

Acquiring Infrared Spectra with Shimadzu IRPrestige-21 ATR-FTIR Spectrometer



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SOP-01	Jorge Plata, Edwin Caballero		University of Puerto Rico at Mayagüez
Effectivity: March/27/2023	Acquiring Infrared Spectra with Shimadzu IRPrestige-21 ATR-FTIR Spectrometer		Revised by:
Revised:			Approved by:

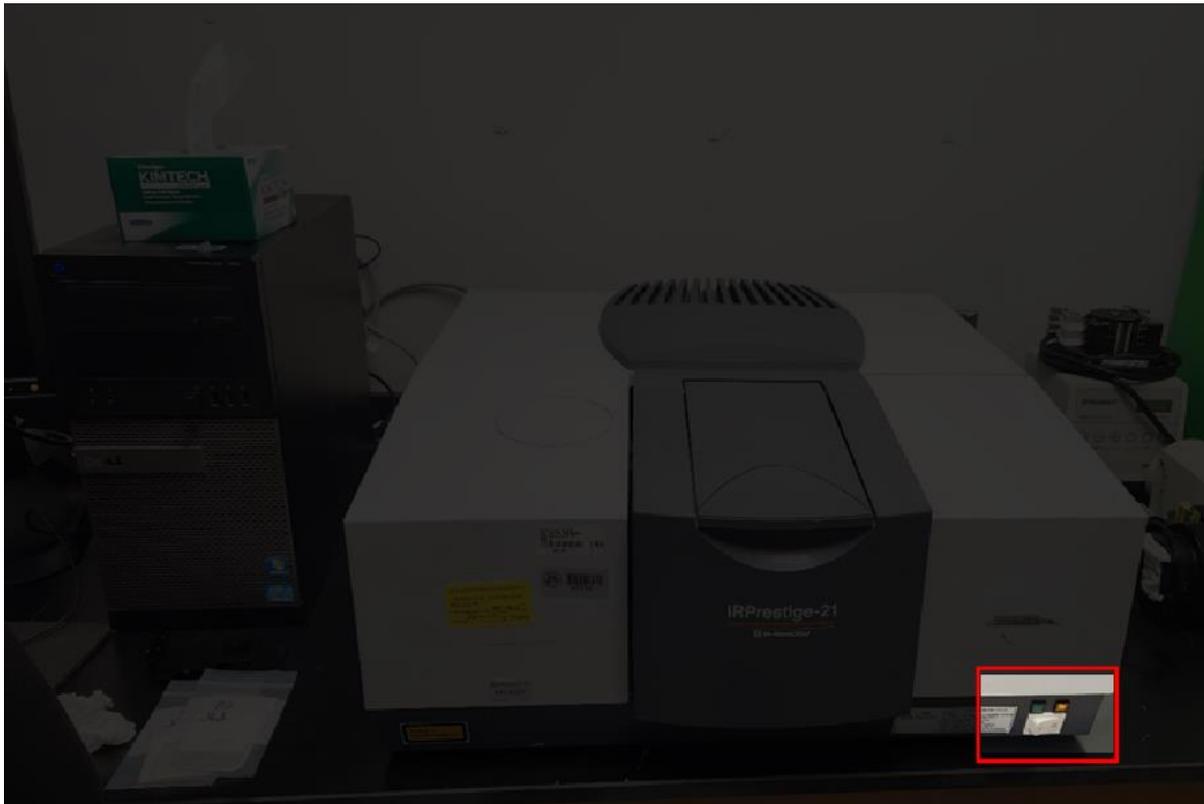
This SOP uses the following:

- Instrument: Shimadzu IRPrestige-21 ATR-FTIR spectrometer
- Program: Shimadzu Lab Solutions



TURNING ON SPECTROMETER

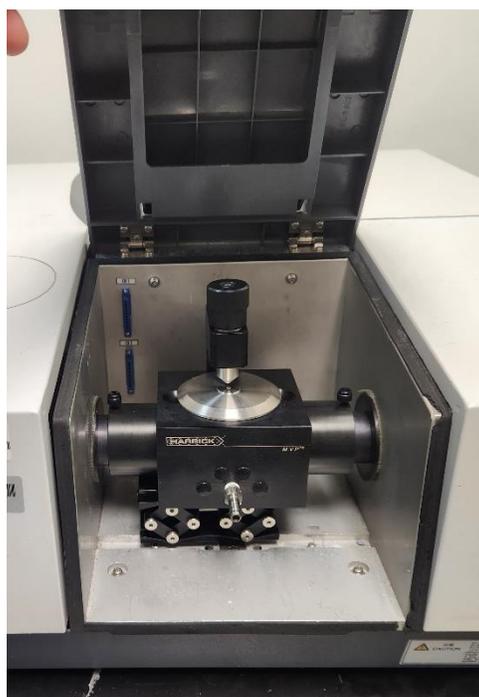
1. Turn on the spectrometer by pressing the ON/OFF button.



