OMNIC Professional Software Suite

The OMNIC Professional Software Suite is the most comprehensive and customizable software for FT-IR and Raman experiment design, data collection, spectral analysis, and reporting. OMNIC software's intuitive design provides an intuitive and flexible tool for

professionals of all spectroscopy experience levels. The OMNIC Professional Software Suite provides all the tools needed to take full advantage of FT-IR and Raman spectroscopy.

Individual Software Data Collection and Manipulation Software	Software Packages			
	Basic	Analytical	Advanced	Research
OMNIC Software	•	•	•	•
Interpretation and Structure Software				
Search and Library Manger	•	•	•	•
Introductory Spectral Library Collection	•	•	•	•
Spectral Interpretation	•	•	•	•
Spectral Interpretation Guide		•	•	•
Application Bibliography		•	•	•
Peak Resolve Spectral Deconvolution		•	•	•
Thermo/ACD Structures			•	•
InterpretIR+				
Automation and Macro Software OMNIC Macros\Basic		•	•	•
OMNIC Macros\Pro				
Time-series Software OMNIC Series				•
Quantitative and Qualitative Software TQ Analyst — Easy Edition				
TO Analyst – Professional Edition			•	
Regulatory Compliance Val-Q FT-IR Spectrometer Validation				
OMNIC DS				
Microscopy Software μView				
OMNIC Atlµs 7.0 (automated mapping)				
Advanced FT-IR Spectroscopy Software SST (Step-scan and dual-channel experiments)				•
SST for TRS (Time-resolved module)				
2D-IR (two-dimensional data correlation)				•
Dedicated Application Software Raman Experiments (FT-Raman Module and Nicolet Almega)				
Integra™ (used oil analysis)				
ECO™ (Silicon wafer analysis)				

Computer Requirements

PC processor with 1 GHz clock speed; 256 Mbytes Ram; 10 Gbyte Hard Drive; 32X CD ROM; 16 Mbytes 4X AGB Video RAM; 15" SVGA monitor (800 x 600); Stereo sound and speakers; 3.5" floppy; Windows 2000 or XP Professional, Mouse and Keyboard.

Some spectrometer functions may require additional computer capabilities. Consult a sales or service representative for more information.

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

Australia +61 2 9898 1244 • analyze.au@thermo.com

Austria

Belgium +32 2 482 30 30 • analyze.be@thermo.com

China +86 10 5850 3588 analyze.cn@thermo.com

France +33 1 60 92 48 00 • analyze.fr@thermo.com

Germany +49 6103 4080 • analyze.de@thermo.com

Japan +81 45 453 9100 • analyze.jp@thermo.com

Netherlands +31 76 587 98 88 • analyze.nl@thermo.com

South Africa +27 11 570 1840 • analyze.sa@thermo.com

Switzerland +41 61 48784 00 • analyze.ch@thermo.com

UK +44 1442 233555 • analyze.uk@thermo.com

www.thermo.com



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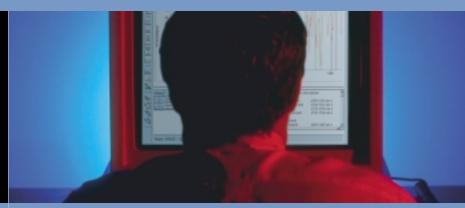
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Specifications, terms and pricing are subject to change. Not all products are available in all countries. Please consult your local sales representative for details.

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Full-featured FT-IR and Raman Spectroscopy Software



