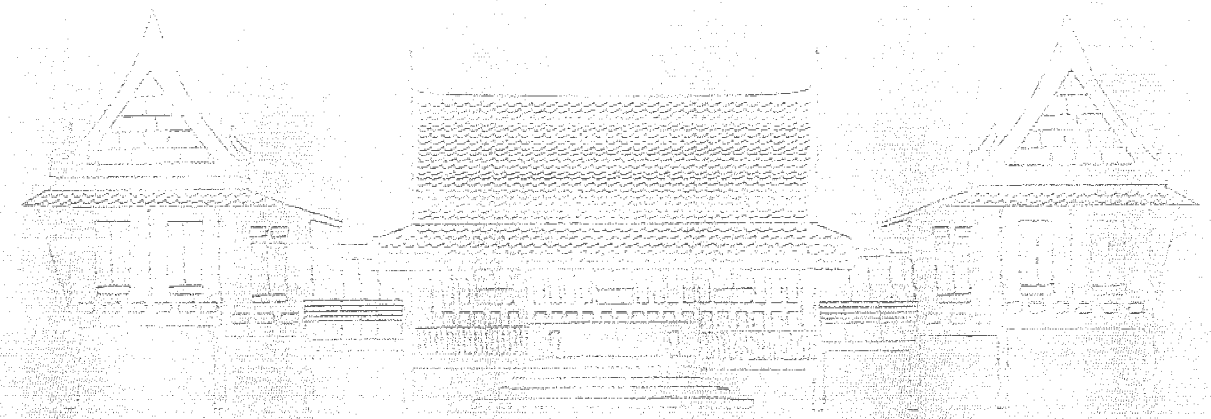

The 3rd Asian Near-Infrared Symposium

May 14-18, 2012

Amari Watergate Hotel, Bangkok, Thailand

Kasetsart University

and

Asian Near-infrared Consortium

Poster (Cont.)

P-49

Relationship Between Volatile Aroma Compounds and Near Infrared Spectroscopy in Ginger Essential Oil

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Abstract

The aim of this study is to demonstrate the potential use of near infrared (NIR) spectroscopy to measure the concentration of volatile aroma compounds in ginger essential oil. By the use of partial least squares (PLS) regression, the quality of the model of calibration and validation statistics could be obtained in the long wavelength region. Results found in this study show the potential use of NIR spectroscopy for quantitative prediction of volatile aroma compounds in ginger essential oil. Further development with a larger data set will be required to test the predictive ability of the NIR calibration models.

Keywords: essential oil, ginger, volatile aroma compound, concentration

Introduction

The spice ginger and its essential oil contain the chemical composition with health promotion and medical value. Among the volatile compounds in fresh ginger, the potent aroma compounds were mainly such monoterpenoids as geraniol, linalool, and geranial by an aroma extract dilution analysis.[1] Furthermore, recent study by GC analysis reported that the major compounds in ginger essential oil (0.510% and 1.1% of fresh and dried ginger, respectively) were camphene (15.9%, 14.1%), α-terpineol (5.8%, 10.9%), farnesene (3.8%, 7.6%), β-cineole (8.4%, 9.4%), pentadecanoic acid (6.0%, 8.0%), β-myrcene (7.7%, 5.0%), pentadecenoic acid (7.9%, zingiberene (7.5%, 8.4%), geranyl isobutyrate (5.1%, 7.0%), 2,7-dimethyl-1,3,7-octatriene (5.7%, 1.9%), 9,12-octadecadienal (4.9%, 2.9%), 9,12,15-octadecatrienal (4.6%,9.1%), limonene (0.6%, 3.3%), neral (4.4%, 2.0%), and α-pinene (1.8%, 1.0%).[2] The application of NIR spectroscopy on the determination of volatile components has not been widely studied.[3-5] To develop NIR spectroscopy for the measurement of those volatile constituents, the purpose of this work was to demonstrate the use of NIR spectroscopy as a rapid tool to determine the volatile chemical constituents in volatile oil of ginger.

Materials and methods

Sample

The commercial essential oil of ginger was purchased from T. N. Chemical Co., Nakhon Ratchasima, Thailand. The sample was diluted with 95% ethanol to various ratios and kept tightly in amber screw-cap bottle at room temperature until used.

Spectral acquisition

The NIR spectrophotometer model NIRFlex Solids with vial adapter (Büchi, CH-9230) was used for spectral acquisition. The NIR spectra were measured in the wavelength region of 4000 nm to 10000 nm with 4 nm intervals. The sample was placed in a light-sealed vial during the measurement to prevent the effect of stray light (Figure 1). The 2-mL sample solutions were prepared under the same condition and controlled at room temperature prior to spectral acquisition.

