Rapid Determination of *cis* and *trans* Content, Iodine Value, and Saponification Number of Edible Oils by Fourier Transform Near-Infrared Spectroscopy

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ABSTRACT: Fourier transform near-infrared (FT-NIR) spectroscopy was evaluated as a means of simultaneously determining the *cis* and *trans* content, iodine value (IV), and saponification number of neat fats and oils. Reference values for these parameters were obtained from oils using a previously developed mid-FTIR Edible Oil Analysis Package. Two partial least squares calibrations were developed for a 5-mm heated flow cell, the first a process calibration based on hydrogenated soybean samples and the second a more generalized calibration based on an oil sample matrix containing many oil types and designed to remove any correlations among the parameters measured. Each calibration performed well with its own validation samples; however, only the noncorrelated calibration was able to analyze oil samples accurately from a variety of sources. It was found that NIR analysis maintained the internal consistency between *cis/trans* and IV, and the accuracy and reproducibility of the predictions were on the order of ±1.5 and ±1.0 units, respectively, for all parameters evaluated. FT-NIR is shown to be a very workable means of determining *cis/trans*/IV values and saponification number for edible fats and oils, and it provides a rapid alternative to the commonly used chemical and physical methods presently employed in the industry.

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KEYWORDS: *cis* content, Fourier transform near-infrared spectroscopy, FT-NIR, iodine value, oil analysis, partial least squares, PLS, saponification number, *trans* content.

Some key factors which determine the chemical and physical properties of edible fats and oils include the relative degree of unsaturation or iodine value (IV), the type of unsaturation (*cis* or *trans*), and the weight-average molecular weight or saponification number (SN). Fats and oils commonly undergo processes such as hydrogenation, which modify the physicochemical characteristics of fats and oils by changing the IV and *cis/trans* ratio, for which specific values are often targeted. Hence monitoring changes in these parameters during a process is important as they define the quality and functionality of the end product. In addition, the *trans* content may become of potential regulatory interest because of its association with arteriosclerosis and heart disease (1) and may one day be a required analysis for labeling purposes. Although AOCS methods are available to measure these parameters, the official methods tend to be laborious, and the industry is always on the alert for more rapid and efficient ways of carrying out routine analyses.

The McGill IR Group has focused on the development of rapid methods for edible oil analysis using Fourier transform mid-infrared (mid-FTIR) spectroscopy (2–5), specifically in relation to industrial quality control applications. A rapid, quantitative mid-FTIR method was developed to simultaneously determine *cis* and *trans* content, IV, and SN, the calibration being based on pure triglyceride standards and using partial least squares (PLS) as the chemometric approach (6). Although mid-FTIR transmission spectroscopy is gaining acceptance as an analytical tool in the edible oil sector, near-infrared (NIR) spectroscopy has seen more use in industrial applications because NIR instruments are more rugged and less energy limited than mid-FTIR spectrometers, can use glass or quartz cells, and have sensitive detectors. In particular, NIR reflectance instruments are widely used by the food industry for the rapid quantitative determination of moisture, lipid, protein, carbohydrates, and fiber in agricultural and food products (7). In the case of edible oils, NIR transmission techniques can be employed; they eliminate many of the difficulties associated with reflectance spectroscopy, especially in relation to calibration development and maintenance. A number of oil processors have expressed an interest in FT-NIR-based edible oil applications, in particular peroxide value, IV, and *trans* analyses. A transmission FT-NIR oil analysis method for the rapid determination of peroxide value (8) has been described previously, and this paper presents the method development protocol, calibration, and validation of an FT-NIR method for the simultaneous determination of *cis*, *trans*, IV, and SN parameters of edible fats and oils.

MATERIALS AND METHODS

Oil samples, calibration standards, and validation samples. Hydrogenated soybean and rapeseed oils with a wide variety

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of *cis/trans* and IV values were obtained courtesy of a major oil processor. Other oils, including coconut oil, soybean oil, olive oil, canola oil, corn oil and sunflower oil, were obtained from retail and commercial outlets. Trisun HB 95, a partially hydrogenated, high-*trans* (65%) sunflower oil (Lot #3R147), was obtained from SVO Specialty Products, Inc. (Eastlake, OH).

