

# McPherson/Princeton Raman Control Software

Developed for the Reznik Lab at the University of Colorado at Boulder  
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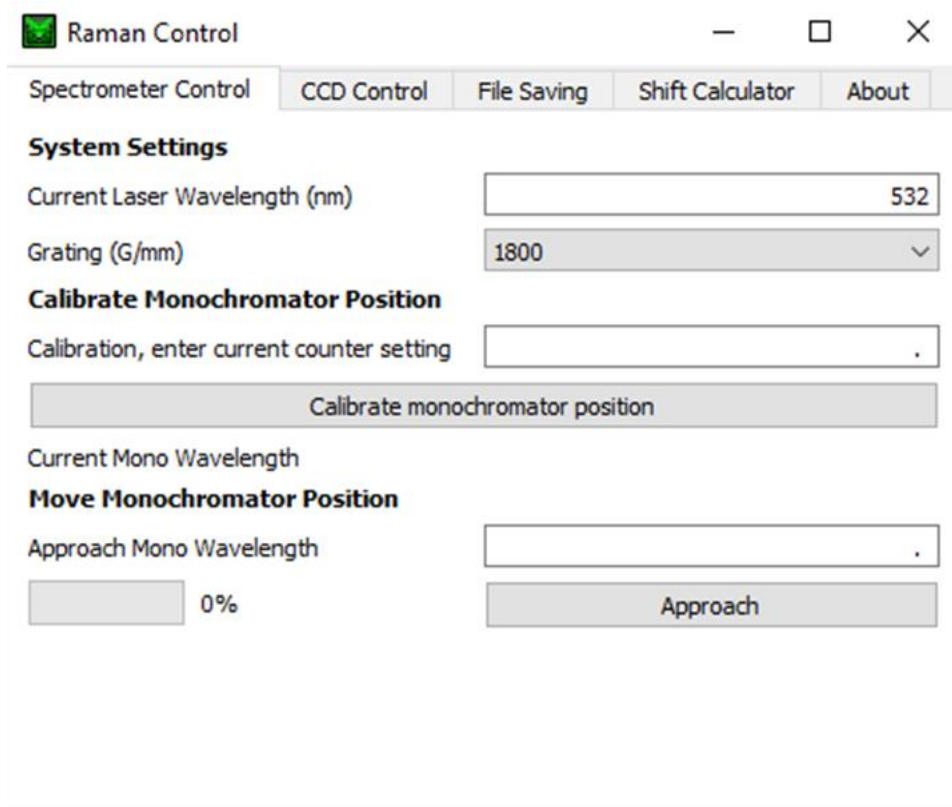


## Getting Started

- For the single monochromator system, ensure that `mono.cfg` is set up as:  
`com_port = COM3`
- For the triple monochromator system operating in single mode:  
`com_port = COM1`
- The Princeton PyLoN CCD must be cooled using liquid nitrogen before data can be collected. To do so, carefully pour LN<sub>2</sub> into the dewar using a funnel according to the PyLoN manual. It will take around 45 minutes for the detector to reach -120 °C.
- The monochromator and CCD must be calibrated when the program is started. If the software is left running this should only need to be performed once, but can also be done at any time.
- Spectra at the current monochromator position can be obtained using the **1D spectrum** and **2D image** buttons. Wider spectra can be obtained by entering start and stop wavenumbers and using the **Raman spectrum** button.
- The most recent spectrum/image can be saved to the desired folder and filename in the **File Saving** tab. All data is automatically saved in the Documents folder.
- The **Shift Calculator** tab provides a convenient calculator for Raman shifts.

## First Tab: Monochromator Control

This tab handles control of the monochromator, which is used to select for different wavelengths/wavenumbers/energies.



The screenshot shows the 'Raman Control' software window. The 'Monochromator Control' tab is active, showing fields for 'Current Laser Wavelength (nm)' (532), 'Grating (G/mm)' (1800), and a 'Calibrate Monochromator Position' section with a 'Calibration, enter current counter setting' field and a 'Calibrate monochromator position' button. Below this is a 'Move Monochromator Position' section with an 'Approach Mono Wavelength' field, a progress bar at 0%, and an 'Approach' button.

### System Settings

System settings include the current grating and laser in the system. These are pre-filled but can be changed as desired.

### Monochromator Calibration

Initial calibration of the software must be performed for correct function. To do this, the current counter number (found next to the PyLoN CCD on the side of the monochromator) must be input. Clicking **Calibrate** will update the current monochromator position in the software to match. Counter and monochromator wavelength are related by a rough factor of 2/3. Note: the monochromator position is the wavelength at the center of the CCD.

