Application Note 127: Multiple Calibration Selection (MCS) software for use on Australian Barley

Introduction:

Measuring protein in whole barley grains has presented a significant problem for the last ten years. Many attempts to develop a universal calibration to cover malting grade and feed grade barley, different varieties, different growing regions and different weather affects, have proven of limited success. In comparison, a stable calibration for protein in whole wheat grains has been developed eight years ago and has proven successful across all states of Australia and even in the USA, Canada and South Africa. As such, we have been looking at new software that can resolve the complex variability that is encountered with barley. This paper introduces a software routine called "Multiple Calibration Selection", ie, MCS, and presents data to illustrate the benefits it offers when measuring protein and moisture in barley.

Description:

Whole wheat and barley grains are generally measured using Near Infrared Transmission in the wavelength range, 720-1100nm. Within this region of the NIR spectrum, protein(N-H), moisture(O-H) and starch(C-O-H) absorb energy. However barley grains have a husk over the endosperm and depending upon the aging and weather affects, the husk becomes separated from the endosperm. This separation of the husk causes a difference in the NIT spectrum, which in effect causes difference in the calibration model required to characterize the protein and moisture in the grains. Figures 1, shows the spectra of two barley samples. The spectrum are called BarleyA and BarleyB. The important spectral difference is at approximately 820nm. In BarleyA, the spectrum shows a distinct minimum, whereas BarleyB shows a slight indent in the spectrum.

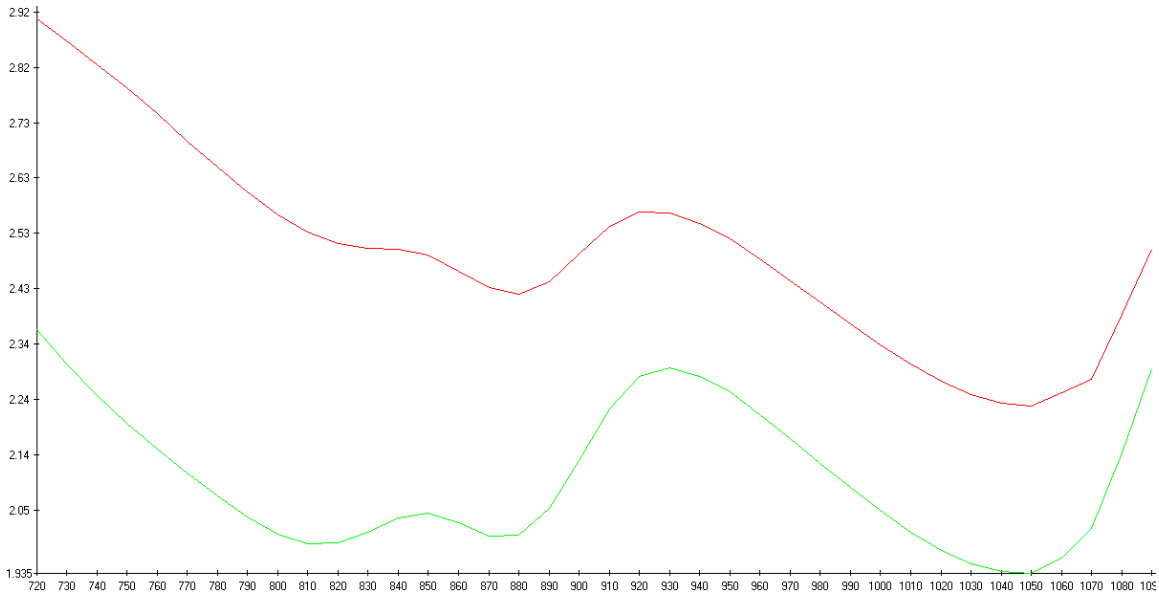

Figure 1. Spectra of BarleyA and BarleyB samples.

This difference in the spectra can be used to select type BarleyA and BarleyB and to apply unique calibrations to each type of barley.

By converting the absorbance spectra into the first derivative spectra, as shown in Figure 2, it can be seen that type BarleyA have a positive value at wavelength 820nm, where as type BarleyB have a negative value at 820nm.

