JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY
ARTICLE

J. Agric. Food Chem. 2009, 57, 9985–9989 9985
DOI:10.1021/jf901730p

Prediction of the Genetic Variety of Extra Virgin Olive Oils Produced at *La Comunitat Valenciana*, Spain, by Fourier Transform Infrared Spectroscopy

Victoria Concha-Herrera,[†] María Jesús Lerma-García,[‡] José Manuel Herrero-Martínez,[‡] and Ernesto Francisco Simó-Alfonso*,[‡]

[†]Unidad Académica de Ciencias Químicas, Universidad Autónoma de Zacatecas, 98160 Zacatecas, México, and [‡]Department of Analytical Chemistry, Faculty of Chemistry, University of Valencia, 46100 Burjassot, Valencia, Spain

Fourier transform infrared spectroscopy (FTIR), followed by multivariate treatment of the spectral data, was used to classify extra virgin olive oils (EVOOs) according to their genetic variety. EVOO samples corresponding to seven different genetic varieties (Arbequina, Borriolenca, Canetera, Farga, Hojiblanca, Picual, and Serrana) were analyzed. The wavelength scale of the FTIR spectra of the oils was divided into 20 regions. The normalized absorbance peak areas within these regions were used as predictor variables. Classification of the EVOO samples according to their genetic variety was achieved by linear discriminant analysis (LDA). A good resolution among all categories was achieved using a LDA model constructed with only nine predictor variables. With this LDA model, 88% of the EVOOs were correctly classified, with assignment probabilities higher than 95%. This method is helpful for olive oil producers because it provides useful information related to the genetic variety of EVOOs, which is required by European Community regulations.

KEYWORDS: Extra virgin olive oil; genetic variety; Fourier transform infrared spectroscopy; linear discriminant analysis

INTRODUCTION

Extra virgin olive oil (EVOO) is a traditional Mediterranean food product, whose market has recently been expanded because of its highly appreciated organoleptic attributes and its health and nutritional properties (*1*). Along the last few years, the consumption of EVOOs has increased considerably in relation to the consumption of virgin and refined olive oils. Owing to its distinctive and peculiar intense taste, EVOOs obtained from some pure genetic varieties are highly appreciated.

To establish the authenticity of edible oils, a number of chromatographic (*2*−*4*), thermal (*5*), and spectroscopic methods, including fluorescence (*6*), near-infrared spectroscopy (*7*, *8*), Fourier transform infrared spectroscopy (FTIR) (*8*−*14*), FT-Raman (*8*), nuclear magnetic resonance (*15*), and mass spectrometry (MS) (*16*−*18*), followed by multivariate statistical analysis of data, have been described. For this purpose, the contents of fatty acids (*2*, *14*), tocopherols (*6*), volatile compounds (*4*), amino acids (*17*), and sterols (*3*, *18*), among others, have been used.

The development of methods to distinguish the genetic variety and also the geographical origin of EVOOs is important because, according to the European Community (EC) regulation 182/2009 (*19*), olive oil producers have to include in their manufactured products the genetic variety and also the geographical origin of the olives. In fact, authentication methods for genetic varieties of EVOO have been mainly addressed by gas chromatography (*20*−*28*) and high-performance liquid chromatography (*20*−*24*). Other techniques, such as MS (*29*), have also been used for these purposes.

FTIR is a rapid and nondestructive powerful analytical tool for the study of edible oils and fats, requiring minimum sample preparation. FTIR is also an excellent tool for quantitative analysis, because the intensities of the spectral bands are proportional to the concentration. For this reason, FTIR has mainly been used to distinguish oils from different botanical origins using non-supervised classificatory techniques (*10*, *11*), to distinguish EVOOs from different geographical origins (*30*, *31*), and to detect olive oil adulteration with other low-cost edible oils (*9*, *12*, *13*). FTIR has also been used to distinguish mixtures of three Turkish monovarietal olive oils using principal component analysis (*32*).

In this work, FTIR, jointly with the application of linear discriminant analysis (LDA), is used to classify EVOOs from seven different genetic varieties, commonly produced at *La Comunitat Valenciana*, Spain. For this purpose, FTIR spectra were divided into 20 wavelength regions, using the normalized absorbance peak areas as predictor variables.

