

Prediction of total solids of oyster sauces by near infrared spectroscopy

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Introduction

Oyster sauce is a seasoning that has long been popularly used in south-east asian countries such as Thailand, China, Korea and Malaysia. In Thailand, the oyster sauce industry is growing continuously, and export value is increasing, therefore the manufacturer must be able to assure the quality standards of oyster sauce. The quality factors of oyster sauce can be identified by the total solids content, which is determined by an oven method. This method is time consuming and requires technical skills. Near infrared (NIR) Spectroscopy has been suggested as a method to resolve these problems. NIR spectroscopy is an effective nondestructive technique that has many potential applications in the seasoning industries for quality control of products such as fish sauce and soy sauce. The purpose of the present study was to use NIR spectroscopy for prediction of total solids in oyster sauce, and to select the optimum wavelength regions for prediction of total solids in oyster sauce, as selected by MWPLSR¹ (moving window partial least squares regression).

Materials and methods

Samples

One hundred oyster sauces were purchased from local markets and supermarkets in Bangkok, Thailand during 2008 to 2009, and kept at 25 °C for 24 hours before analysis and scanning.

Reference analysis

Total solids content was measured in triplicate by oven drying following the AOAC Method 2000.

Table 1. Composition characteristics of oyster sauce samples in NIR calibration and validation sets.

Parameters	Calibration ($n=70$)			Validation ($n=30$)		
	Mean	SD	Range	Mean	SD	Range
Total solids (%)	24.64	6.64	10.48–36.83	23.98	5.24	11.05–33.90

Spectral acquisition

The oyster sauce samples were incubated at 25 °C in water-bath for 15 minutes prior to the NIR measurements. The samples were filled into a Dutch cup for a sample holder, with path length 0.2 mm, and NIR spectra were recorded with an InfraAlyzer 500 spectrometer (Bran+Luebbe, Norderstedt, Germany) in the wavelength region from 1100 to 2500 nm, at 2 nm intervals, using the transmittance mode.

Data analysis

The spectral data of 100 samples were split randomly into two sets for development of the calibration model for predicting the total solids content. The calibration set consisted of 70 samples while the validation set contained 30 samples. Data analysis was carried out using The Unscrambler software. The 1936–1946 nm regions were not employed, in order to avoid heavily overlapping absorption bands. The original spectral data were pretreated with first and second derivatives. Then the calibration equation was developed using partial least square (PLS) regression, and MWPLSR¹ by MATLAB software. Composition characteristics of the calibration and the validation sample sets are given in Table 1.

Results and discussion

Table 2 reports the results of using PLS models before and after raw spectral data were pretreated by derivatives.

The results showed that the second derivative method gave the best model for prediction of total solids in oyster sauce. Further calibration results for predicting total solids are given in Table 3.

Table 2. PLS models predicting the total solids in oyster sauce pretreated with derivative method, using full wavelength range.

Pretreatment	F	Calibration		Prediction			RPD
		R_{cal}	SEC	R_p	SEP	Bias	
Original	5	0.998	0.414	0.996	0.497	−0.002	10.54
First derivative	4	0.998	0.383	0.997	0.459	−0.013	11.41
Second derivative	4	0.998	0.381	0.997	0.379	0.037	13.83

F : The number of factors, R_{cal} : Correlation Coefficient for calibration set, R_p : Correlation Coefficient for prediction set, SEC : Standard error of calibration, SEP : Standard error of prediction, bias: Mean difference between NIR value and reference value, RPD : The ratio of standard deviation of reference data in the validation set to SEP .

Table 3. PLS and MWPLS calibration results for predicting total solids of oyster sauces.

Parameter	Regression	Wavelength (nm)	<i>F</i>	<i>R</i> _{val}	<i>SEC</i>	<i>SEP</i>	Bias	<i>RPD</i>
Total Solids (%)	PLS	1100–2500	4	0.997	0.381	0.379	0.037	13.83
	MWPLS	1490–1682	3	0.998	0.420	0.356	−0.020	14.74

F: The number of factors, *R*_{val}: Correlation Coefficient, *SEC*: Standard error of calibration, *SEP*: Standard error of prediction, Bias: Mean difference between NIR value and reference value, *RPD*: The ratio of standard deviation of reference data in the validation set to *SEP*².

PLS models based on the informative regions selected by MWPLSR gave better performance than that based on the whole spectral region. The wavelength range used (shaded area), and the correlation between reference and predicted results are shown in Figure 1.

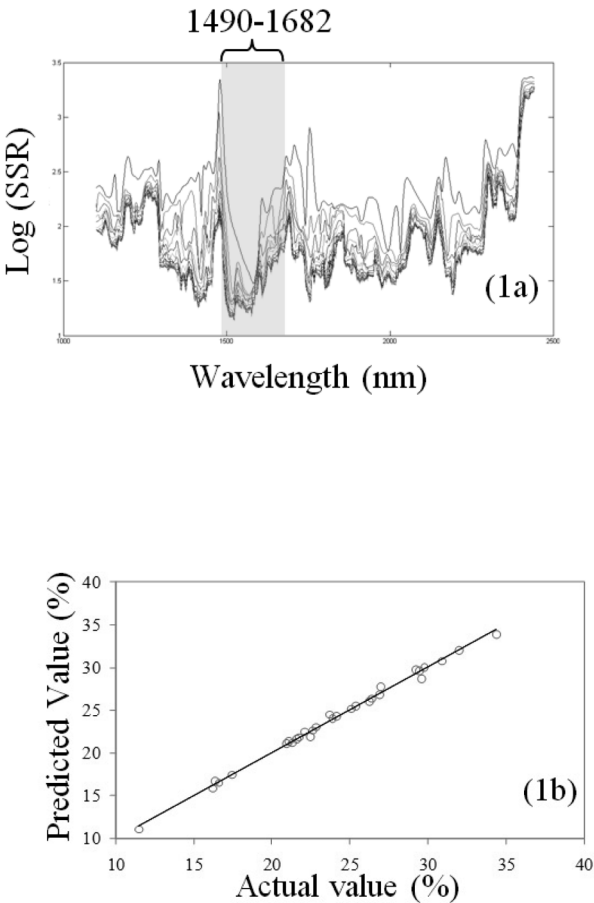


Figure 1. Residual lines (1a) and scatter plot (1b) for total solids of oyster sauces obtained by MWPLSR. The shaded areas represented final informative regions because the methylene first overtone bands occur in the regions 1611–1636 nm.

The results indicated that the NIRS prediction ability of total solids in oyster sauces by PLS and MWPLS calibration models was excellent, and usable for determination of the quality of oyster sauce industries,² based on total solids content.

Conclusion

NIR spectroscopy is very powerful technique for prediction of total solids in oyster sauces. The method is non-destructive of samples, and has a short time for analysis. The technique could be useful to the oyster sauce industry for assuring the quality of their products.

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References

1. J. H. Jiang, R.J. Berry, H.W. Siesler and Y. Ozaki, *Anal. Chem.*, **74**, 3555 (2002).
2. P. Williams, *Near-infrared Technology-Getting the Best out of Light*. PDK Grain, Nanaimo, Canada (2007).