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Screening method for identification of adulterate and fake tequilas by using UV–VIS spectroscopy and chemometrics

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ABSTRACT

Based on UV–VIS spectroscopy and chemometric techniques, a screening method is presented with which the studied brands of white and rested tequila can be differentiated among them and on the other hand, adulterate and fake tequilas can be distinguished from the corresponding genuine brands. Eighty bottles of tequila (39 white type and 41 rested type) were studied and purchased at liquor stores; special care was taken to get different batches. Through the use of support vector machine (SVM), principal component analysis (PCA) and linear discriminant analysis (LDA) the studied tequilas were differentiated and classified into 8 sets: 4 sets of white and 4 of rested tequilas; each set corresponded to a specific tequila brand. Seven additional samples with similar labeling than the 80 samples were used to validate the method and it was found that each sample was located within the ellipse of confidence of the corresponding tequila brand. Furthermore, 14 adulterated samples were generated from 2 bottles of tequila, one white and one rested, and they could be distinguishable from the genuine tequila, i.e., they were outside of the corresponding ellipse of confidence. In addition, the screening method here presented was employed to analyze rested tequilas that were purchased on the street market, i.e., fake tequilas, with the same label than 3 of the used brands in this work. These samples were discriminated from the corresponding genuine tequila brand. The results suggested that the reported method could play an important role when a quick, trustworthy and feasible result on site is needed since the test of the spirit takes minutes, affording robustness, reliability and in addition, a skilled worker is not required necessarily to apply the method.

1. Introduction

During the last four decades the Mexican Industrial Property Institute (IMPI, impi.gob.mx) has registered 5 alcoholic beverages which are protected by appellation *d'origen controlé a.o.c.*, i.e., tequila (1974), mezcal (1994), bacanora (2000), sotol (2002) and charanda (2003) (Lachenmeier, Sohnius, Attig, & López, 2006). These beverages are distilled spirits and the first four are produced with different species of agave while charanda is produced with fermented sugar cane. Tequila is the most popular spirit in Mexico and sales of this spirit have increased worldwide notably during the last years. The Official Mexican Standard (NOM) establishes that tequila must be made only from agave *tequilana Weber*, blue variety (NOM-006, 2005). The production of tequila begins with the cooking of the heads of the agave plant and follows some specific steps to end up with a double distillation (Faria, Loyola, Lopez, & Dufour, 2003; NOM-006, 2005; Mancilla-Margalli & Lopez, 2002). This spirit can be classified in two categories as 100% blue agave when 100% of the sugars come from *tequilana Weber*, blue variety; and as mixed when no more than 49% of other sugars are added (NOM-006, 2005). Usually for mixed spirits, 51% of the sugars come from blue agave and 49% from sugar cane. Within these two categories, tequilas are identified as white and aging spirits. The formers are obtained directly after distillation and the latter kind when the distilled beverages spend some time in wooden barrels before they are bottled; aging spirits can be rested and aged. For rested and aged tequilas the aging must be at least for 2 and 12 months, respectively. Nowadays sales of tequila have been increased and according to the Tequila Regulatory Council (CRT, crt.org.mx) the total production of tequila for blue agave and mixed was about 104 million of litters in 1995 and increased to about 309 million of litters in 2008. The number of producers and brands has been increased too, and it is reported that there are 923 domestic registered tequila brands; however, the number of distilleries is about 111. In addition to the large difference between these numbers it is observed

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that some brands show up in the market while others disappear; these facts might suggest that one distillery produces more than one brand and, therefore some similarities could be observables (and measurable) among specific brands. Prices for single bottle of 750 mL of this beverage run from $5 to $35 USD; however, premium tequilas are more expensive.

