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WITec Suite FIVE

Topography image of a profilometric measurement of an archaeological sample overlaid with the corresponding chemical confocal Raman image.

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Project *FIVE* Control *FIVE* Project *FIVE*+

Data Acquisition, Evaluation and Processing Software

www.witec.de

WITec Suite Powerful Software Tool

Sophisticated data acquisition, evaluation, post-processing and image generation for Confocal Raman Microscopy, AFM, and SNOM.

> Software architecture and graphical user interface enable an integrated functionality incorporating the various techniques and measurement modes.

Suitable for all experience levels and user requirements through customizable user interface.



WITec Control FIVE

• Centralized experiment and instrument settings • Acquisition of imaging and/or spectroscopy data • On- and offline data analysis and image processing •Oi pr •Lie

WITec Project FIVE

• Offline data and image processing • Licensed for an unlimited number of users

WITec Project FIVE+

- Advanced offline data and image processing
- Chemometric post-processing features and superior data analysis tools: Cluster Analysis, Principal Component Analysis, Spectral Demixing, Advanced Spectral Fitting, Image Correlation and many more
- Single user license

Benefits and Highlights





Smart access options

Intuitive and convenient software handling for all principal data acquisition, evaluation, and processing functions.



- User-friendly software interface with smart access options for all principal functions (e.g. circle mouse menu, drag-and-drop actions)
- Accelerated workflow through intuitive menu guidance
- Software Wizard for guidance through the complete investigation, from initial settings and acquisition through data and image post-processing **NEW**
- High-speed data acquisition and processing through intelligent computer resource management (> 1300 Raman spectra per second)
- Large data acquisition volume per measurement
- Microscope objective library: saves and catalogues optical properties with individual measurements; facilitates comparison and reproducibility **NEW**
- RamanTV for direct and fast spectrum-to-image visualization
- Overlay of images from different measurements, for example, AFM/TrueSurface topography with chemical Raman information
- TrueComponent Analysis for automatic identification of the samples' components and representation in the image **NEW**
- Image post-processing possibilities including, among others, 3D imaging and volume visualizations
- Cluster Analysis for automatic identification and visualization of chemical components



Image post-processing

3D Raman image of pollen in honey. Green: Pollen; Red, blue, cyan: Different crystalline phases in the honey; Yellow: Honey.

Image parameters: Size: 50 µm x 50 µm x 50µm, 150 x 150 x 50 = 1,125,000 spectra, Integration time per spectrum: 12.2 ms

The Image Viewer facilitates the overlay of images from different measurements. Example image: Topography image of a profilometric measurement of an archaeological sample overlaid with the corresponding chemical confocal Raman image.



Corresponding Raman spectra of the 3D Raman image.



Ultrafast Raman Imaging option

High speed data acquisition with 0.76 ms/ spectrum = over 1300 spectra/second. The image shows an ultrafast Raman measurement of a toothpaste sample.

Image parameters: 200 x 200 pixels = 40,000 Scan range: 20 µm x 20 µm Total image acquisition time: only 30.4 seconds

Control FIVE

Fast data acquisition combined with full instrument control

Instrument control and experimental setup is made easy with Control FIVE. The user interface changes automatically depending on the measurement mode and includes specialized routines. The clear layout shows all essential control parameters at a glance and facilitates quick access to all measurement tasks, settings and signals. Control FIVE additionally includes all features of the Project FIVE package for on- and offline data evaluation and post processing.

Key Features of Control FIVE

- All measurement modes use one intuitive software package
- Measurements with various techniques (e.g. AFM, Raman) can be applied and controlled simultaneously
- All essential parameters are automatically set when changing between measurement modes
- TrueScan[™] for exact positioning control even at the fastest scan rates
- Capability to measure very large data sets, for e.g. image stacks
- Handheld multifunction controller for tactile and intuitive directing the motorized stages, white light illumination, laser power, autofocus, cantilever positioning and objective selection **NEW**

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- Automated multi-area measurements and time series
- Multi-user management including user-customizable software configurations for individual measurement pre-configurations
- Standard SPM features for AFM and SNOM · High speed, automatic tip approach in all AFM modes · Software-guided cantilever adjustment · Oscilloscope mode for the observation of signals as a function of time

Measurement control and data acquisition with Control FIVE



Imaging of a graphene sample with Raman, AFM, SNOM and Raman-SEM

New control element for all measurement settings and software configurations.

Control FIVE – One software suite to control the measurements and data acquisition for all imaging techniques.





