

OMNIC Software Suite



Full-Featured FT-IR, NIR & Raman Spectroscopy Software

Routine and Quality Control Analysis

Investigative Analysis and Analytical Services

Method Development

Time-based Spectroscopy

Microscopy and Chemical Imaging

Research and Development

Regulatory Compliance

Full-Featured Software with Integrated Tools for FT-IR, NIR and Raman Analysis

For analysts from routine to research, the highly acclaimed Thermo Scientific OMNIC™ software provides an intuitive and customizable graphical environment that allows users to quickly and efficiently acquire, process, analyze, and manage spectroscopy data, providing the best capabilities available to solve your analytical problems.

OMNIC software is the common platform used by all Thermo Scientific FT-IR and Raman laboratory spectrometers and is also available for our line of NIR industrial analyzers. It is at the heart of the Smart System approach to spectroscopy, providing an advanced level of integration between software, spectrometer, and sampling accessory.

OMNIC software provides tremendous functionality in an intuitive interface that can be configured to optimally meet your laboratory's analytical requirements. With OMNIC, it's easy to obtain the right mix of power and simplicity so you can confidently address your analytical needs and get the most out of your spectrometer and spectral data.

The Power of OMNIC

- Total control over experimental parameters to optimize data collection and processing
- Receive immediate feedback with live spectral displays before and during data collection
- Track data changes automatically using file-embedded audit trail
- Maximize the use of spectral libraries with a comprehensive library manager
- Assist data analysis with built-in spectral interpretation
- Create automated analysis routines using powerful and intuitive workflow generator
- Perform advanced peak fitting in overlapping spectral regions using Peak Resolve™
- Develop qualitative and quantitative methods specific to your analysis needs
- Perform advanced experiments, hyphenated techniques or IR or Raman microscopy using OMNIC's integrated add-on software packages

The many integrated add-on software packages offered with the OMNIC suite are designed to accommodate specialized applications in infrared and Raman spectroscopy. They enhance and complement the power of OMNIC software to provide the most complete set of

The Simplicity of OMNIC

- Effortlessly maintain proper experimental conditions with pre-set parameters and Smart Accessories™
- Ensure that both your system and sample analysis is working properly with continuous system performance verification
- Collect high-quality spectral data with no special processing using automatic atmospheric interference suppression
- Configure the toolbar with the most commonly used commands and automated workflows for push-button operation
- Complete QC verification easily using the QCheck spectral correlation routine
- Assemble spectra and associated information using report templates and store in Electronic Laboratory Notebooks
- Rapidly transfer analysis results to office productivity software
- Immediately send spectra to your colleagues using OMNIC's built-in E-mail tool
- Get the most out of your system with interactive multimedia tutorials and context-sensitive Help

spectroscopy tools. These tools provide the flexibility to expand capabilities as requirements grow. See the back cover of the brochure for a complete list of the OMNIC tools and add-on packages.

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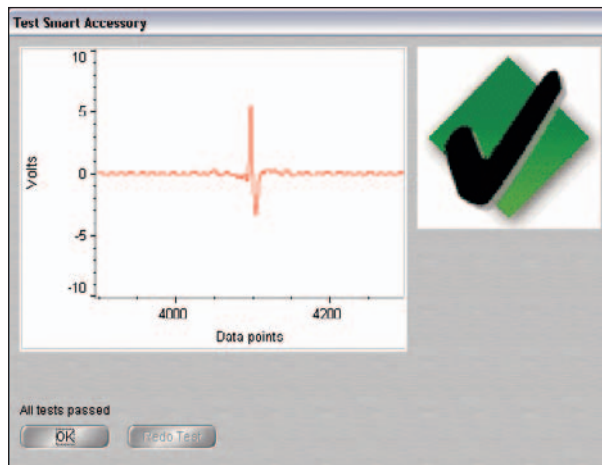
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OMNIC Simplifies Your Job and Builds Your Confidence

For any laboratory using FT-IR, NIR, or Raman spectroscopy, OMNIC has features that make it easy to collect, process, analyze and report spectral data and give you confidence in your results.

OMNIC software communicates with Thermo Scientific spectrometers and accessories, saving time and giving you confidence that the system is working properly and that your analysis results are accurate.

- **System Performance Verification (SPV)** monitors and provides status indication so you know the system is ready for your analysis
- Automatic accessory recognition and experiment set up ensures you get the best possible data

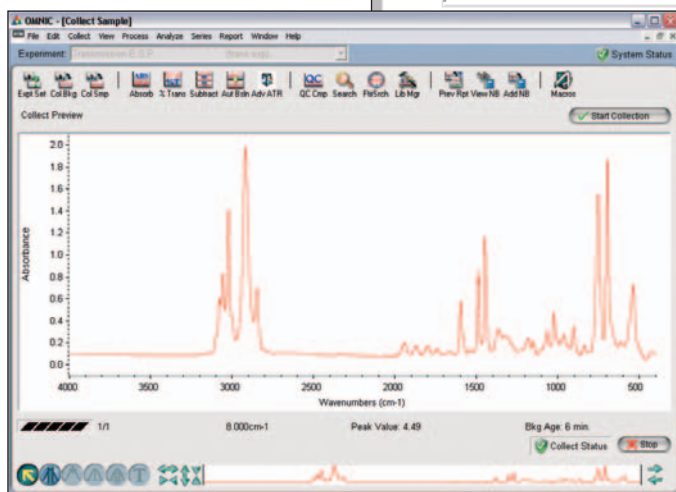


Smart Accessories are automatically recognized and their performance is verified when inserted

The real-time spectral display capabilities of OMNIC provide feedback and assurance that data is accurate. From diagnostic routines for spectrometer alignment to **Preview Data Collect**, OMNIC software provides constant updating of the spectral analysis progress.