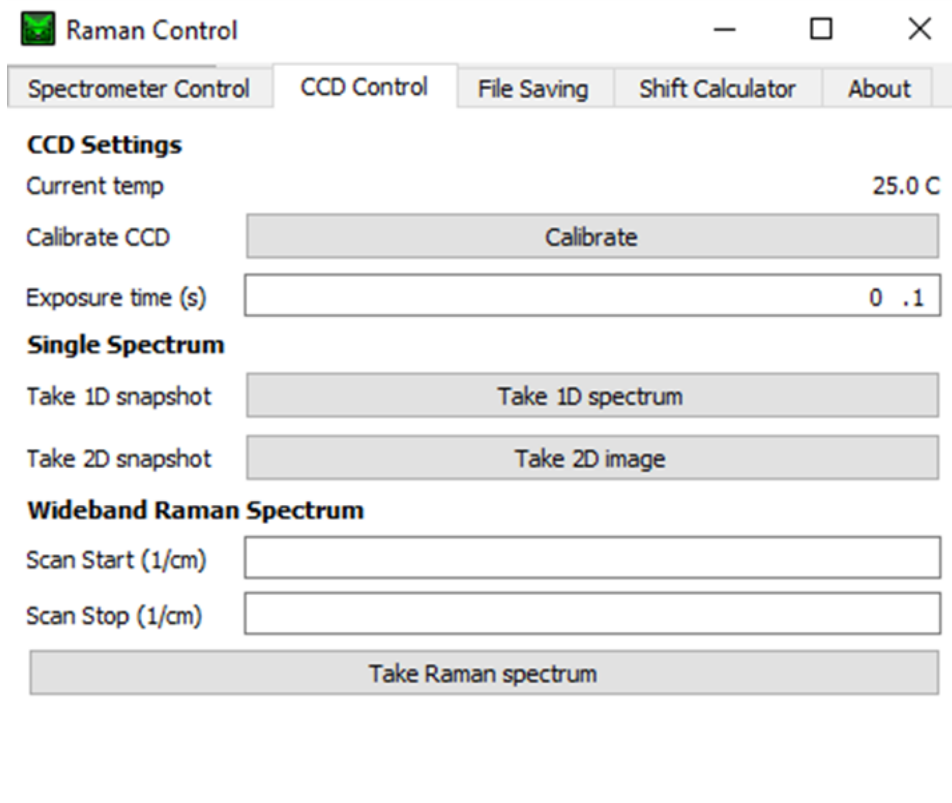
### Monochromator Movement

After calibration has been performed, monochromator can be moved to the desired position by entering a wavelength and using the **Approach** button.

## Second Tab: CCD Control

This tab handles control of the CCD imager which is used to collect data.

The PyLoN CCD is cooled by liquid nitrogen. Carefully pour LN<sub>2</sub> into the dewar according to the PyLoN manual, being aware that some geysering may occur as the dewar walls cool down. Also, LN<sub>2</sub> can easily spill out of the funnel if it is filled too quickly, so slow pours or small amounts at a time are recommended. Cooling of the CCD from room temperature takes about 45 minutes.



The screenshot shows the 'Raman Control' software window with the 'CCD Control' tab selected. The window has a title bar with a green icon, a minus sign, a maximize button, and a close button. Below the title bar are five tabs: 'Spectrometer Control', 'CCD Control' (selected), 'File Saving', 'Shift Calculator', and 'About'. The main content area is divided into three sections: 'CCD Settings', 'Single Spectrum', and 'Wideband Raman Spectrum'. In the 'CCD Settings' section, 'Current temp' is displayed as '25.0 C'. Below it is a 'Calibrate CCD' label and a 'Calibrate' button. Then, 'Exposure time (s)' is shown with a text input field containing '0 .1'. The 'Single Spectrum' section has 'Take 1D snapshot' and 'Take 2D snapshot' labels, each followed by a button labeled 'Take 1D spectrum' and 'Take 2D image' respectively. The 'Wideband Raman Spectrum' section has 'Scan Start (1/cm)' and 'Scan Stop (1/cm)' labels, each followed by a text input field. At the bottom of this section is a 'Take Raman spectrum' button.

### CCD Settings

CCD temperature can be monitored and should be between -100 and -120 °C for best performance.

Calibration of the CCD is necessary for the collection of high precision data. The **Calibrate** button will perform this automatically by shifting the monochromator to center on the laser wavelength. As such, the laser must be on and aligned, and ambient light mitigated via the enclosure and/or dimming the room lights. For correct function, monochromator position must first be calibrated as previously discussed. Calibration spectra are saved in the Documents folder.

CCD exposure time can be changed. For bright samples, values 0.01—1s are sufficient; for dim samples, this can be set up to 9999 seconds (approx. 2.75 hours). If longer scans than this are required, this functionality can be updated in the code.