Two sets of calibration standards were employed in this work. The first set, comprising 32 hydrogenated soybean oil samples and covering a wide range of *trans* values (~0–50% *trans*), was employed to develop a calibration designed to monitor a particular hydrogenation process. For the development of a universal calibration, 29 samples were prepared by mixing a variety of commercial fats and oils of varying *cis*, *trans*, IV, and SN values, Trisun HB 95 being used to extend the *trans* value range of the blends. These samples were combined with 11 commercial hydrogenated soybean and 11 hydrogenated rapeseed samples to produce a calibration set which covered a broader range of *cis/trans,* IV, and SN values than would be found in any single oil type and which obviated *cis/trans* and IV intercorrelations. For validation of the two calibrations developed, hydrogenated rapeseed and soybean oils not used in either calibration set were employed as validation samples. The reference values for *cis* content (expressed as percentage triolein), *trans* content (expressed as percentage trielaidin), IV, and SN for all the calibration standards and validation samples were obtained using the mid-FTIR Edible Oil Analysis Package (EOA Package) developed by the McGill IR Group and described in a previous publication (6).

Instrumentation and sample handling. FT-NIR spectroscopy was carried out using a Bomem FT-NIR spectrometer (Hartmann & Braun MB-Series, Bomem, Inc., Québec, Canada) capable of covering the spectral range of 12,000–2000 cm^{-1}, controlled by an IBM-compatible 486 DX-66 MHz PC running under Windows-based BomemGrams/386 (Galactic Industries Co., Salem, NH) software. The instrument and optical path were purged with a continuous flow of dry air from a Balston dryer (Balston, Lexington, MA) to minimize water vapor and CO_2 interferences. Basic spectroscopic work was carried out using a heated transmission flow cell accessory (5) with quartz windows and a path length of 5 mm; the system was capable of handling preheated fats and oils in their neat state (Dwight Analytical Solutions Ltd., Toronto, Ontario, Canada). The accessory was maintained at 80 ± 0.2°C to ensure that fats were liquefied, the samples being melted in a microwave oven prior to being loaded into the flow cell. FT-NIR spectra of the samples were collected over the range of 10,000–4000 cm^{-1}, an open beam emittance spectrum being collected first, followed by the collection of a sample emittance spectrum (128 co-added scans for each). These were then ratioed and transformed into a conventional absorbance spectrum. Mid-FTIR spectroscopy was carried out using a Nicolet Magna FTIR spectrometer (Nicolet Instrument Corp., Madison, WI) to obtain reference *cis/trans*/IV/SN data using the EOA Package. Data obtained from this system were used as reference values to calibrate the FT-NIR system and validate its predictions.

Calibration. The spectra of the calibration standards together with the *cis/trans*/IV/SN data obtained from the mid-FTIR EOA package were input into the Omnic TQ Analyst chemometrics program (Nicolet Instrument) to develop NIR calibrations. Correlation spectra, which relate spectral changes to the values of the parameter of interest, as well as variance spectra, which illustrate regions of spectral variance in the standards, were generated. These were employed to assist in identifying spectral regions which could be used to develop predictive PLS models for *cis* and *trans* content, IV, and SN. The predicted residual error sum of squares (PRESS) test and the root mean square error (RMSE) associated with the cross validation of the calibrations tested were used to select optimal calibrations. The performance of the calibrations as well as the validations was assessed using linear regression, with accuracy and reproducibility assessed using mean differences (MD) and standard deviations of the differences (SDD) according to the method of Youden and Steiner (9).

