Software Installation

1. Launch the ***SpectraSoft Install*** software. A popup window will appear (Figure 1).
2. Check the box for both ***Required Microsoft Libraries*** and ***Andor Camera Drivers*** if installing SpectraSoft for use with just a spectrograph. For RAMS and portable RAMS check all 3 boxes. Then click next and a new window appears.
3. Select the default destination, which is the Program Files, and then click Install.
4. The software installation process will run and wait until the installation process is completed.

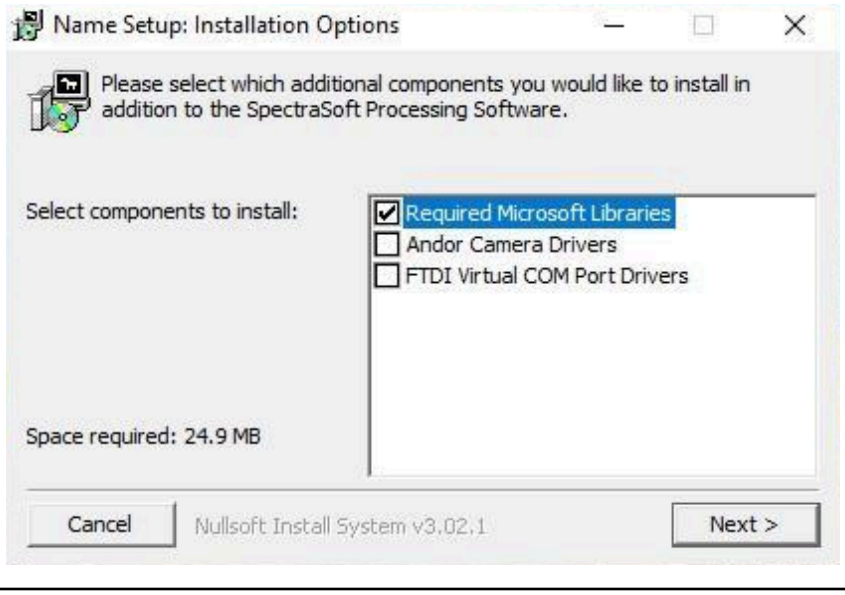

Figure 1. SpectraSoft Installation Window

Starting SpectraSoft

1. Before starting SpectraSoft, make sure that the RAMS instrument is powered up. To start SpectraSoft, click on the Windows Start button and select SpectraSoft in the program list.
2. SpectraSoft will start and a splash screen will appear indicating hardware initialization of the CCD.
3. The main screen window will then appear as shown in Figure 2.
4. Wait for the CCD to reach the set temperature. The CCD temperature is displayed in the bottom right corner. The temperature display color will turn from red to blue when it reaches the set value.

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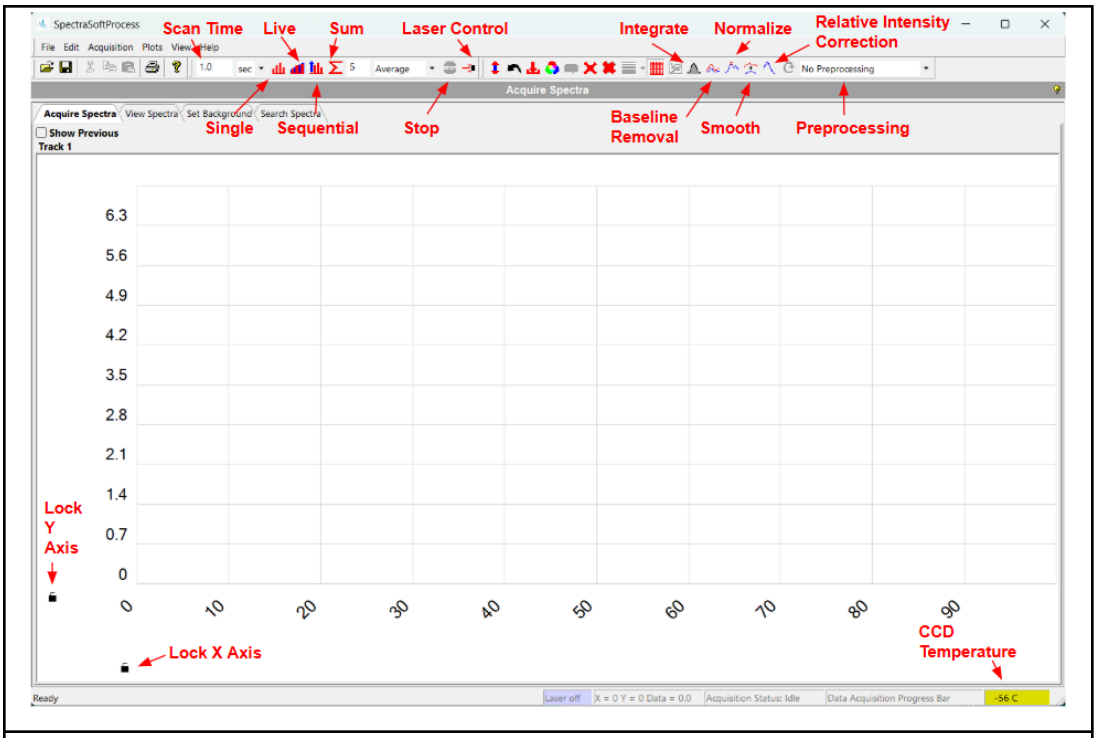

Figure 2. Main window, Acquire Spectra Tab

SpectraSoft Graphical User Interface

1. The SpectraSoft window is divided into tabs: Acquire Spectra, View Spectra, Set Background, Search Spectra and Acquisition Settings.
2. The **Acquire Spectra** tab is where spectral acquisition is performed.
3. The **View Spectra** tab is for displaying saved spectra.
4. The **Set Background** tab is where to acquire background spectra that can be applied (subtracted) instantly to acquired spectra.
5. The **Acquisition Settings** tab allows the user to control the tracks and calibration for the instrument (Access tab with Shift + Fn + Ctrl + F12).

6. A row of icon buttons appears near the top of the window, where different software commands and settings can be selected such as spectral acquisitions, acquisition time setting and stopping running acquisitions. The icon name can be revealed by hovering the mouse pointer on a button.

