Measuring rancidity of brown rice kernels by NIR spectroscopy

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Introduction

The pericarp of brown rice is rich in fat. Under conditions where oxidation can occur rancidity can develop which affects quality, and consumer acceptance. The degree of ageing of rice grain can also be detected by the degree of rancidity that has developed. Rancidity usually increases as the rice is stored for longer periods. Hexanal is a volatile gas that is related to rancidity.¹ However, its determination is time-consuming, requires experienced technicians, and is destructive of the sample. Near infrared (NIR) spectroscopy is a method that could be used to replace the conventional method of analysis for rancidity. The NIR technique has been shown to be effective for evaluation of sweetness in fruits, grain composition, such as protein content of wheat, moisture content of rice, oil content in fish and many other applications. The aim of this experiment was to evaluate the use of NIRS to determine the amount of hexanal in brown rice as an indication of the quality/age of brown rice grains.

Materials and methods

Samples

Brown rice grains of the Khao Dawk Mali 105 variety were treated to establish a range of hexanal content by heating in an oven at 50 °C for varied sampling times. The samples were collected every 3 hours until 48 hrs. All samples were divided to 2 sets, one for calibration and validation

Items	Brown Rice			
	Calibration	Validation		
No. of samples	72	70		
Range in area*P	0.90–15.11	0.94–15.11		
Mean value	5.77	5.56		
SD	4.13	3.93		
Unit used	pA*s	pA*s		

Table 1. Composition characteristics of the rice samples used.



Figure 1. (a) original log 1/R spectra (b) second derivative spectra of brown rice in the wavelength region 800–2500 nm.

for NIRS scanning, and the other for reference analysis. The characteristics of 142 samples were shown in Table 1.

Spectra acquisitions

The first set was scanned in a NIR spectrophotometer and the other set was to determine the amount of hexanal by GC-headspace. NIR spectra of rice samples were measured by a Foss Model 6500 scanning spectrophotometer, operated in reflectance mode over the wavelength region of 800–2500 nm. Figure 1 shows the log 1/R and second derivative spectra of brown rice.

Reference analysis

Hexanal content in rice samples was determined by head space-gas chromatography. The area of the GC hexanal peak was used as reference data in calibration. The measurements were conducted



Figure 2. Regression coefficient plot for PLS calibrations of hexanal content (pA*s).

Wavelength region (nm)	Pretreatment	R	SEC	SEP	Bias	F
800-2500	Original	0.92	1.53	2.07	0.03	10
800-2000	Second derivative	0.94	1.42	1.95	-0.05	15

Table 2. PLS calibration results for prediction of area*P of hexanal measured from brown rice kernels.

F: the number of factors used in the calibration equation; *R*: multiple correlation coefficients; *SEC*: standard error of calibration; *SEP*: Standard error of prediction;

Bias: the average of difference between actual value and NIR value.

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Data analysis

Calibration equations were developed using The Unscrambler software (Camo, Oslo, Norway) for NIR spectra analysis. The samples were grouped into 2 sets, for calibration and validation. Partial least squares regression (PLS) analysis was applied to the second derivative spectra to predict hexanal.

Results and discussion

PLS calibration results developed from original (raw log 1/R) and second derivative spectra for the area*P of hexanal in brown rice are shown in Table 2.



Figure 3. Cross-validation results for prediction of pA*s of hexanal for brown rice kernels.

The model for spectra pretreated with second derivative showed a high correlation (R=0.94), and a low standard error of prediction (*SEP*) of 1.95 pA*s. The regression coefficients showed that variance was important at wavelengths 1140 nm and 1685 nm, which are associated with aromatic compounds, for benzene at 1080 nm, and for CONH₂ at 1428 nm (Figure 2). Figure 3 shows the correlation plot between predicted and actual results for hexanal.

Conclusion

NIR spectroscopy is a useful technique for rough evaluation of the degree of rancidity/age of storage, by prediction of the amount of hexanal in brown rice, over the wavelength 800–2000 nm.

Reference

1. M.G. Shin, S.H. Yoon, J.S. Rhee and T.W. Kwon. J. Food Sci. 51, 460 (2006).