RESULTS AND DISCUSSION

General considerations. NIR spectroscopy differs fundamentally from mid-IR spectroscopy, because the spectral profiles in the NIR region contain less spectral detail and consist of overlapping and poorly defined overtone and combination bands arising from the fundamental absorptions occurring in the mid-IR region. Most of the strong absorption bands in the NIR region are CH overtone and combination bands. The region covering 6200–5500 cm^{-1} comprises the first ν CH overtone, whereas 8500–8200 cm^{-1} is associated with the second ν CH overtone. CH_2 combination bands appear in the 4500–4000 cm^{-1} range. The absorbances near 8475 and 5900 $cm^{-1}$are due to strong -CH=CH- (*cis* double bond) overtones, the respective combination bands being found near 4675 and 4566 cm^{-1}(10). The *trans* overtone and combination bands are very weak and can be difficult to measure, tending to be overwhelmed by stronger absorptions. In terms of edible oils, Sato *et al.* (11) reported that most of the more obvious spectral differences in their NIR spectra were evident in the 6250–5555 cm^{-1} and 4762–4545 cm^{-1} regions. Holman *et al.* (12) related changes in absorbance at 4651 cm^{-1} to the IV of fats and oils, whereas Wetzel (13) correlated NIR absorbance changes at 5952, 4675, and 4529 cm^{-1} to solid-fat index, degree of unsaturation, and SN, respectively. Although these citations indicate that absorptions at selected wavelengths correlate with various physicochemical properties of fats and oils, the absorption bands in the NIR region overlap so extensively that traditional univariate analysis techniques are generally not applicable. Because of this, it is mandatory to make use of advanced chemometric techniques such as PLS to obtain meaningful quantitative data. PLS is a sophisticated multivariate analysis technique that has largely been pioneered for NIR applications and has played a major role in the recent resurgence of quantitative mid-IR spectroscopy. The key difference between PLS and multiple linear regression approaches is that a PLS calibration does not entail es-

tablishing direct relationships between concentration and absorbance measurements at specified frequencies (i.e., peak heights or peak areas), but rather develops a model by compressing the spectral data for a set of calibration standards into a series of mathematical "spectra," known as loading spectra or factors. PLS decomposes the spectrum of each calibration standard into a weighted sum of the loading spectra; and the weights given to each loading spectrum, known as "scores," are regressed against the concentration data for the standards. When the spectrum of an unknown is analyzed, PLS attempts to reconstruct the spectrum from the loading spectra, and the amounts of each loading spectrum employed in reconstructing the spectrum, i.e., the "scores," are then used to predict the concentration of the unknown (14). A PLS calibration can, in principle, be based on the whole spectrum, although in practice the analysis tends to be restricted to regions of the spectrum that exhibit variations with changes in the concentrations of the components of interest. As such, the use of PLS can provide significant improvements in precision relative to methods that use only a limited number of frequencies. In addition, PLS treats concentration rather than spectral intensity as the independent variable and thereby is able to compensate for unidentified sources of spectral interference (e.g., overlapping bands), which are common in NIR spectroscopy.

Certain restrictions are inherent in the PLS method. First, any PLS calibration model will only give accurate predictions for samples that are well represented by the calibration standards. Second, in a multicomponent analysis the predictions obtained from a PLS model will reflect any intercorrelation that exists in the calibration set. Hence, for a generalized calibration it is essential that the values of all parameters measured vary independently. However, in developing a calibration for a specific product line, this may be neither necessary nor readily feasible, as the samples conveniently available for calibration may contain components whose concentrations are inherently correlated. In the present work, two types of calibration models were developed, one based on samples taken from an industrial soybean hydrogenation process and the other based on a wide variety of oil types. For the first calibration, analysis of the calibration standards by mid-FTIR spectroscopy demonstrated that the *cis* and *trans* contents were inversely related and highly correlated (Fig. 1). In contrast, the second calibration was designed to have more variability in all parameters as well as to ensure that there were no intercorrelations between any pair of parameters (Fig. 2). Both calibration approaches are valid, but they differ in the scope of application of the calibrations derived.

Development of a calibration based on process samples. Figure 3 illustrates the mean, variance, and correlation spectra for the calibration set, comprising samples taken from a soybean oil hydrogenation process. The *cis*, *trans* and IV correlation spectra strongly resemble each other because of the inherent correlation between the three parameters in question within this set of process samples. SN was not considered in this analysis, as it is effectively invariant.

