and add columns to the table. See “Creating a sampling sequence” above for information about the Add/Edit Column dialog box.
- **Edit/delete column.** Select any column in the table and then right click to display a shortcut menu that contains options to edit, delete and sort columns in the table. You can sort numeric and alphabetic data in ascending or descending order. See “Creating a sampling sequence” for information about the Add/Edit Column dialog box.
- **Move Row.** To change the order of the entries in your sampling sequence, click a row in the table and drag it to the new location. To move several rows at once, hold down the Shift key while you click sequential rows (or the Control key for split rows) and then drag the selected rows to the new location.
- **Reset.** If you edit a sampling sequence you imported and decide not to keep your changes, you can use the Reset button above the table to display the contents of the original file.
- **Save.** Use the Save button above the table to save your changes to the displayed sampling sequence. You can save the changes in the original file or create a new file and leave the old file unchanged. To save the changes in the original file, select the file name in the Save dialog box and then choose Save. To save the changes in a new file, enter a file name in the File Name box and then choose Save.

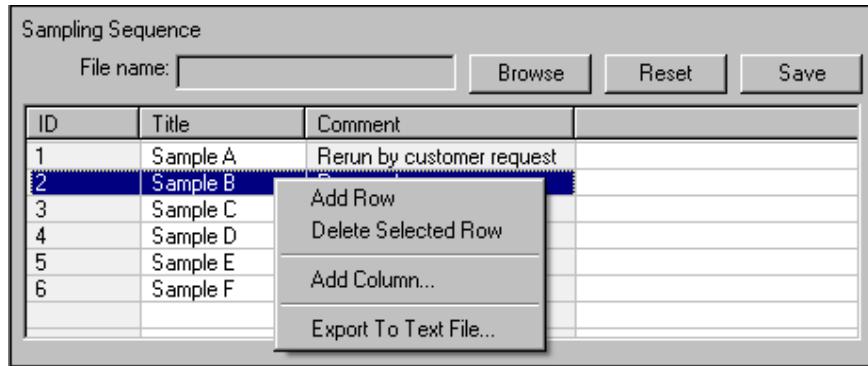
Exporting a sampling sequence

Follow the steps below to export a sampling sequence from a workflow to a text file. Using a text file to store the sampling information allows you to create the file at another computer and easily copy and reuse the sequence in multiple workflows, or quickly switch the sampling sequence in the current workflow. The workflow must contain a Repeat event that is set up to use a sampling sequence (i.e., Number of Repetitions is set to Use Sampling Sequence).

Export To Text File gives you the option to save the sampling sequence information outside the workflow. The contents of the table in the Sampling Sequence group, including any columns you added, is saved in a tab-separated text file (.TXT extension) with the file name you specify.

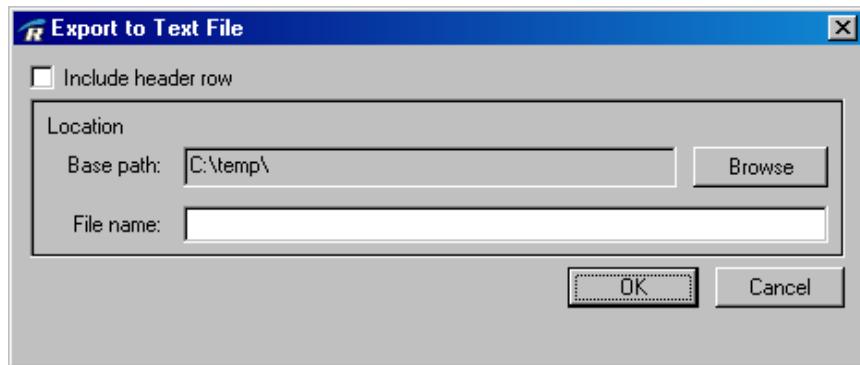
To export a sampling sequence:

1. Right click the table in the Sampling Sequence group.



2. Choose Export To Text File in the shortcut menu.

RESULT displays the following dialog box:



3. Enter a file name for the exported file in the File Name box.

4. Use the Browse button to locate and select a folder for saving the exported file.

5. If you want the table headings to be saved with the data, make sure Include Header Row is selected.

6. When you are finished, choose OK to create the text file.

If Microsoft Excel is installed on the computer, RESULT tries to open the text file in Excel. If you see an error message indicating the file is not in a recognizable format, ignore it and choose OK to display the file's contents.

Note Using the Export To Text File option does not affect the status of the workflow. For example, if the sampling information is saved with the workflow, choosing Export To Text File creates a text file that contains the sampling information but does not associate the text file with the workflow. ▲

Editing a workflow

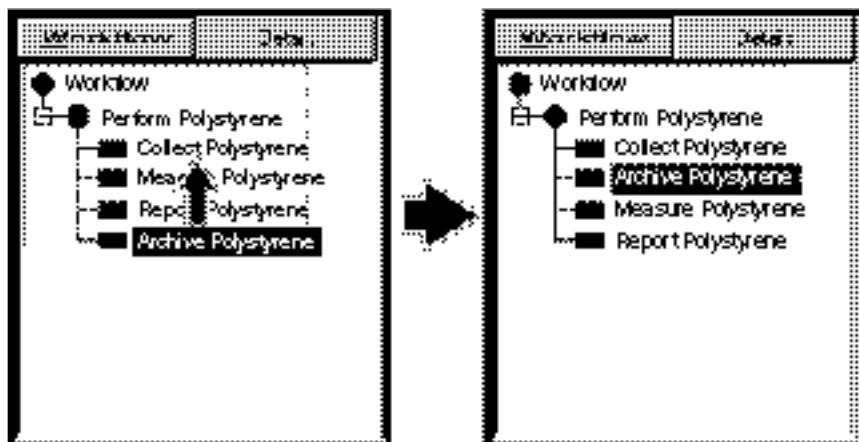
When you run a workflow, the software carries out the events in the order in which they appear in the workflow navigation frame when you display the workflow in RESULT Integration software. You may add and delete workflow events and their associated specifications, arrange them in any order, and move them in and out of event groups. This section explains how to use the commands in the Edit menu and the drag and drop features of RESULT Integration software to add, delete and arrange events to create functional workflows.

Note You cannot edit event and specification names as they are displayed in the workflow navigation frame. To edit the name of an event or specification, select the event or specification in the workflow navigation frame and then edit the name as it appears at the top of the parameters shown in the display area. ▲

Arranging events in a workflow

RESULT Integration software provides Windows drag-and-drop capabilities in the workflow tree, allowing you to easily arrange the events in a workflow.

To move an event, use the mouse to select the event name in the workflow tree and then hold down the mouse button while you drag the item up or down in the list of events.



Drag and drop feature of the workflow tree

To place the event in a specific location in the workflow tree, drag the event to the workflow event that is immediately above the target location. That event should now be highlighted in the workflow tree. Leave the event highlighted while you release the mouse button. The “dragged” event will appear immediately below the highlighted event.

To place the event in an event group, drag and then drop the event on the highlighted event group. The dragged event will be added to the end of the group.

If you want to place the event immediately after (but not in) an event group, drag the event to the highlighted event group and then hold down the Shift key on your keyboard while you release the mouse button. The dragged event will appear immediately below (but not in) the group.

To move an event to the first position in an event group, drag the event to the second position and then drag the first event down to the second position.

Note The drag and drop features do not operate on the specification tree. The positions of the specification groups are fixed and the sequence of the specifications within a group is not relevant to the operation of the workflow. ▲

Moving between screens in a workflow



RESULT Integration software provides tools to help you easily select a previous screen in a workflow.

Use the Back command in the Edit menu to return to the previous screen in the open workflow. The Back command is also available as a button in the RESULT Integration toolbar. After you use the Back command in the Edit menu or the Back button on the toolbar, the Forward command or button becomes available in the software.



Use the Forward command in the Edit menu to return to the screen that was displayed the last time you used Back. The Forward command is also available as a button in the RESULT Integration toolbar.

Cutting items from a workflow

The Cut command in the Edit menu removes the selected event or specification from the open workflow and places the cut item onto a clipboard (replacing the previous contents, if any exist). After you cut an event, you can use Paste to place a copy of the event in another location in the open workflow, or into another workflow. (If you shut off your computer, the cut item will be erased.)

Specifications that have been cut may be pasted back into their original location on the Details tab or into another workflow.

Tip

If a cut event produces results that are used elsewhere in the workflow, you must select each dependent event and/or specification so the software can update them by removing the result for the item that was cut. If the dependent items aren't updated, the workflow may produce errors when you run it, since the dependent events and specifications will be unable to locate the results that were removed. □

Copying items to the clipboard

The Copy command in the Edit menu places a duplicate of the selected event or specification onto a clipboard (replacing the previous contents, if any exist). After you copy an event, you can use Paste to place a copy of the event in another location in the open workflow, or into another workflow. (If you shut off your computer, the copied item will be erased.)

Specifications that have been copied may be pasted back into their original location on the Details tab or into another workflow.

If a copied event has associated specifications, the duplicate event will have the same associated specifications as the original.

Pasting items from the clipboard

After you cut or copy an event or specification, a duplicate of the cut or copied item is on a clipboard. Use Paste in the Edit menu to place a copy of the item in a specified location in the open workflow, or into another workflow. (If you shut off your computer, the cut or copied item will be erased.)

Pasted events are placed after the selected (highlighted) event or, if an event group is selected, after the last event in the group. Specifications that have been cut or copied may be pasted back into their original location on the Details tab or into another workflow.

The pasted event or specification is an exact copy of the item that was cut or copied to the clipboard. For example, if a cut or copied event has associated specifications, the pasted event will have the same associated specifications as the original.

If you paste copied items back into the same workflow, the software appends a number to the item name to indicate that it is a copy of another item in the workflow. For example, if you copy a Collect Polystyrene event and then paste one or more copies back into the same workflow, the copied items will be named Collect Polystyrene (1), Collect Polystyrene (2), etc., so you can tell them apart.

If the copied event produces results that are used elsewhere in the workflow, the duplicate event will produce similar results but those results will not be used by other events in the workflow until you add the results to those events.

You can continue to paste copies until you cut or copy another selected item or turn off your computer.

Tips on pasting items in workflows

- An item that is on the clipboard remains there until you use Cut or Copy again. If you turn off your computer, the contents of the clipboard are erased.
- You may not paste cut or copied items into other applications.

Deleting items from a workflow

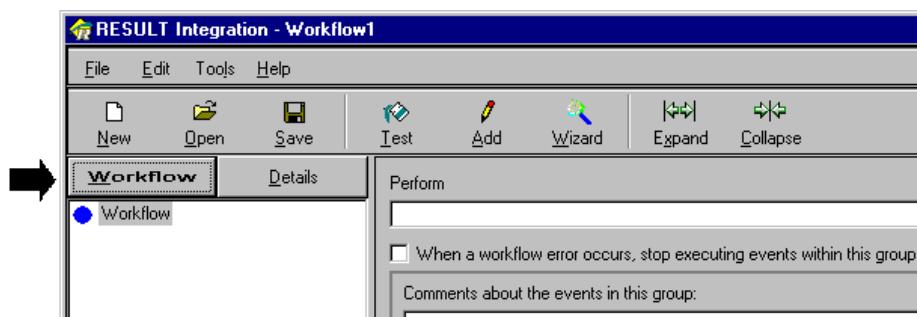
Use Clear in the Edit menu to delete the selected event or specification from the open workflow. Unlike cutting items with Cut, clearing an item does not place a copy of it on the clipboard.

If a deleted event is linked to one or more specifications, those specifications will not be deleted along with the event.

How to delete items from a workflow:

- 1. Make sure the appropriate tab is selected in the workflow navigation frame.**

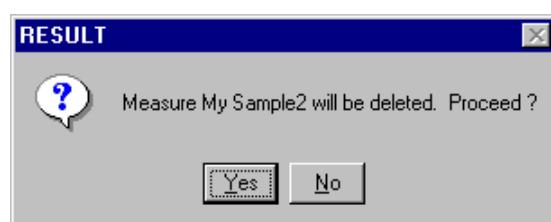
If you want to delete an event, select the Workflow tab, as shown below.



To delete a specification, select the Details tab.

- 2. Select the item or items that you want to delete.**
- 3. Choose Clear from the Edit menu.**

The following dialog box is displayed:



Choose Yes to delete the selected items. If you choose Cancel, the items will not be deleted and will remain in their previous locations in the workflow.

Tip You can press the Delete key on the keyboard instead of choosing Clear to clear the selected event or specification from a workflow. ▲

Undoing an edit

Undo in the Edit menu lets you reverse the effects of various editing operations in a workflow, including Add, Move, Cut, Copy, Paste, and Clear.

For example, if you have just deleted an event, you can restore the original event (and all of its associated specifications and assigned results) by choosing Undo.

To restore the changes you just reversed, choose Redo from the Edit menu.

Choosing Undo multiple times will reverse previous, consecutive editing operations one operation at a time.

The Undo command is available only if you are allowed to undo the operation you just performed. You cannot undo non-editing operations, such as Save Workflow.

Redoing an edit

Redo in the Edit menu lets you reverse the effects of an Undo operation.

For example, if you have just performed an editing operation and then reversed the operation by choosing Undo, you can reverse the Undo operation by choosing Redo, and then continue where you left off.

Resetting to defaults

After editing the parameter settings for a displayed workflow event or workflow specification, you can use the Reset command in the Edit menu to restore those parameters to the settings displayed when you first selected that workflow event or specification. The Reset command is also available as a button in the RESULT Integration toolbar.



The Reset command is also available as a button in the RESULT Integration toolbar.

Adding events to workflows

Workflow events specify a task that will be carried out when the workflow is run. The software implements the tasks in the order in which they appear in the workflow navigation frame when you display the workflow in RESULT Integration software.

Use the Add command in the Edit menu or the Add button on the toolbar to add events to the open workflow. See “Adding events to workflows” in this section for more information.

Using the Workflow wizard to add components to workflows

Use the workflow wizard in the Edit menu or the Wizard button on the toolbar to add the basic components to a workflow in one easy step (i.e., the events and specifications needed to collect, measure, archive, and report a basic spectrum). You choose which components you want to include from a single dialog box. When you close the dialog box, the new workflow events appear in the workflow navigation frame. The new events are placed in a group located at the end of the workflow. See “Using the workflow wizard to create or add to a workflow” in this section for more information.

Testing a workflow

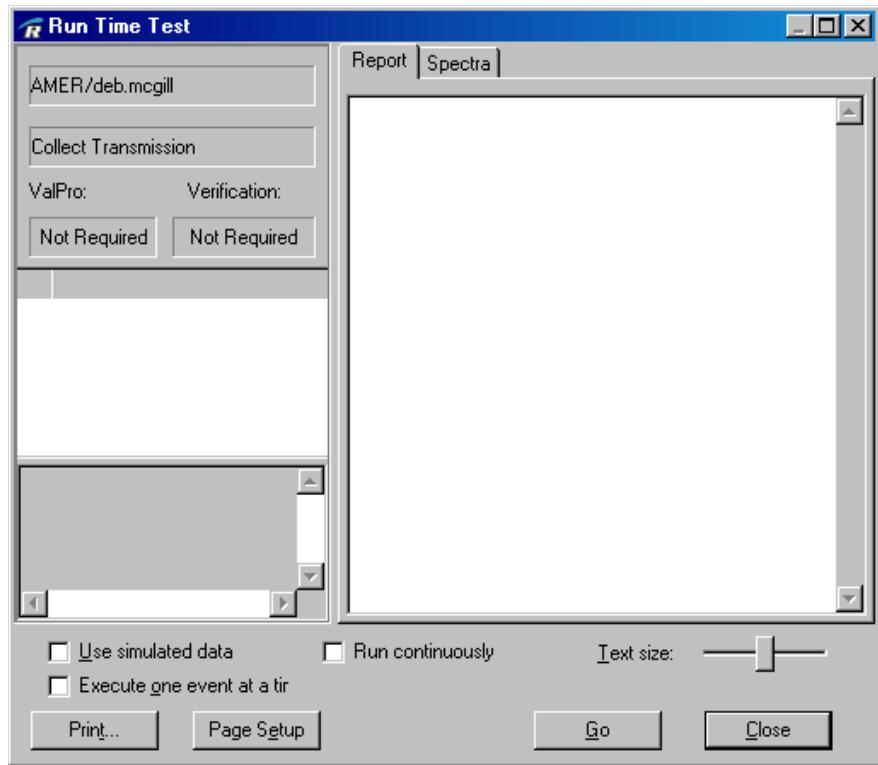
When creating a workflow in RESULT Integration, it is helpful to test the workflow to make sure it functions properly before transferring the workflow to a production system for repeated use. The RESULT Integration toolbar includes a convenient tool for testing a workflow. The RESULT Integration test feature mimics RESULT Operation, so you can see precisely how your workflow will operate in production mode without leaving RESULT Integration.

To test the open workflow:

- 1. Select the Test button on the toolbar in the RESULT Integration main window or choose Test Workflow from the File menu.**

The software displays the Run Time Test window, as shown below.

See “Chapter 1 Getting Started” in the “RESULT Operation User Guide” for detailed descriptions of the features in the Run Time Test window.



This window mimics the main screen for RESULT Operation software. RESULT Operation is the production application for RESULT.

The display boxes show logon information for the current user and the name of the workflow that is being tested.



The ValPro and Verification indicators, which appear below the display boxes, refer to any ValPro instrument qualification and verification workflows that must be run with this workflow. These indicators are meaningful only when the workflow is run in RESULT Operation software. See “Chapter 2 Running Workflows” in the “RESULT Operation User Guide” for more information about qualification and verification workflows.

2. If the workflow contains simulated sample spectra and you want to run the workflow using the simulated spectra, select Use Simulated Data in the Run Time Test window.



Note If the workflow is set up to use simulated data for all workflow runs, this setting in the Run Time Test window has no effect. See “Sample Specifications” in “Workflow Events and Specifications” for more information. □

3. If you want the workflow to pause after executing each event, select Execute One Event At A Time.



4. If you want the workflow to restart each time it completes, select Run Continuously.



The workflow will keep running until you pause or stop it by choosing Pause or Stop in the Run Time Test window.

5. Use the Text Size slider to increase or decrease the size of the text in the display area of the Run Time Test window.



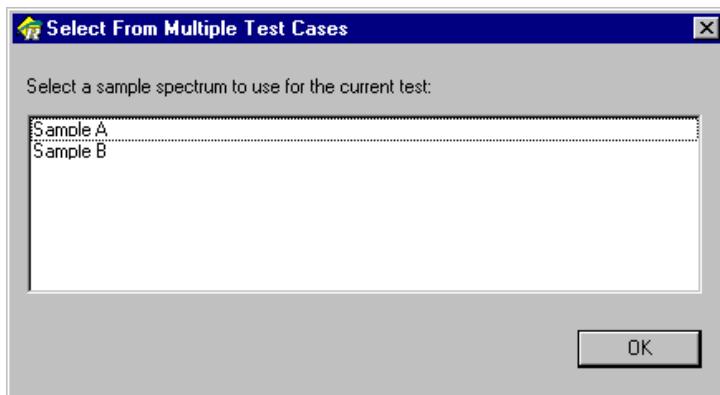
6. Choose the Go button at the bottom of the window to start the workflow.

The content and configuration of the workflow define how it operates. One or more of the following may occur:

- If the workflow is set up to use simulated data for all workflow runs, or if you selected Use Simulated Spectra in the Run Time Test window, the workflow simulates data collection by showing you any prompts or status information that will appear when the

workflow is run normally. However, all workflow events that normally operate on the collected spectrum will use the spectra stored with the workflow instead. See “Sample Specifications” in “Workflow Events and Specifications” for information about requiring simulated data for all workflow runs.

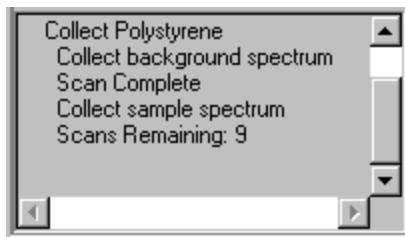
- If the workflow is set up to prompt the operator to select a sample for simulation, the following dialog box appears:



Select a simulation sample and then choose OK to run the workflow using the stored spectrum.

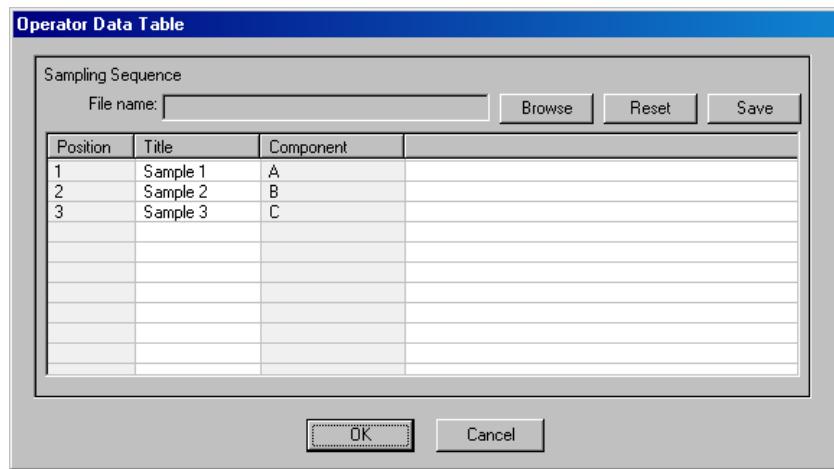
- If the workflow is set up to run using collected data, the workflow begins. Workflow events are carried out in the order in which they appear in the workflow navigation frame when you display the workflow in RESULT Integration software.

