Obtaining Optimum Results With Quick IR®+ Quality Match

Michael P. Fuller, Nicolet Spectroscopy Research Center, Madison, WI, USA

Quality Match is one of the suite of applications included with OMNIC® Quick IR+. In addition to Quality Match, these include Scan and Plot, Basic FT-IR, System Validation, Peak Measurement and Simple Quant. This note is intended to explain the theory, optimization and applications of the Quality Match program. Quality Match is used to determine the degree of similarity between a set of reference materials (known good samples) and a material being tested (the unknown).

HOW DOES THE QUALITY MATCH ALGORITHM WORK?

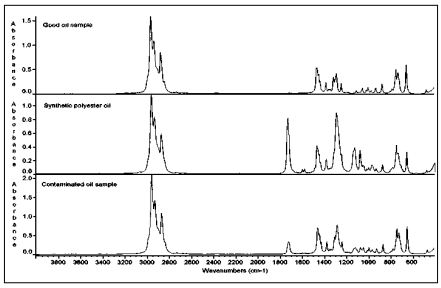
Quality Match compares the unknown spectrum to a list of standard spectra. The algorithm is very similar to the OMNIC correlation search except that unlike a spectral search the derivative of the spectrum is not used in Quality Match. If the unknown spectrum is exactly the same as any of the standard spectra a correlation number of 1.00 is reported. The bigger the differences between the standards and the unknown, the smaller the quality match number becomes. This approach is most useful for large changes in spectral features although, as you will see, it can be used to detect differences in the low percentage composition range.

WHAT PROBLEMS WILL THE QUALITY MATCH PROGRAM SOLVE?

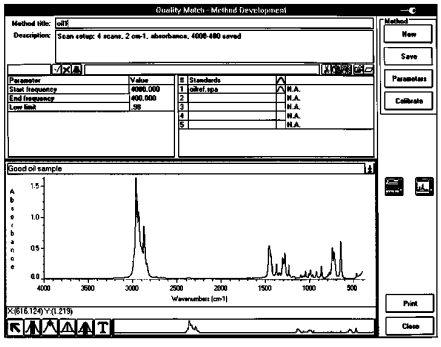
Raw Material Analysis

Often incoming raw materials must be checked to determine if the material is, in fact, what the label or vendor indicates. One example comes from a diesel equipment dealer that stores materials such as various oil types and hydraulic fluids in underground tanks. When a tanker truck shows up with 30W oil, the tractor dealer would like a quick check to determine whether the material is as specified. A Quality Match (QM) method can easily be created to perform this analysis.

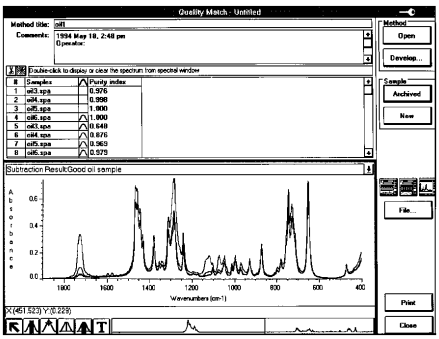
As an example of this experiment the spectra below show a standard petroleum based oil (labeled "good"), a polyester "synthetic" lubricant and the petroleum based oil with a small contamination consisting of the synthetic oil. In this case the QM method is created by using a spectrum of the "good" petroleum oil as the standard. Here we see the region to be used is 4000 - 400 cm^{-1}. Picking the whole spectrum for comparison is usually not the best choice. It is far better to pick a region where changes will be seen such as the fingerprint region from 1200 - 400 cm^{-1}.



Typically reruns of the same or different lots of well controlled materials will give match numbers around 0.999 - 0.990. In the results listed below we find that the contaminated sample gives a match of 0.976 while the spectrum of the pure synthetic oil yields a result of 0.702. Clearly even this low level of contaminant can be spotted through the 0.976 match.

