Application Note
Quality Assurance Library Store and Lookup

Introduction:

The quality assurance library store and lookup application is used to compare a sample to a library of stored spectra and report the closest match and how close the match is in percentage terms. The application consists of two methods, one to store the library spectra and one to compare an unknown sample against the spectra in the library.

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 number of library entries can be increased or decreased to suit the individual's specific testing needs.

The QA library lookup application is useful for functions including incoming quality inspection and product consistency inspections. It is particularly useful when trying to identify an unknown sample within a group of very similar samples where the human eye could easily be deceived. It can be used with any available adaptor for the i-LAB®.

The minimum firmware revision required to run this application is 1.73.11.

Methods:

1. QA_Library
2. QA_Search

Process flow:

1. A series of reference or defined known samples are first acquired and stored into the i-LAB®'s library using the QA_Library method. This method allows the user to store from one to five samples into the i-LAB®'s internal library. The spectra are acquired and a Savitzky-Golay first-derivative calculation is applied to each spectra. The resulting derivative spectra are saved and become the standards against which the sample spectrum's Savitzky-Golay derivative spectrum is compared against.

2. An unknown sample is analyzed using the QA_Search method. QA_Search acquires the sample spectrum and applies the Savitzky-Golay first-derivative calculation. The resulting derivative spectrum is then compared against the reference standards saved by the QA_Library method. A Euclidean Vector Correlation between the sample's derivative spectrum and each standard's derivative spectrum is applied and the HQI values are obtained.

3. The method then displays the library entry with the highest Euclidean Vector Correlation (HQI) value as well as the HQI value and saves the results to the log.

What is displayed to the screen:

QA_Library:

1. Prompt to Scan Blank
2. Prompt to Scan Sample #1
3. Prompt to Press Menu or Scan Sample 2
    a. Menu ends the storing of the library spectra if less than 5 are desired.
    b. Sample 2 scans another sample into the library.
4. Step 3 is repeated for up to 5 samples.

QA_Search:

1. Prompt to Scan Sample
2. The library entry representing the closest match and the HQI correlation value.

What is saved to the Library/Log:

QA_Library: The samples' Savitzky-Golay derivative spectra are saved to the i-LAB®'s internal memory.

QA_Search: The HQI correlation value is saved to the log.

Basic Methodology:

1. QA_Library

The dark current, background and sample (reference standard) spectra are acquired for up to 5 different known samples. These spectra are processed to generate their corresponding Savitzky-Golay derivative spectra and stored into the library. The dark current and background spectrum are also saved to the i-LAB®'s internal library.

The 25-point separation averaging method is employed for the Savitzy-Golay derivative 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.

After each spectrum is acquired and processed, the user is given the option to either exit out of the method (via the menu key) or scan another sample, for up to 5 samples.

The Library of 5-spectra are saved as a group to be used as the reference library for the QA_Search method.

2. QA_Search

The background and dark current saved from the QA_Library method are retrieved from the i-LAB®'s internal library. Next, the sample spectrum is acquired and processed to generate its Savitzky-Golay derivative spectrum, using the 25-point separation averaging method.

This first derivative spectrum is then compared to each first derivative spectrum of the reference standard samples stored in the i-LAB®'s internal library from the QA_Library method . This comparison is achieved using a Euclidean Vector Correlation (HQI) function. The result of the Euclidean Vector Correlation (HQI) is reported to the LAB®'s screen, along with the corresponding library entry.

The HQI results of the Euclidean Vector Correlation are stored to the LAB®'s log.

Usage Examples:

This method allows the user the ability to measure and compare the main spectral features of a sample against a series of known references and report the closest match along with a numerical representation of how close the match actually is.

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.

It allows these comparisons to not only be between two samples but the unknown sample and a series of samples stored in the library. Thus, one can determine which of this series of samples is the closest to the unknown.

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. Euclidean Vector Correlation: A Euclidean Vector Correlation (HQI) is a linear dependence between two variables. It ranges from +1 to -1. An HQI of +1 means that there is a perfect positive linear relationship between variables. An HQI of -1 means that there is an inverse relationship between variables.

4. 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.

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

6. 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.