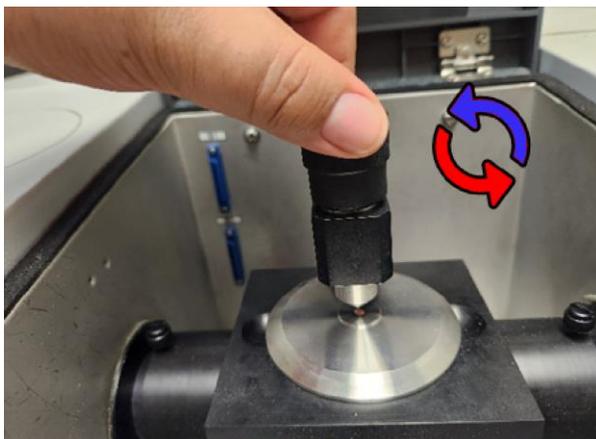
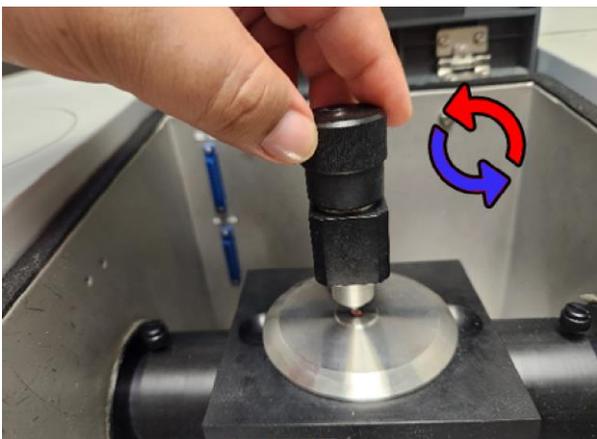
2. Turn on the desktop computer.



3. Open the ATR-FTIR spectrometer compartment.



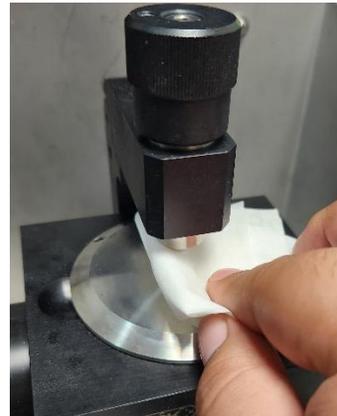
4. **Move** the ATR tip upwards by rotating the knob counterclockwise (CCW).



Or by moving the ATR upwards



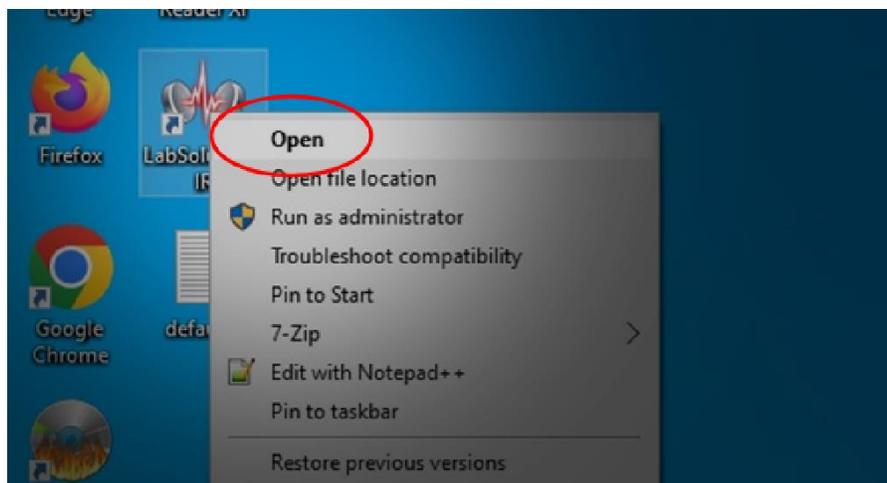
5. Clean ATR tip and plate with Kim Wipes and alcohol.



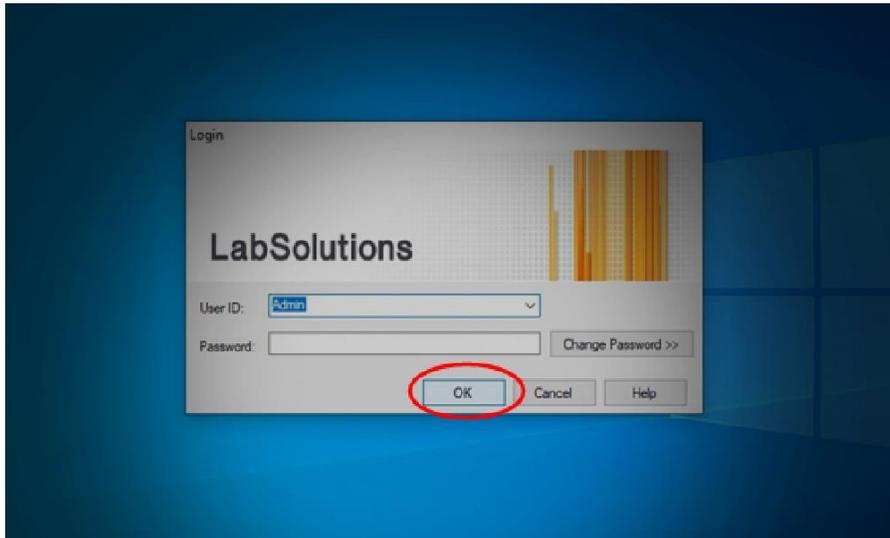
6. Close ATR compartment.



