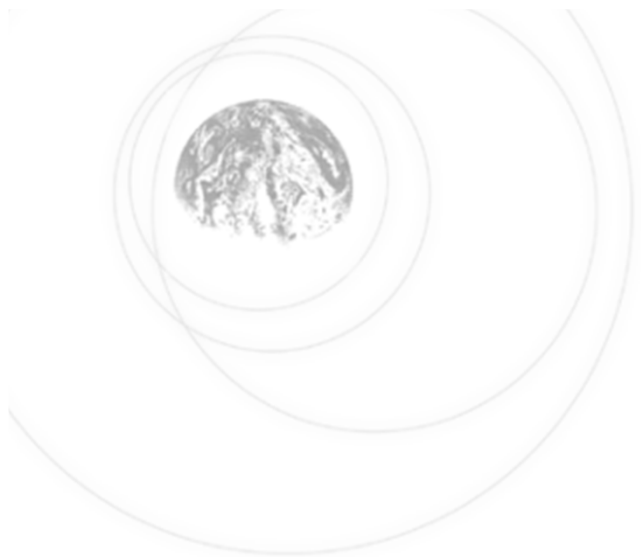




LabSpec 6.2 Tutorials



Explore the future

Automotive Test Systems | Process & Environmental | Medical | Semiconductor | Scientific

HORIBA

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Main Interface

LabSpec 6 - Basic

Graphical manipulation

bar

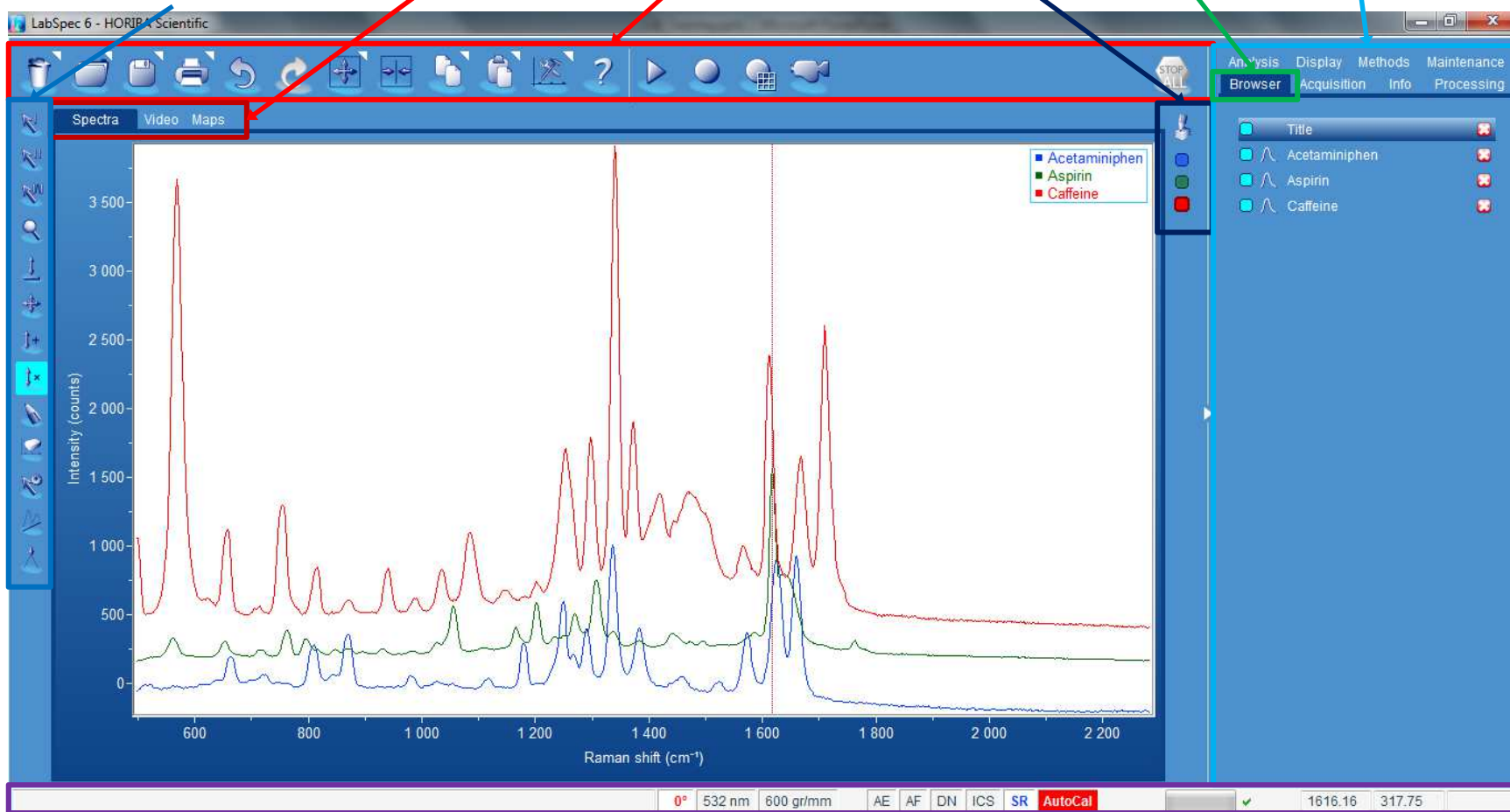
Data tabs

Icon bar

Data bar

Section

Control panel



HORIBA
Scientific

Explore the future

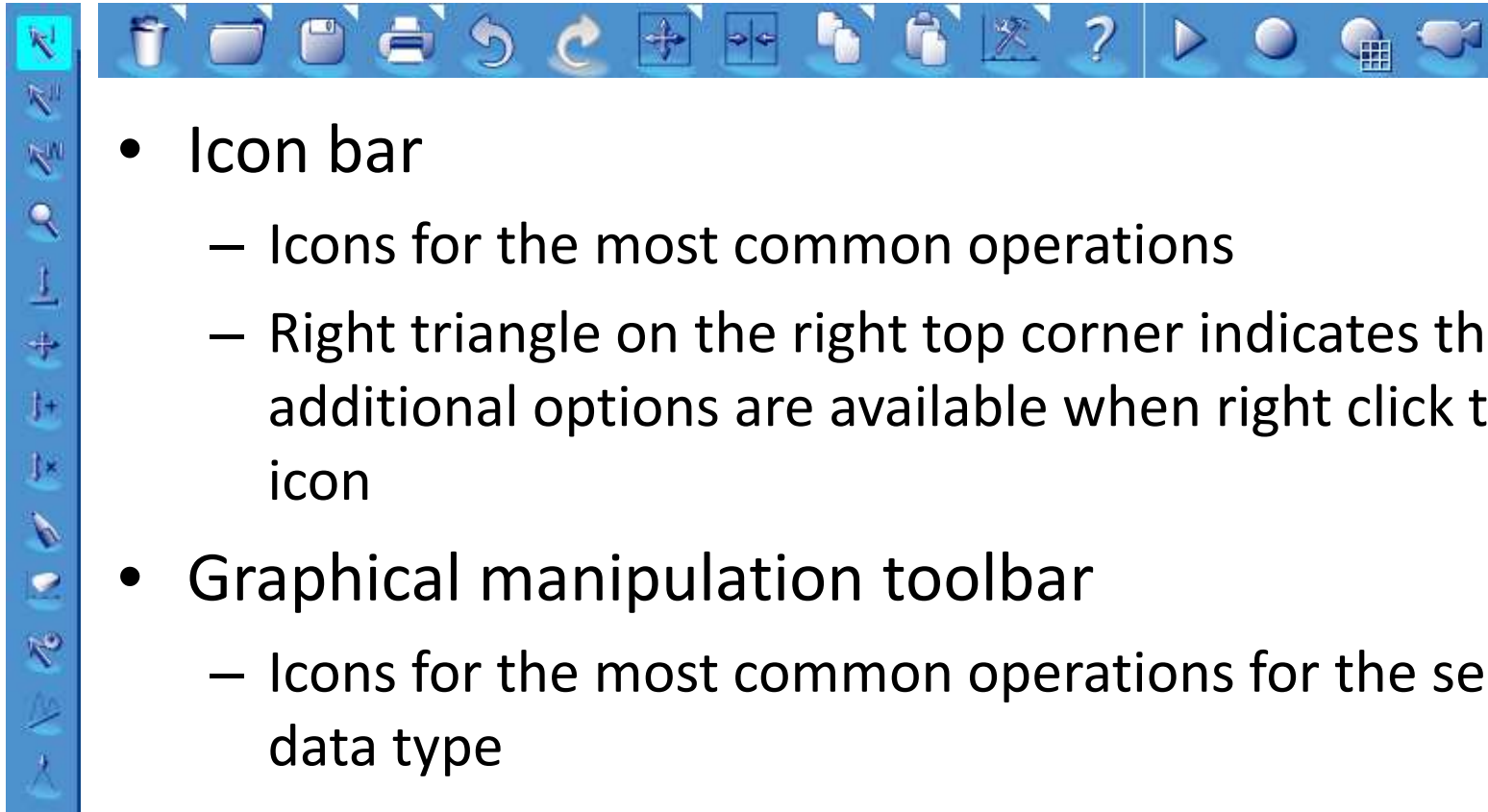
Automotive Test Systems | Process & Environmental | Medical | Semiconductor | Scientific

JOBIN YVON
Technology

HORIBA

Main Interface

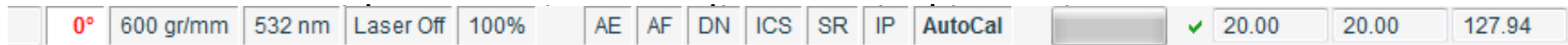
- Data are displayed in the center with multiple tabs (data tabs).
 - Spectra – single point spectra
 - Video – sample images
 - Maps – spectrum arrays + sample image
 - Additional tabs are opened/closed as necessary while data processing and analysis



- Icon bar
 - Icons for the most common operations
 - Right triangle on the right top corner indicates that additional options are available when right click the icon
- Graphical manipulation toolbar
 - Icons for the most common operations for the selected data type

Main Interface

- Status bar at the bottom
 - Detector temperature
 - Selected laser and grating
 - On/Off AutoExposure (AE), AutoFocus (AF), DeNoiser (DN), Intensity Correction System (ICS), Instant Processing (IP) and Spectral Range (SR)
 - Icon for AutoCal
 - Progress bar
 - Values of the selected position
 - Spectrum: Cursor positions, distance between positions, intensity

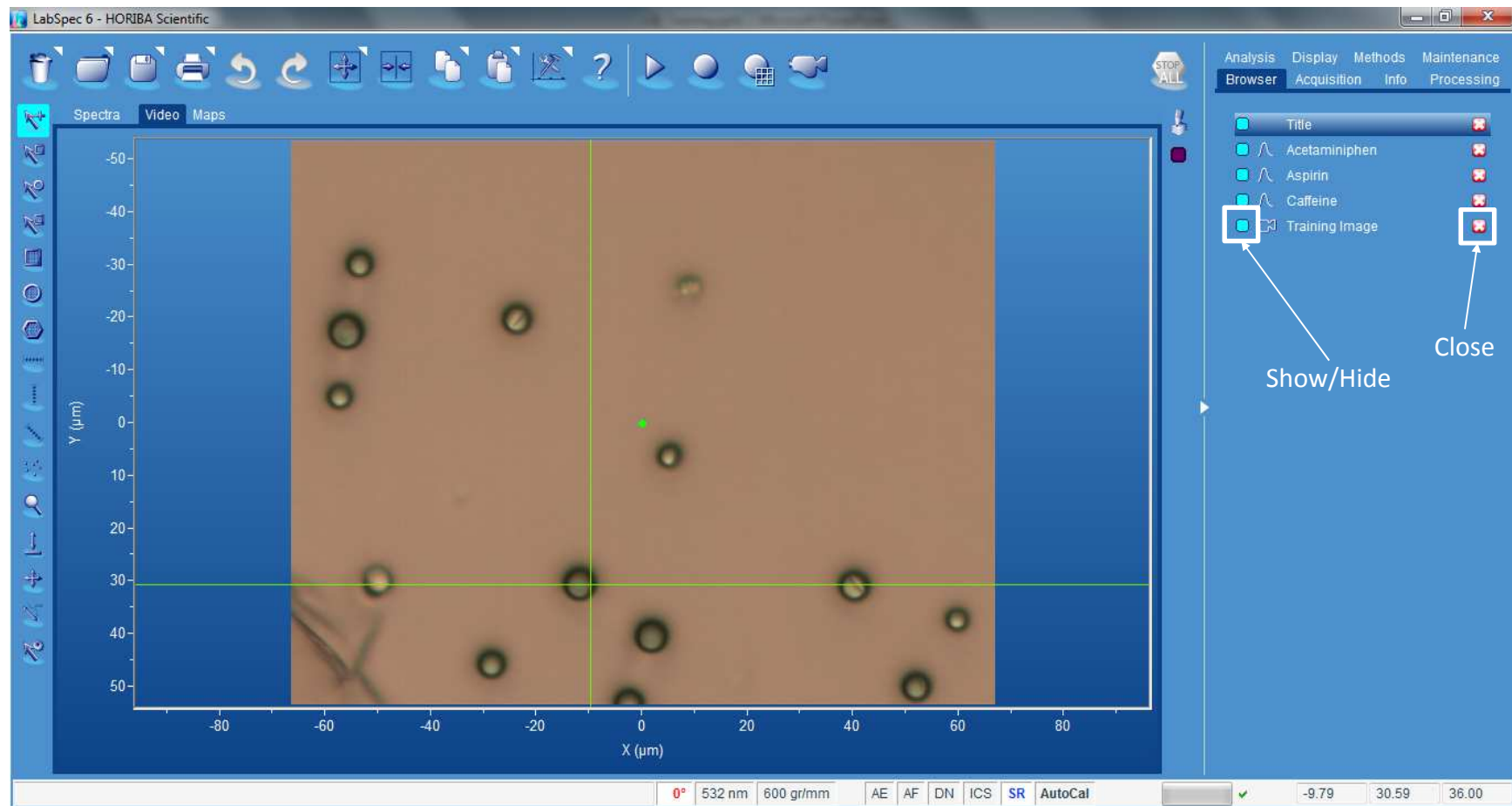


Main Interface

- All instrument and experiment controls are compiled on the right (Control Panel) with multiple tabs (Section).
 - Browser: View and manage data
 - Acquisition: Data acquisition
 - Info: Data information
 - Processing: Data processing
 - Analysis: Data analysis
 - Display: Setup display options
 - Methods: Create, manage and execute macros
 - Maintenance: Perform spectral axis calibration automatically

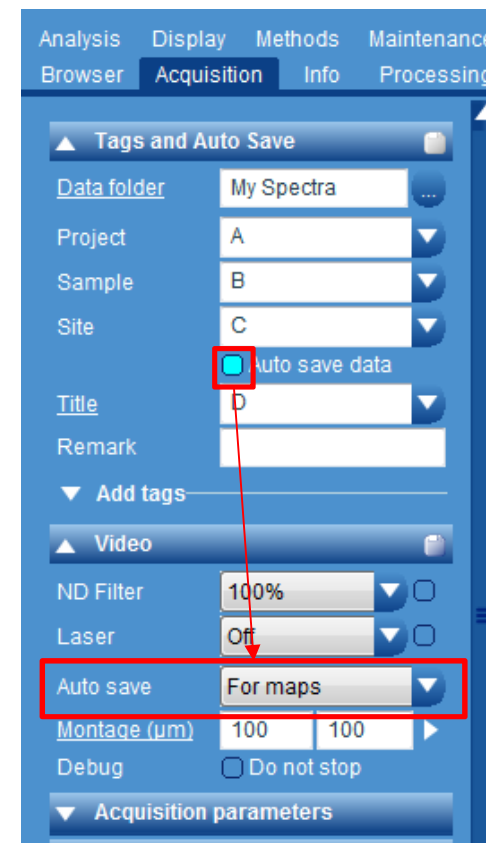


Browser Section



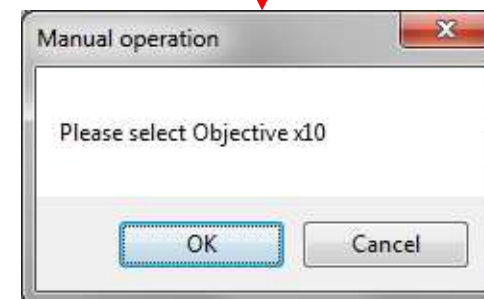
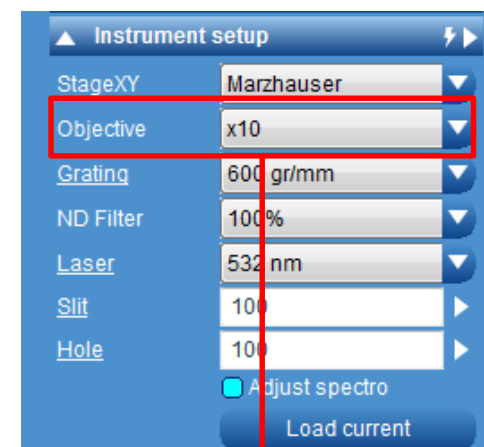
Acquisition Section

- Tags and Auto Save
 - Customize the data storage structure for Auto Save
- Video
 - Montage: Record a large (larger than the field of view) image by stitching multiple images together
 - AutoSave: When Auto Save Data is selected in Tag and Auto Save module, an image of the sample is recorded and saved in the same name as the spectrum or map data file.
- *Underlined text indicates that additional options are available when left click the text*



Record an Image

- Select a sample (e.g. powder)
- Place the sample (e.g. a speck of powder) on a microscope slide
- Place the microscope slide on the stage
- Select a low magnification objective lens (e.g. 10×). Select the matching objective lens from the software, and then click OK when the message for the manual operation appears.



