Capsaicin and Scoville heat units (SHU) determination on Thai sweet sauces by near infrared spectroscopy

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Introduction

Thai sweet sauce, a popular dipping sauce, has the ability to enhance the taste of foods with heat perception, and a sweet taste. It consists of chopped chili, garlic, vinegar, sugar, salt and other additives, such as thickeners and preservatives. Heat sensation influences consumer preference, so capsaicin and Scoville heat units (SHU) determination, using HPLC, are important parameters that are carried out in order to determine and assure quality of the sauce. The HPLC technique requires careful sample preparation and analytical skills. In the present work the application of NIR spectroscopy for measuring capsaicin content and SHU of Thai sweet sauce was investigated, as a possible replacement for HPLC.

Materials and methods

Sample

One hundred and twenty Thai sweet sauce samples consisting of 14 brands were obtained from manufacturing companies, or were purchased from the markets around Kasetsart University, Bangkok, Thailand. The samples were split randomly into two sets. The calibration set consisted of 84 samples while the validation set contained 36 samples. All samples were stored at 4°C before measuring their properties.

Spectral acquisition

The NIR spectra were scanned on an InfraAlyzer Model 500 spectrometer (Bran+Luebbe, Nordertedt, Germany) in the wavelength region of 1100–2500 nm with 2 nm interval and 0.5 mm

Table 1. Composition characteristics of Thai sweet sauces in the calibration and validation sets.

Parameters	Calibration			Validation		
	Mean	*SD*	Range	Mean	*SD*	Range
Capsaicin (mg kg^{-1})	14.96	10.25	3.49–44.92	13.00	7.77	4.42–36.46
Scoville heat units (SHU)	837.12	578.79	181–2642	725.25	444.87	274– 2101

British cup. Prior to spectral measurement, the temperature of the samples was controlled by incubation at 25°C in a water bath for 10 minutes.

Data analysis

Data analysis was performed with the Unscrambler software (version 8.0: CAMO AS, Trondheim, Norway). The wavelength region of 1920–1994 nm was excluded in order to avoid heavily overlapping absorption bands. First, the whole spectral region was treated by Savitzky Golay transformation and smoothing (10 point and second order filtering) as a pre-treatment method. Then the calibration equation was developed using partial least squares regression (the algorithms PLS1 and PLS2). Composition characteristics of Thai sweet sauces are given in Table1.

Reference analysis

Capsaicin content was measured with high performance liquid chromatography (HPLC) and calculation of SHU, following the method of the AOAC (2006);

$$1\ \mu g \text{ total capsaicinoids} g^{-1} \approx 15 \text{ SHU}.$$

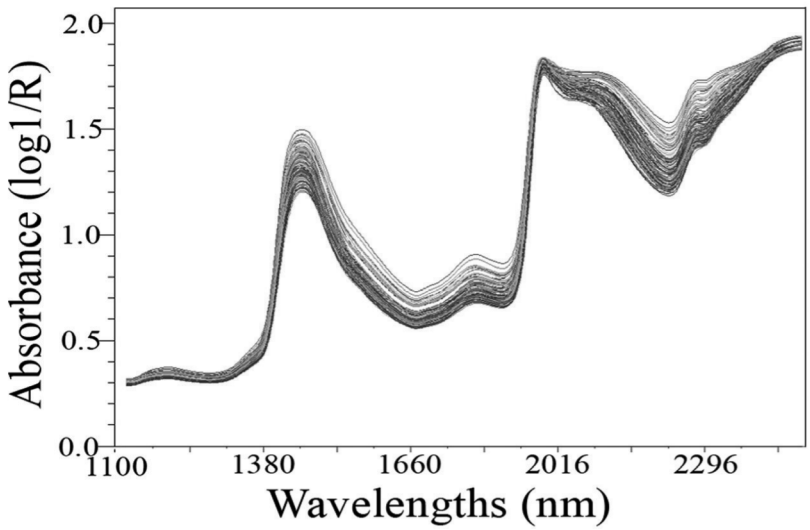

Figure 1. The smoothed NIR spectra of 120 Thai sweet sauces.

Table 2. NIR results for prediction of capsaicin and SHU in Thai sweet sauce.

Parameters	Methods	*F*	*R*	*SEC*	*SEP*	Bias	RPD
Capsaicin (mg.kg^{-1})	PLS1	7	0.84	3.81	4.26	1.34	1.82
	PLS2	7	0.84	3.81	4.23	1.32	1.84
Scoville Heat Unit (SHU)	PLS1	7	0.84	219.47	245.48	80.99	1.81
	PLS2	7	0.84	219.47	245.48	80.99	1.81

F: The number of factors; *R*: Correlation coefficient; *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*

Results and discussion

The NIR spectra of Thai sweet sauces are shown in Figure1.

This figure shows the main absorption bands of water at 1420 nm and 1910 nm. These bands arise from OH stretching.[1] Correlation coefficients (*R*), between capsaicin and SHU at individual wavelengths were observed. High correlations were observed at 1406 nm, 1898 nm and 2012 nm for both capsaicin and SHU. These wavelengths[2] have been related to CH_3 and OH that represent functional groups of the capsaicin molecule.

PLS1 and PLS2 algorithms were used to compute calibration models for the prediction of capsaicin and SHU. Evaluation results are shown in Table 2.

The performances of both capsaicin and SHU models were similar to each other, by either PLS1 or PLS2. The highest *R* value for capsaicin content and SHU values were 0.84. Although the ingredients of Thai sweet sauce are similar to chili sauce, it is a heterogeneous sauce and contains chili and garlic particles. The capsaicin content of Thai sweet sauce is present in only mg kg^{-1} amounts and the samples exhibited a narrow range of capsaicin values. The prediction efficiency for such a trace component was unreliable and only low *RPD* values could be reached. In this study, NIR spectroscopy can be considered as only an approximate method for estimating capsaicin and SHU[3] contents in Thai sweet sauce.

Conclusion

NIR spectroscopy, using PLS1 or PLS2 could be used to develop quantitative models for rough screening of Thai sweet sauce for both capsaicin and SHU contents.

Acknowledgement

The authors thank Kasetsart University Research and Development Institute (KURDI) and Kasetsart Agricultural and Agro-Industrial Product Improvement Institute (KAPI), Kasetsart University, Thailand, for financial supporting and providing us with the InfraAlyzer 500 spectrometer.

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