On the other hand, counterfeiters and fake products is a worldwide problem and the Anti-Counterfeiting Group (ACG, a-cg.org) in the United Kingdom – among others – rises up a warning to consumers about this kind of products. The market of spirits is not free of adulterations or fake brands and the consumer could purchase tequilas at really low price. For the case of tequilas in Mexico, the Federal Prosecutor of the Consumer (PROFECO, mexicanlaws.com/PROFECO/PROFECO.htm) had pointed out that about 40–50% of sales of tequila are adulterated. Thus, the consumer should be aware of these facts and make sure that any given spirit, tequila in particular, is what it is on its label, i.e., its category, quality and/or the authenticity of any specific brand. In this context there is no fast and inexpensive screening method to verify the content of spirit bottles *in situ*. When a beverage is under suspicion some techniques such as gas and/or liquid chromatography have to be used; however, these techniques and the corresponding measurements cannot be performed on site since a fair equipped laboratory is required and achieving results imply time consuming tasks, in many cases of hours.

Some works have shown the effectiveness of applying chemometric methods to different spectroscopic techniques. For example, NIR spectra to estimate the ripeness of wine grapes (Herrera, Guesalaga, & Agosin, 2003), and to FT-IR and UV spectra for the characterization and classification of wine (Guillén, Palma, Natera, Romero, & Barroso, 2005) or the determination of several compounds such as dyes and stimulants in drinks (López-de-Alba, Wróbel-Kaczmarczyk, Wróbel, López-Martínez, & Amador-Hernández, 1996; López-Martínez, López-de-Alba, García-Campos, & León-Rodríguez, 2003). For the case of tequila, chromatic analysis and chemometrics tools have been applied to FT-IR and UV–VIS absorption spectra to discriminate between 100% agave and mixed tequilas as well as among tequilas from different brands (Barbosa-García et al., 2007; Jones, Deakin, & Spencer, 2009a,b; Lachenmeier, Richling, López, Frank, & Schreier, 2005; Muñoz-Muñoz et al., 2010). As of the present time, however, no study has been reported to check the spectroscopic behavior and reproducibility of the final product for a specific brand and to discriminate tequila original brand form adulterate or fake tequila based on the absorption spectra and chemometrics. In this work an alternative method to those based in chromatography techniques is presented in which one builds up a data set of tequilas corresponding to a specific brand; after this has been done and more than one data set is built, a given tequila sample can be identified with its corresponding brand or distillery. For this study one set of white and another of rested tequila were considered. This method is based on the analysis of the UV–VIS absorption spectra of the samples by multivariate methods which points out differences in tequilas between categories (100% blue agave and mixed) and types (white and aging). For this study eight brands of tequila were considered and they were classified and identify accordingly. Furthermore, adulterated and fake samples corresponding to some of the studied brands and well as other 100 samples of different brands to those studied in this work were considered to validate the method. The test can be performed on site since a portable UV–VIS spectrophotometer and a laptop computer can be used; results can be obtained in minutes. It is worth to mention that the aim of this work is not to establish a methodology to differentiate among all brands present in the market (recall that brands easy come and easy go and that there is a large difference between the number of brands and distilleries). However, for selected brands (as shown in this study) it is possible to use this methodology to find significant differences and discriminate among fake, adulterated and original samples of a specific brand.

2. Materials and methods

2.1. Samples of tequila

This study was focused on two types of tequilas, white and rested, since both types are the most popular and easy to get in the liquor store. Thus, 80 bottles of tequila were purchased at the liquor store and 8 sets were defined. Four sets were of white tequila and four of rested tequila. Each set belonged to a specific brand and the sets were labeled as WB1…WB4 for white tequilas and RB1, RB2, RB5 and RB6 for rested tequilas (notice that WB1 and WB2 correspond to the same brand than RB1 and RB2, respectively). All tequila brands were 100% blue agave except for one set of rested tequilas that was mixed. Table 1 shows the 80 used samples according to the labels of the corresponding bottles. The bottles of tequila were purchased in liquor stores and care was taken to get samples belonging of different batches; the purchased bottles come from well-known tequila producers and certified by CRT.

2.2. Instrumentation and software

Broadband spectra of 80 samples of tequila were measured in the 250–500 nm wavelength range in steps of 1 nm and performed by means of a Lambda 900, Perkin-Elmer© spectrophotometer. For each measurement a 1-cm-thick quartz cell was used. The Unscrambler©, MatLab R2009b©, STATGRAPHICS Centurion XV.II.® and Origin7® software were used for the multivariate and statistical analysis.

