

OMNIC Paradigm

Spectroscopy Software

Version 1.9

USER GUIDE

© 2021 Thermo Fisher Scientific Inc. All rights reserved.

Microsoft, Windows and Excel are either trademarks or registered trademarks of Microsoft Corporation in the United States and/or other countries. All other trademarks are the property of Thermo Fisher Scientific Inc. and its subsidiaries.

For technical support, please contact: www.thermofisher.com

Thermo Fisher Scientific Inc. provides this document to its customers with a product purchase to use in the product operation. This document is copyright protected and any reproduction of the whole or any part of this document is strictly prohibited, except with the written authorization of Thermo Fisher Scientific Inc.

The contents of this document are subject to change without notice. All technical information in this document is for reference purposes only. System configurations and specifications in this document supersede all previous information received by the purchaser.

Thermo Fisher Scientific Inc. makes no representations that this document is complete, accurate or error-free and assumes no responsibility and will not be liable for any errors, omissions, damage or loss that might result from any use of this document, even if the information in the document is followed properly.

This document is not part of any sales contract between Thermo Fisher Scientific Inc. and a purchaser. This document shall in no way govern or modify any Terms and Conditions of Sale, which Terms and Conditions of Sale shall govern all conflicting information between the two documents.

Contents

What's new in OMNIC Paradigm v1.9	6
Reprocess spectra	6
Blank regions of spectra	7
Find the average and standard deviation of spectra	7
Add custom logos to reports and template reports	8
Improvements to workflows	8
 Get Started with OMNIC Paradigm Software	 9
Welcome to OMNIC Paradigm Software	10
Install OMNIC Paradigm Software	14
Key Concepts and Features	16
 Configure Your System	 27
Connect to a Spectrometer	28
Connect an Instrument to a Thermo Fisher Connect Account	37
Configure Your Database	40
Set OMNIC Paradigm Options	44
Manage Spectral Libraries	47
 Tutorials and Walkthroughs	 51
Identify an Unknown Sample with ATR	52
Identify an Unknown Sample with Transmission	65
Verify Sample Composition with QCheck	79

Quantify Sample Composition	85
Create and Run Your First Workflow	89
Measure Samples	109
Set and Save Measurement Options	110
Advanced Measurement Settings	115
Measure the Background	120
Measure a Sample	124
Process Data	127
Apply Basic Equations to Acquired Data	128
Advanced Spectral Math	135
Reprocess Spectra	139
Blank a region in your spectra	141
Calculate average and standard deviation spectra	143
Analyze Data	145
Finding Measurements and Reports	146
Search setup	150
QCheck Setup	154
View Measurement History	156
Revert Measurement	157
Duplicate Measurement	158
Use Workflows	161
About Workflows	162
Password Protect a Workflow	168

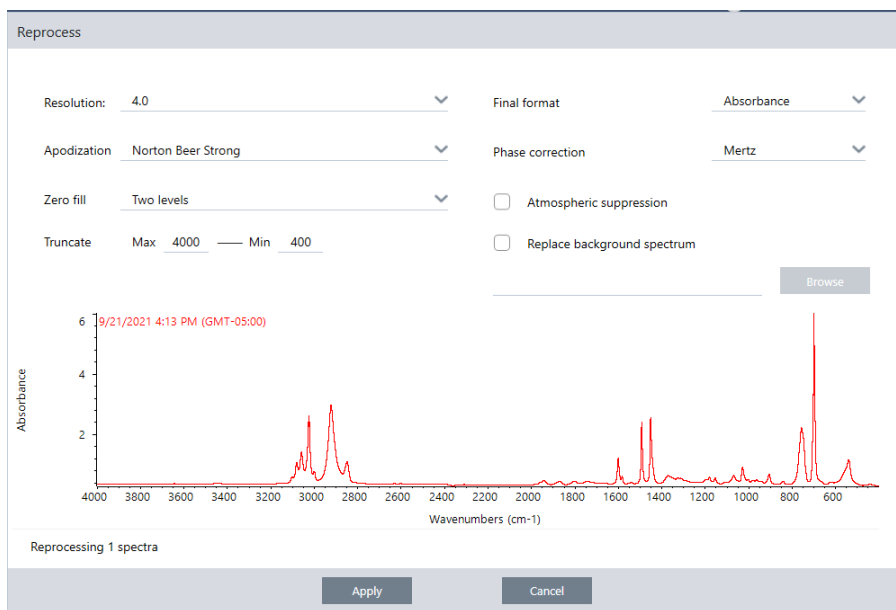
Create a Template Workflow	170
Workflow Tiles Reference	176
Custom Solutions	202
Custom Solutions	203
Create or Edit a Package	206
Operator Administrator	210
Create Reports	213
Create and Share Reports and Export Data	214
Create Historical Spectrum Report	218
Add Labels and Annotations to Spectra	219
Protect Your Data	221
Data Security and Integrity with OMNIC Paradigm Software	222

What's new in OMNIC Paradigm v1.9

The latest version of OMNIC Paradigm software features powerful new ways to process data, updated workflow tiles, and the ability to customize your reports with your organization's logo.

Reprocess spectra

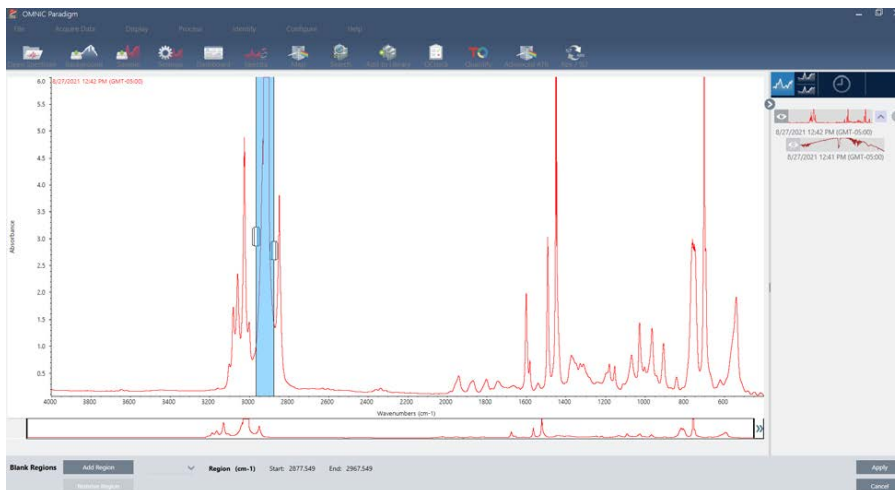
Use Reprocess in the Process menu to transform the original interferogram data for your spectrum with new settings. With Reprocess, you can transform your original data to better match library or other reference spectra, giving you a more accurate comparison.



See ["Reprocess Spectra"](#) for details.

Blank regions of spectra

With Blank Regions in the Process menu, you can clear unwanted data from your spectrum. Blanking a region is useful when your spectrum contains unwanted noise that would otherwise interfere with your analysis. Use Blank Regions to clear, or delete, a region of the spectrum. Blank Regions is also available in the Processing tile in Workflows.



See ["Blank a region in your spectra"](#) for details.

Find the average and standard deviation of spectra

You can now calculate average and standard deviations of spectra using the Statistical Spectra tool in the Process menu. With Statistical Spectra, you can generate new spectra that represent the average or standard deviation of 2 or more spectra. You can also use Statistical Spectra in the Processing tile in Workflows.

See [Calculate average and variance spectra](#) for more information.

Add custom logos to reports and template reports

Go to Configure > Options to use your own company logo in reports and template reports. Your logo replaces the default Thermo Scientific logo on any custom reports you create and any template reports created in a workflow.

Improvements to workflows

With the Peak Analysis tile and Process tile in Workflows, you can now use Find Peaks, Blank Regions, and calculate statistical spectra in your workflows.

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.

In this section:

Welcome to OMNIC Paradigm Software	10
Install OMNIC Paradigm Software	14
Key Concepts and Features	16

Welcome to OMNIC Paradigm Software

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

The screenshot displays the OMNIC Paradigm software interface. At the top is a menu bar with options: File, Acquire Data, View / Display, Process, Identify, Configure, Help, and a Summit button. Below the menu is a toolbar with icons for Open, Background, Sample, Settings, Dashboard, Spectra, Abs / %T, Advanced ATR, OCheck, Quantity, and Add To Library.

The main dashboard area is divided into three sections:

- New Measurement:** This section allows users to set up a new measurement. It includes fields for Measurement name (set to <current date/time>), Tag, Analysis type (set to None), Final format (set to Absorbance), Sample scans (set to 10), Resolution (cm-1) (set to 4), and Sampling accessory (set to None). There are buttons for "Preview and Measure Sample" and "Preview and Measure Background".
- Measurements:** This section shows a list of recent measurements. The table has columns for Measurement Name, Date, and Type. The data shows several measurements from 4/1/2019. To the right of the table is a preview of an FTIR spectrum.
- Workflows:** This section shows a list of workflows. The table has columns for Name, Date Created, and Last Modified. The data shows several workflows created on 3/30/2019. To the right of the table is a preview of a workflow diagram showing steps: Measure, Report, and End.

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.

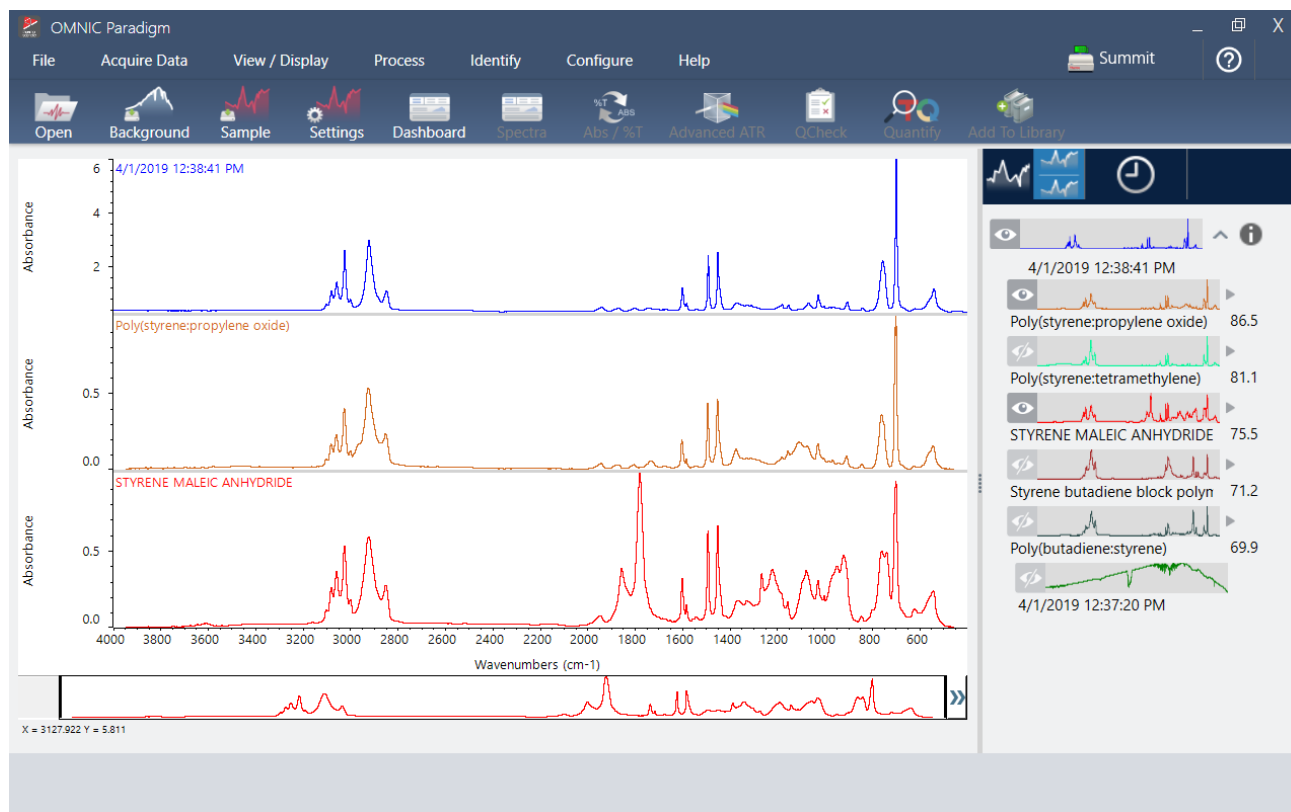
Get Started with OMNIC Paradigm Software

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



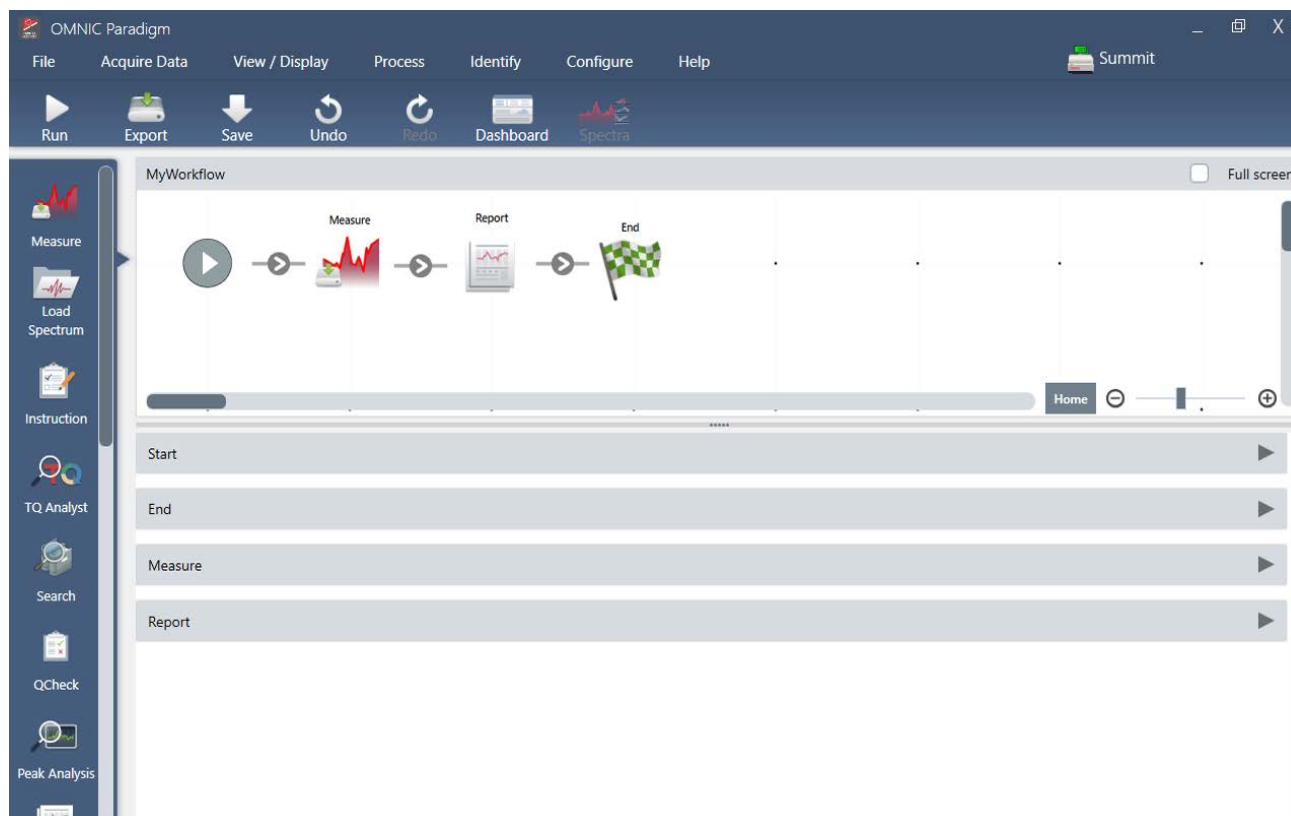
Use the spectral view to process, analyze, or explore your data in depth. Here you can process your data, find and label peaks, and optimize the view so you can more easily compare or analyze spectra.

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



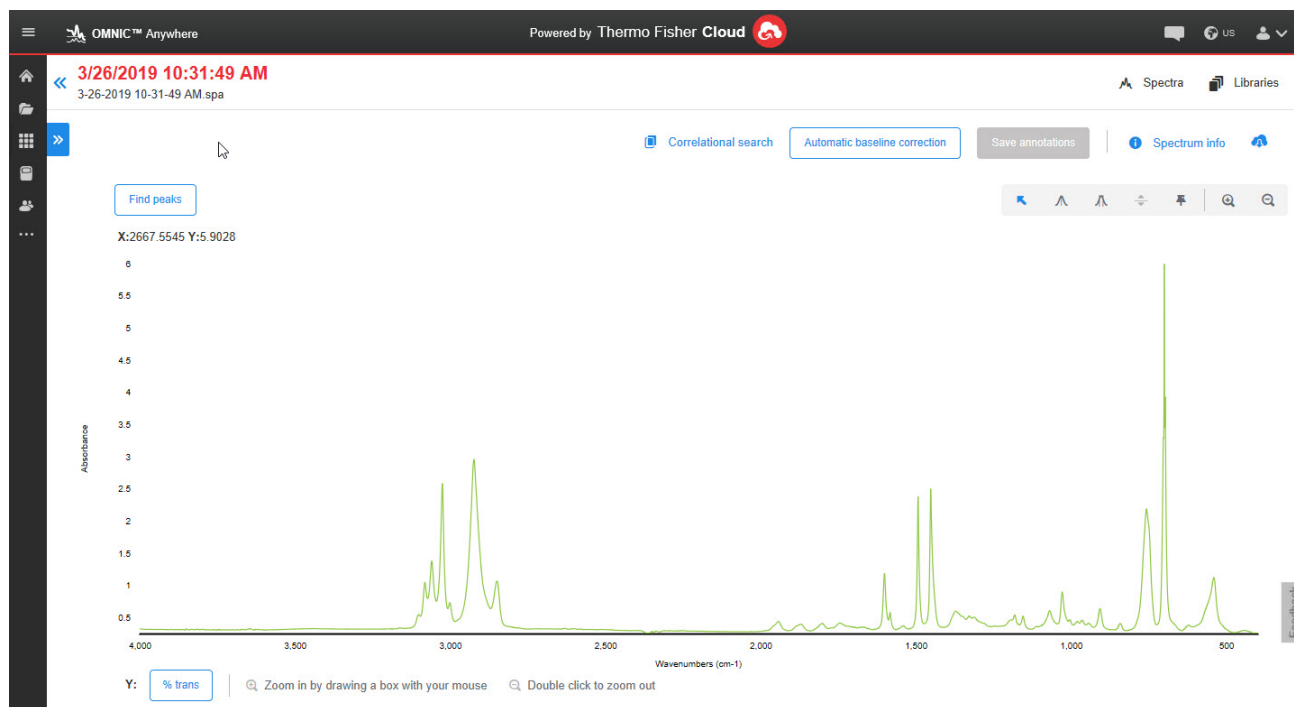
Automate your tasks with a workflow to ensure that measurements are collected and processed in exactly the same way each time. Edit or create a workflow by simply dragging and dropping tiles in the workflow editor, and then run the workflow at the click of a button.

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 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 software on your desktop, laptop, or other device to connect to Summit spectrometers or other instruments, such as Nicolet iS5, over an Ethernet, WiFi, or USB 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 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 software

Installing OMNIC Paradigm software takes only a few minutes.

❖ To install OMNIC Paradigm software

1. Insert the provided installation media (either DVD or flash drive).
2. Run the installer.
 - a. When the download completes, run the start.exe file.
 - b. Follow the on-screen prompts to install OMNIC Paradigm software.

Set Up and Connect OMNIC Paradigm software

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 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.

Key Concepts and Features

This section introduces the core concepts of using OMNIC Paradigm software. The information in this section will help you develop a basic understanding of OMNIC Paradigm software so that you can leverage all of the features and tools to analyze your samples.

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.

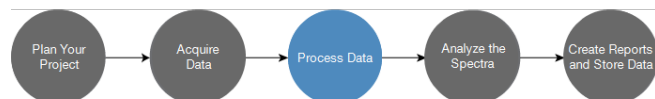
See "[Measure the Background](#)" for a full discussion of when and how to collect a background spectrum.

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 CO₂ or H₂O 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.

OMNIC Paradigm Software Options

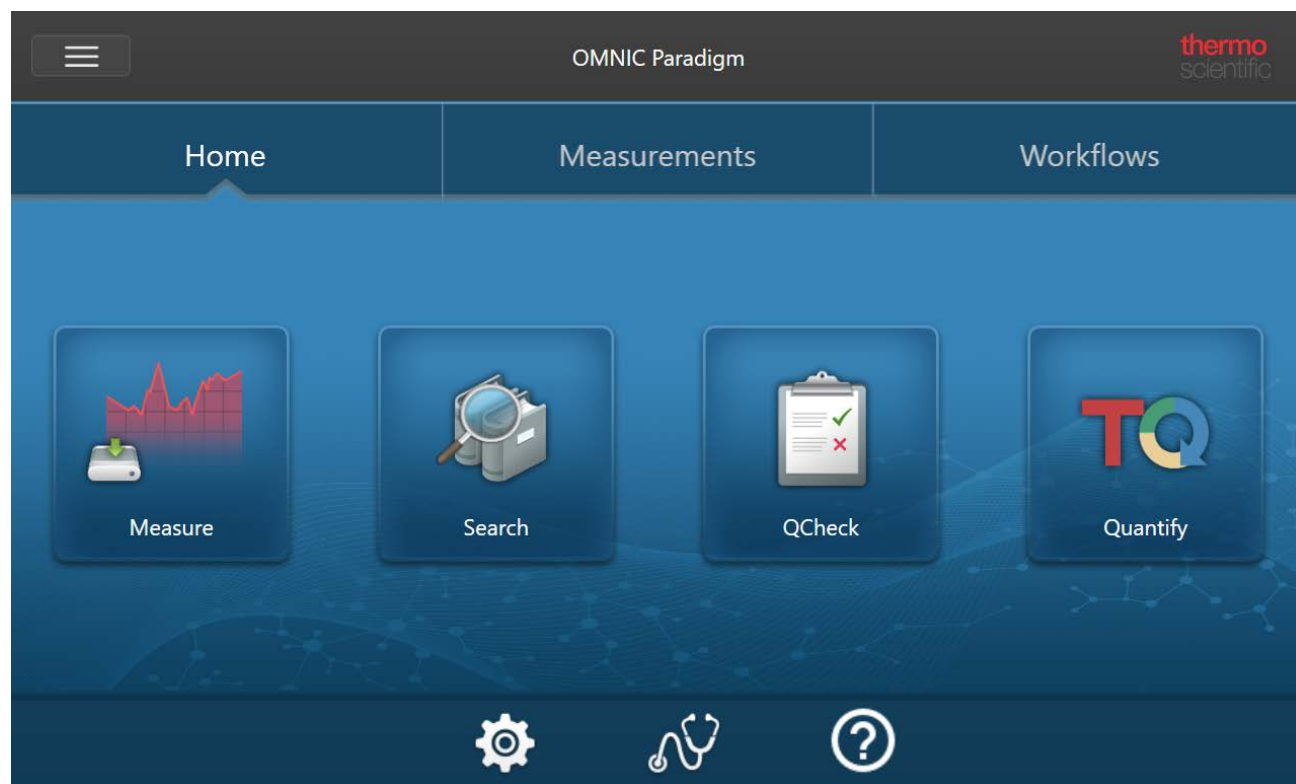
OMNIC Paradigm software features three interfaces to suit your device or task and pairs with other Thermo Scientific software, allowing you to develop and run quantification methods or protect and audit your data.

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 1-1: The touchscreen interface features a simplified interface for streamlined analysis.

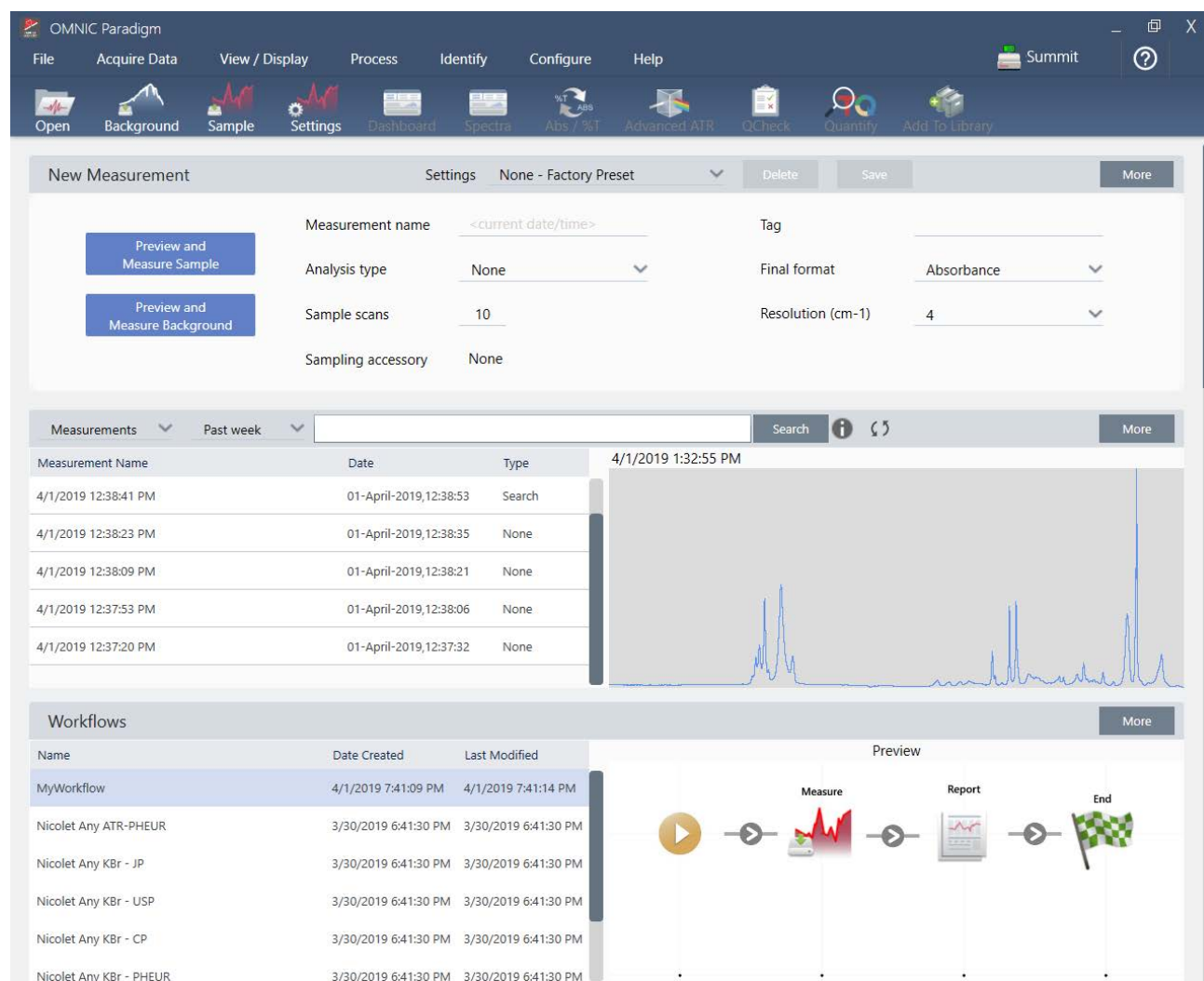


The touchscreen interface is optimized for small screens, such as the Thermo Scientific™ Nicolet™ Summit spectrometer's optional touchscreen device.

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

DESKTOP INTERFACE

Figure 1-2: 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.

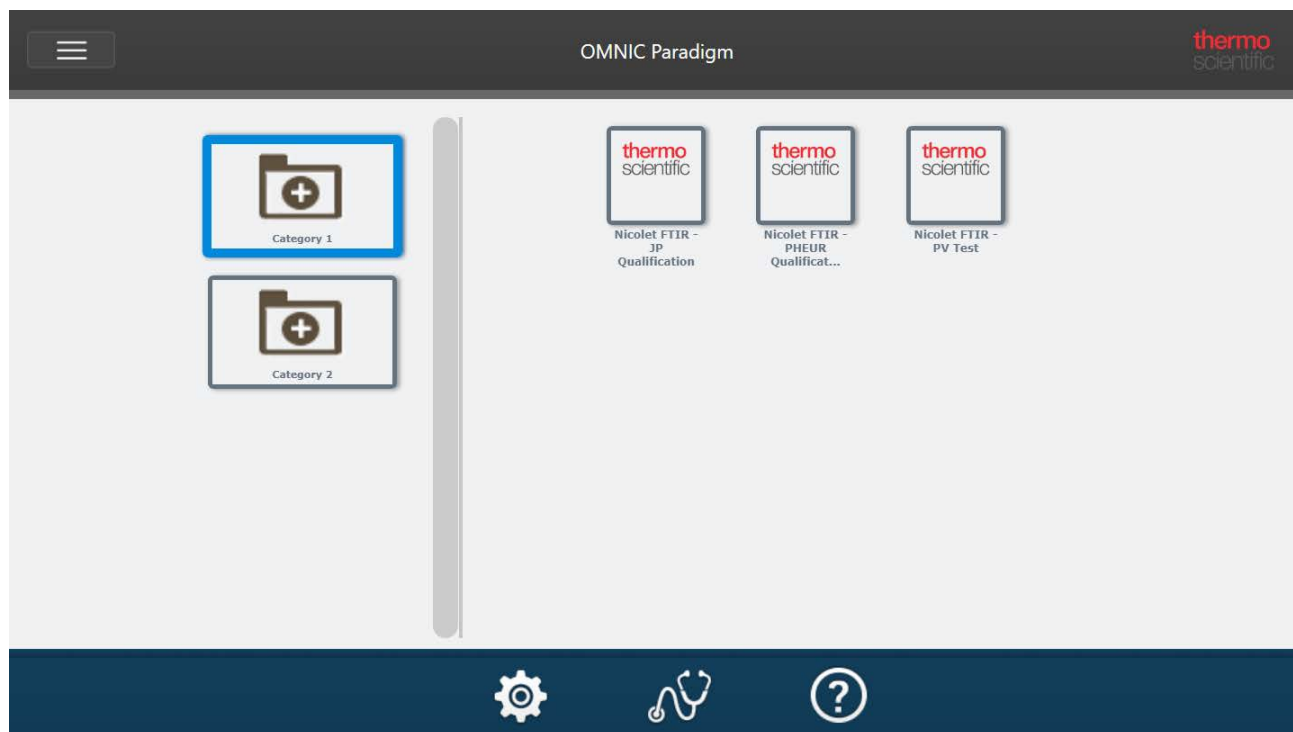
Connect your Summit spectrometer to an external monitor and a USB mouse and keyboard for the best experience using the desktop interface.

OPERATOR INTERFACE

The Operator interface is used for running workflows loaded from packages and for managing packages. After opening a package, operators are presented with a simplified interface designed to

Get Started with OMNIC Paradigm Software

run the package workflows.



For details on using the Operator interface and developing custom solutions, see ["Custom Solutions"](#).

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.

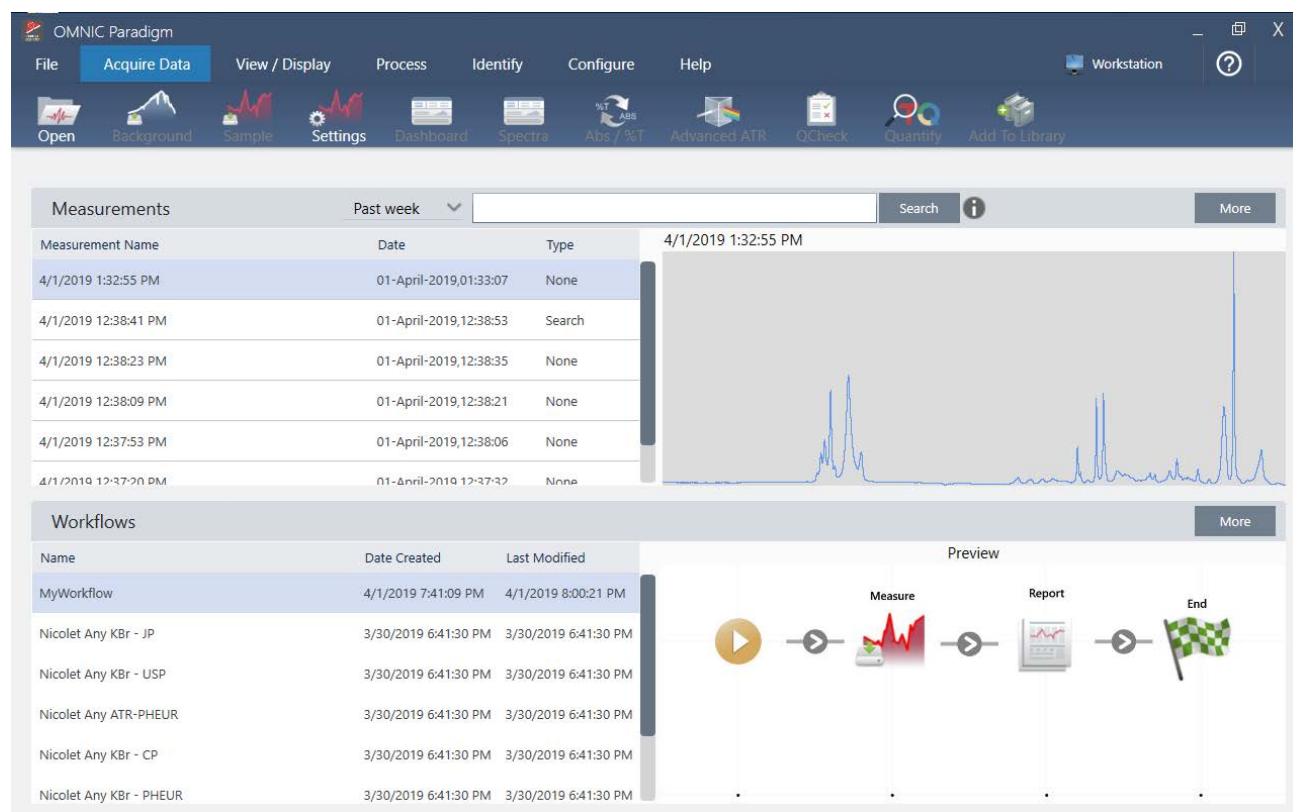
The software will close briefly and re-open with the desktop interface.

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 1-3: 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 version 9.8 or later 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 version 2.2 or later to ensure your data's security and integrity. The Security Suite software ensures 21CFR Part 11 compliance and includes

Get Started with OMNIC Paradigm Software

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.

[This page intentionally left blank]

Configure Your System

In OMNIC Paradigm software, you can configure your instrument connection and database, set up a back up schedule for your database, update your software, or customize display settings and other options.

In this section:

Connect to a Spectrometer	28
Connect an Instrument to a Thermo Fisher Connect Account	37
Configure Your Database	40
Set OMNIC Paradigm Options	44
Manage Spectral Libraries	47

Connect to a Spectrometer

There are three ways to connect your laptop or other device to your spectrometer. The connection you choose depends on the instrument.

- USB
- Network connection
 - local area network
 - wireless network
- Direct Ethernet connection

See the user guides and help content for your instrument for more on setup, installation, and connecting to other devices.

Connect to an instrument using a USB connection

Some instruments can be connected using an USB connection. For example, the Nicolet iS5 and Nicolet Summit LITE spectrometers use this type of connection.

❖ To connect to an instrument using a USB connection

1. Using a USB cable, connect the spectrometer to your computer running OMNIC Paradigm software.
2. In OMNIC Paradigm software, go to Configure and select Connectivity.
3. Select the spectrometer from the list of instruments and click Connect.

Connect to an instrument using an Ethernet or wireless network connection

You can connect to the Nicolet Summit, Summit PRO , or Summit OA spectrometer using an ethernet or wireless network connection. Before you connect to an instrument, make sure you understand database usage and user authentication.

Database Usage

When you connect to an instrument, you will always use the database configured by the client system.

For example, if you are using OMNIC Paradigm software on a laptop and you connect to a Summit spectrometer, you will continue to use the database configured by the software on the laptop. When you disconnect from the spectrometer, the software on the laptop will still show the data that was collected while connected to the spectrometer. If you then work directly on the Summit spectrometer, you will not see any of the data that was collected with the laptop.

When using a shared remote database, the data that is visible depends on which system you are using. For example, if several Summit spectrometers share a remote database with OMNIC Paradigm software that is being run on a laptop, you can use the laptop to view data collected by any of the instruments. However, any individual spectrometer will show only data collected on that machine and not from any other spectrometer.

For more information on configuring your database, see ["Configure Your Database"](#).

User Authentication

When you connect to a Summit spectrometer, the spectrometer needs to authenticate your device to ensure the connection is safe and trusted.

Many organizations manage authentication between devices by using a Windows domain. A domain is a group of computers that share user account information and security settings. With a domain, an administrator can manage many devices, accounts, and policies from a single server called a domain controller. This often allows you to log into many devices on the domain using the same username and password.

When you connect to a spectrometer from your laptop, the spectrometer and your laptop both communicate with the domain controller to make sure that the connection is safe and trustworthy. If either device is not on the domain, you will not be able to make the connection.

If both devices are managed by the same domain, use a local or wireless network connection to connect to the spectrometer.

❖ To connect to a Nicolet Summit spectrometer on a local area network or a wireless network

If your computer and spectrometer are part of a shared domain (recommended), connect using WiFi or Ethernet. Before you begin, make sure the Summit spectrometer and the computer are on the same Ethernet or WiFi network.

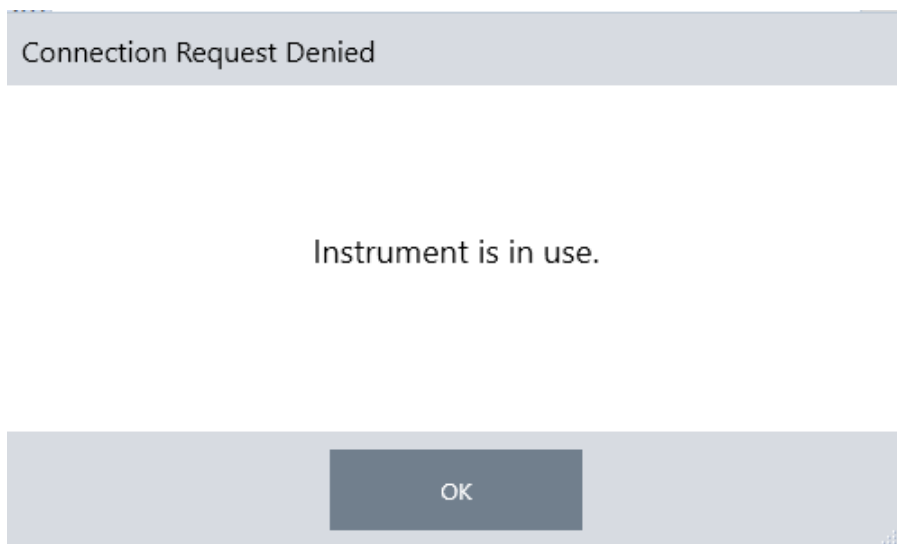
Configure Your System

1. In OMNIC Paradigm software, go to Configure and select Connectivity.
2. Select a spectrometer and click Connect.

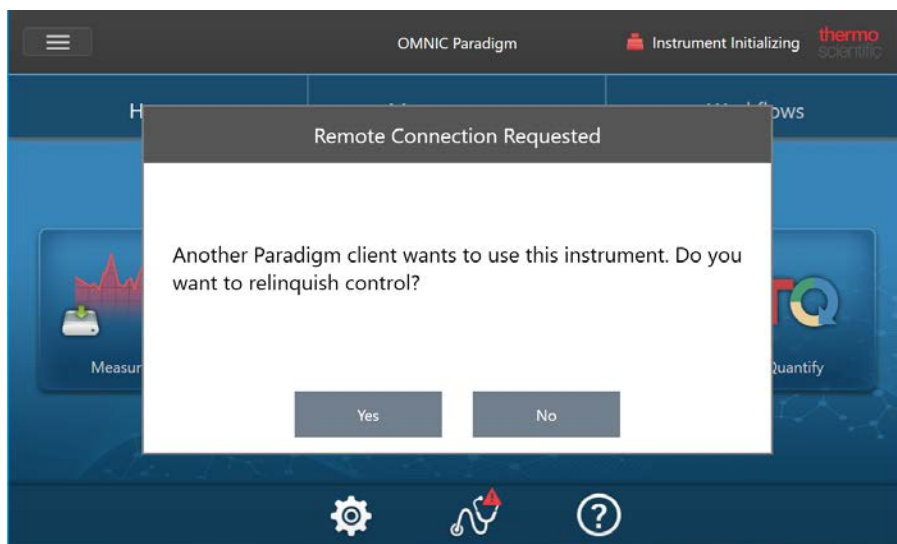
If your spectrometer does not appear on the list of available instruments, you can also enter the IP address or hostname of the instrument and then click Connect.

