

## FTIR (Spectrum One) – Standard Operating Procedure

NOTE: Before reading this you MUST read the 'SOP - Energy and environmental impacts under normal, abnormal and emergency conditions' which is Mills group web site, <https://www.profandrewmills.com/leaf-documents/>. This addresses general energy and environmental impacts under normal, abnormal and emergency conditions considerations which you NEED to be cognisant of before conducting any experiment. If you identify anything in an SOP which can be improved, please contact the LO and PI to discuss the proposed change(s) before putting them into effect.

## FTIR (Spectrum One) – Standard Operating Procedure

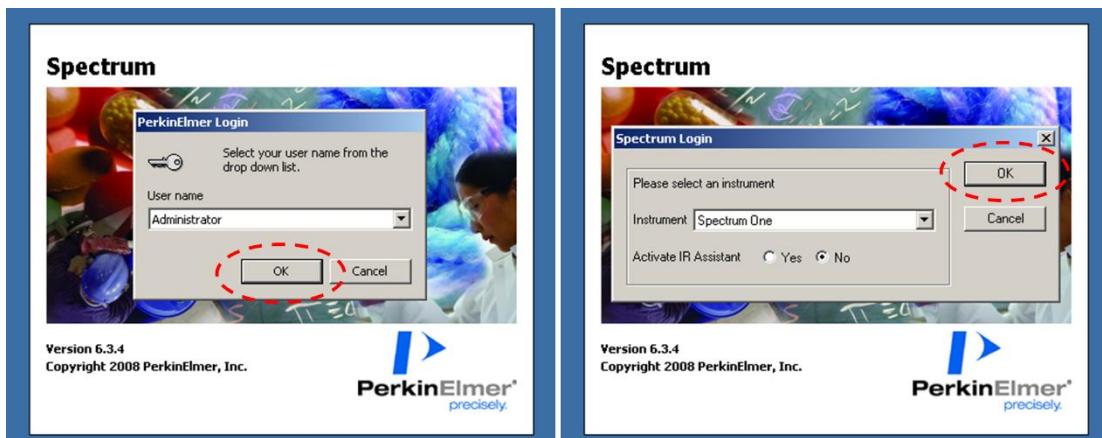
### FTIR (Spectrum One) – Standard Operating Procedure (01.003)



1. The Spectrum One FTIR is always switched on in order to keep the optical components warm and free from moisture. If the spectrometer is ever switched off (no green lights illuminated on the display on the right hand side of the instrument), inform the PI or PDRA.
2. Start up the PC attached to the Spectrum One FTIR.
3. Open the 'Spectrum' software by double clicking the icon below.