### **Single Spectrum**

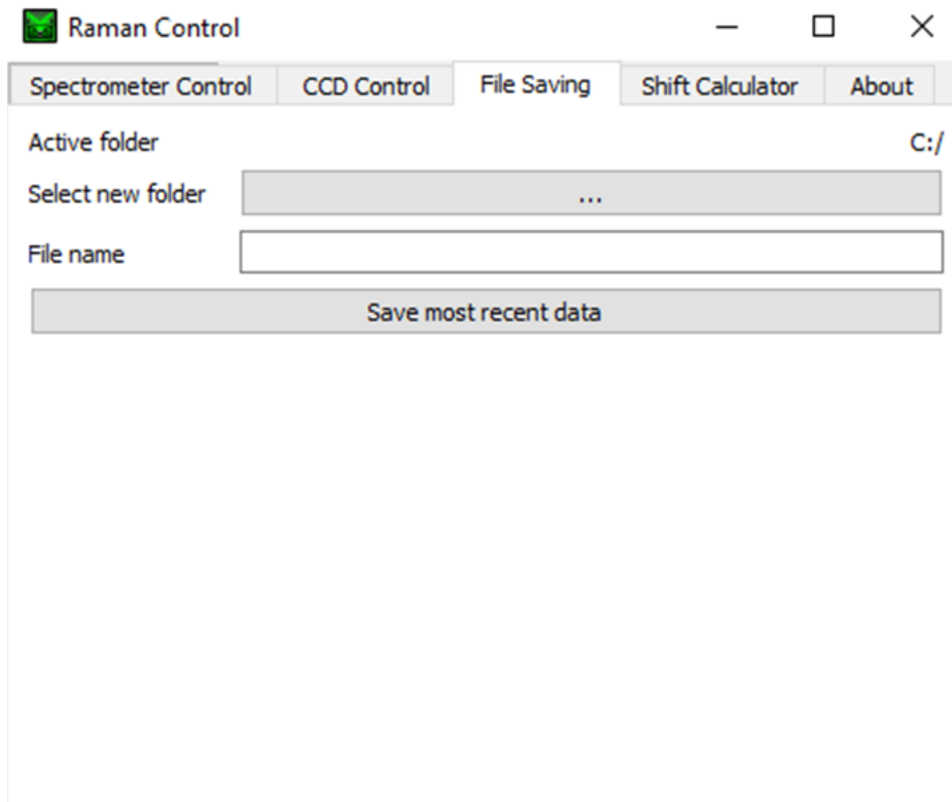
The software offers two snapshot modes, which acquire a 1D spectrum or a 2D image from the detector. These are intended to be used for the collection of high-quality data. The width of these images depends on the grating being used.

### **Wideband Raman Spectrum**

There is also an imaging mode for wider spectra, primarily intended for general mapping of the Raman spectrum for a given sample. This works by taking spectra at different monochromator positions and then stitching them together. There may be some gaps/overlaps in the resulting spectrum, and peak amplitudes may be slightly misrepresented.

### Third Tab: File Saving

This tab handles file saving.