If the spectrometer is already in use when you attempt to connect, the connection may be denied. The request can be denied for two reasons:

- The instrument is busy measuring a sample or processing data and cannot be interrupted.



- Another user is operating the instrument and chose not to relinquish control.



Configure Your System

If the current user does not respond within 30 seconds of the request, the connection is allowed automatically.

If the request is denied automatically or by the current user, you can return to Workstation mode, connect to another instrument, or try to connect again.

Connect directly to the instrument with an Ethernet cable

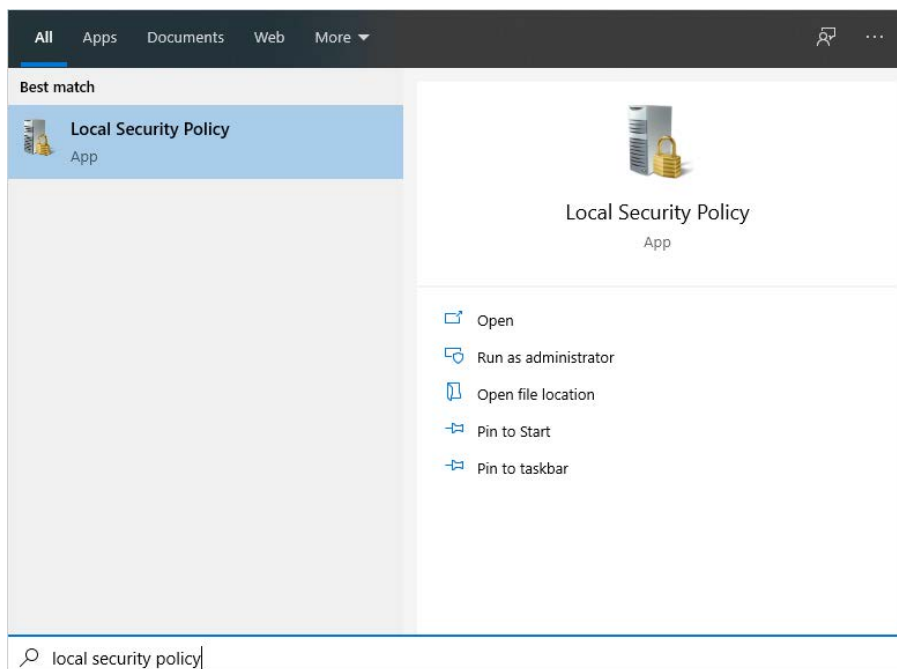
You can also connect to the spectrometer directly using an Ethernet cable.

Using a direct connection requires you to edit the local security policies on the spectrometer. Because the instrument cannot communicate with a domain controller for user authentication when you are using this configuration, you must modify security policies to allow communication between the instrument and your computer.

Note Modifying security policies could pose a security risk to your organization. Follow your organization's security policies.

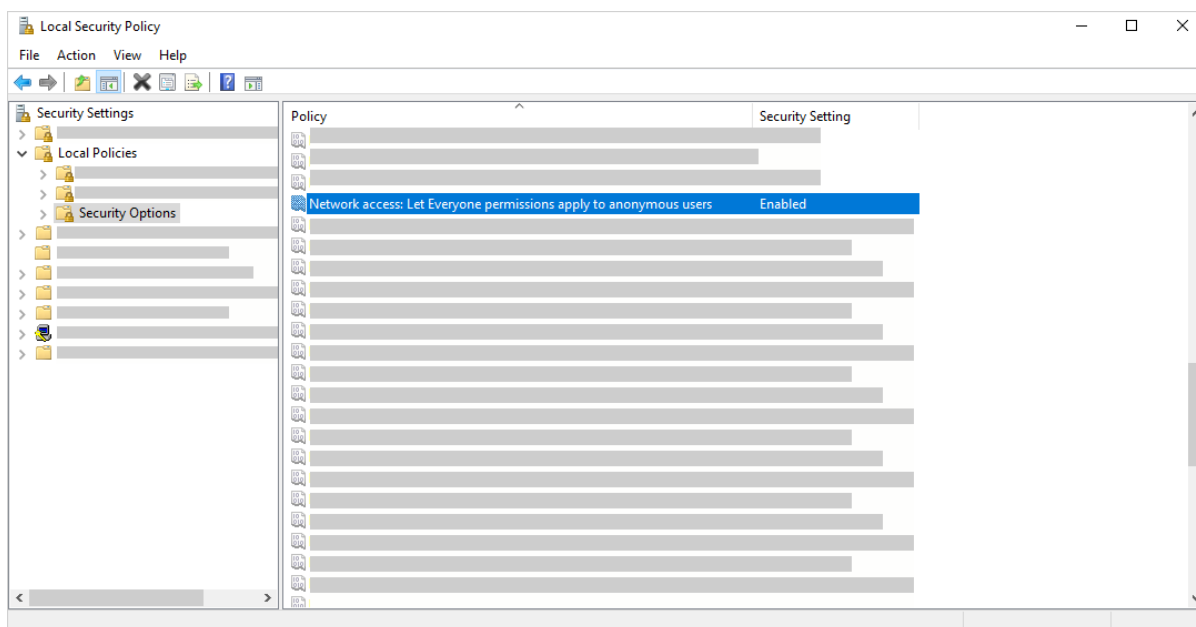
❖ To use a direct connection

1. Modify security policies on the instrument
 - a. On the Nicolet Summit spectrometer, open the Local Security Policy application.



Configure Your System

- b. Navigate to Security Settings > Local Policies > Security Options.
- c. Set Network access: Let Everyone permissions apply to anonymous users to Enabled.



2. Use an ethernet cable to connect the computer directly to the spectrometer.
3. In OMNIC Paradigm software, if the software does not recognize the instrument automatically, go to Configure > Connectivity and connect to the spectrometer.

Preventing Connections from Unsecured Devices

If your spectrometer is using Thermo Scientific Security Suite software to protect and secure your data, you may want to prevent connections from unsecured devices. For example, with the default settings, if a laptop that is not managed by Security Administration software and Audit Manager software connects to a secure spectrometer, any action taken on the laptop would not be managed or logged.

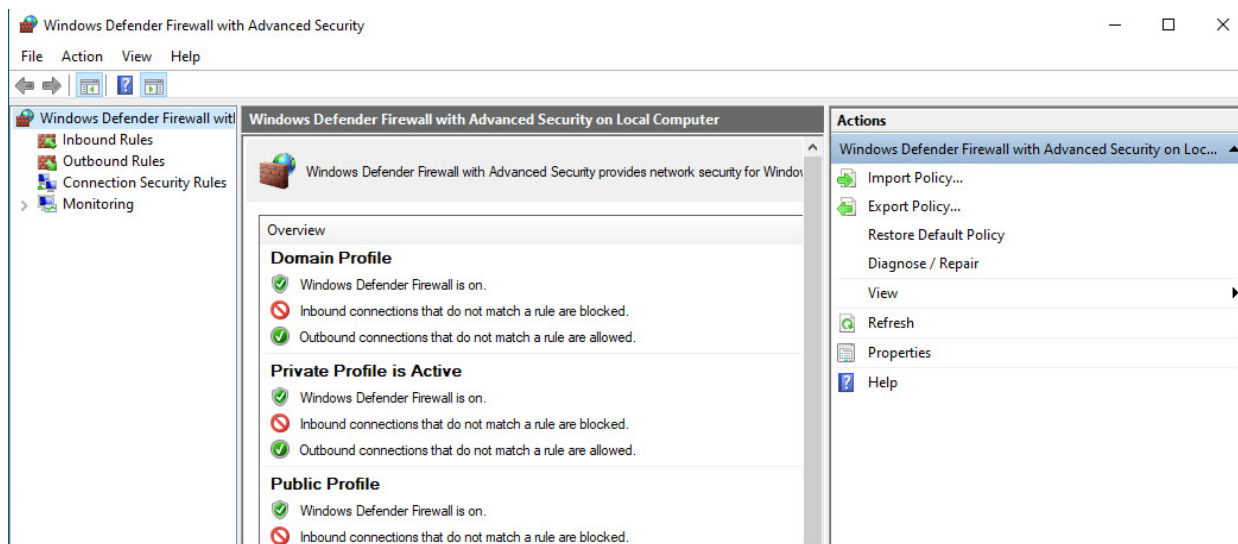
To prevent connections from unsecured devices, you must edit your firewall settings on the secure spectrometer. Disable all Inbound rules that belong to the group RabbitMQ or to OMNIC Paradigm. See ["Firewall Settings"](#) for additional details on these rules.

The following procedure describes disabling the Inbound Rules in Windows Defender Firewall. Your organization may use another application to manage firewall settings.

Configure Your System

❖ To disable Inbound Rules in Windows Defender Firewall

1. Open Windows Defender Firewall with Advanced Security.



2. In the left pane, navigate to Inbound Rules.
3. In the primary pane, under Inbound Rules, select a rule to disable.
4. In the Actions pane, click Disable Rule.

The Enabled column for the rule you have selected changes to No.

To re-enable the rule, click Enable Rule in the Actions column.

Troubleshooting

INSTRUMENT NOT APPEARING IN AVAILABLE CONNECTIONS

If your spectrometer does not appear automatically in the list of available instruments when you go to Configure > Connectivity, check your network connections.

The spectrometer and the computer making the connection must be on the same network for the instrument name to appear in the list. For example, if your organization has several wireless networks, make sure that the spectrometer and computer are on the same network.

If the spectrometer's name doesn't appear in list of instruments, you can attempt to connect by entering the spectrometer's IP address.

Advanced Troubleshooting

If you cannot connect to a spectrometer, you may need to check your firewall settings. Only the IT or network administrator at your organization should edit firewall settings.

FIREWALL SETTINGS

When OMNIC Paradigm software is installed, your firewall settings are updated to allow a connection between a spectrometer and OMNIC Paradigm Workstation software. If you experience problems with your connection, check your firewall settings on both the spectrometer and the connecting computer to confirm that the following ports allow traffic.

The table below reflects the inbound rules as set in Windows Defender Firewall. The available fields may be different depending on the application your organization uses to manage network firewall settings.

Table 2-1: Required inbound rules

Name	Description and Ports Used
Password Management (NB-Name-In)	Description: Inbound rule for Password Management to allow NetBIOS Name Resolution. Group: Thermo Scientific Password Management Program: System Ports: UDP 137 Action: Allow Profile: Domain, Private, Public
Password Management (NB-Session-In)	Description: Inbound rule for Password Management to allow NetBIOS Session Service connections. Group: Thermo Scientific Password Management Program: System Ports: TCP 139 Action: Allow Profile: Domain, Private, Public

Configure Your System

Name	Description and Ports Used
Password Management (SMB-In)	<p>Description: Inbound rule for Password Management to allow Server Message Block transmission and reception via Named Pipes.</p> <p>Group: Thermo Scientific Password Management</p> <p>Program: System</p> <p>Ports: TCP 445</p> <p>Action: Allow</p> <p>Profile: Domain, Private, Public</p>
Thermo Scientific Instrument Discovery	<p>Description: Allows clients to discover this instrument</p> <p>Group: OMNIC Paradigm</p> <p>Program: C:\Program Files\Thermo Scientific\IR Instrument Engine\Instrument.IR.Engine.Service.exe</p> <p>Ports: UDP 50123</p> <p>Action: Allow</p> <p>Profile: Domain, Private, Public</p>
Thermo Scientific Web API Server	<p>Description: Allows client to access a web API</p> <p>Group: OMNIC Paradigm</p> <p>Program: System</p> <p>Ports: TCP 9004</p> <p>Action: Allow</p> <p>Profile: Domain, Private, Public</p>
RabbitMQ - Peer Discovery (EPMD)	<p>Group: RabbitMQ</p> <p>Program: C:\Program Files\erl9.3\erts-9.3\bin\epmd.exe</p> <p>Ports: TCP 4369</p> <p>Action: Allow</p> <p>Profile: Domain, Private, Public</p>

Configure Your System

Name	Description and Ports Used
RabbitMQ - Client Connection (erl)	<p>Group: RabbitMQ</p> <p>Program: C:\Program Files\erl9.3\erts-9.3\bin\erl.exe</p> <p>Ports: TCP 5671, TCP 5672</p> <p>Action: Allow</p> <p>Profile: Domain, Private, Public</p>
RabbitMQ - Management Console (erl)	<p>Group: RabbitMQ</p> <p>Programs:</p> <p>C:\Program Files\erl9.3\erts-9.3\bin\erl.exe</p> <p>C:\Program Files\erl9.3\bin\erl.exe</p> <p>Ports: TCP 15672</p> <p>Action: Allow</p> <p>Profile: Domain, Private, Public</p>
Thermo Scientific History WebAPI	<p>Group: OMNIC Paradigm</p> <p>Program: System</p> <p>Ports: TCP 9002</p> <p>Action: Allow</p> <p>Profile: Domain, Private, Public</p>
Thermo Scientific Workflow Engine	<p>Group: Thermo Scientific Workflow Engine</p> <p>Program: System</p> <p>Ports: TCP 9090</p> <p>Action: Allow</p> <p>Profile: Domain, Private, Public</p>

Connect an Instrument to a Thermo Fisher Connect Account

Connect your instrument to your Thermo Fisher Connect account to view and manage your instruments and data remotely.

For more information on Thermo Fisher Connect and managing your connected instruments, see the Help guide in the Thermo Fisher Connect application.

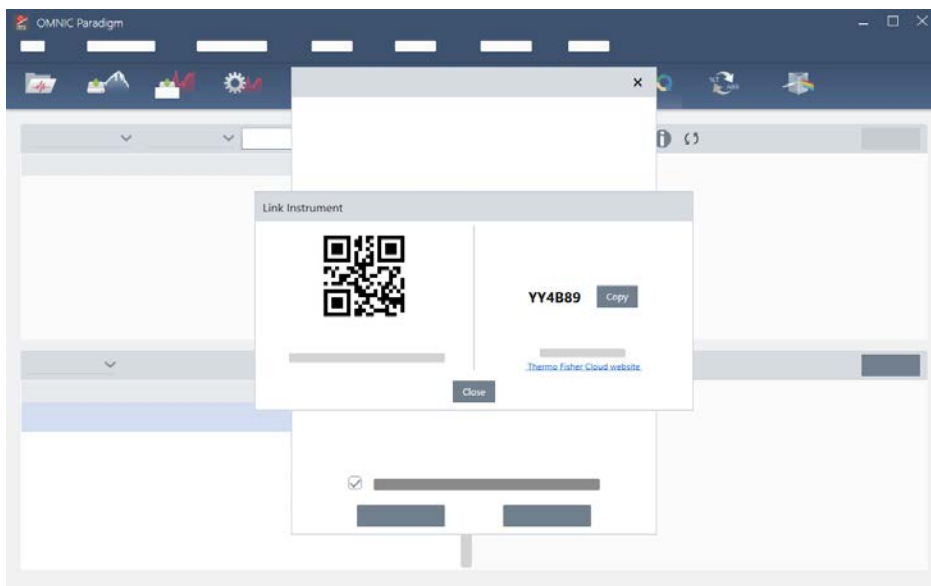
BEFORE YOU BEGIN

To connect your instrument to Thermo Fisher Connect, you need a Thermo Fisher Connect account. To create an account, visit <https://www.thermofisher.com/us/en/home/digital-science/thermo-fisher-connect.html>.

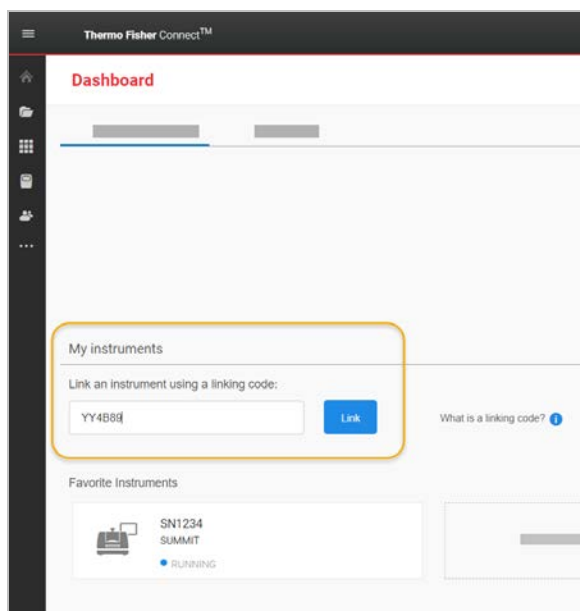
❖ To connect your instrument to your Thermo Fisher Connect account

1. Using the Desktop interface of OMNIC Paradigm software, from the Dashboard, go to Acquire Data > Diagnostics > Instrument Health.
2. Optional: Opt-in to sharing instrument health data.
3. Click Link Instrument.
4. To complete the connection, scan the QR code using the Thermo Fisher Instrument Connect app on your mobile device or use the 6-digit code.

Configure Your System



- To use the 6-digit code
 - a. Click Copy to copy the code to your clipboard.
 - b. Go to Thermo Fisher Connect in your web browser.
 - c. On the dashboard of the Thermo Fisher Connect web application, under My Instruments, paste or enter the 6-digit code and click Link.



Configure Your System

The instrument is now displayed in the InstrumentConnect section of Thermo Fisher Connect.

- To scan the QR code
 - a. Open the Instrument Connect app on your mobile device.
 - b. Touch the + icon in the upper right corner of the screen to add an instrument.
 - c. Select QR Code.
 - d. Use your device to scan the QR code.

The instrument is linked and displayed in the mobile app and online.

Configure Your Database

When you first install OMNIC Paradigm software, the default database is set up on the local device and ready to use. You can continue to use the local database or connect to a remote database in another location on your network. Use a remote database to easily share measurements, settings, and other data across devices.

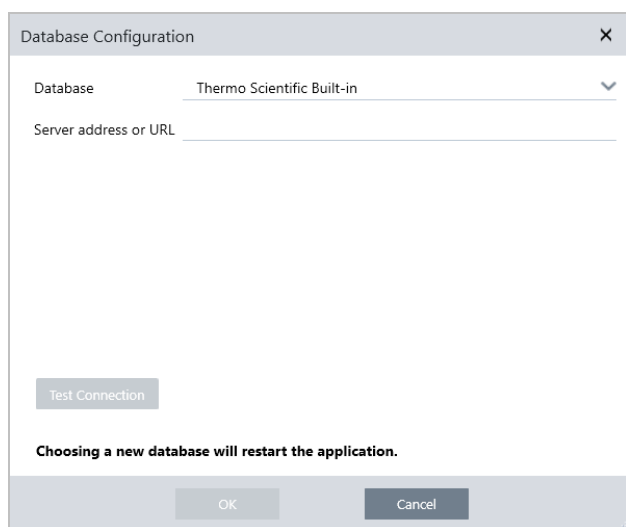
When using OMNIC Paradigm Workstation software, if you connect to a Nicolet Summit spectrometer, data will be stored in the database configured in the workstation software, not the database configured on the spectrometer.

Connect to a Remote Database

Connect to a remote database to easily share measurements, settings, and other data across devices. Change your database configuration at any time to suite your work.

❖ To connect to a remote database

1. Using the desktop interface of OMNIC Paradigm software, go to Configure and select Database.



2. Select the database type from the Database list. The default selection is Thermo Scientific Built-in. To connect to a custom database, enter the database type, version,

name, and port. You may also need to enter a username and password.

3. Enter the IP address or URL for the database server.
4. Click Test Connection to check if the software can connect to the server.
5. If the test reports a valid connection, click OK to connect to the remote database.

The software restarts during connection.

Check the Measurements group on the dashboard to confirm that you are seeing data from the remote database, or return to the Configure > Database menu to view your current connection.

Back Up and Restore a Database

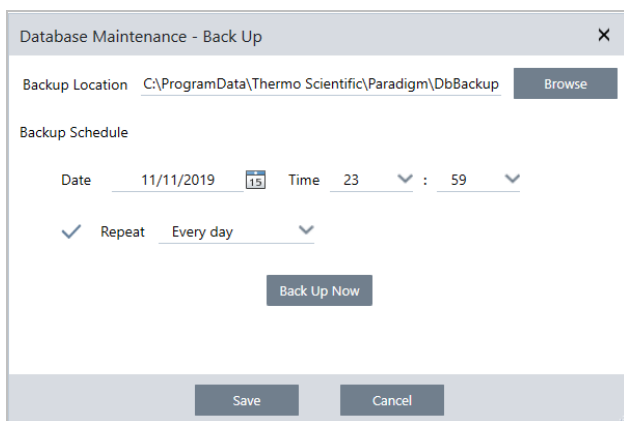
Back up your database periodically to ensure that you can recover your data in the event of hard drive failure. With the database maintenance tools in OMNIC Paradigm software, you can easily backup and restore your data directly from the software.

Back Up Your Database

Back up your database on a separate device in case of hard drive failure. For example, back up the data on a separate computer or external hard drive or in a remote network location.

❖ To back up your database

1. Using the desktop interface of OMNIC Paradigm software, go to Configure > Database Maintenance and select Back Up.



The screenshot shows a dialog box titled "Database Maintenance - Back Up". It has a close button (X) in the top right corner. The "Backup Location" is set to "C:\ProgramData\Thermo Scientific\Paradigm\DbBackup" with a "Browse" button to its right. Below this, the "Backup Schedule" section includes a "Date" field set to "11/11/2019" with a calendar icon, a "Time" field set to "23 : 59" with dropdown arrows, and a "Repeat" section with a checked checkbox and a dropdown menu set to "Every day". A "Back Up Now" button is located below the schedule settings. At the bottom of the dialog are "Save" and "Cancel" buttons.

Configure Your System

2. Select a backup location to save the backup database.
3. To schedule backups, set a date and time for the first backup.
 - a. Ensure that Repeat is selected and choose a repeat option from the list.
 - b. Click Save.

3. To back up the database manually without a schedule, click Back Up Now.

To set a new backup location before backing up, first change the location and save your changes, then reopen the Database Maintenance - Back Up window and click Back Up Now.

4. Click Close to return to the dashboard.

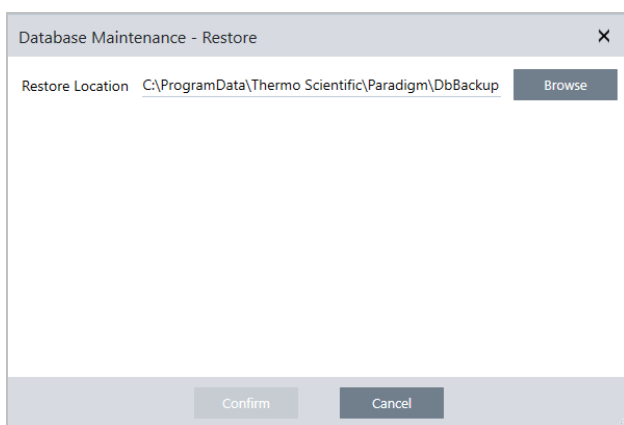
Restore a Database from a Backup

Use the Restore tool in OMNIC Paradigm software to restore your database from a previously saved backup.

Note This action will permanently remove all data currently in your database and will replace it with data from the selected backup.

❖ To restore your database

1. Using the desktop interface of OMNIC Paradigm software, go to Configure > Database Maintenance and select Restore.



2. Click Browse and select the location of the backup database.

Configure Your System

If you are using OMNIC Paradigm software on a Summit spectrometer and you are restoring from a remote backup that is shared with other spectrometers, you can restore data from any individual spectrometer that is using the backup.

To back up data from only a single spectrometer, select a spectrometer from the list of hostnames.

3. Click Confirm.

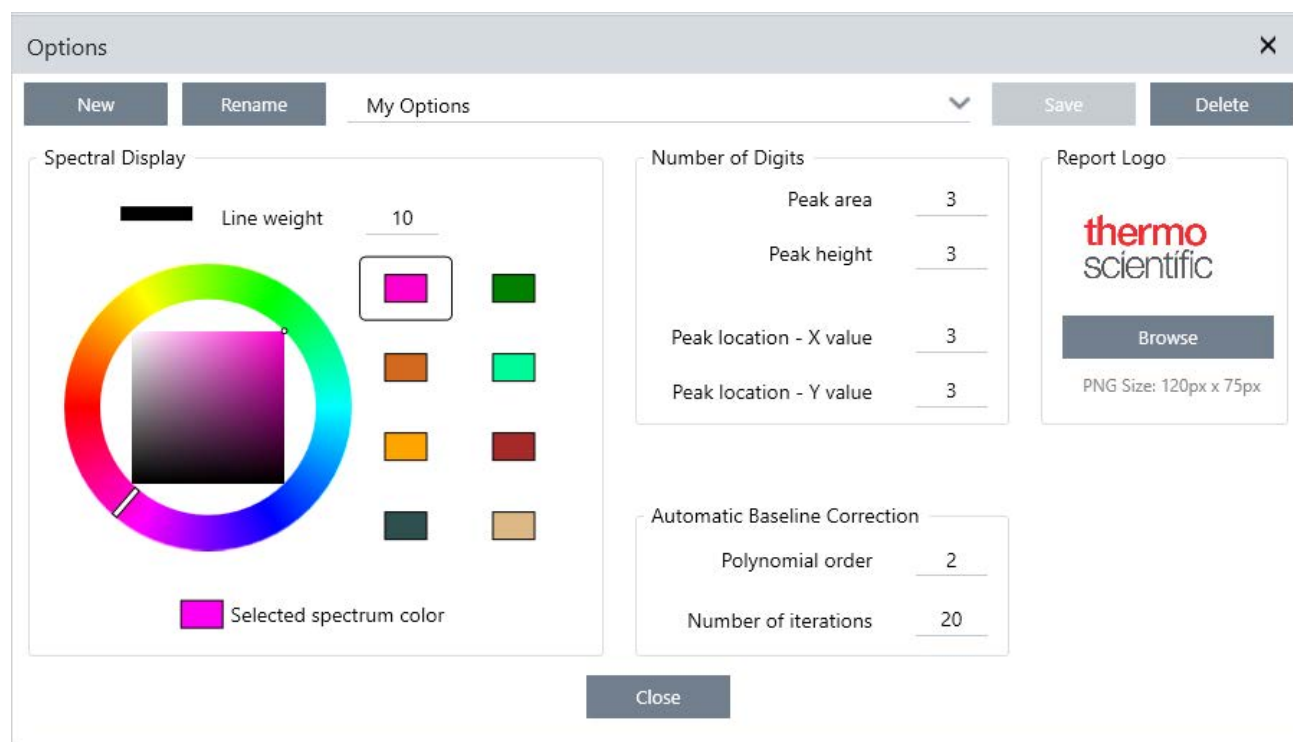
Set OMNIC Paradigm Options

Use the Options dialog to customize the spectral display, to set the number of digits used for peak area, height, and location, and to configure automatic baseline correction.

❖ To set and save OMNIC Paradigm options

1. Open the Options dialog.
 - Desktop interface: open the Configure menu and select Options.
 - Touchscreen interface: Open the settings and navigate to the Options tab.
2. Select New.
3. Enter a name for the new options and click Save.
4. Edit your settings.
5. When you are finished editing settings, select Save to save your changes.
6. Select Close to return to your previous screen.

Figure 2-1: The Options dialog



Customize Spectral Display Settings

The Spectral Display group is used to set the color and line weight of spectra in the Spectra view.

- **Line Weight:** Determines the thickness of the line used to draw the spectrum. Applies to all spectra shown in the Spectra view.
- **Selected Spectrum Color:** Determines the color used to highlight the currently selected spectrum.

The additional colors set the colors of spectra that are not selected.

Set Number of Digits

Use the Number of Digits group to set the limit for the number of digits after the decimal separator. The limit is applied to the following:

- Peak area
- Peak height
- Peak location - X value
- Peak location - Y value

Note that this setting only applies to operations carried out after the setting is adjusted. Numbers in the spectrum information maintain the settings used at the time they were recorded and are not updated to reflect new settings. For example, if you carry out a find peaks operation with settings specifying 3 digits, the spectrum information shows 3 digits. If you then change your settings to use only 1 digit after the decimal, the spectrum information from the earlier find peaks operation will still show the 3 digits.

Configure Automatic Baseline Correction

Use Automatic Baseline Correct in the Process menu to automatically correct tilted or curving baselines.

Set the polynomial order and number of iterations to specify the order of the equation and number of iterations to use for correcting baselines automatically.

Add a custom logo to reports

Use your own logo on reports and template reports. The image is shown on standard reports and reports you create using the Template Report tile in workflows.

Report images must be a PNG file and are automatically resized to be 120 px by 75 px.

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

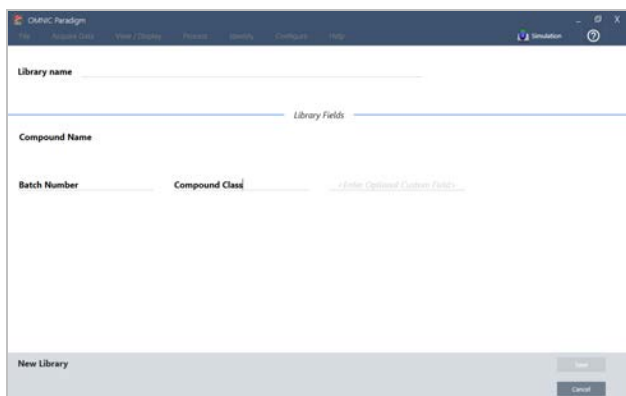
Create a new library to manage your spectral data and to search against your own measured data.

❖ To create a new library in the desktop interface

1. From the menu bar, select Identify > Library Manager.
2. In the Library Manager, select New Library.
3. Enter a name for the library and add any optional fields.

Optional fields are used when you add spectra to a library.


Figure 2-1: Name your library and customize optional fields in the New Library view.



4. Click Save to create the new library.

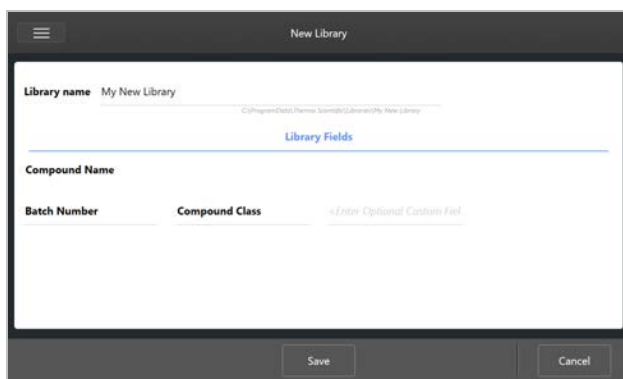
Your new library is listed in the Libraries column of the library manager.

❖ To create a new library in the touchscreen interface

1. From the home screen, open the menu [] and select Library Manager.
2. Select New Library from the toolbar.
3. 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.

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



4. 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

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.

Note Deleted libraries and compounds cannot be recovered.

❖ To delete a compound from a library

- Using the Desktop interface
 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.
- Using the Touchscreen interface
 1. In the Library Manager, select to the compound you want to delete.
 2. Touch Delete in the Spectrum pane.

❖ To delete a library

- Using the Desktop interface
 1. In the Library Manager, select the library to be deleted.
 2. Click Delete in the toolbar, then click Yes to confirm.
- Using the Touchscreen interface
 1. In the Library Manager, select the library to be deleted.
 2. Touch Delete in the main toolbar.

Add Library Locations

Use the Library Locations tab in Search Setup to specify additional library locations. This is useful if your libraries are stored in a shared location such as a network drive. After you add a location, you can use libraries in that location for Search, QCheck, and other analyses.

❖ To add a library location

1. Using the desktop interface, open the Identify menu and select Search Setup.
2. Navigate to the Library Locations tab.
3. Click Add Location.
4. Browse to the location of the additional libraries and click Open.
5. Click Save.

Tutorials and Walkthroughs

The tutorials in this section guide you through some of the most common techniques used with OMNIC Paradigm software, including identifying, quantifying, and verifying samples as well as creating and running a workflow to automate your most common tasks.

These tutorials are intended to be as accessible as possible for those new to OMNIC Paradigm software. If you prefer to get started on your own, see ["Measure the Background"](#) to start measuring your samples. If you prefer a more conceptual overview, see ["Key Concepts and Features"](#).

In this section:

Identify an Unknown Sample with ATR	52
Identify an Unknown Sample with Transmission	65
Verify Sample Composition with QCheck	79
Quantify Sample Composition	85
Create and Run Your First Workflow	89

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.

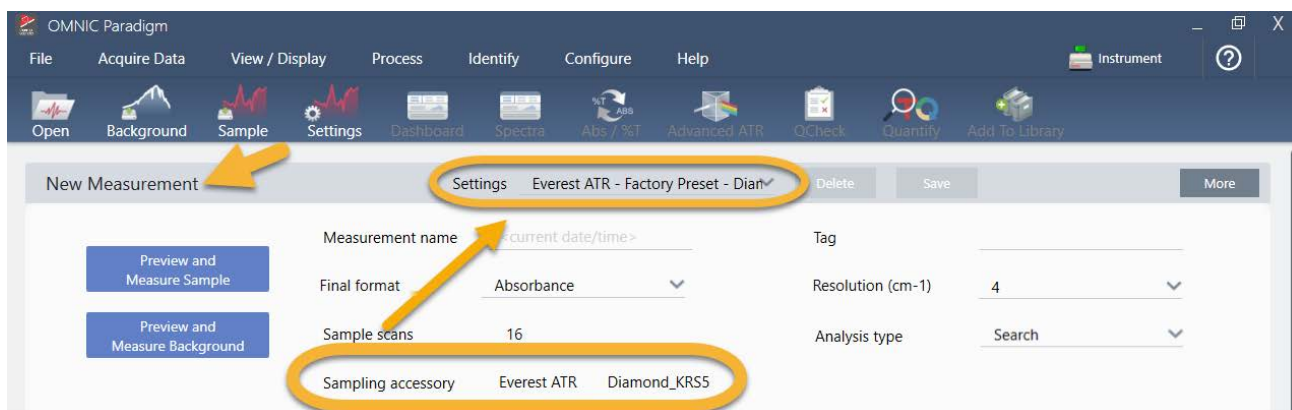
Here is the Thermo Scientific™ Everest ATR accessory with a diamond crystal installed in our Nicolet™ Summit FTIR spectrometer.



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, reseal 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.

Measurement name <current date/time>

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.

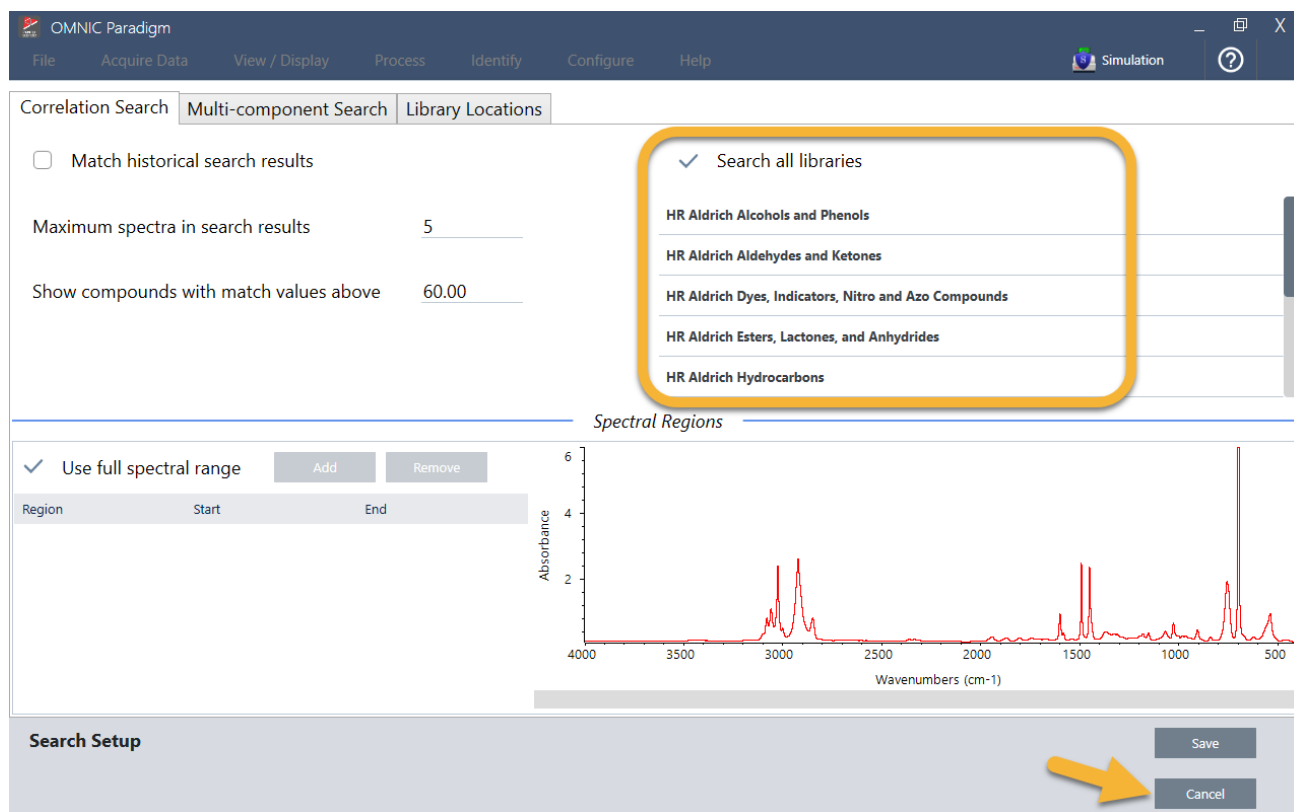
Final format	<u>Absorbance</u> ▼	Resolution (cm-1)	<u>4</u> ▼
Sample scans	<u>16</u>	Analysis type	<u>Search</u> ▼

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.

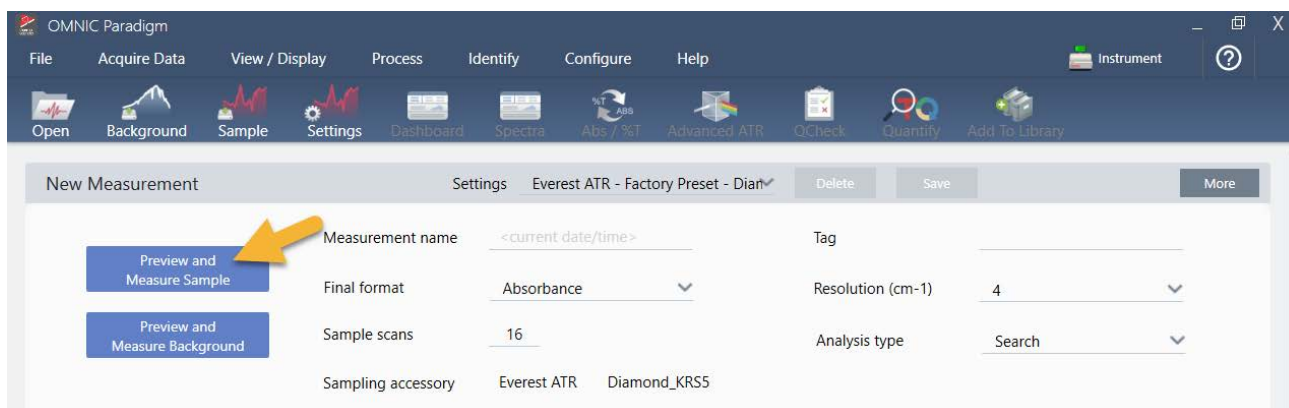
The library spectra are normally the same quality or higher quality than the sample spectrum. It is also helpful if they are acquired using the same sampling technique (ATR in this case). If your library spectra were acquired using the transmission technique, OMNIC Paradigm software has a correction 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.

