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Discriminant analysis of edible oils and fats by FTIR, FT-NIR and FT-Raman spectroscopy

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Abstract

The goals of this study were to use Fourier transform mid-infrared (FTIR), near-infrared (FT-NIR) and Raman (FT-Raman) spectroscopy for discrimination among 10 different edible oils and fats, and to compare the performance of these spectroscopic methods for edible oil/fat study. The spectral features of edible oils and fats were studied and the unsaturation bond (C=C) in IR and Raman spectra was identified and used for discriminant analysis. Linear discriminant analysis (LDA) and canonical variate analysis (CVA) were used for the discrimination and classification of different edible oils and fats based on spectral data. FTIR spectroscopy was found to be the most efficient in classification of oils and fats when used with CVA and yielded about 98% classification accuracy, followed by FT-Raman (94%) and FT-NIR (93%) methods; however, the number of factors were much higher for FT-Raman and FT-NIR methods. Overall, results demonstrated that FTIR, FT-NIR and FT-Raman techniques can be used to rapidly and simply determine the authenticity of edible oils and fats with chemometric analysis.

Keywords: FTIR; FT-NIR; FT-Raman; Discriminant analysis; Oil; Fat

1. Introduction

Authenticity is a very important quality criterion for edible oils and fats, because there is a big difference in prices of different types of oil and fat products. However, determination of authenticity for edible oils and fats is traditionally a time-consuming and laborious process, typically using chromatographic methods. Combined with chemometric methods, vibrational spectroscopy, including infrared (IR) and Raman techniques, is an emerging analytical technique to verify the authenticity of edible oils and fats, due to its simplicity, rapidity, and ease of sample preparation. Both IR and Raman techniques have been used for quantitative and qualitative measurement of edible oils and fats (Baeten, Hourant, Morales, & Aparicio, 1998; Guillén & Cobo, 1997; van de Voort, Sedman, & Russin, 2001). The peaks/bands in the IR and Raman spectra at a specific frequency/wavenumber are characteristics of functional groups that constitute the components in the samples. The IR spectrum is obtained by a change in the molecular dipole moment during vibration, while the Raman spectrum is obtained by a change in polarizability during the vibration (Skoog, Holler, & Nieman, 1998). For example, the C=O and O–H stretching, polar functional groups, have strong absorption in the IR spectrum, while the C=C stretching, non-polar functional group, has strong Raman scattering in the Raman spectra. Therefore, the combined use of IR and Raman spectroscopy can extract comprehensive information from the sample.

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NIR spectroscopy has been applied to qualitatively classify oil and fat products (Bewig, Clarke, Roberts, & Unklwsbay, 1994; Blanco & Pagès, 2002; Hourant, Baeten, Morales, Meurens, & Aparicio, 2000; Li et al., 2000; Sato, 1994). However, the peaks in the NIR region (1100–2500 nm or 9091–4000 cm^{-1}) are broad and weak, while they are combinations and overtones of the sample functional groups. For qualitative analysis, the mid-IR (MIR) spectroscopy has more applications, because the 'fingerprints' of functional groups can be displayed narrowly and intensely in the MIR region (4000–400 cm^{-1}). Fourier transform infrared (FTIR) spectroscopy with attenuated total reflectance (ATR) or transmission cell accessories has been used to authenticate, identify or classify fats and oils (Lai et al., 1994; Dahlberg, Lee, Wenger, & Vargo, 1997; Dupuy, Duponchel, Huvenne, Sombret, & Legrand, 1996; Ozen, Weiss, & Mauer, 2003; Safar, Bertrand, Robert, Devaux, & Genot, 1994). Generally, an ATR accessory is used with the FTIR spectrometer for oil and fat study, due to its ability to handle liquid samples easily.