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Laser Controller

1. In the Main window, the button next to the Stop button (seen in Figure 2) is the Laser Data and Controller button. Selecting this button will bring the window to select and set the laser parameters as shown in Figure 3.
2. Select the laser COM port in the Communication Port drop down menu.
3. In the Controller Type drop down menu, select Luxxmaster or LPCB depending on the laser in the Raman instrument.
4. Hit the Select button to set the instrument laser.
5. The laser is turned on with the Laser On button and turned off with the Laser Off button.
6. The laser power can be adjusted in the Power Level (in mW) field. Hit the Set button to set the selected power level.
7. For instruments with more than one laser, each of the instrument lasers can be selected with the Channel drop down menu. The selected laser can then be controlled according to steps 5 and 6.

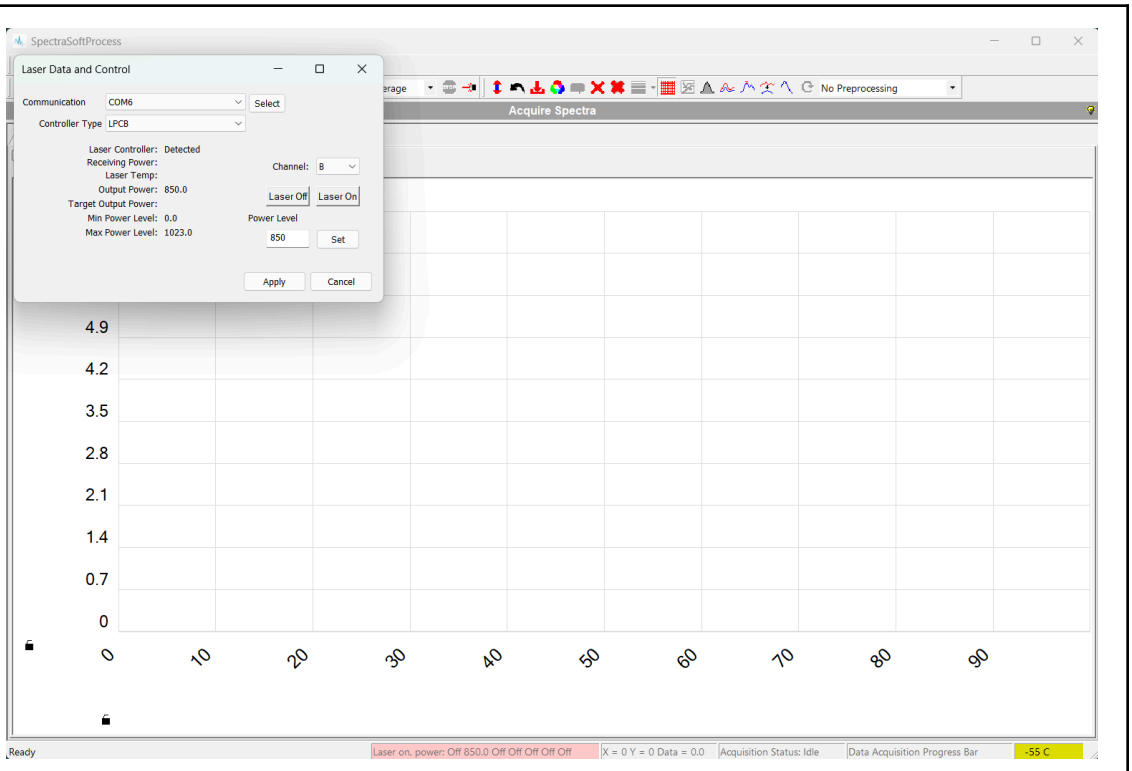

Figure 3. Laser Data and Control window

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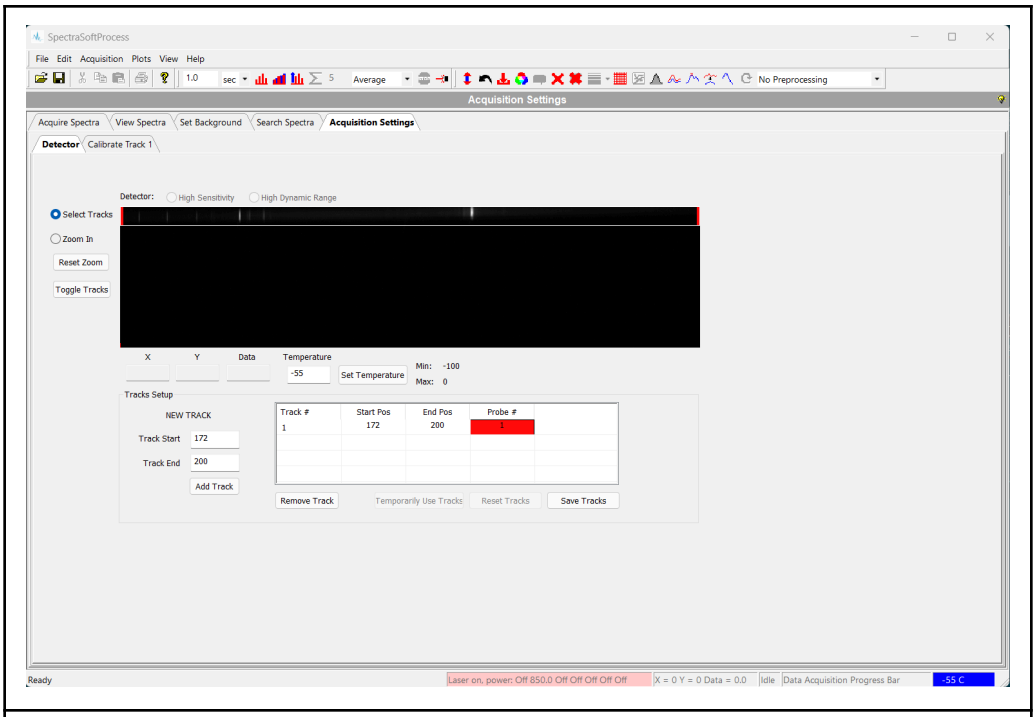

Figure 4. Acquisition Settings Tab

Acquisition Settings

1. ***Detector***
    a. This tab within the acquisition settings tab is used to set the tracks based on the image from the CCD.
    b. Every created track adds a Calibrate Track # tab to the right of the Detector tab in which to calibrate the given track.
2. ***Calibrate Track***
    a. The Calibrate Track tab is where calibration can be set for a given track, seen in Figures 5 and 6.
    a. The x-axis label and regression type can be chosen.
    b. Auto peaks button allows for the program to find discernible peaks in the spectrum and auto populates the pixel column in the data entry text box.
    c. If the Auto Peaks function doesn't get all of the peaks in the reference spectrum, the user can manually add a row and then use the Capture Point button to get the correct peak.
    d. Can choose a reference spectrum to calibrate to which will auto populate in the data entry text box.
    e. The clean up button gets rid of empty rows in the data entry text box.
    f. After setting up the calibration, the user must hit the Save/Apply button to apply the calibration.
    g. This must be done separately for each track.

