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OMNIC Paradigm Software

OMNIC Paradigm

User Guide

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ThermoFisher SCIENTIFIC

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1

Get Started with OMNIC Paradigm Software

Welcome to OMNIC Paradigm software. Learn how to install and update your software, explore software options, and learn the basics of using OMNIC Paradigm software to measure and analyze spectra.

This section includes the following:

Contents

- Welcome

  Introduces some of the main features and tools for using OMNIC Paradigm software.

- Install OMNIC Paradigm Software

  Provides step-by-step instructions on installing OMNIC Paradigm Workstation software.

- Update Your OMNIC Paradigm Software

  Provides instructions on updating OMNIC Paradigm software and configuring your update settings.

- OMNIC Paradigm Software Options

  Using OMNIC Paradigm software with the desktop or touchscreen interface to optimize the software for your work.

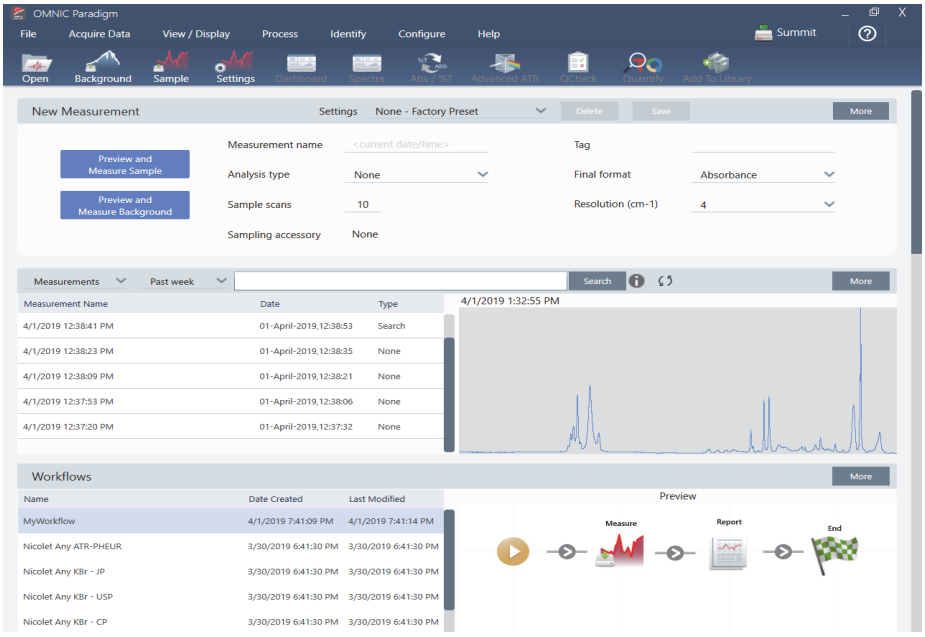
- OMNIC Paradigm Software Basics

  Learn the basics of measure and analyzing spectra using OMNIC Paradigm software.

Welcome

Thermo Scientific™ OMNIC™ Paradigm software for desktop and touchscreen is an advanced software package for FTIR spectroscopy, designed to simplify how you acquire, process, and interpret data and to help you work remotely and collaborate with colleagues around the globe.

Manage New and Recent Work from the Dashboard



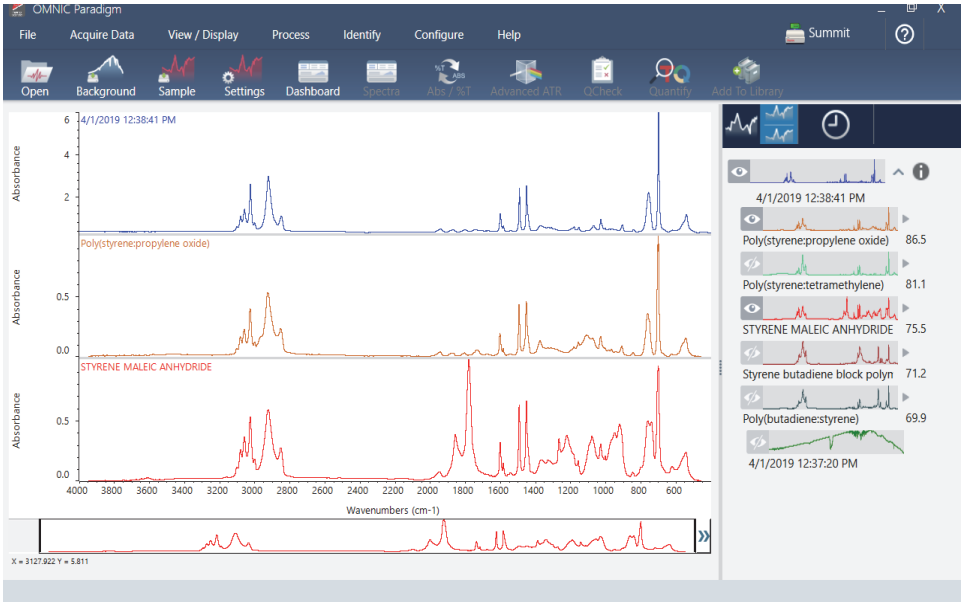
With the new dashboard in OMNIC Paradigm software, you can set and save your measurement settings, measure a new sample, resume your recent work, or run an automated workflow all from the same, convenient screen.

In Paradigm for touchscreen, the home screen provides many of these same tools and features in an even more streamlined, intuitive interface so operators can focus on their work and on the tools they need.

Learn More

- Set and Save Measurement Options
- Measure a Sample
- Create and Run Your First Workflow

Process, Analyze, and Explore Spectra in the Spectral View



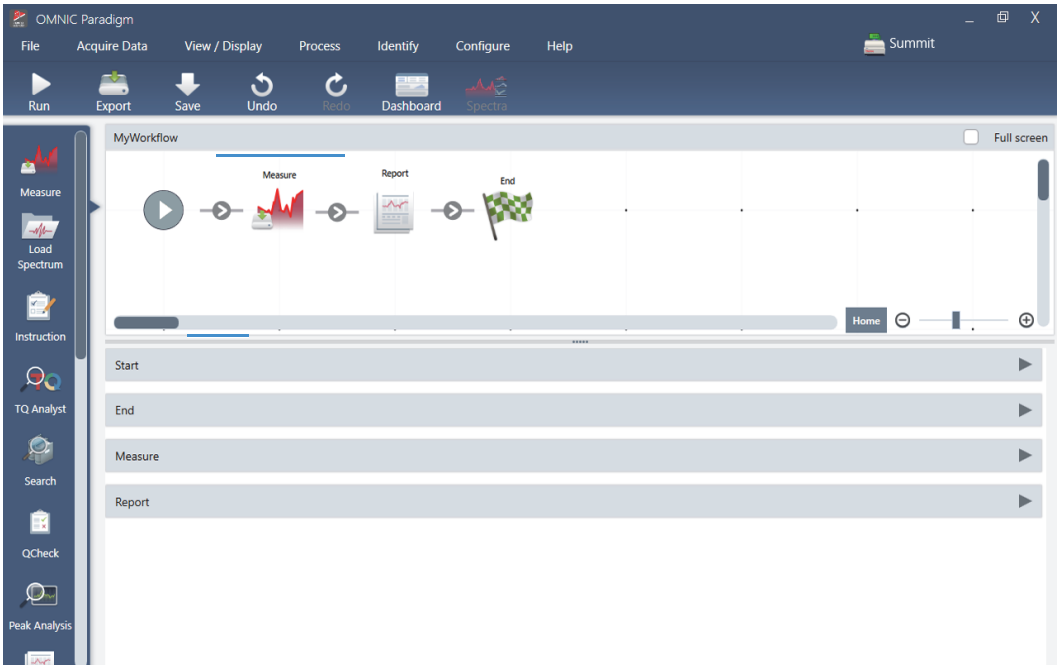
Use the spectral view to process, analyze, or explore your data in depth. Here you can process your data, find and label peaks, and optimize the view so you can more easily compare or analyze spectra.

The results pane allows you to quickly add or remove a spectrum from the main view, explore details of each spectra, or review the change history of your selected spectrum.

Learn More

- Identify an Unknown Sample with ATR
- Identify an Unknown Sample with Transmission

Automate Repetitive Tasks with Workflows



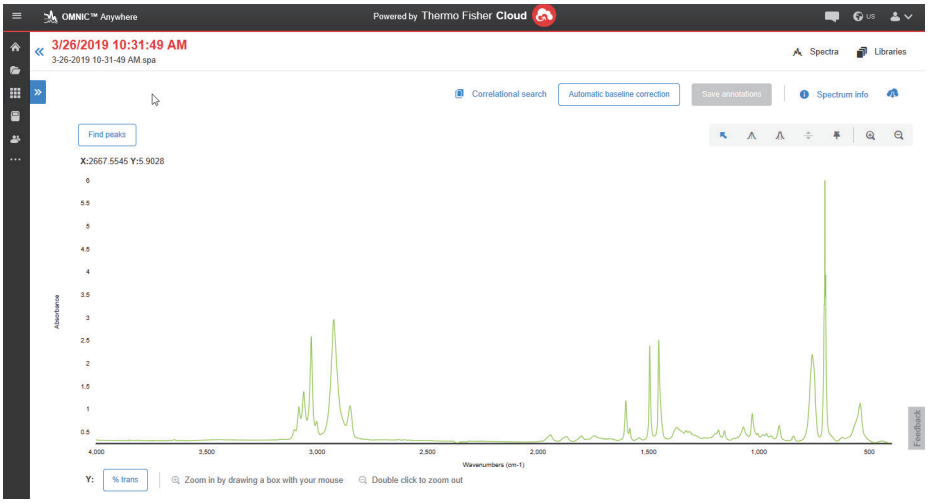
Automate your tasks with a workflow to ensure that measurements are collected and processed in exactly the same way each time. Edit or create a workflow by simply dragging and dropping tiles in the workflow editor, and then run the workflow at the click of a button.

Operators using Paradigm for touchscreen can import and run one of our factory installed performance tests or a custom workflow right from the home screen.

Learn More

- Create and Run Your First Workflow
- Workflow Tiles Reference

Share Your Work Remotely



Upload your data to the cloud and use OMNIC Anywhere to view, analyze or share your data using any connected PC, Apple computer, Android or iOS device.

With a Nicolet™ Summit™ spectrometer and a free Connect account, measure samples in the classroom or lab, upload the data to your Connect account, and view, explore, or share the data on another device in your dorm or workspace.

Learn More

- View Your Data with the OMNIC Anywhere App

Install OMNIC Paradigm Software

OMNIC Paradigm software comes preinstalled on the Thermo Scientific™ Nicolet™ Summit Spectrometer and is ready to use with the attached touchscreen monitor or with an external monitor connected by Mini DisplayPort.

Install OMNIC Paradigm Workstation software on your desktop, laptop, or other device to connect to an instrument over an Ethernet or WiFi connection. Connect to an instrument to measure a sample and disconnect to allow other operators to use the instrument while you analyze your data or develop workflows.

This guide walks you through installing OMNIC Paradigm Workstation software.

Before You Begin

Your system should meet the recommended system requirements outlined below to run and use OMNIC Paradigm Workstation software.

Recommended System Requirements

Operating System	Windows 10 (64-bit)
Processor	Intel Core i5 3.3GHz
RAM	8 GB
Hard Disk	2 GB of available hard-disk space for installation; Additional hard-disk space recommended for storing files. If you are hosting your database on this machine, we recommend 500 GB of hard-disk space.

Install OMNIC Paradigm Workstation

Installing OMNIC Paradigm Workstation takes only a few minutes.

❖ To install OMNIC Paradigm Workstation software

1. Insert the provided installation media (either DVD or flash drive).
2. Run the installer.
   a. When the download completes, run the OMNIC Paradigm.exe file.

b. Follow the on-screen prompts to install OMNIC Paradigm Workstation software.

Set Up and Connect OMNIC Paradigm Workstation

By default, data is saved to the database on your local device. If you connect to a Nicolet Summit Spectrometer, you can continue using your local database, or you can connect to the database on the instrument or another database located on your network.

❖ To connect to a default database

1. Open OMNIC Paradigm Workstation software.
2. Select **Configure > Database.**
3. In the Database Engine list, select **Thermo Scientific Built-in Database**.
4. Enter the server address or URL for your database. The server address or URL is the name of the instrument that you want to connect to on your network.

Update Your OMNIC Paradigm Software

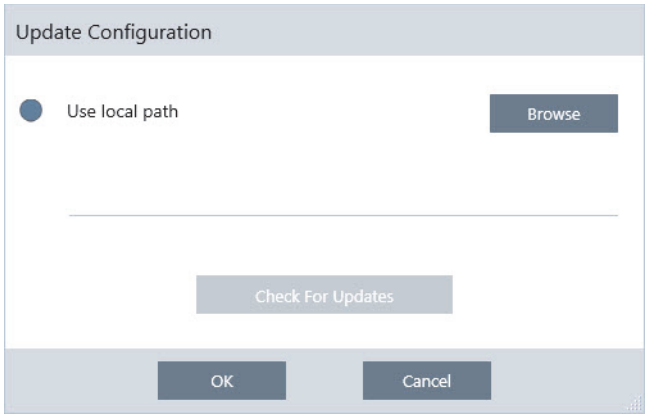
We recommend that you install the latest updates for OMNIC Paradigm software to ensure that you can take advantage of new features and stability improvements.

The latest version of OMNIC Paradigm software is **1.0**.

Note Your spectral data and saved measurement settings will be carried over to the new version. No data will be lost in the update.

❖ To update OMNIC Paradigm software (desktop interface)

1. Using the desktop interface, open the **Configure** menu and select **Update**.



2. In the Update Configuration dialog, click **Browse** and navigate to the local or network directory where updates will be stored.

   Once you have configured the directory for updates, any new versions of OMNIC Paradigm software in this location are automatically recognized. The software automatically checks this location for updates once daily, but you can return to this dialog to manually check for updates at any time.

   A prompt notifies you when new updates are available.

3. Click **Check for Updates**. After a brief scan, a list of available updates is displayed.

4. From the list of available updates, select the version you would like to install and click **Install Update**. Follow the on-screen installation prompts.

You can also configure updates using the touchscreen interface by opening the Settings view and navigating to the Application Updates tab.

OMNIC Paradigm Software Options

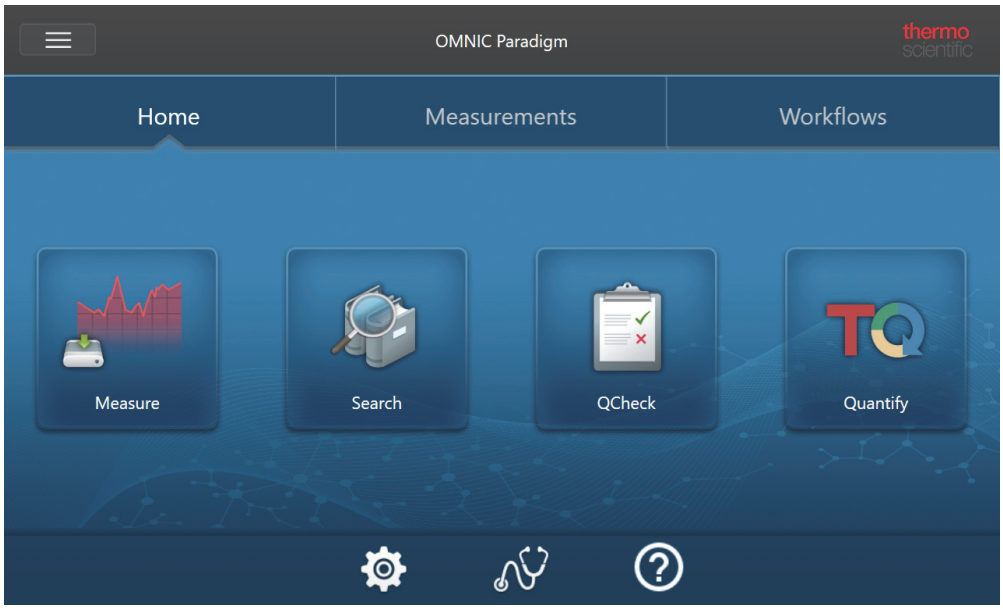
OMINIC Paradigm software features three interfaces to suit your device or task and pairs with other Thermo Scientific software, allowing you to develop and run quantification methods or protect and audit your data.

OMNIC Paradigm Software Interfaces

Switch anytime between OMNIC Paradigm software's touchscreen and desktop interfaces to best suit your device and goals.

Touchscreen Interface

Figure 1. The touchscreen interface features a simplified interface for streamlined analysis.

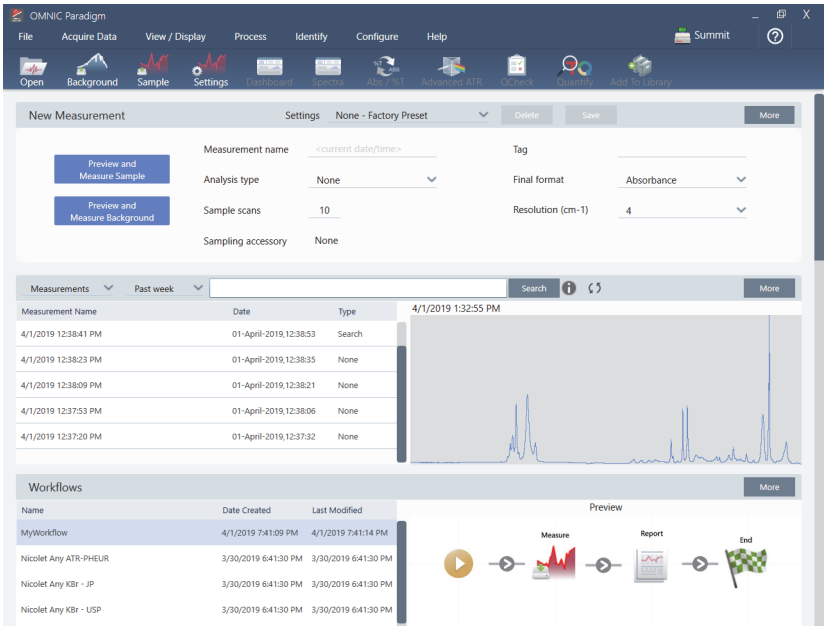


The touchscreen interface is optimized for small screens, such as the Thermo Scientific™ Nicolet™ Summit spectrometer's optional touchscreen device.

Use the touchscreen interface for measuring and analyzing samples or running workflows in a streamlined, simplified interface.

Desktop Interface

Figure 2. The desktop interface includes a wider range of features and tools for more complex measurements and analyses.



Use the desktop interface when working from a larger screen and when you need additional features not available in the touchscreen interface, such as the workflow editor and select spectral processing and analysis tools.

Connect your Summit spectrometer to an external monitor and a USB mouse and keyboard for the best experience using the desktop interface.

Switching Between Interfaces

Although desktop and touchscreen software are optimized for different tasks and devices, you can switch between interfaces at any time.

❖ To switch between the touchscreen and desktop interfaces

- To switch from desktop to touchscreen, select **View / Display > Switch to Touchscreen.**

  The software will close briefly and re-open with the touchscreen interface.

- To switch from touchscreen to desktop, from the home screen, select **Switch to Desktop** from the menu.

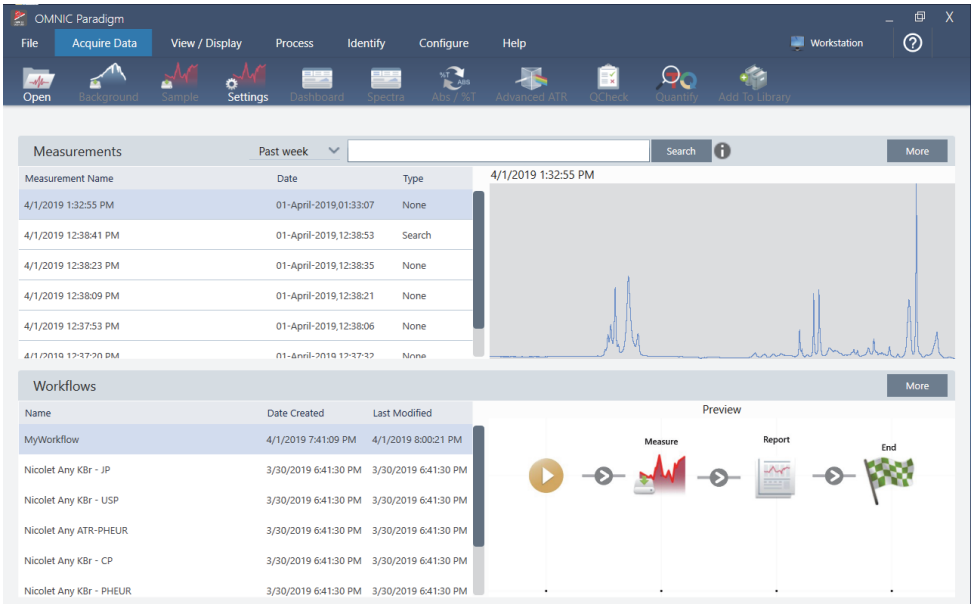
  The software will close briefly and re-open with the desktop interface.

Pairing OMNIC Paradigm with Other Thermo Scientific Software

OMNIC Paradigm software is compatible with other Thermo Scientific software for added flexibility and for quantitative analysis and data security.

OMNIC Paradigm Workstation software

Figure 3. Workstation software lets you analyze spectra or develop workflows while you're away from a spectrometer



When working from a separate computer and not connected to an instrument, use Workstation software to analyze previously collected data, create workflows for later use, or create and share reports.

Quantitative Analysis Software

Pair OMNIC Paradigm software with TQ Analyst™ software to develop and run quantitative analysis methods that you can use in OMNIC Paradigm software.

- TQ Analyst EZ Edition
- TQ Analyst Professional Edition

See "TQ Analyst™ Pro Edition Software" on thermofisher.com for details.

Data Security Software

Use Thermo Scientific™ OMNIC™ Security Suite Software to ensure your data's security and integrity. The Security Suite software ensures 21CFR Part 11 compliance and includes the following:

- Security Administration for controlling system access, handling security policies, and setting digital signatures for responsibility and data integrity

- Audit Manager for creating and managing complete audit trails
- Thermo Software IQ tool to verify your security installation

See "OMNIC™ DS Data Security Software" for more on securing your data with Security Suite software.

OMNIC Paradigm Software Basics

Understanding the core concepts of using OMNIC Paradigm software will help you more efficiently and effectively collect, analyze, and report spectral data.

You may not always carry out every step of the following process, and you can customize OMNIC Paradigm software to meet your specific needs, but in general, you will likely follow a common process:

Plan Your Project

Before getting started with the software, it's important to consider your project goals. Planning in advance will help you decide what type of processing and analysis is appropriate for your work, what measurement settings will yield the best data, and how you can most efficiently carry out your procedures.

Before acquiring data, you should be able to answer the following questions:

- **What are my goals for the project?**

  For example, do you want to identify an unknown sample or verify that your sample is meeting your standards. With OMNIC Paradigm software, you can run different processes and analysis steps depending on how you will use the data. Common goals include the following:

  - Identify a pure sample
  - Identify the components of a mixture
  - Verify that a sample meets your specifications
  - Quantify the components of a sample

- **How will I measure my sample?**

  OMNIC Paradigm software supports a variety of spectrometer sampling accessories and measurement techniques.

  See "FTIR Sample Handling Techniques" on FTIR Spectroscopy Academy for a full discussion of choosing the best collection method for your specific work.

- **Am I planning only a few measurements or will this be a routine, repeated procedure?**

  If you would like to automate a routine procedure, you can create a workflow. With a workflow, you specify settings for data collection, provide instructions to operators, and define data processing, reporting, and archiving in advance. You or other operators can then use the workflow to carry out procedures with the knowledge that exactly the same steps will be taken each time.

  For a step-by-step guide on creating a new workflow, see "About Workflows."

Acquire Data

Once you have a plan for collecting and working with your data, you're ready to start measuring samples. Generally, to measure a sample and collect data, you will follow these steps:

1. **Prepare the spectrometer, sampling accessory, and sample to be measured.**

   Usually, you should make sure your spectrometer, sampling accessory, and sample are ready before you begin. This can mean ensuring the spectrometer is warmed up and functioning well, that the sampling accessory is installed, and that the sample is prepared.

   The specific steps for setting up the spectrometer and accessory will vary depending on the instrument and on your sample. See the user guides and tutorials for your instrument for specifics on preparing your spectrometer. Or, see FTIR Spectroscopy Academy for more on handling and measuring samples.

   Note that you must measure the background without the sample present. The best time to collect a background spectrum will vary by the type of sample you are measuring.

2. **Select or edit your measurement settings.**

   When the instrument is ready, you can adjust settings both for how the software will collect and process the data and for setting up the spectrometer. Select your saved settings from a menu on the dashboard or edit settings individually for a single measurement.

   See "Set and Save Measurement Options," for a discussion of how to edit and save measurement settings.

3. **Measure the background.**

   When you measure a sample, the spectrometer records data from the sample as well as from the environment in the spectrometer. To ensure that your sample spectrum represents only your sample, without any data from the background environment, you must measure the background. The background spectrum is then compared to (or ratioed against) the sample spectrum and any data from the background is accounted for, leaving you with data from only your sample.

   See "Measure the Background," for a full discussion of when and how to collect a background spectrum.

4. **Measure the sample.**

   Finally, you can measure the sample. During the measurement, you can preview the spectrum and refine your measurement settings before proceeding. If you indicated an analysis type in the settings, the data will automatically be processed after collection.

   Once the data are collected, you will be able to view and explore the spectrum in the spectral view.

Process Data

After you measure your sample, it's often helpful to process your data so that it is easier to analyze or compare to other spectra. Common spectral issues that OMNIC Paradigm software can help you correct include the following:

- A sloping, curving, shifted or otherwise undesirable baseline
- Peaks obscured by noise in the data
- Variation in depth of penetration from an ATR measurement
- Totally absorbing peaks from too thick of a sample
- Issues caused by CO_2 or H_2O in the atmosphere

Analyze the Sample

OMNIC Paradigm software has tools designed to help you carry out common analyses and to explore spectral data in-depth. Common types of analysis include the following:

- **Identify an unknown sample or mixture**

  To identify an unknown sample or the components of a mixture, compare the spectrum of your sample to reference spectra that are stored in spectral libraries. Spectral libraries are collections of spectra and usually contain additional information on the stored compounds. Libraries can be created or they can be purchased. When you run a correlation or multi-component search, the software searches your stored libraries and finds spectra that are similar to your sample spectrum and indicates how closely the spectra match.

  For more on spectral libraries, see "Manage Spectral Libraries."

  For more on identifying an unknown sample, see "Identify an Unknown Sample with ATR."

- **Verify the composition of a sample**

  You can quickly verify that a sample meets your specifications by using QCheck. With QCheck, you can compare two selected spectra or compare one or more spectra with a reference spectrum or spectral group. QCheck results show the degree of similarity between the spectra as a match value from 0.0 (no similarity) to 1.0 (the spectra are identical).

- **Find the concentrations of components in a sample**

  Quantitative analysis methods that you have created in TQ Analyst software are available for use in OMNIC Paradigm software. You can select these quantification methods and run the quantification analysis from the OMNIC Paradigm dashboard.

- **Perform custom, in-depth analysis**

  OMNIC Paradigm software features many tools to help you to explore the spectra further. For example, the Find Peaks tool lets you quickly identify and label peaks, or you can subtract one spectrum from another or perform other operations using Spectral Math.

Generate Reports and Save Data

Once you have collected, processed, or analyzed your data, you'll likely want to store or share it. With OMNIC Paradigm software, you can customize how your data is stored or exported.

- **Exporting reports**

  When it's time to share your data, you can generate reports automatically using templates. Templates can include results from library searches, QCheck, quantification methods, and more, or they can be used to send data directly to Microsoft Word, Excel, or PowerPoint.

- **Storing data**

  By default, the software is configured to store data in a MariaDB Server database, but you can also configure the software for other databases, such as Oracle Database or Microsoft SQL Server.

  Additionally, settings, spectra, and workflows can be exported as files that you can backup, store, or share.

  For a discussion of data security options in OMNIC Paradigm software, see "21 CFR Part 11 Compliance."

Next Steps

You may not always follow every step of the process described in this guide, but in general, you will be able to achieve better results by understanding the overall process and capabilities of using OMNIC Paradigm software.

Next, get started by measuring your first samples, reviewing setup of your spectrometer, or creating a workflow to automate routine procedures.

Connect to an Instrument Remotely

Connect to an instrument on your local network to measure a sample or run a workflow while you are away from the instrument.

❖ To connect to a remote instrument

1. In the desktop interface of OMNIC Paradigm software, select **Configure > Connectivity** from the menu.
2. Select an instrument from the list of available instruments or enter the IP address or hostname of the instrument to which you would like to connect.
3. Click **Connect**.

   OMNIC Paradigm software closes and restarts during connection. It may take several moments to re-open and to complete connection to the instrument.

   If the instrument is already in use, click **Request Access** to send a request to use the instrument. The current user can then grant or deny access.

   While you use the instrument remotely, it displays a message indicating that it is in use and allows local users to request access.

Measure Samples

To acquire new data with OMNIC Paradigm software, set and save your measurement settings, collect a background spectrum, and finally measure the sample.

Contents

- Set and Save Measurement Options

  Describes common measurement settings and their values, with suggestions for when you might make changes

- Advanced Measurement Settings

  Describes settings for the instrument and sampling accessory, as well as other less commonly used settings

- Measure the Background

  Provides a brief overview of background spectra and describes the procedure for measuring the background

- Measure a Sample

  Describes the procedure for measuring a sample using OMNIC Paradigm software

Set and Save Measurement Options

Measurement settings allow you to specify how your sample is measured and how the data is processed after the spectrum is collected. Your settings control both how the instrument and sampling accessory measure the sample and how OMNIC Paradigm software processes the data.

After adjusting your measurement settings, you can use them immediately or save them for later use.