Extensions

LabView interface for advanced data evaluation and processing

Project FIVE Sophisticated Data Evaluation and Processing



Statistical Analysis and Data Evaluation



Topography analysis of an AFM measurement.

WITec's multi-user licensing concept allows the installation of Project FIVE on an arbitrary number of computer workstations for data evaluation and post-processing without additional individual licensing.

Software Wizard







Software Wizard



The new software wizard guides the user through the complete investigation, from initial settings and acquisition through data and image post-processing. Presets and highlighted analytical paths accelerate the generation of high-quality images.

Key Features of Project FIVE

Data Evaluation and Processing

- Various pre-configured filters and algorithms for simplified data processing
- Filters and algorithms accessible through simple drag and drop
- Filter Viewer: Fast preview image generation of a filter applied to a data set, also applicable during running measurement
- Multiple algorithms for background subtraction included
- Curve-fitting tool for single spectra
- Various statistical data evaluation options
- Image generation through visualization of corresponding spectra (basis analysis)
- Data export to ASCII, JCamp-DX, SPC, and MatLab possible

Data Representation

- RamanTV: high speed movie-like image presentation of spectral datasets, also functional as preview option simultaneously with data acquisition
- Fast determination of position, time and/or spectral correlation between various data objects
- 2D and 3D color coded representation of any image data set (AFM, Raman, SNOM, etc.) in selectable color schemes
- Image Viewer: 3D overlay of images e.g. AFM topography image with Raman chemical information
- Spectrum peak finder and labelling
- Spectra export to Raman database for convenient identification of sample components
- TrueComponent Analysis for Raman imaging: Automatically establishes the number of components in a sample, locates them in the image, and differentiates their individual Raman spectra NEW





Automated peak labelling

25 x 25 x 20 µm³, 200 x 200 x 50 pixels = 2,000,000 Raman spectra.

(B) Large-area, high-resolution confocal Raman image with 4,194,304 Raman spectra and a raw data file size of 12.5 Gbyte.

(C, D) The consecutive zoom-ins of the same dataset illustrate the extremely high-resolution of the large-area scan.

Project FIVE+ Advanced Data Evaluation and Processing

Project FIVE+ is the software extension for advanced chemometric and microscopic data evaluation and processing. A variety of intelligent algorithms for multivariate data analysis of hyperspectral Raman data files allow the identification of hidden structures automatically. Superior microscopic data analysis tools permit specialized, expert-level evaluation that meets the most demanding requirements.

Key Features of Project FIVE+

All features of Project FIVE+ are included as demo versions in Project FIVE

Cluster Analysis

- Extraordinary automatic identification of similar spectra and classification of multi-spectrum data into a user-defined number of clusters
- Color-coded image generation of user-selected clusters
- Automatic average-spectra generation of cluster areas for further processing

Principal Component Analysis (PCA)

Multivariate analysis method that produces an optimized reduction of a spectral data set to its principal components

Advanced Fitting Tool

- Extensive curve fitting tool for single spectra and 1D and 2D multi-spectral data sets
- · Combinations of various fitting functions
- Generation of individual fitting functions

Data Cropping and Reduction

Selection of image regions and 1D/2D spectral data sets to crop, cut, or combine the data included in these regions

Graph Demixer

Subtraction or addition of spectral information from/to other spectra with a free adjustable weighting factor (weight per spectrum and immediate preview function)

Image Correlation

Easy matching of two or more image objects in a correlation plot and correlative comparison of various object characteristics

Various Filters

e.g. Fourier, anisotropic, edge, sharpen, user-customized filters and many more.

Graph and Image Repair

Data substitution algorithms such as simple interpolations or texture analysis to remove pixel failures (e.g. extreme cosmic rays, hot/dark CCD pixels)

Image Overlay

Image overlay of any combination of two images/bitmaps. Both images may have different sizes, positions or number of pixels

Non Negative Matrix Factorization (NMF)

Automatic unmixing of spectral components and correlation with their distribution.

Image Correlation









Image Overlay function

The Image Overlay function facilitates the correlation of images acquired with different imaging techniques, e.g. Raman/SEM, Raman/AFM, Raman/Profilometry, etc:

(A) Topography profile image (acquired with TrueSurface Profilometry) of a pharmaceutical tablet overlaid with the corresponding confocal Raman image. (A) Raman/SEM image of a geological sample investigated with the correlative RISE Microscope for Raman Imaging and Scanning Electron Microscopy (Raman-SEM).

STIFFNESS TOPOGRAPHY

Advanced Background Subtraction

Sophisticated algorithms for automatic background subtraction. Optimally applicable to large data sets with a varying fluorescence background.