



Chemical analysis and NIR spectroscopy in the determination of the origin, variety and roast time of Mexican coffee

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ABSTRACT

Coffee is a product whose quality and price are associated with its geographical, genetic and processing origin; therefore, the development of analytical techniques to authenticate the above mentioned is important to avoid adulteration. The objective of this study was to compare conventional analytical methods with NIR technology for the authentication of roasted and ground coffee samples from different producing regions in Mexico (origins) and different varieties. A second objective was to determine, under the same processing conditions, if roasting times can be differentiated by using this technology. A total of 120 samples of roasted and ground commercial coffee were obtained from the states of Chiapas, Oaxaca, Tabasco and Veracruz in Mexico, 30 locally available samples per state. Samples from Veracruz included three different varieties, grown on the same farm and processed under the same conditions. One of these varieties was selected to evaluate the chemical composition of samples roasted at 185 °C using four different roasting times (15, 17, 19 and 21 min). Samples from different producing regions showed significant differences ($P < 0.05$) in fat content (from $7.45 \pm 0.42\%$ in Tabasco to $18.40 \pm 2.95\%$ in Chiapas), which was associated with the altitude of coffee plantations (Pearson's $r = 0.96$). The results indicate that NIR technology generates sufficient useful information to authenticate roasted and ground coffee from different geographical origins in Mexico and different varieties from the same coffee plantation, with similar results to those obtained by conventional analytical methods.

1. Introduction

Coffee is the second most consumed beverage in the world and is mainly prepared using two commercial species, *Coffea arabica* L. and *Coffea canephora* Pierre, which account for 60% and 40% of exports from producing countries, respectively. A cup of coffee brewed with *C. arabica* is considered to be of better quality, with lower bitterness and better valued sensory attributes, when compared to one brewed with *C. canephora*. As Arabic coffee is preferred by consumers, its price is higher than *C. canephora* [1]. For this reason, it is categorized into quality grades [2] but can also be adulterated with beans of different species, including lower-priced cereals [3].

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Therefore, supply chain agents such as processors, regulatory authorities and consumers need to have analytical methods available to determine the species, origin and processing of coffee, in order to avoid fraudulent or incorrect labelling [4,5].

Apart from conventional physico-chemical analysis methods, different spectrometric techniques [6–8], combined with statistical methods, have been proposed to determine possible adulterations in coffee. Arboleda [9] and Nallan et al. [10] proposed the combined use of near-infrared spectrometry techniques, associated with neural networks, to detect adulterations in the process and composition of coffee. Other authors [11–13] have applied different modalities of near-infrared technology, supported by hyperspectral images, to assess sensory attributes and identify defects in coffee beans.

Instrumental non-destructive methods, such as near-infrared spectroscopy (NIRS), generate spectral information that, when interpreted by chemometric techniques, yield similar results to conventional methods [7,14], the difference being that the analysis time is within minutes; no reagents are required; no laboratory waste is generated and the physical, chemical, and biological properties of the product are not modified.

Near-infrared spectroscopy has been proposed as a tool for the identification of various quality blends of Arabica coffee [15–17]. It can be used to determine various components of the green bean, such as the total lipid content, the composition of fatty acids present in the lipid fraction and the content of tocopherols [18], as well as the protein content [19] and its relationship with bean origin [20,21] and coffee quality [22]. Furthermore, Baptista et al. [23] and Correia et al. [24] used NIR technology to differentiate the quality of coffee grown in association with different agroforestry species, while Silva et al. [25] reported the feasibility of NIR transmittance spectra for determining the planting density of coffee trees and the maturity level of cherries.

Regarding the roasting process, NIR technology has been proposed for determination of the degree of roasting, related to bean colour [26], for evaluation of blends of different origin and processing (decaffeinated or regular) [27], for determination of metabolites such as chlorogenic acid [28], for predicting the onset and end of first and second cracks [29], for forecasting failures during the roasting process [30] and for quantifying the moisture content of roasted and ground coffee [31].