And for those who can't wait for answers, spectral searches can be performed while scanning!

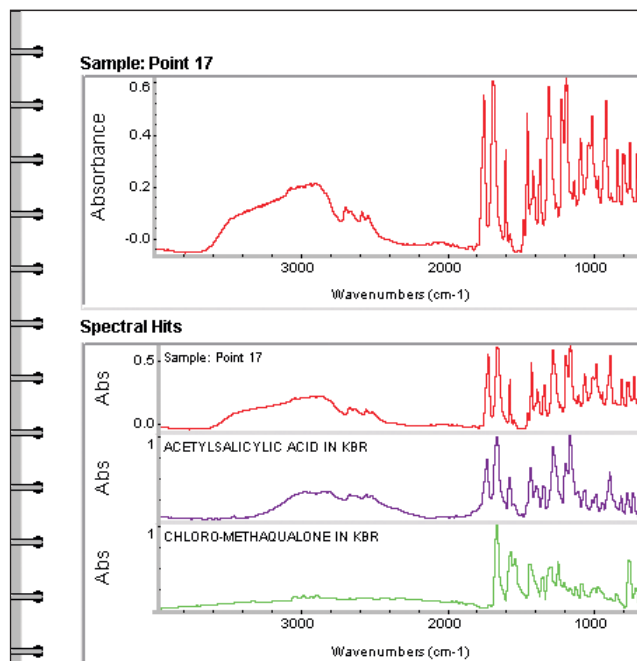
Preview Data Collect saves time so you know your spectrum will be acceptable before you commit the full collection time



OMNIC software has built-in features that allow you to handle your data conveniently and securely and report your results effectively.

- File-embedded audit trails track all collection and processing activity so you know everything that happens to your data
- **Electronic Laboratory Notebooks** with customizable reports make it easy to comply with GLP* guidelines without going out of your way
- Compatibility with popular word processing and presentation software provide convenience by allowing you to format your data and results to fit your needs

*Good Laboratory Practices



KBR
K KBR
EJ IN KBR
ORIDE IN KBR

Electronic Laboratory Notebooks allows you to save your customized results securely in a non-editable format

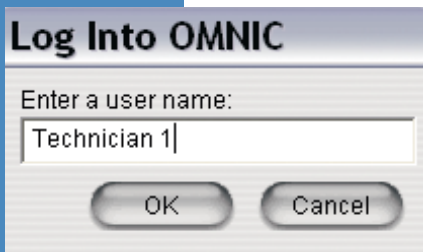
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OMNIC's extensive data compatibility makes it easy to use data files and spectral libraries from a wide variety of spectroscopy software packages. OMNIC can read data files in many common interchange formats such as JCAMP, GRAMS SPC, and CSV as well as data files from many instrument vendors' software. OMNIC can make use of spectral libraries and data files from many different FT-IR and Raman instrument software packages so you don't have to worry about moving to OMNIC and leaving your data behind.

OMNIC for Routine and Quality Control Analysis

In laboratories performing routine and quality control analysis, nobody likes surprises. Users expect reliability and ease of operation from the instruments they use. They must follow pre-set procedures with simple push-button analysis and need to know that their systems are working correctly.

OMNIC has many features designed to address these needs. For easy operation, the OMNIC interface can be configured to provide just what is needed to complete the task at hand. With features like user login, pre-programmed workflows and button-only operation, OMNIC provides the best tools available to obtain the most consistent results, letting you control the operator interface and ensure that your standard operating procedures are followed. System Performance Verification and live spectral displays provide feedback for the operators to let them know the instrument is set up properly and working as expected.

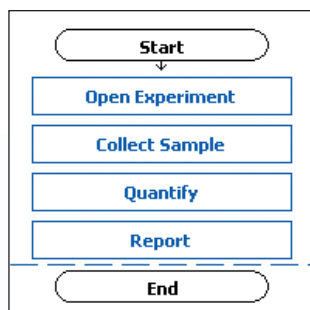


User logins provide a consistent user interface for routine operation

Quality control laboratories have the responsibility of verifying materials used or made in the plant to keep production moving. OMNIC communicates that the instrument results can be trusted, and enables efficient material confirmation with simple reporting of results.

OMNIC Logins let you configure task flow and software functionality assigned to individual users, ensuring consistent operation. OMNIC configurable toolbars and menus allow customization of the interface to meet the needs of the laboratory or individual users.

From method development to SOP automation and enforcement, OMNIC components make creation, deployment, and maintenance of routine analytical methods easy. See the Method Development section for details.

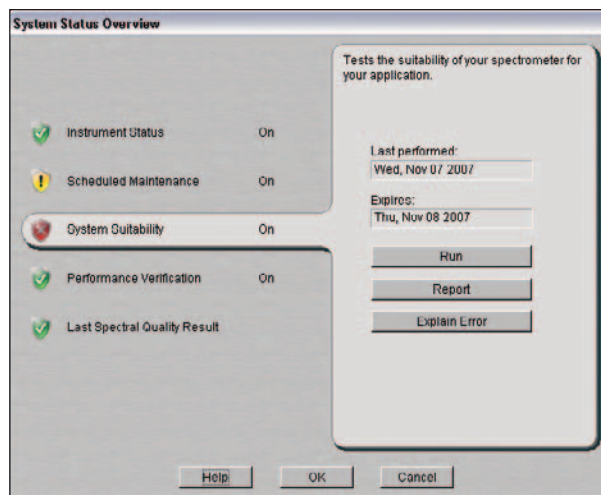


Automated routines and user feedback provide consistent results and build operator confidence



System Performance Verification (SPV) monitors and automatically communicates analyzer health and performance status to give you confidence in the system. The basis for SPV is centered in a System Status monitor that continuously ensures your system is working as expected, alerting you about scheduled tests, maintenance procedures, or other conditions that require attention.