EXPERIMENTAL PROCEDURES

Oil Samples. The EVOO samples employed in this study were mainly produced at *La Comunitat Valenciana*, Spain. Other samples, such as Hojiblanca and Picual, which were not commonly cultivated at *La Comunitat Valenciana*, were also included in this study because, jointly with the Arbequina variety, they are the main varieties in the

*To whom correspondence should be addressed. Telephone: +34-96-354-3176. Fax: +34-96-354-44 36. E-mail: ernesto.simo@uv.es.

Published on Web 10/08/2009

Table 1. Genetic Variety, Number of Samples, Geographical Origin, and Supplier of the EVOOs

genetic variety	number of samples	geographical origin	supplier	crop season
Arbequina	2	Altura (Castellón)	Intercoop	06/07, 07/08
	2	Maestrat comarca (Castellón)	Intercoop	06/07, 07/08
	2	Alicante	Intercoop	05/06, 07/08
	2	Palancia comarca (Castellón)	Intercoop	06/07, 07/08
Borriolenca	3	Alcalatén comarca (Castellón)	Intercoop	05/06, 06/07, 07/08
	4	La Plana comarca (Castellón)	Intercoop	05/06, 06/07, 07/08
Canetera	3	Maestrat comarca (Castellón)	Intercoop	05/06, 07/08
	2	Adzaneta (Castellón)	Intercoop	06/07, 07/08
	3	La Plana comarca (Castellón)	Intercoop	05/06, 06/07, 07/08
Farga	4	Maestrat comarca (Castellón)	Intercoop	05/06, 06/07, 07/08
	3	Alcalatén comarca (Castellón)	Intercoop	06/07, 07/08
	3	La Plana comarca (Castellón)	Intercoop	05/06, 06/07, 07/08
Hojiblanca	2	Estepa (Sevilla)	Carbonell	06/07, 07/08
	2	Luque (Córdoba)	Coosur	06/07, 07/08
	3	Puente Genil (Córdoba)	Borges	06/07, 07/08
	5	Fuente de Piedra (Málaga)	Grupo Hojiblanca	05/06, 06/07, 07/08
	1	Santaella (Córdoba)	Columela	05/06
Picual	2	Martos (Jaén)	Carbonell	06/07, 07/08
	2	Villanueva del Arzobispo (Jaén) and Porcuna (Jaén)	Coosur	06/07
	3	Quesada (Jaén)	Borges	05/06, 06/07, 07/08
	1	Montoso (Córdoba)	Grupo Hojiblanca	06/07
	1	Tabernas (Almería)	Castillo de Tabernas	06/07
	1	Canena (Jaén)	Castillo de Canena	07/08
Serrana	9	Altura (Castellón)	Cooperativa Altura and Intercoop	05/06, 06/07, 07/08
	3	Artana (Castellón)	Intercoop	06/07, 07/08
	3	Jérica (Castellón)	Intercoop	06/07, 07/08
	5	Viver (Castellón)	Intercoop	05/06, 06/07, 07/08

Spanish market. The genetic variety, number of samples, geographical origin, sample suppliers, and crop season are shown in **Table 1**. All Valencian samples were kindly donated by *Intercoop Olival* (Almassora, Castellón, Spain) and the *Cooperativa de Altura* (Castellón, Spain). Other samples were purchased at the local market, with their genetic variety and geographical origin being certified by the suppliers. All of the samples were stored in amber glass bottles at −20 °C prior to their analysis.

FTIR Spectra. FTIR spectra were obtained using a Jasco 4100 type A spectrophotometer (Jasco, Easton, MD) fitted with a single reflection attenuated total reflectance (ATR) accessory. The ATR accessory (ATR-PRO410-S, Jasco) was equipped with a ZnSe reflection crystal. All analyses were carried out at room temperature. Measurements were obtained using 15 scans at 2 cm^{-1} resolution. Spectra were recorded in the absorbance mode from 4000 to 600 cm^{-1}, with only the regions being from 2500 to 750 cm^{-1} considered in this study. Data handling was performed with the Spectra Manager version 2.07.00 software (Jasco).

