

FTIR Virtual Lab

Fundamentals of FTIR spectroscopy

Introduction

The FTIR Virtual Lab contains three learning modules to help teach the fundamentals of FTIR spectroscopy to chemistry students in a remote setting. The Thermo Scientific™ Nicolet™ Summit FTIR Spectrometer includes software workflows and online analysis tools that walk students through the collection and processing steps, which can be done anytime, anywhere, and on any device.

Objectives

Learning module overview

1. **Fundamentals of collection parameters** – FTIR spectroscopy utilizes several data collection parameters that can be changed to optimize a spectrum. This module teaches students about the impact of changing those collection parameters, including number of scans and resolution. See the effects that collection parameters have on signal-to-noise ratios and peak resolution.
2. **Polymer analysis** – Peak locations, peak heights, functional group ID etc., are all important analysis skills for students to learn. The Polymer Analysis module uses the internal polystyrene standard located in the instrument to quickly collect a high-quality polystyrene spectrum. Then, students will conduct basic FTIR processing and analysis steps to correlate the polystyrene spectrum with its chemical structure.
3. **ATR analysis** – Most FTIR systems that students encounter in industry will use an attenuated total reflectance (ATR) accessory. Collecting data through an ATR accessory fundamentally changes the peak intensities, which can impact spectral library searching results. This module clearly shows the difference between transmission and ATR spectra, along with the impact it can have on library searching and material identification.



Thermo Scientific Nicolet Summit FTIR Spectrometer

Materials needed

Material	Details	Helpful links
Educators		
FTIR Virtual Lab set-up instructions Before you begin the FTIR Virtual Lab, it's important to make sure the instrument and software is properly configured. Please download the set-up instructions document.		
Nicolet Summit FTIR Spectrometer with ATR	Thermo Scientific™ OMNIC™ Paradigm Software located on the Nicolet Summit instrument will be used to drive the remote data collection.	Nicolet Summit FTIR Spectrometer
FTIR Virtual Lab Learning Module Workflows	There are 3 learning module workflows available for import into OMNIC Paradigm software. Once imported on the instrument, students will be able to run the workflows remotely.	From your Nicolet Summit Spectrometer, download the FTIR Virtual Lab Folder directly onto the C: drive. This is also the folder where the workflows will export the data.
Standard Remote Desktop Software	Download remote desktop software directly to the Summit FTIR Spectrometer. This enables students to control the Nicolet Summit Spectrometer remotely.	TeamViewer or Google Chrome Remote Desktop
Thermo Fisher Connect account	Data analysis will be done by each student individually in the OMNIC Anywhere cloud-based application located on Thermo Fisher Connect.	Thermo Fisher Connect
Students		
FTIR Virtual Lab set-up instructions Before you begin the FTIR Virtual Lab, it's important to make sure the instrument and software is properly configured. Please download the set-up instructions document.		
Laptop or PC	With a standard remote setup, students will be able to run workflows remotely.	
Standard Remote Desktop Software	Download remote desktop software on to your PC or Laptop. This enables students to control the Nicolet Summit Spectrometer remotely with their laptop or PC.	TeamViewer or Google Chrome Remote Desktop
Thermo Fisher Connect account	Online cloud account for accessing the OMNIC Anywhere application.	Thermo Fisher Connect
OMNIC Anywhere cloud-based application	Data analysis will be done by each student individually in the OMNIC Anywhere cloud-based application located on Thermo Fisher Connect.	Video: Introduction to Connect and OMNIC Anywhere

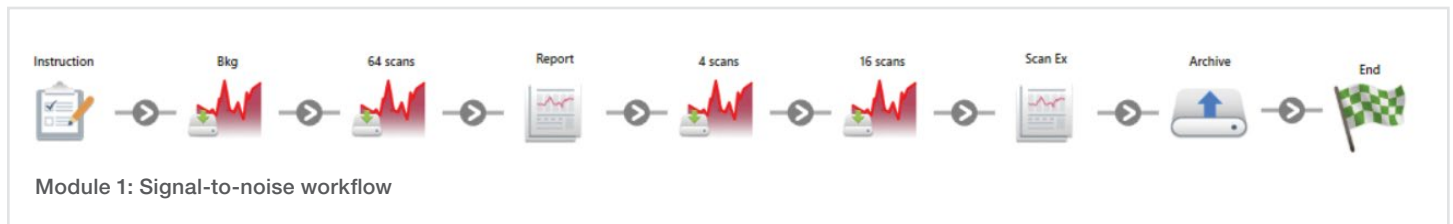
Learning module #1

Fundamentals of collection parameters

Goal: Understand the impact that changing collection parameters, including number of scans and spectral resolution, has on spectral data

Data collection

1. Connect to the Nicolet Summit using the remote desktop application described in the set-up instructions
2. Open OMNIC Paradigm software
3. From the dashboard, locate the *Module 1-SignaltoNoise* workflow, launch it by double-clicking
 - The workflow will walk through several data collection steps, each with a different number of scans. Pay attention to how many scans are collected in each step. Follow the prompts and instructions until the workflow completes



4. Navigate back to the dashboard and launch the *Module 1-Resolution* workflow by double-clicking
 - Follow the workflow prompts and instructions to complete the data acquisition



5. When both workflows are complete, locate and upload your .spa files to your Thermo Fisher Cloud account (for more information on how to do this, see the [FTIR Virtual Lab – Setup Instructions](#))