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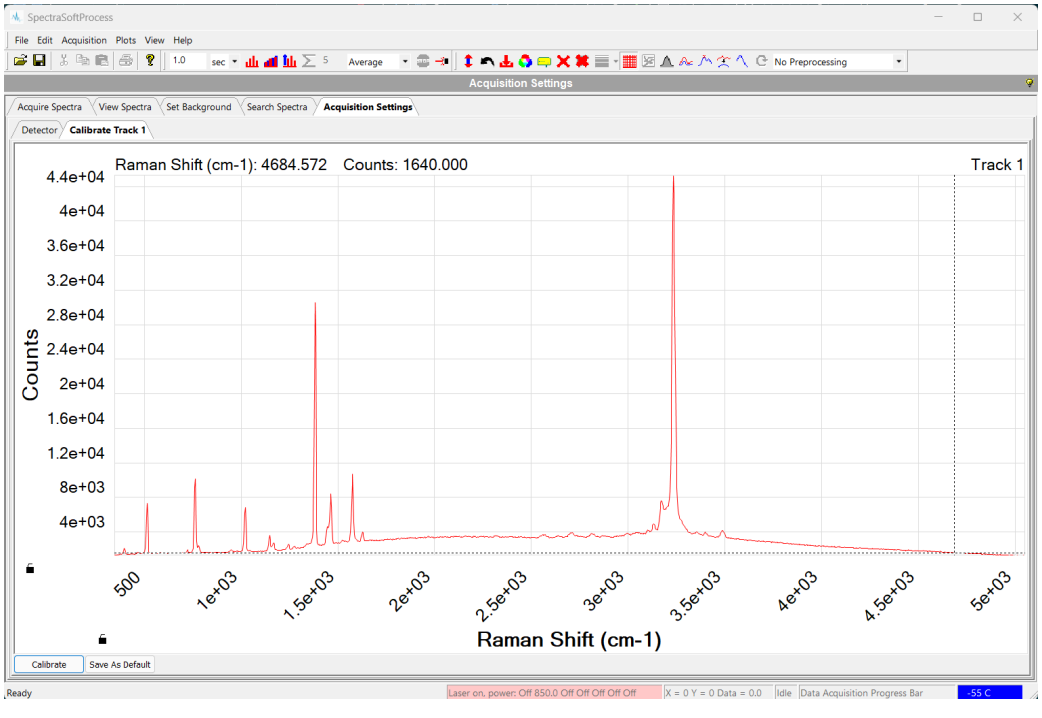

Figure 5. Calibrate Track Tab

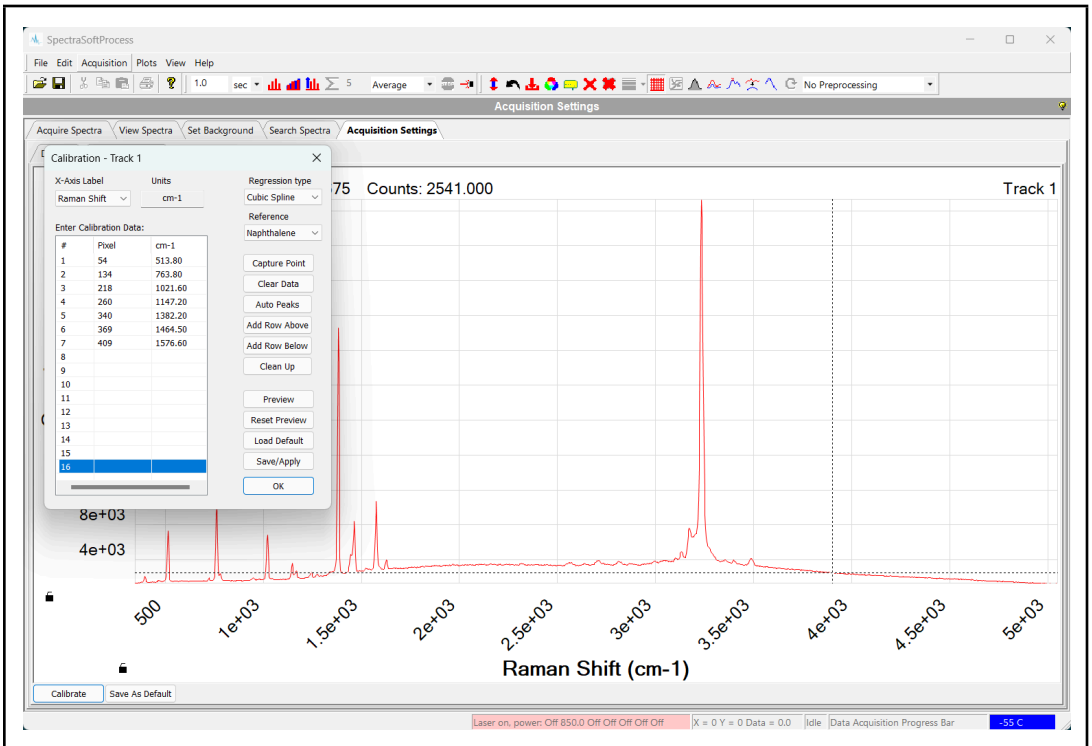

Figure 6. Calibrate Track Window

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Spectral Acquisitions

1. ***Single acquisition***
    a. When this button is selected, the instrument will acquire a spectrum according to the selected CCD integration time (scan time).
    b. The integration time can be changed and set in the scan time field (see Figure 2).
    c. The integration time units (msec, sec and min) can be changed by clicking on the down arrow next to the scan time field and then selecting the desired unit.
    d. When an acquisition (or any acquisition) is started, the Stop button will illuminate red and can be selected to abort the ongoing acquisition.