Record an Image

- Start video 
- Find the desired location and focus
- Select a high magnification objective lens (e.g. 50×).
Select the matching objective lens from the software,
and then click OK when the message for the manual
operation appears.
- Find the desired location and focus
- Stop video 
- Save the image 

Acquisition Section

- Acquisition parameters
 - Range: Record a spectrum over an arbitrary spectral range. When turned on, status bar marks its use with **SR**.
 - Auto Exposure (AE) and Autofocus (AF) are controlled in this module. When turned on, status bar marks their use with **AE** and **AF**.
 - DuoScan is controlled in this module.
- Acquisition options
 - Intensity Correction System (ICS) is controlled in this module. When turned on, status bar marks its use with **ICS**
 - Denoiser: Apply an advanced noise filter to the acquiring spectrum

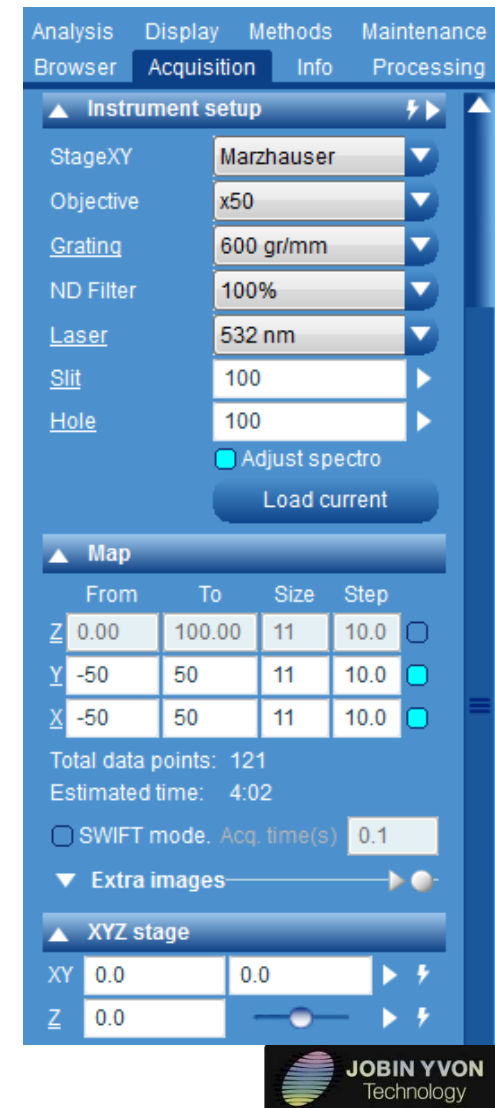
The screenshot displays the 'Acquisition' tab of the LabSpec 6 software. The interface is organized into several sections:

- Acquisition parameters:** This section contains fields for 'Spectro (cm⁻¹)' (1000.18), 'Range' (100 to 4000), 'AE level (cnts)' (1000), 'Acq. time (s)' (1), 'Accumulation' (2), 'RTD time (s)' (1), 'Autofocus' (Off), 'DuoScan Spot' (Off), and 'Title' (D).
- Instant processing:** A section with a single button labeled 'Instant processing'.
- Acquisition options:** This section includes settings for 'Delay time (s)' (0), 'Binning' (1), 'Readout mode' (Signal), 'Shutter mode' (Open/Close), 'Spike filter' (Multiple accum.), 'Denoiser' (Off), 'Laser mode' (Auto), 'ICS correction' (Off), and 'Dark correction' (Off).

The interface features a blue header with tabs for 'Analysis', 'Display', 'Methods', 'Maintenance', 'Browser', 'Acquisition', 'Info', and 'Processing'. A vertical sidebar on the right contains a search icon and a list of icons for various functions.

Acquisition Section

- Instrument setup
 - Adjust spectro: Maintain the spectral position when changing lasers or gratings
- Map
 - Setup to record a spectrum array (e.g. XY-map, Z-profile or t-profile)
 - Control SWIFT in this module
- XYZ stage
 - Reset the position counter at will
 - XYZ positions are with respect to the last counter reset position

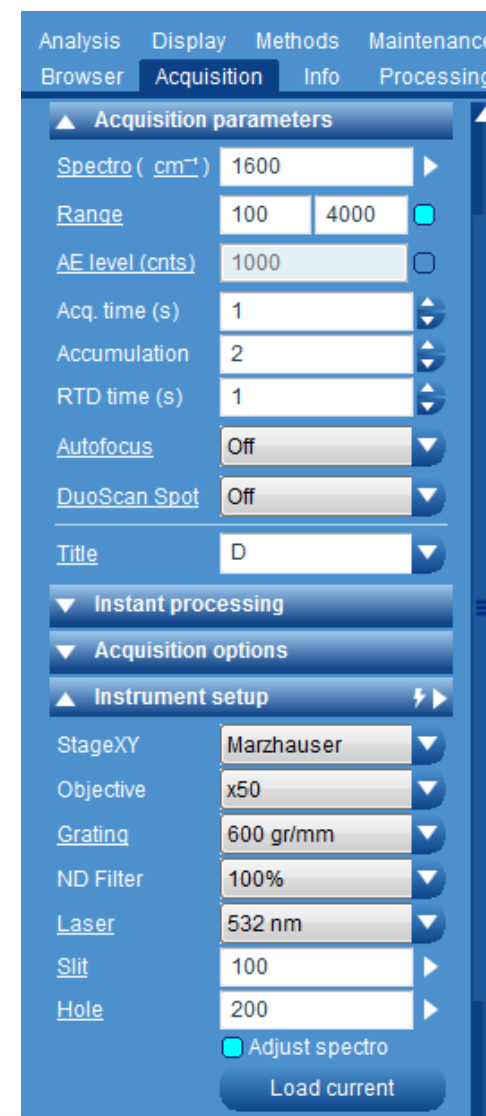


Record a Spectrum

- Select a sample (e.g. polymer)
- Place the sample (e.g. a piece of polymer) on a microscope slide
- Place the microscope slide on the stage
- Select a low magnification objective lens (e.g. 10×).
Select the matching objective lens from the software, and then click OK when the message for the manual operation appears.
- Start video 
- Find the desired location and focus

Record a Spectrum

- Select a high magnification objective lens (e.g. 50×). Select the matching objective lens from the software, and then click OK when the message for the manual operation appears.
- Find the desired location and focus
- Stop video 
- Save the image 
- Select Grating (e.g. 600 gr/mm)
- Select Laser (e.g. 532 nm)
- Set Slit (e.g. 100 μm)
- Set Hole (e.g. 200 μm)
- Set ND filter (e.g. 100 %)



The screenshot displays the HORIBA Scientific software interface with the following settings:

- Analysis Browser:** Acquisition, Info, Processing
- Acquisition parameters:**
 - Spectro (cm^{-1}): 1600
 - Range: 100, 4000
 - AE level (cnts): 1000
 - Acq. time (s): 1
 - Accumulation: 2
 - RTD time (s): 1
 - Autofocus: Off
 - DuoScan Spot: Off
 - Title: D
- Instant processing:**
- Acquisition options:**
- Instrument setup:**
 - StageXY: Marzhauser
 - Objective: x50
 - Grating: 600 gr/mm
 - ND Filter: 100%
 - Laser: 532 nm
 - Slit: 100
 - Hole: 200
 - ☒ Adjust spectro
 - Load current

Record a Spectrum

- Set Spectro (e.g. 1600)
- Set RTD time (s) (e.g. 1)
- Start Real Time Display (RTD) 
- Stop RTD 
- Review the spectral features.
Determine, select and set the Range to record the spectrum (e.g. 100 - 4000)
- Set Acq time (s) (e.g. 1)
- Set Accumulation (e.g. 2)
- Unselect AE level; turn off Autofocus; turn off DuoScan Spot
- Start Spectrum Acquisition 
- Save the spectrum 

Analysis	Display	Methods	Maintenance
Browser	Acquisition	Info	Processing
▲ Acquisition parameters			
Spectro (cm^{-1})		1600 ▶	
Range		100 4000 ☒	
AE level (cnts)		1000 ☐	
Acq. time (s)		1 ▶	
Accumulation		2 ▶	
RTD time (s)		1 ▶	
Autofocus		Off ▼	
DuoScan Spot		Off ▼	
Title		D ▼	
▼ Instant processing			
▼ Acquisition options			
▲ Instrument setup ⚡▶			
StageXY		Marzhauser ▼	
Objective		x50 ▼	
Grating		600 gr/mm ▼	
ND Filter		100% ▼	
Laser		532 nm ▼	
Slit		100 ▶	
Hole		200 ▶	
☒ Adjust spectro			
Load current			

Save and Export

- Left click Save as Data icon 
 - Save As window opens.
 - Save the data in LS6, LS5, LS4, GRAMS, or Text format
 - You can save the entire configuration
- Right click Save as Data Icon
 - Activates the pop-up menu.
 - Batch export to LS4, LS5, LS6, GRAMS or Text format
 - Save to group file: Save all data in the tab to a single file
When opened, individual identity is maintained
 - Save all files: Save all data in the tab to individual files

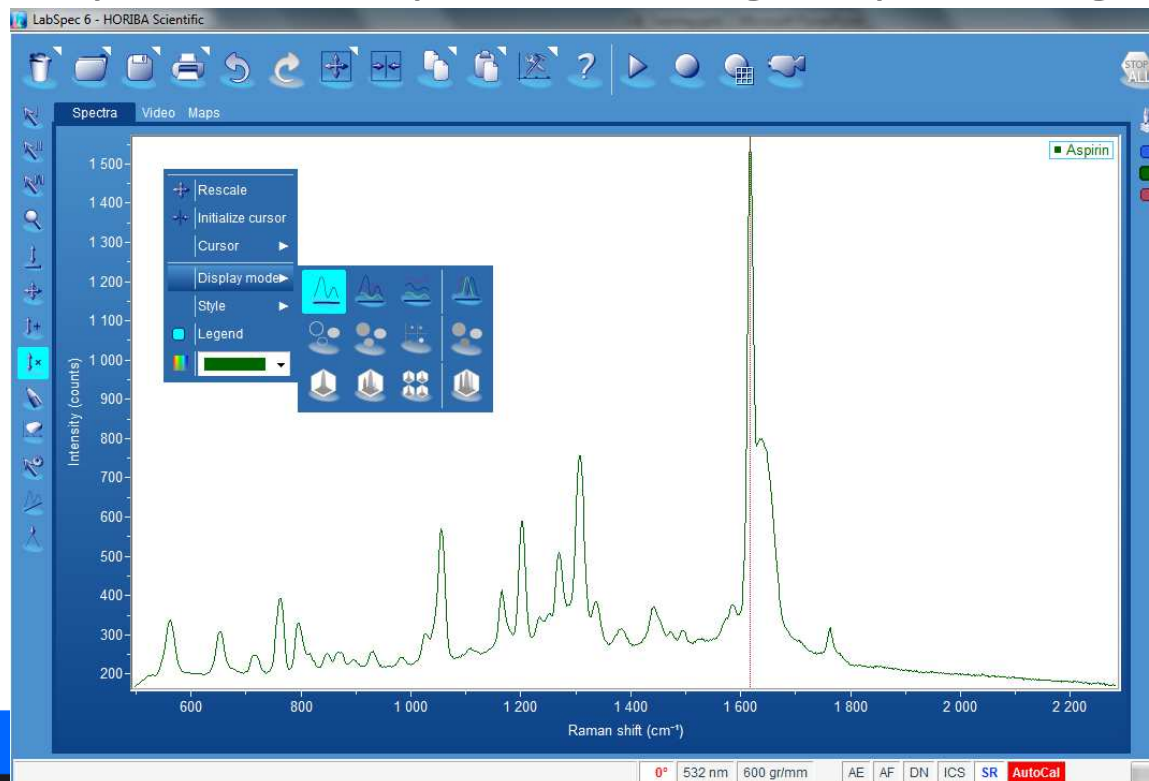


Open and Import

- Left click Open file icon 
 - Open window opens
 - Open a data file
 - Single spectrum in LS4, LS5, LS6, GRAMS or Text format
 - Multi spectrum (or a spectrum array) in LS4, LS5 or LS6 format
 - Image in LS4, LS5, LS6, TIFF, BitMap or JPeg format
 - Arbitrary data in Text format
- Right click Open file icon 
 - Open recently opened files

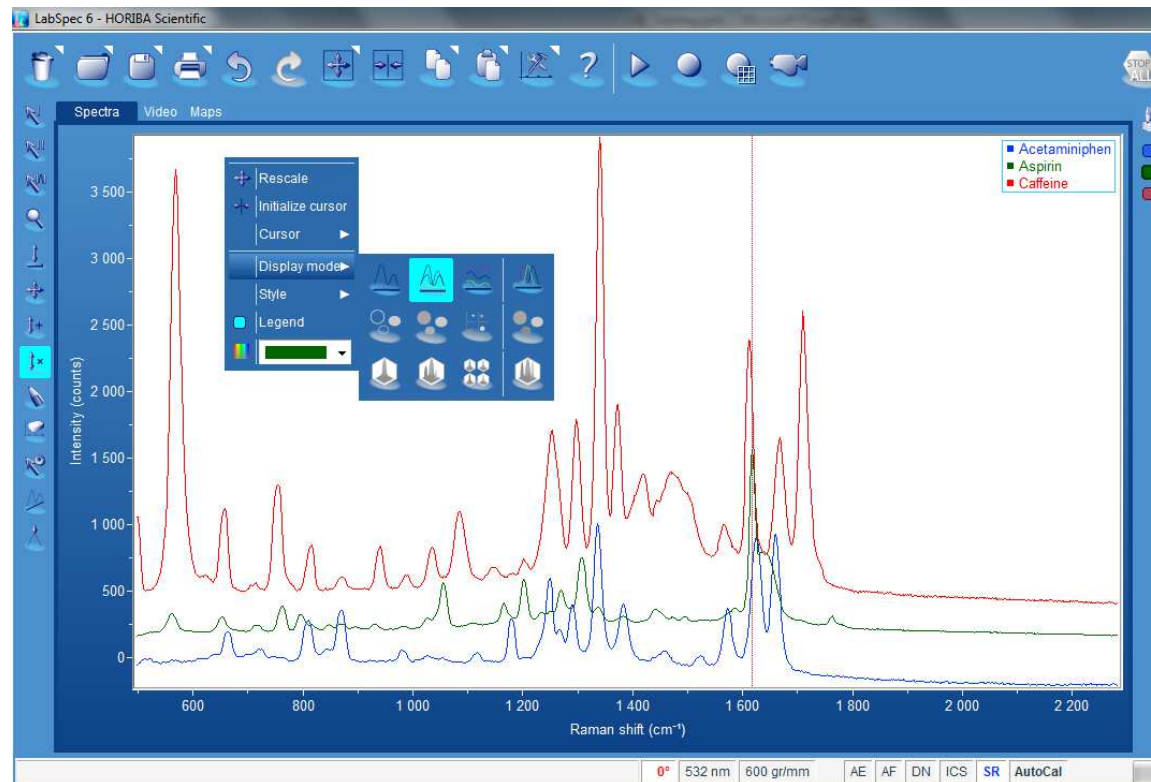
Visualize Spectra

- Open three spectra (e.g. Acetaminophen, Aspirin and Caffeine)
- Right click within Spectra tab, and then bring mouse point to Display mode. Select Single mode to display the currently selected spectrum (e.g. Aspirin in green).



