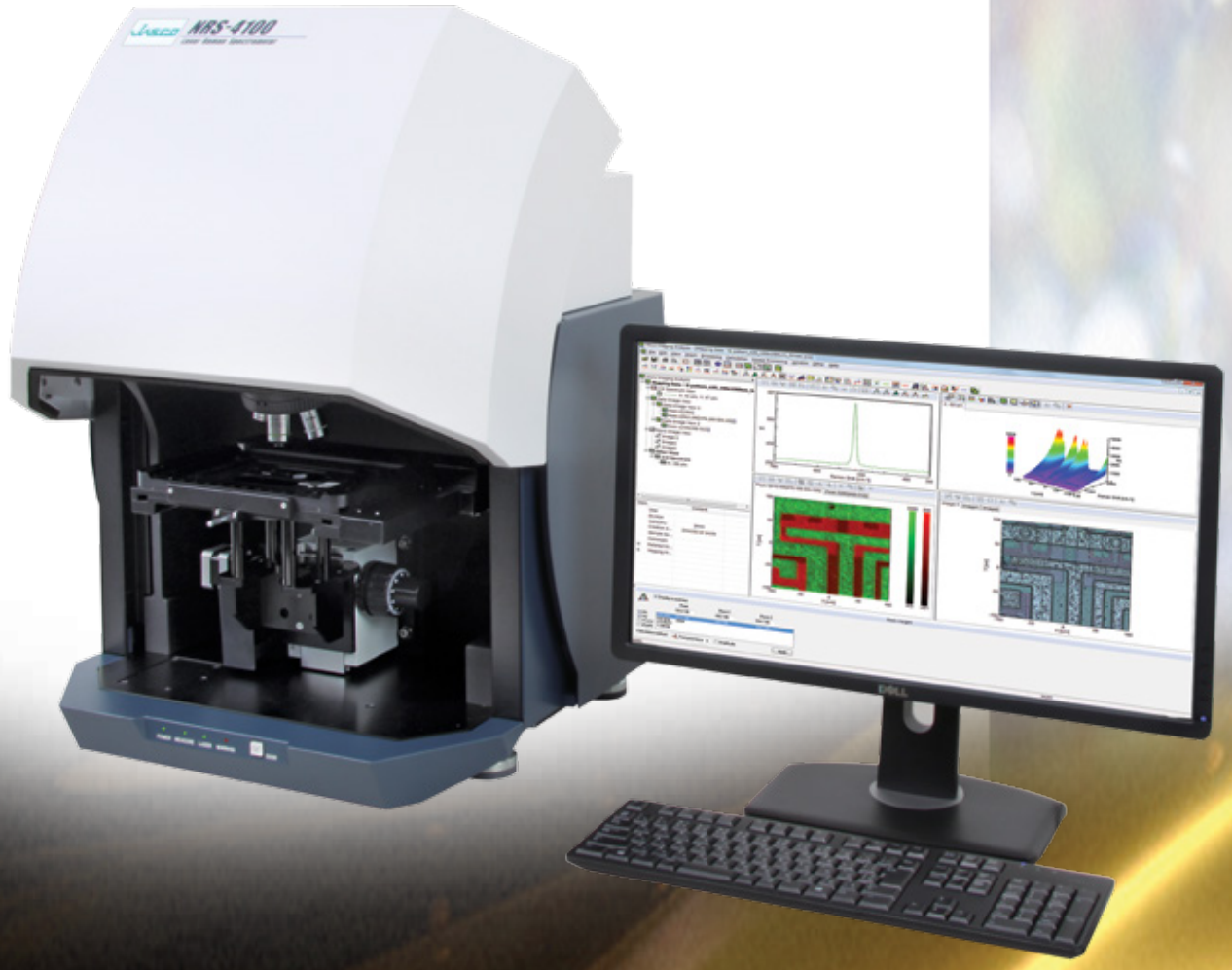
JASCO NRS-4100

Laser Raman Spectrometer



JASCO
Analytical Instruments

The New NRS-4100 Dispersive Laser Raman

The first thing you will notice is the Class 1 safety cabinet for total laser containment more commonly associated with high-end Raman systems, but that is only the beginning.