2. ***Live Acquisition***
    a. When this button is selected, a continuous spectral acquisition is performed and will only stop when the Stop button is selected.
    b. The duration of each acquisition is the time selected in the scan time field.

3. ***Sum Acquisition***
    a. When this button is selected, spectral averaging or median filtering is performed on a number of acquired spectra.
    b. The total number of spectra that are acquired is the number that is entered in the field next to the Sum button.
    c. Spectral averaging or median filtering can be selected by selecting the down arrow next to the number field and selecting the desired averaging algorithm.

4. ***Sequential Acquisition***
    a. This acquisition is used to automate spectral acquisition. The number of spectra that needs to be acquired can be set and a delay time can be inserted between acquisition. Acquired spectra are automatically saved into a folder that is preselected and named sequentially using a selected root file name.
    b. When the sequential button is selected, the popup Sequential window appears as shown in Figure 7.
    c. Selecting the Settings button opens the Sequential Acquisition Setup popup window as shown in Figure 8.
    d. In this window, the folder location to store sequential acquisition data files is entered in the top field.
    e. The base filename that will be used to sequentially name the saved spectra is entered in the Base Filename field.
    f. The delay time between data acquisition is entered in the Delay field and the time units are selected in the down arrow field next to the Delay field.

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g. The number of scans can be either fixed, which can be selected with the radio button and then entering the number of scans or it can be unlimited which is terminated by hitting the Stop button during acquisition.
h. The acquisition type can be selected in the Acquisition per Scan field.
i. Closing the Settings window will bring back the Sequential Acquisition window.
j. Pressing the Start button will commence the sequential acquisition.
k. The Start button then deactivates and the Pause and Stop buttons become active.
l. Pressing the Stop button will abort the sequential acquisition process.
m. The Pause button will pause the sequential acquisition and pressing the Continue button will then continue the sequential acquisition from where it was paused.
n. During the sequential acquisition process, the number of acquired spectra that have been acquired is displayed in the Total Scans field.

