

# **Acquiring Quantum Cascade Laser Infrared Spectra with BlockEngineering LaserTune Spectrometer**

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SOP-01	Jorge Plata Orlando Ruiz Marcos Barreto Giancarlo Vargas Edwin Caballero		University of Puerto Rico at Mayagüez
Effectivity: March/13/2022	Acquiring Quantum Cascade Laser Infrared Spectra with BlockEngineering LaserTune Spectrometer		Revised by: Francheska Colon
Revised:			Approved by:

This SOP uses the following:

- Instrument: BlockEngineering LaserTune QCL IR spectrometer
- Laser: QCL
- Filter:
- Program:

## QCL SPECTROMETER SETUP

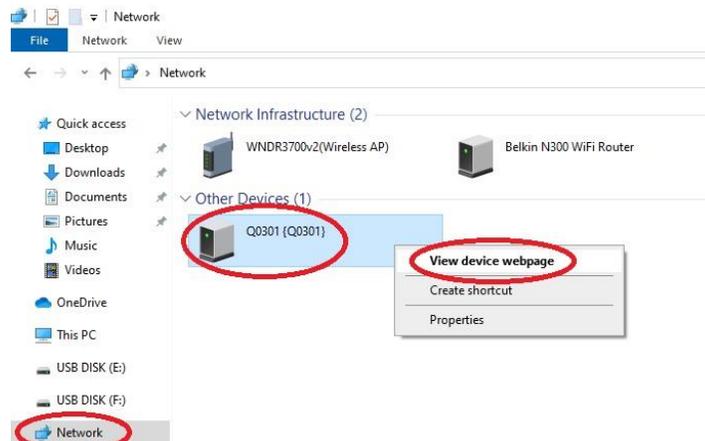
1. Turn on LaserTune spectrometer by pressing its power (I/O) button.