7. Open the Lab Solutions program.



8. Click "OK" only.

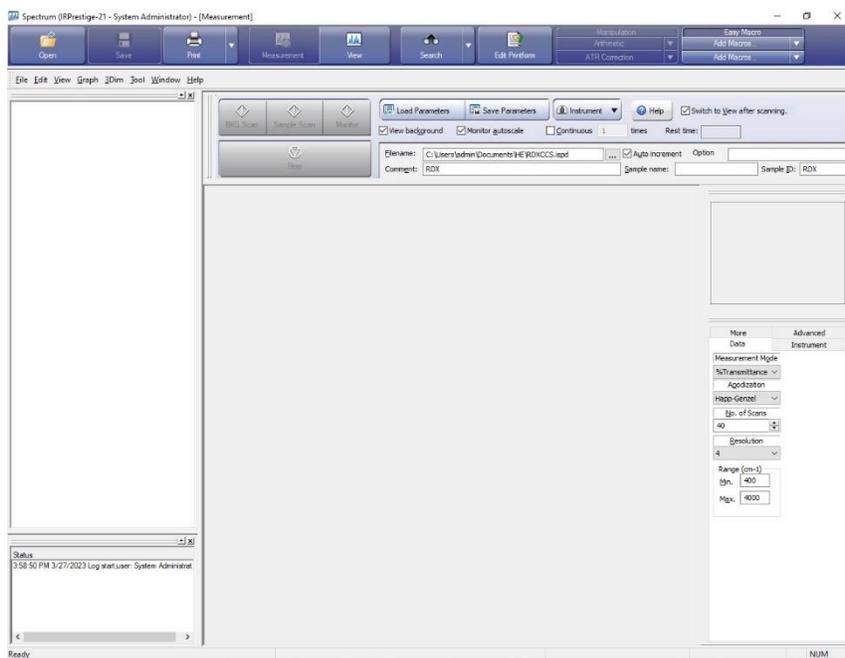


9. Select the "Spectrum" option in the Measurement Program and Postrun tab.

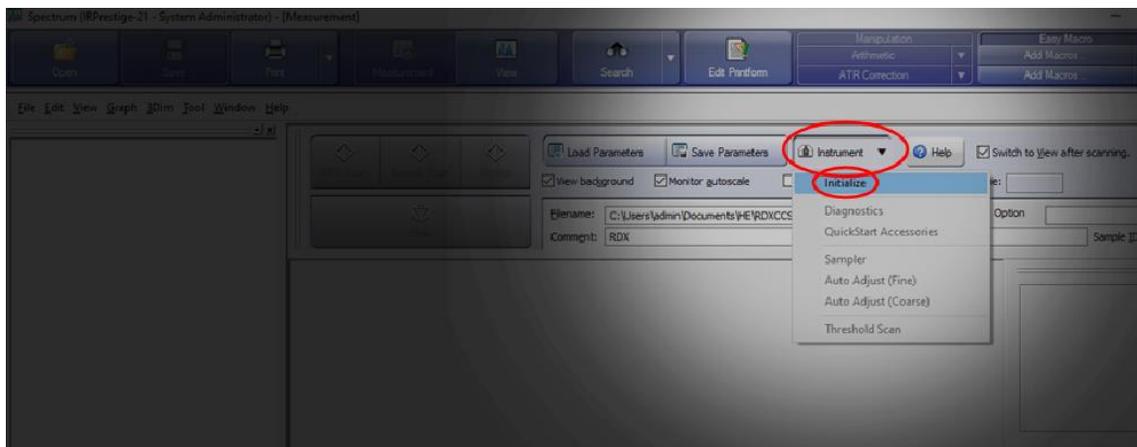




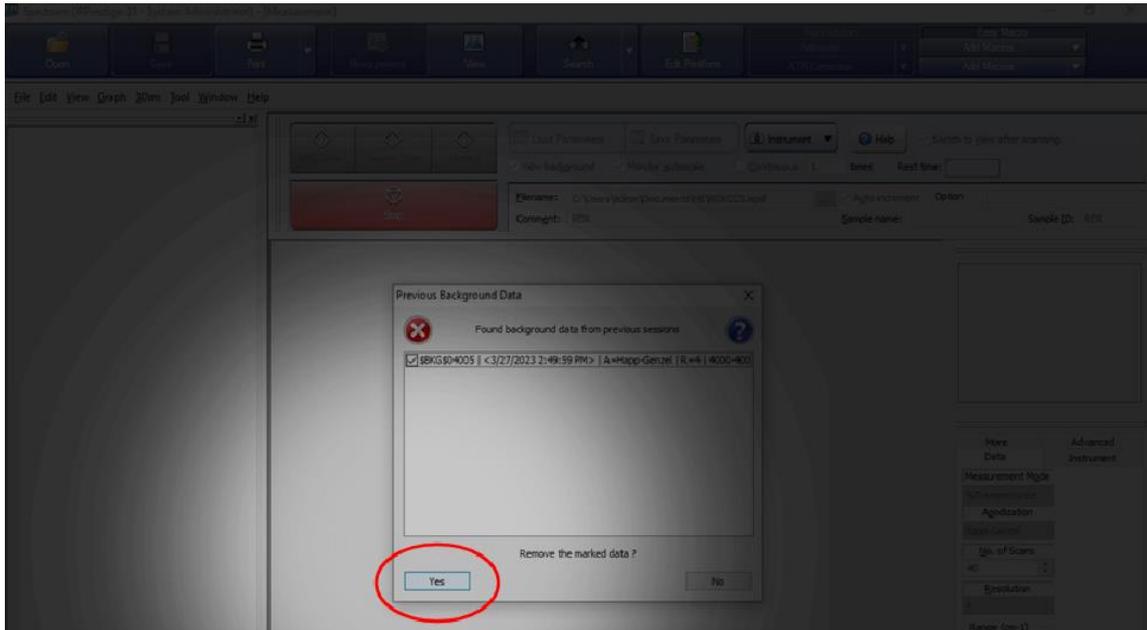
This is the main interface of the program.



