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Discrimination of Cognacs and Other Distilled Drinks by Mid-infrared Spectropscopy

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Mid-infrared spectroscopy was applied to the analysis and discrimination of Cognacs and other distilled drinks (Armagnacs, whiskies, brandies, bourbons, rums, and counterfeit products). Strong correlations were found between dry extract spectra, polyphenolic dry extract spectra, and the total polyphenol concentration of samples, notably of Cognacs. Principal component analysis applied to spectral data made it possible to emphasize the importance of dry extract data when a distinction is made between Cognacs and Armagnacs, whiskies, bourbons, and rums, and of polyphenol concentration when Cognacs, brandies, and counterfeit products are separated. Ninety-six percent of samples in the test set were correctly assigned to Cognacs and non-Cognacs by partial least-squares discriminant analysis.

KEYWORDS: Cognac; distilled drinks; mid-infrared spectroscopy; authenticity; discriminant analysis

INTRODUCTION

Because of the increase in counterfeit products and consumer demand, food industry professionals need to be able to guarantee the authenticity of their products. Cognac is produced within a limited geographical area, using defined white grape varieties and a specific process including fermentation, two distillations, and aging in oak barrels. The age of Cognac is determined by the youngest product introduced into the blend. However, blends contain other older distillates, and then Cognacs exceed the minima required by the regulations.

Several methods have been described to evaluate the authenticity of spirits. Gas chromatography and UV−vis spectrometry are often used to identify strong alcoholic beverages such as whiskies, rums, brandies (*1*), or tequila (*2*). Savchuk et al. (*3*) showed that the chromatographic profiles of Cognacs differed from those of other spirits and could also be used to determine the duration of aging in contact with oak. During the same study, differences in absorbance at 280 nm were recorded for various Cognacs, but the authors considered UV−vis spectrometry as the baseline technique for the discrimination of spirits because some products such as burned-sugar color can cause interference with the UV−vis determination of oak substances in Cognac (*4*). Recently, MacKenzie and Aylott (*5*) successfully tested a hand-held spectrophotometer used to distinguish counterfeit and genuine Scotch whiskies. Goldberg et al. (*6*) emphasized the differences in the levels of phenolic constituents and furan in Cognacs and other distilled spirits analyzed using HPLC. These biochemical compounds showed a trend toward higher values according to the progression VO, VSOP, XO, in line with increasing quality as reflected by longer wood aging. Cognac age has also been evaluated using the concentration of methyl ketones (*7*) or the content of 33 volatile compounds including esters, aldehydes, ketones, alcohols, and lactones (*8*).

During these studies, sample numbers were generally small and data processing was limited.

In recent years, infrared spectroscopy combined with multivariate data analysis has been developed for the rapid quantitative analysis of the most important compounds in wines (*9*, *10*). Infrared spectroscopy quantifies the energy absorbed by molecular bonds and provides spectral data, principally on acids, carbohydrates, and alcohols in wines. On the other hand, white grape musts (*11*), dry extracts of wines from different geographical origins and vintages (*12*), and red wine phenolic extracts from seven cultivars (*13*) were almost completely discriminated using mid-infrared spectroscopy combined with multivariate analytical techniques. Studies of Cognac using infrared spectroscopy are scarce. Palma and Barroso (*14*) reported preliminary results on the classification of Cognacs and other distilled drinks. Cognacs were clearly differentiated from the other samples (Armagnacs and brandies from different countries), by the 3700−4900 cm^{-1} zone and principal component analysis (PCA).

During our study, infrared spectroscopy combined with multivariate data analysis was used to make a discrimination between Cognacs and other distilled drinks such as whiskies, rums, brandies, Armagnacs, bourbons, and counterfeit products. The spectra of raw products, dry extracts, and phenolic extracts

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were recorded. In a first step, correlations between infrared spectra and dry extract and polyphenol levels in Cognac were determined. Then, the products were discriminated by an unsupervised method (PCA) and by a supervised method (partial least-squares discriminate analysis, PLS-DA).

MATERIALS AND METHODS

Samples. One hundred and fifty-one samples, stored in the dark at 4 °C, were selected by the Bureau National Interprofessionnel du Cognac (BNIC): 51 Cognacs, designate C; 24 brandies, designated B; 10 whiskies, designated W; 8 Armagnacs, designated A; 9 rums, designated R; 4 bourbons, designated Bo; and 45 counterfeit products, designated CF. These products were prepared in the laboratory or collected from all over the world.

Physicochemical Analysis. Total dry matter was determined by weight after evaporation of the spirit at 70 °C under low pressure (*15*).