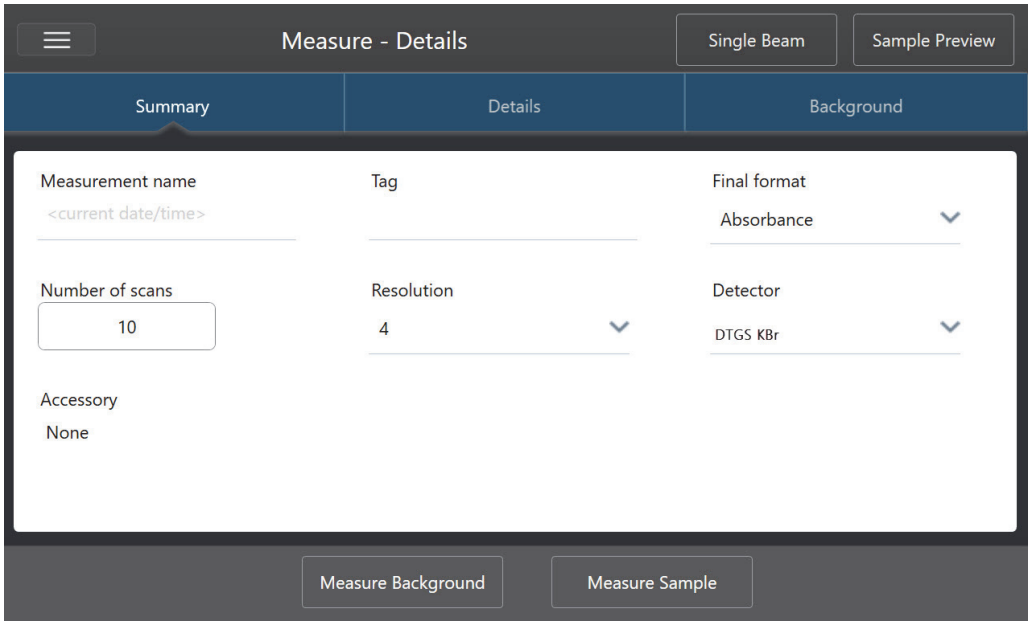
This guide describes how to set, save, and use common measurement options. For a discussion of advanced settings, see "Advanced Measurement Settings."

Set Measurement Options

Set and save your measurement settings or use previously saved settings before starting a measurement.

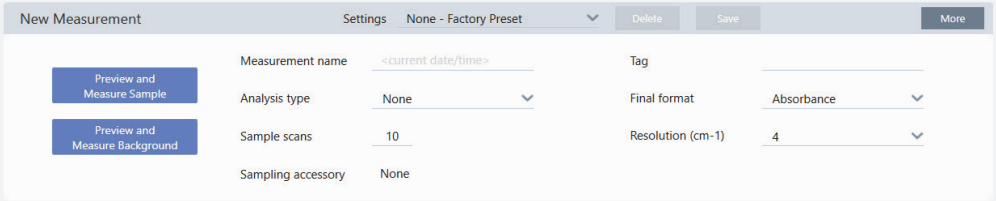
In OMNIC Paradigm software for touchscreen, edit individual settings or import a settings file (.expx) before you measure your sample. To edit or review measurement settings, select an analysis type from the home screen.

Figure 1. Review measurement settings in the Summary, Details, and Background tabs



When using the desktop interface, set and save your measurement settings from the dashboard, or update a few options while previewing a sample spectrum.

Figure 2. Edit measurement settings in the New Measurement pane.



The following table describes the settings you will use most frequently.

Option	Description	Default Setting
Measurement name	The name of your sample data. This name will appear when you save or open this data and in any reports you generate. The default name is the date and time of collection.	Date and Time
Number of sample scans	How many times the sample is scanned during the measurement. The resulting data reflects the average of all the scans. More scans will result in more accurate data but will take longer to measure.	10
Resolution (cm-1)	Like the resolution of a photo or video, a better resolution will mean finer detail in your spectral data. For example, a better resolution will distinguish between two very close peaks while a poor resolution might combine them. A smaller value results in a higher (better) resolution, but also takes longer to measure. Typically, resolutions of 4 are used for solid and liquid samples. For gas samples, use a resolution of 1 or 0.5.	4

Option	Description	Default Setting
Analysis type	With OMNIC Paradigm for touchscreen, you select your analysis type from the home screen rather than selecting from a list. Allows you to automatically process your data after it's collected. Use **None** to measure a sample without additional analysis. **Search** performs a correlation search. Use search to identify an unknown sample. Edit search settings in the Search Setup view. **QCheck** results indicate a match value between your sample and a reference. Use QCheck to verify the composition of a known sample. Edit QCheck settings in the QCheck Setup view. **Quantify** is used to quantify the components of a sample using a pre-selected quantification method. Select Identify > Quantify Setup to specify a quantification method.	None
Tag	Allows you to add a tag to the spectrum. Tags can later be used when searching for a spectrum.	
Final format	Determines the units used for the collected data. You can convert your data to another Y-axis unit after collection in the View/Display menu.	Absorbance
Sampling accessory	The sampling accessory used to measure the sample. Smart accessories are detected automatically.	

Save Your Measurement Settings

You can save, edit, or delete your measurement settings only when using the desktop interface.

Name and save your measurement settings so that you can easily select them from the dashboard for later use. Settings for Search, QCheck, and Quantify analyses are not saved in these settings.

❖ To save your measurement settings

1. Make any desired changes to the settings.

2. Click in the Settings menu at the top of the dashboard.
3. Enter a new name for the settings and click **Save**.

   Saved settings are added to the Settings list for later use.

❖ To make changes to your saved settings

1. Select the named settings that you want to update from the Settings menu.
2. Edit the settings
3. Without entering a new name for the settings, click **Save**.
4. Click **Update** in the confirmation dialog to save your changes.

   Your new settings are now saved under the old setting name and are available in the Settings menu.

❖ To delete your saved settings

1. Select the named settings you want to delete from the Settings menu.
2. Click **Delete**.
3. In the confirmation dialog, click **Yes** to permanently delete the named settings.

Import and Export Saved Settings

Import a settings file to automatically update your current measurement settings to those you saved previously. When importing settings, you can import an OMNIC Experiment file (.exp) or an OMNIC Paradigm settings file (.expx).

OMNIC Paradigm software is compatible with .exp files that were created with OMNIC software. However, with OMNIC Paradigm, you can export only .expx files, which are not compatible with earlier versions of OMNIC software.

Importing an OMNIC Experiment file updates your measurement settings, but does not alter your analysis settings, such as Search Setup or QCheck Setup.

❖ To import a settings file

- If you are using the touchscreen interface
  a. From the home screen, select an analysis type.
  b. While viewing the Summary tab, open the menu and select **Open Settings**.
  c. Select an OMNIC Experiment file (.exp) or OMNIC Paradigm settings file (.expx) file to import and touch **Open**.
- If you are using the desktop interface
  a. In the toolbar, click **Settings**.

b. Select the file to import and click **Open**.

❖ To export a settings file

Settings can be exported only from the desktop interface. Settings files are saved with a .expx file name extension.

1. Choose the settings you wish to export from the **Settings** list
2. Select **Acquire Data > Export Settings**.
3. Enter a name for your settings file, select a directory to save the file, and click **Save.**

   The settings file is now saved and ready for future use.

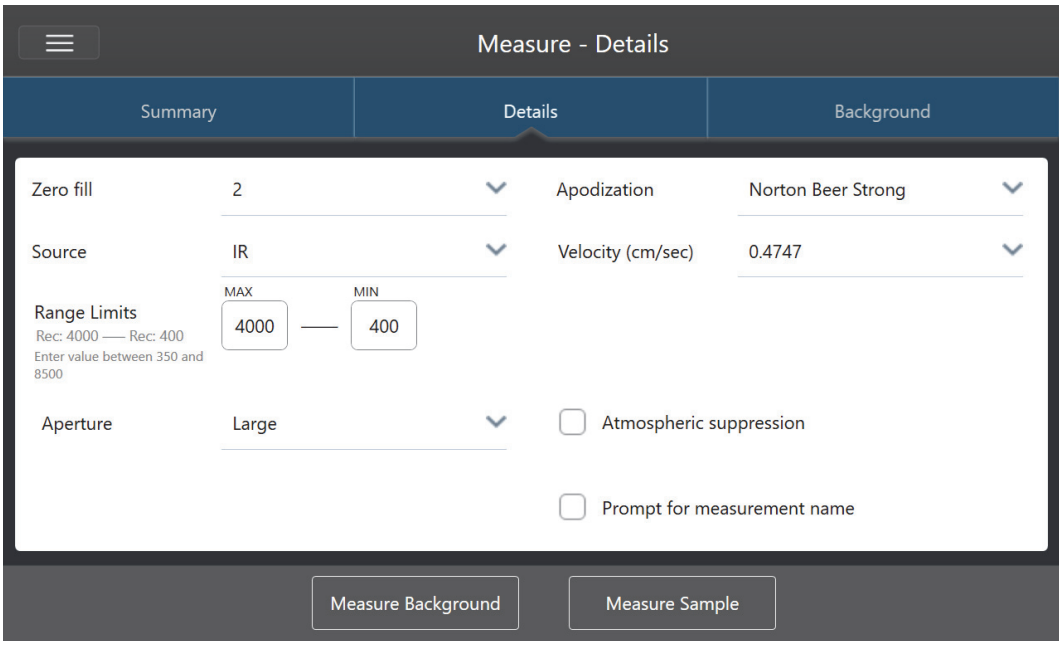
Advanced Measurement Settings

Use advanced measurement settings to control apodization, zero fill, range limits, instrument-specific settings, and more.

These advanced settings should typically be left in their default state. Only in rare or specific circumstances should you edit these settings.

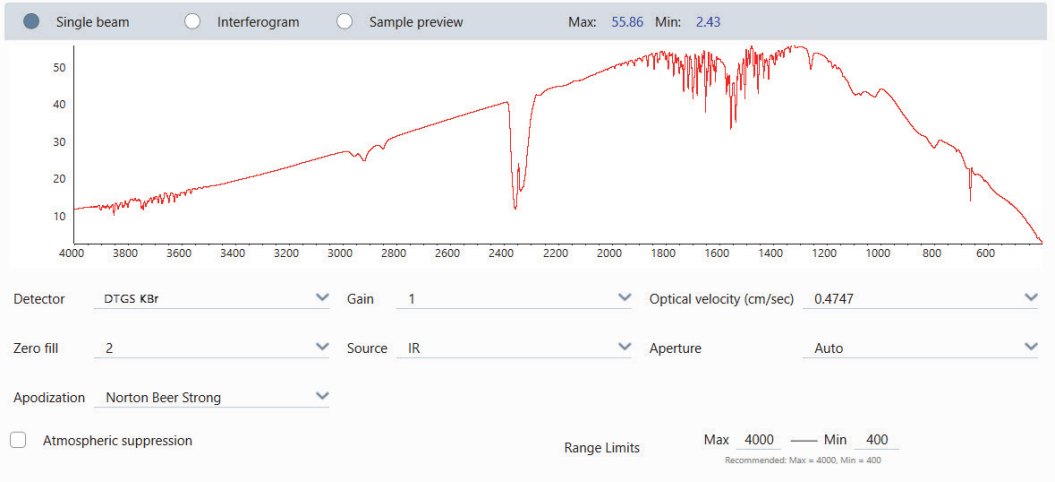
To review or edit advanced settings in the touchscreen interface, open the Details tab.

Figure 1. The Details tab displays advanced measurement settings.



To review or edit advanced settings in the desktop interface, click **More** in the New Measurement pane.

Figure 1. Advanced measurement settings are available from the dashboard



Advanced Measurement Settings

The following table describes each of the advanced settings.

Option	Description	Default Setting
Detector	The detector is a device inside the spectrometer that produces an electrical signal in response to the infrared beam striking it. The detector setting is updated automatically based on your spectrometer setup. • Nicolet Summit: DTGS. • Nicolet Summit Pro: TEC DTGS.	
Gain	Gain is used to increase the intensity of weak detector signals. A greater amount of gain will amplify a weak signal, which can occur with some sampling accessories.	1
Optical velocity	Determines the optical velocity in the interferometer. The default value is determined by the type of detector you are using, and can only be changed on certain spectrometers. On the Nicolet Summit spectrometer, the default value is 0.4747 and cannot be changed.	

Option	Description	Default Setting
Zero fill	Interpolates data points between the collected data points. This doesn't increase the actual resolution of the data, but can smooth out sharp features and improve the line shape of a spectrum. Collect your sample and background spectra using the same Zero Fill setting. Options • None: No zero filling is done. • 1: One data point is added between each collected data point • 2: Three data points are added between each collected data point	2
Source	The component inside the spectrometer that emits the infrared radiation that travels to the detector. The source type is determined by your spectrometer setup. See your spectrometer user guide for details on the source.	
Apodization	Apodization refers to a mathematical function that is applied to the single beam data to reduce or remove peak side-lobes that can occur because the interferogram is not an infinite set of data. Strong apodization reduces more noise but can also reduce the resolution of the data and broaden peaks. You may want to consider weaker apodization, such as Boxcar, if you are measuring spectra with very narrow peaks, such as high-resolution gas spectra. See Apodization Functions for a description of each type of apodization.	Norton-Beer Strong

Option	Description	Default Setting
Automatic Atmospheric Suppression	Suppresses the effects of water vapor and carbon dioxide on the spectra you have collected. In general, it is better to control for atmospheric conditions using a current background spectrum. If you measure the background frequently or if atmospheric conditions change slowly, there is no need to use this feature. Use this feature only if you measure the background infrequently or when atmospheric conditions change rapidly.	Deselected
Range Limits	Sets the limits for the range of frequencies, in wavenumber, included in the collected spectrum.	Max: 4,000 Min: 400
Aperture	Controls the intensity of the infrared radiation that reaches the sample. Aperture can only be changed when using spectrometers with adjustable apertures. In general, larger apertures will result in a better signal-to-noise ratio while smaller apertures result in better stability and accuracy. Small apertures are better for high-resolution measurements. You may need to use small apertures to acquire true high-resolution spectra.	

Apodization Functions

Apodization refers to a mathematical function that is applied to the single beam data to reduce or remove peak side-lobes that can occur because the interferogram is not an infinite set of data.

Strong apodization reduces more noise but can also reduce the resolution of the data and broaden peaks.

See FTIR Spectroscopy Academy for a general introduction to apodization.

The following table describes the available apodization types:

Setting	Description
Boxcar	The interferogram is unweighted; that is, the data are simply truncated at the beginning and end. Use this type when you are measuring a gas sample, want maximum resolution and are not concerned about ringing effects (side lobes). The greatest amount of ringing will be present with this type.
Cosine	This setting suppresses side lobes and only moderately degrades the resolution of the spectrum. This setting is similar to the Happ-Genzel and Norton-Beer medium apodization. Cosine is normally used only to reproduce the results of other experiments that used it.
Happ-Genzel	Suppresses side lobes more effectively than the Triangular type and with less reduction in resolution than that type. (It results in more reduction in resolution than the boxcar type.)
Norton-Beer Weak	This setting has a less pronounced smoothing effect on data than do the Norton-Beer Medium and Norton-Beer Strong types and degrades the resolution less than those types. Side lobes appear on both sides of peaks and are more pronounced for sharper peaks. Use this setting only when the best possible resolution is required. This setting is generally not recommended and is normally used only to reproduce the results of other experiments that used it.
Norton-Beer Medium	This type has a smoothing effect on data which is between that of the Norton-Beer Weak and Norton-Beer Strong types. It suppresses side lobes as much as possible given that it only moderately degrades the resolution of the spectrum. The side lobe suppression is more significant than for Norton-Beer Weak apodization. This setting is suitable for most normal samples; it gives results virtually identical to those obtained with Happ-Genzel.
Norton-Beer Strong	**Norton-Beer Strong is the recommended apodization for the Nicolet Summit and Summit Pro spectrometers.** This setting has a greater smoothing effect on data than do the Norton-Beer Weak and Norton-Beer Medium types and degrades the resolution of the spectrum more. The side-lobe suppression is more significant than for Norton-Beer Medium apodization.

Setting	Description
Triangular	Mathematically weights interferogram data to reduce ringing effects (side lobes), resulting in lower resolution than that obtained with the boxcar and Happ-Genzel types. Some ringing will usually be present with this type. This setting is normally used only to reproduce the results of other experiments that used it.
Blackman-Harris	The 4-term Blackman-Harris function is a strong apodization function that is better than any of the others at suppressing side lobes. However, it results in greater line broadening than any of the others. In practice this has the effect of reducing random noise in a spectrum while causing band broadening.

Measure the Background

Accurate sample spectra require an accurate and current measurement of the background.

When you collect a background spectrum, you are collecting a measurement of the environment in the spectrometer without a sample in place, including characteristics of the detector and atmosphere inside the spectrometer. This background spectrum is then used to eliminate any signals in your sample spectrum that are due to the spectrometer or to the background environment. Without a measurement of the background, there would be no way to know whether you were seeing data from the sample you measured or from the background environment.

When to Measure the Background

Because the background environment in the spectrometer can change over time, you should update your background spectrum frequently.

In addition to collecting a new background spectrum periodically as the environment changes, collect a new background after any of the following circumstances:

- You have changed the hardware in your spectrometer, including changing sampling accessories
- You have changed the settings for measuring samples

Background Settings

There are several options for when and how to measure the background. These options determine when and if you are prompted to collect a new measurement of the background.

To select a different background option in the touchscreen interface, select an analysis option and open the **Background** tab.

To select a different background option in the desktop interface, click **More** in the New Measurement pane of the dashboard and scroll to the Background group.

Figure 1. In the touchscreen interface, select a background setting in the Background tab.

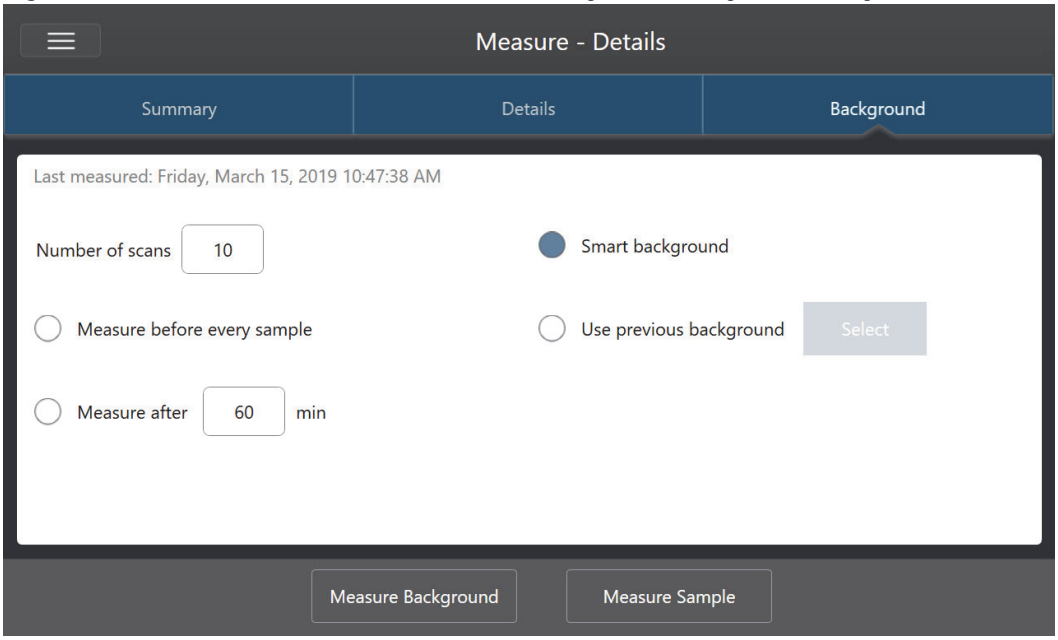
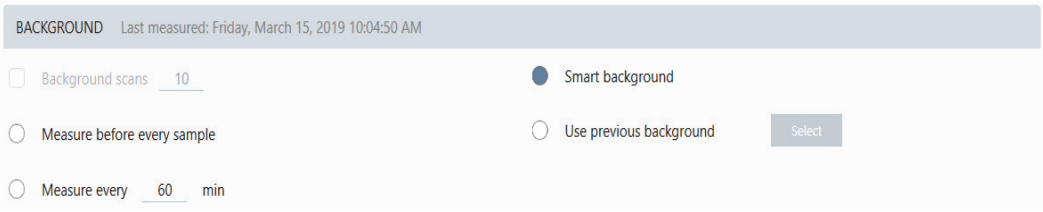


Figure 1. In the desktop interface, select a background setting in the Background pane.



The following table describes the background settings.

Setting	Description
Background scans	How many times the background will be measured. The resulting spectrum represents the average of all scans. More scans will produce a more accurate spectrum but will require a longer collection time. The default is 10.
Measure before every sample	If this option is selected, you will be prompted to collect a new background spectrum before every sample measurement. This is a good option when you are measuring only a few samples, as it ensures a current measurement, but it can slow down the measurement process.
Measure every ___ min	Allows you to measure many samples using the same background spectrum. You can enter any integer value between 1 and 1024, but note that the background environment may change over time and your sample spectra may become less accurate as time passes.

Setting	Description
Smart background	Smart background measures the background automatically, so that you always have a current measurement without having to manually measure the background.
Use previous background	Allows you to select a previous background spectrum. This option should be used only rarely and under unusual circumstances (for example, if it would be impossible to load or remove the sample without changing the system environment). In this case, you would collect and save a background spectrum earlier, using conditions as close as possible to the conditions under which you will measure the sample.

Measure the Background

Measuring the background requires on a few simple steps. If you attempt to measure a sample without a current background spectrum, you will be prompted to measure the background before proceeding.

❖ To measure the background in the desktop interface

1. Remove any sample from the sampling accessory.
2. From the dashboard, select **Preview and Measure Background.**

   The Background Preview window opens, and you can preview the background before continuing with the collection.
3. To continue, select **Start Background Measurement**, or click **Dashboard** in the toolbar to cancel and return to the dashboard.

   During the measurement, you can pause, restart, or stop the collection. If you stop the collection, the partial data will be used. For example, if you plan to collect 8 scans, but you stop after 4, the background spectrum will be used with only 4 scans.

   Once the background spectrum is collected, you can preview the sample spectrum and make any necessary changes to the sample measurement settings, or you can return to the dashboard.

❖ To measure the background in the touchscreen interface

1. From the home screen, select an analysis type**.**
2. Open the **Background** tab to edit or review your background settings.
3. To begin the measurement, touch **Measure Background.**

   The Background Preview opens, and you can preview the background before proceeding.
4. To proceed, touch **Start Background Measurement.**

During the measurement, you can pause, restart, or stop the collection. If you stop the collection, the partial data will be used. For example, if you plan to collect 8 scans, but you stop after 4, the background spectrum will be available with 4 scans.

Once the background spectrum is measured, you can preview the sample spectrum and make any necessary changes to the sample measurement settings, or you can select Home in the menu to return to the home screen.

Measure a Sample

Measuring a sample requires you to prepare your sample, to set and save your measurement settings, to measure a background spectrum, and finally to measure the sample.

❖ To measure a sample using OMNIC Paradigm software for touchscreen

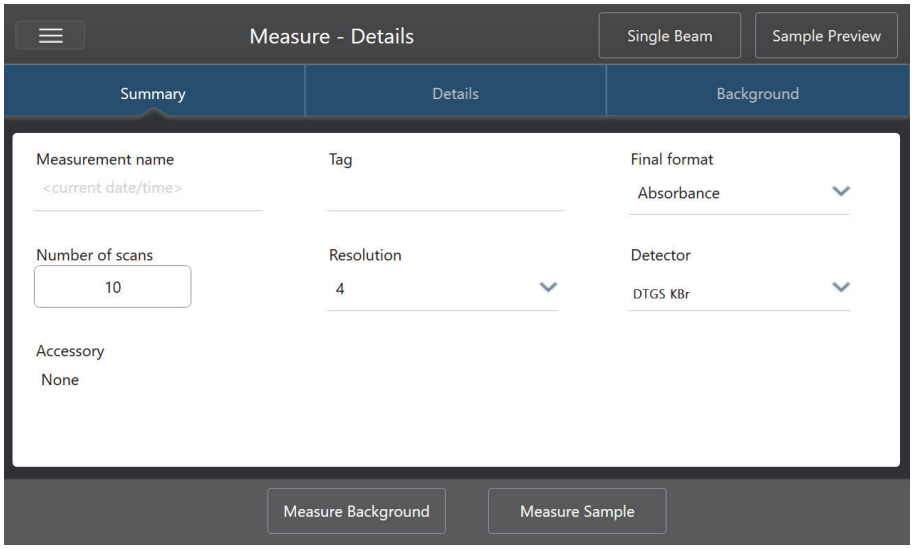
1. Prepare your sample

   How you prepare your sample will depend on your spectrometer and sampling accessory. For details on preparing and loading the sample, see your sampling accessory's user guide.

2. Select the analysis type that reflects the analysis that you are performing. To measure a sample without performing additional analysis, select **Measure**.

   After selecting an analysis type, the settings summary view opens.

   Figure 1. The Summary tab displays common measurement settings.



3. Review and edit your measurement settings.

   Open the **Details** tab to review additional measurement settings or open the **Background** tab to adjust settings for how the background is measured. Depending on your background settings, you may be prompted to measure a new background before measuring the sample.

   See "Set and Save Measurement Options" for a description of each setting.

   For details on setting up your analysis, see "Identify an Unknown Sample with ATR."

4. When you are satisfied with your settings, touch **Measure Sample**. The sample preview opens and displays a live preview of the spectrum.
5. To proceed, touch **Start Sample Measurement**.

   During the measurement, you can pause, restart, or stop and save your measurement. For example, if you feel your data are sufficient and you do not want to wait for more scans, touch **Stop** to save and use the data as is. Touch **Restart** to clear all data and begin scanning from the beginning.

Once your sample is measured, you can process or analyze it in the spectral view, or you can measure another sample. To measure another sample from the Spectral view, touch **Measure New Sample**.

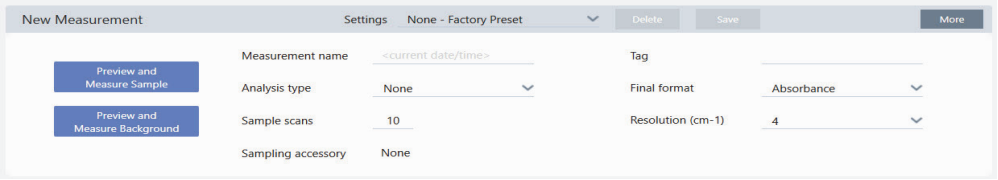
❖ To measure a sample using OMNIC Paradigm software for desktop

1. Prepare your sample

   How you prepare your sample will depend on your spectrometer and sampling accessory. For details on preparing and loading the sample, see your sampling accessory's user guide.
2. To edit the settings for a Search, QCheck, or Quantify analysis, open the **Identify** menu and open the corresponding setup option.
3. Set and save your measurement settings.

   To use previously saved settings, select the settings from the Settings list.

   Figure 1. The Settings list displays your previously saved settings



   See "Set and Save Measurement Options" for a description of each setting.

   For details on setting up your analysis, see "Identify an Unknown Sample with ATR."
4. In the New Measurement pane, click **Preview and Measure Sample**

   Depending on your background settings, you may be prompted to measure a new background. If so, follow the on-screen prompts to measure a new background.

   While measuring the sample, you can pause, restart, or stop and save your measurement. For example, if you feel that your data are sufficient and you do not want to wait for more scans, click **Stop** to save and use the data as is. Click **Restart** to clear all data and begin scanning from the beginning.

Once your sample is measured, you can process or analyze it in the Spectral view, or you can measure another sample. To measure another sample from the Spectral view, click **More** to review common measurement settings, and then click **Measure New Sample** to begin.

Next Steps

Measuring a sample with OMNIC Paradigm software requires only a few simple steps. Before measuring the sample, review your measurement settings and ensure that you have a recent background spectrum in use.

With your spectrum measured, you're ready to identify, verify, or quantity the spectra. See "Identify an Unknown Sample with ATR" for a guide to using a library search to identify your sample.

Process Data

Use the processing tools in OMNIC Paradigm software to better understand your data.

Contents

- Apply Basic Equations to Acquired Data

  Perform basic equations, such as add, subtract, multiply, and divide, with your acquired sample spectrum.

Apply Basic Equations to Acquired Data

You can perform basic equations (add, subtract, multiply and divide) with acquired sample spectra. There are a number of reasons why you might want to do this, especially for subtracting a reference spectrum. For more information, see the sections that follow.

To Perform Any Spectral Math Operation

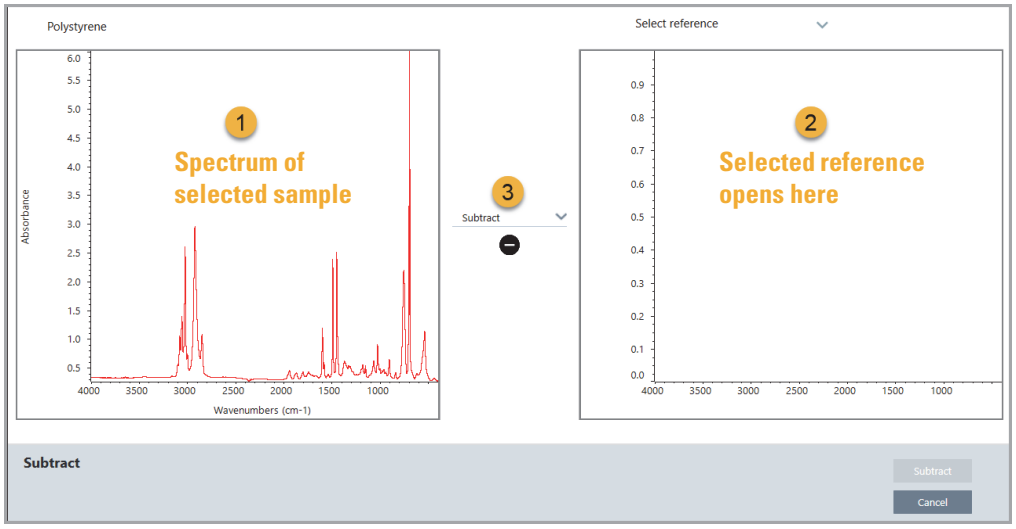
To perform spectral math, the sample and reference spectra must have the same spectral resolution and be in the same Y-axis unit. If they are not, the software automatically converts the selected reference spectrum to match the selected sample spectrum. In order to subtract, multiply or divide spectra, at least a portion of the spectral range (X-axis) of the two spectra must overlap.

❖ To perform any spectral math operation on a spectrum

1. Acquire or open a spectrum of your sample and make sure that spectrum is selected in the spectral view.
2. Choose **Process** (menu) **> Spectral Math**.

   The software opens the Spectral Math setup window with the sample spectrum in the left pane and space for a reference spectrum in the right pane.