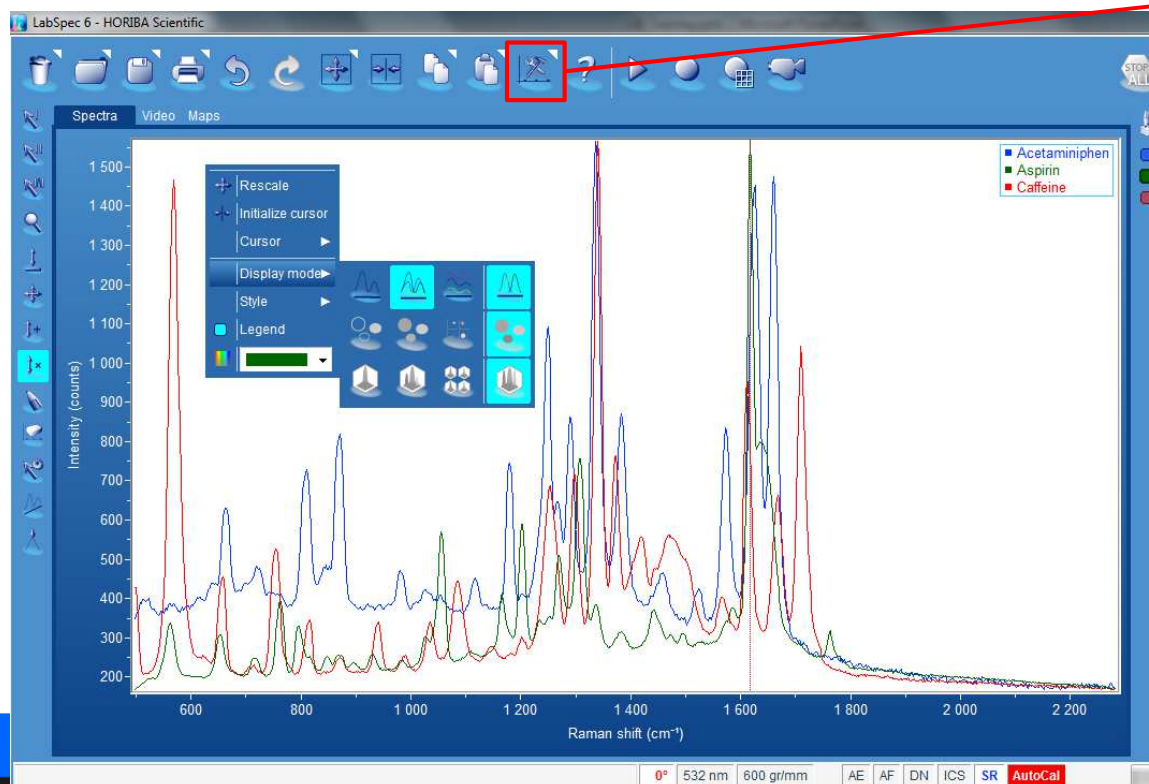
Visualize Spectra

- Right click within the Spectra tab, and then bringt mouse point to Display mode. Select Overlay mode to display all spectra using the same intensity scale



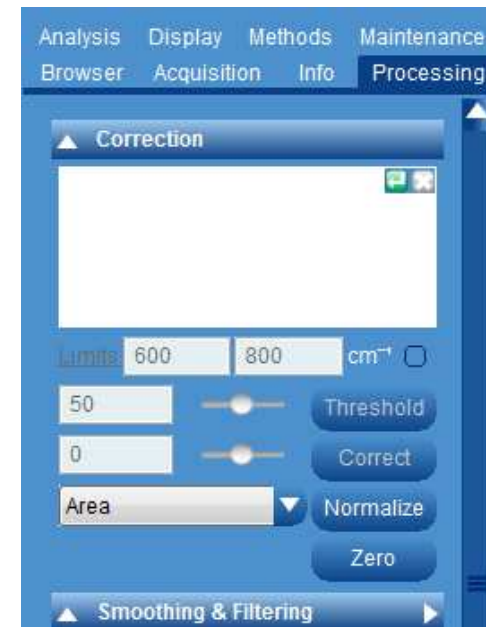
Visualize Spectra

- Right click within the Spectra tab, and then bring mouse point to Display mode. Select Normalize to display all spectra using individual intensity scales.
- *These operations are also accessible by clicking Display Functions icon on the icon bar*



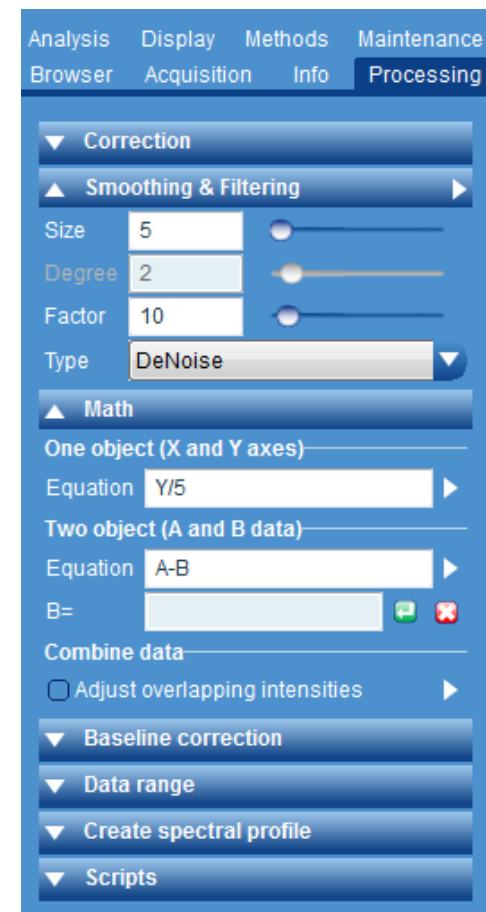
Processing Section

- Correction
 - Threshold: Applicable to a spectrum array only. Reset low intensity spectra to all zeros.
 - Correct: Subtract a spectrum (e.g. a solvent spectrum) from a series of spectra. May apply a scale.
 - Normalize: Normalize to unit intensity sum, unit spectrum area, maximum intensity, unit vector, and normal variate.



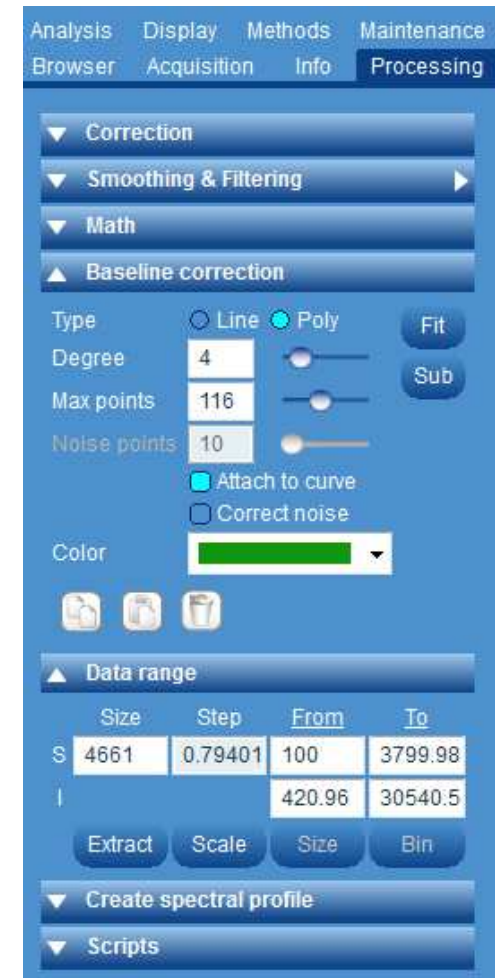
Processing Section

- Smoothing and filtering
 - Denoizer is the identical operation as in Acquisition tab
 - 1st and 2nd derivative
- Math
 - Unary or binary operations
 - Within a spectrum or between spectra



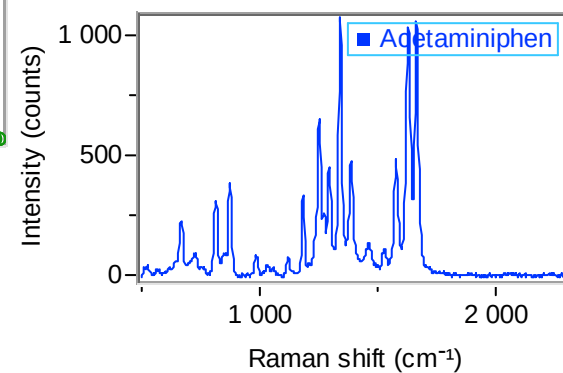
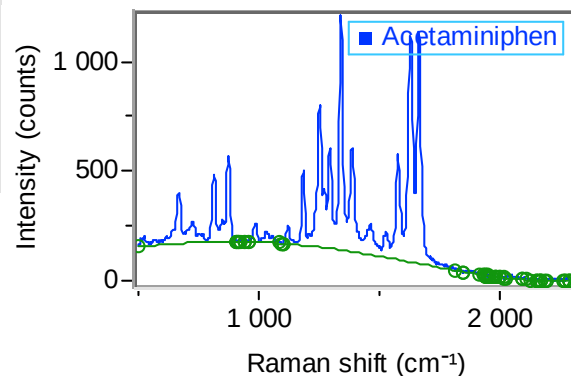
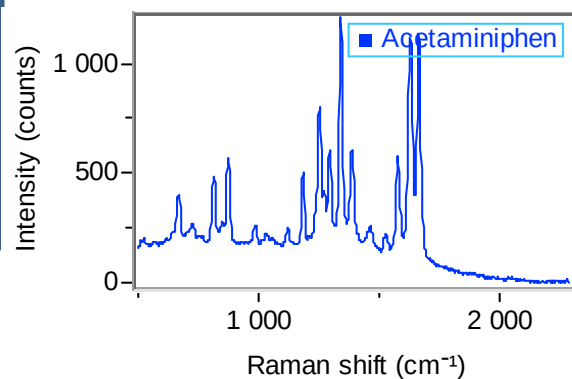
Processing Section

- Baseline correction
 - Polynomial curve or line segments
 - Up to 256 anchor points
 - Copy the baseline of one spectrum, and paste to another spectrum for duplication
- Data range
 - Truncate, rescale or resize data ranges



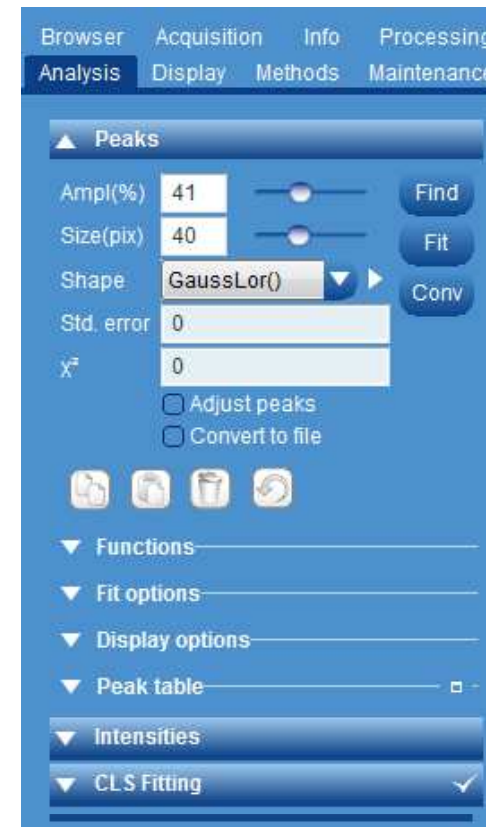
Process a Spectrum

- Baseline correction
 - Select a spectrum (e.g. Acetaminophen)
 - Click Fit
 - Adjust Degree and Max points as necessary
 - Click Sub



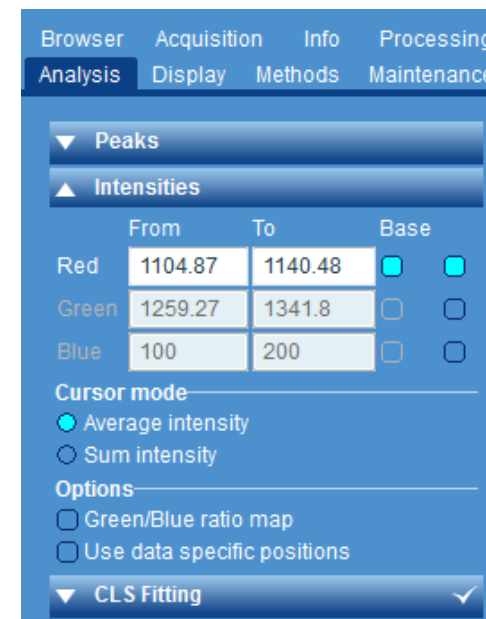
Analysis Section

- Peaks
 - Peak fitting using standard or custom functions
 - Standard functions: Gaussian, Lorentzian, Gaussian+Lorentzian, Asymmetric Gaussian, Asymmetric Lorentzian or Asymmetric Gaussian+Asymmetric Lorentzian
 - Custom functions are operator defined.
 - May fit the baseline while peak fitting
 - Results include peak positions, peak heights, bandwidths (full widths at half maximum) and peak areas



Analysis Section

- Intensities
 - Applicable to a spectrum array only
 - Map the designated peak intensities with or without baseline correction
 - May map a ratio of two peak intensities
 - Use data specific positions
 - When checked, peak designations are applied to, and saved with the target data.
 - When unchecked, peak designates are applied to all data including currently acquiring data.



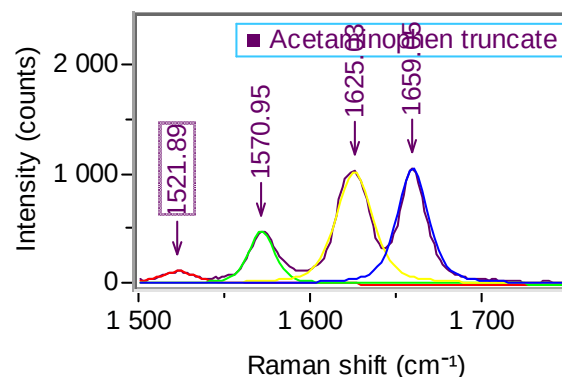
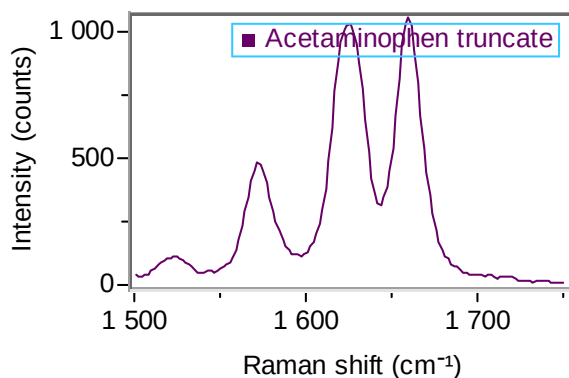
Analysis Section

- CLS fitting
 - Applicable to a spectrum array or a spectrum
 - Require reference spectra. The score indicates the similarity of the target spectrum with respect to the reference spectrum.
 - Use data specific models
 - When checked, reference spectra are applied to, and saved with the target data.
 - When unchecked, reference spectra are applied to all data including currently acquiring data.



Analyze a Spectrum

- Peak fitting
 - Select a spectrum (e.g. Acetaminophen truncate)
 - Select Shape (e.g. GaussLor()) for Gaussian+Lorentzian function)
 - Click Find



Browser Acquisition Info Processing
Analysis Display Methods Maintenance

Peaks

Ampl(%) 10 Find

Size(pix) 15 Fit

Shape GaussLor() Conv

Std. error 12.3457

χ^2 1.40654

☒ Adjust peaks

☐ Convert to file

Functions

Fit options

Iterations 100

Max shift (cm⁻¹) 15

Init width (cm⁻¹) 10

Min width (cm⁻¹) 0.01

Max width (cm⁻¹) 10000

☒ Fit baseline

Display options

Peak table

Analyze a Spectrum

- Peak fitting (cont'd)
 - Click Fit options to expand
 - Iterations: 100
 - Max shift: 15
 - Init width: 10
 - Min width: 0.01
 - Max width: 1000
 - Click Fit. Repeat if necessary until there is no change in Std error and χ^2 .