In the present work, samples from four different producing regions (states) of Mexico were processed under the hypothesis that NIR spectra provide sufficient information to discriminate between producing regions (states) and varieties grown in the same coffee plantation and to differentiate roasting times when samples come from the same coffee plantation, were processed in the same way and are from the same variety.

2. Material and methods

The experimental work was conducted at the Central Analysis Laboratory of the Colegio de Postgraduados Campus Tabasco, Mexico. Prior to analysis, it was verified that green coffee samples had a moisture content, measured using a moisture meter model HG63 (Mettler Toledo, Greifensee, Switzerland), between 10.5 and 11.5%. The moisture content of roasted and ground coffee samples was measured for reference to analysis. Samples intended for NIR spectra determination were sieved with a mesh number 30 (0.60 mm) using a sieve shaker (Endecotts, London, England).

2.1. Samples of roasted and ground coffee to differentiate producing regions

The study was conducted with a descriptive, cross-sectional, prospective and non-experimental design. A total of 120 local produced samples of roasted and ground commercial coffee, locally available in 1 kg presentations, were obtained from four states of the Mexican Republic (Table 1), 30 samples per state, using a non-probabilistic method by convenience sampling. In each state, samples were obtained from coffee growing communities whose farmers process their own coffee and sell it under local brands.

2.2. Green coffee samples to differentiate varieties

From the experimental coffee plantation of the Colegio de Postgraduados Campus Córdoba, 60 kg of cherry coffee samples of the varieties Colombia, Costa Rica 95 and Oro Azteca were harvested separately in triplicate. They were processed separately by wet

Table 1
Origin of the roasted and ground coffee samples.

State	Origin	Geographical reference	Samples
Chiapas	Tziscaco	Latitude: 16° 45' 58" N Longitude: 93° 8' 56" W Altitude: 1500 m.a.s.l.	30
Oaxaca	Ixtepec	Latitude: 16° 33' 41" N Longitude: 95° 5' 51" W Altitude: 160 m.a.s.l.	30
Veracruz	Córdoba	Latitude: 18° 51' 39" N Longitude: 96° 51' 40" W Altitude: 640 m.a.s.l.	30
Tabasco	Huimanguillo	Latitude: 17° 49' 49" N Longitude: 93° 23' 29" W Altitude: 30 m.a.s.l.	30

processing with spontaneous fermentation and dried using a solar dryer. Parchment coffee samples were hulled separately using a sample huller machine (Promor, Xalapa, Mexico).

2.3. Green coffee samples to evaluate roasting time

To determine the effect of roasting times on the chemical composition of coffee samples, a batch of 10 kg of green beans from the same origin (Colegio de Postgraduados Campus Córdoba's experimental coffee plantation, located at 18°51'30"N, 96°51'40"W), the same post-harvest processing (wet processing), production cycle (2015/2016) and Colombia variety were used.

For roasting, an electric sample roaster model CBR-101 (Gene Café, Gyeonggi - Do, Korea) with a 250 g capacity was used, in 100 g roasting batches, the roasting temperature was fixed at 185 °C and the time was automatically controlled. Four roasting times (15, 17, 19 and 21 min) were used, in a duplicate completely randomised design (CRD). Before sample roasting, two batches of 100 g were roasted at 185 °C for 15 min to stabilise the roaster operating conditions. The roasting degree was measured using a CM-600 d colour meter (Konica Minolta, New Jersey, USA).

2.4. Chemical analysis of roasted and ground coffee

For ash and fat content, the conventional analytical methods used were those described in the Mexican standard NMX-F-013-SCFI-2010 [32] for chemical analysis of roasted and ground coffee. Ash content (%) in dry basis was quantified using a muffle furnace at 600 °C for 5 h and crude fat content (%) was quantified using the Soxhlet method. The results of the 120 commercial roasted coffee samples were compared with the reference values of this standard (maximum moisture 6%, maximum ash 6.5% and fat between 8 and 18%), in order to verify the compliance of local coffee brands with Mexican standards in these composition parameters.