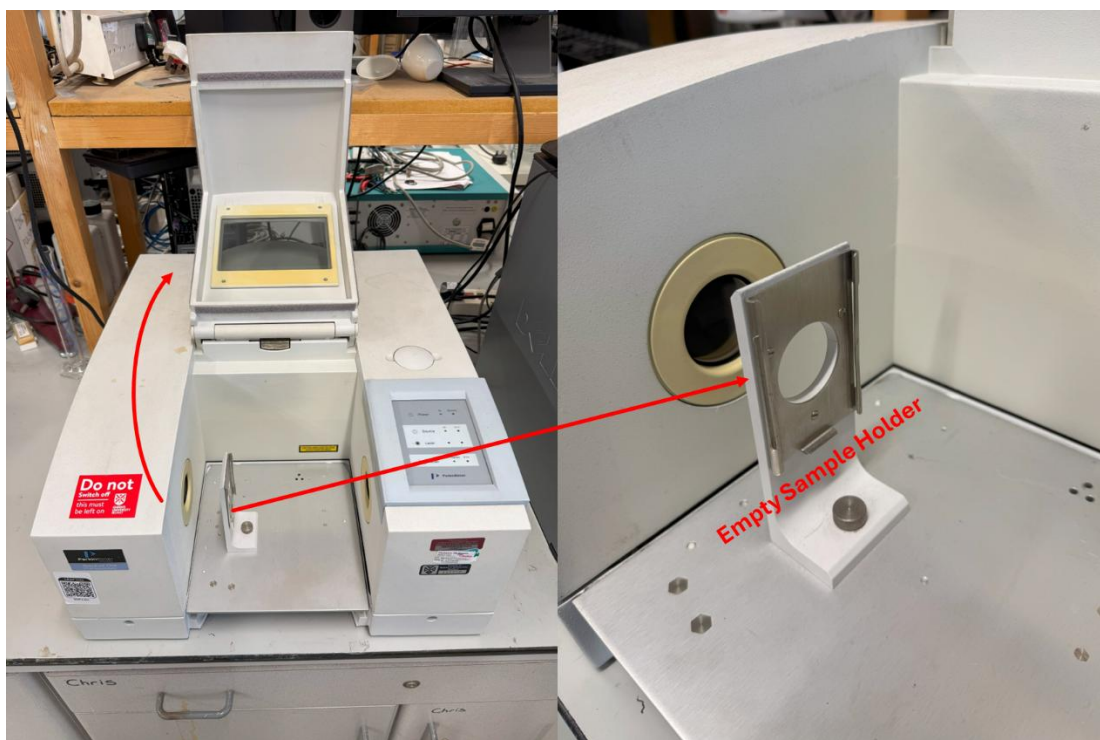


4. Leave the 'User name' as 'Administrator' and click 'OK' on the 2 pop-up boxes.

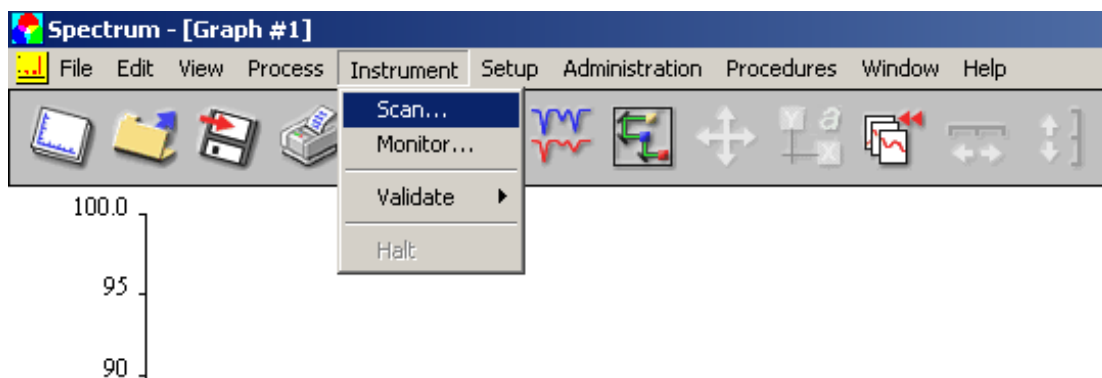


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5. Open the cover of the sample compartment and check that there is nothing in the holder.