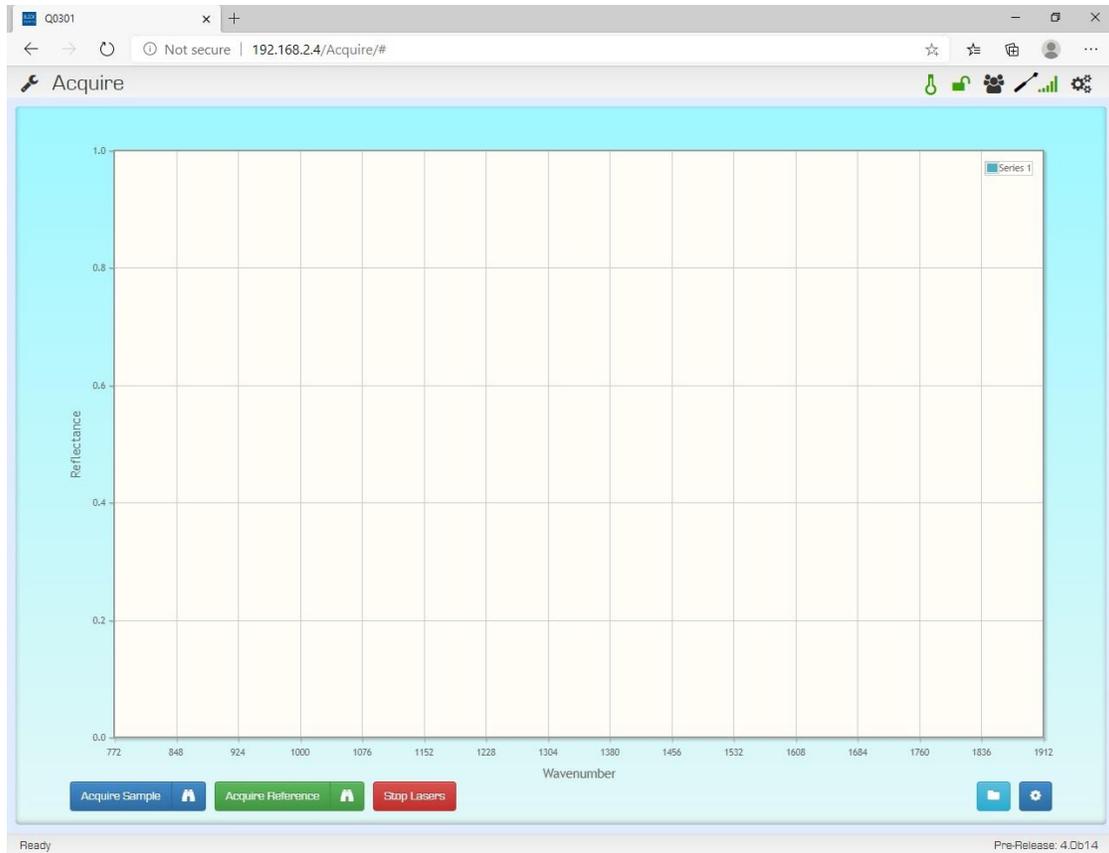


2. Turn on computer connected to the LaserTune.

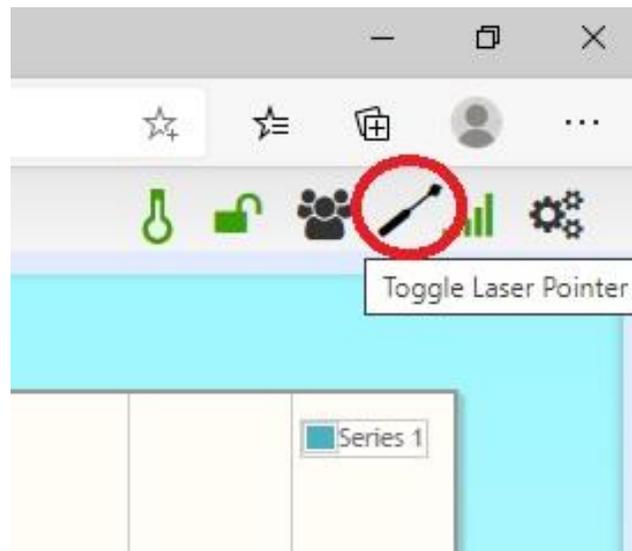


3. Open LaserTune application by going to File Explorer -> Network -> Other Devices -> Q0301 {Q0301}.

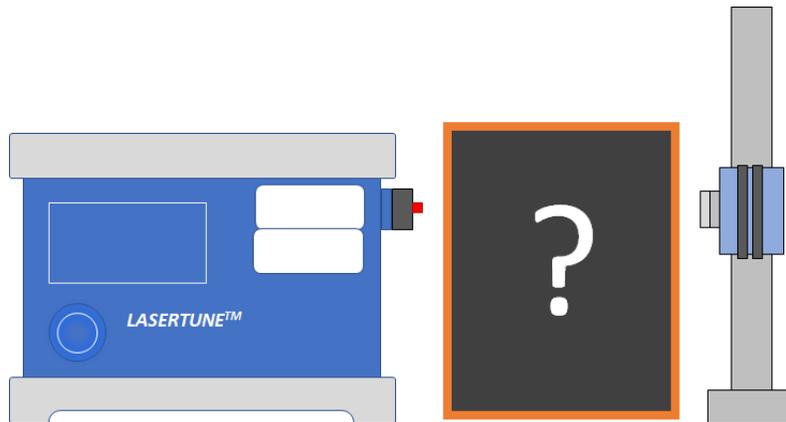




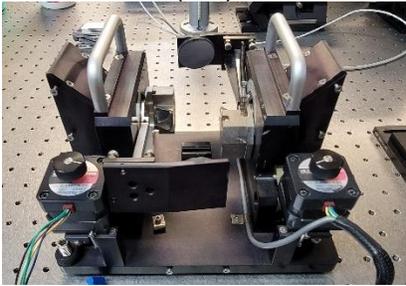
4. Turn on visible laser for aligning by clicking the "Toggle laser" icon.



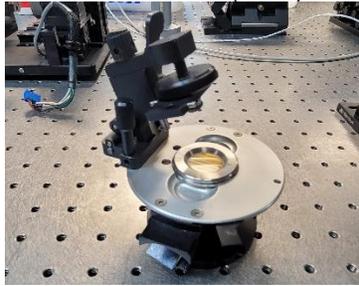
5. Choose and place optical setup for acquisition.



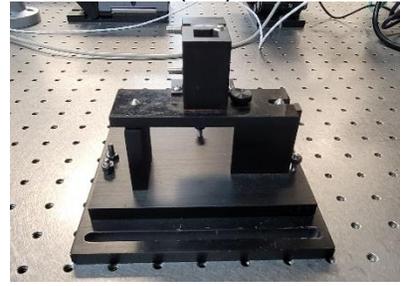
Grazing angle  
(GA)



Attenuated Total  
Reflectance (ATR)



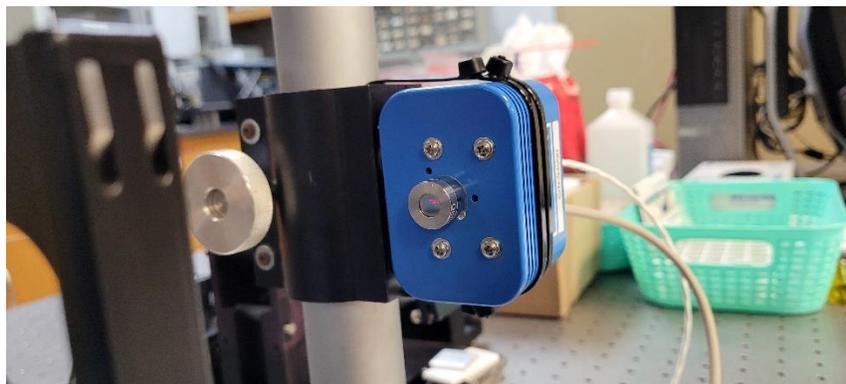
Transmission  
(TR)



Currently grazing angle (GA), Attenuated , and transmission setup are available.