Fourier transform (FT)-Raman spectroscopy can be considered as a complementary method to the IR technique for analysis (Gremlich, 1998). Like FTIR spectroscopy, FT-Raman spectroscopy can also give qualitative and quantitative information of the functional groups in samples. FT-Raman spectroscopy was used to discriminate and classify oils and fats (Aparicio & Baeten, 1998; Baeten et al., 1998; Baeten & Aparicio, 2000; Davies, McIntyre, & Morgan, 2000). FTIR and FT-Raman techniques were compared to determine the authentication of edible oil (Marigheto et al., 1998). With linear discriminant analysis and ANNs, FTIR spectroscopy gave an accuracy of 100% for the authentication of olive oil, while FT-Raman spectroscopy gave 93.1%. Yang and Irudayaraj (2001) compared NIR, FTIR-ATR, FTIR-PAS, and FT-Raman techniques to determine olive pomace oil adulteration in extra virgin olive oil with PLS regression. FT-Raman spectroscopy gave the highest correlation ($R^2 = 0.997$) with the lowest prediction error (SEP = 1.72%). Other NIR and MIR techniques also provided good predictions with an R^2 value greater than 0.99.

Past literature indicates that NIR, FTIR and FT-Raman techniques have been used for discriminant analysis of edible oils and fats, respectively. However, a comparative study of discriminant analysis for a variety of oil and fat samples using different vibrational spectroscopic methods could not be found in the literature. In this study, a variety of fats and edible oils were analyzed by spectroscopic methods and chemometrics, since a mere visual examination of spectra may not be sufficient and hence the need for spectral enhancement or analysis methods. The objective of this study was to compare FTIR, FT-NIR, and FT-Raman spectroscopic methods for rapid discrimination of edible oils and fats. Efforts were also made to correlate the degree of saturation with classification of oils/fats using spectroscopic methods.

2. Materials and methods

2.1. Materials

Butter (Beavers Meadow Creamery Inc., PA and "Finest" Foodhold USA Inc., GA), lard (Hatfield Quality Meats, PA), cod liver oil (E.R. Squibb and Sons Inc., NJ and Roberts laboratory Inc., NJ), extra virgin olive oil ("Sensational" Foodhold USA Inc., GA and "Pompeian" Pompeian Inc., MD), corn oil ("Finest" Foodhold USA Inc., GA and "Mazola" Bestfoods, NJ), peanut oil (Nabisco Inc., NJ and The Hain Food Group Inc., NY), canola (The Hain Food Group Inc., NY and "Crisco" Proctor and Gamble, OH), soybean oil (The Hain Food Group Inc., NY and "Crisco" Proctor and Gamble, OH), safflower oil (The Hain Celestial Group Inc., NY), and coconut oil ("Parachute" Marico Industries Ltd., Mumbai, India) were obtained from a local market. The chemicals and solvents used in our study were of analytical reagent grade.

2.2. FTIR analysis

A Nicolet 870 spectrometer (Nicolet Instrument Corp., Madison, WI) equipped with a deuterated triglycine sulphate (DTGS) detector was used. The same spectrometer was also used for FT-NIR and FT-Raman measurements with additional accessories and detectors. The sampling station was equipped with an overhead ATR accessory (Spectra-Tech, Shelton, CT) comprising of transfer optics within the chamber through which infrared radiation is directed to a detachable ATR zinc selenide crystal mounted in a shallow trough for sample containment. Single beam spectra (4000–400 cm^{-1}) of the samples were obtained against air as a background, to present the spectra in absorbance units at a resolution of 16 cm^{-1} and a total of 256 co-added scans. The ATR crystal was carefully cleaned with pure chloroform to eliminate the presence of oil/fat residues between measurements and dried using nitrogen gas after each experiment to ensure a clean crystal surface so as to obtain the best possible sample spectra. Every oil and fat sample was collected 11 times and used for statistical analysis. The same replication was used for FT-NIR and FT-Raman measurements.