2.5. Near-infrared spectrophotometry (NIRS)

NIR Spectra were generated with a Versatile Agri Analyzer™6500 System II Vertical Type 461008 near-infrared reflectance spectrometer (FOSS; Hillerod, Denmark). Spectra were recorded in the wavelength range from 400 to 2500 nm, at even wavelengths. The programs used were 1) ISISCAN (version 2.81 copyright 2006) for recording spectra, 2) WinISI III (version 2.81) as a bridge program for exporting data to Excel and 3) Excel as a bridge program for exporting data to 4) Pirouette [33]. Chemometric interpretation of the spectra was performed with the latter.

2.6. Statistical analysis

Analyses of variance were carried out for chemical parameters with origin, variety and roasting time as factors, separating means ad hoc with Tukey's test ($\alpha = 0.05$) [34]. A principal component analysis (PCA) and a biplot representation with scores and factor loadings were performed. Before chemometric techniques were applied to the NIR spectra, data were pretreated applying a Savitzky-Golay [35] filter to find a second order derivative, based on a quadratic polynomial and 11-point window size. Data analysis included principal component analysis (as a reduction dimension technique), hierarchical clustering and a supervised classification method named Soft Independent Modelling of Class Analogy (SIMCA) for the identification (classification) of regions and varieties.

3. Results and discussion

3.1. Chemical analysis of roasted and ground coffee samples

The ash and moisture content evaluated in the coffee samples from Chiapas, Oaxaca, Veracruz and Tabasco (Table 2) comply with the reference values established for roasted and ground coffee in the NMX-F-013-SCFI-2010 standard, whereas for fat content, the samples from Tabasco present values below the limit established in the standard (8.0% dry basis), and those from Chiapas exceed the maximum percentage of fat established in the standard (18% dry basis). A review of the data on the origins of the samples revealed that they originated from a wide range of altitudes (m.a.s.l.). With the exception of samples from low altitudes (<200 m.a.s.l.), the results obtained for fat were similar to those reported by Zhu et al. [19] for Arabic coffee samples from Colombia, Guatemala and Honduras (from 13.37% to 16.29%), countries that produce coffees of quality similar to those produced in Mexico.

Table 2
Chemical characterisation of roasted and ground coffee (mean \pm SD).

Origin (Reference)	Moisture (%)	Ash (%)	Fat (%)
	Max 6.0	Max 6.5	8–18
Chiapas	1.19 \pm 0.19 b	4.20 \pm 0.07 ab	18.4 \pm 2.95 a
Oaxaca	1.55 \pm 0.17 ab	3.89 \pm 0.05 c	11.0 \pm 2.11 c
Veracruz	1.57 \pm 0.13 ab	4.15 \pm 0.12 b	13.1 \pm 1.88 b
Tabasco	1.91 \pm 1.57 a	4.23 \pm 0.10 a	7.45 \pm 0.42 d

Within each column, different letters indicate significant differences (Tukey, 0.05). SD = standard deviation.

All samples were statistically different in fat content: the fat content increased with increasing altitude of production. Pearson's correlation coefficient between altitude and fat content was 0.96, coinciding with the information generated by Menchu and Ibarra [36], who indicated that fat is associated with the altitude at which the coffee is produced. Data from this study yielded the model $Y(\text{fat}) = 0.0067 X(\text{altitude}) + 8.5383$ ($R^2 = 0.9424$), which explains fat content as a function of the altitude at which the coffee was produced. However, more research is needed on the relationship between plantation altitude and coffee fat content, as well as possible interactions with the variety and shade level (agronomic management).

3.2. Principal component analysis (PCA)

Using data from moisture, ash and fat analyses, a principal component analysis was performed for the 120 coffee samples from Tabasco, Oaxaca, Veracruz and Chiapas. Principal component one (PC1) explained 99.7% of the variance in the original data, so only the first two components were used to plot the clusters (Fig. 1) by sample group according to their geographical origin.

Data on Table 2 shows significant differences between the four origin groups due to fat. This becomes evident when looking at the factor loadings for PC1: moisture 0.10, ash 0.28 and fat 0.95. Therefore, fat was a deciding factor in authenticating samples from four Mexican regions when analyzed by conventional chemical methods.

