Near infrared spectroscopic determination of capsaicin and Scoville heat units in chilli sauces

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Introduction

Chilli sauce is used as a dipping sauce in a wide variety of foods. The seasoning sauce market in Thailand is expanding. Nowadays, Thailand produces sauces as an important export product. Quality control is essential to maintain this market. Capsaicin and Scoville heat units (SHU) are two of the parameters associated with chilli sauce quality and consumer acceptance. The reference methods for determination of these are expensive and time-consuming. Because of these disadvantages, non-destructive analysis methods, such as near infrared (NIR) spectroscopy, have been investigated as replacement methods. In the present study, NIR spectroscopy in combination with partial least squares (PLS1 and PLS2) regression was used to measure the capsaicin and SHU contents of chilli sauce. The predictive ability of the PLS2 model was compared with the results obtained by PLS1 models for each parameter.

Materials and methods

Samples

One hundred and forty eight samples of chilli sauces were collected, partly from manufacturing companies, and partly purchased from the markets in Bangkok, Thailand during 2007 and 2008. All samples were separated randomly into two groups: 104 samples of calibration and the remaining 44 for validation. The samples were kept at 4°C for 24 hours.

Reference analysis

Capsaicin and SHU were measured by High-performance liquid chromatographic method according to the method of the AOAC 2005.

Table 1. Composition characteristics of chilli sauce samples.

Analysed	Calibration set ($n=104$)			Validation set ($n=44$)		
	Mean	*SD*	Range	Mean	*SD*	Range
Capsaicin *(ppm)*	28.72	26.97	3.38–110.20	26.35	19.38	7.98–81.78
Scoville heat units (SHU)	1560.1	1450.5	143–6088	1425.2	1077.2	407–4537

Spectral acquisition

Samples were filled into a Dutch cup and NIR transflectance spectra were recorded over the wavelength range from 1100 nm to 2500 nm, with 2 nm intervals using an InfraAlyser 500 spectrometer (BRAN + LUEBBE, Norderstedt, Germany). Chilli sauce samples were incubated at 25°C in a water-bath prior to the NIR measurement.

Data analysis

The spectra data obtained were transposed into the Unscrambler (Version 8.0: CAMO, Oslo, Norway). The 1936–1946 nm regions were excluded in order to avoid heavily overlapping absorption bands. The spectral data were preprocessed by multiplicative scatter correction (MSC) after Savitsky-Golay smoothing, Calibration equations were developed using Partial least squares (PLS1 and PLS2) regression. Validation was performed using a separate test set. Composition characteristics of the calibration and the validation sample sets are shown in Table 1.

Results and discussion

Table 2 shows a comparison between the best models obtained using PLS2 and those which presented the best predictive abilities using PLS1 for each property.

It can be seen that PLS2 presented slightly better predictive abilities for capsaicin and SHU than the PLS1 model. The results of the PLS2 method with highest correlation coefficients (*R*) for

Table 2. Comparison between PLS1 and PLS2 models with the best predictive abilities.

Analysed	Method	*F*	*R*	*SEC*	*SEP*	*RPD*
Capsaicin (ppm)	PLS1	10	0.88	10.92	9.26	2.09
	PLS2	9	0.89	11.11	9.07	2.14
SHU	PLS1	10	0.87	570.40	541.48	1.99
	PLS2	9	0.87	577.23	526.47	2.05

PLS: Partial least squares regression, *F*: The number of factors; *R*: correlation coefficient of prediction; *SEC*: standard error of calibration, *SEP*: standard error of prediction; *RPD*: the ratio of standard deviation of reference data in the validation set to *SEP*.

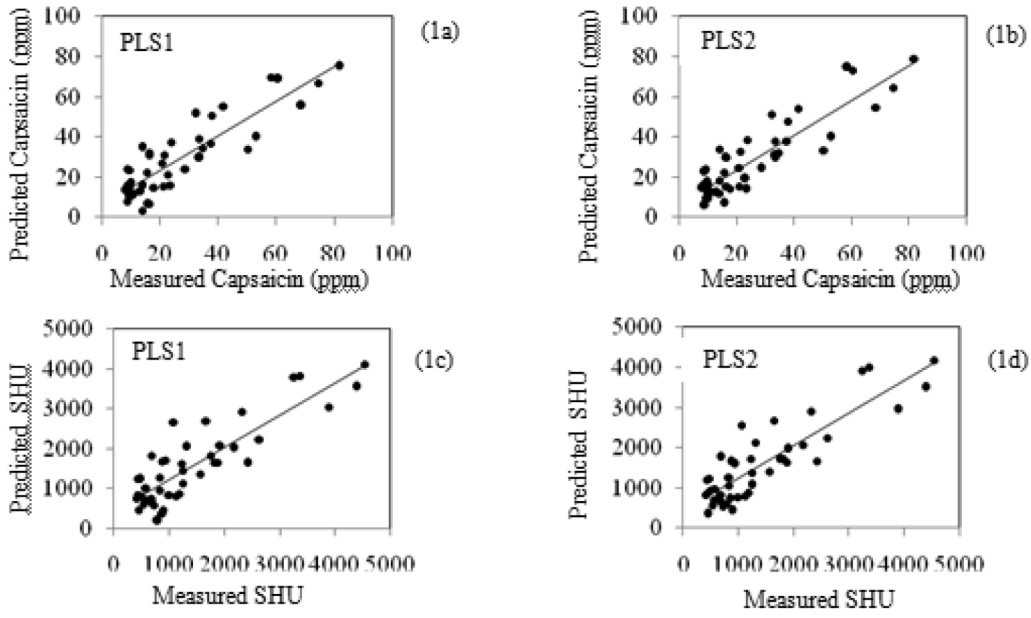

Figure 1. Relationship between NIR and measured value of capsaicin (a) and (b) and SHU(c) and (d).

capsaicin and SHU were 0.89 and 0.87, the lowest *SEP*s were 9.07 ppm and 526.47 SHU, and the highest *RPD*s were 2.14 and 2.05, respectively.

Figure 1 shows the relationships between NIRS and measured values of capsaicin and SHU.

The results indicated that both PLS1 and PLS2 calibration models had potential for rough screening and determination of the approximate levels in the samples,[1] but that the PLS2 model was slightly the better.

Conclusion

NIR spectroscopy with PLS2 models could be used for estimation of capsaicin and Scoville Heat Units (SHU) in chilli sauce, and could be a useful analytical tool for the chilli sauce industry.

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Reference

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