Total phenol content was determined using the Folin−Ciocalteu method (*16*) and expressed as milligrams per liter of gallic acid.

Infrared Spectroscopy. *Sampling.* Three sampling methods were used to analyze the spirits.

(i) ATR. Raw product was deposited on the attenuated total reflection cell with a 12 reflections zinc selenide crystal. Each sample single-beam spectrum was ratioed to a single-beam spectrum of the ATR plate covered with water.

(ii) Transmission of Dry Extract. One hundred and fifty microliters was deposited on a type 61 3M microporous polyethylene membrane (Spectra Tech Inc.) usable in the spectral range from 4000 to 400 cm^{-1}, except in the 2918−2849 and 1430−1480 cm^{-1} regions. The spectrum of the card was recorded before sample application and was used as blank for the acquisition of the sample spectrum. The samples were dried to eliminate water, ethanol, and volatile components in a desiccator under vacuum at 30 °C.

(iii) Transmission of Dry Phenolic Extract. The method was derived from that of Edelman et al. (*12*). Three milliliters of sample was diluted 1:6 with distilled water and loaded onto C18 Bond elute SPE cartridges (Varian). The cartridges were washed with 20 mL of water and dried by air flow. The retained compounds were eluted by 3 mL of acidic methanol (0.01% HCl) and concentrated to 0.5 mL. One hundred and fifty microliters was deposited on polyethylene membrane as previously described.

Equipment and Spectral Acquisition. A Nicolet Magna 750 purged spectrophotometer (Thermo) equipped with a DTGS detector was used. Thirty-two interferograms were collected at an optical resolution of 4 cm^{-1}.

VAL Q software (Thermo Nicolet) was used to verify that the spectrometer was working consistently over time.

The single-beam spectra of products were transformed in absorbance units using the background spectra of the membrane or of the ATR cell. The spectra were derivatized twice. Except for ATR, spectra were normalized on the integrated spectral area because the optical path length of the dry extract was unknown. All samples were analyzed three times, and the average spectrum was introduced in the data set.

Data Analysis. The Statistica software, version 6.1 (Statsoft, Tulsa, OK) was used in the data treatment. Stepwise multiple regression analysis (forward stepwise selection with p values = 0.05) was performed between the chemical data (dry matter and total phenol concentration) and the infrared spectroscopy data.

PCA was applied to the spectral data to show the existence of differences according to Cognac and non-Cognac groups. This linear dimensionality reduction technique identifies orthogonal directions of maximum variance in the original data and projects the data into a lower dimensionality space formed of a subset of the highest variance components.

Classifications according classes defined as Cognac and non-Cognac were carried out by PLS-DA. The samples were coded 1 (samples belonging to the Cognac class) or 2 (samples belonging to the non-Cognac class) and were divided into three sets: training (85 samples), validation (43 samples), and test (23 samples). A sample was assigned to the Cognac group when its predicted value fell within the 95% confidence interval around the mean μ of the predictions for Cognac samples in the training and validation sets (*17*). Samples with a predicted value outside this interval were assigned as non-Cognac. The 95% confidence limit is given by the expression $\mu \pm 1.96\sigma$, where σ is the residual standard deviation.

RESULTS AND DISCUSSION

Infrared Spectra of Cognac, Dry Extract, and Phenolic Dry Extract. Normalized mean spectra of Cognacs, dry extracts, and phenolic dry extracts from the same products and the second derivatives of signals are shown in **Figure 1**, panels **A** and **B**, respectively.

As can be seen from the ATR spectrum of raw product, ethanol dominated the spectrum and masked the absorption bands of other compounds. Peaks at 1085 and 1045 cm^{-1} were characteristic of the asymmetric stretching of the primary alcohol group. The peak at 878 cm^{-1} was assigned to symmetric stretching of the same group.

The dry extract of spirits was made up of carbohydrates, caramel, and extractable material from oak wood (*18*). The mean transmission mean spectrum exhibited highest absorption levels between 950 and 1150 cm^{-1}. Peaks and shoulders in this region could be attributed to specific vibrations such as primary alcohol stretching (1061 and 1078 cm^{-1}) or secondary alcohol stretching (1103 and 1140 cm^{-1}), functions found in carbohydrates.

The transmission spectrum of the dry phenolic extract included a large number of peaks between 900 and 1700 cm^{-1}, as previously described for wine extracts (*12*, *13*). The region between 950 and 1150 cm^{-1} was assigned to the aromatic fingerprint and C−O valence vibrations (*13*). However, the most important spectral changes appeared between 1500 and 1800 cm^{-1} (**Figure 1B**). According to Coates (*19*), the region between 1450 and 1615 cm^{-1} can be assigned to the aromatic ring stretch and that between 1160 and 2000 cm^{-1} to aromatic combination bands.