3.3. NIR second derivative spectra of coffees of four origins

Each spectrum of the 120 roasted and ground coffee samples is made up of 1050 variables (scans every 2 nm, from 400 to 2500 nm), resulting in a matrix of 126,000 numerical variables, to which the PCA dimension reduction technique was applied. It was found that the first two components explained 99.88% of the total variability observed in the 120 samples which, as observed in Fig. 2, formed groups defined by geographical origin (Tabasco, Chiapas, Oaxaca and Veracruz). Clustering was obtained with greater precision than that reported by Santos et al. [37] and by Giraudo et al. [20], who obtained a cumulative variance in the first two components of 92% and 95.3%, respectively, when analysing the NIR spectra of samples from the states of São Paulo and Rio Grande do Norte, Brazil, as well as from several coffee-producing countries. Samples from Veracruz showed the largest dispersion, but class boundaries were maintained between all coffee origins (Fig. 2).

The origin determination, using NIR technology, of coffee by producing region within a country has been reported by different authors [20,37]. In this work, the usefulness of this technology to discriminate between coffees of different regional origin in Mexico was confirmed. This is important for a country with around 60 coffee growing regions [38], whose distinctive conditions of climate, soil, management, altitude, latitude, among other factors, give identity to the coffee coming from each of these growing regions.

3.4. Soft independent modelling of class analogy (SIMCA)

Soft Independent Modelling of Class Analogy (SIMCA) was applied to the NIR spectra, generating the six Coomans diagrams in Fig. 3, where samples of commercial roasted coffee from different producing states in Mexico were placed in a different and unique class with a correct classification observed in 100% of the cases (Table 3), a better result than when it is known that samples come from different origins but are classified by different criteria, as reported by Santos et al. [37], who examined samples of Arabica, robusta and blends of both species from the states of São Paulo and Rio Grande do Norte, Brazil, and used SIMCA to model the classification into

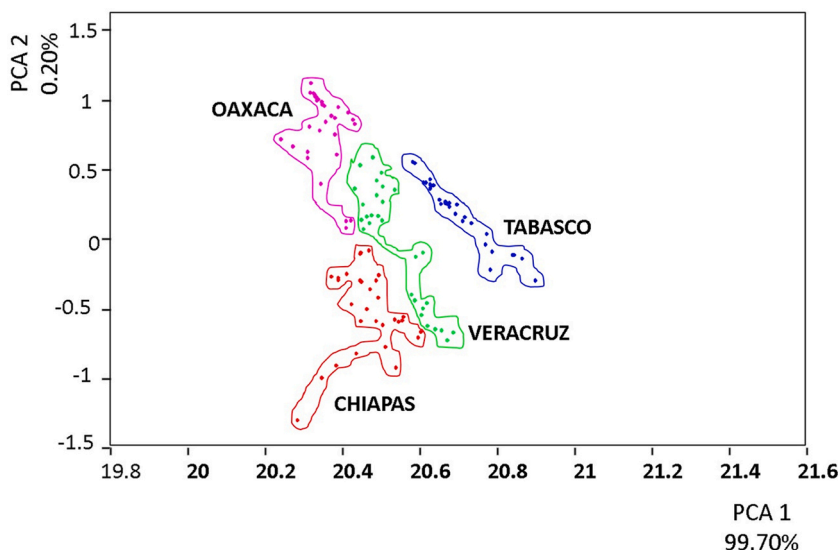


Fig. 1. PCA biplot of commercial roasted and ground coffee samples separated by geographical origin based on chemical analysis.

