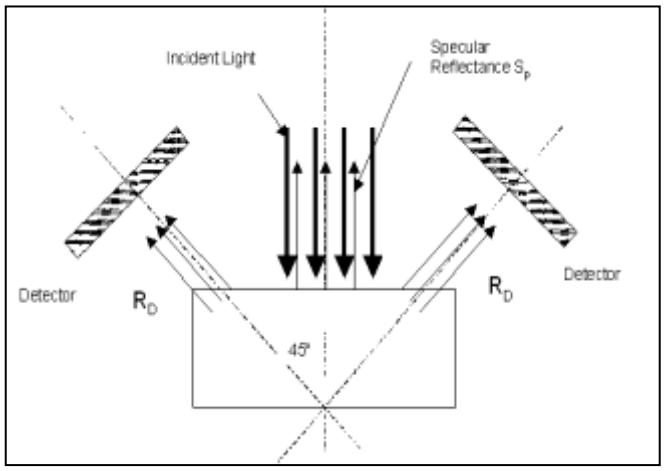
Application Note 179. A comparison between for protein and moisture in animal, fish and feather meals using the Series 4000 FTNIR using spectra at 64cm-1 and 16cm-1 resolution.

Introduction:

Near Infrared Reflectance spectroscopy is best performed in the 1900 to 2500nm region of the electromagnetic spectrum. Within this spectral region, Protein (N-H 2120nm), Moisture (O-H, 1940nm) and Fat (C-H, 2350nm) absorb NIR energy. Using 0 – 45 degree illumination and detection optics, as shown in figure 1, provides a means of collecting NIR spectra from samples such as Hemp Powder. Using a Fourier Transform (FTNIR) spectrometer to collect diffuse reflectance spectra from powdered samples provides a very accurate and precise means of developing NIR calibrations for a number of parameter, including: Protein, Moisture, Fat and Ash.



A FTNIR Spectrometer offers several advanced features including superior wavelength precision, variable resolution, faster scanning speed and immunity to stray light or external light.

A feature of the MultiScan Series 4000 FTNIR Spectrometer is the ability to collect spectra at 1, 2, 4, 8, 16, 32, 64cm-1*. However the question arises whether higher resolution spectra improve or degrade a calibration.

Procedure:

To test this idea, a set of meal samples, ie, 3 feather meal, 3 animal protein meal and 3 fish meal samples were scanned using the Series 4000 FTNIR Spectrometer at 64cm-1 and 16m-1 resolution. NTAS software was used to perform a Partial Least Squares Regression for protein and moisture against the spectra.

Results:

Figure 1 shows the 64cm-1 resolution spectra and figure 2 shows the 16cm-1 resolution spectra.