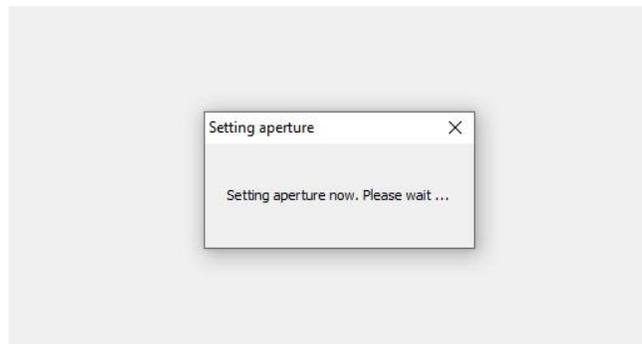
10. Initialize the instrument by going to Instrument > Initialize.



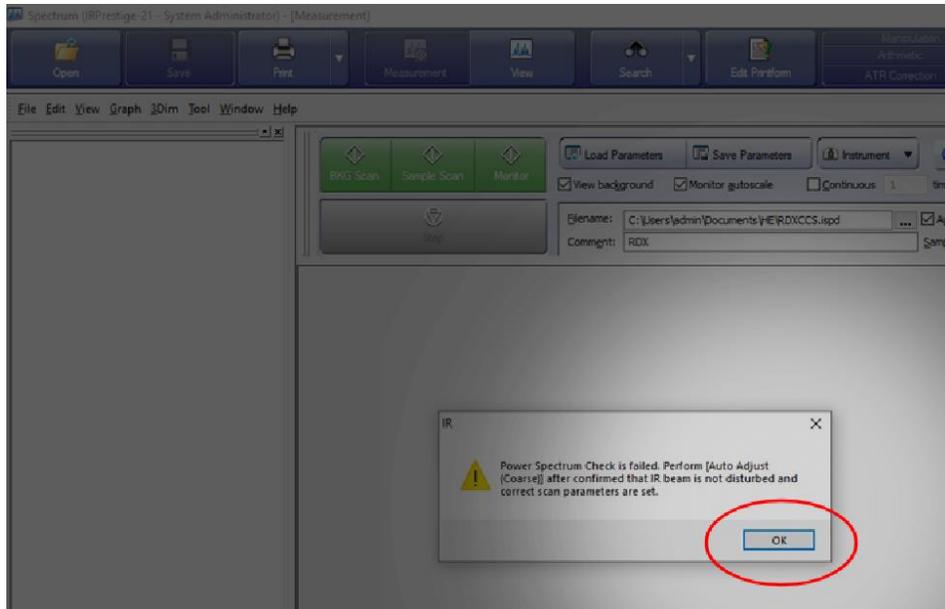
11. Click "Yes" on the following window that will pop up.



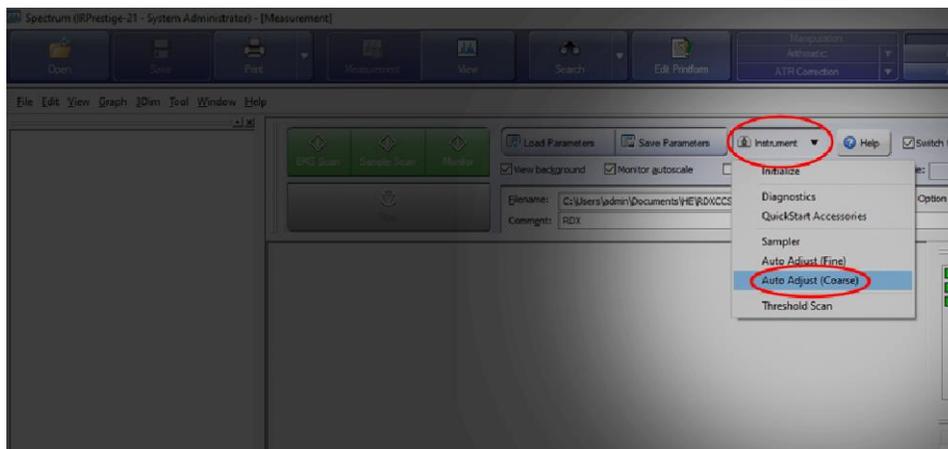
Instrument will start setting aperture.