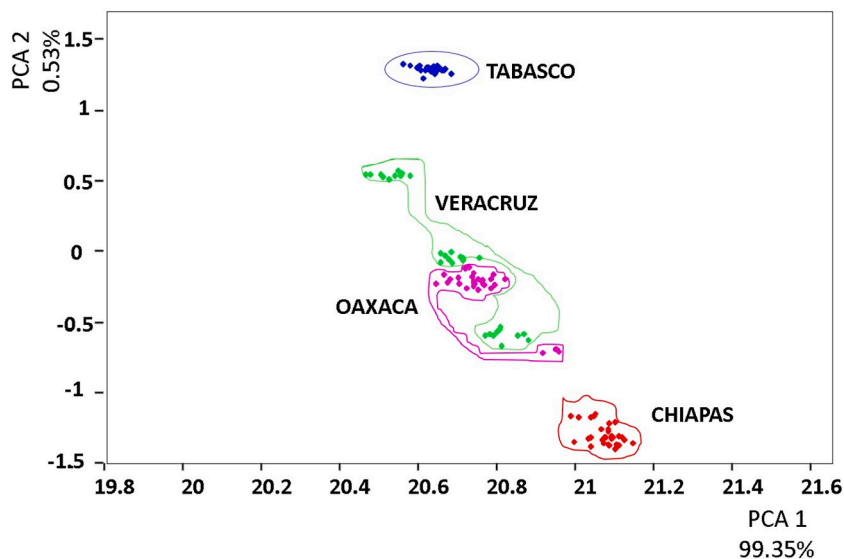


Fig. 2. NIR spectra PCA biplot of commercial coffee samples from four Mexican states.

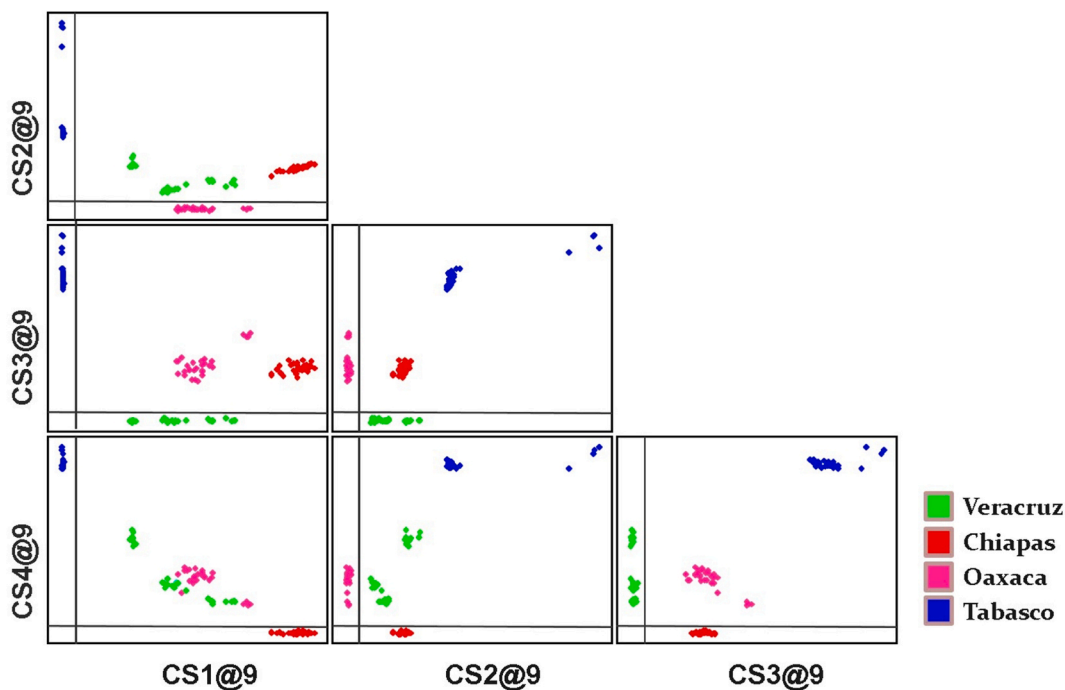


Fig. 3. Coomans plot constructed with SIMCA class modelling.

Table 3

Results of the SIMCA classification method based on origin.