2.3. Methodology

The spectra data from the UV–VIS absorption of tequila samples are inherently multivariate; therefore, multivariate methods such as principal component analysis (PCA) were used to reduce data dimensionality while the support vector machine method (SVM) was used for classification (Abe, 2005; Brereton, 2003; Cristiannini & Shawe-Taylor, 2000; Jobson, 1991). To calculate the principal components (PC) a multivariate data matrix containing tequila samples as rows (80 rows) and spectral data as columns (251 columns) was used. Thus, PCA linearly combined the 251 spectral data characterizing each sample to produce new variables, i.e., principal components. Full cross-validation technique was used in all PCA calculations and spectral data were centered. The broadband spectrum for each tequila sample was smoothed with the use of five-point moving average algorithm to improve the signal-to-noise ratio. Reproducibility (for absorption value and wavelength shift) was corroborated in white and rested samples. We define the same baseline (zero value) for all broadband spectra.

Table 1
The 8 sets of tequila grouped by brands, white tequilas (WB1, …, WB4) and rested tequilas RB1, RB2, RB5, RB6.

Samples					
White tequilas			Rested tequilas		
Label brand	No. of samples	$Abs_{max} \pm \Delta Abs$ at λ_{mean}	Label brand	No. of samples	$Abs_{max} \pm \Delta Abs$ at λ_{mean}
WB1	9	0.95 ± 0.10 at 276 nm	RB1	11	2.16 ± 0.20 at 274 nm
WB2	13	1.55 ± 0.59 at 280 nm	RB2	10	5.87 ± 1.15 at 275 nm
WB3	10	0.93 ± 0.31 at 279 nm	RB5	10	3.98 ± 0.85 at 278 nm
WB4	7	1.25 ± 0.21 at 278 nm	RB6	10	3.53 ± 0.48 at 275 nm

Abs_{max}, the mean peak absorbance (a.u.).
ΔAbs, standard deviation.
λ_{mean}, mean wavelength.

3. Results and discussion

3.1. Spectral characteristics of tequila samples

Fig. 1 illustrates the measured broadband absorption spectra of 20 tequila samples; 9 belonging to samples of the WB1 set and the other 11 to RB1. By comparing the spectra of the WB1 set to those of RB1 it is observed that they show different absorbance characteristics. The set of tequilas WB1 show low absorption peak while the set of tequilas RB1 shows about twice that absorption. That is, the peak of white tequilas is between 0.7 and 1.1 and for rested tequilas between 1.8 and 2.6. Further, white tequilas show a single well-defined absorption band with nearly a Gaussian shape with no absorption at wavelengths larger than 350 nm, meanwhile rested tequilas still exhibit absorption in the range 350–425 nm. Similar behavior is observed for those other brands of tequila studied in this work. For white and rested tequilas each absorption peak is at about 278 nm and show small shifts in wavelengths, see Table 1. Table 1 also shows the mean peak absorbance with the corresponding standard desviation at the calculated mean wavelength for each set of tequilas. Furthermore, Table 1 shows that for white and rested tequilas the largest standard desviation value is for the set WB2 and RB5, and the peaks shift from 276 to 280 nm and from 274 to 278 nm, respectively.

3.2. Chemometric study

Since the samples were of two different types (white and rested), the study begun by looking for an easy way to diffentiate one type from the other. Thus, PCA was applied to the 80 samples and it was found that two principal components accounted for 99.99% of total spectral variation and 97% accounted for the first component. Fig. 2 shows a two dimensional subspace of the calculated components, PC1 and PC2, where the scores of all tequilas are plotted. SVM was used to calculate the line border decision to classiffy the spirit samples in white and rested tequilas, and 50% of the samples were used for training and the rest for prediction (Abe, 2005; Acevedo, Saturnino, Domínguez, & Narváez, 2007). The solid line in Fig. 2 is generated by an SVM calculation where 24 support vectors were used. White tequilas are bottled just after the double distillation, so the beverage is colorless and transparent. The corresponding spectra are located in the UV region and at glimpse minor differences among different white brands are observed, Fig. 1. Therefore in Fig. 2 most of the spectra data are concentrated in a small area of the PC plot. In contrast, rested tequilas are bottled after an aging process for at least two months that increases the number of organic compounds. Due to this process the spectra data are more dispersed than the spectra data of white tequilas, Fig. 2. (Mangas, Rodríguez, Moreno, Suárez, & Blanco, 1996; Muñoz-Muñoz, Grenier, Gutiérrez-Pulido, & Cervantes-Martínez, 2008). The statistical analysis (ANOVA) was performed to see if white and rested tequilas show statistical differences. It is found that the p-value is less than 0.05, which indicates that the two tequila types under study denote a statistically significant difference in agreement with the results given by SVM. Therefore, white and rested tequila samples will be analyzed and discussed in an independent way.