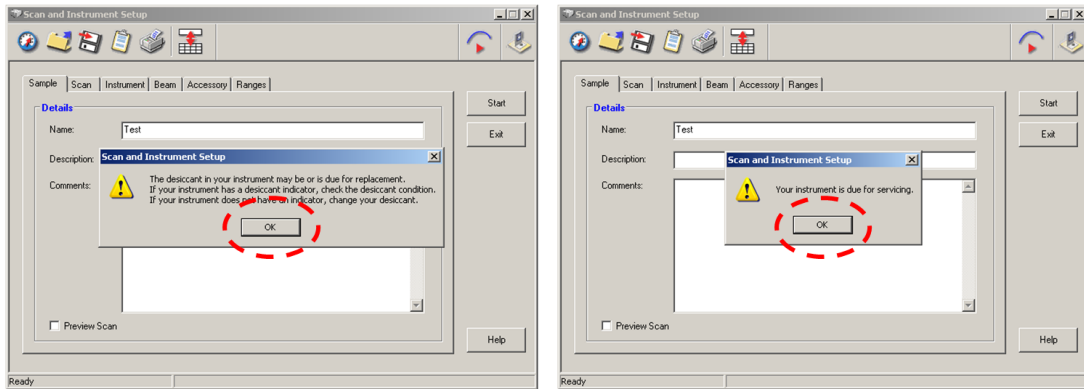


6. Click on the 'Instrument' dropdown tab at the top of the screen and select 'Scan'.

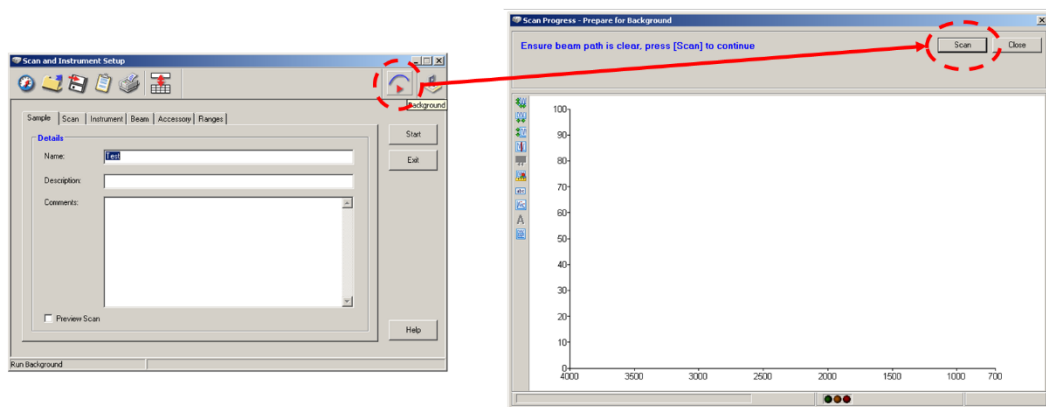


7. Two boxes will appear saying that the desiccant needs changed and the instrument is due to be serviced. This can be ignored by clicking 'OK'. The instruments are regularly maintained in-house by the PDRA.

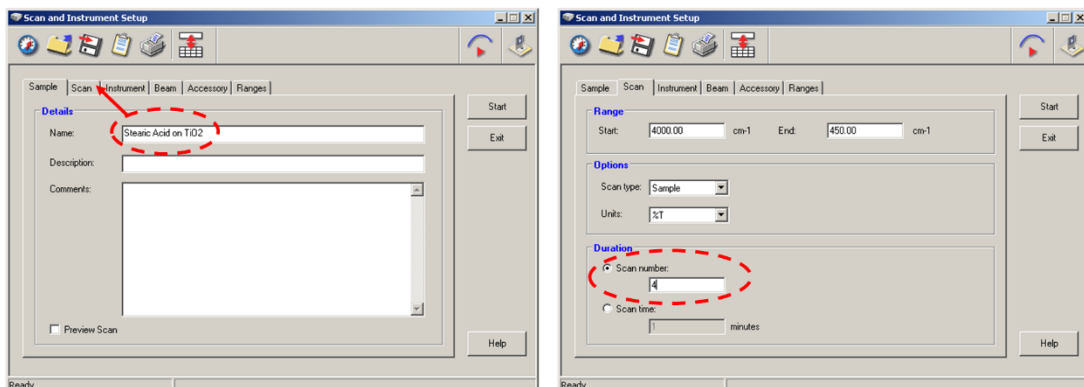
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8. Before running any samples, a background scan has to be performed. Click on the background button highlighted below and then click 'Scan' on the following screen.

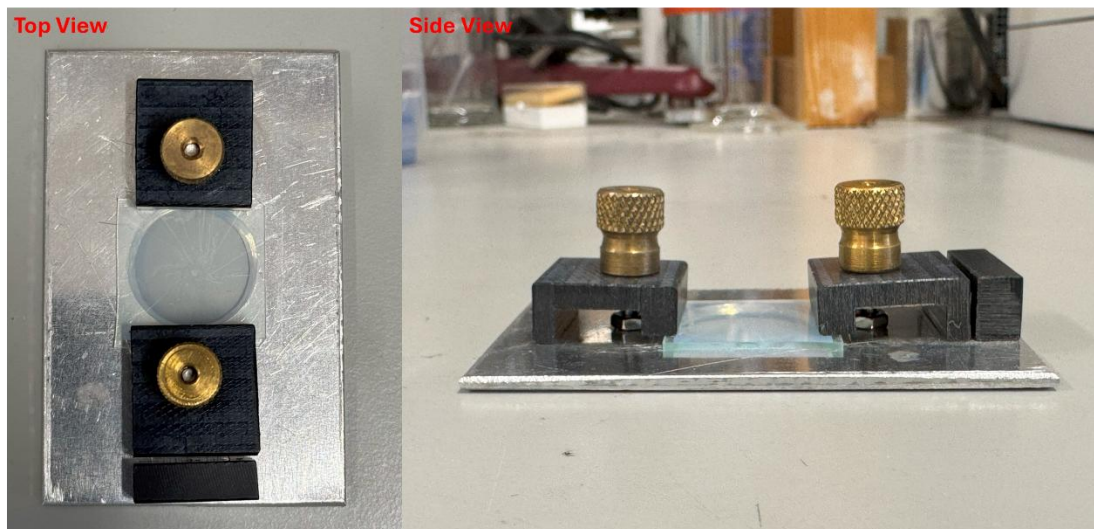


9. You will then be taken back to the 'Scan and Instrument Setup' window. Type in your sample name in the highlighted box and then click on the scan tab. On the scan tab you can change the scan range and units, i.e. %transmittance, absorbance etc., however, these are usually left as default (450 – 4000  $\text{cm}^{-1}$ ). It is recommended to increase the scan number to at least 4 to help average out any noise (useful when looking at thin films with weak signals).