Instrument Control and Diagnostics



Data Collection and Processing



Spectral Interpretation Tools



Intuitive Interface with Customizable Operation

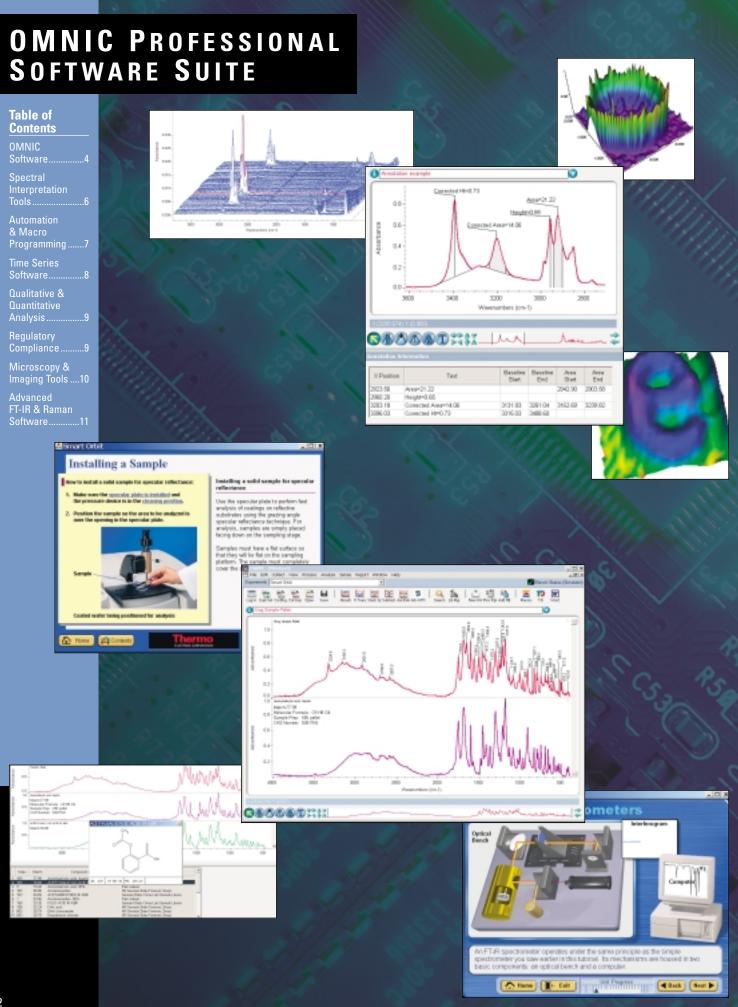


Regulatory Compliance



Expert Help





A Full-Featured Software Package that Provides Integrated Tools for FT-IR and Raman Analysis

OMNIC software from Thermo allows the user to quickly and easily acquire, process, analyze, and manage FT-IR or Raman data in a graphical environment that is intuitive and customizable.

OMNIC™ software is the common platform used by all Nicolet™ FT-IR and Nicolet Raman laboratory spectrometers. It is at the heart of the unique Smart System approach to spectroscopy, providing an advanced level of integration between software, spectrometer, and sampling accessory.

In addition to the standard operations available in OMNIC software, many integrated add-on and ancillary software packages are available. These packages are designed to accommodate a wide variety of specialized applications in infrared and Raman spectroscopy. They enhance and complement the power of OMNIC software to provide the most complete set of spectroscopy tools available. These tools provide the flexibility to expand capabilities as requirements grow.

OMNIC Professional Software Suite Benefits

- Continuous spectrometer and spectral data diagnostics ensure both system and sample analysis are working properly
- Smart Accessories[™] maintain proper experimental conditions
- Real-time spectral display provides immediate analysis feedback
- Automatic atmospheric interference suppression provides high-quality spectral data with no special processing
- Interactive multimedia tutorials and a context-sensitive Help function provide information to maximize system output
- Full-featured spectroscopic analysis tools address data processing needs
- Spectral History automatically tracks data changes providing an embedded audit trail
- Complete library manager function that maximizes the use of spectral libraries

- Built-in spectral interpretation feature assists with data analysis
- Report generation and digital laboratory notebooks provide storage of spectra and associated information
- Intuitive compatibility with Microsoft®
 Office and other common desktop software allows for quick spectral and data
 analysis information transferability
- Built-in ability to e-mail spectra directly from OMNIC software to colleagues for rapid-information transfer
- Powerful and intuitive programming capabilities to create automated analysis routines which ensure consistency of results
- Seamless compatibility with TQ Analyst™ chemometrics software
- Integrated add-on software packages increase system power for advanced experiments and infrared microscopy



OMNIC Professional Software Suite – Standard Features

The standard features of OMNIC software provide tremendous functionality in an intuitive Windows®-style interface. The user can configure the interface and features so that only functions best suited to their analytical requirements are seen. If requirements exceed those offered in the standard feature set, a host of integrated add-on capabilities are available. Advanced spectral interpretation, programming, data collection, chemometric, regulatory and imaging add-on packages provide the user the tools needed to make the most of their vibrational spectroscopy experiments.

