The powerful WiRE™ software driving Renishaw's Raman systems

#renishaw

A high definition Raman image of a volcanic rock section from Mount St Helens generated from 2.7 million spectra. The colours indicate the many different minerals present. Rock section courtesy of Dr Claire Horwell and David Damby, University of Durham, UK.

Powerful Raman software

Renishaw's Windows®-based Raman Environment (WiRE™) software is dedicated to Raman spectroscopy and is the power behind Renishaw's Raman spectrometers.

WiRE™ software is the interface between you and your Raman instrument. It controls the acquisition of Raman data and provides users with dedicated data processing and analysis options. You can, for example, use the WiRE software to identify an unknown spectrum, remove its background, or determine the distribution of particles in megapixel-sized Raman images.

Our WiRE software suite has been produced by Renishaw's international team of software experts, guided by our experienced application specialists and users worldwide.

When used within a suitable environment, the WiRE software complies with 21 CFR Part 11 (the U.S. Food and Drug Administration's part 11 of Title 21 of the Code of Federal Regulations; Electronic Records; Electronic Signatures).

Access WiRE™ software training

We have produced a library of detailed WiRE software training documents and videos. These give step-by-step instructions and are available for download from our dedicated training portal. To gain access please visit:

renishaw.com/ramantraining
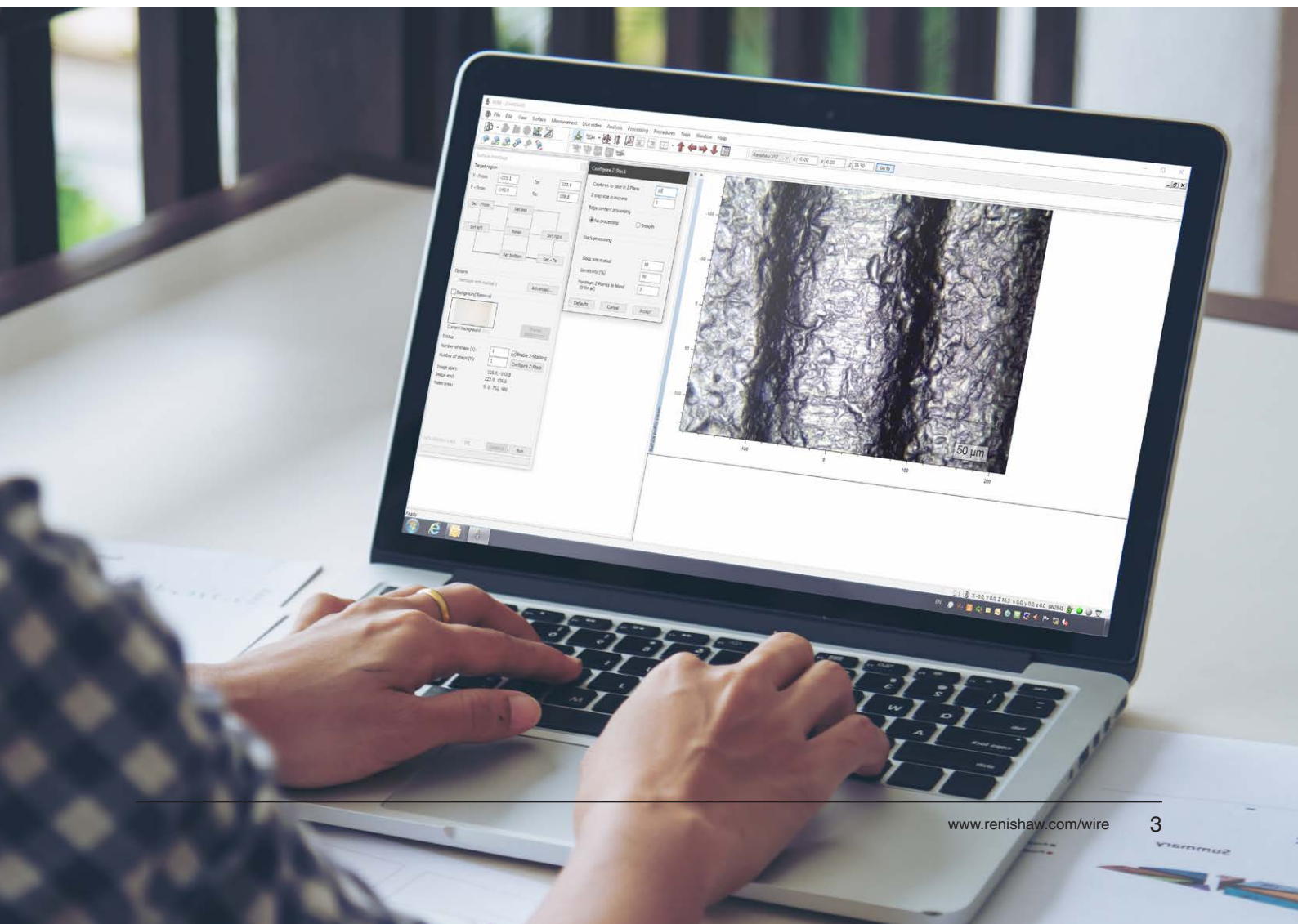
Control your Raman system