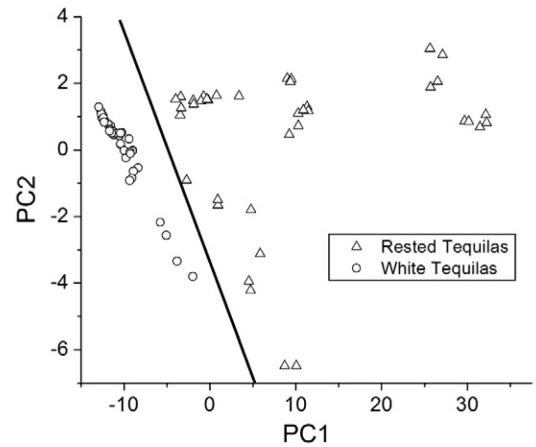

Fig. 2. PC1–PC2 subspace obtained from the absorption spectra of tequilas from 250 to 500 nm. The solid line represents the classification of white and rested tequilas using support vector machines, SVM.

3.2.1. Analysis of white tequilas

When the PCA was applied to the 39 samples of white tequilas, leaving out the samples of rested tequilas, two principal components preserved the 99% of spectral variation and the 98% of variance corresponded to the first component; the results on a PCA score plot are shown in Fig. 3. This figure shows that white tequilas are grouped into 4 sets and each set corresponds to one specific brand of tequila. To enhance this result, the ellipse of confidence for each set was calculated and encloses 95% of the plotted data according to a bivariate normal distribution (Brereton, 2003, Jobson, 1991). Notice that the major and minor axis of the ellipse coresponding to samples

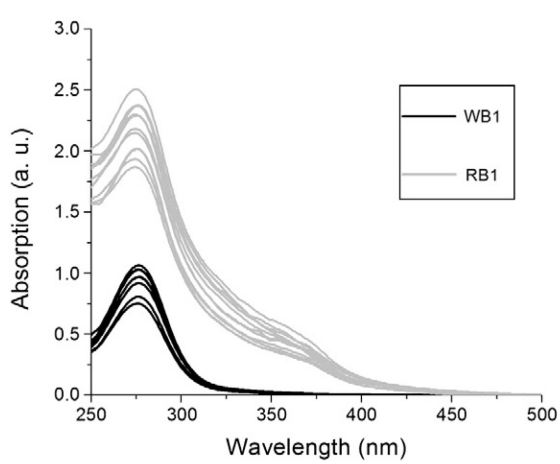

Fig. 1. Broadband spectra for the sets WB1 (nine with samples) and RB1 (eleven rested samples).

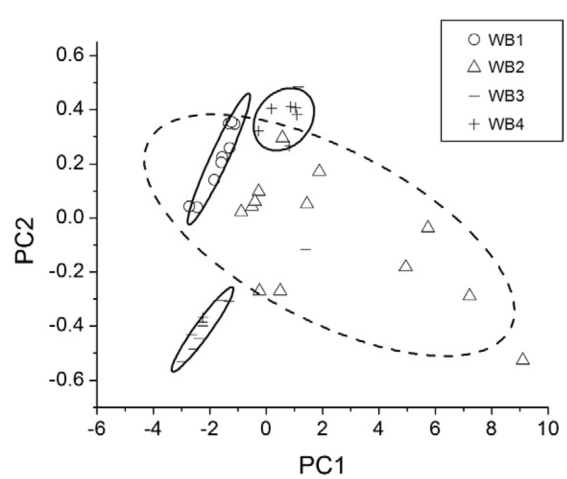

Fig. 3. PC1–PC2 subspace generated by 39 white tequila samples. All spectra data are grouped into 4 sets (brands) and each enclosed by ellipses of confidence.