2.3. FT-NIR analysis

The Nicolet 870 spectrometer equipped with the DTGS detector was used for FT-NIR analysis. The sampling station was equipped with a transmission cell from Specta-Tech (CT, USA). White light was used as

a source and the sample was contained in a quartz cuvette. A total of 256 co-added scans were collected for each sample at a resolution of 16 cm^{-1}. The spectra were collected in the range between 2000 and 8000 cm^{-1}, corrected against the background spectrum of air and presented in absorbance units. The quartz cuvette was cleaned with pure chloroform after successive measurements and dried using nitrogen gas to ensure the best possible sample spectra.

2.4. FT-Raman analysis

FT-Raman spectra were obtained using the Nicolet 870 spectrometer with the Nicolet Raman module 32B (Madison, WI) and HeNe laser with a maximum power of 2.0 W. The system was equipped with an InGaAs (Indium-Gallium Arsenide) detector, XT-KBr beam-splitter with 180° reflective optics with a fully motorized sample position adjustment feature. The laser output power of 2.0 W used for analysis was low enough to prevent possible laser induced sample damage yet provided a high signal to noise ratio. Data were collected at 32 cm^{-1} resolution with 256 scans. Spectra were obtained in the Raman shift range between 400 and 3700 cm^{-1}. The system was operated using a OMNIC software (Version 5.1, Madison, WI).

2.5. Discriminant analysis

The Win-DAS (Wiley, Chichester, UK) software package was used for qualitative analysis. Area normalization of spectroscopic data was done to compensate for gross differences in the spectral response that were caused by physical effects, such as instrumental artifacts. Two methods of discriminant analysis were used for the purpose of multiple group classification: these are linear discriminant analysis (LDA) and canonical variate analysis (CVA) (Kemsley, 1998). Since multi-dimensional data (arising when the numbers of variates are larger than the number of observations) cannot be directly used in the above methods, principle component analysis (PCA) and partial least square (PLS) analysis were employed for data compression, to transform the original data set comprising of a large number of inter-correlated variates (wave numbers) into a reduced new set of variates before CVA or LDA. This process is, respectively, denoted by PCA-CVA and PLS-CVA in the text. This procedure was applied to classify edible oils and fats in to different groups by using whole spectra as well as spectral regions known for vibrations of unsaturated C=C bonds. Eleven replications of each oil/fat were used for calibration and validation models. For each sample, eight of 11 measurements were used for the development of calibration model and rest for validation. Hence a total of 80 individual samples were used for calibration and 30 for validation.

2.6. Determination of iodine number

Iodine absorption number for oil and fat samples were determined by Hanus method (AOAC, 1984).

3. Results and discussion

It is well known that every oil/fat differs in composition, length and unsaturated degree of the fatty acids as well as their positions in the chain. IR and Raman spectra represent a combined fingerprint pattern unique to each oil/fat and were used for discriminant analysis. A second set of analysis was conducted using regions specific to the C=C bond vibration. The double bond considered is an unsaturated bond and the intensities, areas or heights of its peak in this region might indicate the degree of unsaturation in fatty acids, sterols, and vitamins.

Fig. 1 shows the FTIR spectra of 10 edible oils and fats. The triglyceride, which is a major component in edible oils and fats, was dominant in the spectra. The major peaks that represent triglyceride functional groups could be observed around 2937 cm^{-1} (C–H stretching (asymmetry)), 2856 cm^{-1} (C–H stretching (symmetry)), 1749 cm^{-1} (C=O stretching), 1454 cm^{-1} (C–H bending (scissoring)), 1166 cm^{-1} (C–O stretching and C–H bending), and 709 cm^{-1} (C–H bending (rocking)) (Guillén & Cobo, 1997). There was a very weak peak around 1650 cm^{-1} (Fig. 1) in IR spectra, which is C=C stretching (*cis*). It was very difficult to differentiate these oils and fats based on the spectra from observation. Therefore, the chemometric techniques, such as PCA and PLS, were adopted to systematically classify edible oils and fats based on their FTIR spectra.

