

Verify samples quickly

Using reference samples and automated workflows

One of the most popular applications of FTIR spectroscopy is mathematically comparing the spectrum from one sample to that of a known, good reference material. The process of comparing two spectra is used as a verification technique for incoming materials, evidence in a court of law and even proof that a patented chemical is unique. The most simple and reliable metric for measuring the similarity between infrared spectra is determining the correlation value. A perfect correlation results in a value of 100 and any small differences between the two spectra reduces the value. Even with modern FTIR spectrometers, it is extremely rare to have a perfect correlation of 100. Most labs consider a correlation value of 95 or better to indicate a strong spectral match. In a typical industrial environment, the goal is to verify that the sample falls within an acceptable level of purity relative to the good reference material.



Figure 1. Installing the Everest Diamond ATR in the Nicolet Summit with integrated touchscreen.

In the Thermo Scientific™ OMNIC™ Paradigm Software, a function called QCheck makes it easy to compare one spectrum to one or more reference spectra. In this example, we use QCheck to verify that a plastic sample is actually the specified material, polystyrene.

In the OMNIC Paradigm Software shown in Figure 2, we overlaid the polystyrene reference material and our plastic sample. Visually, the two spectra look similar. The peak

locations and intensities overlap well. The QCheck function mathematically calculates the correlation of these two spectra. The results of the QCheck analysis are shown in the report (Figure 3) with a correlation value of 99.81, which is very good.

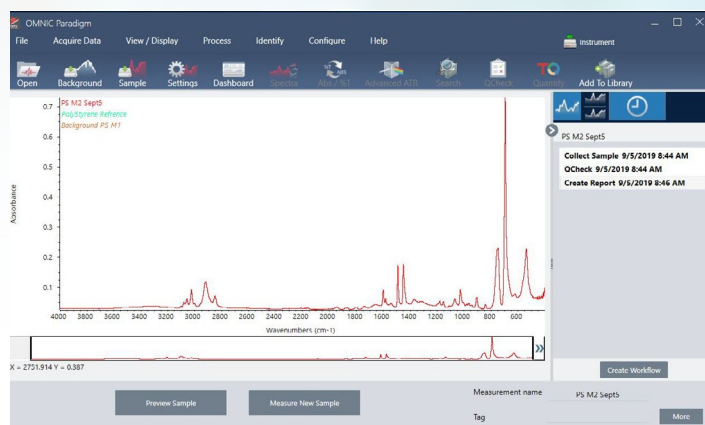


Figure 2. Sample spectrum and best match from QCheck analysis.

QCheck results

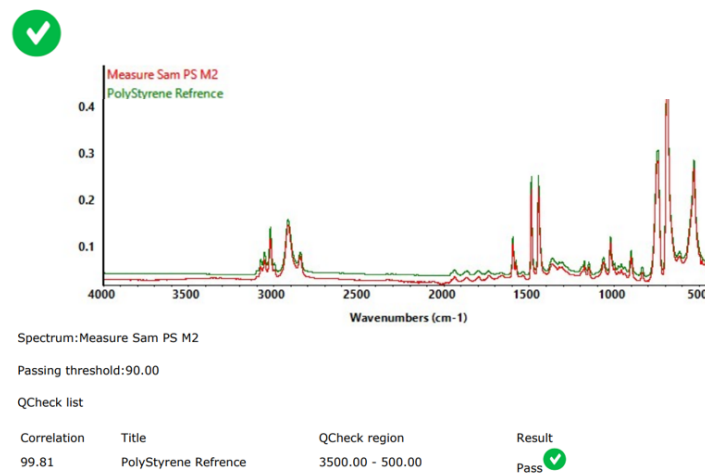


Figure 3. The report from the QCheck analysis.

The QCheck analysis is fast and reliable. Users can also optimize the algorithm to fit their needs, such as selecting the best spectral region for the application, choosing the spectral resolution, determining how much signal averaging is required to produce an acceptable spectrum, and deciding on a Pass/Fail correlation value. Figure 4 shows the different variables that can be optimized in the QCheck function, the most popular of which is selecting specific regions to conduct the correlation comparison.