Optical setup used = \_\_\_\_\_

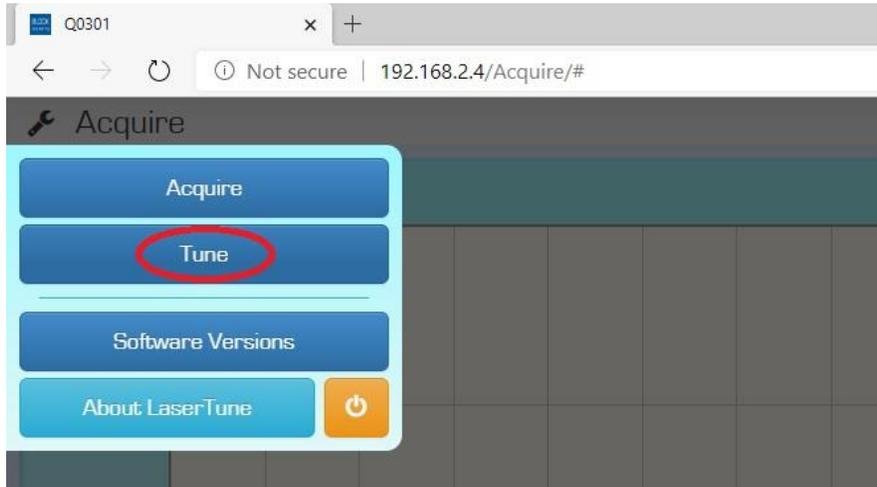
6. **Adjust** arrangement optics to ensure that the laser hits the center of the detector.