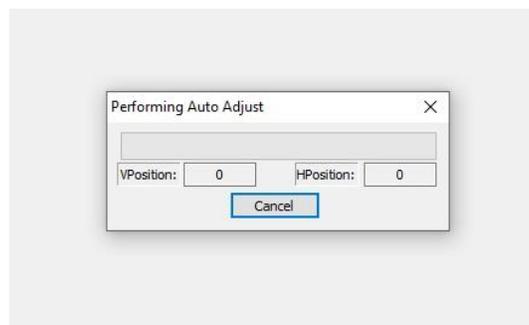
12. Click "OK" on the IR window pop-up.



13. Click Auto Adjust (Coarse) by going to Instrument > Auto Adjust (Coarse).

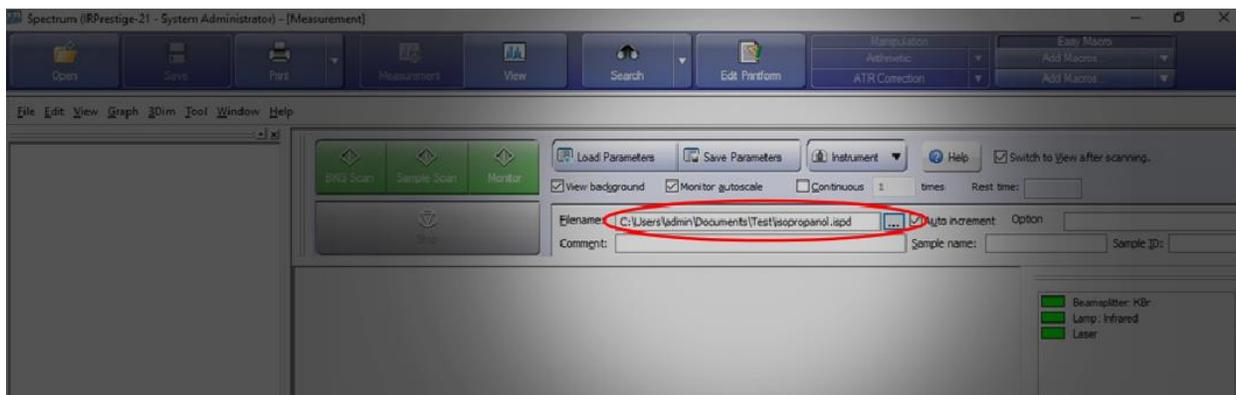


Instrument will start performing Auto Adjust

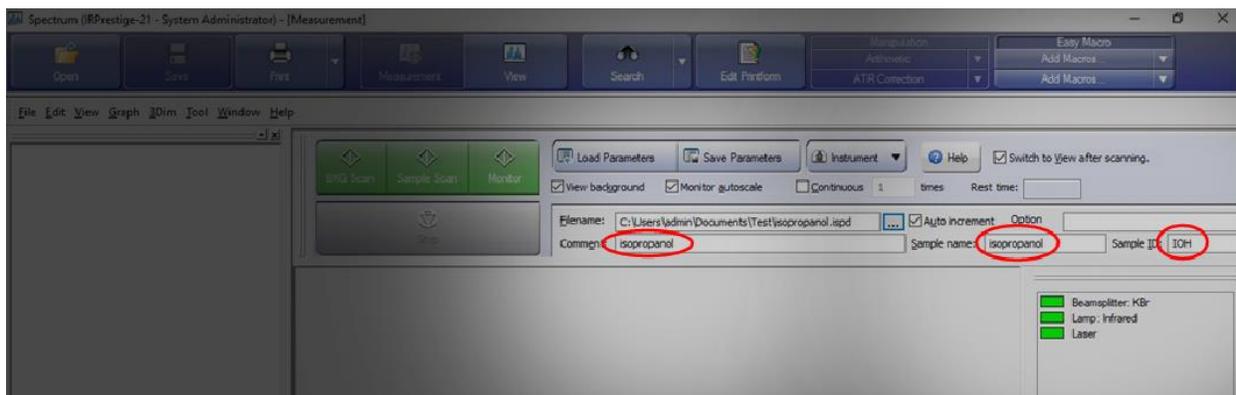


14. Browse where the files will be stored by clicking the "..." box at the right the "Filename:" text box. Alternatively, you can write the path for the files.

C:\Users\admin\Documents\Your folder\name-of-spectrum.ispd.



