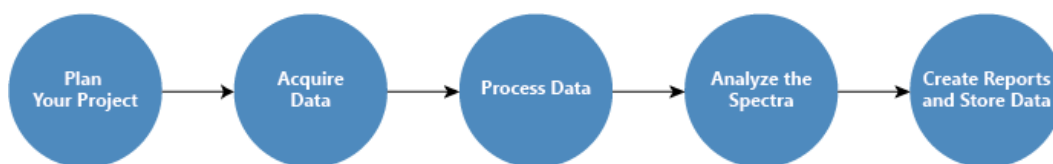


OMNIC Paradigm Software Basics

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 “[Measurement Settings,](#)” 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 Libraries.”](#)

For more on identifying an unknown sample, see [“Identify an Unknown 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.

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269-335800_Revision A