



Using spectra libraries for your quality control lab

Library FAQs

Why do spectral libraries matter?

Spectral library searching has long been an extraordinarily valuable tool in the analytical chemist's toolbox. The vibrational spectrum of a compound is a kind of "fingerprint" of its component functional groups that can help an FTIR user determine the chemical's make-up. Spectral library searching based on digital matching of spectral signatures is a very effective way of performing qualitative identification of compounds. Thermo Scientific Nicolet's series of spectral libraries includes information relevant to various applications, industries, or spectral techniques.

Why are libraries important in routine FTIR applications?

FTIR libraries are essential to efficient and effective use of Thermo Scientific™ Nicolet™ FTIR applications, especially for identification of compounds and for quality control. By comparing a sample's spectrum against a library of data, the spectroscopist can identify an unknown sample or judge a sample of known identity against an accepted standard.

Users may possess their own libraries, or they might purchase commercial libraries. In either case, the analysts would use these libraries for comparison standards against their samples. Routine users of FTIR spectra libraries would expect to receive either a PASS/FAIL result (for quality control purposes) or an IDENTIFICATION result in the form of the sample's name or CAS (Chemical Abstracts Service) number.

Our Thermo Scientific Nicolet FTIR instruments can be utilized with a wide range of libraries for either of these applications.

How are libraries involved when routine users receive a FAIL result during testing?

Library searches become even more important when a user witnesses a FAIL result for an analyzed sample. When this happens, the situation can be handled in two ways:

1. Attempt to find the closest match to the sample by searching other libraries beyond those applied in the current protocol. (This is still not guaranteed to find a good match, especially if the sample contains contaminating components or is some sort of mixture.)
2. Send the sample out for some other type of analysis that could confirm its identity.

Either of these scenarios—further library searches or alternative analyses—can lead to bottlenecks or even stoppages in production or processing. There is even a chance that the sample in question might need to be quarantined pending a final QC test, causing even further slowdowns. A user's ability to make a quick choice regarding how to proceed with the substandard sample could greatly impact downstream processes and overall efficiency and costs.

Thermo Scientific™ OMNIC™ Paradigm Software with contaminant search and multicomponent search functionality would, in this case, help the analyst make a timely decision. At the touch of a button, this functionality will make use of spectral libraries to search for a mixture of components or find the possible contamination present in the sample.

What different types of spectral libraries are available?

Spectral libraries are broadly categorized as general or specific. Many Thermo Fisher Nicolet libraries would fall under the general category, as they contain the FTIR, FT-NIR, and Raman spectra of a wide variety of common compounds across a variety of fields—a sort of “greatest hits” or “sampler platter” of spectra, if you will.

Specific libraries cover a narrower range of compounds but contain a much more in-depth survey of that range. A specific library might focus on providing spectra for a given niche of industry, such as environmental science, inorganic chemistry, or pharmaceuticals. There are also specific user-created and validated libraries that may be company-specific or contain trade secrets. For example, certain specific libraries are required for USP and EP pharmaceutical raw materials release testing.

Searching general libraries has advantages and disadvantages. Because FTIR and Raman spectroscopic signatures are based on molecular functional groups, even if the exact compound is not present in the libraries, the list of matching compounds from a general spectral library search can often lead to identification, or at least classification, of the material. One can almost always find an answer or a near-match close to the answer when searching through broad libraries.

However, if the user is querying spectra for a compound like a particular active pharmaceutical component or an explosive, broad libraries may not help. In cases like these, specific libraries related to the user’s industry will be more useful.



Figure 1. DXR3xi Raman Imaging Microscope.

Verifier, Identifier, Validator

Users in a QA/QC lab in any industry using vibrational spectroscopy solutions are categorized as either verifier, identifier, or validator.

- The verifier is the user who observes the PASS/FAIL result for a raw material QC check.
- The identifier looks at identity of the substance if the QC test FAILED; they may subsequently be interested in the mixture search test or contaminant search test.
- The validator double-checks that the methods outlined above have been validated and deliver consistent answers with negligible false positives.

For any of these users, OMNIC Paradigm Software, combined with OMNIC Specta Software, will ensure consistent results for your quality control lab using Nicolet FTIR spectrometers.



Figure 2. Nicolet Summit X FTIR Spectrometer.



Figure 3. Nicolet iS20 FTIR Spectrometer.

Learn about the promotions with spectra libraries at thermofisher.com/ftirpromos