Data analysis

1. Log into your Thermo Fisher Connect Account
2. Open the three spectra that you uploaded earlier (4 scan, 16 scan, 64 scan) and view them in the OMNIC Anywhere application
3. View spectra in % transmittance and place them on common scale
4. Zoom into specific regions and make note of the difference in spectral noise
 - Generate a report that clearly shows the difference in noise between the three spectra. Export the report to PDF and save
5. Open the three resolution spectra (Res 05, Res 4, Res 16) and view them in the OMNIC Anywhere application
6. View spectra in % transmittance and place them on common scale
7. Find a set of peaks that shows the difference in spectral resolution
 - Generate a report that clearly shows the resolution difference. Export the report to PDF and save

Questions and observations

Include answers to these questions in the submitted lab report

■ Signal-to-noise

1. What did you notice about the relative noise intensity of the three spectra? Rank them in order from most to least noisy.
2. Is the decrease in noise exactly proportional to the number of scans? Explain.
3. How many additional scans must be collected to reduce the noise of a spectrum by 3x?
4. What is the benefit of less noisy data? What is the “cost”?
5. Besides increasing the number of scans, what other ways can we reduce the spectral noise?

■ Resolution

1. What impact does resolution have on the spectral features?
2. Does improved resolution have an impact on every spectral feature, or just some?
3. What is the benefit of higher resolution? Would you run every sample with high resolution?
4. Is higher resolution most important for solid, liquid, or gas analysis? Why?
5. Why does it take longer to collect higher resolution data?

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Learning module #2 Polymer analysis

Goal: Correlate spectral peak locations with chemical structure / functional groups of polystyrene and explain the significance of peak heights and peak areas

Data collection

1. Connect to the Nicolet Summit using the remote desktop application described in the set-up instructions
2. Open OMNIC Paradigm software
3. From the dashboard, locate the *Module 2-Polystyrene* workflow, launch it by double-clicking
 - The workflow will walk through the data collection steps. A small piece of polystyrene is located inside the Nicolet Summit instrument. During the workflow, the software will automatically place the polystyrene sample into the beam path at the appropriate time



4. Follow the prompts and instructions until the workflow completes
5. When the workflow is complete, locate and upload your .spa file to your Thermo Fisher Cloud account (for more information on how to do this, see the [FTIR Virtual Lab – Setup Instructions](#))

Data analysis

1. Log into your Thermo Fisher Cloud Account
2. Open the polystyrene spectrum and view it in the OMNIC Anywhere application
3. Place the spectrum in % transmittance view
4. Using the Find Peaks function in OMNIC Anywhere, determine the wavenumber locations of the prominent spectral features
5. Using the free-standing annotation feature, label the peaks with their corresponding functional group (i.e. CH stretching)
6. Use the peak area tool to find and annotate the area of two separate peaks, one with a small area and one with a large area
7. Use the peak height tool to find and annotate the height of two separate peaks, one with a small height and one with a large height
8. Generate a report that clearly shows all annotations. Export the report to PDF and save

Questions and observations

Include answers to these questions in the submitted lab report

1. What main functional groups are present in the chemical structure of polystyrene? List each functional group and its corresponding peak location(s).
2. Explain the differences in the two annotated peak areas. Why is one area larger than the other? What does that indicate?
3. Explain the differences in the two annotated peak heights. Why is one height larger than the other? What does that indicate?
4. Why are there two CH stretching peak locations near 3000 cm^{-1} ? If they are all CH stretching peaks, why do they appear at slightly different locations?

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Learning module #3 ATR analysis

Goal: Understand why ATR analysis changes the relative peak intensities of a spectrum and investigate the impact of ATR correction on spectra library searching



The diagram illustrates the ATR (Attenuated Total Reflectance) setup. A pressure device tip is shown pressing a sample against an ATR crystal. The sample is held in a crystal mount. The ATR crystal is mounted on a crystal mount. The diagram shows the incident light beam and the reflected light beam, with the sample thickness labeled as d_p .

[Introduction to ATR basics, sample prep and data collection](#)

Data collection

1. Connect to the Nicolet Summit using the remote desktop application described in the set-up instructions
2. Open OMNIC Paradigm software

- From the dashboard, locate the *Module 3-ATR* workflow, launch it by double-clicking
 - The workflow will walk through the data collection steps. First, a background of the instrument will be taken. Then, a pre-collected spectrum of polycarbonate will be uploaded into the workflow.



- Follow the prompts and instructions until the workflow completes
- When the workflow is complete, locate the generated report and spectral files, upload your two .spa files to your Thermo Fisher Cloud account (for more information on how to do this, see the [FTIR Virtual Lab – Setup Instructions](#)).

Data analysis

- Log into your Thermo Fisher Cloud Account
- Open the two polycarbonate spectra and view them in the OMNIC Anywhere application
 - One spectrum shows the results before the ATR correction and the other spectrum shows the results after the ATR correction
- View the spectra in absorbance and overlay them to compare relative peak intensities
- Generate a report that shows both spectra and their relative peak intensities. Export the report to PDF and save

Questions and observations

Include answers to these questions in the submitted lab report

- Explain the change in relative peak intensities from the ATR correction. Which peak heights increase and which ones decrease when a spectrum is collected in ATR vs. transmission mode?
- Why do relative peak intensities change when a spectrum is collected with an ATR accessory? (Hint: consider the ATR depth of penetration equation)
- From your OMNIC Paradigm report, identify which spectrum has the ATR correction applied. How much of an improvement in the library match value was observed?
- Why is it important to correct an ATR spectrum before comparing it to a transmission-based spectral library? How else could you achieve a high library match without having to perform an ATR correction?

Find out more at thermofisher.com/FTIRVirtualLab