



SPECTROview User Manual

(updated 25.02.2026)

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1. Introduction

Spectroscopy techniques (such as Raman, Photoluminescences, XRD, XPS...) are widely used in various fields, including materials science, chemistry, biology, and geology. In recent years, these techniques have increasingly found their place in cleanroom environments, particularly within the microelectronics industry, where they serve as critical metrology tools for wafer-scale measurements. The data collected from these in-line measurements (wafer data) require specific processing, but existing software solutions are often not optimized for this type of data and typically lack advanced plotting and visualization capabilities. Additionally, the licensing requirements of these software solutions can restrict access for a broader community of users.

SPECTROview addresses these gaps by offering free, open-source software that is compatible with both in-line data (wafer-map) as well as standard spectroscopic data (discrete spectra, 2D maps). It also features a built-in visualization tool, enabling users to streamline both data processing and visualization in a single application, making the workflow more efficient.

More details regarding the latest updates and features of the SPECTROview can be found in the Github repository : <https://github.com/CEA-MetroCarac/SPECTROview>

Dont forget to cite the tool when it is used for your data processing , data visualization on your publication:

Le, V.-H., & Quémésré, P. (2025). SPECTROview : A Tool for Spectroscopic Data Processing and Visualization. Zenodo. <https://doi.org/10.5281/zenodo.14147172>

Highlighted features:

- Cross-platform compatibility (Windows, macOS, Linux).
- Supports processing of spectral data (1D) and hyperspectral data (2D maps or wafer maps).
- Ability to fit multiple spectra or 2Dmaps using predefined custom fit models.
- Collect all best-fit results with one click.
- Optimized user interface for easy and quick inspection and comparison of spectra.
- Dedicated module for effortless, fast, and easy data visualization.
- Each module will be described in detail in the following sections.

2. Installation

Ensure that Python (version between v3.8 and v3.12) is already installed on your PC.

The installation of SPECTROview can be performed via the command line (CMD):

```
pip install spectroview
```

You can also install directly via the GitHub repository by copy and paste following line in CMD:

```
pip install git+https://github.com/CEA-MetroCarac/SPECTROview.git
```

To open SPECTROview, Open CMD then type:

```
spectroview
```

to update to the newest version:

```
pip install --upgrade spectroview
```

or update to the specific version:

```
pip install --upgrade spectroview==num-of-version
```

example: `pip install --upgrade spectroview==26.6.1`



3. Supported data by SPECTROview

Examples of all supported data types can be found in the `/examples` folder within the [GitHub repository](https://github.com/CEA-MetroCarac/SPECTROview/tree/main/examples):

<https://github.com/CEA-MetroCarac/SPECTROview/tree/main/examples> .

Users can download these files to understand the supported files format and data structures; practice using the SPECTROview application with real examples.

3.1 .wdf (Renishaw) and .spc format

Since version **26.7.1**, Spectroview natively supports the `.wdf` and `.spc` file formats:

- **.wdf** — recorded with WiRE software from Renishaw instruments
- **.spc** — recorded with LabSpec 6 software from HORIBA instruments

Both discrete spectra and hyperspectral datasets (2D maps) are fully supported. These files can be opened directly in Spectroview without any prior conversion. In addition to spectroscopic data, Spectroview also reads and imports the associated metadata, including experimental parameters such as: *excitation wavelength (nm)*, *gratings (gr/mm)*, *objective used*, *laser power*, *slit/hole*, *acquisition timestamp*, etc... This ensures full access to both measurement data and experimental conditions within a single workflow.

3.2 Spectroscopic data (.txt, .csv)

SPECTROview supports spectroscopic data (TXT or CSV format). The files must consist of two columns, separated by *semicolon* or *space*, or *tab*. Data files can contain or not column headers:

- **Column 1:** Raman shift (cm^{-1})
- **Column 2:** Corresponding Raman intensity (a.u.)

header	header
R ₁	Intensity
R ₂	Intensity
...	...
R _{n-1}	Intensity
R _n	Intensity

3.3 Hyperspectral data (.txt, .csv)

SPECTROview supports hyperspectral data (2D maps or wafer maps) in TXT or CSV format, with the data structure arranged as follows:

		R ₁	R ₂	R ₃	...	R _{n-1}	R _n
X1	Y1	I ₁	I ₁	I ₁	...	I ₁	I ₁
X2	Y2	I ₂	I ₂	I ₂	...	I ₂	I ₂
...
Xn	Yn	I _n	I _n	I _n	...	I _n	I _n

- The first row (R₁ → R_n) is the **Raman shift (cm^{-1})** of all spectrum
- Two first columns listing the **X** and **Y** coordinate of the spectrum within the maps.
- The remaining columns contain the corresponding **intensity** values for each spectrum (I₁ → I_n), from the second row to the last.

Note: 2D map formats from Renishaw tools must be converted before they can be used in SPECTROview. An integrated conversion tool is provided in SPECTROview application for this purpose (see Section 4, File Convert Tool)



3.4 Datasheet (Excel or CSV files)

Excel files (.xlsx, .xls) containing one or multiple sheets, or CSV file can be directly loaded into SPECTROview.

3.5 Formats saved by SPECTROview application

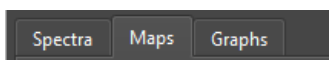
Depending on the active workspace, SPECTROview saves files with specific extensions so work can be resumed later:

- Maps workspace → .maps
- Spectra workspace → .spectra
- Graphs workspace → .graphs

4. User Interface Overview

The SPECTROview application is designed for the efficient processing of spectroscopic data and the easy visualization of fitted results. The interface features three main **workspaces**, each developed for a

specific purpose:



- **Spectra**: For processing one or multiple discrete spectra.
- **Maps**: For processing one or multiple hyperspectral datasets, including wafer data and 2D maps.
- **Graphs**: For plotting and visualizing data.

Tooltip: Most GUI elements in SPECTROview (buttons, text boxes, dropdowns, etc.) feature **tooltips**. → To see a brief explanation of its function : hover the mouse cursor over an element for 1second.

Toolbar : a horizontal toolbar is located at the top edge of the application containing the following buttons:

	Loads all supported data types as listed in section 3. The application will automatically switch to the appropriate workspace based on the loaded file type.
	Saves the current active workspace to a file, allowing the user to reopen it later and resumes the work. As detailed in Section 3.5, the file extension will be .maps , .spectra , or .graphs depending on the active workspace.
	Clears the current active workspace to start a new session. All loaded data will be removed.
	Opens the File Convert Tool to convert hyperspectral data (2D maps) from the Renishaw WiRE format into a format supported by SPECTROview:
	“Settings” : Opens the Settings Panel to adjust fitting parameters and define the storage folder for user-defined fitting models

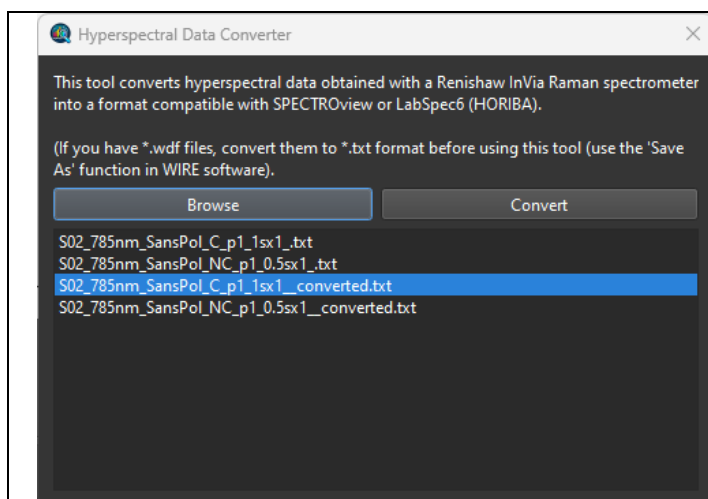


Figure 1: Interface of “Hyperspectral Data Converter”

How to use (see Figure 1): Load the file(s) to convert
 → Click button “Convert” (4.2) → The new converted
 file(s) is created in the same folder with the suffix
converted (4.3).