The screenshot displays the 'Analysis' tab of the HORIBA Scientific software. The 'Peaks' section is expanded, showing parameters for peak fitting. The 'Fit options' section is also expanded, showing various settings for the fitting process.

Parameter	Value
Ampl(%)	10
Size(pix)	15
Shape	GaussLor()
Std. error	12.3457
χ^2	1.40654
Iterations	100
Max shift (cm ⁻¹)	15
Init width (cm ⁻¹)	10
Min width (cm ⁻¹)	0.01
Max width (cm ⁻¹)	10000

Buttons: Find, Fit, Conv, Adjust peaks, Convert to file, Functions, Fit options, Display options, Peak table.

Analyze a Spectrum

- Peak fitting (cont'd)
 - Click Peak table to expand, and then click the button on the right top corner to popup the peak table
 - Click Show options to expand. In Value row of Show options, check p (peak position), a (peak height), w (FWHM) and ar (peak area)
 - Click Conv to convert the data to the fitted result if desired.

Peaks

	p	a	w	ar
1	1520.51	92.8779	22.7153	2207.9
2	1572.05	478.636	19.0642	13304.4
3	1623.86	1009.05	21.4537	24211.5
4	1659.16	1053.44	17.8391	25369.4

▲ Show options

	p	a	g	w	ar
Value	☒	☒	☐	☒	☒
Fix	☐	☐	☐	☐	☐
Map	☐	☐	☐	☐	☐
Min	☐	☐	☐	☐	☐
Max	☐	☐	☐	☐	☐

Browser Acquisition Info Processing
Analysis Display Methods Maintenance

▲ Peaks

Ampl(%) 10 Find

Size(pix) 15 Fit

Shape GaussLor() Conv

Std. error 12.3457

χ^2 1.40654

☒ Adjust peaks

☐ Convert to file

▼ Functions

▼ Fit options

▼ Display options

▲ Peak table

	p	a	w
1	1520.51	92.8779	22.7153
2	1572.05	478.636	19.0642
3	1623.86	1009.05	21.4537
4	1659.16	1053.44	17.8391

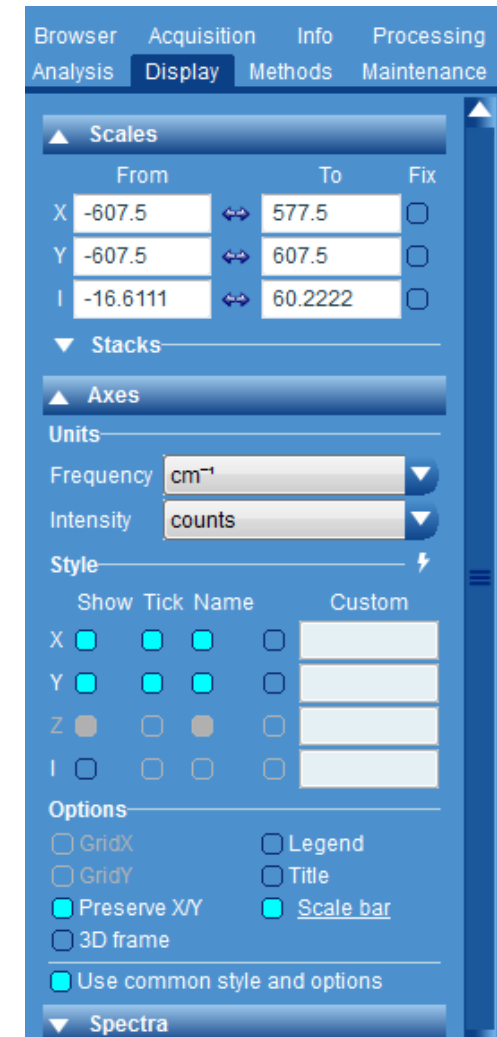
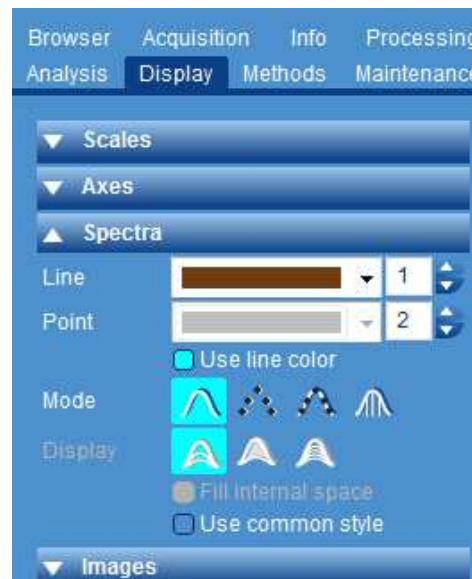
▼ Show options

▼ Intensities

▼ CLS Fitting

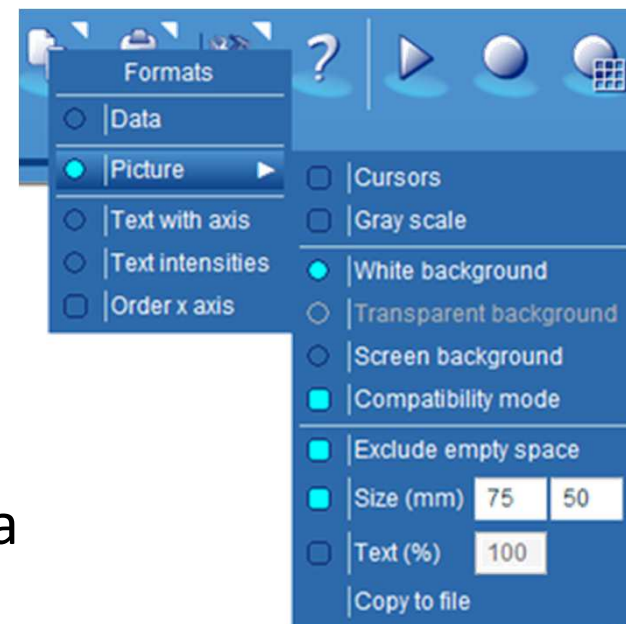
Display Section

- Scales
 - May fix or reverse the axis scales
- Axes
 - Select axis units for spectrum
 - On/Off axis
- Spectra
 - Adjust line thickness



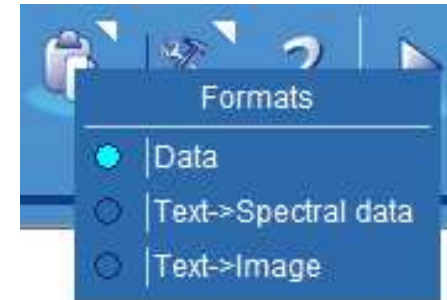
Copy

- Right click Copy icon 
 - Setup the copy options
 - Data: Copy the current data set as the same data type. Paste to the same tab/window
 - Picture: Copy the current tab (Spectra, Video or Map) display as a picture. Paste to another software (e.g. PowerPoint)
 - Text: Copy the current data set to the text format. Paste to another tab (e.g. Spectra Tab) or another software (e.g. Excel)



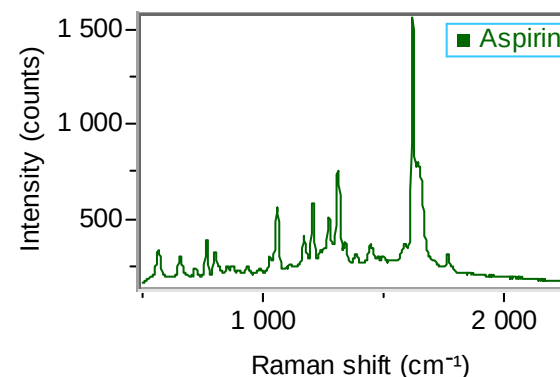
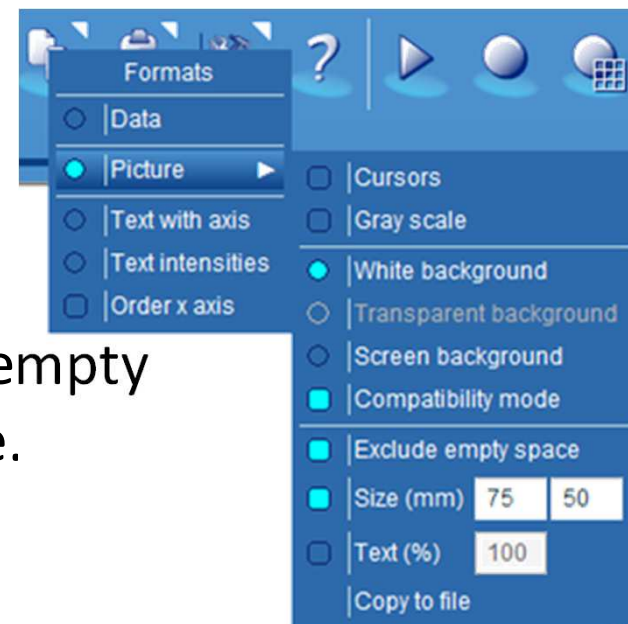
Paste

- Right click Paste icon 
 - Setup the paste options
 - Data: Paste the data in the memory to the same tab/window as the original data
 - Text → Spectral data: Paste the text in the memory as a spectra or a spectrum array.
 - Text → Image: Paste the text in the memory as an image.



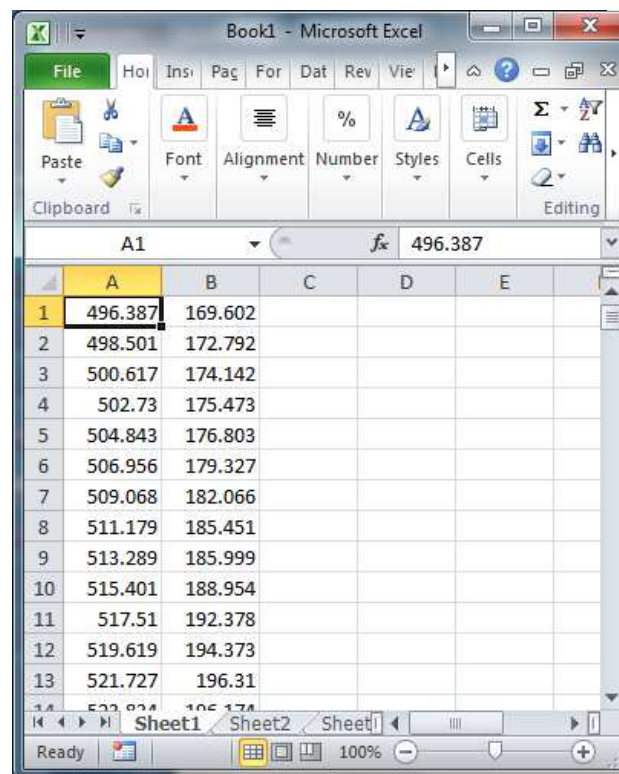
Copy and Paste a Spectrum as a Picture

- Select a spectrum (e.g. Aspirin)
- Right click Copy icon
 - Select Picture
 - Check White background, Exclude empty space, Compatibility mode and Size. Uncheck the rest
 - Input 75 and 50 for Size
- Left click Copy icon
- Open PowerPoint and paste



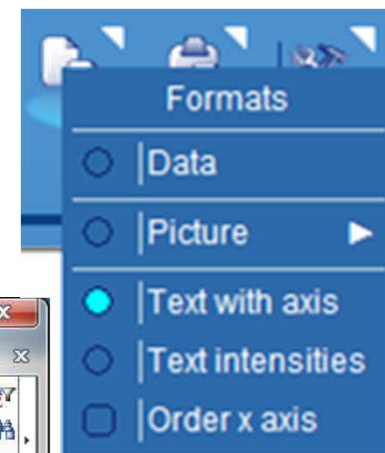
Copy and Paste a Spectrum as Text

- Select a spectrum (e.g. Aspirin)
- Right click Copy icon
 - Select Text with axis
- Left click Copy icon
- Open Excel and paste



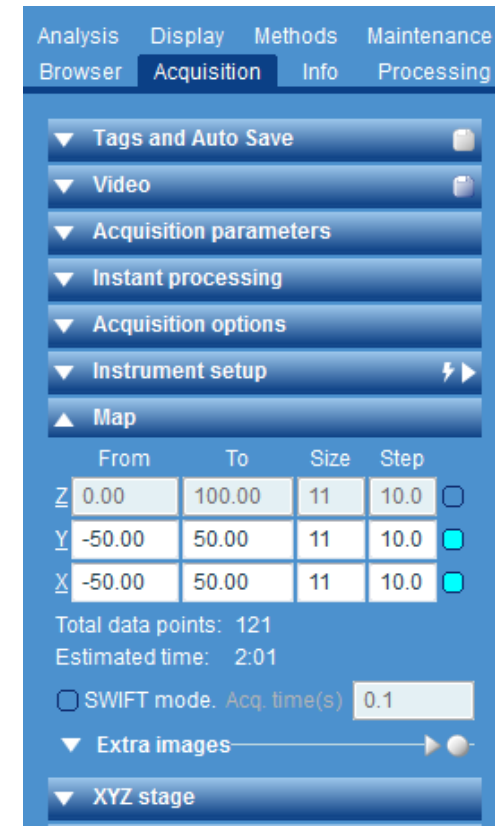
Book1 - Microsoft Excel

	A	B	C	D	E
1	496.387	169.602			
2	498.501	172.792			
3	500.617	174.142			
4	502.73	175.473			
5	504.843	176.803			
6	506.956	179.327			
7	509.068	182.066			
8	511.179	185.451			
9	513.289	185.999			
10	515.401	188.954			
11	517.51	192.378			
12	519.619	194.373			
13	521.727	196.31			



Spectrum Array

- Spectrum array is a collection of spectra, typically acquired over a range of a variable (or variables) at a regular interval.
- Types of a spectrum array include
 - XY-map: a collection of spectra recorded over an area
 - Z-profile: a collection of spectra recorded over a range of height
 - t-profile: a collection of spectra recorded over a length of time
- Spectrum array is typically setup in Map module of Acquisition section



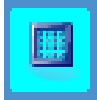
Record a XY-Map

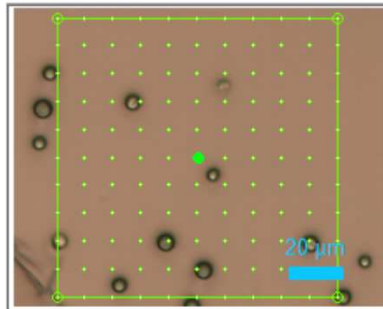
- Select a sample (e.g. tablet)
- Place the sample (e.g. a tablet) on a microscope slide
- Place the microscope slide on the stage
- Select a low magnification objective lens (e.g. 10×).
Select the matching objective lens from the software, and then click OK when the message for the manual operation appears.
- Start video 
- Find the desired location and focus

Record a XY-Map

- Select a high magnification objective lens (e.g. 50×). Select the matching objective lens from the software, and then click OK when the message for the manual operation appears.
- Find the desired location and focus
- Stop video 
- Save the image 

Record a XY-Map

- Select the map shape (e.g. rectangle) from the graphical manipulation toolbar .
- The cursor of the selected shape appears. Drag, stretch and/or drop the cursor to mark the location and area of the map.