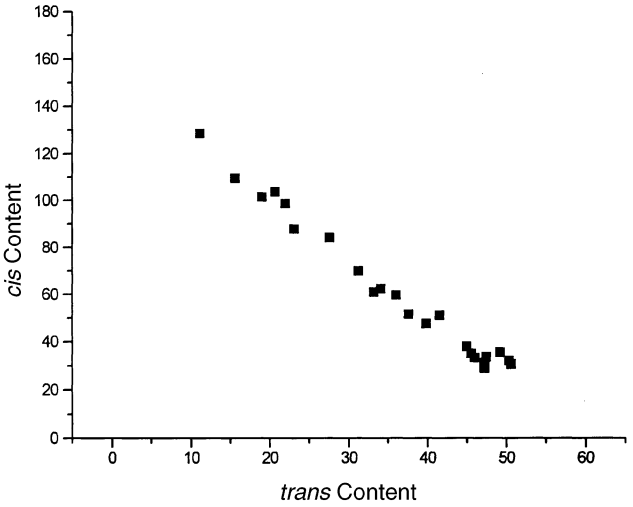

FIG. 1. *Cis* and *trans* values for the soybean process calibration set, illustrating their intercorrelation.

The variance spectrum shows that there are three main regions in which there are significant spectral variations, 8700–8000 cm^{-1}, 6100–5350 cm^{-1} and 4900–4500 cm^{-1}, with some minor variations around 7200 cm^{-1}. The correlation spectra, which relate the changes in the values of each parameter to spectral changes, are more complex; however, the regions of high correlation correspond to those in which the most spectral variation is observed. These regions basically correspond to the first and second CH overtone regions (6200–5300 and 8900–8000 cm^{-1}) and the corresponding CH combination band regions (4900–4500 and 7400–6700 cm^{-1}). A number of calibrations were assessed using each of these regions and combinations thereof. On the basis of the RMSE of the predictions for a separate set of validation samples, the first combination band region encompassing 4777–4553 cm^{-1} using a single-point baseline at 4800 cm^{-1}

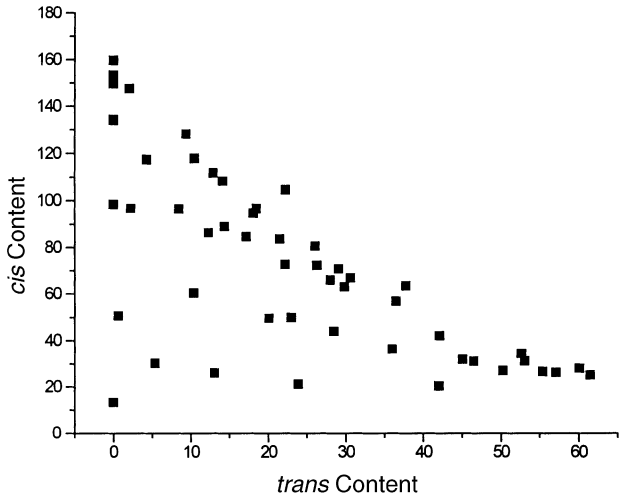

FIG. 2. *Cis* and *trans* values of the generalized calibration set, illustrating how intercorrelation was avoided, thereby ensuring that these variables would be evaluated independently.

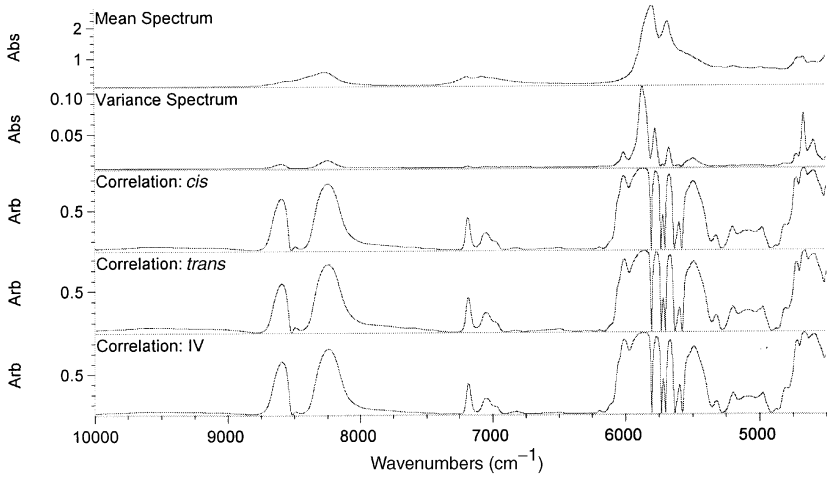

FIG. 3. Mean, variance, and *cis/trans*/iodine value (IV) correlation spectra of the soybean calibration standards.