SPV includes instrument diagnostics, ASTM based performance verification for the instrument* and system suitability tests for your specific methods**. You can also schedule system maintenance, and review spectral quality check results to make sure your samples are being run correctly.



If there's a problem with your system the System Status Monitor lets you know.



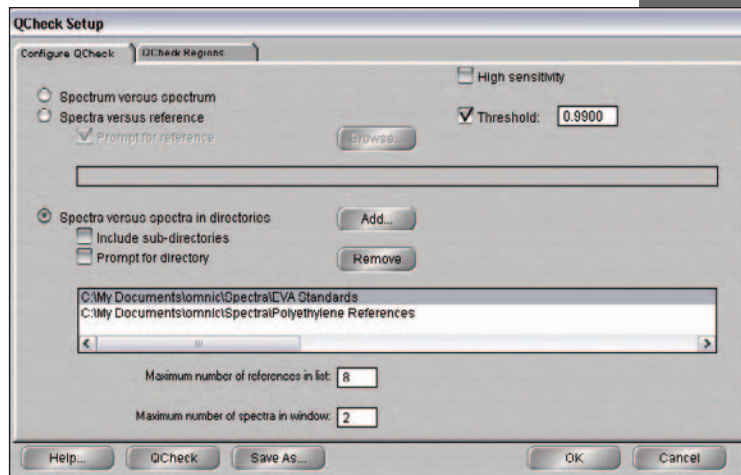
Automated routines implemented using OMNIC MacrosBasic™ become single-button workflows that ensure consistent analysis of your samples

* Performance verification tests not available for all spectrometers
 ** System suitability tests not available for all spectrometers



QCheck provide spectral correlation results with pass/fail limits

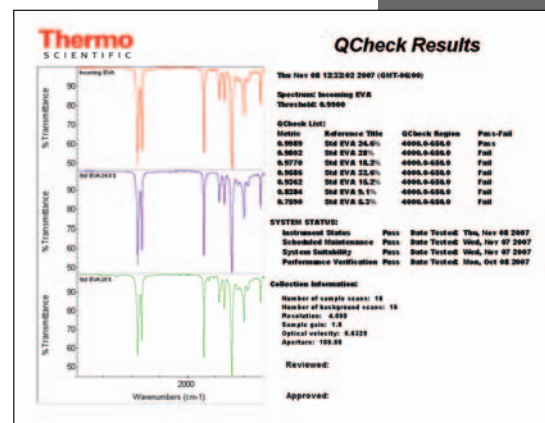
QCheck spectral correlation is an ideal tool for the verification of incoming materials, in process materials, or finished goods. With QCheck you can compare your test sample to one or more spectral files, allowing you to make the best comparison without needing to create reference libraries. If you are developing methods for routine use, QCheck lets you easily compare correlations in different regions so you can optimize comparisons for your specific materials to obtain the best results.



QCheck's unique High Sensitivity Correlation allow better differentiation of very similar materials

Unlike other spectroscopic QA/QC software routines, OMNIC's QCheck can operate in Normal and High Sensitivity mode. For products and processes where extremely small compositional variability can mean the difference between passing and failure, these differences are typically undetected or treated as passing in standard QA/QC comparison software. The QCheck high sensitivity mode brings unprecedented screening and discriminating power to identify small material differences and can be an invaluable safeguard for manufacturers' products and reputations.

The **OMNIC Report** feature makes it simple to communicate and archive your results flexibly and professionally. Reports include important elements such as spectral displays, search or quant results, collection parameters, and even your company's logo. And you can paste reports and other OMNIC results directly into popular office productivity software for printing or archiving.



Results are reported consistently using the OMNIC report templates

21 CFR Part 11

For those who need compliance with 21 CFR Part 11 regulations, OMNIC DS Data Security with Thermo Security Administration is ready for the most demanding security and accountability requirements.

System Qualification

For labs in regulated environments, or for those who want a higher level of documented and traceable performance verification, ValPro System Qualification provides cGMP and Pharmacopoeial level qualification and is available for all FT-IR, NIR, and Raman systems.

See *OMNIC and Regulatory Compliance* page for details.

Key OMNIC Components

System Performance Verification (SPV)
Login & Toolbars
OMNIC Macros\Basic
QCheck

OMNIC for Investigative Analysis and Analytical Services

The world of the investigative analyst is filled, literally, with unknowns. For samples that come in the door and must be identified quickly and efficiently, OMNIC offers everything you need. From the powerful and easy to use OMNIC software to the all new OMNIC Spectra™ material characterization software plus our extensive offering of spectral libraries, OMNIC provides all the tools to get to answers with confidence.

OMNIC software includes a full suite of spectral investigation tools such as Advanced ATR correction, interactive Kramers-Kronig correction, baseline correction, math functions, peak labeling, Peak Resolve advanced spectral peak fitting, Library Manager, IR spectral interpretation, and spectral navigation and display tools. OMNIC is the benchmark to which all other analytical spectroscopy software is compared.

For the investigative user requiring heavy use of searching and identification of unknowns and spectral data management, **OMNIC Spectra** is a new software tool that redefines investigative spectroscopy by combining a powerful set of spectral identification tools with a logical interface that steps through data analysis efficiently.