Smart Technology

Enhanced Synchronization Protocol (E.S.P.) allows OMNIC software to communicate with Thermo spectrometers and accessories. OMNIC software monitors every step of an experiment, saving time and providing confidence that analysis results are accurate.

- Automatic accessory recognition of E.S.P. and Smart Accessories set parameters and ensure system readiness
- Automatic experiment set up and system optimization saves time
- Intelligent spectral data quality checks ensure the best possible data
- Real-time bench status indicator monitors system functionality, significantly decreasing downtime
- Integrated diagnostics and context-sensitive video help for trouble shooting and parts replacement
- Interactive tutorials provide instruction on software, spectrometer, and accessory use, as well as theory and sampling techniques

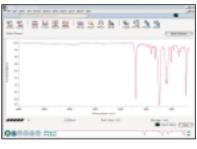
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Real-Time Spectral Display

The real-time spectral display capabilities of OMNIC software are second to none for providing feedback and assurance that data is accurate. From the diagnostic routines for spectrometer alignment, to the preview data collection option, OMNIC software provides constant monitoring of the spectral analysis progress.

- Bench set-up and diagnostic displays provide information on bench status and performance
- Freeze display allows monitoring of changes to optimize experimental conditions
- Continuous updates during data collection provide visual feedback of the signal averaging effect on spectral results
- Preview data collect allow results to be viewed before committing precious time to numerous scans – particularly useful for ATR or infrared microscope analyses

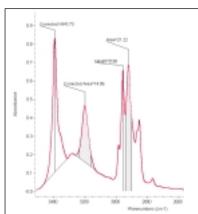
And for those who can't wait for answers, spectral searches can be performed while scanning.



Data Analysis Tools

OMNIC software has the tools needed to process and analyze data. It also ensures data integrity by recording all spectral operations in the spectral history, and allowing raw data to be stored automatically.

- Peak measurement tools, including height, area, and location with annotation and automatic logging of results in the spectral history
- Intelligent atmospheric interference suppression, without altering original data, guarantees both data quality and integrity
- Baseline, ATR, Kramers-Krönig, Kubelka-Munk, and other specialized data correction algorithms
- Exclusive, advanced ATR correction allows adjustment of ATR accessory parameters to improve searches when using transmission libraries
- Spectral subtraction, component autosubtract, and advanced spectral math operations
- Fourier self-deconvolution and multiple spectral derivative options



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Customized Interface and Built-In Audit Trail

OMNIC software tools help make it easier than ever to customize the user interface and provide proof of results.

- Completely customizable toolbar and menus for flexible configuration to each user's preference
- Entire test procedures can be run by single, push-button macros, ensuring consistent and proper operation
- File-integrated spectral data audit trail logs all collection parameters, analysis conditions, data manipulations and modifications to the data
- · Log-in and user-level access control

Spectral Library Manager

Spectral Library Manager is a powerful spectral database management tool that allows the user to browse and maintain spectral libraries from a single interface.

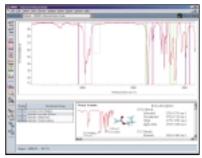
- Easily sort, view, merge, compress, retrieve, and find text among the spectra in all spectral libraries
- Library Creation Wizard
- All data is stored with full resolution for the x-axis and y-axis, providing greater accuracy
- Full retention of all collection parameters in user-created libraries



Total Solution Tools for Identification and Interpretation

OMNIC software provides multiple search and spectral interpretation tools to maximize data output, regardless of whether the user is identifying unknowns, confirming quality, or doing research.