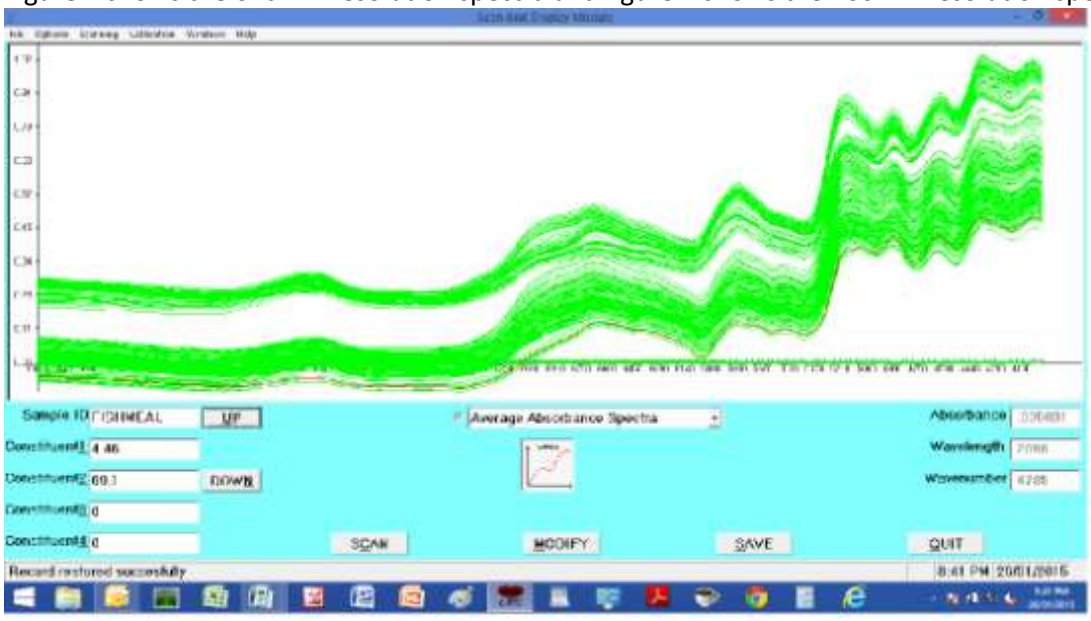


Figure 1. Meal Spectra at 64cm-1

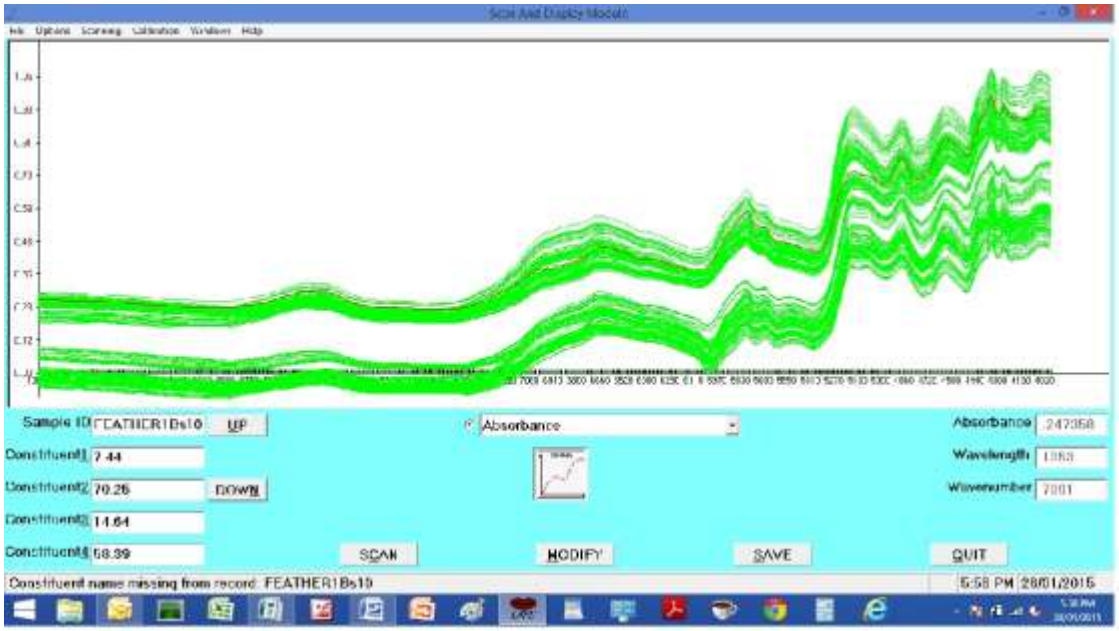


Figure 2. Meal Spectra at 16cm-1

Although the spectra look similar, the 16cm-1 spectra have more defined peaks, especially for the oil bands at 5790-5690cm-1 and 4350-4250cm-1 regions.

Figures 3 and 4 show the calibration plots for protein using the 64cm-1 and 16cm-1 spectra.