Classification of edible oils and fats was performed by discriminant analysis using the FTIR spectra between 400 and 4000 cm^{-1} and between 1400 and 1800 cm^{-1}, respectively. The whole spectra between 400 and 4000 cm^{-1} are the combination of many constituents of oil/fat whereas the region selected between 1400 and 1800 cm^{-1} mostly represents the combination of C–H bending, C=O stretching, and C=C stretching and hence is directly related to unsaturated C=C bond. When data from both spectra (i.e., between 400 and 4000 cm^{-1} and spectra between 1400 and 1800 cm^{-1}) were used in the analysis CVA with PLS data compression method was found to give the highest classification accuracy than the other methods (i.e., PCA-LDA, PCA-CVA, and PLS-LDA). Results of the discriminant analysis are shown in Table 1. The factor numbers for discriminant analysis were only three for spectra between 1400 and 1800 cm^{-1} compared to five for spectra between 400 and 4000 cm^{-1}. It demonstrated that vibrations of C–H bending, C=O stretching, and C=C stretching played a very important role in discriminant analysis.

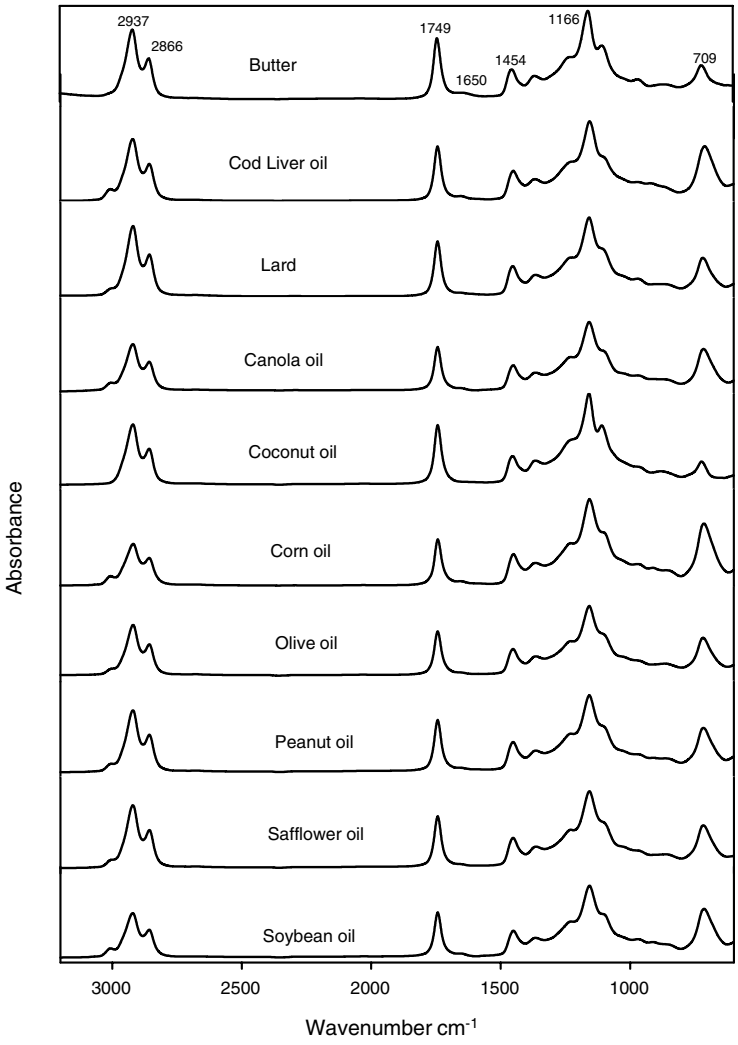

Fig. 1. FTIR spectra of different edible oils and fats.

Table 1
Discrimination analysis of FTIR spectra of oils and fats

	Factors	% Correct discrimination of calibration samples	% Correct discrimination of validation samples
(400–4000 cm^{-1})			
PCA compression method			
LDA	5	96.3	97.8
CVA	5	94.2	95.6
PLS compression method			
LDA	5	96.3	97.8
CVA	5	94.6	95.6
(1400–1800 cm^{-1})			
PCA compression method			
LDA	3	94.2	96.7
CVA	3	92.1	98.9
PLS compression method			
LDA	3	94.2	96.7
CVA	3	92.1	98.9

The correct classification for calibration as well as validation models for both the regions were found to be greater than 92%.