was found to produce good calibrations for all three parameters with a minimum predictive error. Figure 4 illustrates the one-to-one correspondence between the NIR IV predictions for a set of soybean validation samples and the mid-FTIR reference values. Similar validation plots were obtained for *cis* and *trans* content, and Table 1 summarizes the MD_a and SDD_a for the three parameters measured.

Another basis for evaluating the calibrations is to assess whether they are internally consistent, as there is a defined relationship (Equation 1) between *cis*/*trans* content and IV, as has been discussed elsewhere (6):

$$IV = 0.8601\ cis + 0.8601\ trans \qquad [1]$$

This relationship was assessed by calculating IV from the FT-NIR *cis* and *trans* predictions using Equation 1 and comparing these values to the FT-NIR IV predictions. The relation between the calculated and predicted IV values was:

$$CalcIV = 1.005\ PredIV \qquad SD = 0.93 \qquad r = 0.999 \qquad [2]$$

indicating that the internal consistency expected to exist between the *cis*, *trans,* and IV predictions is maintained for the soybean validation set.

As noted earlier, one can expect that a calibration based on a set of process samples will not be generally applicable because the built-in correlations between *cis* and *trans* content are a potential source of predictive error. To evaluate the magnitude of this effect, samples of hydrogenated rapeseed oil were analyzed. Table 2 presents the linear regression equations and statistics of the FT-NIR predictions for these samples regressed against their mid-FTIR reference values. As can be seen from the data in Table 2, there are definite changes in MD and SDD values relative to those noted in Table 1. In particular, the MD values for the *cis* and IV parameters indicate that the FT-NIR rapeseed predictions are significantly biased while the SDD for IV and *trans* is three to four times greater for the rapeseed than for the soybean validation samples. The IV predictions are graphically shown in Figure 5 and illustrate the magnitude of the errors which can result when a calibration model with a built-in correlation is applied to samples that do not reflect that correlation.

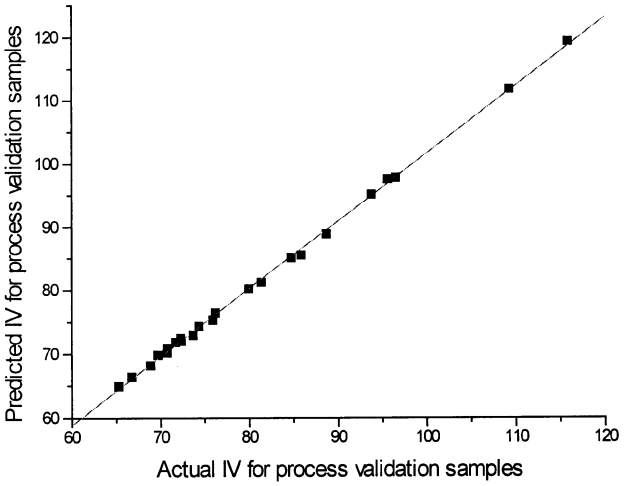

FIG. 4. Plot of predicted vs. actual IV for the process validation samples. Linear regression equation forced through the origin is $y = 1.005x$, SD = 0.99, $r^2 = 0.999$. For abbreviation see Figure 3.

TABLE 1
MD_a, SDD_a, and CV for Process Soybean Validation Samples Relative to the Mid-IR Reference Values[a]

Parameter	*n*	MD_a	SDD_a	CV
Cis	23	–0.26	0.96	1.03
Trans	23	–0.02	0.39	0.93
IV	23	–0.28	1.04	0.57

[a]MD, mean difference; SDD, standard deviation of the differences: CV, coefficient of variation; mid-IR, mid-infrared; *n*, number of samples; IV, iodine value; *a*, accuracy.