The status of the workflow appears in the status box at the lower left corner of the window, as shown below.



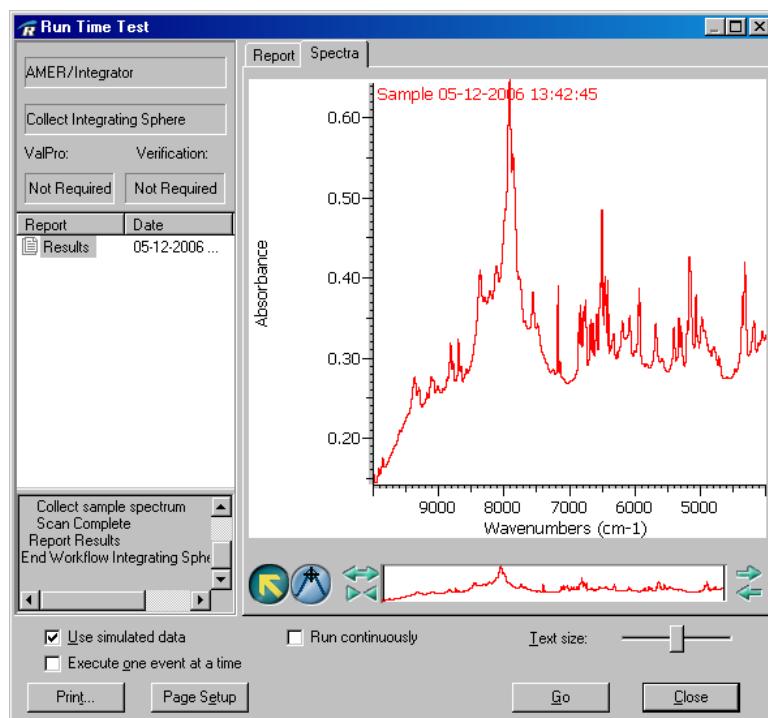
Any operator prompts that were set up in the workflow, instructing the operator to prepare for background or sample collection for example, will appear on the screen at the appropriate time.

- If the workflow is set up to use a sampling sequence that requires confirmation from the operator, the following dialog box will appear on the screen before the sequence begins:



Use the features in the Sampling Sequence box to edit, import or create a valid sampling sequence. See “Creating a sampling sequence” and “Importing a sampling sequence” in the previous section for more information.

- If you want to view the spectral data during data collection, select the Spectra tab at the top of the Run Time Test window.

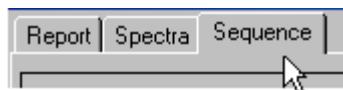


The first spectrum will be displayed as it is collected. As new spectra are added to the spectral window, the spectra are overlaid. The most recent spectrum is shown in red.

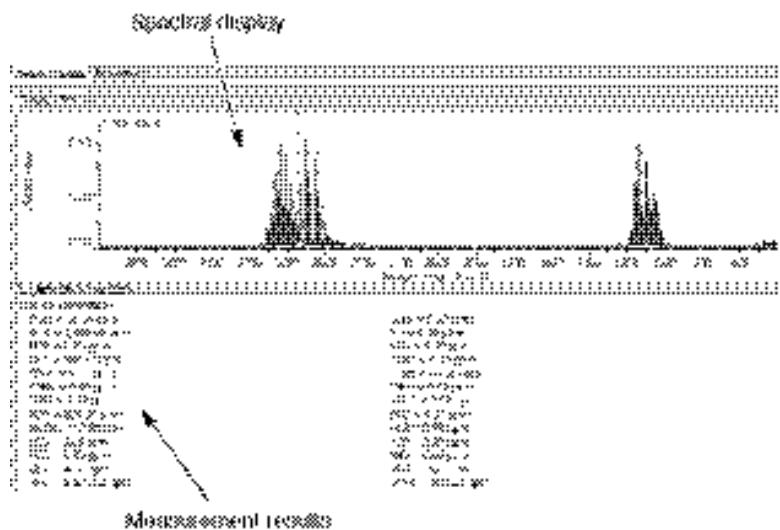
When viewing the spectral data, RESULT provides a variety of options for configuring the display window and manipulating displayed spectra. See “Chapter 2 Running Workflows” in the “RESULT Operation User Guide” for more information about these features.

- If the workflow contains a run sequence event, the Sequence tab appears in the Run Time Test window. The run sequence event configures RESULT software to collect and process spectra continuously. Continuous data collection provides information about samples that change composition over time.

If you want to view the sequence data during collection, select the Sequence tab.



The Sequence tab is divided into two main display areas for showing spectral data and measurement results.



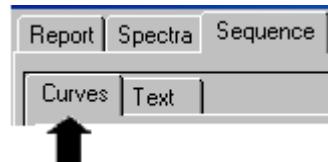
The spectral display appears in the upper part of the tab and shows the most recent spectrum. The spectral display updates each time the instrument collects and processes a new spectrum. The rate of

data collection is determined by the resolution, mirror velocity and number of scans collected for each spectrum. The spectra are displayed in sequence; each spectrum represents a “snapshot” of the sample at a particular moment in time. The vertical axis shows intensity (the workflow defines the data format) and the horizontal axis is in wavenumbers (cm⁻¹).

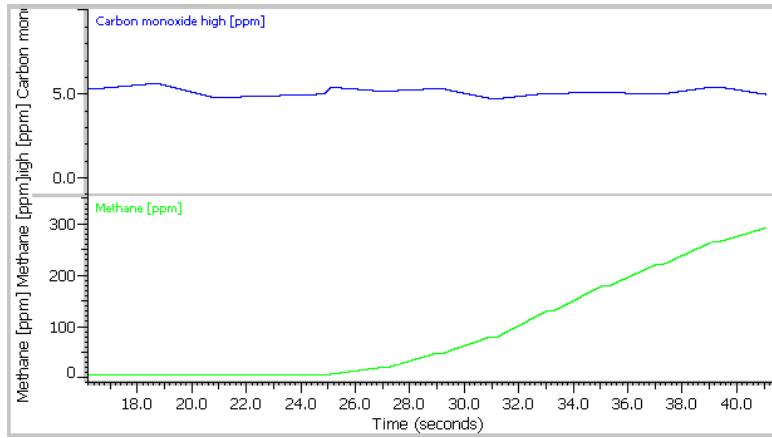
Depending upon how the run sequence event is configured in the workflow, the lower portion of the Sequence tab may show the measurement results calculated by the workflow over the time of the data collection. The measurement results can be component concentrations from a quantitative analysis, a match value or class number from a classification analysis, or peak heights or areas. The available results and types depend on the analysis method or methods associated with the run sequence event in the workflow.

You can choose between a text format and a run chart format for displaying the measurement results. The text format (shown above) provides a running list of the calculated values over the time of the data collection. Each time the software collects a new spectrum, it recalculates the results and then displays the new values.

To display the measurement results in a run chart format, select the Curves tab at the top of the sequence display.



When the Curves tab is selected, the lower display area may be divided into one or more panes.

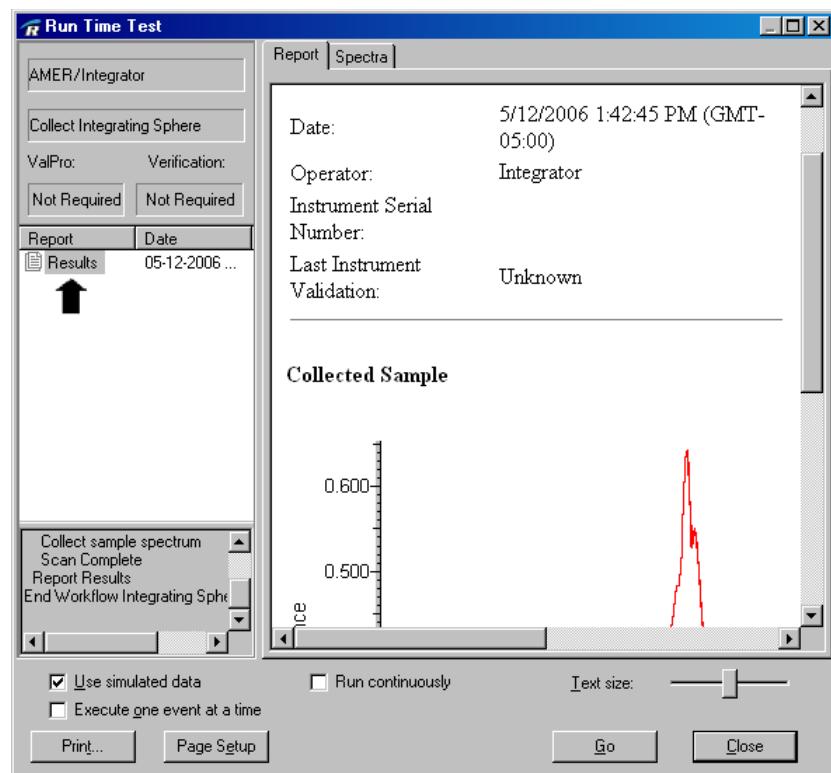


Each pane shows a measurement calculated by the workflow over the time of the data collection. The vertical axis shows sample concentration (the analysis method defines the component name and unit) and the horizontal axis is in seconds. The software adds data points to the concentration curves each time it collects a new spectrum.

The run sequence event in the workflow specifies the information displayed on the Sequence tab. See “Viewing sequence data while running a workflow” in “Chapter 2 Running Workflows” of the “RESULT Operation User Guide” for more information about the sequence display.

- If Execute One Event At A Time is selected in the Run Time Test window, the workflow executes the first event and then stops. The Go button flashes to the Pause button, and then changes to the Resume button. When you are ready for the workflow to execute the next event, press Resume. Continue pressing Resume until all the events have been executed.
- If the workflow is set up to create a sample report, the report will appear in the display area when the workflow is completed. The name of the report and the date and time it was created are displayed in the report navigation frame to the left of the report as shown below.

To print the report, use the Page Setup and Print buttons at the bottom of the window, or move the mouse cursor over the display area and click the right mouse button to display a shortcut menu. Then choose Print from the shortcut menu. Page Setup displays a standard Windows printer setup dialog box. Print sends the data to the specified printer.



The software adds one of the following disclaimers to the end of the report, depending on whether you ran the workflow normally or with simulated data.

- Generated in diagnostic mode (if you ran the workflow with simulated data).
- Generated in off-line production mode (if you ran the workflow normally).

This allows you to easily distinguish reports that are created by workflows run in RESULT Integration from reports created by workflows run in production mode in RESULT Operation.

- If workflow errors occurred, the errors will be listed in a table in the display area, as in the example below.

Event Name	Error Description
Collect Polystyrene	RESULT is unable to communicate with the analyzer. Check the following: Interface cable is connected to analyzer and computer.

Read the descriptions provided in the table and the suggestions for resolving the errors. See “Chapter 6 Troubleshooting” for more information about errors that may occur when testing workflows in RESULT Integration software.

7. When you are finished testing the workflow and reviewing the report, choose the Close button in the lower right corner of the window to close the Run Time Test window.

Saving a workflow

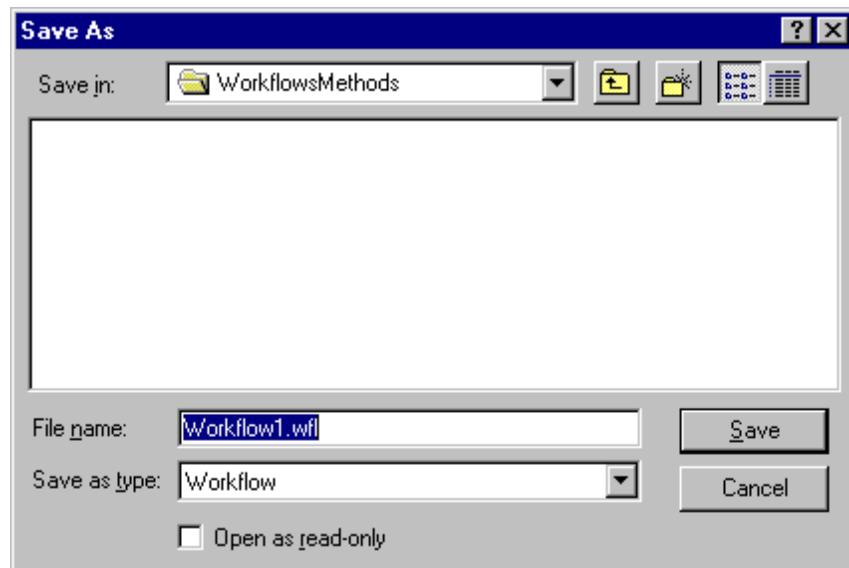
Use Save Workflow in the File menu or the Save button on the toolbar to save the open workflow on a disk.

To save the open workflow:



1. Choose Save Workflow As from the File menu or choose the Save button on the toolbar.

The Save As dialog box is displayed.



The default folder is the currently selected location for storing workflows and methods. See “Setting RESULT Integration Options” in “Chapter 1 Getting Started” for information about setting this and other directory paths in RESULT Integration software.

2. Select a folder for storing the new workflow or create and then select a new folder.
3. Enter a descriptive name for the new workflow in the File Name box and then choose Save.

The extension “.WFL” is automatically added to the file name.

After you choose Save, the file name for the new workflow appears in the title bar at the top of the RESULT Integration main window, as shown below.



Signing workflow files

Before transferring a new workflow to a production system, you should digitally sign the workflow file. You may want to sign other files associated with the workflow, such as the method files, to completely secure the workflow. Applying digital signatures to your files can help ensure their authenticity.

Note The digital signature features of RESULT software comply with 21 CFR Part 11 (Title 21 – Food and Drugs of the Code of Federal Regulations; Electronic Records; Electronic Signatures; Final Rule, Federal Register 62, no. 54, 1997). ▲

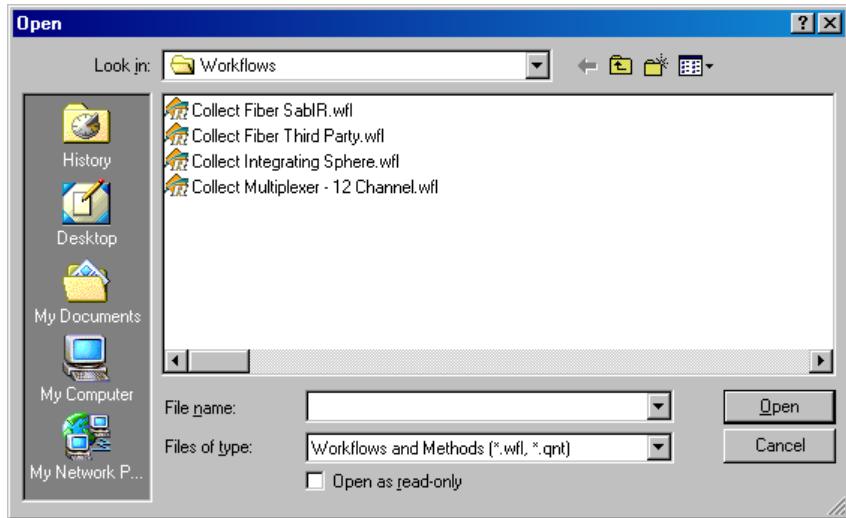
You must enter a valid Windows user name and password to digitally sign a file.

Note The user name and password must match your Windows user name and password exactly, including the letter case. ▲

To sign a file:

- 1. Choose Sign File from the File menu in RESULT Integration.**

The following dialog box appears.



2. Use the Files Of Type drop-down list box to select the type of file you want to sign.

The following types of files may be signed:

- Workflow files (*.wfl)
- TQ Analyst method files (*.qnt). (Method library files (*.lbd and *.lbt) are considered signed when their associated method file has been signed, since the library files can only be altered through the associated method file.)
- Spectral data files (*.spa, *.jdx, *.spc, *.csv)
- Sequence data files (*.srs, *.sri, *.cnc)
- Report files (*.htm).

Note Spectral and report files are typically signed before they are archived by a workflow. The archive event may be configured to require digital signatures. See “Archive events” in “Workflow Events and Specifications” for more information. ▲

3. Select the file you want to sign and then choose Open.

After you choose Open, the following dialog box is displayed.

If you choose Cancel from the Digital Signature dialog box, the file will not be digitally signed.



4. Select the User Name box and enter your Windows user name.

The name must match your Windows user name exactly.

5. Select the Password box and enter your Windows password.

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

6. Open the Reason For Signature combo box and select an option that describes your purpose for signing this file, or select the combo box and type a description.

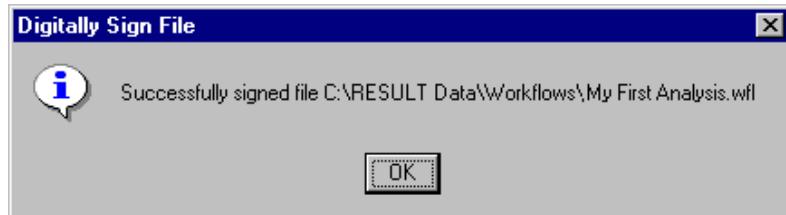
The options provided in the software are described below.

- **Authorship**, to indicate that you created the file.
- **Review**, to show that you reviewed the file.
- **Approval**, to confirm that you reviewed and approved the file.
- **Responsibility**, to indicate that you are responsible for the file but didn't necessarily create it.

Note If RESULT is running with the Security Administration application, the RESULT administrator may customize the list of reasons based on an operator's job function. ▲

7. Select OK to close the dialog box.

The software should display a message indicating that the file has been successfully signed, as shown below.



Your user name is now archived with the file and the file's contents are “stamped” so that any changes which occur after this date and time will be detected.

Note You can sign a file multiple times by using Sign File again. However, only the two most recent signatures will be visible when you view a file's signature information. ▲

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



After you choose OK, the following message appears:



If you see these error messages, the file was not digitally signed. To retry, use Sign File again to select the file and then enter the correct user name and password.

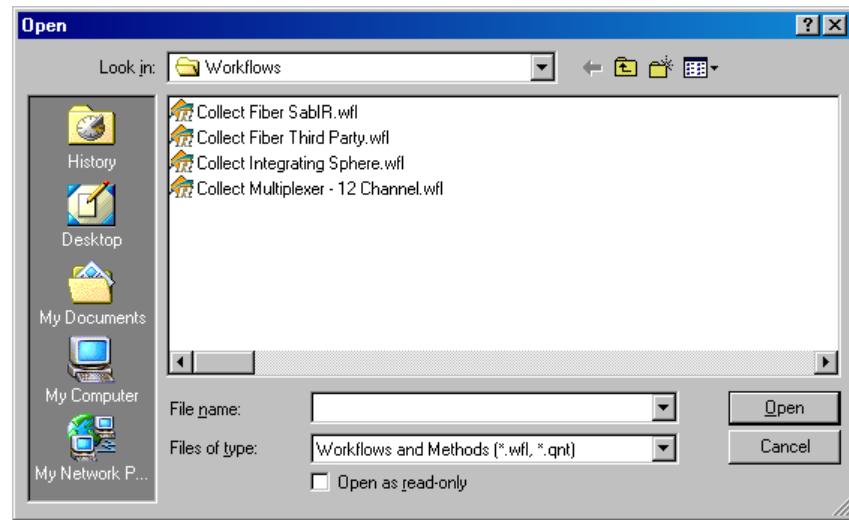
Checking file signatures

RESULT Integration allows you to easily check whether a file that was produced in RESULT software has been digitally signed.

To check whether a file has been signed:

1. Choose Check Signature from the File menu in RESULT Integration.

The following dialog box appears.



2. Use the Files Of Type drop-down list box to select the type of file you want to check for signature.

The following types of files may contain signatures:

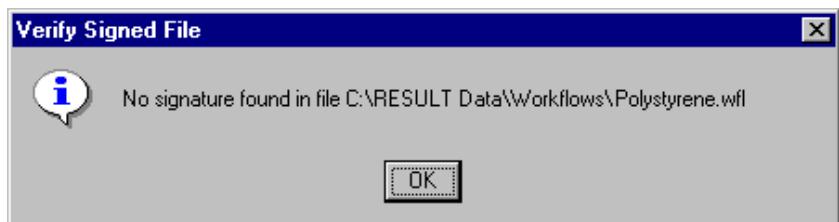
- Workflow files (*.wfl)
- TQ Analyst method files (*.qnt)
- Spectral data files (*.spa, *.jdx, *.spc, *.csv)
- Sequence data files (*.srs, *.sri, *.cnc)
- Report files (*.htm).

3. Select the file you want to check for signature and then choose Open.

If the file contains one or more digital signatures, an information box appears showing the file name and file location, the names of the last two people who signed the file, the date and time the file was signed, and the reason it was signed, if one was specified, as shown below.



The software displays the following message instead if the file does not contain a signature, or if the file was altered after it was signed.