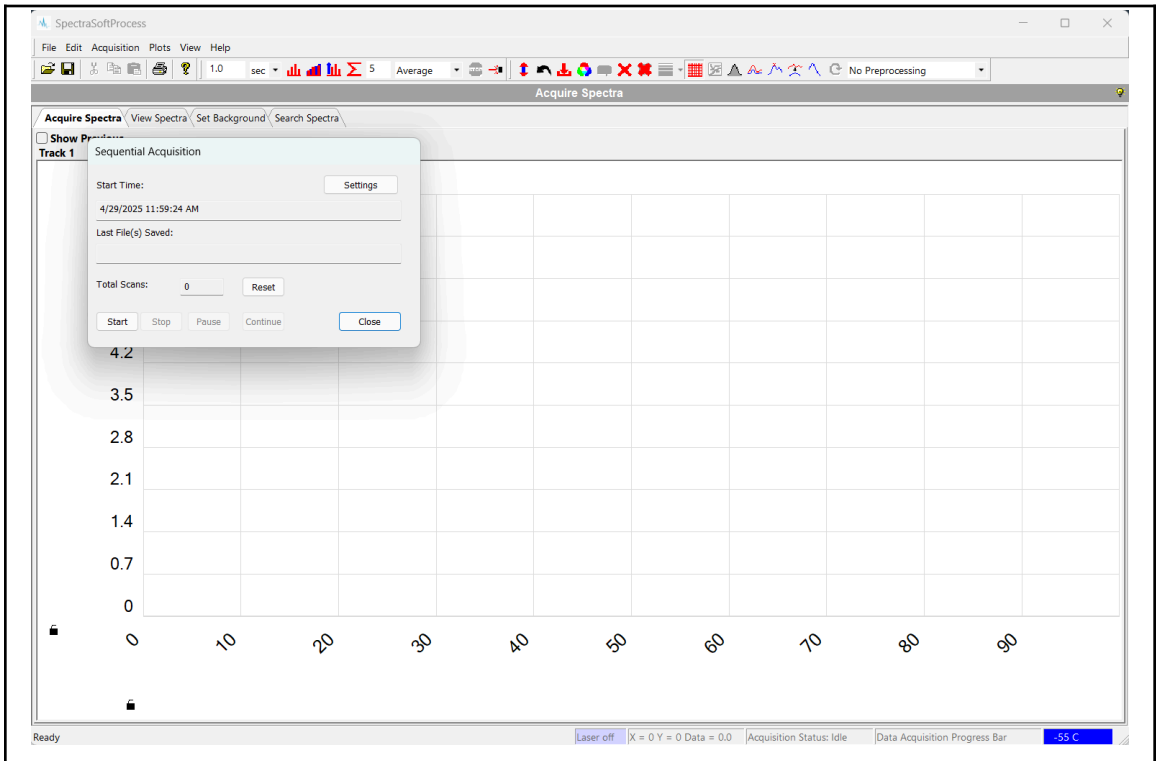

Figure 7. Sequential Acquisition Window

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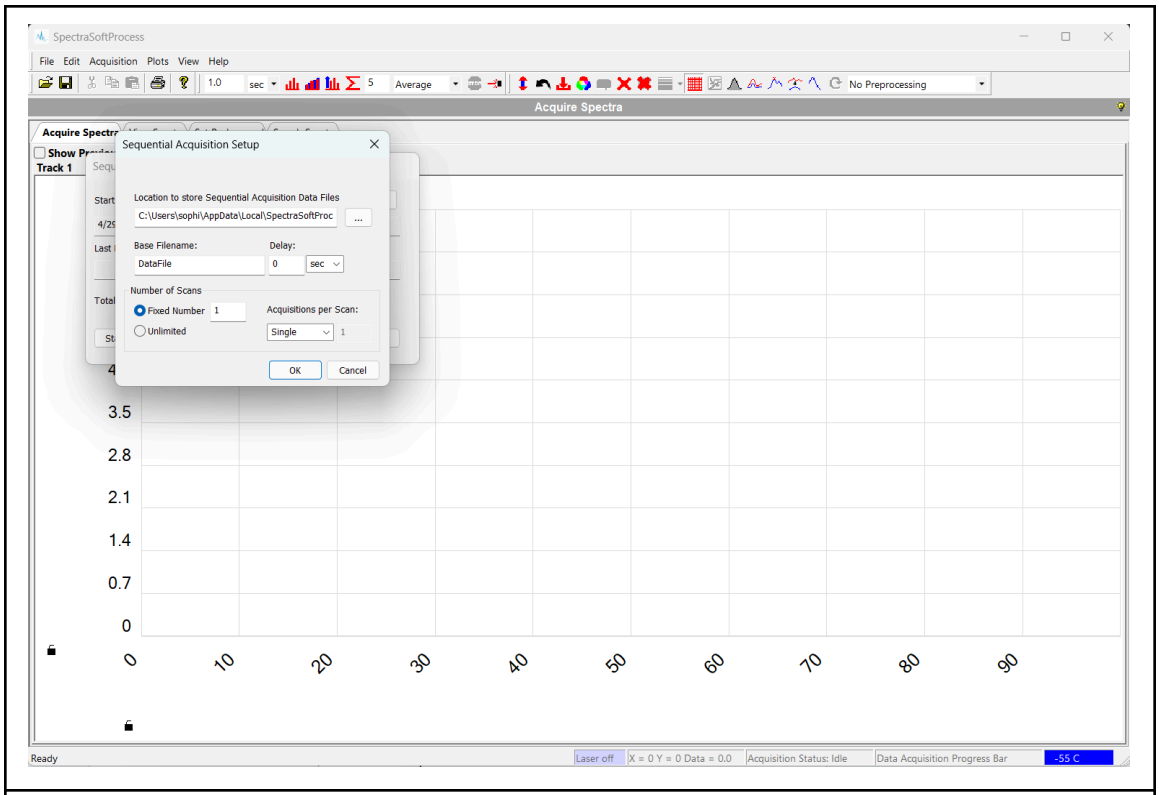

Figure 8. Sequential Acquisition Settings Window

Preprocessing

1. Different preprocessing methods (baseline removal, normalization, smoothing, background subtraction, normalized background subtraction) can be set from the drop down menu on the toolbar, seen in Figure 2.
2. Background correction can be performed on acquired spectra by acquiring and saving the background spectrum in the Set Background tab seen in Figure 9.
3. Background acquisition is scaled to whatever acquisition time is set for the single scan.
4. Once a background spectrum is obtained, it will need to be saved to memory and this is done by selecting the Saved Background button.
5. The Load Default button will recall a previously saved background.
6. The Reset/Clear button will clear the background in memory and will disable background removal in subsequent acquisitions.
7. For baseline removal, the bubble width set in the popup window will be applied to the acquired spectra.
8. For smoothing, the window size and smoothing algorithm set in the popup window will be applied to the acquired spectra.

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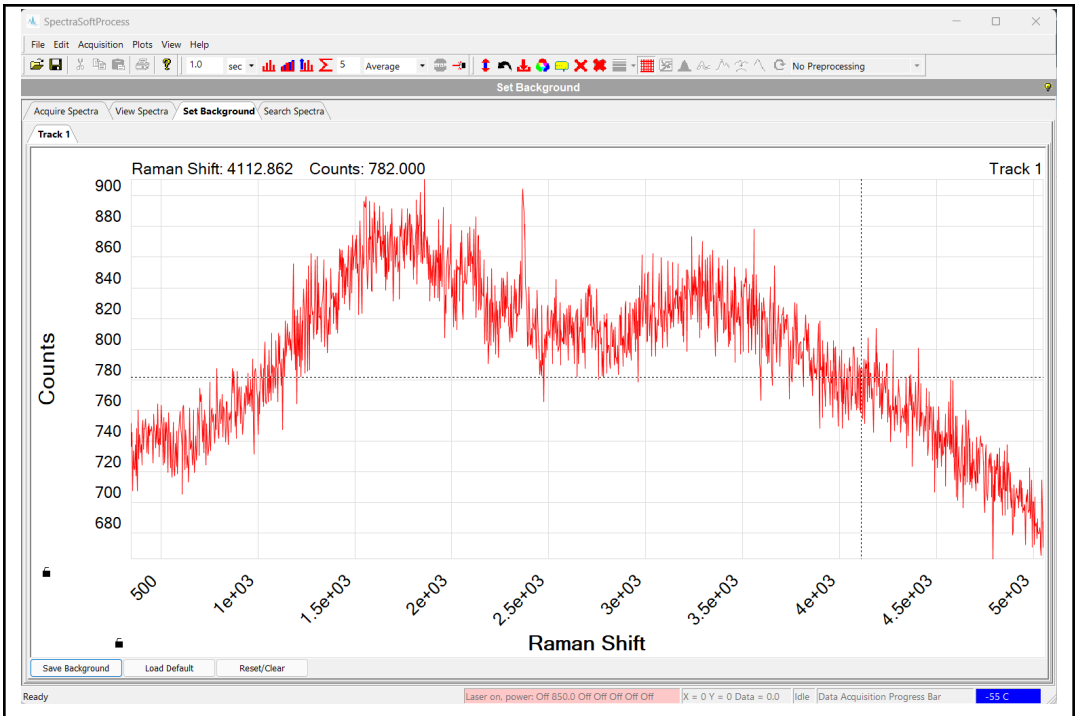

Figure 9. Set background tab window.

Saving Acquired Spectrum

1. For each spectral acquisition, the acquired spectrum is displayed on the screen once the acquisition is finished.
2. The acquired spectrum can be saved by clicking on the Saved file icon or going to the file menu and selecting Save.
3. A finder window will appear and type the file name for the spectrum and then navigate to the folder where the file will be stored.
4. The acquired Raman spectrum can be saved in Galactic SPC and/or text (CSV) file formats.
5. To select the saved spectrum file format, click on the Save Formats in the File menu.
6. The file format can be selected by checking the appropriate boxes.
7. If SPC is checked, the files will only be saved in SPC and vice versa if CSV is checked.
8. If SPC and CSV are both checked, the spectrum will be saved in both CSV and SPC files.