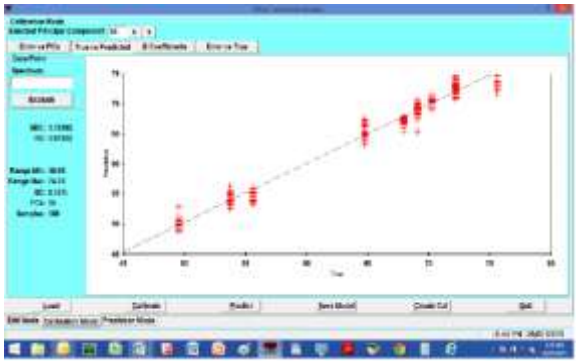


Figure 3. Protein Cal Plot at 64cm-1

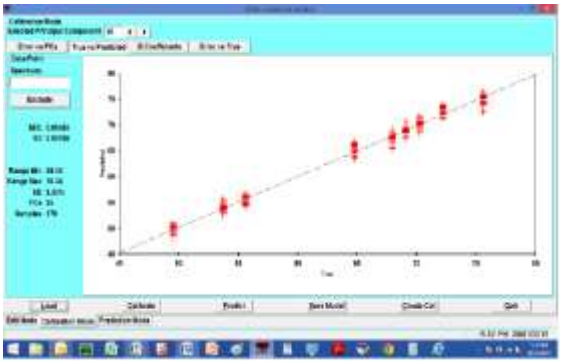


Figure 4. Protein Cal Plot at 16cm-1

Figures 5 and 6 show the calibration plots for moisture using the 64cm-1 and 16cm-1 spectra.

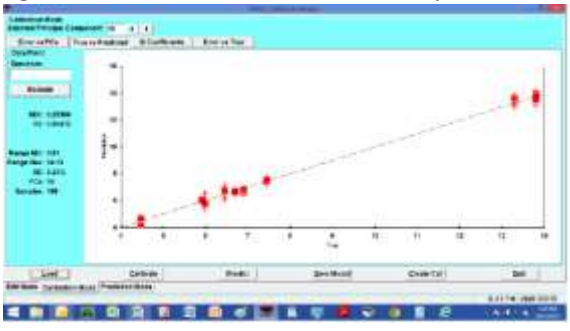


Figure 5. Moisture Cal Plot at 64cm-1

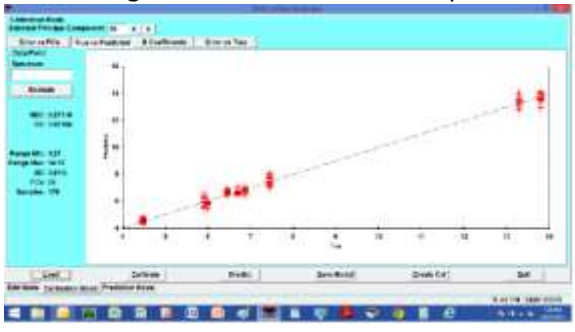


Figure 6. Moisture Cal Plot at 16cm-1

To ensure that the calibrations were equivalent, 10 Principal Components, ie, PC's, were used for all regressions.

Summary Table:

Constituent	64cm-1		16cm-1	
	SEC	R^2	SEC	R^2
Protein	1.18%	.979	.95	.987
Moisture	.25	.994	.27	.997

Conclusion:

Although there are a small number of samples used in this study, the purpose is not to seek the least SEC, but to compare the two sets of calibration data and assess whether using a higher resolution spectra, ie, 16cm-1 vs 64cm-1, reduces the SEC. The data presented above shows that for protein there is a benefit of using higher resolution spectra where as for moisture there is not.

The observation that an improvement for protein was found is consistent with the difference in absorptivity, ie, the relative absorption of light at each wavelength, for protein and moisture. The N-H bonds that characterize protein are weaker absorbers of light than the O-H bonds in water. Also the water bond has an absorption band at 1940nm that is well isolated from the other bands, ie, starch, fat and protein. As such, the calibration of moisture can be achieved with low resolution spectra or higher resolution spectra, where as protein and fat calibrations can be improved by using higher resolution spectra.

NIR Technology Systems
366 Edgar Street, Condell Park, NSW, 2200, Australia
Tel: 612 9771 5444 Fax: 612 9771 5255
Email: sales@nextinstruments.net Web: www.nextinstruments.net