Instrument control

WiRE software is the communication interface between you and your Raman instrument. Quickly and easily configure your experiment, harnessing the high degree of automation of Renishaw's Raman systems. WiRE software:

- Automatically references and positions motorised components during instrument start-up.

- Moves key optics to their pre-determined positions when you change instrument configuration. You don't need to manually align components.

- Synchronises mechanical components and electronics during precision operations (such as SynchroScan™ spectrum acquisition and StreamLine™ technology rapid chemical image generation).

- Performs health checking and calibration of the instrument.

Sample viewing

The WiRE software can control video cameras and mapping stages to provide enhanced views of your samples.

- Automatically capture white light images from reflected or transmitted white light. These images can be stored with your spectral data.

- Create high resolution white light images over large areas by using the WiRE software's white light montaging (tiling).

Data collection

Use WiRE software to define and optimise key parameters of your data collection. You get your data quickly and save valuable instrument time.

- Choose the laser, grating and detector configuration using simple measurement templates.

- Easily configure measurements, such as:
  - multiple discrete sample points (1D multi-file).
  - linear profiling (1D multi-file: time, temperature, distance, etc).
  - fast spatial area analysis (2D multi-file).
  - complete sample volume (3D multi-file).

- Collect as many or as few data as you need. You can collect over 50 million spectra in one dataset if you want.

- All instrument and measurement parameters are stored with your data; you do not need to take handwritten notes.

- Sometimes you don't know the exact measurement conditions to use. Rather than having to manually try them one by one, you can use WiRE software's queuing capability. Configure the measurements all at once and then leave WiRE software to run them for you.

- Automate Raman data collection positions using contrast from optical or 3rd party images.

- Raman analyse specific positions already analysed with other techniques.
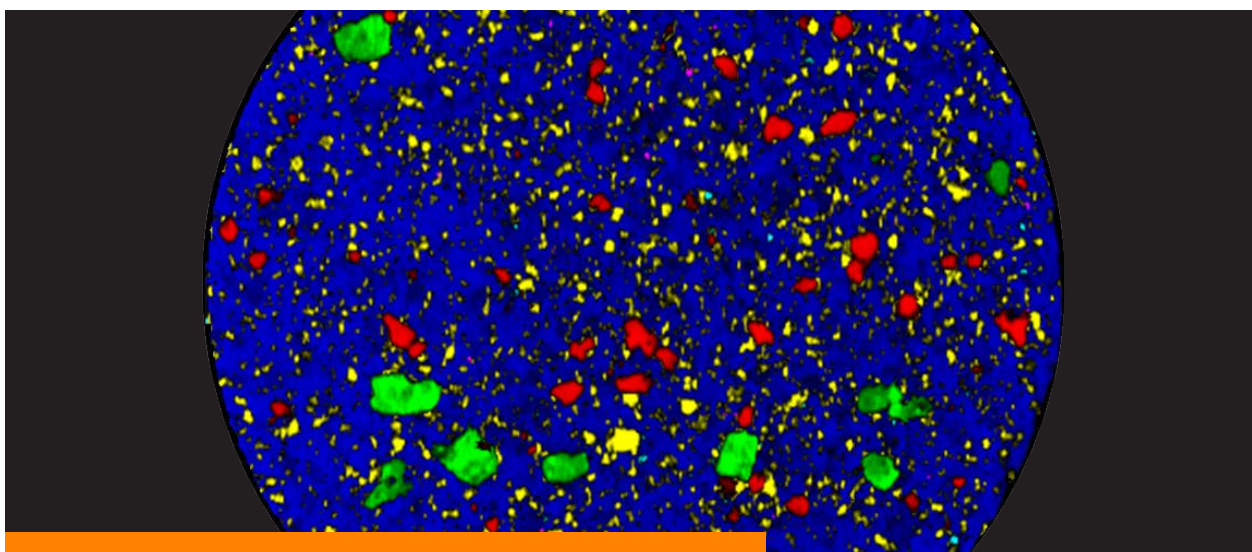
StreamLine technology Raman image of a tablet used for the treatment of Parkinson's disease. StreamLine technology enables users to produce Raman chemical images rapidly.