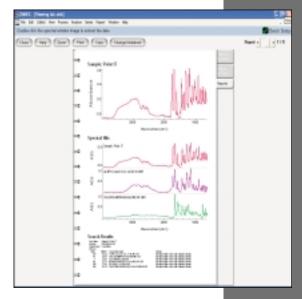
- Label peak locations on spectra using the Find Peaks function to aid spectral interpretation
- Search Expert uses artificial intelligence for simplified searching, and interpreted results
- Flexible, powerful, and easy-to-use Full Spectrum Search
- Single- and multiple-region search eliminates the need for complex manipulations
- Search result stacking or one-at-a-time overlay for detailed spectral comparison
- IR spectral interpretation for functional group identification
- QC Compare Search for routine quality testing and confident, day-to-day material verification
- Introductory Spectral Library Collection containing over 600 infrared and Raman spectra of common compounds



Reporting and Data Archival

OMNIC software includes an electronic Report Notebook that organizes and archives FT-IR and Raman experiment results, following GLP* guidelines.

- All operations are recorded without the paperwork and can not be edited
- Multiple notebooks can be set up for different users, applications, or time periods
- Retrievable storage of data and collection parameters
- Reports can include peak tables, quant results, library search matches, data collection information, images, and many other elements
- Flexible customization of templates for reporting
- Individual reports can be digitally signed
- Reports can be exported to popular word processing and presentation software
- * Good Laboratory Practice

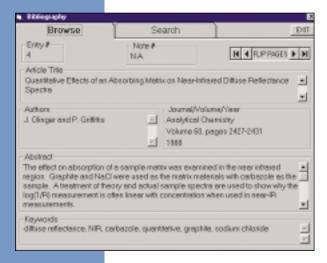




Spectral Interpretation Tools

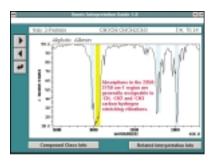
IR Bibliography

OMNIC software's IR Bibliography is a searchable on-line reference database containing information from over 3,000 journal articles books and papers. This extensive collection includes the title, author, publisher, abstract, and keywords for all entries. The search feature enables the user to locate, view, and print entries based on a variety of data fields.



IR Interpretation Guide

The OMNIC IR Interpretation Guide is a valuable learning tool for developing infrared interpretation skills. This software package contains spectral information on more than 600 compounds, including aliphatic ketones, alkyl aromatics, and more. Each spectrum has a set of "hot buttons"—highlighted regions where characteristic absorption bands are located. Simply moving the mouse pointer to a highlighted region displays useful vibrational assignment information about the spectrum. Additionally, the program has detailed spectral and chemical class information.



InterpretIR+™ for Infrared and Raman Spectral Data

InterpretIR+ is Thermo's interactive spectral interpretation software package. It provides useful information on all major chemical compound classes for both infrared and Raman data, allowing the user to interpret the collected spectra with OMNIC software, or other spectroscopy software packages. The program's extensive database includes over 115 chemical compound classes for infrared and over 90 classes for Raman.



InterpretIR+ and OMNIC software work together to seamlessly display spectra from the active window. Using InterpretIR+ in conjunction with OMNIC software's integrated infrared spectral interpretation tool allows for thorough interpretation by providing both functional group and compound class information. InterpretIR+ can be used in conjunction with OMNIC software, or as a stand-alone package. It is compatible with OMNIC software and JCAMP file formats.

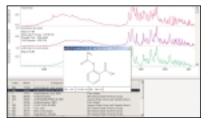
Peak Resolve Spectral Deconvolution

OMNIC software's Peak Resolve function is a fast and powerful tool for spectral deconvolution analysis. It allows users to detect and separate unresolved peaks with speed and efficiency. The application provides valuable

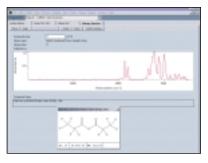
information, including peak positions, widths, heights, and areas of overlap in an easy-to-use graphical interface. It fits Gaussian, Lorentzian, mixed Gaussian-Lorentzian, Log Normal, Pearson VII, and Voigt line shapes. Peak Fitting uses the Fletcher-Powell-McCormick, non-linear peak fitting algorithm to iteratively adjust every variable to find the best solution.