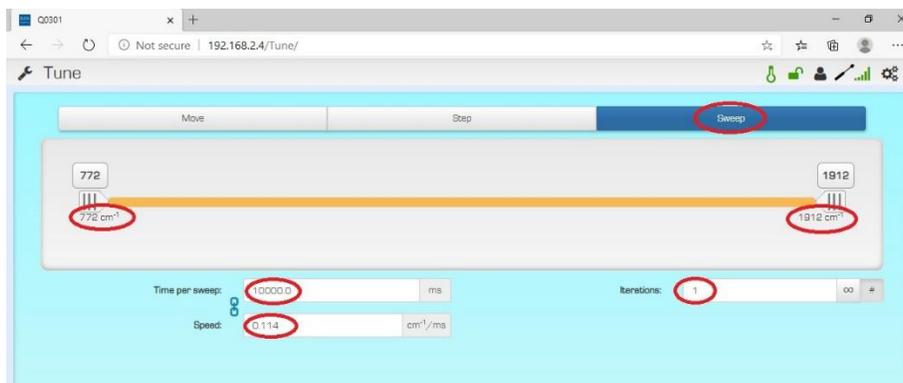


## SETTING PARAMETERS

1. Select the tool icon at the upper left side of the software and select “Tune”.

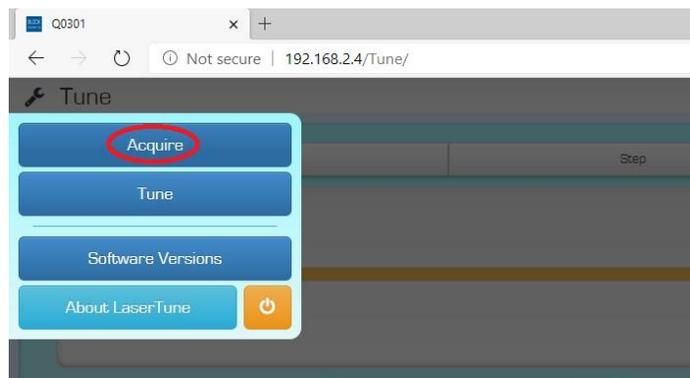


2. Adjust wavenumber range using “Sweep” option.

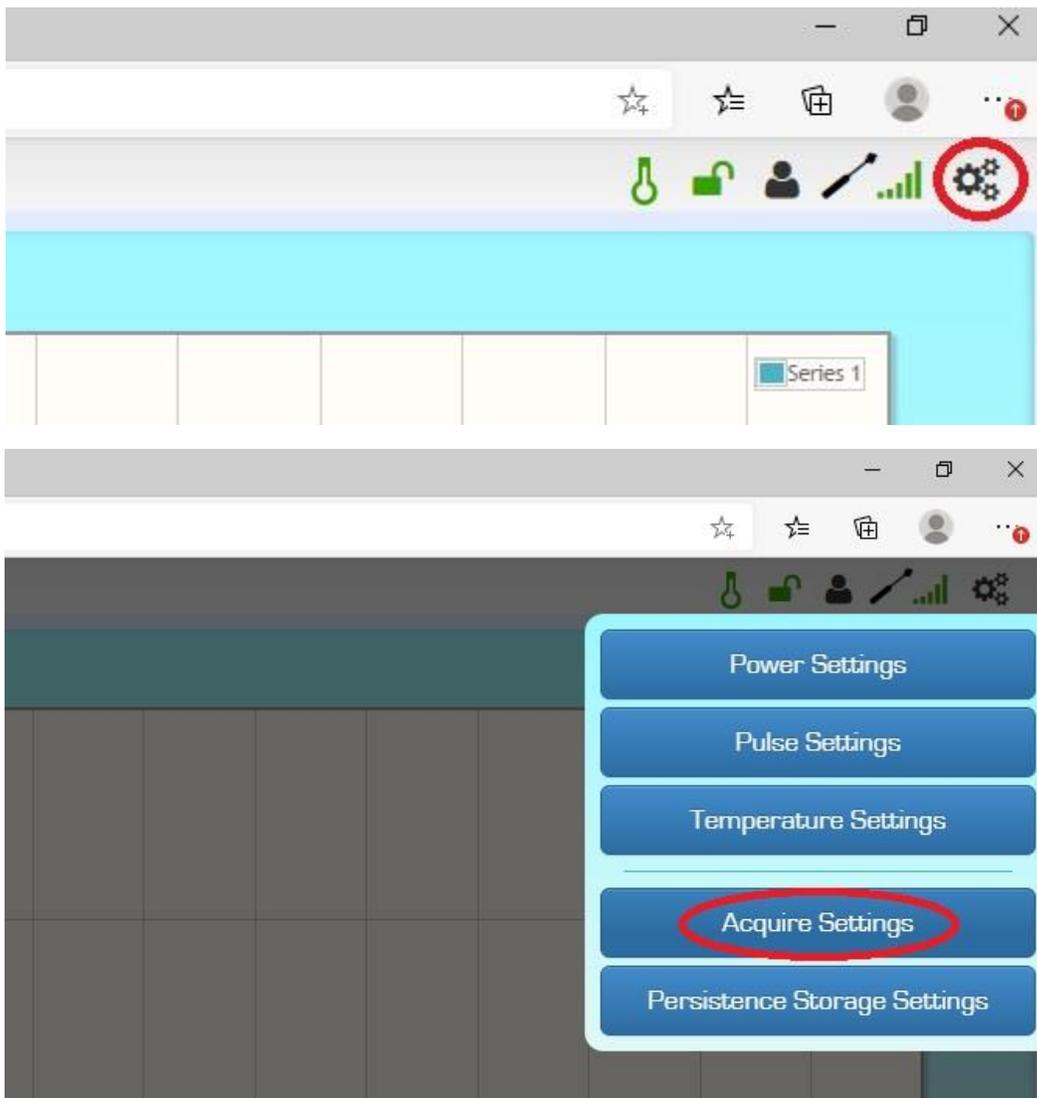


Wavenumber range = \_\_\_\_\_

3. Select the tool icon at the upper left side of the software and select “Acquire”.



4. **Adjust** acquisition parameters by choosing the gear icon for “Settings” in the upper right side and then “Acquire Settings”.

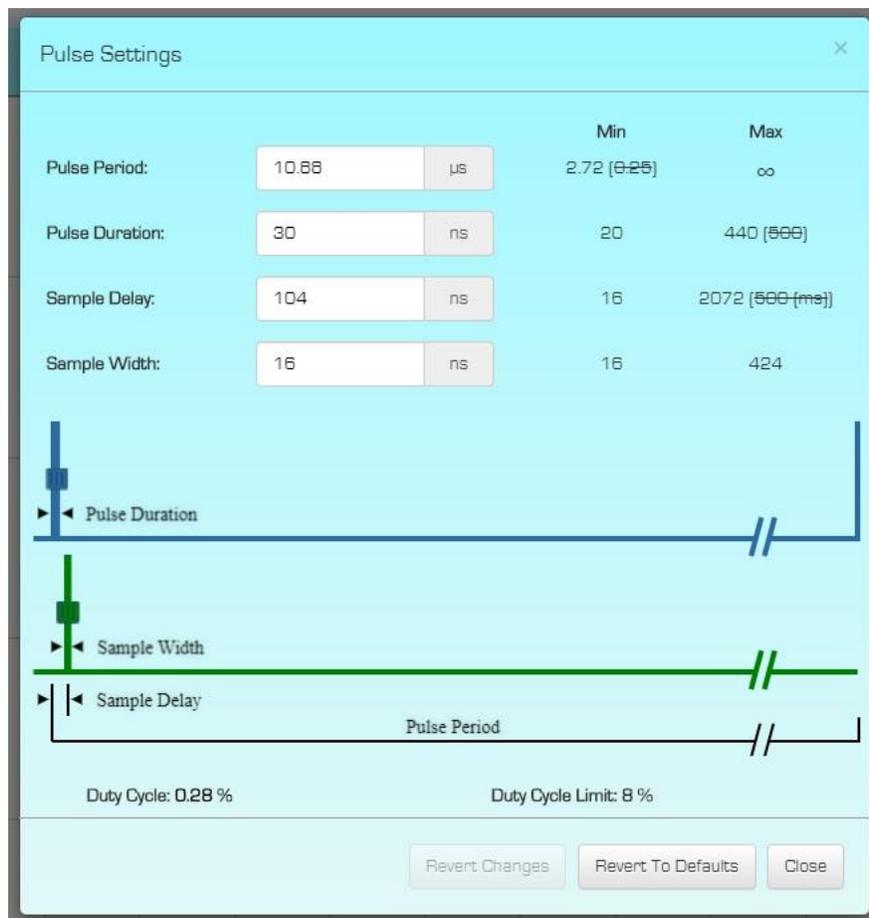
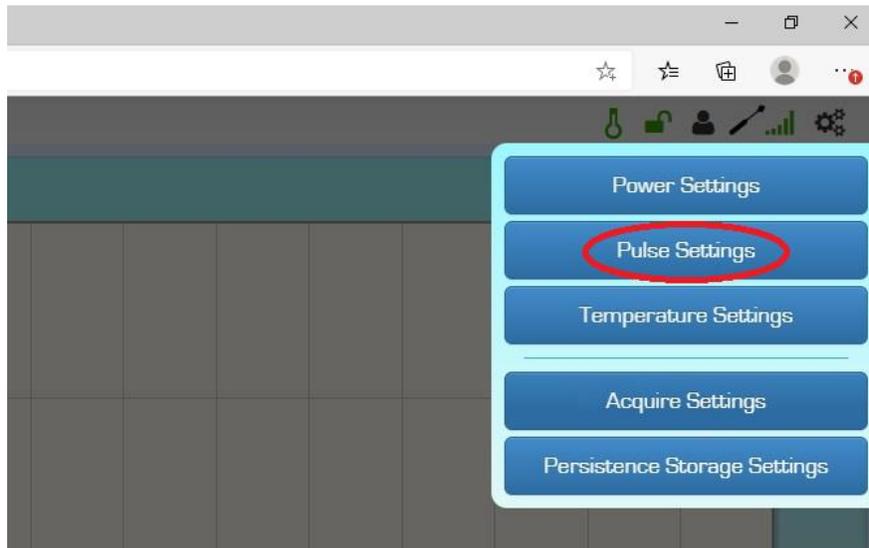