Additional features of WiRE software

- Multiple mapping regions can be configured to run unattended with WiRE software's batch mapping capability.

- Choose the laser power level you want with automated and repeatable power control options.

- Ensure focus is perfect. The WiRE software has a range of focus maintaining options. Use these when studying samples with uneven surfaces or samples shifting out of focus (for example when your sample changes phase in a temperature control cell).
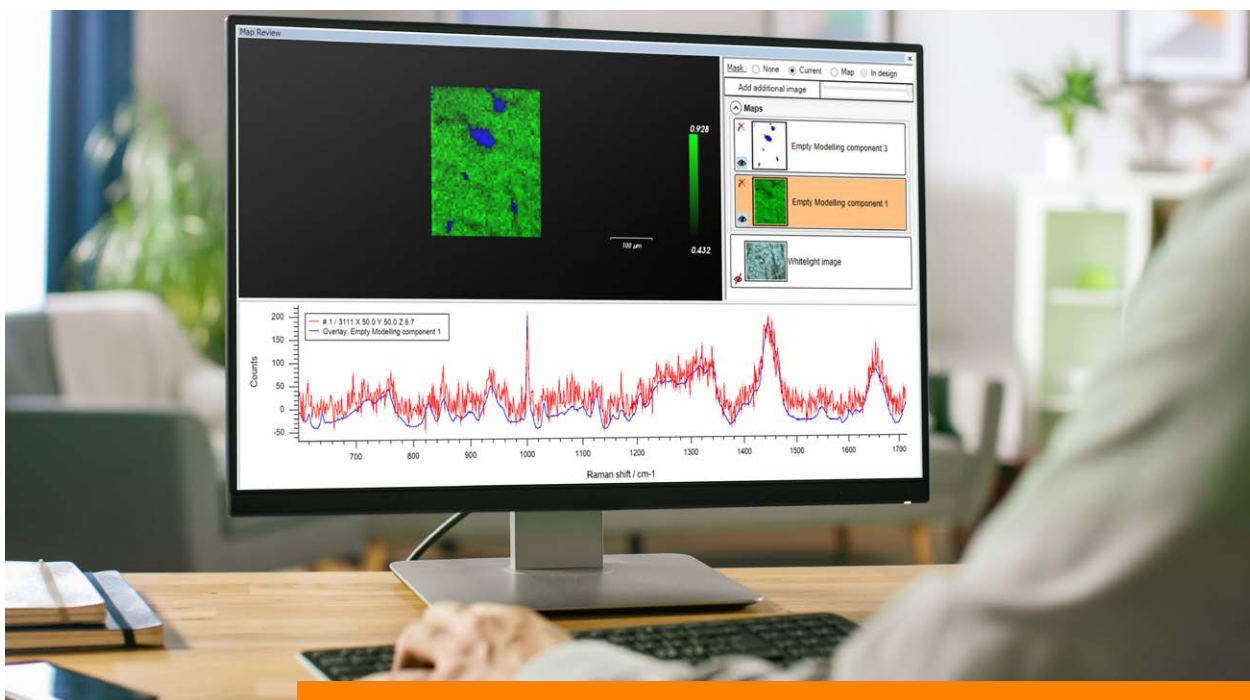
The Empty Modelling™ method can—in seconds—identify the chemical species present from millions of spectra and generate chemical images of their distribution, even when individual spectra may represent mixed components.

Analyse your Raman data

Data processing and analysis

WiRE software is a dedicated software package for Raman spectroscopy. It is designed by experienced Raman users. As a result, it has the specific tools you need to get information from Raman data.

- Process your data to get the most accurate and representative information during analysis.

- Analyse your Raman data to extract the wealth of information contained within.

Key WiRE software features

The software has a range of processing options for single spectra and multi-files focused on:

- Background fluorescence removal (including patented intelligent fitting baseline subtraction).

- Subtraction of spectral features originating from substrates and solvents.