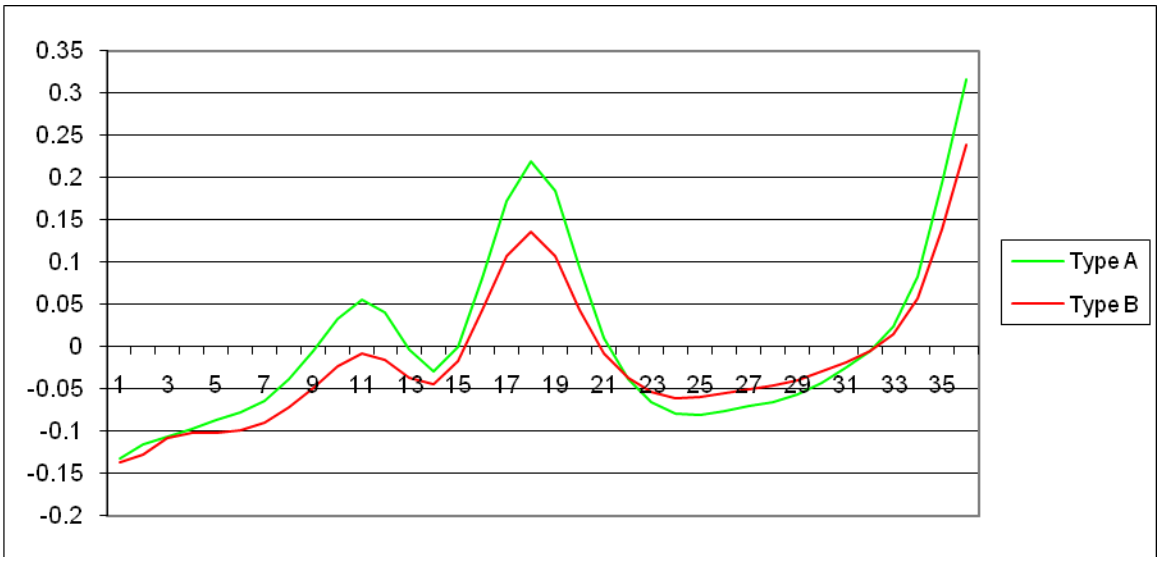

Figure 2. 1st Derivative Spectra showing type BarleyA and type BarleyB samples.

Calibration Development:

141 samples of barley were collected from around Australia. 109 samples were determined to be type BarleyA and 32 samples were determined to be type BarleyB. Figure 2. shows the plot of the 141 samples, each scanned in duplicate, to generate 282 spectra.

