FT-IR and Raman Spectrometers

Series

Getting Started

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Getting Started

Congratulations on your purchase of Thermo Scientific OMNIC™ Series software! You can use the software to collect, display and process time series data for GC, TGA, FT-IR, FT-Raman, rapid scan, kinetics and other applications in a graphically rich and interactive format.

This document will get you started using the software. These topics are covered:

Contents

- Starting the Software
- Series Data Sets
- Collecting Series Data
- Displaying Series Data
- Processing and Analyzing Your Data
- Finding Information
- Glossary

Once you are familiar with the basics, you can explore the more advanced features. Full instructions for OMNIC Series features are available through Series Help Topics in the Help menu and from within dialog boxes and task windows. See “Finding information” near the end of this manual for details. A helpful glossary of common terms is also provided at the end of this manual.

NOTICE Be sure that all persons operating this system read the site and safety manual first.

Starting the Software

❖ Follow these steps to start OMNIC Series

1. Double-click the OMNIC program icon on your computer desktop.

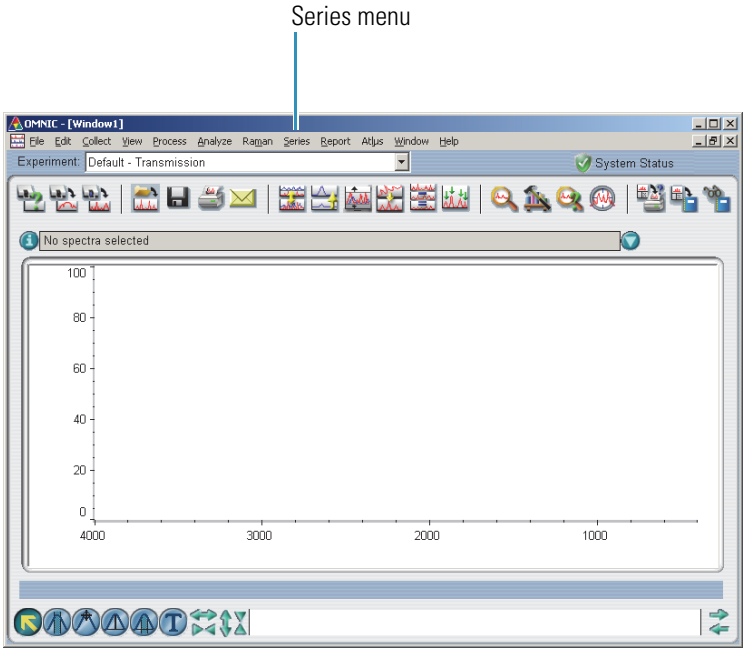
- If you have the DS option, you are asked to enter a password. Type the password for the user currently logged into Windows™ software and then choose OK.
- If you do not have the DS option but the log-in feature is turned on, you are asked to enter a user name. You may also be asked to enter a password. Type a user name (normally your name) and password, if required, in the appropriate text box and then choose OK.

  If you entered a name that is not recognized by OMNIC's log-in feature, a message informs you. Choose OK and then enter a valid name.

  If the configuration file associated with the entered user name has a password, a prompt asks for the password. Type the correct password in the text box and choose OK. (If you fail to enter the correct password after three attempts, OMNIC starts but only the Log In and Exit commands in the File menu are available.)

When OMNIC starts, the OMNIC window appears. Here is an example:

Figure 1. Series menu in OMNIC software



Notice that the Series menu is available in the menu bar, indicating that the Series features were installed with OMNIC.

You are now ready to use the features of OMNIC Series.