Adding operator instructions to a workflow

You can create an associated document that contains instructions or a standard operating procedure (SOP) for running a workflow. The document can then be converted to a portable document format (PDF) file and attached to the workflow in RESULT Operation software. You must have a copy of Adobe® Acrobat® software and a current version of Adobe Reader installed on your computer to create instructions for use in RESULT software and to view those instructions using RESULT.

If an operator running RESULT Operation selects a workflow that has an attached instruction file, then the file will be loaded along with the workflow and the operator will be able to view the instructions before running the workflow. See “Chapter 1 Getting Started” in the “RESULT Operation User Guide” for information about viewing operator instructions when running a workflow.

You can use any word processing or text editor application to create the instructions document. When the document is complete, use the Adobe Acrobat software application to convert the document to the portable document format (PDF).

Note Adobe Acrobat provides tools to sign *.pdf files if you need to have these documents signed to comply with regulations or procedures. ▲

Store the pdf file (*.pdf extension) in the same directory as the workflow for now. When you transfer the workflow to RESULT Operation software, make sure you transfer the PDF file along with the workflow. See “Transferring Workflows To RESULT Operation Software” in the next section for more information.

See “Setting Up A New Workflow” in the “RESULT Software Administration” manual for information about attaching instructions to a workflow. You can attach one instruction file to each workflow.

Transferring a workflow to RESULT Operation

After you have completed and signed a new workflow, the workflow is ready to be transferred to RESULT Operation, which is the production application for RESULT software. RESULT Operation can be running on the same workstation as RESULT Integration or on a different workstation or a production system.

You can transfer workflows to RESULT Operation by copying the workflow and its associated files to the proper workstation and placing the files in the proper directory and path.

A workflow can have an associated document that contains instructions or a standard operating procedure (SOP), images for HTML reports, analytical methods, simulation data, and verification workflows. These items must be transferred along with the workflow in order for the workflow to function properly in RESULT Operation software. We recommend collecting and storing the workflow and its associated files in one directory to facilitate the transfer.

To move a workflow in order to run the workflow in RESULT Operation software, copy the files listed below to the proper workstation and place them in the current directory path in RESULT Operation.

- Workflow file (*.wfl).** If possible, store the workflow in the directory designated for workflows and methods, as specified in the RESULT Options dialog box in RESULT Operation software. If the workflow cannot be stored in that directory, make sure the workstation has access to the directory where the workflow is actually stored.
- Verification workflow file (*.wfl).** If the workflow requires a verification workflow, then store the verification workflow in the same directory as the workflow.

Note When setting up workflows in RESULT Operation, set up the verification workflow before setting up the associated production workflow. See “Chapter 6 Managing Workflows” in the “RESULT Software Administration” manual for information about setting up a new workflow in RESULT Operation software. ▲

- Method files (*.qnt).** If the workflow has associated TQ Analyst or other method files, store the method files in the same directory as the workflow.
- Method library files or other run-time files.** If using a TQ Analyst method, store the methods’ associated library files (*.lbd and *.lbt) in the same directory as the method. (There is no need to copy the spectral data files for the method standards to RESULT Operation software. Copies of the standards used to calibrate a TQ Analyst method are automatically stored in the method library files.)

If using a third-party method, copy the proper run-time files to the same directory as the third-party method. See “Using third-party methods with RESULT” in Chapter 4 Tools for Building Methods and Viewing Spectra” for more information.

- Image files (*.bmp, *.gif, *.jpeg, *.png, etc.).** If the workflow contains a report event that specifies one or more image files, to be placed in a report heading or table for example, store the image files in the directory designated for HTML images, as specified in the RESULT Options dialog box in RESULT Operation software.
- Instructions file (*.pdf).** If the workflow has an associated document with instructions or a standard operating procedure (SOP), store the document in the directory designated for instructions, as specified in the RESULT Options dialog box in RESULT Operation software. If the

instructions cannot be stored in the standard directory, then make sure the workstation has access to the directory where the instructions file is actually stored. The instructions document must be converted to portable document format (PDF) before it can be attached to the workflow. See “Operator Instructions” in the previous section for information about creating instructions files and converting them to the portable document format.

- **Simulation files for sequence collection (*.sri).** If the workflow contains a run sequence event that has an associated simulation sample (used for simulated runs of the workflow), store the interferogram (*.sri) data for the simulation sample in the same directory as the workflow.

Note Other types of data (*.spa and *.spg files) selected for simulated runs of a workflow are automatically stored with the workflow and need not be present as a separate file in order to run the workflow in simulation mode. ▲

Note To determine the proper directory paths for the above items in RESULT Operation software, see “Chapter 4 Setting RESULT Operation Options” in the “RESULT Software Administration” manual. ▲

Use the Windows Explorer program in your Programs menu to transfer the files. The Programs menu is available from the Start menu on your Windows taskbar. See your Windows documentation for information about using Windows Explorer.

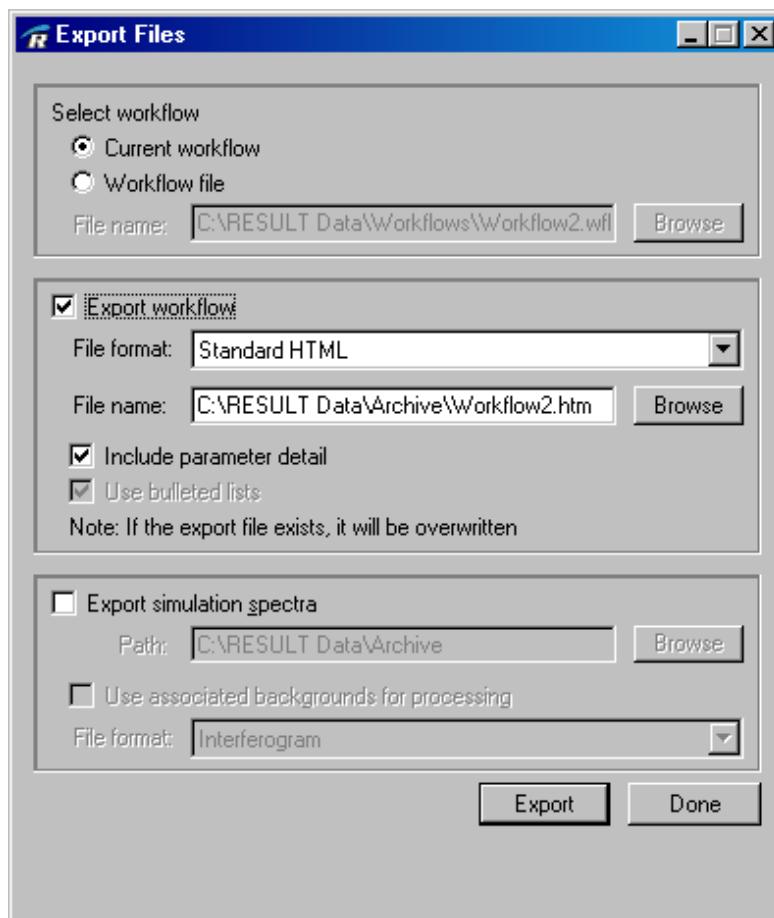
Exporting workflow files

The RESULT Integration File menu includes an Export command, which allows you to export workflows or the simulation spectra attached to a workflow to separate files in various formats so they can be viewed or printed from other applications.

Read this section to learn about the Export Files dialog box and the options for exporting workflows and their associated spectra.

Export Files dialog box

To export files from a workflow, first start the RESULT Integration application. From the RESULT Integration main window, open the File menu and then choose Export. The Export Files dialog box is displayed, as shown below.



You can use this dialog box to export a workflow to a text file or the simulation spectra for a workflow to individual spectral files. The exported workflow files can be set up to show only the workflow contents and structure for both the Workflow tab and the Details tab, or the structure and a complete listing of the parameter settings for each workflow event and specification. You can export files from the open workflow or select a workflow file saved on a disk. The simulation spectra will be exported to individual spectral data files in the Nicolet spectrum file format (*.spa file name extension).

Exporting a workflow

Follow these instructions to export a workflow to a text file.

To export a workflow to a text file:

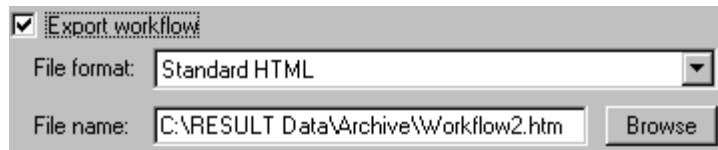
1. Select a workflow.

To export the open workflow, select the Current Workflow option in the Select Workflow group.



To select a different workflow, select the Workflow File option and then use the Browse button to select a workflow file. Workflow files have the *.wfl file name extension. You may browse to any disk or directory to locate a workflow file.

2. Select the Export Workflow check box.



3. Choose a file format for the exported workflow.

The available file formats are described below:

- **Standard HTML**, which creates a standard hypertext markup language (HTML) text file with an *.htm file name extension. HTML documents are viewable by RESULT software, as well as web browsers and other applications that can open HTML files.
- **Text file**, which creates a standard text file with a *.txt file name extension. Text files can be viewed from any text file editor such as NotePad.

- **Unicode HTML**, which creates a Unicode HTML text file with an *.htm file name extension. You may prefer the Unicode HTML format if your document contains text from double-byte character sets such as Kanji.
 - **Unicode text file**, which creates a Unicode text file with a *.txt file name extension. Unicode text files can be viewed from any text file editor such as Notepad.
- 4. Specify a path and file name for the exported workflow or leave the default path and file name.**
- You can enter a path and file name in the File Name box or use the Browse button to specify the path and file name. If you leave the default path and file name, the exported workflow file will be saved in the C:\\RESULT Data\\Archive folder using the same name as the workflow file but with a *.htm or *.txt extension.
- Note** If you leave the default file name and that file already exists in the specified location, the software will overwrite the existing file. ▲
- 5. If you want the exported file to include the parameter settings for each workflow event and specification, select the following check box.**
- Include parameter detail**
- If you leave this check box cleared, the software exports the workflow's basic contents and structure for both the Workflow tab and the Details tab, but not the parameter settings.
- 6. If you selected one of the text file formats in step 3 above, use the following check box to indicate whether you want the text file to include bullet symbols.**
- Include bullet symbols**
- 7. Choose the Export button at the bottom of the dialog box to create the exported file.**

8. Select another workflow to export or, if you are finished exporting files, choose Done.

The software saves the file using the directory, path and file name you specified in the Export Files dialog box in step 4 above. You can use any text editing application, such as the Windows Notepad program, to open, edit, and print an HTML or text file.

Exporting simulation spectra

RESULT allows you to attach spectra to a workflow in order to run the workflow without stopping to collect data. Follow the instructions in this section to export the simulation spectra attached to a workflow to individual spectral data files. You can export the simulation spectra from the open workflow or select a workflow file saved on a disk. When exporting simulation spectra, keep in mind that the software automatically exports all the simulation spectra for all the sample and background specifications included in the workflow. Depending upon the format you select for the exported sample data, the software may need an appropriate background spectrum to complete the processing. If the selected format requires a background but the simulation spectra do not have associated backgrounds, the software displays an error message.

The simulation spectra will be exported to individual spectral data files in the Nicolet spectrum file format. Each file is named with the spectrum title and a *.spa file name extension.

To export the simulation spectra saved with a workflow:

1. Select a workflow.

To export the simulation spectra from the open workflow, select the Current Workflow option in the Select Workflow group.



To select another workflow, select the Workflow File option and then use the Browse button to select a workflow file. Workflow files have the *.wfl file name extension. You may browse to any disk or directory to locate a workflow file.

2. Select the Export Simulation Spectra check box as shown below.



3. Specify a path for the exported files.

You can enter a path name, or use the Browse button to select the path name, or leave the default path name.

4. If the simulation spectra in the selected workflow have associated background spectra and you want to use the associated backgrounds to reprocess the simulation spectra to another data format, select the following check box.



If this check box is cleared, the software exports the simulation spectra as interferograms and the option to select the data format (see step 5 below) is unavailable in the software.

Note If this check box is selected and you choose a data format that requires background spectra but the simulation spectra do not have associated backgrounds, the software displays an error message. □

5. Choose a data format for the exported simulation spectra.

The following options are available:

- Interferogram
- Single beam
- % Transmittance
- Absorbance
- % Reflectance

- Log 1/R
- Kubelka-Munk
- Single beam raw

See “Collect events” in “Workflow Events and Specifications” for descriptions of these data formats.

6. **Choose the Export button at the bottom of the dialog box to create the data files.**
7. **Select another workflow or, if you are finished exporting simulation spectra, choose Done.**

The files are saved in Nicolet spectrum format in the directory and path you specified in the Export Files dialog box in step 3 above. Each file is named with the spectrum title and a *.spa file name extension. You can use the TQ Analyst method development application to view or print a Nicolet spectral file. Exported files can also be used as method standards or representative samples for development purposes.

Chapter 4 Tools for Building Methods and Viewing Spectra

RESULT Integration is designed to work hand-in-hand with Thermo Scientific TQ Analyst™ method development software for seamless method creation and design, including the collection of standards. TQ Analyst is a sophisticated yet easy-to-use software package for developing analytical methods for near-infrared (NIR) and other spectroscopic applications. RESULT is also compatible with several method development applications created by other manufacturers.

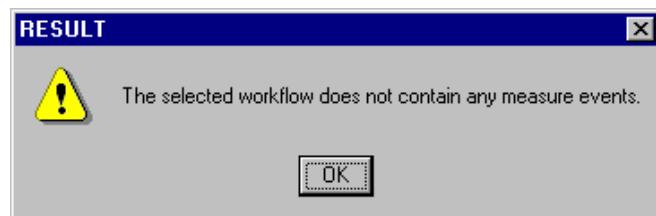
This chapter describes how to use the commands in the Tools menu of RESULT Integration software and your TQ Analyst or other compatible method development software to build an analytical method and assign the method to a measure event in a workflow. You will learn how to configure and collect the method standards and, if using TQ Analyst software, to import the method standards, select the analysis type, specify the analysis region or regions, and calibrate, save and test the method. The chapter also covers the Quick Collect and View Spectra tools, which may be used to collect and view spectra using RESULT Integration software.

Configuring standards

Standards are samples of known composition used to develop a quantitative or qualitative (classification) model. Use Configure Standards in the RESULT Integration Tools menu to configure and then collect standards in order to use those standards to build a quantitative or qualitative method for use with a measure event in a workflow.

To configure standards in RESULT Integration, simply specify any user prompts that will be needed for collecting the spectra of the standards, such as a prompt to request concentration values from the operator or a sampling sequence, and define how and where the spectra will be saved. You may configure standards differently for each measure event that is included in a workflow. You can also configure and collect the same set of standards for use by two measure events in a workflow.

Note In RESULT Integration software, standards are based on a measure event in a workflow (and its associated collect event). You must first open an appropriate workflow before you can configure the standards and begin collection. If you attempt to configure or collect standards without opening a workflow that contains at least one measure event, the software displays the following message. ▲



The measure event requires an associated collect event. The measure event should also be linked to a functional measurement specification. See “Workflow Events and Specifications” for information about setting up collect and measure events in a workflow.

Setting up the collection of standards

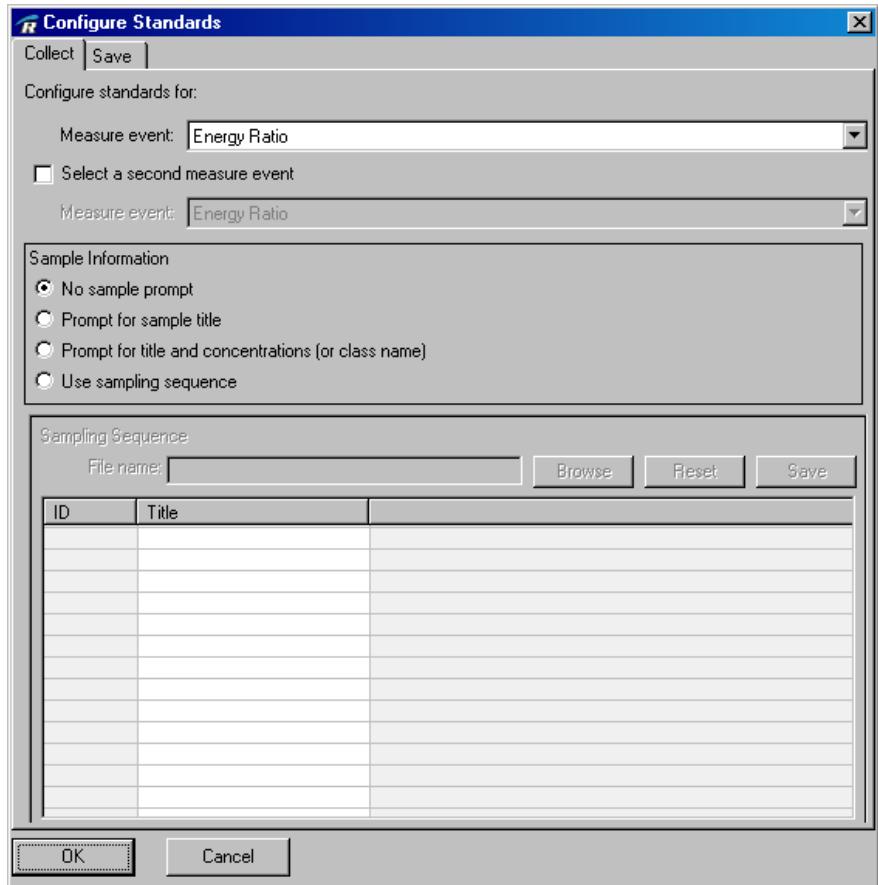
To specify how to collect the spectral data for the standards for a given workflow:

1. Open the workflow that requires standards.

The workflow must contain at least one measure event.

2. In the RESULT Integration main window, open the Tools menu and choose Configure Standards.

The software opens the Configure Standards dialog box with the Collect tab selected.

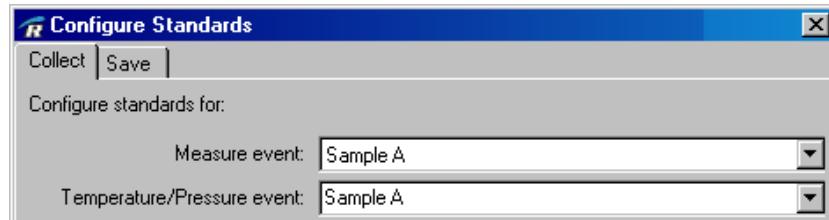


3. Select the measure event that requires standards by choosing an option in the Measure Event drop-down list.

The list includes the name of every measure event in the current workflow.

Note The selected measure event should be linked to a functional measurement specification. See “Measurement Specifications” in “Workflow Events and Specifications” for information about setting up measurement specifications in a workflow. ▲

If the workflow contains a Configure Temperature/Pressure event, a Temperature/Pressure Event list box appears on the Collect tab.



The Configure Temperature/Pressure event defines the temperature and pressure values that will be used to calculate the component concentrations of the standards.

4. If the Temperature/Pressure Event list box appears on the Collect tab, use the list box to select the appropriate Configure Temperature/Pressure event for the standards.
5. If the current workflow contains multiple measure events and you want to use the same standards for a second measure event, select the following check box.

Select a second measure event

When you select the check box, the Measure Event list box directly below the check box is enabled. The drop-down list includes the names of the remaining measure events in the workflow.

Choose a name in the Measure Event drop-down list.

Measure event: Incoming Material

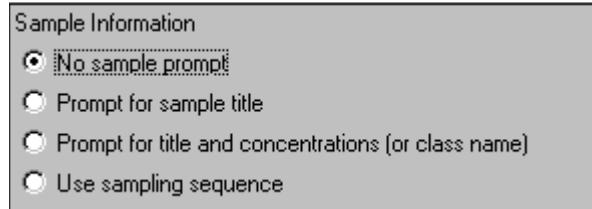
The second measure event can occur anywhere in the workflow. If both measure events operate on the same collection result, the software collects one set of spectra and uses both measure events for the analysis. If the second measure event operates on the spectra (results) from a different collect event, then the software will collect two spectra from each standard and use the first collect/measure event pair to analyze the first set of spectra and the second collect/measure event pair to analyze the second set of spectra.

This feature allows you to use the same set of standards to collect spectra for two different measure events, or two collect/measure event pairs, at the same time. This is useful for measuring a combination of

sample characteristics that aren't (or can't be) combined in one analytical method, such as collecting both transmission and diffuse reflection data using the MultiPro Autosampler.

6. Choose a method the operator will use to specify information about the standards at run time by selecting an option in the Sample Information group.

When Configure Standards is set up to collect standards for two measure events (see step 4 above), you must use a sampling sequence to specify information about the standards at run time.



The options include:

- **No sample prompt.** The software collects each standard without prompting the operator to enter a title or other information.

Notice If you plan to use a compatible third-party application to develop your method, set Sample Information to No Sample Prompt. The sample prompt features are available only for methods developed using TQ Analyst software. ▲

- **Prompt for sample title.** Before collecting each standard, the software displays a prompt asking for the title of the standard. The user must enter a title before the software will continue. Keeping this feature selected is helpful if your organization has specific naming conventions you want to use when titling each standard.