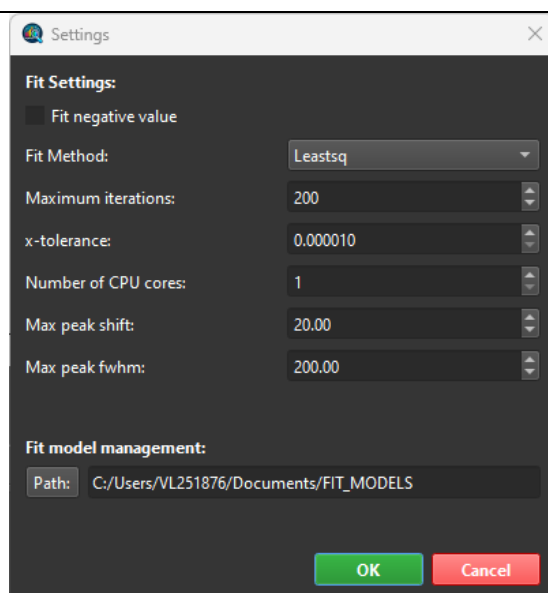


Figure 2: Setting Panel

	Theme Toggle: Switches the application GUI between Dark and Light modes.
	To Open this User Manual document.
	To displays version information and details about the application..

5. Spectra and Maps workspaces

The Maps and Spectra workspaces are very similar. They share many common features, with the Maps workspace containing additional specific features designed to handle multiple hyperspectral datasets (see Figure below). The following section details the GUI of the Maps workspace:

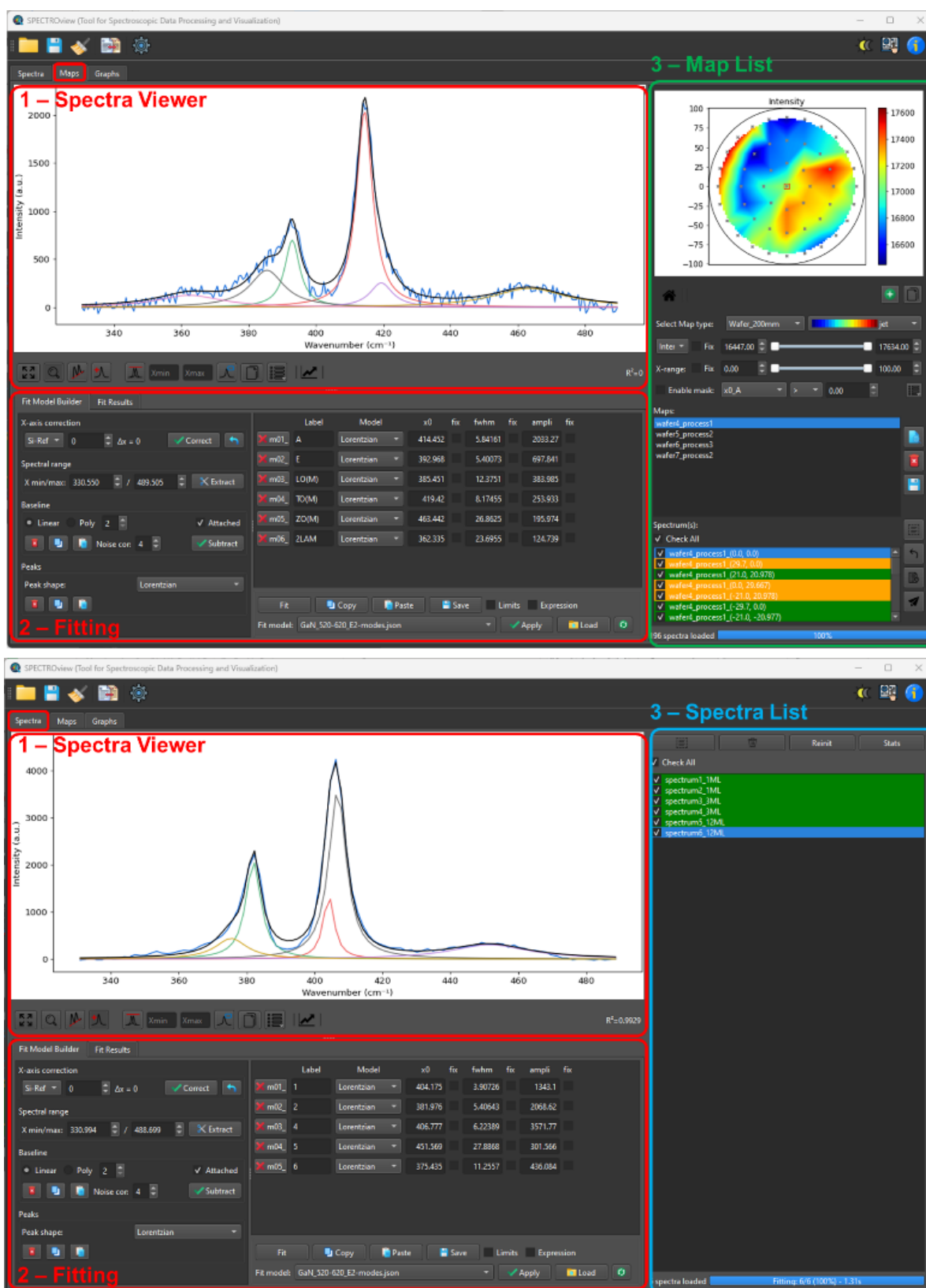


Figure 3: Interface overview of Spectra (left) and Maps (right) workspaces. The interface is divided into three main sections. Section 1-SpectraViewer and 2-FittingPanel are identical in both workspaces, whereas section 3-SpectraList (in Spectra workspace) or 3-MapList (in Maps Workspace) are different.



5.1 SpectraList and MapList

As showed in Figure 3, the **SpectraList** and **MapList** sections are designed differently for **Spectra** and **Map** workspaces in order to efficiently navigate between spectral or hyperspectral (maps) data.

In the following, the **MapList** section of the **Maps** workspace (which also contains also a **SpectraList** module) is described in detail (Figure 4).