State	Total Spectra	Spectra in the Training Set	Spectra in the Test Set	PC used in the Training Set	Correct Classification Rate
Chiapas	30	15	15	3	100%
Oaxaca	30	15	15	3	100%
Veracruz	30	15	15	3	100%
Tabasco	30	15	15	3	100%
Total	120	60	60		60/60

PC = Principal components.

three quality categories (traditional, gourmet and decaffeinated), obtaining a classification error of 9%, and by Monteiro et al. [39], who used NIRS to evaluate samples from five different states in Brazil to differentiate the farming system (organic or conventional), obtaining a classification rate of 85% using partial least-squares discriminant analysis.

The results obtained with NIR technology were the same as those of conventional chemical analysis. Commercial coffee samples are separated according to their geographical origin using both analytical techniques, with the advantage that NIRS analysis takes minutes, while conventional methods can take hours and in some cases, days. In addition, NIRS does not generate laboratory waste, the analytical error is only the uncertainty of the instrument calibration (the sample is not weighed, and no analytical manipulation is performed) and less analyst involvement and use of laboratory infrastructure are required.

3.5. Varieties from a single origin and process

With the moisture, ash and fat content data, a PCA was performed for the varieties from Córdoba, Veracruz (Oro Azteca, Colombia and Costa Rica 95). The results are shown in Fig. 4a, where the formation of three groups corresponding to each variety can be observed. Note that the first two extracted components explain almost 100% of the total variability observed in the samples. A similar result was obtained using the NIR spectra from the readings of the 30 coffee samples (1050 variables per sample), as shown in Fig. 4b.

3.6. Soft independent modelling of class analogy

In the Coomans diagrams (Fig. 5) each variety is located in its own class area, showing a 100% correct classification of samples (Table 4). So far, the successful use of NIRS has been reported to discriminate between *Coffea* species and mixtures of species [4]. Fig. 5 corroborates that NIR technology also provides sufficient information to differentiate coffee samples from the same coffee plantation and process by variety.

The advantage of NIR technology is that coffee samples retain their physical, chemical and biological properties, and the analysis can be applied in real time. With chemometric techniques, recognition patterns are obtained to classify similar materials into defined groups and to discriminate unknown samples, as established by Abdelwareth et al. [40]. Chemical spectra differences between two coffee samples could be explained by a number of factors, the most relevant of them are the genetic material from which coffee samples come from, the environmental conditions in which coffee plants were grown, including the culture management practices applied, but of prime importance is the post-harvest management of the coffee bean, including the sample preparation for analysis. These factors pose a challenge for the NIR technology, whose main disadvantage is that it requires large libraries of composition spectra representing different regions, countries, cultivation or process conditions, with which to compare an unknown sample and determine whether its spectrum matches any of the spectra stored in the library.

It was pointed out earlier in the document that roasted and ground coffee samples from different geographical origins in Mexico differ, suggesting differences in the fat contents of the samples as possible causes and associating such contents with the altitude of the coffee plantations. Attention was also drawn to the fact that samples from the same altitude and with the same agronomic and post-harvest management can differ in their chemical composition spectra if they come from different varieties. Next, it was demonstrated that the chemical spectra of coffee samples from the same coffee plantation, of the same variety and with the same agronomic management and post-harvest processing, can differ when roasted at the same temperature but for different times (Fig. 6).

3.7. Roasting time

The chemical composition spectra of samples from the same coffee plantation and variety, processed in the same way, can differ depending on the roasting time, even if the roasting temperature is kept constant. Carvalho et al. [26] processed samples of the same