Large resolution for solids, low resolution for gases.

Amount of Co-Adds increases precision, however, it also increases acquisition time.

<b>Scan Type</b>	
<b>Resolution (<math>\delta\lambda</math>) [<math>\text{cm}^{-1}</math>]</b>	
<b>Scan Time (ST) [ms]</b>	
<b>Co-Adds (CA) [N/A]</b>	

5. **Adjust** laser parameters by choosing the gear icon for “Settings” in the upper right side and then “Pulse Settings”.



Long pulse duration can affect biological samples.

Study what type of pulse is needed for specific sample. Optimization experiment is recommended.

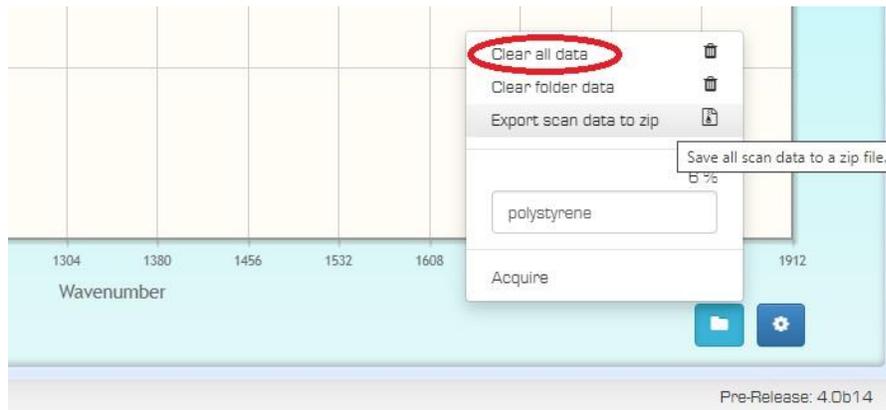
Pulse period (PP) [ $\mu$ s]	
Pulse duration (PD) [ns]	
Sample delay (SD) [ns]	
Sample width (SW) [ns]	

## ACQUIRING SAMPLE SPECTRUM

1. Create table with the first column indicating the order of acquisitions and the second column the label for said spectrum.

Sample Number	Sample Name
1	Substrate
2	Sample with substrate Position 1
3	Sample with substrate Position 2
4	Sample with substrate Position 3

2. Place substrate if present on the optical setup.
3. Clear all spectral data by going to the lower right corner, clicking on the folder logo, clicking on “Clear all data”.



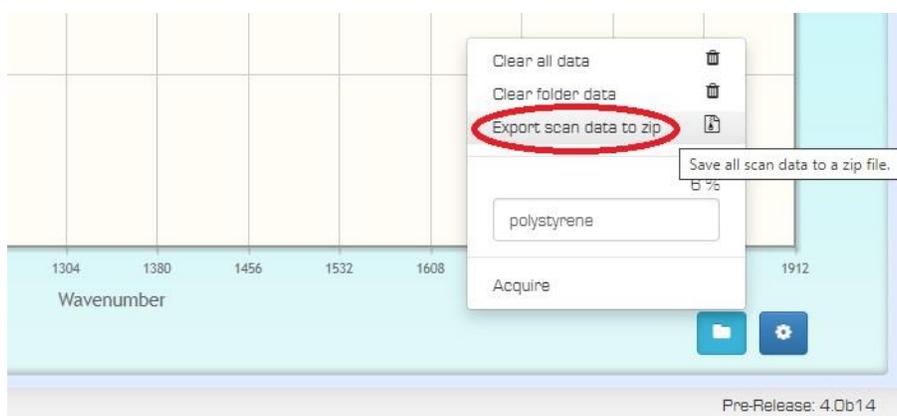
4. Acquire background spectrum by going to “Acquire” and “Acquire Reference”.



