Evaluation of aromatic compound (2-acetyl-1-pyrroline : 2AP) by near infrared spectroscopy

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Introduction

2-Acetyl-1-Pyrroline (2AP) is an aromatic compound that occurs in many crops, such as rice, pandan leaf, pop corn, and others. The aroma is caused by a volatile gas (2AP), which can disappear easily during long storage (six months or more), or under unsuitable conditions, such as high temperature.

Aromatic rice is preferred to non-aromatic rice for export, as a result of its more favourable price. Customers need to know how well the aroma is maintained during cooking. But the standard method is time-consuming, and is destructive of the samples. NIR spectroscopy has been introduced to determine the amount of 2AP in real time.

NIR Spectroscopy has enjoyed widespread use in the food and agriculture industries due to its ability to perform rapid, non-destructive analyses on samples with little or no sample preparation. Analytical, quality control, and research and development laboratories that support industrial manufacturing processes for fine and specialty chemicals, pharmaceutical formulations, petrochemicals and solid or liquid resins, share similar needs with the food and agriculture industries for rapid, non-destructive testing. NIR spectroscopy is one of the simpler non-destructive, rapid, accurate and precise methods. It is used effectively to analyse many characteristics of crops, including moisture and protein in wheat, sweetness in apples, oranges, and other fruits. This study was to determine the efficacy of NIR Spectroscopy as an analytical technology for 2AP in rice.

Materials and methods

Samples

Samples of whole brown rice grain of the Khao Dawk Mali 105 variety were oven dried at 50°C and sampled every two hours for a total period of 48 hours, to prepare samples with various levels of 2AP. The measurements were conducted at the Postharvest and Processing Research Development Office in the year 2009. Sample characteristics are shown in Table 1.

Table 1. Composition characteristics of the rice samples used.

Items	Brown Rice	
	Calibration	Validation
No. of samples	72	70
Range	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

Reference analysis

Analysis of 2AP of the rice grain samples was determined by headspace-gas chromatography (GC) with a flame ionised detector.[1] Whole brown rice grains were used in this study. The peak area data were used in calibration. Data were reported as pA*s (peak area at the releasing time of 2AP).

NIR spectra acquisition

Samples were scanned by a Foss NIRSystems Model 6500 NIR instrument operated in reflectance mode over the wavelength region of 800–2500 nm. Original spectra were recorded (Figure 1).

Second derivative pre-treatment was performed using the Savitsky-Golay algorithm at 10 nm averaging for left and right sides (Figure 1).

Data analysis

The samples were grouped into calibration and validation sets. PLS calibration was used to evaluate the calibration equations developed using the Unscrambler software (Camo, Oslo, Norway).

Results and discussion

PLS calibration results developed from the original spectra, and for the pA*s of 2AP in brown rice are shown in Table 2.

An effective model with high correlation (r) of 0.89, and low standard error of prediction (SEP) of 0.96 pA*s was developed. The regression coefficients shown at wavelength 1143, 1410, 1540, 1705 and 1920 nm were interpreted to be involved with aromatic compound (Figure 2).