Preliminary Study. A preliminary study had been carried out to assess the sampling and measurement methods: ATR of raw product, transmission of dry matter, transmission of dry phenolic extract. The spectra of 40 samples (30 Cognacs, 5 other distilled drinks, and 5 counterfeit products) were acquired and discriminated using PCA.

On the basis of the ATR spectra, only one product could be separated from the others because its ethanol concentration was lower and reduced the level of absorption in the region between 850 and 1150 cm^{-1}. This method could be useful to discriminate products with different alcoholic strengths.

On the basis of the transmission spectra of dry extracts, counterfeit products could be separated from the other distilled drinks and Cognacs. Using the transmission spectra of phenolic extracts, the three groups could be separated in score scatter plots of the first and third components of PCA (data not shown).

As a result of these findings, ATR measurement of raw product was abandoned.

Correlations between IR Spectra, Dry Matter, and Polyphenol Concentrations. The mean values for dry matter and total polyphenol concentrations in the seven studied groups are shown in **Table 1**.

Levels of polyphenol compounds in Cognacs, Armagnacs, rums, and bourbons were high (>300 mg/L) when compared with those of whiskies, brandies, and counterfeit products, which contained <200 mg/L. Polyphenol concentration increased markedly from the youngest qualities of Cognac to the older, these results agreeing with those published by Goldberg et al. (*5*).