- Removal of artefacts caused by cosmic rays. (including automated nearest neighbour options).

- Noise removal and reduction (including automated PCA noise removal).

- Mask spectra from map data to target sub-areas for further processing/analysis.

A range of analysis options for single spectra:

- Spectral identification (choose from an extensive range of libraries or build your own).

- Accurate reporting of band parameters (such as position, width and area, to reveal material properties).

A range of univariate and chemometric analysis options for multi-files and Raman images:

- Location of known and unknown species using a choice of supervised and unsupervised analysis options, such as Raman optimised component analysis (NNLS) and Empty Modelling™.

- Empty Modelling™ can be used to de-mix map datasets. It produces chemical images which correlate to pure components present within the data. You can then use library searching to identify these unknowns.

- Mixture fraction quantification.

- Understand the change in material properties through the fitting of accurate theoretical bands (curve fitting) or reference spectra (DCLS), to help understand changes in material properties.

- Domain size and distribution analysis from Raman/optical images.

- Use Correlate to view overlaid images from your sample collected using different techniques.

Getting your data out

The WiRE software can export results, spectra and images to other applications, for use in reports and scientific papers

- Export of single and multiple spectra to different spectral formats.

- If you need more specialised analysis, you can import the WiRE software wdf data format into Matlab* (Mathworks*).

Flexible solutions

The core WiRE software package includes all the features most users need. You can add optional modules which provide extra capabilities or, if necessary, Renishaw can work with you to develop a custom solution.

Additional modules

Customise the WiRE software by adding modules which contain specialist features:

- Microplate mapping - automated pharmaceutical and biological data collection where you have a large number of similar samples.

- Custom Analysis Package (CAP) module - for process monitoring, QA and QC.

- Dedicated SEM-SCA controller - for combined SEM-Raman systems.

- Particle analysis - flexible approach to locating, analysing and automating measurements on multiple particles.

- Batch converter - convert data between file formats.

- Temperature cell controller - advanced and interruptible control of temperature ramps for temperature cells.

- Particle statistics - produce morphology metrics from white light and Raman images.

- Data Classifier - Group Raman spectra based on major or minor spectral differences.

- Process monitoring - Use Monitor™ software module or the Custom Analysis Package (CAP) module for QA and QC.

Particle analysis automates Raman analysis and reporting of multiple particles in an intuitive and highly automated workflow.

Custom software for your experiment

We pride ourselves on our ability to provide you with bespoke solutions, if required. We can do this because our Raman systems are flexible and fully automated. WiRE software plays a key role in supplying a complete solution. It ensures custom hardware changes are fully integrated and easy to use.

*Mathworks and Matlab are registered trademarks of Mathworks.

Key features

Instrument control and data collection		Compatibility		
Name	**Details**	**inVia**	**Virsa**	**RA800**
Fully integrated instrument control	Full control of all key features, including:			
	• Automatic wavenumber and response calibration	✔	✔	✔
	• Auto system alignment maintenance	✔	-	-
	• Performance qualification (system performance checking utility)	✔	-	✔
Motorised lenses and mirrors	Motorised control of spectrometer lenses and mirrors, for convenient optimisation of system performance in all configurations.	✔	-	-
Configuration change automation	Fully automatic switching of excitation wavelength, Rayleigh filter selection, and spectral coverage.	✔	✔	-
Secondary detector support	For additional camera support e.g. Ingas and EMCCD. Others available on request.	✔	-	-
Automated mode switching	Automatic switching between sample viewing and Raman acquisition modes.	✔	✔	✔
Easy measurement setup	• Single acquisition measurements	✔	✔	✔
	• Multiple acquisition measurements	✔	✔	✔
	• Triggered time series acquisitions	✔	✔	-
	• Area	✔	✔	✔
	• Line, depth mapping, and depth slices	✔	✔	-
Measurement templates	Easy storage and recall of conditions for repeat measurements. Applicable to singe spectrum and map measurements.	✔	✔	✔
Measurement queuing	Multiple measurements can be queued for sequential unsupervised acquisition. For example, this enables users to fully utilize the instrument by running a series of measurements overnight.	✔	✔	✔
Measurement repeat	Ability to automatically repeat the same measurement a user definable number of times.	✔	✔	✔
SynchroScan™	Renishaw's patented method for producing seamless, artefact-free, large wavelength coverage spectra - removing the need to join multiple spectra. This synchronises and scans Renishaw's high precision grating stage and Centrus multichannel detector continuously.	✔	✔	-
Sample stage support	Integrated control of XYZ stages, for manual and automated motion.	✔	✔	✔
System video	Integrated live video viewing and image capture, including white light image processing.	✔	✔	✔
High resolution/trinocular microscope video	Integrated support for high resolution and trinocular video with digital zooming. With appropriate microscope hardware, enables other optical contrast methods such as polarisation and dark field.	✔	-	✔
Image montaging	For the creation of large area composite white-light-illumination images, rather than just the objective's field of view. These visible light images greatly facilitate the analysis of larger samples, simplifying the logging of points of interest and the definition of regions to Raman image.	✔	✔	✔
Optical image Z stack	Enables an 'in-focus' image to be generated from an image stack.	✔	✔	✔
Integrated support for multiple microscopes	Enhanced Sample Review option to automatically control settings for different microscope and fibre optic probes including the SEMSCA SEM-Raman option.	✔	-	-
Fully configurable interface	Includes customisable toolbars and procedures.	✔	✔	✔
Remote support	Remote access to the system, by the Renishaw support team, for remote servicing diagnostics. (requires internet connection).	✔	✔	✔