Tutorials and Walkthroughs



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.

Tutorials and Walkthroughs



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 3-1: Measure a liquid with ATR



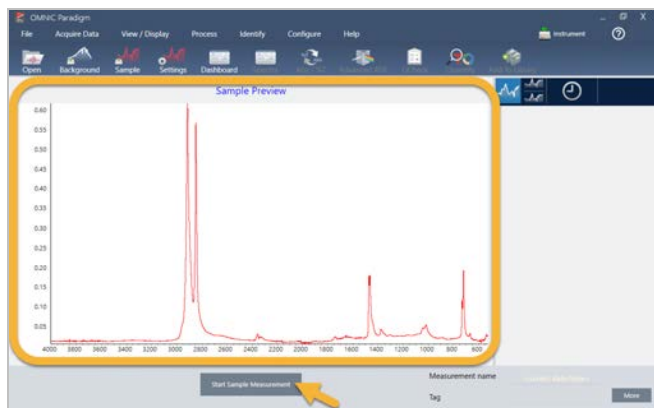
Tutorials and Walkthroughs

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 card.

Figure 3-2: 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.



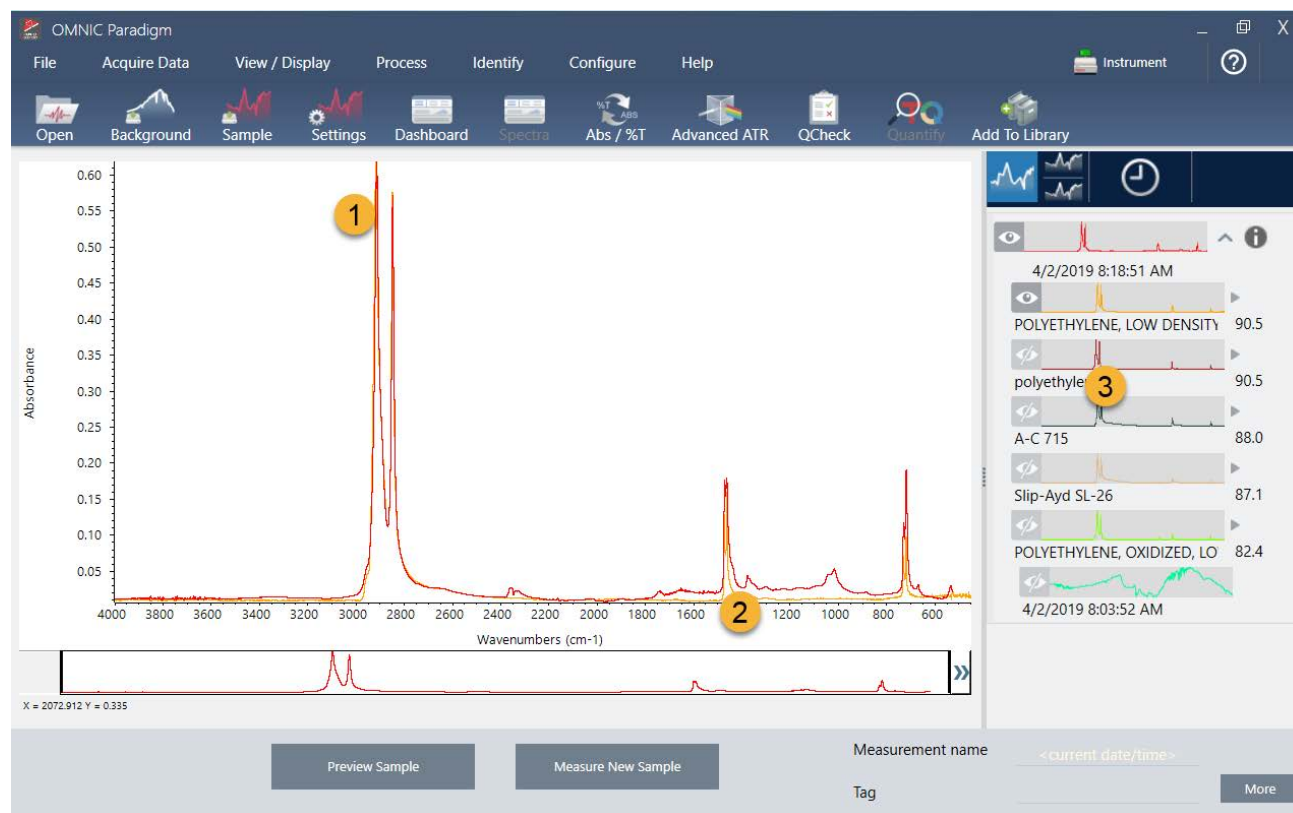
If the spectrum has no sample peaks, check that the sample material absorbs energy in the infrared region of the light spectrum. If you observe extra peaks in the spectrum, make sure the crystal is clean.

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

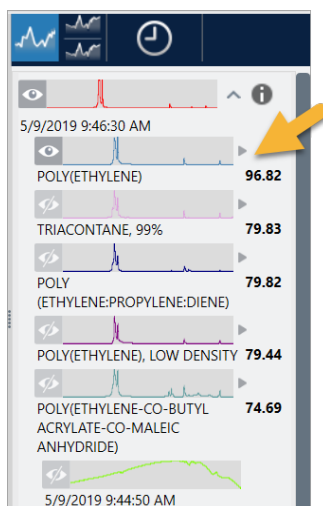


1. Sample spectrum (red)
2. Best match (yellow)
3. Results panel

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.

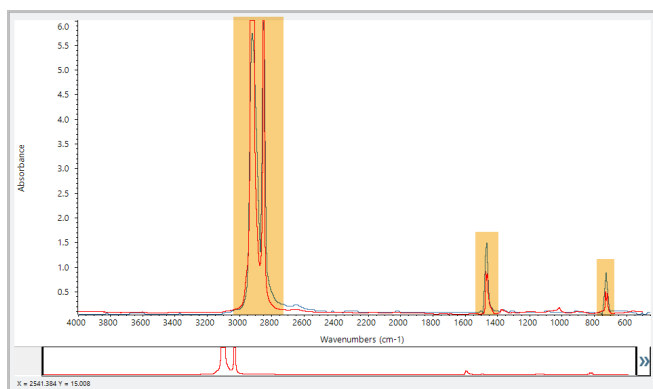
In this example, the top match has a match value that is above 90, which indicates a good match. The match value for the next spectrum in the list is well below that.

Figure 3-4: Match values showing a clear best match



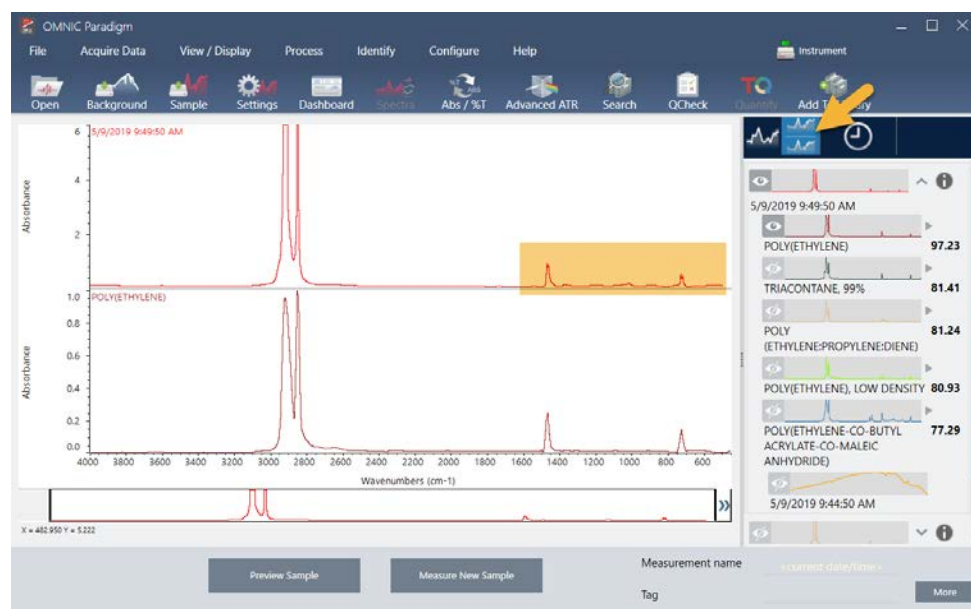
If we look at the overlaid spectra in the spectral pane, the positions of the main peaks line up along the X-axis, and they differ only in their peak heights.

Figure 3-5: Overlaid spectra showing a clear match



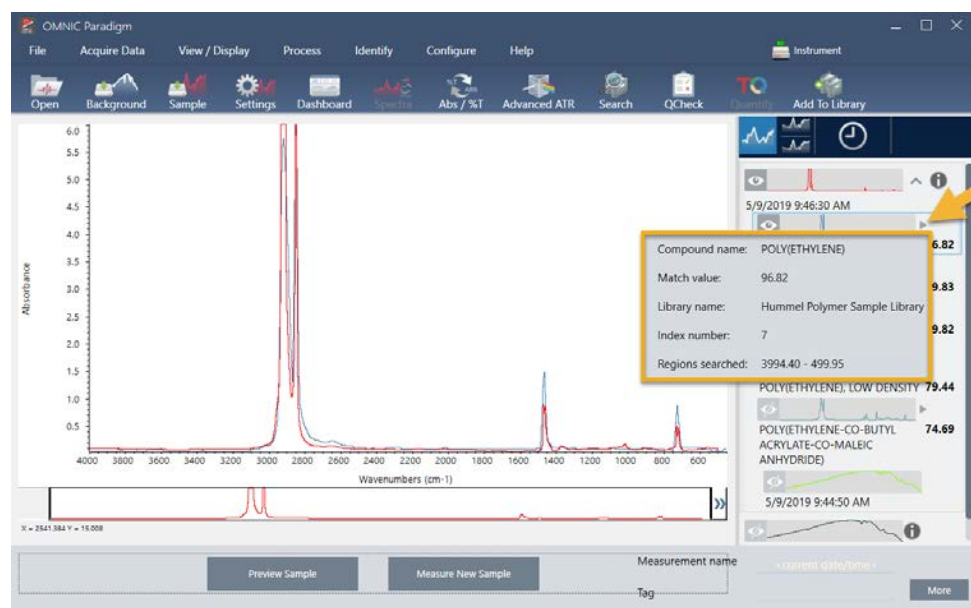
Click the Stack button to see the two spectra scaled to fill each Y-axis. Again, the spectra are well matched except for the slightly raised baseline in the sample spectrum's low frequency region. As a result, we can conclude that the sample is polyethylene and the analysis is complete.

Figure 3-6: 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, hover over the spectrum's grey arrow in the results panel.

Figure 3-7: 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.

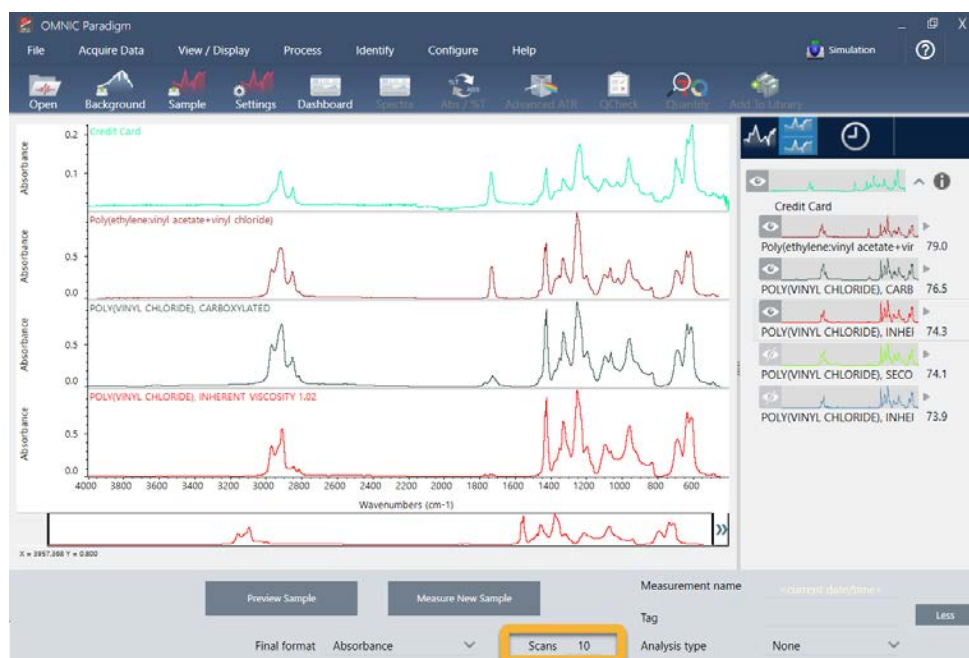
Figure 3-8: Stacked spectra showing several similar matches



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 3-9: 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.

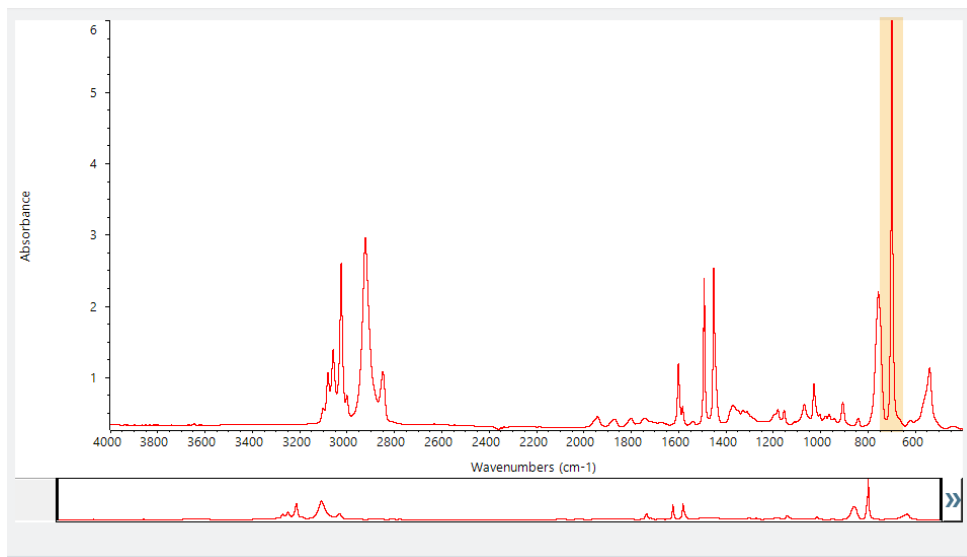
If the sample spectrum has a tilted or curved baseline, try applying Automatic Baseline Correction (Process menu) to your sample spectrum and then restart the analysis.

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 3-10: 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, open the search settings, de-select Use full spectral range, and specify the regions to search that exclude the totally absorbing region.

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

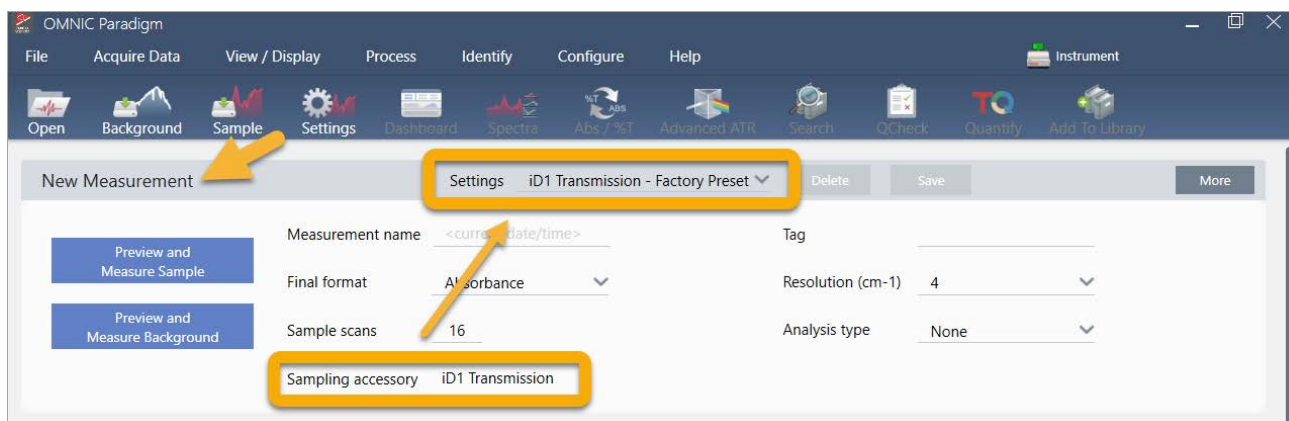
To begin, make sure your transmission accessory or sample holder is inserted in the spectrometer sample compartment. Here is the Thermo Scientific™ iD1 Transmission Accessory in our Nicolet™ Summit FTIR Spectrometer.



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.)

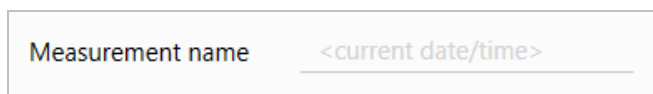
Set Up the Analysis

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.

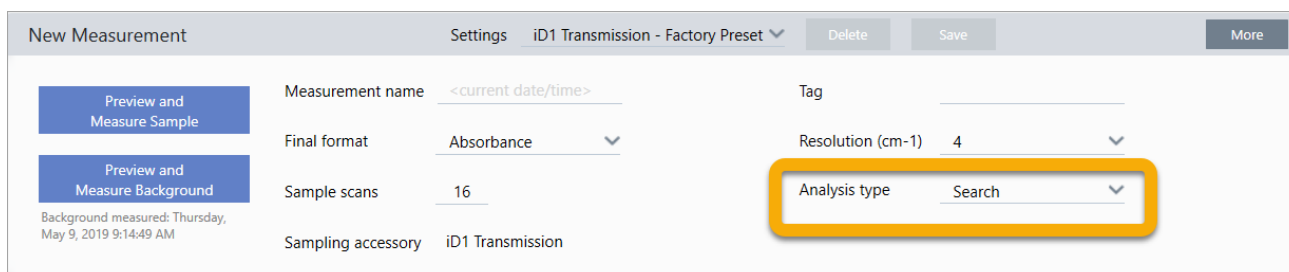


First, make sure the Sampling Accessory readout shows the installed accessory. If it doesn't, reseal the accessory. Notice that the factory presets for that accessory appear under "Settings."

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.

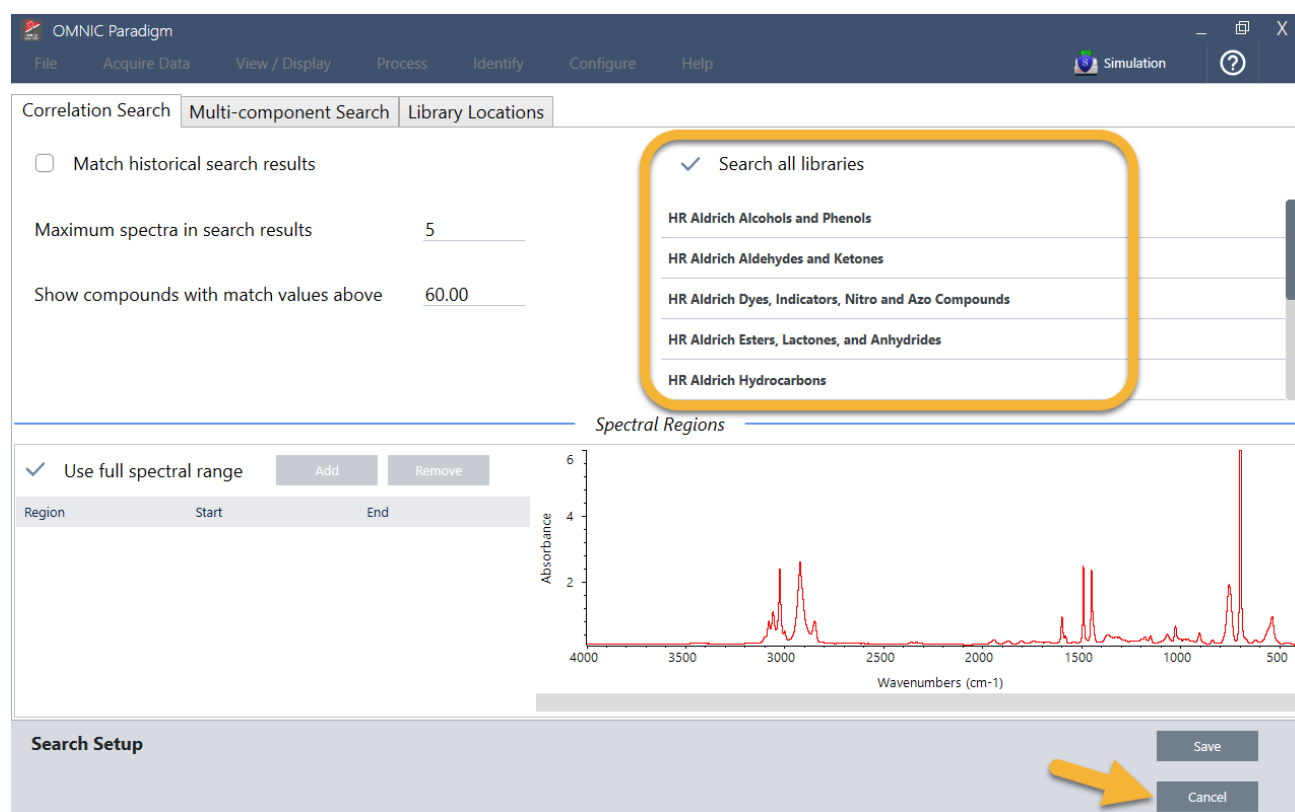
Tutorials and Walkthroughs

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.

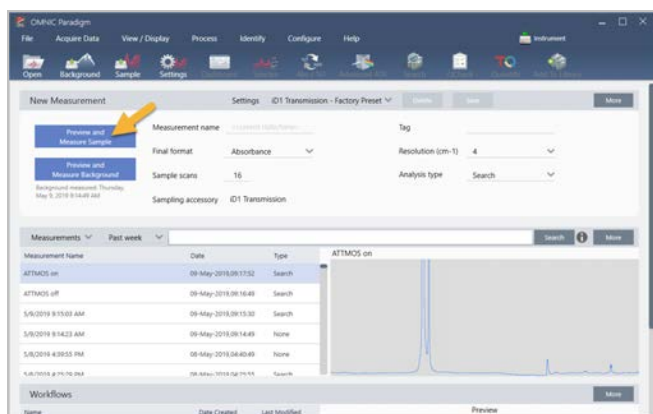
You can also use the Library Manager in the same menu to easily create a spectral library. Any libraries you create should be from pure materials that represent what you expect to find in your unknown samples.

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.

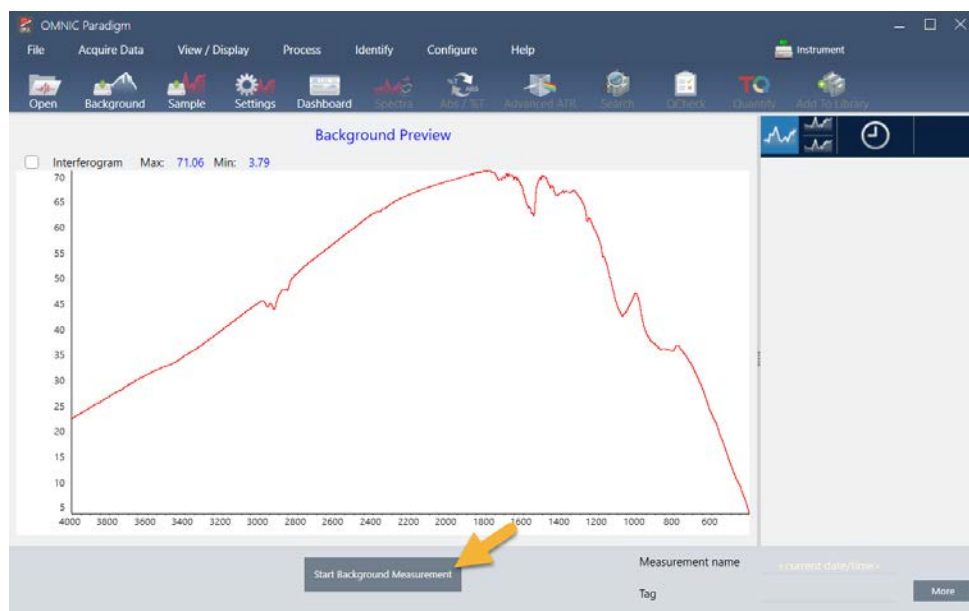
The software shows a preview of the current background spectrum in the spectral pane. The examples below show typical background spectra for transmission analysis using a transmission accessory that has not been purged with dry air or nitrogen, and one that has been purged.

Figure 3-1: Background spectrum from a transmission accessory that has not been purged

Tutorials and Walkthroughs



Figure 3-2: 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.



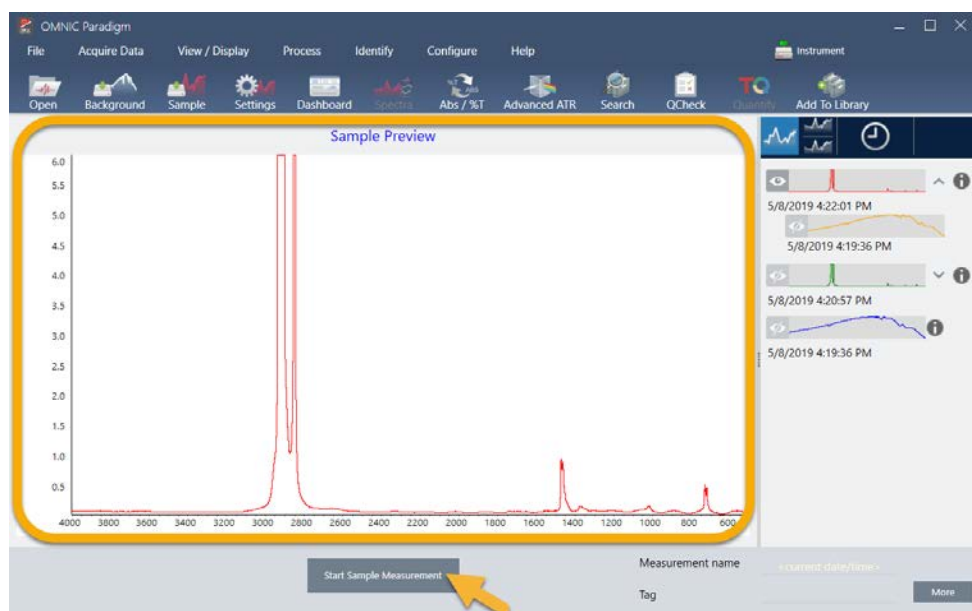
To install a mounted film sample, open the cover for the transmission accessory and slide your sample or sample holder into a slot that best fits the sample or sample holder width. If your sample or holder allows it, choose a slot that is close to the beam's focal point (for the iD1 accessory, this is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

Figure 3-3: iD1 Transmission Accessory beam focal point

Tutorials and Walkthroughs



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 3-4: Sample and top search result displayed together using the same Y-axis scale

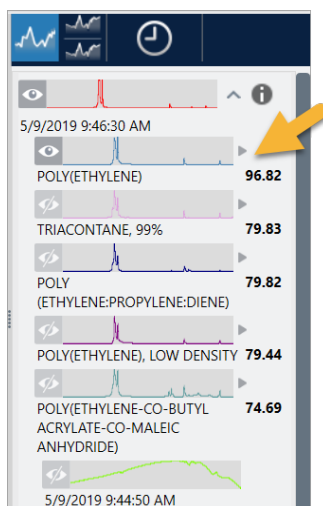


1. Sample spectrum (red)
2. Best match (blue)
3. Results panel

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.

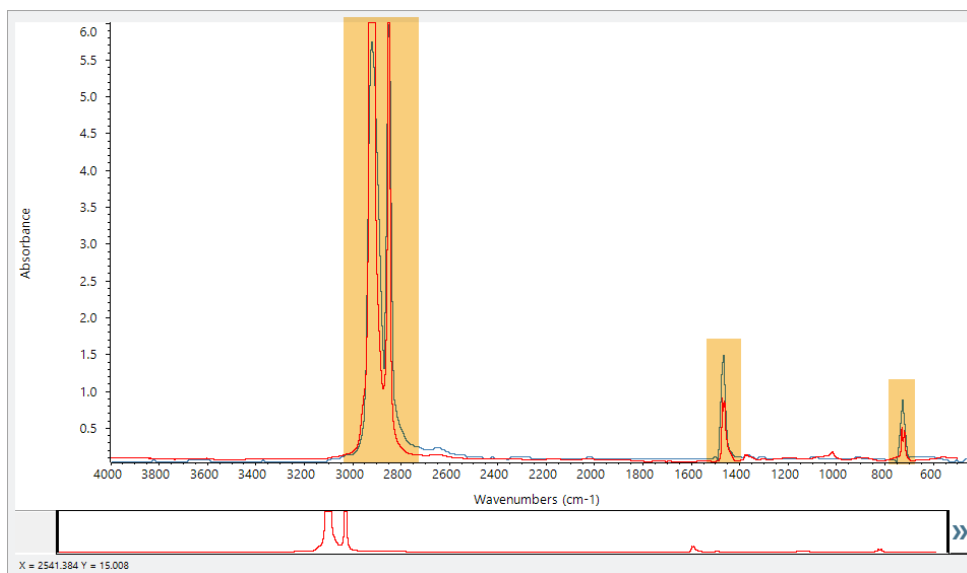
In this example, the top match has a match value that is above 85, which indicates a good match. The match value for the next spectrum in the list is well below that.

Figure 3-5: Match values showing a clear match



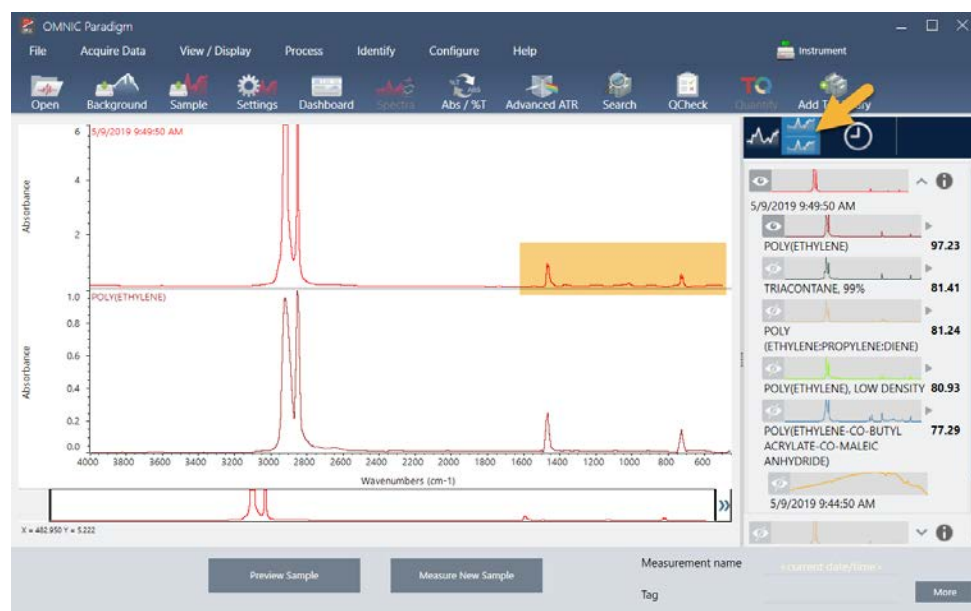
If we look at the overlaid spectra in the spectral pane, the positions of the main peaks line up along the X-axis, and they differ only in their peak heights.

Figure 3-6: Overlaid spectra showing a clear match



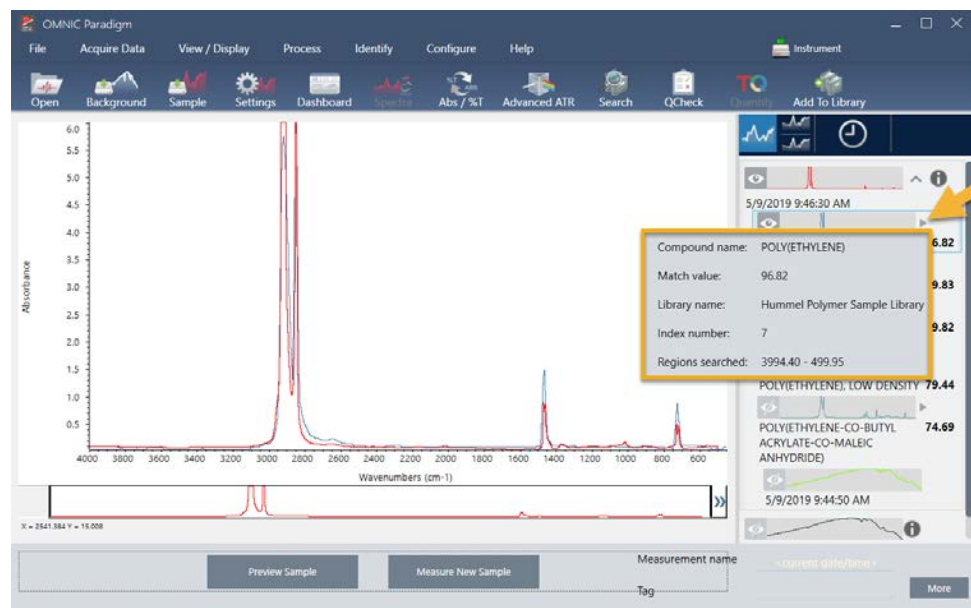
Click the Stack button to see the two spectra scaled to fill each Y-axis. Again, the spectra are well matched except for the slightly raised baseline in the sample spectrum's low frequency region. As a result, we can conclude that the sample is polyethylene and the analysis is complete.

Figure 3-7: 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, hover over the spectrum's grey arrow in the results panel.

Figure 3-8: 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 3-9: 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.)

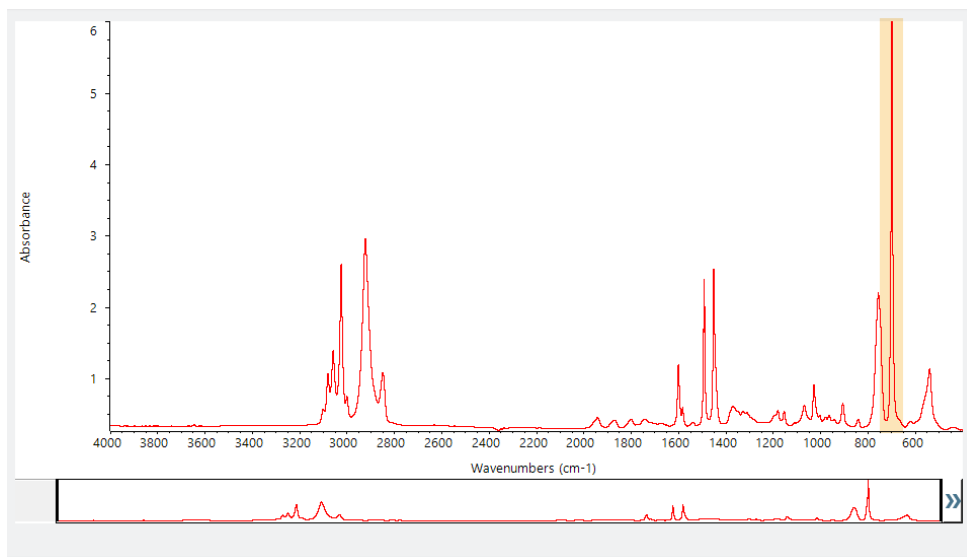
For starters, you can return to the dashboard and adjust the Resolution setting for the unknown sample. For example, you can acquire the spectrum at a higher resolution by using a lower Resolution setting. If the sample peaks are sharper or more numerous, you may get a better analysis result. You can 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 3-10: 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, 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 3-11: Tools for selecting the regions to search

Correlation Search | Multi-Component Search | Library Locations

☐ Match historical search results ☒ Search all libraries

Maximum spectra in search results: 5

Show compounds with match values above: 60.00

HR Aldrich Alcohols and Phenols

HR Aldrich Aldehydes and Ketones

HR Aldrich Dyes, Indicators, Nitro and Azo Compounds

HR Aldrich Esters, Lactones, and Anhydrides

HR Aldrich Hydrocarbons

Spectral Regions

☐ Use full spectral range Add Remove

Region	Start	End
1	2279.900	2119.900

Search Setup Save Cancel

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

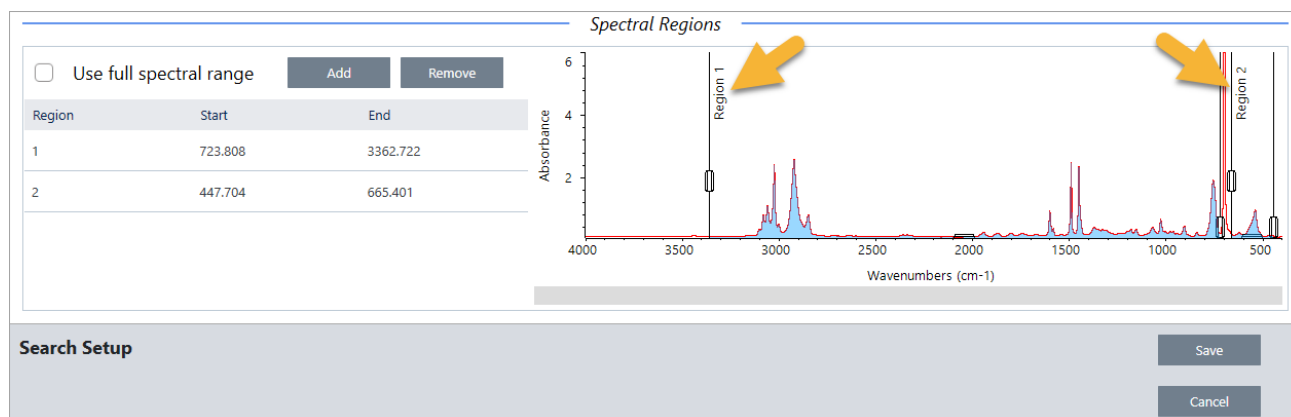
☐ Use full spectral range Add Remove

Region	Start	End
1	723.808	3362.722

Search Setup Save Cancel

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.

Tutorials and Walkthroughs



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.

Tutorials and Walkthroughs

File

Acquire Data

View / Display

Process

Identify

Configure

Help

Summit

☐ High sensitivity

☒ Pass/fail threshold

Maximum spectra in QCheck results

☒ Prompt for reference

Add

Remove

Measurement Name	Date	Type

☐ Blank diamond ATR region (2200 - 1955)
 ☐ Blank CO₂ region (2390 - 2240)

☒ Use full spectral range

Add

Remove

Region	Start	End

6

4

2

Absorbance

4000

3500

3000

2500

2000

1500

1000

500

Wavenumbers (cm-1)

Test Sample for Paradigm

X = 2669.691 Y = 0.554

QCheck Setup

Save

Cancel

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.

Setting	Description
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.
Blank CO2 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.