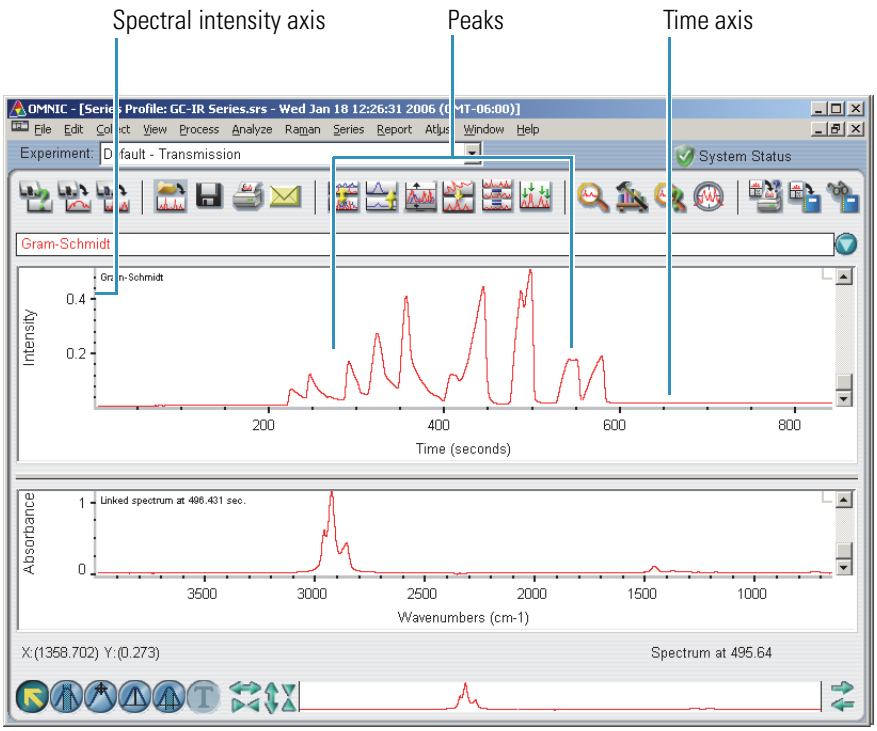
Series Data Sets

When you collect data using OMNIC Series, individual spectra are collected at intervals and saved automatically in a single file called a data set. In addition to the spectra, the data set includes the parameter settings for the collection, and the profiles created from the series data.

A profile is a plot showing spectral response, the result of a specified spectral calculation, or other data as a function of time. For example, a commonly used profile is a Gram-Schmidt reconstruction, a plot showing how overall spectral intensity changed during the experiment.

In the GC-IR example below, the peaks in the Gram-Schmidt plot indicate when different compounds in the sample eluted from the GC column, passed through the spectrometer beam path and absorbed infrared energy. This plot is the equivalent of an infrared absorbance chromatogram.

Figure 2. Gram-Schmidt reconstruction



Notice that the X-axis of the plot represents the elapsed time. In this case the time is measured in seconds, but minutes can also be used. The Y-axis represents relative infrared absorbance intensity.

In the case of Raman analysis, the intensity axis represents relative Raman energy emittance.

Once a data set is collected, you can do many things with series data. Here are a few examples:

- Display it in different ways to reveal spectral information.
- Create new profiles from it.

- Convert it to different units.
- Perform mathematical operations on it.
- Split it into separate spectral data files.
- Run a Mercury GC or Mercury TGA analysis.

Collecting Series Data

While the basic concept of series data collection is the same for all applications—spectra are collected at equal intervals over a span of time—there are some differences between FT-IR, FT-Raman and visible Raman collections. The summary below gives the general steps of series data collection.

Step 1: Set up the equipment.

In addition to the spectrometer, you may need to set up a gas chromatograph and GC-IR module or interface, a thermogravimetric analyzer and TGA-IR interface, or other equipment for time-based analysis.