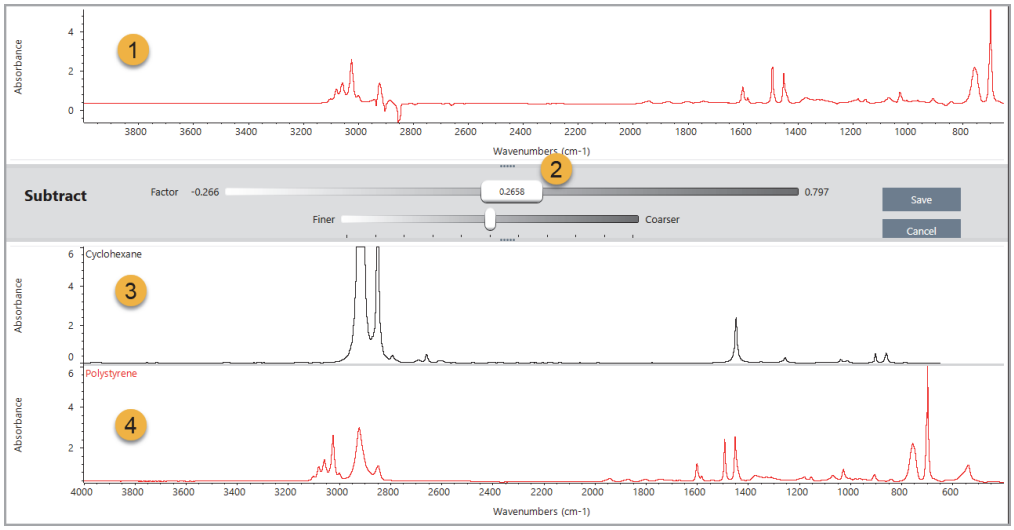
Figure 1. Spectral Math Setup Window



1. Spectrum of selected sample
2. Selected reference opens here
3. Selected math operation

3. Use the settings list between the two panes to select a spectral math operation (Subtract, Add, Multiply or Divide).
4. Use the Select Reference list to search for a spectrum in the current project, another project, or from a spectral library.
5. Click **Subtract** (Add, Multiply, Divide) to start the operation.

   The software opens the Spectral Math operation window with the two original spectra (bottom) and the current result with a factor slide bar (top). Here is an example showing a subtraction result:



1. Current subtraction result
2. Factor
3. Reference
4. Sample

6. Adjust or enter a factor as needed to increase or decrease the intensity of the reference in the result spectrum.

   See the sections below for tips on adjusting the factor for each math type.

   Note Use the bottom bar to change the Factor's adjustable range.

7. Choose **Save**.

The software shows the spectral view with the subtraction result in the spectral pane and at the top of the results panel, with the original sample and reference spectra directly below it.

1. Spectral math result
2. Sample
3. Reference

Note The result has the same name as the original sample with the type of math operation performed (for example, add, subtract, etc.) appended to it.

Subtract One Spectrum from Another (A-B)

Use Subtract to subtract one spectrum from another. Spectral subtraction is useful in a variety of situations. Here are some examples:

- If you measure a sample that is dissolved in a solvent, the spectrum will contain peaks due to the solvent. By subtracting a spectrum of the pure solvent from the sample spectrum, you can eliminate the solvent peaks and produce a "clean" spectrum of the sample material.
- When you measure a sample that is a mixture of two or more components, the spectrum is, theoretically, the sum of the spectra of all the components. By subtracting a spectrum of a pure component from the sample spectrum, you can produce a simpler mixture spectrum with that component removed. You can then search that spectrum against a library to identify the remaining components. (In this case, you might want to try using the Multi-Component Search option instead.)
- If you measure a sample that contains an unknown contaminant, the spectrum will contain peaks due to the contaminant. By subtracting a spectrum of uncontaminated sample material from the first spectrum, you can produce a residual spectrum of the contaminant. You can then search that spectrum against a library to identify the contaminant.

- If you collect spectra to monitor the quality of a material being produced, you can more easily detect changes from one batch to the next by subtracting one sample spectrum from the next (or vice versa) than by just comparing the spectra visually.

Tips on subtracting spectra

- To determine the subtraction factor, watch the changes in the common peaks as you change the factor. The common peaks in the result spectrum should become smaller. The optimum factor is one which produces nulled (or zeroed) common peaks in the subtraction result without subtracting other important spectral information. If you use the correct factor, the peaks present in the result will be due solely to the sample material of interest.
- The initial subtraction factor is automatically calculated from the displayed region. If you display a different spectral region and perform the subtraction again, the difference spectrum will probably be different because the subtraction factor changed.
- When you subtract a reference spectrum from a sample spectrum, the baseline regions are subtracted along with the regions that contain peaks. If the sample spectrum's baseline is not flat and at zero absorbance (or 100% transmittance), the baseline of the subtraction result will have the same undesirable characteristics. If you correct the baseline first, you can obtain a “clean” subtraction in which corresponding peaks are subtracted out, without baseline problems in the result.
- When you subtract the spectrum of a pure reference material from that of a mixture, the peaks may not subtract cleanly. This is because the reference spectrum does not account for any changes that may occur due to molecular interactions with the other components in the mixture or differences in relative concentrations of components. These conditions may cause some peaks to shift slightly or change shape.

Add Two Spectra Together (A+B)

Use Add to add two spectra together. Adding spectra can be useful in the following situations:

- Add can be used to join together two spectra of different spectral ranges.
- By adding two pure component spectra together, you can produce a theoretical composite spectrum that is the sum of the two component spectra. This theoretical composite spectrum can be compared with an unknown mixture spectrum in a quantitative analysis.

Tips on adding spectra

- Use the Factor setting to scale the reference spectrum up or down before adding it to the sample spectrum.
- If only one of the spectra contains data points in a spectral region, the Y value of the other spectrum is considered to be zero in that region when the spectra are added.

Multiply One Spectrum by Another (A*B)

Use Multiply to multiply two spectra. Most people use divide rather than multiply for most applications. But multiplying spectra can be useful for reprocessing a spectrum with a different background. For example, if you measure a sample that is adhered to a matrix, you can acquire a single beam spectrum of just the matrix and use that spectrum to cancel out the original background and replace it with the new one. Here is the equation:

$S * B_1/B_2$

Where:

S= sample spectrum (processed with original background)
B_1 = original background
B_2 = new background

Divide One Spectrum by Another (A/B)

Use Divide to divide one spectrum by another. Dividing spectra can be useful for reprocessing a spectrum with a different background. For example, if you measure a sample that is adhered to a matrix, you can acquire a single beam spectrum of just the matrix and use that spectrum to cancel out the original background and replace it with the new one. Here is the equation:

$S / (B_2/B_1)$

Where:

S= sample spectrum (processed with original background)
B_1 = original background
B_2 = new background

Tips on dividing spectra

- Data points that have zero absorbance values in the original sample spectrum will produce very strong absorbance values in the resulting spectrum.

Using Spectral Math with Data Security

When “Require reason for change for Spectral Math” is enabled in the Thermo Scientific Security Suite, Spectral Math requires a change reason and signature before the results can be saved, and the following change event is recorded in the audit log:

- Date and time
- Operation performed: subtract, add, multiply, divide
- Sample spectrum title
- Reference spectrum title
- Factor

4

Analyze Data

Use the analysis tools in OMNIC Paradigm software to identity unknown samples and to verify the components of your sample.

This section includes the following:

Contents

- Manage Spectral Libraries

  Learn to view, select, and create spectral libraries to use in your analyses.

- Identify an Unknown Sample with ATR

  This tutorial provides detailed instructions on using OMNIC Paradigm software to identify and unknown sample using the Attenuated Total Reflection (ATR) sampling technique.

- Identify an Unknown Sample with Transmission

  This tutorial provides detailed instructions on using OMNIC Paradigm software to identify an unknown sample using the infrared transmission.

Manage Spectral Libraries

Libraries contain lists of compounds and related information and can be purchased or created from your own data. When you perform a correlation or multi-component search, the analysis compares your sample spectrum to compounds stored in the libraries you specify in your search settings.

Use the library manager to view information about your libraries and stored compounds and to create or delete libraries.

Create a New Library

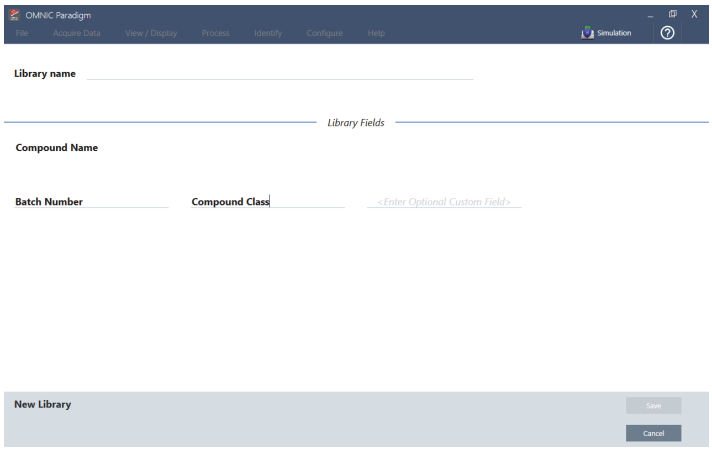
Create a new library to manage your spectral data and to search against your own measured data.

❖ To create a new library in the desktop interface

1. From the menu bar, select **Identify** > **New Library.**
2. In the New Library view, enter a name for the library and add any optional fields.

   Optional fields are used when you add spectra to a library. For example, Figure 2 shows a library with two optional fields. When adding spectra to My New Library, users can provide a batch number and compound class.

   Figure 1. Name your library and customize optional fields in the New Library view.



3. Click **Save** to create the new library.

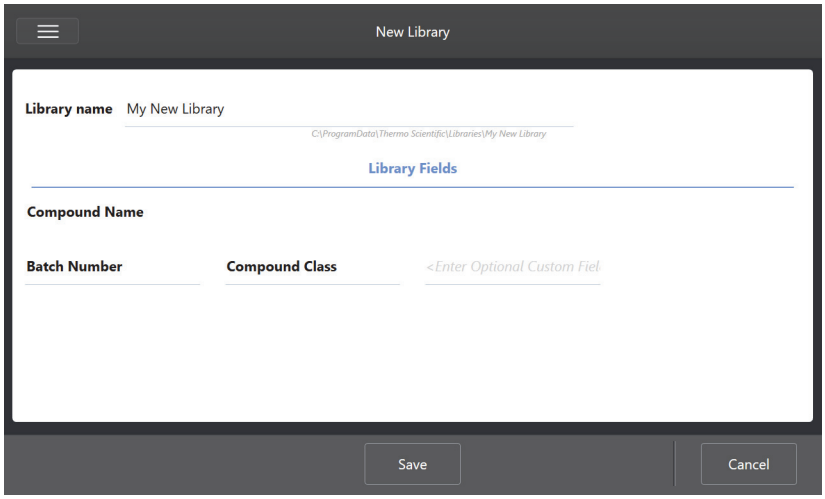
   Your new library is listed in the Libraries column of the library manager.

❖ To create a new library in the touchscreen interface

1. From the home screen, open the menu [☰] and select **Library Manager**.Open the menu and select **New Library.**
2. In the New Library view, enter a name for the library and add any optional fields.

   Optional fields are used when you add spectra to a library. For example, Figure 2 shows a library with two optional fields. When adding spectra to My New Library, users can provide a batch number and compound class.

   Figure 2. Name your library and customize optional fields in the New Library view.



3. Touch **Save** to save your new library.

Add Spectra to a Library

Add spectra to a library to use your own sample data in other Search analyses.

❖ To add spectra to a library in the desktop interface

1. In the spectral view, select the spectrum you want to add to a library.
2. From the menu bar, select **Identify > Add to Library** to open the Add to Library view.
3. Select the library you want to add the spectrum to from the list of libraries.
4. Make any adjustments to the spectrum information and set a name for the compound. The default name will be the measurement name used when the sample was measured.
5. Click **Save**. Your spectrum is now available in the library, and you can view it in the library manager.

❖ To add spectra to a library in the touchscreen interface

1. In the spectral view, select the spectrum to add to a library.

2. Select **Add to Library** from the menu.
3. In the Add to Library view, select a library from the Libraries column.
4. Name the compound, specify any optional fields and touch **Save**. The spectrum will now be available in your selected library.

Extract Spectra from Libraries

Extract spectra from libraries to use them as references in your analyses or workflows. Extracted spectra are stored with your measurements in the database, but cannot be renamed, tagged, or exported.

❖ To extract a spectrum from a library

1. Navigate to **Library Manager**.
2. Select a compound to extract.
3. In the toolbar, select **Extract**. A message confirms that the spectrum has been extracted successfully. View your measurements to find the extracted spectrum.

Delete Libraries and Compounds

Libraries and compounds in libraries can be deleted only in the desktop interface.

When you delete a compound, that compound is no longer used in search analyses and is crossed out in the list of compounds. The index position of other compounds in the library is maintained.

You can delete or edit only the libraries that you have created. Commercial libraries and their compounds cannot be deleted.

CAUTION Deleted libraries and compounds cannot be recovered.

❖ To delete a compound from a library

1. In the Library Manager, navigate to the compound you want to delete.
2. Right-click the compound and select **Delete**. In the dialog box, click **Yes** to confirm.

❖ To delete a library

1. In the Library Manager, select the library to be deleted.
2. Click **Delete** in the toolbar, then click **Yes** to confirm.

Identify an Unknown Sample with ATR

Your FTIR spectrometer and OMNIC Paradigm software can help you determine what's in an unknown sample. This article demonstrates how to measure and analyze a sample using the Attenuated Total Reflection, or ATR, sampling technique. It is a common and "mess-free" technique for acquiring FTIR data from a sample material. This article includes a number of examples to help you build confidence in interpreting your analysis results.

You will learn how to:

- Prepare the ATR accessory
- Set up and run the analysis, and
- Evaluate and confirm the results

Follow these instructions to measure and analyze an unknown pure sample using the ATR sampling technique.

Prepare the ATR Accessory

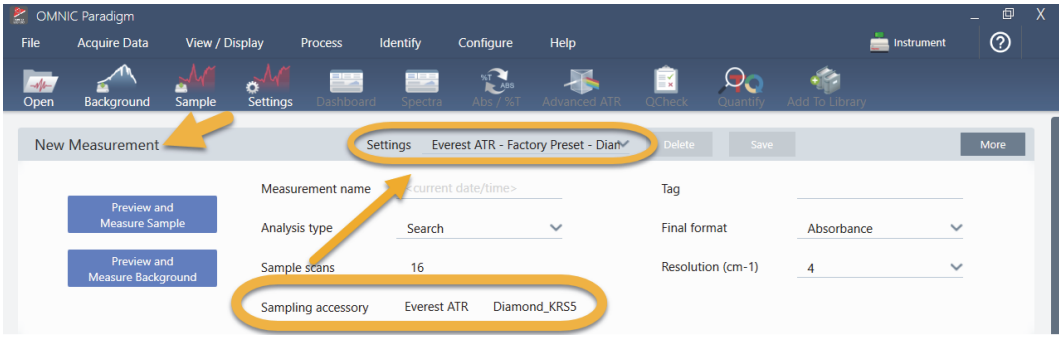
To begin, make sure your ATR accessory is inserted in the spectrometer sample compartment and that it has an appropriate crystal installed. Each crystal material provides some kind of sampling advantage such as a wider spectral range, a higher energy throughput, or more durability. The correct choice depends on what crystals are available, which one works best with your sample material, and which one produces the needed information. See the information that came with your ATR accessory for more information.

Here is the Thermo Scientific™ Everest ATR accessory with a diamond crystal installed in our Nicolet™ Summit FTIR spectrometer.

Make sure the crystal is clean so the spectrometer can take an accurate background measurement when it's ready. To clean the crystal, dab it with a soft cloth. If the crystal requires more rigorous cleaning, check the user guide that came with your ATR accessory. The guide should list appropriate cleaning solvents for each crystal type.

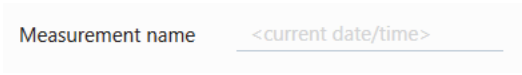
Set Up the Analysis

The next step is to set up the OMNIC Paradigm software. After you open the software, you see the dashboard in the main window. The important measurement settings are at the top.



First, make sure the Sampling Accessory readout shows the installed accessory. If it doesn't, reseat the accessory. Notice that the factory presets for that accessory appear under "Settings."

Then enter a measurement name, or you can leave the suggested name, which is the exact date and time of the measurement.



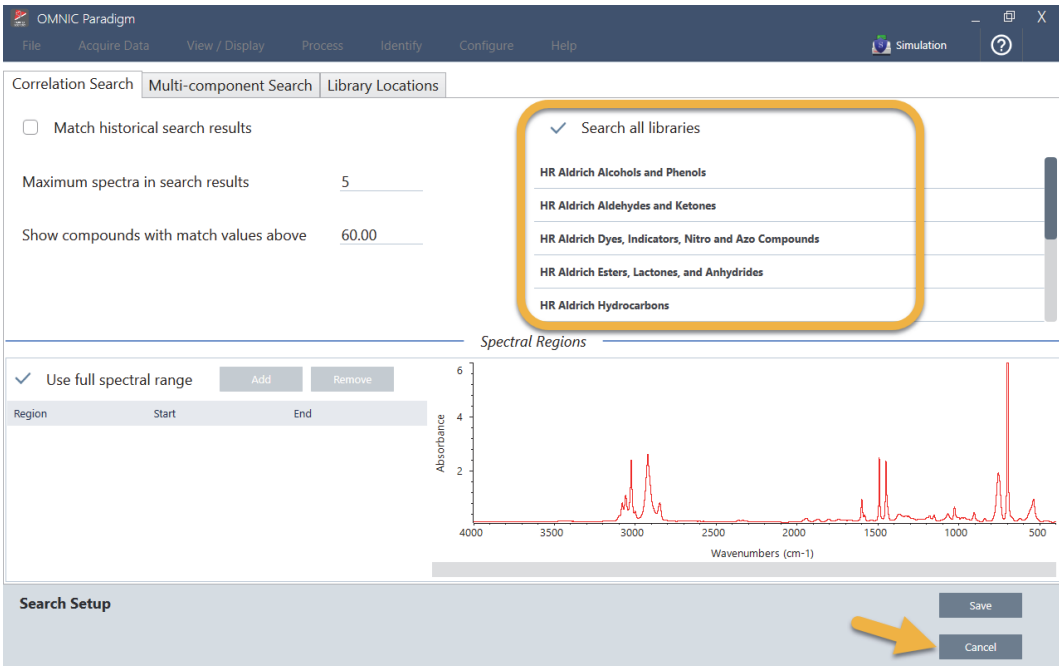
Next make sure the Analysis Type is set to Search. This performs a point-by-point comparison of the sample spectrum against FTIR library spectra. The quality of the output depends on the source and quality of the spectra in the selected libraries.

Finally, check the acquisition settings (sample scans, resolution and final format). The settings shown above are all good starting values for this analysis.

It's important to note that the quality of the sample data you acquire will affect the analysis results. For example, speeding up the analysis by measuring fewer scans, or decreasing the resolution could lead to a less certain analysis result.

Consider Your Spectral Libraries

All existing spectral libraries are selected automatically by default. Choose **Search Setup** in the Identify menu to view or change your library selections.



For this demonstration, we are using the free libraries provided with OMNIC Paradigm software.

Choose **Cancel** to close the Search Setup window.

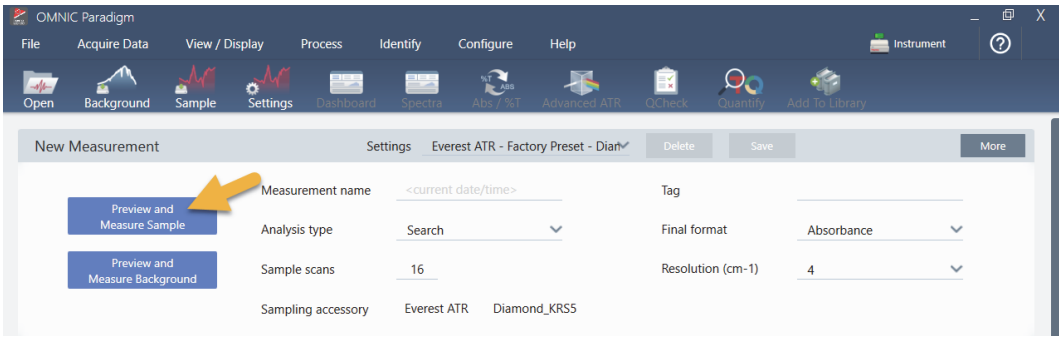
You can also use the Library Manager in the same menu to easily create a spectral library. Any libraries you create should be from pure materials that represent what you expect to find in your unknown samples.

The library spectra are normally the same quality or higher quality than the sample spectrum. It is also helpful if they are acquired using the same sampling technique (ATR in this case). If your library spectra were acquired using the transmission technique, OMNIC Paradigm software has a correction that can be applied to the sample spectrum to improve the results. You'll learn more about that later in this article.

There is no need to perform conversions such as final format, resolution or spectral range on the sample data before performing a search—the software does that for you.

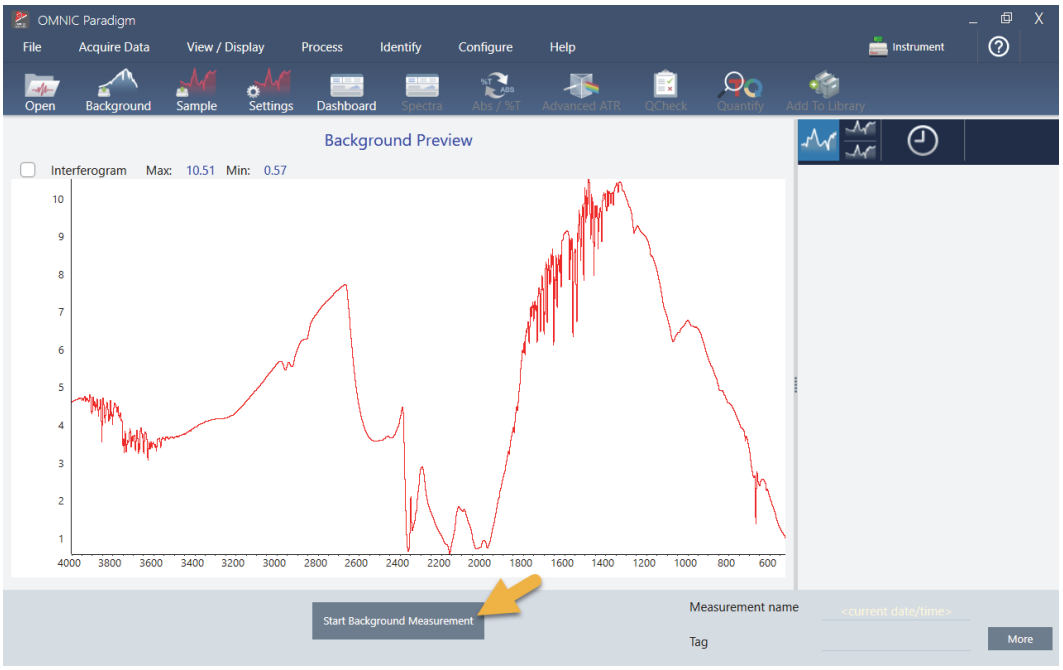
Measure and Analyze the Sample

To start the analysis, click **Preview and Measure Sample**.



The analysis starts with a background measurement. The only requirement for an ATR background is to make sure the crystal is clean. The background spectrum is used to eliminate any signals in the sample data that are due to the spectrometer, the ATR crystal, or the background environment.

The software shows a preview of the current background spectrum in the spectral pane. The background shape shown below is typical for a diamond crystal.

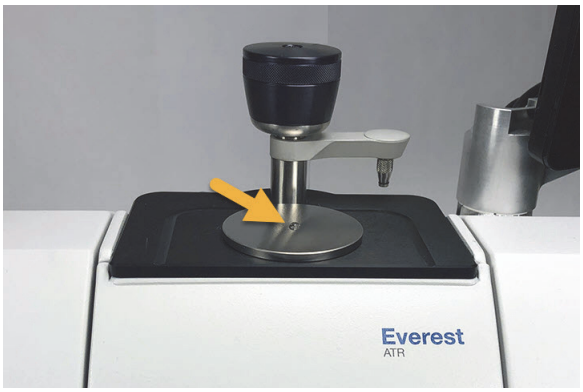


Click **Start Background Measurement**.

When the background measurement is completed, its image appears in the results panel and in the spectral pane.

If your sample is a liquid, raise the pressure tower and rotate it out of the way. Use a clean pipette to place a single drop on the crystal. Keep in mind that crystal types vary in size and some may require more sample. Use just enough sample to cover the crystal completely.

Figure 1. Measure a liquid with ATR

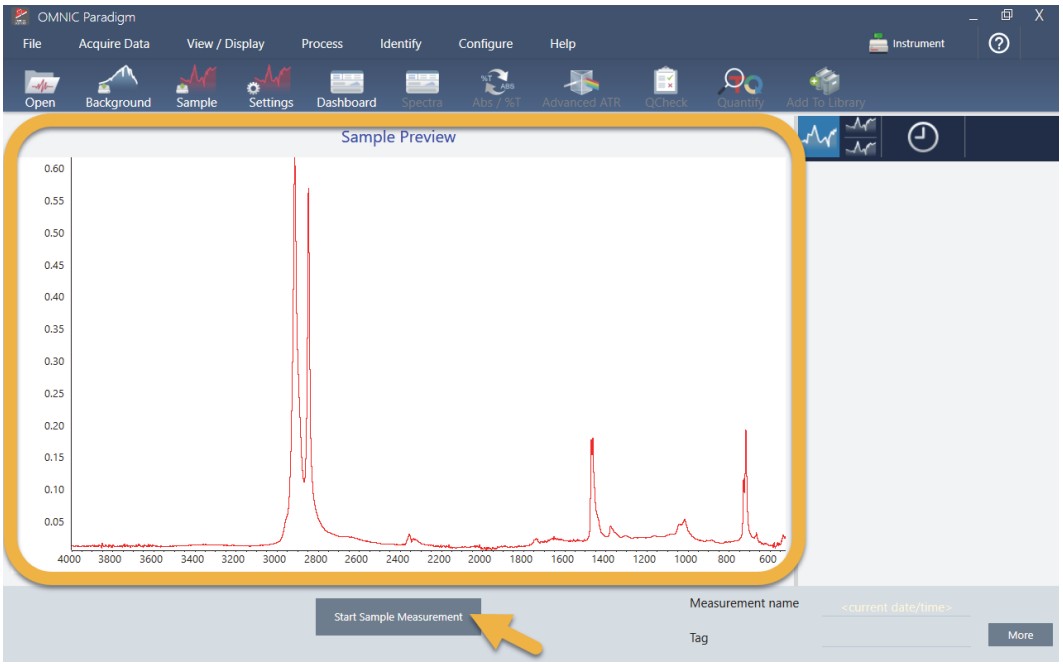


The pressure tower should not be used when analyzing a liquid sample

For a solid sample, rotate the knob on the pressure tower counterclockwise to raise the arm. Then place the sample on the crystal and rotate the knob clockwise to lower the arm. Continue to rotate the knob until clicks. For this demonstration, we are measuring a plastic bag.

Figure 2. Measure a solid with ATR

Once a sample is in place, click **Preview Sample** to preview the sample data in the spectral pane. If the peaks in the preview spectrum are very small, use a more concentrated liquid sample. If you are measuring a solid, reposition the sample on the ATR crystal and reapply pressure.



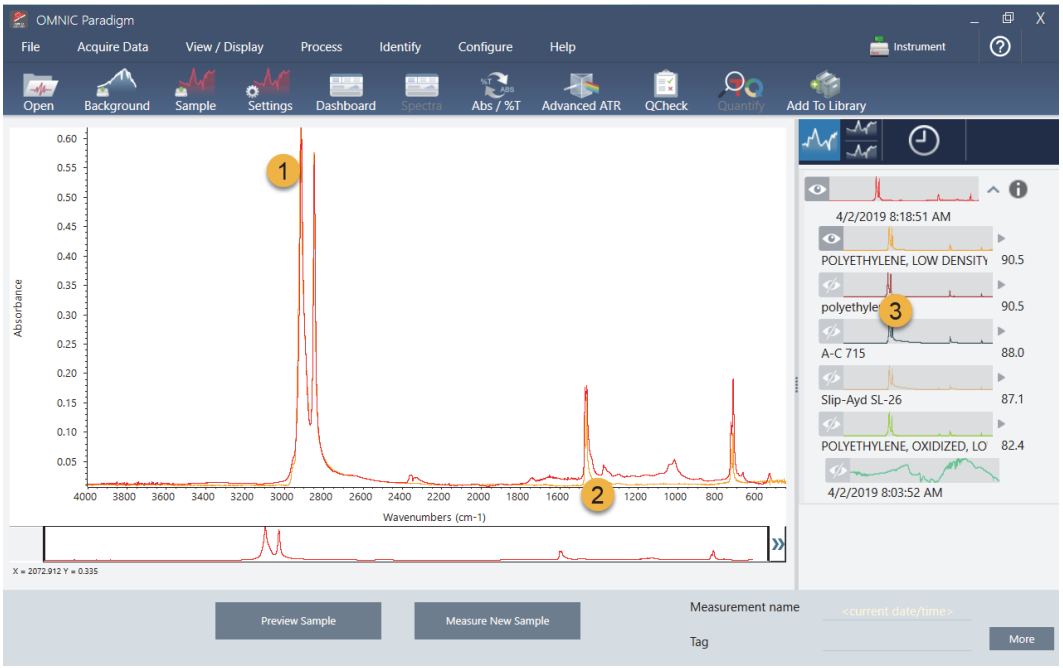
If the spectrum has no sample peaks, check that the sample material absorbs energy in the infrared region of the light spectrum. If you observe extra peaks in the spectrum, make sure the crystal is clean.

When you are ready to continue, choose **Start Sample Measurement** (see the previous image) and wait for the progress bar to complete. The software quickly compares the sample spectrum to the selected library spectra and shows you the results.

What's in My Sample?

The spectral pane shows the sample spectrum along with the best matched spectrum from the selected libraries. The two spectra are overlaid with the same Y-axis scale so you can compare the results visually. (If the spectra are very similar, as in this case, there are other views that will highlight the differences. We'll talk more about that later.) The results panel shows a list of the 5 best matched spectra, along with their match values.