The titles are saved along with the spectral data for the standards. The titles also appear in the TQ Analyst standards table in default mode, after the standards have been imported to that application, and in the TQ Analyst spectral windows when the spectra are displayed.

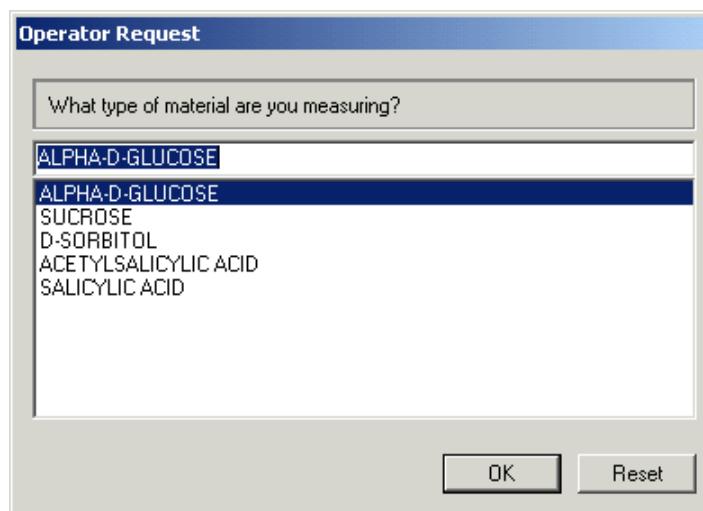
Note The title is a descriptive name saved within a spectral file; it is not the file name. ▲

- **Prompt for title and concentrations (or class name).** This option operates differently depending on whether the selected measure event is linked to a quantitative, qualitative, or spectral measurement method.

For quantitative methods. Select this option if you want the operator to enter the concentration values of the components in each standard as they are being collected. The software will display a dialog box prompting the user to enter the concentration value of each component before collecting each standard. After the concentration values have been entered, the software displays a second dialog box requesting a title for the standard.

If you don't select this option, then the concentration values for the standards will need to be entered when developing the method in TQ Analyst or other method development application.

For qualitative methods. Select this option if you want the operator to specify the correct class for each standard as it is being collected. The software will display a dialog box prompting the user to indicate the type of material he or she is measuring and present the class names from the qualitative method associated with the measure event specified in the Configure Standards dialog box. The operator dialog box will look something like the following:



The operator must indicate the sample material being analyzed by selecting a material in the list and then choose OK.

If you don't select this option to prompt for the spectrum title and class, then the correct classes for the standards will need to be specified when developing the method in TQ Analyst or other method development application.

For spectral measurement methods. If the selected measure event is linked to a measurement specification for a spectral measurement method, select one of the other Sample Information options.

Note Spectral measurement methods do not require standards. However, you can still use Configure Standards and Collect Standards to set up and test a spectral measurement method. ▲

- **Use sampling sequence.** The software uses the sample titles and concentration data (or class index numbers) listed in the table at the bottom of the Configure Standards dialog box (see the next step for details). This option is selected automatically when the Configure Standards dialog box is set up to collect standards for two measure events in a workflow. See step 5 above to learn how to configure standards for two measure events.

7. If you selected the Use Sampling Sequence option in the previous step, use the Sampling Sequence group to enter the sample information.

The group is enabled only when the Use Sampling Sequence option is selected for Sample Information. If you are collecting standards for a quantitative method created with TQ Analyst software, the names of the components in the associated method are listed in the table as shown in the example below.

If collecting standards for a qualitative method that contains multiple classes, a class index column appears in the table instead of the component names.

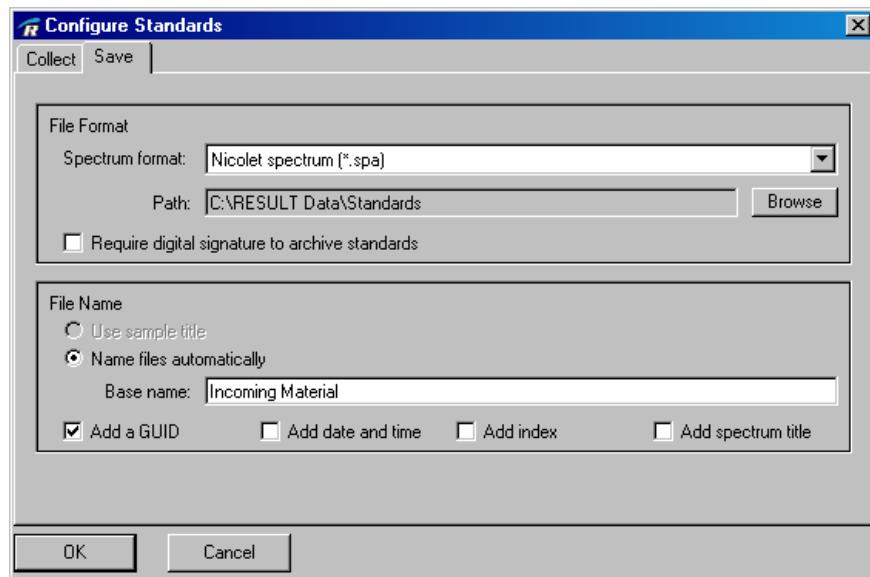
The sampling sequence must specify a sample name, a sample identification code (or position number if using an autosampler), and component concentrations (or a class index number) for each standard. The information may be entered manually or imported from a text file. Right click in the table to display a shortcut menu with options for adding rows and columns to the table. See “Using a Sampling Sequence to collect standards” in the next section for more information.

Setting up the archiving of standards

To specify how to save the spectral data for the standards:

1. Select the Save tab.

The following information is displayed.



2. Use the Spectrum Format list box to select a format for archiving the spectra of the standards.

The following options are available:

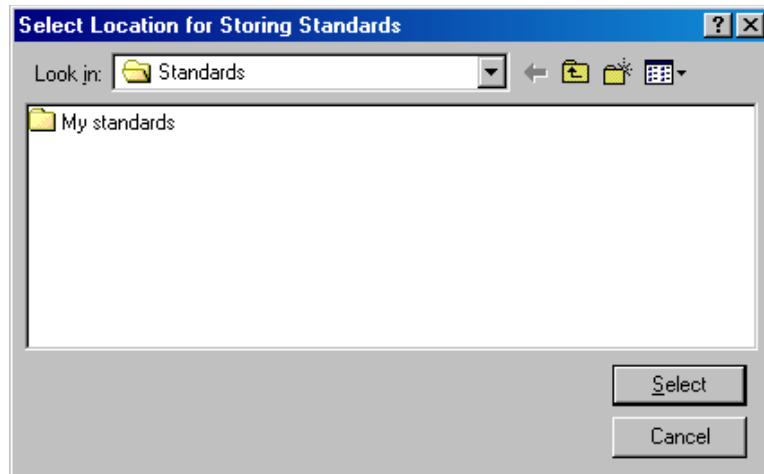
- **Nicolet (*.SPA)**. This is the preferred format for spectra, and is compatible with Thermo Scientific spectroscopy applications including TQ Analyst and RESULT. Data that are stored in the Nicolet spectrum format contain complete information about the conditions used for data collection as well as the archived sample and background interferograms, and are compatible with the digital signature features of RESULT software.
- **JCAMP-DX (*.JDX)**. This file format is compatible with other software applications used in the industry, allowing exchange of spectral data between various instruments. JCAMP-DX uses printable ASCII characters and provides some file header information.
- **Galactic (*.SPC)**, 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 header information.

Notice

If you plan to use a compatible third-party application to develop your method, select the Galactic option for Spectrum Format. Galactic works with third-party method development applications that are compatible with RESULT. ▲

- **Comma-Separated Values (*.CSV)**. This option creates 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.
3. **Use the Path text box to enter the path and folder that will be used to archive the spectra, or use the Browse button to locate, or create and then select an appropriate folder.**

When using Browse to choose a directory path, spectral files do not appear in the Browse dialog box.



Creating a folder for a set of standards can help you easily locate and select those standards when importing them into TQ Analyst or other method development application.

4. If you want to require digital signatures to archive the spectral files, select the **Require Digital Signature** check box.

Notice

If you plan to use a compatible third-party application to develop your method, clear the **Require Digital Signature** check box. The digital signature features are available only for methods developed using TQ Analyst software. ▲

Using digital signatures for spectral files can help ensure the authenticity of the data. When this feature is selected, after you collect the spectrum of each standard, the software will open a dialog box prompting the user to enter his or her Windows user name and password to sign the file. The software will request the digital signature when the standards are collected in RESULT Operation or RESULT Integration software.

You have three attempts to enter your password correctly when digitally signing a file. If you are unable to correctly enter your Windows password or if you cancel the Digital Signature dialog box, the following error message appears:



If you see this error message, the files are not archived.

You can use the Check Signature feature in the File menu of RESULT Integration software to determine whether a specific file has been signed. See “Checking File Signatures” in “Chapter 3 Creating and Editing Workflows” for more information.

To check for signatures in spectral files from RESULT Operation software, use the query feature to display the archived spectra 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.

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

Note If you collect unsigned standards, you can ensure the authenticity of the data after you import the standards into TQ Analyst by signing the TQ Analyst method file. ▲

5. Use the File Name group to specify how the spectral files will be named.

The following options are available:

- **Use sample title.** This option is available in the software only when the Sample Information feature on the Collect tab is set to Prompt For Sample Title or Use Sampling Sequence. If you elect to use the sample 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 file names of the archived spectra will match the titles exactly.

- **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), date stamp, index, spectrum title or any combination of these will be added to the file name.

Base name. If you want to include a base name when the files are named automatically, enter a name in the Base Name box. If you specify a base name, the software will include that name at the beginning of the file name of each standard. This step is recommended because creating a base name for a set of standards can help you easily identify those standards after they are archived. The base name is also used by RESULT Integration to identify which standards to import into TQ Analyst when building an analytical method. If you don't specify a base name, the files will be named with any file name options selected in the File Name group, such as a GUID or date stamp, and no prefix.

Add GUID. If you want the software to add a globally unique identifier (GUID) to the file names of the standards, select Add A 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.

Add date and time. If you want the software to add a date stamp to the file names of the standards, select Add Date And Time. The software adds the date stamp immediately after the base name.

Add index. If the software is set up to collect multiple standards without operator intervention, you can use the Add Index option to add an index number to the file names of the standards. 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.

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 spectrum title. If you want the software to add the spectrum title to the file names of the standards, select Add Spectrum Title. 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.

Note For detailed examples of how these automatic file naming option can be used to archive spectral data, see “Archive events” in “Workflow Events and Specifications.” ▲

6. When you are finished configuring the standards, choose OK to close the Configure Standards dialog box.

Choose Cancel to close the dialog box without saving your settings.

When you are ready to collect the standards, in the RESULT Integration main window open the Tools menu and then choose Collect Standards. RESULT Integration collects standards based on how they were configured in the Configure Standards dialog box, along with the parameters specified in a collection and measure event in a workflow. See “Collecting Standards” in the next section for more information.

Collecting standards

Use Collect Standards in the RESULT Integration Tools menu to collect the standards for a quantitative or qualitative method. Standards collected in RESULT Integration may be used to build a TQ Analyst or other method for use with a measure event in a workflow. You may also use Collect Standards to update a method model by adding standards to the method.

RESULT Integration collects standards based on how they were configured in the Configure Standards dialog box, along with the parameters specified in a collection and measure event in a workflow. The procedure for collecting a standard involves collecting a background spectrum and then collecting sample data to produce a spectrum. A background is a reference spectrum that accounts for the unique optics of the sampling module or accessory and the instrument. The background spectrum is the result of the output of the source, the response of the beamsplitter optics, sampling module or sample holder, and detector and any atmospheric absorptions inside the instrument. Each sample spectrum is ratioed against a background so that the final spectrum is free of these features.

Note In RESULT Integration software, standards are based on a measure event in a workflow. You must first open an appropriate workflow and configure the standards before you can begin collection. See Configuring Standards in the previous section for more information. ▲

To collect the standards for a measure event in a workflow:

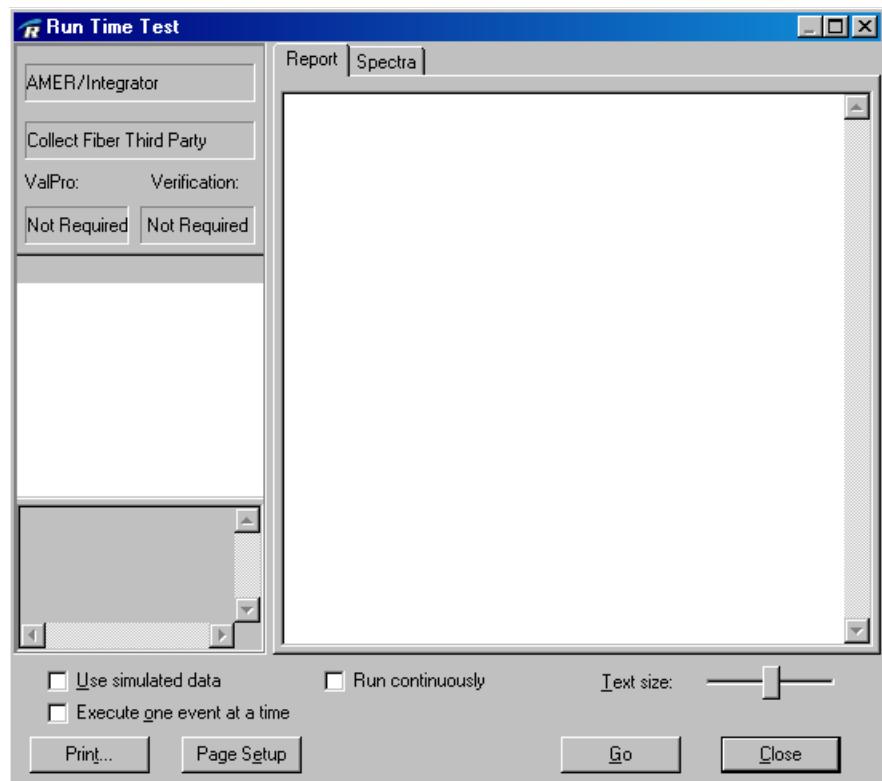
- 1. Make sure an appropriate workflow is open and configured for collecting standards.**

See “Configuring Standards” in the previous section for instructions.

- 2. Choose Collect Standards from the Tools menu in the RESULT Integration main window.**

The software opens the Run Time Test window, as shown below:

See “Testing a Workflow” in “Chapter 2 Creating and Editing Workflows” and “Chapter 2 Running Workflows” in the “RESULT Operation User Guide” for descriptions of the features in the Run Time Test window.

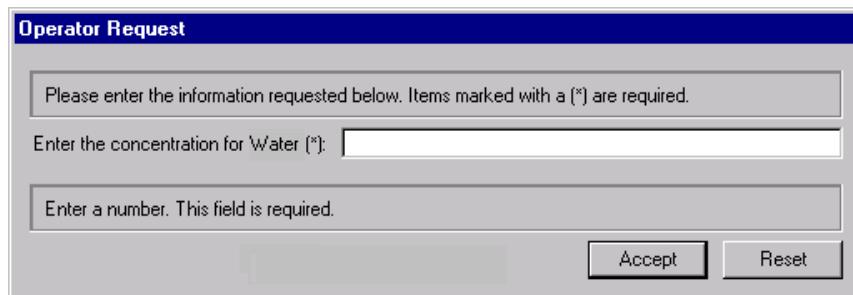


3. When the instrument and sample material are prepared for data collection, choose Go.

Note RESULT Integration collects standards based on how they were configured in the Configure Standards dialog box, along with the parameters specified in the collect event associated with the measure event that requires standards. If you are unfamiliar with data collection, find the appropriate chapter for the sampling module you plan to use in your *Antaris User's Guide* and run the procedure for Your First Experiment. ▲

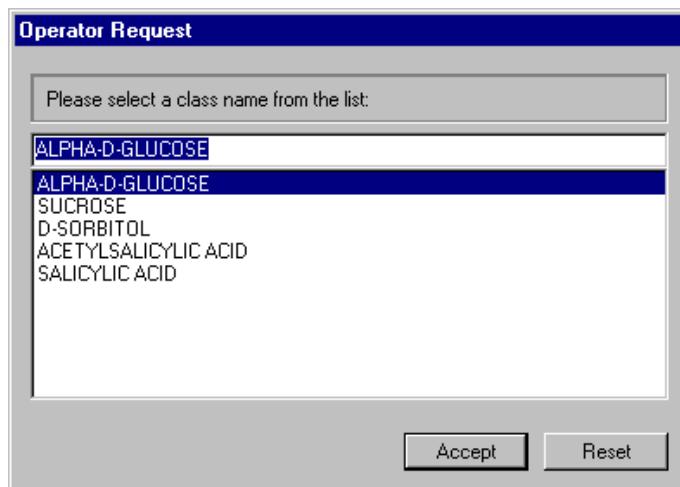
4. If the standards are configured to prompt for concentration values or class names, enter those items when requested by the software.

An example of a concentration amount prompt is shown below.



Enter a real number (a number that can include a decimal point). Always enter the value in the unit requested in the dialog box.

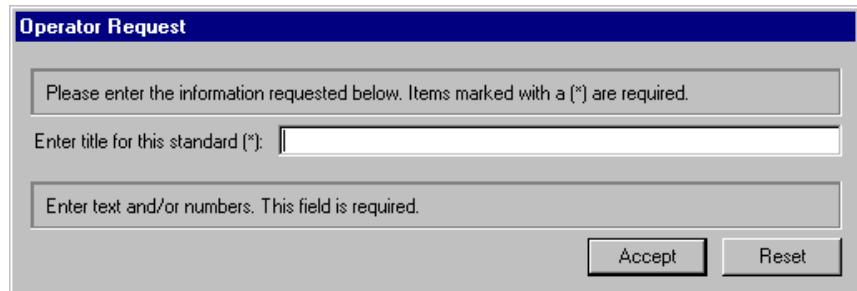
An example of the dialog box for selecting a class name is shown below.



Select the appropriate class name from the list, and then chose Accept. Choose Reset to clear the selection if you have chosen the wrong class name.

5. If the standards are configured to prompt for titles, enter the title of the standard at the software prompt, as shown below.

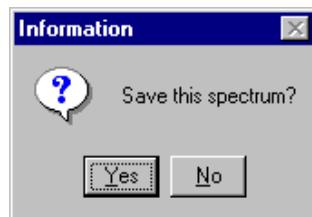
The titles are saved along with the spectral data for the standards. The titles also appear in the TQ Analyst standards table in default mode, after the standards have been imported to that application, and in the TQ Analyst spectral window when the spectra are displayed.



Enter the title in the text box. Choose Accept to save the title and close the dialog box, or choose Reset to clear the text box if you have made an error.

The software begins collecting data using the parameters set in the workflow. You can view the status of the collection in the status indicator at the lower left corner of the Run Time Test window.

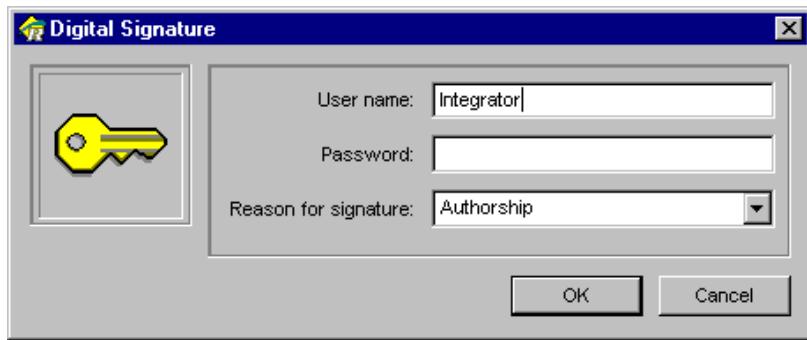
When the software has finished collecting data, it displays the spectrum in the display area of the window and opens the following dialog box:



6. Choose “Yes” to save the spectrum you just collected.

If you believe an error occurred during sample preparation or collection, or if the spectrum does not look reasonable, choose No.

7. If the standards were configured to require digital signatures for archiving, the software displays the following dialog box.

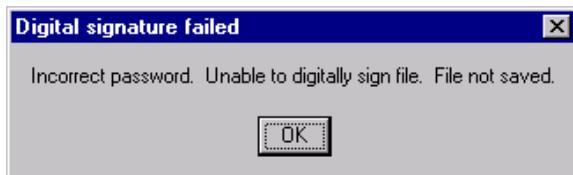


Enter your Windows user name in the User Name text box, and your password in the Password text box. The user name and password must match your Windows user name and password exactly, including the letter case.

Select the Authorship option from the Reason for Signature drop-down list, or enter another appropriate reason for the signature, and choose OK.

The spectrum is given a unique file name based on the file base name, if one exists, along with a globally unique identifier (GUID), date stamp, or other file name suffix selected in the Configure Standards dialog box. The file is stored in the location that was specified in the Configure Standards dialog box in the previous chapter.

Note You have three attempts to enter your password correctly when digitally signing a file. If you are unable to correctly enter your Windows password, or if you choose Cancel from the Digital Signature dialog box, the file will not be saved and the software will display the following message:



Choose OK to close the message. □

8. If you are collecting standards manually, prepare the instrument and the next standard for data collection and then choose Go in the Run Time Test window.

