

Application Note 129: Spectral discrimination of flour premix using a Series 3000 Food Analyser.



Introduction:

The purpose of this study is to determine if flour premixes can be identified as within specification or not, using their NIT spectrum. This study is not meant to create a calibration or to prove the method, but to demonstrate that these products can be discriminated between the in or out of specification.

Description:

Fifty samples of flour premixes were provided for this study. Each sample was packed into a 5mm petri dish and 10 scans were collected using the Series 3000 Food Analyser, between 720 and 1100nm. 12 samples from each of the in and out of specification batches were then combined into two library files called "Good" and "Bad" respectively.

Figure 1 below shows the standard absorbance spectra for all flour premixes.

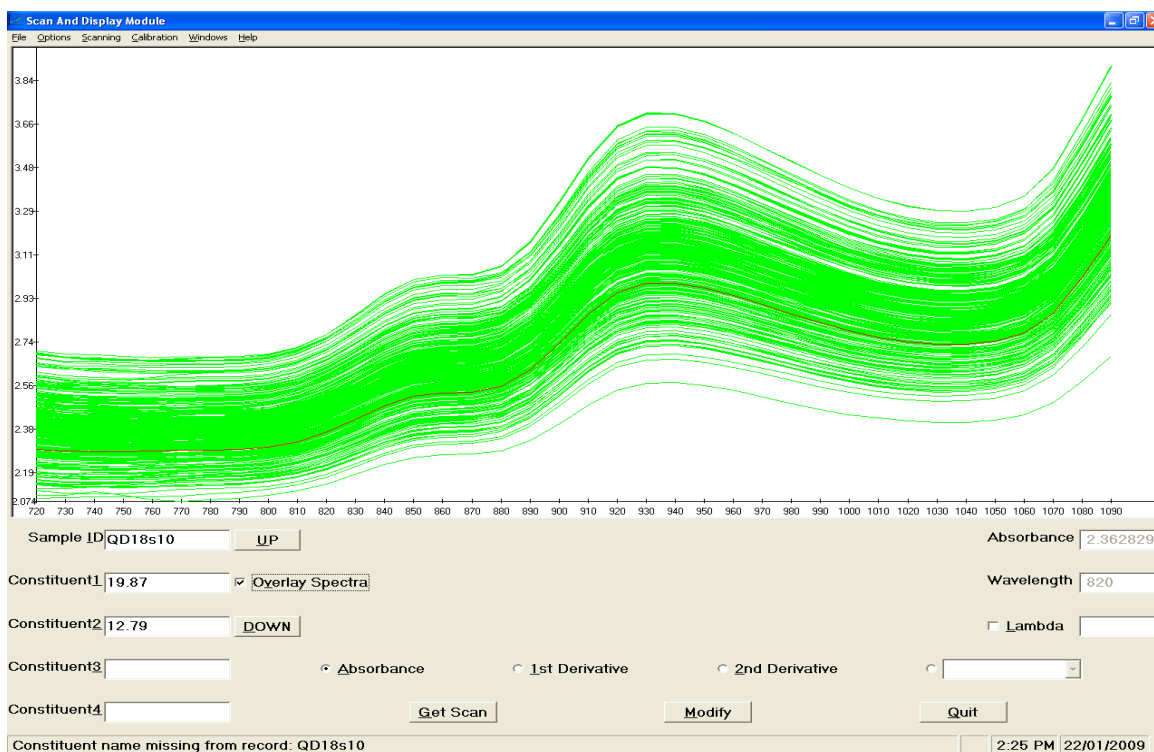


Figure 1: Absorbance Spectra for all flour premixes.

The remaining samples were then analysed using the NTAS Discriminant Analysis software include in NTAS(NIR Technology Analysis Software). The Discriminant Analysis software calculates the Mahalanobis Distances between the unknown sample spectrum and the library files. The library file with the lowest Mahalanobis Distance is selected as being the closest match.

Figure 2 below shows results of the Discriminant Analysis routine of an "In specification" or "Good" sample.