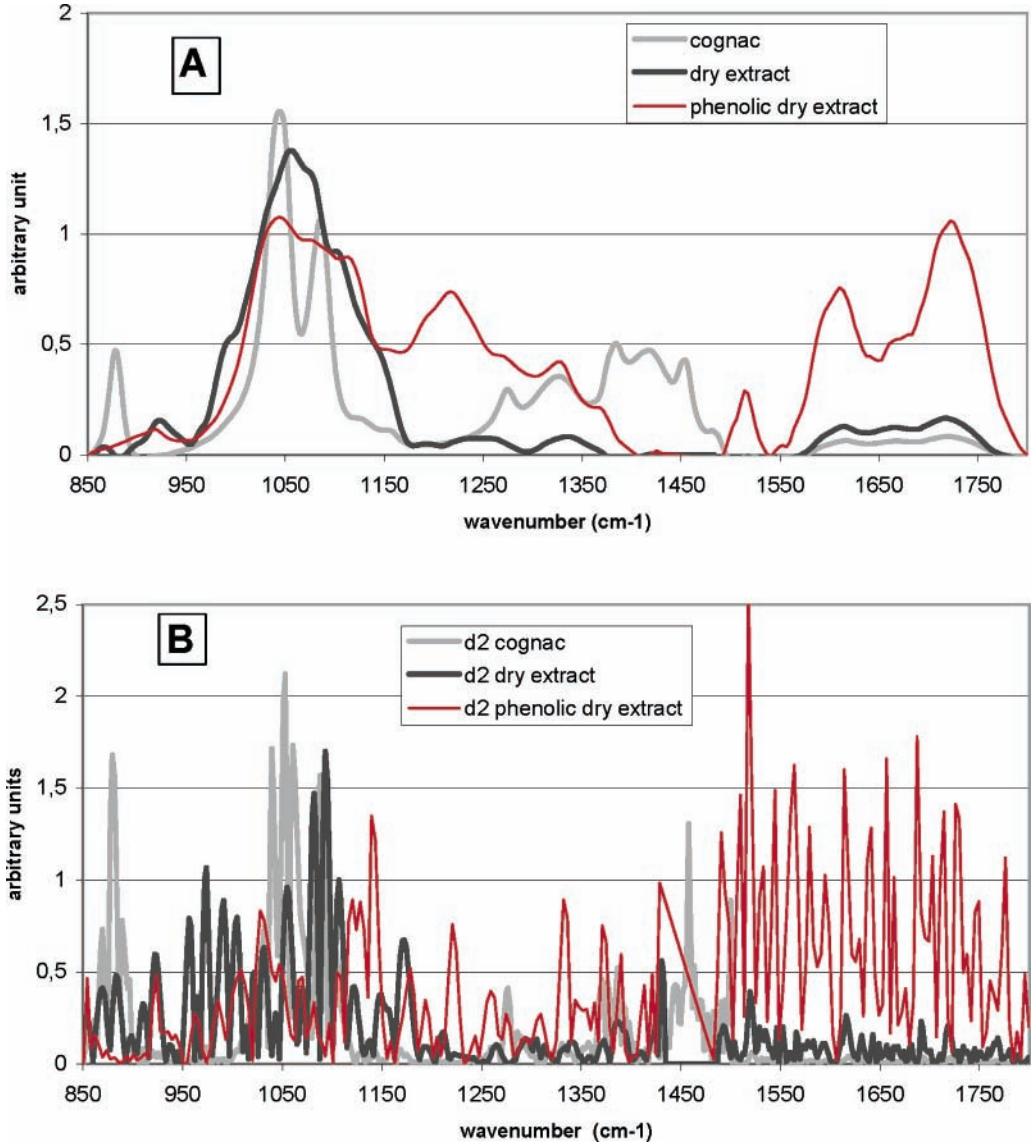

Figure 1. Normalized mean spectra of 41 Cognacs obtained by ATR, of dry extract and phenolic dry extract of the same products obtained by transmission (**A**) and the second derivatives of the signals (**B**).

Table 1. Means and Standard Deviations (SD) of Dry Matter and Total Polyphenol Concentration of the Seven Groups of Products

		polyphenol concn (mg/L)		dry matter (g/L)	
product	samples	mean	SD	mean	SD
Cognac	51	374	118	11.165	1.858
Armagnac	8	389	178	6.575	3.344
whiskey	10	104	67	1.090	0.490
rum	9	341	185	4.775	6.330
brandy	24	114	89	11.617	7.317
counterfeit	45	195	220	7.591	4.199
bourbon	4	350	88	2.025	0.545

The highest concentrations of dry extract were measured in Cognacs, brandies, and Armagnacs. Dry extracts of bourbons and whiskies were very low, between 1 and 2 g/L, and 3−10-fold lower than in the former spirits. No notable difference could be seen in the dry extract levels of Cognac samples.

The high level of the standard deviations calculated for counterfeit products (for dry extracts and polyphenol concentrations) was due to the broad diversity of samples, which included products collected from all over the world as well as specific homemade solutions.

Stepwise multiple regressions were carried out to build a linear model of the observed values for dry matters and polyphenol concentrations and IR spectral data (**Table 2**).

In all samples, the calculated values for dry matter in the dry extract spectra or phenolic dry extract spectra were poor. The correlation coefficients were low, at 0.65 and 0.49, respectively (**Table 2**). If only Cognac samples were taken into account, the regression results were similar (**Table 2**).

Models predicting the polyphenol concentrations in all of the samples were better, notably with respect to polyphenolic dry extract spectra. The correlation coefficients were 0.71 and 0.88 and the standard errors of calibration were 101 and 65 mg/L, respectively, for dry extract spectra regression and phenolic dry extract spectra regression (**Table 2**).

The same type of linear regression calculated for Cognacs produced excellent results. The correlation coefficients were >0.9 and the errors near 30 mg/L for a range of concentrations from 120 to 630 mg/L. Graphs of calculated values versus expected values (**Figure 2**) confirmed these results. The good correlations between polyphenol concentrations and infrared spectra were thus emphasized, notably with respect to Cognac samples.

Table 2. Correlation Coefficients and Standard Errors (SE) of Calibration of Multiple Linear Regressions between Dry Matter, Polyphenol Concentration, and IR Spectra for All of the Samples and for Cognacs

	predicted values				
	range	sample numbers	spectral data set	corr coeff	SE
dry matter (g/L)	1–34	all (151)	dry extract spectra	0.65	3.3
			phenolic dry extract spectra	0.49	3.9
	7–15	Cognacs (151)	dry extract spectra	0.51	1.3
			phenolic dry extract spectra	0.45	1.4
polyphenol concn (mg/L)	0–780	all (151)	dry extract spectra	0.71	101
			phenolic dry extract spectra	0.88	65
	120–630	Cognacs (51)	dry extract spectra	0.96	29
			phenolic dry extract spectra	0.93	35