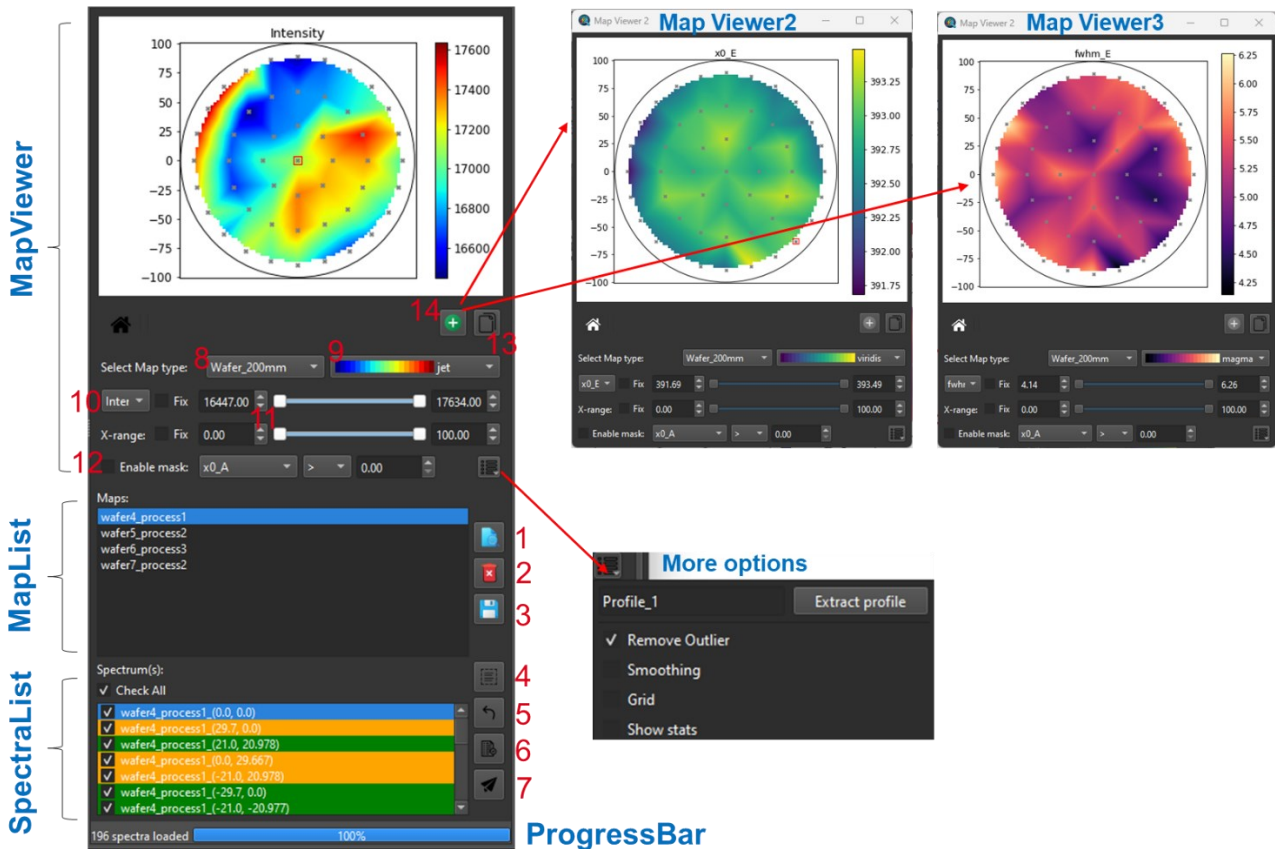


Figure 4: (Left) **MapList** section within the **Maps** workspace. On the right: (top) additional **MapViewer** module(s) can be added as floating window(s); (bottom) **More Options** to adjust and customize the heatmap display.

MapList: The MapList displays all loaded map files, including wafer maps and 2D map types. Three buttons located on the right side of the MapList allow the user to (1) **view** the selected map data, (2) **delete** the selected map, or (3) **save** the selected map to an Excel file (see Figure 4).

SpectraList: all loaded spectra in the Spectra workspace, or all spectra associated with the map selected in the MapList (in the Maps workspace). Users can select one or multiple spectra simultaneously. The selected spectra are displayed in the SpectraViewer (cf. section 5.2). Four buttons associated with the SpectraList allow the user to (4) **Select all available spectra in the list**, (5) **reset (reinit) the selected spectra**, (6) **display the fit statistic report** or (7) **send the selected spectra to the Spectra workspace** (see Figure 4).

MapViewer: displays the heatmap of the selected map (wafer or 2D map type) chosen from the **MapList**. Several options are available to customize the heatmap:

- (8) **Map type:** 2D map or wafer map with different diameters.
- (9) **Color palette** selection for the heatmap.
- (10) **Displayed parameter:** maximum intensity, area, or any fitted parameter.
- (11) **Range sliders:** two sliders are available to adjust the X-axis range and the color bar limits.



- (12) **Mask feature**: allows the user to define specific regions of the heatmap based on user-defined filters.
- (13) **Copy button**: copies the heatmap to the clipboard, allowing it to be pasted elsewhere.
- (14) **Multiple MapViewers**: users can add additional MapViewer windows as floating windows, enabling comparison between different fitted parameters of the same map (see Figure 4) (see Figure 4).

ProgressBar: placed under the SpectraList (see Figure 5) displays the number of spectra available in the SpectraList, and the progress of the fitting process (number of fitted spectra / total spectra, percentage (%), and elapsed time (s)). The Stop button allow to stop the fitting process at anytime.

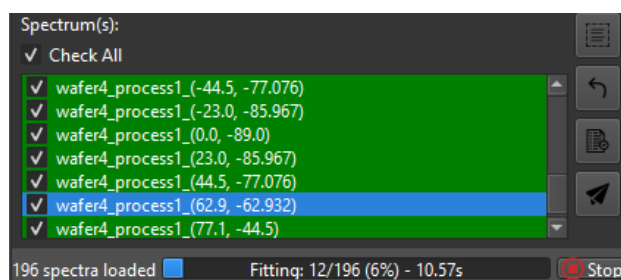


Figure 5: SpectraList and ProgressBar

5.2 Spectra Viewer

SpectraViewer plot all spectra (and it best fit curves) selected via the SpectraList (cf. section 5.1)