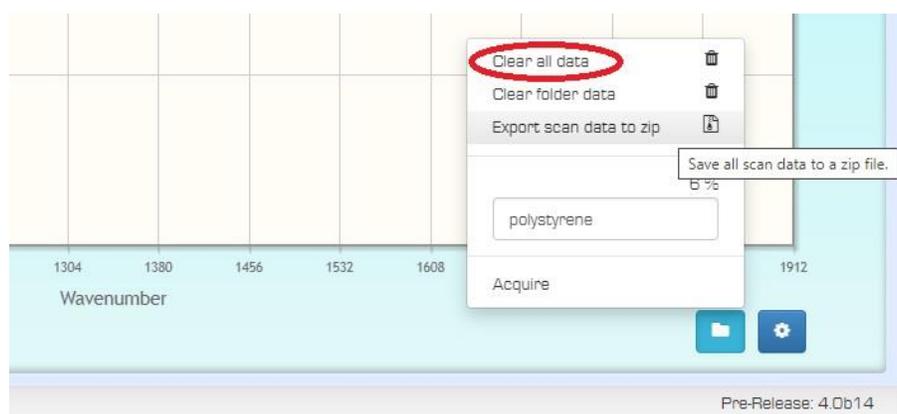
5. **Acquire** sample spectrum by going to “Acquire” and “Acquire Sample”.



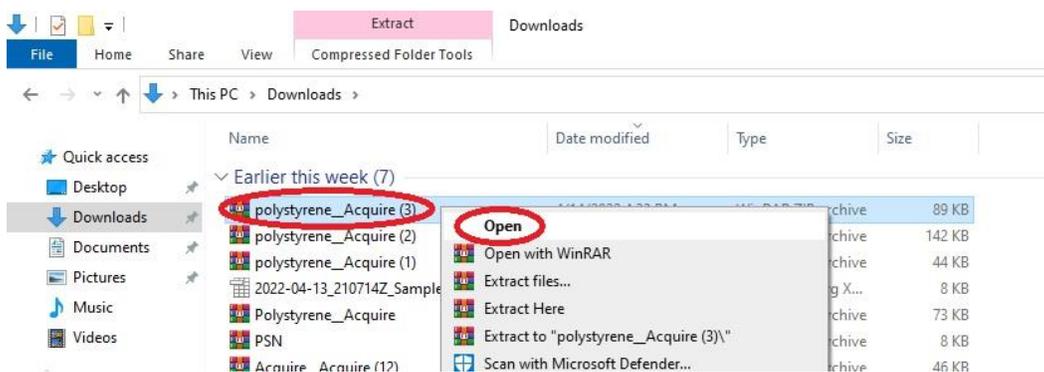
6. **Export** spectra by going to the lower right corner, clicking on the folder logo, clicking on “Export scan data to zip”. Files are exported in \*.csv file.



7. **Clear** all spectral data by going to the lower right corner, clicking on the folder logo, clicking on “Clear all data”.



8. Open \*.zip folder in the Downloads window.



9. Rename each \*.csv file containing one spectrum.

*TNT\_RA\_dL4\_ST5000\_CA5\_PP10.88\_PD30\_SD104\_SW16\_01\_01*

e.g.

The above name indicates that a spectrum of TNT was taken in Ratio scan type (RA), 4 cm<sup>-1</sup> resolution (dL), 5000 ms Scan Time (ST), 5 Co-Adds (CA), 10.88 s Pulse Period (PP), 30 ns Pulse Duration (PD), 104 ns Sample Delay (SD), 16 ns Sample Width (SW), replicate 01 (01), and block 01 (01).

Additionally, or alternatively, document the information of each sample in the table below.

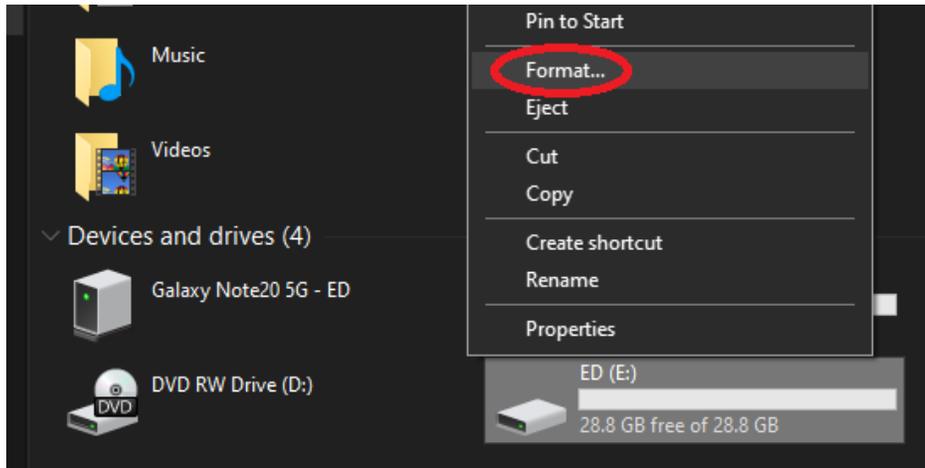
**Acronyms**

Single Beam (SB) or Ratio (RA); Resolution ( $\delta\lambda$ ); Scan Time (ST); Co-Adds (CA)