Instrument control and data collection

Name	Details	Compatibility		
		inVia	Virsa	RA800
Correlate™	This module aids users who want to combine Raman data with data from other microscopes (such as SEM, AFM, fluoresence and confocal microscopes). Correlate relates the coordinate systems of the two microscopes to provide effortless sample navigation and acquisition after you move your sample to your Renishaw Raman microscope. • Coordinate manager - acquire Raman data in the correct sample location • Image alignment tool - overlay and register images and data Can be combined with batch mapping optional module.	✔	✔	✔
Japanese language support	The WiRE software automatically runs on Japanese versions of Microsoft Windows®. Other languages may be available on request.	✔	✔	✔

Data processing and analysis

Name	Details	inVia	Virsa	RA800
Cosmic ray removal	Fast and targeted removal of cosmic ray features using 'nearest neighbour' and 'width of feature' methods. Control the sensitivity of data to cosmic ray features. Use results presented in sortable tables to confidently remove large numbers of cosmic ray features at the same time.	✔	✔	✔
Zapping	Manually remove unwanted spectral features such as those produced from cosmic rays.	✔	✔	✔
Noise filtering	Uses principal component analysis (PCA) to rapidly and effectively enhance data by removing noise - with preview and residuals option. Enhanced option where user can select individual loadings for removal.	✔	✔	✔
Smoothing	Several options, including Savitsky-Golay and Adaptive smooth.	✔	✔	✔
Truncate spectra	Terminate the ends of spectra to remove extraneous data points. Remove unwanted features such as the Rayleigh filter transmission edge profile.	✔	✔	✔
Baseline subtraction	Removal of unwanted background from spectral data (including automatic 'intelligent baseline removal' option). Applicable to single spectra and multi-files.	✔	✔	✔
Masking	Enables one or more pixels (spectra) from a map dataset to be ignored for future processing and analysis operations. Masks can be defined by: selecting individual spectra; drawing on a white light or Raman image; thresholding a white light or Raman image; flagged from any saturated data. Average spectra can be generated and saved for regions masked in or out.	✔	✔	✔
Arithmetic operations applied to spectra, profiles and images	Use a range of simple and complex arithmetic functions, that can be applied to single data files or multiple data files. This enables, for example, the subtraction of substrate spectra data from mixed spectra, and the re-scaling of spectral information.	✔	✔	✔
Peak picking	Automatic or manual labelling of Raman band positions.	✔	✔	✔
Curve fitting	Produce information on the position, width, intensity and area of Raman bands to a much higher accuracy than manual measurement. Apply these metrics to multi-files to generate profiles and images. Use multiple curves to 'deconstruct' complex band systems.	✔	✔	✔