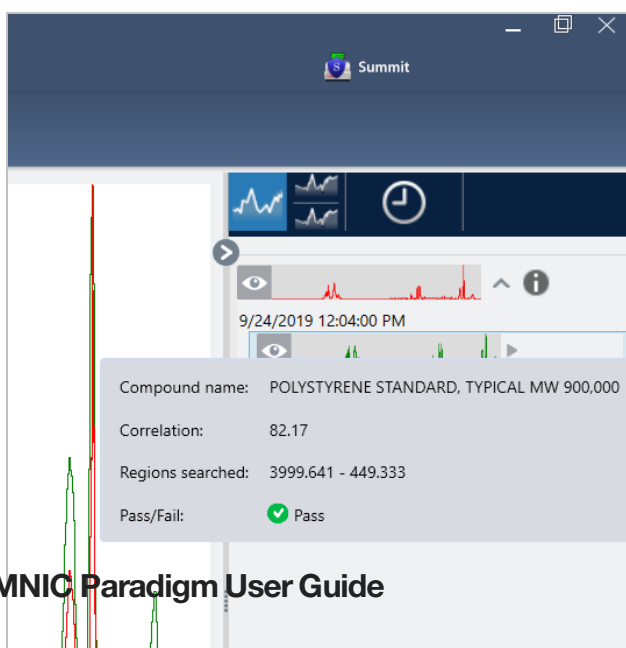
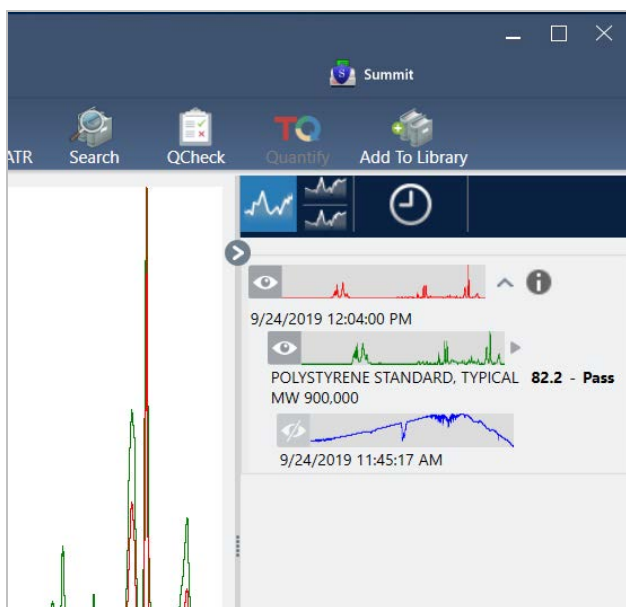
- d. Select one or more reference spectra to use in the analysis and click OK.

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 QCheck 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.

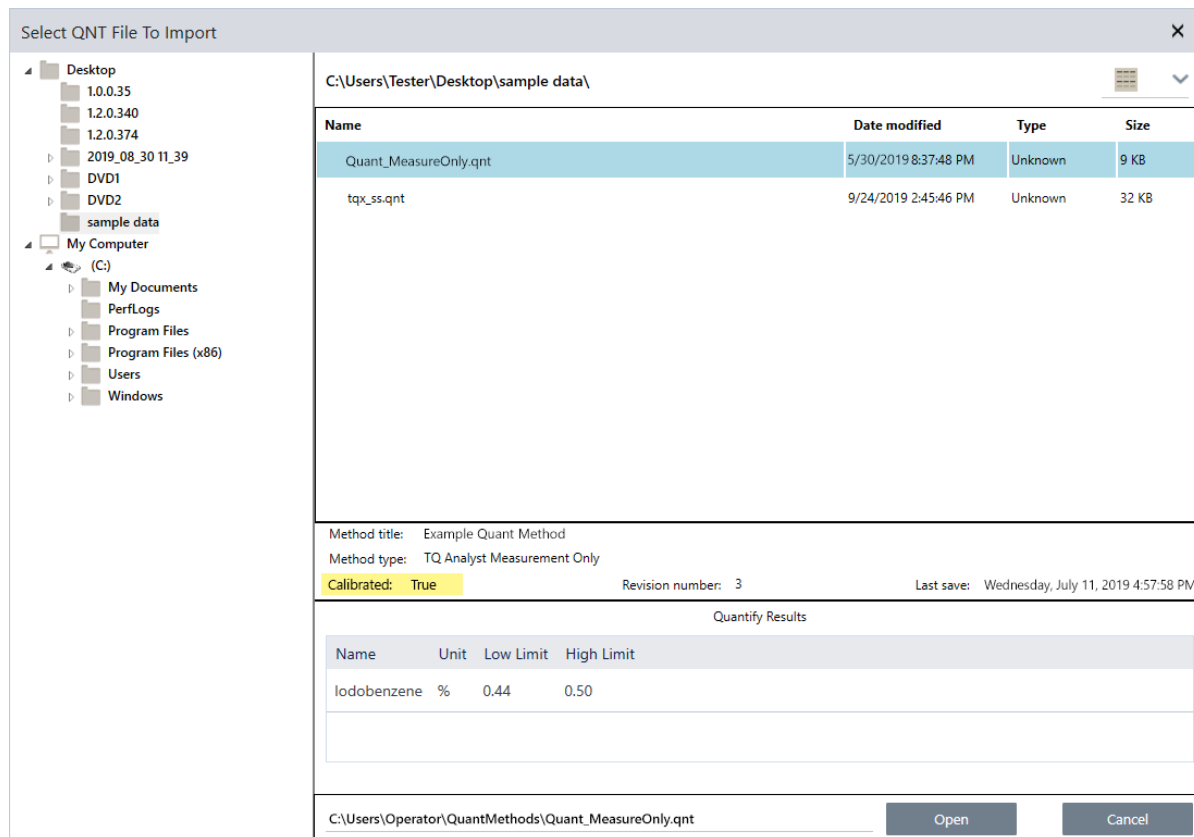
- c. To import the method, click Open.
- d. In the Analysis type list, select Quantify. A symbol indicates that you have imported a valid



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.

- Click Preview and Measure Background.
- Click Start Background Measurement. When the background measurement is complete, the spectrum is added to the results panel.

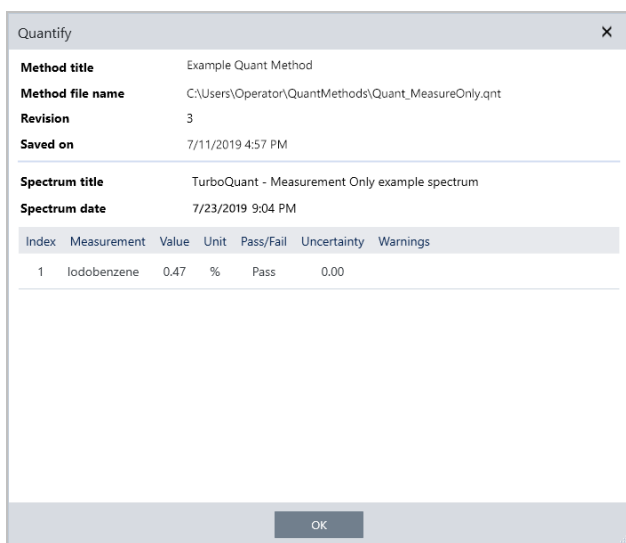
3. Measure the sample.

- 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.



The Quantify dialog box displays the following information:

Method title	Example Quant Method					
Method file name	C:\Users\Operator\QuantMethods\Quant_MeasureOnly.qnt					
Revision	3					
Saved on	7/11/2019 4:57 PM					
<hr/>						
Spectrum title	TurboQuant - Measurement Only example spectrum					
Spectrum date	7/23/2019 9:04 PM					
<hr/>						
Index	Measurement	Value	Unit	Pass/Fail	Uncertainty	Warnings
1	Iodobenzene	0.47	%	Pass	0.00	

At the bottom of the dialog box is an OK button.

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.

Create and Run Your First Workflow

This tutorial 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

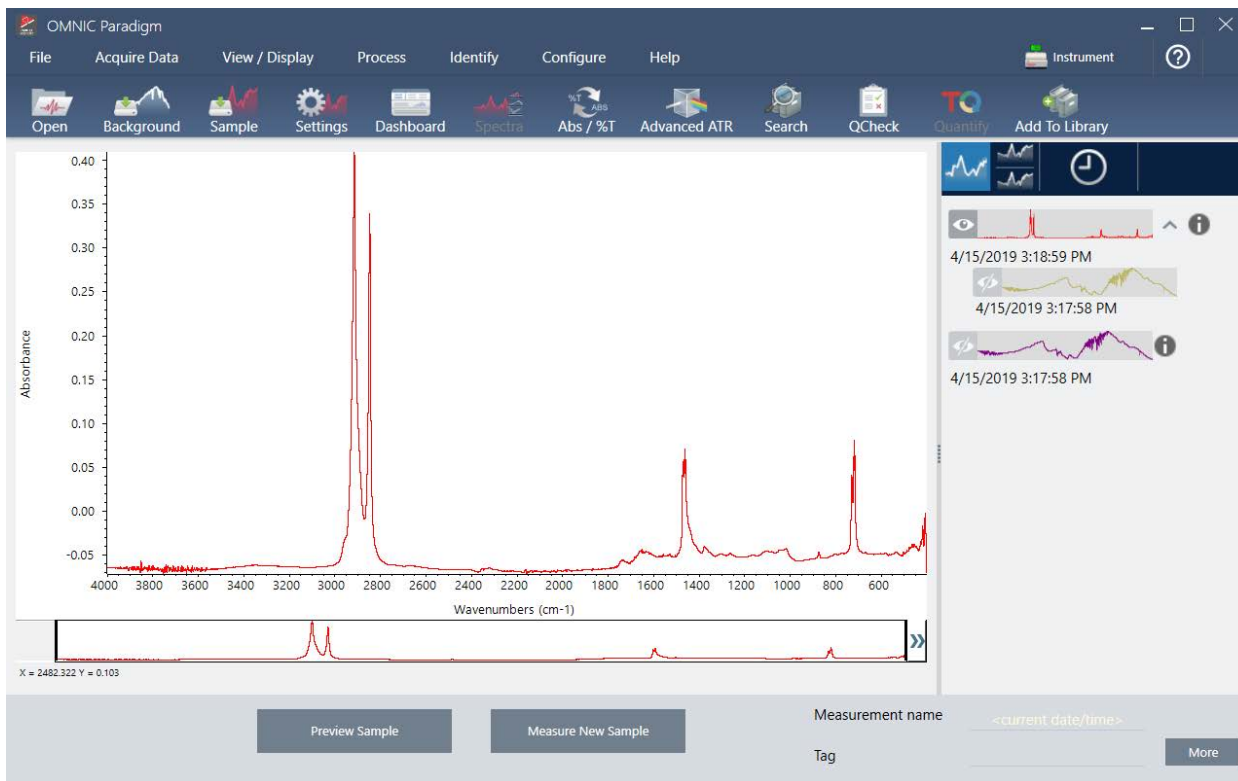
❖ To create a new workflow from an acquired spectrum

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.

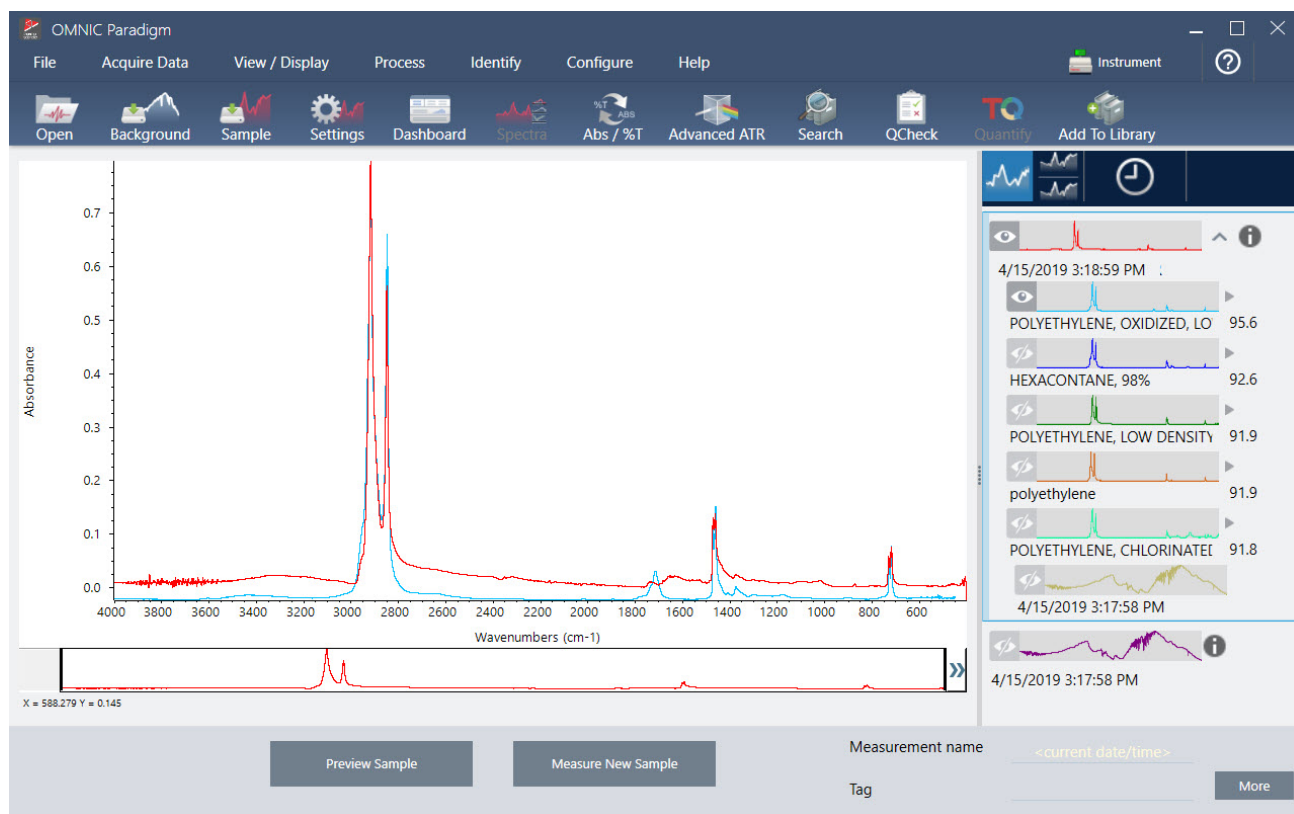
Tutorials and Walkthroughs

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

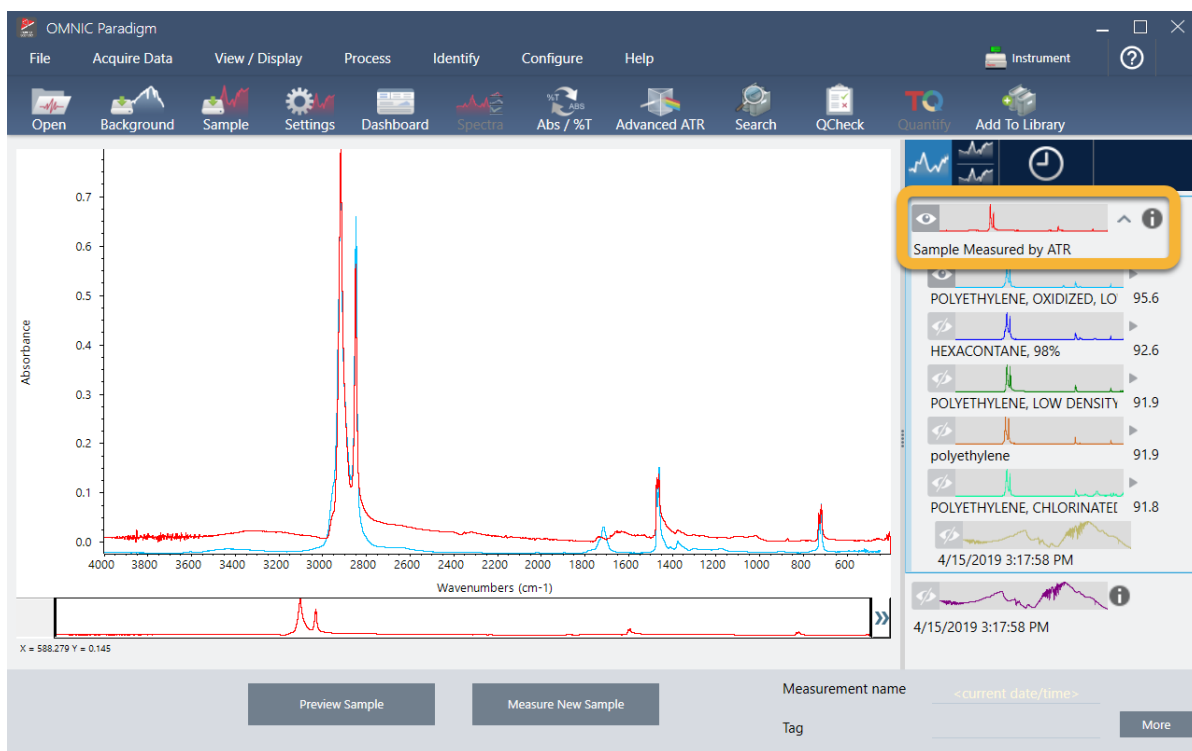


2. Make sure the spectrum is selected in the spectral pane and then perform any processing or analysis steps you like (for example, subtraction, baseline correction, correlation search, etc.).

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



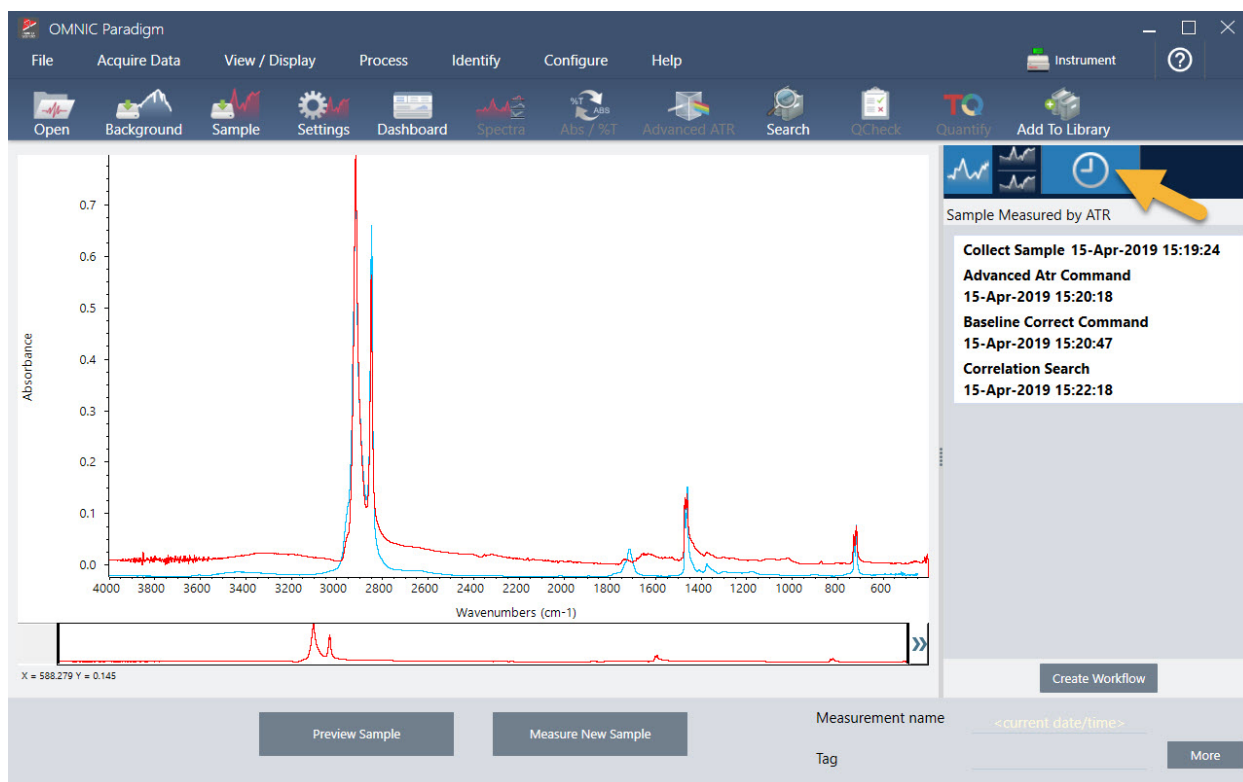
3. Give your spectrum a descriptive name (the software will use this name for the created workflow as the default, or you can give the workflow a new name).
 - a. Right click the image of the original spectrum in the results panel and choose Rename Spectrum.
 - b. Replace the default name with a descriptive name for your workflow and choose OK. Here is our renamed example spectrum.



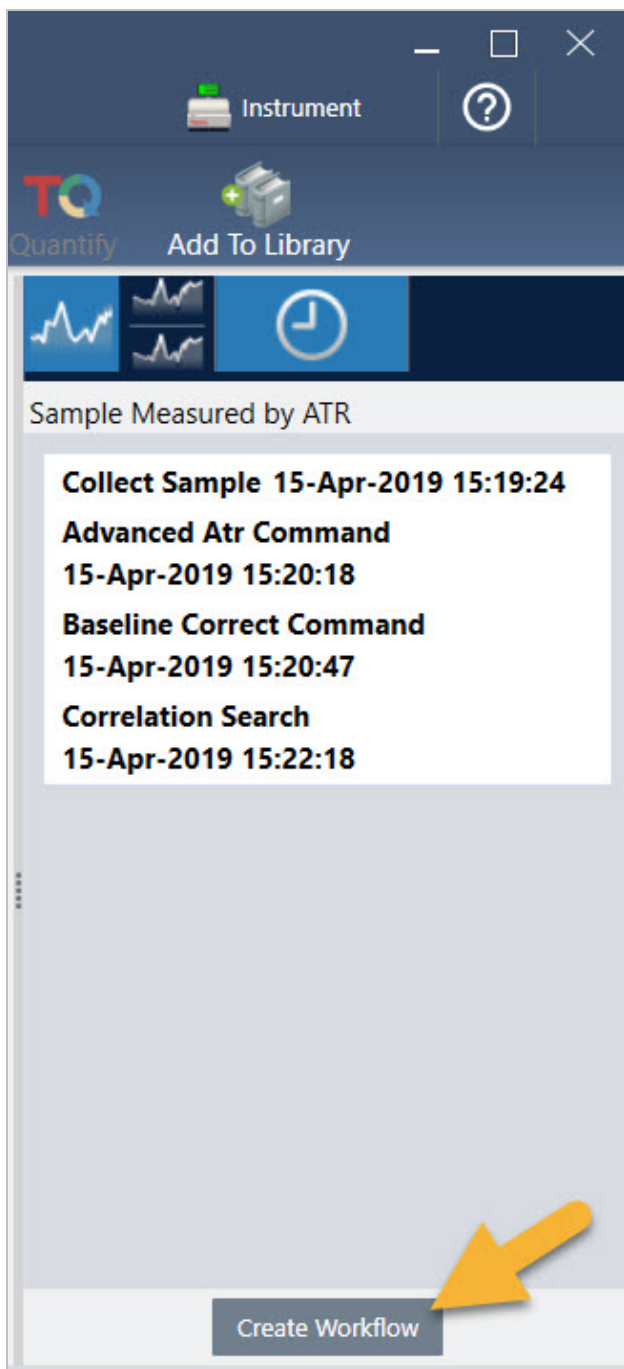
- Once you have completed your processing and analysis steps, click the History button in the results panel.

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.

Tutorials and Walkthroughs

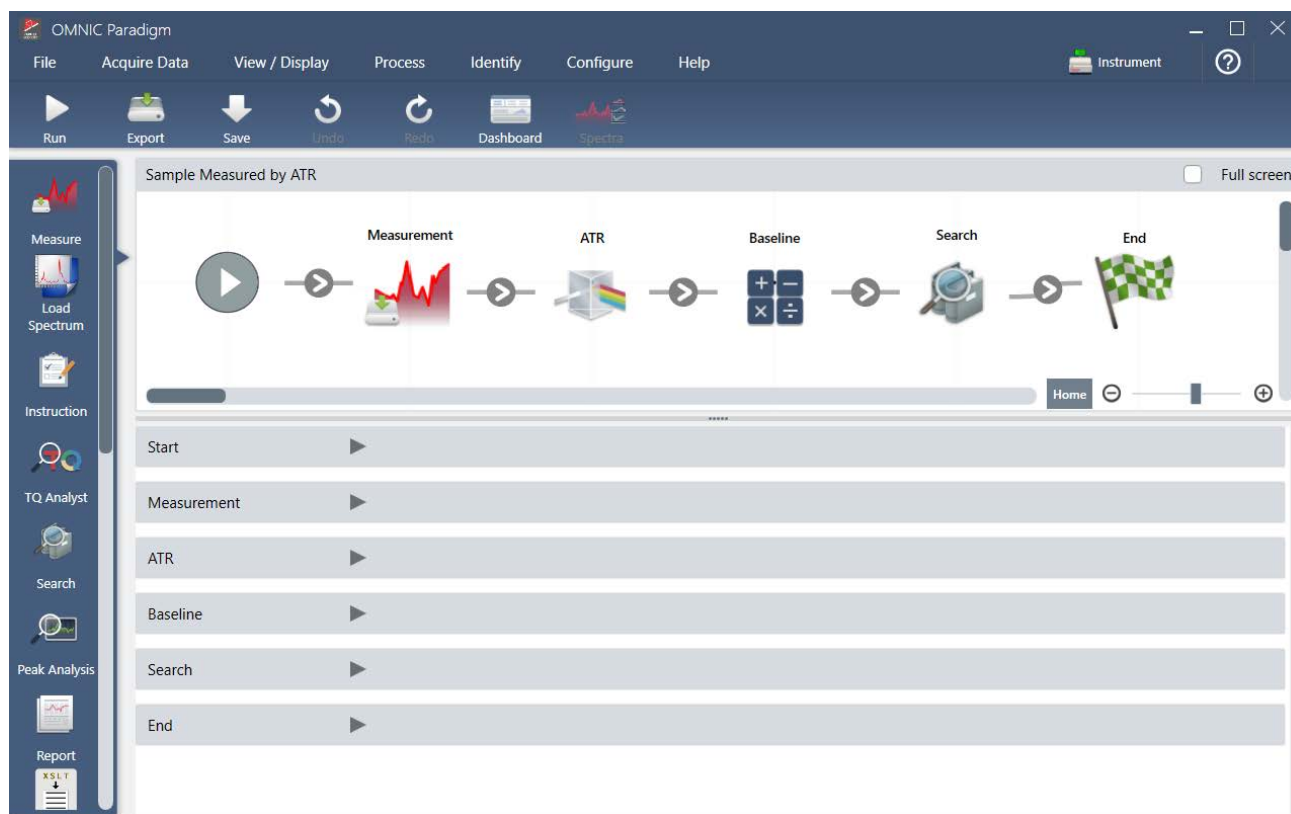


5. At the bottom of the history panel, click Create Workflow.

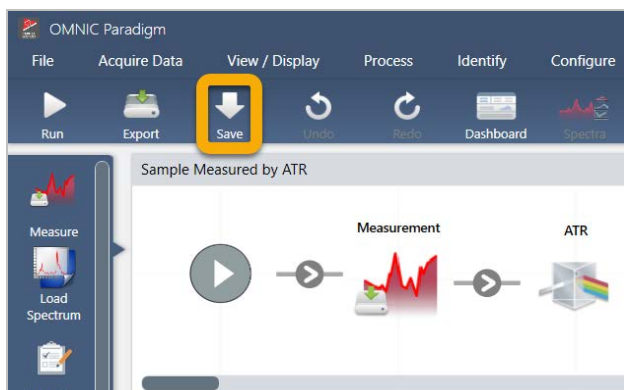


The software creates a workflow that includes all of the steps you just performed. The workflow is displayed in the workflow editor. Each performed task is represented by a colorful tile. Depending on which steps you performed, your workflow may look different from our example below:

Tutorials and Walkthroughs



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.

Tutorials and Walkthroughs

- 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.

The screenshot displays the OMNIC Paradigm software interface. The top menu bar includes File, Acquire Data, View / Display, Process, Identify, Configure, and Help. The toolbar below the menu contains icons for Open, Background, Sample, Settings, Dashboard, Spectra, Abs / %T, Advanced ATR, Search, QCheck, Quantify, and Add To Library. The main window is divided into two sections: Measurements and Workflows.

Measurements

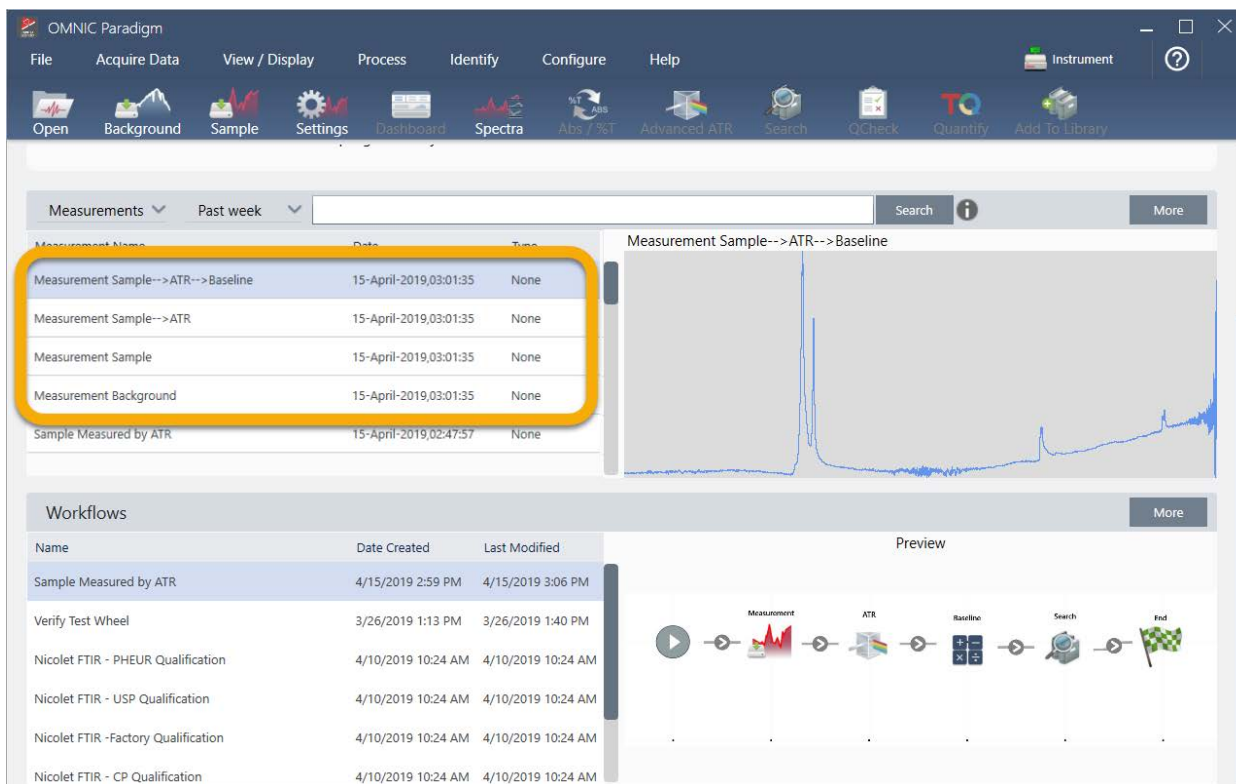
Measurement Name	Date	Type
Measurement Sample-->ATR-->Baseline	15-April-2019,03:01:35	None
Measurement Sample-->ATR	15-April-2019,03:01:35	None
Measurement Sample	15-April-2019,03:01:35	None
Measurement Background	15-April-2019,03:01:35	None
Sample Measured by ATR	15-April-2019,02:47:57	None

Workflows

Name	Date Created	Last Modified
Sample Measured by ATR	4/15/2019 2:59 PM	4/15/2019 3:06 PM
Verify Test Wheel	3/26/2019 1:13 PM	3/26/2019 1:40 PM
Nicolet FTIR - PHEUR Qualification	4/10/2019 10:24 AM	4/10/2019 10:24 AM
Nicolet FTIR - USP Qualification	4/10/2019 10:24 AM	4/10/2019 10:24 AM
Nicolet FTIR - Factory Qualification	4/10/2019 10:24 AM	4/10/2019 10:24 AM
Nicolet FTIR - CP Qualification	4/10/2019 10:24 AM	4/10/2019 10:24 AM

The **Sample Measured by ATR** workflow is highlighted with a yellow arrow. To the right of the Workflows list is a **Preview** box showing a sequence of steps: Measurement, ATR, Baseline, Search, and End. Above the preview box, a spectrum plot is displayed with the title "Measurement Sample-->ATR-->Baseline".

- 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.

Tutorials and Walkthroughs

The screenshot shows the OMNIC Paradigm software interface. The top menu bar includes File, Acquire Data, View / Display, Process, Identify, Configure, and Help. Below the menu is a toolbar with icons for Open, Background, Sample, Settings, Dashboard, Spectra, Abs / %T, Advanced ATR, Search, QCheck, Quantify, and Add To Library. The main area is divided into two sections. The top section, titled 'Measurements', shows a table of recent measurements. The bottom section, titled 'Workflows', shows a list of workflows with a context menu open over the 'Sample Measured by ATR' workflow, highlighting the 'Edit' option. An orange arrow points to the 'Edit' option in the context menu.

Measurement Name	Date	Type
Measurement Sample-->ATR-->Baseline	15-April-2019,03:01:35	None
Measurement Sample-->ATR	15-April-2019,03:01:35	None
Measurement Sample	15-April-2019,03:01:35	None
Measurement Background	15-April-2019,03:01:35	None
Sample Measured by ATR	15-April-2019,02:47:57	None

Workflows

Name	Date Created	Last Modified
Sample Measured by ATR	4/15/2019 3:06 PM	4/15/2019 3:06 PM
Verify Test Wheel	3/26/2019 1:40 PM	3/26/2019 1:40 PM
Nicolet FTIR - PHEUR Qualification	4/10/2019 10:24 AM	4/10/2019 10:24 AM
Nicolet FTIR - USP Qualification	4/10/2019 10:24 AM	4/10/2019 10:24 AM
Nicolet FTIR - Factory Qualification	4/10/2019 10:24 AM	4/10/2019 10:24 AM
Nicolet FTIR - CP Qualification	4/10/2019 10:24 AM	4/10/2019 10:24 AM

Preview

Measurement ATR Baseline Search End

The workflow opens in the workflow editor.

The screenshot shows the OMNIC Paradigm workflow editor. The top menu bar includes File, Acquire Data, View / Display, Process, Identify, Configure, and Help. Below the menu is a toolbar with icons for Run, Export, Save, Undo, Redo, Dashboard, and Spectra. The main area is divided into two sections. The top section, titled 'Sample Measured by ATR', shows a visual representation of the workflow steps: Start, Measurement, ATR, Baseline, Search, and End. The bottom section, titled 'Instruction', shows a list of instructions for each step: Start, Measurement, ATR, Baseline, Search, and End.

Sample Measured by ATR

Start Measurement ATR Baseline Search End

Instruction

Start Measurement ATR Baseline Search End

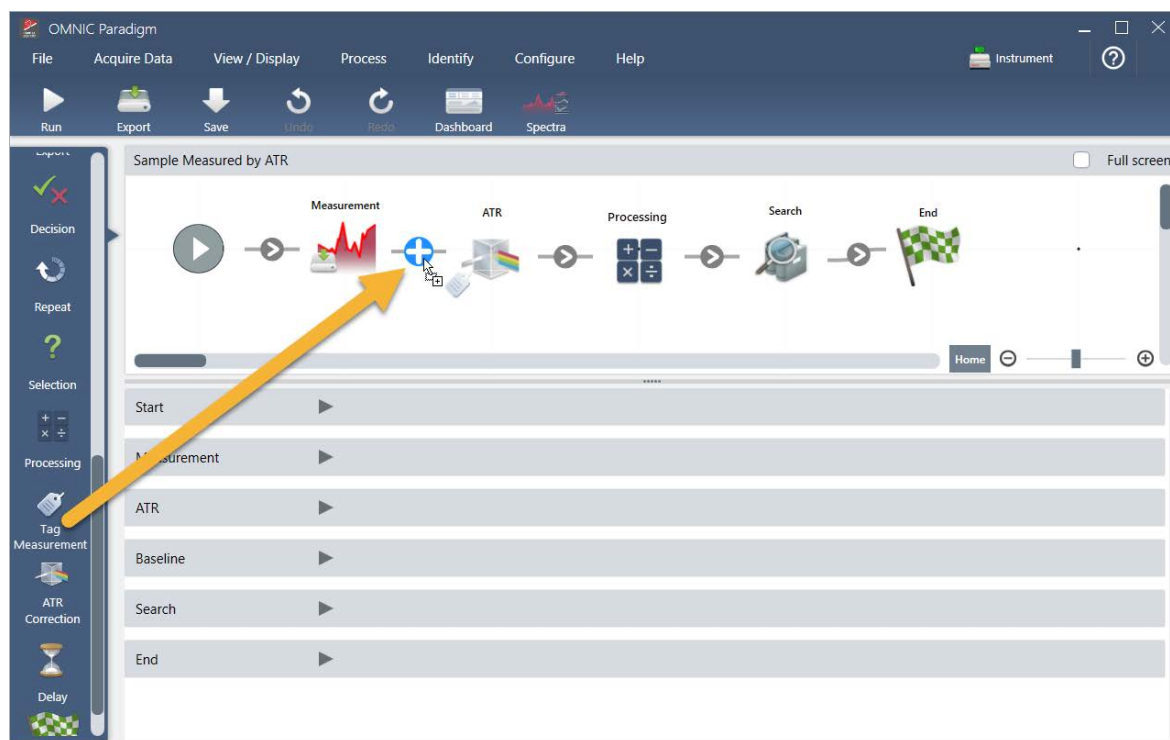
Tutorials and Walkthroughs

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.

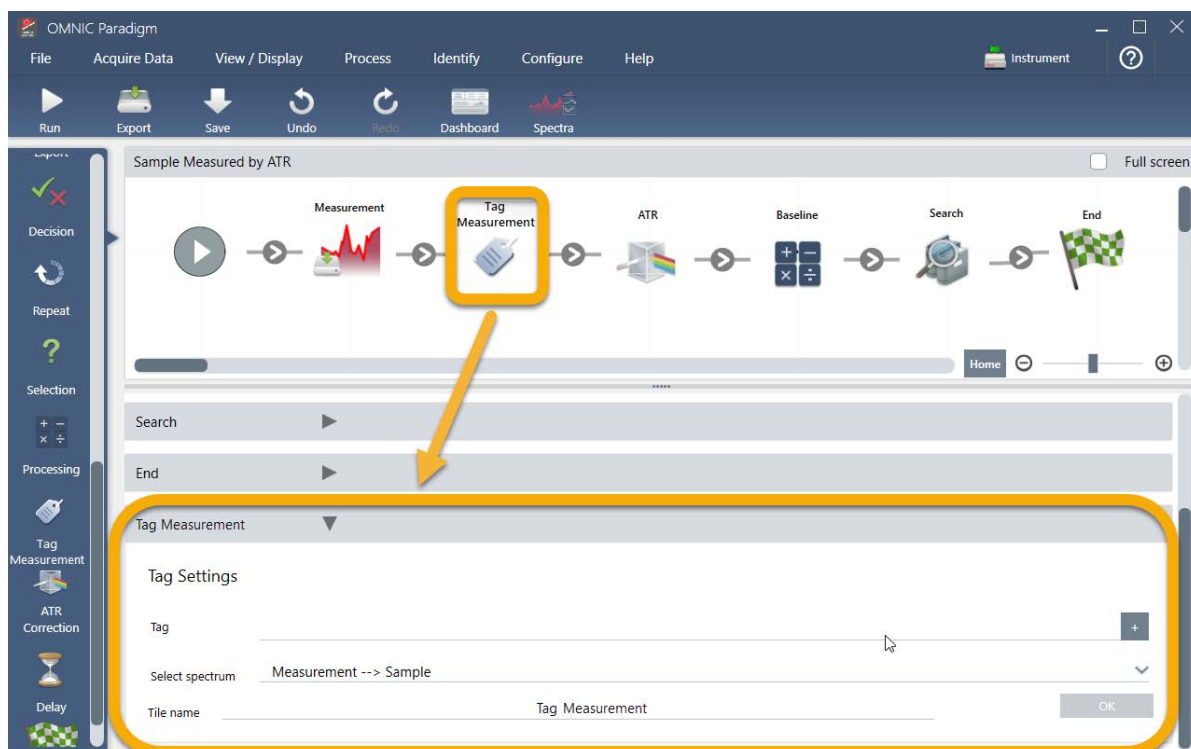
- a. In the workflow editor, drag the Tag Measurement tile from the selection bar to the canvas so that your mouse cursor hovers over the grey arrow ➡ between the Measurement and ATR Correction tiles.