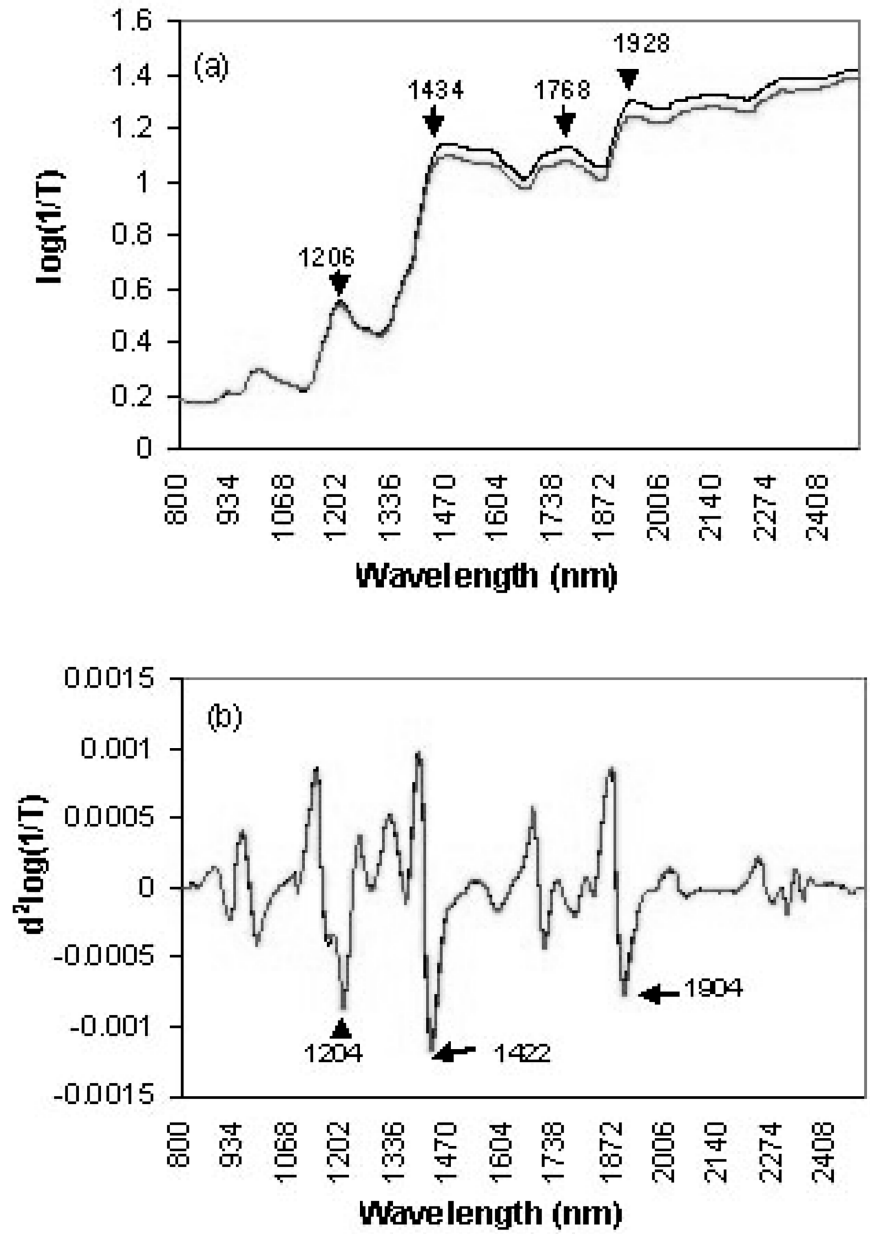

Figure 1. (a) original spectra (b) second derivative spectra of aromatic rough rice in the wavelength region 800–2500 nm.

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

Wavelength region (nm)	Pretreatment	*R*	*SEC*	*SEP*	Bias	*F*
800–2000	Original	0.86	0.75	0.98	0.19	10
800–2000	Second derivative	0.89	0.68	0.96	0.14	9

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.

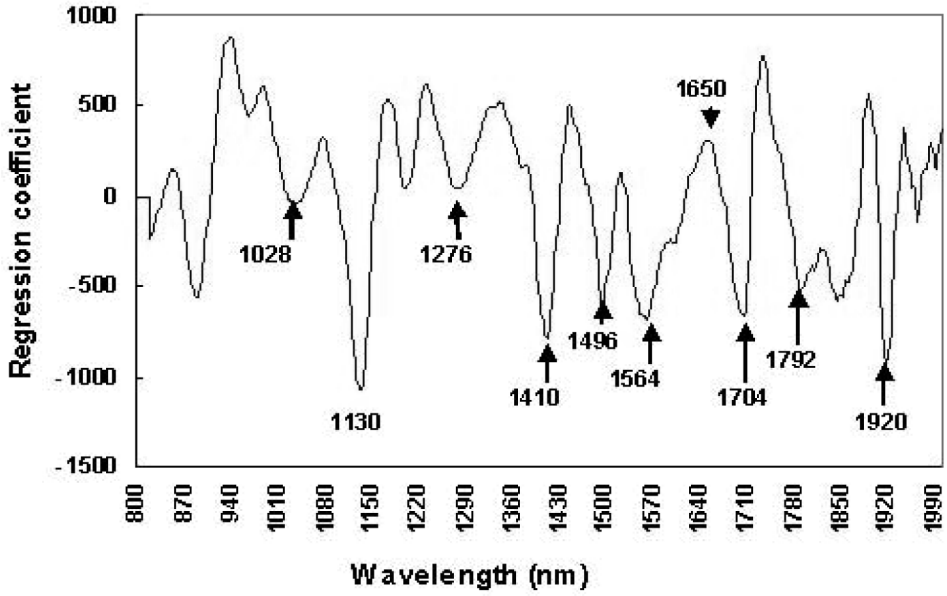

Figure 2. Regression coefficient plot for PLS calibrations for 2AP content (pA*s).

Conclusion

NIR Spectroscopy was shown to be an effective technique to detect the amount of aromatic compound (2AP) in intact brown rice kernels. The model was developed over the wavelength range of 800–2000 nm in reflectance mode. The spectral data were treated with second derivative for development of the calibration model. The range covered the wavelengths at 1410 and 1685 nm, which are related to aromatic C-H absorbers.

Reference

1. S. Wongpornchai, T. Sriseadka and S. Choonvisage, *J. Agric. Food Chem.* **51,** 457 (2003).