TABLE 2
MD_a, SDD_a, and CV for Rapeseed Validation Samples Relative to the Mid-IR Reference Values[a]

Parameter	*n*	MD_a	SDD_a	CV
Cis	15	−6.53	1.41	2.46
Trans	15	0.00	1.89	4.14
IV	15	−4.62	1.50	1.81

[a]For abbreviations see Table 1.

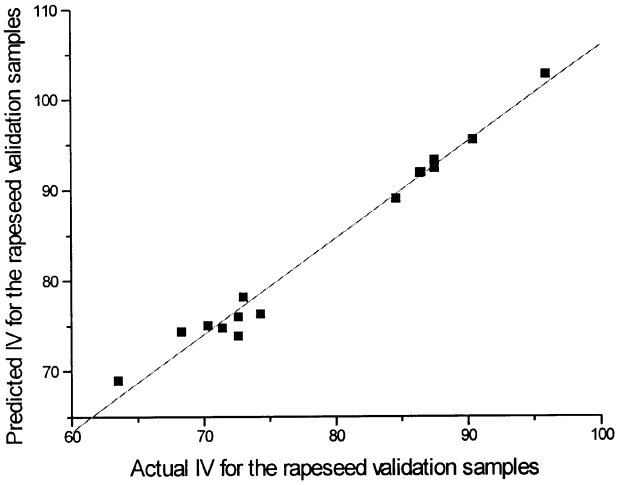

FIG. 5. Plot of predicted vs. actual IV for the rapeseed validation samples. Linear regression equation is $y = -0.291 + 1.062x$, SD = 1.43 r^2= 0.991. For abbreviation see Figure 3.

Generalized calibration. To minimize the potential errors introduced by developing a calibration based on samples having intercorrelated variables, a calibration set was designed to remove all intercorrelations between the parameters of interest. This set consisted of 29 samples prepared by mixing various oils along with 22 samples of hydrogenated soybean and rapeseed oils. Figure 6 presents the mean, variance and correlation (for *cis*, *trans*, IV, and SN) spectra for this calibration set. The mean and variance spectra presented in Figure 6 appear to be quite similar to the corresponding spectra in Figure 3 for the process calibration set. However, Figure 6 differs from Figure 3 in that substantial differences between the *cis*, *trans*, and IV correlation spectra now exist because there are no intercorrelations between these parameters. As a result, it can be expected that the optimum spectral regions for calibration will be different for each parameter and thus have to be determined independently, making the development of the calibration a more time-consuming process.

Table 3 presents the optimal regions chosen for the calibration of each parameter on the basis of the RMSE obtained from a leave-one-out cross-validation, and Table 4 presents the cross-validation MD and SDD statistics for accuracy for both the process-based and the generalized calibrations. It can be seen that the process-based calibrations perform somewhat better, likely owing to the supporting intercorrelation of the three parameters measured. In the generalized calibration approach, PLS has to evaluate each of the parameters independently, resulting in some loss of accuracy; however, this approach has the advantage that the calibration devised can readily be applied to a wide variety of samples, rather than being restricted to samples having particular characteristics. The generalized calibration was validated with a set of 61 samples of hydrogenated soybean and rapeseed oils. A plot of IV predictions vs. the reference IV values for the validation samples is presented in Figure 7. Table 5, which summarizes the accuracy and reproducibility statistics for the four parameters, shows that the accuracy of the generalized cali-