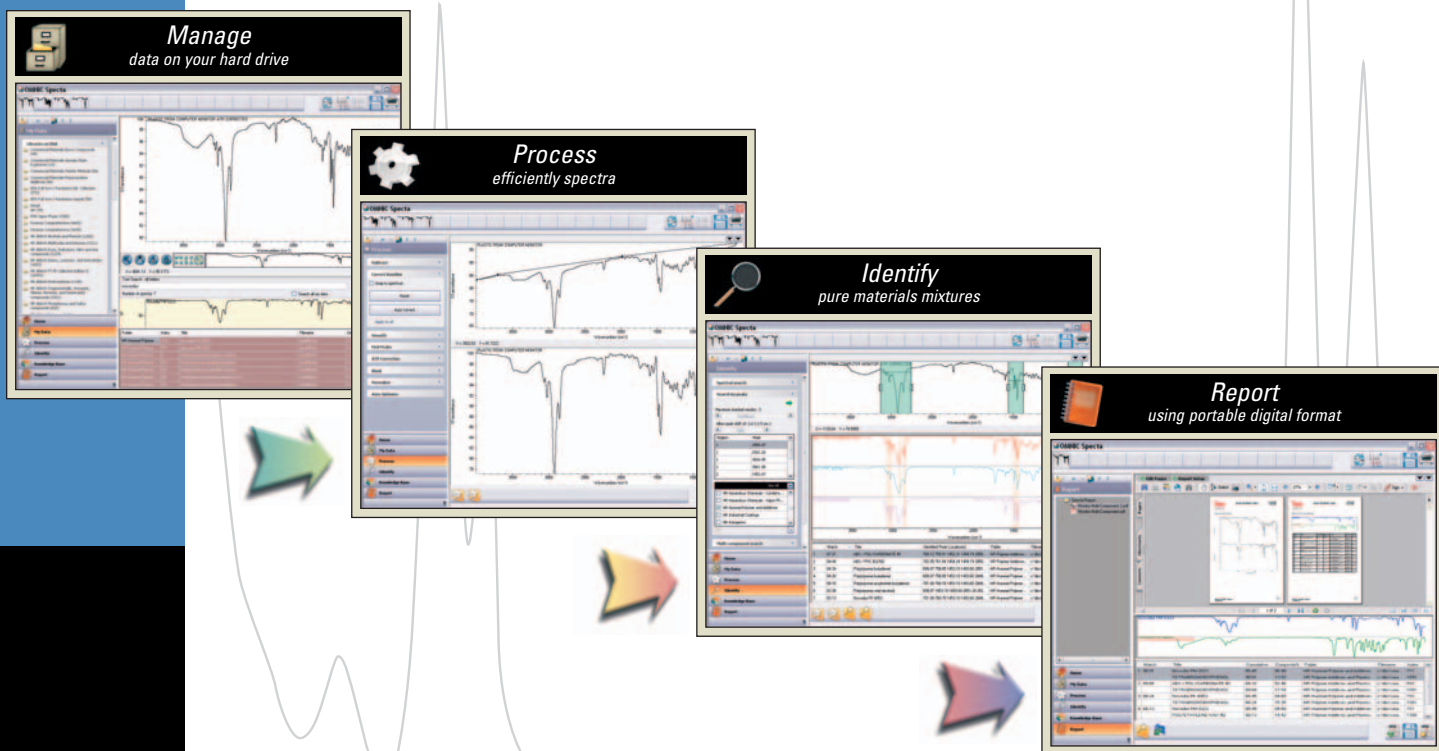
OMNIC Spectra includes revolutionary multi-component mixture searching, interpretation algorithms and a knowledge-base of scientific documentation. The software indexes spectral data on the workstation and organizes it for immediate availability and use in reviews, searches, measurements, and reports. With OMNIC Spectra your hard drive becomes a spectral database, eliminating the need to create libraries and improving data access efficiency.

With OMNIC Spectra at your command, you leave behind the often labor-intensive operations found in most spectroscopy software. Tasks flow naturally without sacrificing power where you need it. OMNIC Spectra allows you to focus your efforts towards getting the answers you need and taking the required actions.

OMNIC Spectra Empowers You To:

- Manage data on your hard drive easily
- Process information with ease and confidence
- Identify and interpret pure materials and mixtures
- Present reports in a portable digital format
- Expand your infrared problem-solving skills with an extensive spectral data collection included with the software

No molecular spectroscopy problem solving toolkit is complete without spectral databases. We offer an extensive offering of FT-IR and Raman spectral libraries that range from general chemical to forensic and industry-specific collections designed to assist in your analytical investigations.



Key OMNIC Components

- OMNIC Process Functions
- OMNIC Analyze Functions
- OMNIC Spectra
- FT-IR and Raman Spectral Libraries

OMNIC for Method Development

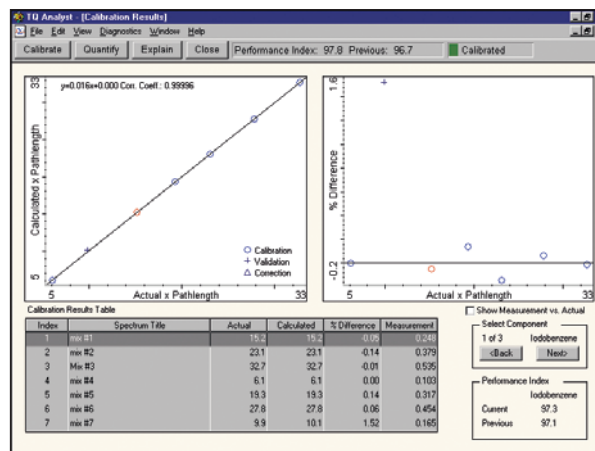
Behind the scene of quality control or routine analysis lies qualitative or quantitative methods that extract answers from the spectra of the materials you analyze. Whether spectroscopy is used for routine analysis, quality control, or process control, the development chemist needs the right tools to create, verify, and implement these methods.