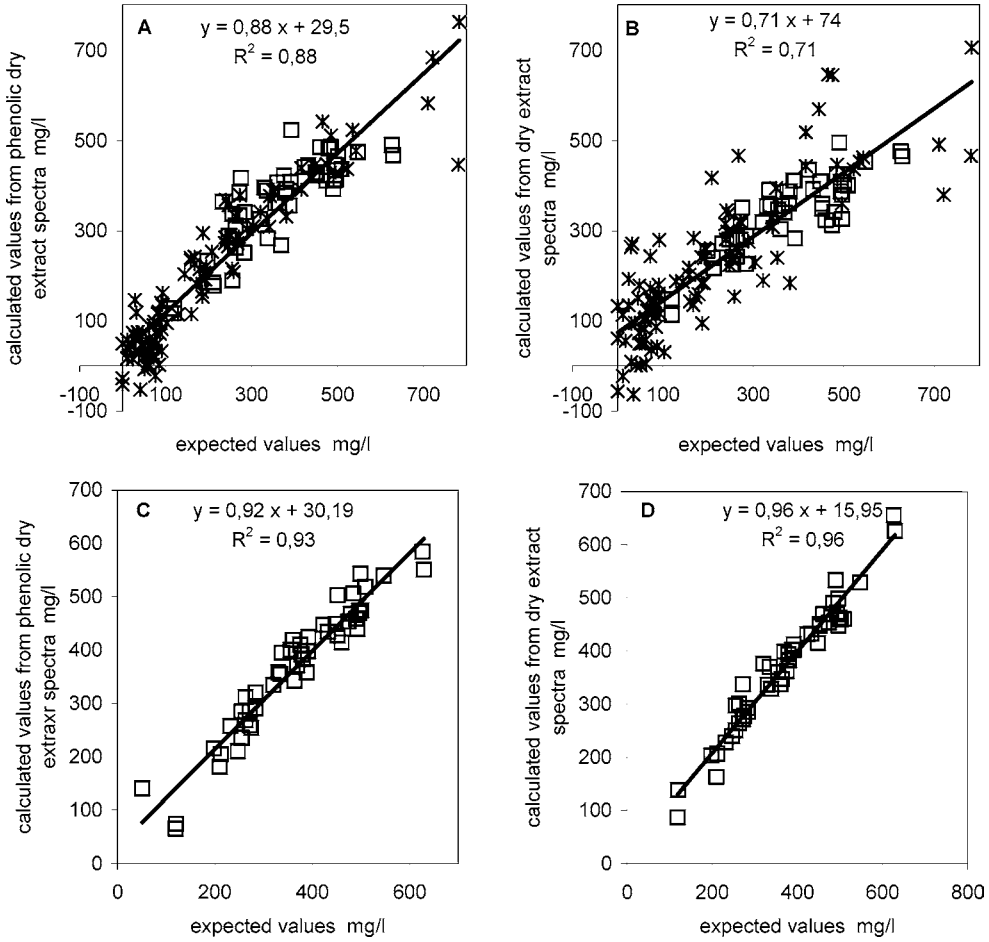

Figure 2. Calculated values of polyphenol concentrations from phenolic dry extract IR spectra (**A**–**C**) and dry extract IR spectra (**B**–**D**) versus expected values using multiple linear regression for all of the samples (**A**, **B**) and for Cognacs only (**C**, **D**): (*) non-Cognac samples; (□) Cognac samples; (—) linear regression between expected values and calculated values.

Discrimination between Cognac and Non-Cognac Samples Using Principal Component Analysis. PCA was applied to the 151 spectra obtained from dry extracts and phenolic dry extracts to discriminate among the 7 specific groups and most particularly to distinguish Cognacs from the other spirits.

The PCA results for dry extract spectra indicated that the first three principal components could explain 69% of the variance in the data and that 13 components were necessary to explain 95% of the total variance. For PC1, the highest values of eigenvectors were found in the 850−1400 cm^{-1} region related to alcohol vibrations of carbohydrates and in the 1500−1650 cm^{-1} region assigned to aromatic ring stretch. For PC2 and PC3, the highest values of eigenvectors were found between 1500 and 1800 cm^{-1} and between 850 and 1250 cm^{-1}, respectively. **Figure 3A** shows the PCA scores (PC1 versus PC2) calculated from the second derivative of the spectra for samples. Cognacs formed a homogeneous group on the right of the score plot. Whiskies, bourbons, and rums are completely separated from the Cognac group and display a considerable dispersion in the factorial space. Several counterfeit samples were clearly separated from the Cognac group, although some of them were close.

Whiskies, bourbons, and rums, discriminated from Cognacs on the component 1 of the first factorial space, presented the lowest dry extract concentrations. The well-separated homemade counterfeit products also exhibited a low dry extract (mean = 1.386 g/L versus mean value = 4.775 g/L for all counterfeit products, **Table 1**).