- Expand Map module, and set the number of measurement points (e.g. Size = 11). Measurement points are marked in the rectangle shaped cursor

Analysis Display Methods Maintenance
Browser Acquisition Info Processing

▼ Tags and Auto Save 

▼ Video 

▼ Acquisition parameters

▼ Instant processing

▼ Acquisition options

▼ Instrument setup ⚡▶

▲ Map

	From	To	Size	Step	
Z	0.00	100.00	11	10.0	☐
Y	-50	50	11	10.0	☒
X	-50	50	11	10.0	☒

Total data points: 121
Estimated time: 28:14

☐ SWIFT mode. Acq. time(s) 0.1

▼ Extra images ▶◀

▼ XYZ stage

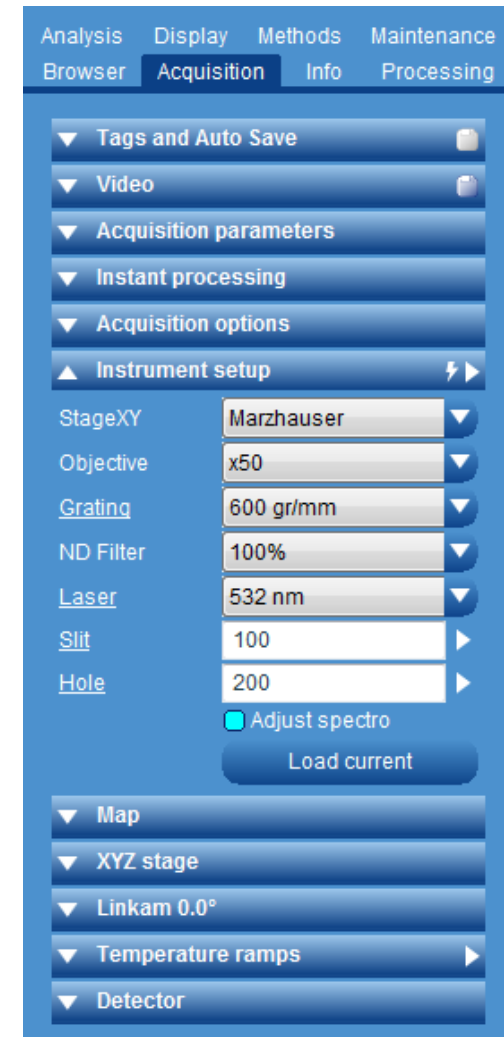
▼ Linkam 0.0°

▼ Temperature ramps ▶

▼ Detector

Record a XY-Map

- Select Grating (e.g. 600 gr/mm)
- Select Laser (e.g. 532 nm)
- Set Slit (e.g. 100 μm)
- Set Hole (e.g. 200 μm)
- Set ND filter (e.g. 100 %)



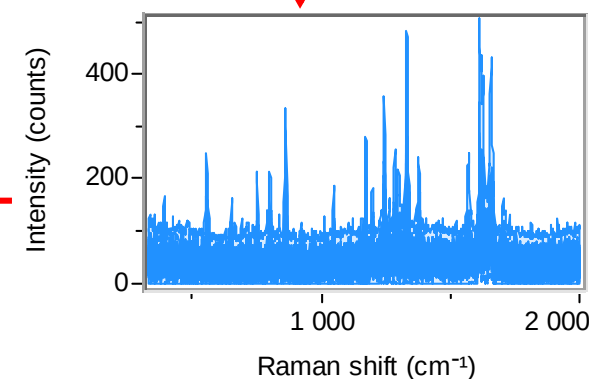
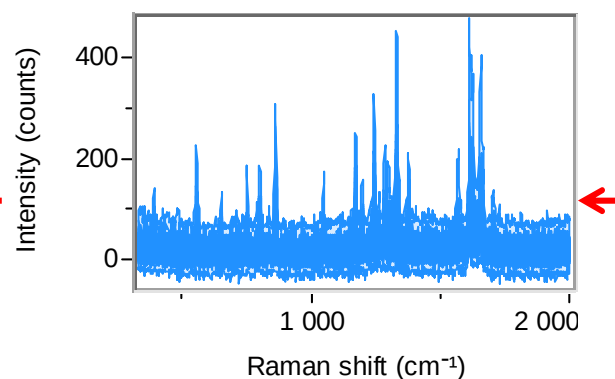
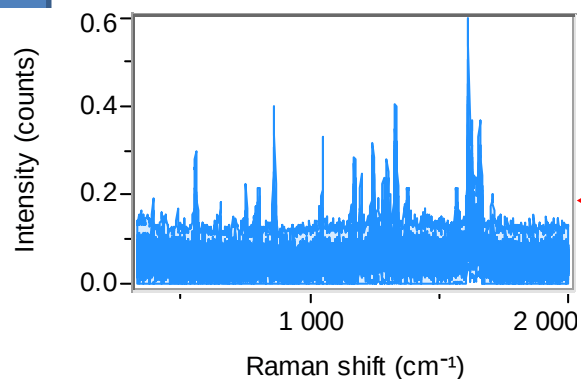
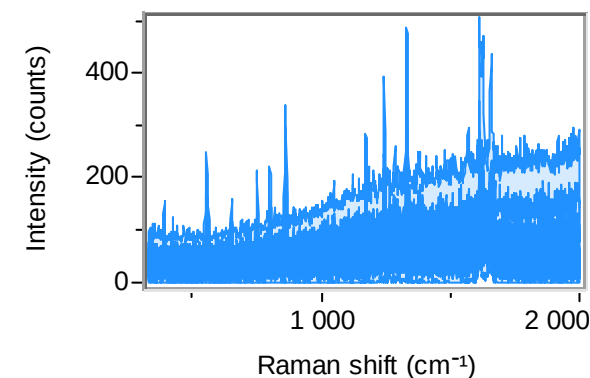
Record a XY-Map

- Set Spectro (e.g. 1600)
- Set RTD time (s) (e.g. 0.5)
- Start and stop RTD  
- Review the spectral features. Adjust Spectro if necessary
- Set Acq time (s) (e.g. 1)
- Set Accumulation (e.g. 2)
- Unselect range; unselect AE level; turn off Autofocus; turn off DuoScan Spot
- Start map acquisition 
- Save the map 

Analysis	Display	Methods	Maintenance
Browser	Acquisition	Info	Processing
▼ Tags and Auto Save			
▼ Video			
▲ Acquisition parameters			
Spectro (cm^{-1})		1600	
Range		100	4000 ☐
AE level (cnts)		1000	☐
Acq. time (s)		1	▲ ▼
Accumulation		2	▲ ▼
RTD time (s)		0.5	▲ ▼
Autofocus		Off	▼
DuoScan Spot		Off	▼
Title		D	
▼ Instant processing			
▼ Acquisition options			
▼ Instrument setup ⚡▶			
▼ Map			
▼ XYZ stage			
▼ Linkam 0.0°			
▼ Temperature ramps ▶			
▼ Detector			

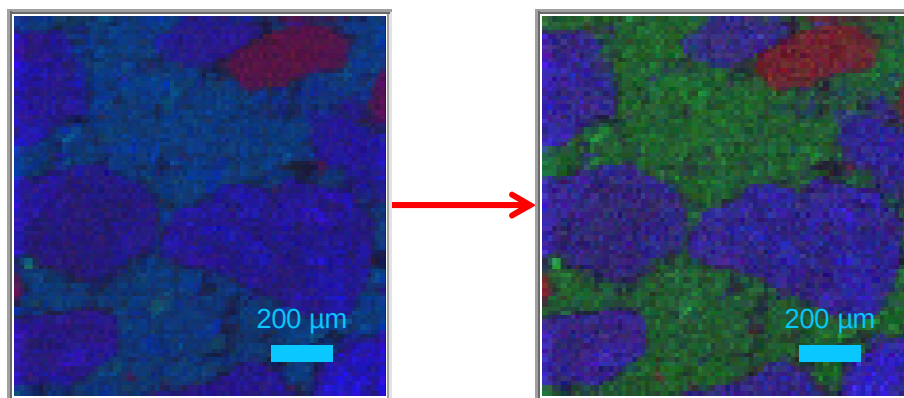
Process the XY-Map

- Select a spectrum array file (e.g. Training Map)
- Select the spectrum array window
- Apply Baseline correction
- Apply Zero
- Apply Normalize to unit area



Process the XY-Map

- Intensities
 - Select the spectrum array window
 - Select red map cursor. Double red lines become solid. Bracket the band $\sim 555 \text{ cm}^{-1}$
 - Select green map cursor. Double green lines become solid. Bracket the band $\sim 857 \text{ cm}^{-1}$
 - Select blue map cursor. Double blue lines become solid. Bracket the band $\sim 1608 \text{ cm}^{-1}$
 - Check Base for Red, Green and Blue



Browser Acquisition Info Processing
Analysis Display Methods Maintenance

▼ Peaks
▲ Intensities

	From	To	Base	
Red	540	570	☒	☒
Green	845	875	☒	☒
Blue	1600	1615	☒	☒

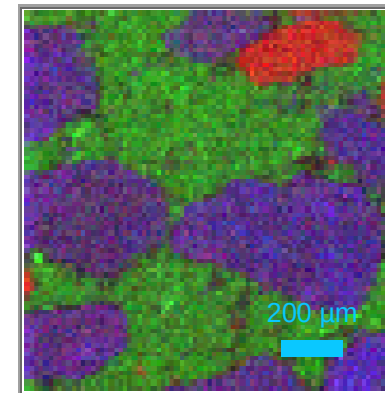
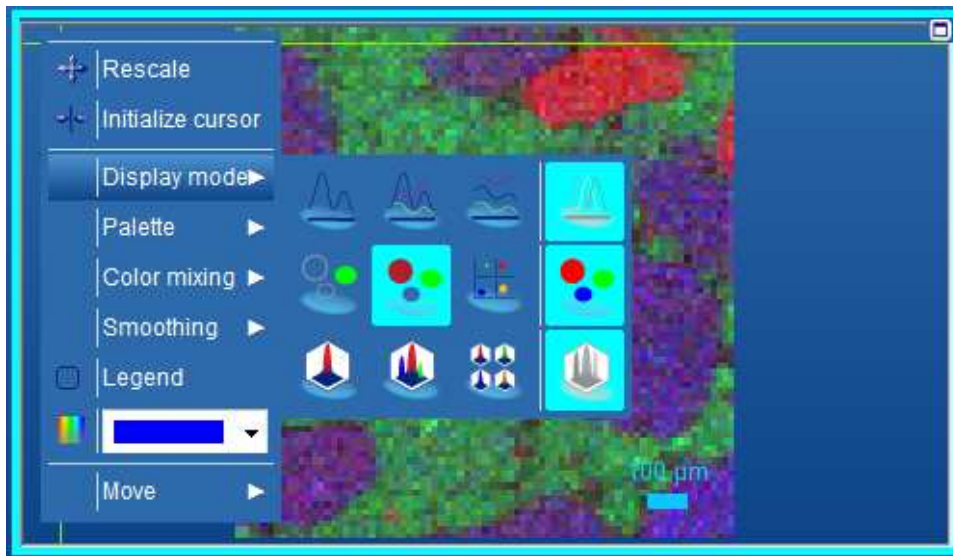
Cursor mode
☒ Average intensity
☐ Sum intensity

Options
☐ Green/Blue ratio map
☒ Use data specific positions

▼ CLS Fitting ✓

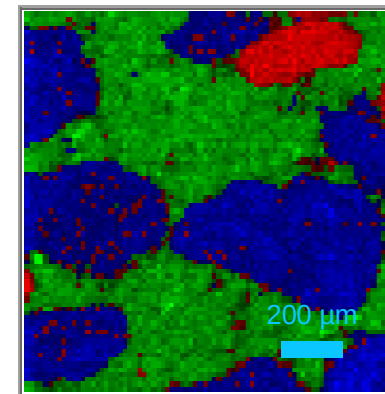
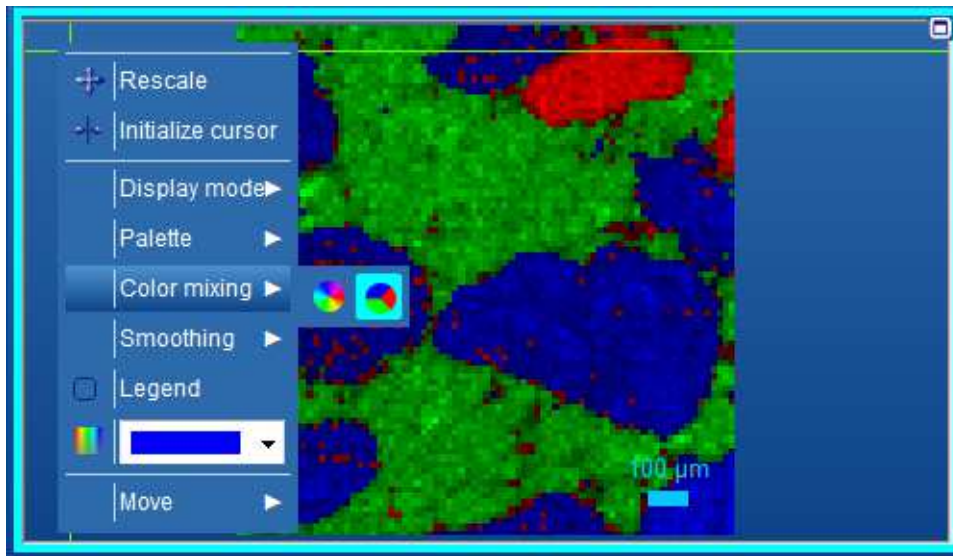
Visualize the XY-Map

- Right click within Map window, and then bring mouse point to Display mode. Select Normalize to display all intensity maps using individual intensity scales.



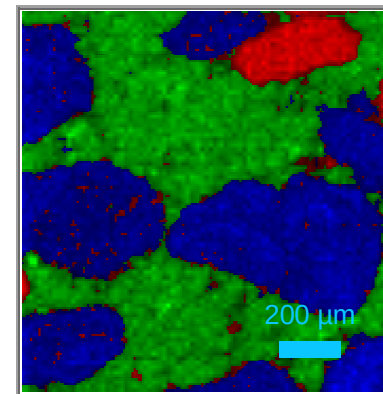
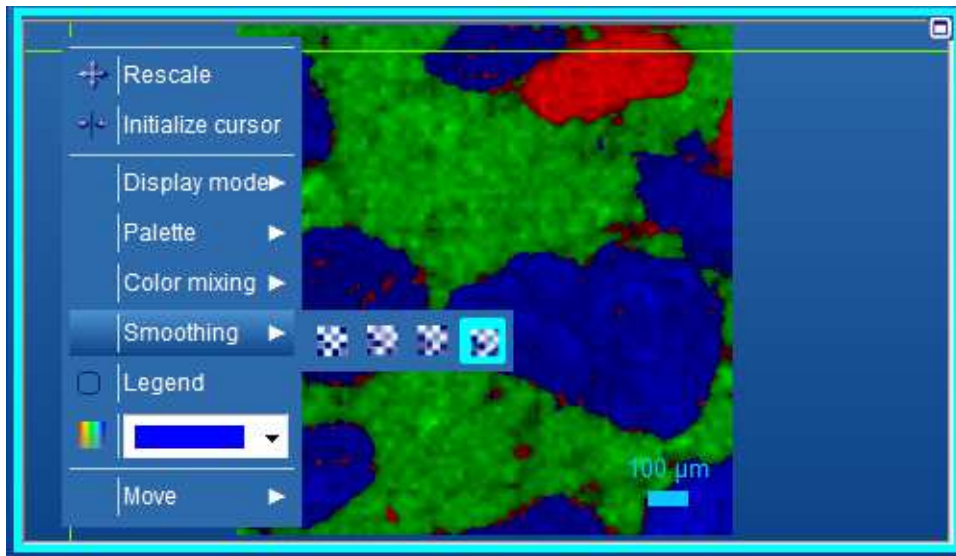
Visualize the XY-Map

- Right click within Map window, and then bring mouse point to Color mixing. Select Unmixed to display each pixel in the color of the highest intensity.



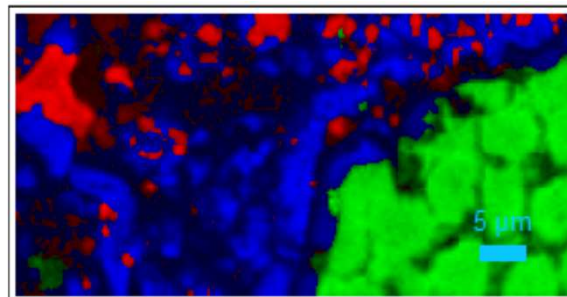
Visualize the XY-Map

- Right click within Map window, and then bring mouse point to Smoothing. Select Smoothed to interpolated display.



