Technical Note: 51507

Rapid, Accurate Quality Verification with QCheck

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Key Words

- QCheck
- High-sensitivity Scaling
- Product Verification
- Quality Assurance
- Quality Control
- SOP

Introduction

The primary operation in a quality control and assurance laboratory involves verifying that a material meets specifications. This means assuring the material is what it is supposed to be, or that the level of impurity is below a threshold. Given the high throughput of the typical QC/QA laboratory and the potential for sampling errors, the demand for a simple, fast and error-free analysis tool has become more pronounced.

Thermo Fisher Scientific has worked extensively with QC laboratory personnel to develop the Nicolet™ iS™ 10 FT-IR spectrometer and add enhancements to its OMNIC™ spectroscopy software. At the core of these efforts are new tools for the QC laboratory, including the powerful Spectrometer Performance Verification (SPV) feature and the quality check routine QCheck. Described in detail in Technical Note 51508,[1] SPV provides the QC laboratory with the highest level of confidence in the spectrometer system.

QCheck is designed to permit a rapid quality check of materials. A spectrum of the test material can be compared against another spectrum of the material, against a stored reference (gold standard) or against a stored directory of files. There is no need for constructing libraries – directories containing spectra and their subdirectories can be used without special treatment. Even spectra taken under different conditions (different resolutions, for instance) can be compared without difficulty.

QCheck can be used to compare two materials or, in a more exacting analysis, to discriminate based on subtle differences. Comparison involves a basic quality check method, which will return high comparison values even if there is some variation. Natural products are a good candidate for this procedure, as variation is expected depending upon the natural source, but there is still an underlying similarity. Further, the basic method of comparison gives users of present commercial packages a similar analysis result.

Differentiating materials of slightly different composition requires a higher level of discrimination power. QCheck's high-sensitivity scaling option, unique to OMNIC software, increases the ability to tell these materials apart. Where current quality routines would return multiple answers or pass criteria that are too wide, the high-sensitivity option clearly makes a distinction, providing an even higher level of confidence.

Discrimination in the QC Laboratory: Ethylene Vinyl Acetate (EVA)

Polymer blends of polyethylene and ethylene vinyl acetate (EVA) are used for making food packaging films and hot melt adhesives. In the application discussed here, a target value for the raw material was set at 15% EVA, with a very high pass/fail criterion required.

A simple data base of spectra from samples with a range of EVA concentrations were obtained and saved – neither processing or library creation was needed. A new incoming material was then run through QCheck using the basic algorithm. Figure 1 shows that the sample matched two possible EVA values – 15% and 18% – at a high level. The latter value placed the sample outside of the allowed variation, lowering the confidence of the operator in the method. Confusion of this kind is not satisfactory in the quality control laboratory, where critical decisions can rest on small sampling sets.

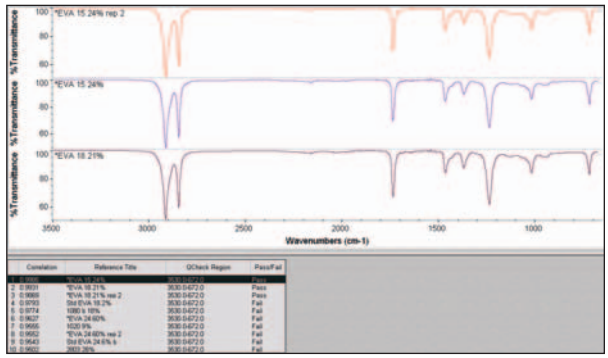

Figure 1: EVA raw material of 15% expected concentration. Result in normal sensitivity correlation mode leaves some room for debate.

Enabling the high-sensitivity option in QCheck provides the much more exacting result, as shown in Figure 2. Now, only the 15% match is within the allowed tolerance limit (0.980 match index), and the next closest is considerably lower. The algorithm stresses small differences, giving the QC lab a much higher level of confidence in the incoming materials verification process. While QCheck is a valuable tool for raw materials inspection, it can be used for finished goods, final inspection or intermediates, enhancing the confidence on materials quality in various stages of the production cycle.

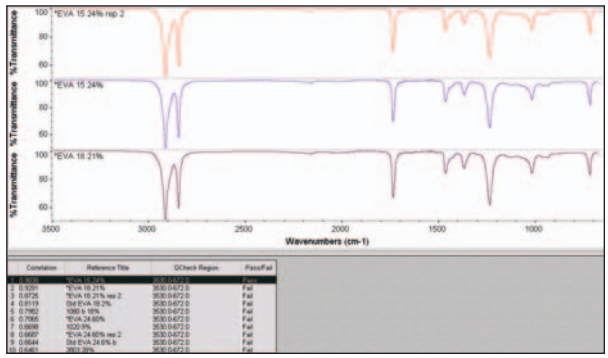

Figure 2: EVA raw material of 15% expected concentration. Result with High-Sensitivity turned on in QCheck is unambiguous.

As a counter example, another EVA copolymer, for a different production line, was first run using the basic method. QCheck returned a range of possible grades for the material, including the pass-criteria of 28%, as seen in the top of Figure 3. However, activation of the high-resolution option causes this material to fail, (as seen in the lower portion of Figure 3), allowing the QC laboratory to reject the incoming material before entering the production cycle. Further analysis of the rejected material reveals that the EVA copolymer is a 32% type, which is not within the specifications range.