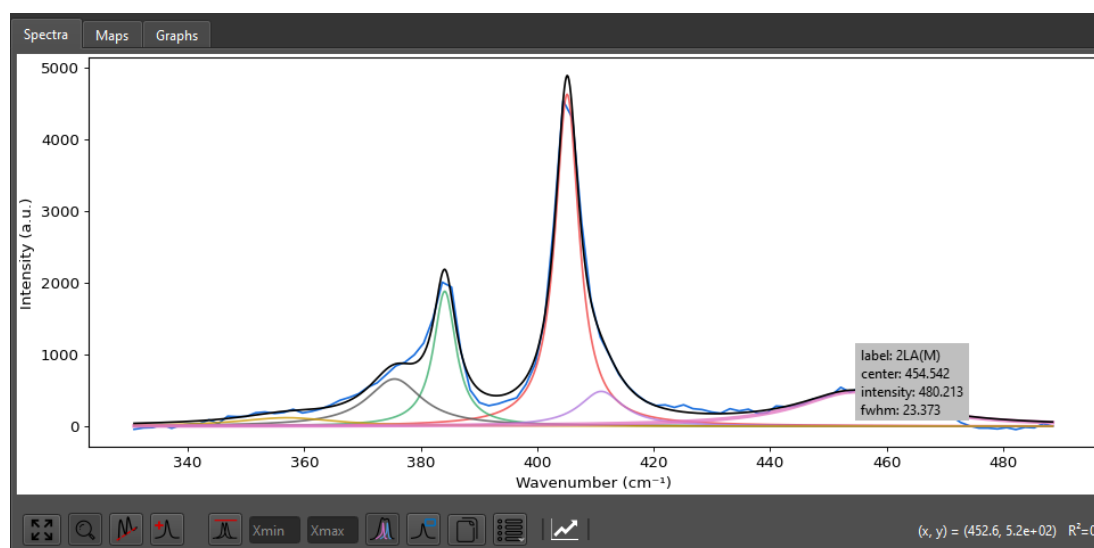



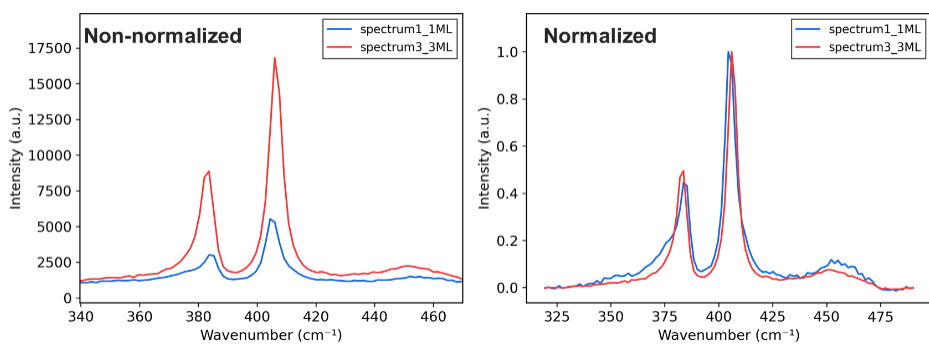

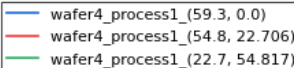
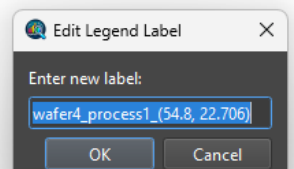


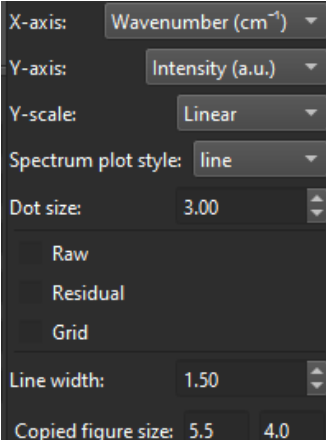


Figure 6: Spectra Viewer (left) widget and View Options Menu (right).

	Rescale : to rescale the spectra plot. Shortcut: Ctrl + R
	Zoom : when active, enables the "zoom" feature of spectra plot using the left mouse click & drag
	Baseline : when active, allows the user to define baseline point(s) using the left mouse click.
	Peaks : when active, allows the user to define peak(s) on the spectra using the left mouse click.




  	<p>Normalization: when clicked, displays all selected spectra normalized to the maximum peak intensity. If the user wants to normalize to a specific spectral range or specific peak → type the corresponding spectral range into text box 'min' and 'max' (see Figure 7).</p> <div data-bbox="367 280 1300 627">  </div> <p>Figure 7: Example of Raw spectra (left) and spectra normalized to the maximum intensity within the 400-420 cm⁻¹ range (right) to facilitate the inspection of peak shifts.</p>
	<p>Legend: displays the legend for all selected spectra.</p> <p>Once the legend is shown, the user can click directly on the legend box to change the color or labels (see figure on the right).</p> <p>Note: This feature only works when the Zoom button is disabled (by selecting Baseline or Peak button).</p> <div data-bbox="1077 739 1388 1030">   </div>
	<p>Copy: copies the spectra plot to the clipboard as an image. The user can then paste it into other applications (PowerPoint, Excel, etc.).</p> <ul style="list-style-type: none"> - Ctrl + Click (or Cmd + click on macOS): Copies the numerical data of the spectra (including RAW data and best-fit curves) to the clipboard.
	<p>More options: opens a pop-up window with several view options (cf. figure on the right).</p> <ul style="list-style-type: none"> - X-axis unit : available option (Wave number (cm⁻¹), wavelength (nm), Emission energy (eV), binding energy (eV), Frequency (Hz), 2θ (°), time (ns). - Y-axis unit : available option (Intensity (a.u.), (Intensity (a.u./s)). - Y axis-scale: Linear or log scale. - Spectrum plot style : line or dot (Dot Size adjutement) - Raw : Toggles the visibility of the raw data. - Residual: Displays the residual (Raw - bestfit). - Grid: adding grids on the plot. - Line width: to adjust the line with of the spectra plot. - Figure size: to adjust the ratio (high-width) of copied figure. <div data-bbox="1061 1232 1404 1691">  </div>

Other features of SpectraViewer:

- **Show Peak Parameters** on the spectra plot: by hovering the mouse cursor over a peak displays a pop-up with the peak parameters (peak label, intensity, FWHM, position), as shown in Figure 6.



- **Add/Remove Peaks**: Right-click to remove the current peak, or left-click to add a new peak (ensure the Peak button  is active).
- **Adjust peak by dragging**.
- **Quick re-scale** of the y axis: Use the mouse wheel to quickly adjust the Y-axis (intensity scale).

5.3 Fit Model Builder

The FitModelBuilder Tab widget contains three main panel : Fitting, PeakTable Panel, FitModelControl Panels (Figure 8).

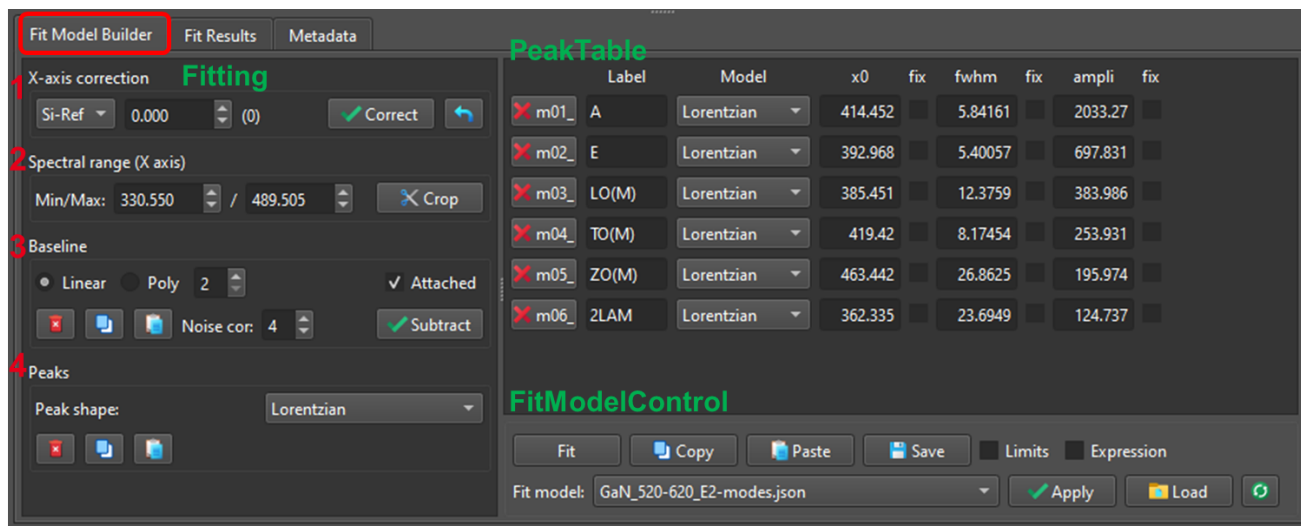


Figure 8: FitModelBuilder tab widget containing three main panels: (1) Fitting, (2) PeakTable and (3) FitModelControl.

5.3.1 Fitting Panel

The FittingPanel (left panel of Figure 8) is divided four small sections, each corresponding to the key steps in the fitting process or in the construction of the fit model.

Step 1: x-axis Correction (optional) : This step is used to perform an x-axis correction based on measurements from a well-known reference sample. In SPECTROview, this feature is currently implemented for a **silicon reference sample**, which has a theoretical Raman peak position at 520.7 cm^{-1} . Support for additional reference samples will be added in future versions.