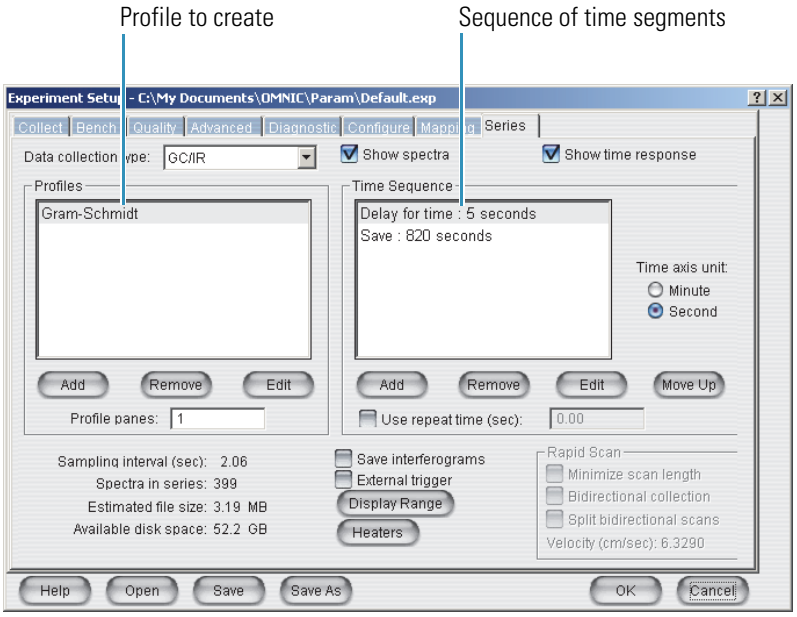
CAUTION Be sure to follow all safety precautions in the provided documentation whenever you use the equipment.

Step 2: Start OMNIC Series and set the parameters.

Use Experiment Setup in the Collect menu to set the experiment parameters. Those that are special to series data collection are on the Series tab of Experiment Setup. This tab lets you specify the profiles to create from the collected data.

In the example below, a Gram-Schmidt reconstruction has been specified in the Profiles box.

Figure 3. Selecting a profile



The Series tab also lets you configure the experiment as a sequence of time segments during which data is collected or discarded. This allows you to limit the data set to only the data that is of interest—and saves disk space. In the example above, two time segments have been specified in the Time Sequence box.

You can set other parameters for the collection on the Collect tab, Bench tab and other tabs in Experiment Setup. These parameters specify the number of scans, how backgrounds are handled, the spectral range, etc.

You can save your settings in an experiment file that can be opened later to set all the parameters in one step. Be sure to enter a unique and descriptive title for your experiment on the Collect tab so that you can identify it easily later.

Step 3: Prepare the sample.

As you prepare the sample and sampling device for the analysis, take into consideration how the background data, if any, will be collected.

Step 4: Start collecting data.

Choose Collect Series from the Collect menu to start collecting preliminary data. Typically a background and a set of basis vectors are collected first. The background serves as a reference to compare with the sample data that is collected over time. The basis vectors are used to calculate the Gram-Schmidt profile if that profile setting is used.

Step 5: Start the experiment.

The software prompts you to do this at the appropriate time. If a background was collected, the software waits for you to initiate the sample scan once the sample is ready to be analyzed. You can use an external trigger to synchronize the start of data collection.

For more information about collecting series data, choose Series Help Topics from the Help menu, find "data collection" in the Index, and go to the "Collecting series data" topic.

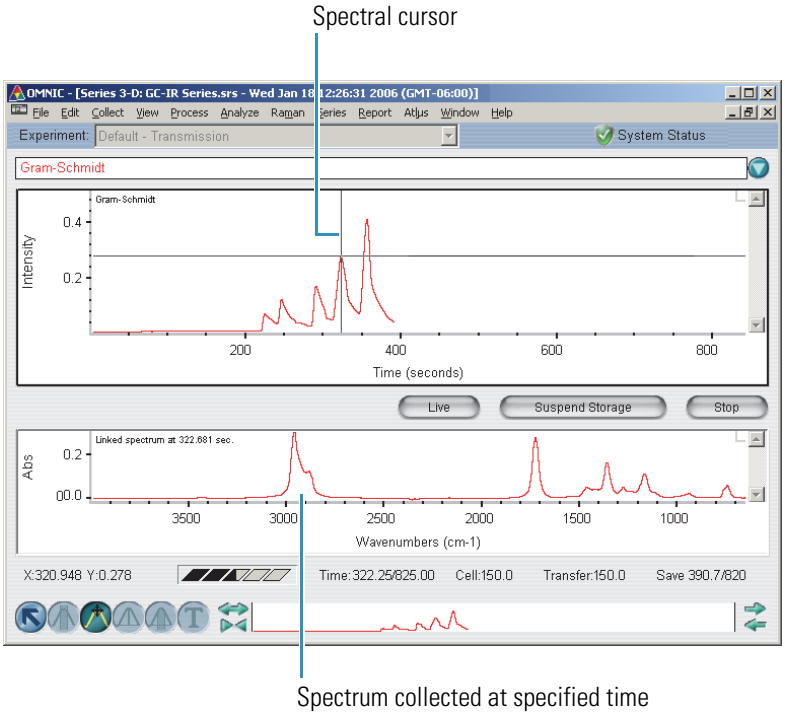
What happens during data collection?