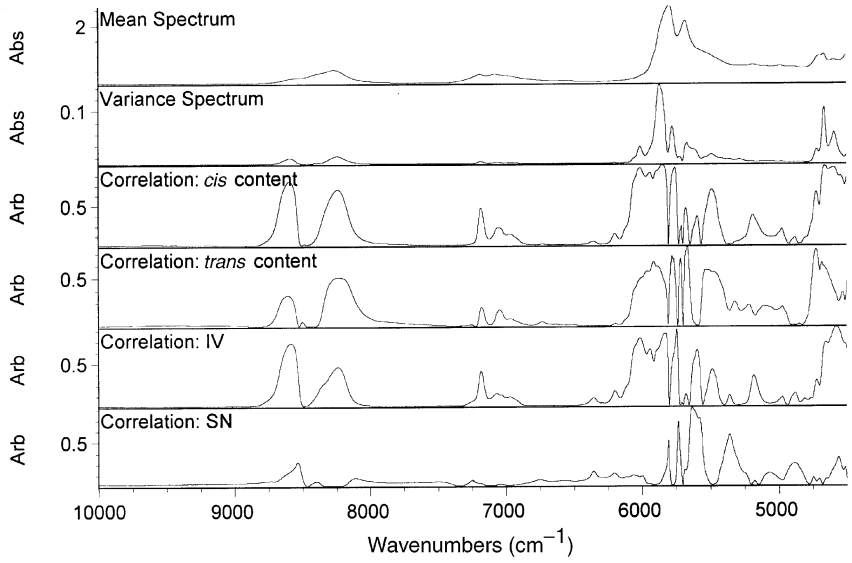

FIG. 6. Mean, variance, and *cis/trans*/IV/saponification number (SN) correlation spectra of the noncorrelated calibration standards.

TABLE 3
Optimized Calibration Regions for *cis/trans*/IV/SN Calibrations

Region (cm^{-1})	Baseline (cm^{-1})	*cis*	*trans*	IV	SN
4698–4553	4825	+[a]		+	
6085–5938	6638	+		+	
8975–7189	7575	+	+	+	
4779–4564	4800		+		
5238–5056	3563		+		
8441–7582	7575				+
8857–8477	7575				+

[a]The plus symbol indicates that the associated spectral region and baseline were used in the calibration model for the parameter. SN, saponification number; for other abbreviation see Table 1.

TABLE 4
Cross-Validation Data for Calibrations Based on Correlated Process Samples and for Generalized Calibrations Based on Noncorrelated Calibration Standards[a]

	Process-based calibration			Generalized calibration		
Parameter	*n*	MD_a	SDD_a	*n*	MD_a	SDD_a
Cis	25	0.015	0.75	51	–0.046	1.58
Trans	25	0.069	0.49	51	0.009	1.44
IV	25	0.059	0.69	51	–0.070	1.00
SN	25	NA	NA	51	0.001	1.93

[a]NA, not applicable. For other abbreviations see Table 1.

brations is largely in line with the leave-one-out cross-validation results (Table 4), indicating that *cis*, *trans*, IV, and SN can be measured to within 1.3 units of the mid-IR reference values. The reproducibility of the predictions, evaluated using a subset of 20 of the validation samples analyzed 2 wk apart, is within one unit for each of the four parameters.

Based on the results obtained in this study, it is apparent that FT-NIR is capable of providing high-quality *cis*, *trans*, IV, and SN data from edible oils if the system is properly calibrated. With the use of a heated flow cell accessory, a typical analysis takes about 2 min per sample, and analysis can be carried out "at-" or "on-line". The critical issue is of course calibration, as FT-NIR is a secondary method of analysis. In this study, reference data were conveniently obtained by mid-IR spectroscopy using our EOA Package. In the industrial setting such data would be obtained using standard chemical methods or by gas chromatography. We have demonstrated the inherent limitation associated with the use of process samples as standards for the development of PLS calibrations if the measured parameters are highly correlated. This does not prevent one from calibrating on such samples; however, it is important to ensure that the standards used are representative of the samples to be analyzed and that the limited scope of applicability of the calibrations be recognized. Our preference is to employ a generalized calibration approach and prepare calibration samples in which the parameters are not correlated, thereby providing the capability to analyze a wide range of oil samples. In conclusion, IV, SN, *cis,* and *trans* content of fats and oils can be determined by FT-NIR analysis, providing a more rapid and convenient alternative to conventional chemical and physical methods of analysis.