The grey arrow changes to a plus sign.

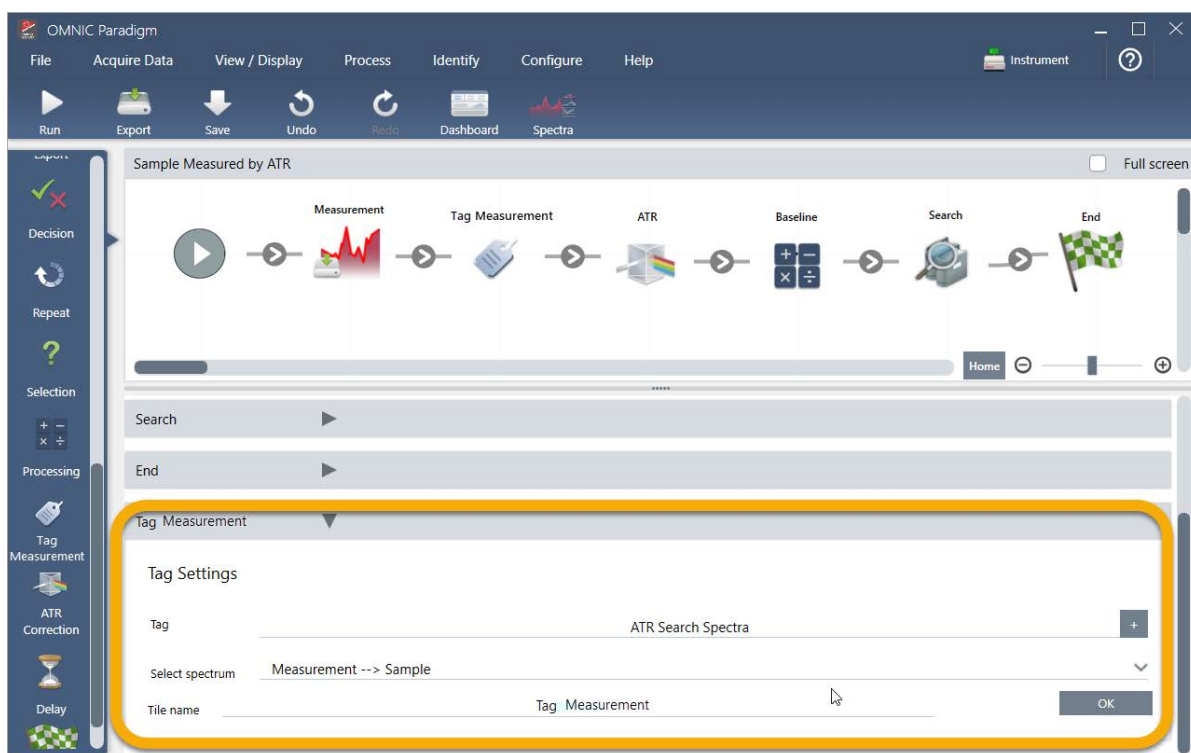


- b. Release the mouse button.

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.

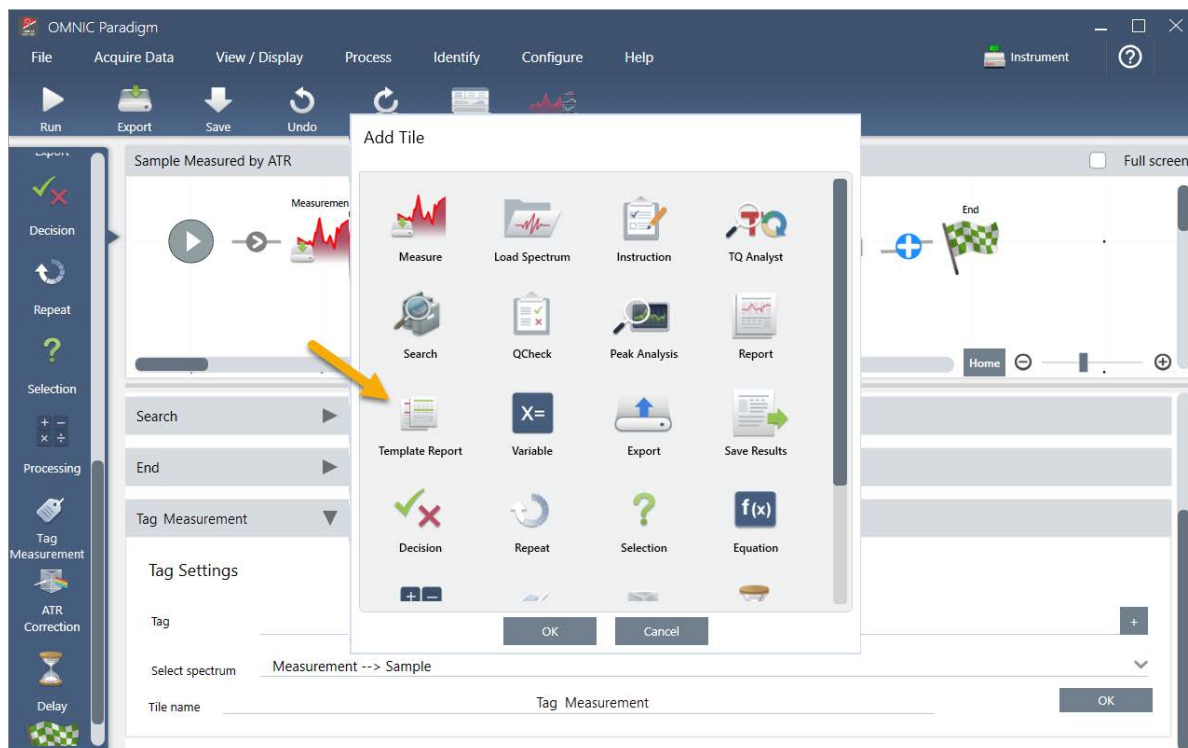


Tutorials and Walkthroughs

The Tag Measurement 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.

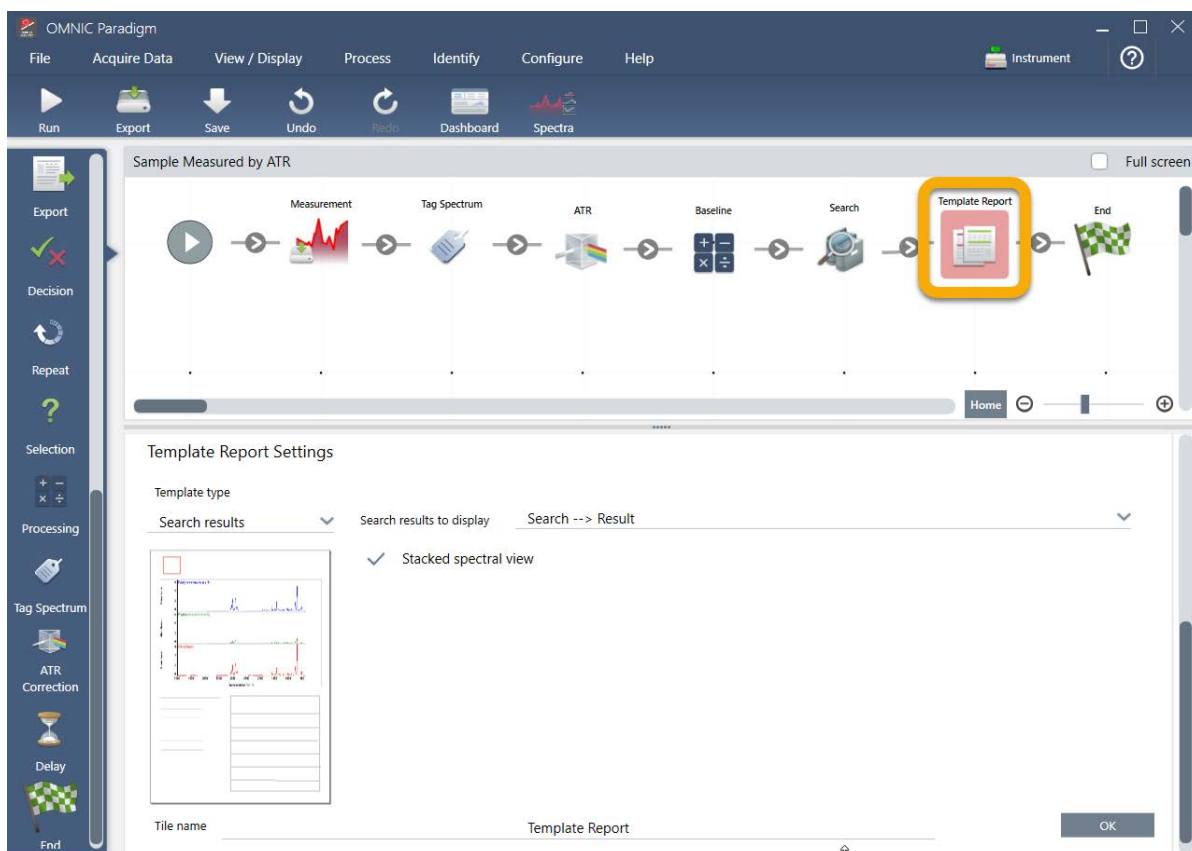
3. Add a Report Template tile to the workflow.
 - a. In the workflow editor, use the mouse to hover over the grey arrow between the Search and End tiles (arrow changes to a plus (+) sign) and then click the mouse button. The software opens the Add Tile box. (This is another easy way to add tiles.)



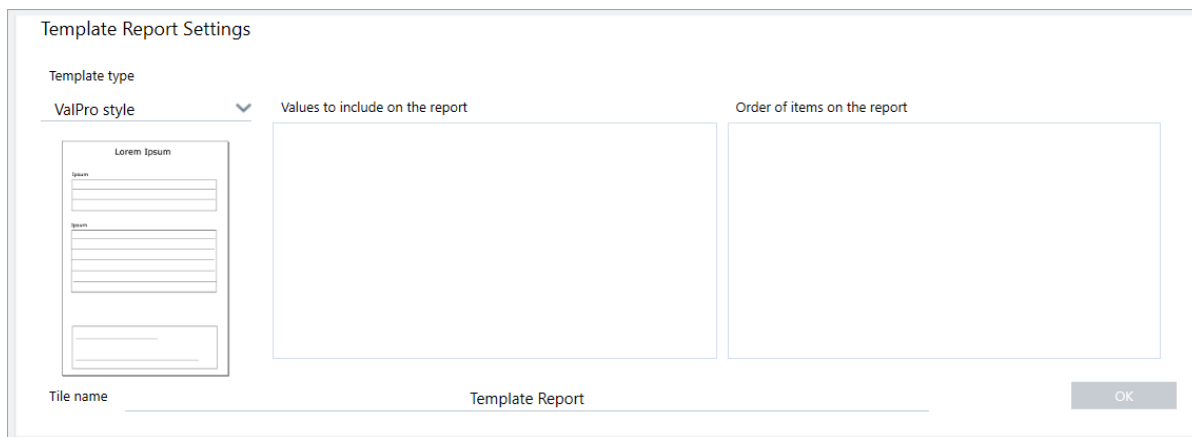
- b. In the Add Tile box, select the Template Report and choose OK.

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

Tutorials and Walkthroughs



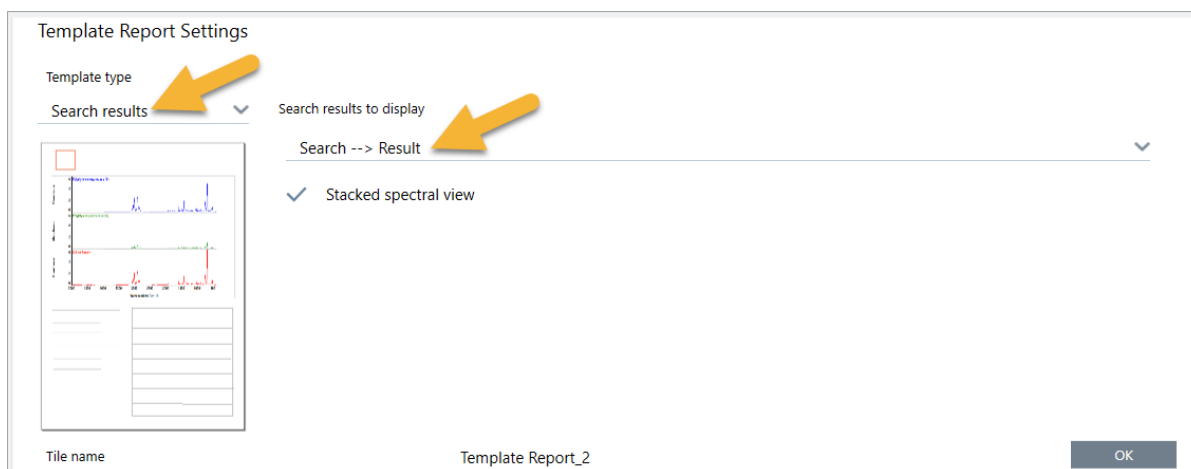
Notice that the Report Template tile has a red border, which indicates the workflow won't run successfully right now. If we view the Report Template settings, the boxes are all blank.



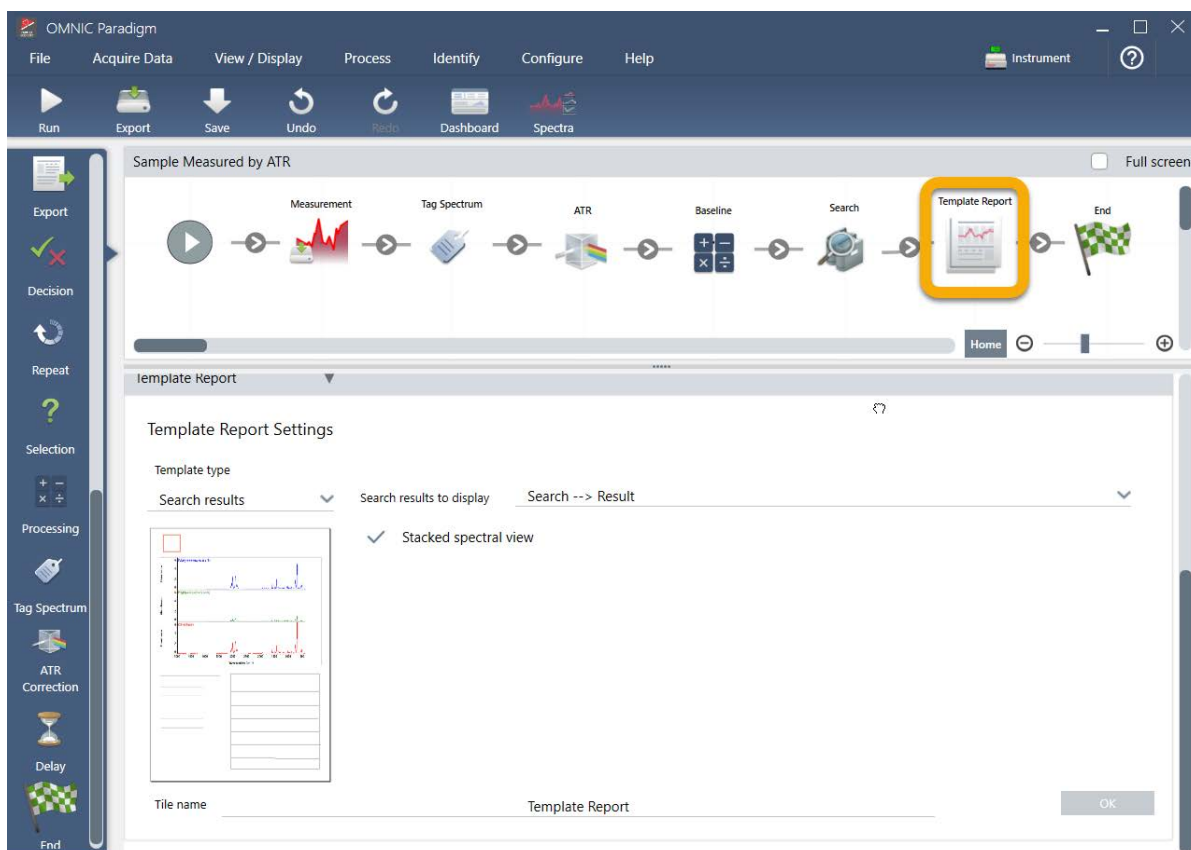
To fix the problem, we need to specify a template for the report and which results to include.

- 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.

Tutorials and Walkthroughs



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.

Tutorials and Walkthroughs

The screenshot shows the OMNIC Paradigm software interface. The top menu bar includes File, Acquire Data, View / Display, Process, Identify, Configure, and Help. Below the menu is a toolbar with icons for Open, Background, Sample, Settings, Dashboard, Spectra, Abs / %T, Advanced ATR, Search, QCheck, Quantify, and Add To Library. The main window displays the 'Measurements' tab with a table of measurement data. The 'Measurement Sample' column is highlighted, and a spectrum plot is shown on the right. The 'Workflows' tab is also visible, showing a list of workflows and a 'Preview' section with a flowchart of the measurement process.

Measurement Name	Date	Type
Original Sample Measurement	16-April-2019,03:52:26	None
Measurement Sample-->ATR	16-April-2019,03:44:15	None
Measurement Background	16-April-2019,03:44:15	None
Measurement Sample-->ATR-->Baseline	16-April-2019,03:44:15	None
Measurement Sample	16-April-2019,03:44:15	None

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

The screenshot shows the OMNIC Paradigm software interface. The top menu bar includes File, Acquire Data, View / Display, Process, Identify, Configure, and Help. Below the menu is a toolbar with icons for Open, Background, Sample, Settings, Dashboard, Spectra, Abs / %T, Advanced ATR, Search, QCheck, Quantify, and Add To Library. The main window displays the 'Measurements' tab with a table of measurement data. The 'Measurement Sample' column is highlighted, and a spectrum plot is shown on the right. The 'Workflows' tab is also visible, showing a list of workflows and a 'Preview' section with a flowchart of the measurement process.

Measurement Name	Date	Type
Measurement Sample-->ATR-->Baseline	15-April-2019,03:01:35	None
Measurement Sample-->ATR	15-April-2019,03:01:35	None
Measurement Sample	15-April-2019,03:01:35	None
Measurement Background	15-April-2019,03:01:35	None
Sample Measured by ATR	15-April-2019,02:47:57	None

Tutorials and Walkthroughs

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.”

The screenshot shows the OMNIC Paradigm software interface. The top menu bar includes File, Acquire Data, View / Display, Process, Identify, Configure, and Help. Below the menu is a toolbar with icons for Open, Background, Sample, Settings, Dashboard, Spectra, ATR, Advanced ATR, Search, QC check, Quantify, and Add To Library. The main window displays the Measurements list on the left and the Workflows section on the right. An orange arrow points to the 'More' button in the Measurements list. The Measurements list contains the following data:

Measurement Name	Date	Type
Original Sample Measurement	16-April-2019,03:52:26	None
Measurement Sample-->ATR	16-April-2019,03:44:15	None
Measurement Background	16-April-2019,03:44:15	None
Measurement Sample-->ATR-->Baseline	16-April-2019,03:44:15	None
Measurement Sample	16-April-2019,03:44:15	None

The Workflows section on the right shows a list of workflows and a preview of the workflow process. The workflow list includes:

Name	Date Created	Last Modified
Sample Measured by ATR	4/16/2019 3:42 PM	4/16/2019 3:50 PM
ATR Accessory - PHEUR Qualification	4/9/2019 12:11 PM	4/9/2019 12:11 PM
Nicolet FTIR - CP Qualification	4/9/2019 12:11 PM	4/9/2019 12:11 PM
Nicolet FTIR - USP Qualification	4/9/2019 12:11 PM	4/9/2019 12:11 PM
Nicolet FTIR - PHEUR Qualification	4/9/2019 12:11 PM	4/9/2019 12:11 PM

The preview section shows a sequence of steps: Measurement, Log Lockdown, ATR, Baseline, Search, QC check, Quantify, and End. The 'More' button is located at the bottom right of the Workflows section.

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.

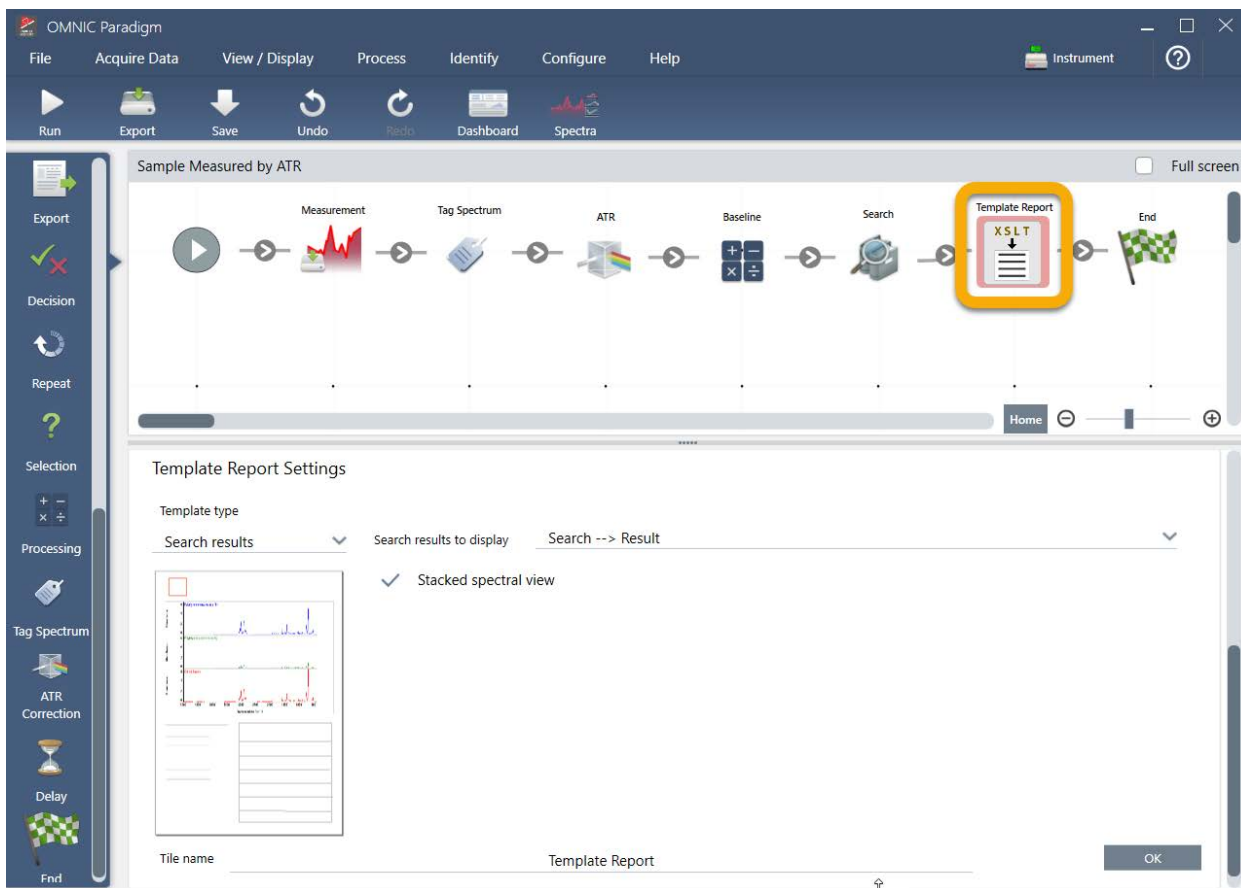
- Is the order in which the tiles appear in the workflow important? Yes, the order of the tiles is important. Each workflow tile builds on the previous tiles, and all the tiles are interconnected by their input requirements and their output results. For example, if you add a Measure tile, it creates an output result (a spectrum), which can only be accessed by tiles positioned after the Measure tile in the workflow. If you want to correct the baseline of an acquired spectrum, you would need to add a Processing tile after the Measure tile, and then set the Processing tile input to the Measurement output (i.e., the spectrum). Otherwise, the Processing 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 Export 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 Export 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 Processing tile *before* a Measure tile in a workflow, the Processing tile will have a red border and the workflow will contain an unresolvable error because there is no output spectrum to baseline correct.

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.

In this section:

Set and Save Measurement Options	110
Advanced Measurement Settings	115
Measure the Background	120
Measure a Sample	124

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 (.exp) before you measure your sample. To edit or review measurement settings, select an analysis type from the home screen.

Measure Samples

Figure 4-1: Review measurement settings in the Summary, Details, and Background tabs

Measure - Details

Single Beam

Sample Preview

Summary

Details

Background

Measurement name

<current date/time>

Tag

Final format

Absorbance

Number of scans

10

Resolution

4

Detector

DTGS KBr

Accessory

None

Measure Background

Measure Sample

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 4-2: Edit measurement settings in the New Measurement pane.

New Measurement

Settings

None - Factory Preset

Delete

Save

More

Preview and Measure Sample

Preview and Measure Background

Measurement name

<current date/time>

Analysis type

None

Sample scans

10

Sampling accessory

None

Tag

Final format

Absorbance

Resolution (cm-1)

4

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

Option	Description	Default Setting
Number of sample scans	<p>How many times the sample is scanned during the measurement. The resulting data reflects the average of all the scans.</p> <p>More scans will result in more accurate data but will take longer to measure.</p>	10
Resolution (cm-1)	<p>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.</p> <p>A smaller value results in a higher (better) resolution, but also takes longer to measure.</p> <p>Typically, resolutions of 4 are used for solid and liquid samples. For gas samples, use a resolution of 1 or 0.5.</p>	4
Analysis type	<p>With OMNIC Paradigm for touchscreen, you select your analysis type from the home screen rather than selecting from a list.</p> <p>Allows you to automatically process your data after it's collected.</p> <p>Use None to measure a sample without additional analysis.</p> <p>Search performs a correlation search. Use search to identify an unknown sample. Edit search settings in the Search Setup view.</p> <p>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.</p> <p>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.</p>	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 New near the Settings menu at the top of the dashboard.
3. Enter a 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. Click Save.

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 OK 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).

Measure Samples

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 4-1: The Details tab displays advanced measurement settings.

The screenshot shows the 'Measure - Details' screen with three tabs: Summary, Details (selected), and Background. The settings are organized into two columns. The left column includes 'Zero fill' (set to 2), 'Source' (set to IR), 'Range Limits' (MAX: 4000, MIN: 400, with a note 'Rec: 4000 — Rec: 400' and 'Enter value between 350 and 8500'), and 'Aperture' (set to Large). The right column includes 'Apodization' (set to Norton Beer Strong), 'Velocity (cm/sec)' (set to 0.4747), and two checkboxes: 'Atmospheric suppression' and 'Prompt for measurement name', both of which are unchecked. At the bottom, there are two buttons: 'Measure Background' and 'Measure Sample'.

Setting	Value
Zero fill	2
Source	IR
Range Limits	MAX: 4000, MIN: 400
Aperture	Large
Apodization	Norton Beer Strong
Velocity (cm/sec)	0.4747
Atmospheric suppression	<input type="checkbox"/>
Prompt for measurement name	<input type="checkbox"/>

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

Figure 4-2: 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	<p>The detector is a device inside the spectrometer that produces an electrical signal in response to the infrared beam striking it.</p> <p>The detector setting is updated automatically based on your spectrometer setup.</p> <p>Nicolet Summit: DTGS.</p> <p>Nicolet Summit Pro: TEC DTGS.</p>	
Optical velocity	<p>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.</p> <p>On the Nicolet Summit spectrometer, the default value is 0.4747 and cannot be changed.</p>	

Option	Description	Default Setting
Zero fill	<p>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.</p> <p>Collect your sample and background spectra using the same Zero Fill setting.</p> <p>Options</p> <p>None: No zero filling is done.</p> <p>1: One data point is added between each collected data point</p> <p>2: Three data points are added between each collected data point</p>	2
Source	<p>The component inside the spectrometer that emits the infrared radiation that travels to the detector.</p> <p>The source type is determined by your spectrometer setup. See your spectrometer user guide for details on the source.</p>	
Apodization	<p>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.</p> <p>Strong apodization reduces more noise but can also reduce the resolution of the data and broaden peaks.</p> <p>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.</p> <p>See "Apodization Functions" for a description of each type of apodization.</p>	Norton-Beer Strong
Automatic Atmospheric Suppression	<p>Suppresses the effects of water vapor and carbon dioxide on the spectra you have collected.</p> <p>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.</p> <p>Use this feature only if you measure the background infrequently or when atmospheric conditions change rapidly.</p>	Deselected

Option	Description	Default Setting
Range Limits	Sets the limits for the range of frequencies, in wavenumber, included in the collected spectrum.	Max: 4,000 Min: 400
Aperture	<p>Controls the intensity of the infrared radiation that reaches the sample.</p> <p>Aperture can only be changed when using spectrometers with adjustable apertures.</p> <p>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.</p> <p>You may need to use small apertures to acquire true high-resolution spectra.</p>	

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.

Setting	Description
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	<p>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.</p> <p>Use this setting only when the best possible resolution is required. This setting is generally not recommended and is normally used only to reproduce the results of other experiments that used it.</p>
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	<p>Norton-Beer Strong is the recommended apodization for the Nicolet Summit and Summit Pro spectrometers.</p> <p>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.</p>
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.

Measure Samples

Figure 4-1: In the touchscreen interface, select a background setting in the Background tab.

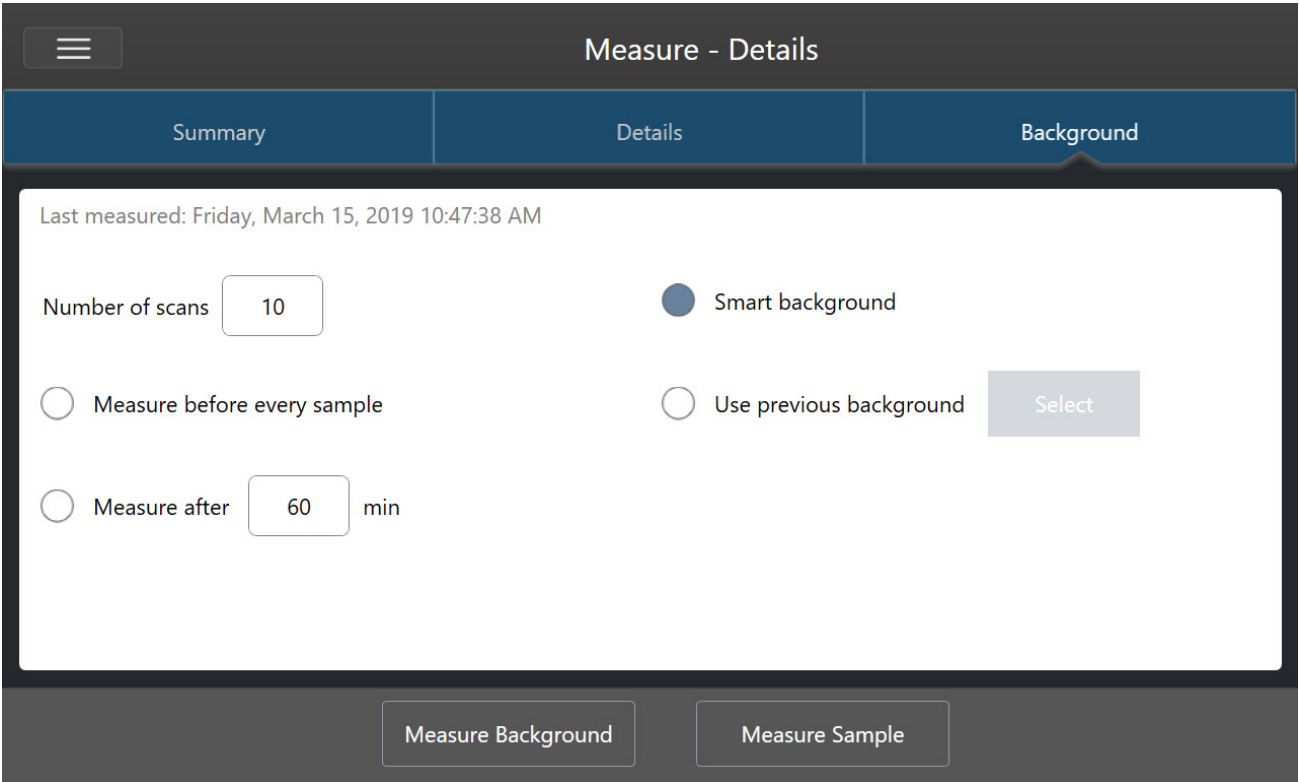
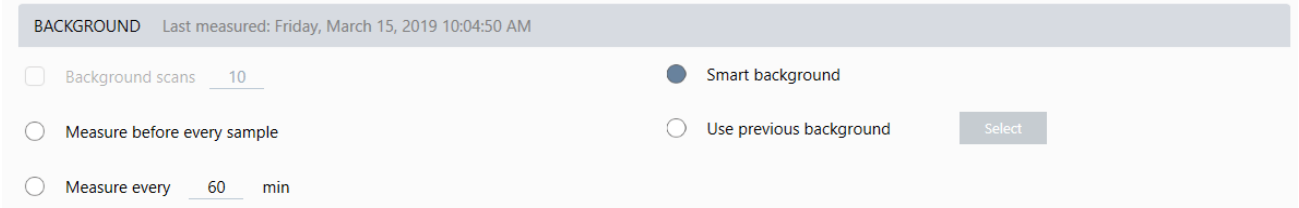


Figure 4-2: In the desktop interface, select a background setting in the Background pane.



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.

Setting	Description
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.
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 only 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.

Measure Samples

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 4-1: The Summary tab displays common measurement settings.

The screenshot displays the 'Measure - Details' interface. At the top, there is a dark header bar with a menu icon on the left, the title 'Measure - Details' in the center, and two buttons, 'Single Beam' and 'Sample Preview', on the right. Below the header is a tabbed interface with three tabs: 'Summary' (which is selected and highlighted with a blue underline), 'Details', and 'Background'. The 'Summary' tab contains a white card with the following settings:

Measurement name <current date/time>	Tag	Final format Absorbance
Number of scans 10	Resolution 4	Detector DTGS KBr
Accessory None		

At the bottom of the screen, there is a dark bar containing two buttons: 'Measure Background' and 'Measure Sample'.

3. Review and edit your measurement settings.

Measure Samples

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 4-2: The Settings list displays your previously saved settings

New Measurement		Settings	None - Factory Preset	Delete	Save	More
<div>Preview and Measure Sample</div> <div>Preview and Measure Background</div>	Measurement name	<current date/time>		Tag		
	Analysis type	None		Final format	Absorbance	
	Sample scans	10		Resolution (cm-1)	4	
	Sampling accessory	None				

See ["Set and Save Measurement Options"](#) for a description of each setting.

Measure Samples

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.

In this section:

Apply Basic Equations to Acquired Data	128
Advanced Spectral Math	135
Reprocess Spectra	139
Blank a region in your spectra	141
Calculate average and standard deviation spectra	143

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

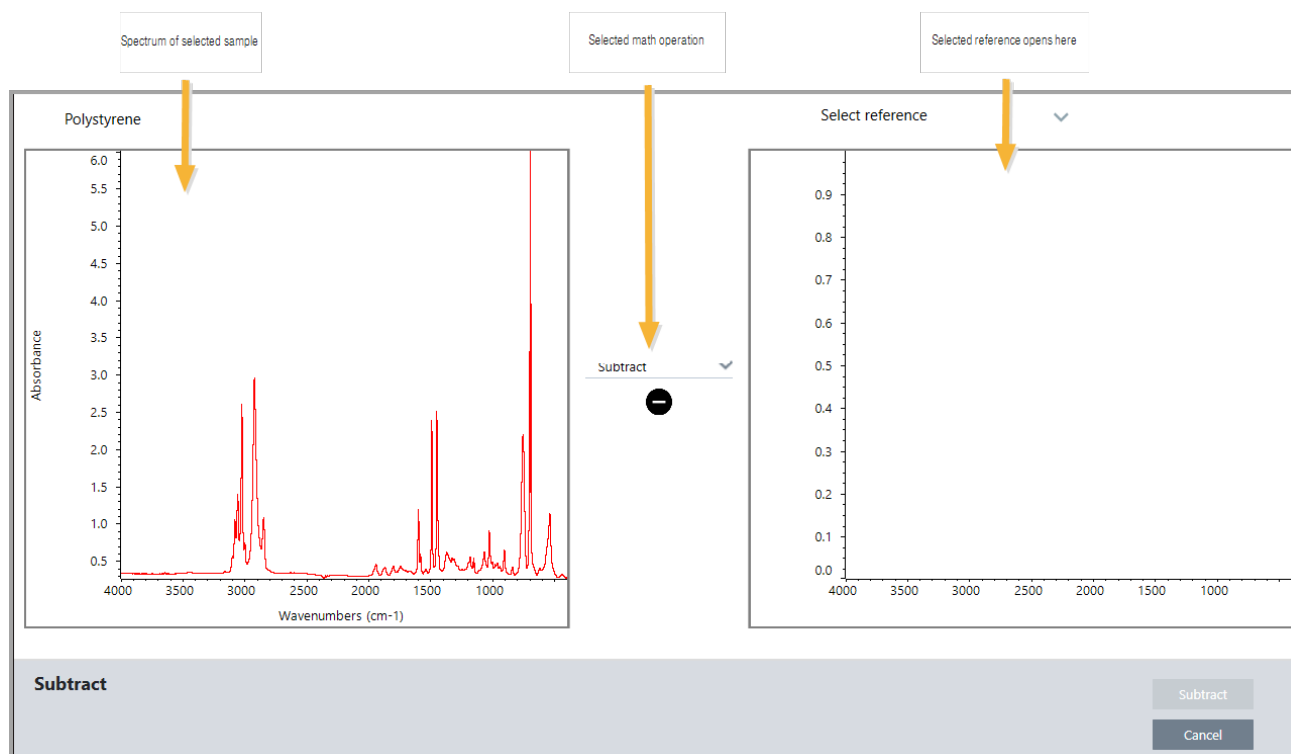
To perform spectral math, the sample and reference spectra must have the same spectral resolution and be in the same Y-axis unit. If they are not, the software automatically converts the selected reference spectrum to match the selected sample spectrum. In order to subtract, multiply or divide spectra, 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.

