USING A DA 7200 DIODE ARRAY HIGH SPEED ANALYSIS SYSTEM TO ANALYZE DRIED CRANBERRIES

BACKGROUND

Fifteen samples of dried cranberries were sent to Decagon Devices and Perten Instruments. The purpose of the samples was to test the feasibility of using the DA 7200 Diode Array NIR Analysis system to measure the Water Activity, Oil Content, and Karl Fisher Moisture Content of Cranberries in 6 seconds.

MATERIALS & METHODS

Instrumentation

A DA7200 diode array based spectrometer was used for optical data collection on all samples. The DA7200 spectrometer consists of a stationary grating for wavelength dispersion and 256 pixel Indium-Gallium-Arsenide (InGaAs) detector operating in the wavelength range 950-1650 nm for energy detection. The spectrometer records 180 absorbance spectra in a typical analysis time of 6 seconds. A built-in ceramic reference and patented emission lamp ensure spectrum and wavelength reproducibility.

Figure 1. – DA7200

A unique feature of the spectrometer is its ability to collect spectra in ambient room light precluding the need for a light-tight sample enclosure. The DA7200 uses open faced sampling dishes for presentation to the instrument eliminating any instrument to sample contact. Closed faced sample cups or cells are significant sources of error and are difficult to clean. Sample cups exhibit significant variability in results from cup to cup and are subject to operator influence by packing differences, damage, or cup rotation. The sample cups/cells are difficult to clean – particularly when fatty or high moisture products are analyzed. The DA7200 eliminates the needs for these cups providing more accurate, real world results and significantly shortening analysis time.

Samples **(***Note: all samples were analyzed as received with no further sample preparation required***)**
Each sample consisted of enough cranberries to fill a 5" diameter sample dish. A sample consisted of all of the cranberries packaged together in the individual plastic bags. There were 15 total bags resulting in 15 total samples. The DA 7200 rotates the sample dish during analysis collecting spectral data on the full sample. 180 individual spectra are collected during the 3 second rotation and averaged together. Each sample was re-packed and spectra collected again to measure sample homogeneity and reproducibility. Two samples were not used to develop the calibration for oil content due to missing data.

Figure 2. – Aqualab

After spectra collection, a sub-sample of cranberries was immediately placed into a Decagon cup and analyzed for Water Activity using an Aqualab Series 3TE. Each sample was analyzed in duplicate on the Series 3TE as well. The average of the two values was used as the reference value for calibration development.

DEFINITION OF TERMS

PLS – Partial Least Squares, a calibration algorithm that finds patterns in the spectra which are a cross between the pattern of the analyte and the pattern which describes the largest variability in the spectrum.

R^2 – The square of the correlation coefficient R; a measure of the variance described by the model to the total sample variance.

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SECV – Standard Error of Cross-Validation; the expected error or accuracy of the calibration. SECV is calculated by leaving each sample out of the calibration, calibrating the rest of the samples, and then predicting the one left out.

MSC – Multiplicative Scatter Correction; a technique for correcting spectra using a baseline offset and slope for each spectrum.

RESULTS & DISCUSSION

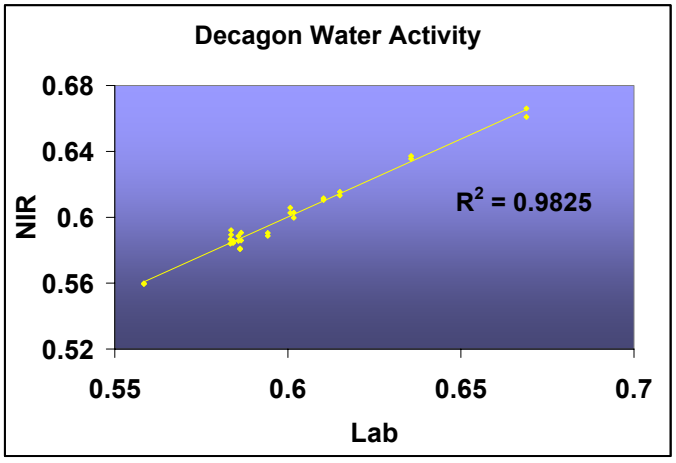
PLS 1 with Multiplicative Scatter Correction was used to develop a calibration for Water Activity, Oil Content, and Karl Fisher Moisture Content. Table 1 lists the calibration statistics for all of the parameter and Figure 1 shows the predicted vs. actual concentrations. Included in the statistics are the range of lab analytical values, the R^2, SECV (Standard Error of Cross Validation), and the number of samples used.

Table 1. Calibration statistics for all 4 constituents.

Parameter	Range	Samples	R^2	SECV*
Water Activity	0.558-0.669	15	0.982	0.0035
Oil	0.210-0.690	13	0.707	0.075
Karl Fisher Moisture	13.0-20.5	15	0.754	0.863

Figure 1. Actual lab values vs. predicted NIR values

Water Activity
The results are very good for Water Activity and much better than Karl Fisher Moisture..



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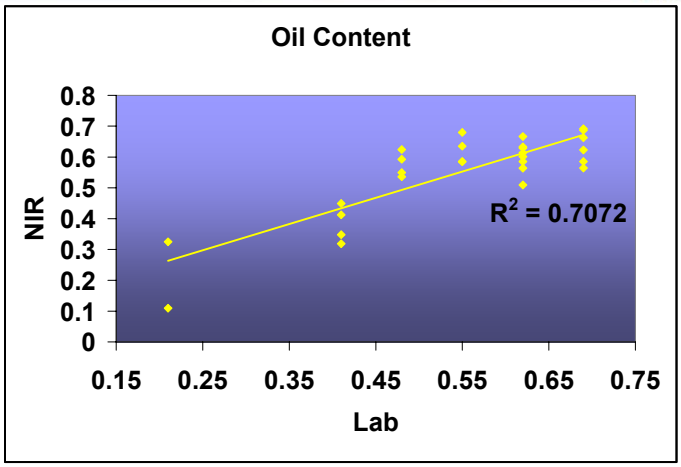
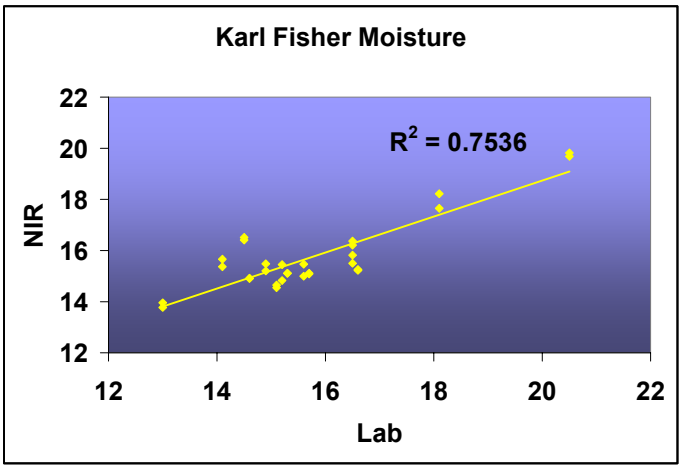
Oil Content
The results were not as good for oil content, but similar to other calibrations for oil content. One problem is the low resolution of the reported values.



Karl Fisher Moisture Content
The results were not as good for Karl Fisher Moisture either. It is interesting how much better the results are for water activity vs. moisture content



COMMENTS & CONCLUSIONS

The results of this preliminary study indicate that NIR has huge potential in accurately measuring Water Activity. The results for Oil Content and Karl Fisher were not as good, but similar to calibrations for these constituents for other products. It is very interesting to note how much better the results were for Water Activity than moisture content.

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