Key features

Data processing and analysis

Name	Details	inVia	Compatibility Virsa	RA800
Data viewing	2-D and 3-D views of data, including spectra, images, and mapped sections.	✔	✔	✔
Data merging	Merge data from a set of measurements and view as a higher dimension object (e.g. merge and view a series of 2D chemical images as a volume).	✔	✔	✔
Time/temperature series	Enables the generation of Raman profiles from non-spatial variables:			
	• 1D time series	✔	✔	✔
	• 1D temperature series (requires optional temperature feature with temperature hardware	✔	✔	-
	Supports alternate profile axes, useful for correlating spectral changes against temperature or time (enabling hysteresis-type plots).			
Profile and image generation	Image generation and display based on analysis of: • Spectral intensities • Integrated spectral intensities • Curve-fit results • Sample topography / morphology • Image arithmetic (ratio, subtraction, etc.) Optional image generation modules available.	✔	✔	✔
Live profile and image generation	Raman profile/image generation and display can be performed during data acquisition, rather than solely by post processing. This enables users to review information as it is collected ('live'), and can be performed using both univariate methods and multivariate component analysis methods.	✔	✔	✔
Dynamic image viewing	Interact with Raman mapping data to produce live Raman images based on intensity at a point, signal to baseline and signal to axis methods.	✔	✔	✔
Image overlay	Multiple image (Raman and microscope image) overlay with transparency and opacity. Enables users to generate colour-coded information-rich images.	✔	✔	✔
Normalise spectra	Linearly rescales the intensity data from a spectrum to satisfy a defined criterion.	✔	✔	✔
Differentiation	Calculates a gradient at each point of a given spectrum or line profile. Provides an option to remove background from Raman features or to estimate the spatial resolution of the system by differentiating a line profile across a feature.	✔	✔	✔
Integrate individual spectra	Calculate and display the area beneath user selectable regions of a spectrum.	✔	✔	✔
Chains	Option to combine specific processing and/or analysis functions to a single step and apply to a new data file.	✔	✔	✔
Integrated display system	Fully configurable display of spectral, image and mapping data.	✔	✔	✔
Labelling of spectra	Customisable labelling of spectra with simple text labels, dynamic labels consisting of data 'mined' from within WiRE data files (file name, measurement parameter, user, etc.), and images.	✔	✔	✔
Data import/export	Data transfer using the Windows clipboard, and by file (Galactic SPC and text formats). Ability to import Renishaw 'wdf' format into Matlab®. Ability to export a white light image/montage up to 530 Mpixel in size.	✔	✔	✔
Piezo stage support	Support for selected piezo sample stages.	✔	-	-

Help

Name	Details	inVia	Virsa	RA800
Online help system	Extensive context-based help system with training modules.	✔	✔	✔

Data assurance

Name	Details	Compatibility		
		inVia	Virsa	RA800
Report export	Export Raman data, white light images, Raman images and measurement information to Microsoft® Word and Microsoft PowerPoint programs.	✔	✔	✔
Full data recording	Full measurement details and instrument state settings are recorded with all collected data. Data file history (audit log) records all changes to the file since creation.	✔	✔	✔
Software audit log	Full traceability of system operations: Data traceability: full listing of data operations recorded in file Calibration traceability: full audit log of instrument operations	✔	✔	✔
Microsoft® Windows 10 compatible	Operation on Microsoft® Windows 10 x64	✔	✔	✔

Optional modules

Name	Details	inVia	Virsa	RA800
FocusTrack™	Maintain focus iteratively point by point by using signal intensity for non flat samples.	✔	-	-
Surface	Enables the user to manually define in-focus points on their sample, producing a 3D surface used to determine where mapping data is collected.	✔	✔	✔
LiveTrack™	Live automated focus tracking technology enables the analysis of samples with uneven, curved or rough surfaces and maintains focus in both white light video and Raman modes. Simple workflow driven interface. Supplied with LiveTrack configured instruments only.	✔	✔	✔
Motorised sample position control and mapping	When used in conjunction with the Renishaw high speed encoded stage (HSES), this enables accurate and repeatable sample positioning direct from the video or XYZ stage control toolbar. Includes point mapping options:			
	• 1D line profiles (X,Y)	✔	✔	✔
	• 1D depth profiles (Z)	✔	✔	
	• 2D area mapping (XY)	✔	✔	✔
	• 2D depth slices (XZ, YZ)	✔	✔	
StreamHR™ mapping	Fast imaging technique for spot-focus lasers. It can exploit the very high resolution of Renishaw's encoded stage to reveal sample features much smaller than the laser spot.	✔	✔	-
Line Focus	Option to collect multiple spectra, simultaneously, along a laser line, whilst maintaining spatial information.	✔	-	✔
StreamLine imaging	StreamLine fast Raman imaging technology enables users to produce Raman chemical images rapidly. Line focus illumination, with parallel data collection, enables higher laser powers to be employed.	✔	-	✔
Rapide	Ultra-fast StreamLine and StreamHR mapping options which use 2 MHz detector readout and constant velocity stage motion. Rapide Time Series for static high speed spectroscopy e.g. reaction kinetics.	✔	-	✔
Batch mapping	Uses a defined set of coordinates to centre the same measurement and collect data at multiple locations. This is compatible with any measurement type including mapping measurements, and with Correlate™.	✔	✔	✔