Figure 3. Sample and top search result displayed together using the same Y-axis scale

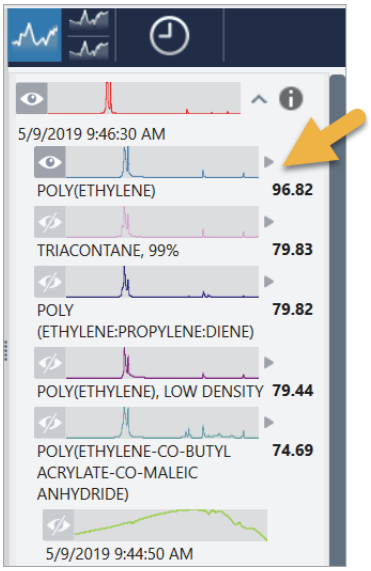


1. Sample spectrum (red)
2. Best match (yellow)
3. Results panel
4. Stack button

The match values tell you how well each library spectrum matches the unknown sample. The closer this value is to 100, the better the match.

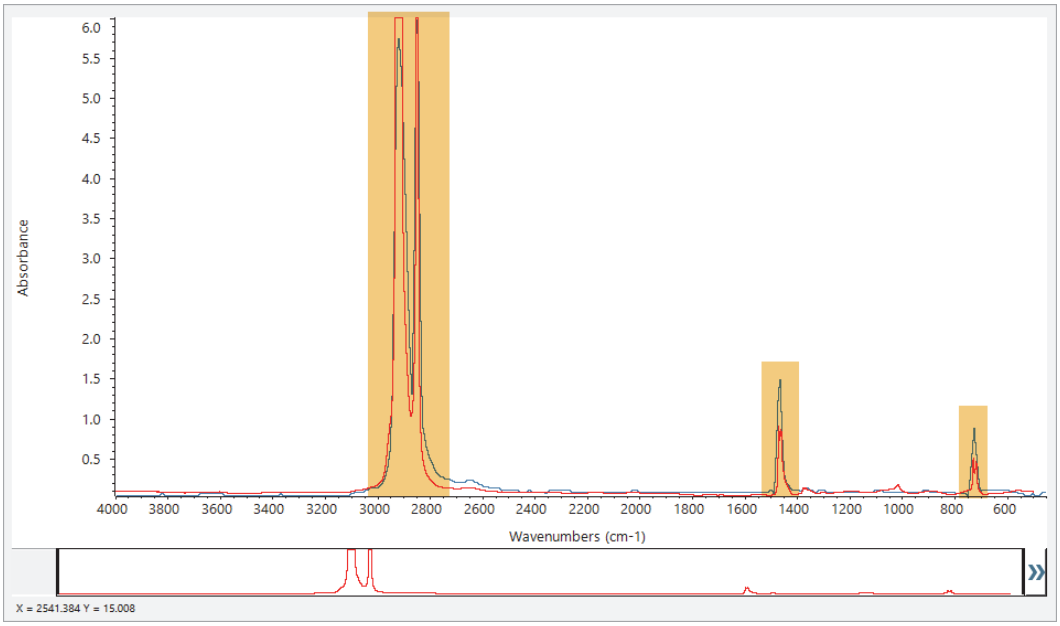
In this example, the top match has a match value that is above 90, which indicates a good match. The match value for the next spectrum in the list is well below that.

Figure 4. Match values showing a clear best match



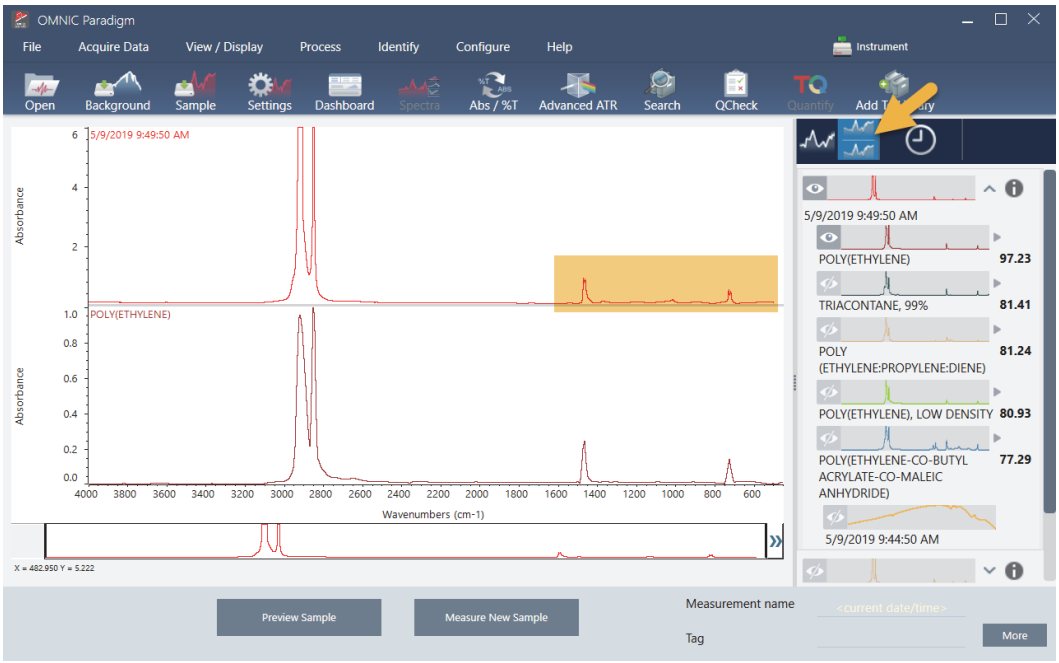
If we look at the overlaid spectra in the spectral pane, the positions of the main peaks line up along the X-axis, and they differ only in their peak heights.

Figure 5. Overlaid spectra showing a clear match



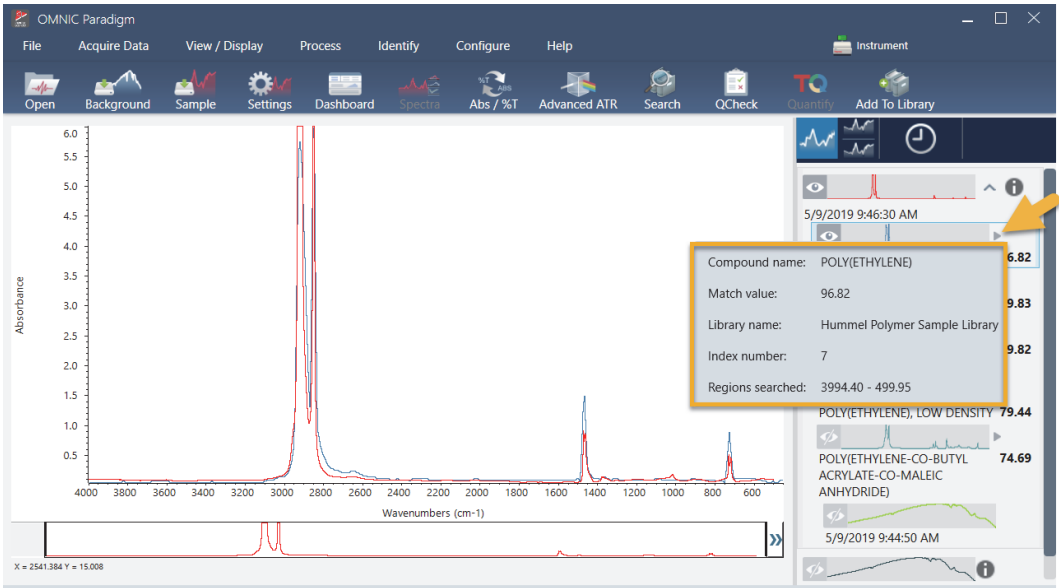
Click the Stack button to see the two spectra scaled to fill each Y-axis. Again, the spectra are well matched except for the slightly raised baseline in the sample spectrum's low frequency region. As a result, we can conclude that the sample is polyethylene and the analysis is complete.

Figure 6. Stacked spectra showing a minor difference in the low frequency region



To get more information about a spectrum in the match list, including the library it came from and its identification number, click the spectrum's grey arrow in the results panel.

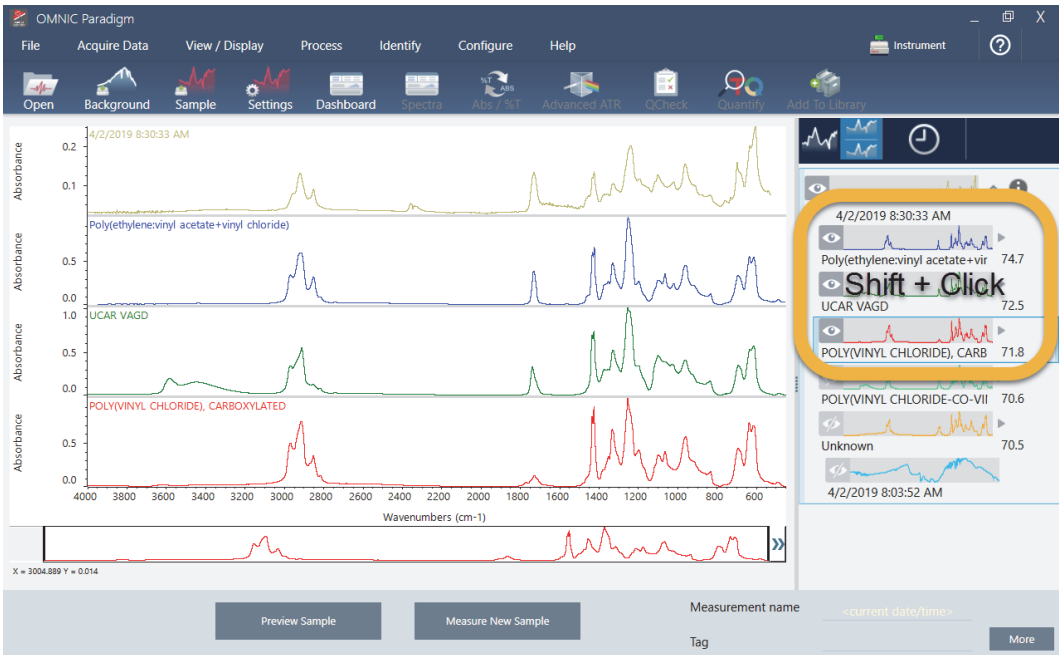
Figure 7. Information button for a library spectrum



What if there isn't a clear (single) match?

If the analysis results show several matches that all have similar match values, as in this example, Shift + click the three matches in the results panel to add all three spectra to the spectral pane.

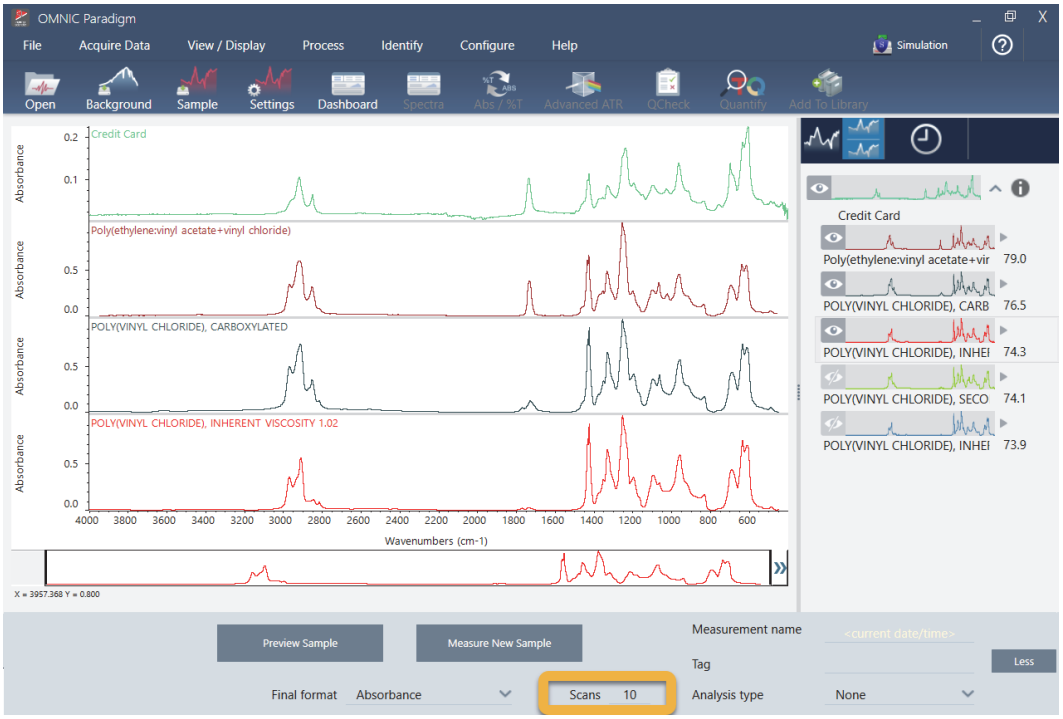
Figure 8. Stacked spectra showing several similar matches



How can I improve my analysis results?

If no clear match appears, there are a number of options to consider that may improve your results. (Some setting adjustments will require a new background measurement.)

Figure 9. Search results with changeable measurement settings displayed



For starters, you can return to the dashboard and adjust the Resolution setting for the unknown sample. For example, you can acquire the spectrum at a higher resolution by using a lower Resolution setting. If the sample peaks are sharper or more numerous, you may get a better analysis result.

You can also acquire more scans (see image above) to reduce spectral noise, which can also affect the results. Then restart the analysis by choosing **Identify** (menu) > **Correlation Search** or click the **Search** button on the toolbar.

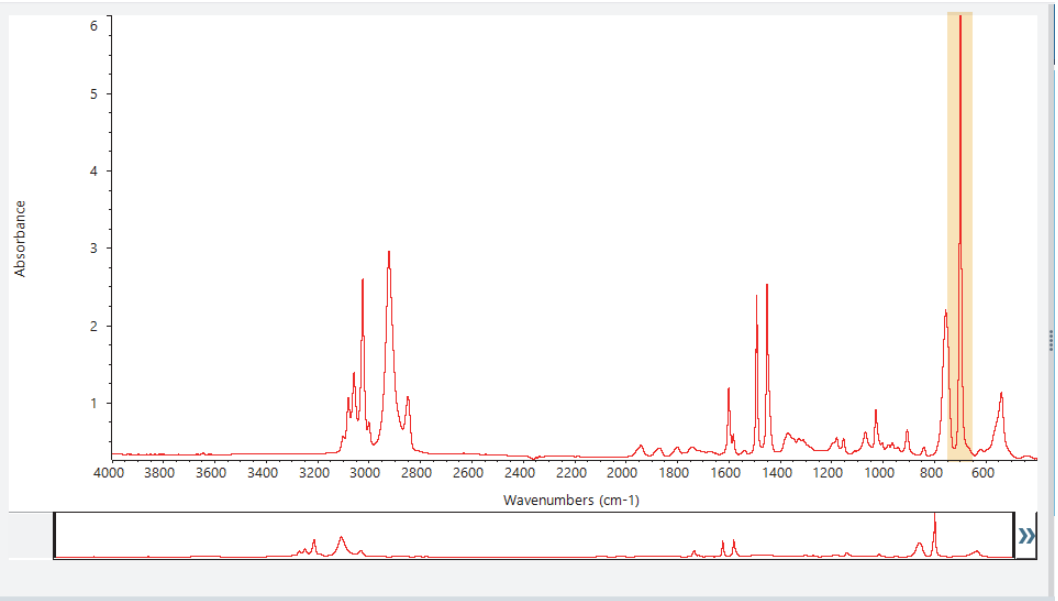
If the sample spectrum has a tilted or curved baseline, try applying Automatic Baseline Correction (Process menu) to your sample spectrum and then restart the analysis.

If you need to search against transmission spectra, try using the Advanced ATR Correction (Process menu) and then repeat the analysis. This correction adjusts an ATR spectrum so that it looks more like a transmission spectrum, which can improve the results.

How to Specify the Spectral Region for the Analysis

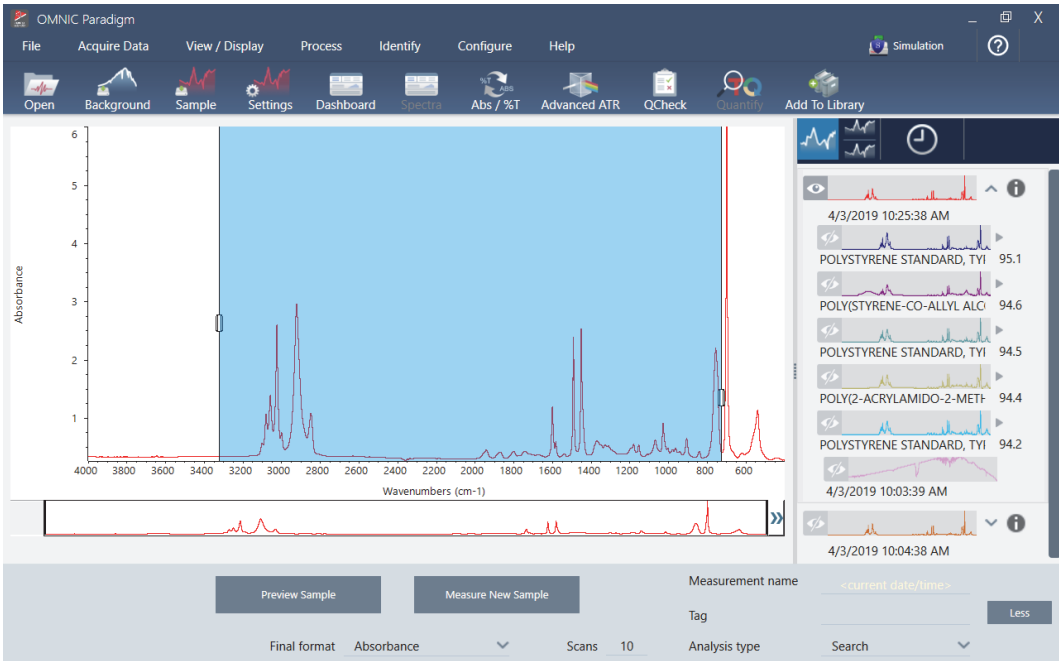
If your sample spectrum has a peak that is so large it is off the Y-axis scale, you may want to exclude that peak from your analysis. Here is an example:

Figure 10. Example of a totally absorbing peak



These “flat topped” peaks are referred to as “totally absorbing” and can contain excessive spectral noise, which affects the analysis results. To exclude a totally absorbing peak, right-click the sample spectrum and choose **Add Region**. Use the vertical bars to select a region that excludes the peak in question and then rerun the analysis.

Figure 11. Using Add Region to exclude a peak from the search



Identify an Unknown Sample with Transmission

Your FTIR spectrometer and Thermo Scientific™ OMNIC Paradigm software can help you identify the chemical composition of an unknown sample. This article demonstrates how to measure and analyze a sample using infrared transmission. By "transmission" we mean that the infrared beam passes directly through the sample. Transmission is a common technique for acquiring FTIR data. This article includes a number of examples to help you build confidence in interpreting your analysis results.

You will learn how to:

- Prepare the transmission accessory
- Set up and run the analysis, and
- Evaluate and confirm the results

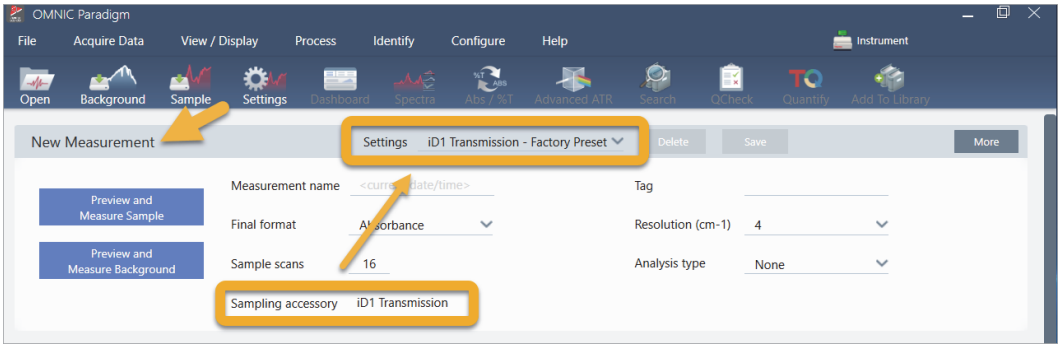
Prepare the Transmission Accessory

To begin, make sure your transmission accessory or sample holder is inserted in the spectrometer sample compartment. Here is the Thermo Scientific™ iD1 Transmission Accessory in our Nicolet™ Summit FTIR Spectrometer.

Remove any sample from your accessory or sample holder so the spectrometer can take an accurate background measurement when it's ready. The iD1 accessory cover can be open or closed. (If your transmission accessory is purged with dry air or nitrogen, keep the cover closed unless you are adding or removing a sample.)

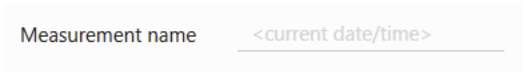
Set Up the Analysis

The next step is to set up the OMNIC Paradigm software. After you open the software, you see the dashboard in the main window. The important measurement settings are at the top.

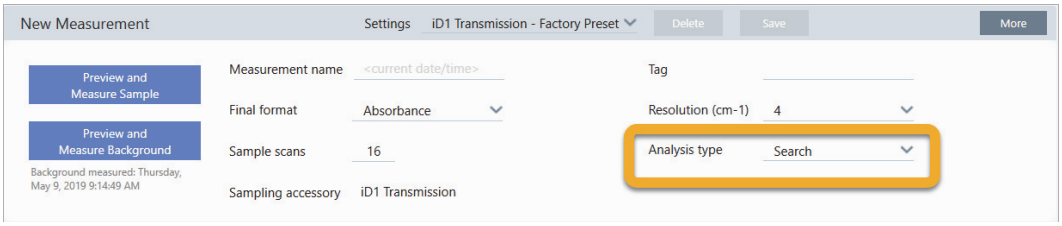


First, make sure the Sampling Accessory readout shows the installed accessory. If it doesn't, reseat the accessory. Notice that the factory presets for that accessory appear under "Settings."

Then enter a measurement name, or you can leave the suggested name, which is the exact date and time of the measurement.



Next make sure the Analysis Type is set to Search.



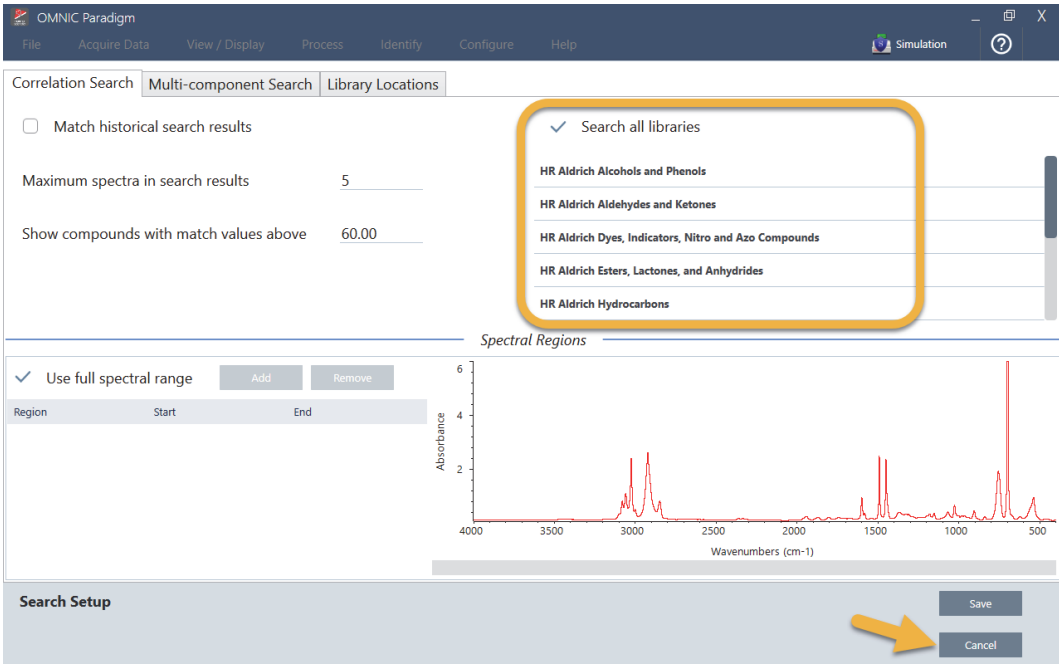
This performs a point-by-point comparison of the sample spectrum against FTIR library spectra. The quality of the output depends on the source and quality of the spectra in the selected libraries.

Finally, check the acquisition settings (sample scans, resolution and final format). The settings shown above are all good starting values for this analysis.

It's important to note that the quality of the sample data you acquire will affect the analysis results. For example, speeding up the analysis by measuring fewer scans, or decreasing the resolution could lead to a less certain analysis result.

Consider Your Spectral Libraries

All existing spectral libraries are selected automatically by default. Choose **Search Setup** in the Identify menu to view or change your library selections. For this demonstration, we are using the free libraries provided with OMNIC Paradigm software and the Nicolet Summit Pro spectrometer.



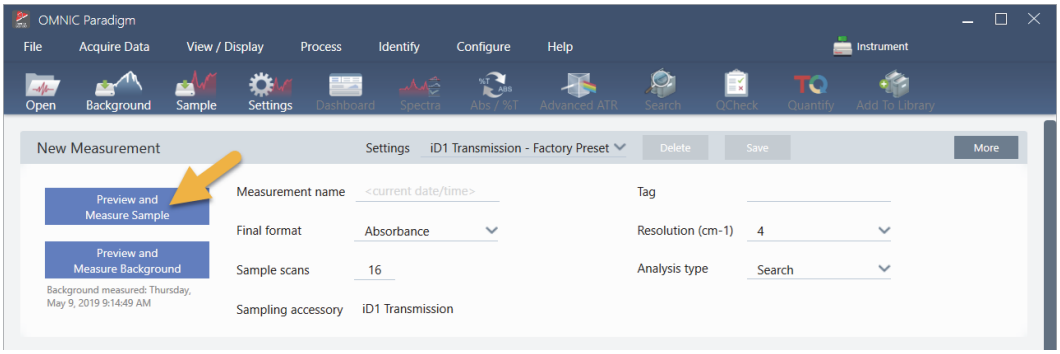
Choose **Cancel** to close the Search Setup window.

You can also use the Library Manager in the same menu to easily create a spectral library. Any libraries you create should be from pure materials that represent what you expect to find in your unknown samples.

The library spectra are normally the same quality or higher quality than the sample spectrum. It is also helpful if they are acquired using the same sampling technique (transmission in this case). There is no need to perform conversions such as final format, resolution or spectral range on the sample data before performing a search—the software does that for you.

Measure and Analyze the Sample

To start the analysis, click **Preview and Measure Sample**.

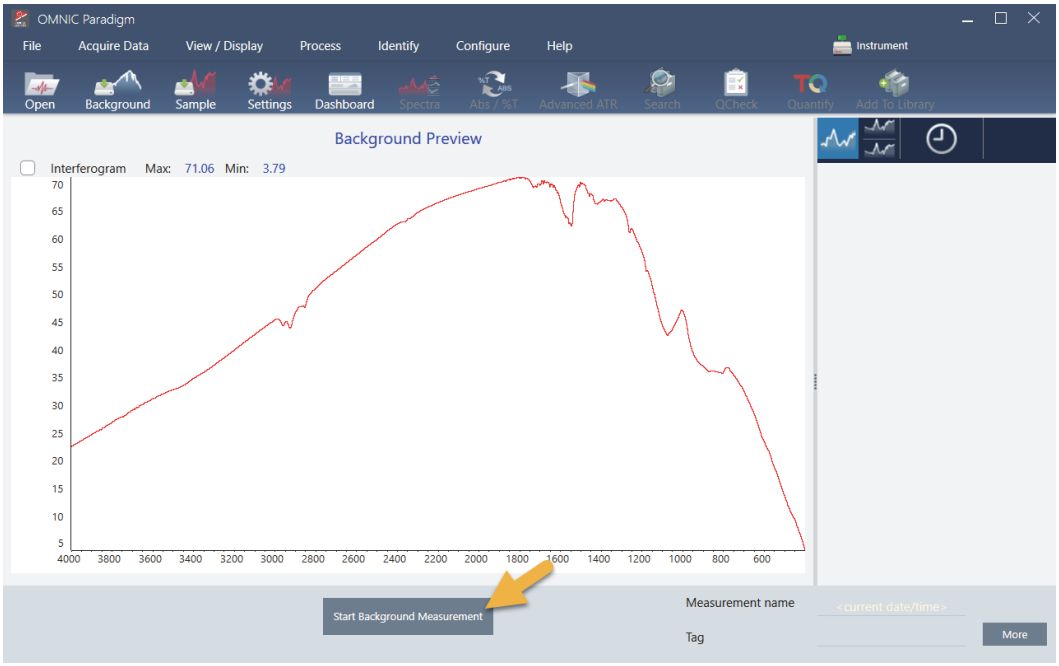


The analysis starts with a background measurement. The only requirement for a transmission background is to remove any sample from the path of the infrared beam. The background spectrum is used to eliminate any signals in the sample data that are due to the spectrometer, your transmission accessory or sample holder, or the background environment.

The software shows a preview of the current background spectrum in the spectral pane. The examples below show typical background spectra for transmission analysis using a transmission accessory that has not been purged with dry air or nitrogen, and one that has been purged.

Figure 12. Background spectrum from a transmission accessory that has not been purged

Figure 13. Background spectrum from a transmission accessory that has been purged

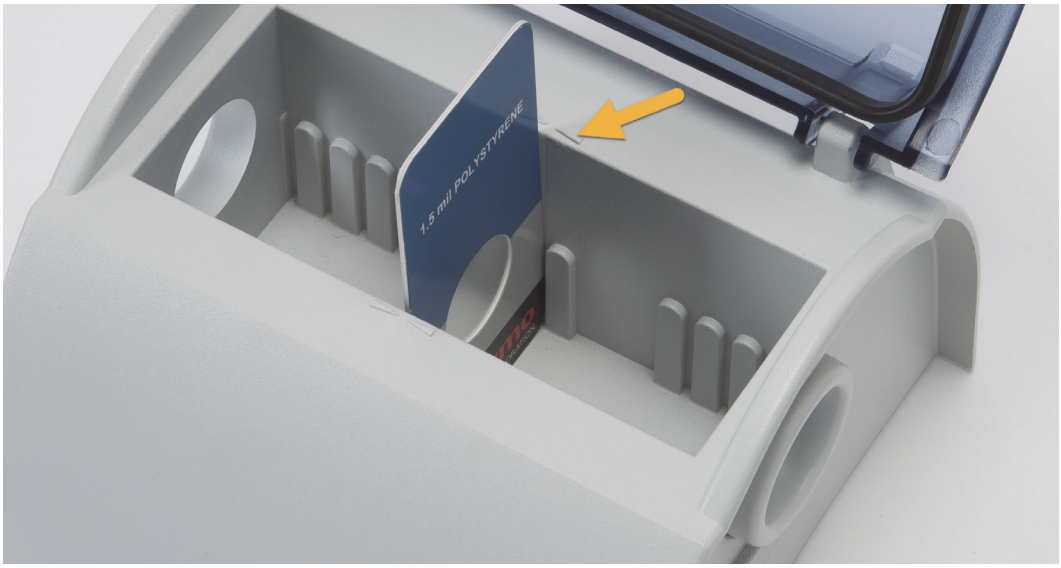


Click **Start Background Measurement**.