Expanding Spectral Region (Zoom) in Display

1. A region of a spectrum can be expanded by clicking and dragging the computer pointer over the region that needs to be expanded. This will form a square boundary over the region and when the mouse is released, it will expand and display this region.
2. To get back to full display, right click on the mouse and a popup window appears. Select Undo Zoom in the window, or in the toolbar at the top of the program.

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Displaying Saved Spectra

1. Selecting the View Spectra tab will bring the spectral display window where saved spectra can be displayed as shown in Figure 10.
2. Single or multiple spectra can be displayed in this window.
3. To open a file, select the open file icon or go into the file menu and select open.
4. A finder window will appear.
5. Navigate to the folder where the file or files are stored and select the desired file(s).
6. The spectra of the files that were selected will then be displayed in the View Spectra window.
7. On the right-hand side of the display, the displayed spectra file names are listed with the corresponding plot color.
8. Right clicking the mouse button (Figure 11) will show a popup window where various operations on the displayed spectra can be performed.

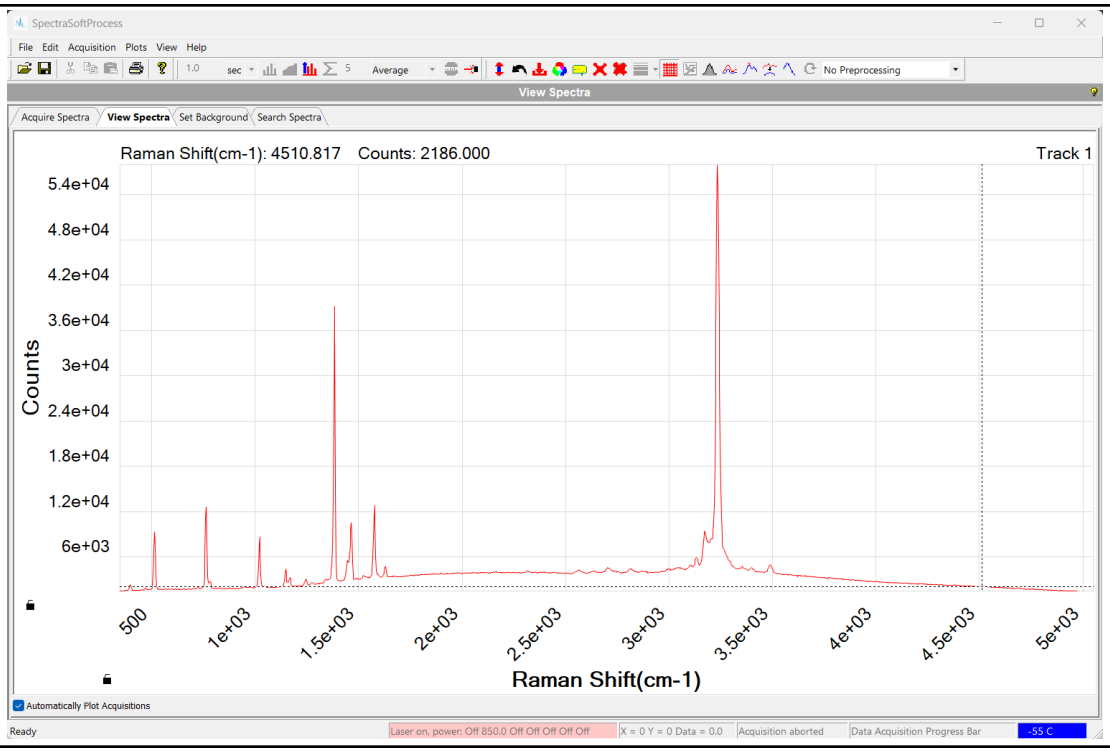

Figure 10. View Spectra tab

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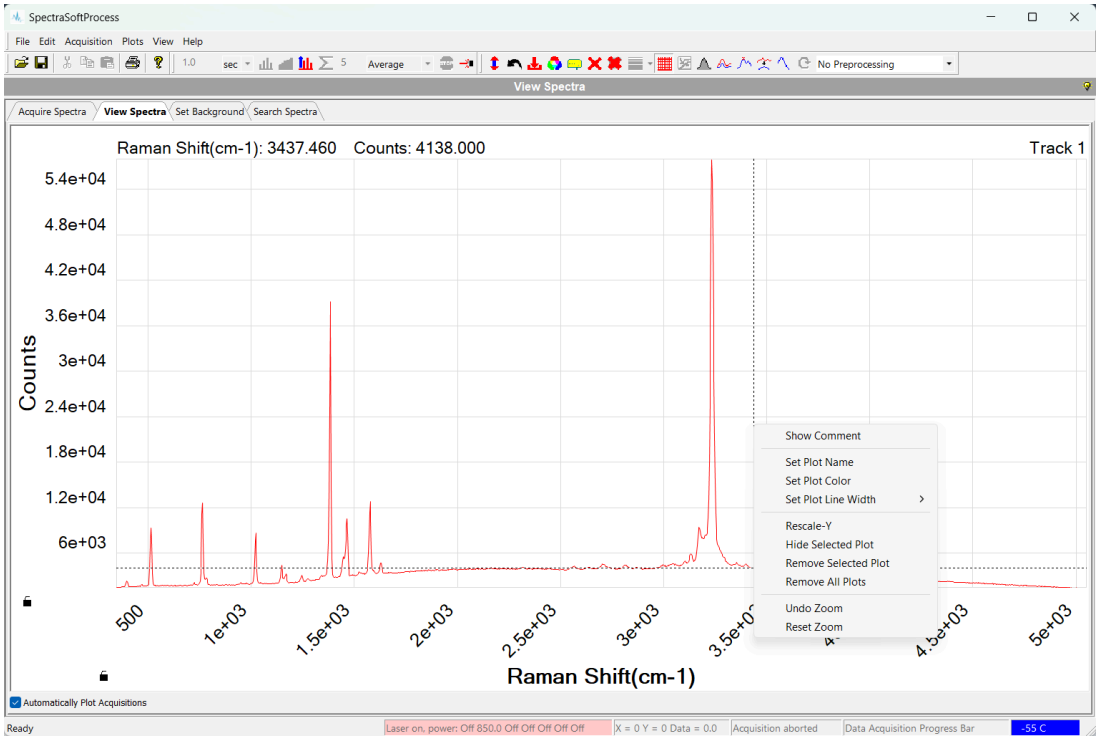

Figure 11. View Spectra tab with right click options shown

Spectra Manipulation

1. ***Integration***
    a. Gaussian integration under the spectrum can be done by clicking the Integrate button in the toolbar, seen in Figure 2.
    b. This brings up the Integrate Under Spectra window, where the user can input a Threshold Factor (how much the peak is above surrounding points), a Minimum Peak Distance and a Window Size in order to find the peaks in the spectrum and integrate under them.