of WB2 have larger values compared to the axis of the other ellipses and, therefore, its data are more dispersed. In general, the nature of this dispersive behavior is difficult to explain since several parameters might be in play when producing tequila. For example, some of those parameter would be the variability in the raw material such as geographical origin, maturity of agave plants and pest control; the time at which the sugar is fermented; or the times involved for cutting off the distillation process, i.e., heads and tails, and so on (Cedeño, 1995). As shown in Fig. 3 the ellipse of confidence of WB2 encloses the total spectra data belonging to WB1 and two samples of WB4. This overlaping of ellipses is observed because each ellipse was calculated based on the previous knowledge of the samples. However, the overlaping does not matter because the aim of this paper is built up a spectral database of a particular brand and afterwards to differentiate among fake and adulterated samples. Furthermore, when linear discriminant analysis (LDA) was applied to the derivative spectra for the analysis of these 39 samples of white tequilas no overlaping was obtained among brands; results from LDA are reported in Fig. 4. That is, the change of chemometric technique improves the differentiation among brands which shows the potential of chemometric methods for discrimination, in this case among tequila brands. Thus, when overlapping among some brands is obtained other chemometric techniques could be used and afterwards one could be allowed to follow the reported methodology to identify fake and adulterated tequilas as explained below.

3.2.2. Analysis of rested tequilas

On the other hand, when similar PCA was performed for rested tequila samples, leaving out the white samples, two principal components preserved the 99.4% of the spectral variation and the 93.2% of variance corresponded to the first component. PCA score plot for rested tequilas shows four groups corresponding to the four considered brands as it can be seen in Fig. 5. To enhance this result, the ellipses of confidence were also calculated. For this case no overlaping among the ellipses is observed, so the use of another multivariate technique was not required and three outliers can be observed in the plot. As discussed above, after double distillation white tequilas can be aging at least for 2 months to obtain rested tequilas. Therefore, through the aging process each factory gives distintive color, flavor and smell to tequilas and these issues depend on the nature and age of the used barrels. These other issues should be added to those described above for white tequilas if the nature of the dispersion of the spectral data shown in Figs. 3–5 would be explained.

Therefore, through the analysis of spectra data of white and rested tequilas with the use of chemometric techniques the studied samples

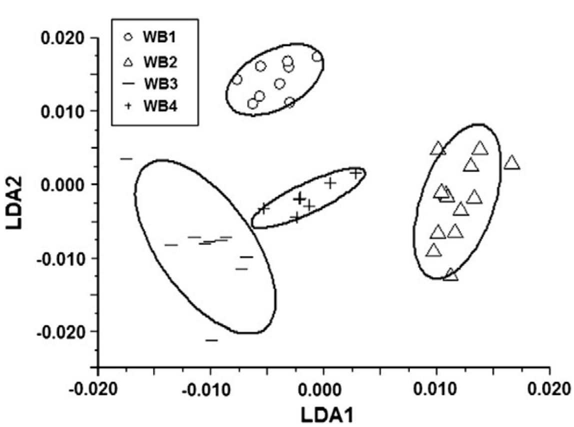

Fig. 4. LDA1–LDA2 subspace generated by 39 derivative spectra of white tequila samples. All spectra data are grouped into 4 sets (brands) and each enclosed by ellipses of confidence.