As the experiment proceeds, data for the specified profiles gradually appears, left to right, in the time response display. The data is automatically saved as it is collected.

The spectrum currently being collected appears in the spectral data display. To display a spectrum collected at a particular time, first select the spectral cursor tool…

…and then choose the desired time location in the profile in the time response display. Here is an example showing the cursor located at the top of a peak in the time response display and the corresponding spectrum in the spectral data display:

Figure 4. Using the spectral cursor tool to display the spectrum collected at a specific time in the series data



To return to a "live" display that shows the spectrum currently being collected, choose the Live button.

Notice that the profile in this example is a Gram-Schmidt reconstruction, which was specified before data collection on the Series tab of Experiment Setup (see step 2 in the preceding section).

If you minimize the Collect Series window during the experiment, you can perform other tasks that don't exceed your computer's capabilities.

You can stop the collection at any time by choosing the Stop button. You can then proceed to process the data collected up to that point. If you do not stop the experiment manually, data collection proceeds until the specified run time is reached.

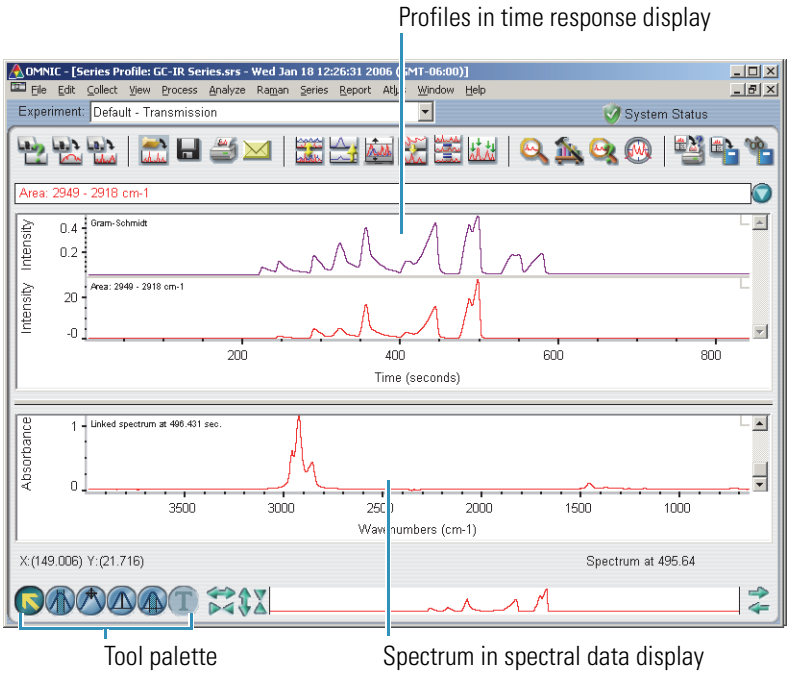
Displaying Series Data

Immediately after a series experiment, the collected data appears in a series profile window. This type of window is also used when you open a saved data set with Open in the File menu. When you open a data set, set Files Of Type in the Open dialog box to Series Files (*.SRS) and then locate and select the desired file.

Note An example data set named GC-IR Series.srs was installed in the OMNIC\Spectra folder when you installed OMNIC Series. You may wish to open this data set before learning about the display features described below.