TQ Analyst™ qualitative and quantitative analysis software is a comprehensive method development platform for users of all experience levels. It employs an intuitive interface and program flow not available in similar packages. TQ Analyst enables even users with minimal training or familiarity with chemometrics to create high performance methods.

The comprehensive set of method development tools for qualitative and quantitative analysis in TQ Analyst include search, distance match, similarity match, QC Compare, discriminant analysis, Simple Beer's law, stepwise multiple linear regression (SMLR), classical least squares (CLS), partial least squares (PLS) and principal component regression (PCR).

TQ Analyst has all the performance and flexibility you need to develop robust methods and is available in Professional and EZ Editions.

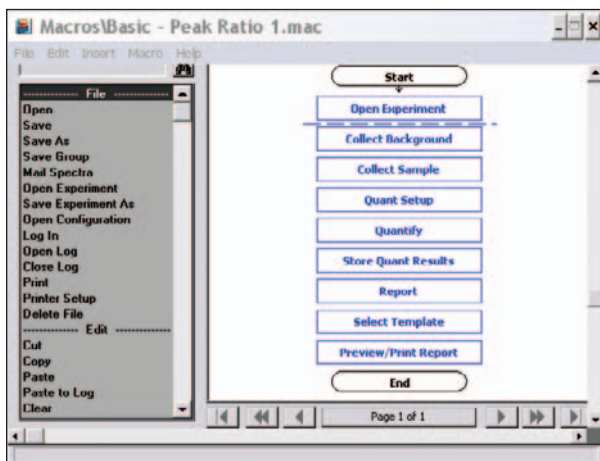
Once a method is built in TQ Analyst, deployment for routine operation typically follows. **OMNIC Macro\Basic** is ideal for creating routine analysis workflows that set system parameters and instruct the operator, saving time and ensuring that the analysis is consistent and reproducible. This gives you the confidence you need in the end results.



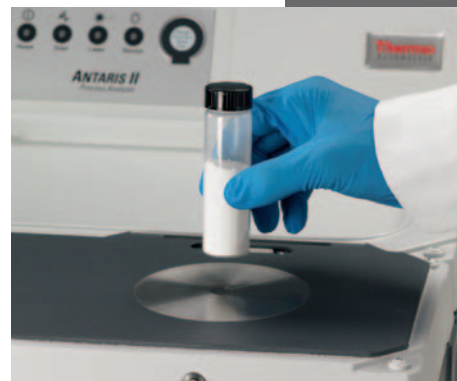
TQ Analyst's calibration results window shows how well the method performs

OMNIC Macro\Basic, with its intuitive, point-and-click environment, allows you to assemble the tasks required to analyze and process samples following your standard operating procedures. With OMNIC Macro\Basic even novice users can implement methods, since there is no need for programming skills. Results can be output in reports, saved in an OMNIC Electronic Laboratory Notebook, or sent directly to your LIMS software.

Once developed, your OMNIC Macro\Basic procedures may be added to the OMNIC interface for routine execution. OMNIC Macro\Basic is the right solution for automating tasks, allowing all operations to be performed with the simple push of a button.



OMNIC Macro\Basic intuitive graphical interface allows easy implementation of automated routines.



Key OMNIC Components

- TQ Analyst
- OMNIC Macro\Basic

OMNIC for Spectroscopy of Dynamics Events

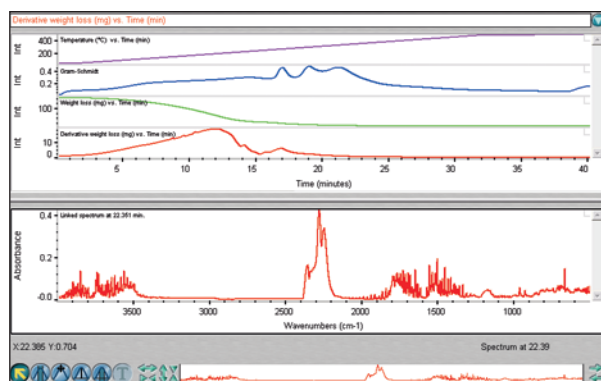
For laboratories that analyze chemical features changing or evolving over time, OMNIC has the capability to collect and process data at sufficient speeds to elucidate the nature of the changes. OMNIC Series software includes the most useful features to handle dynamic FT-IR and Raman spectral data efficiently. Combining OMNIC Series software with TQ Analyst and automated workflows created in OMNIC Macro\Basic, gives you everything you need to handle even the most demanding kinetics or flowing stream analysis application.

OMNIC Series software is a powerful data collection and processing tool designed to couple FT-IR or Raman spectroscopy with other analytical techniques to address applications where spectra change with respect to time, temperature, or other phenomena. Techniques commonly monitored using FT-IR include gas chromatography (GC), thermogravimetric analysis (TGA), automotive exhaust gas, fire chemistry, surface plasmon resonance (SPR), and kinetics experiments. OMNIC Series can also be used for Raman experiments such as kinetics studies.