Display Section

- Images
 - Adjust brightness and contrast of RGB format
 - Adjust hue, lightness and saturation of HLS format
 - For an unmixed image, calculate the area ratio of each color in RGB format



Browser Acquisition Info Processing
Analysis **Display** Methods Maintenance

▼ Scales
▼ Axes
▼ Spectra
▲ Images

Palette 

Mode 

Smoothing 

▲ Area

	Area %	Area (μm²)
	14.9	266.126
	29.6	526.752
	55.5	987.255

▲ Options

Brightness  ⚡

Contrast  ⚡

    ⚡

Hue  ⚡

Lightness  ⚡

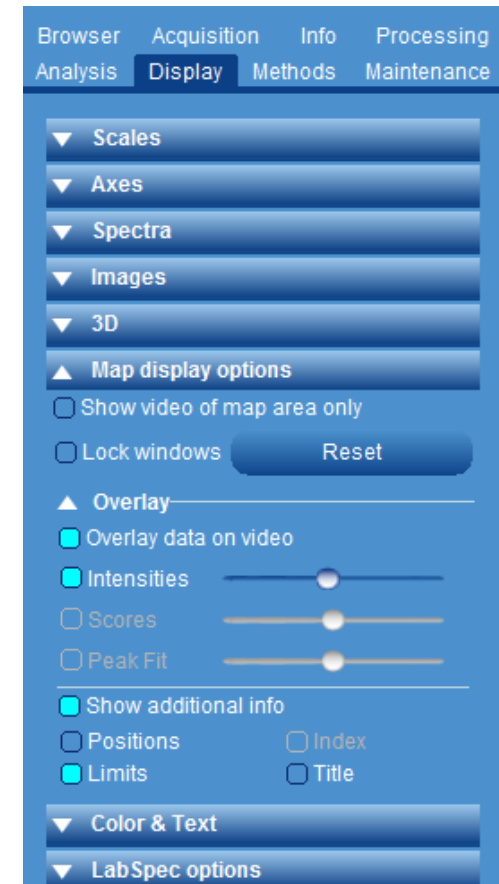
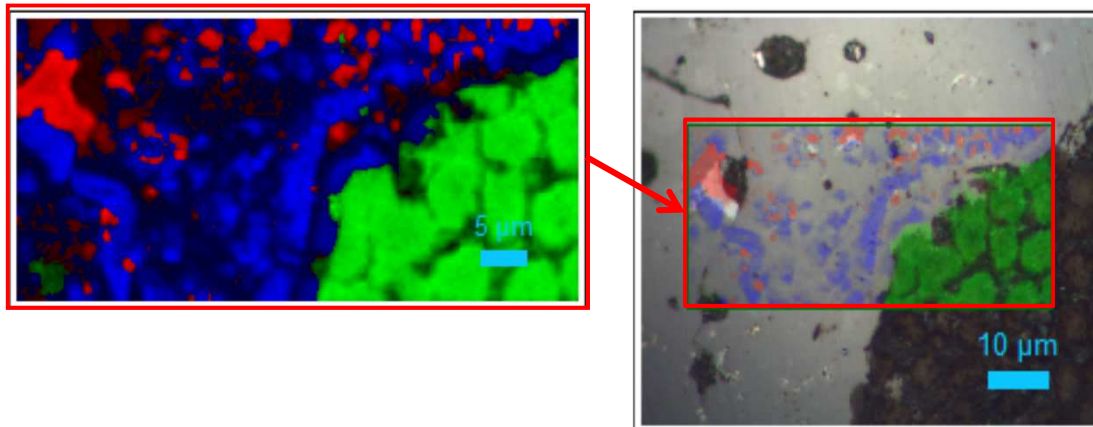
Saturation  ⚡

▼ Histogram

▼ 3D

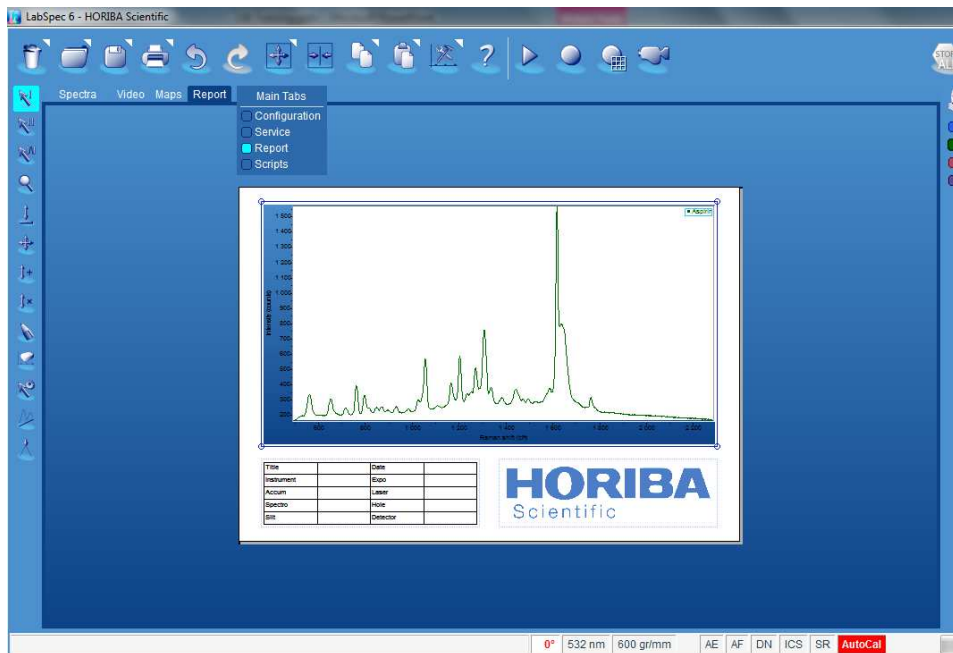
Display Section

- Map display options
 - Overlay the microscopy image (e.g. brightfield image) with the chemical image (e.g. intensity map or score map)



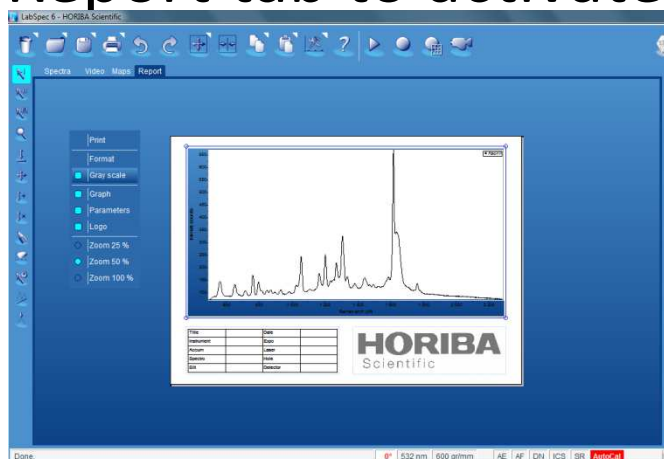
Report Tab

- Right click on Data tabs, and select Report
- Display data, parameters and log in one page for printing



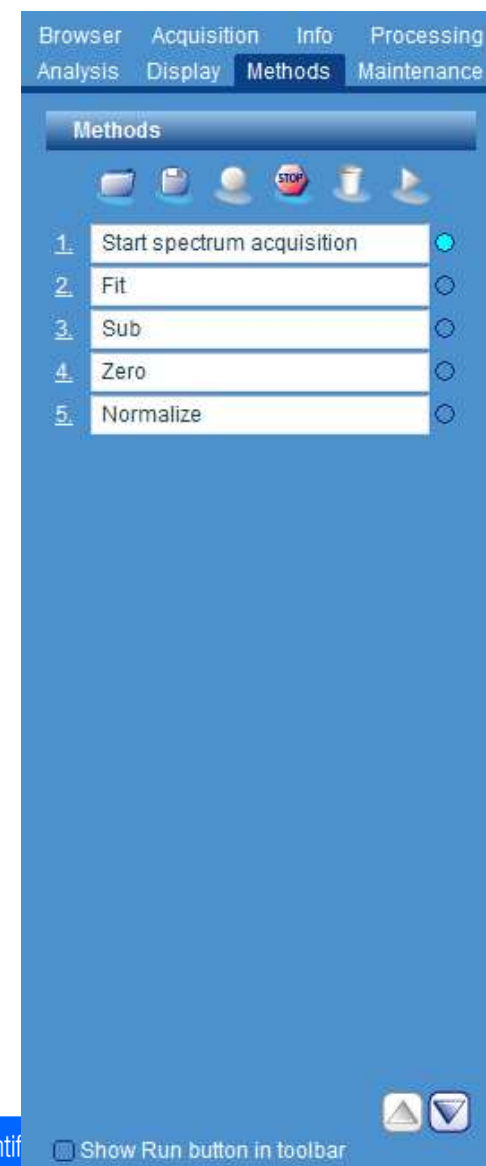
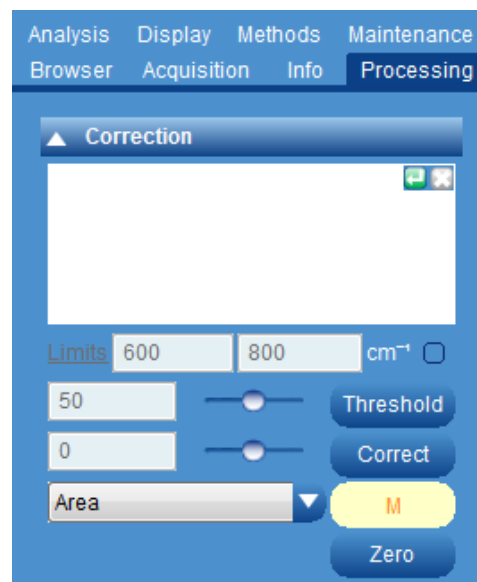
Report Tab

- Select a spectrum (e.g. Aspirin)
- Right click on Data tabs, and select Report to open Report tab.
- Right click within Report tab to activate the popup menu
- Select Zoom 50%
- Select Gray scale
- Select Print
- Right click on Data tabs, and unselect Report to close Report tab



Method Section

- Records and perform the operator selected operations in sequence.
- Method compatible operations turn M when the mouse point hovers. Click to add to Method
- Acquisition, Processing and Analysis operations are Method compatible.



Automation

- Take a tablet, and shave the top surface flat if necessary
- Place the sample on the stage using a microscope slide
- Select a low magnification objective lens (e.g. 10×).
Select the matching objective lens from the software.
- Start video 
- Find the desired location and focus
- Select a high magnification objective lens (e.g. 50×).
Select the matching objective lens from the software.
- Find the desired location and focus
- Stop video 

Automation

- Select Acquisition section
- Expand Tab and Auto Save
 - Select Auto Save Data
 - Data folder: Select a location on the hard drive
 - Project, Sample, Site and Title: Input appropriate texts
 - Expand Add Tags, and select Operator. Input your name

The screenshot displays the 'Acquisition' tab in the software's top menu bar. Below the menu, the 'Tags and Auto Save' section is expanded, showing fields for 'Data folder' (C:\Users\lelee.HOR...), 'Project' (Training), 'Sample' (Test), 'Site' (Position), 'Title' (Try), and 'Remark' (This is for training). The 'Auto save data' checkbox is checked. Below this, the 'Add tags' section is expanded, showing fields for 'Operator' (HORIBA), 'Power', 'Type', 'Formula', and 'Solvent', each with a corresponding checkbox. The 'Edit names' checkbox is also visible at the bottom.

Automation

Exercise

- Expand Instrument setup
 - Objective: 50×
 - Grating: 600 gr/mm
 - Laser: 532 nm
 - Slit: 100
 - Hole: 200
 - ND filter: 100 %
- Expand Acquisition parameters
 - Spectro: 1600
 - Range: Select, and input 100 and 4000
 - AE level: Unselect
 - Acq. time: 1
 - Accumulation: 2
 - Autofocus: off

The screenshot displays the HORIBA Scientific software interface. At the top, there are tabs for Analysis, Display, Methods, Maintenance, Browser, Acquisition, Info, and Processing. The 'Acquisition' tab is selected. Below the tabs, there are several sections: 'Acquisition parameters' (expanded), 'Instant processing', 'Acquisition options', and 'Instrument setup' (expanded). The 'Acquisition parameters' section includes fields for Spectro (cm⁻¹) set to 1600.14, Range (100 and 4000), AE level (cnts) set to 1000, Acq. time (s) set to 1, Accumulation set to 2, RTD time (s) set to 0.5, Autofocus set to Off, and DuoScan Spot set to Off. The 'Instrument setup' section includes fields for StageXY (Marzhauser), Objective (x50), Grating (600 gr/mm), ND Filter (100%), Laser (532 nm), Slit (100), and Hole (200). At the bottom of the 'Acquisition parameters' section, there are checkboxes for 'Adjust spectro' and 'Load current'.

Parameter	Value
Spectro (cm ⁻¹)	1600.14
Range	100 4000
AE level (cnts)	1000
Acq. time (s)	1
Accumulation	2
RTD time (s)	0.5
Autofocus	Off
DuoScan Spot	Off
Title	Try
StageXY	Marzhauser
Objective	x50
Grating	600 gr/mm
ND Filter	100%
Laser	532 nm
Slit	100
Hole	200

Automation

- Select Methods section
 - Select Record Method
 - From Icon Bar, click Start Spectrum Acquisition
 - From Processing section, click Fit and then Sub in Baseline correction
 - From Processing section, click Zero and then Normalize in Correction
 - Select Stop method recording



Automation

Exercise

- Expand Acquisition parameters
 - Spectro: 1600
 - Range: Unselect
 - AE level: Unselect
 - Acq. time: 0.5
 - Accumulation: 2
 - Autofocus: off
 - DuoScan Spot: off
- Expand Map
 - Select Y; From = -50; To = 50; Size = 11; Step = 10 (automatically set)
 - Select X; From = -50; To = 50; Size = 11; Step = 10 (automatically set)

The screenshot displays the HORIBA Scientific software interface. The top navigation bar includes tabs for Analysis, Display, Methods, Maintenance, Browser, Acquisition (selected), Info, and Processing. The main panel is titled 'Acquisition parameters' and contains the following settings:

- Spectro (cm^{-1}): 1600
- Range: 100 to 4000 (checkboxes for 100 and 4000 are present)
- AE level (cnts): 1000
- Acq. time (s): 0.5
- Accumulation: 2
- RTD time (s): 0.5
- Autofocus: Off
- DuoScan Spot: Off
- Title: Try

Below the acquisition parameters, there are expandable sections for 'Instant processing', 'Acquisition options', 'Instrument setup', and 'Map'. The 'Map' section is expanded, showing a table with the following data:

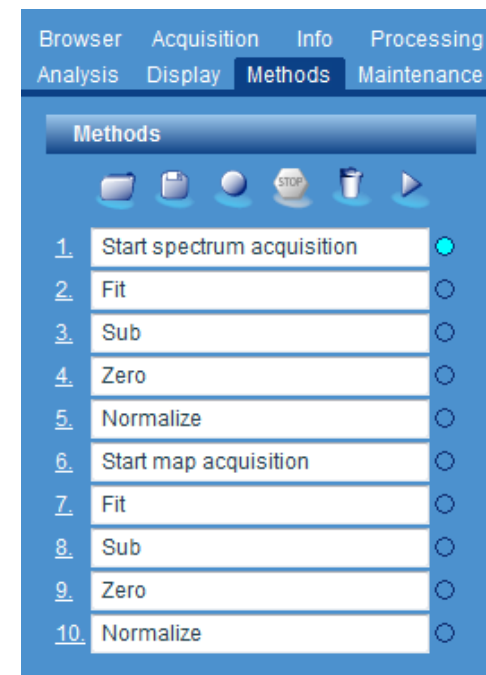
	From	To	Size	Step	
Z	0.00	100.00	11	10.0	☐
Y	-50	50	11	10.0	☒
X	-50	50	11	10.0	☒

Below the table, the following information is displayed:

- Total data points: 121
- Estimated time: 2:01
- ☐ SWIFT mode. Acq. time(s) 0.1
- Extra images: (slider bar)

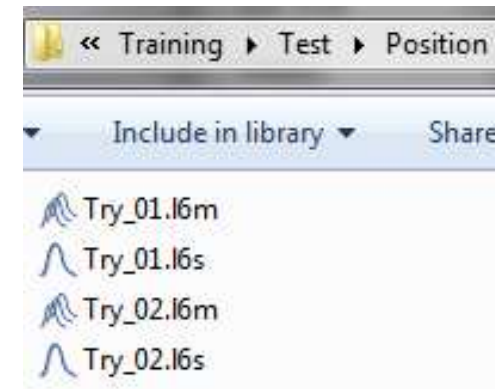
Automation

- Select Methods section
 - Select Record Method
 - From Icon Bar, click Start Map Acquisition
 - From Processing section, click Fit and then Sub in Baseline correction
 - From Processing section, click Zero and then Normalize in Correction
 - Select Stop method recording