Data analysis

Data analysis was performed with the Unscrambler® version 9.8 (CAMO software AS, Oslo, Norway). First, spectral pretreatments of smoothing and second derivative (segment = 20 nm, gap = 0 nm) were applied. Then the calibration equation was developed using PLS regression. The wavelength region at 4 nm intervals was used for the calculation. Validation was performed by a randomized test set. Statistical characteristics of the calibration and the validation sample sets are shown in Table 1.

Reference analysis

Reference concentration of the ethanolic solutions of ginger essential oil was calculated to percentage by volume. A 95% ethanolic solution was measured as blank.

Results and discussion

The calibration results for predicting concentration of total volatile compounds in ginger essential oil were shown in Table 2. The wavelength region of 6000 nm to 10000 nm could provide better results (Figure 2) compared with those with the short wavelength regions. The regression coefficient plots of the calibration

equation reveal that the calibration uses the information regarding to the volatile constituents absorption at 8570 nm. The NIR spectra show the maximum absorption of the essential oil solutions around 7500 and 9000 nm. These obtained results could be developed to extensively study on the qualitative and quantitative chemical constituents of the essential oil.

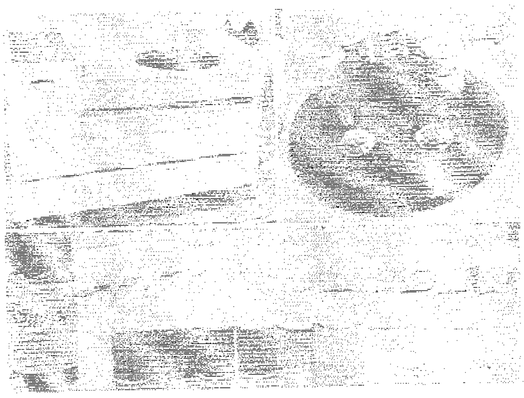

Figure 1. NIR measurement of ginger essential oil.

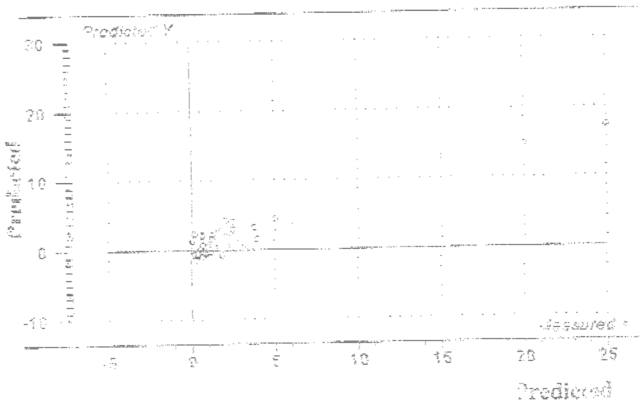

Figure 2. The second derivative NIR spectra of the concentrations of ginger essential oil.

Table 1. Statistical characteristics of the calibration and the validation sample sets

Items	Calibration set	Validation set
Averaged	2.67	[illegible].67
Standard deviation	[illegible].20	14.02
Minimum	17.[illegible]9	1[illegible]5.02
Maximum	-1.[illegible]	[illegible].55
Number of samples	40	6[illegible]

Table 2. PLS calibration results for predicting concentration of volatile aroma compounds in ginger essential oil. The calibration equation was developed on the second derivative NIR spectra.

Wavelength region (nm)	F	Correlation	R^2	SEC	SEP	Bias	RPD
4000-10000	5	0.96	0.80	3.6[illegible]	1.97	-1.20	3.7[illegible]
5000-10000	[illegible]	0.94	0.80	3.67	1.33	-0.60	3.68
6000-10000	7	0.89	0.87	1.86	2.20	0.24	1.85
7000-10000	12	0.94	0.87	1.9[illegible]	1.19	-0.68	2.02

F: The number of factors; R^2: the coefficient of multiple determination, SEC: standard error of calibration, SEP: standard error of prediction; Bias: the average of differences between reference value and NIR value; RPD: the ratio of standard deviation of reference data in the validation set to SEP; Unit: %

Conclusion

NIR spectroscopy can be used as an easy and rapid tool to determine the volatile aroma compounds in ginger essential oil in transmission mode and the long wavelength regions. The optimization of wavelength region used to develop a calibration equation could help improving the calibration results.

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