Armagnacs and brandies were close to the Cognac group. However, when the PC1 versus PC3 scores plot was considered, Armagnacs were differentiated from Cognacs, and a separation

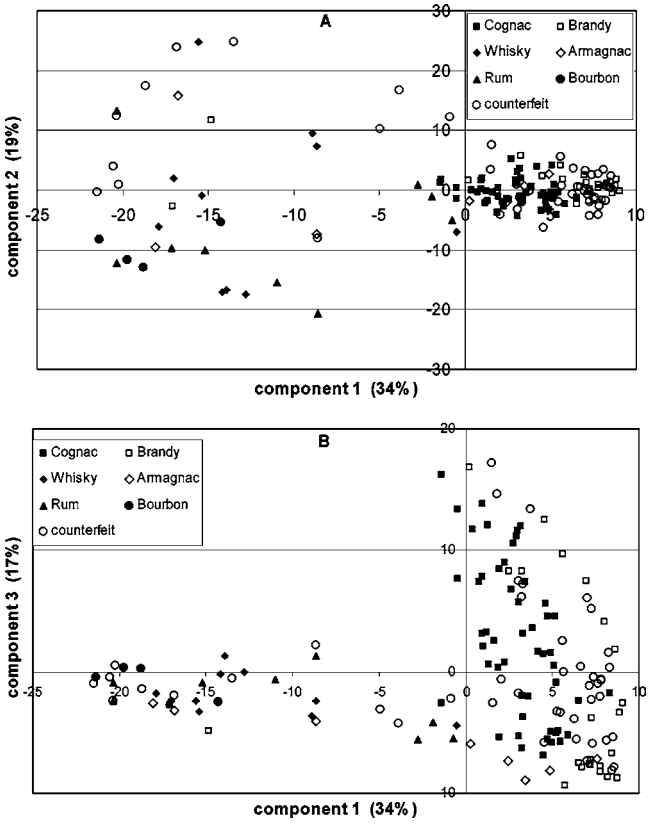

Figure 3. PCA scores scatter plot [PC1 vs PC2 (**A**) and PC vs PC3 (**B**)] of the FTIR spectra of dry extract of Cognac, whiskey, rum, brandy, Armagnac, bourbon, and counterfeit products.

between brandies and counterfeit products versus Cognacs appeared more clearly (**Figure 3B**).

From phenolic dry extract spectra, it could be seen that 15 principal components accounted for 95% of the total variance of data with 28, 16, and 12%, respectively, for PC1, PC2, and PC3. The highest values of eigenvectors were found in spectral regions similar to those described for dry extract PCA, that is, 850−1700 cm^{-1} for PC1 and 1500−1800 cm^{-1} for PC2.

Projection of the sample coordinates in the factorial space formed by the first two PCs showed that Cognacs formed a homogeneous group, little dispersed except for two samples (**Figure 4A**). Many brandies and counterfeit products were separated from the Cognac group. The other samples in the same groups (eight brandies and six counterfeit products) were integrated in the Cognac group. Bourbons and rums formed homogeneous groups remaining close to the Cognac group. In this setting, Armagnacs and Cognacs were not correctly separated, and whiskies were distributed around the Cognacs. Analysis of the factorial space formed by PC1 and PC3 (44% of the variance) produced identical observations (data not shown). This observation was confirmed by visualization of the factorial space formed by PC2 and PC3. This space enabled better discrimination of whiskies (**Figure 4B**). Exploration of other spaces made it is possible to visualize better separations of rums and bourbon from Cognacs in the score plot of PC4 versus PC5 (16% of variance) and between Armagnacs and Cognacs in the score plot of PC6 versus PC7 (11% of variance) (data not shown).

The samples of brandies, counterfeit products, and the two Cognacs separated in the first factorial space displayed low concentrations of polyphenol, <200 mg/L. It was surprising that whiskies were not better separated in this space even though