"Once you operate the interlock switch, the door opens to reveal a wealth of powerful automation tools making Raman accessible for all users"

NRS-4100 Dispersive Raman Spectrometer

In Raman spectrometry, sample preparation is generally considered to be much easier than for infrared spectroscopy and unlike FTIR microscopy, Raman offers greatly improved spatial resolution. As a result, the use of Raman spectrometry is rapidly spreading as the analytical technique of choice for materials analysis. One of the factors which has previously held back the adoption of laser Raman instruments is the skill set required for optical adjustment, measurement optimization and data analysis. The NRS-4100 will change the way Raman is used for so many different applications from QA, to academic teaching, to cutting edge research.

"FOR THE FIRST TIME, THE NEW NRS-4100 BRINGS TOGETHER A NUMBER OF CRITICAL ELEMENTS TO MAKE RAMAN SPECTROSCOPY ACCESSIBLE NOT ONLY TO EXPERIENCED SPECTROSCOPISTS, BUT ALSO TO FIRST-TIME USERS."

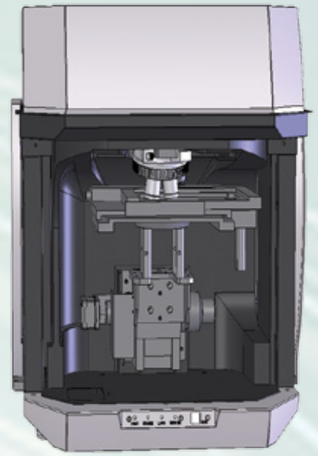
Rigid optical bench and laser image

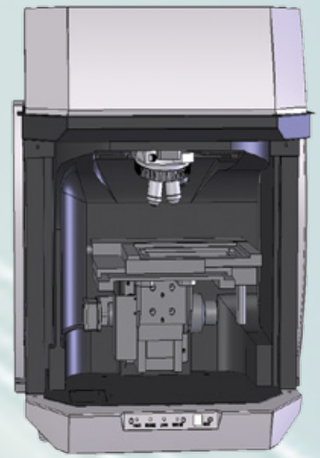
The purposed-designed microscope is completely rigid to prevent flexing; this is not the case with other systems built around an optical microscope. The NRS-4100 also offers direct observation of the laser spot (not generally available) to ensure it is perfectly aligned to the target sample and with XY spatial resolution down to only to 1 µm (Z=1.5 µm). Switching between observation and measurement modes is completely automatic and can be done with the safety cabinet closed.

Flexible sampling options

With a choice of refractive objectives, both micro and macro measurements are possible as well as options for long working distance objectives for heated sample stages and other sampling accessories. The NRS-4100 can also be specified with a manual sample stage or with the PC-controlled, automated XYZ mapping stage, and with the option of the large sample stage (80 mm working distance) to accommodate a variety of heating and cooling sample accessories. With options for macro sampling and for probe based measurements, the NRS-4100 has everything you will need for virtually any type of Raman experiment.

Standard stage





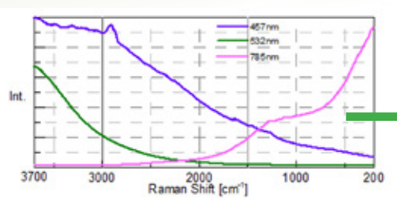
80 mm stage for larger samples and optional heated stage

Standard Configuration with 532/785nm lasers with matching notch or edge filters

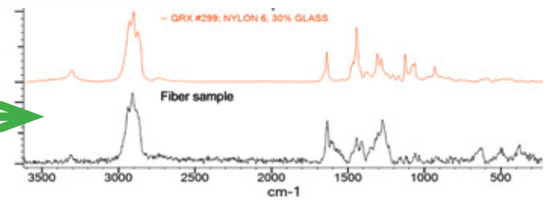
The NRS-4100 offers standard configurations that include the typical 532/785nm laser combination with matching edge or notch filters and an option for a third laser. All laser wavelengths are automatically selected in the software with matching notch or edge filter and, once selected, the optical system including the laser is automatically aligned for optimal throughput and resolution. Four software selectable gratings control the spectral range and resolution from 8000 to 100 cm^{-1} as standard (8000 to 50 cm^{-1} as an option). With a direct-drive rotary encoder, the wavelength reproducibility is ±0.2cm^{-1}

Laser choices and the New 457nm laser for improved fluorescence rejection and patented fluorescence rejection algorithm