For each sample (ca. 20 μL were put on the crystal surface), the absorbance spectrum was collected against a background obtained with a dry and empty ATR cell. Two spectra were recorded for each sample. Before each spectrum was acquired, the ATR crystal was cleaned with a cellulose tissue soaked in *n*-hexane, rinsed with acetone, and dried.

Data Treatment and Construction of Data Matrices. FTIR spectra were divided into the 20 wavelength regions described in **Table 2**. Each selected region corresponds to a peak or a shoulder, which represent structural or functional group information, either about the lipids or minor components of the oil samples (see **Table 2**). For each region, the peak/shoulder area was measured. To reduce the variability associated with the total amount of oil sample used and to minimize other sources of variance also affecting the intensity of all of the peaks, such as the radiation source intensity, normalized rather than absolute areas were used. To normalize the variables, the area of each region was divided by each one of the areas of the other 19 regions; in this way and because any pair of areas should be considered only once, $(20 \times 19)/2 = 190$ normalized variables were obtained.

A matrix containing 76 objects, which corresponded to the average of 2 replicates (**Table 1**), and 190 predictors, was constructed. A response column, containing the categories corresponding to the 7 genetic varieties of the oils, was added to this matrix. Only the means of the replicates of the samples were included in this matrix; in this way, the internal dispersion of the categories was reduced, which was important to reduce the number of variables selected during model construction. The matrix was randomly divided into two groups, training and evaluation sets. The training set was composed of 6 samples for each genetic variety ($6 \times 7 = 42$ objects), while the evaluation set was performed with the remaining samples (34 objects). Statistical data treatment of the normalized variables was performed using the SPSS package (version 12.0.1, Statistical Package for the Social Sciences, Chicago, IL).

RESULTS AND DISCUSSION

FTIR spectra of the 76 EVOO samples shown in **Table 1** were collected. **Figure 1** shows the spectra of seven oils, corresponding to the seven genetic varieties. As it can be observed, FTIR spectra were closely similar. To enhance small differences that were not appreciated straight away in the spectra of oils obtained from different genetic varieties, the peak areas of the 20 selected regions were conveniently handled by multivariate statistical techniques.

Classification of EVOOs According to Their Genetic Variety Using LDA. LDA, a supervised classificatory technique, is widely recognized as an excellent tool to obtain vectors showing the maximal resolution between a set of previously defined categories. In LDA, vectors minimizing Wilks' lambda, λ_w, are obtained (*35*). This parameter is calculated as the sum of squares of the distances between points belonging to the same category

Table 2. FTIR Spectral Regions Selected as Predictor Variables for Statistical Data Treatment

identification number	range (cm^{-1})	functional group	nominal frequency	mode of vibration
1	2393−2347	alcane[a]		
2	2347−2279	alcane[a]		
3	1870−1712	−C=O (ester)	1746[b]	stretching
4	1712−1693	−C=O (acid)	1711[b]	stretching
5	1693−1671	−C=O	[a]	stretching
6	1671−1590	−C=C− (*cis*)	1654[b]	stretching
		−C−H (CH_2)	1465[a]	bending (scissoring)
7	1467−1426	−C−H (CH_3)	1450[a]	bending (asym)
8	1426−1407	=C−H (*cis*)	1417[b]	bending (rocking)
9	1407−1380	=C−H	1400[a]	bending
		−C−H (CH_3)	1377[b]	bending (sym)
10	1380−1336	O−H	1359[a]	bending (in plane)
11	1336−1309	non-assigned	1319[b]	bending
12	1309−1292	=C−H (*cis*)	1294[c]	bending
13	1292−1257	=C−H	−[c]	bending
14	1257−1216	−C−O		stretching
		$-CH_2-$	1238[b]	bending
		−C−O	1163[b]	stretching
15	1216−1127	$-CH_2-$	1163[b]	bending
		−C−O	1138[a]	stretching
16	1127−1109	−C−O	1118[b]	stretching
17	1109−1045	−C−O	1097[b]	stretching
18	1045−998	−C−O	1033[b]	stretching
		−HC=CH− (*trans*)	968[b]	bending (out of plane)
19	998−883	−HC=CH− (*cis*)?	914[b]	bending (out of plane)
20	883−796	$=CH_2$	850[a]	wagging

[a] According to ref *34*. [b] According to ref *33*. [c] According to ref *8*.

divided by the total sum of squares. Values of λ_w approaching 0 are obtained with well-resolved categories, whereas overlapped categories made λ_w approach 1. Up to $N-1$ discriminant vectors are constructed by LDA, with N being the lowest value for either the number of predictors or the number of categories.