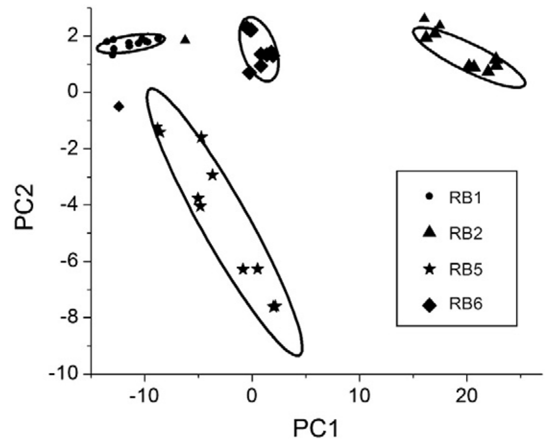

Fig. 5. PC1–PC2 subspace generated by 41 spectra data of rested tequilas. All spectra data are grouped and each group enclosed by ellipses of confidence.

are distinguishable and grouped by brands. Furthermore, with a similar method white tequilas were studied before and it was reported that 100% blue agave and mixed tequilas were distinguishable too (Barbosa-García et al., 2007). This method can be extended to other beverages and will be of great help to identify one given spirit, with a given brand, by having the corresponding data set. Thus, the reported method based on UV–VIS spectroscopy and multivariate analysis might play an important role when a quick, trustworthy and feasible result on site is needed.

3.3. Validation of the proposed method

Four experiments were performed in order to validate and prove the robustness of the method; furthermore, it is shown that adulterated and fake tequilas can be distinguishable from the genuine spirit brand.

3.3.1. Analysis of different samples

For one experiment 100 additional tequila samples were considered: 52 were white, 39 rested and 9 aged; all tequila brands were different to those of Table 1. This new set of samples was considered with the reported modeling in section 4.2 and the spectra data were projected in the corresponding PCA score plot. Figs. 6 and 7 show the result for white and rested samples, respectively, and the ellipses of

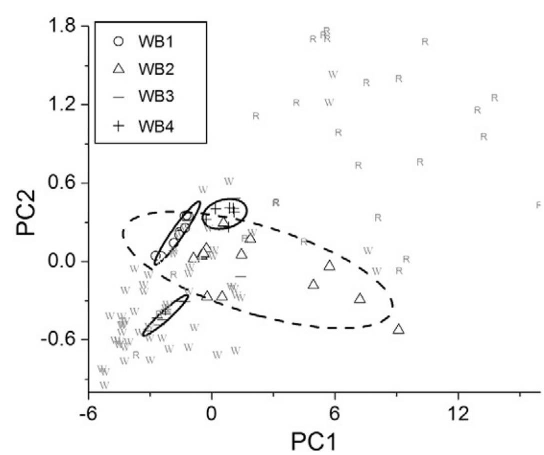

Fig. 6. The 100 tequila samples mapped over the PC1–PC2 subspace with the corresponding spectra data of sets WB1, WB2, WB3 and WB4. The letters W, R and A are for white, rested and aged tequila, respectively.

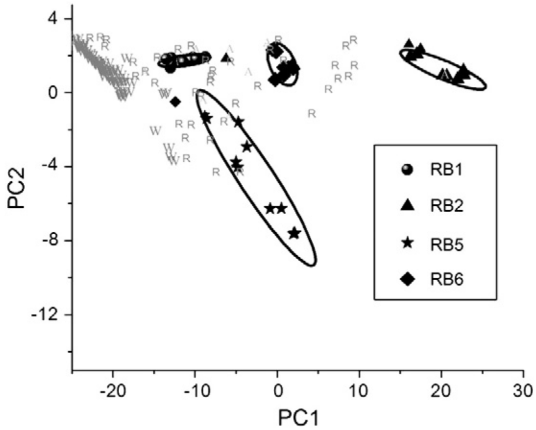

Fig. 7. The 100 tequila samples mapped over the PC1–PC2 subspace with the corresponding spectra data of sets RB1, RB2, RB5 and RB6. The letters W, R and A are for white, rested and aged tequila, respectively.

Table 3
Samples of WB1 and RB1 tequila were adulterated with mixtures of tequila, RON, ethanol (EtOH) and desionized water (H_2O); % V/V. (EtOH:H_2O, 40:60, v/v).