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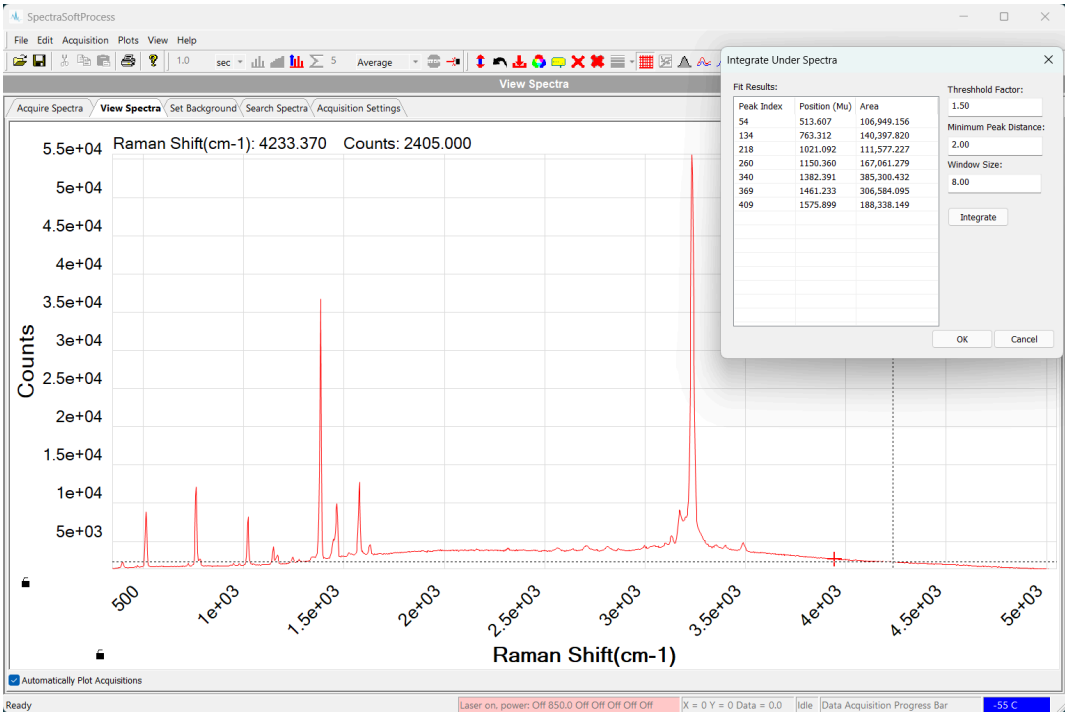

Figure 12. Integrate Under Spectra window

2. ***Baseline Removal***
    a. Baseline Removal is done by clicking the Baseline Removal button in the toolbar, shown in Figure 2 or by setting it as a preprocessing method in the drop down menu, also shown in Figure 2.
    b. Baseline Removal is done using a function called BubbleFill, which uses the parameter of minimum bubble width to determine the baseline of the spectrum and remove it.
    c. Tuning of this parameter can be done in the Baseline Removal popup window (seen in Figure 13) using the minimum bubble width slider.

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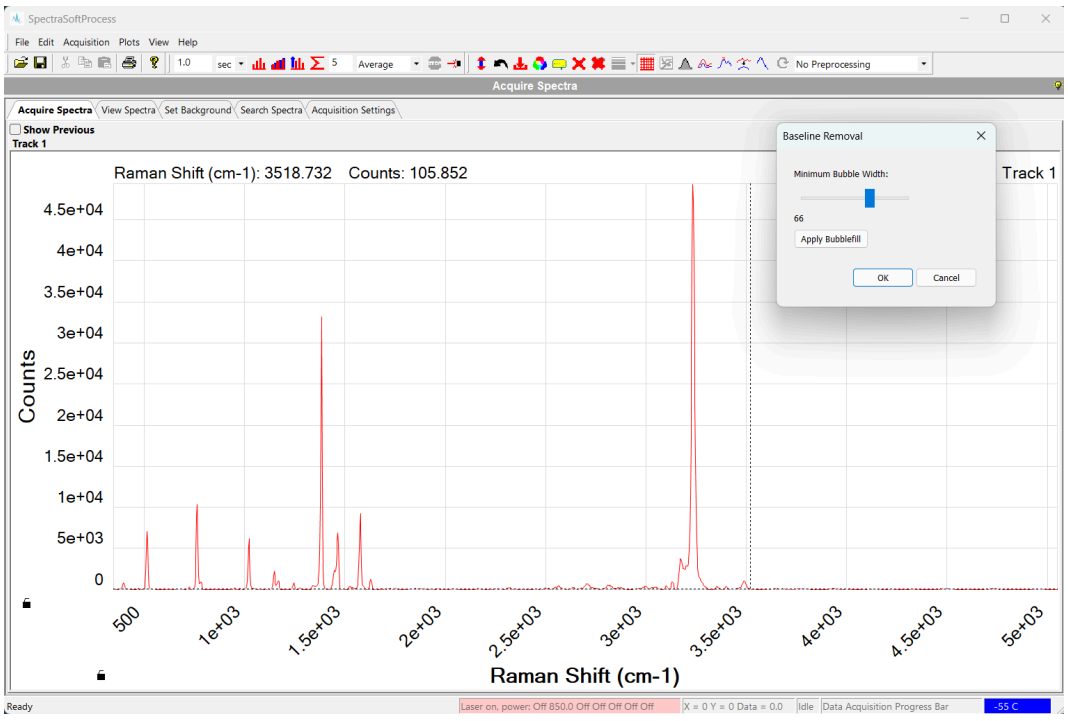

Figure 13. Baseline Removal window

3. ***Normalization***
    a. Normalization to the highest peak can be done using the Normalize button in the toolbar, shown in Figure 2.
4. ***Smoothing***
    a. Different smoothing algorithms can be applied to a given spectra using the Smooth Spectra button shown in Figure 2.
    b. Different algorithms are listed, such as Moving Average, Savitzky-Golay, Gaussian, and Median Filter.
    c. The window size can be changed for all of these algorithms using the slider in the Smoothing window, seen in Figure 14.