Using the normalized variables, a LDA model capable of classifying the EVOO samples according to their genetic varieties was constructed. To select the variables to be included in the model, the SPSS stepwise algorithm was used. According to this algorithm, a predictor is selected when the reduction of λ_w produced after its inclusion in the model exceeds F_{in}, the entrance threshold of a test of comparison of variances or F test. However, the entrance of a new predictor modifies the significance of those predictors that are already present in the model. For this reason, after the inclusion of a new predictor, a rejection threshold, F_{out}, is used to decide if one of the other predictors should be removed from the model. The process terminates when there are no predictors entering or being eliminated from the model. The default probability values of F_{in} and F_{out}, 0.05 and 0.10, respectively, were adopted.

A good resolution between the seven categories was achieved when the LDA model was constructed ($\lambda_w = 0.576$). This λ_w value was higher than those previously reported in our previous work (*29*); however, in this previous study, just three categories were simultaneously distinguished. The variables selected by the SPSS stepwise algorithm and the corresponding standardized coefficients of the model, showing the predictors with large discriminant capabilities, are given in **Table 3**. According to this table, the main IR regions selected by the algorithm to construct the LDA model corresponded to −C=O (acid, stretching), −C−H (CH_2, bending scissoring), −C−H (CH_3, bending sym), =C−H (bending), −C−O (stretching), and $-CH_2-$ (bending).