Follow steps 3 through 7 for each standard you need to collect.

If you are using an autosampler with a sampling sequence to collect the standards, the software will automatically position the next standard for data collection and begin collecting the data as defined in the sampling sequence and the Configure Standards dialog box.

9. When you are finished collecting standards, choose Close in the Run Time Test window.

You can collect standards again with the same settings as long as the workflow is open. If you close the workflow, you will need to configure standards again before collecting them.

Building a TQ Analyst method

Use Build TQ Analyst Method in the RESULT Integration Tools menu to build a new TQ Analyst method for use with a measure event in a workflow. RESULT Integration begins by building a core method based on a set of standards, along with the parameters specified in the measure event and its associated measurement specification. Then it opens the TQ Analyst application, allowing you to specify the spectral region for the analysis and to calibrate and save the new method. You can collect the standards in RESULT Integration or RESULT Operation software or another spectroscopy application that is compatible with RESULT and TQ Analyst.

Note In RESULT Integration software, methods are based on a measure event in a workflow. You must first open an appropriate workflow and configure and collect the standards before you can begin building a method. See “Configuring Standards” and “Collecting Standards” in the previous sections for more information. ▲

Note The Build TQ Analyst Method command in the RESULT Integration Tools menu works only for methods created using TQ Analyst method development software. ▲

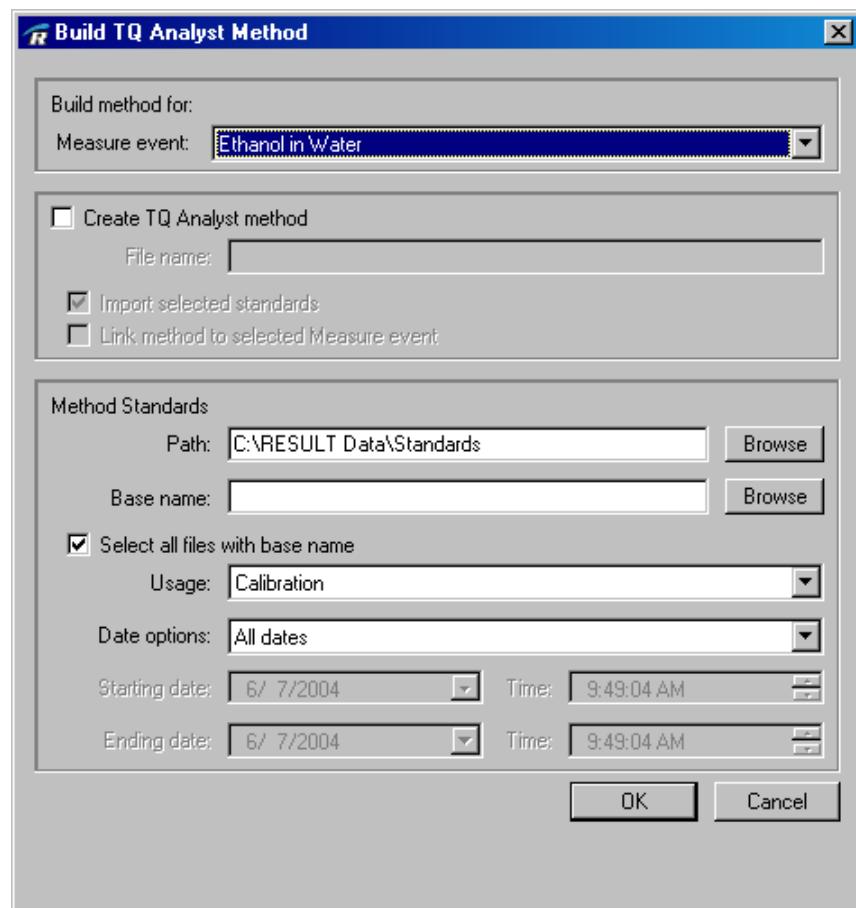
To build a TQ Analyst method for a measure event in a workflow:

- 1. Make sure the correct workflow is open and appropriate standards have been collected.**

See “Configuring Standards” and “Collecting Standards” in the previous sections for more information.

- 2. Choose Build TQ Analyst Method from the Tools menu in the RESULT Integration main window.**

The software opens the Build TQ Analyst Method dialog box.



- 3. Select the measure event that requires a TQ Analyst method by choosing an option in the Measure Event drop-down list.**

The list includes all of the measure events in the current workflow.

Note The selected measure event should be linked to a functional TQ Analyst measurement specification. See “Measurement Specifications” in “Workflow Events and Specifications” for information about setting up measurement specifications in a workflow. ▲

4. If you want to create a new TQ Analyst method for the selected measure event, select Create TQ Analyst Method.

Leave the check box cleared if the selected measure event and its associated measurement specification point to an existing TQ Analyst method, and you simply want to add standards to that method.

When Create TQ Analyst Method is selected, the rest of the parameters in the group become available, as shown below.



- **File Name.** Use this text box to specify a file name for the new TQ Analyst method. If you leave the File Name box blank, the software will use the name of the selected measure event for the method file name.
- **Import Selected Standards.** Select this option if you want to import standards to your new method. To use this option, before building the method, you must collect the spectrum of each standard and save the spectrum in a separate file on a disk. All of the standards must be collected using the same parameter settings and conditions.

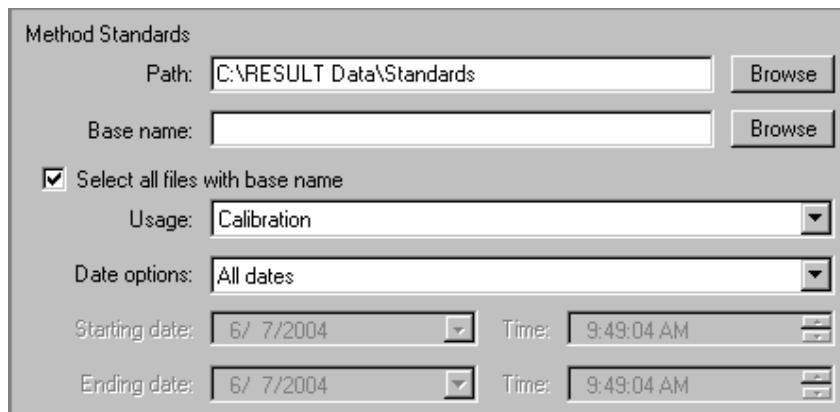
If you clear this option, the software creates the method but doesn't import standards. You will need to import the standards directly into TQ Analyst after the method has been created.

- **Link Method To Selected Measure Event.** Select this option if you want to link the new method to the selected measure event. When this option is selected, the software automatically selects the file name of the new TQ Analyst method in the TQ Analyst File Name list box, which is located on the measurement specification

associated with the selected measure event. If you clear this option, then the new method will still be created based on the selected measure event, but it won't be linked to a measure event in a workflow.

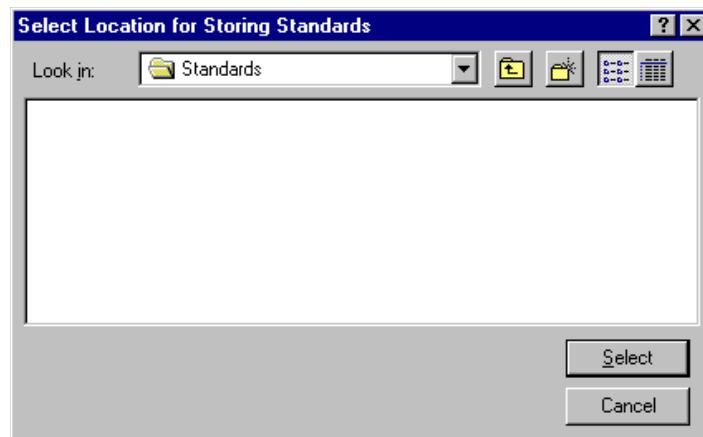
5. If you are importing standards, use the features in the Method Standards group to specify the standards you want to import.

If you are not importing standards, then skip to step 5.



- **Path.** Use this entry box to specify the path where the method standards are located, or choose Browse and select a path. The default path is the path specified in the Options dialog box in RESULT Integration software (see “Setting RESULT Integration options” in “Chapter 1 Getting Started” for details). However, you can select standards that are located in a different path by typing the path in the text box or by choosing Browse to open a standard Windows Browse dialog box, as shown below.

Spectral files do not appear in the Browse dialog box when choosing a directory path.



If you choose Browse, navigate to the correct path in the Browse dialog box, and then choose Select. The dialog box closes and the selected path appears in the Path text box in the Build TQ Analyst Method dialog box.

- **Select All Files With Base Name.** If importing multiple standards that all have the same base name, leave this check box selected. If you want to import a single standard or a group of standards that have unique file names, clear Select All Files With Base Name.
- **Base Name.** If the file names of all the standards have the same base name, you can use the base name feature to quickly select those standards. Make sure Select All Files With Base Name is selected (see above) and then enter the base name in the Base Name box, or choose Browse to search for a representative standard. After you select a standard, its base name appears in the Base Name box in the Build TQ Analyst Method dialog box.

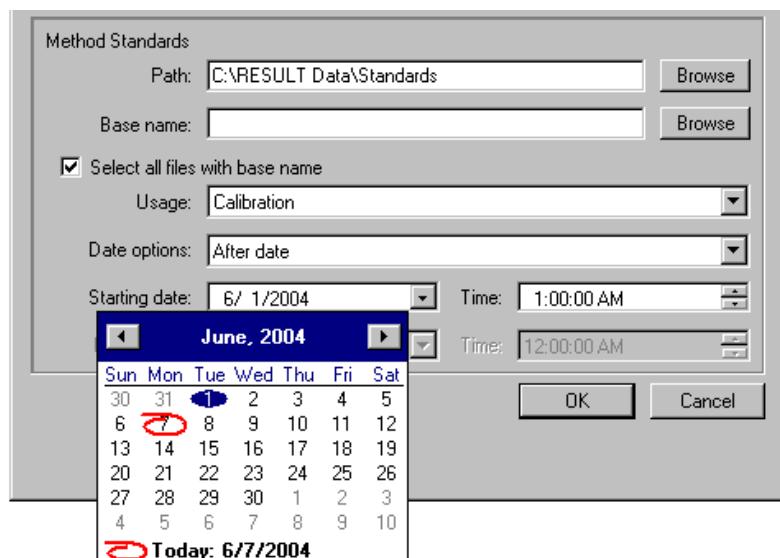
If you want to import a single standard, make sure Select All Files With Base Name (see above) is cleared and then use the Base Name box to specify the standard. You can type the file name of the standard in the Base Name box or choose Browse to search for the standard. After you choose Browse, the software opens a standard Windows Open dialog box that points to the appropriate path, and you can select the standard. After you select the standard, its file name appears in the Base Name box in the Build TQ Analyst Method dialog box.

If you want to import a group of standards that have unique file names, make sure they are located in the specified path and leave the Base Name box blank. The software will add all the standards located in the specified directory and path or use Date Options to limit the selected standards in that directory.

- **Date Options.** Use the Date Options to broaden or limit the selected standards. Leave the default setting (All Dates) for Date Options to select all standards that have the specified base name, if one was entered, and are located in the specified directory and path. If you want to limit the selected standards to include only those files which were collected on a certain day or time, or in a date or time range, set the date or time option by selecting an item in the Date Options drop-down list. Depending on the selection you

make, the Starting Date and/or Ending Date boxes may become available. You can change the dates in these boxes by:

- *Typing* the appropriate dates(s) in the boxes;
- *Selecting* a portion of the date and using the arrow keys on your keyboard to adjust the date; or
- *Selecting* the drop-down arrow to the right of the box. If you select the drop-down arrow on one of the date boxes, the software opens a calendar, as shown below.



Choose the date from the calendar with your cursor. Use the arrow buttons at the top of the calendar to navigate to the next and previous months.

You can change the time by typing the appropriate time in the box, or by selecting a portion of the time and using the arrow keys on your keyboard or the Up and Down buttons to the right of the box to change the time.

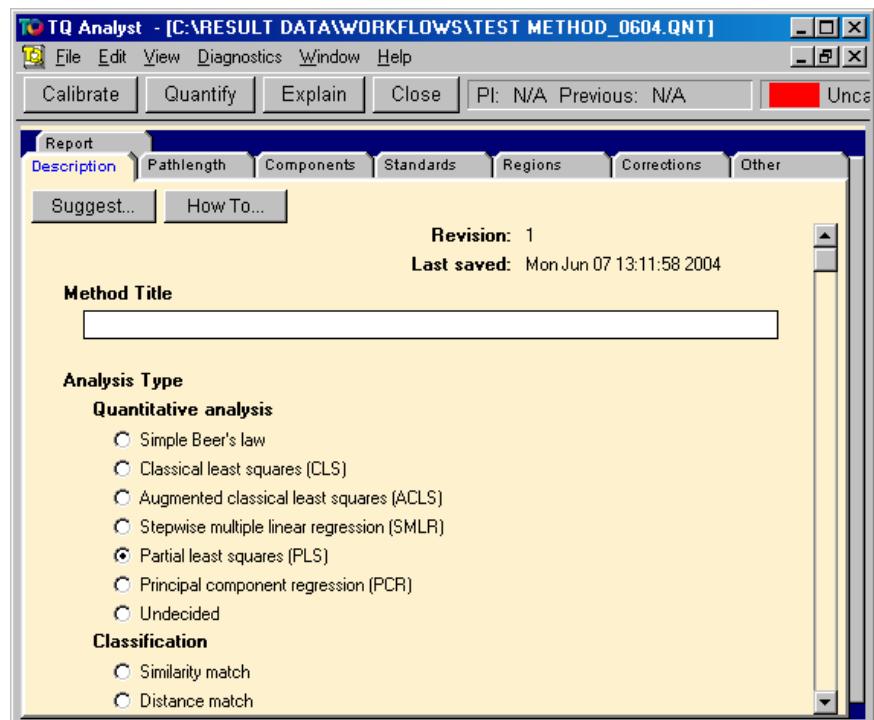
- **Usage.** Specify the usage of the selected standards by selecting an option in the Usage drop-down list. Select one of the following options.
 - *Calibration.* Calibration standards will be used to create the method model during calibration.

- *Validation*. TQ Analyst uses validation standards to calculate a performance index after the method is calibrated.
- *Correction*. Correction standards may be used to create a correction curve for a TQ Analyst quantitative method.
- *Ignore*. Standards that have the Usage property set to “Ignore” are not used for calibration, performance index, or other calculations in a TQ Analyst method.

The standards will have this property set when they are imported to TQ Analyst. When working with a method in TQ Analyst, you may change the usage setting for a standard at any time.

6. When you are finished specifying the method parameters and selecting standards, choose OK.

RESULT Integration starts the TQ Analyst method development application and displays the application’s main screen.



7. Make sure the Analysis Type is set correctly for the type of method you want to create.

The following Analysis Type options are available in TQ Analyst.

For quantitative analysis:

- **Simple Beer's Law**, which uses the classic Beer-Lambert-Bouguer law (absorbance increases proportionally with concentration) to create a calibration model.
- **Classical Least Squares (CLS)**, which looks at many regions of the spectra to find relationships between absorbance and concentration.
- **Augmented Classical Least Squares (ACLS)**, which is a combination of the CLS and PCR techniques and it uses additional factors to facilitate method transfer. This option appears in the software only if you purchased the optional ACLS add-on for TQ Analyst software. See one of our sales representatives for more information.
- **Stepwise Multiple Linear Regression (SMLR)**, which expresses concentration as a function of the absorbance at specific frequencies.
- **Partial Least Squares (PLS)**, which uses a partial least squares statistical analysis to determine which spectral regions vary as a function of component concentration.
- **Principal Component Regression (PCR)**, which uses a principal component regression statistical analysis to determine which spectral regions vary with component concentration.

For qualitative (classification) analysis:

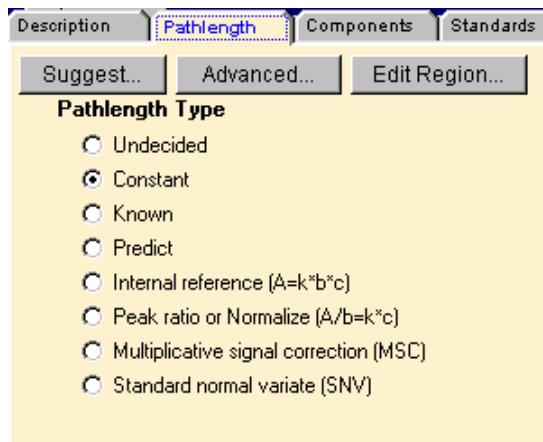
- **Similarity Match**, which uses multiple standards that define one class to determine how closely an unknown material matches a known material. Reports a match value, which indicates the quality of the match.
- **Distance Match**, which uses multiple standards that define multiple classes to determine how closely an unknown material matches each class. Reports a list of classes ranked from best match to worst match, and a match value for each class.

- **Discriminant Analysis**, which uses multiple standards that define multiple classes to determine the class or classes of known materials which are most similar to an unknown material. Reports a list of classes ranked from best match to worst match, and a distance value for each class.
- **Search Standards**, which uses multiple classes and one standard per class to determine which known material is most similar to an unknown material. Reports a list of standards ranked from best match to worst match, and a match value for each standard.
- **QC Compare Search**, which uses multiple standards that define multiple classes to determine which standard and class is most similar to an unknown material. Reports the best matched standard in each class, and a match value for each standard. The classes are ranked from best match to worst match.

For spectral measurements:

- **Measurement only**, which measures the unknown sample spectrum and reports the measured value(s). You can specify up to 50 measurements in a spectral measurement method. A spectral measurement method can be configured to do any of the following:
 - Measure the height or area of a peak.
 - Measure the ratio of two spectral peaks.
 - Measure the random noise in a given region.
 - Measure the width at half maximum of the largest peak in a region.
 - Locate the largest peak in a specified region.
 - Find where a peak is reduced to a specified percentage of its maximum height.

8. Select the Pathlength tab along the top of the window and make sure Pathlength Type is set correctly for the new method.



Sample pathlength, defined as the distance a beam of incident energy travels within a sample, affects only quantitative and qualitative (classification) analyses. When analyzing samples that are in the solid state, sample pathlength is often referred to as “sample thickness.” The pathlength of a liquid sample is defined by the distance between the internal walls of the holder used to place the liquid in the light beam.

If sample pathlength is constant, or assumed to be constant, set Pathlength Type to Constant. When the Constant pathlength option is selected, sample pathlength is not a factor in the analysis.

If sample pathlength is variable or unknown, one of the other pathlength settings is appropriate. See your *TQ Analyst User’s Guide* for a general discussion of sample pathlength considerations for quantitative and qualitative measurements in spectral analysis applications.

Note If you are setting up a spectral measurement method, set Pathlength Type to Constant for no pathlength correction. If you want the method to calculate the ratio of two spectral peaks, set Pathlength Type to Peak Ratio and specify the denominator peak or region as the pathlength peak. See your *TQ Analyst User’s Guide* for more information about calculating peak ratios in a spectral measurement method. ▲

9. If you are setting up a qualitative or quantitative method, select the Standards tab and make sure you imported the correct files for the standards.

The titles of the standards that were imported from RESULT Integration software are listed in the standards table, as shown below.

Index	Select	Spectrum Title	Usage	% ET
1	●○○	glucose 1	Calibration ▾	0.00
2	●○○	glucose 2	Calibration ▾	0.00
3	●○○	glucose 3	Calibration ▾	0.00
4	●○○	sucrose 1	Calibration ▾	1.00
5	●○○	sucrose 2	Calibration ▾	1.00
6	●○○	sucrose 3	Calibration ▾	1.00
7	●○○	sorbitol 1	Calibration ▾	2.00
8	●○○	sorbitol 2	Calibration ▾	2.00
9	●○○	sorbitol 3	Calibration ▾	2.00

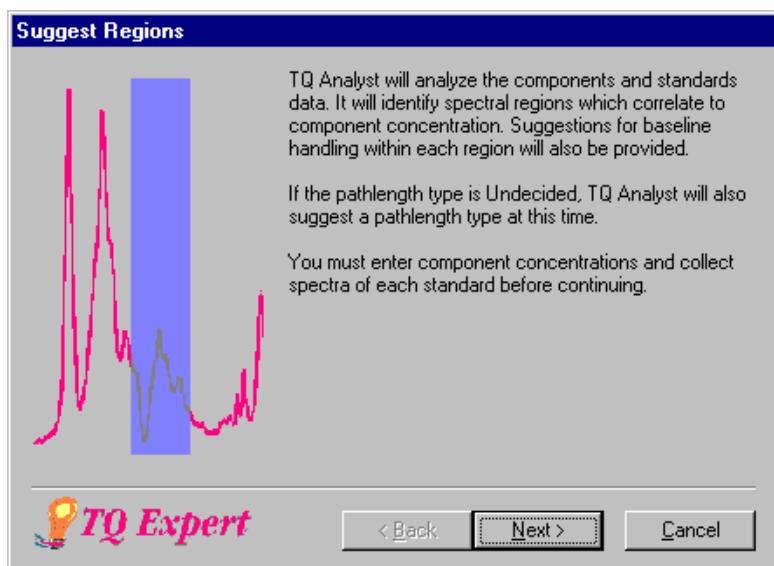
If you want to see the file names of the standards, select Show Spectrum File Names in the list of options that appears above the table. When Show Spectrum File Names is selected, the software expands the standards table to include a File Name column.