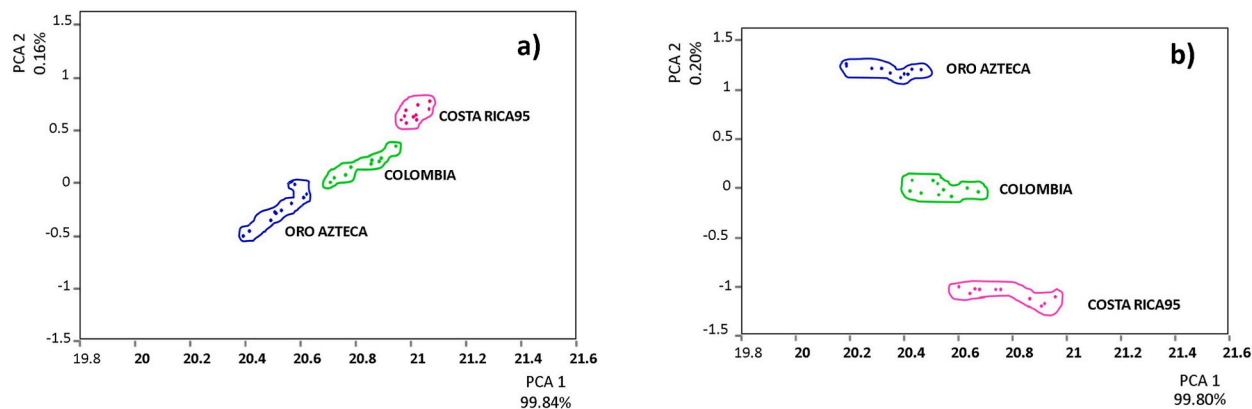


Fig. 4. Groups of roasted and ground coffee samples from Córdoba, Veracruz, (a) separated by variety based on conventional analysis, (b) separation of the spectral fingerprints (NIR) of varieties with the same origin and processing.

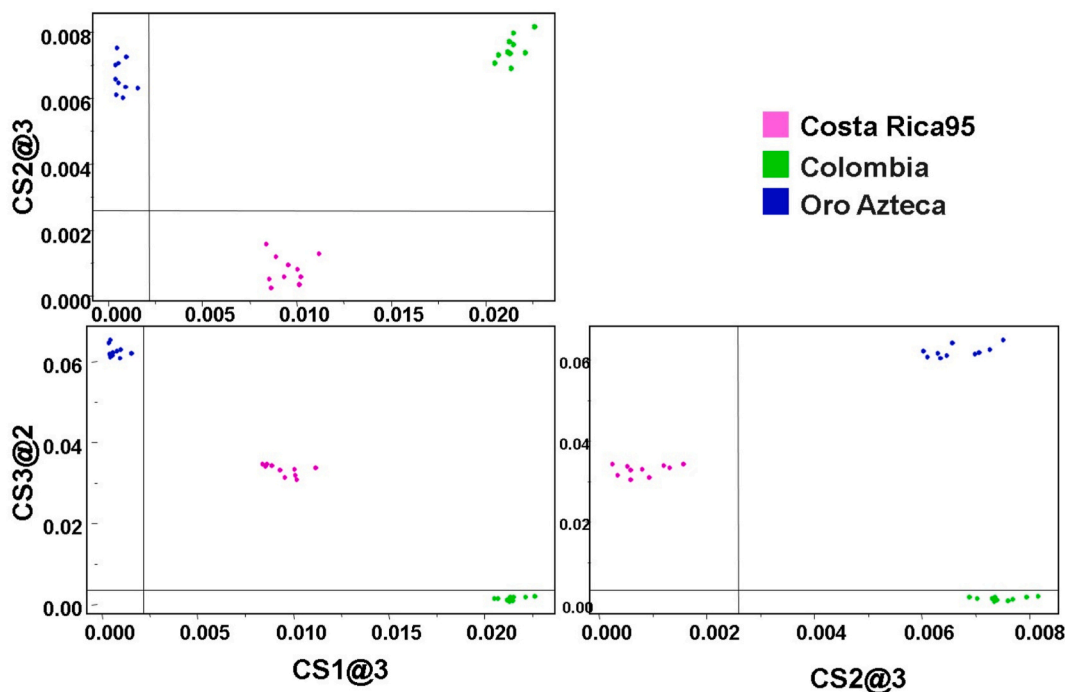


Fig. 5. Groups of roasted and ground coffee samples from Córdoba, Veracruz, divided into variety groups with SIMCA class modelling and NIR spectra.

Table 4

Results of the SIMCA classification method based on variety.