Automation

- Select Methods section
 - Select Run method
 - After completion of the first run, select Run method one more time
- Results
 - Select Spectra tab, and confirm two spectra (Try_01 and Try_02) are recorded
 - Select Map tab, and confirm two maps (Try_01 and Try_02) are recorded
 - Open Data Folder location. Confirm subdirectories are created, and data files saved



Maintenance Section

0°

532 nm

600 gr/mm

AE

AF

DN

ICS

SR

AutoCal

✓

1484.35

122.97

- AutoCalibration
 - Use Si standard provided by HORIBA with the system.
 - Click AutoCal button in the status bar or Run button in AutoCalibration module
 - Setup AutoCalibration: Available only to administrator level operators.
 - Current AutoCalibration: Current laser + current grating
 - Full AutoCalibration: All lasers + all gratings
 - Show log: Display AutoCalibration log

Browser

Acquisition

Info

Processing

Analysis

Display

Methods

Maintenance

▲ Instrument calibration

Offset shift < 0 > Zero

Coeff 0.0120636 Apply

▲ AutoCalibration

Last run on : 2012-12-7 8:17

Status : Undefined

AutoCalibration

Please choose your AutoCalibration operation

Current AutoCalibration

Full AutoCalibration

Custom AutoCalibration

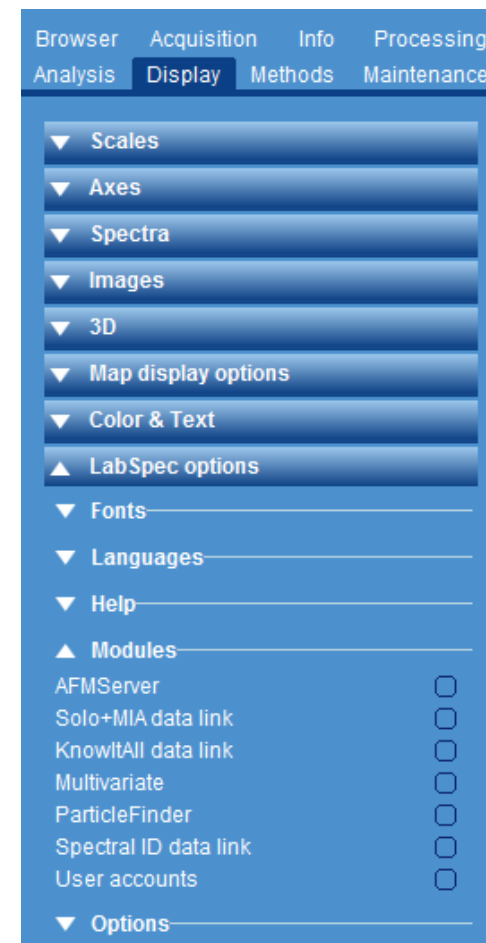
Setup AutoCalibration

Exit

Date_Time	Operator	Methods	Grating	Laser	Peak_Position(tolerance)	Peak_Intensity	New_Offset	Old_Offset	New_Coeff	Old_Koeff	New_Laser_WL	Old_Laser_WL	
2013-02-28_11:17:34		AutoCalibration	600 gr/mm	532 nm	644.75 cm-1 (517.65 - 523.75)	174 cnt/s	FAIL	0	N/A	N/A	N/A	N/A	Could not f
2013-02-22_08:32:53		AutoCalibration	600 gr/mm	532 nm	636.62 cm-1 (517.66 - 523.74)	159 cnt/s	FAIL	0	N/A	N/A	N/A	N/A	Could not f
2013-01-15_13:35:49		AutoCalibration	600 gr/mm	785 nm	440 cm-1 (517.83 - 523.57)	149 cnt/s	FAIL	0	N/A	N/A	N/A	N/A	Could not f

Display Section

- LabSpec options
 - Available only to administrator level operators
 - Activate/deactivate advanced/optional functionality



User Accounts

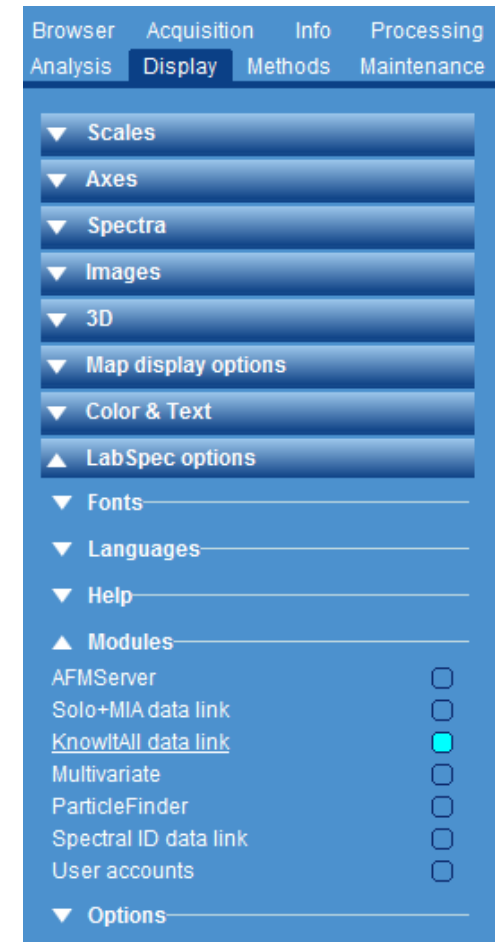
- Administrator only
 - Manage user accounts
 - Full access to Processing and Analysis sections
 - Full access to Display section including custom module management
 - Setup AutoCalibration
 - Access to Service and Configuration functions
- Expert and higher
 - Full access to Acquisition
 - Access to advanced functions in Processing and Analysis sections
 - Access to Display section except for custom module management
 - VBS scripting for advanced customization

User Accounts

- Operator (full) and higher
 - Acquire spectrum arrays
 - Access to Processing and Analysis functions for spectrum arrays
 - Access to Image and Map display parameters in Display section
- Operator (basic) and higher
 - Acquire spectra and microscope images
 - Access to Processing and Analysis functions for spectra
 - Access to Spectrum display parameters in Display section
 - Perform AutoCalibration, and view AutoCalibration log file

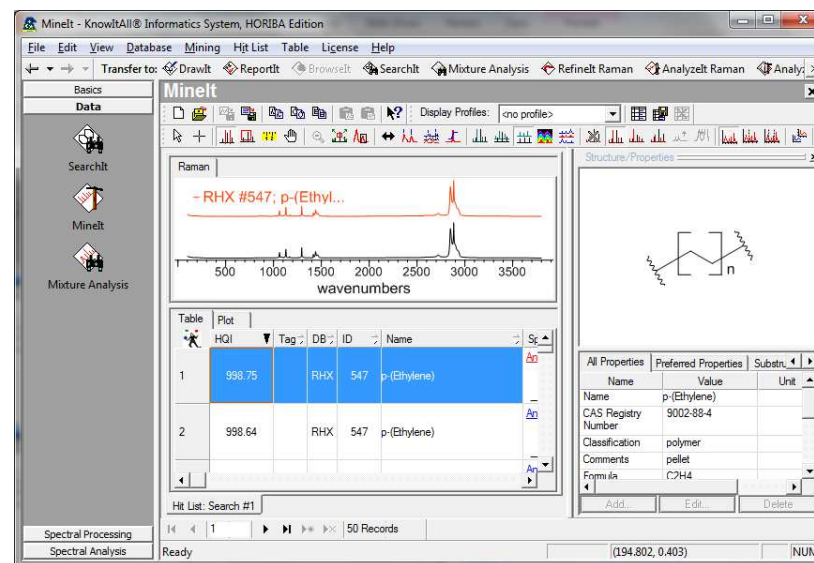
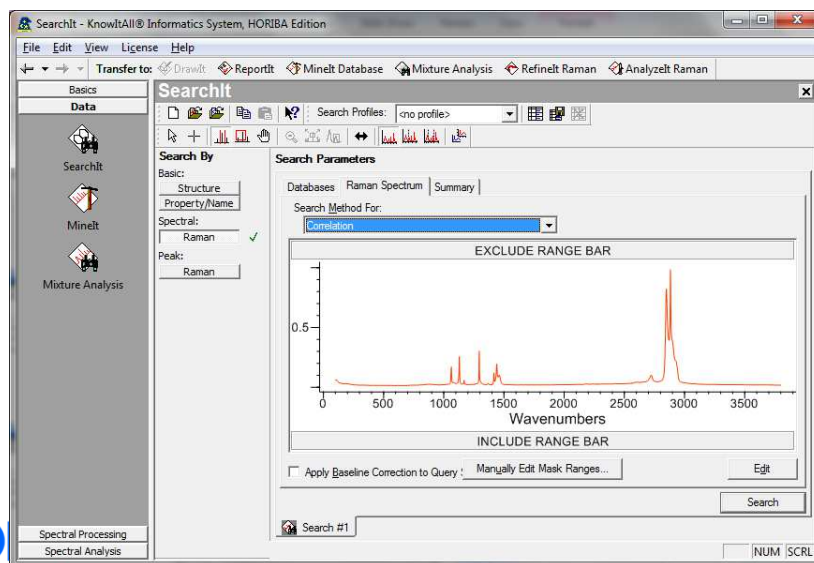
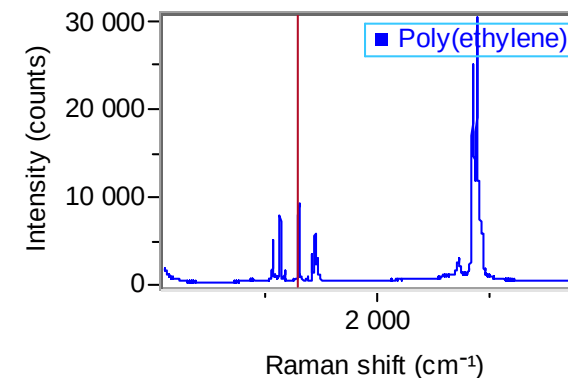
KnowItAll

- An optional module for LS 6
- Available in LS 6.1 and higher
- Library search engine by BioRad
- After installation of KnowItAll (KIA), direct link from LS 6 to KIA is  activated from LabSpec options module in Display section. The procedure requires a separate license.



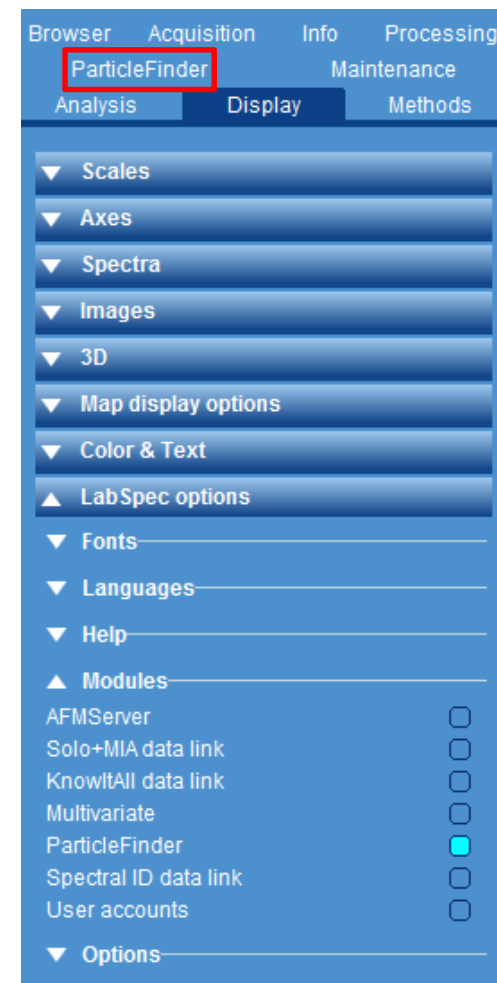
Search Library

- Select a spectrum (e.g. polyethylene)
- Click the link to KIA 
- KIA opens with the spectrum imported, and ready to search.
- Click Search. The first hit/best fit is polyethylene



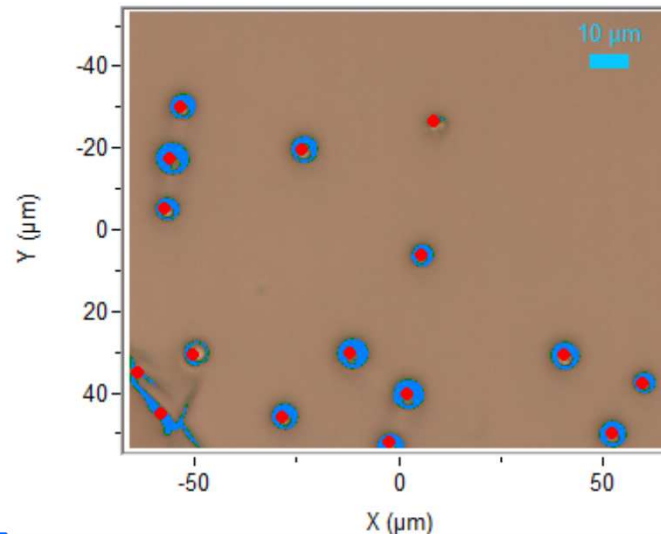
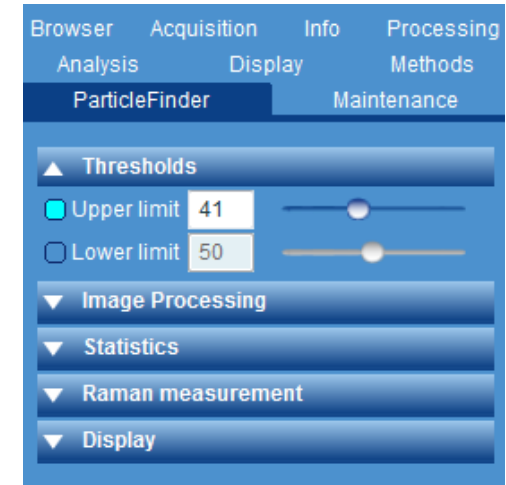
Particle Finder

- An optional module for LS 6
- Available in LS 6.2 and higher
- Analyze the sample image to identify, and analyze particles. Morphological and Raman analyses.
- After installation, Particle Finder section is activated from LabSpec options module in Display section. The procedure requires a separate license.