JASCO has developed new, patented mechanisms to reduce sample fluorescence. As with other Raman systems, we can utilize laser wavelengths of 785nm and up to 1064nm, but we have recently incorporated a 457nm laser option that offers higher Raman signal, improved spatial resolution and much lower fluorescence for many different sample types than with the conventional 532nm laser. Selecting optional excitation laser wavelengths is only one of the ways JASCO minimizes fluorescence interference. The Fluorescence Rejection algorithm (patented) included in the Spectra Manager II collection and analysis software effectively removes or minimizes fluorescence, regardless of the laser wavelength used.



improved Raman intensity

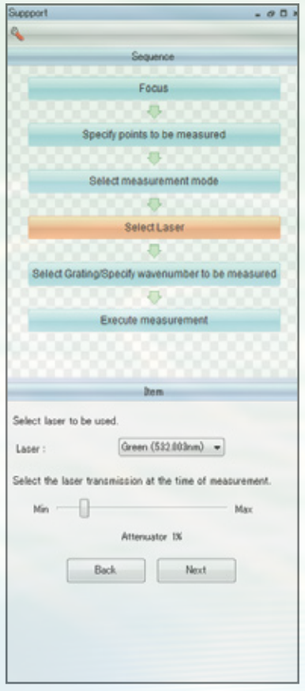


results in better sample identfication

Spectra Manager II spectroscopy data analysis

Powerful 'UserAssist' control for experienced spectroscopists and new users alike

The 'UserAssist' guide aids the user in setting up the NRS-4100 for sample measurement; a simple sequence takes you through setup and optimization of measurement parameters with helpful advice and tips, such as a warning if you have the laser intensity set too high. When each of the parameters has been set, the NRS-4100 automatically selects the laser and matching notch filter, the grating for the appropriate resolution, focuses on the sample and then the sample measurement is performed.



Real-time 'User-Assist'

Guides you through set-up and sample measurement

CHOOSE THE SAMPLE AREA TO BE MEASURED

SELECT THE LASER AND FILTER

SLIDER BAR TO SET THE LASER ATTENUATION

SET THE GRATING

WAVELENGTH RANGE

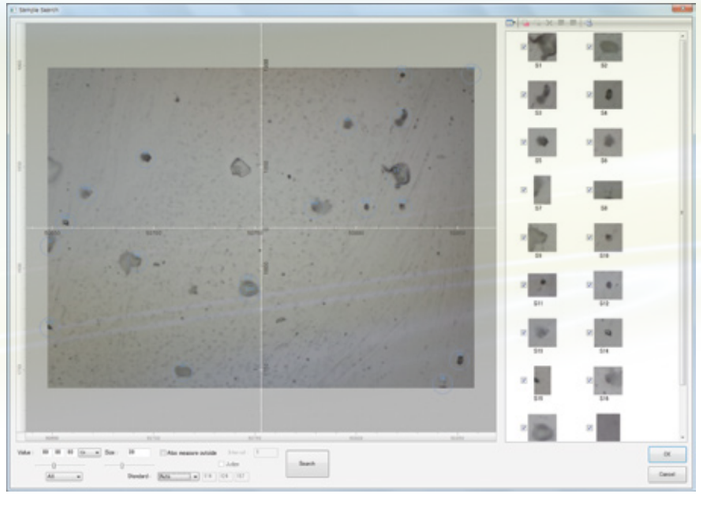
And 'Execute'

'Simple Search' function

The new 'Simple Search' function is used with the automated XYZ stage. A new algorithm developed by JASCO (patent pending) analyzes the microscopic image and automatically selects measurement position(s) based on the size, contrast and/or color of the target material described by the user, then simply click the measurement button to execute spectral measurements of the automatically identified sample positions.

