Application Note
Quality Control and Sample Verification

Introduction:

The quality control/quality assurance application is used to determine the closeness of an unknown sample to a reference sample. The result is displayed as a percentage match. The method is setup so that the user first scans the reference sample and then can make an unlimited amount of comparisons against the reference.

This application is meant as a basic example of the capabilities of the i-Lab. While it is very useful in its generic form, it can be modified to suit the individual needs of the user. For instance, the Pass/Fail criteria can be changed to a different percentage or instructional messages can be displayed prompting the user to take an action based on the comparison result.

The QAQC application is useful for functions including incoming quality inspection and product consistency inspections. It is also very useful for color matching applications, such as paint matching. It can be used with any available adaptor for the i-LAB.

Methods:

1. QAQCStd
2. QAQCSamp

Process flow:

1. A reference or defined known sample is first analyzed using the method "QAQCStd".
   The spectrum is acquired and a Savitzky-Golay first-derivative calculation is applied to the spectrum. The resulting derivative spectrum is saved and becomes the standard against which the sample spectrum's Savitzky-Golay derivative spectrum is compared against.

2. An unknown sample is analyzed using the method "QAQCSamp". "QAQCSamp" acquires the sample spectrum and applies the Savitzky-Golay first-derivative calculation. The resulting derivative spectrum is then compared against the reference standard derivative spectrum saved by the "QAQCStd" method. A Pearson's Correlation between the sample's derivative spectrum and the standard's derivative spectrum is applied and an R-Squared (R^2) value is obtained.

3. The method then uses the Pearson's Correlation (R^2) value to determine what is displayed. First it checks to see if the R^2 is less than 0.95. If it is, the method reports to the i-LAB® screen "Fail <0.95". Then the program will end.

4. If the R^2 is greater than 0.95 the method will check to see if the R^2 is less than 0.98. Being less than 0.98 means the R^2 is between 0.95 and 0.98. If it is in this range the method will report to the iLAB Screen "Pass 0.95 R^2". Then the program will end.

5. If the R^2 is greater than 0.98 the method will report to the i-LAB® screen "Pass 0.98 R^2". Then the program will end.

What is displayed to the screen:

As the method "QAQCSamp" is run on the i-LAB®, the user will observe the sample being acquired. After which, the user will observe the results of the Pearson's Correlation comparison displayed to the screen.

What is saved to the Library/Log:

During the methods, the "X SPECTRUM UDF" and "Y SPECTRUM UDF" spectra are saved to the Log (for both methods), where they can be downloaded and viewed with the i-LAB® Spectrum Software after the method has been completed. The Savitzky-Golay derivative spectrum (from QAQCStd) is saved to the library – where it is available to be retrieved and compared against the sample's derivative spectrum (from QAQCSamp). The Savitzky-Golay derivative spectra are not accessible to the user.

Basic Methodology:

1. QAQCStd:

The dark current, background and sample (reference standard) spectra are acquired. These spectra are processed to produce a y-Spectrum-UDF format (400-700nm, 1 nm resolution). This spectrum is saved to both the i-LAB®'s internal library as well as the log.

This y-Spectrum UDF is processed into a first derivative spectrum using the Savitzky-Golay derivative function. The 25-point separation averaging method is employed for this derivation calculation. The first derivative spectrum format is a resolution enhancement format that allows increased differences between spectra to be observed. This spectrum is saved to the i-LAB®'s internal library – where it is available to be retrieved and used by other programs.

2. QAQCSamp:

The background, dark current and sample spectra are acquired. These spectra are processed to produce a y-Spectrum-UDF format (400-700nm, 1 nm resolution). This spectrum is saved to the i-LAB®'s log.

This y-Spectrum UDF is processed into a first derivative spectrum using the Savitzky-Golay derivative function. The 25-point separation averaging method is employed for this derivation calculation.

This first derivative spectrum is compared to the derivative spectrum of the reference standard sample stored in the i-LAB®'s internal library obtained using the method "QAQCSamp". This comparison is obtained using a Pearson's Correlation function. The result of the Pearson Correlation is then used to determine if the sample has a <95% match to the reference standard, a match between 95% and 98%, or a match >98% and reports the result to the screen as a pass or fail condition.

Usage Examples:

This method allows one the ability to measure and compare the main spectral features of a sample against a known reference. It will allow the determination how closely these features are to each other.

This method will also allow one the ability to measure if the concentration (qualitatively) of a component in the sample is different from that of the reference. The lower or higher the concentration of this component, the farther apart the match is between the two samples.

Additional Information:

1. i-LAB® Internal Storage: There are two locations within the i-LAB® that one can store information – the Library and the Log. The library is an internal location that can be used by future analyses. The library is not accessible to the user under normal operations. These two methods use the library to store and retrieve the reference sample information – allowing additional unknown samples to be analyzed by "QAQCSamp" against this reference sample. The Log is an internal storage location that can be used to allow the user access to the data. Spectra and results can be stored to this location by a method. These spectra and results can then be downloaded and reviewed using the i-LAB® Spectrum or Datalog Software after the method has been completed.

2. Savitzky-Golay Derivative: The Savitzy-Golay derivative technique is a method commonly used to pre-process spectra before performing additional analysis. The Savitzy-Golay derivative analyzes the rate of change in intensity versus wavelength throughout the spectrum. A sharp peak has a fast rate of change, while the very top of the peak will have no rate of change. By generating the Savitzky-Golay derivative spectrum, additional spectral features are highlighted that are not readily observed from the raw spectrum. This is especially useful for visible spectra, where the peaks tend to be broad.

   The Savitzky-Golay technique obtains the derivative by using the convolution arrays derived from the coefficients of a least square fit formula. Effectively, the technique is a moving average fit to a polynomial, using a defined number of points in the moving average array. Additional information on the Savitzky-Golay derivative can be obtained in the following references:

   1. A. Savitzky and M.J.E.Golay, Anal. Chem, 36(8), 1627 (9164).
   2. J. Steinier, Y. Termonia and J. Deltour, Anal. Chem, 44(11), 1906 (1972)
   3. H.H. Madden, Analytical Chem, 50(9). 1383, 1978.

3. Pearson Correlation: A Pearson's Correlation (R^2) is a linear dependence between two variables. It ranges from +1 to -1. An R^2 of +1 means that there is a perfect positive linear relationship between variables. An R^2 of -1 means that there is an inverse relationship between variables.

4. X Spectrum UDF: The spectrum generated by the normalization of the X axis values into standard universal data format of 400-700nm.

5. Y Spectrum UDF: The spectrum generated by the normalization of the X axis and Y axis into standard universal data format with the X axis representing the wavelength and the Y axis representing the transmission or absorbance value. This is the native spectrum format used in the i-LAB® and Spectrum Software.