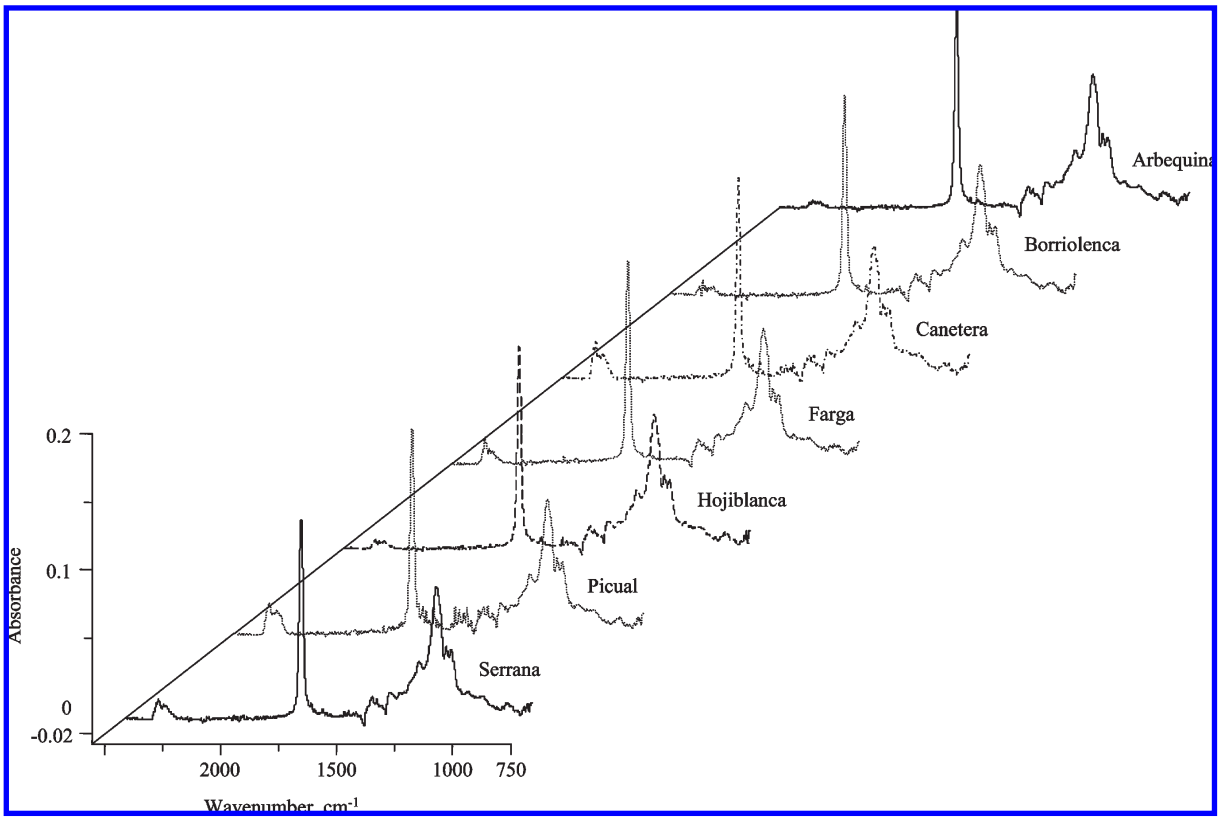

Figure 1. FTIR spectra of EVOO samples of (A) Arbequina from Alicante (crop season 05/06), (B) Borriolenca from Alcalatén comarca (crop season 07/08), (C) Canetera from La Plana comarca (crop season 06/07), (D) Farga from Maestrat comarca (crop season 06/07), (E) Hojiblanca from Luque, Córdoba (crop season 07/08), (F) Picual from Martos, Jaén (crop season 06/07), and (G) Serrana from Altura, Castellón (crop season 05/06).

Table 3. Predictors Selected and Corresponding Standardized Coefficients of the LDA Model Constructed To Predict the Genetic Variety of EVOOs

predictors[a]	f_1	f_2	f_3	f_4	f_5	f_6
1/5	0.13	−0.91	−0.96	−0.06	−0.60	−2.04
1/7	5.85	4.36	−1.51	4.00	4.07	−2.22
1/9	−6.01	−3.57	3.91	−3.71	−3.11	4.03
3/6	−0.13	0.30	0.47	0.58	0.95	0.76
4/12	9.48	15.43	12.74	16.47	−7.05	−6.22
4/14	−9.00	−14.54	−12.66	−16.58	7.15	6.35
12/15	0.85	1.32	1.25	1.30	−0.89	0.35
13/16	−0.28	−0.55	0.69	−0.11	1.03	−0.48
14/17	1.06	−0.10	−0.37	−0.32	−0.41	0.43

[a] Pairs of wavelength regions were identified according to **Table 2**.

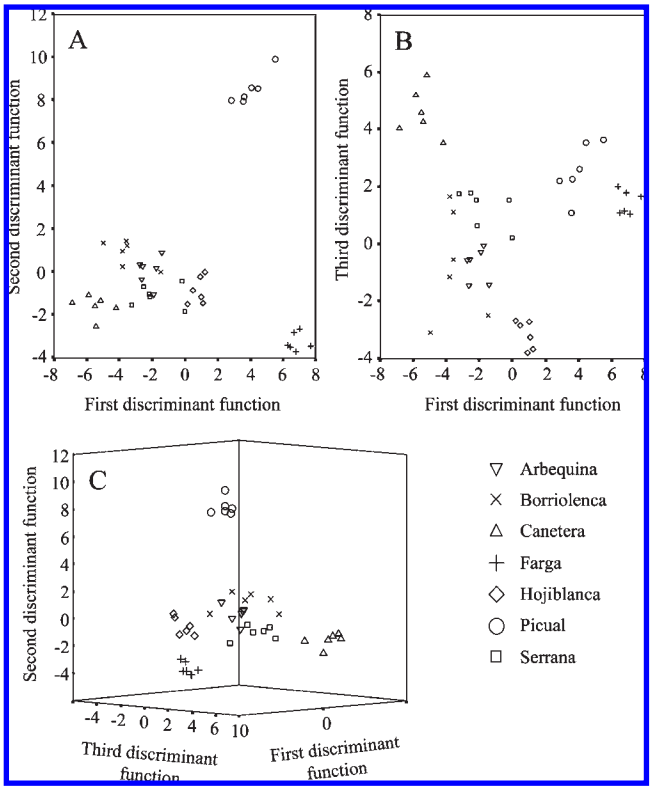

Figure 2. Score plots on the planes of the (A) first and second and (B) first and third discriminant functions and (C) an oblique perspective of the 3D space defined by the three discriminant functions of the LDA model constructed to classify EVOOs according to their genetic variety.

