Near infrared spectra of rice grains with normal and extremely low phosphorus concentrations

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Introduction

The ability of NIR calibrations to predict phosphorus (P) is, at best, moderately reliable (R^2 ~ 0.7–0.9). This raises the question "How does P influence an NIR spectrum of plant tissue?" I am not aware of a publication which has examined the basis of a P calibration. This raises the concern that NIR spectroscopy is only able to determine P by an as yet unidentified inter-correlation effect. In cereal grains (such as wheat, rice and barley) and some other grains (maize), the majority (50 to 80%) of the P is in an organic form called phytate and this is found in the aleurone layer in the cereals. This raises another question when developing P calibrations for cereal grains. "Are NIR calibrations for P actually calibrations for phytate-bound- P with the estimation of total P being based on the high correlation (R^2 = 0.98)[1] between phytate-P and total-P?"The aim of this study was to compare spectra of grains with contrasting total P and, by association with phytate-P, levels.

Materials and Methods

Rice grains were obtained from the fertilized (control; normal) and the No-P fertilizer plots at the 2008 harvest of the long term (86 years) rice plots at Aichi Prefecture Experiment Station in Japan.[2] The grains were dehulled and 100 single grains from each treatment were analysed using a Foss NIRSystems 6500 spectrometer fitted with a transmittance single kernel sample presentation attachment. The scans (1100 – 2500 nm) for each treatment were averaged and the difference between the treatments plotted.

Results and Discussion

Grains from the control plot contained 0.33% P while grains from the No-P plots only contained 0.16% P. The raw, average, 2nd derivative and difference spectra were examined and are presented as Figures 1-4

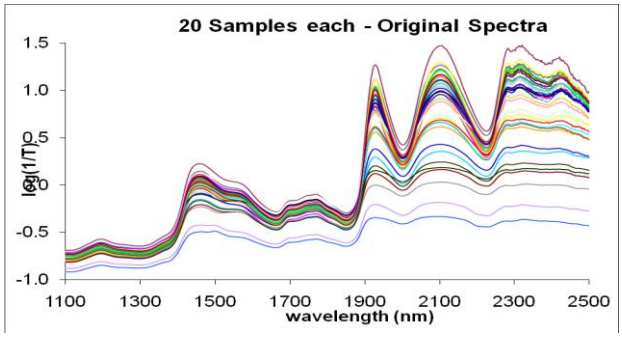

Figure 1. 20 spectra (log1/R) of control and low-P grains.

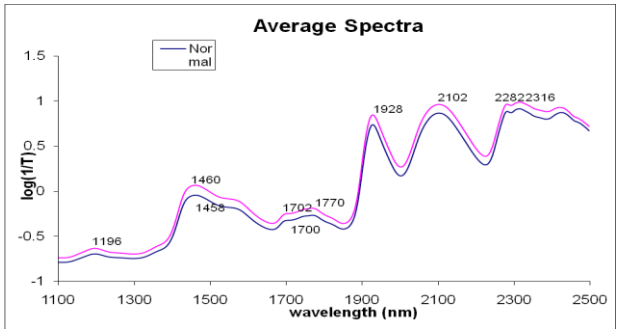

Figure 2. Average spectra (log1/R) of control and low-P grains.

Reference paper as:
G.D. Batten (2012).NIR spectra of rice grains with normal and extremely low phosphorus concentrations,
in: Proceedings of the15th International Conference on Near Infrared Spectroscopy, Edited by M. Manley, C.M. McGoverin, D.B. Thomas and G. Downey, Cape Town, South Africa, pp. 372-374.

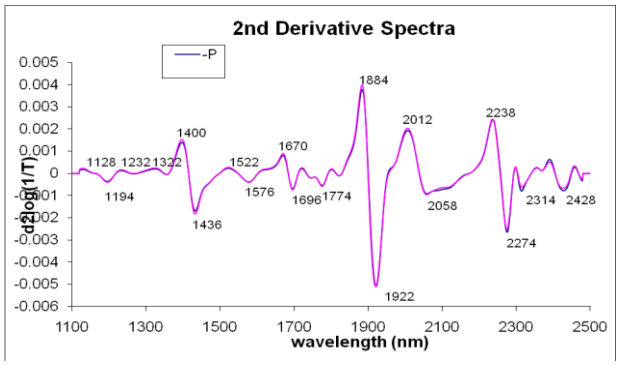

Figure 3. Average 2-Der spectra of control and low-P grains

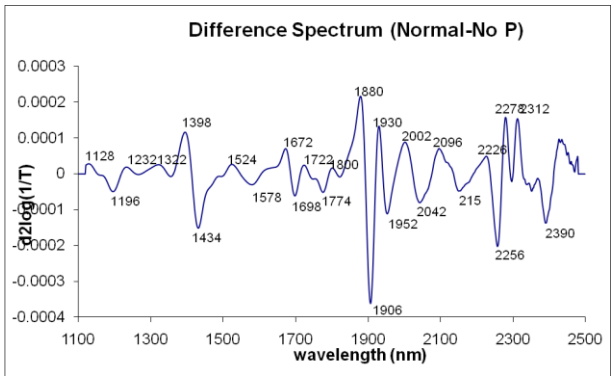

Figure 4. Difference between 2-Der spectra of control and low-P grains

There were differences between the average spectra of the control and No-P grains at about 25 wavelengths. The chemical bonds which are related to these wavelengths include mainly functional groups of carbohydrates and, to a lesser degree, protein (Table 1).

Table 1. Preliminary assignment of absorption bands.

Peak (λ)	Assignment	Structure
1128	-	
1196	C-H str. second overtone	CH_3
1232	C-H str. second overtone	CH
1322	-	
1398	2xC-H str. + C-H def.	CH_2
1434	N-H str. first overtone	$CONH_2$
1524	N-H str. first overtone	ROH
1578	O-H str. first overtone	Starch, glucose
1672	-	
1698	C-H str. first overtone	CH_3
1722	C-H str. first overtone	CH_2
1774	C-H str. first overtone	cellulose
1800	-	
1880	-	
1906	O-H str. first overtone	POH
1930	-	
1952	C=O str. second overtone	$-CO_2R$
2042	N-H sym. str. + amide II	Protein
	N-H sym. str. + amide III	$CONH_2$
2096	2xO-H def. + 2xC-O str.	starch
2150	2xamide I + amide III	$CONH_2$
2226	-	
2256	O-H str. + C-C str.	starch
2278	O-H str. + C-C str.	starch
2312	C-H str. + C-H def.	CH_3
2390	O-H def. second overtone	ROH

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P is believed to regulate the deposition of K and Mg into grains and in this study, the grains from the No-P plots also had lower K and Mg.[2] Some influence on the spectra due to low levels of these minerals cannot be discounted. The difference spectra of the grains suggest that grains with lower concentrations of P have associated changes mainly in starch properties and to some extent protein. This is consistent with reports that inorganic P is maintained within narrow limits to maximise starch metabolism in developing grains. In this study, grains low in P were associated with slightly smaller grain weight and higher protein concentrations.

Conclusions

Using unique samples, this study has provided support for the hypothesis that P-calibrations based on NIR spectra rely on changes in the carbohydrate and protein in the tissues. Studies are required to assess the impact of changing the phyate-P : total-P ratio on the NIR spectra of cereal grains.

Acknowledgements

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References

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Reference paper as:
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