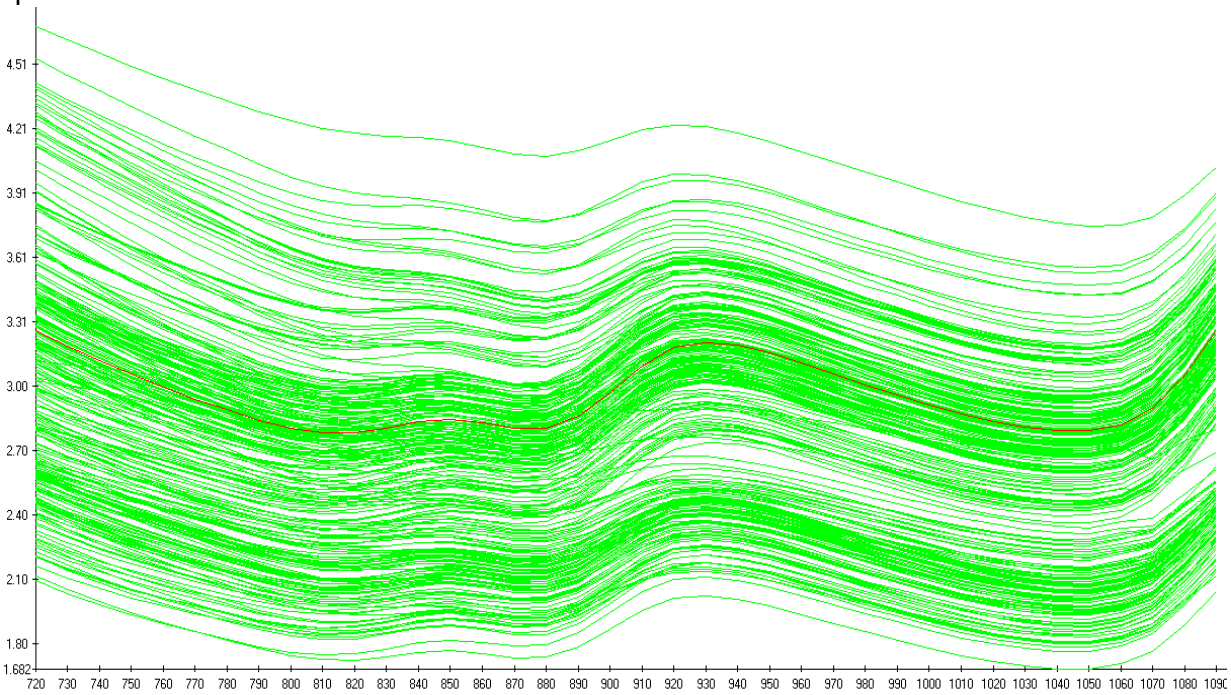

Figure 2: NIR spectra of scanned barley samples.

Figure 3. Shows the calibration plot for protein using Partial Least Squares regression, NTAS, NIR Technology Analysis Software, NIR Technology Systems, Sydney, Australia. The standard error of calibration(SEC) was computed to be 0.40% and the correlation coefficient(R^2) was computed to be .879. Considering that the desired SEC would be 0.30%, this calibration model is not acceptable.

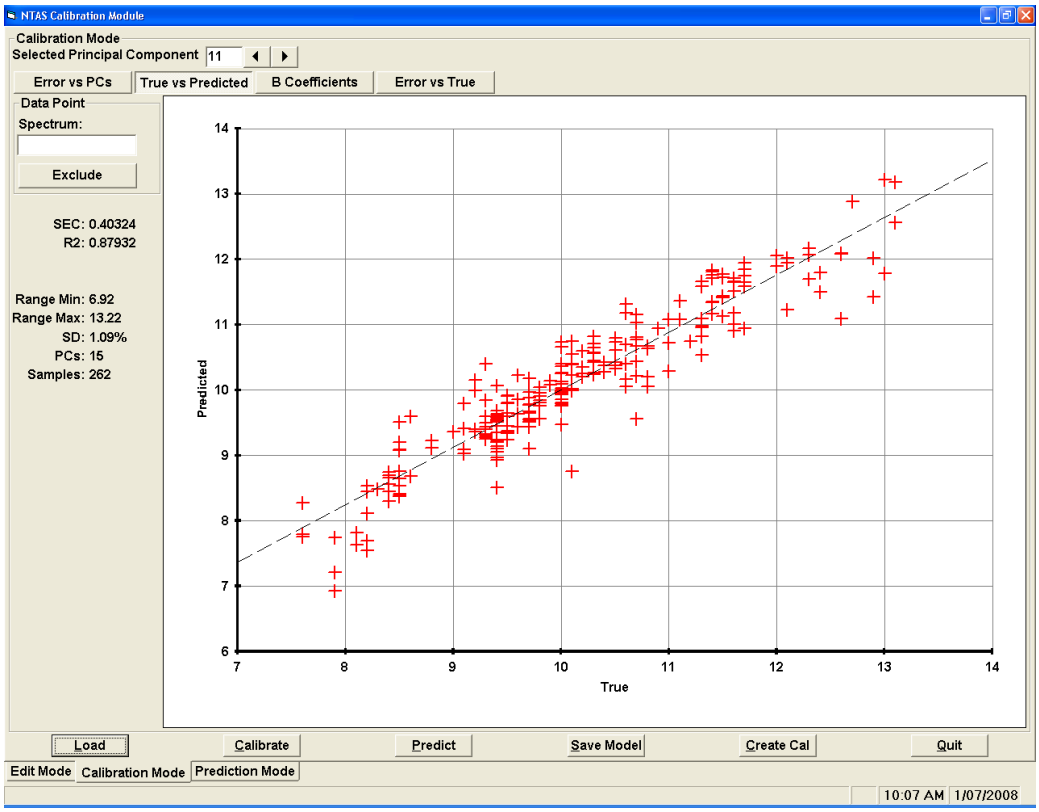

Figure 3: Calibration plot for Protein.