Using a QCheck workflow

The OMNIC Paradigm Software makes it easy to analyze single samples, as shown above. QC laboratories will often document those steps in a Standard Operating Procedure to ensure that multiple samples can be analyzed consistently. OMNIC Paradigm Software includes a feature set called workflows to automate those steps for busy laboratories that need consistent answers (Figure 5).

A workflow can be easily created from the spectral processing history. Take a closer look at Figure 2. On the right side of the screen, you can see the spectral processing history, which shows that the spectrum was collected, a QCheck was performed, and a report was created. By clicking on the Create Workflow button in the lower right, OMNIC Paradigm will automatically create a workflow based on the spectral processing history. Each step in the spectral processing history becomes a tile in the workflow (Figure 6).

Once the basic workflow is created, users can manipulate the workflow to run multiple samples and save the results in a file that can be opened in Microsoft Excel. If more than one sample needs to be analyzed, users can insert a repeat loop to measure multiple samples in a row. In Figure 6, we added a Repeat tile that repeats the workflow 20 times. To save time, our workflow collects a single background to use with all the other measurements. We then add the Export Tile to append the results to a text file and we can also add an Exit tile to allow users to exit the workflow if they have less than 20 samples to run that day.

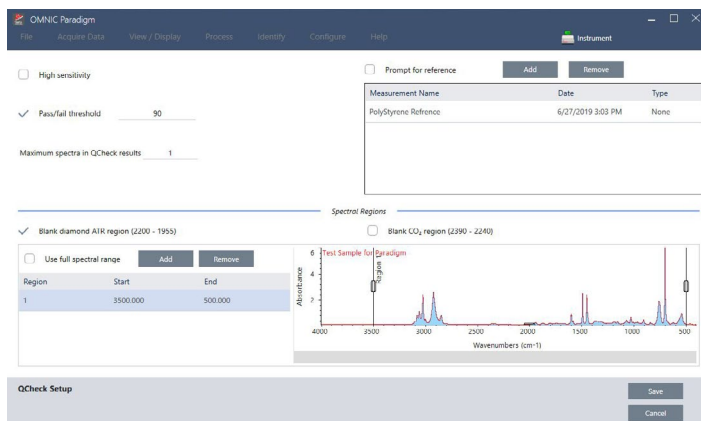


Figure 4. The setup screen for the QCheck analysis.

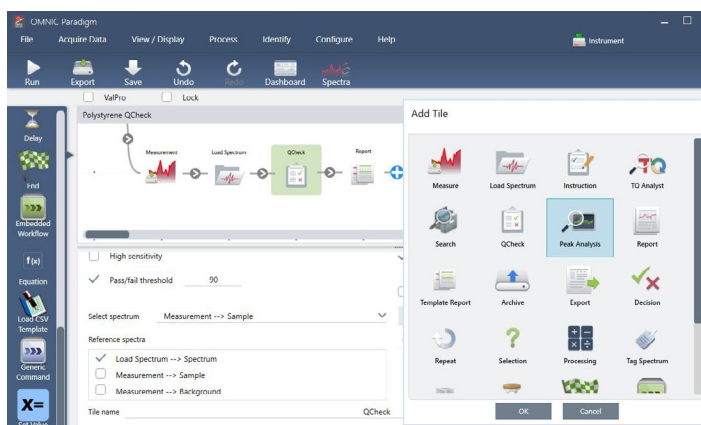


Figure 5. Workflow template and list of possible functions.



Figure 6: A schematic overview of the final workflow. The workflow, spectra, results, and reports are all automatically saved.

OMNIC Paradigm is a modern FTIR spectroscopy platform that makes it easy to mathematically compare one spectrum to another. To automate the process further, OMNIC Paradigm helps users automatically create workflows based on the spectral processing history. If you have OMNIC Paradigm Software, **download the workflow** from the resources section at the bottom of the page to get started!

Find out more at thermofisher.com/paradigm