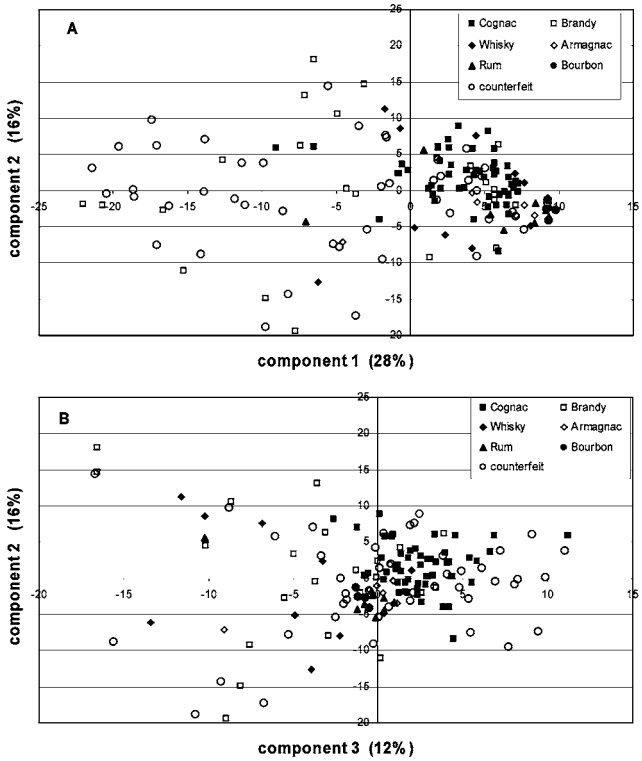

Figure 4. PCA scores scatter plot (PC1 vs PC2 and PC2 vs PC3) of the FTIR spectra of phenolic dry extract of Cognac, whiskey, rum, brandy, Armagnac, bourbon, and counterfeit products.

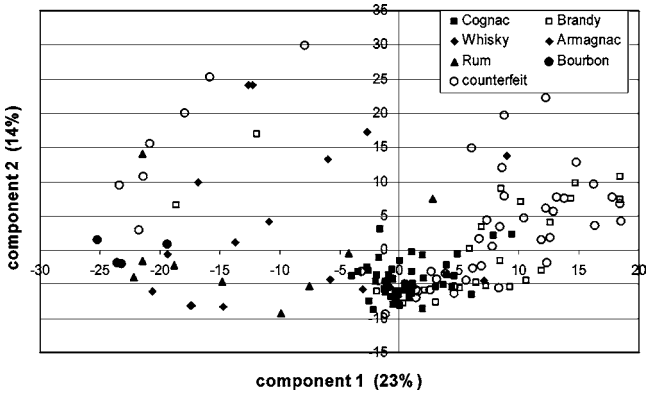

Figure 5. PCA scores scatter plot (PC1 vs PC2) of the concatenated FTIR spectra (dry extract and phenolic dry extract) of Cognac, whiskey, rum, brandy, Armagnac, bourbon, and counterfeit products.

the mean polyphenol concentration was 104 mg/L. It could be assumed that the information provided by the polyphenol content was complex and played a role in other eigenvectors, as shown with PC3 (**Figure 4B**).

PCA of concatenated spectra of dry extract and phenolic dry extract confirmed the previous results. The two-dimensional score plots in the space defined by PC1 and PC2 demonstrated good discrimination between Cognacs and other distilled drinks (**Figure 5**). Except for two samples (those found with PCA of phenolic dry extract spectra), Cognacs formed a homogeneous group in the middle of the factorial space. As for PC1, which accounted for only 23% of the total variance, spirits with the lower dry extracts (whiskies, rums, and special counterfeit products) had negative score values. Spirits with lower polyphenol concentrations, brandies and counterfeit products, all had positive score values.

Table 3. Classification Table between Cognac (C) and Non-Cognac (NC) Samples for Dry Extract Spectra and Phenolic Dry Extract Spectra of Training, Validation, and Test Sets

	sets					
	dry extract spectra		phenolic dry extract spectra		phenolic and dry extract spectra	
sample numbers	incorrect classification	% of correct classification	incorrect classification	% of correct classification	incorrect classification	% of correct classification
training: 85 (30 C, 55 NC)	5 (2 C, 3 NC)	94	1 (1 C)	99	4 (2 C, 2 NC)	95
validation: 43 (16 C, 27 NC)	7 (1 C, 6 NC)	84	1 (1 C)	98	4 (1 C, 3 NC)	91
test: 23 (5 C, 18 NC)	3 (3 NC)	87	1 (1 NC)	96	1 (1 NC)	96