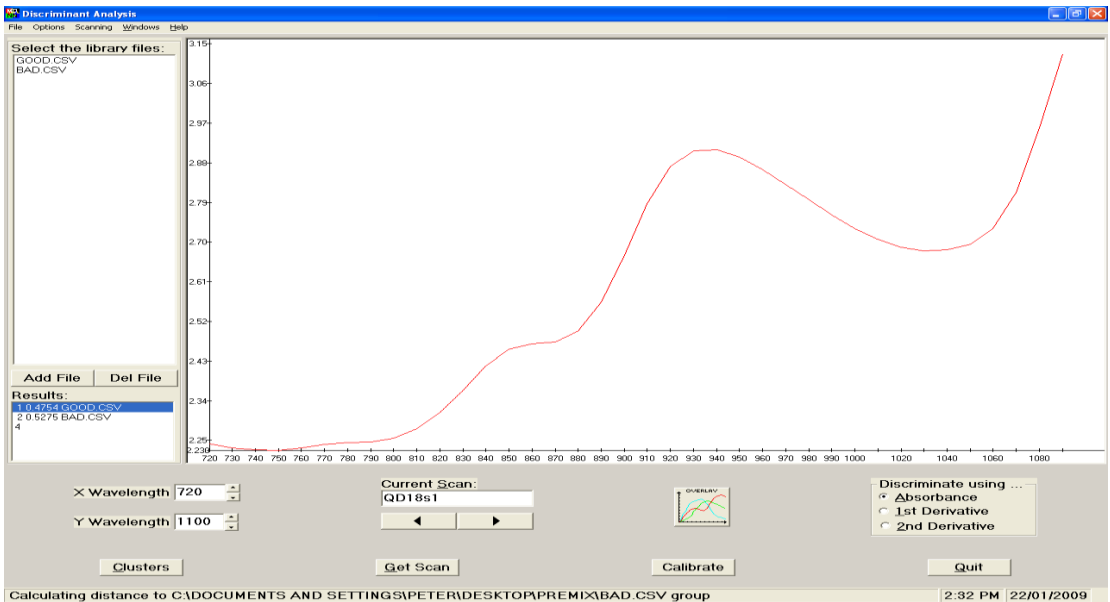


Figure 2: Discriminant analysis results for a good product.

Figure 3 below shows Discriminant analysis of an “out of specification” or bad sample.

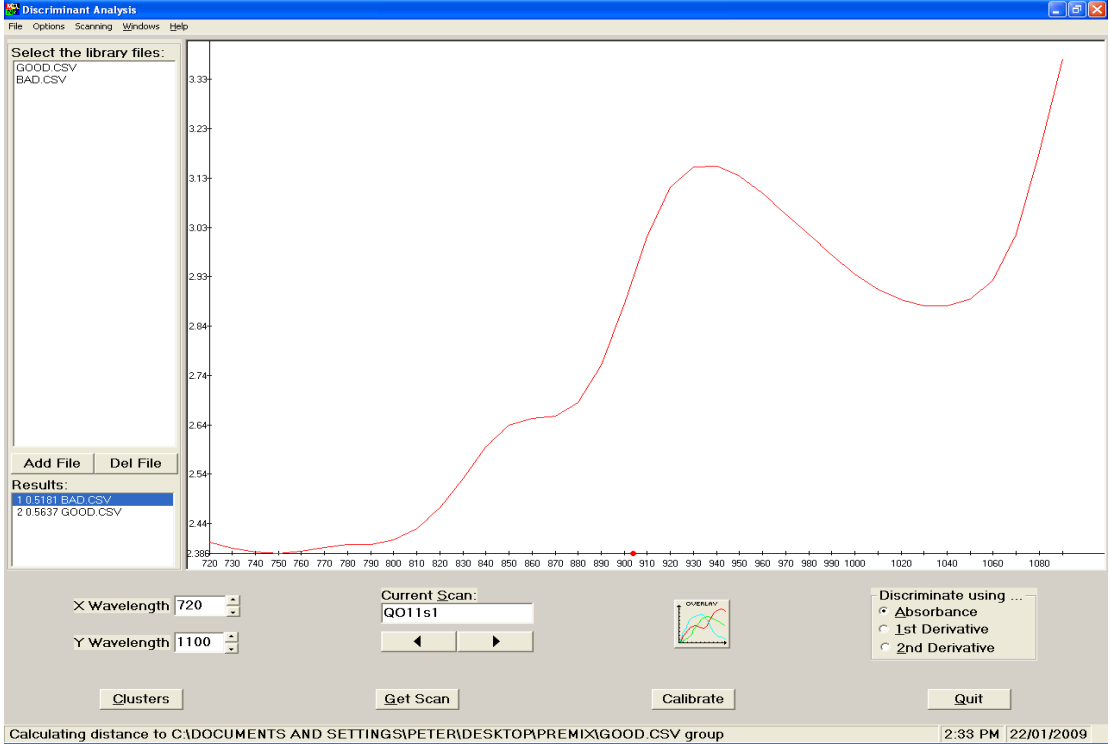


Figure 3: Discriminant Analysis of a “Bad” sample or “Out of Specification” product.

The table below shows the full list of samples and whether the sample was “Good” or “Bad” according to Discriminant Analysis routine.

Sample ID	Group
QD10	Good
QD12	Good
QD16	Good
QD17	Good
QD23	Good
QD30	Good
QD31	Good

QD13	Good
QD18	Good
QO20	Bad
QO23	Bad
QO24	Bad
QO11	Bad
QO12	Bad
QO15	Bad
QD32	Good
QD33	Good
QO03	Bad
QO04	Bad
QO07	Bad
QO08	Bad
QD24	Good
QD25	Good
QD26	Good
QD27	Good
QO16	Bad
QO19	Bad

Table 1: List of Validation Set Results.

Conclusion:

The spectra for both in and out of specification products cannot be visually identified from their spectra. However, the Discriminant Analysis software was able to accurately and reproducibly categorise the products into the correct groupings.

This analysis could be conducted on several of the range of analysers on offer by NIR Technology Systems that operates in the 720-1100nm spectral region. The Series 3000 Food Analyser was chosen because of the ease of sample loading.

It can therefore be concluded that the Series 3000 food analyser is capable of discriminating between the in and out of specification flour premixes supplied.