Thermo/ACD Structures

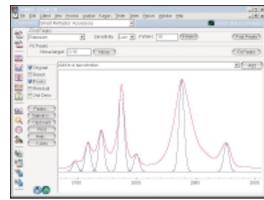
Thermo and ACD Inc. have a unique partnership that utilizes the powerful library search function of OMNIC software to retrieve both spectral information and structural information from commercial and user-created libraries. This capability expands the power of OMNIC software by not only assisting with spectral confirmation of a library search, but also providing access to CAS numbers, physical data, and chemical structures.



In addition to obtaining chemical structures when searching the extensive offering of Thermo spectral databases, Thermo/ACD Structures software provides a powerful drawing package that allows 2D or 3D structures to be created from within OMNIC software.



After a structure is created, OMNIC software's Library Manager automatically adds the structural information to any user-generated library selected.



Automation and Macro Programming Packages

Using a macro program to set system parameters and quide the user through an experiment saves time and guarantees that the end results are reproducible.

Macros can be created in an intuitive, point-and-click environment using OMNIC Macros\Basic™, or written with the advanced programming capabilities of OMNIC Macros\Pro™.

OMNIC Macros\Basic

OMNIC Macros\Basic software is the ideal package for multi-user environments and operators with varying levels of expertise. From QC laboratories to R&D departments, OMNIC Macros\Basic software is the solution for automating tasks and operations in the OMNIC software package.

It also allows OMNIC software to be customized so all operations can be performed with the push of a button. Simply assign the macro to the tool bar or menu, and users of any level of expertise can run the most complicated analyses.

The benefit of OMNIC Macros\Basic software is that it allows even the computer novice to construct and execute macro programs. The click and drag graphical environment makes it easy to string together a series of menu commands. Most standard commands are available and OMNIC Macros\Basic software supports other OMNIC software products, such as TQ Analyst.

Results can be output into a specific report template and printed or stored automatically in a digital laboratory notebook. Results can also be made part of the spectrum, added to a text file, or even sent to another software package, such as Microsoft Excel or Microsoft Word, using Dynamic Data Exchange (DDE).

OMNIC Macros\Pro

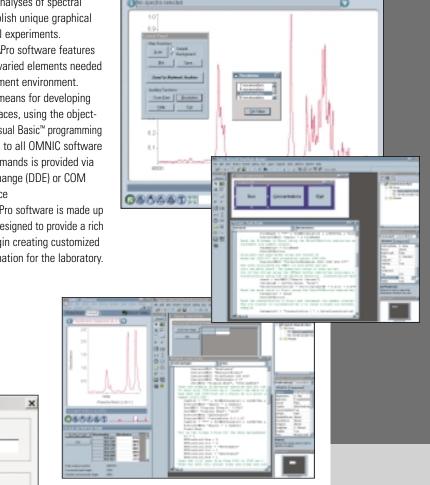
OMNIC Macros\Pro software picks up where OMNIC Macros\Basic software leaves off, providing greater control over OMNIC software while addressing advanced programming needs. Macros can be created that perform complex numerical analyses of spectral information, or establish unique graphical interfaces for special experiments.

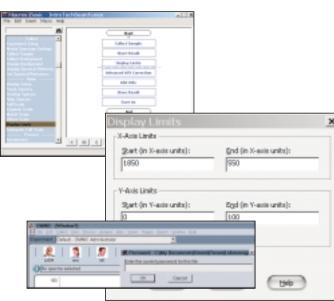
OMNIC Macros\Pro software features many essential and varied elements needed for a macro development environment. It provides intuitive means for developing graphical user interfaces, using the objectoriented Microsoft Visual Basic™ programming environment. Access to all OMNIC software parameters and commands is provided via a Dynamic Data Exchange (DDE) or COM programming interface

OMNIC Macros\Pro software is made up of four components designed to provide a rich tool set to easily begin creating customized interfaces and automation for the laboratory.