AUTOMATED SAMPLE IDENTIFICATION FOR SPECTRAL MEASUREMENT

SPECTRA MANAGER IDENTIFIES A TARGET AREA AND THE USER SIMPLY CHOOSES TO INCLUDE IT FOR MEASUREMENT



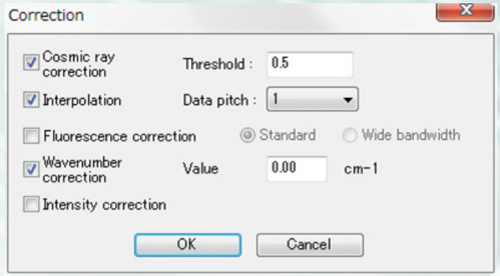
Real time data processing functions

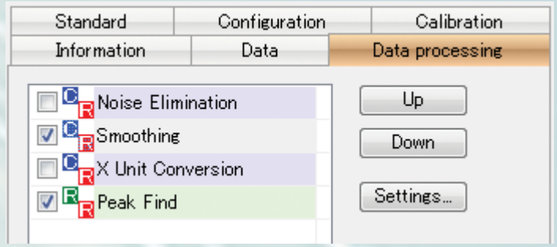
Spectra Manager II includes a wealth of user-selectable options for data analysis; as well as the usual tools like opening single or multiple spectra, zooming, normalization and a range of arithmetic data processing functions. In addition, there are a variety of Raman specific tools and analysis functions which can be applied during Raman spectrum collection, immediately after Raman data collection as a post-collection processing algorithm, or independently using the Micro Spectra Analysis software.

Useful Corrections for Raman spectrosopy

There are a number of different spectral processing functions available for Raman spectra, some of which are required to eliminate interference that may obscure the Raman peaks, others can be used to 'enhance' the Raman spectra, providing data for further calculations. The most common correction functions are listed in order below.

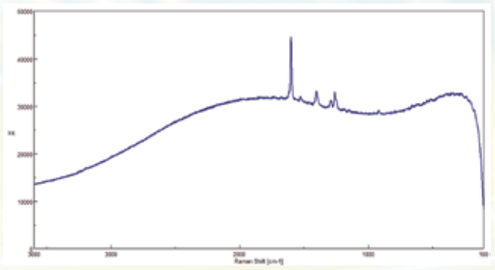
- Cosmic Ray, Fluorescence, Wavenumber and Intensity Corrections.
- Smoothing and Peak find
- Automated operations for routine use
- Expanded PL measurement



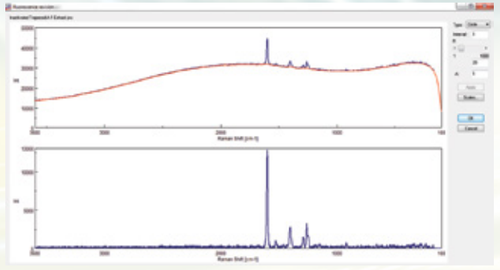


Fluorescence correction

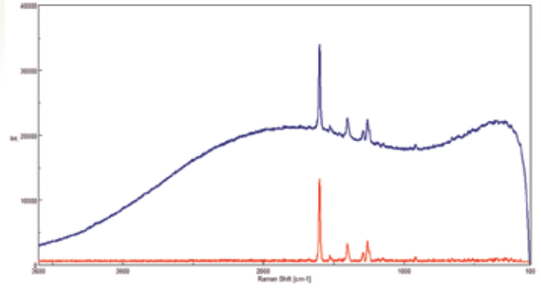
Fluorescence correction algorithm (JASCO patent). The NRS-4100 has two physical methods of reducing fluorescence - confocal aperture size to limit the amount of the surrounding matrix being measure for a sample, and changing the excitation wavelength to one which minimizes sample fluorescence. A fluorecence correction algorithm (JASCO patent) is also included which is highly effective at removing fluorescence after data collection.