By separating the barley samples into BarleyA and BarleyB, the calibration was significantly improved. Figure 4. shows the calibration plot for BarleyA samples and figure 5. shows the calibration plot for BarleyB samples.

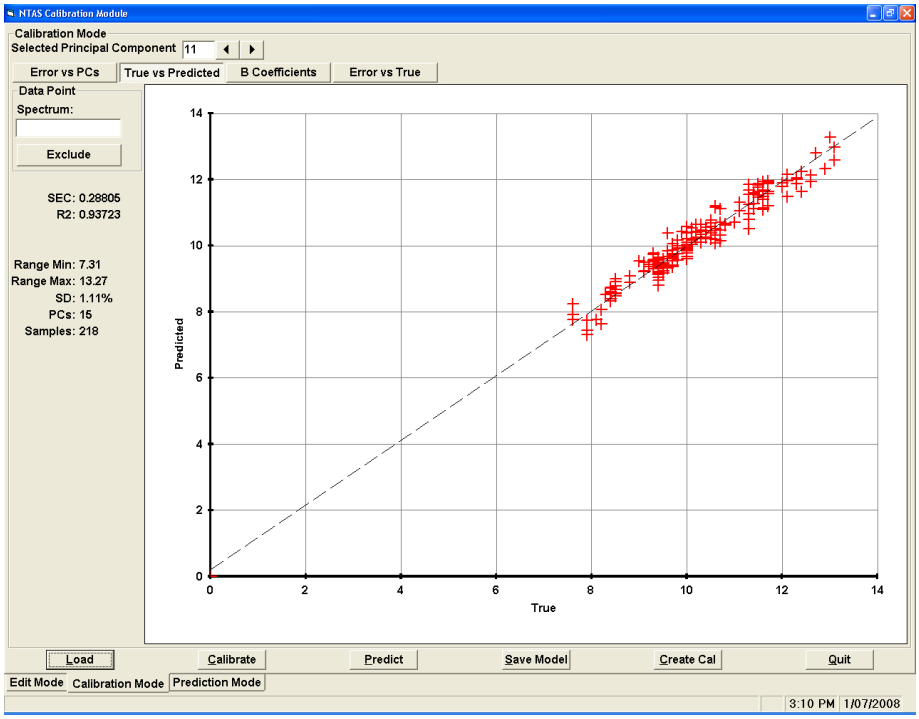

Figure 4: Calibration plot for protein in type BarleyA.

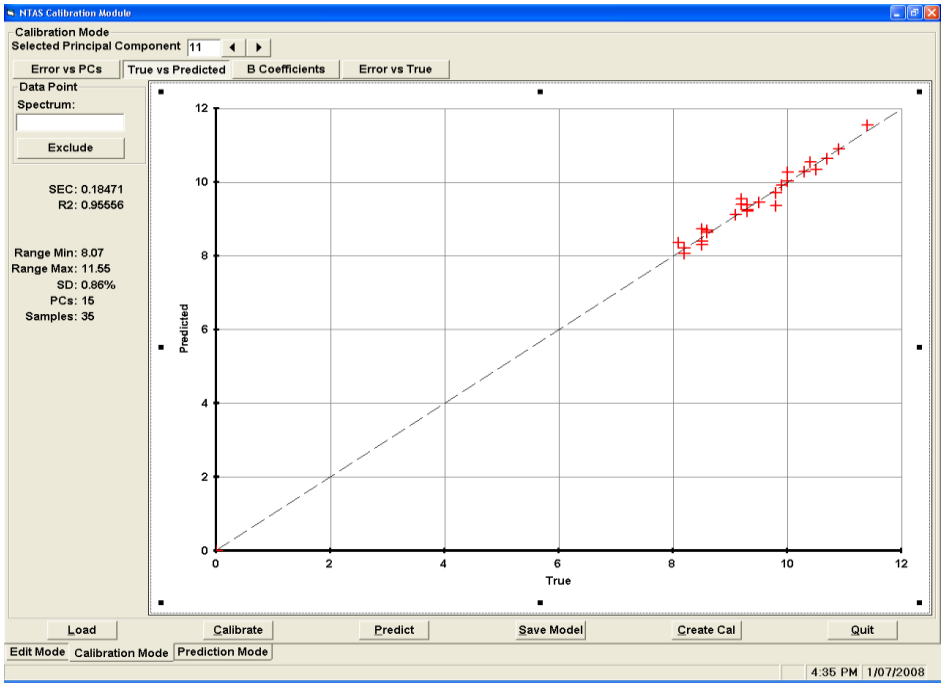

Figure 5: Calibration plot for protein in type BarleyB.