The Usage column shows how the standards will be used in the method, as discussed in step 5 of this procedure. You may change the Usage setting for a standard at any time.

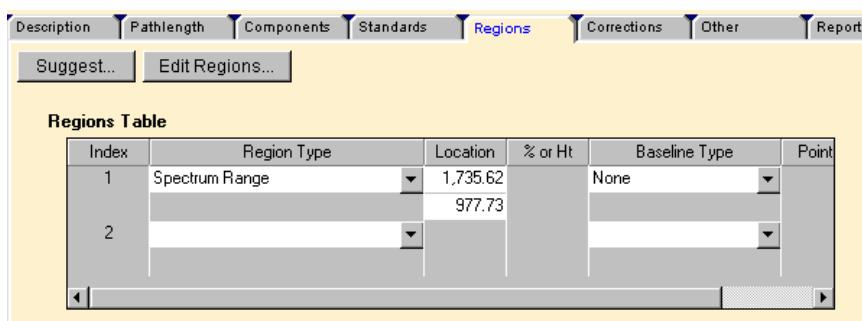
Note If you entered class names or concentration values for the standards, those characteristics will also be imported to TQ Analyst and reported in the Standards table. □

10. Select the Regions tab and specify the spectral region or regions that will be used for the analysis.

If you are setting up a quantitative or qualitative (classification) method, the Regions wizard starts automatically. The initial screen displayed by the Regions wizard is shown below.

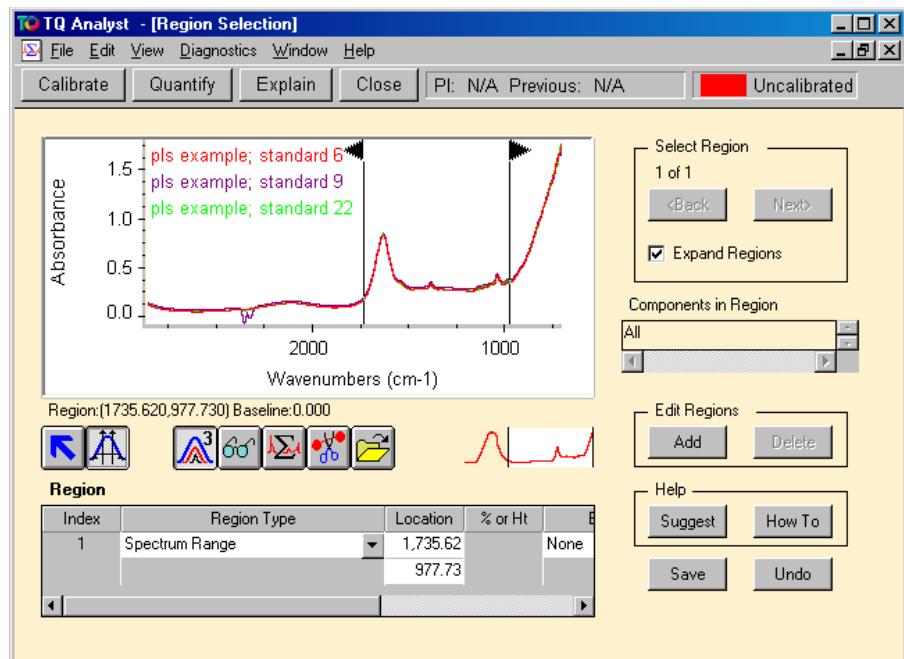


Choose Next in the wizard dialog boxes and then choose Finish to complete the wizard. TQ Analyst displays the Regions tab, as shown below.



The end points of each spectral region that is currently selected for the analysis and the assigned “region type” are displayed in a table. To view the selected regions in a graphical display, choose Edit Regions. The software opens the Region Selection window, as shown below.

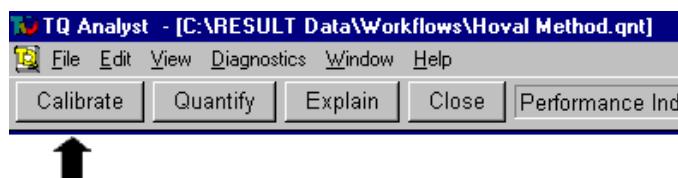
See your TQ Analyst User's Guide for information about selecting regions for quantitative, qualitative, and spectral measurement methods, or choose the How To button in the Region Selection window to view the instructions on-line.



Use the tools in the Region Selection window to make any adjustments to the selected regions, and the selected measurement type for each of those regions.

Note If you are setting up a spectral measurement method, you must select the peaks or regions to be measured manually using the tools in the Region Selection window. To display the Region Selection window, choose Edit Regions on the Regions tab. The software displays a Windows Open dialog box. Select the spectrum of a representative sample that will be analyzed with this method and then choose OK. The Region Selection window opens with the selected spectrum shown in the graphical display. Use the tools in the Region Selection window to select the peaks or regions to be measured and set the measurement type for each peak or region. ▲

11. When you are finished setting up the method, select the Calibrate button on the TQ Analyst toolbar to calibrate the method.



For quantitative and some qualitative methods, TQ Analyst uses the calibration step to analyze the method standards in order to calculate a method model. The model is then used to predict component concentrations or class similarities in unknown samples.

Note Spectral measurement methods and some classification methods do not require a method model. However, the software uses the “calibration” step to test the method for consistency and proper experimental design. If you neglect to calibrate a TQ Analyst method, the method will cause an error in your workflow when you test or run the workflow in RESULT software. ▲

12. Choose Save Method from the File menu to save the new method.

Three files are created when you save a new TQ Analyst method. All three files will use the method file name you entered in step 4 above. The method specifications are saved in the file methodname.QNT. The spectral data for the method standards are stored in two associated library files (methodname.LBD and methodname.LBT). All three method files are saved in the same directory and path as the open workflow.

13. Choose Exit from the File menu to quit TQ Analyst software.

TQ Analyst closes and control is returned to RESULT Integration. The current workflow appears in the workflow navigation frame.

14. If you configured the new method to be linked to a measure event in this workflow (see step 4 above), choose Save on the RESULT Integration toolbar to save the workflow.

The TQ Analyst method files are now linked to the workflow.

Using third-party methods with RESULT

RESULT supports add-in options for method development software applications from other software companies as well as our TQ Analyst method development software. The supported third-party applications include the following.

- Thermo Scientific PLSplus/IQ method development software for GRAMS/32° AI.
- The Unscrambler® method development software from Camo AS.
- Pirouette method development software from InfoMetrix, Inc.

Note

Please refer to the release notes for RESULT software (located on your Antaris Documentation disk) for information about the versions numbers for these software packages that are compatible with TQ Analyst and RESULT software. ▲

Read this section to learn how to create and save analytical methods that are compatible with RESULT using one of the third-party method development applications listed above. The chapter also demonstrates how to link a third-party method to a workflow created in RESULT Integration. After linking a third-party method to a RESULT workflow, you can save, test and run the workflow in RESULT Integration or RESULT Operation software the same way you do for workflows that are linked to methods created using TQ Analyst method development software.

Before you begin

Before you begin creating methods that will be linked to RESULT workflows, consider the following points:

- Make sure the third-party method development application and any required run-time files are properly installed and configured on the computer you use to run RESULT. See *Installing Your Software* for more information.
- Make sure the RESULT add-in option for your third-party method development software is installed on your computer. Use Instrument Status to determine whether the proper software components are installed. To view the instrument status report, choose Instrument Status from the Maintenance menu of RESULT Operation software. If you need to install an add-in option, see *Installing Your Software* for instructions.

- Workflows and their associated method files must be stored in the same directory or the workflows will not run. If a method has associated library or other run-time files, store those files in the same directory as the corresponding method. To determine which files are required to run a third-party method from another location or another software package such as RESULT, see the documentation that came with your third-party method development software.

To locate workflows and methods, RESULT uses the directory and path specified in the Options dialog box in RESULT Integration software and in the RESULT Options dialog box in RESULT Operation software. To learn how to specify paths for storing workflows and methods in RESULT software, see ‘Setting RESULT Integration Options’ in this manual and “Setting RESULT Operation Options” in the “RESULT Software Administration” manual.

- When configuring and collecting standards for methods developed using third-party software, use the Configure Standards and Collect Standards commands in RESULT Integration or RESULT Operation software to configure and collect the method standards. In the Configure Standards dialog box, set the Sample Information feature on the Collect tab to “No Sample Prompt” and clear Require Digital Signature on the Save tab. Those features work only for methods developed using TQ Analyst software. You should also set the file format to Galactic (*.spc extension). Galactic is a binary file format that is compatible with The Unscrambler, PLSplus/IQ and Pirouette method development applications. See “Collecting Standards for Third-Party Methods” in the next section for more information.

When you are finished collecting the methods standards, use the third-party application to build your new method. (The Build TQ Analyst Method command in the RESULT Integration Tools menu works only for methods created using TQ Analyst software.)

- You cannot use RESULT software to digitally sign methods created using third-party method development software. Only TQ Analyst method files can be signed from RESULT software.

- You may use a request event to set up a class-selection dialog box for qualitative (classification) methods created in TQ Analyst software (see “Request events” in “Workflow Events and Specifications” for more information). This feature is not available for methods created using third-party method development software.

Collecting standards for third-party methods

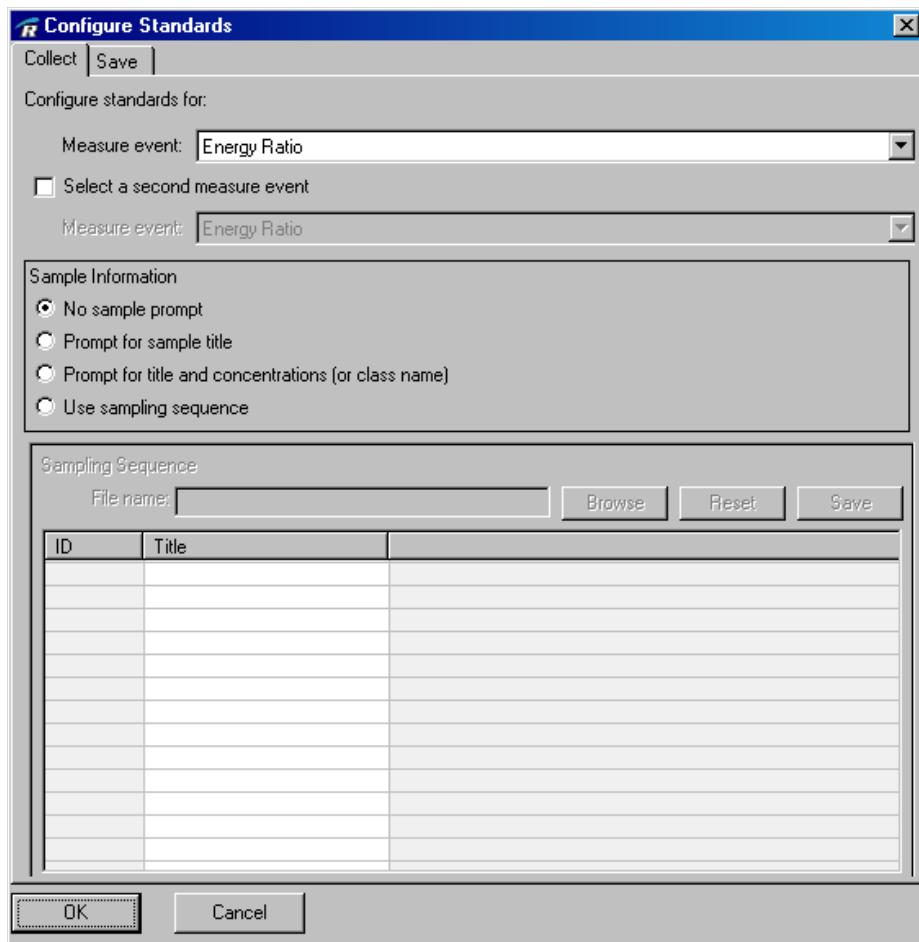
Before creating a new method for a RESULT workflow, create the basic workflow, including at least one collect event and a subsequent measure event, set up the collection parameters in the corresponding sample and background specifications, and then use the Configure Standards and Collect Standards commands in the RESULT Integration Tools menu to configure and collect the method standards.

Note

Standards may also be run from RESULT Operation software using the Configure Standards and Collect Standards commands in the Standards menu. Before you are able to run standards in RESULT Operation, the RESULT administrator must give you the privilege to access the Standards menu. ▲

The Configure Standards dialog box allows you to define how the standards will be collected and archived. Use the Collect tab shown below to select the measure event(s) that requires standards.

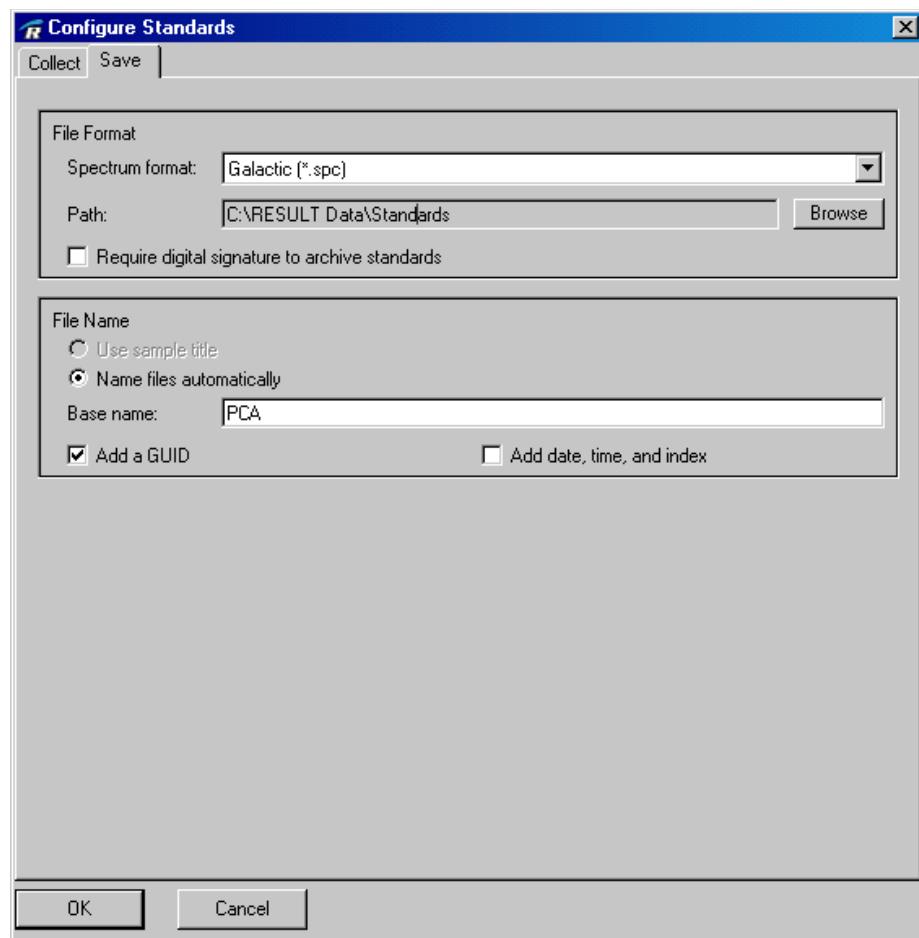
See “Setting up the collection of standards” in this chapter for descriptions of the features in this dialog box.



When configuring standards for methods developed using third-party software, set Sample Information to “No Sample Prompt” as shown above and use your third-party method development application to enter the sample titles and concentration values or class names. The sample information feature works only for methods developed using TQ Analyst method development software.

Use the Save tab shown below to define the file format, path and base name for the new standards.

See “Setting up the archiving of standards” in this chapter for descriptions of the features in this dialog box.

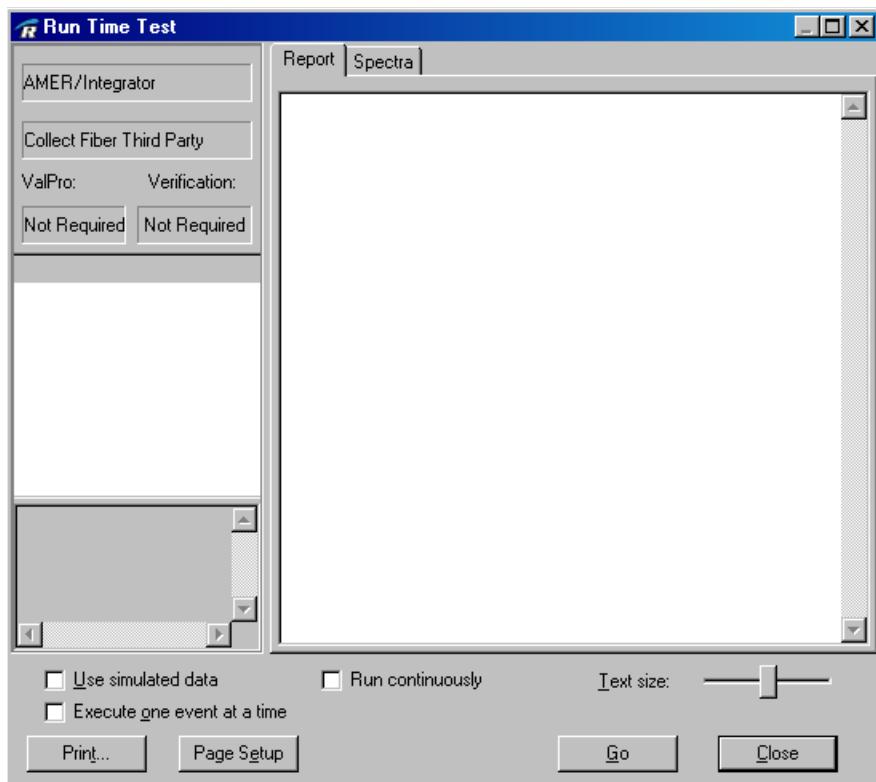


When configuring standards for methods developed using third-party software, follow these steps:

- **Set the file format to Galactic (*.spc extension).** Galactic is a binary file format that is compatible with The Unscrambler, PLSpplus/IQ, and Pirouette method development applications.
- **Clear Require Digital Signature.** This feature works only for methods developed using TQ Analyst software.

When you are ready to collect the standards, in the RESULT Integration main window open the Tools menu and then choose Collect Standards. The software displays the Run Time Test window, as shown below.

See “Testing a Workflow” in “Chapter 2 Creating and Editing Workflows” for descriptions of the features in the Run Time Test window.



RESULT Integration collects standards based on how they were configured in the Configure Standards dialog box, along with the parameters specified in a collect and measure event in a workflow. See “Collecting Standards” in this chapter for more information.

Building a third-party method for use with RESULT software

After collecting the method standards, use your third-party software to build the new method. (The Build TQ Analyst Method command in the RESULT Integration Tools menu works only for methods created using TQ Analyst software.) When the method is completed, save it and then copy the method file and any other required run-time files to the directory and path for workflows and methods specified in the Options dialog box in RESULT Integration software or the RESULT Options dialog box in RESULT Operation software.

To determine which files are required to run a third-party method from another location or software package such as RESULT, see the documentation that came with your third-party method development software. For information about specifying paths for storing workflows and methods in RESULT software, see “Setting RESULT Integration Options” in this manual and “Setting RESULT Operation Options” in the “RESULT Software Administration” manual.

Note You must have the Unscrambler ON-LINE Classifier (OLUC) application installed on your computer to run an Unscrambler classification method from RESULT software and the Unscrambler ON-LINE Predictor (OLUP) application to run quantitative methods from RESULT. See *Installing Your Software* for more information. ▲

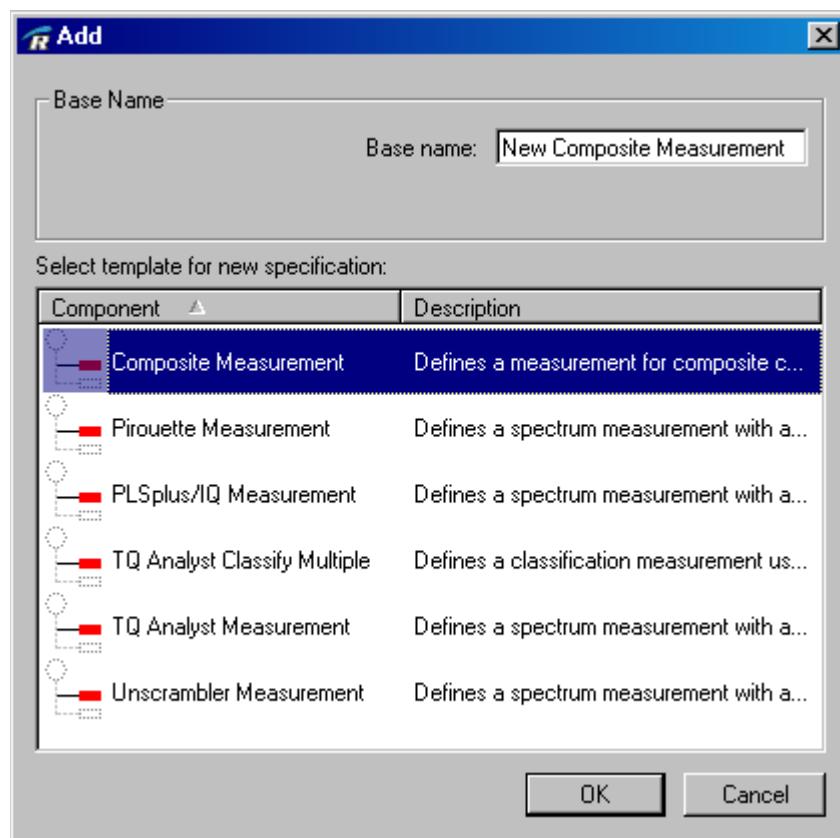
Note You must have the full version of Pirouette software installed on your computer and Pirouette correctly configured for proper operation with RESULT. See *Installing Your Software* for more information. ▲

Linking a third-party method to a RESULT workflow

When creating workflows in RESULT Integration software, use a measurement specification to link your workflow to an existing third-party method. You can create a measurement specification two ways: from the Workflow tab (by choosing the New button at the right of the Measurement Specification list box) or from the Details tab (by selecting the Measure Specifications group and then choosing Add from the toolbar in the RESULT Integration main window). After you choose Add, the following dialog box appears.