Here is an example of a data set displayed in a series profile window:

Figure 5. Series profile window



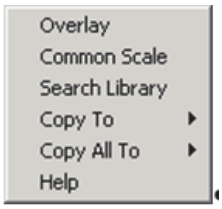
The **time response display** contains the profiles created for the data set during collection and those created using Profile Setup in the Series menu. A profile shows spectral response or the result of the specified spectral calculation as a function of time. The horizontal axis represents elapsed time, and the vertical axis is in a unit of relative intensity or other specified unit.

The **spectral data display** contains the series spectrum or interferogram collected at a specified time during the experiment or a spectrum created by coadding a time region of a profile. You can use the spectral cursor tool as explained in the "What happens during data collection?" section to display any spectrum or interferogram collected during the experiment.

The **tool palette** contains tools that let you display spectra, zoom in or out on the data, select a spectral region for processing, measure peaks in spectra, and perform other operations.

You can change the display limits for the axes in the active display by using Display Limits in the View menu.

When you right-click a pane in the window, a pop-up menu appears. Here is an example:

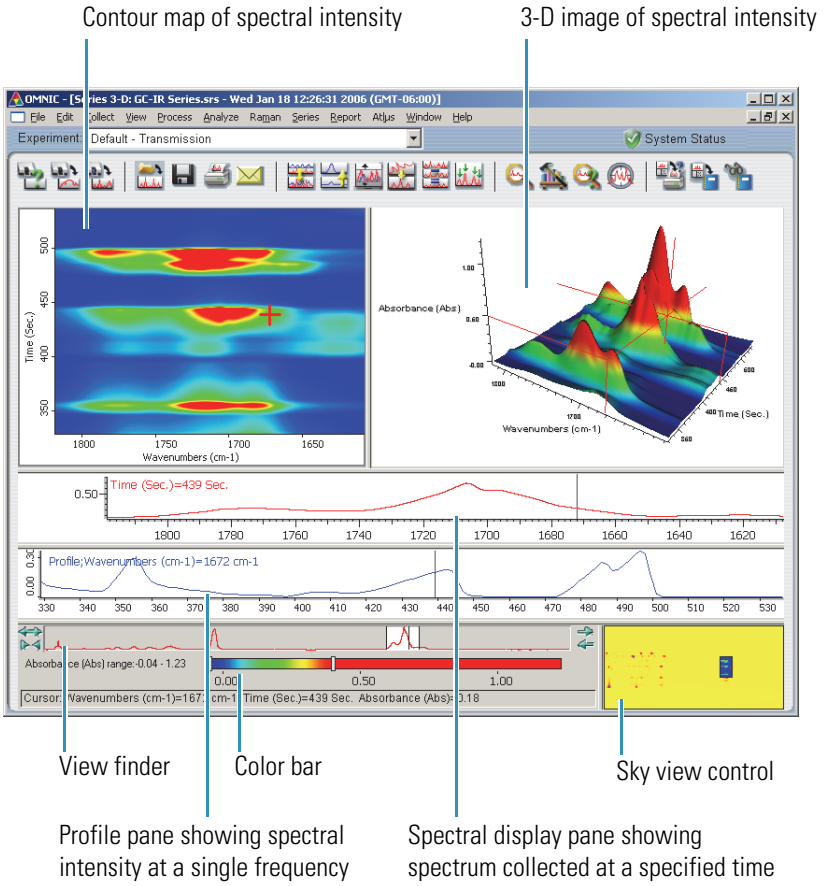


The features in the pop-up menus let you copy items, change the display scale of the data and perform other operations.

For more detailed information about series profile windows, choose Series Help Topics from the Help menu, find "series profile window" in the Index, and go to the "Using series profile windows" topic.

Another way you can display any series data is in a series 3-D window. It lets you view and extract useful information from your data with the help of an enhanced display. The window appears when you choose Show Series 3-D Window from the Series menu.
Here is an example:

Figure 6. Series 3-D window



This window lets you see different views of the data at the same time. Because the panes of the window are "linked," manipulating or interacting with the data displayed in one affects the others. For example, clicking a point in the contour map displays the corresponding spectrum in the spectral display pane. These features can help you reveal spectral information of interest, even in a very large data set.