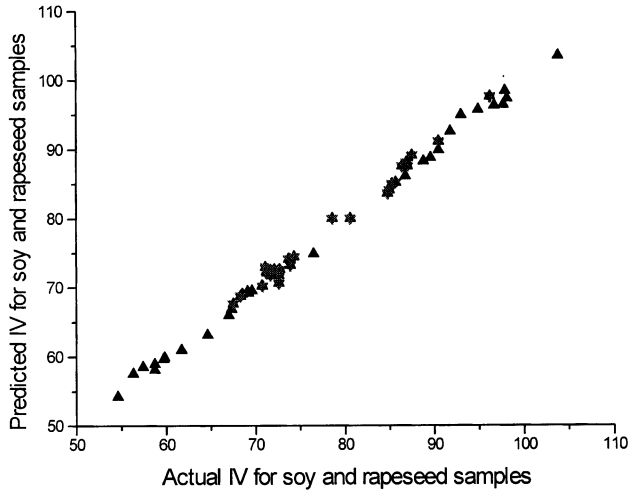

FIG. 7. Plot of predicted vs. actual IV for the soybean (▲) and rapeseed (▼) validation samples.

TABLE 5
Validation Data for the Soybean and Rapeseed Oil Samples Predicted Using the Generalized Calibrations[a]

Parameter	MD_a	SDD_a	N_a	MD_r	SDD_r	N_r
Cis	–0.346	1.184	60	0.263	0.778	20
Trans	–0.272	1.028	60	–0.455	0.451	20
IV	–0.030	0.889	60	0.891	0.686	20
SN	–0.453	1.345	60	0.625	1.074	20

[a]N_a, number of samples for which accuracy was evaluated; N_r, number of samples for which reproducibility was evaluated; for other abbreviations see Table 1.

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REFERENCES

1. Haumann, B.F., Dietary Fats Still Spark Controversy, *INFORM 5*:358 (1994).
2. van de Voort, F.R., J. Sedman, G. Emo, and A.A. Ismail, Rapid and Direct Iodine Value and Saponification Number Determination of Fats and Oils by Attenuated Total Reflectance/Fourier Transform Infrared Spectroscopy, *J. Am. Oil Chem. Soc. 69*:1118–1123 (1992).
3. Ismail, A.A., F.R. van de Voort, J. Sedman, and G. Emo, Rapid Quantitative Determination of Free Fatty Acids in Fats and Oils by FTIR Spectroscopy, *Ibid. 70*:335–341 (1993).
4. van de Voort, F.R., A.A. Ismail, J. Sedman, J. Dubois, and T. Nicodemo, The Determination of Peroxide Value by Fourier Transform Infrared Spectroscopy, *Ibid. 71*:921–926 (1994).
5. van de Voort, F.R., A.A. Ismail, J. Sedman, and G. Emo, Monitoring the Oxidation of Edible Oils by FTIR Spectroscopy, *Ibid. 71*:243–253 (1994).
6. van de Voort, F.R., A.A. Ismail, and J. Sedman, A Rapid Deter-

mination of *cis* and *trans* Content of Fats and Oils by FTIR Spectroscopy, *Ibid. 72*:873–880 (1995).
7. Dunmire, D., and R. Williams, Automated Qualitative and Quantitative NIR Reflectance Analysis, *Cereal Foods World 35*:913 (1990).
8. Dong, J., Kangming Ma, F.R. van de Voort, and A.A. Ismail, Stoichiometric Determination of Hydroperoxides in Oils by Fourier Transform Near-Infrared Spectroscopy, *JAOAC Int. 80*:345–353 (1997).
9. Youden, W.J., and E.H. Steiner, *Statistical Manual of the AOAC*, Association of Official Analytical Chemists, Arlington, 1975.
10. Cast, J., Infrared Spectroscopy of Lipids, in *Developments in Oils and Fats*, edited by R.J. Hamilton, Blackie, Glasgow, 1995, pp. 224–263.
11. Sato, T., S. Kawano, and M. Iwamoto, Near-Infrared Spectral Patterns of Fatty Acid Analysis from Fats and Oils, *J. Am. Oil Chem. Soc. 68*:827–833 (1991).
12. Holman, R.T., and P.R. Edmondson, Near-Infrared Spectra of Fatty Acids and Some Related Substances, *Anal. Chem. 28*:1533–1538.
13. Wetzel, D.L., Lipid Structures and NIRA, presented at the 4th International Symposium NIRA, Kansas State University, Manhattan, 1983.
14. van de Voort, F.R., FTIR Spectroscopy in Edible Oil Analysis, *INFORM 5*:1038–1042 (1994).

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