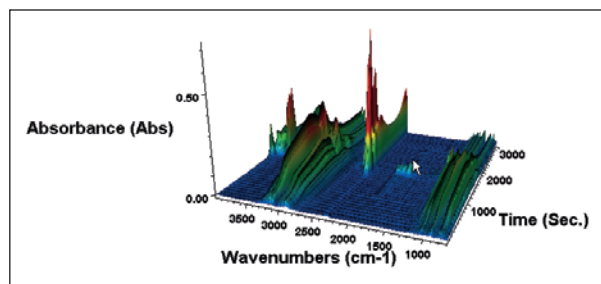
OMNIC Series software is fully integrated with OMNIC and puts experimental control at your fingertips. Real-time display of IR spectra and up to five different pre-programmed spectral profiles is available, providing a continuous update of chemical changes with respect to time. Spectra can be viewed and searched during data collection providing the analyst immediate feedback.

Beyond data collection, OMNIC Series has many features to process data to help reveal, isolate and extract useful information including:

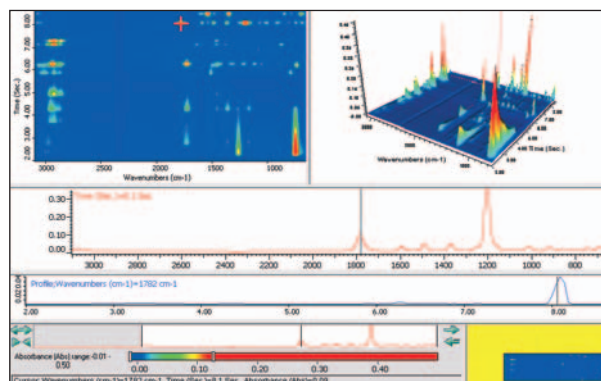
- State-of-the-art 2- and 3-dimensional interlinked views allow optimal navigation and provide information critical to understanding the results
- Data optimization tools, including co-addition and basis vector addition, improve results and eliminate baseline effects or isolate overlapping components
- Profile reconstructions to assess specific functional groups, quantitative analysis results, or peak ratios as a function of time
- Batch processing using a wide array of OMNIC functions
- Creation of series sets from existing spectra or splitting data sets into smaller ones



OMNIC Series Profile window can be used to view real-time data or for data analysis after the collection is done



OMNIC Series 3D window allows the analyst to navigate the data to assist with information discovery



OMNIC Series interlinked 2D and 3D display of TGA-IR data

Key OMNIC Component

OMNIC Series

OMNIC for Microscopy and Chemical Imaging

In a world where materials are getting smaller every day, the ability to obtain chemical information from small samples is critical. OMNIC Atlus™ imaging software offers an attractive and efficient means to aid in the collection and processing of data from microscopic samples to verify chemical distribution in homogenous samples or locate defects or contaminants on a heterogeneous sample.

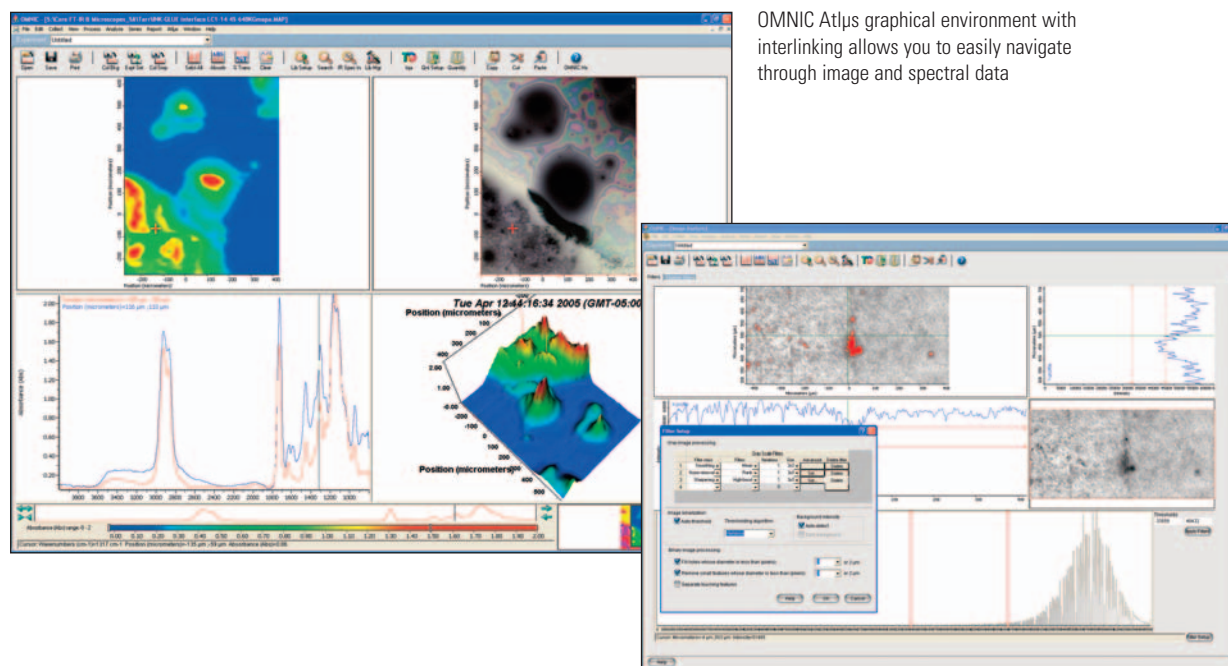
OMNIC Atlus provides data collection, processing, and visualization with powerful, easy to use software that is fully integrated with OMNIC. It provides the very best in spectral manipulation, spectral searching, and chemometrics, and supports multiple microscope stages. OMNIC Atlus is compatible with all Thermo Scientific FT-IR and Raman microscopes.

