OMNIC Software Suite Specifications

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

For analysts from routine to research, the award-winning Thermo Scientific OMNIC software provides an intuitive and customizable graphical environment that allows users to quickly and efficiently acquire, process, analyze, and manage FT-IR, NIR or Raman 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 NIR industrial analyzers. The heart of the Smart System approach to spectroscopy, OMNIC integrates software, spectrometer, and sampling accessory. OMNIC can be configured to optimally meet your laboratory’s analytical requirements. With OMNIC, it is 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 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 spectroscopy tools. These tools provide the flexibility to expand capabilities as requirements grow.

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
- Create automated analysis routines using powerful and intuitive workflow generator
- Perform advanced experiments, hyphenated techniques or IR or Raman microscopy using OMNIC’s integrated add-on software packages

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
- Configure the toolbar with the most commonly used commands and automated workflows for push-button operation
- Get the most out of your system with interactive multimedia tutorials and context-sensitive Help

Part of Thermo Fisher Scientific
OMNIC Software Suite Specifications

OMNIC Standard Features

User Interface (Overview)

Navigation is simple in OMNIC with intuitive and configurable tools and layout.

- Experiment and spectral selection dropdown list, and Spectral Information button
- Spectral Selection, Cursor, Region, Peak Height, Peak Area, and Annotation tools
- X-axis Viewfinder, Spectral Positioning & Expansion tools, Box and click spectral zooming, and Roll and Zoom buttons

OMNIC Display features allow convenient processing and review of spectral data.

- Window-based interface allowing multiple data files and operations to be used at the same time
- Change windows any time, even during data collections
- Display setup and limit controls, Stack/Overlay mode, Hide
- Data scaling options including Automatic Full, Full, Common, Match, and Offset

OMNIC Customization allows users to view only needed features, making their job easier.

- Each user may have their own interface with access via configuration files or optional log-in names and/or passwords
- Includes interface and software behavior options, plus menu and toolbar configuration
- External programs or pre-programmed workflows can be added to the menu or toolbar
- Option to use toolbar-only mode for completely push-button operation

1. Instrument Interface

OMNIC Live Display features give users confidence in the instrument by showing them their data as it collects.

- Diagnostic and experiment setup displays show operators that the instrument is working as expected
- Data collection displays provide immediate spectral quality feedback and show collection status
- Preview data collection shows what the sample spectrum looks like before collection, allowing adjustments to optimize the data

Smart System approach recognizes installed components reducing setup and operation errors.

- Information about key components, like detectors, beamsplitter, and sources, is reported to the operator for diagnostic and setup ease.
- Accessories are recognized when inserted, appropriate parameters set and performance is verified

Experiment Setup provides easy configuration of parameters to optimize experiments.

- Set sample collection conditions like preview data collection, automatic atmospheric suppression, saving of interferogram data, and background handling
- See live spectrometer data output for diagnostic feedback, system alignment and operational verification
- Select instrument interface conditions like sample compartment, detector, source, accessory, data range, and the use of optical components like filters and screens
- Spectral Quality checks set minimum performance requirements for data collection to ensure good quality spectral data
- Set parameters for optional application software like Series and Atlus™

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Customize the OMNIC toolbar for easy access to commonly used features or automated workflows

Smart Accessories are automatically recognized and their performance is verified when inserted.
2. Data Assurance/Security
System Performance Verification (SPV) with System Status Monitor continuously monitors the system and provides tests to ensure it’s working correctly.

- Instrument status checks provide warning of hardware diagnostic failure
- Spectral Quality is monitored live during data collection and reported in the status monitor
- System Suitability tests are configurable for any instrument configuration or accessory using any desired test sample and can be scheduled to run at a selected interval
- Performance Verification tests based on ASTM E1421 FT-IR can be scheduled to run unattended overnight
- System Maintenance status allows scheduled maintenance timing to be programmed and operator warning interval set
- Optional ValPro™ System Qualification is available to provide additional qualification tests and procedures for DQ/IQ/OQ/PQ with test intervals programmed and tests launched through the System Status Monitor

Automatic file-embedded audit trails ensure data integrity.