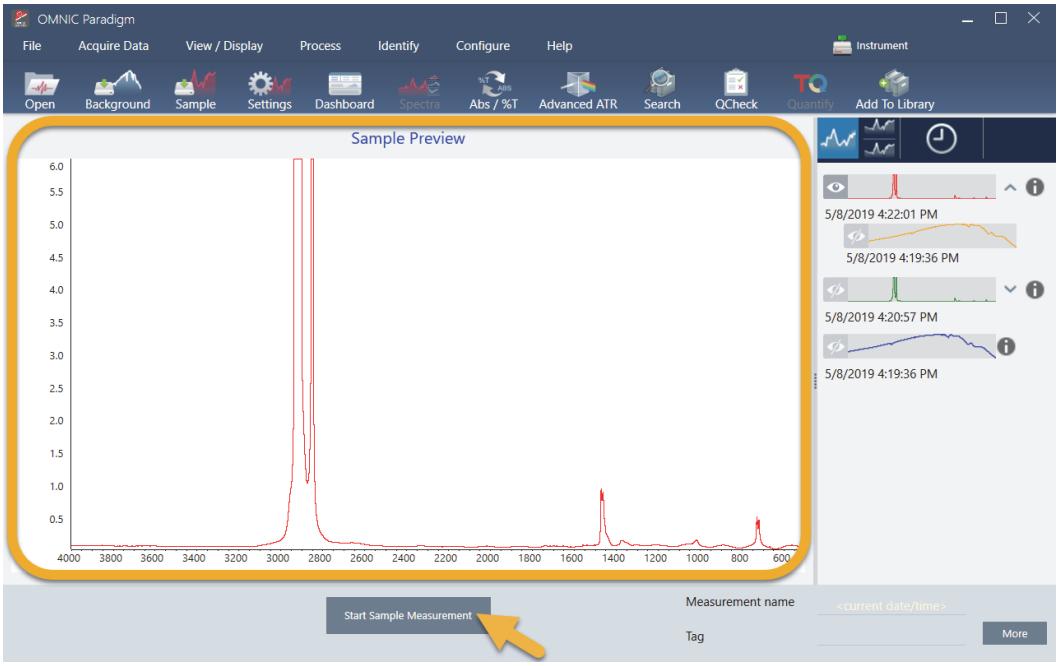
When the background measurement is completed, its image appears in the results panel and in the spectral pane.

To install a mounted film sample, open the cover for the transmission accessory and slide your sample or sample holder into a slot that best fits the sample or sample holder width. If your sample or holder allows it, choose a slot that is close to the beam's focal point (for the iD1 accessory, this is roughly in the center of the sample compartment). For this demonstration, we are measuring a plastic film mounted on a sample card.

Figure 14. iD1 Transmission Accessory beam focal point



Once a sample is in place, click **Preview Sample** to preview the sample data in the spectral pane.



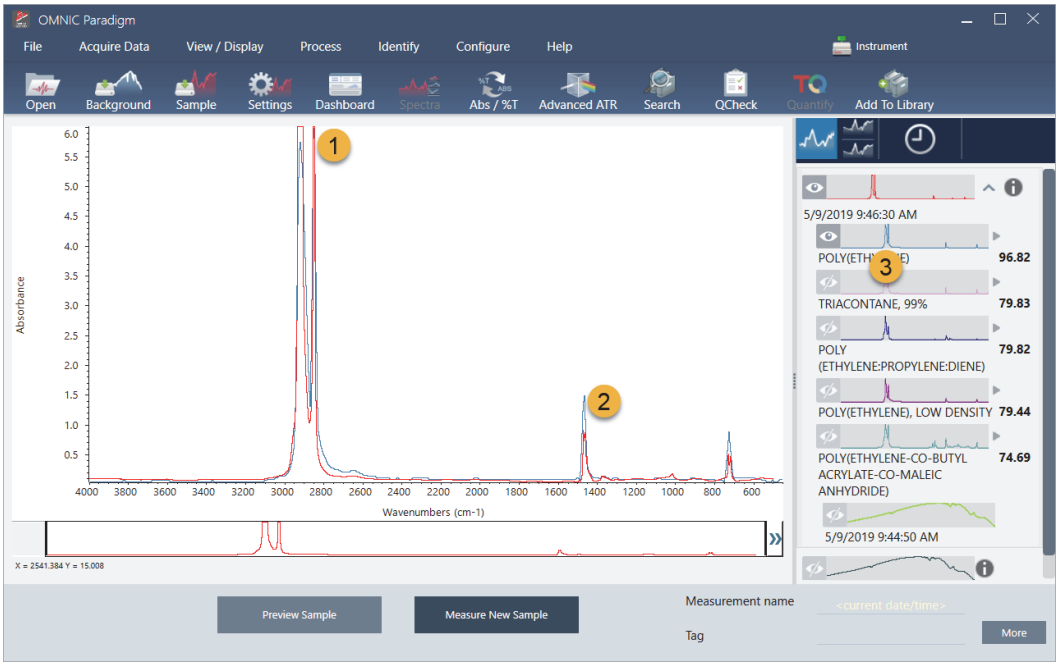
If the peaks in the preview spectrum are very small, try using a thicker sample. If the spectrum has no sample peaks, check that the sample material transmits energy in the infrared spectrum.

When you are ready to continue, choose **Start Sample Measurement** (see the previous image) and wait for the progress bar to complete. The software quickly compares the sample spectrum to the selected library spectra and shows you the results.

What's in My Sample?

The spectral pane shows the sample spectrum along with the best matched spectrum from the selected libraries. The two spectra are overlaid with the same Y-axis scale so you can compare the results visually. (If the spectra are very similar, as in this case, there are other views that will highlight the differences. We'll talk more about that later.) The results panel shows a list of the 5 best matched spectra, along with their match values.

Figure 15. Sample and top search result displayed together using the same Y-axis scale

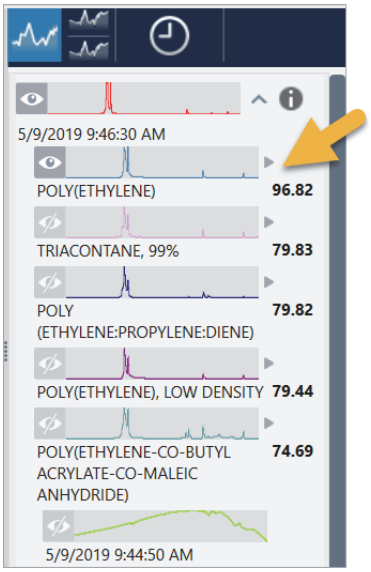


1. Sample spectrum (red)
2. Best match (blue)
3. Results panel

The match values tell you how well each library spectrum matches the unknown sample. The closer this value is to 100, the better the match.

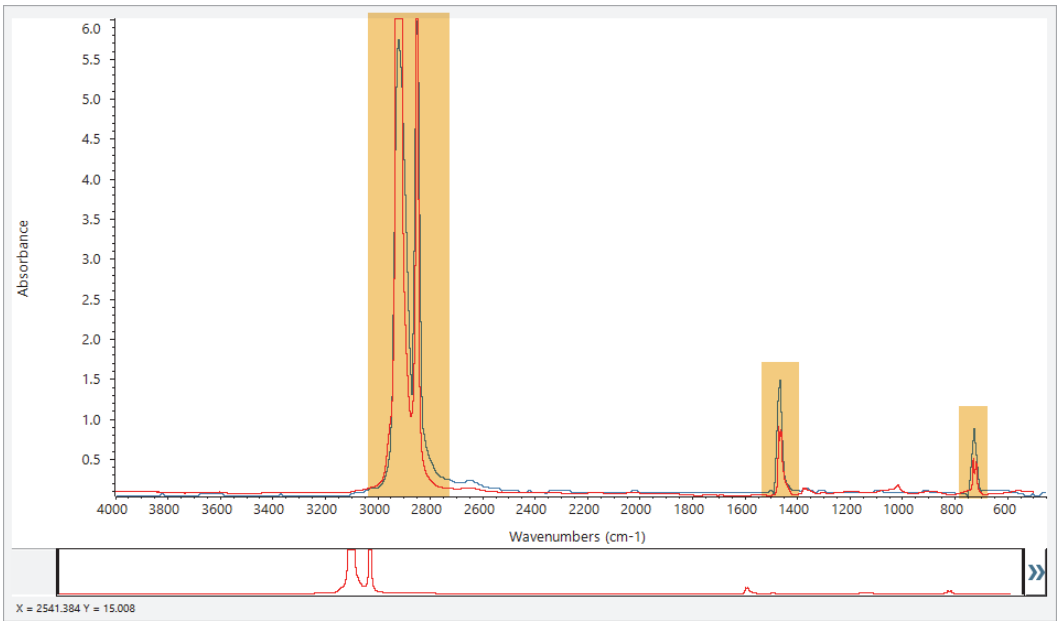
In this example, the top match has a match value that is above 85, which indicates a good match. The match value for the next spectrum in the list is well below that.

Figure 16. Match values showing a clear match



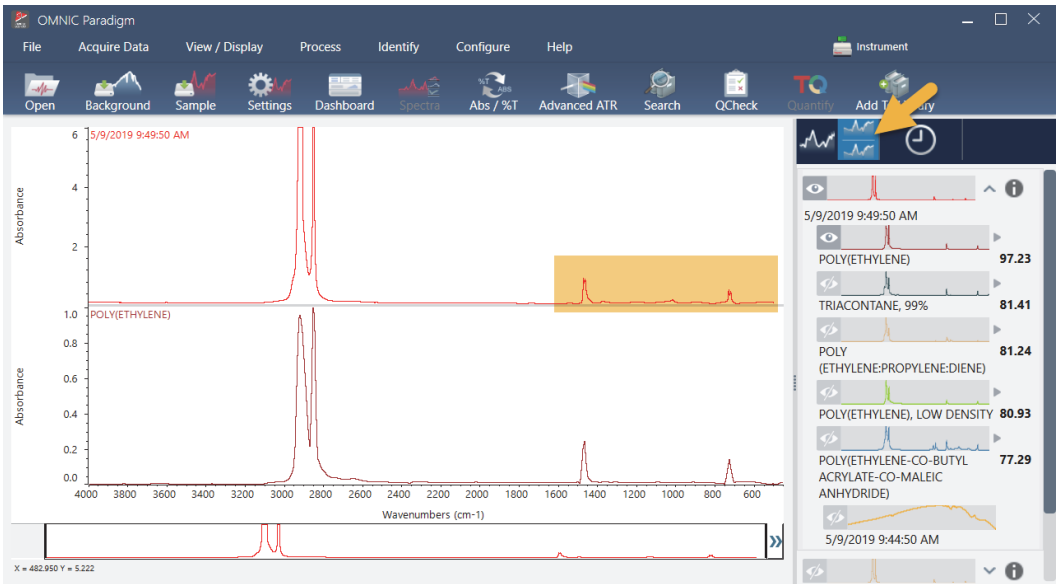
If we look at the overlaid spectra in the spectral pane, the positions of the main peaks line up along the X-axis, and they differ only in their peak heights.

Figure 17. Overlaid spectra showing a clear match



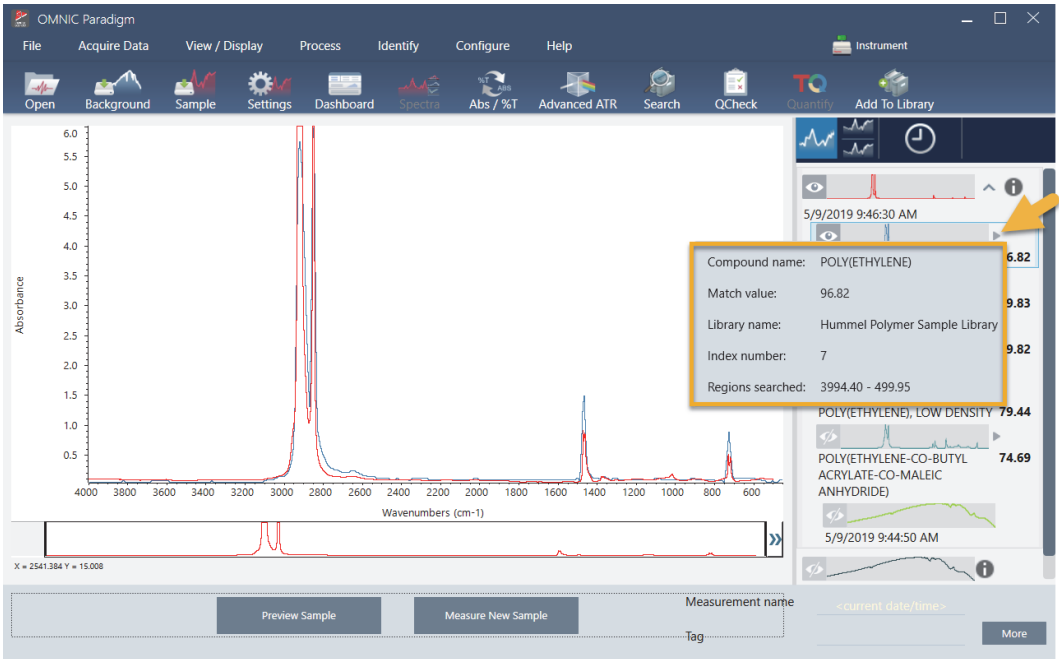
Click the Stack button to see the two spectra scaled to fill each Y-axis. Again, the spectra are well matched except for the slightly raised baseline in the sample spectrum's low frequency region. As a result, we can conclude that the sample is polyethylene and the analysis is complete.

Figure 18. Stacked spectra showing a clear match



To get more information about a spectrum in the match list, including the library it came from and its identification number, click the spectrum's grey arrow in the results panel.

Figure 19. Information button for a library spectrum



What if there isn't a clear (single) match?

If the analysis results show several matches that all have similar match values, as in this example, Shift + click the three matches in the results panel to add all three spectra to the spectral pane for a detailed comparison.

Figure 20. Stacked spectra showing several similar matches

How can I improve my analysis results?

If no clear match appears, there are a number of options to consider that may improve your results. (Some setting adjustments will require a new background measurement.)

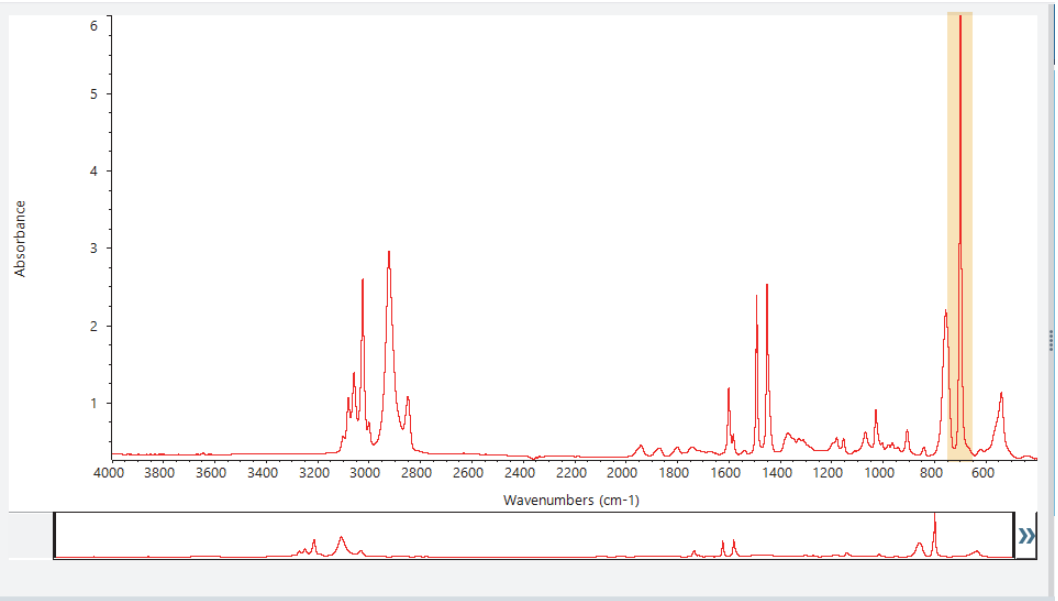
For starters, you can return to the dashboard and adjust the Resolution setting for the unknown sample. For example, you can acquire the spectrum at a higher resolution by using a lower Resolution setting. If the sample peaks are sharper or more numerous, you may get a better analysis result. You can also acquire more scans to reduce spectral noise, which can also affect the results.

If the sample spectrum has a tilted or curved baseline, try applying Automatic Baseline Correction (Process menu) to your sample spectrum. Then restart the analysis by choosing **Identify** (menu) > **Correlation Search**, or click the **Search** button on the toolbar.

How to Specify the Spectral Region for the Analysis

If your sample spectrum has a peak that is so large it is off the Y-axis scale, you may want to exclude that peak from your analysis. Here is an example:

Figure 21. Example of a totally absorbing peak

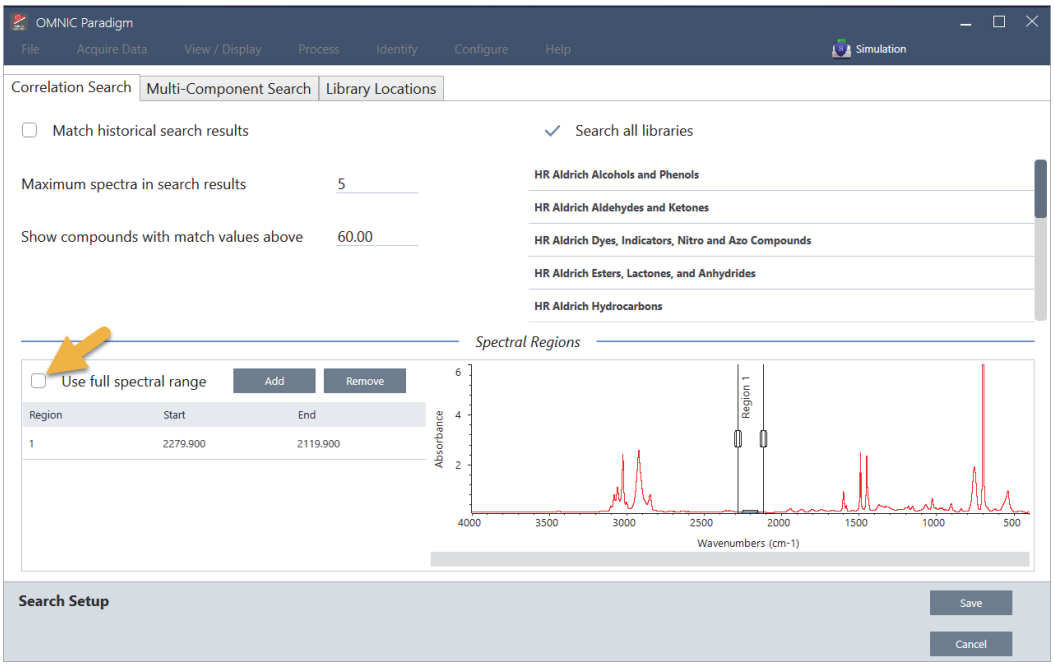


These “flat topped” peaks are referred to as “totally absorbing” and can contain excessive spectral noise, which affects the analysis results.

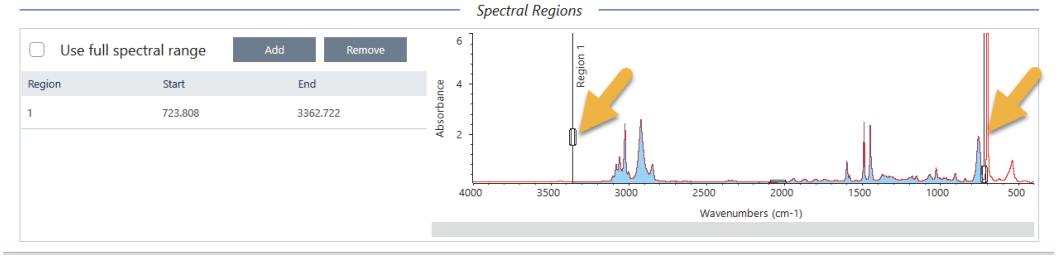
To exclude a totally absorbing peak, choose **Identify** (menu) **> Search Setup** and use the tools to select the regions to search.

First, clear the "Use Full Spectral Range" check box to enable the region tools.

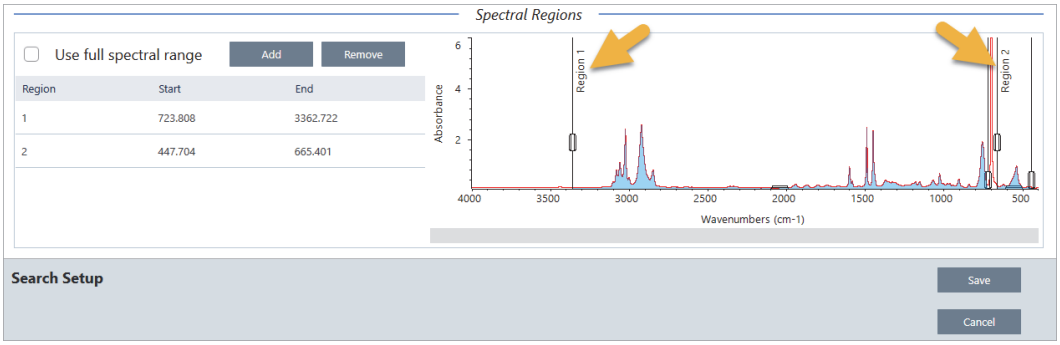
Figure 22. Tools for selecting the regions to search



Then position the vertical bars to select the first region to search.



To add a search region, click the **Add** button and use the second set of vertical bars to select the next region. Here we used the first set of vertical bars to select the region to the left of the fully-absorbing peak. And then we added a region and used the second set of vertical bars to select the region to the right of the fully-absorbing peak.



When you are finished selecting regions, click **Save** to return to the Dashboard view, and then click the **Search** button on the toolbar to re-run the search.

Verify Sample Composition with QCheck

Verify your sample quality with a QCheck analysis. With QCheck, your sample is compared to a known reference, and the results report a correlation value between your sample and the reference, giving you quick verification that your sample meets your specifications.

This guide walks you through an example QCheck analysis.

Prerequisites

This guide assumes that you have already set up your instrument and sampling accessory. For instructions on installing a sampling accessory, see the documentation that came with your instrument.

You will also need at least one spectrum to use as a reference. You can specify any spectrum in your database as the reference spectrum. To use a spectrum from a library, first extract the spectrum from the library so that it is available in the database. For details, see Extract a Spectrum from a Library

Performing a QCheck Analysis

Running a QCheck analysis requires you to set up your analysis and measurement settings, measure the background, measure your sample, and interpret your results. Finally, when your analysis is complete, you can create and save a report.

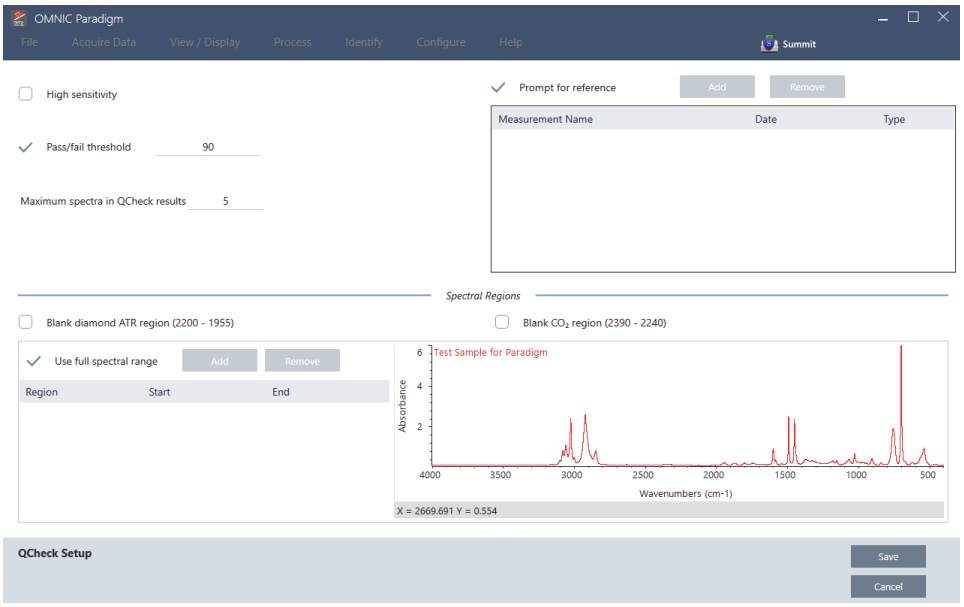
❖ **To verify your sample composition with QCheck**

1. **Set up the analysis.**

   Before measuring your sample, review your analysis settings.

   a. Navigate to **Identify > QCheck Setup**.

   b. Review the QCheck Setup options.



Setting	Description
High Sensitivity	Select high sensitivity for more exact results between a sample that is very similar to the reference. You may want to de-select high sensitivity if you are measuring samples with some natural variation.
Pass/fail threshold	Set a threshold for pass or failure. Enter an integer between 0 and 100. A correlation value of 100 indicates a perfect match. If you de-select this option, all results will show Pass.
Maximum spectra in QCheck results	Sets the number of results shown in the results panel. For example, if you set the value to 2, only the two best matches will be shown in the results panel.
Prompt for reference	Select to choose a reference during the measurement. De-select to specify one or more reference spectra in advance. If you are planning to compare several samples to the same references, it is convenient to set them in advance to avoid having to keep selecting the same reference every time you measure a sample.
Blank diamond ATR region (2200 - 1955)	Select to exclude data in the region from 2200 wavenumbers to 1955 wavenumbers, where diamond ATR crystals absorb radiation.

Setting	Description
Blank CO_2 region (2390 - 2240)	Select to exclude data in the region from 2390 wavenumbers to 2240 wavenumbers, where carbon dioxide absorbs radiation.
Use full spectral range	Select to use the full range in the analysis. De-select to specify only a limited range to use for the analysis.

c. To save your settings and return to the dashboard, click **Save**.

d. On the dashboard, review your measurement settings, and confirm that the listed sampling accessory matches the accessory you are using.

e. From the Analysis Type list, select **QCheck**.

Once you are satisfied with your measurement and analysis settings, you are ready to measure the background.

2. Measure the background.

Before measuring your sample, you need to have a current measurement of the background.

The background spectrum is used to eliminate any signals in the sample data that are due to the spectrometer, the sampling accessory, or the background environment.

a. Click **Preview and Measure Background**.

b. Click **Start Background Measurement**. When the background measurement is complete, the spectrum is added to the results panel.

3. Measure your sample.

a. Load your sample. For instructions on loading a sample, see the documentation that came with your instrument or sampling accessory.

b. Click **Preview Sample**. The Sample Preview displays a live preview of your sample spectrum. The preview gives you the opportunity to correct any potential issues before measuring the sample.

c. When you are ready to continue, click **Start Sample Measurement.**

If Prompt for Reference is selected in your analysis settings, the Select Reference Spectrum dialog opens after the measurement is complete.

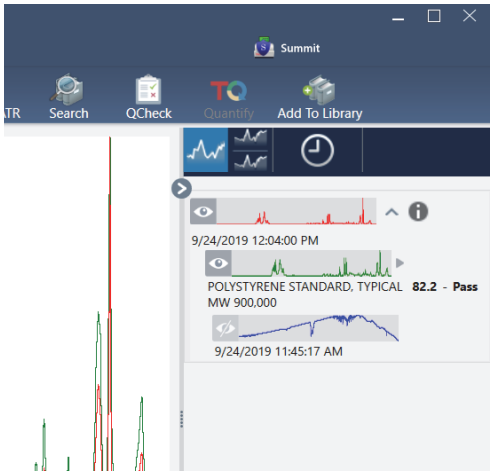
d. Select one or more reference spectra to use in the analysis and click **OK**.

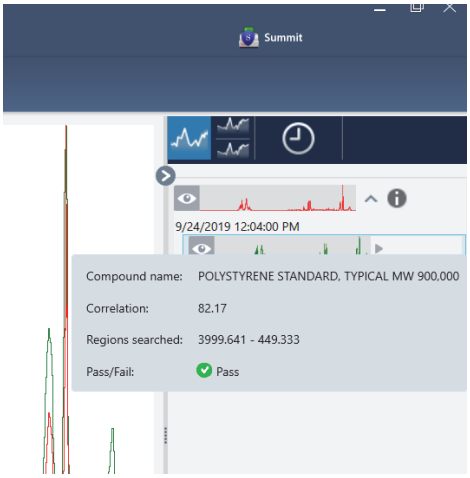
Hold Ctrl and click to add a spectrum to your selection.

Hold Shift and click to add a group of spectra to the selection.

4. **Interpret your results.**

   When the measurement and analysis are complete, your results are displayed in the results panel. Hover over the gray arrow for additional details.





5. **Create a report**

   When you are finished with your analysis, create a report to export your results to Microsoft™ Word™, PowerPoint™ or Excel™ or to print or save your results.

   a. Navigate to **File > Create Report.**

   b. Give your report a title.

   c. Select a format from the Format list and choose the Quantify template. A preview of the report is shown in the right panel.

   d. Click **Create**.

Improving Your Results

If your correlation value is lower than expected, there are several options to consider that may improve your results.

- Return to the dashboard and adjust the Resolution settings for your measurement. For example, you can measure the sample at a higher resolution by selecting a smaller value, such as 1 or 2. If the sample peaks are sharper or more numerous, you may get a more accurate analysis result.
- Increase the number of scans in your measurement, which may reduce spectral noise.
- If the sample spectrum has a tilted or curved baseline, try applying Automatic Baseline Correction to your sample and then restart the analysis from the Identify menu.