Variety	Total Spectra	Spectra in the Training Set	Spectra in the Test Set	PC used in the Training Set	Correct Classification Rate
Colombia	10	5	5	2	100%
Costa Rica 95	10	5	5	2	100%
Oro Azteca	10	5	5	2	100%
Total	30	15	15		15/15

PC = Principal components.

origin and variety, different roasting degrees and the same roasting temperature and proposed models to associate roast colour (Agron values) with NIR spectra. In this work, the colour value of roasted coffee changed with roasting time (luminescence values $L^* = 14.69 \pm 3.56$, 10.78 ± 1.15 , 9.87 ± 0.31 and 9.00 ± 1.31 for 15, 17, 19 and 21 min of roasting time, respectively), and the chemical composition of the samples was also modified, as shown in Fig. 4.

4. Conclusion

Near infrared spectroscopy generates useful and sufficient information to authenticate commercial roasted and ground coffee from different producing regions in Mexico and to separate by variety coffee from the same coffee plantation which has undergone the same post-harvest processing. It is also a useful tool to differentiate roasting times when beans come from the same variety and coffee plantation and have received the same post-harvest treatment. Results with NIR technology are similar to those obtained by conventional analytical methods. This confirms the validity of NIR technology, not only to differentiate origins, species, qualities and roasting degrees, but also varieties and bean roasting times.

Author contribution statement

Armando Guerrero-Peña: Conceived and designed the experiments; Analyzed and interpreted the data; Wrote the paper.

Lorena Vázquez-Hernández: Performed the experiments; Analyzed and interpreted the data; Wrote the paper.

Adolfo Bucio-Galindo: Analyzed and interpreted the data; Wrote the paper.

Victorino Morales-Ramos: Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

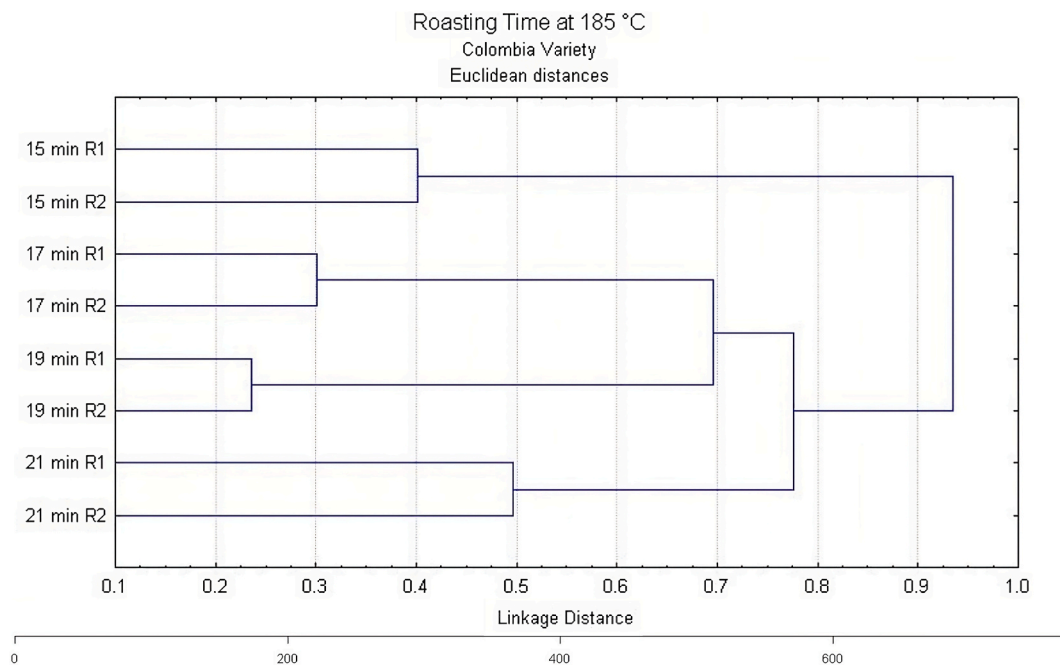


Fig. 6. Hierarchical clustering of samples from the same coffee plantation, of the same variety, processed in the same way and roasted at 185 °C, using four different roasting times.

Data availability statement

Data associated with this study has been deposited at <https://doi.org/10.17632/t8wjfxm5cc.1>.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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