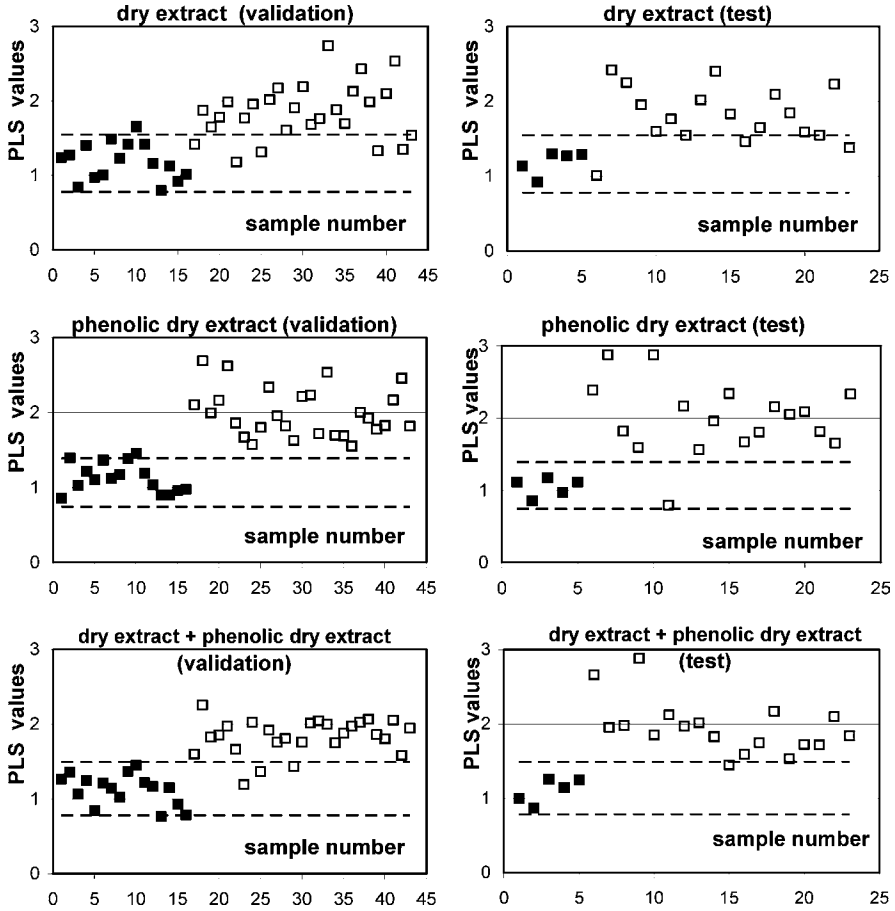

Figure 6. Predicted values by PLS-DA for the samples in validation and test sets from the dry extract spectral data, phenolic dry extract spectral data, and concatenated data: (- - -) 95% confidence limits around the mean predicted value for the Cognac samples in training and validation sets; (■) Cognac; (□) non-Cognac.

Discrimination between Cognac and Non-Cognac Samples Using PLS-DA. PLS-DA was performed on the three sets of spectra: (i) dry extract spectra, (ii) phenolic dry extract spectra, and (iii) concatenated spectra from the two previous sets. The numbers of components were 12, 15, and 7, respectively, for the three sets of spectra. At these levels, it was possible to claim that there was no overfitting (*20*).

Ninety-five percent confidence limits around the mean predicted values for the Cognac group were the lowest for polyphenolic spectra: $\mu = 1.08 \pm 0.32$ versus 1.16 ± 0.38 and 1.14 ± 0.35 for the two others. Samples with a score included within these limits were considered to be Cognac.

Whatever the spectral data, the models correctly predicted between 94 and 99% of the training samples (**Table 3**). For validation sets in comparison with training sets, the percentage of correct classification remained similar for phenolic dry extract spectra and associated spectra but decreased by 10% for dry extract spectra. For test sets, the levels of correct answers remained high: 87% from dry extract spectra and 96% from phenolic dry extract spectra and from associated spectra.

The best result was obtained from the phenolic dry extracts spectra. Just one sample was misclassified whatever the data set, training, validation, or test.

Calculated values for validation and test sets of the three types of spectral data and the Cognac acceptance region are plotted in **Figure 6**. A clear separation can be seen between Cognacs and non-Cognacs regarding validation and test sets, and the best quality of results obtained from the phenolic dry extract spectra was evident when compared with other spectral data.

Conclusions. Dry extract spectra and polyphenolic dry extract spectra were strongly correlated with total polyphenol concentrations in the samples, notably in the case of Cognac ($r^2 > 0.9$). These infrared spectra could be used to calculate the concentrations of other compounds and constitute a simple and rapid method to evaluate the Cognac composition and its evolution during the aging. The potential for mid-infrared

spectroscopy associated with multivariate analysis has been shown to differentiate Cognac from other distilled drinks. The infrared spectra of dry extracts and polyphenolic dry extracts provided additional information and allowed good discrimination between Cognac and non-Cognac drinks. Ninety-six percent of samples in the test set were correctly assigned. The analysis of more specific polyphenol fractions, obtained by the use of other types of chromatographic cartridges or new conditions of elution, may provide further information and enhance the discrimination between Cognacs. On the other hand, the combination of mid-infrared spectra with other analytical determination such as UV−visible spectra and/or other data analysis such as neural network may also enhance the separation of counterfeit products from Cognac and other products.

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