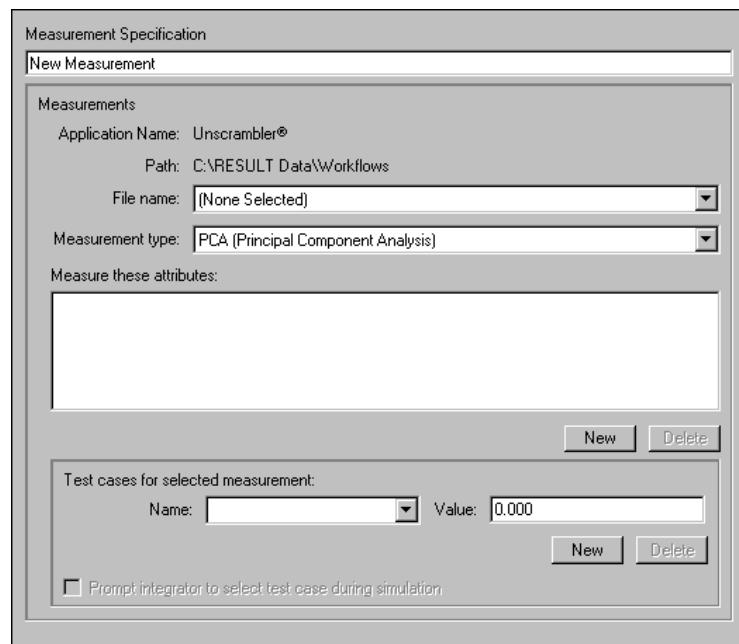
If you don't see a measurement specification that matches your method development application, make sure the

application and any required run-time files are properly installed and configured on the computer you use to run RESULT. In addition, check that the RESULT add-in option for your method development software is installed. Use Instrument Status to determine whether the proper software components are installed. To view the instrument status report, choose Instrument Status from the Maintenance menu of RESULT Operation. If you need to install a run-time file or add-in option, see "Installing Your Software" for instructions.



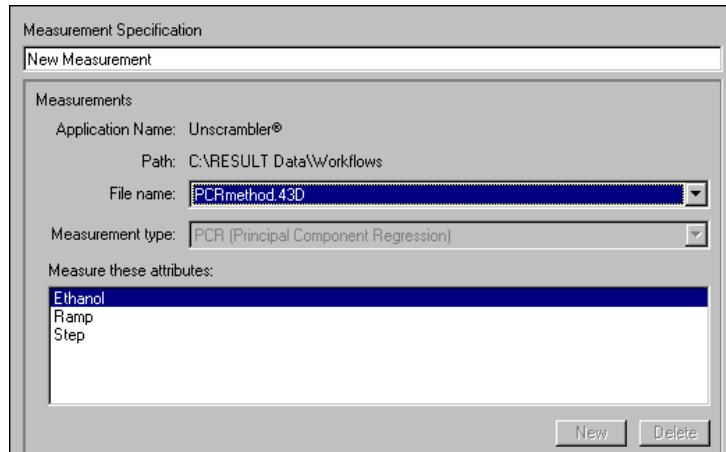
Select the template that matches the method development software application you used to create your analytical method. The software adds a new measurement specification for that software application to the workflow.

The following illustration shows a measurement specification for methods creating using The Unscrambler software.



Use the File Name list box to select a method file to link to your workflow. Only methods created using the selected software application appear in the drop-down list. For example, when using the Unscrambler measurement specification, only Unscrambler methods appear in the drop-down list. (If your method doesn't appear in the drop-down list, copy it to the directory and path listed above the File Name list box.)

After you select a method file, the measurement type and the RESULT component or other attribute names appear below the method file name, as shown below.



Use the Test button on the RESULT Integration toolbar to test the new workflow. See “Testing a Workflow” in “Chapter 2 Creating and Editing Workflows” for more information.

For each third-party method development software package and method type supported in RESULT, the following table lists each output variable and its corresponding RESULT attribute name. The attribute names appear in the Attribute list boxes throughout RESULT software so they can be added to logical test specifications, calculations, and sample reports in a workflow.

Application Name	Application Method Type	Application Variable Name	RESULT Attribute Name
PLSplus/IQ	PLS1	Concentration	Concentration
		Spectral F ratio (calculated)	F-Ratio
		Distance	Mahalanobis distance
	PLS2	Concentration	Concentration
		Spectral F ratio (calculated)	F-Ratio
		Distance	Mahalanobis distance

Application Name	Application Method Type	Application Variable Name	RESULT Attribute Name
Unscrambler	PCR	Concentration	Concentration
		Spectral F ratio (calculated)	F-Ratio
		Distance	Mahalanobis distance
	Discriminate	Residual	Concentration
		Spectral F ratio (calculated)	F-Ratio
		Distance	Mahalanobis distance
Pirouette	PLS1	yPredicted	Concentration
		yDeviation	Confidence value
	PLS2	yPredicted	Concentration
		yDeviation	Confidence value
	PCR	yPredicted	Concentration
		yDeviation	Confidence value
PCA	PCA	Si	Concentration
		Si/S0	Distance result
	PLS	Y Predictions	Value
		F Ratio	F-Ratio
	PCR	Mahalanobis Distance	Mahalanobis distance
		yPredicted	Value
CLS	PCR	F Ratio	F-ratio
		Mahalanobis Distance	Mahalanobis distance
	CLS	Y Predictions	Value
		F Ratio	F-ratio
	KNN	Mahalanobis Distance	Mahalanobis distance
		Predicted class	Class name
SIMCA	SIMCA	Class Distances	Value
		Predicted class	Class name

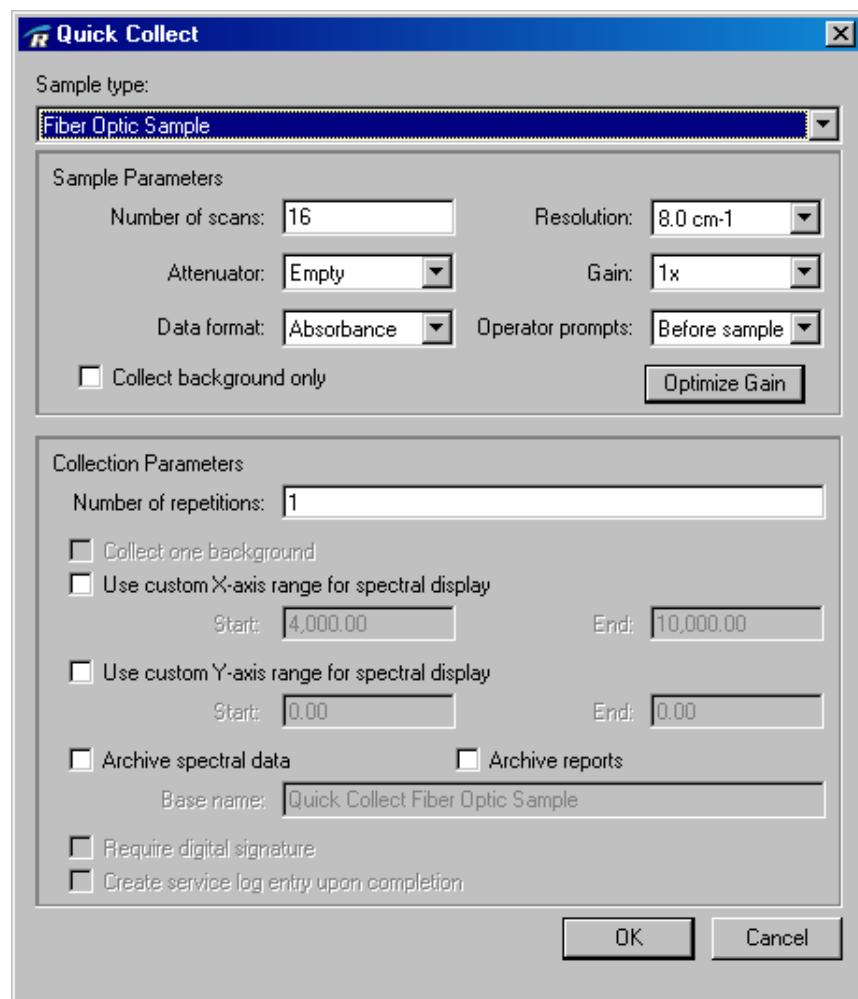
Collecting data using Quick Collect

The Quick Collect feature allows you to collect background and sample spectra without the necessity of creating or selecting a workflow. This is a helpful feature if you simply want to produce a viewable spectrum from a sample or background collection.

To use the Quick Collect feature:

1. Choose Quick Collect from the Tools menu in the RESULT Integration main window.

The software opens the Run Time Test window, along with the Quick Collect dialog box, as shown below.



2. Select the sampling module you plan to use from the Sample Type drop-down list.

The options in the drop-down list will vary, depending upon the instrument your software was configured to use. Once you select a sampling module, the Sample Parameters box will display the default settings for that module.

3. Change any default settings in the Sample Parameters box.

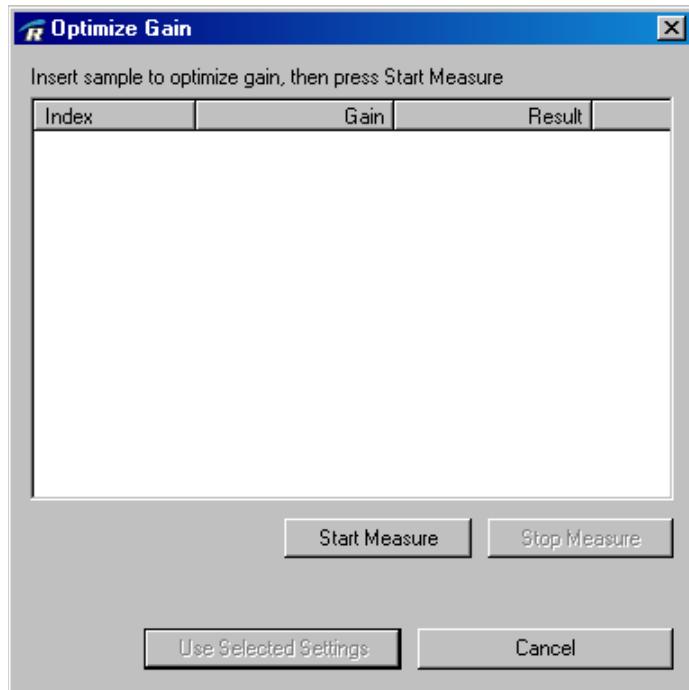
These parameters are described in the “Collect events,” “Sample Specifications,” and “Background Specifications” sections of “Workflow Events and Specifications.”

Recommended settings for the collection parameters are also provided for each sampling module. See the appropriate section for your sampling module in your *Antaris User’s Guide* for more information.

Note When deciding what to select in the Operator Prompts drop-down list, the selection you make should depend on the sampling module you are using and whether you are collecting background data using an internal or external reference. See the appropriate section for your sampling module in your *Antaris User’s Guide* for more information about specifying operator prompts in the Quick Collect feature. ▲

If you need to determine appropriate gain and attenuation settings for your samples, choose Optimize Gain in the Quick Collect dialog box. When you choose Optimize Gain, the following dialog box appears:

For detailed information about the Optimize Gain feature, see “Sample specifications” in “Workflow Events and Specifications.”



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. When the measurements are completed, the results appear in a table in the Optimize Gain dialog box.

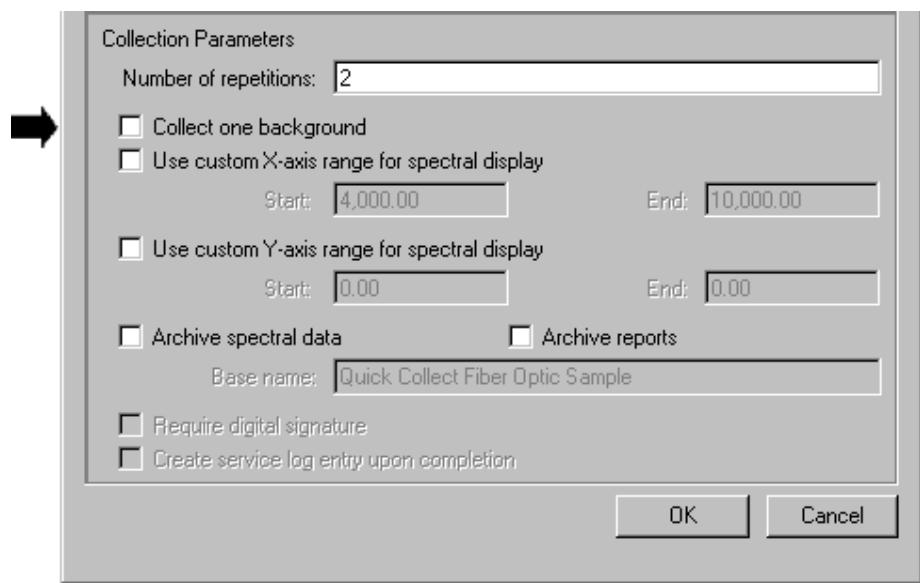
If you want the software to automatically reset the Attenuator and Gain parameters in the Quick Collect dialog box to the recommended settings (or simply reset Gain to the highest voltage value), choose Use Selected Settings in the Optimize Gain dialog box. The dialog box closes and the new Gain setting appears in the Quick Collect dialog box.

4. If you are collecting a background spectrum only, select Collect Background Only.

When this option is cleared, the software collects both a background and sample spectrum.

5. If you want to collect multiple spectra from the same sample (recommended for samples that are not homogeneous), enter the number of collections you want to perform in the Number Of Repetitions text box.

If Number Of Repetitions is greater than 1, then the Collect One Background feature will become available, as shown below.



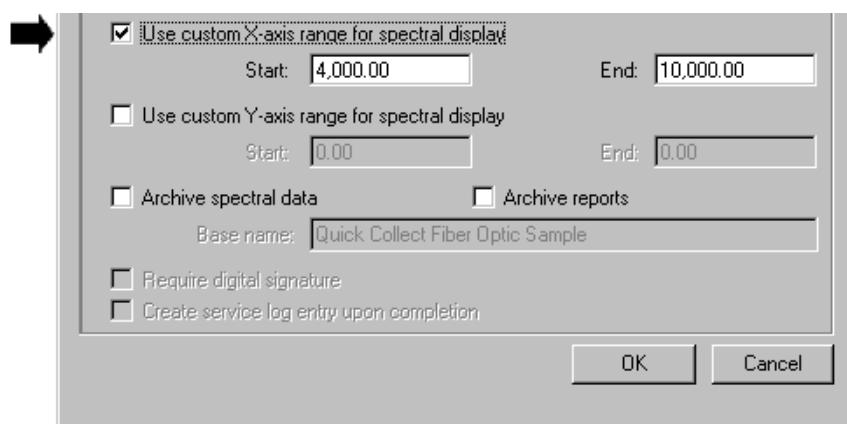
Select Collect One Background if you want to collect only one background spectrum for the experiment. If you want to collect a background spectrum for each sample collection, then do not select this check box.

Note If you use the option to collect multiple spectra, then those spectra will not be displayed until all of the repetitions are completed. If you elect to archive the spectral data and/or report from multiple collections, the spectra will be saved in separate data (*.spa) files and overlaid in a spectral plot in a report (*.htm) file. ▲

6. If you want to specify custom X- and/or Y- axes for the spectral display, select the Use Custom X-axis Range For Spectral Display and/or the Use Custom Y-axis Range For Spectral Display check box(es).

If you do not select custom axes, then the software will use the default spectral range and data format range (the data will be autoscaled). If you select one or both of the custom axis check boxes, then you need to enter the beginning and ending ranges in the appropriate entry boxes, as shown below.

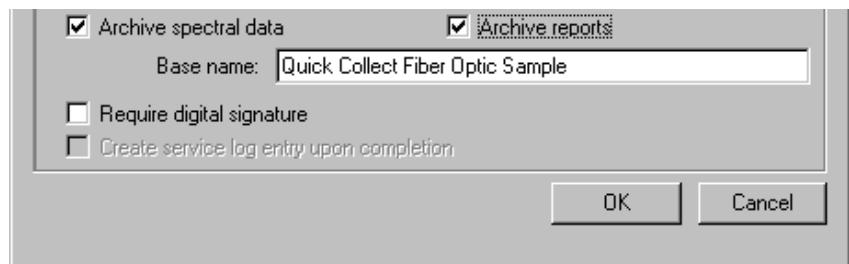
The Start and End entry boxes become available if you select one of the custom axes check boxes. Enter the starting and ending values in the appropriate entry boxes.



7. Select any archive options.

You can elect to archive a spectrum and/or report by selecting the appropriate check boxes. The Archive Spectral Data check box directs the software to save the spectrum as a spectral file (*.spa), which is compatible with many Thermo Scientific spectroscopy software packages, including RESULT Integration and TQ Analyst. Archive Reports directs the software to save the report as an HTML file (*.htm), which is viewable by Web browser applications and RESULT Integration and Operation software. If the report includes a spectrum, it also saves a bitmap image of the spectrum (*.png) in the same directory as the report. The bitmap image is required to properly display the report in RESULT software. If you open the report file and the bitmap image isn't available, the report will have a blank box where the spectrum should be.

If you elect to archive the spectrum or report, then the Base Name box and Require Digital Signature check box become available, as shown below.



The software automatically completes the Base Name box based on the type of module you are using. However, you can change this base name or delete it.

If you use a base name, the files will be saved with that base name, plus a globally unique identifier (GUID) and the appropriate extension. If no base name is entered, the files will be archived using the GUID and the appropriate extension.

You can also elect to digitally sign the archived item by selecting the Require Digital Signature check box.

8. After you have selected the appropriate options, choose OK.

The software closes the Quick Collect dialog box. If you close the dialog box without choosing OK, your settings will not be saved and collection will not begin. Choose Cancel to close the dialog box without saving your settings.

9. Choose Go from the Run Time Test Window to begin collection.

After you choose Go, the software begins data collection. If you are prompted to prepare for a background and/or sample collection, after you have prepared the appropriate items, choose OK at the software prompt to continue the collection process.

When data collection is complete, the spectrum appears in the display area of the Run Time Test window. If you elected to archive the spectra and/or report files but did not require digital signatures, the

file(s) are automatically archived. Archived data produced using the Quick Collect feature of RESULT Integration are placed in a Quick Collect subdirectory, which is located in the current directory for archiving spectra and reports as specified in the RESULT Options dialog box. See “Setting RESULT Integration Options” in “Chapter 1 Getting Started” for information about specifying the directory for archiving spectra and reports.

If you elected to archive items and require a digital signature, the software opens the Digital Signature dialog box, as shown below.



Enter your Windows user name in the User Name box, and your password in the Password box. The user name and password must match your Windows user name and password exactly, including the letter case.

Select the Authorship option from the Reason for Signature drop-down list, or enter another appropriate reason for the signature, and choose OK.

The spectrum is given a unique file name based on the base name, if one exists, along with the date and time the spectrum was collected and a globally unique identifier (GUID). The file is stored in the location that was specified in the Configure Standards dialog box in the previous chapter.

Note You have three attempts to enter your password correctly when digitally signing a file. If you are unable to correctly enter your Windows password, or if you choose Cancel from the Digital Signature dialog box, the file will not be digitally signed. The software will create a report of workflow errors indicating that the file has not been signed. □

Viewing Spectra

The View Spectra feature in RESULT Integration software allows you to view a spectrum or spectra using the TQ Analyst software package. You can view spectral files that have been saved in one of the following formats:

- **Nicolet (*.spa)**, which is the standard format for spectra for use with Thermo Scientific spectroscopy applications, including RESULT Integration, RESULT Operation, and TQ Analyst.
- **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 header 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.