With the most powerful infrared and Raman image analysis tools available on the market, OMNIC Atlus allows extraction of physical, chemical, and spatial information from your sample. While image analysis is widely used in microscopy to provide dimensions, shape and distribution of sample features, OMNIC Atlus extends this powerful capability by applying image analysis to both video and chemical images of the sample. Data acquisition includes image mosaic collection, discrete points, line maps and area maps in transmission, reflectance, or ATR. OMNIC Atlus shows contour display, 3D display, video image, and spectral data view all interlinked in a single easy to use interface.

Image analysis applied to optical and chemical images extracted from the sample provides physical and chemical information specifically for each component including:

- **Number and size of sample features** – particles, fibers, and irregularly shaped objects
- **Physical information** – length, diameter, area, and much more
- **Analysis of a chemical image** – for each material identified in a sample
- **Total distribution of each material** – semi-quantitative with no need for calibration

Chemical images can be based on spectral frequency, functional group, correlation to a reference spectrum, Principal Component Analysis, Multivariate Curve Resolution or a chemometric model derived from TQ Analyst. These capabilities allow users to obtain the most useful information from their materials to help them find the answers they need to problems big and small.



OMNIC Atlus graphical environment with interlinking allows you to easily navigate through image and spectral data

OMNIC Atlus image analysis tools extract detailed information from video and chemical images

Key OMNIC Component

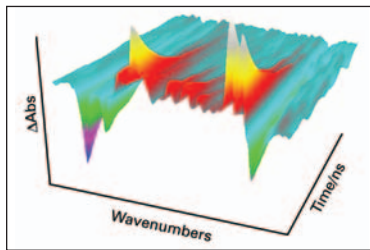
OMNIC Atlus

OMNIC for Research and Development

Research spectroscopists need maximum power and flexibility to configure, analyze and process data from cutting-edge studies. With step-scan, time-resolved, and dual channel data collection, plus SpectraCorr 2-dimensional spectral correlation software, OMNIC has the most comprehensive set of tools for the researcher. The development chemist needs tools designed to accelerate the discovery process. In applications such as drug discovery or combinatorial chemistry, OMNIC offers software such as Array Automation that brings high throughput screening capabilities to FT-IR and Raman analysis.

OMNIC Advanced FT-IR Research Tools

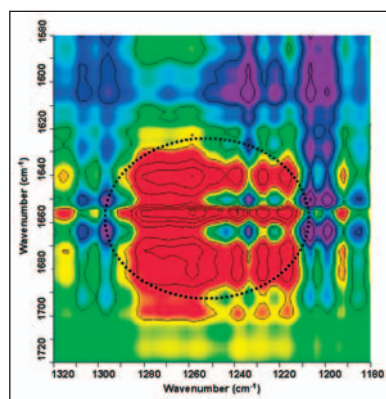
- Step scan amplitude modulation for emission experiments such as electroluminescence
- Step scan phase modulation for photoacoustic depth profiling analysis
- Step scan multiple modulation for sample modulation such as polymer stretching
- Step scan time resolved for high-speed, time-resolved kinetic measurements
- Dual-channel polarization modulation for linear and circular dichroic measurements, such as IRRAS, VLD and VCD
- Phase array operations for dynamic FT-IR interferometric data manipulation
- VCD Calibrate for calibrating VCD intensities



Step-scan time-resolved FT-IR spectra of the pp* triplet obtained after irradiation of 4-phenyl benzophenone. The IR spectra were taken in 500 ns time slices. *Courtesy of Dr. Michael George of the University of Nottingham, UK.*

OMNIC SpectraCorr software provides the means of correlating

both classic orthogonal in-phase and quadrature spectral data, and time-dependent spectral series of an arbitrarily perturbed system. Synchronous and asynchronous correlation maps are generated rapidly and displayed with a choice of fourteen, high-resolution imaging-quality modes.



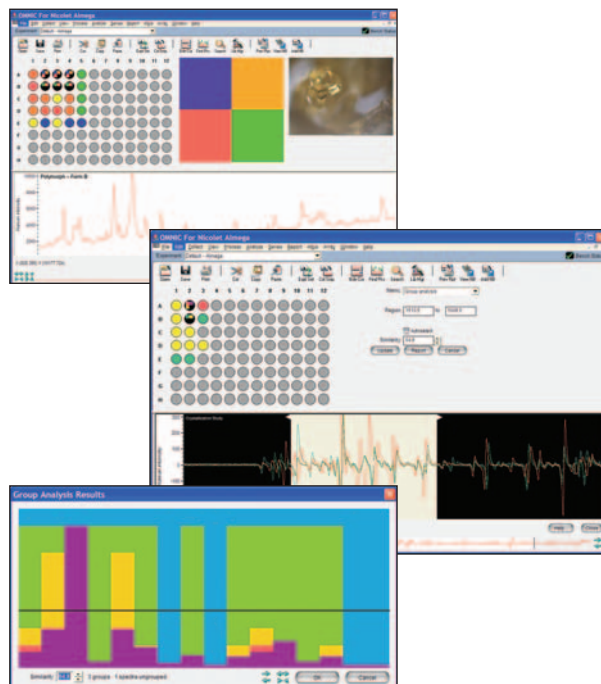
Asynchronous correlation of FT-IR imaging data of human cartilage generated using SpectraCorr software

OMNIC Array Automation for High Throughput Screening

OMNIC Array Automation software enhances R&D productivity by automating the collection and analysis of FT-IR and Raman spectra from microtiter well plates and other array-based sample sets. Compatible with Thermo Scientific FT-IR, FT-Raman or dispersive Raman spectrometers, Array Automation can handle everything from a few samples to high-throughput applications employing robotic sample delivery.