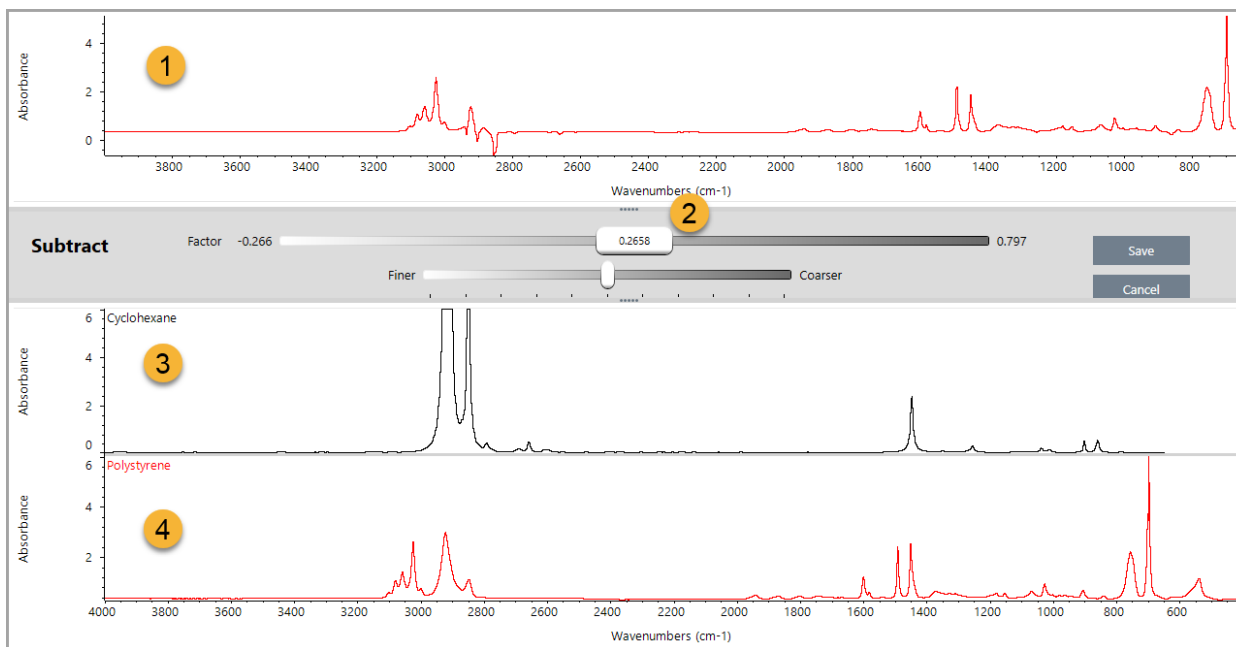
The software opens the Spectral Math setup window with the sample spectrum in the left pane and space for a reference spectrum in the right pane.

Figure 5-1: Spectral Math Setup Window



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:



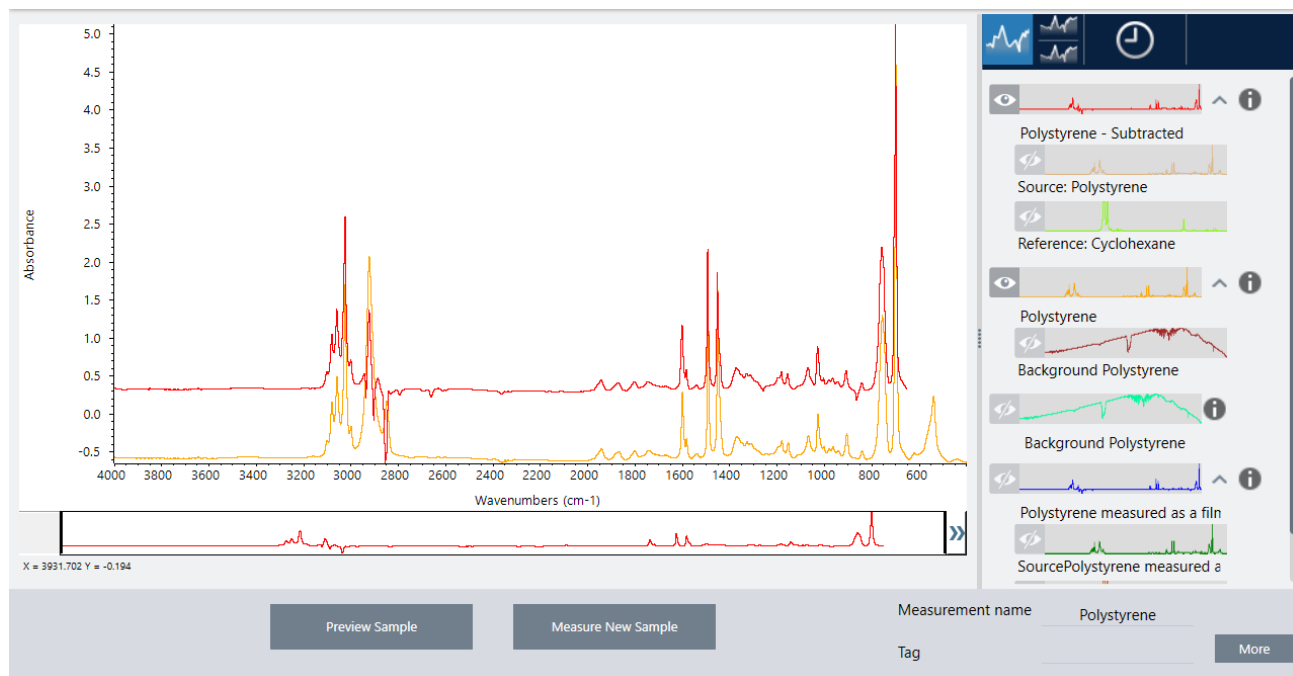
1. Current subtraction result
2. Factor
3. Sample
4. Reference
6. Adjust or enter a factor as needed to increase or decrease the intensity of the reference in the result spectrum.

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.



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)

B₁ = original background

B₂ = 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)

B₁ = original background

B₂ = 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

Advanced Spectral Math

Advanced Spectral Math provides more flexibility and power than standard spectral math. While standard spectral math supports spectral subtraction, addition, multiplication, and division using a single reference spectrum, Advanced Spectral Math allows you to build custom equations using up to 10 reference spectra and using a wider range of operations.

For many applications, using the standard subtract, add, multiply, and divide functions in spectral math is simple and sufficient. However, if your analysis requires a more complex equation, Advanced Spectral Math may be required.

Both forms of spectral math are available only in the Desktop interface of OMNIC Paradigm software.

When choosing between the two methods, consider the following differences to decide which tool is right for you:

- Standard Spectral Math
 - Supports only subtraction, addition, multiplication, and division using a single reference spectrum with a slider to adjust the factor
- Advanced Spectral Math
 - Flexible equation builder using basic subtraction, addition, multiple, and division as well as derivatives, exponents, and more
 - Can include up to ten different reference spectra in the equation

Carrying Out Advanced Spectral Math

When you use Advanced Spectral Math, you will typically add spectra that you will use in the equation, build your equation, preview the results, and finally review the result in the Spectral View.

❖ To perform advanced spectral math

1. In the Spectral View, select a measurement to use in Advanced Spectral Math.
2. Open the Process menu and select Advanced Spectral Math. The equation builder opens.

Figure 5-1: The Advanced Spectral Math view



3. Add reference spectra to use in the equation.

You can add up to 10 spectra, and you do not need to use every spectrum that you open. You may find that it is easier to add the spectra first so that they are available while you focus on the equation, or you may prefer to add them only as needed.

a. Select reference or library spectra. When you add a spectrum, a new tab opens automatically.

- If you use a spectrum from a commercial (locked) library in the equation, you cannot export the result.

4. Build the equation.

a. Click an operator to add it to the equation.

b. Once the operator is added, you can click any of the open ? spaces to insert a spectrum or another operator.

- To add a spectrum, with the open space selected, choose a spectrum and click Insert into Equation.
- To add an operator, click the operator. If you have an open ? space selected, the operator is inserted into that location. If you do not have any spaces selected, the new operator is wrapped around the the current equation.
- You can also save your equation or load a previous equation.

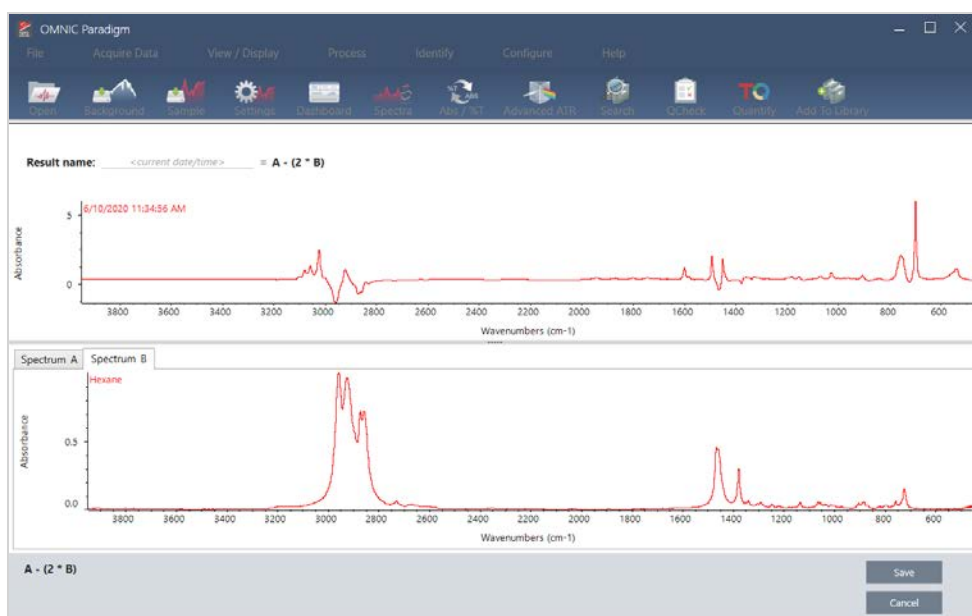
Process Data

- To save the equation, simply click Save. The equation is added to the list of available equations.
- To load a previous equation, you must first open the correct number of spectra used in the equation. For example, if the equation used 3 spectra (A, B, and C), open at least 3 spectra. Your open spectra will automatically be inserted into the equation in their corresponding position, but you can edit the equation as needed or replace the spectra.

c. When you are satisfied with the equation, click Calculate to preview the result.

5. Preview the result.

Figure 5-2: The shows the result on top and your reference spectra below

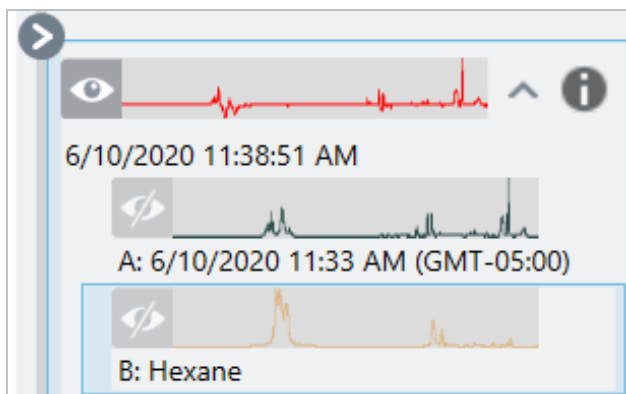


The result preview displays the spectrum resulting from your equation as well as each of the spectra used in the equation. The result is shown in the top pane and your reference spectra are shown in the bottom pane.

- To edit the equation, click Cancel to return to the previous screen.
- To save the results of the equation, enter a name for the resulting spectrum or leave the default and click Save.

6. View the result in the Spectral View.

The resulting spectrum is listed in the Results pane. Spectra used in the equation are shown in the sub-panes below the result spectrum with a label indicating their use in the equation.



Functions Available in Advanced Spectral Math

Function	Description
k	Constant
? + ?	Addition
? - ?	Subtraction
? * ?	Multiplication
? / ?	Division
log(?)	Logarithm. Returns the base 10 log
exp(?)	Returns the result of the constant e (2.7182818) raised to the power of the specified value
sqrt(?)	Square root of the value
deriv(?)	Derivative
savderiv (?)	Savitsky-Golay Derivative
norderiv (?)	Norris Derivative

Reprocess Spectra

You can transform the original interferogram data for your spectrum with new settings by using Reprocess.

When comparing your spectrum to a reference, you can get a more accurate comparison if both spectra were processed using the same settings. For example, if your spectrum was collected using a broader range than the reference or if it used a different apodization technique, your comparison may be inaccurate. Reprocessing allows you to transform the original data to match your reference spectrum, resulting in better results for your correlation, QCheck, or quantification analyses.

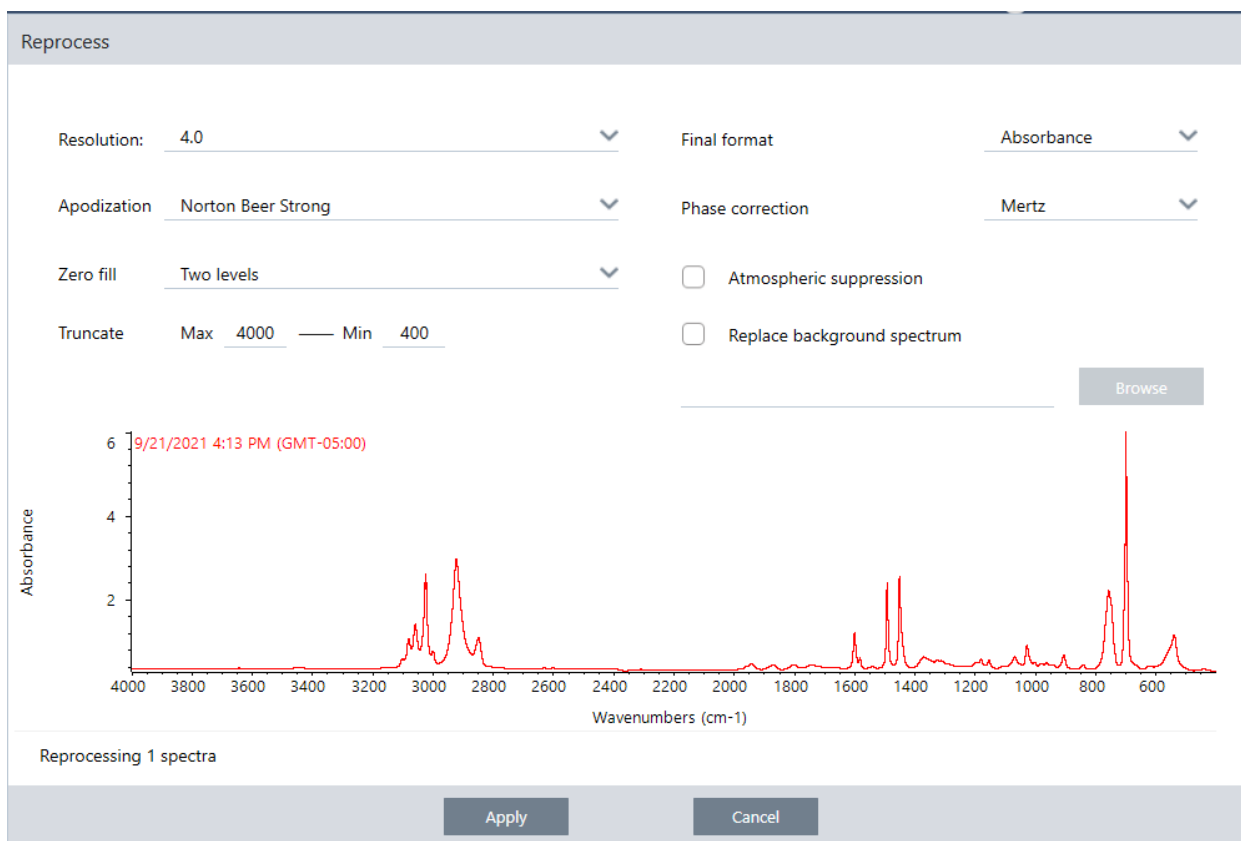
You cannot reprocess to a finer resolution than was originally used. Reprocessing can transform your data but cannot fill in data that was never collected.

If you reprocess multiple spectra, the options show only the values that they share. For example, if one spectrum was measured at a finer resolution, you can select only the shared, lower resolution for reprocessing. This is also true for range. You can set the max and min values for Truncate to only the shared, overlapping range.

❖ To reprocess your spectra

Reprocess is available only in the Desktop view of the software.

1. In the Spectra view, select one or more spectra.
2. Go to the **Process** menu and select **Reprocess**. The Reprocess dialog shows the settings used for reprocessing and a preview of your resulting spectrum. If you are reprocessing more than one spectra, the preview shows only the first spectrum.



3. Change your reprocessing settings. To reprocess the spectrum using a different background spectrum, select **Replace background spectrum** and then select a new spectrum to use.
4. Click Apply to reprocess the spectra.

You can undo the reprocessing by viewing the History panel and reverting to an earlier state. If you reprocessed more than one spectrum, you will have to revert each one individually.

Blank a region in your spectra

Clear data from a region of your spectrum with the Blank Regions tool in the Process menu. You can also blank regions in workflows with the Processing tile.

The Blank Regions tool is a great way to get rid of noisy data that would interfere with your analysis. For example, blanking a region helps in the following situations:

- Your spectrum has totally absorbing peaks because the sample is too thick. The random noise at the top of these peaks will cause poor results when you search the spectrum against a library or when you quantify or subtract the spectrum.
- Your spectrum includes the region below the cutoff of an MCT detector (around 700 wavenumbers) or the cutoff of an ATR crystal. These regions contain only noise, since there is no spectral information present. If you don't exclude these regions, they will interfere with library searches and spectral processing.

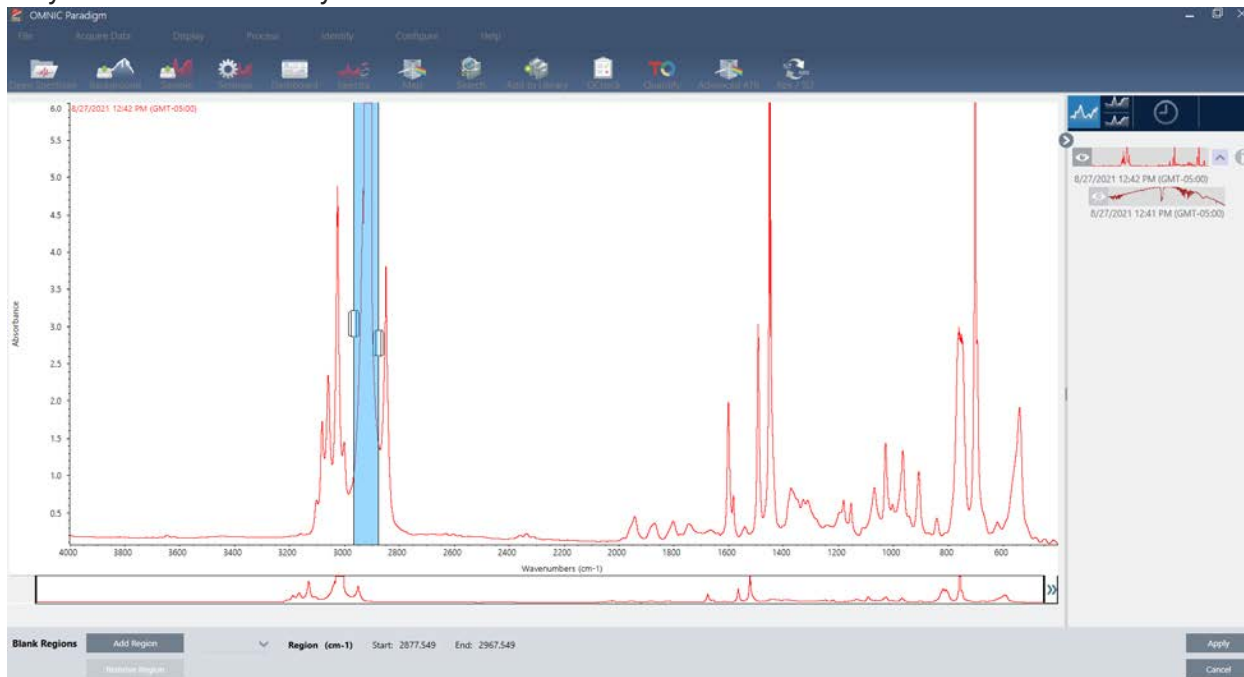
Blanking a region

You can blank regions on one or more spectra.

1. Select the spectra that have regions you want to blank. Hold CTRL and click to select more than one spectrum or press CTRL + W to select all spectra.

Process Data

2. Go to the **Process** menu and select **Blank Regions**. If you have more than one region selected, they are shown in overlay view.



3. Use the region selector to select the region you want to delete. Click **Add Region** to delete more than one region, and click **Apply** to blank the regions.

To undo the change, view the spectrum's history and revert to a previous state.

Calculate average and standard deviation spectra

To find the average or standard deviation of spectra, use the Statistical Spectra tool in the Process menu.

For each X value of your spectrum, you can find the average or standard deviation of the Y value. This creates a new spectrum.

- **Average:** Finds the arithmetic mean of the Y value for each data point. If you have taken several measurements of a sample material, you can calculate the average spectrum to reduce the effect of measurement variations. The average spectrum is also useful as a reference spectrum since it may be more representative of a compound than any single measurement.
- **Standard Deviation:** Finds the standard deviation of the Y values for each data point. By comparing the variance of peaks, you can detect if impurities were introduced during a production process.

You can also use the standard deviation to compare spectra of a standard sample that you measured at different times. This is a useful way to test the repeatability of the measurement.

You can calculate statistical spectra only in the Desktop view of the software. Use the Processing tile to calculate statistical spectra in workflows.

❖ To calculate statistical spectra

1. From the Spectral view, select 2 or more spectra to use in the calculation.
2. Go to the Process menu and select **Statistical Spectra**.
3. Select the calculation you want to perform and the data format to use for the calculation and then select **Calculate**. The resulting spectrum is added to the Results panel. You can see which spectra were used to generate the new spectrum in the new spectrum's Measurement Information.

[This page intentionally left blank]

Analyze Data

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

This section includes the following:

Finding Measurements and Reports	146
Search setup	150
QCheck Setup	154
View Measurement History	156
Revert Measurement	157
Duplicate Measurement	158

Finding Measurements and Reports

When looking for saved measurements and reports, use tags and search keywords to filter the measurements and reports lists.

Searching

When you search for a measurement, the search term is checked against information such as the spectrum tags, title, last modified date, identified compounds, custom strings, serial numbers, etc. If you search for a report, fields used for the search include report name, date created, and the template type.

Tip Click a column header, such as Measurement Name or Type, to sort the measurements. By default, measurements are sorted to show the most recently modified item first.

❖ To search for measurements and reports

1. Select either Reports or Measurements from the list.
2. Select a time to limit the search results.
3. Enter your search terms and click Search.

Use the following search techniques to refine your results.

Search Technique	Description	Example
Quotation Marks ("")	Use quotation marks to return only exact matches from the tags. This is useful if you are searching for a two-word tag and do not want to see spectra tagged with only one of the words.	"red blue" Returns: only spectra with the tag "red blue". Does not return spectra with tags "red" or "blue" separately.

Search Technique	Description	Example
* (asterisk)	<p>Add an asterisk (*) to the end of your search terms to return all results that include the text preceding the asterisk</p> <p>Note: The * can be appended to the end of the search terms but cannot come before other terms.</p>	<p>Poly*</p> <p>Returns: Any measurement with a term beginning with poly, such as polystyrene.</p>
AND, OR, NOT operators	<p>These keywords must be in all capital letters, as shown.</p> <p>AND: Returns only results that contain both terms.</p> <p>OR: Returns results that contain either keyword.</p> <p>NOT: Returns only results that contain the first term but do not include the term after NOT.</p>	<p>Sample AND Background</p> <p>Returns: Only measurements that have both Sample and Background in the searched fields.</p> <p>Sample OR Background</p> <p>Returns: Measurements with either sample or background in the data are returned.</p> <p>Sample NOT background</p> <p>Returns: Measurements or reports that have sample in the data and do not have background in the terms.</p>
title:<keyword>	<p>Use to specify that the keyword must be in the measurement or report title.</p>	<p>title:poly</p> <p>Returns: measurements with poly in their name, but those with poly elsewhere (such as identified compounds) are ignored.</p>

Search Technique	Description	Example
tags:<keyword>	<p>Use to specify that the keyword must be a tag.</p> <p>If the tag is two words, use an underscore instead of a space.</p>	<p>tags:blue</p> <p>tags:blue_powder</p> <p>Returns: measurements with blue as a tag, but those with blue elsewhere (such as the measurement name) are ignored. “blue_powder” searches for the two word tag “blue powder”.</p>


Tagging

Tags give you another convenient way to locate measurements and reports in your database. For example, if you are collecting many measurements related to a single project, you might tag each of those measurements with the same “Project A” tag. Later, you can use this tag to filter your measurements to show you only measurements with the “Project A” tag.

❖ To add or delete a tag in the desktop interface

1. Right-click a measurement in the Measurements list and select Manage Tags.


Tags currently assigned to the measurement are listed under Current Tags.

- To add a new tag, enter text in the New Tag field and click Add. The new tag is added to the current tags.
 - To delete a current tag, click the delete icon () in the upper right corner of the tag. The tag is removed immediately.
2. To save your changes, click OK. Click Cancel to exit the Manage Tags dialog without saving the changes.

❖ To add or delete a tag in the touchscreen interface

1. From the Home screen, navigate to the Measurements tab.
2. Select a measurement and touch the more options icon.
3. Touch Manage Tags.

Analyze Data

- To add a tag, enter text in the New Tag field and touch Add. The new tag is added to the current tags list.
 - To delete a tag, touch the delete icon () in the upper right corner of the tag.
4. To save your changes, touch OK. Touch Cancel to exit the Manage Tags dialog without saving the changes.

Search setup

Configure settings for correlation search and multi-component search using Search Setup. These settings are used automatically when you select Correlation Search or Multi-component Search from the Identify menu in the desktop interface or from the main menu in the touchscreen interface.

Using the desktop interface, you can also use Search Setup to specify the location of additional libraries on your system. See ["Add Library Locations"](#) for details.

Correlation Search Settings

A correlation search compares your measurement to compounds in your libraries and returns the closest matches. The results include the match value for each compound with a value between 0 and 100, with 100 indicating a perfect match.

Figure 6-1: Correlation search settings

The screenshot shows the OMNIC Paradigm software interface with the Search Setup dialog box open. The dialog has three tabs: Correlation Search (selected), Multi-Component Search, and Library Locations. In the Correlation Search tab, there are several settings: 'Match historical search results' is unchecked, 'Search all libraries' is checked, 'Maximum spectra in search results' is set to 5, and 'Show compounds with match values above' is set to 60.00. Below these settings is a section titled 'Spectral Regions' which includes a table with columns 'Region', 'Start', and 'End'. The table is currently empty. To the right of the table is a spectral plot titled 'Test Sample for Paradigm' showing Absorbance vs. Wavenumbers (cm⁻¹) from 4000 to 500. The plot shows several peaks, with the most prominent one around 1700 cm⁻¹. At the bottom of the dialog, there are 'Save' and 'Cancel' buttons.

OMNIC Paradigm

File Acquire Data View / Display Process Identify Configure Help

Correlation Search Multi-Component Search Library Locations

☐ Match historical search results ☒ Search all libraries

Maximum spectra in search results 5

Show compounds with match values above 60.00

HR Nicolet Sampler Library

Spectral Regions

☒ Use full spectral range Add Remove

Region	Start	End
--------	-------	-----

Absorbance

Wavenumbers (cm⁻¹)

Test Sample for Paradigm

Search Setup

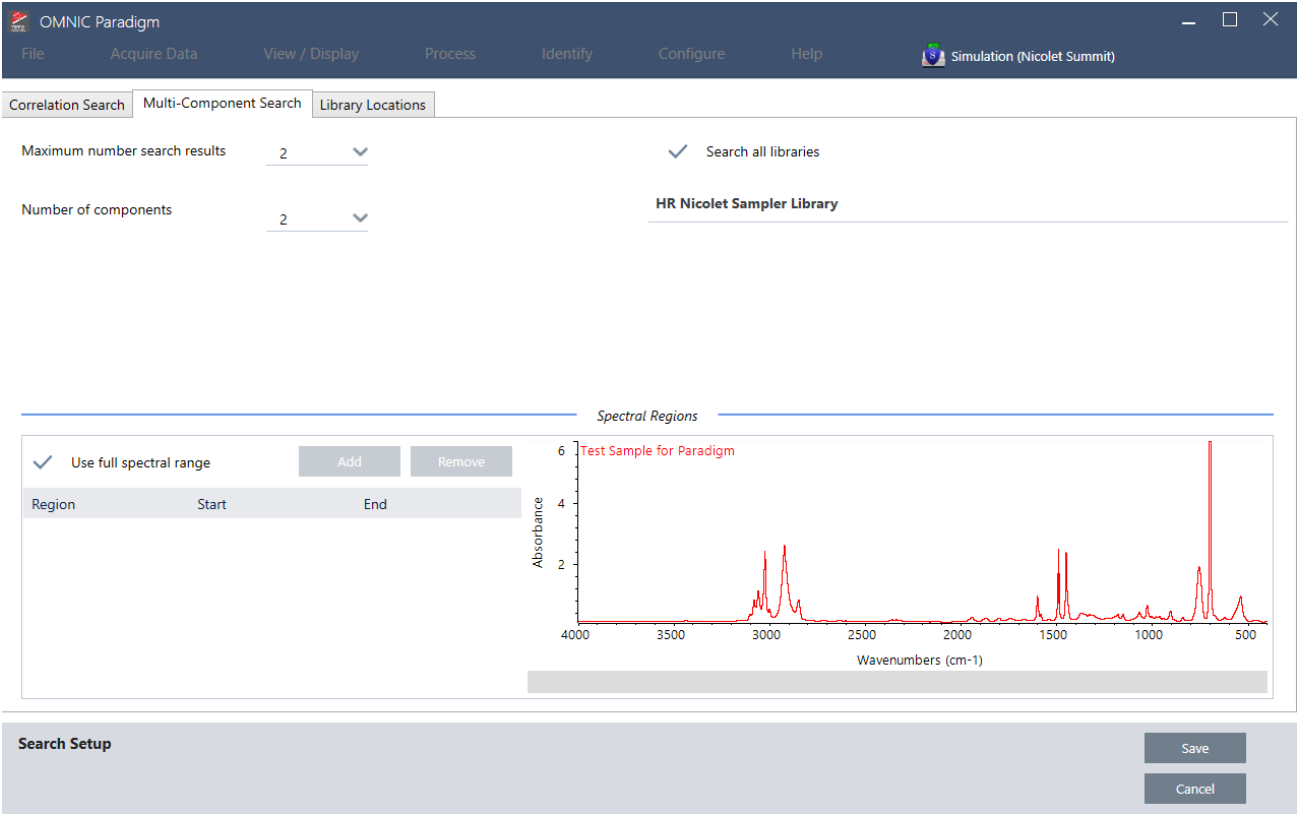
Save Cancel

Setting	Description
Match historical search results	<p>Select to have search results match those of legacy OMNIC applications. The improved algorithm used in OMNIC Paradigm software scales large peaks to reduce the effects of totally absorbing spectra.</p> <p>Select only if you are comparing new measurements with older data collected using legacy OMNIC software.</p>
Maximum spectra in search results	<p>Limit the number of search results. For example, with a maximum of 5, the search will return only the 5 best matches.</p> <p>You can enter a value from 1 to 20.</p>
Show compounds with match values above ____	<p>Set a threshold for which matches are returned by the search. For example, with a value of 60, the correlation search will return only matches with a match value above 60.</p>
Search all libraries	<p>Select to search all of your libraries. Clear the selection to specify only specific libraries to use for the search.</p>
Use full spectral range	<p>Select to use the full spectral range for the search. Clear the selection to specify one or more limited ranges for the search.</p> <p>You can use multiple regions to exclude another region from the search. For example, include a region on either side of a totally absorbing peak to exclude it from the search.</p>

Multi-Component Search Settings

Use multi-component search to identify the components making up your sample.

Figure 6-2: Multi-component search settings



Setting	Description
Maximum number of search results	Limit the number of composite search results.
Number of components	Set the number of components to return for each composite.
Search all libraries	Select to search all of your libraries. Clear the selection to specify only specific libraries to use for the search.

Analyze Data

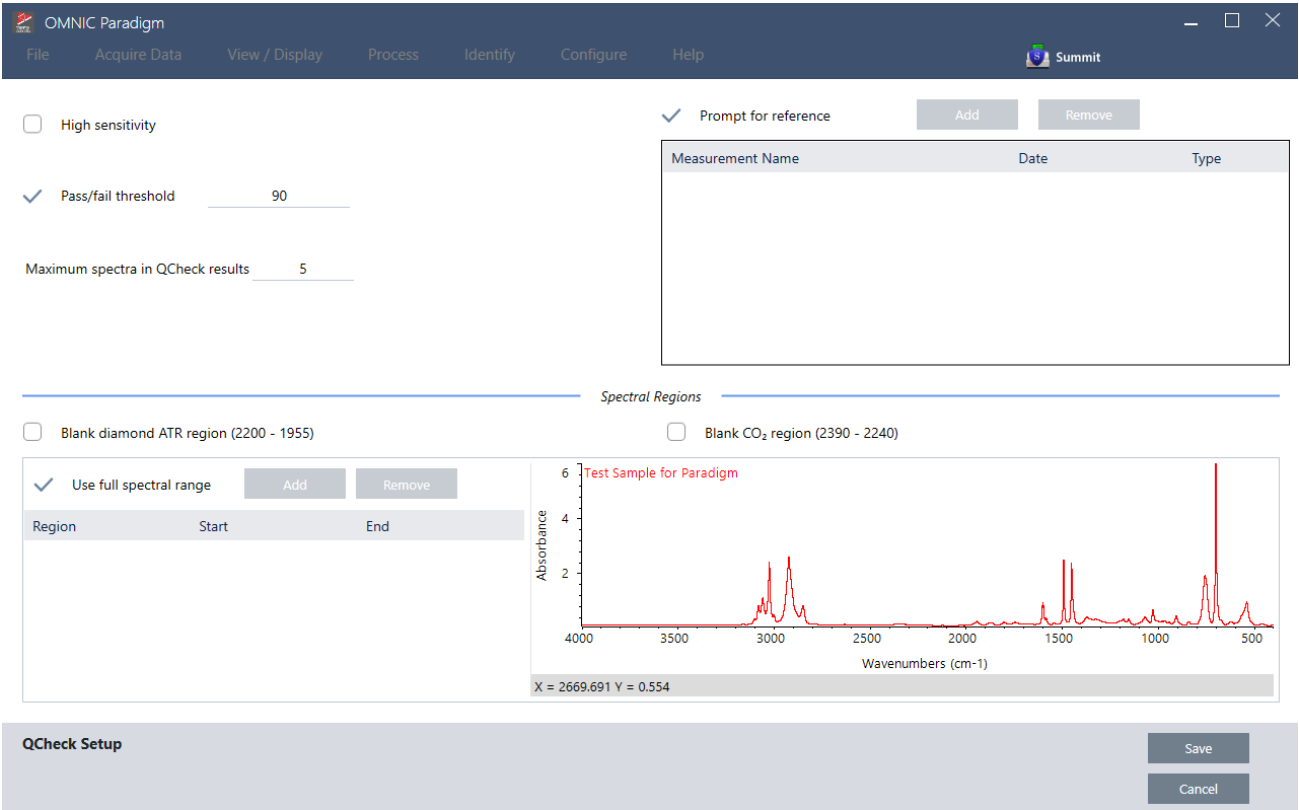
Setting	Description
Use full spectral range	<p>Select to use the full spectral range for the search. Clear the selection to specify one or more limited ranges for the search.</p> <p>You can use multiple regions to exclude another region from the search. For example, include a region on either side of a totally absorbing peak to exclude it from the search.</p>

QCheck Setup

Use QCheck Setup to configure your QCheck analysis. Your saved QCheck settings will be used automatically when you select QCheck as your analysis type before measuring a sample or when you select QCheck from the Identify menu.

For more on using QCheck, see ["Verify Sample Composition with QCheck"](#).

Figure 6-1: The QCheck setup screen



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 deselect 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.

Analyze Data

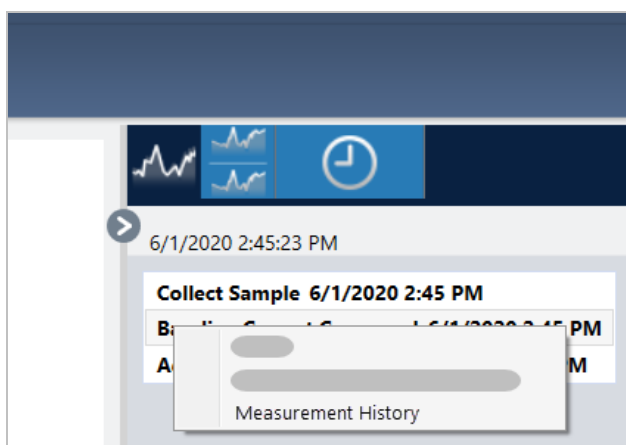
Setting	Description
Maximum spectra in QCheck results	Sets the number of results shown in the results panel. For example, if you set the value to 2, only the two best matches will be shown in the results panel.
Prompt for reference	<p>Select to choose a reference during the measurement. De-select to 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.</p> <p>To use a compound from a library as your reference, first extract the compound so that it is available in your database.</p>
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.
Blank CO2 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	<p>Select to use the full range in the analysis.</p> <p>De-select to specify only a limited range to use for the analysis.</p>

View Measurement History

View the measurement history to visually compare a spectrum at different stages of processing and analysis. For example, after applying automatic baseline correction, view the measurement history to quickly see how the spectrum changed.

❖ To view the measurement history

1. From the Spectral View, navigate to the history panel.
2. Right-click any item in the history and select Measurement History.



The historical data displays the spectrum at each stage in your processing and analysis.

- To create a report of the historical data, open the File menu and select Create Report. Select the Historical Spectrum template, edit your report settings, and click Create.
- To exit the measurement history, click Close Measurement History.


Revert Measurement

Use Revert to undo one or more steps when processing or analyzing a measurement. For example, if a processing step degraded the quality of your measurement data, instead of starting over and collecting a new sample measurement, use Revert to return to an earlier step.

When you revert to an earlier state, any actions taken after the step you are reverting to are lost. In other words, there is no way to undo a revert.

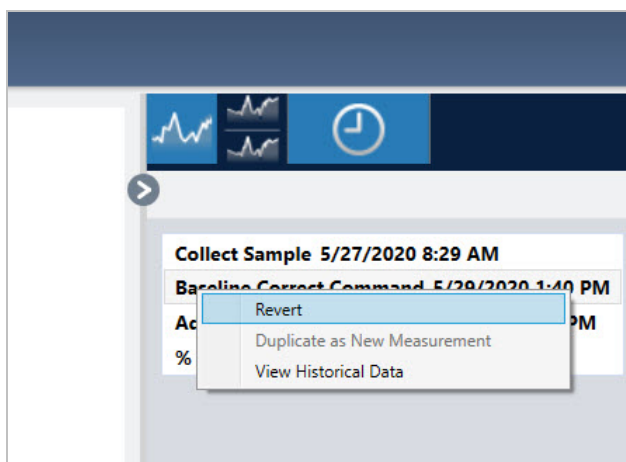
If you are in a secure environment, Revert is not available. However, you can instead use the Duplicate tool to create a copy of the measurement as it was at an earlier step. You can then work with the duplicated measurement without having to remeasure your sample. See ["Duplicate Measurement"](#) for details.

❖ To revert to an earlier step

1. In the Spectral View, select your measurement from the results panel.
2. Click the  icon to view the history panel.

Click any item in the history to preview the measurement at that stage.

3. In the list of events, right-click the step you want to revert to.
4. In the context menu, select Revert.



5. Click Yes to revert or No to cancel.

Duplicate Measurement

Create a copy of a measurement by using Duplicate as New Measurement. You can duplicate a measurement from its current state or from an earlier step in its history.

Tip Duplicate can be useful as an alternative to Revert. For example, while reverting discards the current data and returns the measurement to an earlier state, with Duplicate, you can copy the measurement from an earlier state and keep your current data.

You might also use Duplicate to save a copy of your measurement at specific stages while you work. For example, you might duplicate your measurement immediately after collecting data to save a copy of the measurement without any further processing, and then work with only one copy of the measurement.

When you duplicate a measurement, not all of the measurement information is copied to the new measurement. Most information is duplicated, but there are some differences:

- If the original measurement has tags, the tags will not be copied to the new measurement.
- The measurement history is copied, but the history panel in the spectral view does not display any steps prior to the point at which the measurement was duplicated. Open the Measurement Information and view the History tab to review the measurement history.

❖ To duplicate a measurement

- From the dashboard

Duplicate from the dashboard to copy the measurement in its current state.

1. Right-click a measurement in the Measurements pane.
2. Select Duplicate as New Measurement.
3. Enter a name for the new measurement or keep the default name.
4. Click OK.