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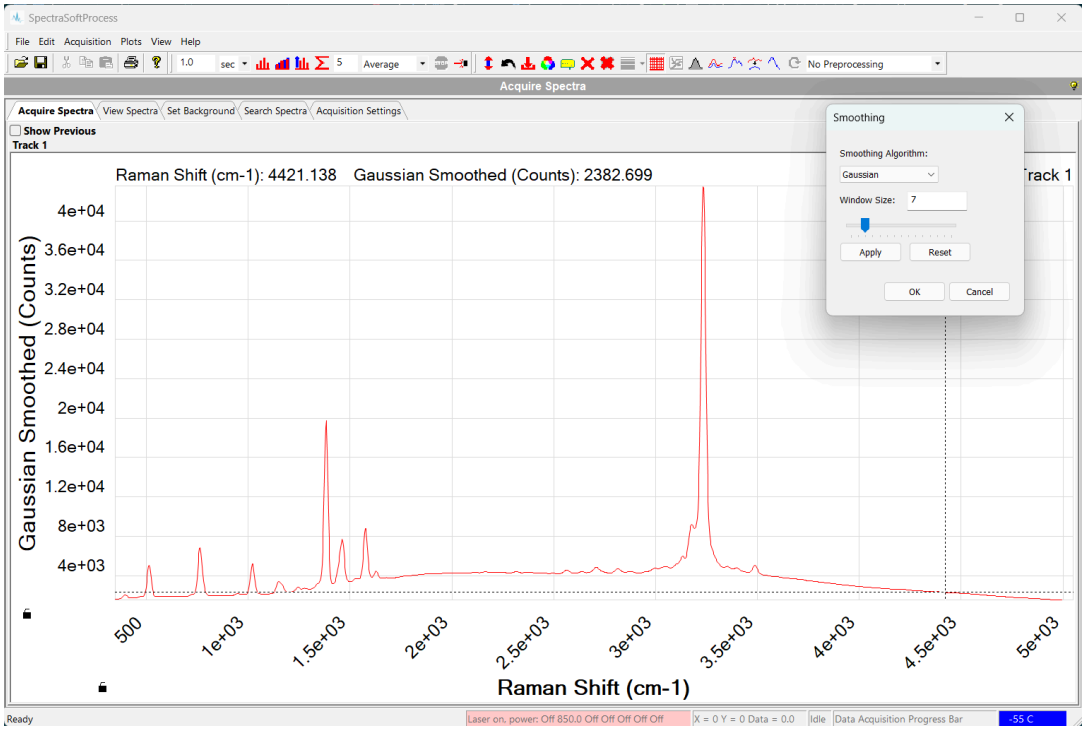

Figure 14. Smoothing window

5. ***Relative Intensity Correction***
    a. Relative Intensity Correction can be done for 532 nm instruments using the button in the toolbar, seen in Figure 2.
    b. In order to apply the correction, the user must select the wavelength they are using, as well as take a reference using the standard reference material and upload that using the Load Reference button (Figure 15).
    c. Then the user can apply the correction to acquired spectra using the Apply Correction button.

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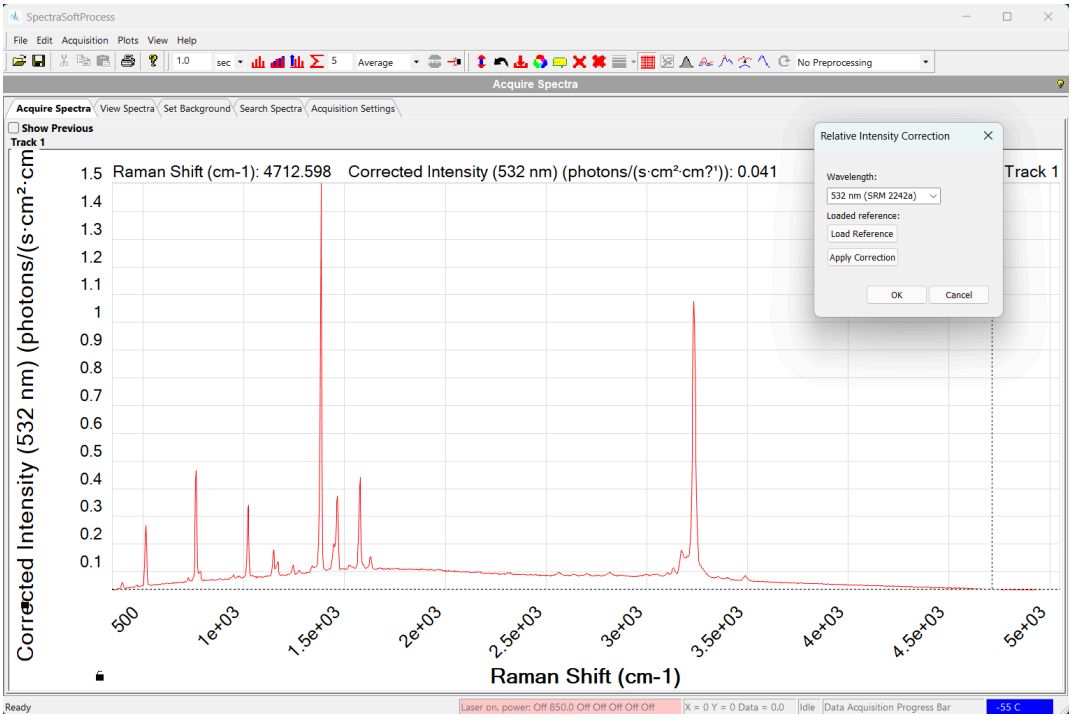

Figure 15. Relative Intensity Correction window

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