Key features

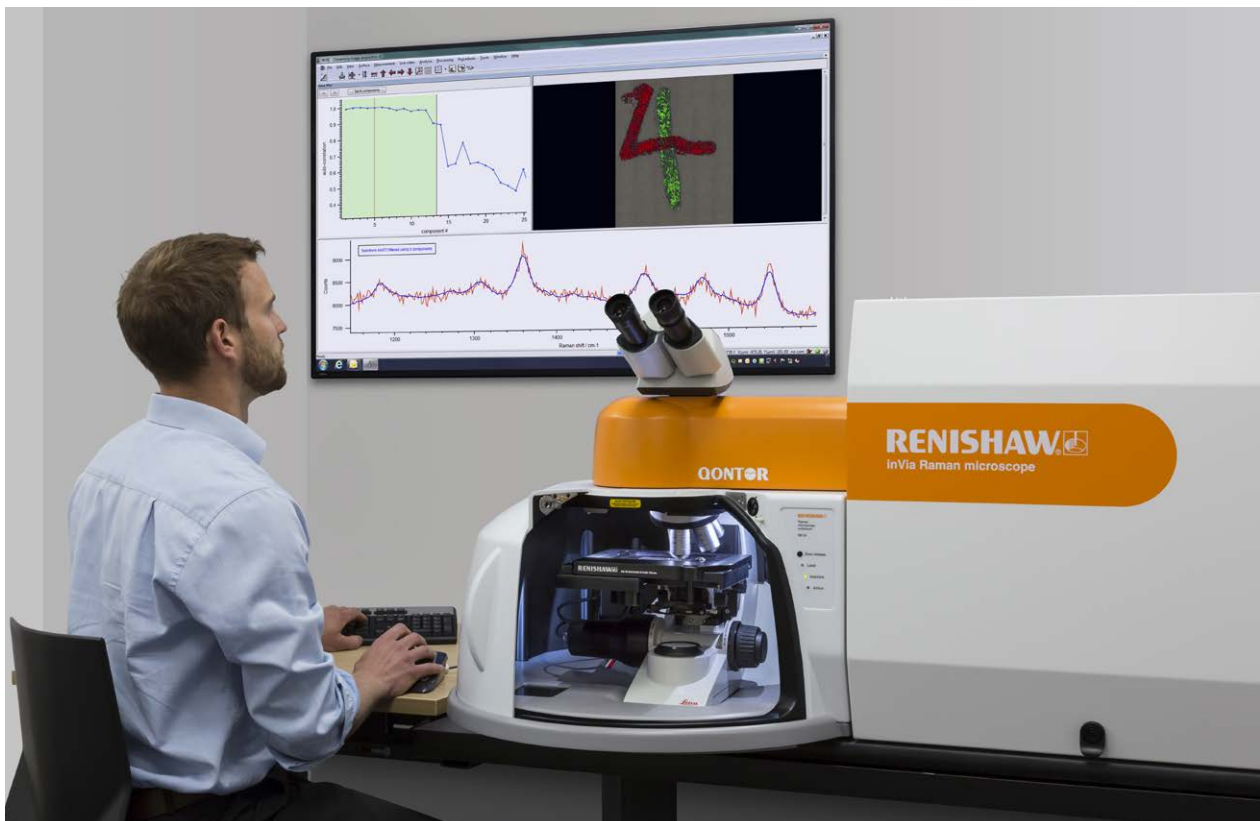| Optional modules		Compatibility		
Name	**Details**	**inVia**	**Virsa**	**RA800**
3D data collection and viewing	Use of StreamHR mapping and StreamHR Rapide to collect 3D (XYZ) datasets. Processing and analysis is performed in WiRE on the entire dataset, not just individual planes. Viewing is performed using the Renishaw volume viewer, where planes, slices, and volumes can be viewed for single and multiple volumes. Including opacity control and animation scripting. Planes can be saved as a new data file. Videos can be exported to AVI format.	✔	-	-