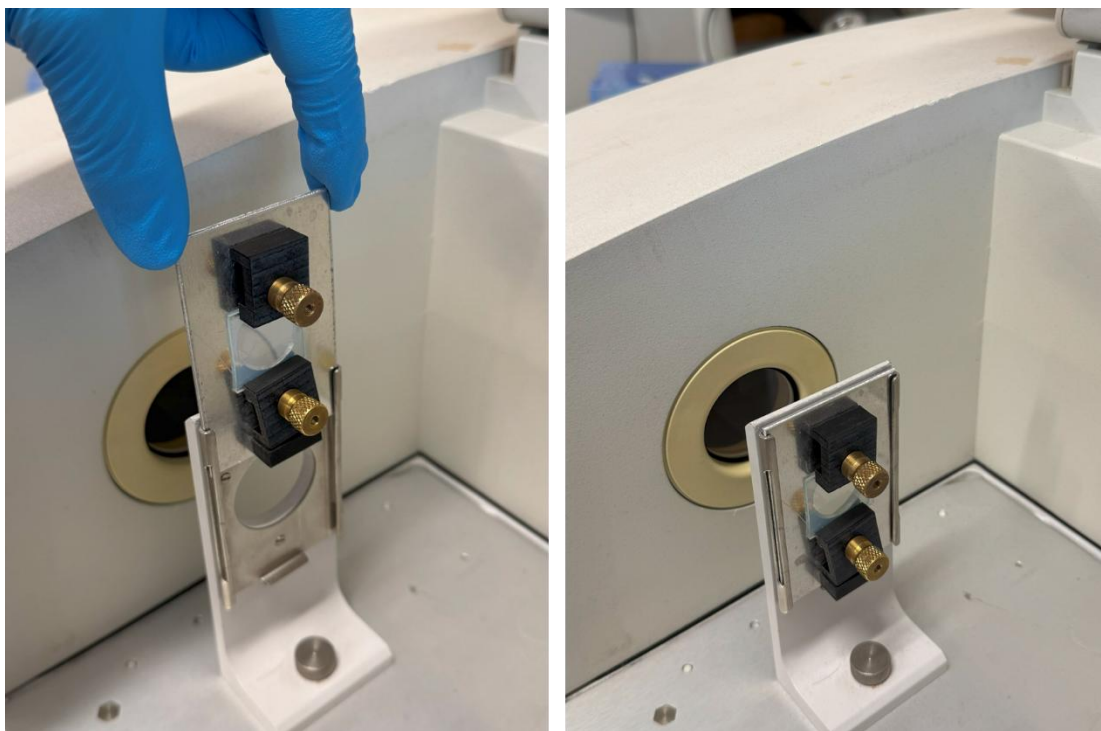


10. Place your sample in a FTIR holder such as the one shown below. The sample below is stearic acid on a  $\text{TiO}_2$  film, supported on a 2.5 cm square microscope slide. This is held in place by the 2 clamps/retainers.

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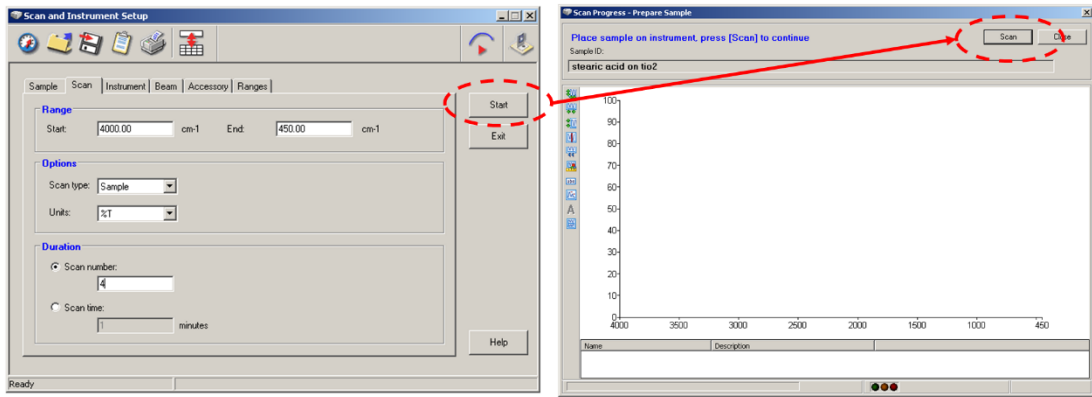


