OMNIC Array Automation Software

Automated collection and analysis software for array-based sample sets for Raman and FT-IR

OMNIC Array Automation is optional software fully integrated into the OMNIC Professional Software suite from Thermo Fisher Scientific. OMNIC software provides advanced chemometrics, rigorous qualification tools, and extensive spectral libraries for Raman and infrared spectroscopy. OMNIC Array Automation draws on and enhances the resources embedded in OMNIC software, providing an interface that is easy to understand and use.

Automating both data collection and analysis of array-based sample sets, OMNIC Array Automation reduces tasks that previously required hours of manual analysis into ones that can be accomplished in a matter of minutes. Such productivity gains facilitate applications such as high-throughput screening and crystallization studies.

OMNIC Array Automation Provides Support for a Variety of Sample Formats

OMNIC Array Automation includes predefined templates for many standard array-based sample formats, including standard 96-, 384-, and 1536-well microtiter plates. A standard template is also provided for the capillary tube array sample holder from Thermo Fisher Scientific, and the package provides an interface to define and store templates for custom sample arrays.

Automated Data Collection

OMNIC Array Automation automates all aspects of data collection – positioning the microscope over each sampling point, optimizing the focus, collecting Raman spectra and video images, applying specified spectral processing functions, and storing results. Direct operator involvement is needed only to load the samples and start collecting data.

Automated Data Analysis

Most autosampling packages just manage data collection. OMNIC Array Automation takes automation a step further by also automating data analysis. Simple analyses, such as identity verification, are easily performed by directly linking to TQ Analyst™ quantification methods. In addition, OMNIC Array Automation can execute sophisticated screening methods on all the samples in a data set. Group analysis flags samples with significant spectral differences, thereby saving hours of manual data analysis time.

Bidirectional Communication with LIMS

OMNIC Array Automation supports communications to and from LIMS (Laboratory Information Management System) platforms, allowing the LIMS to specify samples and analytical methods for incoming sample sets. OMNIC Array Automation also reports the results of the analysis back to the LIMS for archiving and decision making.

Compatibility with Multiple Instrument Platforms

OMNIC Array Automation is compatible with Thermo Scientific Nicolet™ Almega™ XR dispersive Raman microscopes, Nicolet FT-Raman spectrometers with either a MicroStage FT-Raman microscope or a ViewStage accessory, and Nicolet Series FT-IR spectrometers configured with well-plate reading accessories.
OMNIC Array Automation Software

Illicit Drug Analysis in Forensic Drug Labs

Raman is being used more and more frequently for illicit drug identification in high volume forensic drug labs. It offers rapid, non-destructive identification with almost no sample preparation. The ease of setup, ability to store analytical methods, and minimal operator interaction, make OMNIC Array Automation on Raman platforms particularly appealing for this application.

Common Applications for OMNIC Array Automation Software

Graphical Data Display

The interactive graphical data display provided by OMNIC Array Automation makes it easy to explore the results of an analysis with one click of the mouse. Displayed on the left of the screen is the multi-well array, which is updated in real time during data collection. A click on a well reveals the spectra obtained from that well. A visual representation of the results is readily available, since OMNIC Array Automation is able to color-code the wells based on a quantitative metric, a spectral property, correlation with a reference well, or as a result of a spectral classification algorithm. The user can decide whether to code all the wells with the same metric or to use an assortment of metrics for different wells.

Flexible Collection Options

OMNIC Array Automation gives you the flexibility to collect data in a format best suited to your needs. Not only can you specify the wells to analyze, but also the collection parameters for each well. Options include the ability to collect single or multiple points, average data from multiple points, search and select for the strongest signal in a well, and map the bottom of each well. Templates for 96-, 384-, and 1536-well plates are provided, together with the ability to design custom templates. OMNIC Array Automation supports visual and spectral-based autofocusing to ensure optimal response during unattended operation. Automatic background subtraction and real-time quantitative metrics are also available to speed data analysis.

Graphical Analysis Selection Tool

High Throughput Crystallization Studies in Pharmaceutical Drug Discovery

A valuable tool for crystallization screening applications, Raman microscopy is an excellent means by which to identify organic materials, and is particularly well-suited to discrimination between amorphous material and different crystal polymorphs – even between free bases and their related salts. Automated grouping functions found within OMNIC Array Automation software are particularly useful for high-throughput analysis of the very large data sets typically found in this type of application, making it a powerful new tool in the rapid identification of potentially new polymorphs.
Chemical Synthesis Experiments
Raman and FT-IR both generate excellent molecular structure information to help elucidate the progress of an organic synthesis. Performing a synthesis in parallel in an array format permits the simultaneous study of the influences of several parameters. The kinetics feature within OMNIC Array Automation software can be particularly useful in tracking the progress of slow reactions.

Biological Screening Studies
Raman is an emerging technique for biological screening. Measurement of samples deposited within grids on microscope slides is easily automated using OMNIC Array Automation software.

Powerful Data Analysis and Review Tools
Comprehensive analytical tools make it easy to extract valuable information. Designed for flexibility, OMNIC Array Automation enables you to tailor your analysis to your precise requirements. Automatically apply spectral preprocessing techniques such as baseline correction, multiple order derivatives, data smoothing, and reference file subtraction to the entire data set. All of the reanalysis tools provided by OMNIC software may be applied manually to individual spectra, or to groups of spectra. Data sets may be reanalyzed automatically by correlation with a reference well, by a quantitative metric applied either to the entire spectrum or to a selected region, or by principal component analysis. OMNIC Array Automation makes it easy to place spectra from multiple wells into a review window, enabling a closer inspection of entire columns or rows.