- File-embedded non-editable spectral data history records collection conditions and tracks data changes, including SPV status.
- User logins and passwords are available to ensure proper system use
- OMNIC customization and experimental conditions can be assigned to specific user login names and passwords are available to prevent changing settings or unauthorized use

21 CFR Part 11 tools are also available that go beyond OMNIC standard features for an extra level of access control and data security.

- Optional OMNIC DS Data Security provides a higher level of access control, digital signatures and an audit trail that monitors file use even when OMNIC is not running, to ensure compliance with 21 CFR Part 11 Electronic Records regulations

3. Data Management
OMNIC offers extensive data compatibility to make it easy to use data files and spectral libraries from a wide variety spectroscopy software packages.

- File open formats include OMNIC spectra, groups, series, and maps; Nicolet™ legacy; Mattson legacy; JCAMP DX, Spreadsheet (CSV); GAML, GRAMS, PerkinElmer, Bruker, Shimadzu, JASCO
- File save formats include OMNIC spectra, groups, series, and maps; Nicolet legacy; Mattson legacy; JCAMP DX, Spreadsheet (CSV); GAML, GRAMS, Shimadzu, Windows® Metafile, TIF
- Library conversion is available to import user libraries in formats that include GRAMS, Bruker, PerkinElmer, SearchMaster, Mattson

OMNIC includes convenient Microsoft® Windows-style editing tools that allow data to moved between different windows and external programs.

- Functions include Cut, Copy, Paste, Clear, Select All, Delete Annotations, Undo

4. Data Processing
OMNIC offers extensive data conversions and corrections for the most effective comparisons between data formats from different sampling techniques.

- Conversions available include Absorbance, %Transmittance, Kubelka-Munk, Photoacoustic, % Reflectance, Log (1/R), Delta absorbance, Wavenumbers, Micrometers, Nanometers, ATR
- Corrections include the exclusive Advanced ATR Correction that takes into account depth of penetration, crystal type, sample refractive index and number of bounces; plus Atmospheric Suppression, Interactive Kramers-Kronig, and PAS Linearize

Data clean-up tools in OMNIC may be used to improve data for better search and analysis results.

- Spectral clean-up features include Baseline correct – automatic or interactive, Blank, Straight line generate, Smooth – automatic or interactive

The wide array of math functions in OMNIC help users extract more information from spectral data.

- Math functions include Subtract, Region Subtract, Add, 1st or 2nd Derivative, Multiply, Spectral Math Tool, Fourier Self-Decconvolution, and Normalize Y-scale

OMNIC has several data adjustment functions allowing operators to view data using different parameters or compare data collected under different conditions

- Users can retrieve and reprocess interferograms, change data spacing, normalize the x-axis
5. Data Analysis

OMNIC offers extensive analysis features that allow users to get the most from their spectral data.

- Label peak locations on spectrum based on intensity threshold and slope sensitivity. Peak labels are saved with the spectrum and result tables can be added to reports or copied to the clipboard.
- Peak to Peak and RMS Noise calculations in selected spectral regions for diagnostic information.
- Statistical spectra calculator generates average, variance, and range results from a group of spectra to see how spectra vary.
- Peak Resolve is a full-featured, advanced peak fitting routine that extracts individual peaks from overlapping spectral regions.

Spectral library and data comparison tools in OMNIC facilitate a wide range of material verification and investigative analysis.

- Library setup configures search and QC Compare parameters including libraries to search, algorithms, output format, combined text and spectral searching, and multiple region selection.
- Search Algorithms include Correlation ($r^2$), Difference, Squared Difference (Euclidean distance), Derivative, and Squared Derivative.
- Library Manager makes spectral database creation and handling easy and convenient. Viewing library content and doing text searches makes good use of databases when spectral searching is not an option.
- QC Compare is a special searching routine that applies a correlation search to QC Compare libraries created with compound classes. The best hit from each class is reported if above the threshold value, with a spreading function used to differentiate very similar materials.
- QCCompare is a unique spectral comparison routine that allows direct comparison to one or many spectra not in spectral libraries. Correlation values are provided along with pass/fail if a threshold is set. High sensitivity correlation can be used to help differentiate very similar materials.
- OMNIC includes 1400 library spectra in multiple starter libraries.
- IR Spectral Interpretation is built right in to OMNIC to provide supporting information when looking at unknowns.
- OMNIC interpretation function provides chemical class information about your spectral data and includes interpretation details available through an embedded HTML database.