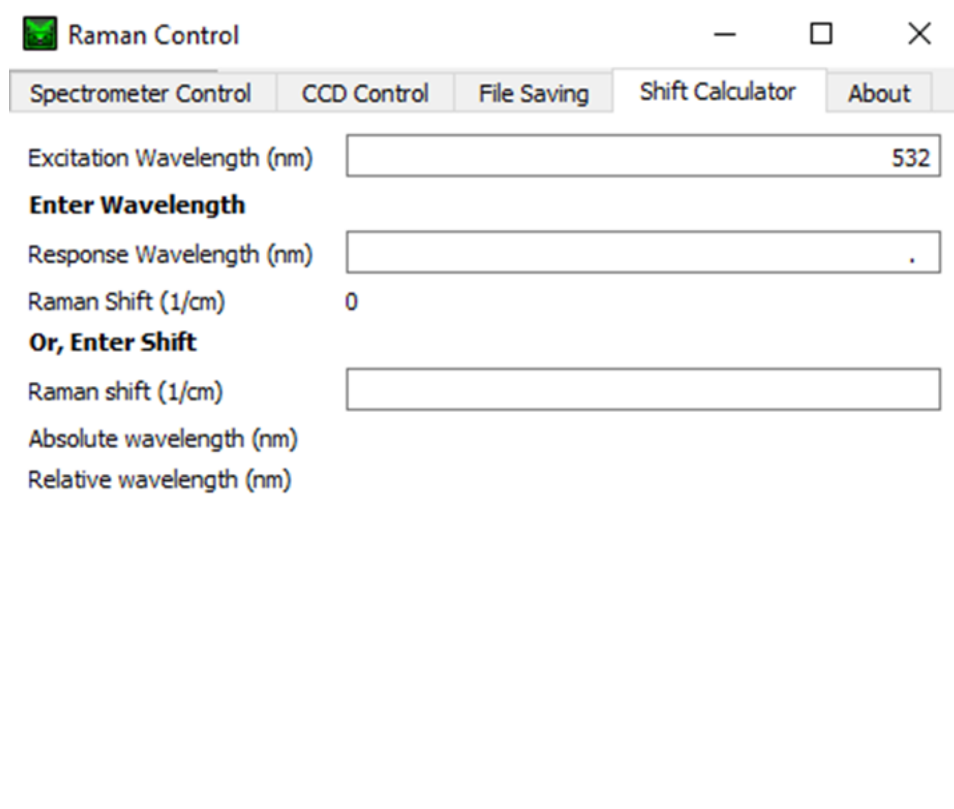


First, an active folder must be selected. This is the location that any selected data will save to. A valid file name (no extension) must be entered. Ensure that the intended file does not already exist, or errors including crashing may occur.

Note: All data is saved to the Documents folder under a timestamp so that it may be recovered later if it is not saved manually.

#### Fourth Tab: Shift Calculator

This tab provides a convenient means of calculating Raman shift, going from wavenumber to wavelength or vice versa.



The screenshot shows a software window titled "Raman Control" with standard Windows window controls (minimize, maximize, close). The window contains five tabs: "Spectrometer Control", "CCD Control", "File Saving", "Shift Calculator" (which is the active tab), and "About".

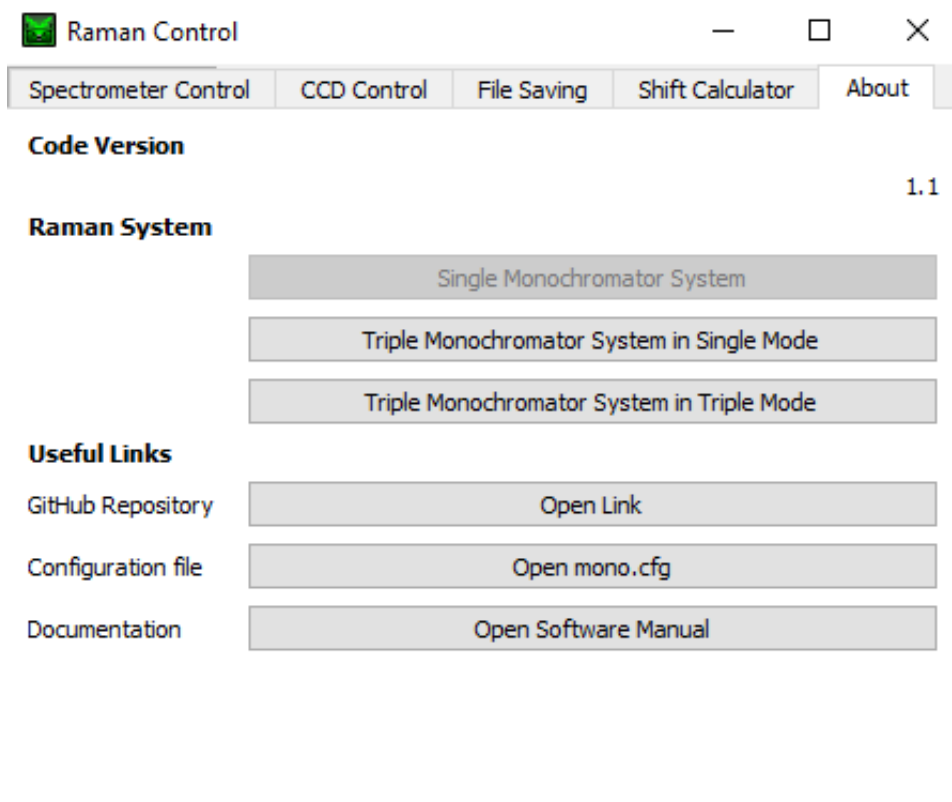
Under the "Shift Calculator" tab, the following fields and labels are visible:

- "Excitation Wavelength (nm)" with a text box containing the value "532".
- A bold label "Enter Wavelength" below the first field.
- "Response Wavelength (nm)" with a text box containing a decimal point ".".
- "Raman Shift (1/cm)" with a text box containing the value "0".
- A bold label "Or, Enter Shift" below the second field.
- "Raman shift (1/cm)" with an empty text box.
- "Absolute wavelength (nm)" with an empty text box.
- "Relative wavelength (nm)" with an empty text box.

## Fifth Tab: About

This tab provides useful information and links.

such as version number and a link to the GitHub repository where the underlying code is housed.



## Raman System

This section allows selection of the system in use. Currently this does not do anything other than update the configuration file, but in the future, this may enable seamless use of this software with a variety of different setups.

## Useful Links

This section contains links to the GitHub repository, where underlying code and files are hosted; the configuration file, for manual updating or verification of the values housed there; and this software manual.

**Planned Updates:**

- Live acquisition mode
- Cryo-/temperature control