Analyze Data

- Duplicate from the measurement history

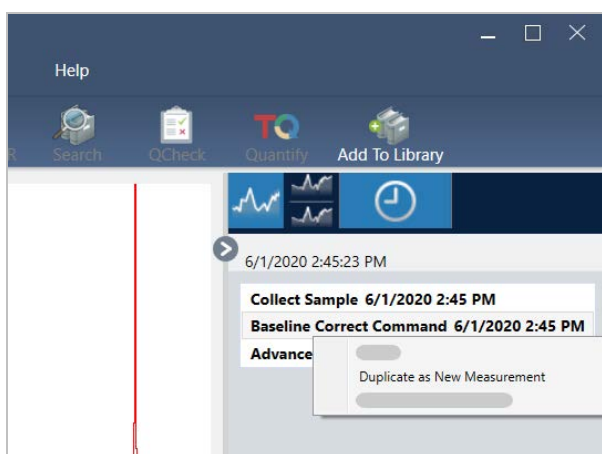
Duplicate from the Spectral View to copy the measurement from a previous point.

1. In the Spectral View, select the measurement in the Results pane.
2. With the measurement selected, navigate to the history panel.

Click any item in the history to preview the spectrum at that point.

3. Right-click the step at which you want to duplicate the measurement.

Events that did not change the spectrum, such as Add to Library or Create Report, cannot be duplicated as a new measurement.



4. Select Duplicate as New Measurement.
5. Enter a name for the new measurement or keep the default name.
6. Click OK.

[This page intentionally left blank]

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:

In this section:

About Workflows	162
Password Protect a Workflow	168
Create a Template Workflow	170
Workflow Tiles Reference	176

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.

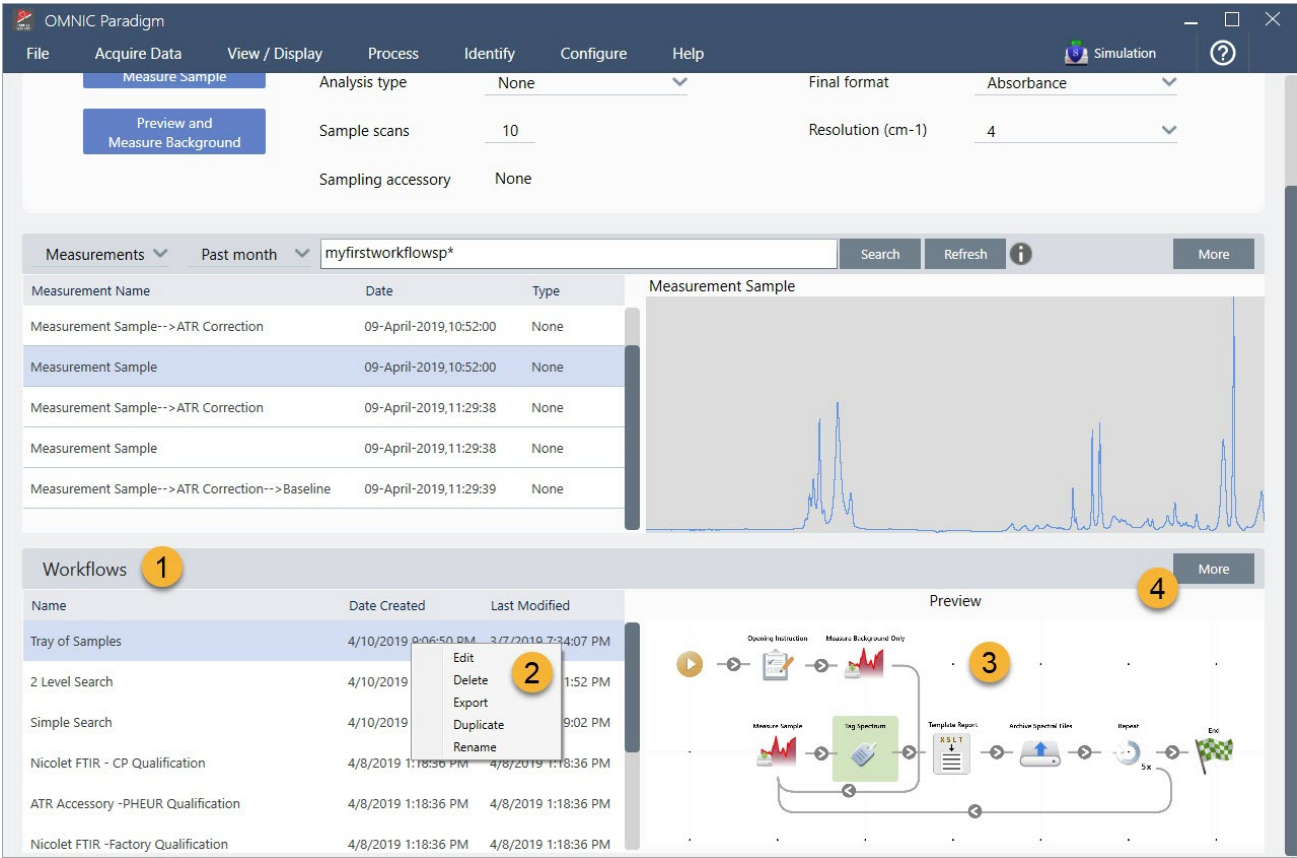
This article provides an overview of these basic workflow features and tools:

- Workflow pane
- Run 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 run workflows you've created, and to open the workflow editor to edit or create a new workflow.

Figure 6-1: Workflow Pane on the OMNIC Paradigm Dashboard



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

Table 6-1:
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	Right-click the workflow and select Run. This opens the Run Workflow window where you can step through the workflow tasks.

To do this...	Take this action
Edit, rename, duplicate, delete or export the selected workflow	Right-click the workflow and choose an option from the shortcut menu.

Run Workflow Window

Use the Run Workflow window to test or run a workflow. To open the run Workflow window, right-click a workflow and select Run.

Figure 6-2: Right-click a workflow and select Run

The screenshot displays the OMNIC Paradigm software interface. The top menu bar includes File, Acquire Data, View / Display, Process, Identify, Configure, and Help. Below the menu bar is a toolbar with icons for Open, Background, Sample, Settings, Dashboard, Spectra, Abs / %T, Advanced ATR, QCheck, Quantify, and Add To Library. The main window is divided into two sections: 'Measurements' and 'Workflows'. The 'Measurements' section shows a table of measurement data. The 'Workflows' section shows a table of workflow data, with the 'Tray of Samples' workflow selected and highlighted by a yellow circle with the number 1. To the right of the 'Workflows' table is a 'Preview' section showing a flowchart of the workflow steps: Opening Instrument, Measure Background Only, Measure Sample, Tag Spectrum, Sample Report, Archive Spectral File, Export, and Exit.

Measurement Name	Date	Type
Mon Jan 14 16:04:32 2019 (GMT-06:00)	04-April-2019, 11:47:54	None
4/4/2019 11:30:45 AM	04-April-2019, 11:30:57	None
4/4/2019 11:30:32 AM	04-April-2019, 11:30:44	None
4/4/2019 8:14:14 AM	04-April-2019, 08:14:28	None
*PTFE	03-April-2019, 05:07:00	None

Name	Date Created	Last Modified
Tray of Samples	4/8/2019 12:31:12 AM	3/7/2019 7:34:07 PM
Simple Search	4/8/2019 12:31:01 AM	3/7/2019 7:19:02 PM
Measure Only Quant with Poly	4/8/2019 12:30:37 AM	3/7/2019 7:32:57 PM
Nicolet Any KBr - Factory	4/3/2019 1:50:48 PM	4/3/2019 1:50:48 PM
Nicolet Any KBr - CP	4/3/2019 1:50:48 PM	4/3/2019 1:50:48 PM
2 Level SearchCopy	4/5/2019 4:56:55 PM	4/5/2019 5:06:01 PM

Workflow Preview:

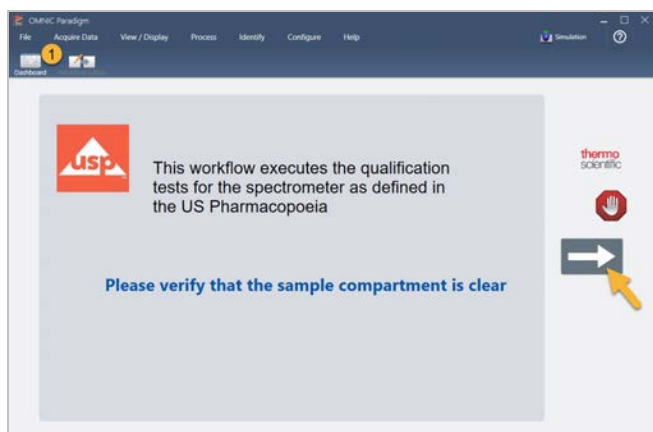
```

graph LR
    Start(( )) --> Opening[Opening Instrument]
    Opening --> MeasureBg[Measure Background Only]
    MeasureBg --> MeasureSample[Measure Sample]
    MeasureSample --> TagSpectrum[Tag Spectrum]
    TagSpectrum --> SampleReport[Sample Report]
    SampleReport --> ArchiveSpectralFile[Archive Spectral File]
    ArchiveSpectralFile --> Export[Export]
    Export --> Exit((Exit))
  
```

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

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

Figure 6-3: Run Workflow Window



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

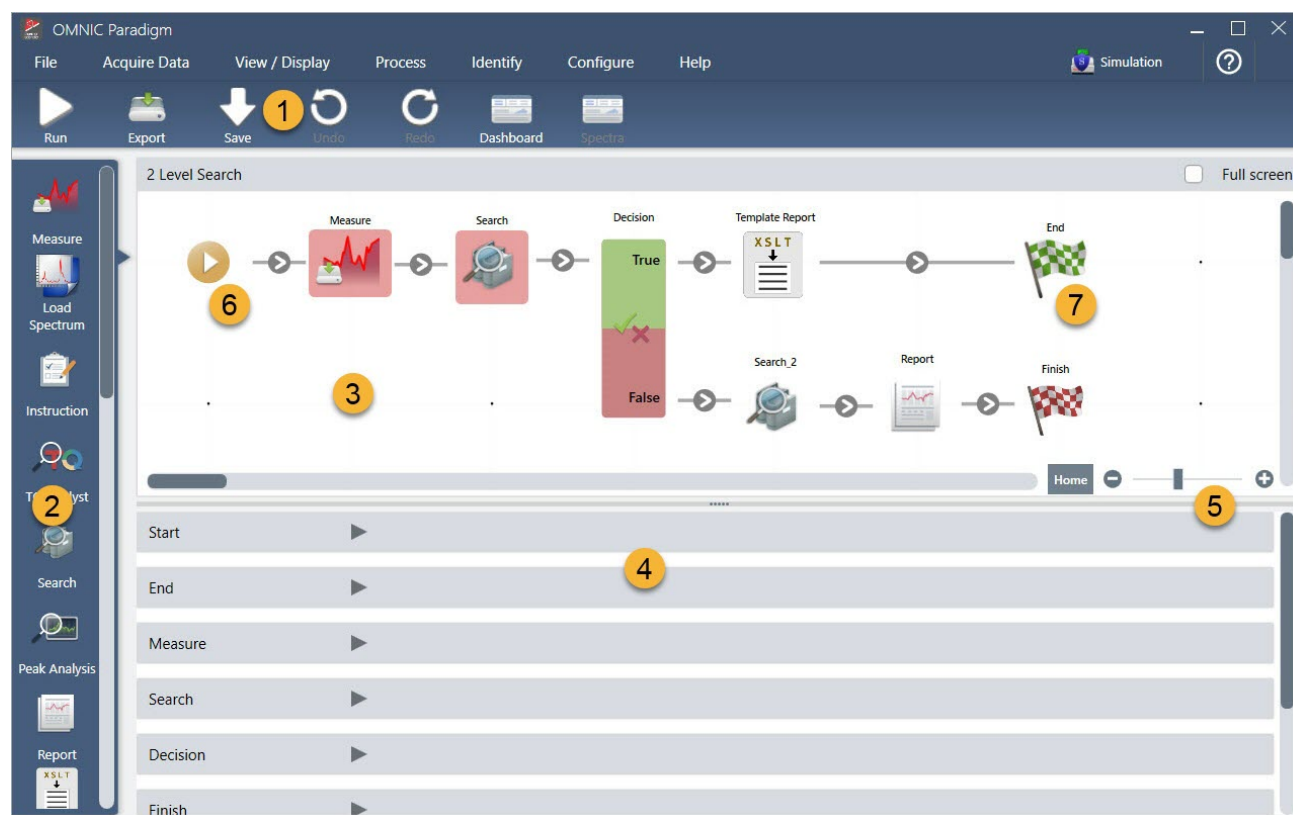
The workflow editor contains all the tools for creating workflows, including the workflow menu, toolbar, tile selection bar, and canvas. To open the workflow editor, right-click a workflow name on the dashboard and choose Edit from the shortcut menu.

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 6-4: Workflow Editor



1. Toolbar
2. Tile selection bar
3. Canvas
4. Tile settings
5. Tools to adjust and reset the canvas
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:



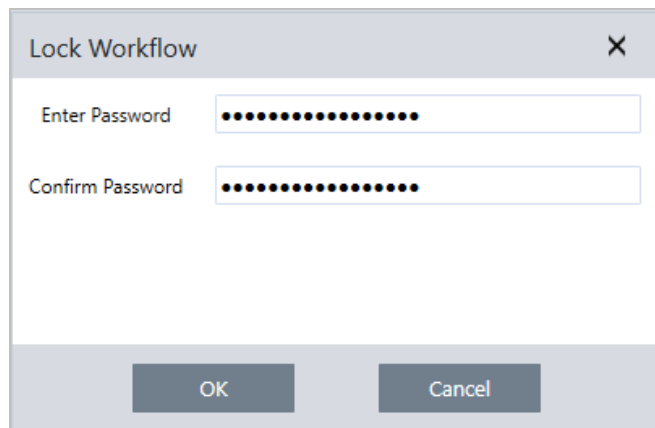
Use Workflows

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."

Password Protect a Workflow

Lock a workflow with a password so that it cannot be edited by others. A locked workflow cannot be edited, deleted, or duplicated and will not display a preview. When a workflow is locked, it can still be renamed or exported.

A screenshot of a 'Lock Workflow' dialog box. The dialog has a title bar with 'Lock Workflow' and a close button (X). Inside, there are two text input fields. The first is labeled 'Enter Password' and the second is labeled 'Confirm Password'. Both fields contain a series of black dots representing a password. At the bottom of the dialog, there are two buttons: 'OK' and 'Cancel'.

Lock and Unlock a Workflow

You can lock and unlock workflows only from the desktop interface of OMNIC Paradigm software.

❖ To lock a workflow

1. In the Workflow Editor, select Lock.
2. Enter and confirm the password and click OK.
3. Save your changes.

❖ To unlock a workflow

1. On the dashboard, right-click the workflow and select Unlock.
2. Enter the correct password and click OK.

Reset a Lost Password

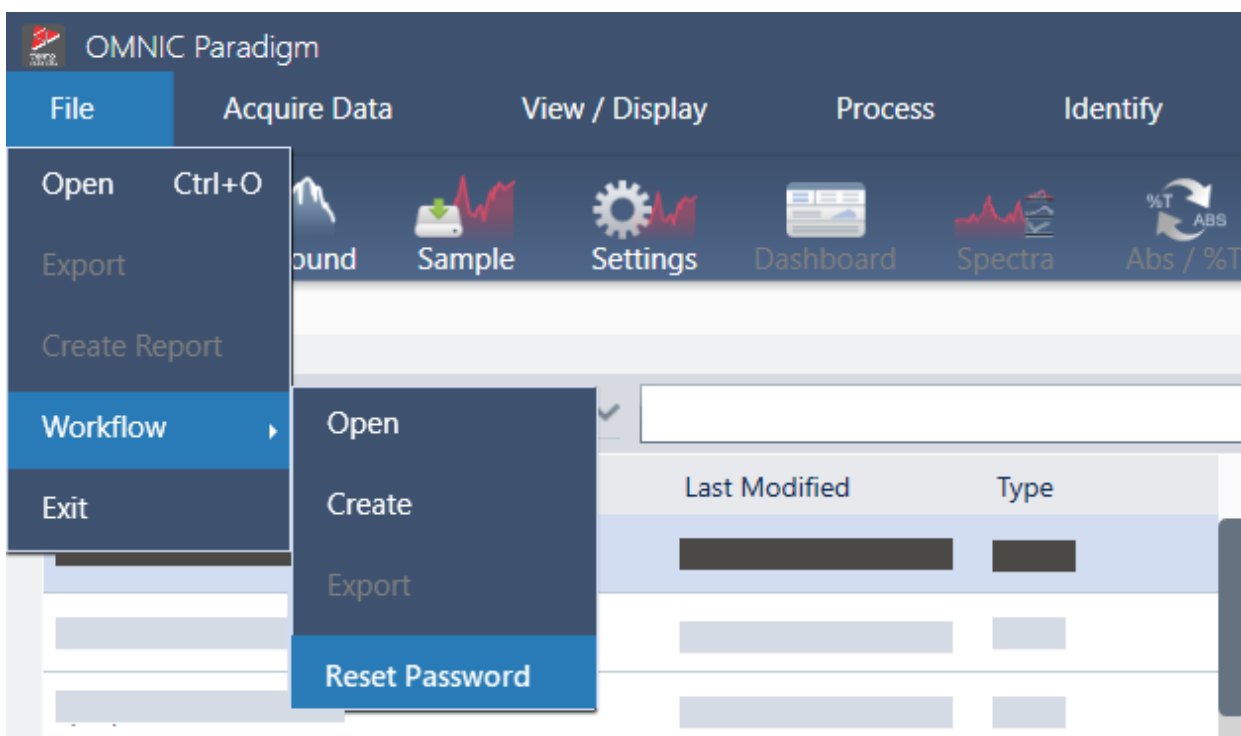
If you lose or forget the password to a workflow, you can reset the password to unlock the workflow.

Use Workflows

You can only reset a workflow password with an Administrator account type in Windows. To reset a password, run OMNIC Paradigm software as an Administrator. Note that if you are using Security Suite software, even if you grant an account access to the Reset Workflow Password control, the user must still run OMNIC Paradigm as an administrator.

❖ To reset a workflow password

1. From the Windows desktop, in the Start menu, navigate to Thermo Scientific > OMNIC Paradigm. Right click OMNIC Paradigm and select Run as administrator.
2. In OMNIC Paradigm, using the desktop interface, select the locked workflow with the password to be reset.
3. Select File > Workflow > Reset Password. This option appears only if you run OMNIC Paradigm software as an Administrator.



The password is removed from the workflow and the workflow is unlocked.

Create a Template Workflow

A template workflow allows you to create a single workflow that can be run using dynamic values depending on the situation. For example, with a template workflow, you can create a single workflow that can be run using several different sampling accessories. The operator can select an accessory and the workflow will be updated automatically to use images, quantification methods, and variables that match the accessory.

To create a template workflow, use the Workflow Table tile. With the Workflow Table tile, you import a table of options and corresponding values from a CSV file. Then use the values throughout the workflow.

With a Workflow table tile, you can ...

- import many files and variables at once
- allow the operator to select from a list of options or automate the selection
- import custom variables or reference external files, such as images or QNT files

Using the Workflow Table tile requires you to build a CSV file of the options and data you want to include, configure the Workflow Table tile, and use the included data.

❖ To create a template workflow with the Workflow Table tile

Step 1: Create a CSV file for your data

1. Create a CSV file to import with the Workflow Table tile.

Figure 6-1: The following example shows a table with three accessory options

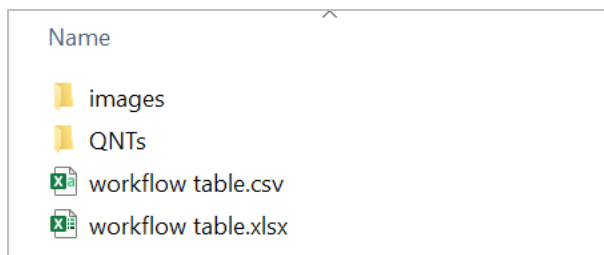
	A	B	C	D	E	F
1	Accessory	images	values	quants		
2	Everest ATR	Everest.jpg	5	HexadecaneCoverage.qnt		
3	iD7 ATR	iD7.jpg	10	HexadecaneMatchR.qnt		
4	iD1 Transmission	iD1.jpg	20	PathlengthHexadecaneR.qnt		

- Structuring the table. When creating the table, each row reflects an option or a category of related values. For example, you might use each row for an accessory, with the columns for data and files associated with that accessory. When developing your workflow, the column headings are used as variables. You can create the table directly as a CSV file, but it may be

easier to work with a table in a spreadsheet program and then export the data as a CSV file.

- Organizing your external assets. When referencing external assets, such as image or QNT files, keep your files very organized. This will make them easier to import in the Workflow Table tile and to update later.

Figure 6-2: Keep referenced assets organized



2. Save the table as a CSV file.

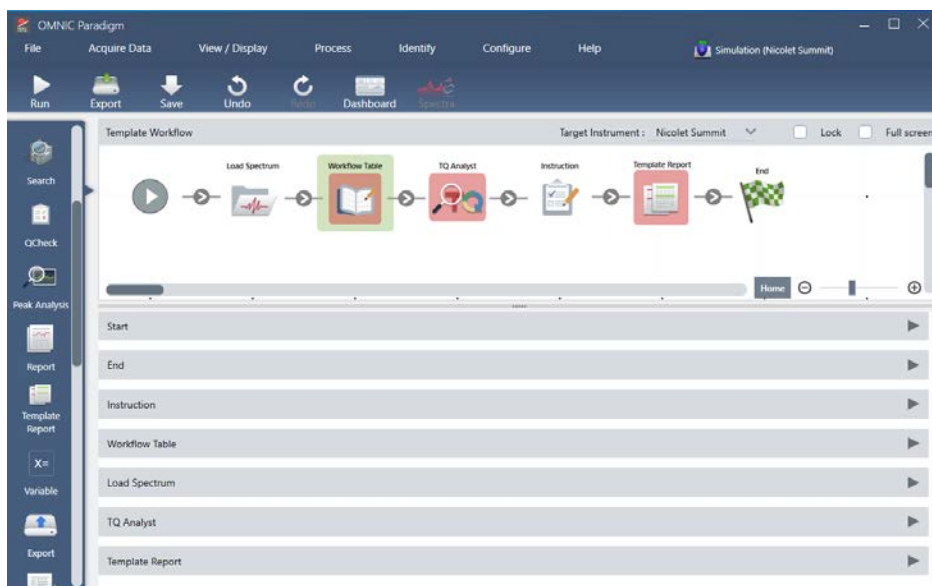
Figure 6-3: This image shows the table as a CSV file

```
1  Accessory,images,values,quants
2  Everest ATR,Everest.jpg,5,HexadecaneCoverage.qnt
3  iD7 ATR,iD7.jpg,10,HexadecaneMatchR.qnt
4  iD1 Transmission,iD1.jpg,20,PathlengthHexadecaneR.qnt
```

Step 2: Create the workflow and configure the Workflow Table tile.

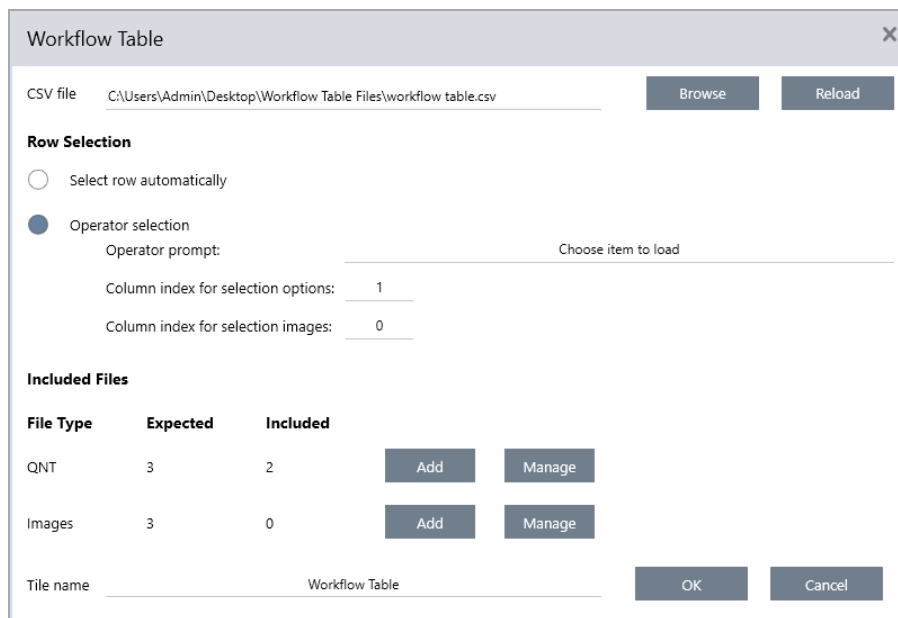
1. In OMNIC Paradigm software, go to File > Workflows > Create. Name the workflow and select OK to open the Workflow Editor.
2. Add any desired tiles to the workflow.
3. Add the Workflow Table tile to the workflow. The placement of the Workflow Table tile depends on your individual requirements.

Figure 6-4: This example workflow uses the workflow table tile near the start



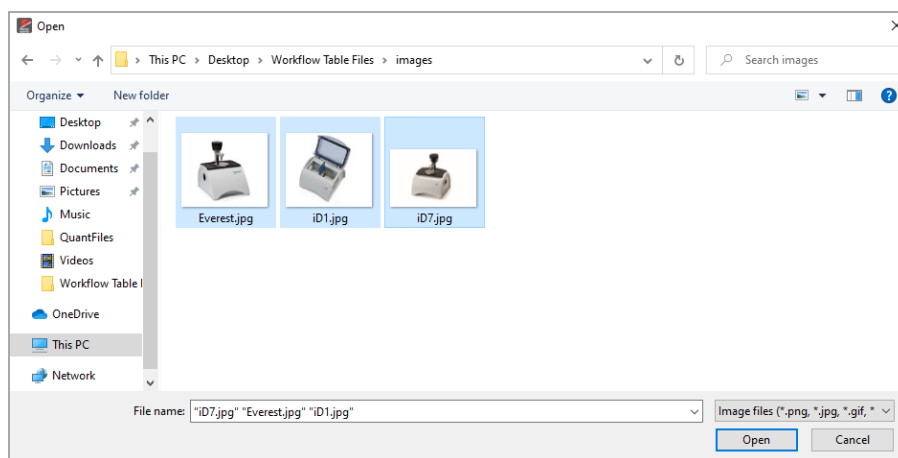
4. Double-click the Workflow Table tile to open the tile settings.
5. Configure the Workflow Table tile.
 - a. Select Browse and open your CSV file.

If the CSV file included references to image, QNT, or SPA files, the tile indicates that the template expects additional files and provides a button to add and manage files.



- b. For each category of required files, select Add and open the associated files that you listed in the CSV file. The file name must match exactly what you included in the CSV file.

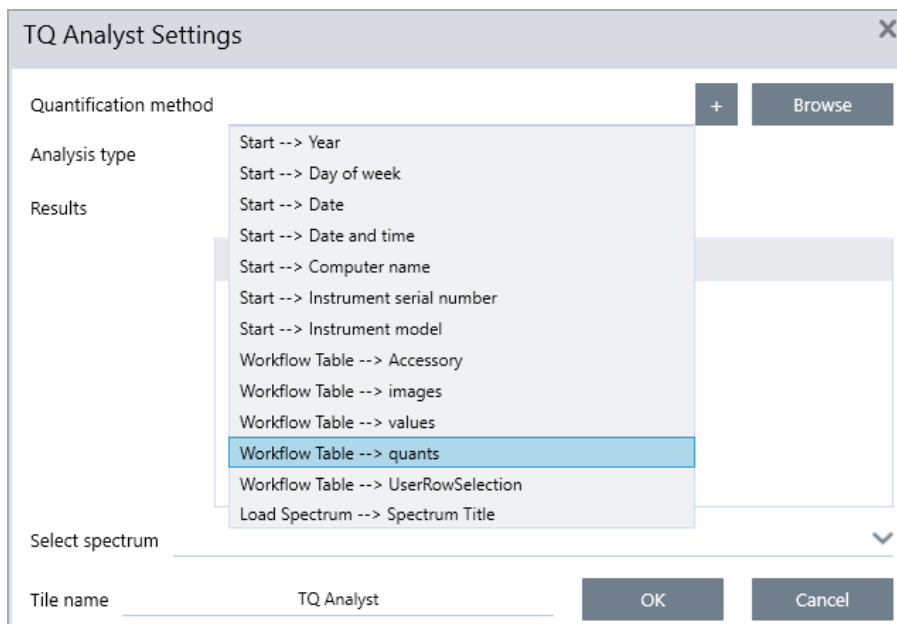
Figure 6-5: These image files match the filenames in the CSV file



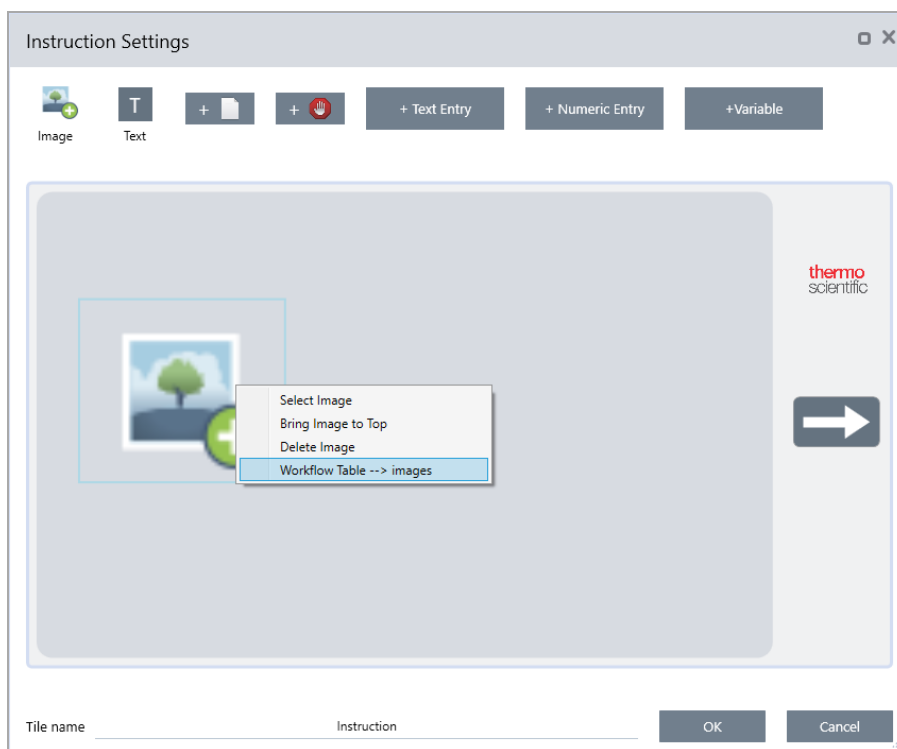
- c. To prompt the operator to select an option, select Operator Selection and choose a column. The column index of options determines which column of data is used for the options presented to the operator. The first column is column 1. You can also specify a column of images to display with the options. Set the index to 0 if you do not want to show an image. To choose a row automatically, select Select row automatically. The first row is row 1. You can enter a specific value or use a variable. For example, use the Variable tile to increase the Repeat_Count variable from a Repeat tile by 1, then use the new variable to automatically loop through all of the options.

Step 3: Use the imported files and variables

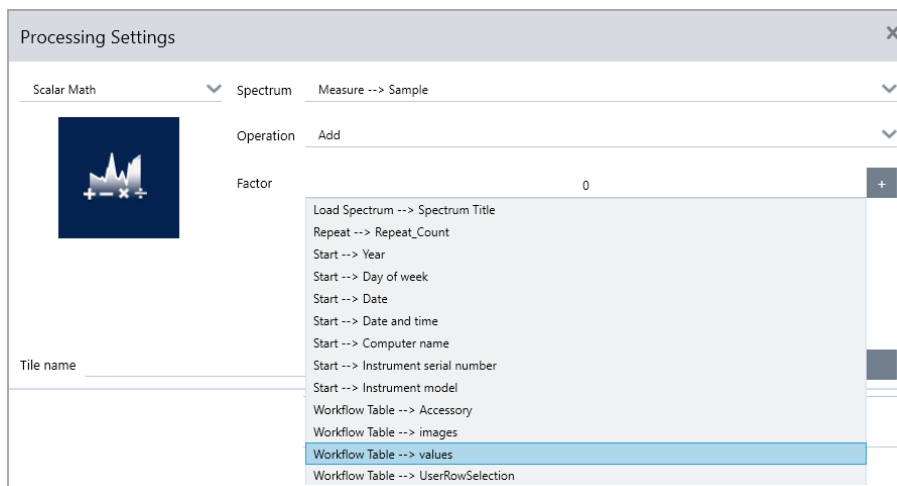
1. Select another tile where you would like to use data from the Workflow Table tile. How you use values from the Workflow Table tile depends on your specific needs. Consider the following examples:
 - To use a QNT file: In the TQ Analyst tile settings, select the + icon to select a variable. Select the Workflow Table variable that corresponds to the QNT files in your CSV file.



- To use an image in an Instruction tile. In the Instruction tile, click Image to add an image. Right-click the image placeholder and select the appropriate Workflow Table value.



- To use a value as a variable. Select the + icon in the tile settings and select a Workflow Table variable.



2. Save the workflow.

Step 4: Test your Workflow

It is a good idea to test your workflow to be sure that everything is loaded and working as expected.

If you workflow includes measuring data, you may want to use the Simulator mode to simplify the test.

1. (optional). Switch to Simulator mode.
 - a. Return to the dashboard.
 - b. Go to Configure > Connectivity.
 - c. Select Simulator and select Connect.
 - d. Choose an instrument to Simulate and select OK. It may take a moment for the software to switch to the new simulated instrument.
2. Open your workflow in the Workflow Editor.
3. Select Run to run the workflow.

Note that if your workflow measures data, the measurements will be saved to your database just as they would during a normal workflow. You may wish to delete these measurements that use simulated data.

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.

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	<p>Select a pass/fail decision type to use a previously generated pass/fail result as the decision criteria.</p> <p>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.</p>
Numeric Value	<p>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.</p> <p>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.</p>
String Value	<p>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.</p> <p>With a string value, you can check if the selected value is equal to or contains your test string.</p> <p>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.</p>
Spectrum Age	<p>Control the flow of the workflow depending on the age of a spectrum.</p> <p>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.</p>
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.

EMBEDDED WORKFLOW

Use the Embedded Workflow tile to include one workflow in another.

Using the Embedded Workflow tile, you can create one workflow for a subset of common tiles or processes and then reuse that workflow in many other workflows. If you want to change a setting or update a tile in the embedded workflow, you can make the change once rather than having to manually edit the settings in every workflow.

You can update any embedded workflows in the Workflow Editor. Open the workflow that includes the Embedded Workflow tile, right-click an empty space on the canvas and click Update Embedded Workflow(s). Then select any embedded workflows that you want to update.

It is recommended that you always keep embedded workflows up to date to ensure the workflows behave as expected.

Setting	Description
Select a Workflow file to import	<p>Browse to a workflow file to use as the embedded workflow.</p> <p>If you update the embedded workflow, you must browse to the workflow and reload it or the changes will not be reflected in this workflow.</p>

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.

Setting	Description
Tile name	Sets the name of the tile in the workflow canvas.

EQUATION

The Equation tile is an advanced tile for evaluating complex equations. You can include variables from other tiles in the equation and use built-in functions for common problems, such as calculating an average or rounding a value. You can also use functions to find peak height or peak location or to perform other operations on a spectrum.

The tables below list valid operators and functions.

Table 6-1:

Arithmetic Operations

Operator	Description	Example
+	Addition	$15 + 4 = 19$
-	Subtraction	$15 - 4 = 11$
*	Multiplication	$15 * 4 = 60$
/	Division	$15 / 4 = 3.75$
-	Negation	$-15 + 4 = -11$
mod	Modulo division (returns the remainder)	$15 \text{ mod } 4 = 3$
&	Text concatenation	"abc" + "def" = "abcdef"

Comparison operators return 0 for false or 1 for true.

Table 6-2:

Comparison Operations

Operator	Description	Example	Result
<	Less than	$2 < 3$	true
>	Greater than	$3 > 2$	true
<=	Less than or equal to	$2 <= 3$	true

Operator	Description	Example	Result
>=	Greater than or equal to	3 >= 2	true
=, ==	Equals	3 = 3, 3 == 3	true, true
!=, <>	Does not equal	3 != 3	false
true		true = 1	true
false		false = 0	true

Table 6-3:

Logical Operations

Operator	Description	Example
AND	True if both operands are true	x AND y
OR	True if either of the operands is true	x OR y

In the table below, parameters surrounded by square brackets ([]) are optional.

Table 6-4:

Functions

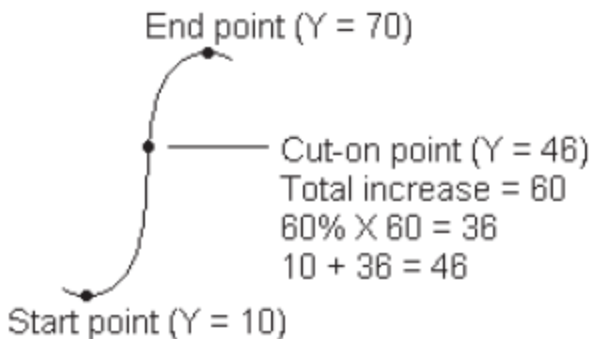
Operator	Description
Average(list)	The average of a list of numbers (sum divided by the number of items)
Avg(list)	The average of a list of numbers (sum divided by the number of items)
Max(list)	The highest value in the list
Min(list)	The lowest value in the list
AMax(list)	The absolute value of the maximum value
AMin(list)	The absolute value of the minimum value
Sum(list)	The sum of a list of numbers
StdDeviation (list)	The standard deviation
Std(list)	The standard deviation
acos(number)	Arcosine of a number in radians

Use Workflows

Operator	Description
asin(number)	Arcsine of a number in radians
atan(number)	Arctangent of a number in radians
aTan2(X1,X2)	Arctangent of X1 divided by X2 in radians. The signs of both arguments are used to determine the quadrant of the returned value.
cos(radians)	Cosine of an angle measured in radians.
cosh(radians)	Hyperbolic cosine of an angle measured in radians.
sin(radians)	Sine of an angle measured in radians.
sinh(radians)	Hyperbolic sine of an angle measured in radians.
tan(radians)	Tangent of an angle measured in radians.
tanh(radians)	Hyperbolic tangent of an angle measured in radians
Pi()	Ratio of the circumference of a circle to its diameter
abs(number)	Absolute value of a number.
Ceiling (number)	Smallest integer greater than or equal to <number>. Example: Ceiling(2.2) is 3.0
Floor(number)	Largest integer less than or equal to <number>. Example: Floor(2.7) is 2.0
Round (number)	Rounds a floating point value to the nearest integer value. (tie rounds to the nearest even integer. 3.5 -> 4; 4.5 -> 4
sqrt(number)	Square root of a number.
Truncate (number)	Truncated number. Everything to the right of the decimal point is removed, leaving only the integer portion of the number. The returned value is not rounded.
Random()	Random fractional number between 0 and 1
exp(number)	Result of the constant e (2.7182818) raised to the power of the specified number (e^<number>)
pow(base, power)	The base value raised to the power. Example: pow(2,3) = 8
log10(number)	Base 10 log of number

Operator	Description
log(number)	Base 10 log of number
ln(number)	Natural logarithm (base e logarithm) of a number
expneg(power)	Result of the constant e (2.7182818) raised to the negative power of the specified number ($e^{-\text{number}}$)
ten(power)	10 raised to the power
tenneg(power)	10 raised to the negative power
negln(number)	Negative natural log
neglog (number)	Negative base-10 log
invsqrt (number)	Inverse square root
toNumber(text)	Converts a text number to a numeral that can be used in equations. ("10" to 10)
textLength(text)	Number of characters, including spaces, in the specified text. A CRLF is counted as two characters.
Y(location [,baseline] [,baseline2])	Y-axis value at the given location with a two-point baseline
Area(start,end [,baseline] [,baseline2])	Area between two spectral limits using a two-point baseline
Pmin(start,end [,baseline] [,baseline2])	Corrects the spectrum with a two-point baseline and then reports the minimum Y-axis value between two spectrum limits
Pmax(start,end [,baseline] [,baseline2])	Corrects the spectrum with a two-point baseline and then reports the maximum Y-axis value between two spectrum limits
Ploc(start,end [,baseline] [,baseline2])	Corrects the spectrum with a two-point baseline and then report the location (X-axis value) at which the maximum Y-axis value occurs between two spectral limits

Operator	Description
Pavg(start,end [,baseline] [,baseline2])	Determines the average value of the spectrum between two spectral limits
PkHgt(start,end [,baseline] [,baseline2])	Finds the height of a peak
PkArea (start,end [,baseline] [,baseline2])	Area between two spectral limits using a two-point baseline
PkLoc (start,end [,baseline] [,baseline2])	Corrects the spectrum with a two-point baseline and then report the location (X-axis value) at which the maximum Y-axis value occurs between two spectral limits
PkMin (start,end [,baseline] [,baseline2])	Corrects the spectrum with a two-point baseline and then reports the minimum Y-axis value between two spectrum limits
PkMax (start,end [,baseline] [,baseline2])	Corrects the spectrum with a two-point baseline and then reports the maximum Y-axis value between two spectrum limits
Pwidth(start, end [, %height])	Determines the peak width between two spectral limits. Report the width at which the peak reaches a specified percentage of the peak maximum.