	Correlation	Reference Title	Pass/Fail
1	0.9915	Std EVA 28%	Pass
2	0.9899	Std EVA 28% b	Pass
3	0.9621	Std EVA 24.6%	Fail
4	0.9525	Std EVA 24.6% b	Fail
5	0.8760	Std EVA 18.2%	Fail
6	0.7943	Std EVA 15.2%	Fail
7	0.7821	Std EVA 15.2% b	Fail
8	0.6490	Std EVA 9.1%	Fail

	Correlation	Reference Title	Pass/Fail
1	0.9137	Std EVA 28%	Fail
2	0.8993	Std EVA 28% b	Fail
3	0.7034	Std EVA 24.6%	Fail
4	0.6560	Std EVA 24.6% b	Fail
5	0.4690	Std EVA 18.2%	Fail
6	0.4011	Std EVA 15.2%	Fail
7	0.3939	Std EVA 15.2% b	Fail
8	0.3246	Std EVA 9.1%	Fail

Figure 3: EVA copolymer for second production line. Result with normal QCheck is unclear (top, not multiple passes), while the high-sensitive setting clearly makes a discrimination (bottom, only one pass).

Allowable Variation: Natural Products

Natural products will exhibit slight variations due to differences in source materials and growing conditions. Nutraceutical base components will display this inherent variability, while still being acceptable for commercial use. There are definitive characteristics of the components which can be used to make commercial products, so QCheck can be used to clear materials for use.[2] However, the natural variation implies that some flexibility for a pass/fail condition must be allowed.

Samples of nutraceutical materials (Gold Seal Leaf) were analyzed using diamond ATR. The spectra of the different classes of materials are different, but there is also some variation seen within the classes. The spectra from each class were stored in separate directories for organizational purposes. Figure 4 shows the complete set up menu for this analysis. No spectral processing or method development was done. The top-level directory where the spectra are stored is selected, and the option for subdirectories turned on. Nothing more need be done.

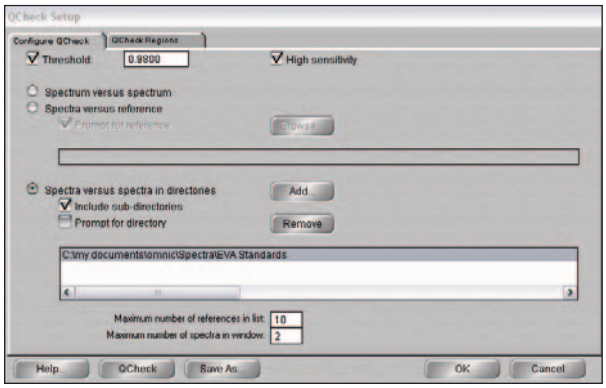

Figure 4: QCheck Setup menu. All options are set here – no method development is needed.

Leaf was first analyzed using the high sensitivity QCheck method. The results, shown in Figure 5, are correct, but the match results are low, due to small variations between the various Gold Seal Leaf samples that are not detrimental to the usability of the material.

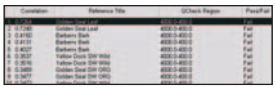

Figure 5: Nutraceutical material analyzed with the high-sensitivity option turned on. The correct material appears at the top of the list, but the analysis fails due to natural variability in the sample.

Switching to the normal QCheck method gives the results shown in Figure 6. The results now show a very high confidence that this material is Gold Seal Leaf. Given the expected variations in natural products, this provides excellent affirmation for the use of this material in the production of nutraceuticals.

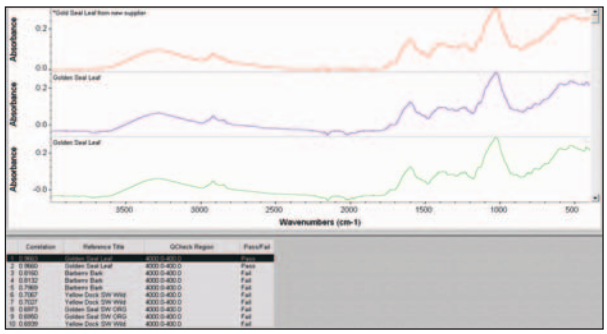

Figure 6: Nutraceutical material analyzed with normal sensitivity setting. There is now a clear pass condition.

QCheck: Flexibility without Complexity

QCheck requires no complex set-up routines. There is no need to build libraries, pick spectral regions or perform complex spectral manipulations to achieve a level of performance which will satisfy the toughest quality laboratory standards. All of these tools are available in the single Setup menu.

The dual analysis algorithms provide tools for your SOP development within a simple interface. The standard algorithm provides confidence for classification of materials, by comparing the spectrum to a group of spectra. QCheck with high sensitivity can investigate the differences between similar materials, providing in some cases semi-quantitative results such as shown here.

Coupling QCheck with the SOP development software included in OMNIC, Macros\Basic™, provides an enormously powerful productivity tool. Automation of SOPs can be built in minutes, removing the variability of the test results from user to user.

Reference

1. Garry, M., Bradley, M. "Confident Data Collection in the QC Lab: Spectrometer Performance Assurance," Thermo Scientific Application Note: 51508
2. Ciorciari, J., Bradley, M. "Classification of Nutraceutical Herbal Powders by FT-IR Using ATR and Discriminant Analysis," Thermo Scientific Application Note: 51254

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TN51507_E 01/08M