Acquiring Quantum Cascade Laser Infrarred Spectra with BlockEngineering LaserTune Spectrometer



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Effectivity: March/13/2022	Acquiring Quantum Cascade Laser Infrarred 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.

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5	^	-		Q°
		Тод	gle Laser	Pointer
		Series 1		

5. Choose and place optical setup for acquisition.





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.







- 8. Adjust optics to ensure that the laser hits the sample in the desired manner. Work without light in the room to observe laser.
- 9. Verify mirrors are free of dust or oils from fingers.
- **10. [OPTIONAL]** Clean mirror with compressed air if needed.



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.

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772 cm-1)					(191	2 cm ⁻¹	
		_		~				
		0.0	ms	Iterations:			00	#
	Time per sweep:							

Wavenumber range =

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



- Ð X ∿≣ 回 公 J Series 1 ٥ \times 公 ☆ 田 0 O. Power Settings Pulse Settings Temperature Settings Acquire Settings Persistence Storage Settings
- **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.

Scan Type	
Resolution ($\delta\lambda$) [cm ⁻¹]	
Scan Time (ST) [ms]	
Co-Adds (CA) [N/A]	

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) [µs]	
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".

0	772	848	924	1000	1076	1152	1228	1304 Waven	1380 Jumber
Act	quire Samp	ole 👗	Acquire	Reference	A	Stop Lasers			
Ready									

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.

	Clear all data 🛍 Clear folder data 🛍 Export scan data to zip 🚯
	Save all scan data to a zip t 8 % polystyrene
1304 1380 1456 1532 1608 Wavenumber	Acquire 1912

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.

🖓 📙 🖛 I		Extract	Downloads		
le Home	Share View	Compressed Folder Too	ols		
→ * ↑ ↓	> This PC > Do	wnloads >			
	Name		Date modified Ty	pe	Size
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Downloads	👷 👎 polys	tyrene_Acquire (3)	Onen	chive	89 KB
Documents	👷 🔛 polys	tyrene_Acquire (2)	Open with WinBAR	rchive	142 KB
Distance	polys	tyrene_Acquire (1)		rchive	44 KB
Pictures	1 2022-	-04-13_210714Z_Sample	Extract files	g X	8 KB
Music	Polys	tyrene_Acquire	Extract Here	chive	73 KB
Videos	PSN		Extract to "polystyrene_Acquire (3)\"	chive	8 KB
	Acqui	ire Acquire (12)	Scan with Microsoft Defender	chive	46 KB

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

*TNT_RA_dL4_ST*5000_*CA5_PP*10.88_*PD*30_*SD*104_*SW*16_01_01

e.g.

The above name indicates that a spectrum of TNT was taken in Ratio scan type (RA), 4 cm-1 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> =	$Scan Type = \\delta\lambda [cm^{-1}] = \ST [ms] = \CA = \$	$\begin{array}{l} PP \ [\mu s] = ___\\ PD \ [ns] = ___\\ SD \ [ns] = ___\\ SW \ [ns] = ___\\ \end{array}$
2		Tune =	$Scan Type = \\delta\lambda [cm^{-1}] = \ST [ms] = \CA = \$	$\begin{array}{l} PP \ [\mu s] = ___\\ PD \ [ns] = ___\\ SD \ [ns] = ___\\ SW \ [ns] = ___\\ \end{array}$
3		Tune =	$Scan Type = \\delta\lambda [cm^{-1}] = \ST [ms] = \CA = \$	$\begin{array}{l} PP \ [\mu s] = ___\\ PD \ [ns] = ___\\ SD \ [ns] = ___\\ SW \ [ns] = ___\\ \end{array}$

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

	Pin to Start
Music	Format
	Eject
Videos	Cut
	Сору
 Devices and drives (4) 	Create shortcut
Galaxy Note20 5G - ED	Rename
	Properties
💿 DVD RW Drive (D:)	ED (E:)
	28.8 GB free of 28.8 GB

11. Connect usb pen-drive in LaserTune PC.



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

polystyrene_Acquire (3).zip (only 1 days left to buy a licens e Commands Tools Favorites Options Help	e)		- 0
Add Extract To Test View Delete Find	Wizard Info	VirusScan Comment SFX	
polystyrene_Acquire (3).zip - ZIP archive, unpack	ed size 267,314 bytes		
ame	Size	Packed Type	Modified
		File folder	
2022-04-14_193533Z_Sample1_Reference.csv	7,957	3,289 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
2022-04-14_193613Z_Sample1_Sample.csv	14,230	4,996 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
2022-04-14_193744Z_Sample2_Sample.csv	14,225	5,285 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
2022-04-14_193905Z_Sample3_Sample.csv	14,228	5,129 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
2022-04-14_194022Z_Sample4_Sample.csv	14,073	5,160 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
2022-04-14_200311Z_Sample5_Sample.csv	14,080	5,176 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
2022-04-14_202512Z_Sample6_Sample.csv	14,140	5,205 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
2022-04-14_202820Z_Sample7_Sample.csv	50,132	15,873 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
2022-04-14_202916Z_Sample8_Sample.csv	98,140	29,455 OpenOffice.org XML 1.0 Spreadsheet	4/14/2022 4:24 PM
	26 100	9.927 OpenOffice are VML 1.0 Server deheet	A/1A/2022 A-24 DM

- 13. Merge all *.csv files into one Excel file.
- 14. Create new Sheet inside the merge Excel file.

A I	В	с	D	E	F	G	н	1	J	К	L	М	N	0	P	Q	
1 Sample	Class	Acronym	can 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	
2 1	Air	AIR	Ratio	4	5000	5	10.88	30	104	16	0.998946	1.001204	0.999399	1.00047	0.999981	0.999886	
3 2	Polystyrene	PSE	Ratio	4	5000	5	10.88	30	104	16	0.151699	0.29919	0.467569	0.599851	0.681587	0.761614	
4 3	Polyethylene	PEE	Ratio	4	5000	5	10.88	30	104	16	0.952139	0.948046	0.940192	0.932534	0.907543	0.880886	
5 4	Acetone	ACE	Ratio	4	5000	5	10.88	30	104	16	0.001721	0.002633	0.003518	0.004412	0.005326	0.006472	
6 5	Water	WAT	Ratio	4	5000	5	10.88	30	104	16	0.009531	0.010461	0.01158	0.013728	0.015421	0.017611	
7 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					

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

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

Co-Advisor Signature