- Documentation of OMNIC Macros\Pro DDE needed to set parameters, issue commands, and retrieve results
- Microsoft Visual Basic programming environment
- A set of subroutines that make DDE simple to understand and implement
- Example Visual Basic programs, showing the user how to create powerful programs that interact with OMNIC software

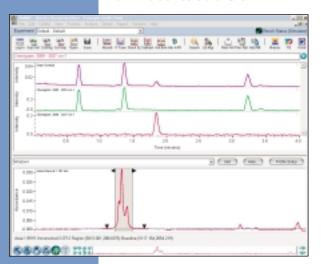
OMNIC Macros\Pro software enables modifications to OMNIC software that fit with the user's needs, making it ideal for program flexibility.





Time Series Software

OMNIC Series Software



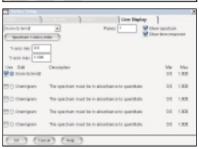
If a material changes or evolves over time, OMNIC Series software adds time-based resolution to the spectral resolving power of FT-IR spectroscopy to better characterize and understand the changes. OMNIC Series software is a powerful data collection and processing tool for a wide variety of applications where spectra change with respect to time, temperature, or other phenomena. OMNIC Series software collects an ordered set of spectra that relate to a specific event, or series of events. It then provides reconstructions of the chemical changes and specialized display options to reveal even the smallest molecular transformations. The result is an integrated series of individual, time-stamped spectra in a format that allows samples to be picked out at individual times during the experiment, or chemical changes to be characterized as a function of time.

OMNIC Series software can be used when coupling FT-IR spectroscopy with other analytical techniques, such as gas chromatography (GC), thermogravimetric analysis (TGA), or various slow or rapid kinetics experiments for real-time spectral information that make the original experiment far more valuable. It integrates seamlessly into OMNIC software, putting experimental control at the user's fingertips, with intuitive command over the spectrometer's true power.

Real-time display of fully processed IR spectra and Gram-Schmidt Reconstruction (GSR) is available providing a continuous update of chemical changes with respect to time. However, successful analysis goes beyond data collection. It requires a complete toolkit of data processing features that allow the user to reveal, isolate, and highlight the information sought after in time-based data. Toolkit features include:

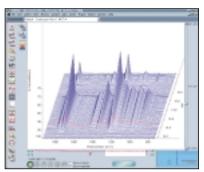
- GSR provide a total IR response chromatogram displayed in real-time during data collection
- Data optimizing tools, including co-addition and basis vector addition, to maximize signal-to-noise, eliminate baseline effects or isolate overlapping components
- Chemigram reconstruction provide specific functional group presence, quantitative analysis (using TQ Analyst chemometric software), or specific measurement profiles as a function of time
- Data group and batch processing, including time region co-adding, series batch reprocessing, spectral format, and range options
- Build or split series data sets, adding a dimension of information to existing data





Visualization of results is critical to understanding time-based spectroscopic data. OMNIC Series software includes several, intuitive options for displaying results for both maximum meaning and presentation content.

- Series processing display Simultaneous display of individual or multiple GSR or Chemigram reconstructions, and spectral data file, allowing for clean interpretation of reconstructed data
- Color contour display Provides an Interlinking[™] topographical view of the time series and the individual spectra associated with points the user interactively selects
- Waterfall display Provides a threedimensional view of real spectra, stacked as a function of time



The IR spectra of a fragrance oil collected by coupling a gas chromatograph with FT-IR. Chromatography allows the physical separation of the components, which are uniquely identified by the FT-IR system as they are eluted from the sample and exit the GC column.

TQ Analyst Qualitative and Quantitative Analysis Software

Professional and EZ Editions

TQ Analyst software is a comprehensive method development platform for users of all experience levels. It has all the performance and flexibility to develop robust methods.