OMNIC Array Automation is fully integrated into OMNIC to provide seamless collection and processing of spectral data. It includes templates for microtiter plates and also can be custom configured to meet most array sampling needs. Graphical set-up and analysis tools, including group and cluster analysis, combined with bidirectional LIMS communication, make Array Automation an ideal tool for the modern high throughput screening laboratory.

Common high throughput applications include polymorph screening and chemical synthesis studies.



OMNIC Array Automation presents the results of parallel screening experiments in easily understood visual formats

Key OMNIC Components

- Advanced Experiments
- OMNIC SpectraCorr
- OMNIC Array Automation

OMNIC and Regulatory Compliance

Whether your laboratory must comply with government regulations for full system validation, qualification and electronic records, or you have a quality system in place that requires documented evidence of system performance, Thermo Scientific FT-IR, NIR, and Raman systems and OMNIC software offer the right mix of compliance tools. When your needs go beyond the standard performance verification capabilities offered in OMNIC, ValPro™ System Qualification and OMNIC DS Data Security with Thermo Security Administration Server offer best in class tools to meet or exceed any level of compliance requirements.

ValPro System Qualification

Our full system approach to the qualification of your FT-IR, NIR, or Raman spectrometer and accessories is the most comprehensive offering in the industry. Whether your laboratory is in a highly regulated pharmaceutical company or an ISO certified facility, the products and services offered by ValPro provide the most time and cost effective method of addressing your compliance needs so you can get your system commissioned faster and start getting results sooner.



ValPro System Qualification goes beyond the standard performance verification tests offered in OMNIC by providing Pharmacopoeial test methods, extensive documentation and procedures for DQ, IQ, and OQ, recommended PQ test protocols, plus control charts to track your system's performance. With ValPro

products and services you are confident that your system will provide accurate and consistent results throughout its lifetime and have the documented evidence required to prove it.

OMNIC DS Data Security

With the security and data integrity tools provided in OMNIC via the **DS Data Security** option, full 21 CFR Part 11 compliance can be readily achieved. OMNIC DS uses the Thermo Security Administration Server to control access and set policies for OMNIC based on Microsoft® Windows® user authentication protocols. This lets OMNIC DS give you complete 21 CFR Part 11 compliance without the hassle of many other instrument companies' offerings.



OMNIC DS works within the operating system's security environment to address the requirements of the regulation so you can rest assured your system is being used according to your policies and your precious data is secure.

And for large enterprises with multiple systems Thermo Security Administration Server allows you to manage user policies over the network so system use is consistent.

Advantages OMNIC DS Provides:

- No need to create new user names and passwords
- Digital signatures establish record responsibility and ensure data integrity, something electronic signatures can't do
- Spectral data audit trails and raw data storage travels with the data to provide traceability
- Unique log within the Windows Event Viewer tracks software use and OMNIC file events, even when OMNIC is not running

Complete Compliance Portfolio for Molecular Spectroscopy

Thermo Scientific offers a portfolio of solutions to meet your compliance needs so you can select exactly what you require. This reduces your time and resource investment to commission your system and keep it running properly.

ISO Certified Quality System: Thermo Scientific FT-IR, NIR and Raman systems are designed and manufactured under an ISO 9001:2000 certified quality system to give you confidence in the design and construction of the spectrometer and software

Complete System IQ/OQ: Each package is tailored for specific techniques, instruments and accessories to shorten the qualification cycle and provide reliable checks for system performance.

Certified Installation: Factory trained and certified technicians plus factory-supplied test data ensure fast, accurate and fully documented installation and qualification.

Custom Validation: Turn-key plans and documented procedures, executed by experts, lowers the hassle factor and time commitment of validation.

Operator Training: On-site training and supplemental courses offered at Thermo Fisher Scientific training centers ensure operators learn proper system operation procedures.

21 CFR Part 11: Software tools and expertise in configuring systems for complete compliance with FDA requirements for data security and traceability.

Key OMNIC Components

ValPro System Qualification
OMNIC DS Data Security
Thermo Security Administration

OMNIC Software Suite

The OMNIC Software Suite is the most comprehensive and customizable software for FT-IR, NIR and Raman experimental design, data collection, spectral analysis, and reporting. OMNIC software provides an intuitive and flexible toolset for operators at all spectroscopy experience levels. The feature-rich OMNIC Software Suite provides all of the tools needed to get the most out of your Thermo Scientific FT-IR, NIR or Raman spectrometer.

OMNIC software is compatible with Windows Vista™ and XP (service pack 2 minimum)



OMNIC Spectroscopy Standard Tools

- Data collection and analysis
- File and library conversion tools
- Search
- Library Manager
- 1400 Compound Introductory Library Collection
- Spectral Interpretation Tool
- Peak Resolve Spectral Peak Fitting
- Report generator
- Electronic Laboratory Notebooks
- Thermo/ACD Structures



Advanced Material Characterization

- OMNIC Spectra



Method Development

- TQ Analyst EZ Edition
- TQ Analyst Professional Edition
- OMNIC Macros\Basic
- OMNIC Macros\Pro™



Dynamic Spectroscopy

- OMNIC Series



Microspectroscopy and Imaging

- OMNIC Atlas mapping and image analysis



Research Spectroscopy

- SST (Step-scan and dual-channel experiments)
- SST for TRS (Time-resolved module)
- SpectraCorr (Two-dimensional spectral correlation)
- OMNIC Array Automation



Regulatory Compliance

- ValPro System Qualification for FT-IR and Raman
- OMNIC DS with Thermo Security Administration (for 21 CFR Part 11 compliance)



Dedicated Application Software

- OMNIC FT-Raman Experiments
- OMNIC for Dispersive Raman

In addition to these offices, Thermo Fisher Scientific maintains a network of representative organizations throughout the world.

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