Procedure:

- Record the silicon reference spectrum during the same experimental session as the other samples, using identical measurement parameters.
- Fit the Si-Ref spectrum to determine the measured silicon peak position.
- Enter the measured position into the text box.
- Select one or more spectra to correct → the x-axis correction is applied based on the difference between the measured position and the theoretical value (520.7 cm^{-1}).

Step 2: Define the fitting range : to define the x-axis range to be used for the fitting process.

Step 3: Baseline definition:

Two baseline modes (**Manual** or **Auto**) can be chose by user for baseline definition and substraction.

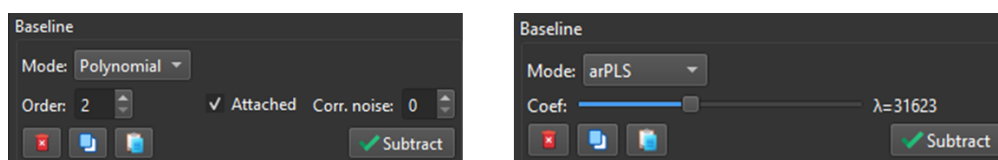



Figure 9: baseline mode selection: (left) Manual vs. (right) Auto mode


Regarding **Manual** modes: user can choose between “Linear” or “Polynomial” options. Once these mode are selected user must define baseline points (anchor points) and other parameters (attached, correct noise).

- **Baseline points** are defined directly in the spectra plot (**SpectraViewer** widget) by left-clicking. The Baseline button  must be active (cf. section 0).
- **Attached checkbox** : When checked, the baseline points remain attached to the spectrum curve.
- **Correct noise**: Calculates each baseline point as the average of the specified number of neighboring data points, ensuring it sits in the center of the noise level.

Regarding **Auto** mode, user can choose between **airPLS** and **asLS** options. Baseline curve will be automatically defined and evaluated. Adjust the slider to further adapt the baseline curve to the selected spectrum data.

- **airPLS (Adaptive Iteratively Reweighted PLS)**: Zhang, Z. M., Chen, S., & Liang, Y. Z. (2010). “Baseline correction using adaptive iteratively reweighted penalized least squares”. **Analyst**, 135(5), 1138-114: It is “aggressive.” It tries to force the baseline to the very bottom. This makes it great for high-fluorescence samples but risky if you have very weak signals that might be mistaken for background.
→ This method is specifically developed and validated using Raman data (Zhang et al., 2010). It handles high-intensity fluorescence better than AsLS.
- **AsLS (Asymmetric Least Squares)**: Eilers, P. H. C. (2005). “Baseline Correction with Asymmetric Least Squares Smoothing”. Unstable Baselines in Spectroscopy. [Note: Often cited as Eilers & Boelens, 2005]: It is a “blunt instrument.” Because the weight p is the same for a tiny bump and a massive peak, it doesn't distinguish between noise and actual signal well.
→ This method is best for very clean, simple spectra with consistent background. It is the most “stable” but the least “intelligent” regarding large peaks.

Step 4: Peak definition:

- Peaks can be defined directly on the spectrum plot (**SpectraViewer**) by left-clicking on the desired position. The Peak button () must be enabled (cf. section 0). Once a peak is added to the active spectrum, it can be adjusted interactively by hovering over the peak and dragging the mouse cursor to modify its position and/or intensity.
- Added peaks are automatically listed in the **PeakTable** panel (see below). Users can further modify or fine-tune peak parameters directly within the PeakTable. (fixing, changing limits or linking between peak(s)).
- Supported peak shapes include: **Lorentzian**, **Gaussian**, **PseudoVoigt**, **LorentzianAsym**, **GaussianAsym**, **Fano**, **DecaySingleExp** and **DecayBiExp** (for Single-Exponential Decay, and Bi-Exponential Decay).



5.3.2 PeakTable Panel

The **PeakTable** displays all available peaks defined of the selected spectrum.

Peak properties (*label*, *model*, *position*, *FWHM*, *intensity*) are dynamically updated as user modifying via SpectraViewer plot (with mouse *click* or *dragging*). Users can also remove peak(s) or manually adjust their parameters directly via PeakTable.

	Label	Model	X0	fix X0	Fwhm	fix Fwhm	Ampli	fix Ampli
<input checked="" type="checkbox"/>	m01_ A	Lorentzian	414.258	<input type="checkbox"/>	5.888	<input type="checkbox"/>	2709.714	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m02_ E	Lorentzian	392.946	<input type="checkbox"/>	5.045	<input type="checkbox"/>	970.902	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m03_ LO(M)	Lorentzian	386.016	<input type="checkbox"/>	11.105	<input type="checkbox"/>	592.371	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m04_ TO(M)	Lorentzian	418.887	<input type="checkbox"/>	8.277	<input type="checkbox"/>	345.69	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m05_ ZO(M)	Lorentzian	463.469	<input type="checkbox"/>	25.345	<input type="checkbox"/>	301.522	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m06_ 2LAM	Lorentzian	364.236	<input type="checkbox"/>	25.078	<input type="checkbox"/>	164.159	<input type="checkbox"/>

Figure 10: PeakTable panel

Constraints: For each peak, one or more parameters can be fixed by selecting the corresponding checkbox. For more advanced constraints, two additional options (via checkboxes **Limit** or **Expression**) are proposed:

- **Limits** checkbox: When enabled, **min** and **max** value columns are displayed for each parameter, allowing the user to restrict parameter variations within a defined range (as opposed to the **Fix** option, which keeps the value constant).

	Label	Model	min X0	X0	max X0	fix X0	min Fwhm	Fwhm	max Fwhm	fix Fwhm
<input checked="" type="checkbox"/>	m01_ A	Lorentzian	393.68	414.258	433.68	<input type="checkbox"/>	0	5.888	200	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m02_ E	Lorentzian	369.29	392.946	409.29	<input type="checkbox"/>	0	5.045	200	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m03_ LO(M)	Lorentzian	360.17	386.016	400.17	<input type="checkbox"/>	0	11.105	200	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m04_ TO(M)	Lorentzian	398.61	418.887	438.61	<input type="checkbox"/>	0	8.277	200	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m05_ ZO(M)	Lorentzian	437.78	463.469	477.78	<input type="checkbox"/>	0	25.345	200	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m06_ 2LAM	Lorentzian	338.74	364.236	378.74	<input type="checkbox"/>	0	25.078	200	<input type="checkbox"/>

- **Expression** checkbox: when enabled, **expression** column it allows parameters from different peaks to be linked through mathematical expressions.
 - o Example 1: To constrain the position of peak **m02_** to be 17 units less than **m01_** → type: **m01_x0 - 17**.
 - o Example 2: To constrain the intensity of peak **m03_** to be half that of **m02_** → type: **m02_ampli / 2**

	Label	Model	X0	expression X0	fix X0	Fwhm	expression Fwhm	fix Fwhm	Ampli	expression Ampli	fix Arr
<input checked="" type="checkbox"/>	m01_ A	Lorentzian	409.725	None	<input type="checkbox"/>	0.001	None	<input type="checkbox"/>	6.431	None	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m02_ E	Lorentzian	392.725	m01_x0 - 17	<input type="checkbox"/>	5.424	None	<input type="checkbox"/>	1038.248	None	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m03_ LO(M)	Lorentzian	385.352	None	<input type="checkbox"/>	10.362	None	<input type="checkbox"/>	519.124	m02_ampli/2	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m04_ TO(M)	Lorentzian	414.523	None	<input type="checkbox"/>	6.666	None	<input type="checkbox"/>	2822.882	None	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m05_ ZO(M)	Lorentzian	463.381	None	<input type="checkbox"/>	26.637	None	<input type="checkbox"/>	296.755	None	<input type="checkbox"/>
<input checked="" type="checkbox"/>	m06_ 2LAM	Lorentzian	364.862	None	<input type="checkbox"/>	26.493	None	<input type="checkbox"/>	167.265	None	<input type="checkbox"/>



5.3.3 FitModelControl Panel

Once the desired fit model has been defined (as shown in the **PeakTable** panel), click the button **Fit** to start the fitting process (Figure 11).