Figs. 2 and 3 systematically show the classification model of PLS-CVA for edible oils and fats based on FTIR spectra between 400 and 4000 cm^{-1} and spectra between 1400 and 1800 cm^{-1}, respectively. A total of 10 different classes of edible oils and fats are displayed in Figs. 2 and 3. More clear separation of clusters was observed in the case of spectra between 1400 and 1800 cm^{-1} (Fig. 3) than the spectra between 400 and 4000 cm^{-1} (Fig. 2). Iodine numbers for the oil and fat samples were determined and tabulated (Table 2). They were in the range reported in the literature. Upon comparison (Fig. 3 and Table 2), coconut oil and butter separate clearly in the PLS-CVA cluster analysis from the rest of oils and fats considered because their iodine numbers are less than 50 or a lower degree of unsaturation (i.e., C=C bond). Validation tests are performed and values of R^2 are more than 0.95 for all discriminant analyses.

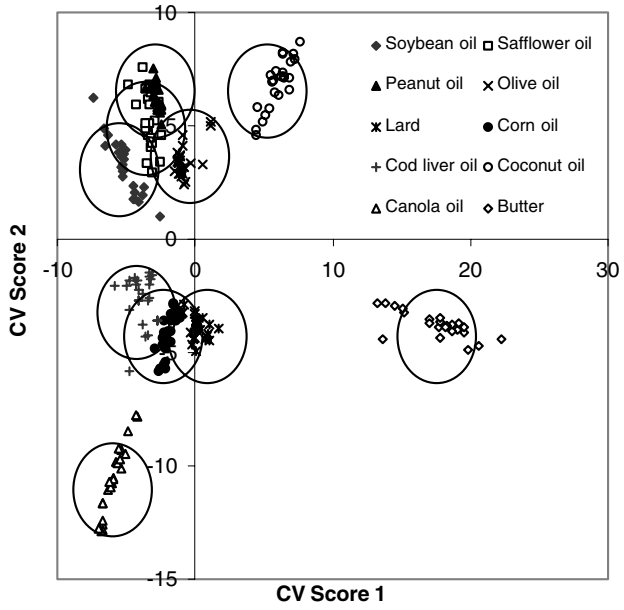

Fig. 2. PLS-CVA plot for classification of edible oil and fats using FTIR spectra in the region 400–4000 cm^{-1}.

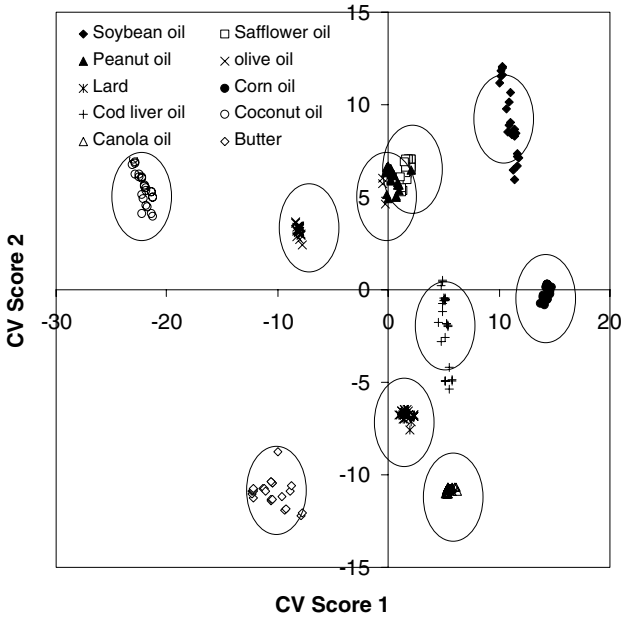

Fig. 3. PLS-CVA plot for classification of edible oil and fats using FTIR spectra in the region 1400–1800 cm^{-1}.