Operator	Description
Pcut(start, end [, %height])	<p>Determines the location (X-axis value) of the cut-on or cut-off point in the specified spectral region. For example, for a region with increasing Y value, a cut-on point occurs where the increase reaches the specified percentage of total increase across the region. Here is an example showing a cut-on point with “percent” set to 60:</p>  <p>End point (Y = 70)</p> <p>Cut-on point (Y = 46)</p> <p>Total increase = 60 $60\% \times 60 = 36$ $10 + 36 = 46$</p> <p>Start point (Y = 10)</p>
Ghalfwidth (start, end)	Finds the width of a peak at half the peak height
Slope(x1, y1, x2, y2, x3, y3, ...):	Returns the slope ($y=mx+b$)
Intercept(x1, y1, x2, y2, x3, y3, ...):	Returns the intercept point
ZSlope(x1, y1, x2, y2, x3, y3, ...):	Returns the zslope ($y=mx$)
CorCoef(x1, y1, x2, y2, x3, y3, ...):	Correlation coefficient

Use Workflows

Operator	Description
Laser(x1, y1, x2, y2, x3, y3, ...)	<p>Calculates the best laser frequency for the instrument under the conditions in which the spectrum was measured.</p> <p>x1, x2, x3 ... refer to the measured values of a peak or feature of the spectrum.</p> <p>y1, y2, y3 ... refer to the true values of the corresponding peak or feature.</p> <p>The output of the function is the value of the laser frequency that would move the measured value as close as possible to the true, actual value.</p>
DoesFileExist (filename):	<p>Accepts a full file path in quotes and returns true(1) or false(2).</p> <p>Example: DoesFileExist("C:\Users\MyFiles\MyMethod.qnt")</p>

Table 6-5:

TQ Functions: These functions allow you to work with information from a TQ method

Operator	Description
M(name)	Returns the measurement method used
V(name)	Returns the composite component
C(name)	Returns the concentration of the component (name)
U(name):	Returns the uncertainty associate with the concentration of component (name)
TQ_Y(value):	Enter the index value for the Y file. The first element is index 1.
TQ_Z(value)	Enter the index value for the Z file. The first element is index 1.
U_Set(index, value)	Sets the value at the index
TQ_UU(value)	Access the user values attached to a TQ method
UU_Set(index, value)	Sets the user value at the specified index

EXPORT

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	<p>The base name is prepended to the full file name.</p> <p>When the file is archived, it is named according to the following template:</p> <p><base name>_<workflow name>.<tile name of data creation>.<variable name>_YYYY_MM_DD_HHMMSS_<time zone in GMT>.<file extension></p> <p>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:</p> <p>“example_my workflow.Measure.Sample_2019_06_25_104928_GMT-0500.spa”</p>
Append date and time to file name	<p>If selected, the system appends the date and time that the data are saved to the file name. This ensures that a new file is created every time the workflow is run.</p> <p>If not selected, every time you run the workflow, the previously exported file will be overwritten with a new file. This is useful if you want to update one file, rather than create new files.</p>
File location	The directory in which the file will be archived.
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	<p>Add an image that the operator will see on the instructions screen during the workflow. Valid file types include:</p> <p>.PNG .JPG .GIF .BMP</p>

Use Workflows

Setting	Description
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.
+ 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.

Setting	Description
From database	<p>Select to load a spectrum from the database.</p> <p>Selected spectrum: Choose a spectrum from the database.</p> <p>Choose during workflow execution: Allow the operator to select a spectrum during the workflow.</p> <p>Show only experiments containing this text: Limit the operator's choice to only spectra that contain the specified text in the title or tags.</p>
Import spectrum every run	<p>If selected, the spectrum is imported from the file system when the workflow is run. If the spectrum file is updated, the workflow will always use the latest version of the spectrum.</p> <p>If not selected, a copy of the spectrum file is imported when the workflow is created. This spectrum only changes if you manually edit the workflow and update spectrum files.</p> <p>Note that if you share this workflow or add it to a package, you will need to share the SPA file separately, and it must be saved on any other systems in the exact same file path specified in the Import Spectrum tile.</p>
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.

Use Workflows

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	<p>Customize the measurement settings used in this workflow or match the settings used with another spectrum.</p> <p>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.</p> <p>Atmospheric suppression: Used to suppress the effects of CO₂ and H₂O.</p> <p>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.</p> <p>Spectrum Title: Select to append variable data to the spectrum title.</p> <p>See Measurement Settings and Advanced Measurement settings for a description of additional settings.</p>
Tile name	Sets the name of the tile in the workflow canvas.

PEAK ANALYSIS

Find peak locations or analyze the Peak Height or the Peak Ratio of a spectrum.

Setting	Description
Peak Height	<p>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."</p> <p>Peak position: Enter the wavenumber of the peak to be measured.</p> <p>Corrected: Select to measure the peak height from the spectral baseline rather than from zero absorbance (or 100% transmittance)</p> <p>Reference point: Select for single-point correction, using one point as the baseline reference.</p> <p>Reference range: Select for two-point correction, using a point on either side of the peak to calculate the baseline.</p> <p>Generate pass/fail result: Select to create a pass/fail result that can be used in a Decision tile.</p>
Peak Ratio	<p>Find the ratio of height between two peaks. Peaks can be calculated from zero absorbance units or from a corrected baseline.</p> <p>Not corrected: The peak heights are measured from zero absorbance (or from 100% transmittance)</p> <p>Single-point corrected: The peak height will be measured from the baseline at the wavenumber you entered.</p> <p>Two-point corrected: A point on either side of the peak will be used to calculate the baseline.</p> <p>Generate pass/fail result: Select to create a pass/fail result that can be used in a Decision tile.</p>
Find Peaks	Find the locations of peaks in your spectrum. The resulting spectrum with labeled peaks is available as a spectrum in the Report tile and as a template option in the Template Report 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
Spectral Math		Perform basic operations using a sample spectrum and a reference spectrum. For more on spectral math, see "Apply Basic Equations to Acquired Data"
	Sample spectrum	The starting spectrum to which the operation will be applied.
	Reference spectrum	The reference spectrum used in the operation.
	Operation	Add Subtract Divide Multiply
	Spectral Math Type	Select a type of spectral math. Available options include <ul style="list-style-type: none"> • Factor • Pathlength • Range
Normalization		<p>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.</p> <p>After a spectrum is normalized, you cannot use it for quantitative analysis unless you know the scaling factor and adjust the quantitative results accordingly.</p>

Setting		Description
	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.
Derivative		Convert the spectrum to either its first or second derivative to help you find the location or intensity of peaks.
	Select spectrum	The spectrum to which the operation will be applied.
	Order	Select either first or second order derivative.
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.
	Spectral range	Use the spectral range to exclude totally absorbing peaks from the correlation search.
Scalar Math		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.

Use Workflows

Setting		Description
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.
Conversion		Convert a spectrum to another unit.
	Select spectrum	Select the spectrum to convert.
	Conversion type	Convert to one of the following: <ul style="list-style-type: none"> • Absorbance • % Transmittance • % Reflectance • Log 1/Reflectance • Kubelka-Munk
Blank regions		Clear the data from one or more regions of your spectrum. See "Blank a region in your spectra" for more information about blanking regions. Set the start and end points for the region to blank. Click Add to add more regions.
Statistical spectra		Calculate the average and standard deviation of 2 or more spectra. View the resulting spectra in the Report tile. See "Calculate average and standard deviation spectra" for more information about calculating the average or standard deviation of spectra. Select 2 or more spectra, the calculation to perform, and the data format used in the calculation.
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.
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 variable	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 table	display a table of results, such as from TQ Analyst / Quant method or peak analysis. Displays results from previous instances of running the workflow, not just from the current run.
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

RUN PROGRAM

Use the Run Program tile to have your workflow run an executable file. For example, use this tile to create a step in your workflow that runs a third-party automated sampling accessory.

Combine this tile with the Variable tile or other tiles to create powerful workflows. For example, use the count variable from the Repeat tile to automatically increment an argument passed to the executable.

The Run Program tile can run only executable files that do not require any user interaction and that do not have a user interface.

Setting	Description
File name	The executable to run. Note that if you run this workflow on another computer, that computer must have this same EXE in the exact same file path.
Arguments	<p>Pass arguments to the executable. To include variables in the command, select a variable from the list and click Add to Arguments List. When entering arguments, observe the following syntax requirements:</p> <ul style="list-style-type: none"> • Each argument must be enclosed in double quotes (“”) • Separate arguments with spaces <p>Example: “-p 6” “workflowname.variable.myVariable”</p>
Verify program file integrity at run time	<p>Ensures that the executable is exactly the same file during runtime.</p> <p>When you create the workflow, the software stores the location and name of the executable file.</p> <p>If the file is replaced by a new executable with the same name, that file will be run instead. Select this option to ensure that the file is exactly the same file you selected when you created the workflow.</p> <p>We recommend leaving this selected to ensure that the exe has not been replaced with another file. If you update the exe intentionally, you must update the workflow as well.</p> <p>Turning this setting off is useful if you expect to update the EXE periodically and do not want to update the workflow. However, this may pose a security risk.</p>

SAVE RESULT

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.
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.

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.

Use Workflows

Setting	Description
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	<p>Determines the image that is displayed when the workflow is run. Accepts a file path to an image file.</p> <p>The following file types are valid:</p> <p>.PNG .JPG .GIF .BMP</p>
Desired aspect ratio	<p>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.</p> <p>Examples: 4:3 for older computer monitors</p> <p>16:9 is the standard for high-definition video and is common for current computer monitors</p> <p>Accepts the following:</p> <p>1:1 4:3 5:4 16:9 16:10 3:2 2:1</p>

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.

VARIABLE

Use the Variable tile to assign a new value to an existing variable or to create a new, custom variable. Variables created or edited with the variable tile can be used in other tiles.

Setting	Description
Operation	<p>Select an operation type. The operation you select determines the other settings that are available.</p> <p>Set Variable: Use to set the value of a current variable.</p> <p>Create Variable: Use to create a new variable.</p>
Set Variable	<p>Variable to set: Select a variable to change the value.</p> <p>Current variables: Provides a list of current variables in the workflow. Select one and click Add to Expression to include the variable in the expression.</p>
Create Variable	<p>Numeric or Text: Select a type for the value of this variable. The type determines what operations are valid for this variable. For example, if you set the type to Text, you will not be able to use the value of this variable for calculations.</p> <p>Variable name: Enter a name for the variable</p> <p>Initial value: Enter a starting value for this variable</p>

WORKFLOW TABLE

Import a CSV file to use as a template for your workflow.

With the Workflow Table tile, you can import a table of options to use throughout the workflow. For example, with this tile, you can select one option when you begin the workflow and then automatically load specific variables, methods, and images throughout the workflow that correspond to that option.

Setting	Description
CSV file	<p>Browse to a CSV file to import.</p> <p>Browse to select a new file. Reload to check the file for updates.</p>
Select row automatically	Automatically select a row from the CSV file.

Setting	Description
Operator selection	<p>The workflow operator selects a row manually during the workflow.</p> <p>Operator prompt: Text instruction to display to the operator.</p> <p>Column index for selection options: Specify the column to use as available options. The first column is index 1.</p> <p>Column index for selection images: You can also display an image along with the selection options. Set the index to 0 if you are not using images.</p>
Included files	<p>Shows what files are expected based on the CSV file and how many have been included in the workflow.</p> <ul style="list-style-type: none"> • Select Add to add one or more files. • Select Manage to view or remove included files
Tile name	Sets the name of the tile in the workflow canvas.

Custom Solutions

Bundle and share workflows using the Package Editor and open and run packages using the Operator interface.

In this section:

Custom Solutions	203
Create or Edit a Package	206
Operator Administrator	210

Custom Solutions

This page offers a brief overview of using packages and the Operator interface in OMNIC Paradigm software to develop and run custom solutions. When available, follow the links to find more detailed information about using specific features.

What Are Custom Solutions?

With custom solutions in OMNIC Paradigm software, you can design and bundle workflows for other operators to use.

A developer designs workflows and bundles them with all their required files into Packages and then shares the packages as RDEP files.

An Administrator then opens the packages so that the workflows can be run using the Operator interface.

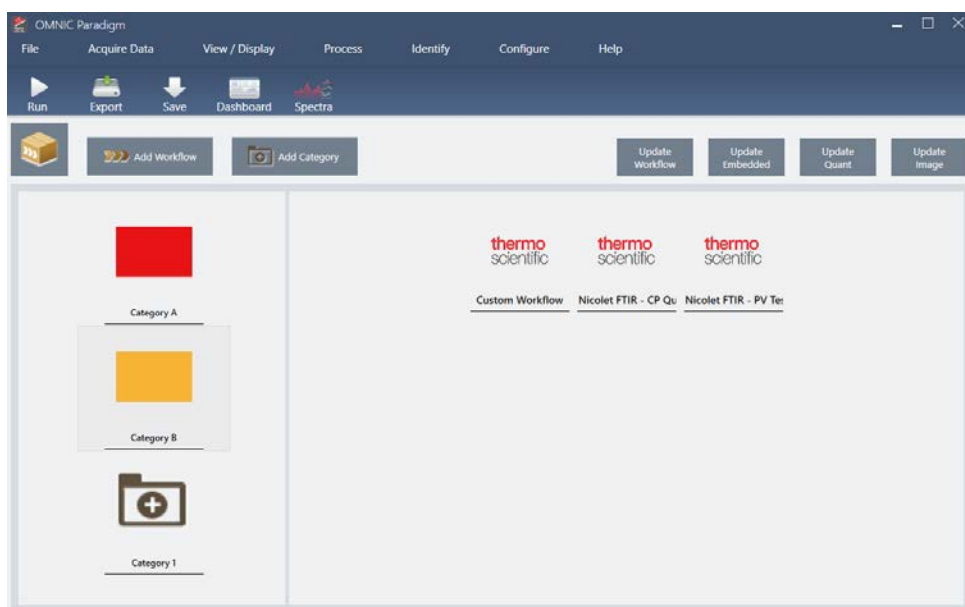
Packages and the Package Editor

A package is an organized collection of workflows that can be easily shared. When you bundle workflows into a package, the package includes all of the files and information necessary to run the workflow on another system, including any reference spectra, images, and QNT files.

When you create and export a package, an Administrator at another site can open the package in the Operator interface so that users can run all of the included workflows.

For details on creating and exporting packages, see ["Create or Edit a Package"](#)

Figure 6-1: The Package Editor



There are two major elements to a package:

- **Workflows:** A workflow is a pre-determined set of procedures and settings that ensure that procedures are carried out in exactly the same way each time. For more on workflows, see ["About Workflows"](#).
- **Categories:** In a package, workflows are organized into categories. You can group workflows into categories in any way that makes sense for your organization; however, a workflow can be included in only one category. The same workflow cannot be included in more than one category.

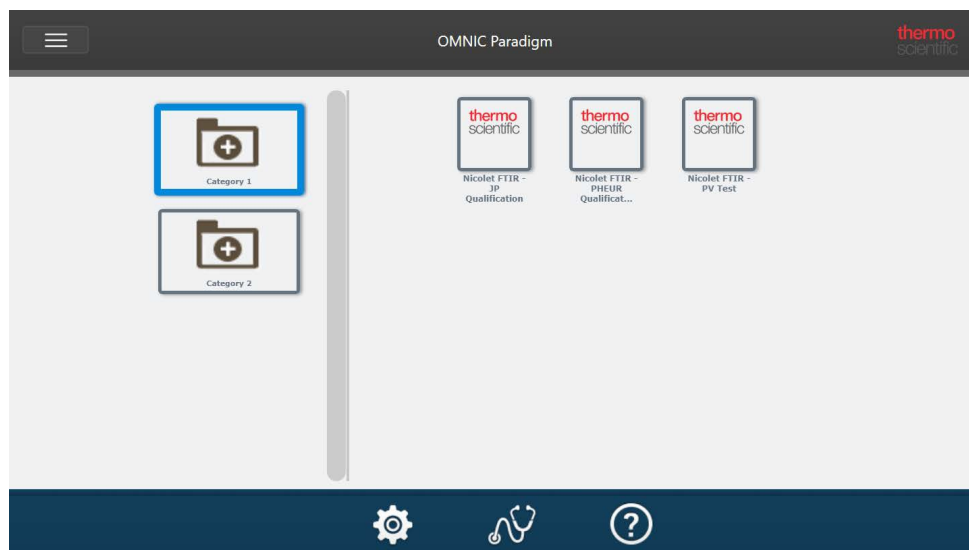
When you export a package, all of the required files used in the workflows are packaged as well, ensuring that operators have all the files they need to run the workflows when they open the package.

The Operator Interface

The Operator interface is used for running workflows loaded from packages and for managing packages. After opening a package, operators are presented with a simplified interface designed to run the package workflows.

The Operator Administrator can control which workflows are available by opening or deleting packages.

Figure 6-2: The Operator Interface



The Operator interface is similar to OMNIC Paradigm software's touchscreen interface but presents only workflows from opened packages.

An Operator Administrator can open, update, and delete packages using the administrator controls. For details on opening and deleting packages, see ["Operator Administrator"](#)

Tips for Working with Packages

When creating workflows and packages, it can be challenging to keep track of dependencies, such as quant methods and embedded workflows. The following tips may help you manage your files and ensure your workflows are up to date and easy to maintain.

- Organize your files so that they are easy to update and maintain. For example, you may want to create a single folder for resources used in your workflows. Then, within that folder, create specific folders for related items, such as quant methods, images, and spectra files. Then, keep the folder in the same location and keep the file names the same. You can then use the Update commands in the Workflow Editor to quickly update all of the workflow's dependencies.
- Keep your workflows as simple as possible. For example, the Embedded Workflow tile is a powerful tool, but it adds greater complexity to your project. Whenever the embedded workflow is updated, you will need to manually update every other workflow that uses it.

Create or Edit a Package

You can create a new package or open and edit an existing package with the Package Editor.

Before you create a package, you will need at least one workflow. For more on creating and using workflows, see ["About Workflows"](#).

Packages can be created only in the Desktop interface of OMNIC Paradigm software.

Create a New Package

◆ To create a new package

1. Using the desktop interface, go to File > Packages > Create.
2. Enter a name for the package and select OK. The package editor opens with one default category. You can add more categories or add workflows to the category.
3. To add a workflow, select a category and select Add Workflow.

Workflows can be included in only a single category. You cannot use the same workflow in multiple categories.
4. To add a category, select Add Category.
5. Select Save to save the package. The saved package is available in the Packages pane of the dashboard. The package is saved automatically when you return to the dashboard but is not saved automatically if you exit the software from the Package Editor.
6. To share the package, select Export. When you export the package, it is saved with an .rdep file name extension.

Tips for Organizing Workflows and Categories

There are a few important factors to consider when organizing your workflows and categories in packages.

- A workflow can be included in only one category. You cannot use the same workflow in more than one category. If you have workflows that you want to share across categories, you may want to create a separate category only for these shared workflows. This is true even with multiple packages. If a previously loaded package already includes a workflow with the same name, the operator Administrator will not be able to open a new package if it includes that workflow in

another category.

- Categories must also have a unique name. When the operator opens a package, any category that uses the same name as a category from a previous package will be merged. For example, if a new package includes a category named Category A, and a previous package already included a Category A, the categories will be merged into a single category including all of the workflows from both categories.

Consider the following example:

- Category A (First Package)
 - Workflow 1
 - Workflow 2
- Category A (Second Package)
 - Workflow 3

Is displayed as :

- Category A
 - Workflow 1
 - Workflow 2
 - Workflow 3

Edit a Package

You can open and edit a package either from the Packages pane on the dashboard or from a saved RDEP file.

❖ To edit a package

- From the dashboard of the desktop interface
 1. Scroll to the Workflows pane and select Packages from the list.
 2. Right click a package and select Edit. The package opens in the package editor.
- From a saved RDEP file

1. From the dashboard, go to File > Packages > Open.
2. Select a RDEP file and select Open. The file is added to the list of packages on the dashboard.
3. In the Packages pane, right click the package and select Edit.

If you open a RDEP file from the Package Editor, the package is opened in the Package Editor automatically.

Update Workflows

The Package Editor includes several tools for updating workflows and their associated files.

When you add a workflow to a package, the workflow file is copied to the package. Any updates apply only to this package copy and are not reflected in the original file or any other packages that have copied the workflow file.

To keep the workflow files and their associated files (such as images or QNT files) synchronized, you must update them in the Workflow Editor manually. To avoid unexpected behaviors or results, you may want to update the workflow directly using the Workflow Editor and then use only the Update Workflow command in the Package Editor.

Command	Description
Update Workflow	Reloads the selected workflows and updates any changes, including any files included in the workflow (for example, changed image files)
Update Embedded	Updates any workflows embedded using the Embedded Workflow tile.
Update Quant	Reloads any .QNT files that were included in the workflows.
Update Image	Reloads any image files used in the workflows.

Test Packages

Use the Run command to test the package before exporting it. By running the package, you can view and run categories and workflows as they will be shown in the Operator interface.

Note When you run the package, if you run any workflows that collect data, the measurements are added to your database just as if you ran the workflow normally.

Run Workflows Automatically

You can set a workflow to run automatically using Auto Run. If automatic running is enabled, the workflow will run without any operator input. The workflows will run in the background while you use the software. If a workflow is running in the background, the operator will need to wait for it to complete before running another workflow.

You can set workflows to auto run only if they do not require any user input.

If multiple workflows are scheduled to run with Auto Run, they are added to a queue. For example, if one workflow runs every hour and another every two hours, they will both run on the overlapping hours and will not interfere with one another.

◆ To enable Auto Run

1. In the Package Editor, right-click a workflow and select Set Up Auto Run.
2. Select Enable automatic running for this workflow and enter a value for the frequency in hours. You can also enter partial hours. For example, entering 0.5 will cause the workflow to run every 30 minutes.
3. Select OK.

The workflow will run automatically after the package is opened in the Operator interface.

Operator Administrator

Use the Administrator controls in the Operator interface to manage packages, to change the Administrator password, and to return to the Desktop interface.

To access the administrator controls, select Administrator from the menu in the Operator interface and enter the correct password. The default password is `Password`. The Administrator should change the password immediately after installing the software.

Manage Packages

Use the Package Maintenance tab in the Administrator view to manage packages.

Open a Package

Opening a package loads the package categories and workflows into the Operator interface. Once the package is opened, operators can select categories and run workflows. Any workflows set to run automatically will begin running as scheduled.

When you open a new package, new categories and workflows are added to the categories and workflows from previously opened packages. For example, if the administrator opens "Package A" and then later opens "Package B", the operator will see the categories and workflows from both packages.

◆ To open a package

1. Using the Operator interface, open the menu and go to Administrator.
2. Enter the password to access the administrator controls.
3. In the Package Maintenance tab, select Open.
4. Select a package file and select Open. Package files have a `.rdep` file name extension.

Update a Package

When you open a package with the same name as a previously opened package, the package is updated.

For example, if you have already opened a package called "Package A" in the past, when you open a new package that is also called "Package A", the new package replaces the previous package.

Delete a Package

Deleting a package removes that package's categories and workflows from the Operator interface.

❖ To delete a package

1. Using the Operator interface, open the menu and go to Administrator.
2. Enter the password to access the administrator controls.
3. Select one or more packages from the list of packages.
4. Select Delete and confirm your choice in the confirmation dialog.

Change Administrator Password

Use the Change Password tab to change the password for the Operator Administrator.

[This page intentionally left blank]

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.

In this section:

Create and Share Reports and Export Data	214
Create Historical Spectrum Report	218
Add Labels and Annotations to Spectra	219

Create and Share Reports and Export Data

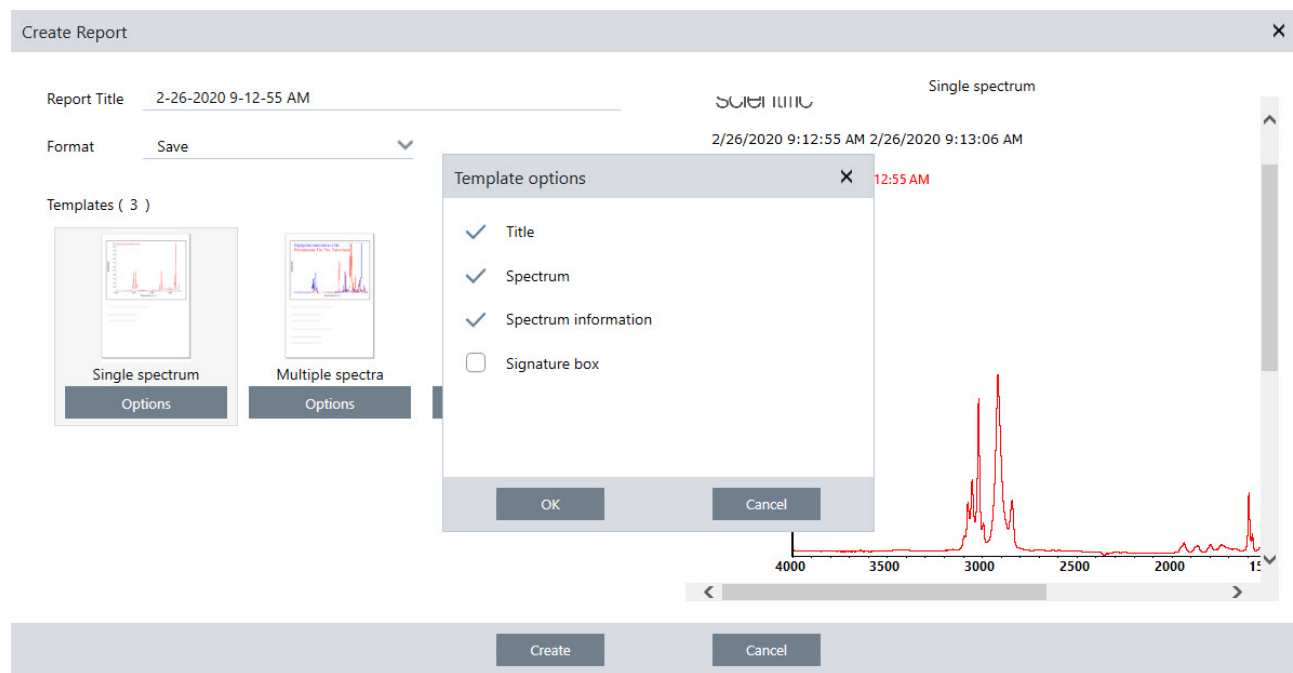
Generate reports from templates to quickly save or share your data as Microsoft™ Word™, PowerPoint™, or Excel™ files, or export your spectra, workflows, or settings.

❖ To create a report from the desktop interface

1. From the Spectra view, select File > Create Report.
2. 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. To configure the template, click Options and select items to include. Click OK to save your selection.



4. Click Create.

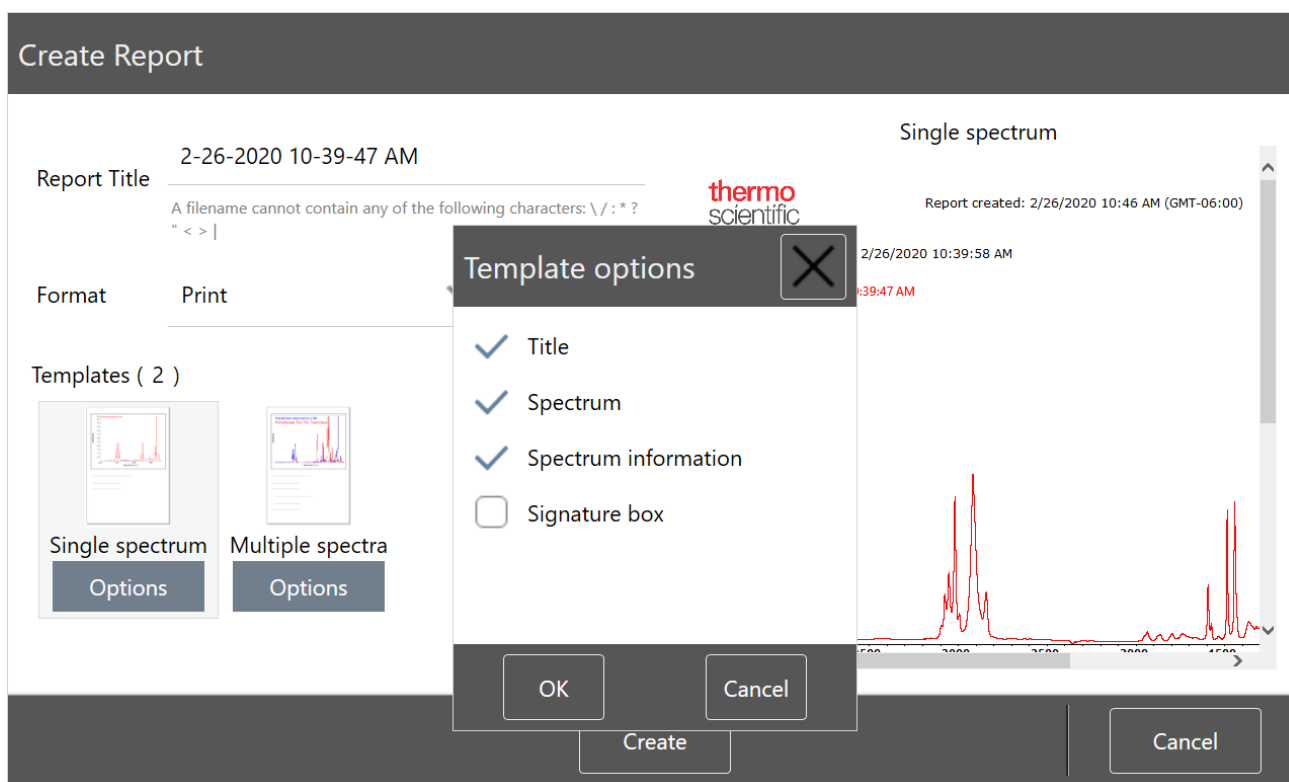
Create Reports

❖ To create a report from the touchscreen interface

1. From the spectral view, open the menu and select Create Report.
2. 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. To configure the template, touch Options and select items to include. Touch OK to save your selection.



4. 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.
 - c. Workflow files are saved with a .rwfl file extension.
- If you are using the touchscreen interface
 - a. In the Workflows tab, select the workflow you wish to export and select the more options menu.
 - b. Select Export.
 - c. Name your workflow file and touch Save.
 - d. Workflow files are saved with a .rwfl file extension.

❖ To export measurements

- If you are using the desktop interface
 - a. In the Measurements pane, right-click the spectrum you wish to export and select Export.
 - b. 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.

Create Reports

- c. Touch Save. Spectra are saved with a .spa file extension.

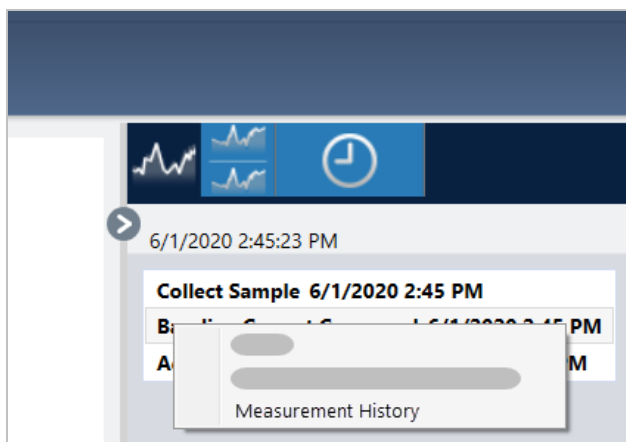
Create Historical Spectrum Report

A Historical Spectrum report includes detailed information about how a measurement changed over time as you carried out processing and analysis. The report shows the spectrum at each step in the history.

Creating a report of the measurement history is similar to creating other reports but requires you to first open the Historical Data view. The Historical Spectrum template will not be available if you open Create Report from the normal Spectral View.

❖ To create a Historical Spectrum template report

1. Using the desktop interface, open a measurement in the Spectral View.
2. Navigate to the measurement history tab.
3. Right-click any item in the history and select Measurement History.



4. Open the File menu and select Create Report.
5. In the Create Report dialog, enter a title for the report, select a format, and edit any template options. Only the Print and Save formats are available for Historical Spectrum template reports.
6. Click Create.

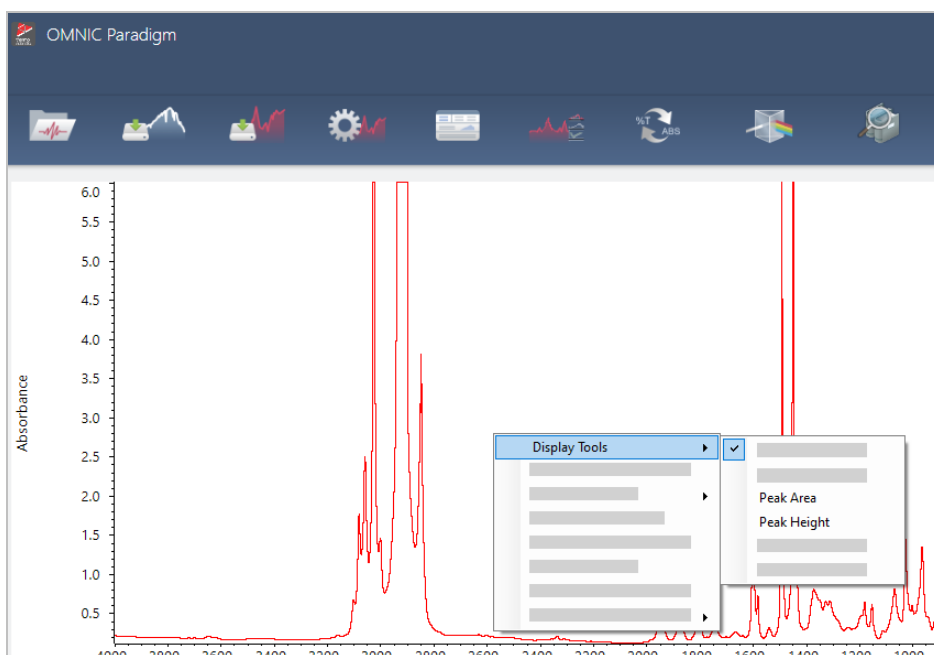
Add Labels and Annotations to Spectra

Use the Annotation Tools to add custom labels or to highlight features of a spectrum. Annotations are great for adding extra information to reports when presenting or sharing your data.

You can create annotations only in the Desktop interface.

❖ To add peak annotations to a spectrum

1. In the Spectral view, select a spectrum.
2. Right-click the spectral pane, select Display Tools, and select either Peak Area or Peak Height.

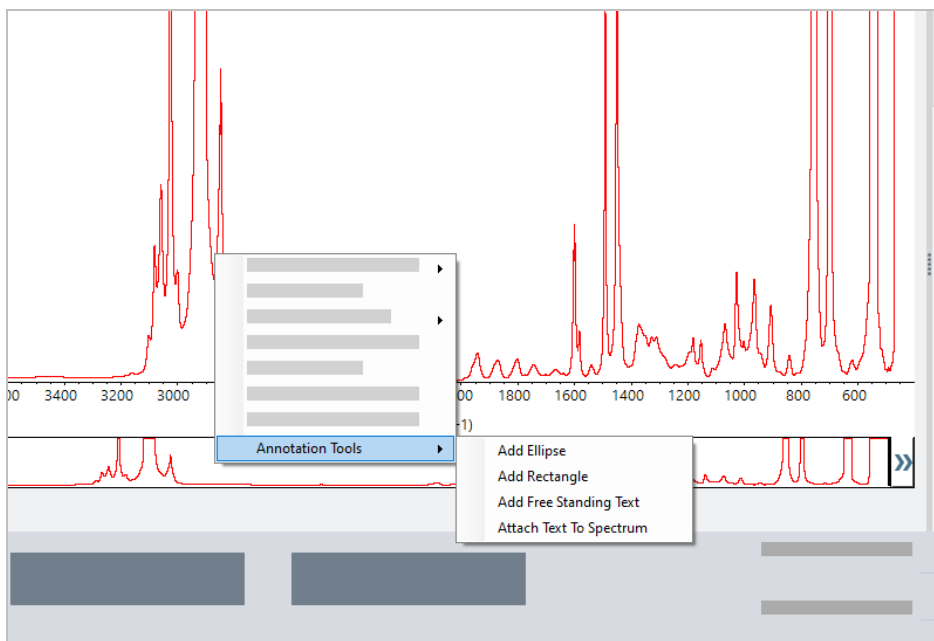


3. Adjust the settings for the peak tools and click Save.
4. To move the annotation, click and drag the text.

Peak height and peak area annotations cannot be edited or deleted using the right-click menu. To remove them, use the history to revert to an earlier processing step.

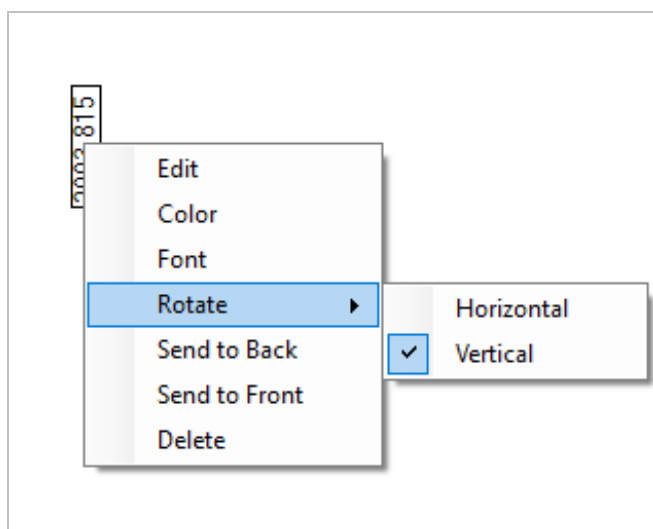
❖ To add custom labels and annotations to a spectrum

1. In the Spectral view, select a spectrum.
2. Right-click the spectral pane, select Annotation Tools, and select an annotation option.



3. To move the annotation, click and drag the text or, for an Ellipse or Rectangle, click and drag the top of the shape.

Right-click an annotation for additional customization options.



Protect Your Data

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

In this section:

Data Security and Integrity with OMNIC Paradigm Software	222
---	------------

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.