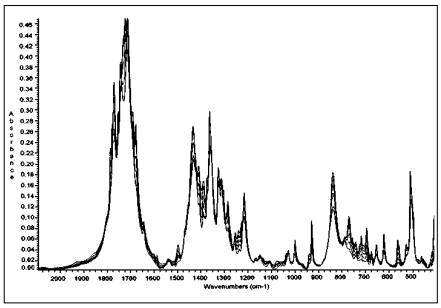


As mentioned above, it is often possible to improve the discrimination power of the QM method by narrowing the region used for the comparison. In the following table the first four values are calculated using the entire spectrum while the second four results are obtained using a region from 1200 - 1000 cm^{-1}. It is clear that the smaller region containing representative bands for the material yields a much more sensitive method even when the polyester contaminant is at a very low level (all spectra are on the same scale)

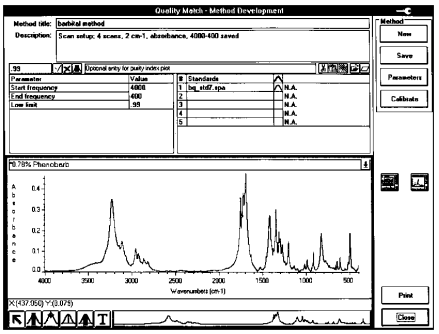


Analyses of Mixtures

The QM approach can also be used when comparing samples containing mixtures of very similar compounds. The following QM method was created to analyze barbiturates. The mixture spectra range from 0.78-16.4% by weight secobarbital. The overlaid spectra below indicate that there is essentially total overlap of the absorptions from the two compounds.



Here the 0.78% secobarbital standard was used to calibrate the QM method. In the first example the complete 4000 - 400

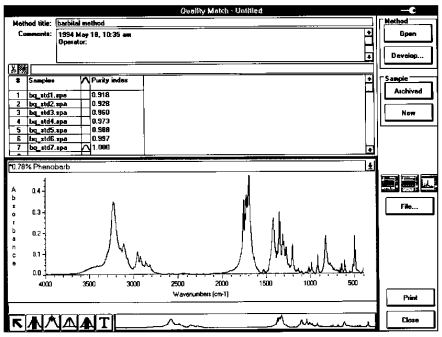


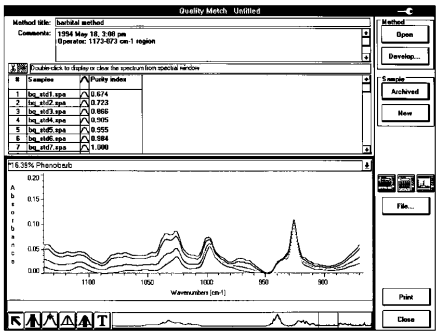
cm^{-1} region was used for the method. Using this approach it is difficult to distinguish the 1.98% mixture from the 0.78% standard. If, however, the 1137 - 873 cm^{-1} region is used we can clearly distinguish even the 1.98% sample from the 0.78% standard. This indicates that with careful analysis range selection differences as low as a few percent can be clearly determined.

CONCLUSIONS

Incoming QC and mixture analyses are just two of many potential uses for the Quick IR+ Quality Match program. In both cases the QM approach was able to distinguish problem samples from reference "good" materials. The QM algorithm is simple to use and is a strong indicator of the similarity of the infrared spectra of materials. What the QM program does not tell you is what match number represents an adequate match value to accept a material under a quality control or quality assurance program. This is left for the user to determine based upon the performance of the product as a function of the match number. Try the QM program sometime and see how easy it is to distinguish similar materials!

Quick IR and OMNIC are registered trademarks of Nicolet Instrument Corporation.





Nicolet Analytical

5225 Verona Road, Madison, WI 53711-4495 • 608-276-6100 • 800-356-8088 • FAX 608-273-5046

Nicolet
ANALYTICAL