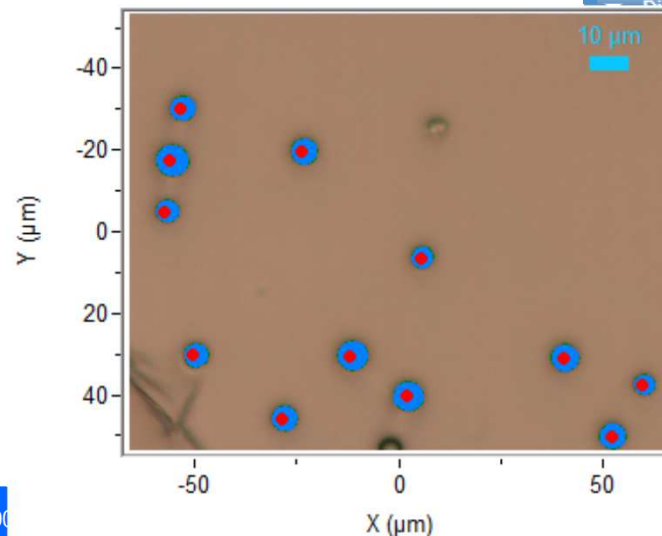
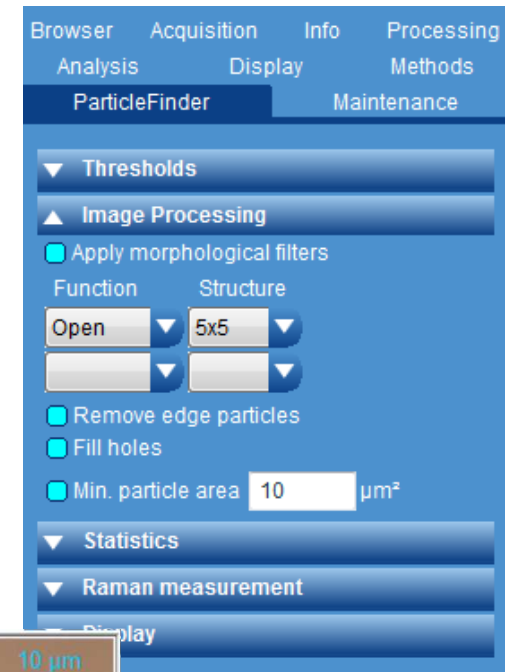
Particle Finder

- Open an image (e.g. Training Image)
- Select ParticleFinder section
- Expand threshold
 - Select Upper limit. Threshold is applied interactively
 - Adjust the threshold to your satisfaction (e.g. 41)



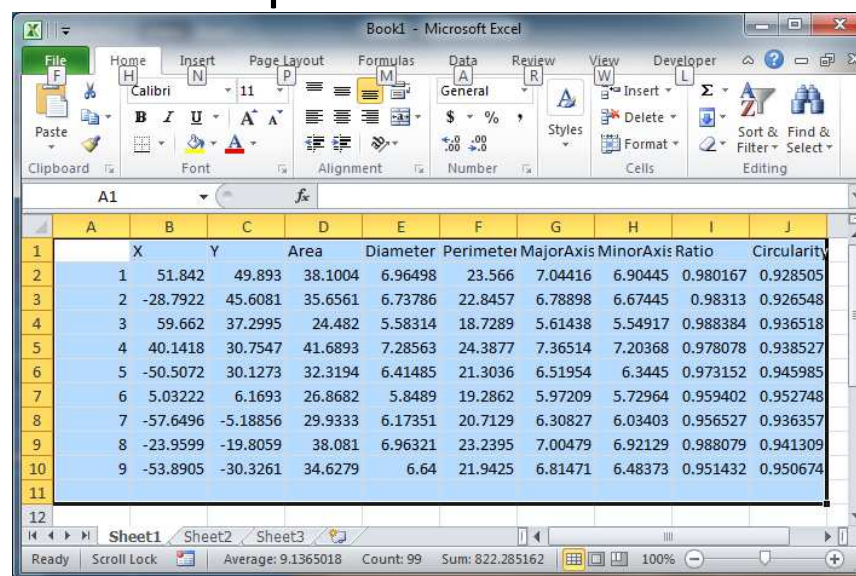
Particle Finder

- Expand Image Processing
 - Select Apply morphological filters.
 - Select a filter (e.g. Open) or filters from Function
 - Select Remove edge particles and Fill holes
 - Select Min. particle area, and input the threshold (e.g. 10)



Particle Finder

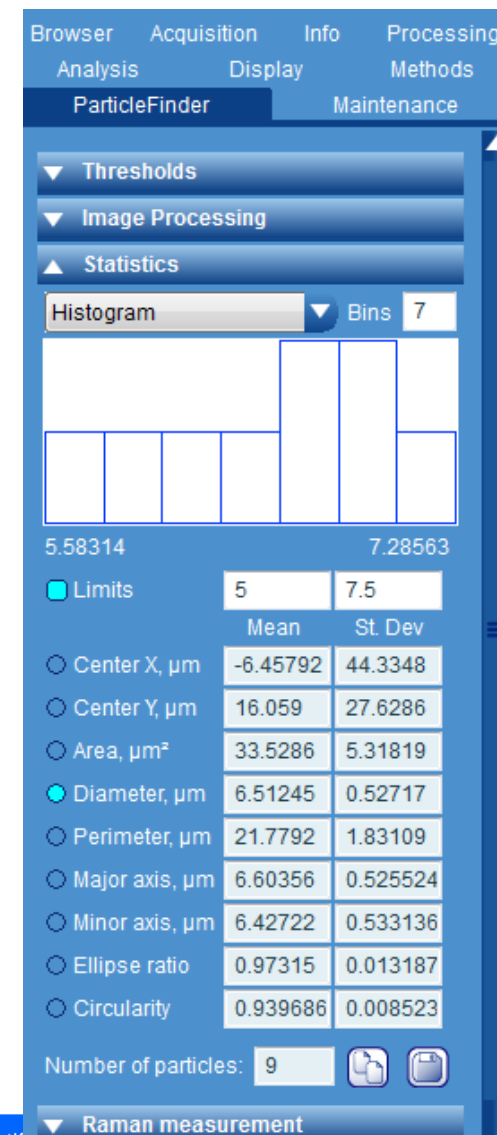
- Expand statistics
 - Further select particles based on the morphological characteristics (e.g. $5\text{ }\mu\text{m} < \text{Diameter} < 7.5\text{ }\mu\text{m}$)
 - Select Copy button to copy full statistics
 - Open Excel and paste



Book1 - Microsoft Excel

	A	B	C	D	E	F	G	H	I	J
1	X	Y	Area	Diameter	Perimeter	MajorAxis	MinorAxis	Ratio	Circularity	
2	1	51.842	49.893	38.1004	6.96498	23.566	7.04416	6.90445	0.980167	0.928505
3	2	-28.7922	45.6081	35.6561	6.73786	22.8457	6.78898	6.67445	0.98313	0.926548
4	3	59.662	37.2995	24.482	5.58314	18.7289	5.61438	5.54917	0.988384	0.936518
5	4	40.1418	30.7547	41.6893	7.28563	24.3877	7.36514	7.20368	0.978078	0.938527
6	5	-50.5072	30.1273	32.3194	6.41485	21.3036	6.51954	6.3445	0.973152	0.945985
7	6	5.03222	6.1693	26.8682	5.8489	19.2862	5.97209	5.72964	0.959402	0.952748
8	7	-57.6496	-5.18856	29.9333	6.17351	20.7129	6.30827	6.03403	0.956527	0.936357
9	8	-23.9599	-19.8059	38.081	6.96321	23.2395	7.00479	6.92129	0.988079	0.941309
10	9	-53.8905	-30.3261	34.6279	6.64	21.9425	6.81471	6.48373	0.951432	0.950674

Sheet1 | Sheet2 | Sheet3 | Average: 9.1365018 | Count: 99 | Sum: 822.285162



Browser Acquisition Info Processing
Analysis Display Methods
ParticleFinder Maintenance

▼ Thresholds
▼ Image Processing
▲ Statistics

Histogram Bins 7

5.58314 7.28563

☒ Limits 5 7.5

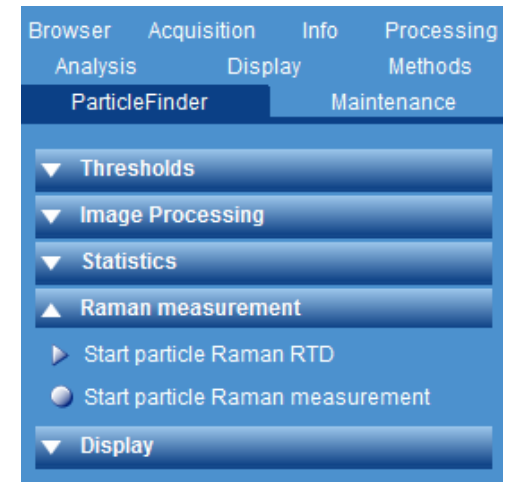
	Mean	St. Dev
Center X, μm	-6.45792	44.3348
Center Y, μm	16.059	27.6286
Area, μm^2	33.5286	5.31819
☒ Diameter, μm	6.51245	0.52717
Perimeter, μm	21.7792	1.83109
Major axis, μm	6.60356	0.525524
Minor axis, μm	6.42722	0.533136
Ellipse ratio	0.97315	0.013187
Circularity	0.939686	0.008523

Number of particles: 9

▼ Raman measurement

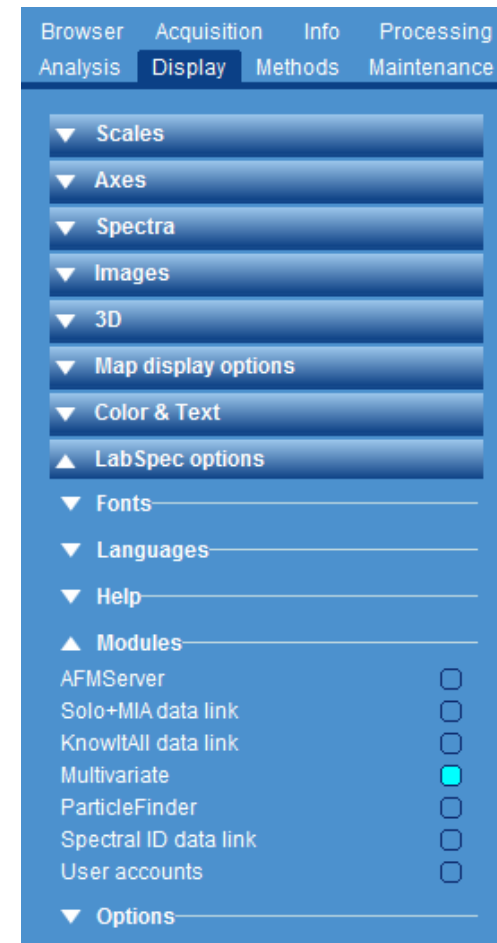
Particle Finder

- Expand Raman measurement
 - Click Start particle Raman measurement
 - Stage moves to center each particle in turn, and record a spectrum from the red dotted position
 - The result is a map as a collection of all particle spectra



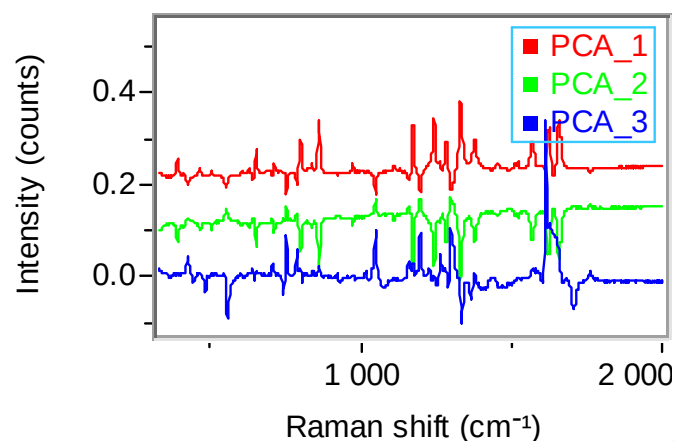
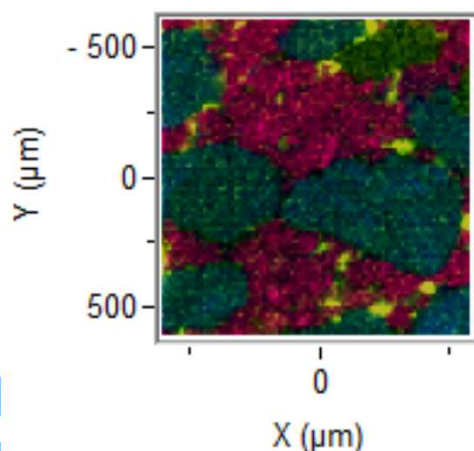
Multivariate Analysis

- An optional analysis methods for LS 6
- Selected methods are available in LS 6.2 with more in development
- Multivariate analysis (MVA) engine by Eigenvector Research
- After installation, MVA methods are activated from LabSpec options module in Display section. The procedure requires a separate license.
- MVA methods are added to Analysis section.



Multivariate Analysis

- Select a map (e.g. Training Map)
 - Select Spectrum Array window
- From Analysis section, expand PCA
 - Expand Preprocessing, and select Mean center
 - Set Components to 3
 - Click Apply



Browser Acquisition Info Processing
Analysis Display Methods Maintenance

▼ CLS Fitting ✓
▲ PCA ✓

▲ Preprocessing

☐ Normalize
☒ Mean center
☐ Autoscale
☐ Save preprocessed data

Components : 3

☐ Show score scatter plot

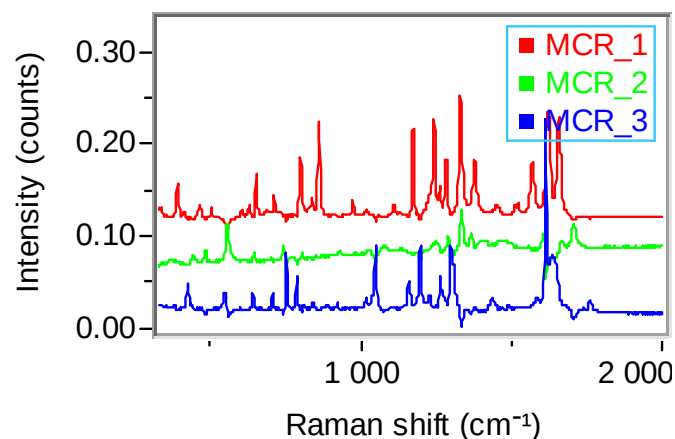
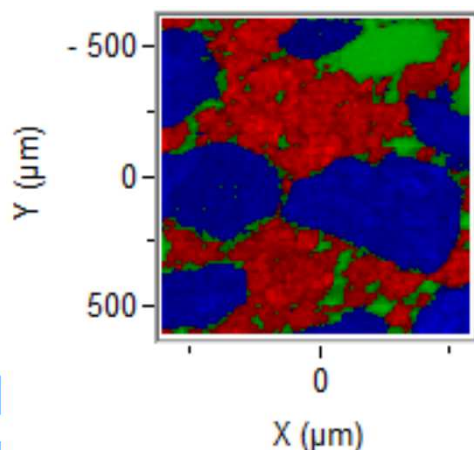
1 PCA_1
2 PCA_2
3 PCA_3

▲ Statistics

Component	% variations	accum. % variation
1 PCA_1	38.10	38.10
2 PCA_2	19.58	57.68
3 PCA_3	4.54	62.23

Multivariate Analysis

- Select a map (e.g. Training Map)
 - Select Spectrum Array window
- From Analysis section, expand MCR
 - Expand Preprocessing, and select Normalize
 - Set Components to 3
 - Click Apply



Browser Acquisition Info Processing
Analysis Display Methods Maintenance

▼ PCA ✓
▲ MCR ✓

▲ Preprocessing
☒ Normalize
☐ Save preprocessed data
 Loadings : 3

☐ Show score scatter plot

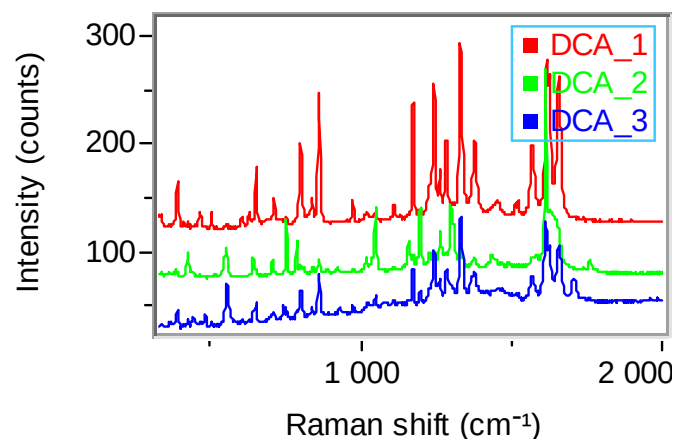
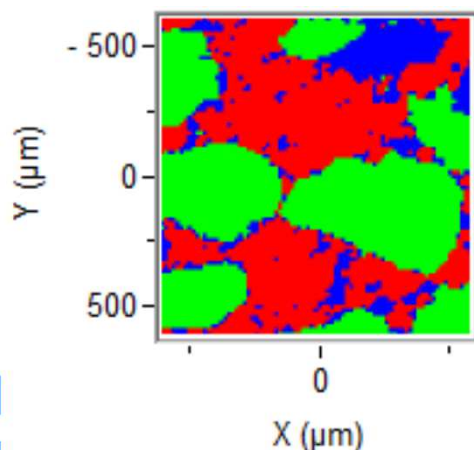
1 MCR_1
 2 MCR_2
 3 MCR_3

▲ Statistics

	Loading	% variations	accum. % variation
1 MCR_1	36.75		36.75
2 MCR_2	23.92		60.67
3 MCR_3	34.20		94.87

Multivariate Analysis

- Select a map (e.g. Training Map)
 - Select Spectrum Array window
- From Analysis section, expand DCA
 - Expand Preprocessing, and select Normalize
 - Set Components to 3
 - Click Apply



Browser Acquisition Info Processing
Analysis Display Methods Maintenance

▼ PCA ✓
▼ MCR ✓
▼ HCA ✓
▲ DCA ✓

▲ Preprocessing

☒ Normalize
☐ Mean center
☐ Autoscale
☐ Save preprocessed data

Number of classes 3 Apply

1 DCA_1 [Red]
2 DCA_2 [Green]
3 DCA_3 [Blue]

▲ Statistics

	class	counts	%
1	DCA_1	2633	41.15
2	DCA_2	2792	43.63
3	DCA_3	974	15.22