

Getting Started

This manual provides the information you need to get started collecting spectra with your Thermo Scientific™ Smart Raman spectrometer and DXR™ Raman or Thermo Scientific™ DXR3 Flex™ Raman microscopes.



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Your First Experiment

Detailed information about software features and operations is available in the Help system or the instrument documentation on your media (installed with the software).

Prepare the System

1. Turn on the instrument.
2. Start Thermo Scientific™ OMNIC™ software.
3. Align the instrument.

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- a. Click Expt Set () in the toolbar.
 - b. Choose the Diagnostic tab of the Experiment Setup dialog box.
 - c. Click Align  .

For more information, see OMNIC Help Topics in the Help menu.

Prepare and Install the Sample

Your sample may be one you provide or one you obtain from us.

- If you have a microscope, it will be a slide that is compatible with the microscope stage.
 - Place the sample on the microscope stage.
- If you have a spectrometer, the sample will be configured in a way that is appropriate for the accessory you are using.
 - Place the sample in the accessory you are using
- Move the stage to position and focus on the sample.

For detailed information on positioning and focusing, refer to *Using Your DXR Raman Instrument* located on the documentation set that came with your system.

Collect the Sample Spectrum

Before you collect a sample spectrum be aware:

- The experiment file sets the data collection parameters to appropriate values for your instrument and configuration.
 - When you choose an experiment from the Experiment drop down list box in OMNIC, the appropriate experiment file will open automatically.
 - If you wish, you can browse through the parameters to see how the system has been set up.

Choose Experiment Setup from the Collect menu.

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- Before you collect a sample spectrum, a background is normally collected so that it can be subtracted from the sample data.

This ensures that the peaks in the final spectrum are due solely to the sample.

- The background for your first experiment will be collected automatically by the software.
- After your first experiment, you can use the Collect tab of the Experiment Setup dialog box to specify how and when the background will be collected.
- Your options are:
 - collect a background before each sample collection
 - collect a background when a specified number of exposures is reached
 - use a smart background, which is a stored, high quality reference background
- A smart background takes about 40 hours to generate, so this feature is not available on the Collect tab until your system has been running for at least 40 hours and an initial smart background has been generated.
- The Auto Exposure feature, located on the Collect tab of the Experiment Setup dialog box, allows you to automatically set the exposure time and the number of exposures based on the desired signal to noise ratio.

This feature requires a smart background, so it is not available until a smart background has been generated.

❖ To collect the sample spectrum

1. Close the sampling area doors (if there are any).

2. Click **Collect Sample** () in the toolbar.

3. Type a title in the Collect Sample dialog box and click **OK**.

Preliminary data is collected and displayed. This lets you evaluate the spectral data or adjust the sample focus before starting the actual data collection.

4. Click **Start Collection** to start collecting sample data.

The button is in the upper-right corner of the window. When the sample data has been collected, the Confirmation dialog box asks whether to add the spectrum to a spectral window:

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5. Click **Yes** to add the sample spectrum to the window.

No ends the procedure without saving the spectrum.

Cancel returns you to the Collect Sample window.

Save the Spectrum

You can save your spectrum by using either of two commands, **Save** or **Save As**.

Search a Spectral Library

If you were unsure of your sample's composition, you could identify it by comparing the sample spectrum to the reference spectra in a spectral library.

❖ To search a spectral library

1. Select the sample spectrum.
2. Choose **Library Setup** from the **Analyze** menu.

The dialog box that appears contains a list of the directories that are currently being used for spectral searches.

3. Add the `My Documents\OMNIC\LIBS` directory to the list of directories if it is not already in the list.

This is the directory that contains the Raman sample library. To add the directory to the list, choose **Add Directory**. In the dialog box that appears, locate and select the `My Documents\OMNIC\LIBS` directory; click **OK**.

4. Add the library called "**Raman Sample Library**" to the list of libraries to search.

Click the library in the **Available Search Libraries And Groups** box; click **Add**.

5. Open the **Search Results** tab and select **Use Search Expert**.

Using the search expert saves time because it always searches the region from 2600 to 450 wavenumbers.

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6. Choose **Search** from the **Analyze** menu.

This opens the Search window. As library matches are found, the closest matches are added to the search results list in order of match value, with the best match listed first.

When the search is finished, the sample spectrum and the library spectrum that best matches it are displayed in panes in the upper portion of the window.

Comments about your search appear in the lower portion of the window.

7. Click **Close** to close the Search window.

Other Operations

Other useful operations that you may want to perform once you have collected a spectrum:

- Labeling peaks
- Creating and printing reports
- Creating user libraries
- Adding a spectrum to a user library

Information about these operations can be found in the software Help system.

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