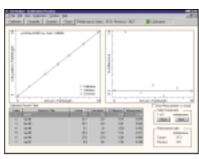
- Spectral preprocessing and selection
- Pathlength treatment
- · Complete diagnostics
- Data handling
- Full set of qualitative and quantitative tools
- Correction and transferability tools

Advanced features are also provided to help develop high performance methods without having extensive experience. Smart tutorials with artificial intelligence referred to as "wizards" guide the user through method development.



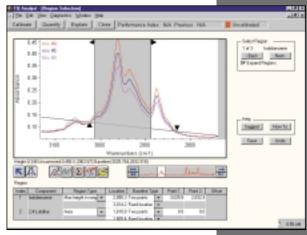
Assess Feasibility feature indicates if the method is likely to be successful.

TQ Analyst Professional Edition can be used to develop methods using classification techniques, which include search standards, distance match, similarity match, QC Compare, and discriminant analysis. Quantitative models include measurement only, Simple Beer's law, stepwise multiple linear regression (SMLR), classical least squares (CLS), partial least squares (PLS), and principal component regression (PCR).



The calibration Results window shows how well the method performs by displaying the calculated values compared to the actual values, the relative difference, and the method Performance index.

TQ Analyst EZ Edition has a more limited set of methods options, which include search standards, similarity match, measurement only, Simple Beer's law, and classical least squares (CLS). It still provides the same method development assistance as the Professional Edition.



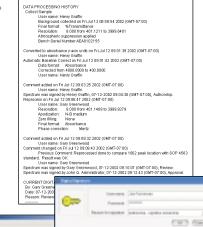
The Region Selection window gives full control to set up analytical regions. Use the graphical tools to place region boundaries and set baseline points.

Regulatory Compliance

Advanced Security, Data Integrity, and Regulatory Compliance Tools

By adding the OMNIC DS option, full 21 CFR Part 11 compliance can readily be achieved.

- Thermo's Security Administration Server controls access, sets policies, and configures digital signature meanings on a per user basis.
- User authentication to control system access and ensure secure system use
- Digital signatures establish record responsibility and ensure data integrity
- Spectral data audit trails and interferogram storage provide data traceability and experiment reproduction
- Unique Thermo log within the Windows® Event Viewer tracks all software use and OMNIC software file events, even when the software is not running





In addition to security and access control, Thermo offers qualification tools to help validate the system.

- Val-Q software for DQ, IQ and OQ for FT-IR spectrometers
- OMNIC software OQ package with detailed software functionality protocols and algorithm documentation
- Installation and Operational Certification services

OMNIC Atlus Microscopy and Imaging Tools

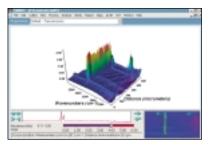
Automated Microscopy Software for Infrared and Raman

OMNIC Atlµs software provides an elegant and efficient means to automate infrared and Raman microscopic sampling analysis. Repetitive analysis tasks can be reduced to an effective, unattended operation that frees time and minimizes user error. The spectral data relates to a specific position on the sample, allowing the user to verify distribution of a homogenous sample or locate defects or contaminants on a heterogeneous sample based on the spectral results.

The software integrates the spectrometer, microscope, sampling stage, and data analysis into a single, powerful system. It is compatible with all IR and Raman instruments from Thermo that have motorized sampling stages. OMNIC Atlµs supports multiple microscope stages that offer the flexibility of stage travel, positional accuracy, and speed.