FT-NIR spectra of edible oils and fats are displayed in Fig. 4. The peaks/bands in FT-NIR were much broader and weaker, compared to those in the FTIR spectra (Fig. 1). The FTIR spectrum contains more isolated bands, while the NIR spectrum contains more overlapped bands. The region between 5500 and 6000 cm^{-1} is the first overtone of the C–H stretching from $–CH_2$, $–CH_3$ and –CH=CH– functional groups of edible oils and fats (Hourant et al., 2000). The region between

Table 2
Iodine numbers for different edible oils and fats.

Oils/fats	Iodine numbers	Normal ranges[a]
Coconut	11.3 ± 1.28	8–10
Soybean	132.8 ± 2.19	125–140
Canola	122.5 ± 0.911	110–126
Safflower	135 ± 2.01	130–140
Olive	86.1 ± 2.90	75–95
Corn	124 ± 3.82	115–130
Pea	100 ± 2.60	85–100
Cod liver	160 ± 0.85	120–180
Butter	40.0 ± 3.88	25–40
Lard	73.3 ± 4.25	45–70

[a] Reported values.

4500 and 4800 cm^{-1} is the combination of C–H stretching related to *cis* double bonds, while the intensity of this area increases with the degree of total unsaturation (Hourant et al., 2000).

Table 3 shows the results of discriminant analysis based on FT-NIR spectra. The values of R^2 for calibration samples were from 0.85 to 0.94, while the values of R^2 for validation samples were 0.84 to 0.93. The rate of correct classification obtained from discriminant analysis of the spectra between 2000 and 8000 cm^{-1} was found to be better than the data from the spectral region between 4000 and 6500 cm^{-1}. The number of factors used in the model was also found to be more for the model with data from the region between 4000 and 6500 cm^{-1} compared with the whole spectra between 2000 and 8000 cm^{-1}. This may be due to the fact that factors other than the degree of saturation may be contributing more towards the classification of oils and fat. Results from FT-NIR were not as good as those from FTIR. This may be due to the differences of vibrational features of functional groups in the NIR and MIR regions. It is well known that functional groups have strong and narrow absorbances (peaks/bands) in the MIR region but very broad and weak absorbances in the NIR region. Therefore, NIR spectroscopy is more commonly used for quantitative analysis while FTIR spectroscopy, on the other hand, is more commonly used for qualitative analysis.

The FT-Raman spectra of oils and fats are shown in Fig. 5. Major peaks included 3013 cm^{-1} (=C–H stretching (asymmetry)), 2909 cm^{-1} (C–H stretching (asymmetry)), 1750 cm^{-1} (C=O stretching), 1660 cm^{-1} (C=C stretching), 1447 cm^{-1} (C–H bending), and 1294 cm^{-1} (=C–H bending (*cis*)) (Baeten et al., 1998). The spectra between 400 to 3700 cm^{-1} and 1600 to 1700 cm^{-1} were used for discriminant analysis. It should be noted that the region between 1600 and 1700 cm^{-1} contains the stretching vibration of the C=C bond which is very distinctive around 1660 cm^{-1} in FT-Raman spectra (Fig. 5) but not in FTIR spectra (Fig. 1). It demonstrated that FT-Raman