The projections of the samples on the six discriminant functions allowed for the distinction of at least a different category. As shown in **Figure 2A**, a large resolution between Farga, Picual, and the other categories was achieved along f_1. On the other hand, the variance gathered by f_2 was mainly associated with the resolution between Picual and the rest of categories as a whole. According to **Figure 2B**, Canetera, Picual, and Hojiblanca were resolved from the rest of categories along f_3. Finally, **Figure 2C** shows a score plot from an oblique perspective of the 3D space defined by the three first discriminant functions. When this 3D figure was rotated, the separation between all of the different categories was evident. Because of the fact that a large number of categories (seven) were included in this work in relation to the three categories described in our previous work (*29*), it is logical that it was more difficult to appreciate separation between categories when represented in a plane. When the leave-one-out validation method was applied to the training set, all of the points were correctly classified. Concerning the evaluation set, all of the objects were correctly assigned to an assignment probability higher than 95%, except four objects, which corresponded to two Borriolenca, one Hojiblanca, and one Arbequina samples.

Thus, the possibility of classifying EVOO samples according to their genetic variety using FTIR data has been demonstrated. Using only nine predictors, all of the EVOO samples belonging to seven different genetic varieties mainly produced at *La Comunitat Valenciana* were correctly classified with a good resolution among the categories. According to the EC regulation (*19*), this reliable procedure provides useful information regarding the genetic varieties, which is important for olive oil producers.

On the other hand, this method is faster than other methods described in the literature (*20*−*23*, *26*), which are based on chromatographic separations, using fatty acids (*20*−*22*, *26*), sterols (*21*), *n*-alkanes (*23*), and triglycerides (*22*) as variables. For classification purposes, these methods have used both nonsupervised and supervised statistical tools. The first one just led to a preliminary distribution according to the genetic varieties (*20*). The second approach produced satisfactory resolution among the categories (*21*−*23*, *26*); however, in these studies, no more than five categories were simultaneously resolved.

ABBREVIATIONS USED

EVOO, extra virgin olive oil; LDA, linear discriminant analysis; MS, mass spectrometry.

LITERATURE CITED

(1) Bendini, A.; Cerretani, L.; Carrasco-Pancorbo, A.; Gómez-Caravaca, A. M.; Segura-Carretero, A.; Fernández-Gutiérrez, A.; Lercker, G. Phenolic molecules in virgin olive oils: A survey of their sensory properties, health effects, antioxidant activity and analytical methods. An overview of the last decade. *Molecules* **2007**, 12, 1679–1719.

(2) Brodnjak-Voncina, D.; Kodba, Z. C.; Novic, M. Multivariate data analysis in classification of vegetable oils characterized by the content of fatty acids. *Chemom. Intell. Lab. Syst.* **2005**, 75, 31–43.

(3) Mariani, C.; Bellan, G.; Lestini, E.; Aparicio, R. The detection of the presence of hazelnut oil in olive oil by free and esterified sterols. *Eur. Food Res. Technol.* **2006**, 223, 655–661.

(4) de Koning, S.; Kaal, E.; Janssen, H.-G.; van Platerink, C.; Brinkman, U. A. T. Characterization of olive oil volatiles by multi-step direct thermal desorption−comprehensive gas chromatography−time-of-flight mass spectrometry using a programmed temperature vaporizing injector. *J. Chromatogr., A* **2008**, 1186, 228–235.

(5) Chiavaro, E.; Vittadini, E.; Rodriguez-Estrada, M. T.; Cerretani, L.; Bendini, A. Differential scanning calorimeter application to the detection of refined hazelnut oil in extra virgin olive oil. *Food Chem.* **2008**, 110, 248–256.

(6) Sikorska, E.; Górecki, T.; Khmelinskii, I. V.; Sikorski, M.; Koziol, J. Classification of edible oils using synchronous scanning fluorescence spectroscopy. *Food Chem.* **2005**, 89, 217–225.