The results of separating the types of barley are shown in table 1.

Table 1.

	Protein	
	SEC	R^2
BarleyA	0.29%	0.923
BarleyB	0.18%	0.955

Another set of barley samples were used as a prediction set to evaluate the two separate calibration models. Figure 6. shows the prediction plot for BarleyA samples and

figure 7. shows the prediction plot for BarleyB samples. Table 2. shows the prediction data.

Table 2. Protein

	SEC	R^2
BarleyA	0.21%	0.976
BarleyB	0.36%	0.985

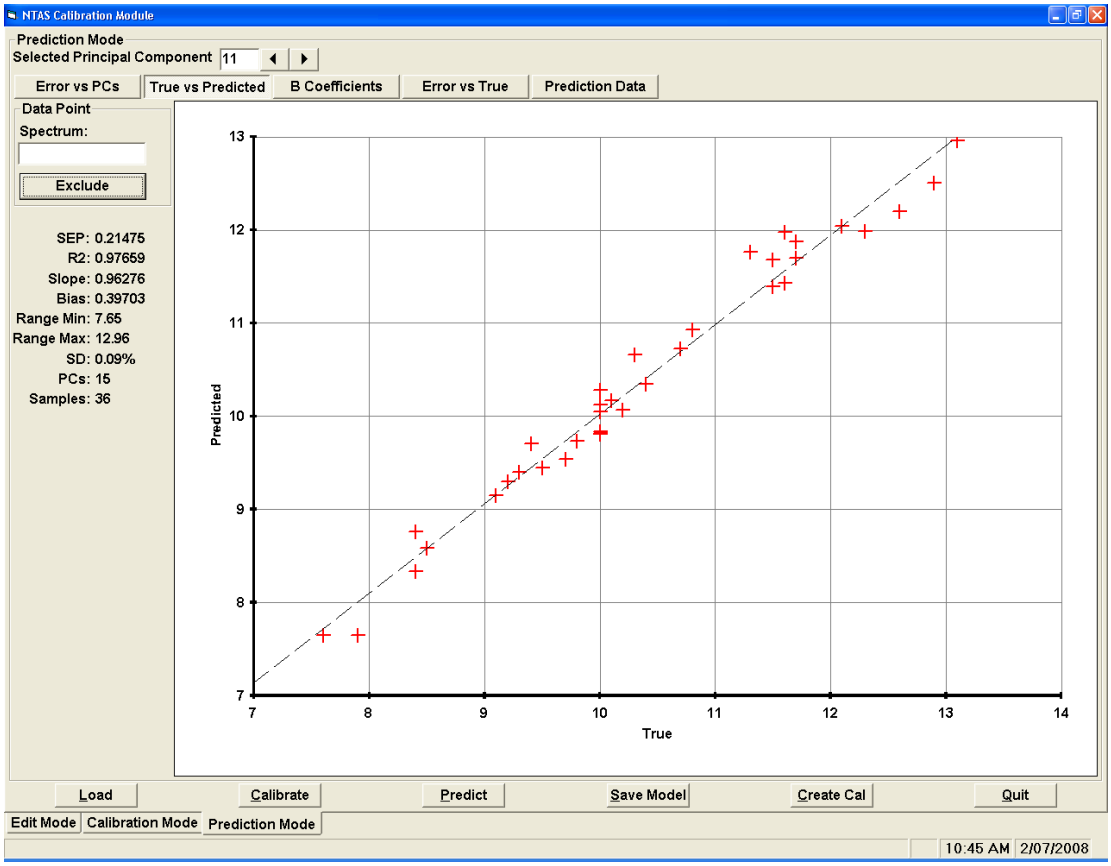

Figure 6: Prediction plot for protein in type BarleyA.

