Empa
Materials Science and Technology

Spectra Analysis App – Quick-Start Guide

Purpose

This application loads a space-delimited text file containing spectral data (exported from WITec), plots the **average** spectrum, then generates **heatmaps** of peak centers and intensities **along with** an Excel results file.

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1. Prepare Your Data in WITec

1. **Locate Your Raman Mapping Data** in the WITec Project.
2. **Right-Click** on the mapping data entry in WITec.
3. Select **Export** → **Table**.
4. In the "Export Filter File Info" dialog, set your **x-axis units** (e.g. rel. 1/cm or nm—whatever you prefer).
5. Choose to **export into one file** and give it a filename (e.g. Export File.txt).
6. Click **OK** to finalize the export.
    - This creates a space/tab-delimited .txt file with:
        - **First column**: x-axis (wavenumbers, wavelength, etc.)
        - **Subsequent columns**: intensities for each spectrum in the map
7. **Note the Points per Line and Lines per Image used in your WITec scan.**
   You can find these parameter values in the **Info** text object (the green "T" icon) directly under the mapping data in the WITec project tree. You'll need these values to generate correct heatmaps in this app.

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2. Launch the App

1. **Double-click** the .exe (on Windows)
2. You will see a small window with two fields:
    1. **Select .txt File**
    2. **Select Output Directory**

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3. Select the Input .txt File

1. Click **Browse** next to "Select .txt File."
2. Navigate to the **.txt** file you exported from WITec.
    - **Data Format Reminder**:
        - First column = x-axis (e.g. wavenumber or wavelength)
        - All subsequent columns = intensities for each spectrum
3. Click **Open**.

The program will then show a temporary message:

"**Plot is being generated, please wait…**"

Once loading is complete, the window resizes to display the **average spectrum** plus additional fields (Region Start/End, Points per Line, etc.).

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4. Select the Output Directory

1. Click **Browse** next to "Select Output Directory."
2. Choose any folder where you want the **heatmaps** (.png) and **Excel** results (.xlsx) to be saved.

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5. Specify Parameters

Four boxes now appear underneath the average spectrum:

1. **Region Start** – The lower bound of your region of interest (e.g. 240).
2. **Region End** – The upper bound of your region of interest (e.g. 254).
3. **Points per Line** – The number of spectra points in each horizontal line of your map.
    - *(This matches the "Points per Line" from WITec's "Image Scan" panel.)*
4. **Lines per Image** – How many horizontal lines make up each 2D map.
    - *(This matches the "Lines per Image" from WITec's "Image Scan" panel.)*

Tip: If you are unsure about these numbers, check your WITec scan setup or the exported file's metadata. They **must** match the actual layout of your Raman map to produce correct heatmaps.

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6. Click "Analyze"

When you press **Analyze**, the software:

1. Reads each column of the input data within the specified **Region Start–End**.
2. Finds the **top 3 highest intensities** in that region (for each column).
3. Calculates:
    - **Peak Center** = the x-axis position of the highest among those top 3 peaks
    - **Average Intensity** of those top 3 peak values
4. Displays a **Progress Bar** to indicate processing progress.

When finished, the program:

- **Saves** two heatmaps (center_heatmap.png and intensity_heatmap.png) in the chosen output folder.
- **Saves** an Excel file (results.xlsx) listing each column's center and intensity.
- Shows a popup message:
  "**Analysis complete! Results saved.**"

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7. Review Your Outputs

- **Average Spectrum**
  Displayed in the main window, with a Matplotlib toolbar (zoom/pan/save).
- **Center Heatmap** (center_heatmap.png)
  Visualizes the peak center position across your scanned 2D area.
- **Intensity Heatmap** (intensity_heatmap.png)
  Visualizes the peak intensity across your scanned area.
- **results.xlsx**
  Spreadsheet with two columns:
  1. **Center (X-axis)**
  2. **Intensity**

Troubleshooting & Tips

- **Export Format**: Ensure the .txt is space/tab-delimited. Double-check the first column is indeed your x-axis.
- **Long Load Times**: Large .txt files can take a while to load. You'll see "Plot is being generated…" while waiting.
- **Points/Lines Mix-up**: If the heatmaps look incorrect or throw a reshape error, verify you used the correct **Points per Line** and **Lines per Image** from WITec.
- **Missing File/Directory**: An error prompt appears if you forget to choose both a .txt file and output directory.
- **Invalid Inputs**: If Region Start/End or Points/Lines are not numeric, an error prompts you to correct them.