(7) Kasemsumran, S.; Kang, N. Partial least squares processing of near-infrared spectra for discrimination and quantification of adulterated olive oils. *Spectrosc. Lett.* **2005**, 38, 839–851.

(8) Yang, H.; Irudayaraj, J.; Paradkar, M. M. Discriminant analysis of edible oils and fats by FTIR, FT-NIR and FT-Raman spectroscopy. *Food Chem.* **2005**, 93, 25–32.

(9) Baeten, V.; Fernández Pierna, J. A.; Dardenne, P.; Meurens, M.; García-González, D. L.; Aparicio-Ruiz, R. Detection of the presence of hazelnut oil in olive oil by FT-Raman and FT-MIR spectroscopy. *J. Agric. Food Chem.* **2005**, 53, 6201–6206.

(10) Dupuy, N.; Duponchel, L.; Huvenne, J. P.; Sombret, B.; Legrand, P. Classification of edible fats and oils by principal component analysis of Fourier transform infrared spectra. *Food Chem.* **1995**, 57, 245–251.

(11) Lai, Y. W.; Kemsley, E. K.; Wilson, R. H. Potential of Fourier transform infrared spectroscopy for the authentication of vegetable oils. *J. Agric. Food Chem.* **1999**, 42, 1154–1159.

(12) Ozen, B. F.; Mauer, L. J. Detection of hazelnut oil adulteration using FT-IR spectroscopy. *J. Agric. Food Chem.* **2002**, 50, 3898–3901.
(13) Vlachos, N.; Skopelitis, Y.; Psaroudaki, M.; Konstantinidou, V.; Chatzilazarou, A.; Tegou, E. Applications of Fourier transform-infrared spectroscopy to edible oils. *Anal. Chim. Acta* **2006**, 573−574, 459–465.
(14) Maggio, R. M.; Kaufman, T. S.; Del Carlo, M.; Cerretani, L.; Bendini, A.; Cichelli, A.; Compagnone, D. Monitoring of fatty acid composition in virgin olive oil by Fourier transformed infrared spectroscopy coupled with partial least squares. *Food Chem.* **2009**, 114, 1549–1554.
(15) Dais, P.; Spyros, A. ^{31}P NMR spectroscopy in the quality control and authentication of extra-virgin olive oil: A review of recent progress. *Magn. Reson. Chem.* **2007**, 45, 367–377.
(16) Lay, J. O.; Liyanage, R.; Durham, B.; Brooks, J. Rapid characterization of edible oils by direct matrix-assisted laser desorption/ionization time-of-flight mass spectrometry analysis using triacylglycerols. *Rapid Commun. Mass Spectrom.* **2006**, 20, 952–958.
(17) Lerma-García, M. J.; Ramis-Ramos, G.; Herrero-Martínez, J. M.; Simó-Alfonso, E. F. Classification of vegetable oils according to their botanical origin using amino acid profiles established by direct infusion mass spectrometry. *Rapid Commun. Mass Spectrom.* **2007**, 21, 3751–3755.
(18) Lerma-García, M. J.; Ramis-Ramos, G.; Herrero-Martínez, J. M.; Simó-Alfonso, E. F. Classification of vegetable oils according to their botanical origin using sterol profiles established by direct infusion mass spectrometry. *Rapid Commun. Mass Spectrom.* **2008**, 22, 973–978.
(19) Commission regulation (EC) number 182/2009 of 6 March 2009 amending regulation (EC) number 1019/2002 on marketing standards for olive oil. *Off. J. Eur. Union* **2009**, *L63*, 6−8.
(20) Stefanoudaki, E.; Kotsifaki, F.; Koutsaftakis, A. Classification of virgin olive oils of the two major Cretan cultivars based on their fatty acid composition. *J. Am. Oil Chem. Soc.* **1999**, 76, 623–626.
(21) Bucci, R.; Magri, A. D.; Magri, A. L.; Marini, D.; Marini, F. Chemical authentication of extra virgin olive oil varieties by supervised chemometric procedures. *J. Agric. Food Chem.* **2002**, 50, 413–418.