Acquired spectrum



Applying fluorescence rejection, using simple parameters

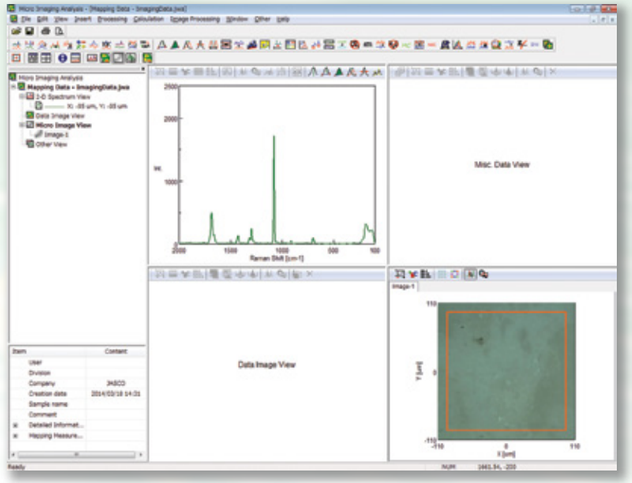


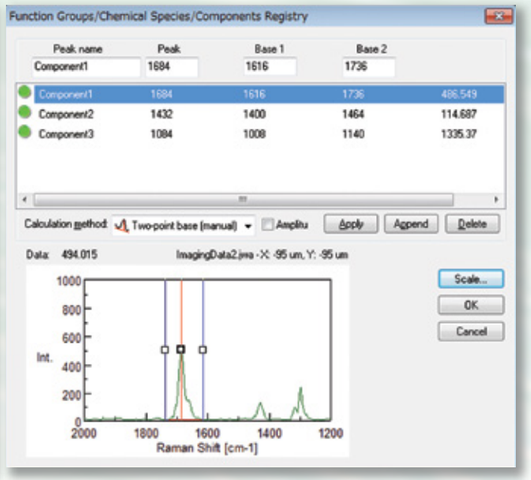
Overlay showing data before and after fluorescence rejection. The background is completely eliminated without loss of data integrity or change in signal to noise.

Spectra Manager II spectroscopy imaging analysis

Chemical Image identification and functional groups registry

To provide faster Raman image processing, the Imaging Analysis software includes a 'Registry' of functional groups or other relevant compound information based on peak height or area calculations. After a peak height or area calculation has been developed, it can be saved to the Component Registry for use in future analysis. The registry includes the peak calculation information and a 'label' describing the relevant vibrational motion. The registered functional group(s) can be monitored in real time to evaluate the mapping of a sample area.





CHARACTERIZE THE PEAKS OF INTEREST

↓

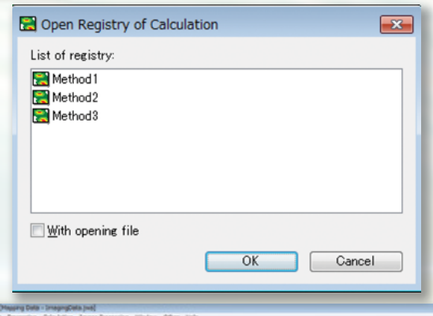
ASSIGN NAMES OR FUNCTIONAL GROUPS

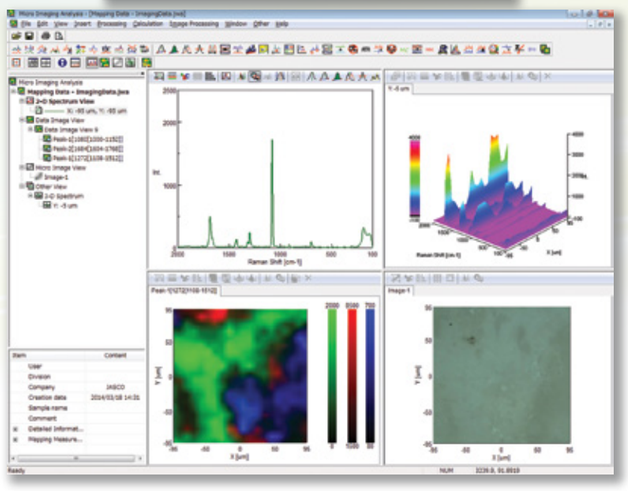
↓

SAVE THE COMPONENTS TO A METHOD IN THE REGISTRY

↓

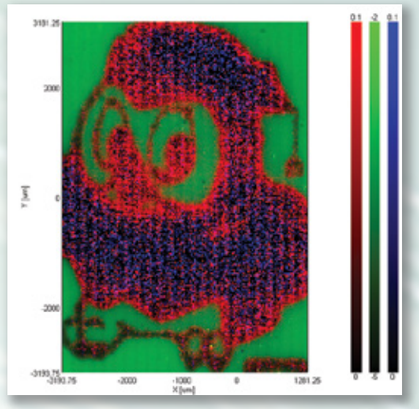
SELECT THE COMPONENTS FROM THE REGISTRY TO MAP THE SAMPLE

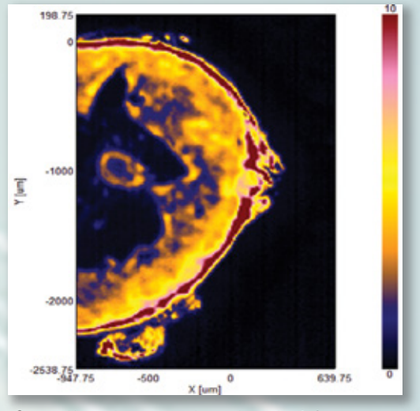




Creative Color Mapping

The large amount of spectral data obtained by Raman mapping/imaging operations can be overwhelming. Color image maps provide a simplified 'picture' of the spectral data, based on the Raman peak intensity for selected functional groups. Images maps are developed from the mapping data by simply clicking on a specified registered calculation, which can be based on the peak height/peak height ratio or the peak area/peak area ratio of selected Raman peaks. Up to 10 functional groups or molecular vibrations can be selected simultaneously to create descriptive image patterns of the sample being analyzed.