Pulse Period (PP); Pulse Duration (PD); Sample Delay (SD); Sample Width (SW)

Sample Number	Sample Name	Tune Settings	Acquisition Settings	Pulse Settings
1		<i>Tune</i> = _____	<i>Scan Type</i> = ____ <i><math>\delta\lambda</math></i> [cm <sup>-1</sup> ] = ____ <i>ST</i> [ms] = ____ <i>CA</i> = ____	<i>PP</i> [ $\mu$ s] = ____ <i>PD</i> [ns] = ____ <i>SD</i> [ns] = ____ <i>SW</i> [ns] = ____
2		<i>Tune</i> = _____	<i>Scan Type</i> = ____ <i><math>\delta\lambda</math></i> [cm <sup>-1</sup> ] = ____ <i>ST</i> [ms] = ____ <i>CA</i> = ____	<i>PP</i> [ $\mu$ s] = ____ <i>PD</i> [ns] = ____ <i>SD</i> [ns] = ____ <i>SW</i> [ns] = ____
3		<i>Tune</i> = _____	<i>Scan Type</i> = ____ <i><math>\delta\lambda</math></i> [cm <sup>-1</sup> ] = ____ <i>ST</i> [ms] = ____ <i>CA</i> = ____	<i>PP</i> [ $\mu$ s] = ____ <i>PD</i> [ns] = ____ <i>SD</i> [ns] = ____ <i>SW</i> [ns] = ____

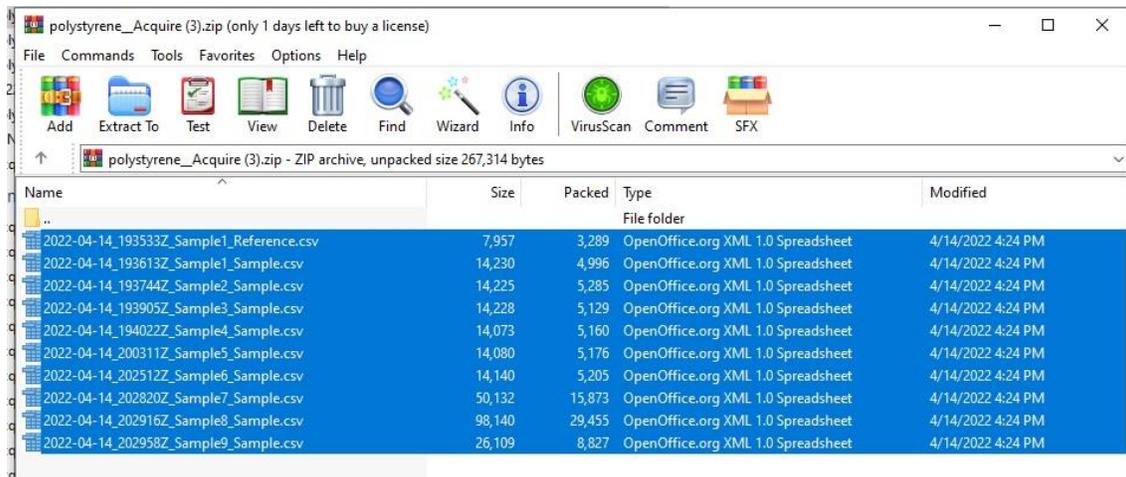
10. Format usb pen-drive before inserting on the LaserTune PC.



11. Connect usb pen-drive in LaserTune PC.



12. Click and drag \*.csv files from the \*.zip folder to the usb pen-drive.



13. Merge all \*.csv files into one Excel file.

14. Create new Sheet inside the merge Excel file.

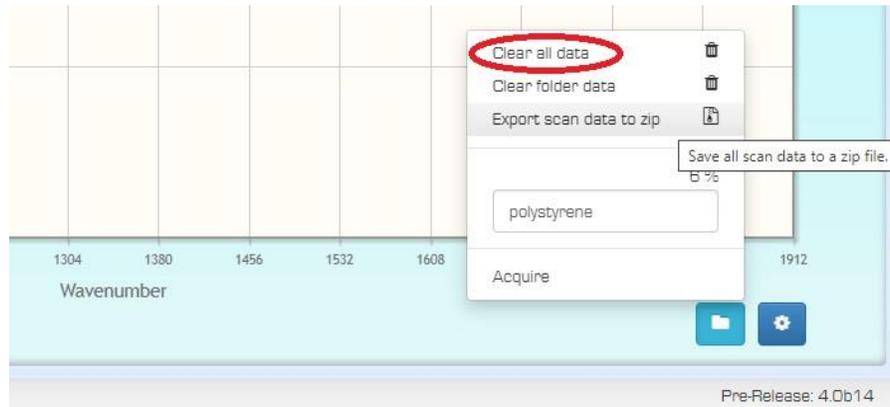
15. Add all relevant information regarding spectra (Instrument, parameters, etc.).