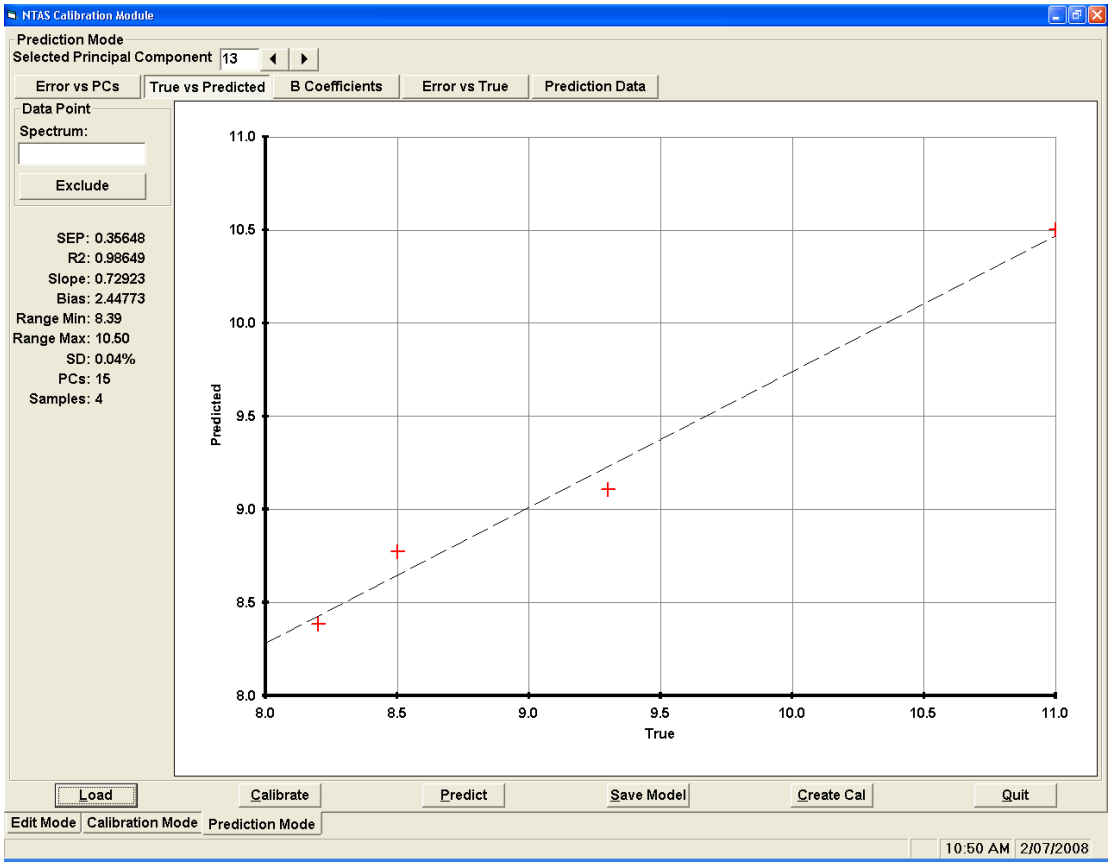

Figure 7: Prediction plot for protein in type BarleyB.

Discussion:

MCS software is a simple routine that is part of the operating software included in the Cropscan 1000B and 2000B range of NIT analyser. This software scans the barley sample and computes the 1st derivative spectrum. If the spectrum at wavelength 820nm is positive, the sample is assessed as BarleyA and if the spectrum is negative or zero, the sample is assessed as BarleyB. The software then applies the appropriate model for protein and moisture.

The data presented above is limited because of the number of samples available for the study. Most significant is the small number of BarleyB samples. However similar studies were performed on barley samples collected in Italy and The Netherlands. In these cases, there were more BarleyB samples than BarleyA, however the results were very similar. The use of the MCS resulted in a significant reduction in the SEP for protein for both BarleyA and BarleyB samples.

Moisture measurements can be significantly improved using MCS, however the problem has always been about the variability in protein data where as moisture measurements have been considered acceptable.

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