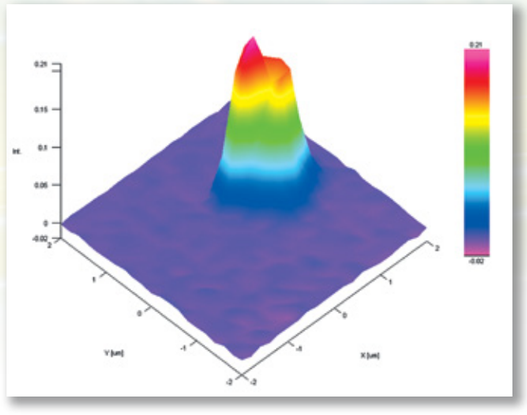




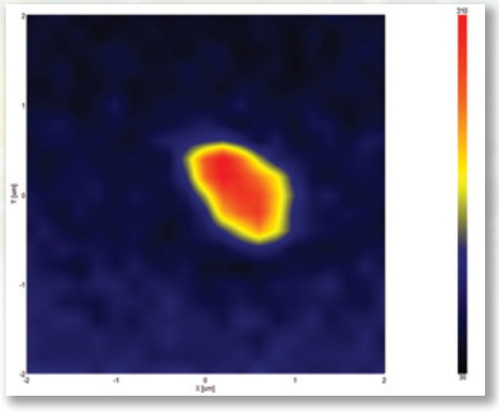
Use color overlays for up to 10 different bond conformations to map a target material

Color Data Display

There are numerous methods for display of the calculated image maps, including contour, false-color images, line images and 3-D image maps. All of the displayed images can provide fine detail based on the high resolution imaging capability of the NRS-4100 Raman instrument.



3D color map of a 4µm x 4µm sample with excellent spatial resolution.



2D contour map of the same data show the spatial resolution down to about 1µm

KnowItAll® JASCO Edition Informatics for Raman Spectroscopy

The industry standard KnowItAll informatics package with JASCO edition Raman library provides not only an excellent search tool, but also includes a range of analysis, molecule modeling and reporting tools.

AnalyzeIT™ Raman

Identification of Raman spectra of unknown compounds.
Classification/pattern characterization of chemicals.
Supplemental to other methods of spectral interpretation.

Key Features

- Knowledgebase of over 200 functional groups
- Knowledgebase contains hundreds of interpretation wavelengths
- Import experimental spectral data
- Determine if a structure matches a spectrum
- Intelligent “Suggest a Peak” feature
- Summarize negative or positive interpretations
- Browse knowledgebase by chemical class
- Peak overlay display
- Display & highlight structural bonds
- Link to additional functional group information in Sadtler Handbook
- View notes for functional groups when available
- Build your own knowledgebase to use in analyses
- For those expert and non-expert in spectral interpretation alike

SearchIT™ Database Searching

SearchIt™ - import data and search against KnowItAll user-generated or reference databases. Searches are fully customizable and are driven by powerful algorithms and can be performed by name, structure, substructure, properties, spectra and peak—in any combination.

Advanced Spectral Searching
SearchIt permits both full spectrum searching, as well as peak searching. Euclidean Distance, First Derivative Euclidean Distance, Second Derivative Euclidean Distance, and Correlation algorithms are available for full-spectrum searches.
For peak searches, manually select peaks or use the automated peak picking capability.

MineIt™ Database Viewing & Mining

With MineIt you can view reference or user created databases or search results

Advanced Datamining Capabilities
With KnowItAll’s MineIt application, users can view reference databases, user-created databases, or hit lists generated by the companion SearchIt application. This interface allows the user to access databases containing many types of data, such as IR, UV-Vis, Raman, NIR, structures, chromatograms, physical properties, and more. MineIt also includes the capability to compare variables in databases using a scatter-plot diagram.