- Exclude selected regions from the analysis. If your sample spectrum has a peak that is so large it is off the Y-axis scale, you may want to exclude that peak from your analysis. These "flat topped" peaks are referred to as "totally absorbing" and may affect the analysis results. Open QCheck Setup, de-select Use Full Spectral Range, and select ranges that exclude the sample spectrum's totally absorbing peak. Then, rerun the QCheck analysis.

Extract a Spectrum from a Library

Extract a spectrum from a library to use it as a reference in a QCheck analysis. Spectra extracted from commercial libraries can be used for analysis, but cannot be renamed, tagged, or exported.

❖ To extract a spectrum from a library

1. From the dashboard of the desktop interface of OMNIC Paradigm software, navigate to **Identify > Library Manager**.
2. Select a compound to extract.
3. Click **Extract**. A confirmation message states that the spectrum was successfully extracted.

Next Steps

In this guide, you set up and ran a QCheck analysis to verify that your sample matched a known reference within a pre-set threshold.

Next, see Create and Run Your First Workflow for a guided tutorial on using workflows to create routine, repeatable procedures.

Quantify Sample Composition

Find the concentrations of components in your sample using a Quantify analysis. A Quantify analysis uses a previously created quantitative analysis method and reports the concentration of components in the sample or other kind of information, such as peak height or match value.

This guide walks you through setting up and running a Quantify analysis using the desktop interface of OMNIC Paradigm software.

Prerequisites

This guide assumes that you have already set up your instrument and sampling accessory. For instructions on installing a sampling accessory, see the documentation that came with your instrument.

You will also need a valid quantification method saved as a QNT file. The quantitative analysis method must be calibrated using Thermo Scientific TQ Analyst software. See the documentation that came with that software for information on calibrating quantitative analysis methods.

Performing a Quantify Analysis

Running a Quantify analysis requires you to import a QNT file, review your measurement settings, measure the background, and finally measure your sample. When analysis is complete, you can create a report to save or share your results.

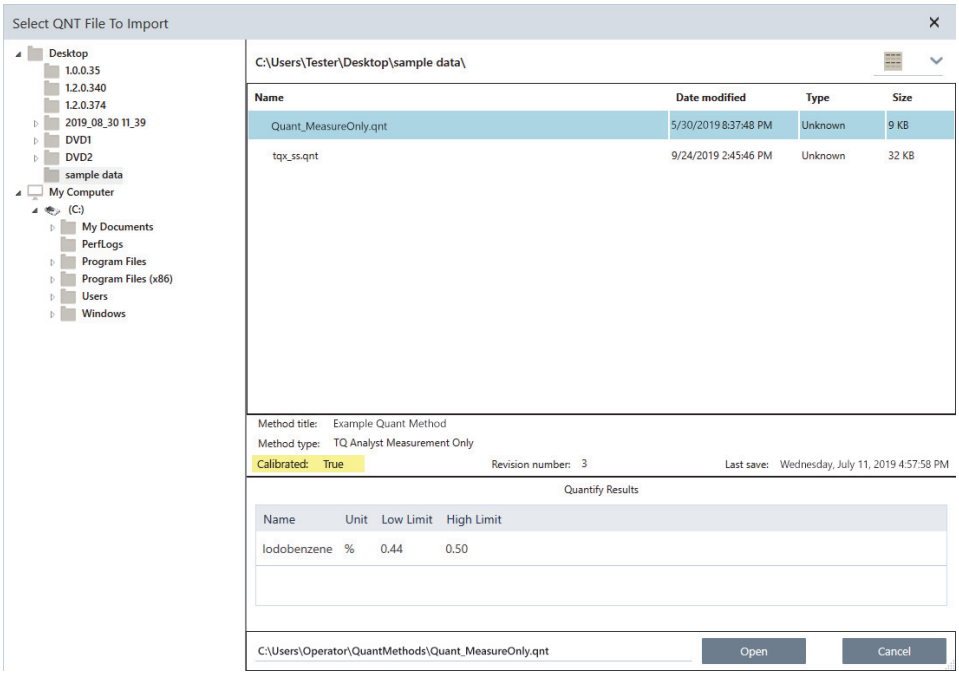
❖ **To perform a Quantify analysis**

1. **Set up the analysis.**
   a. On the dashboard of the desktop interface of OMNIC Paradigm software, confirm that the settings display your sampling accessory.
   b. Navigate to **Identify > Quantify Setup** and browse to the QNT file you would like to use in the analysis.

      The file explorer displays additional information about the QNT file that you have selected, such as the method title, method type, and whether the method has been calibrated.
   c. To import the method, click **Open**.

d. In the Analysis type list, select **Quantify**. A symbol indicates that you have imported a valid QNT file. A red circle with an X [ ] indicates that a valid method has not been imported.

When selecting a QNT file, the file explorer displays additional information to help you make a selection, including the method title and type and whether the method has been calibrated. Only methods that have been calibrated with TQ Analyst software are valid.



2. **Measure the background.**

Before measuring your sample, you need to have a current measurement of the background.

The background spectrum is used to eliminate any signals in the sample data that are due to the spectrometer, the sampling accessory, or the background environment.

a. Click **Preview and Measure Background**.

b. Click **Start Background Measurement**. When the background measurement is complete, the spectrum is added to the results panel.

3. **Measure the sample.**

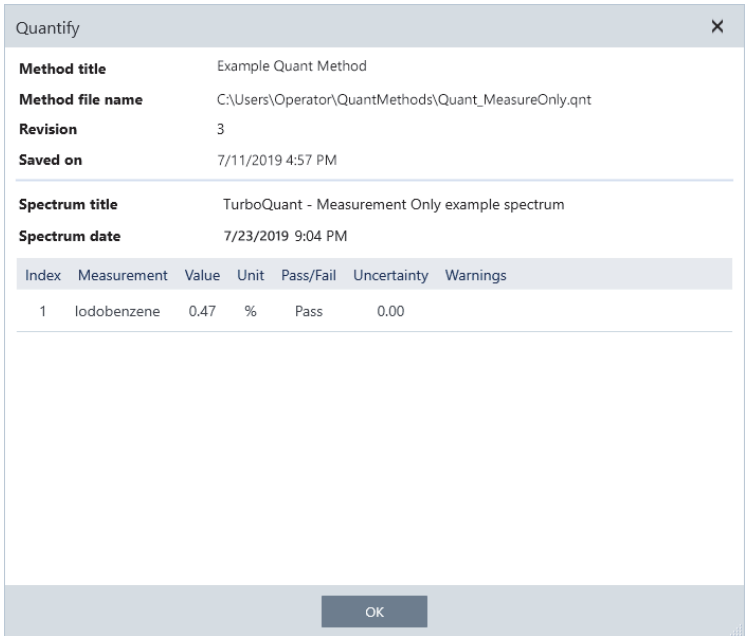
a. Load your sample. For instructions on loading a sample, see the documentation that came with your instrument or sampling accessory.

b. Click **Preview Sample**. The Sample Preview displays a live preview of your sample spectrum. The preview gives you the opportunity to correct any potential issues before measuring the sample.

c. When you are ready to continue, click **Start Sample Measurement.**

4. **Interpret your results.**

   When the sample measurement is complete, the Quantify dialog box displays results of the analysis. The results shown depend on the settings in the quantitative analysis method used in the analysis. The results shown below show a measurement only result indicating a passing value.



   After clicking OK to close the Quantify dialog box, you can view the analysis results by clicking the information icon [ ] next to the spectrum in the results panel. In the Spectrum Information dialog, navigate to the History tab and see the Quantify Results section.

5. **Create a report**

   When you are finished with your analysis, create a report to export your results to Microsoft™ Word™, PowerPoint™ or Excel™ or to print or save your results.

   a. Navigate to **File > Create Report.**

   b. Give your report a title.

   c. Select a format from the Format list and choose the Quantify template. A preview of the report is shown in the right panel.

   d. Click **Create**.

Improving Your Results

If your results are unclear or problematic, there are several options to consider that may improve your data.

- Return to the dashboard and adjust the Resolution settings for your measurement. For example, you can measure the sample at a higher resolution by selecting a smaller value, such as 1 or 2. If the sample peaks are sharper or more numerous, you may get a more accurate analysis result.
- Increase the number of scans in your measurement, which may reduce spectral noise.
- If the sample spectrum has a tilted or curved baseline, try applying Automatic Baseline Correction to your sample and then restart the analysis from the Identify menu.

Next Steps

In this guide, you set up and ran a Quantify analysis.

Next, see Create and Run Your First Workflow for a guided tutorial on using workflows to create routine, repeatable procedures.

5

Use Workflows

Use workflows to automate your tasks, ensuring that your analysis and processing will be carried out in exactly the same way each time.

This section includes the following:

Contents

- About Workflows

  Provides an overview of using workflows to automate important procedures and frequent tasks

- Create and Run Your First Workflow

  This tutorial walks you through the process of creating and running your first workflow

- Workflow Tiles Reference

  This reference describes available workflow tiles and their settings

About Workflows

You can use the workflow features in OMNIC Paradigm software to automate important procedures and frequent tasks. A workflow is a series of software operations that can be initiated with the click of a button. The software operations are represented by tiles, which you drag and drop onto the workflow canvas in OMNIC Paradigm software. You can specify settings for data collection, provide instructions for operators, and define data processing, reporting, and archiving in advance. Once a workflow has been created, operators can use it repeatedly to complete the steps the same way every time.

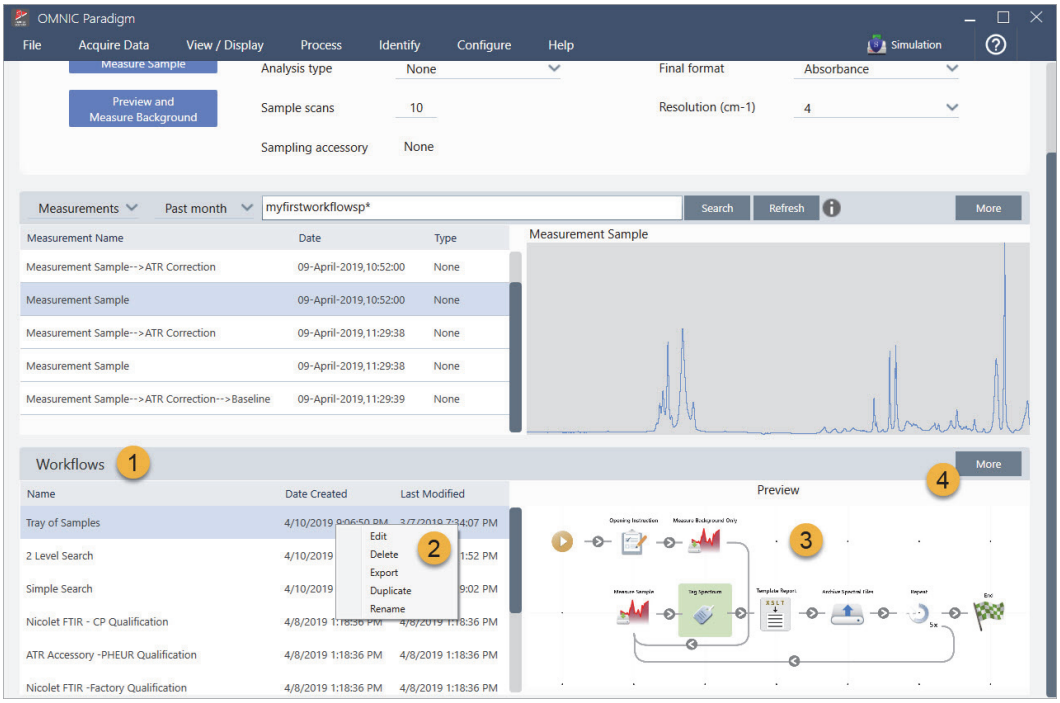
This article provides an overview of these basic workflow features and tools:

- Workflow pane
- Play Workflow window
- Workflow editor

Workflow Pane

The workflow pane is always available at the bottom of the OMNIC Paradigm dashboard. Use this space to preview and play workflows you've created, and to open the workflow editor to edit or create a new workflow.

Figure 1. Workflow Pane on the OMNIC Paradigm Dashboard



1. Most recent workflows (click once to preview a workflow; click twice to play it)
2. Right-click a workflow for more options
3. Preview of selected workflow
4. Enlarge or reduce the Workflows pane

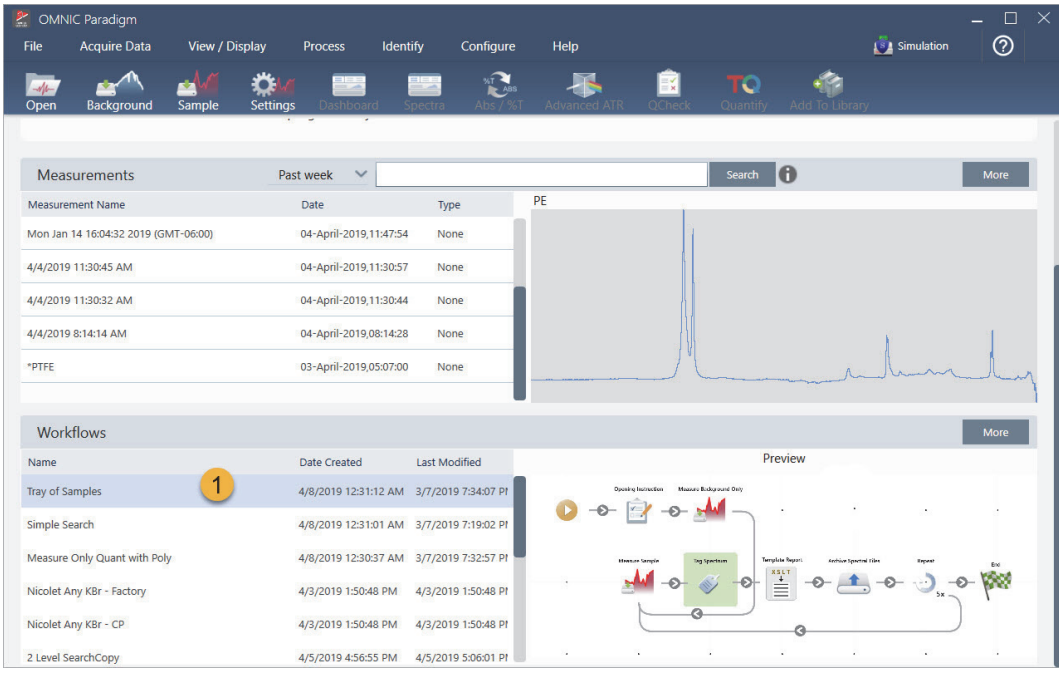
Table 1. Work with existing workflows from the workflow pane

To do this...	Take this action
Select and preview a workflow	Click once on the workflow name
Test or run a workflow	Double-click the workflow name. This opens the Play Workflow window where you can step through the workflow tasks.
Edit, rename, duplicate, delete or export the selected workflow	Right-click the workflow and choose an option from the shortcut menu.

Play Workflow Window

Use the Play Workflow window to test or run a workflow. To open the Play Workflow window, double-click a workflow name in the Workflows list on the dashboard.

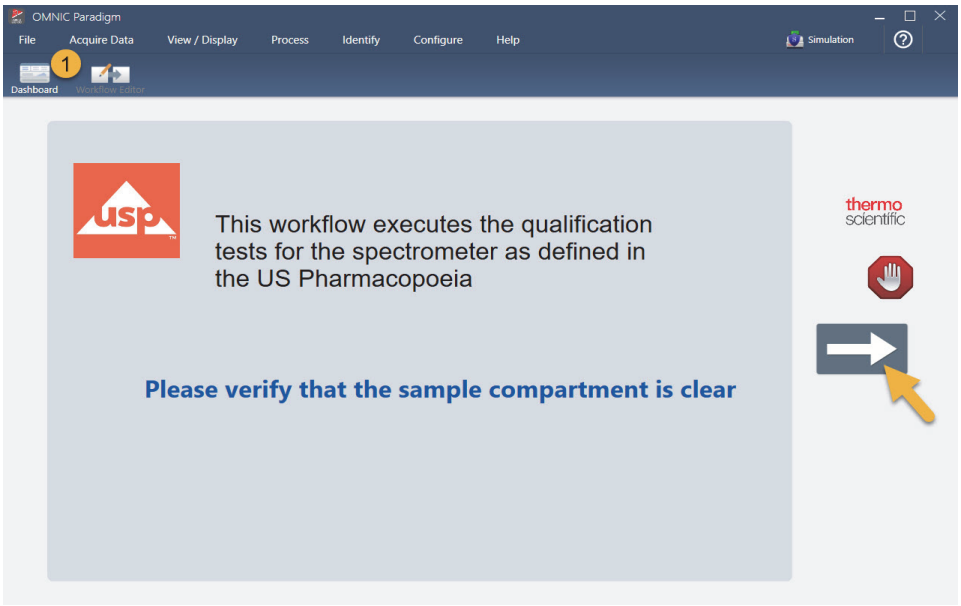
Figure 2. Double-click a Workflow Name to Run the Workflow



1. Selected workflow (double-click to open and run this workflow)

From the Play Workflow window, use the arrow button to move to the next task in the workflow. The workflow will play exactly as it has been designed, with tasks and operator messages displayed as indicated by the workflow.

Figure 3. Play Workflow Window



1. Toolbar

To stop the workflow and return to the dashboard, click the Stop button in the Play Workflow window. (If the workflow doesn't have a Stop button, click the Dashboard button on the toolbar to stop the workflow.)

Workflow Editor

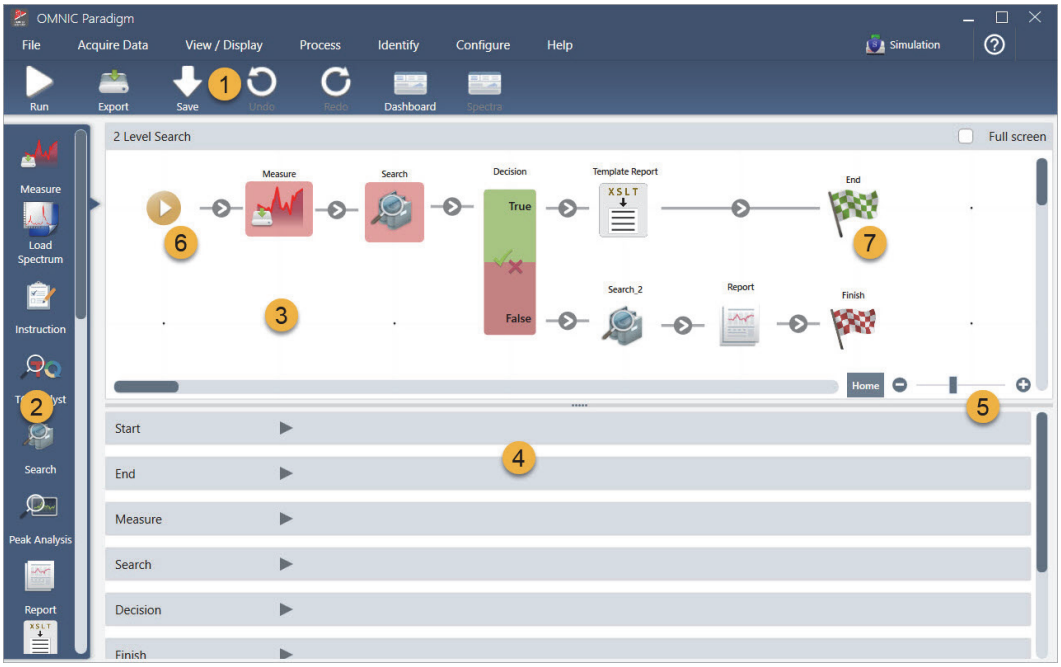
The workflow editor contains all the tools for creating workflows, including the workflow menu, toolbar, tile selection bar, and canvas. To open the workflow editor, right-click a workflow name on the dashboard and choose **Edit** from the shortcut menu.

You can also open the workflow editor from the OMNIC Paradigm main window by choosing:

File (menu) > **Workflows** > **Create Workflow**

The workflow canvas is where you select and set up the tasks you want the workflow to perform and join tasks together to create the workflow. The workflow editor opens with the mandatory “Workflow Start” and “Workflow End” tiles displayed on the canvas. Available settings for each tile in the current workflow are in the expandable sections below the canvas. Tools for scrolling, zooming and resetting the canvas view are at the right. A handy toolbar is above the canvas.

Figure 4. Workflow Editor



1. Toolbar
2. Tile selection bar
3. Canvas
4. Tile settings
5. Tools to adjust and reset the canvas view
6. Start tile
7. End tile

Each task is represented by a colorful tile in the tile selection bar. Here are some commonly used examples:

Tools for creating, opening, and exporting workflows are located in the Workflow submenu (available from the OMNIC Paradigm File menu). Example workflows, available here, are a good place to start, or you can create a workflow from a spectrum’s history. See “Create and Run Your First Workflow” for details.

Tiles can be added, moved, copied and deleted to create the desired workflow. For more information, see the article titled "Edit a Workflow."

Create and Run Your First Workflow

This article explains a simple way to create workflows in OMNIC Paradigm software. For basic information about workflows and brief descriptions of the workflow features and editing tools, see the article titled "About Workflows" in the OMNIC Paradigm online help.

Note The software operations to create workflows are available only in the desktop version of OMNIC Paradigm software (not the touchscreen version).

There are several ways to create workflows. Some approaches may work better than the others, depending on the steps you are trying to automate and how you want to start. For example, you can create a new workflow by:

- building a workflow from scratch
- editing a workflow that someone gave you
- duplicating an example workflow provided with the software
- performing the measurement tasks you want to automate and letting the software create the workflow from the spectrum's history information

This article shows how the software can create a workflow automatically based on the history of an acquired spectrum. It also demonstrates how to:

  – run a workflow from the workflow editor or dashboard
  – identify workflow generated spectra
  – edit a workflow by adding tiles, and
  – fix a common workflow error

The last section provides useful tips for creating and editing workflows.

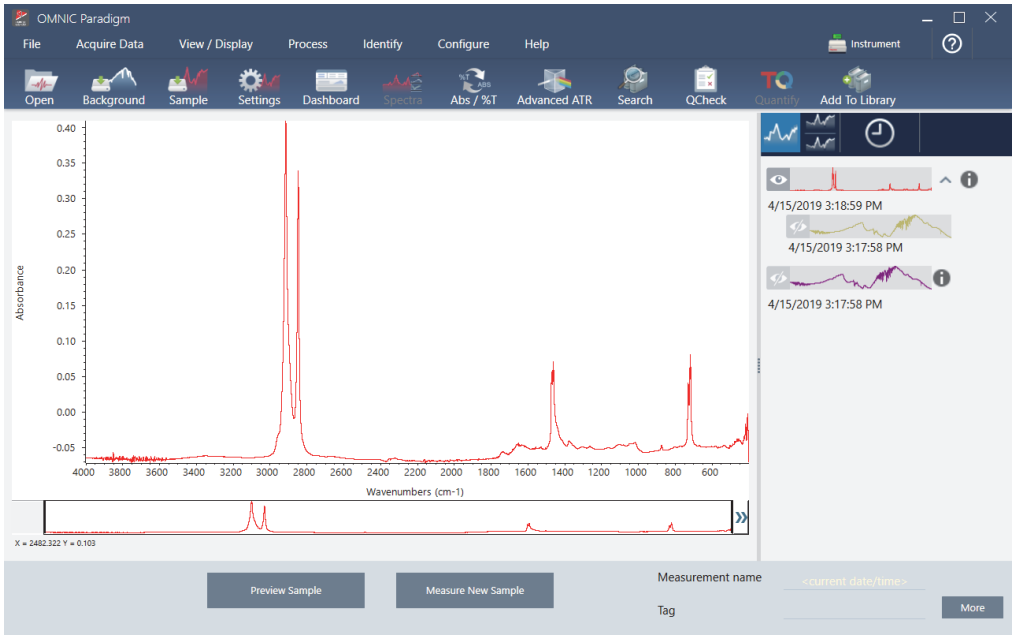
Create a Workflow

❖ To create a new workflow from an acquired spectrum

1. From the OMNIC Paradigm dashboard, acquire a spectrum of a sample material.

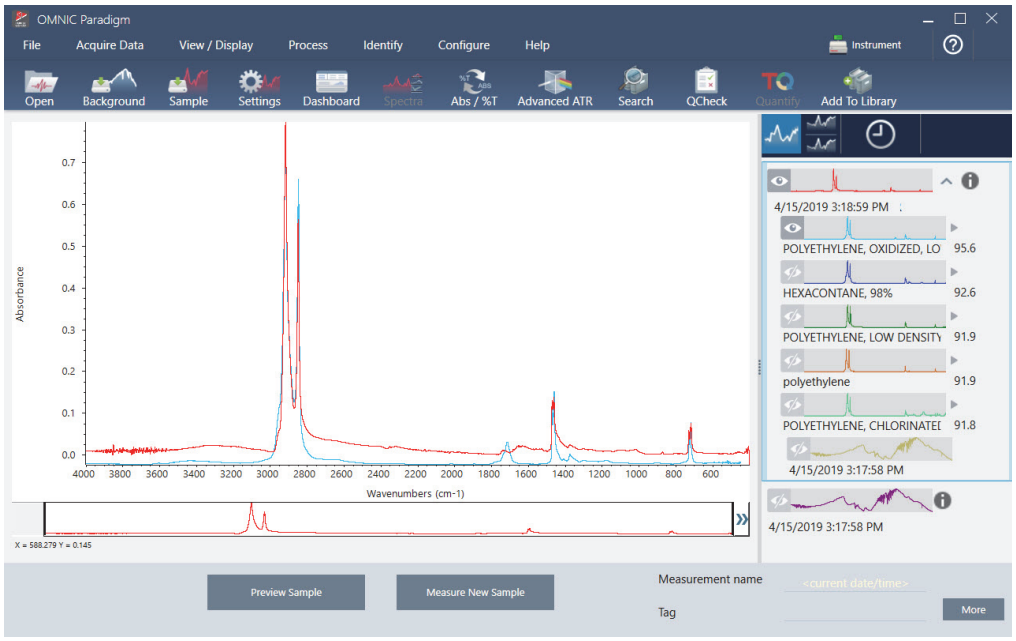
   It doesn't matter what kind of material or sampling technique you use. If the software requires a new background measurement, go ahead and do that first. When the sample measurement is completed, the sample spectrum is displayed in the spectral view.

   Here is our example spectrum (plastic bag measured with an Attenuated Total Reflectance, or ATR, accessory) displayed in the spectral view:



2. Make sure the spectrum is selected in the spectral pane and then perform any processing or analysis steps you like (for example, subtraction, baseline correction, correlation search, etc.).

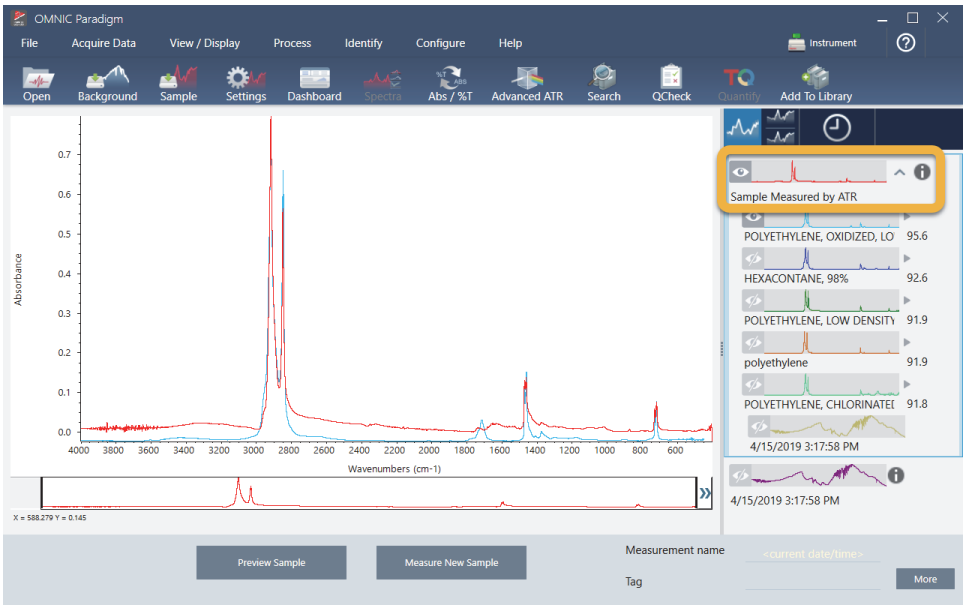
Here is our example spectrum after applying Advanced ATR Correction and Automatic Baseline Correction and then performing a Correlation Search.



3. Give your spectrum a descriptive name (the software will use this name for the created workflow).

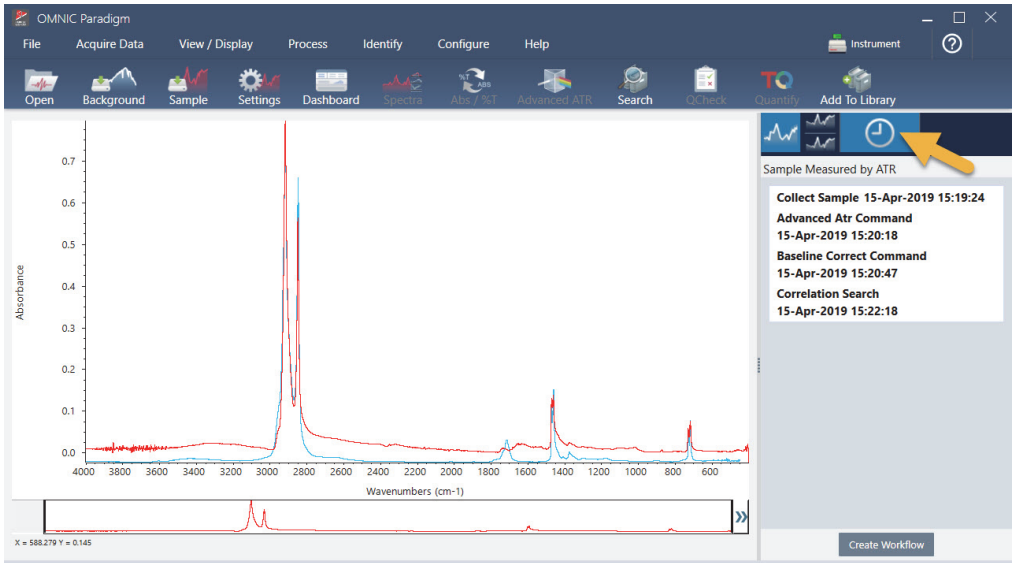
   a. Right click the image of the original spectrum in the results panel and choose **Rename Spectrum**.

   b. Replace the default name with a descriptive name for your workflow and choose **OK**. Here is our renamed example spectrum.