OMNIC allows users to predict qualitative and quantitative results using methods developed through TQ Analyst™ or other external programs which expands OMNIC data analysis capabilities for maximum flexibility.

- Methods created using TQ Analyst can be executed from OMNIC, providing results directly from the OMNIC interface, simplifying the analysis process.

6. Reporting

The OMNIC report template and electronic laboratory notebook features allow users to format and archive results with the most useful information.

- With OMNIC report generation using custom report templates users can create and edit reports using spectra in the current window. Once created reports provide consistent data output.
- Archiving reports in the OMNIC Electronic Laboratory Notebook creates a non-editable record of the analysis results. Reports in the notebook include spectral data that can be extracted for future work.

The many output options offered by OMNIC provide the flexibility to meet the needs of any laboratory.

- Print hard copy spectra, reports, notebook pages and other useful information or send to PDF with the included PDF print driver.
- Export data via copy and paste functions. Applies to spectra, reports, notebook pages, and other useful information.
- E-mail spectra function launches e-mail program and attaches spectrum so they can be sent directly to customers or colleagues.

7. Help

OMNIC provides comprehensive help that goes beyond software and hardware operation to teach the fundamentals of instrument operations and sampling techniques plus provides applications assistance.

- Tutorials teach operators how to run the spectrometer, software, and sampling accessories including Beginners Guide, Getting Started, Learning OMNIC, sampling techniques and a long list of tutorials for sampling accessories.
- Context sensitive Help in the software allows operators to get answers when and where they need them.

The flexible reporting options in OMNIC allow you to present your data in the best possible light, like this report showing pass/fail results from a QCspectral correlation analysis.
**OMNIC Add-on Software**

**OMNIC Spectra™**
OMNIC Spectra is next generation spectral analysis software that redefines IR sample identification.
- Unique and powerful data management, processing, identification and reporting features that work the way you do. OMNIC Spectra:
  - Uses your entire hard drive as a spectral database so you don’t need to hunt for spectra or libraries
  - Allows you to get answers faster by reducing extra time-consuming steps and operator effort.
  - Builds your confidence in your results with innovative search routines, like the exclusive Multi-Component Search feature, and integrated spectral interpretation.
  - Allows you to compile results directly into PDF reports or export data directly to word-processing programs.
- Includes a high quality database of over 9000 spectra

**TQ Analyst**
TQ Analyst Qualitative and Quantitative Analysis is a comprehensive method development platform that allows users of all experience levels to create high performance methods.
- Available in Professional and EZ Editions, TQ Analyst has an extensive list of analysis types and data treatments plus diagnostics to help create robust analytical methods. To simplify method creation for less experienced users there are Suggest Wizards and an Explain function plus comprehensive Help.
- TQ Analyst EZ analysis types include measure-only (peak height, area, & ratio), search standards, similarity match, QC Compare, Simple Beer’s law, classical least squares (CLS)
- TQ Analyst Professional analysis types include those in the EZ Edition plus distance match, stepwise multiple linear regression (SMLR), partial least squares (PLS) and principal component regression (PCR)
- TQ Analyst EZ Edition included with the OMNIC Standard Suite

**OMNIC Macros®Basic™**
From QC to R&D, OMNIC Macros®Basic is the best solution for creating automated sequences of everyday tasks to streamline operations and allow any user to get the right answers consistently and improve your laboratories productivity.
- Using routines created in OMNIC Macros®Basic, OMNIC software can be customized so all operations can be performed with the push of a button allowing users of any level of expertise to run the most complicated analyses by assigning the macro to the toolbar or menu.
- OMNIC Macros®Basic included with the OMNIC Standard Suite

**OMNIC Macros®Pro™**
OMNIC Macros®Pro picks up where OMNIC Macros®Basic leaves off, providing greater control of OMNIC software while addressing advanced programming requirements.
- Working through Microsoft Visual Studio or other programming environments, OMNIC Macros®Pro provides COM control over OMNIC allowing developers to create unique graphical interfaces or control multiple hardware devices.