11. Lower the sample into the holder of the FTIR and then close the cover.

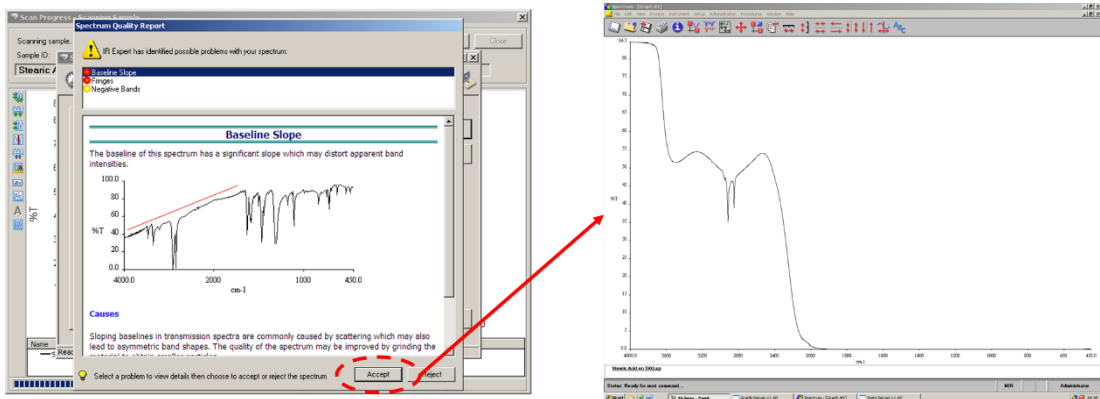


12. Go back to the software and click 'Start' and then click 'Scan' on the following screen.

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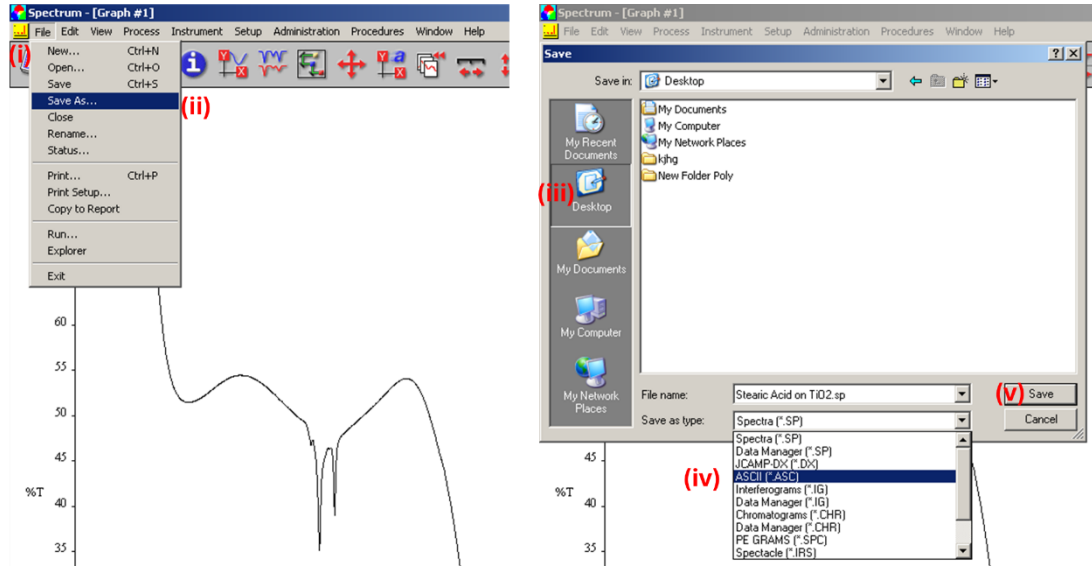
13. Depending on your sample, you may get a warning pop up regarding, sloping baselines, water content etc. Usually, this can just be ignored by clicking 'Accept'. It's normally due to weak signals, or the fact that the  $\text{TiO}_2$  is blocking half the scan range. You will be taken to the main window in the software where your spectra will be displayed.