Temperature cell support	Support for selected sample heating and cooling cells:
	• Temperature ramping
	• Advanced temperature control (ATC)
	  ◦ White light viewing during temperature change
	  ◦ Automatic recording of white light images
	  ◦ Pause and adapt temperature ramps
	  ◦ Adapt any data collection parameter
		✔	✔	-

Library manager and spectrum search	Module for the creation and use of spectral libraries to identify unknown materials. Includes automatic and interactive methods for identifying the chemical consituents of both pure and mixed spectra, by matching to spectral libraries.	✔	✔	✔
Spectral libraries	Spectral libraries for the identification of unknown materials: Other 3rd party libraries available on request.			
	• Inorganic materials and minerals	✔	✔	-
	• Polymeric materials	✔	✔	-
	• Excipient materials	✔	✔	✔
	• Forensic materials	✔	✔	-
Chemometrics	Powerful supervised and unsupervised multivariate image generation methods, to help users rapidly create meaningful images, including: • Component analysis (DCLS, NNLS) • Principle component analysis (PCA) • Empty Modelling™ (MCR-ALS) • Cluster analysis (k-means and HCA) Component analysis of single spectra. Quantify mixture composition from average spectra. Partial least squares (PLS) option. To enable the prediction of a value from an 'unknown' spectrum, based on a model incorporating a set of known values spanning a suitable set.	✔	✔	✔
Particle statistics	Quantification of image domains based on Raman and white light images within WiRE. Revealing: number of particles, total particle area, area percentage, centre of mass displacement, D90, D50, D10, perimeter, equivalent circle diameter, eccentricity, orientation, solidity, nearest-neighbour distance, centre of mass X, centre of mass Y, length, width, aspect ratio, circularity, elongation. Also enables the generation of map measurements to analyse discrete domain locations. Particle positions can be exported for subsequent analysis.	✔	✔	✔
Particle Analysis	Automates Raman analysis and reporting of multiple particles in an intuitive and highly automated workflow. It uses images generated using the microscope's different contrast modes (or using images imported via Correlate) to guide Raman data collection from those particles. Data processing, data analysis, and reporting options are all inclusive within the module.	✔	✔	-

Optional modules

Name	Details	inVia	Virsa	RA800
		Compatibility		
Monitor	Monitor software performs complex spectral analysis, giving simple readouts of concentrations and trends during experiments. This makes it easy for you to monitor changes and reactions in real time and pass them to third party applications.	✔	✔	✔
Data classifier	Separate module dedicated to the classification of Raman data using PCA-LDA. Includes integrated data processing, model building, cross-validation and classification of unknowns.	✔	✔	✔
AFM	Support for selected AFM systems.	✔	-	
TERS hot spot mapping	Automated alignment to locate the TERS hot spot on a TERS active AFM tip using a volume image. Laser is aligned at the optimal hot spot point for subsequent TERS data collection.	✔	-	-
Support for 3rd party hardware	The WiRE software supports the triggering of Raman data collection from 3rd party hardware. Enables map data to be plotted against 3rd party values (programmable via TCP/IP).	✔	-	-
Andor Rapide	Support for ultra-fast EM-enabled detector.	✔	-	-
Photocurrent mapping	Enables the generation of simultaneous Raman and photocurrent spectra and images, when used with the necessary additional hardware.	✔	-	-
Microplate mapping	Analyse, rapidly and easily, material contained in microarrays and multiple-well plates.	✔	-	-
CAP – Custom Analysis Package	CAP is aimed at users who want to employ their Raman instruments for quality-assurance/quality-control (QA/QC) and other applications that require repeat measurements to be performed in a controlled manner. CAP enables users to configure both data acquisition and data analysis, with features such as a TCP/IP interface for external control.	✔	✔	-
21 CFR Part 11	Module adding features required for compatibility with 21 CFR Part 11 Electronic Records regulations. Also supports peak position and peak area ratios for Pharmacopoeia performance verification.	✔	✔	✔
Remote Access	Remote instrument access and control via TCP/IP.	✔	✔	✔

When performance really matters, choose Renishaw

We launched our first Raman spectroscopy product in 1992, and have been continuously developing Raman instrumentation ever since. Decades of experience ensure that our products can be trusted to deliver the results you need.

Our Raman systems are built with many parts manufactured in-house. These are put through extensive and rigorous testing to ensure they are highly stable and reliable.

To find out more about WiRE Raman software, please contact your local representative or visit **www.renishaw.com/wire**