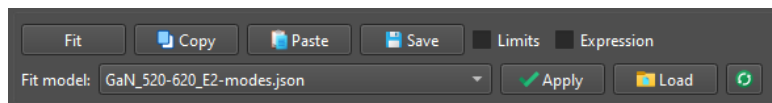


Figure 11: Interface of FitModelControl

If the result is unsatisfactory, adjust the parameters (via **PeakTable** or **SpectraViewer**) and click **Fit** again.

Copy / Paste Fit Models: The entire fit model (including spectral range, baseline, and peaks) can be copied and pasted between spectra:

- Select the fitted spectrum and click **Copy**.
- Select one or multiple target spectra and click **Paste**.

Saving Fit Models: Users can save the fit model for later use by clicking **Save**. It is recommended to store all models in a predefined folder, which can be specified in the **Settings Panel** (Figure 2). Saved models can then be quickly accessed using the "Fit Model" dropdown menu.

To using a pre-define fit model :

- Select the fit model via the drop-down list. Then click to the **Apply** button to perform the fitting for selected spectra.
- Use can also load a fit model store anywhere in the PC via **Load** button.

5.4 Collect & Save Fit Results

SPECTROview provides simple and efficient access to fitted data. To collect best-fit results from all fitted spectra or maps. To save bestfit data:

- Switch to the **Fit Results** tab.
- Click to the Collect button **Collect Fit Results**.
- Results are then aggregated into a table and displayed in the GUI (Figure 12).

	Filename	x0_A1g	x0_E1_2g	x0_LO(M)	x0_ZO(M)	x0_LA(M)	x0_2LA(M)	fwhm_A1g	f
1	wafer4_(-54.8, -22.706)	414.126	392.663	383.5	419.0	362.0	463.152	5.688	6
2	wafer4_(-42.0, -41.955)	414.154	392.73	383.5	419.0	362.0	462.678	5.735	5
3	wafer4_(-22.7, -54.817)	414.247	392.719	383.5	419.0	362.0	462.496	5.726	5
4	wafer4_(0.0, -59.333)	414.362	392.683	383.5	419.0	362.0	463.629	5.646	6
5	wafer4_(22.7, -54.817)	414.433	392.385	383.5	419.0	362.0	463.071	5.573	6
6	wafer4_(42.0, -41.955)	414.838	392.439	383.5	419.0	362.0	463.327	5.842	6
7	wafer4_(54.8, -22.706)	414.827	392.477	383.5	419.0	362.0	461.344	5.778	6
8	wafer4_(89.0, 0.0)	414.882	392.193	383.5	419.0	362.0	464.356	5.693	6
9	wafer4_(86.0, 23.035)	415.077	392.207	383.5	419.0	362.0	463.112	5.925	6

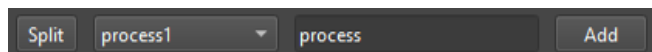
Figure 12: Collect_fit_results panel



5.4.1 Splitting filename features

This feature enables the extraction of metadata from filenames and automatically adds it as new columns in the results table. For optimal use, files should be named consistently, with underscores used to separate relevant information or parameters intended for subsequent analysis (e.g., `Sample1_ProcessA_Temp25`).

- **Example:** In the figure below, the process type (`process1`, `process2`) is extracted from file name of each spectra; and added as a new column named "Process"..



5.4.2 Compute and add new columns

The **Computed Column** feature allows you to create new columns in the Fit Results table via mathematical expressions that reference existing columns. This is useful for calculating derived quantities, ratios, differences, or any mathematical combination of your fit parameters.

Basic Steps

- **Collect Fit Results:** First, click the "Collect Fit Results" button to populate the fit results table with data from your fitted spectra.
- **Enter Column Name:** In the "New Column Name" field, type a descriptive name for your new computed column (e.g., `Peak_Ratio`, `Total_Area`, `Normalized_Position`).
- **Enter Mathematical Expression:** In the expression field, type a mathematical formula using existing column names (e.g., `x0_p1 - x0_p2`).
- **Compute:** Click the "Compute & Add" button to evaluate the expression and add the new column to your results

Supported Operations: the expression evaluator supports standard mathematical operations:

Operation	Symbol	Example
Addition	+	column1 + column2
Subtraction	-	column1 - column2
Multiplication	*	column1 * 2
Division	/	column1 / column2
Power	**	column1 ** 2
Modulo	%	column1 % 10
Parentheses	()	(column1 + column2) / 2

⚠ Important: Column Names with Special Characters

If your column names contain special characters like parentheses (), spaces (), hyphens-, or operators (+ - * /), you must wrap them in **backticks** (`):

Column Name	Correct Syntax	Incorrect Syntax
<code>x0_LO(M)</code>	<code>`x0_LO(M)`</code>	<code>'x0_LO(M)'</code> or <code>x0_LO(M)</code>
<code>Peak Area</code>	<code>`Peak Area`</code>	<code>'Peak Area'</code> or <code>Peak Area</code>
<code>x0-Alg</code>	<code>`x0-Alg`</code>	<code>'x0-Alg'</code> or <code>x0-Alg</code>
<code>area_p1+p2</code>	<code>`area_p1+p2`</code>	<code>area_p1+p2</code>

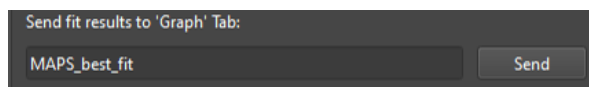



Complete expression examples:

```
(x0_Alg - x0_E1_2g) * `x0_LO(M)`  
`Peak Area` / `Background Area`  
(`x0-A1g` + `x0-E1g`) / 2
```

5.4.3 Saving or Visualizing

Name bestfit dataset and click “**send**” it to the **Graphs** workspace for plotting (cf. Section 0) :



Or, export the results as an Excel file .

5.5 More TAB

The Metadata contain three main sections:

- on the left: Showing all metadata with settings parameters information of the loaded file (.wdf or .spc format only), including *excitation wavelength (nm)*, *gratings (gr/mm)*, *objective used*, *laser power*, *slit/hole*, *acquisition timestampe*, etc...
- In the middle: more information of the selected spectra.
- On the left: additional features for data processing : *intensity normalization*, *cosmic ray dection*.