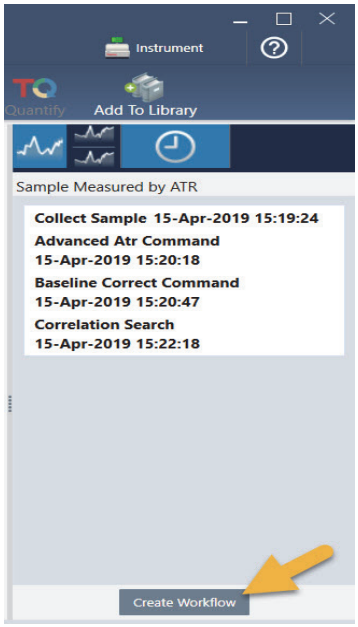


4. Once you have completed your processing and analysis steps, click the **History** button in the results panel.

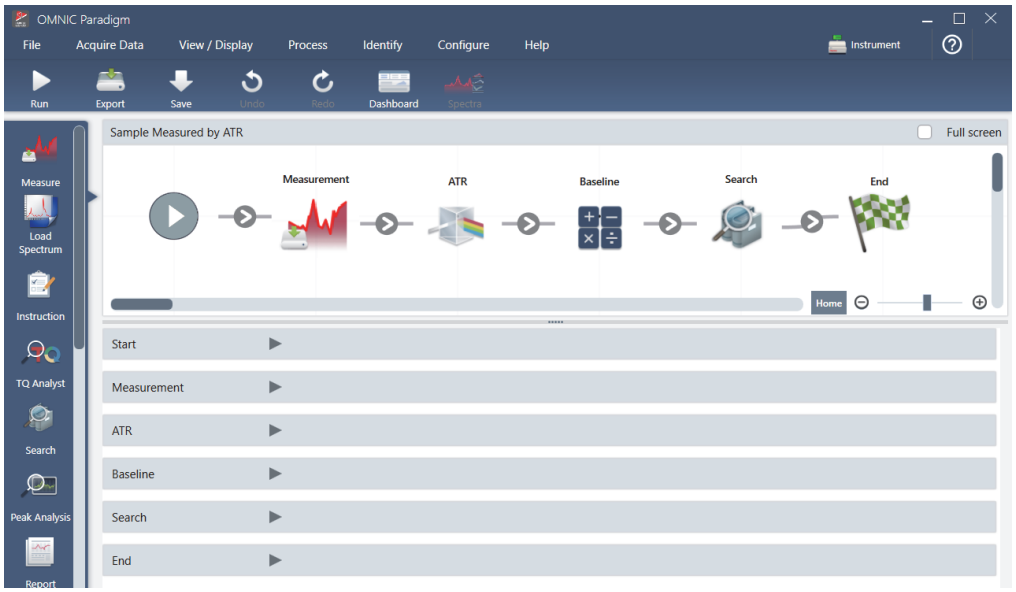
   The history panel shows all the tasks performed on the selected spectrum in the order in which they were performed. Here is the history information for our example spectrum.



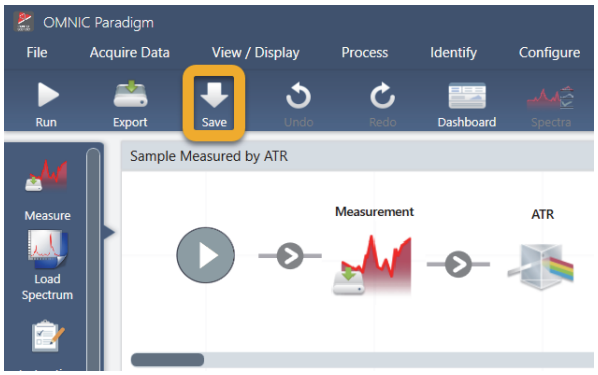
5. At the bottom of the history panel, click **Create Workflow**.



The software creates a workflow that includes all of the steps you just performed. The workflow is displayed in the workflow editor. Each performed task is represented by a colorful tile. Depending on which steps you performed, your workflow may look different from our example below:



6. To save your new workflow, click the **Save** button on the toolbar.



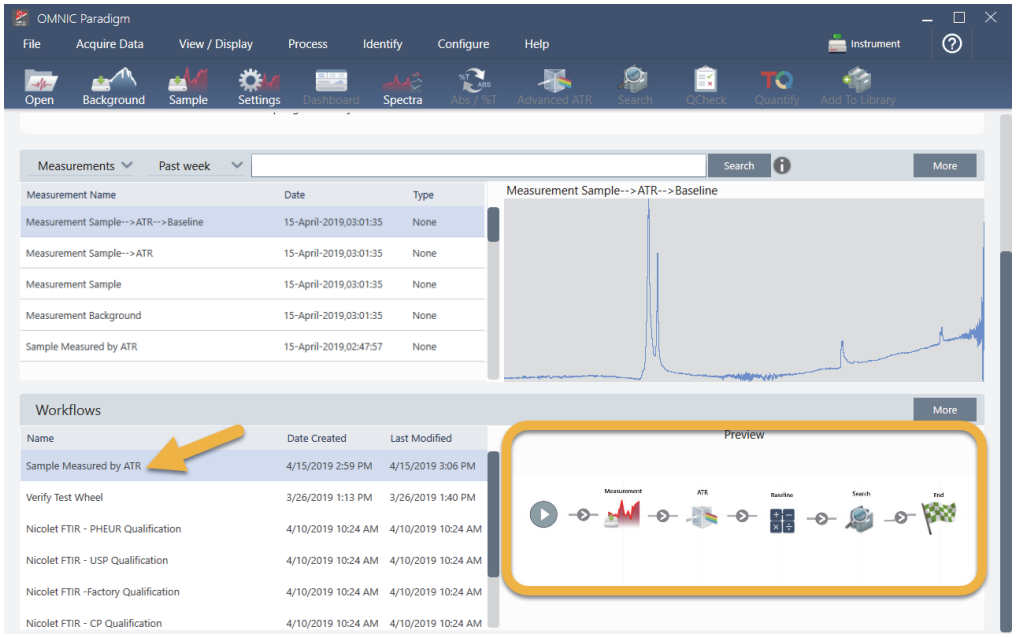
7. To run the workflow, click the **Run** button on the toolbar.

   The workflow performs the same tasks you completed manually in exactly the same sequence. In our case, we measured a spectrum, performed an Advanced ATR Correction, corrected the spectral baseline, and performed a correlation search.

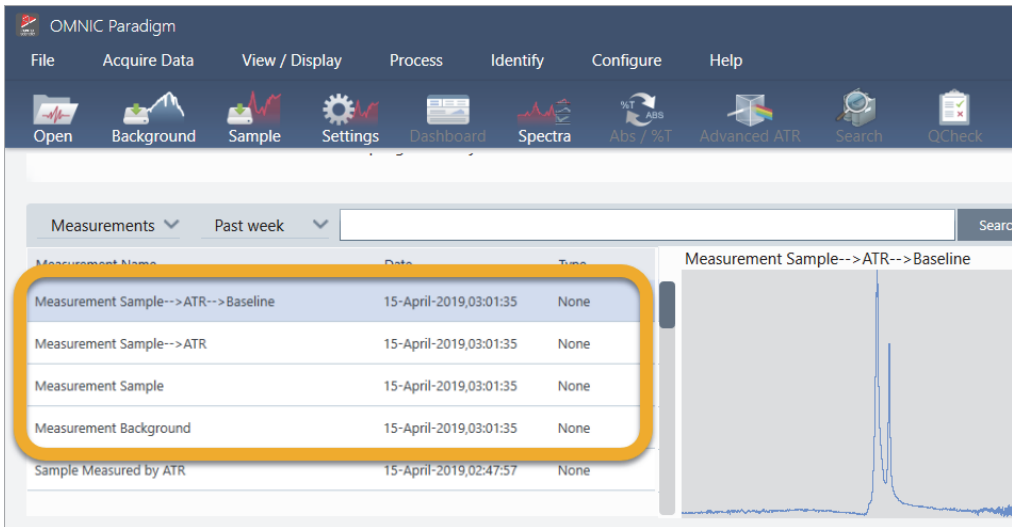
   When the workflow is done, the software returns to the Workflow Editor.

8. Click the **Dashboard** button on the toolbar to see your newly created workflow in the Workflows list.

   The workflow is named automatically based on the name of the spectrum used to create it. Here is our newly created example workflow in the Workflows list and a preview of the workflow in the preview box.



9. The workflow-generated spectra appear in the Measurements list.

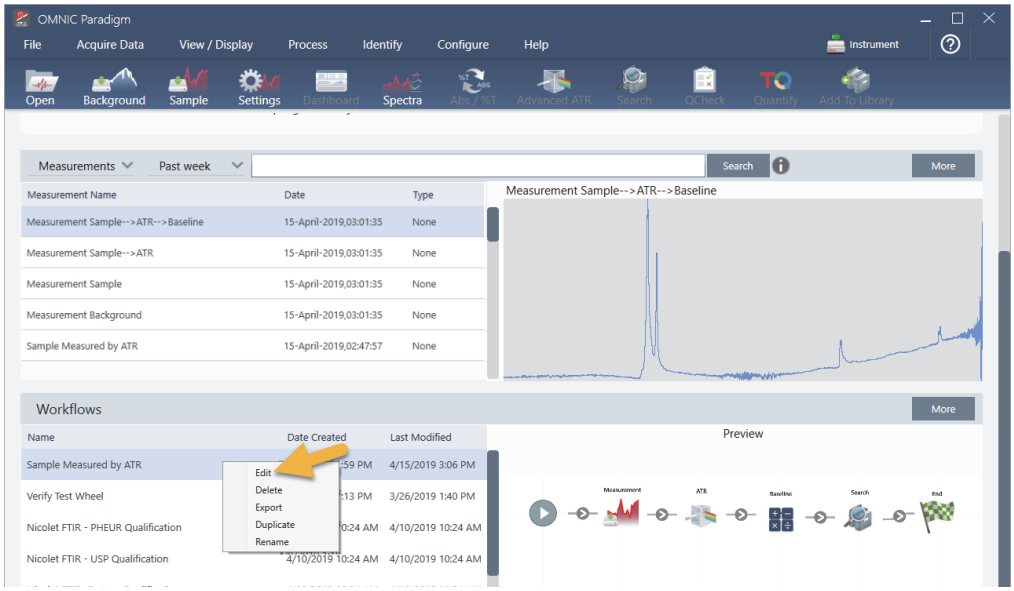


Our example workflow created four spectra, the measured background spectrum, the measured sample spectrum, the ATR corrected sample spectrum, and the ATR and baseline corrected sample spectrum with the search results. The workflow-generated spectra are named with the Tile Name properties of their associated workflow tiles.

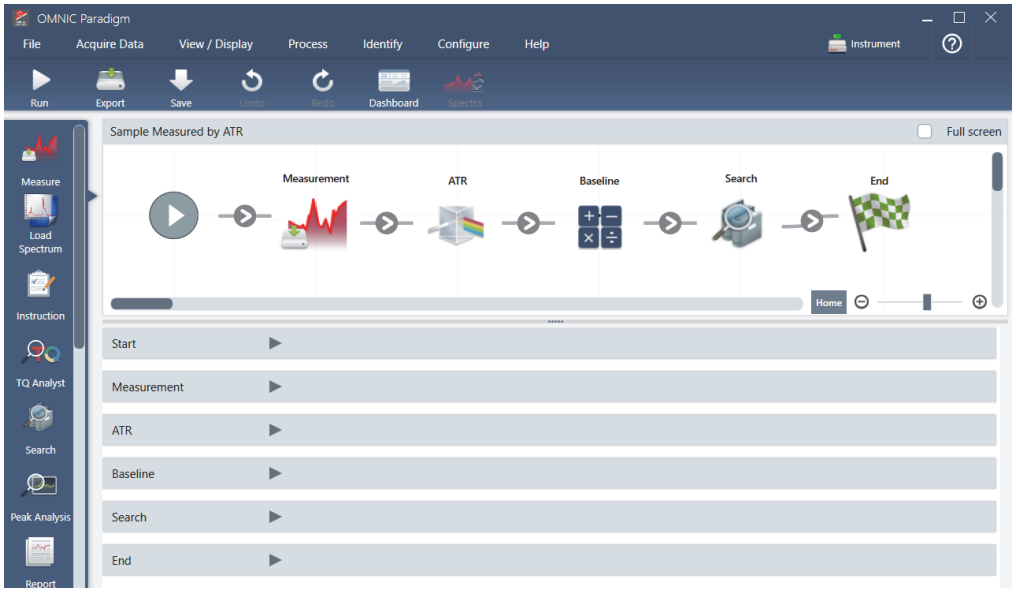
Add Tiles to a Workflow

This section demonstrates how to use the workflow editing tools to add tiles to your auto-generated workflows.

1. From the dashboard, right-click the workflow name and choose **Edit**.



The workflow opens in the workflow editor.

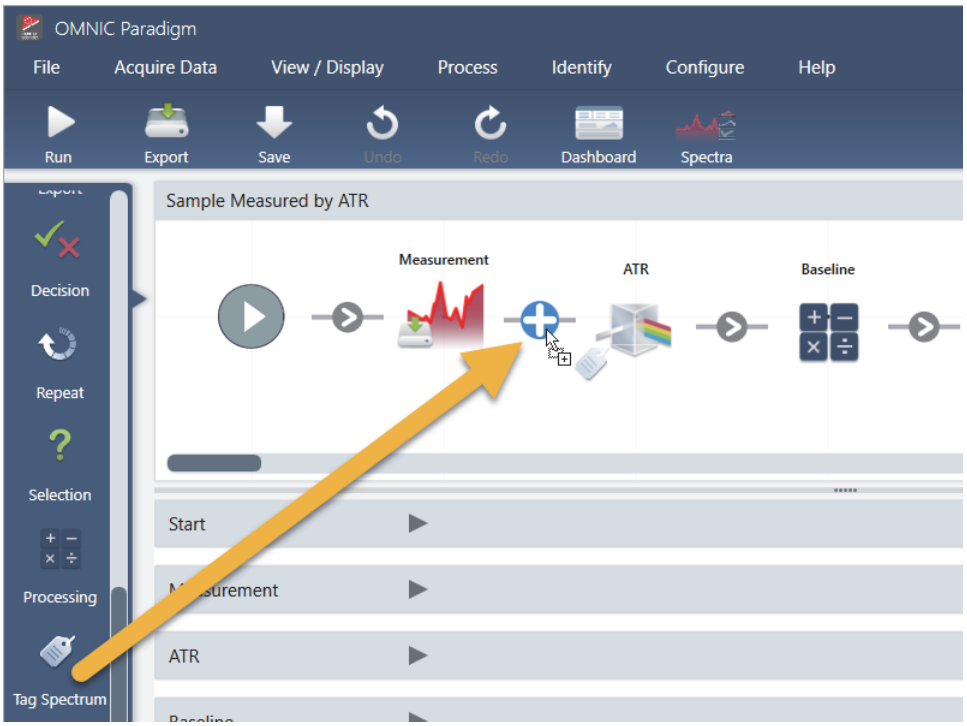


2. Add a Tag Spectrum tile to the workflow.

   Workflow-generated spectra are saved in the OMNIC Paradigm database along with any data acquired manually. Let's tag the workflow spectra to associate them with our workflow. This makes it easy to open and view them later.

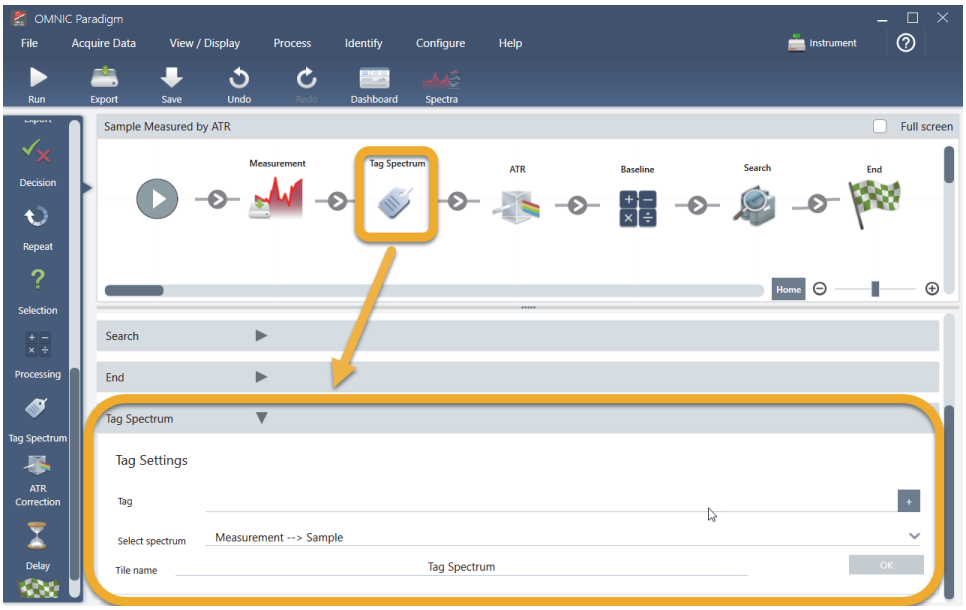
   a. In the workflow editor, drag the Tag Spectrum tile from the selection bar to the canvas so that your mouse cursor hovers over the grey arrow  between the Measurement and ATR Correction tiles.

      The grey arrow changes to a plus sign.

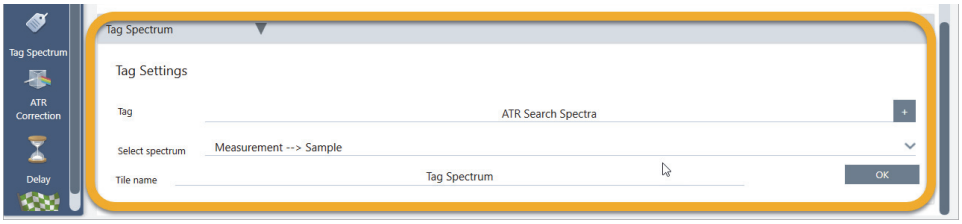


b. Release the mouse button.

The tile is added to that location in the workflow and its settings box is opened below the canvas.



c. In the Tag Settings enter a base name for your workflow-generated spectra, such as "ATR Search Spectra", make sure Select Spectrum is set to your measured spectrum ("Measurement - Sample"), and choose **OK**.

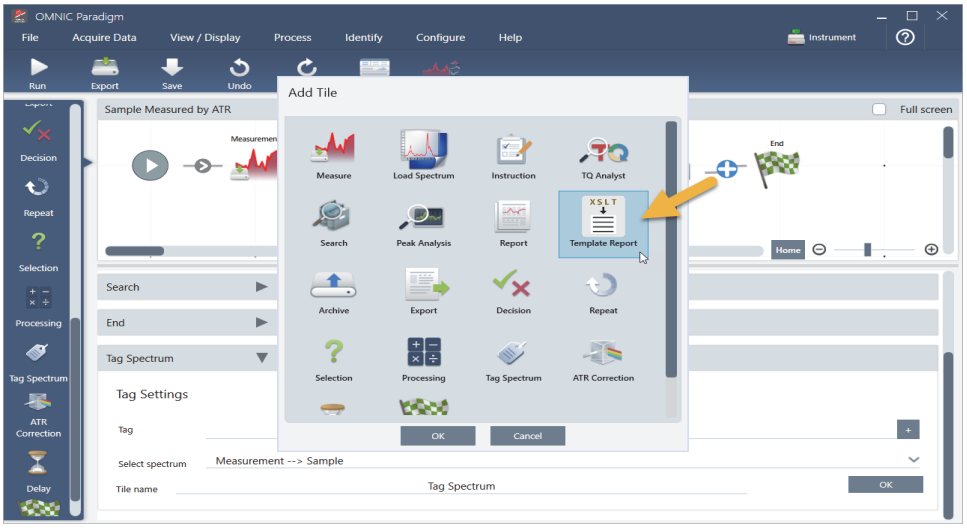


The Tag Spectrum tile will automatically add the "ATR Search Spectra" tag to each spectrum generated by the workflow. We'll explain how to search for those spectra later.

Now let's explore what happens when we add a tile that flags an error.

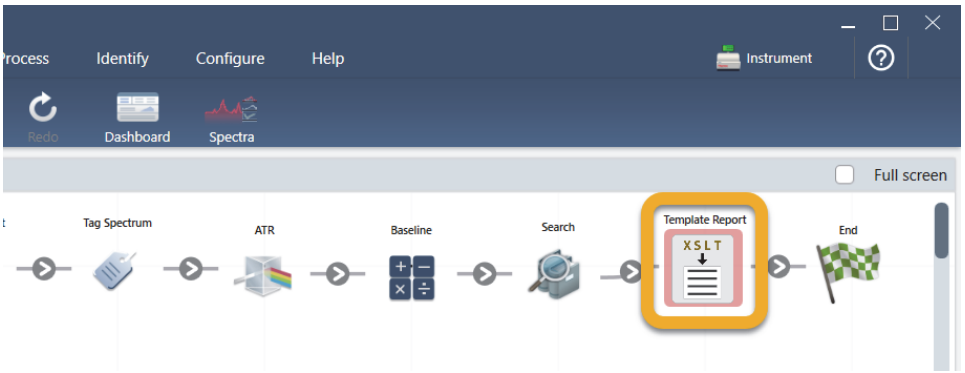
3. Add a Report Template tile to the workflow.

   a. In the workflow editor, use the mouse to hover over the grey arrow between the Search and End tiles (arrow changes to a plus (+) sign) and then click the mouse button. The software opens the Add Tile box. (This is another easy way to add tiles.)

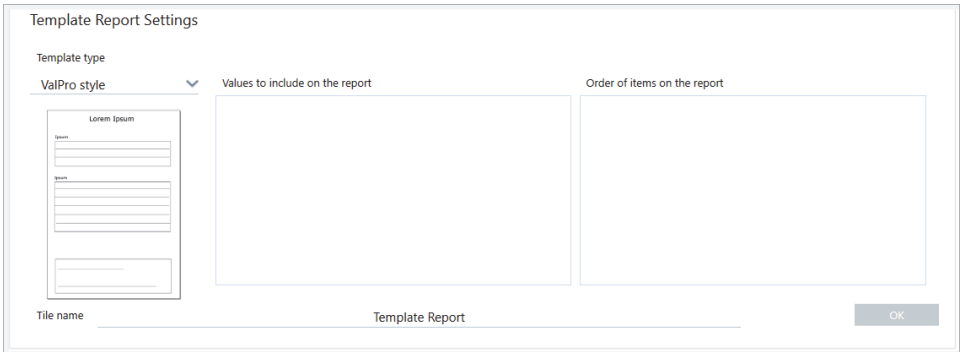


   b. In the Add Tile box, select the Template Report and choose **OK**.

   The tile is added to that location in the workflow and its settings box is opened below the canvas.

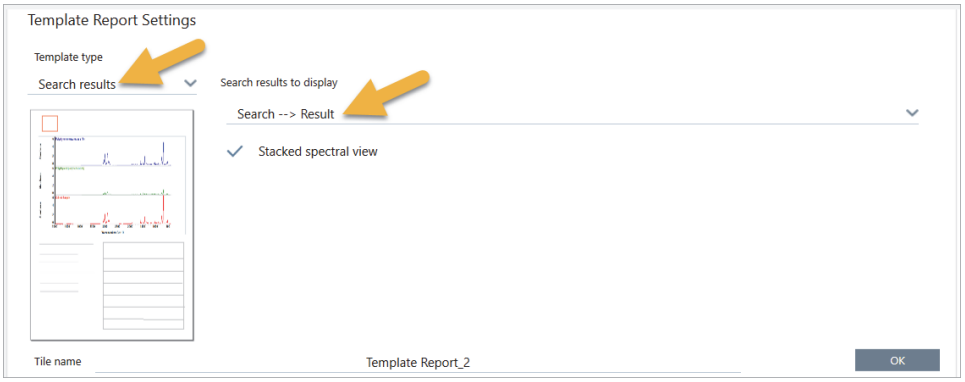


Notice that the Report Template tile has a red border, which indicates the workflow won't run successfully right now. If we view the Report Template settings, the boxes are all blank.

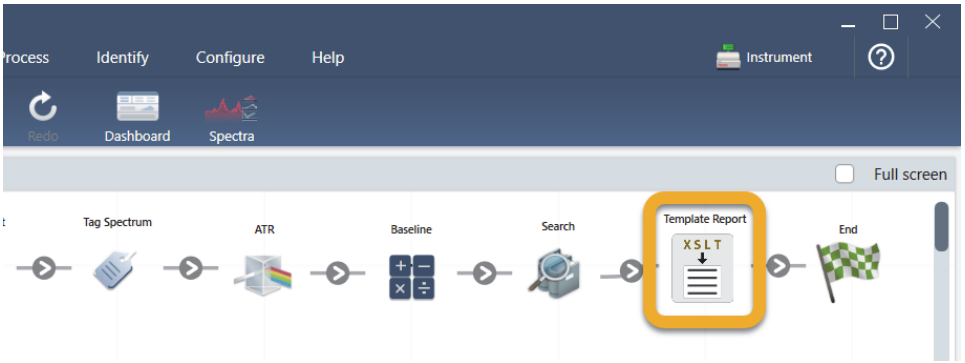


To fix the problem, we need to specify a template for the report and which results to include.

c. Set **Template Type** to your preferred report style (we are using the Search Results template), set **Search Results To Display** to your workflow's output ("Search Result" in our example) and choose **OK**.



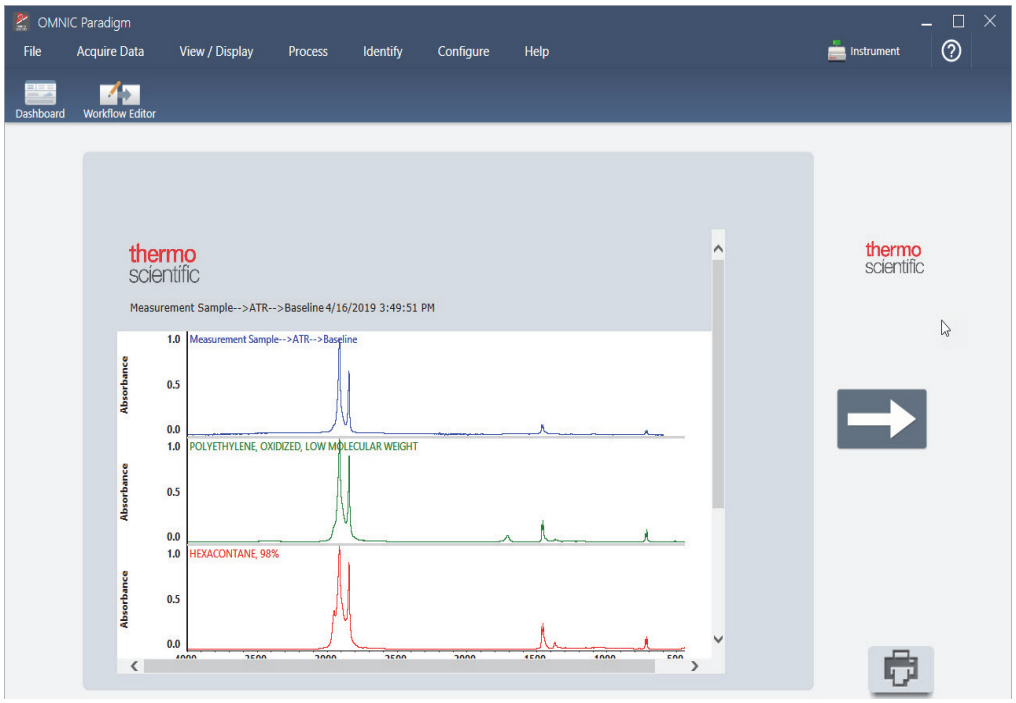
Notice that the red border is no longer there.



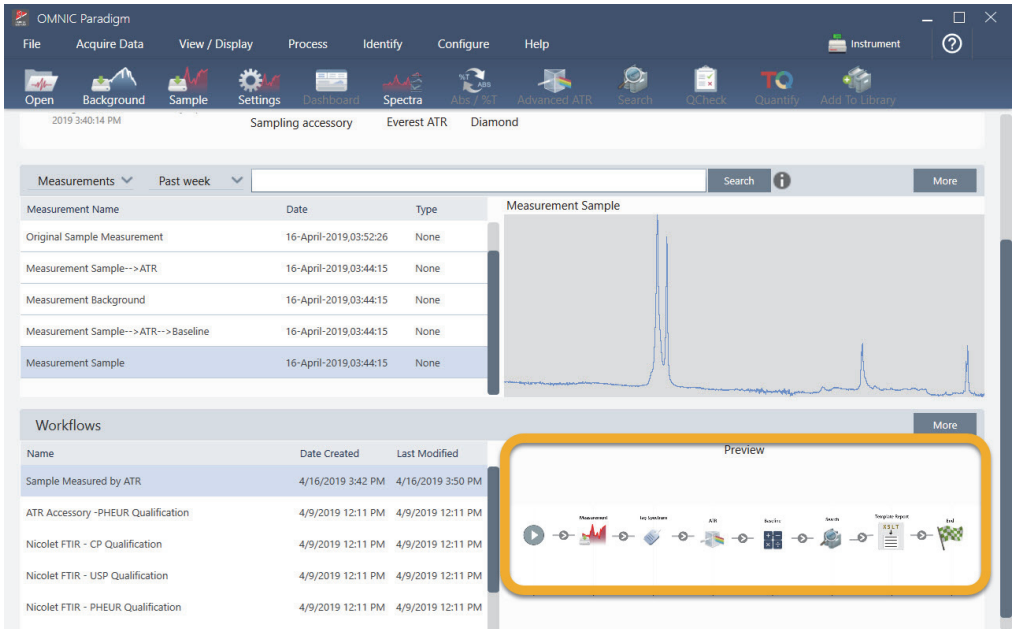
4. To save the updated workflow, click the **Save** button on the toolbar.
5. To run the workflow, click the **Run** button on the toolbar.

   The workflow runs through all the steps and then displays the final report.