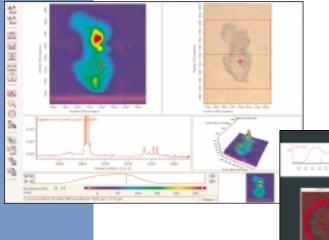
- Full automation for the collection of point, line and area maps using the single-element or array detector
- Fully integrated into OMNIC software
- Window panes can be resized or hidden to customize display.
- Pane contents can be copied to the clipboard
- Chemometric tools for image/data processing: Principal Component Analysis, rotating 3-D image, animation tool for scanning through spectral data, and profile tools
- Spectral processing functions for maps

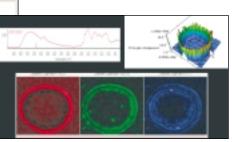


MicroView Microscope Image and Control Software

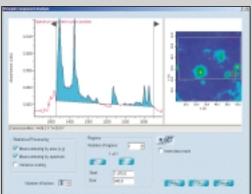
For those infrared microscope users who don't need the advanced mapping and data manipulation capabilities offered by OMNIC Atlµs software, Microview image and control software provides image viewing and storage tools. This package allows users to view the visible microscope image on their computer screen.

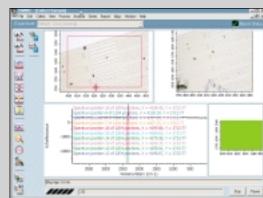
- Intuitive video microscopy software for new systems
- Support for advanced video microscopy and autofocus
- Functions for documentation and use of video image data
- Ability to annotate, print, and save video images
- Cut and paste operations for easy report generation
- · Graphical measurement tools











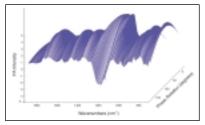
Advanced FT-IR Spectroscopy Experiments

Advanced Spectroscopy Experiments

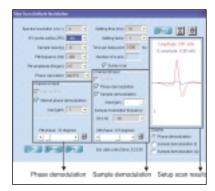
Advanced FT-IR experiments and spectral correlation analysis are performed by OMNIC Simultaneous Sampling Techniques (SST™), and OMNIC 2D-IR software.

- 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 experiments
- Step scan time resolved for highspeed, time-resolved chemical 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

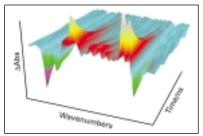
The enhanced OMNIC 2D-IR software packages provide the means of correlating both classic orthogonal in-phase and quadrature spectral data, and time-dependent spectral series of an arbitrarily perturbed system. Synchronous and asynchronous correlation maps are generated rapidly with improved algorithms and displayed with a choice of any fourteen, high-resolution imaging-quality modes.



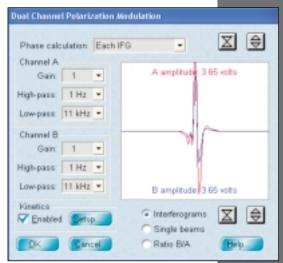
Phase rotation 3D plot of photoacoustic spectra of Kapton™ collected at a phase modulation step-scan FT-IR mode with modulation frequency of 400 Hz.



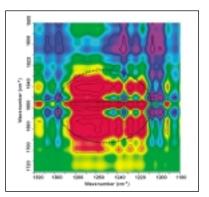
OMNIC SST setup screen for simultaneous DSP double modulation (SDM) and demodulation process.



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 SST setup screen for dual-channel polarization experiments (PM-IRRAS, VLD, and VCD). Two channels of interferograms (or spectra) are collected and displayed simultaneously, and thus, eliminate the moisture effect on the final spectra. Dual channel kinetic mode is also available to collect time-resolved spectra for any of these experiments.



Asynchronous correlation of FT-IR imaging data of human cartilage sample from superficial to deep zones.

Raman Experiments

The Raman experiment module adds essential functionality to the OMNIC software interface that is optimized for FT or dispersive Raman analysis. This capability, integrated seamlessly into OMNIC software, allows users to exploit the power and versatility of the Raman technique, while providing access to a host of data collection, manipulation, and viewing functions. In addition to the wide array of standard OMNIC software features there are many specific features for dispersive

and FT Raman that allow users to control the conditions of their analysis to obtain the best possible results.

Thermo also offers the most complete collection of high-quality Raman spectral databases to aid identification of unknowns. These databases can be used to search FT or dispersive Raman spectra.

Raman Experiment Setup