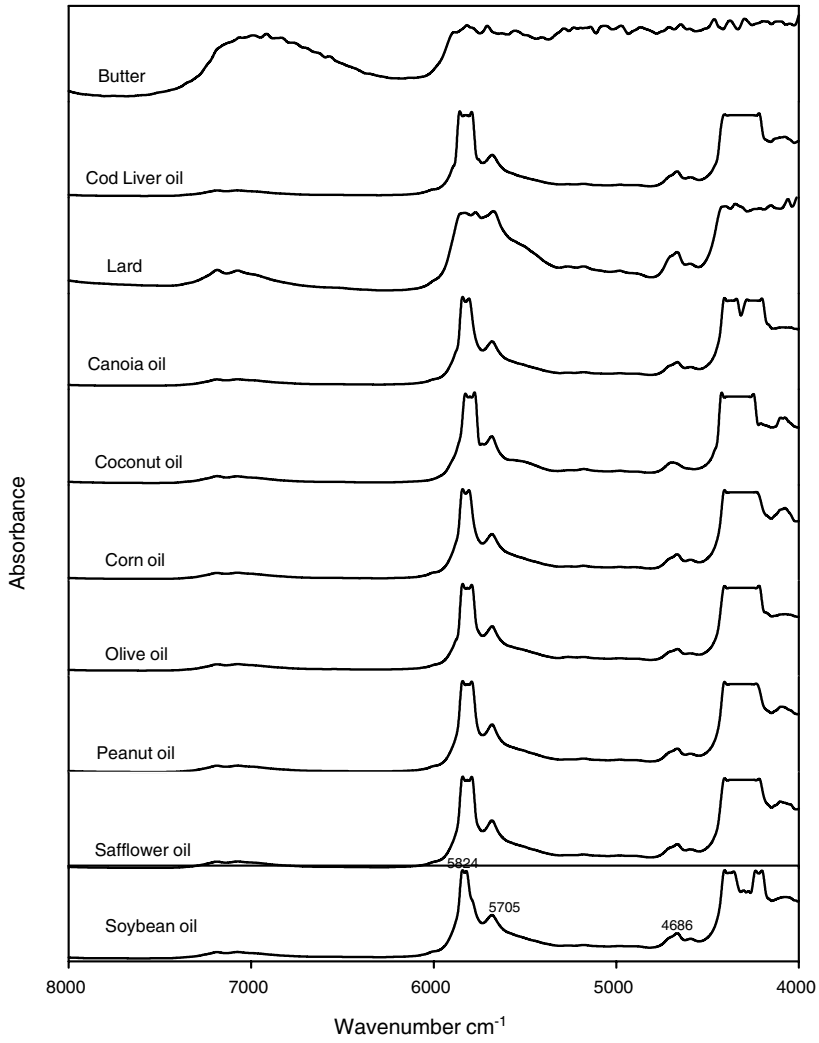

Fig. 4. FT-NIR spectra of different edible oils and fats.

Table 3
Discrimination analysis of FT-NIR spectra of oils and fats.

	Factors	% Correct discrimination of calibration samples	% Correct discrimination of validation samples
(2000–8000 cm^{-1})			
PCA compression method			
LDA	5	93.8	85.6
CVA	5	90.0	92.2
PLS compression method			
LDA	6	93.8	90.0
CVA	6	91.3	91.1
(4000–6500 cm^{-1})			
PCA compression method			
LDA	7	85.4	84.4
CVA	10	92.1	90.0
PLS compression method			
LDA	10	85.4	86.7
CVA	10	90.0	93.3

spectra can display non-polar groups of samples, which are very weak in IR spectrum.

Table 4 showed that the results obtained for both the regions were almost same. The rate for correct classification with CVA methods was found to be more than 91% for both the calibration and validation samples due to the degree of unsaturation (i.e., C=C bond). Results from FT-Raman measurements were not as good as these from FTIR. Normally, peaks/bands of bending vibrations, such as C–H, in Raman spectra are much weaker than these of stretching vibrations (Baeten et al., 1998). Vibrations from polar groups, such as C=O and O–H, are very weak in Raman spectra. Therefore, the lower correct classifying rate from FT-Raman spectra was obtained due to some important vibrations missing or weak in Raman spectra, such as C–H bending and C=O stretching, which could play very important roles in discriminant analysis. It could also be caused by the lower signal-to-noise ratio of FT-Raman, compared to that of FTIR (Marigheto et al., 1998). Baeten et al.