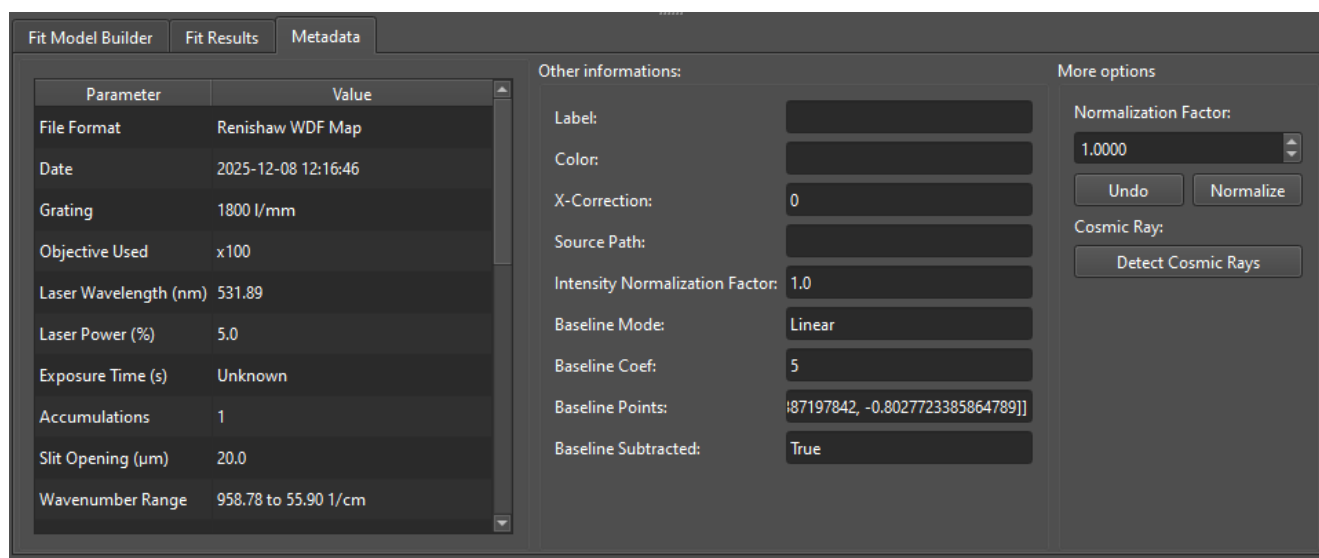


Figure 13: More Tab's user interface.



6. Graphs workspace

The **Graphs Workspace** is dedicated to data visualization, with an emphasis on simplicity and speed. The graphical user interface (GUI) of this workspace is shown in Figure 14:

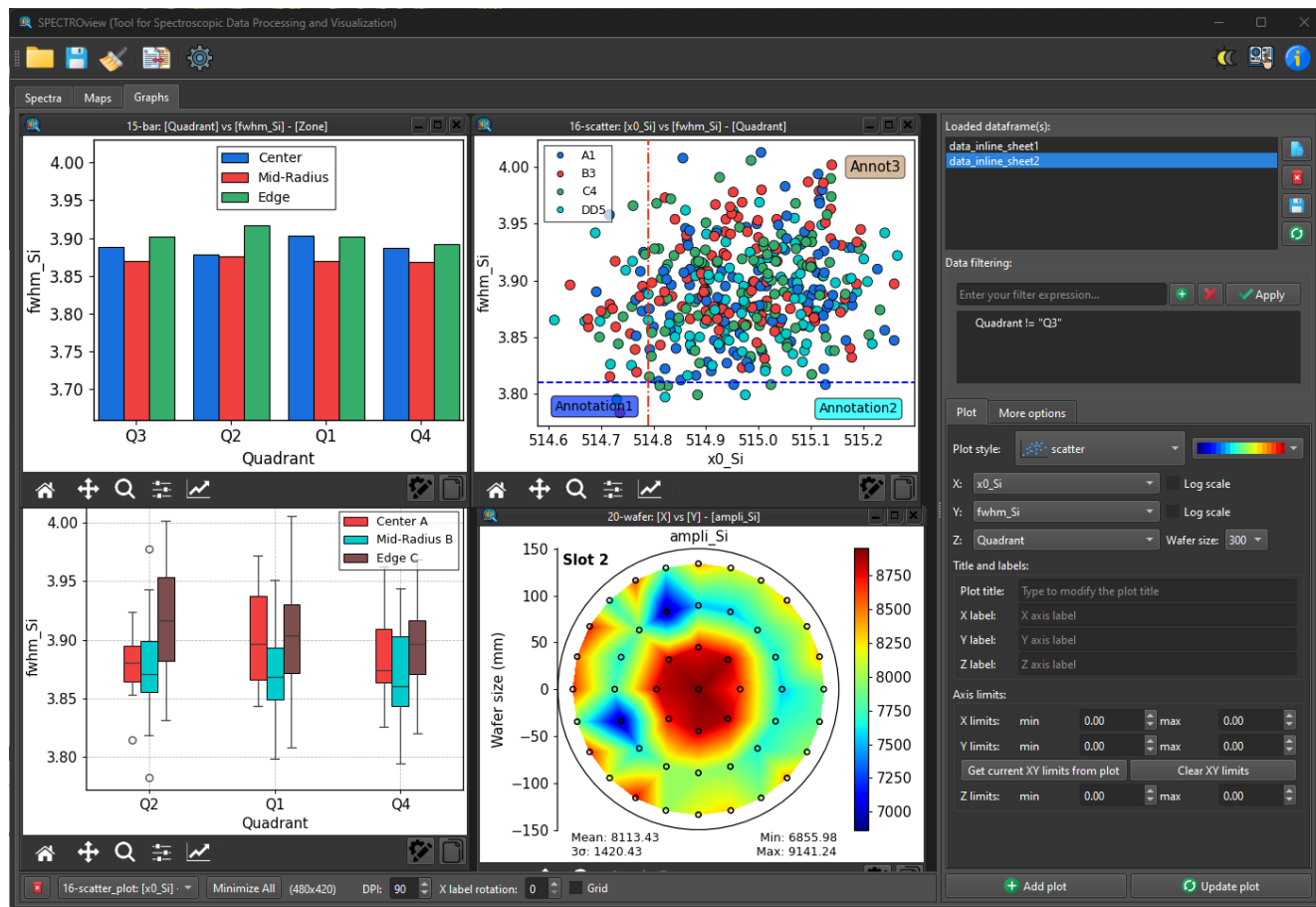


Figure 14: Graphs Workspace's interface. The Control Panel is located on the right side, while the Graph Viewer is displayed on the left side.

6.1 Loading data

Datasets (dataframes) can be sent directly from other workspaces (**Spectra** or **Maps**) or loaded from Excel or CSV files. Excel files may contain one or multiple worksheets; each worksheet is loaded into the Graphs Workspace as an independent dataset. Multiple datasets can be loaded simultaneously.

All loaded datasets are displayed in a list widget (Figure 15) from which the user can select the dataset to work with. On selected a dataset, user can click on the buttons of right side :

- **View:** Display selected dataset
- **Delete:** Remove selected dataset
- **Save:** Save selected dataset
- **Refresh:** Reload the dataset if it was originally loaded from a CSV or Excel file (not sent from other workspaces like Graphs or Maps). This is particularly useful when the user modifies the source file (e.g., adding or removing columns, or editing headers) directly in Excel or Text Reader application. Clicking the Refresh button updates the loaded dataset to reflect these changes.

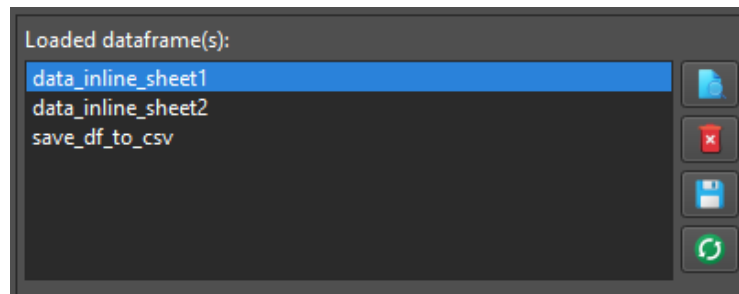
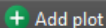


Figure 15: List of loaded dataframe(s) from Excel file(s) or CSV file(s).