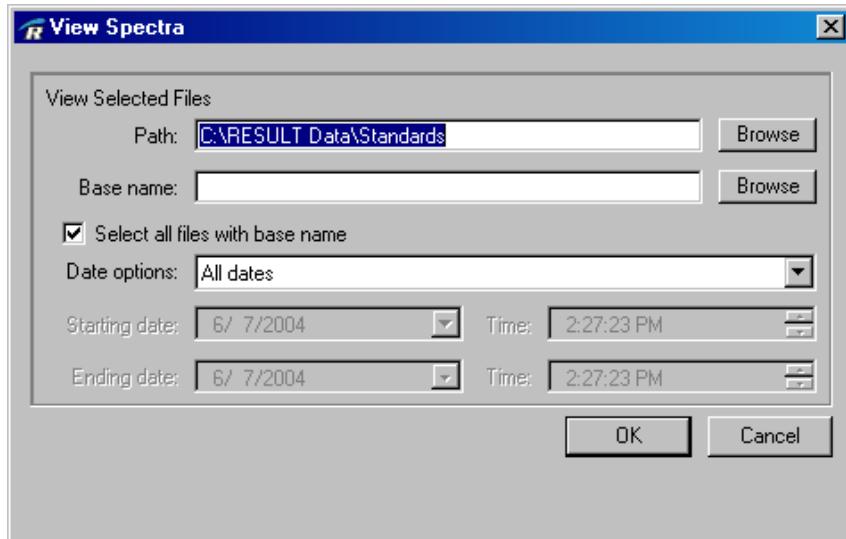
The View Spectra feature allows you to open a spectrum or group of spectra based on a file base name and/or date range.

Note In order to use the View Spectra feature, you must have TQ Analyst software installed on your system. TQ Analyst is included on your RESULT disk. ▲

To view a spectrum or spectra:

1. **Select View Spectra from the Tools menu in the main window of RESULT Integration software.**

The software opens the View Spectra dialog box, as shown below.

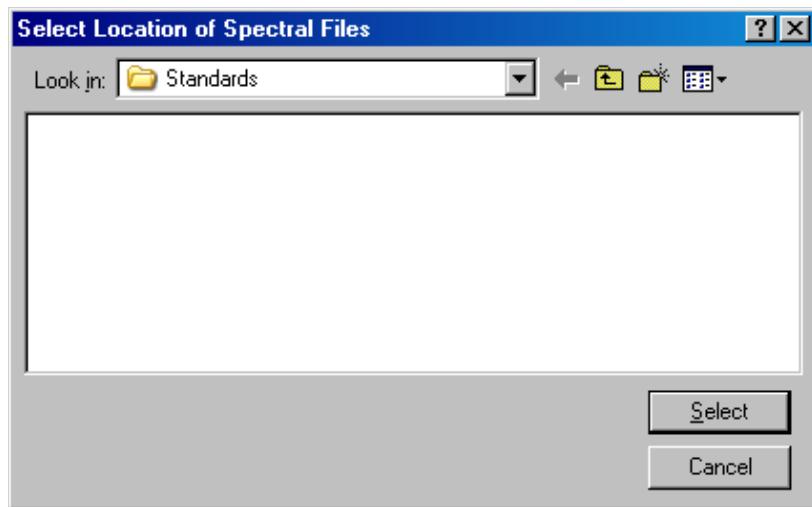


2. Enter the path where the spectrum or spectra are located in the Path text box.

If the correct path does not already appear in the box, you can type the path in the text box, or choose Browse to open a standard Windows Browse dialog box.

If you choose Browse, navigate to the correct path in the Browse dialog box, and then choose Select, as shown below.

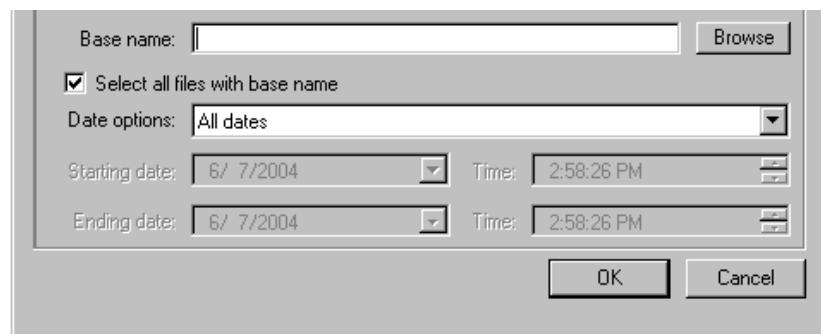
Spectral files do not appear in the Browse dialog box when choosing a directory path.



The dialog box closes and the selected path appears in the Path box in the View Spectra dialog box.

3. Select the standards you want to view.

Use the Base Name and Date Options features to select the standards.



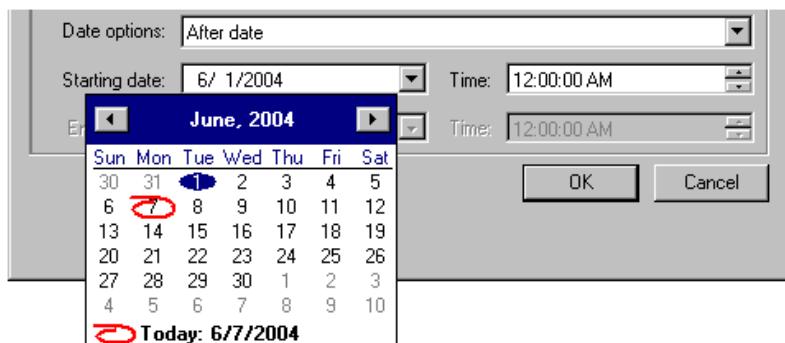
- **Select All Files With Base Name.** To select multiple standards that have the same base name, leave this check box selected. If you want to select a single standard or a group of standards that have unique file names, clear Select All Files With Base Name.
- **Base Name.** If the file names of all the standards have the same base name, you can use the base name feature to quickly select those standards. Make sure Select All Files With Base Name is selected (see above) and then enter the base name in the Base Name box, or choose Browse to search for a representative standard. After you select a standard, its base name appears in the Base Name box in the View spectra dialog box. The software will select all the standards that have the specified base name and are located in the specified directory and path, or use Date Options to limit those standards.

Note Using a base name to select the spectra to view can cause a delay if you have many spectra with the same base name. ▲

If you want to select a single standard, make sure Select All Files With Base Name (see above) is cleared and then use the Base Name box to specify the standard. You can type the file name of the standard in the Base Name box or choose Browse to search for the standard. After you choose Browse, the software opens a standard Windows Open dialog box that points to the appropriate path, and you can select the standard. After you select the standard, its file name appears in the Base Name box in the View spectra dialog box. The software will select only that standard.

If you want to select a group of standards that have unique file names, make sure they are located in the specified path and leave the Base Name box blank. The software will select all the standards located in the specified directory and path or use Date Options to limit those standards.

- **Date Options.** Use the Date Options to broaden or limit the selected standards. Leave the default setting (All Dates) to select all standards that have the specified base name, if one was entered, and are located in the specified directory and path. If you want to limit the selected standards to include only those files which were collected on a certain day or time, or in a date or time range, set the date or time option by selecting an item in the Date Options drop-down list. Depending on the selection you make, the Starting Date and/or Ending Date boxes may become available. You can change the dates in these boxes by:
 - *Typing* the appropriate date(s) in the boxes;
 - *Selecting* a portion of the date and using the arrow keys on your keyboard to adjust the date; or
 - *Selecting* the drop-down arrow to the right of the box. If you select the drop-down arrow on one of the date boxes, the software opens a calendar, as shown below.



Choose the date from the calendar with your cursor. Use the arrow buttons at the top of the calendar to navigate to the next and previous months.

You can change the time by typing the appropriate time in the box, or by selecting a portion of the time and using the arrow keys on your keyboard or the Up and Down buttons to the right of the box to change the time.

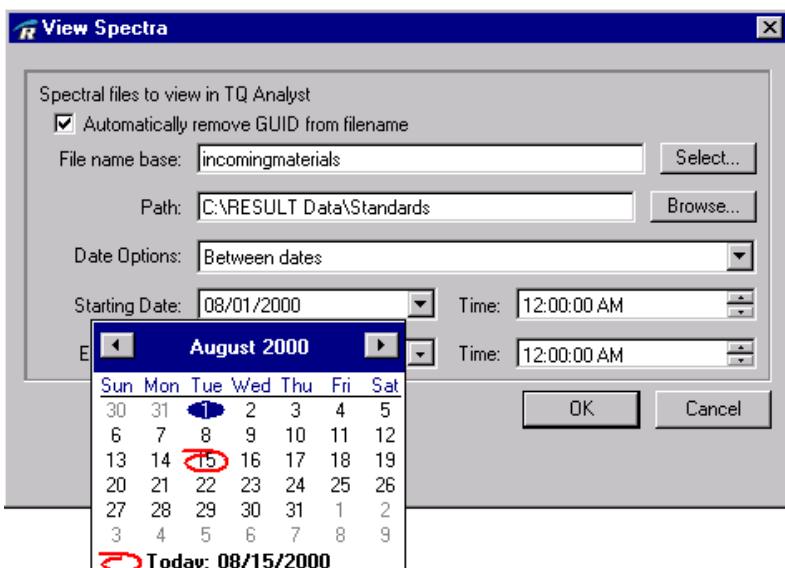
4. Use the Date Options to broaden or limit the selected spectra.

Leave the default setting (All Dates) for Date Options to select all spectra that have the specified base name, if one was entered, and are located in the specified directory and path.

If you want to limit the selected spectra to include only those files which were collected on a certain day or time, or in a date or time range, set the date or time option by selecting an item in the Date Options drop-down list.

Depending on the selection you make, the Starting Date and/or Ending Date boxes may become available. You can change the dates in these boxes by:

- *Typing* the appropriate dates(s) to the boxes;
- *Selecting* a portion of the date and using the arrow keys on your keyboard to adjust the date; or
- *Selecting* the drop-down arrow to the right of the box. If you select the drop-down arrow on one of the date boxes, the software opens a calendar, as shown below.



Choose the date from the calendar with your cursor. Use the arrow buttons at the top of the calendar to navigate to the next and previous months.

You can change the time by typing the appropriate time in the box, or by selecting a portion of the time and using the arrow keys on your keyboard or the Up and Down buttons to the right of the box to change the time.

5. Choose OK to view the spectrum or spectra you have specified.

The software closes the View Spectra dialog box and opens TQ Analyst. Depending upon the number of spectra you have chosen to view, it may take several minutes for the software to load the spectra into TQ Analyst.

Once the software has finished loading the spectra, you can view each spectrum by selecting it from the drop-down list, as shown below.



See your TQ Analyst documentation for information about working with the features in the spectral window.

Chapter 5 System Maintenance

The Maintenance menu in RESULT Integration contains diagnostics and other features to assist you with troubleshooting and maintenance of the system. The features in the maintenance menu include:

- **Test Sample**, which allows you to perform a diagnostic run of a sample collection event in a workflow.
- **Test Background**, which allows you to perform a diagnostic run of a background collection event in a workflow.
- **Test Measurement**, which allows you to perform a diagnostic run of a measurement event in a workflow.
- **Instrument Status**, which produces a report of the status of the laser, source, detectors, and power supply. The instrument status report also contains serial numbers and firmware version information.
- **Align Instrument**, which calibrates the gain, aligns the laser, and optimizes the interferogram position for the instrument.
- **Instrument Check**, which uses the main analyzer transmission detector to produce a series of spectra for diagnostic purposes. The spectra produced by running the instrument check include an interferogram, a single-beam, 100% line, and polystyrene (if the system has an internal attenuator wheel that includes a polystyrene sample).

All of these features are also available in the Maintenance menu of RESULT Operation. For detailed information about using a maintenance feature, see the feature name in “System Maintenance” in the *RESULT Operation User Guide*.

Chapter 6 Troubleshooting RESULT Integration

This chapter describes some possible problems you may encounter when developing and testing workflows in RESULT Integration software and offers some suggestions for resolving them.

If you are unable to resolve a problem or have questions or concerns, call one of our service representatives or use the information at the beginning of this document to contact us.

Notes The information in this chapter pertains to troubleshooting issues within RESULT Integration software only. Troubleshooting information can also be found in other sections of this user's guide pertaining to RESULT Operation software, software administration, and sampling modules.

Updated troubleshooting information can also be found in the release notes issued for the software on your installation disks.

Because they are self-explanatory and contain suggestions for resolution, workflow errors are not covered in this troubleshooting chapter. If you receive workflow errors when testing a workflow, follow the suggestions in the error table for resolving the situation. ▲

When testing workflows, additional troubleshooting information may be found in the troubleshooting chapter in "RESULT Operation Software," since the test mimics how the workflow will be run in RESULT Operation software. ▲

Logging on to the workstation/software

Problem	Possible Causes	Suggestions
A Service Control Manager message appears when you log on to the workstation, stating that at least one service or driver failed during startup.	The analyzer is not connected to the workstation.	If an analyzer is supposed to be connected to the computer, make sure the instrument is properly connected to the computer. Log off the computer and restart before running any workflows. If an analyzer is not supposed to be connected to the computer (if the computer is for software use only), then you do not need to perform any action in order to use the software. However, you may want to have your Windows administrator reinstall the software without loading the bench driver to avoid receiving this message each time you log on to the workstation.

Using the Workflow wizard

Problem	Possible Causes	Suggestions
The sampling module you want to use does not appear in the Sample Specification drop-down list.	The instrument model is specified incorrectly in the software's options.	Choose Options from the Edit menu. In the Target Instrument Options, make sure the proper model is selected from the Model drop-down list.
The Validation Wheel Sample option does not appear in the Sample Specification drop-down list.	The software was not set up to develop customer qualification workflows.	Choose Options from the Edit menu in RESULT Integration software. Make sure the Instrument Has ValPro Option Installed check box is selected in the Target Instrument Options. Note: Your system must have the ValPro System Qualification software package and the internal validation wheel in order to develop customer qualification workflows.

Problem	Possible Causes	Suggestions
The TQ Analyst method does not appear in the TQ Analyst method drop-down list.	The method file is not stored in the directory specified for locating workflows and methods.	<p>Choose Options from the Edit menu. Make sure the directory path for locating workflows and methods points to the file where the method is stored.</p> <p>-or-</p> <p>Locate the method file and move it into the directory for storing workflows and methods as shown in the software's options.</p>

Developing workflows

Note Events and specifications are dependent on each other and must be developed and appear in the proper order to work effectively. See “Workflow Events and Specifications” for specific information about how a particular event or specification is dependent on and related to other events and specifications.

Normally, if an item does not appear in a drop-down list when working with an event or specification, a related event or specification has not yet been created. See the section specifically describing the event or specification for more information about items related to them. ▲

Problem	Possible Causes	Suggestions
You receive an error message stating, “Invalid Setting. Please Check Required Fields.”	A required field in the software is not completed. Usually, the required field is the text box containing the title of the event or specification.	Enter the name of the event or specification in the appropriate text box. If the name already appears, check other text boxes in the software window to determine which required field needs to be completed before progressing further.

Problem	Possible Causes	Suggestions
Specifications are no longer linked to events.	<p>When using copy & paste features to paste items from a workflow in one session of RESULT Integration into a workflow in another session of the software, specifications do not stay linked to workflow events.</p>	Go into each workflow event and attach the appropriate specifications.
Specifications do not appear in workflow events that you have copied from one workflow into another.	<p>When using copy & paste features to paste items from a workflow in one session of RESULT Integration into a workflow in another session of the software, linked specifications are not copied along with events.</p>	Go into the Details tab, copy the appropriate specification(s), and paste them into the new workflow.
The Validation Wheel Sample option does not appear in the New Specification dialog box.	The software was not set up to develop customer qualification workflows.	<p>Select Options from the Edit menu in RESULT Integration software. Make sure the Instrument Has ValPro Option Installed check box is selected in the Target Instrument Options.</p> <p>Note: Your system must have the ValPro System Qualification software package and the internal validation wheel in order to develop customer qualification workflows.</p>

Problem	Possible Causes	Suggestions
<p>You are unable to attach a spectrum to use as a simulated sample in a Sample Specification.</p>	<p>The spectrum's collection parameters do not match the workflow parameters.</p> <p>-or-</p> <p>The spectrum does not have an associated background spectrum.</p>	<p>A spectrum for simulation must have been taken using the same parameters as specified in the workflow in RESULT Integration (except for the Number Of Sample Scans parameter).</p> <p>Collect a spectrum by running the actual workflow and using the intended sample material. Be sure the workflow is set up to archive the spectrum. After running the workflow, choose the archived spectrum to use for simulated data for future workflow tests.</p> <p>-or-</p>
<p>The method name does not appear in the File Name drop-down list in the Measurement Specification.</p>	<p>The method is not stored in the directory specified in the software for locating workflows and methods.</p> <p>The directory path for storing workflows and methods is incorrect.</p>	<p>Copy the method file into the appropriate directory for locating workflows and methods (this information can be found in RESULT Integration options).</p> <p>Choose Options from the Edit menu, and change the path for locating workflows and methods to the appropriate directory.</p>

Problem	Possible Causes	Suggestions
The name of an image file does not appear in the Select An Image text box (in the Add/Edit Header Item dialog box when adding a heading section to a report) after you have chosen to display a custom image from the Select Data Type drop-down list.	The image is not stored in the directory specified in the software for locating HTML images.	Copy the image file into the appropriate directory for locating HTML images (this information can be found in RESULT Integration options).
Images do not appear in reports.	<p>The directory path for locating HTML images is incorrect.</p> <p>The image is not located in the same directory as the report.</p> <p>The image format is not supported by your web browser.</p>	<p>Choose Options from the Edit menu, and change the path for locating HTML images to the appropriate directory.</p> <p>Copy the image file into the same directory as the report.</p> <p>Using another graphic program, save the image in a format that is supported by your web browser, such as *.jpg, *.gif, *.bmp, or *.png.</p>
When testing a workflow, you receive a message stating "Too many bad scans occurred, so collection was aborted."	The gain setting is too high, and you are collecting multiple samples with only one background collection.	<p>In the Sample Specification, lower the Gain to 1x or 2x.</p> <p>-or-</p> <p>In the Collect Event, change the Background Frequency to collect Before Every Sample.</p>
When testing a workflow, you receive a workflow error stating, "Interferogram peak location not found within expected range. An alignment of the instrument may be necessary."	If aligning the instrument does not solve the problem, the gain setting is too high and you are collecting multiple samples with only one background collection.	<p>In the Sample Specification, lower the Gain to 1x or 2x.</p> <p>-or-</p> <p>In the Collect Event, change the Background Frequency to collect Before Every Sample.</p>

Digitally signing files

Problem	Possible Causes	Suggestions
The software is unable to recognize the password you entered when digitally signing a file.	The letter case of your password does not match your password stored on the computer. Another user is logged into the workstation.	Make sure you type the password correctly, including matching letter case (for example, all capital letters, all lower case letters, or a mixture of capital and lower case letters). Be sure the Caps Lock key is not turned on. Close the software and point to Shut Down from the Start menu on the Windows Taskbar. Select the Close All Programs And Log On As A Different User Option, and choose OK. Log onto the workstation using your user name and password.
You receive other types of errors when attempting to digitally sign a file.	Your password has been changed or forgotten Windows Workstation files are missing or were overwritten with different versions when installing other software applications.	See your Windows administrator to reset your password. Have a Windows administrator install or reinstall the latest Windows Service Pack.

Building a TQ Analyst method

Note If you experience other problems with building methods than the ones described below, or if any of the below suggestions do not help resolve the problem you are experiencing, refer to your TQ Analyst documentation for more assistance with building methods. ▲

Problem	Possible Causes	Suggestions
You receive an error message: Failed to read the selected method.	The TQ Analyst method has not been created.	When using the Build TQ Analyst Method dialog box, make sure to select the Create TQ Analyst Method check box and enter a name for the method in the File Name text box.
You cannot add standards to your method.	The method is a measurement only method type.	Standards are not required for a measurement only method type. Double-check the method type to make sure you have selected the correct type.

Viewing spectra

Problem	Possible Causes	Suggestions
The process of opening TQ Analyst to view spectra is taking too long, or the feature stopped working before all spectra were opened.	Too many spectra have been selected to be viewed.	Reduce the number of spectra you are opening with this feature. You can do this by clearing the Automatically Remove G UID From File Name check box in the View Spectra dialog box. Clearing this check box will allow you to open only the spectrum you select (as opposed to all spectra that contain the same file base name).

Configuring and collecting standards

Problem	Possible Causes	Suggestions
While configuring standards, you receive a message stating that the workflow does not contain any measure events.	The appropriate workflow is not loaded in the software.	Select and load the appropriate workflow.
	The workflow does not contain a measure event.	Add a measure event to the workflow.

Running Quick Collect

Problem	Possible Causes	Suggestions
You receive a message stating “Too many bad scans occurred, so collection was aborted.”	The gain setting is too high, and you are collecting multiple samples with only one background collection.	Lower the Gain to 1x or 2x. -or- Clear the Collect One Background only check box so the software will collect a background spectrum for each repetition of the experiment.
You receive a message stating, “Interferogram peak location not found within expected range. An alignment of the instrument may be necessary.”	If aligning the instrument does not solve the problem, the gain setting is too high and you are collecting multiple samples with only one background collection.	Lower the Gain to 1x or 2x. -or- Clear the Collect One Background only check box so the software will collect a background spectrum for each repetition of the experiment.

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