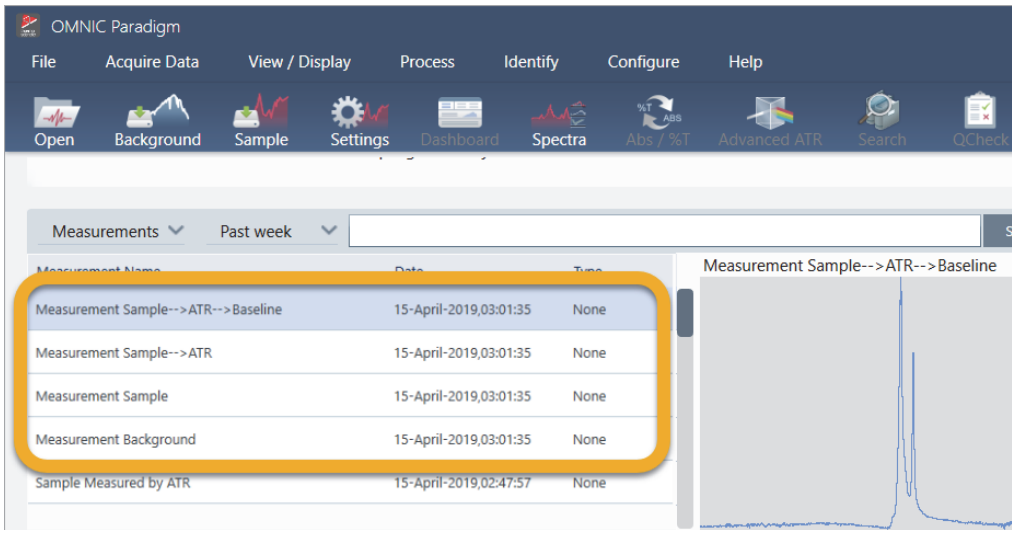
Click the arrow button to end the workflow.



6. Click the **Dashboard** button on the toolbar to return to the dashboard.
7. If you select the workflow in the Workflows list, the preview has been updated.

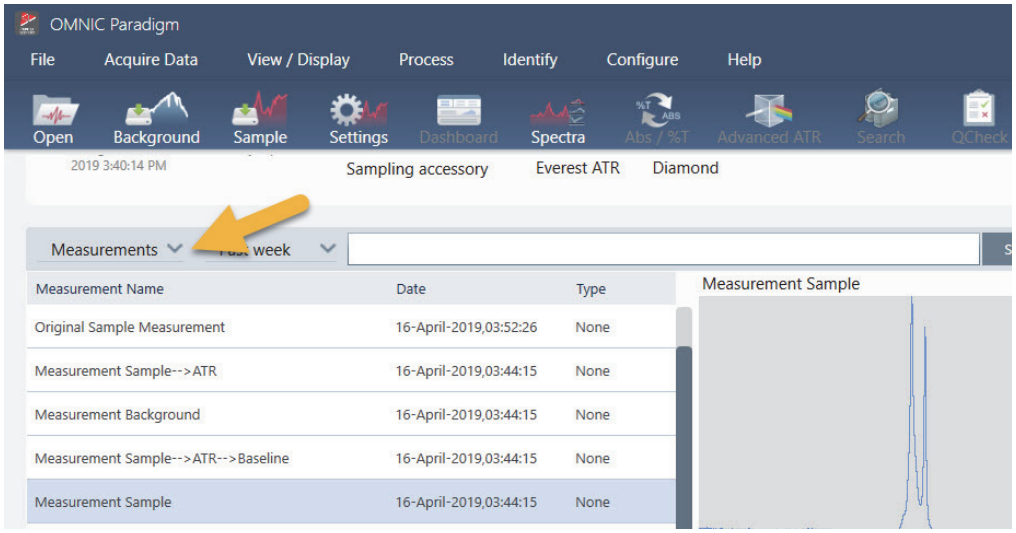


8. If you enter your tag in the Search box, the software shows you the workflow-generated spectra in the Measurements list.



To view the spectra in the spectral pane, use Shift + Click to select all four in the Measurements list, then right-click and choose "Open Selected Measurements."

9. To see the workflow-generated report, click this arrow button and select "Reports."



Tips on Creating Workflows

Before you head off to create more workflows, read through these answers to common questions about workflows and tips for solving any problems that may occur.

- **Is the order in which the tiles appear in the workflow important?** Yes, the order of the tiles is important. Each workflow tile builds on the previous tiles, and all the tiles are interconnected by their input requirements and their output results. For example, if you add a Measure tile, it creates an output result (a spectrum), which can only be accessed by tiles positioned after the Measure tile in the workflow. If you want to baseline correct the

acquired spectrum, you would need to add a Baseline tile after the Measure tile, and then set the Baseline input to the Measurement output (i.e., the spectrum). Otherwise, the Baseline tile will have a red border, indicating it contains options that must be set before the workflow will run. If you see a tile that has a red border, use the mouse to hover over that tile for help finding the source of the problem.

- **Do I need to add a background measurement to my workflow?** Not unless you want the workflow to perform an operation only on the background spectrum. If you only need a background spectrum in order to process your measured sample data, then you just need to add a Measure tile to the workflow and use the Measure tile settings to define the background measurement.
- **Can I change the titles of the workflow tiles?** Each workflow tile has a setting that specifies the tile name. (Double-click the tile in the workflow editor to open its associated settings.) The Tile Name setting can be used to add detail to your workflow. This can help the workflow developer keep things organized, especially when creating workflows that contain multiple paths or loops, or multiple tiles of the same type (several Measure tiles, for example, in the same workflow).

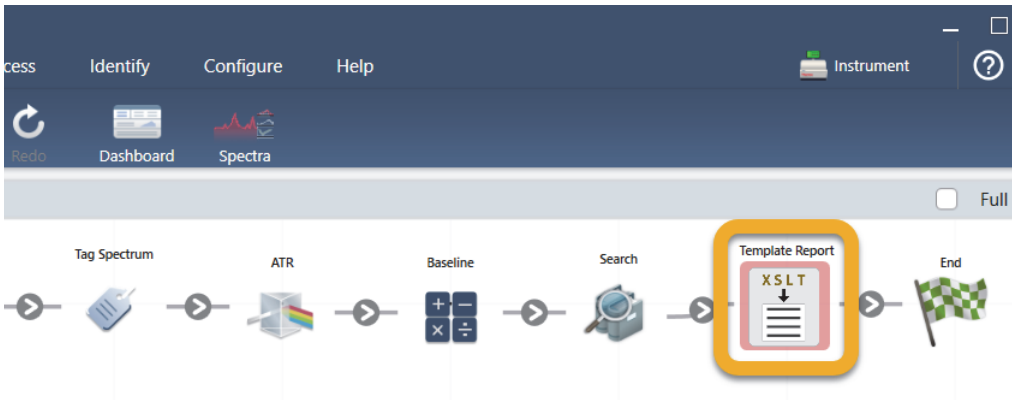
  The tile names may also be used to name output files when the workflow is run. Here are some examples:

  – **Measure tile.** This tile acquires background and sample spectra. When the workflow is run, the sample spectrum is saved with the tile name of its associated Measure tile.

  – **ATR Correction Tile, Process Tile, etc**.. Tiles that operate on acquired spectra generate output spectra that are saved along with the final sample spectrum when the workflow is run. Each interim "processed" spectrum is saved with the tile name of the workflow tile that generated it.

  – **Report tile**. This tile creates a sample report. When the workflow is run, the report is saved with the tile name of its associated Report tile.
- **Should every workflow have an Archive tile?** The answer to this question is "no." Any spectra and reports generated from a workflow are saved automatically in the OMNIC Paradigm database, along with all the other spectra and reports that are created manually with the spectrometer (that is, not from a workflow). If you want to save your workflow-generated spectra and reports as files that can be archived or opened elsewhere (from your OMNIC Paradigm workstation software, for example), use an Archive tile to create those files automatically.

- **Why doesn't my workflow run?** Before you run a newly created workflow, ensure there are no tiles with a red border. Here is an example:



The workflow will not run to completion if it contains a tile with a red border.

If your workflow has a red bordered tile, use the mouse to hover over the tile for tips on how to solve the problem. Typically, the red border indicates the tile contains required options that have not been set. However, it can also mean the tile is "illegal." For example, if you place a Baseline tile *before* a Measure tile in a workflow, the Baseline tile will have a red border and the workflow will contain an unresolvable error because there is no output spectrum to baseline correct.

Workflow Tiles Reference

Workflow tiles are icons that represent the tasks a workflow can perform. Each tile has settings that define what the tile does when the workflow runs. To see a tile's settings, add the tile to your workflow on the workflow canvas, then double-click the tile.

This reference of workflow tiles is organized alphabetically. Each tile description includes a description of available settings.

Archive

Send data and reports to a user specified location. This location can be on your local system or on a network or flash drive for alternate storage.

Setting	Description
Select data to archive	Choose from available spectra and reports created or imported during the workflow.
File base name	The base name is prepended to the full file name. When the file is archived, it is named according to the following template: <base name>_<workflow name>.<tile name of data creation>.<variable name>_YYYY_MM_DD_HHMMSS_<time zone in GMT>.<file extension> For example, with a base name of "example" and a workflow called "my workflow", a spectrum collected on the Measure tile would be archived as the following: `"example_my workflow.Measure.Sample_ 2019_06_25_104928_GMT-0500.spa"`
File location	The directory in which the file will be archived.
Tile name	Sets the name of the tile in the workflow canvas.

ATR Correction

Corrects ATR spectra for the effects of variation in the depth of penetration and the shifting infrared absorption bands that occur with the ATR technique.

Setting	Description
Crystal type	Select the type of crystal used to measure the sample.
Angle of incidence	Enter the angle of incidence that was used to measure the sample. See the specifications for the accessory to obtain this value. The Everest ATR Accessory: 45° The default value is 45.00
Sample refractive index	Enter the refractive index of the sample at 1000 cm^{-1}. Most organic materials range between 1.45 and 1.55 at 1000 cm^{-1}. Materials that contain carbon black have higher refractive index values (1.7 or higher). If you do not know the refractive index of your sample material at 1000 cm^{-1}, we recommend using the default value of 1.5.
Number of bounces	Enter the expected number of internal reflections of the infrared beam that occurred in the ATR crystal. See the documentation for your ATR accessory for information about crystal material, angle of incidence, and the number of bounces. The default value is 1.00
Select spectrum	ATR Correction is applied to the specified spectrum.
Tile name	Sets the name of the tile in the workflow canvas.

Decision

With a Decision tile, you can control the flow of the workflow based on criteria that you specify. For example, you can provide two separate paths based on whether or not a correlation search result had a match value above a specified threshold.

Setting	Description
Pass/Fail	Select a pass/fail decision type to use a previously generated pass/fail result as the decision criteria. For example, the Peak Analysis tile can generate a pass/fail result based on the measurement of the peak height. For instance, you can specify that if the peak height is above a given value, generate a pass result, and if it was below that value, generate a fail result. Then, you can use the decision tile to continue the workflow in two separate paths, depending on that result.
Numeric Value	Select a numeric value to be used in the decision. The value can be data generated in a previous workflow tile or it can be a value that the operator entered using the Instruction tile. For example, you can check if the match value of a search result was above a specified threshold and continue the workflow based on that criteria.
String Value	Select a string value to be used in the decision. The string can be data generated in a previous workflow tile or it can be text entered by the operator using the Instruction tile. With a string value, you can check if the selected value is equal to or contains your test string. For example, if you select Contains and provide “Poly” as the test string, the decision tile will evaluate to True if the selected value is Polystyrene.
Spectrum Age	Ccontrol the flow of the workflow depending on the age of a spectrum. For example, you can check if a background spectrum is more than 20 minutes old before moving on to another step in the workflow and then measuring a new background if necessary.
Tile name	Sets the name of the tile in the workflow canvas.

Delay

Pauses the workflow for the indicated amount of time before proceeding.

Setting	Description
Delay (seconds)	The number of seconds that the workflow will remain paused.
Message	The message is displayed to the operator during the delay.
Tile name	Sets the name of the tile in the workflow canvas.

End

Every workflow has at least one End tile. If your workflow includes Decision or Selection tiles, there may be more than one possible ending.

Setting	Description
End type	Choose Success or Failure for a visual indication of the workflows end state. The end type does not affect data in the workflow. It only provides a visual cue to the workflow developer.
Note	Use the note field to enter text for a tooltip that appears when hovering over the tile in the workflow canvas. This is useful for providing a reminder to the workflow developer. For example, if used with a Failure end type, the note could summarize the test that caused the failure.
Tile name	Sets the name of the tile in the workflow canvas.

Export

Exports collected data to a CSV file.

Setting	Description
Select data to export	Select available data that can be exported to the CSV file, such as peak heights or search result match values.
Append to file	If selected, will append the exported data to an existing CSV file. To append the data to an existing file, enter the name of the file in the File Name field. If the file doesn't exist, a new file will be created with the name you entered.
File name	(only available if Append to File is selected) Enter the name of the file that the data will be appended to. If the file does not already exist, a new file will be created.

Setting	Description
File base name	(only available if Append to File is not selected) The file base name is added to the file name before the date and time.
File location	The directory in which the file will be appended or created.
Tile name	Sets the name of the tile in the workflow canvas.

Instruction

Use the Instruction tile to provide additional instructions to the workflow operator. The Instruction tile can also include entry fields for the operator to enter text or numeric data. These entries can later be used in the workflow. For instance, text entered by the operator can be added to a custom report.

Setting	Description
Add Image	Add an image that the operator will see on the instructions screen during the workflow. Valid file types include: .PNG .JPG .GIF .BMP
Add Text Box	Use to add text. This is useful for providing instructions to the operator and for adding labels to text and numeric entry fields.
Add or Remove PDF	Provide a button that operators can click or touch to view a specified PDF. After adding the document button, click the button to specify the PDF file.
Add or Remove Cancel Button	Provides a cancel button that the operator can click or touch to stop the workflow.
+ Text Entry	Allows the operator to enter text which can be used later in the workflow. For example, the operator can enter a file path which can be used in the Archive tile.
+ Numeric Entry	Allows the operator to enter a numeric value which can later be used as a variable in other tiles. For example, the numeric value entered can be used in the Decision tile as the condition in a Numeric Value decision.

Setting	Description
+ Value	Display data from a variable, such as match value of a result from a correlation search.
Tile Name	Sets the name of the tile in the workflow canvas.

Load Spectrum

Load a SPA file to use during the workflow. You can browse to a file location on the instrument computer or on a flash drive or network location or you can load a spectrum from the database.

This can be useful for importing a saved spectrum to use as a reference. For instance, you may want to import a reference spectrum to use in a subtraction operation.

Setting	Description
From file	Load a SPA file from a location on your system or your network. **File name:** Browse to a SPA file to include a spectrum.
From database	Select to load a spectrum from the database. **Selected spectrum:** Choose a spectrum from the database. **Choose during workflow execution:** Allow the operator to select a spectrum during the workflow. **Show only experiments containing this text:** Limit the operator's choice to only spectra that contain the specified text in the title or tags.
Tile name	Sets the name of the tile in the workflow canvas.

Measure

Use the measure tile to measure the background and a sample and to set the measurement settings. Spectra and reports created during the workflow are saved to the database and can be archived with the Archive tile.

Setting	Description
Background settings	Specifies whether the workflow will prompt the operator to acquire a new background, use a spectrum from another tile in the workflow, or measure a background only, without measuring a sample.
Use internal polystyrene sample	If selected, an internal polystyrene reference sample installed in the instrument will be used to validate the instrument's performance.
Use background prompt	Select to provide instructions to the operator before measuring the background. It is a good idea to instruct the operator to prepare to measure the background.

Setting	Description
Use sample prompt	Select to provide instructions to the operator before measuring the sample. You may want to instruct the operator to insert the sample.
Allow other workflows to access result of measurement	If selected, you can include spectra from this workflow in other workflows. For example, once this workflow is run and has measured a sample, a separate workflow could use the collected spectra as a reference spectrum or in a report.
Show spectrum during measurement	Select to view the spectrum during the measurement. If not selected, operators see only a progress indicator.
Progress text	Provide a custom message to operators during the background and sample measurement.
Other Measurement Settings	Customize the measurement settings used in this workflow or match the settings used with another spectrum. **Number of scans:** The number of times that the sample will be scanned. More scans typically means for accurate data, but will take longer to measure. **Atmospheric suppression:** Used to suppress the effects of CO_2 and H_2O. **Match Settings:** Select to match the measurement settings used with a specified SPA or QNT file. Select All Settings to review all of the settings used with this measurement. **Spectrum Title:** Select to append variable data to the spectrum title. See Measurement Settings and Advanced Measurement settings for a description of additional settings.
Tile name	Sets the name of the tile in the workflow canvas.

Peak Analysis

Analyze the Peak Height or the Peak Ratio of a spectrum.

Setting	Description
Peak Height	Measure the height of a peak from zero absorbance (or 100% transmittance), without regard to the position of the baseline, or from the baseline. If measured from the baseline, the measurement is called the "corrected peak height." **Peak position:** Enter the wavenumber of the peak to be measured. **Corrected:** Select to measure the peak height from the spectral baseline rather than from zero absorbance (or 100% transmittance) **Reference point:** Select for single-point correction, using one point as the baseline reference. **Reference range:** Select for two-point correction, using a point on either side of the peak to calculate the baseline. **Generate pass/fail result:** Select to create a pass/fail result that can be used in a Decision tile.
Peak Ratio	Find the ratio of height between two peaks. Peaks can be calculated from zero absorbance units or from a corrected baseline. **Not corrected:** The peak heights are measured from zero absorbance (or from 100% transmittance) **Single-point corrected:** The peak height will be measured from the baseline at the wavenumber you entered. **Two-point corrected:** A point on either side of the peak will be used to calculate the baseline. **Generate pass/fail result:** Select to create a pass/fail result that can be used in a Decision tile.
Select spectrum	Select the spectrum that will be used in the peak analysis. You can choose from spectra generated in the workflow or imported with the Load Spectrum tile.
Tile name	Sets the name of the tile in the workflow canvas

Processing

The Processing tile includes several tools for processing spectral data, including subtraction, normalization, correlation, basic spectral math, and baseline correction.

Setting	Description
Subtraction	Subtract one spectrum from another. Spectral subtraction is useful in many instances. For example, if you are measuring a sample that is dissolved in a solvent, you can subtract a reference spectrum of the pure solvent to remove any peaks from the solvent. You can also identify an unknown contaminant in your sample by subtracting a known reference material, leaving you with only the contaminant. You can then use a correlation search to identify the contaminant.
Sample spectrum	The starting spectrum to which the operation will be applied.
Reference spectrum	The reference that will be subtracted from the starting spectrum.
Subtraction type	There are three types of subtraction available. Choose from subtraction by Factor, Pathlength, or Range.
Normalization	Use Normalize to change the Y-axis scale of the selected spectra to a "normal" scale in which the Y values of the data points range from 0 absorbance units for the lowest point to 1 absorbance unit for the highest peak (for an absorbance-like spectrum) or from 10% to 100% transmittance (for a transmission-like spectrum). These normal scales are typical of spectra in commercial spectral libraries. After a spectrum is normalized, you cannot use it for quantitative analysis unless you know the scaling factor and adjust the quantitative results accordingly.
Select spectrum	The starting spectrum to which the operation will be applied.
Max range (cm^{-1})	Use to set the range used in the normalization.
Min range (cm^{-1})	Use to set the range used in the normalization.
Target value	Target value is specified in absorbance units.
Correlation	Returns the match value between the first and second spectrum. Like QCheck, the match value is given between 0.0 and 1.0, with 1.0 reflecting a perfect match.
First spectrum	Select the starting spectrum that the second spectrum is being compared to.
Second spectrum	Select a reference spectrum.

Setting	Description
Spectral range	Use the spectral range to exclude totally absorbing peaks from the correlation search.
Basics	Apply an operation to a single spectrum.
Spectrum	Select the spectrum to which the operation will be applied.
Operation	Add Subtract Divide Multiply
Factor	Increases or decreases the amplitude of the spectrum so that it can be better compared to another spectrum.
Baseline Correction	Use to correct a baseline that is shifted.
Select spectrum	Select a spectrum for which the baseline will be corrected.
Polynomial order	Specify the polynomial order for the correction.
Tile name	Sets the name of the tile in the workflow canvas

Repeat

Loop a portion of the workflow to repeat steps.

Setting	Description
Repeat ___ times	Sets the number of times that the looped portion of the workflow will repeat.
Tile name	Sets the name of the tile in the workflow canvas.

Report

Create a custom report that can be stored, archived, or printed. Reports generated in the workflow are available in the Reports section of the dashboard.

Setting	Description
Add image	Add an image that the operator will see on the report screen during the workflow. Valid file types include: .PNG .JPG .GIF .BMP
Add text	Use to add text. This is useful for providing instructions to the operator and for adding labels to text and numeric entry fields.

Setting	Description
Add or remove document	Provide a button that operators can click or touch to view a specified PDF. After adding the document button, click the button to specify the PDF file.
Add spectrum	Add a spectrum to the report. Select any spectrum generated or loaded earlier in the workflow.
Add value	Add a value from another workflow tile to the report. For example, if the workflow included a measurement and a search, you can include data from the results of the search.
Add or remove print button	With a print button, operators can print the report while viewing the report screen.
Tile name	Sets the name of the tile in the workflow canvas

Search

Perform a correlation or a multi-component search.

Setting	Description
Available libraries	Drag libraries from the Available Libraries column to the Selected Libraries to use them in the search. Click Refresh to update the list of available libraries.
Search type	Set the type of search that will be performed. **Correlation:** Use to identify an unknown sample. **Number of results:** Set the number of results that will be shown. **Multi-component:** Use to identify the components of a sample. **Number of components:** Set the number of components that will be shown.
Spectral Ranges	Add a start and end value for the region that will be searched.
Select spectrum	Specify the spectrum that will be used in the search.
Tile name	Sets the name of the tile in the workflow canvas

Selection

With a Selection tile, the operator chooses which path the workflow should follow.

Setting	Description
Add image	Add an image that the operator will see on the selection screen during the workflow. Valid file types include: .PNG .JPG .GIF .BMP
Add text	Use to add text. This is useful for providing instructions to the operator.
Add value	Add a value from another workflow tile to the report. For example, if the workflow included a measurement and a search, you can include data from the results of the search.
Selection label	Edit the selection label to change the text that appears on the workflow canvas.

Start

This is the first tile in every workflow. The Start tile is added to the workflow canvas automatically each time a new workflow is created.

Setting	Description
Workflow image	Determines the image that is displayed when the workflow is run. Accepts a file path to an image file. The following file types are valid: .PNG .JPG .GIF .BMP
Desired aspect ratio	Specify an aspect ratio to optimize the appearance of the workflow when it is run. The aspect ratio should match the display used by the operator as closely as possible. Examples: 4:3 for older computer monitors 16:9 is the standard for high-definition video and is common for current computer monitors Accepts the following: 1:1 4:3 5:4 16:9 16:10 3:2 2:1

Tag Spectrum

Apply a tag to spectra created during the workflow.

Setting	Description
Tag	Apply a tag to a spectrum.
Select spectrum	Choose the spectrum to which the tag will be applied.
Tile name	Sets the name of the tile in the workflow canvas.

Template Report

Generate a report from a template. Reports generated in the workflow are available in the Reports section of the dashboard. Most of the settings for a template report depend on the template type that is selected.

Setting	Description
Template type	Choose from the following template types: • ValPro style • Single spectrum • Multiple spectra • Search results • Single quantification • QCheck • Multiple run quantification
Automatically advance workflow after displaying report for 5 seconds	If selected, the workflow will advance after displaying the report for 5 seconds. If not selected, the operator manually continues the workflow.
Generate pass/fail result	If selected, specify text that will trigger a fail result. For example, if you specify “fail,” the template report tile will generate a fail result if the report includes the text “fail.”

TQ Analyst

Quantify the components of the sample using a specified quantification method.

Setting	Description
Quantification method	Select a QNT file for the quantification method.
Select spectrum	Select the spectrum that will be used for the quantification.
Tile name	Sets the name of the tile in the workflow canvas.

6

Create Reports

Generate reports from template to quickly save and share your data as Microsoft Word, PowerPoint, or Excel files. Or, export your spectra, workflows, and settings to share with your colleagues.

- Create and Share Reports and Export Data

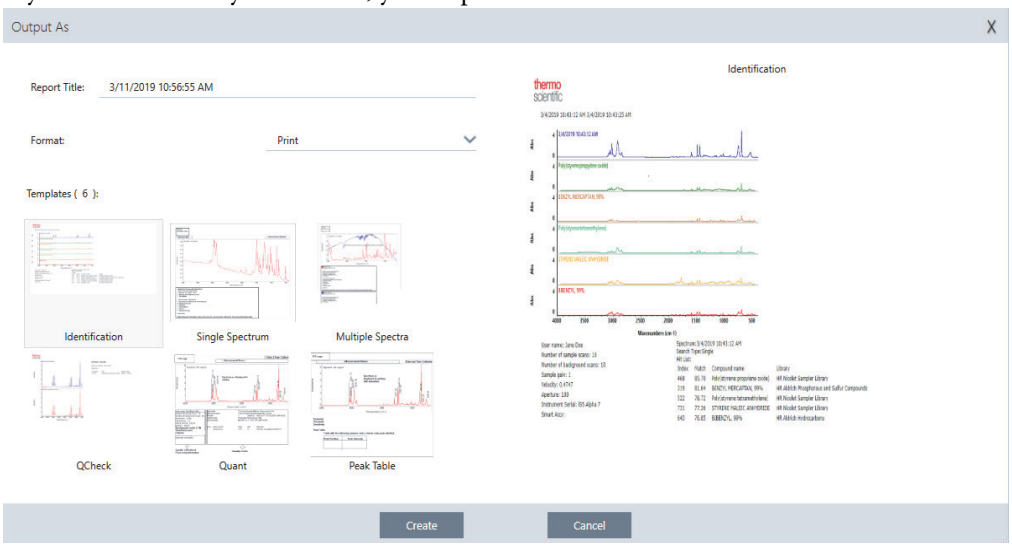
Create and Share Reports and Export Data

Generate reports from templates to quickly save or share your data as Microsoft™ Word™, PowerPoint™, or Excel™ files, or export your spectra, workflows, or settings.

❖ To create a report from the desktop interface

1. Select **File > Create Report**.
2. In the Output As dialog box, enter a title for your report and select a format and template option.The preview updates to match your selections.

   If you select Save as your format, your report data is saved to the database.

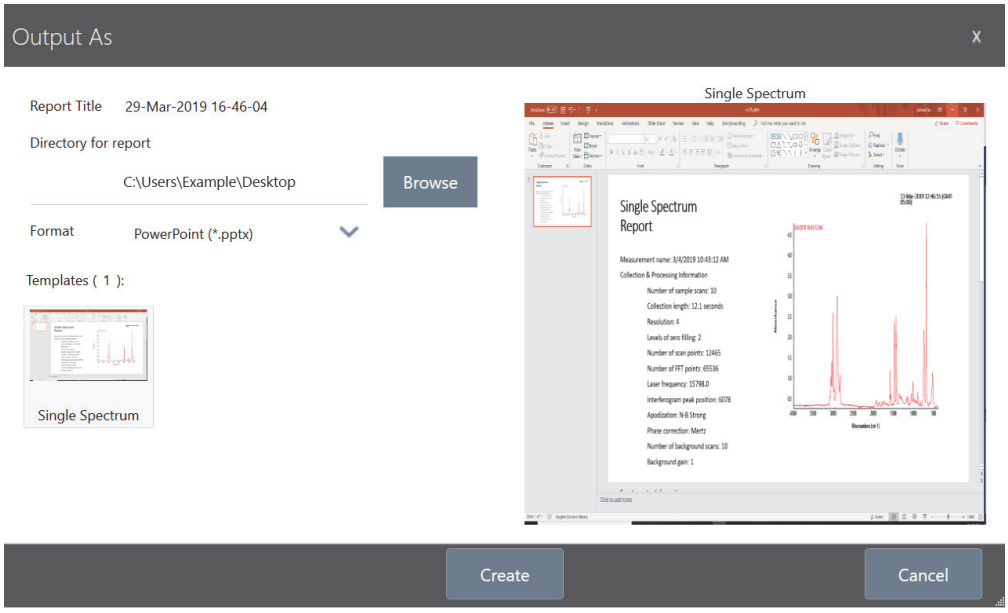


3. Click **Create**.

❖ To create a report from the touchscreen interface

1. From the spectral view, open the menu and select **Create Report**.
2. In the Output As dialog box, enter a title for your report, select a directory to save the report to, choose a format, and finally select a template. The preview updates to match your format and template selection.

If you select Save as your format, your report data is saved to your database.



3. Touch **Create**.

Export Settings, Spectra, or Workflows

Use OMNIC Paradigm software for desktop to export settings and workflows. Export spectra in either desktop or touchscreen mode.

❖ To export settings

1. Select the settings you wish to export from the Settings list.
2. Select **Acquire Data > Export Settings**.
3. Name the settings file and click **Save**.

   Settings are saved with a .expx file extension. These settings files store your measurement settings but not Search, QCheck, or Quantification settings. Settings files with a .expx file extension are not compatible with previous versions of OMNIC software.

❖ To export workflows

- If you are using the desktop interface
  a. In the Workflows pane, right-click the workflow you wish to export and select **Export** from the menu.
  b. Name your workflow file and click **Save**.

     Workflow files are saved with a .rwfl file extension.
  c. In the Measurements pane, right-click the spectrum you wish to export and select **Export**.
  d. Name your spectrum file and click **Save**. Spectra are saved with a .spa file extension.
- If you are using the touchscreen interface
  a. From the home screen, select the **Measurements** tab.
  b. Open the more options menu [ ] and select **Export**.
  c. Touch **Save**. Spectra are saved with a .spa file extension.

7

Protect Your Data

OMNIC Paradigm software pairs with Security Suite software to ensure your data integrity and security.

- Data Security and Integrity with OMNIC Paradigm Software

Data Security and Integrity with OMNIC Paradigm Software

To ensure the security and integrity of your data and to help your lab comply with 21 CFR Part 11 or other regulations, pair the OMNIC™ Paradigm software with Thermo Scientific Security Suite software.

Security Suite is a comprehensive data security toolset, allowing you to perform the following tasks:

- Limit and control access to features and tools in the OMNIC Paradigm software and other instrument applications.
- Set and manage security policies to ensure proper data handling.
- Customize and enforce digital signatures to establish responsibility.
- Log and view security events.

You can purchase Security Suite software to manage a single system or to manage multiple instruments distributed on a network. After installation, configuring the OMNIC Paradigm application for security takes only moments.

For a discussion of how Security Suite software can help you comply with 21 CFR Part 11, see 21 CFR Part 11 Compliance.