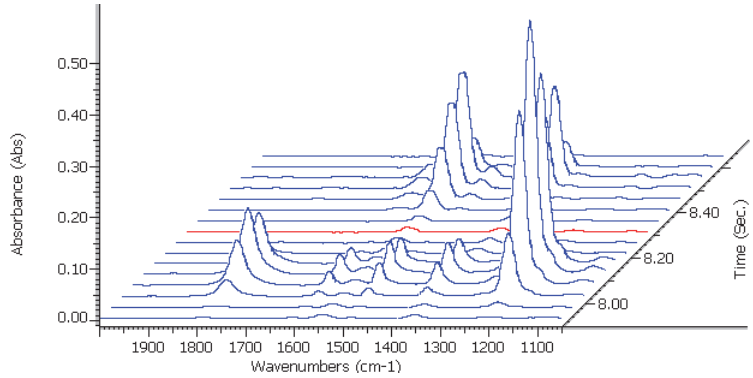
The **contour map** is a graphical representation of the spectral intensity of the series spectra. The "contours" in the map are areas of similar intensity displayed using the same color. The map is useful for locating high and low spectral intensities, because they stand out as areas of different colors. The X-axis is in wavenumbers or Raman-shifted wavenumbers and represents the frequencies at which spectral bands occur. The Y-axis is in time units and represents the time after the start of the experiment that each spectrum in the series was collected.

Initially the contour map shows data from the entire data set. To see more detail for a portion of the data, you can draw a box around an area of interest and click inside the box to expand it. The other panes are updated to reflect the new view of the data. Our example shows the result of zooming in on an area of the contour map. Notice that the 3-D image, contour map and profile pane contain only data from the expanded area, and the peaks in this portion of the data are easier to see.

The **3-D image** shows series data in three dimensions: time since the start of the experiment (Time axis), frequency (Wavenumbers axis) and spectral intensity (vertical axis). There are two kinds of 3-D images that can be displayed in this pane.

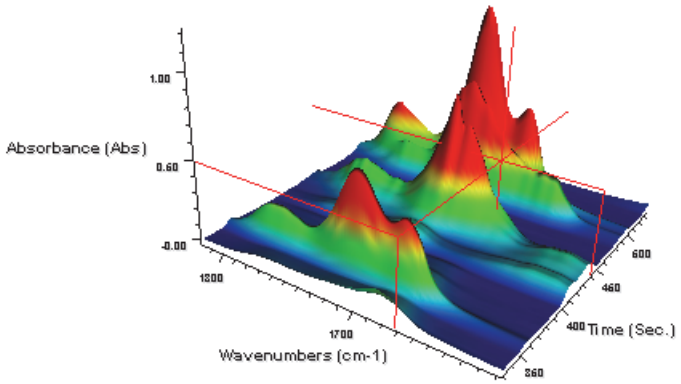
Waterfall view shows series spectra in the form of a link plot, a three-dimensional arrangement that makes it easy to see changes in absorbance response over time. This view is useful when viewing a narrow region of the data.

Figure 7. Waterfall image



Terrain view shows series data in the form of a three-dimensional surface plot (a smooth, interpolated surface.)

Figure 8. Terrain image



These images are useful for locating high and low spectral intensities, because they appear as upward or downward pointing peaks—and typically also appear in different colors in Terrain view. You can rotate the image to see the data from any angle.

The **spectral display pane** shows the spectrum collected at the time indicated by the vertical line in the profile pane. You can display a different spectrum by clicking the desired location in the 3-D image or contour map. You can display multiple spectra by holding down the Shift key while you click locations.

The **profile pane** shows spectral intensity at the currently specified frequency versus time. This is useful for finding when significant spectral response at a particular frequency occurred during an experiment; for example, a peak indicative of a chemical functional group in a GC experiment.

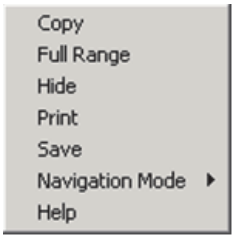
The **sky view control** lets you quickly change the display of series data by adjusting the size, shape and position of the box inside it.