KnowItAll® Informatics for Raman JASCO Edition includes over 600 spectral library

Spectral Searching & Analysis

Analytical Data Management

Structure Drawing & Reporting

SearchIt™	Database searching (full spectrum, structure, peak, property, etc.)
MineIt™	Data display and mining: Build databases with Raman spectra and structures
Overlap	Density Heatmap (Patented) for visual datamining and analysis
Mixture Analysis	Analyze spectral data of mixtures
AnalyzeIt™Raman	Raman spectral interpretation
RefineIt™ Raman	Raman spectrum processing
DrawIt™	2D structure drawing
ReportIt™	Publish professional reports, with structures, spectra, and more
BrowseIt™	Web portal for users with links to training resources and latest product information

DrawIT™

- A fully-featured 2D structure drawing program using ChemWindow® Technology
- DrawIt provides an advanced set of drawing tools—just click and drag to draw any chemical structure. Access the most comprehensive set of tools to draw rings, bonds, atoms, electrons, charges, chains, arrows, and more.

Key Features

- Customizable toolbars with tools to draw chemical structures easily, including bonds, rings, atom labels, charges, etc.
- Chemical recognition features such as hot keys, chemical syntax checker, tools to calculate mass and formula, etc.
- Stereochemical recognition including R/S and E/Z isomers
- OLE technology for in-place editing in word processing and presentation software
- Predefined styles for captions and structures

ReportIt™ create standard reports, presentations, and publications

- Create reports that include structures, spectra, chromatograms and other chemical data
- Use one of several pre-defined templates or create custom templates
- Easy-to-use tools to draw chemical reactions, such as arrows, text boxes, shapes, etc.
- Import chemical structures in common formats
- Import spectra and chromatograms in common native file formats
- Annotation tool to add captions to objects
- Table tool to enter and organize data easily
- Pen tool for freehand drawings
- Multi-spectrum display: overlay, stack, and offset
- OLE technology (Object Linking and Embedding) for in-place editing in word processing and presentation software (Word, Powerpoint, etc.)
- MS fragmentation tool to display a mass for each fragment; allows multifragmentation in one step
- 3D chemical structure visualization (spacefill, ball & stick, stick, wire frame display options)
- Clip art libraries with laboratory glassware drawings and engineering symbols
- Directly import chemical structures drawn in KnowItAll’s DrawIt applications

System configurations

The NRS-4100 is a flexible fully configurable optical system. We can build any system to your specification including laser and matching rejection notch or edge filters, matching grating(s), optimal CCDs and a range of stage options.

We have also created several dedicated systems designed for a variety of commonly used QC and research applications.

Impurity analysis system

Features

- Multiple lasers for avoiding fluorescence interference
- Auto-stage and objective carousel for preventing contamination.
- For measurement of biological samples, 457nm may be useful.
- KnowItAll Infromatics with 600 compound Raman spectra library

Item	Description
Laser	457, 532, 785nm
Options	Auto-stage, Automated objective carousel, optional Sadtler databases
Target user	Analysis division, QC department, technology center etc.

Carbon analysis system

Features

- Addition of 2400 gr/mm gratings which can measure G and D band at one time with high resolution.
- Also possible to add 1800 (1200) gr/mm gratings for measuring G and 2D band (such as Graphene)
- Assist function for carbon analysis
- Versatile analysis and measurement with highest resolution

Item	Description
Laser	532, 785nm
Grating	Addition of 2400 (1800,1200) gr/mm
Options	Carbon analysis program Auto-stage
Target User	Carbon materials manufacture, Graphene research, nanotubes, etc.

Item	Description
Laser	532, 785nm
Gratings	900, 1800 gr/mm
Options	manual stage
Target user	Academic teaching

Simple academic teaching system

Features

- Typical 532/785nm laser combination
- Multiple gratings
- Manual stage
- Standard Spectra Manager II software with User Assist and Sample Search
- Fully automated set-up and alignment

Item	Description
Laser	532, 785nm
Options	Macro measurement unit
Target user	Analysis of foreign material, measurement of liquid samples, chemical manufacture, R&D (for routine measurement of liquids, consider the RMP-500)

Macro measurement system

Features

- Mounting of macro measurement unit. (There are no obstacles for the samples when rotating the objective carousel)
- When working with larger samples, it is possible to adjust the length of the stand for the stage (option) to provide improved clearance

Pharmaceutical R&D

Features

- Multiple lasers for avoiding fluorescence interference
- Macro measurement unit for measuring liquid sample or sediment in drug solution
- Contactless analysis through glass bottles by using a 20x long working distance objective lens
- Thermal change measurement using Linkam accessories
- Imaging analysis of tablet samples with multivariate analysis
- Analysis of crystal polymorphism using E grade edge filters