(22) Aranda, F.; Gómez-Alonso, S.; Rivera del Álamo, R. M.; Salvador, M. D.; Fregapane, G. Triglyceride, total and 2-position fatty acid composition of Cornicabra virgin olive oil: Comparison with other Spanish cultivars. *Food Chem.* **2004**, 86, 485–492.
(23) Koprivnjak, O.; Moret, S.; Populin, T.; Lagazio, C.; Conte, L. S. Variety differentiation of virgin olive oil based on *n*-alkane profile. *Food Chem.* **2005**, 90, 603–608.
(24) Krichene, D.; Taamalli, W.; Daoud, D.; Salvador, M. D.; Fregapane, G.; Zarrouk, M. Phenolic compounds, tocopherols and other minor components in virgin olive oils of some Tunisian varieties. *J. Food Biochem.* **2007**, 31, 179–194.
(25) Luna, G.; Morales, M. T.; Aparicio, R. Characterisation of 39 varietal virgin olive oils by their volatile compositions. *Food Chem.* **2006**, 98, 243–252.
(26) D'Imperio, M.; Dugo, G.; Alfa, M.; Mannina, L.; Segre, A. L. Statistical analysis on Sicilian olive oils. *Food Chem.* **2007**, 102 (3), 956–965.
(27) Baccouri, O.; Bendini, A.; Cerretani, L.; Guerfel, M.; Baccouri, B.; Lercker, G.; Zarrouk, M.; Ben Miled, D. D. Comparative study on volatile compounds from Tunisian and Sicilian monovarietal virgin olive oils. *Food Chem.* **2008**, 111, 322–328.
(28) Ben Temime, S.; Manai, H.; Methenni, K.; Baccouri, B.; Abaza, L.; Daoud, D.; Sánchez-Casas, J.; Osorio-Bueno, E.; Zarrouk, M. Sterolic composition of Chétoui virgin olive oil: Influence of geographical origin. *Food Chem.* **2008**, 110, 368–374.
(29) Lerma-García, M. J.; Herrero-Martínez, J. M.; Ramis-Ramos, G.; Simó-Alfonso, E. F. Prediction of the genetic variety of Spanish extra virgin olive oils using fatty acid and phenolic compound profiles established by direct infusion mass spectrometry. *Food Chem.* **2008**, 108, 1142–1148.
(30) Bendini, A.; Cerretani, L.; Di Virgilio, F.; Belloni, P.; Bonoli-Carbognin, M.; Lercker, G. Preliminary evaluation of the application of the FTIR spectroscopy to control the geographic origin and quality of virgin olive oils. *J. Food Qual.* **2007**, 30, 424–437.
(31) Galtier, O.; Dupuy, N.; Le Dréau, Y.; Ollivier, D.; Pinatel, C.; Kister, J.; Artaud, J. Geographic origins and compositions of virgin olive oils determinated by chemometric analysis of NIR data. *Anal. Chim. Acta* **2007**, 595, 136–144.
(32) Gurdeniz, G.; Tokatli, F.; Ozen, B. Differentiation of mixtures of monovarietal olive oils by mid-infrared spectroscopy and chemometrics. *Eur. J. Lipid Sci. Technol.* **2007**, 109, 1194–1202.
(33) Guillén, M. D.; Cabo, N. Relationships between the composition of edible oils and lard and the ratio of the absorbance of specific bands of their Fourier transform infrared spectra. Role of some bands of the fingerprint region. *J. Agric. Food Chem.* **1998**, 46, 1788–1793.
(34) Silverstein, R. M.; Bassler, G. C.; Morrill, T. C. In *Spectrometric Identification of Organic Compounds*; John Wiley and Sons: Chichester, U.K., 1981.
(35) Vandeginste, B. G. M.; Massart, D. L.; Buydens, L. M. C.; De Jong, S.; Lewi, P. J.; Smeyers-Verbeke, J. In *Data Handling in Science and Technology Part B*; Elsevier Science B.V.: Amsterdam, The Netherlands, 1998; p 237.

Received for review February 25, 2009. Revised manuscript received September 11, 2009. Accepted September 22, 2009. This work was supported by Project CTQ2007-61445 (MEC and FEDER funds). V. Concha-Herrera thanks the University of Valencia for a contract. M. J. Lerma-García also thanks the Generalitat Valenciana for a FPI grant for Ph.D. studies.