15. Write sample name, ID, and comments on the sample in the text boxes below the "Filename:" text box.



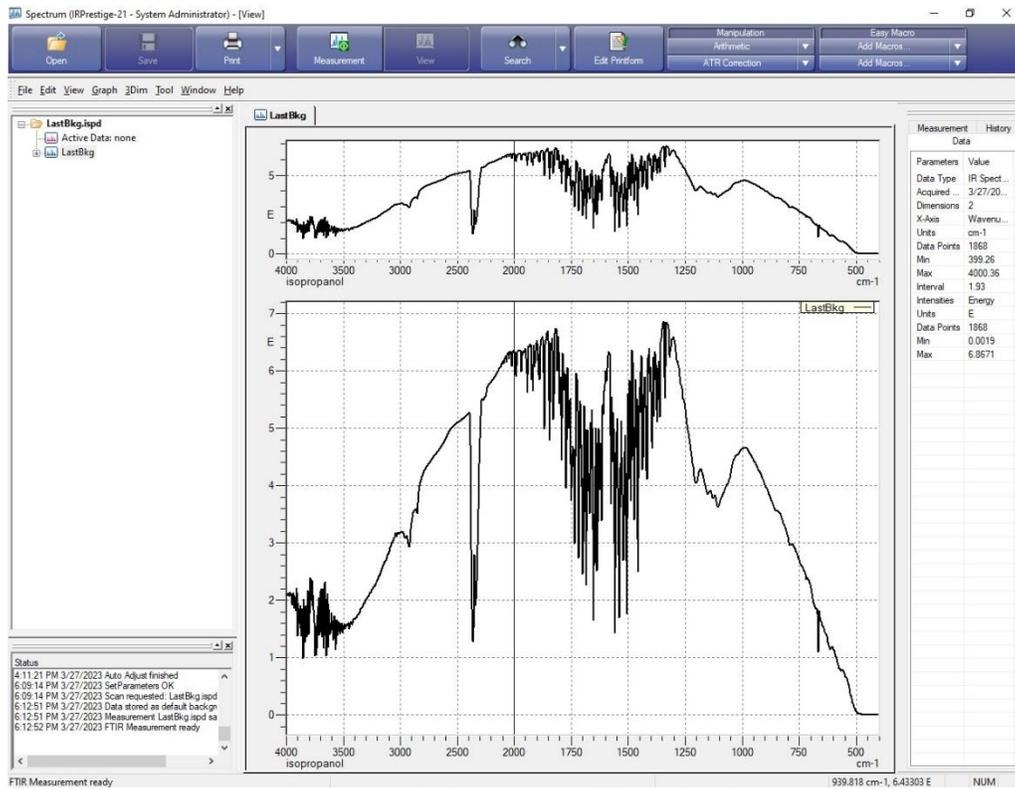
16. Click on the "BKG Scan" button to acquire background sample.

The background sample counts as the blank.

- If you do not want to see the spectral information of a solvent in your sample, place the solvent in the ATR and acquire the background sample.
- If you only have a pure sample, do not place any sample on the ATR and acquire the background sample.



The interface will change from “Measurement” to “View” when the spectra is acquired.