Productivity-Oriented Screening Tools
In the absence of automated data analysis, it can take hours to compare and classify the spectra from large sample arrays. The powerful tools provided by OMNIC Array Automation software reduce the time to perform an analysis to a matter of minutes. Automatic group and cluster analysis tools, combined with vivid graphical representation, permit rapid identification of outliers in a data set, elucidate relationships between spectra at a glance, and quickly draw attention to the interesting spectra in large data sets.
Flexible Array-based Sample Formats Supported

- Templates for 12-, 96-, 384-, and 1536-well formats included for simple experimental setup
- Ability to design custom templates for any array-based sample format accommodated by hardware. Includes sample grids on microscope slides or filter paper.
- 10 µm minimum step size for mapping within wells
- Capillary tube arrays†

Fully Integrated with OMNIC Software Suite

Compatible with:
- Nicolet Almega XR dispersive Raman microscopes, with motorized stages
- FT-Raman ViewStage accessory
- MicroStage FT-Raman microscope
- FT-IR well-plate sampling accessory

Interactive Graphical Data Display

- Rapid data review in easily understood formats
  - Ability to click directly on well to view spectra obtained from that well
  - Ability to color-code wells based on a quantitative metric, spectral property, correlation to a reference well, or spectral classification algorithm
  - Ability during collect to code all wells using the same metric or use different metrics for different wells
  - Graphical display updated in real-time during collect using autoranging option
  - Easy reanalysis post data collection

Flexible Data Collection Options

- Collect spectra from all wells or select wells only
- Optional collection modes: Automatically collect a single point in a well, specify one or more collection points in a well, calculate an average from multiple points in a well, search for the strongest signal in a well, collect from an array of points in order to map a well
- Apply quantitative metrics real-time during collection to save time when processing large numbers of samples
- Apply individual quantitative metrics to individual wells.
- Load and save collection methods for repetitive, routine analyses

- Supports video and spectral-based autofocusing, depending on hardware, ensuring maximum response during unattended operation
- Data preview window available during method setup facilitates selection of optimal data collection parameters
- Automatic background subtraction option available
- Estimated collection time for entire data set is automatically displayed in method setup window and is updated as changes are made to the method, facilitating workflow planning
- Kinetics collection mode allows repeated data collection from each specified well at specified time intervals
- Video images stored automatically with the spectral data for full sample documentation

Powerful Built-in Analysis and Review Tools

- Spectra from multiple wells, whole columns, or whole rows are easily placed into the review window for closer inspection and comparison
- Automatic data set reanalysis based on six different spectral properties; by correlation to a reference well, by a quantitative metric applied to the entire spectrum or just a selected region, or by principal component analysis, group analysis, or cluster analysis
- Graphical tools for specifying reanalysis of spectral properties
- Dataset analysis results easily exported to .csv files for communication with in-house databases (LIMS)
- All OMNIC reanalysis tools may be applied manually to individual spectra or groups of spectra
- Automatic spectral preprocessing techniques applied to entire data set:
  - Baseline correction (select polynomial order)
  - Smoothing
  - Blank regions
  - Replace regions with straight lines
  - Multiple order derivatives (First Difference, Savitsky-Golay, and Norris types)
  - Subtract a reference file (automatically or based on a pre-selected factor)
  - Convert between different IR data types (Abs, %T, %R, log (1/R), Kubelka-Monk)
  - Normalize

Automatic Group and Cluster Analysis

- Rapid analysis of large data sets reduces analysis time from hours to minutes
- Provides rapid identification of outliers in data set
- Graphic tools elucidate relationships between spectra at a glance
  - Group analysis tool
  - Hierarchical cluster analysis tool
- Draws analyst attention to interesting spectra in large data sets
- May be applied over entire spectra or over a defined spectral region

Support for Automated Sampling Stages

- Software-controlled loading and ejection of well plates, as well as illumination control on microtiter well-plate accessory
- Compatible with OMNIC macros used to integrate robotic sample delivery systems

Nicolet 6700 FT-IR configured with NXR FT-Raman module and MicroStage FT-Raman microscope

Comprehensive Data Archiving Options

- Save entire data set in one file
- Export all or part of the data set to individual spectral files
- Saved selected spectra individually
- Data headers on all data files with all collection parameters stored in them.

Regulated Environment Usage

Supports extended functionality of OMNIC Digital Signature (DS) software when this package is installed. The ValPro System Qualification package is available for both the Nicolet Almega XR dispersive Raman microscope, and the Nicolet NXR FT-Raman modules and spectrometers. ValPro System Qualification provides a thorough set of qualification tools for instrument compliance with commonly accepted regulatory requirements. The ValPro System Qualification package includes all the necessary components for compliance with Design Qualification (DQ), Installation Qualification (IQ), Operational Qualification (OQ) and Performance Qualification (PQ) testing.

† Requires appropriate hardware.

©2007 Thermo Fisher Scientific Inc. All rights reserved. All trademarks are the property of Thermo Fisher Scientific Inc. and its subsidiaries.

Specifications, terms and pricing are subject to change. Not all products are available in all countries. Please consult your local sales representative for details.