The **color bar** shows the colors used in the contour map and Terrain view image. You can adjust the color bar to change the distribution of the colors for optimum viewing.

The **view finder** lets you adjust the displayed spectral region.

You can change how data is displayed in the current series 3-D window by using Display Setup in the View menu. For example, you can select the items to display, adjust the use of color in the contour map and Terrain view image, and specify a cursor style.

When you right-click most major features in the window, a pop-up menu appears. Here is an example:



The features in the pop-up menus let you copy items, display the full range of data, print items, save an image of the pane, and perform other operations.

For more detailed information about series 3-D windows, choose Series Help Topics from the Help menu, find “series 3-D window” in the Index, and go to the “Using series 3-D windows” topic.

Processing and Analyzing Your Data

The Process menu contains commands that let you process the active series data set. For example, you can convert the data to different units or correct the baselines of the series spectra. The available commands depend on the type of data displayed in the current window.

Processing operations change the data. The changes are not saved until you save the data using Save or Save As in the File menu. For more detailed information about saving series data, choose Series Help Topics from the Help menu, find “data set” in the Index, and go to the “Saving a data set” topic.

The Analyze menu includes features that let you analyze the active data set. Unlike the Process menu features, these features do not change the data. For example, you can use the Search feature to search the displayed spectrum against one or more spectral libraries to identify it. To quickly identify all the unknown material in a gas chromatography sample, use the Mercury GC feature which compares the spectrum at each retention time that shows a maximum spectral response against the selected spectral libraries and finds the closest match.

If you are working with data from a thermogravimetric analysis, the Mercury TGA feature in the Analyze menu can help you quickly identify the primary sample components, even if the material is a mixture. The software looks for a mathematical combination of reference spectra that best describes the unknown.

If you have installed OMNIC Specta™ software, you can export the selected spectra to that program by choosing Sent To OMNIC Specta from the Analyze menu. See the OMNIC Specta Help system for complete information about analyzing the exported data.

Finding Information

OMNIC Series includes the standard features of OMNIC plus additional features for working with time-series data. Each of these features is explained in OMNIC Series Help. To find information, choose Series Help Topics from the Help menu and then use the Index tab, Contents tab or Search tab just as you would in other Windows applications.

If a dialog box or window contains a Help button, you can choose it to see information about all the displayed features. To view information about an item in a series profile window or series 3-D window, right-click the item and choose Help (if present) from the pop-up menu.

To see information about regular OMNIC features, use the Help button as explained above, choose OMNIC Help Topics from the Help menu, or open the OMNIC User Guide in your OMNIC documentation set.For an overview of OMNIC, point to Getting Started in the Help menu and choose Getting Started With OMNIC.

Glossary

Becoming familiar with the important series terms defined below will help you learn to use the features of OMNIC Series.

basis vector – Spectral data used to generate a Gram-Schmidt reconstruction. Basis vectors are also used to eliminate unwanted features from the Gram-Schmidt reconstruction, such as baseline tilt or peaks due to water, carbon dioxide or contaminants.

Chemigram – A plot that shows the sample's integrated spectral response over a specified region as a function of time.

coadd – To average together each data point of the spectra in a time region to produce a spectrum with reduced noise.

contour map – A graphical representation of the spectral intensity of the series spectra, with intensities indicated by areas of a single color.

data set – A group of spectral data files collected during a series experiment, the parameter settings for the collection, and any profiles created from the series data.

Gram-Schmidt reconstruction – A plot of series data showing how relative spectral response changed over the duration of the experiment.

profile – A plot showing spectral response, the result of a specified spectral calculation, or other data as a function of time.

3-D image – An image that shows series data in three dimensions: time since the start of the experiment, frequency and spectral intensity.

Terrain image – A type of 3-D image in the form of a surface plot.

time segment – A period of time during a series experiment when data is either saved or discarded according to your specifications.

Waterfall image – A type of 3-D image in which lines connect points having the same intensity value.