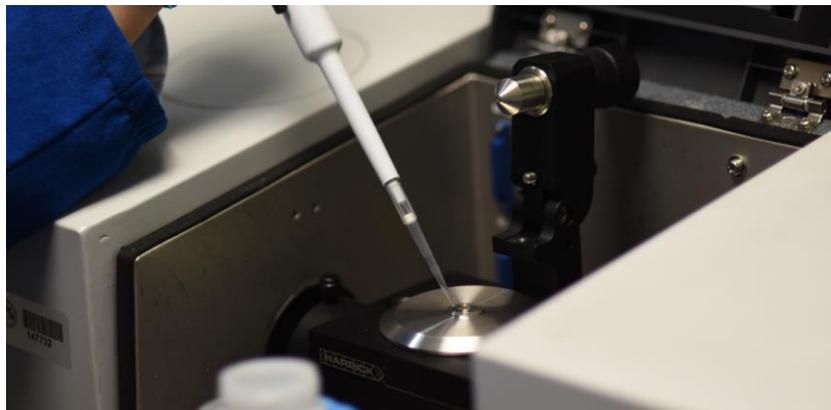


ACQUIRING SPECTRA

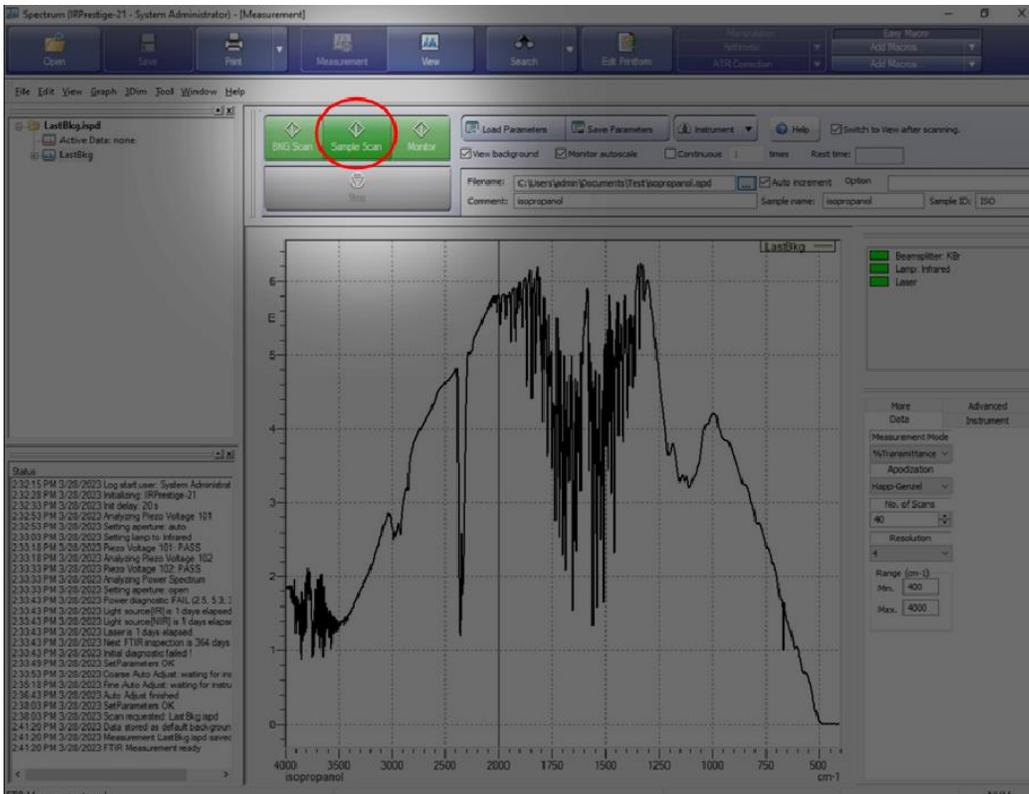
1. **Clean** ATR plate and tip.



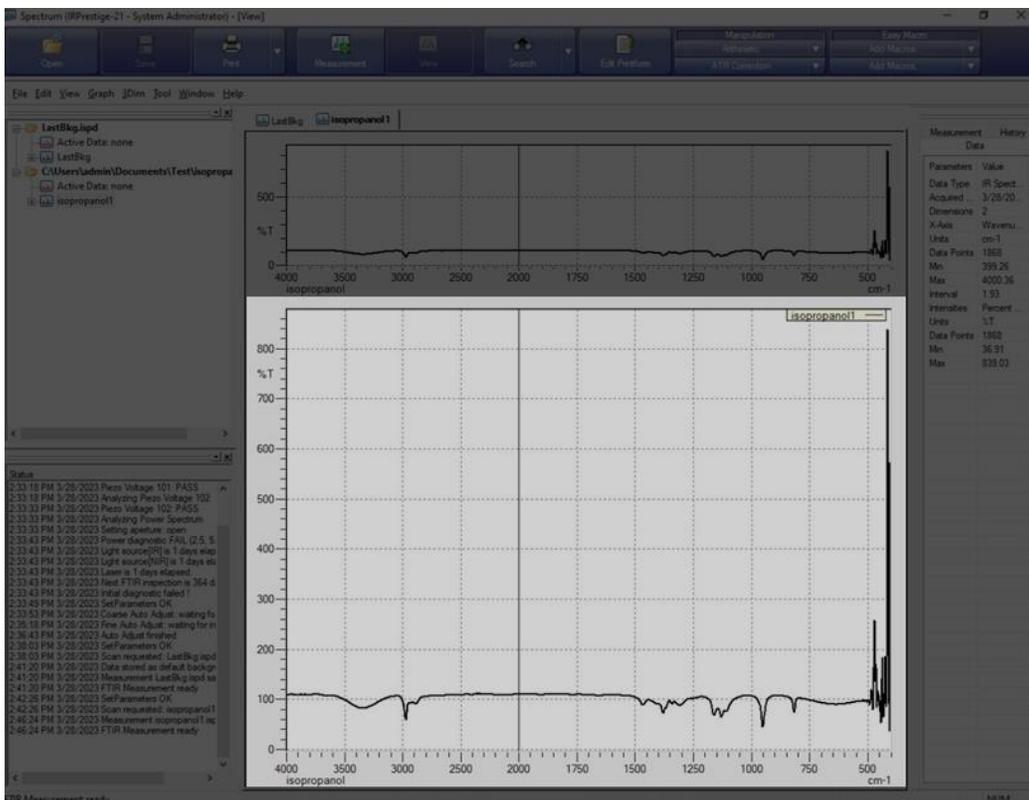
2. **Place** sample in ATR plate and adjust tip.



