Evaluation of oil deterioration by near infrared spectroscopy

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Introduction

Near infrared (NIR) absorptions derived from overtones and combinations of the fundamental vibrations of molecules found in mid-IR region. Especially, the absorptions by C–H, O–H, and N–H groups are major. Therefore, NIR technique has been widely used for food, agriculture, medicine, etc. In our laboratory, spectral analysis for protein determination,[1–5] lipid oxidation,[6] moisture content,[7] and water pollution[8,9] by NIR has been studied for years. In this work, we analyzed oil deterioration in detail.

Oil and foods of oil are needed quality control in factory. Therefore, the development of simple and easy methods for the determination of lipid oxidation is required. The indices of oil deterioration are acid value (AV), carbonyl value (COV), viscosity, polar compounds, and polymers. However, determinations of AV, COV, viscosity, polar compounds, and polymer need a long time, hazardous reagents, and skill. In this work, we analyzed the relationship between oil deterioration indices and NIR spectra in a model system of oil deterioration by using several oils in order to develop a method for determination of the oil deterioration indices by NIR spectroscopy.

Materials and methods

Sample preparation

Canola, soybean, safflower, rice bran and cottonseed oils were deteriorated by heating at 210°C for 0–21 h with deep frying of frozen French fries.

Determination of NIR spectra

NIR transmittance spectra (680–1235 and 1100–2500 nm) of the drainage were determined in 10 mm cuvette cell by using the NIRSystems (Pacific Science) Model 6250 Research Composition Analyzer at 30°C. Statistical analysis was performed with NSAS Ver. 3.27 (NIRSystems).

Determination of deterioration index

Colour was determined by Gardner method. AV was determined by potassium hydroxide titration. COV was determined by colorimetry using 2,4-dinitrophenylhydrazine. Viscosity was determined by Brookfield viscosity meter. Polar compounds and polymers were determined by Iatroscan (TLC/FID) and HPLC, respectively.

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Regression analysis

A partial least squares (PLS) regression analysis was used for calibration and prediction.

Results and discussion

NIR raw spectra of fresh and deteriorated soybean oil

Figure 1 shows the NIR raw spectra of fresh and deteriorated soybean oil. Other oils showed similar spectra in the region of 685–1230 nm. However, the spectra in the region of 1100–2500 nm were too noisy to use. Hence, we used the spectra in the region of 685–1230 nm.

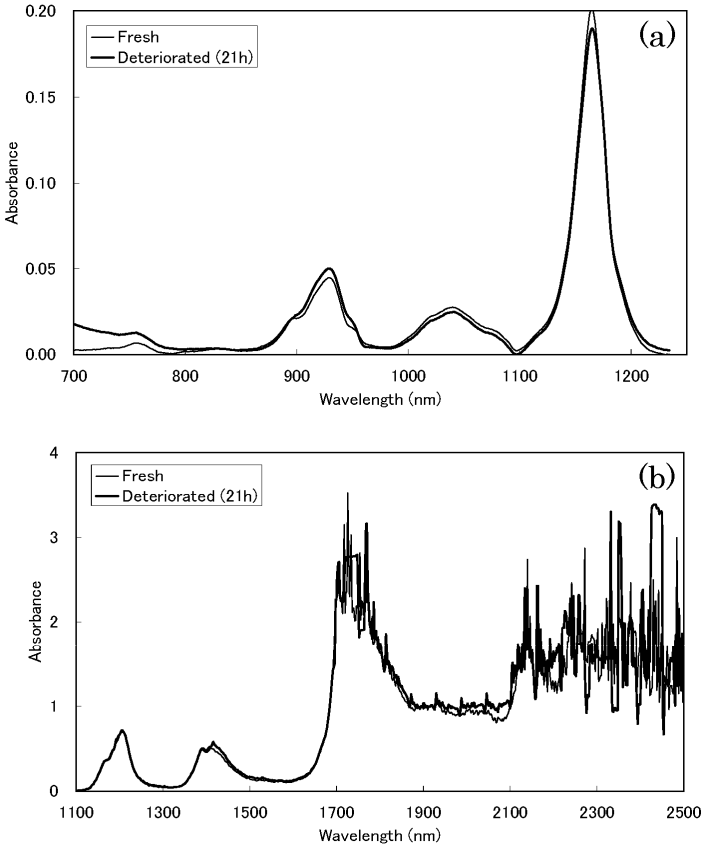

Figure 1. NIR raw spectra of fresh and deteriorated soybean oil in the region of (a) 685–1250 nm and (b) 1100–2500 nm.

Correlation between NIR raw spectra and deterioration indices

Table 1 shows the correlation between NIR raw spectra in the region of 685–1230 nm and deterioration indices of various oils. Colour, AV, COV, and polymers were highly correlated with NIR raw spectra.

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Table 1. Correlation between NIR raw spectra and deterioration indices.

Index	Range	Factor	*R*	*SEC*
Colour	0–10	9	0.965	0.866
AV	0–1.2	9	0.928	0.144
COV	0–53.1	12	0.966	5.07
Viscosity	0–117.5	2	0.839	19.9
Polor compounds	0–16.1	3	0.875	2.34
Polymers	0–30.4	13	0.989	1.76

Prediction statistics of NIR raw spectra for deterioration indices

Table 2 shows the prediction statistics of NIR raw spectra in the region of 685–1230 nm for deterioration indices of various oils. Good predictions were obtained for colour, AV, COV, and polymers.

Table 2. Prediction statistics of NIR raw spectra for deterioration indices.

Index	Range	*R*	*SEP*
Color	0–10	0.971	0.739
AV	0–1.2	0.928	0.126
COV	0–53.1	0.966	4.22
Viscosity	0–117.5	0.839	19.4
Polor Compounds	0–16.1	0.875	2.25
Polymers	0–30.4	0.989	1.44

Conclusion

Good calibration and predictions were obtained for colour, AV, COV, and polymers of deteriorated oils. These results suggest that NIR spectroscopy can be used to evaluate the deterioration of frying oils.

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