6.2 Add a new plot

- Selected datasheet among the loaded dataset via the Listbox → X, Y, Z dropdown menu will be populated with all columns available in the selected dataset.
- Select the plot styles : scatter, point, bar, box, line, 2Dmap, wafer
- Specify the label of the x and y axis, as well as the title of the plot (optional).
- Set the limits of the x and y axis (optional)
- Define the label as well as the z limit range (for the heatmap type only) (optional).
- For wafer plot type: → define the wafer size: 100, 200, 300 (mm).
- Click to the Add plot button 

6.3 Modify existing plot

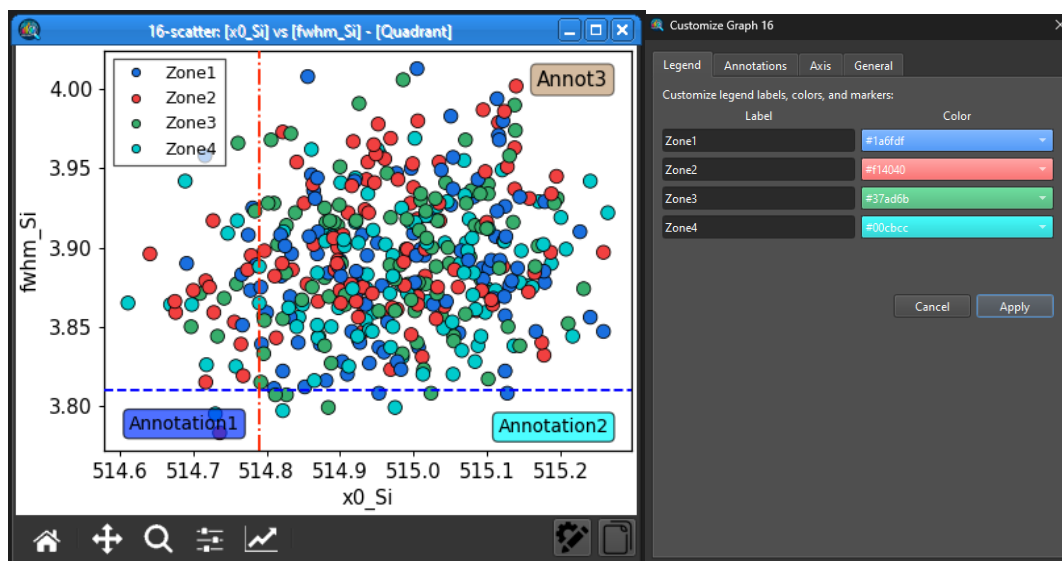



Figure 16: Example of a plot widget. The toolbar includes two buttons on the right: “Customize” and “Copy”, allowing further plot customization or copying the plot to the clipboard.

Once a plot is added by clicking the “Add Plot” button , a plot widget is displayed in the left panel of the GUI, as shown in Figure 16 (left). User can customize/modify further by :

- Click the “Customize” button in the toolbar to open the Customize Dialog (Figure 16, right), from where user can perform difference modification related to **Legend, Annotation, Axis, General**.
- Double-click the legend box or any existing annotation to edit its content.
- Adjust plot settings (plot style, axis labels, axis limits, DPI, axis label rotations, grid) via **ControlPanel** on the right side.



- After making changes, click the “Update” button  to apply the modifications to the plot.

Copying a Plot : Click the “Copy” button  to copy the selected figure to the clipboard. The image can then be pasted into external applications (e.g., documents or presentations).

6.4 Data filtering feature

The **pandas.DataFrame.query()** method allows you to filter rows from a DataFrame based on a boolean expression. It's a powerful and flexible way to subset your DataFrame to include only the rows that meet specific conditions.

In **SPECTROview**, User can work with the entire dataset or a part of the dataset by using **filtering feature** (Figure 17). The selected dataset can be filtered by typing as following syntax:

(column_name) (operator) (value):

- (column_name): is the exact header of the column containing the data to be filtered. When the column header contain 'space', you need to enclose them in single or double quotes (see example below).
- (operator): it could be comparison operators (e.g., ==, <, >, <=, >=, !=) and logical operators (e.g., and, or, not) to build complex and multiples conditions.
- (value): it could be numeric or string values. String value must be enclosed in double quotes (cf. example below)

Examples of using Filter features: Assuming that the datasheet containing several columns, including the columns whose headers are : Confocal, Thickness, a3_LOM, Laser Power and other columns....

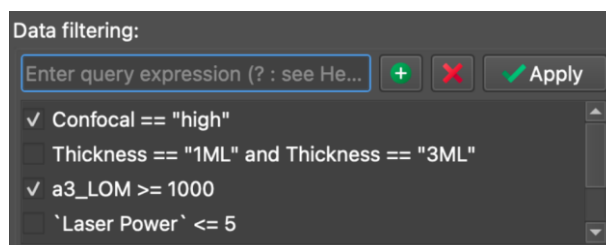


Figure 17: Example of the use of filters for dataframe within SPECTROview

Filter expression	Meanning
Confocal != "high"	→ selected all values within column “Confocal” that is different to “high”
Thickness == "1ML" or Thickness == "3ML"	→ selected all values within column “Thickness” that is equal to 1ML OR 3ML
a3_LOM >= 1000	→ selected all values within column “a3_LOM” that is superior to 1000
`Laser Power` <= 5	→ selected all values within column “Laser Power” that is superior or equal to 5.



6.5 Annotation features & other plot customization

Additional view and customization options are available in the **MoreOptions** tab (Figure 18). Users can also add/customize the annotation (lines and text) for each curve directly from the plot by clicking on the legend box (Figure 19).

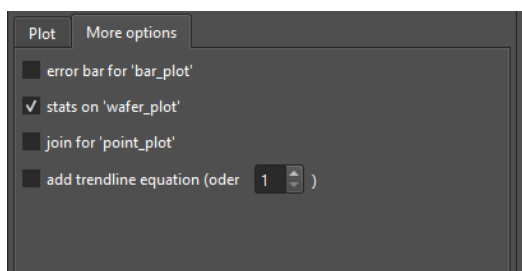


Figure 18: MoreOptions Panel

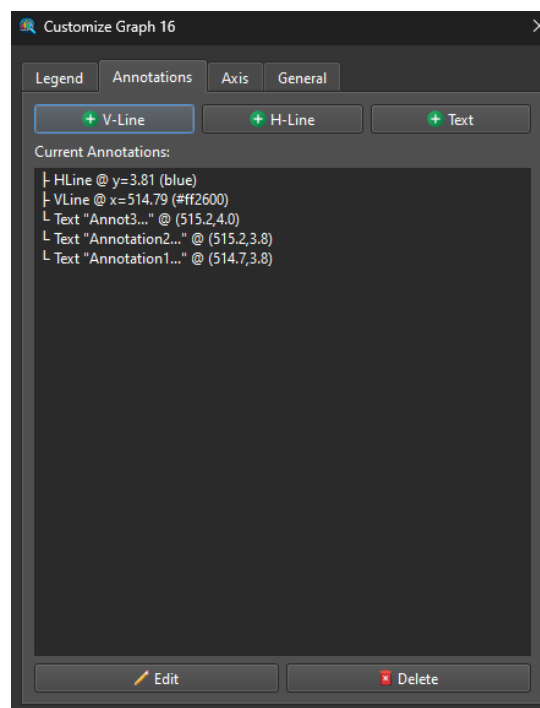


Figure 19: Annotation (line & text) Customization Panel.

7. Save workspace.

To save the current active workspace, click the **Save** button (2) in the toolbar.



Depending on the active workspace, the file will be saved with a different extension :

(Maps workspace → .maps; Spectra workspace → .spectra; Graphs workspace → .graphs).