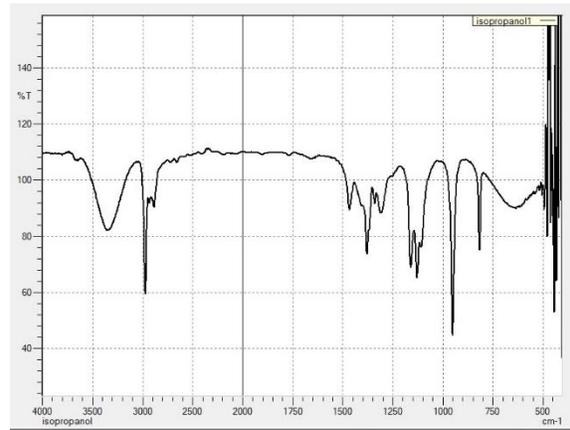
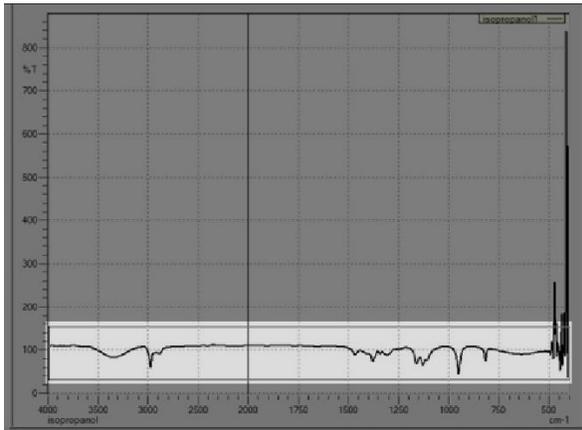
3. **Select** "Sample Scan" to acquire spectrum of the sample in the ATR plate.
Set the desired number of scans in the "No. of Scans" box on the data tab.
Set the resolution in the "Resolution" box on the data tab.



The resulting spectrum



4. **Zoom in** on the spectrum by left clicking on one side and dragging a box around the spectrum, then clicking left click again.

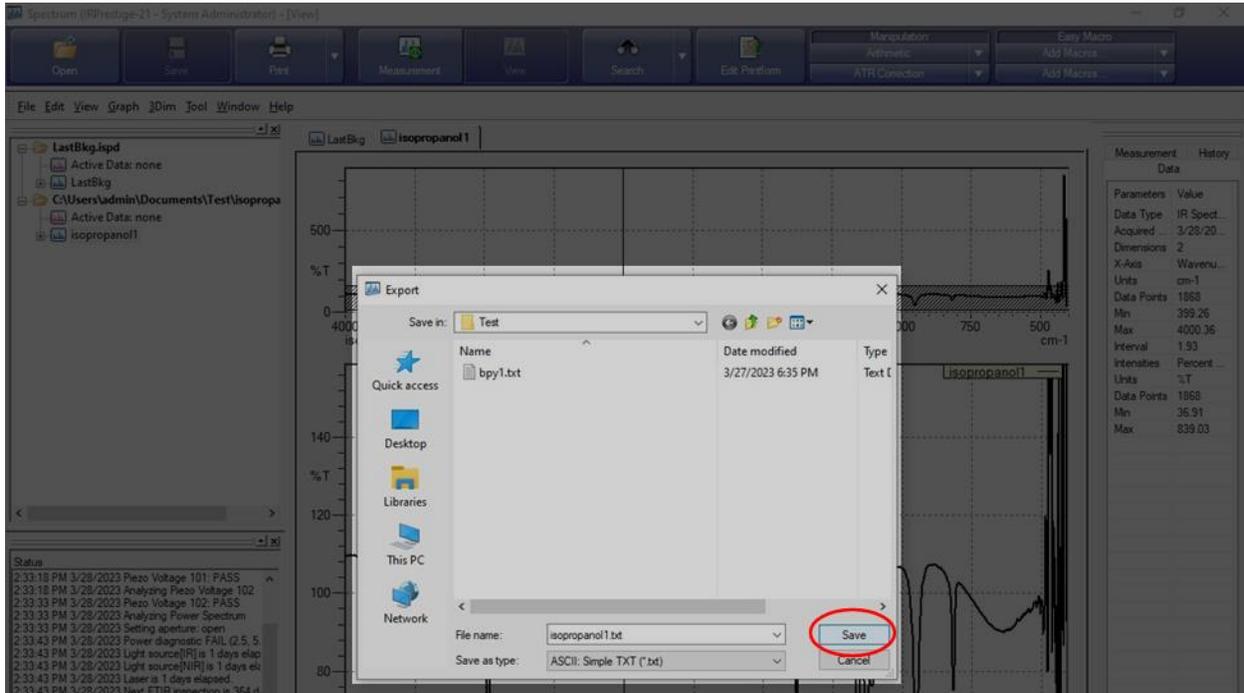


5. **Export** spectrum by going to File > Export...

The screenshot shows the Spectrum (IRPrestige-21) software interface. The 'File' menu is open, and the 'Export...' option is highlighted with a red circle. The main window displays two IR spectra plots for 'isopropanol1'. The top plot shows the full spectrum from 4000 to 500 cm-1, and the bottom plot is a zoomed-in view of the same data. On the right side, there is a 'Measurement Data' table with the following information:

Parameters	Value
Data Type	IR Spect...
Acquired	3/28/20...
Dimensions	2
X-Axis	Wavenu...
Units	cm-1
Data Points	1868
Min	399.26
Max	4000.36
Interval	1.93
Intensities	Percent ...
Units	%T
Data Points	1868
Min	36.91
Max	839.03

6. Save the spectrum in “.txt” format.



TURNING OFF SPECTROMETER

1. Verify ATR plate and tip are clean.



2. Turn off the spectrometer by pressing the ON/OFF button.



TROUBLESHOOT

Advisor Signature

Co-Advisor Signature