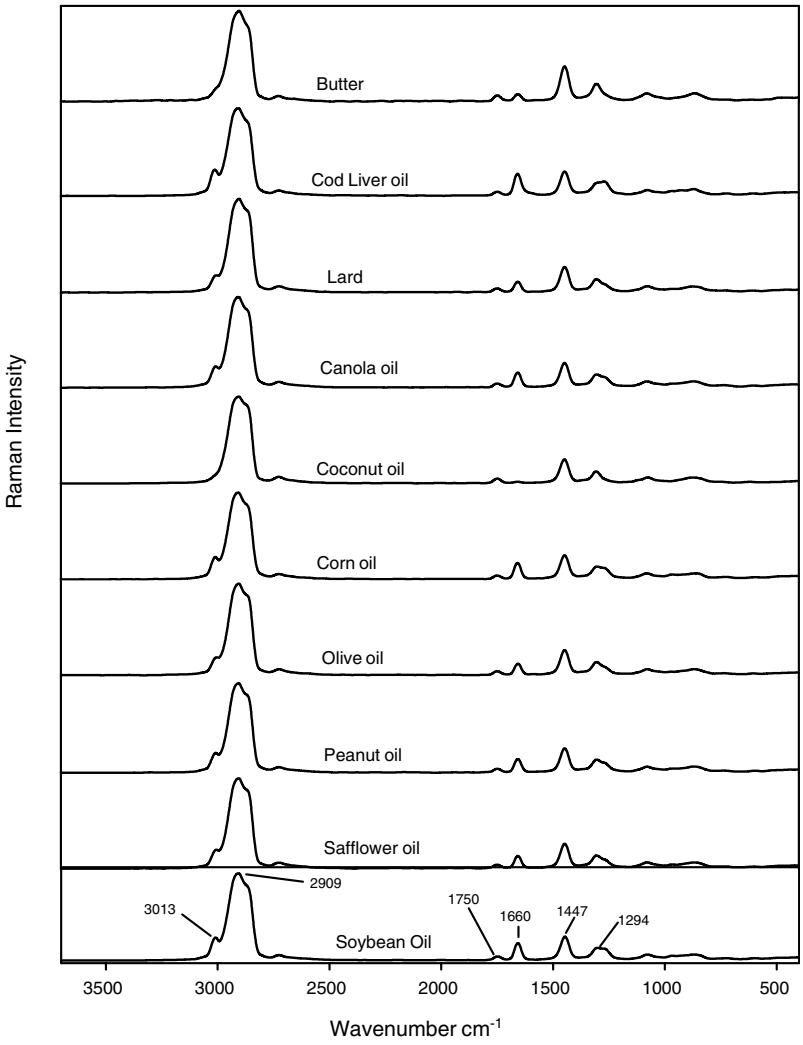

Fig. 5. FT-Raman spectra of different edible oils and fats.

Table 4
Discrimination analysis of FT-Raman spectra of oils and fats.

Adulterants	Factors	% Correct discrimination of calibration samples	% Correct discrimination of validation samples
(400–3700 cm^{-1})			
PCA compression method			
LDA	8	90.0	85.6
CVA	8	92.5	91.1
PLS compression method			
LDA	8	93.8	88.9
CVA	8	93.3	94.4
(1600–1700 cm^{-1})			
PCA compression method			
LDA	8	90.0	85.6
CVA	8	92.1	91.1
PLS compression method			
LDA	8	93.8	88.9
CVA	8	92.5	94.4

(1998) reported that FT-Raman spectroscopy had problems in classifying soybean, corn and sunflower oils into clear separate groups.

4. Conclusion

Generally, FTIR, FT-NIR and FT-Raman spectroscopy techniques can be used for rapid classifying edible oils and fats without the need for sample preparation. Both FTIR and FT-Raman spectroscopy techniques provided exquisite structural insights into functional groups of oils and fats for discriminant analysis. FTIR spectroscopy was found to be the most superior for discrimination and classification of edible oil and fats followed by the FT-Raman method. The FT-NIR method, although capable of discriminating and classifying oils and fats, was found to be less efficient than the other two spectroscopic methods.

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