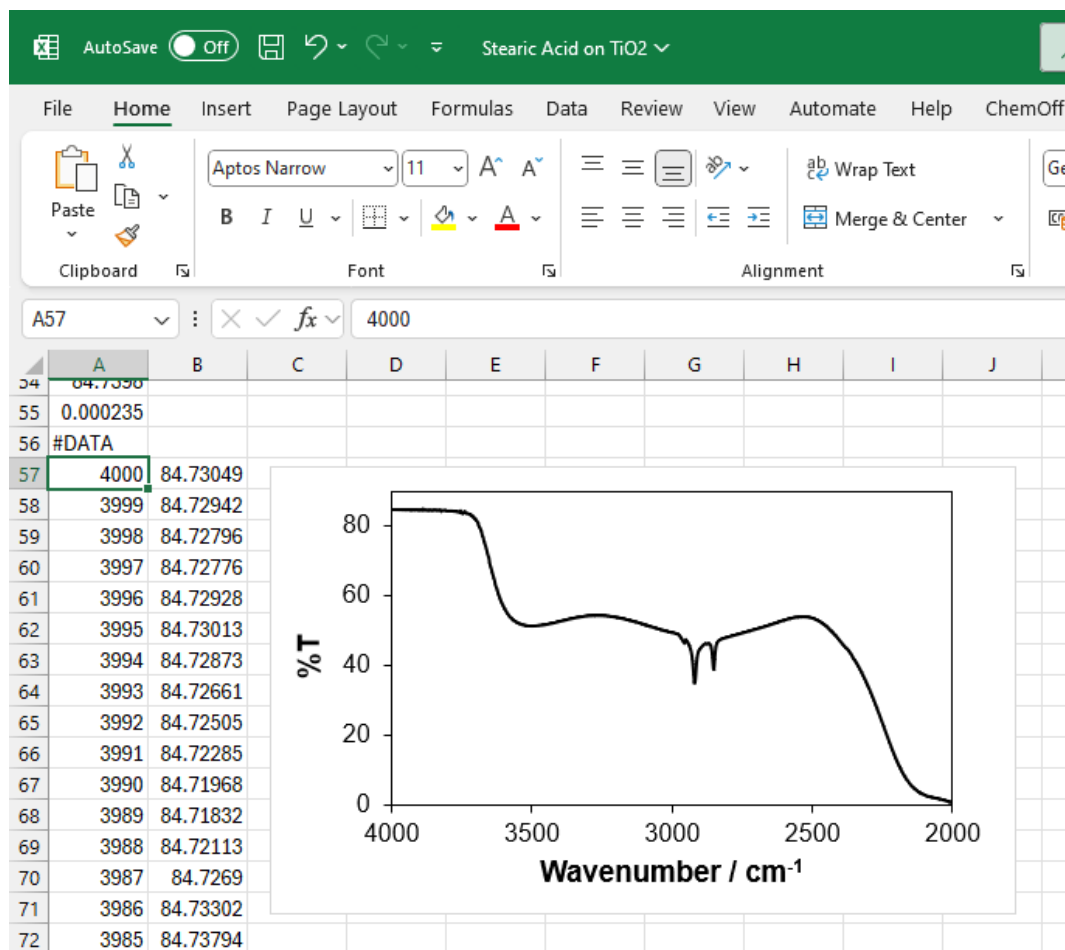
14. If you are recording multiple spectra, simply place in your next sample and click the 'Instrument' dropdown tab again at the top of the screen and select scan. Enter your next file name and click 'Start' and then 'Scan' just as before (step 12). All spectra will be overlaid in the main window.

15. Although all the data is automatically saved, it will have to be saved again in a format that can be read by Excel. **(i)** Click the 'File' dropdown tab and **(ii)** select 'Save As...'. **(iii)** Click on the 'Desktop' button and then you'll have to change the **(iv)** 'Save as type:' to 'ASCII (\*.ASC)' before clicking **(v)** 'Save'. If you have multiple spectra, the 'Save' window will keep reappearing to save the next file until the end of the list is reached. **NOTE:** Each time, you will have to change the 'Save as type:' to 'ASCII (\*.ASC)' before clicking 'Save'.

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16. The ASCII files can be opened directly by Excel. The data can be found by scrolling down to row 57.



17. When finished, ensure that no sample is left inside the spectrometer. The software should be closed and the PC shut down. The FTIR should remain switched on.