**OMNIC Series**
OMNIC Series includes the most useful features to handle dynamic FT-IR and Raman spectral data efficiently and help elucidate the nature of the changes.
- Fully integrated into OMNIC with data collection types for GC/IR, TGA/IR, Kinetics, Rapid Scan or Real-time analysis.
- Provides real-time display of fully processed spectra plus up to five different pre-programmed spectral profiles giving a continuous update of chemical changes with respect to time.
- Spectra can be viewed and searched during data collection providing the analyst immediate feedback.
- State-of-the-art 2D and 3D views interlinked to allow optimal navigation through the data and provide information critical to understanding the results.
- Assess functional groups, quantitative results, or peak ratios; batch process using spectral processing functions; or build a series set from existing spectra.

**OMNIC Atlµs Imaging**
OMNIC Atlµs Imaging 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 contaminants on heterogeneous samples.
- Unprecedented integration with the spectrometer, microscope, stage control, data processing, and image analysis to provide everything needed at your fingertips.
- Data acquisition includes video image mosaic collection, discrete points, line maps and area maps in transmission, reflectance, or ATR.
- Contour display, 3D display, video image, and spectral pane in a single easy to use interface.
- Image analysis provides physical and chemical information specifically for each component.
- Chemical images based on frequency, functional group, correlation a reference, or a chemometric model derived from quantitative methods, Principal Component Analysis or Multivariate Curve Resolution.

**OMNIC Array Automation**
OMNIC Array Automation significantly enhances productivity by automating the collection and analysis of FT-IR and Raman spectra from microtiter well plates and other array-based sample sets.
- Fully integrated with and draws upon the many capabilities of OMNIC with an easy to use interface ideal for handling array-based sample sets.
- Includes standard templates and can be custom configured for any array format.
- Interactive graphical data display and flexible data collection, processing, and review options allow users to obtain the most useful information from sample sets.
- Automatic group and cluster analysis plus LIMS output reduces analysis times from hours to minutes for highly efficient analysis of large data sets.
OMNIC Add-on Software (continued)

OMNIC Advanced Experiments
OMNIC Advanced Experiments allow research spectroscopists to maximize the power and flexibility to configure, analyze and process data from their cutting-edge studies.
- Simultaneous Sampling Techniques (SST) provide the functions needed to address Step-Scan amplitude, phase, multiple, and time-resolved modulation; dual-channel polarization modulation, phase array, and VCD calibrate experiments
- OMNIC SpectraCorr™ software provides the means of correlating both classic orthogonal in-phase and quadrature spectral data, and time-dependent spectral series

OMNIC FT-Raman Experiments
OMNIC FT-Raman Experiments add features to OMNIC to facilitate analysis for systems with FT-Raman capabilities.
- Raman-focused experiment parameter setup including spectral quality checks to ensure high quality data collection.
- Live hardware control with visual feedback and active diagnostics for optimized data collection
- Raman instrument correction plus data conversions for shifted and unshifted spectra
- Access to all OMNIC data viewing, processing, analysis, and reporting features

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

OMNIC FT-NIR Analyzers
OMNIC for FT-NIR Analyzers provides all of the power and flexibility of OMNIC with features specially designed to address the needs of customers using Thermo Scientific FT-NIR analyzer systems.
- Built-in features for control of FT-NIR analyzers allow users of these systems to use OMNIC software for method development and take advantage of the wide array of spectroscopic analysis features offered in OMNIC
- All other OMNIC features and Add-on software are available

OMNIC DS Data Security
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 Windows user authentication protocols on a local computer or over a network
- No need to create new user names or passwords so there is no need for users to remember special ones
- Digital signatures establish record responsibility and ensure data integrity, something electronic signatures can’t do
- Unique log within the Windows Event Viewer tracks all software use and OMNIC software file events, even when OMNIC software is not running

OMNIC Customized Versions

OMNIC for Dispersive Raman
OMNIC for Dispersive Raman provides all of the power and flexibility of OMNIC with features specially designed to address the needs of customers using Thermo Scientific dispersive Raman systems.
- Smart System approach recognizes installed components reducing setup and avoiding operation errors and configuration memory retains alignment and calibration settings when lasers are changed
- Embedded capabilities like Autoexposure, Autofocus, Smart Background, white-light correction, laser power control at the sample, spot size reporting, and Automatic Fluorescence correction optimize and simplify dispersive Raman analysis
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