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
Sample	Class	Acronym	Scan Type	Resolution [cm-1]	Scan Time [ns]	Co-Adds	Pulse Period [mcs]	Pulse Duration [ns]	Sample Delay [ns]	Sample Width [ns]	774	778	782	786	790	794
1	Air	AIR	Ratio	4	5000	5	10.88	30	104	16	0.998946	1.001204	0.999399	1.00047	0.999981	0.999886
2	Polystyrene	PSE	Ratio	4	5000	5	10.88	30	104	16	0.151699	0.29919	0.467569	0.599851	0.681587	0.761614
3	Polyethylene	PEE	Ratio	4	5000	5	10.88	30	104	16	0.952139	0.948046	0.940192	0.932534	0.907543	0.880886
4	Acetone	ACE	Ratio	4	5000	5	10.88	30	104	16	0.001721	0.002633	0.003518	0.004412	0.005326	0.006472
5	Water	WAT	Ratio	4	5000	5	10.88	30	104	16	0.009531	0.010461	0.011158	0.013728	0.015421	0.017611
6	Hydrogen peroxide	PER	Ratio	4	5000	5	10.88	30	104	16	0.006544	0.007924	0.009589	0.011876	0.013575	0.017161

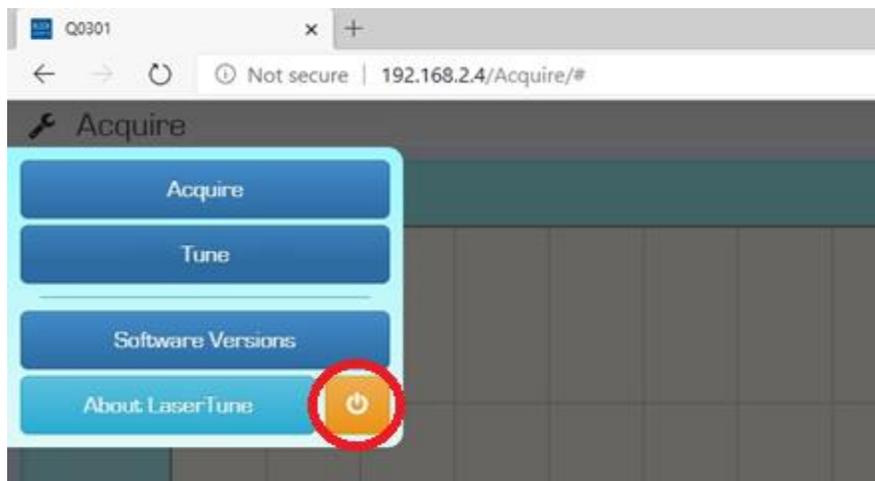
Sample information      Acquisition Settings      Pulse Settings      Spectral Data

## TURNING OFF SPECTROMETER

1. **Clear** spectral data on the spectrometer.



2. **Turn off** spectrometer by clicking on the tool menu and selecting the power button.



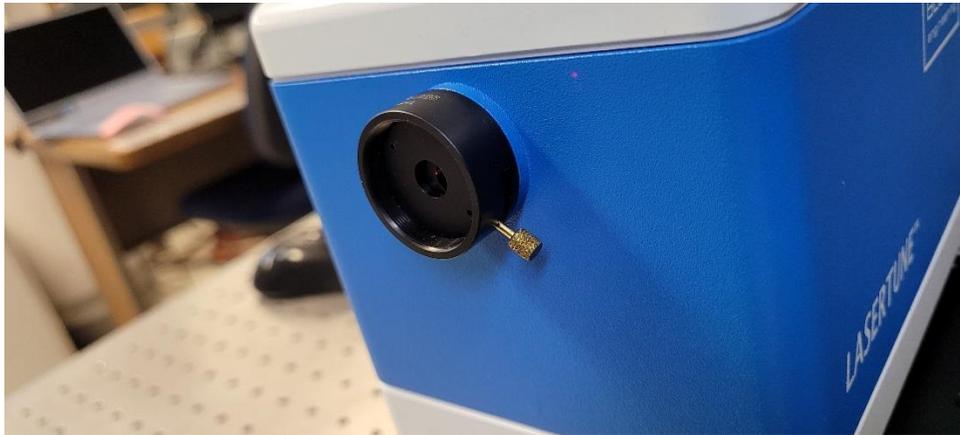
**NEVER TURN OFF BY PRESSING THE BUTTON  
ON THE SPECTROMETER!!!**

**IT IS ONLY PRESSED TO TURN ON THE SPECTROMETER**

## TROUBLESHOOTING

### 1. Laser spot appears as two circles.

Change the aperture of the LaserTune by moving the part shown below clockwise and counterclockwise.



Advisor Signature

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Co-Advisor Signature

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