Item	Description
Laser	457, 532, 785nm
Additional lens	Macro measurement unit 20x long working distance objective
Options	Auto-stage, heated stage, E grade edge filters, Thermal control measurement
Target User	Reaction studies

Specifications

Model	NRS-4100
Monochromator	
Monochromator:	Aberration-corrected, Czerny-Turner mount single monochromator, f = 200 mm
Wavenumber scanning mechanism:	High-accuracy direct-drive type (with rotary encoder) Wavenumber repeatability: ± 0.2 cm^{-1}
Wavenumber range:	8000 to 100 cm^{-1} (standard) 8000 to 50 cm^{-1} (option, required 532 nm E grade edge filter)
Resolution:	2 cm^{-1}/pixel (standard, 100 to 3900 cm^{-1}) 0.7 cm^{-1}/pixel (option, 100 to 1350 cm^{-1}, 532 nm, 2400 gr/mm grating, 1650 pixel CCD)
Grating:	Standard: 900 gr/mm Selectable from 2400, 1800, 1200, 600, 300, 150 gr/mm (Max. 4 gratings can be mounted simultaneously)
Optical alignment:	Auto-Alignment (Laser light) Raman light path auto alignment function Automatic switching of imaging lens for optimized spectrograph illumination.
Rejection filter switching:	Automatic filter switching mechanism (up to 4 filters) as standard Notch filter: 5 years warranty Edge filter: 3 years warranty
Detector	
Detector:	Air-cooled Peltier CCD detector (Max. -60°C), 1650 x 200 pixel, 16 µm x 16 µm, Visible to NIR
Optional Detectors:	Visible high sensitivity type, NIR high-sensitivity type, High-resolution type, InGaAs etc.
Laser	
Laser:	Standard: 532 nm, 20 mW Optional laser: 405, 442, 457, 488, 514.5, 532, 633, 785, 1064 nm, etc. *Red wavelengths are recommended lasers. *In case of 1064 nm, detector needs to be changed to InGaAs.
Number of mountable lasers:	Maximum 3 lasers (3 internal or 2 internal and 1 external)
Microscope	
Sample observation:	High resolution CMOS camera (200 M pixel)
Confocal optical system:	Standard
Spatial resolution:	XY= 1 µm, Z= 1.5 µm
Objective lens:	5x, 20x, 100x, (Plan Achromat objective lens) Manual 6 position objective carousel as standard Electronic drive 6 position carousel as option. Long working distance type, NIR type, water immersion lenses are also available as options
Sample stage:	Manual stage (standard) Automatic XYZ stage with auto-focus function (option)
Imaging measurement:	Option, Automatic stage imaging with auto focus, XYZ 0.1 µm step, 3D imaging, omni- focus
Laser safety Classification and Safety mechanism:	Class I Interlock mechanism by software and hardware, Laser optical path protection
Macro measurement:	Option, Carousel type macro-measurement unit is available as local upgrade option
Fiber probe:	Option (Manual switching)
Other hardware options:	Dichroic mirror, Polarized observation, differential interference contrast, transmitted illumination
Software	
Standard program:	Microscope spectra measurement, Validation, Spectra analysis, Imaging analysis, Wavenumber correction, Sensitivity correction, Fluorescence correction, JASCO canvas
Imaging program (option):	Sample search function, Multiple focus function, Focused view, 3-D structure observation, Peak calculation, PCA mapping, Refractive index correction
Correction program:	Standard, Auto-fluorescence correction, Sensitivity correction, Wavenumber correction (Ne lamp and Std sample are included.)
Optional program:	Interval measurement analysis, Thermal change measurement, Imaging analysis, Stress analysis, Carbon analysis
Others	
Anti-vibration table:	Option (air source for anti-vibration table: nitrogen gas or air source, secondary pressure 0.25 - 0.3 MPa)
Dimension and weight:	Main Unit 550 (W) × 610 (D) × 800 (H) mm, approx. 80 kg - Power Supply : 220 (W) × 320 (D) × 70 (H) mm, approx. 3 kg AC 100 V ±10 V, AC 200 V ±20 V, 200VA

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For more information, please contact :

LRA-1404-P Printed in Japan

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MADE IN TOKYO, JAPAN