Samples								
WB1				RB1				
1	90% WB1	0%	10% EtOH-H_2O	8	80% RB1	0%	10% EtOH-H_2O	10% RON
2	80% WB1	0%	20% EtOH-H_2O	9	60% RB1	0%	30% EtOH-H_2O	10% RON
3	70% WB1	0%	30% EtOH-H_2O	10	40% RB1	0%	50% EtOH-H_2O	10% RON
4	50% WB1	0%	50% EtOH-H_2O	11	40% RB1	20% RB5	40% EtOH-H_2O	0% RON
5	70% WB1	20% WB2	10% EtOH-H_2O	12	40% RB1	0%	50% EtOH-H_2O	10% RON
6	30% WB1	0%	70% EtOH-H_2O	13	20% RB1	10% RB5	60% EtOH-H_2O	10% RON
7	10% WB1	30% WB2	60% EtOH-H_2O	14	10% RB1	20% RB5	60% EtOH-H_2O	10% RON

confidence are those reported in Figs. 3 and 5, respectively. In Fig. 6 most of the white samples are located in the lower left of the plot meanwhile the rested tequila samples are in the upper right. However, as expected, very few rested samples (5) are located within the region of the white samples and vice versa, 2 white samples within the region were the rested samples are located. For the case of Fig. 7 similar results can be observed. Therefore, the percentage of white samples within the 4 ellipses of confidence in Fig. 6 is 13.0% and for the case of rested and aged tequilas the percentage of samples within the ellipses of confidence in Fig. 7 is 8.0%. That is, these percentages correspond to the misclassified samples when the 100 tequila samples were considered for the modeling of Section 4.2. On the other hand, Table 2 shows the percentage of samples properly classified, i.e., as not belonging to the tested brands. The first column on the left lists the 100 tequila samples according to the type of tequila, that is, white, rested and aged, meanwhile the other columns on the right give the percentage of the properly classified samples. The worst classification result, as expected, is for WB2 for the case of white samples with 73%.

3.3.2. Analysis of adulterated samples

For a second experiment, 14 adulterated samples were obtained from 2 new tequila bottles purchased at the liquor store. These two bottles were from the same brand than those of the sets WB1 and RB1; we used ethanol, water, rum and other tequilas as adulterants. Table 3 points out the adulterated samples and the used amounts of adulterants. Samples 1 to 7 in Table 3 were obtained from the new bottle of WB1 and samples 8 to 14 from the new bottle of RB1. Figs. 8 and 9 show the results on the PCA score plot for white and rested modeling, respectively. The PC plots in these figures show the spectra data of the 4 sets of white and rested tequilas as reported in Figs. 3 and 5; the numbers from 1 to 14 in each plot represent the spectral data of the adulterated samples according to Table 3. In Fig. 8 sample 1 is located within the ellipse of validation of WB1, this is so because 90% of this sample is pure tequila and only 10% of ethanol and water. That is, the added compounds were not enough to differentiate this sample from the samples of the set WB1. Contrary to sample 1, sample 7 has only 10% of pure tequila and 90% is adulterated according to Table 3. For this case the modeling distinguishes sample 7 easily from the spectra data of the set WB1. Similar to sample 7, samples 2–6 are not within the confidence ellipse of WB1 because the added compounds. Notice that each sample from 2 to 7 is “different” from any of the samples that define the spectra data of set WB1 and, furthermore, they are “different” each other as shown in Fig. 8. In this figure, the adulterated samples 8–14 are outside the ellipse of confidence of WB1 since they were obtained from the new bottle of the set RB1. For the case of Fig. 9, similar results were obtained. Samples 8–14 are located outside of the ellipse of confidence of RB1 due to the added compounds according to Table 3. Since samples 1–7 were obtained from WB1, they are outside the ellipse of confidence of RB1. It is worth to observe that none of the adulterated samples 2–14 are located within any of the other ellipses of confidence of the studied sets in Figs. 8 and 9.

Table 2
Percentage of classification of 100 additional tequila samples (different brands) as not belonging to the tested brands. The number between parentheses indicates the number of samples.

Different brandsgrouped by types	Tested brands							
	WB1	WB2	WB3	WB4	RB1	RB2	RB5	RB6
White (54)	94	73	96	98	100	100	100	100
Rested (39)	100	95	97	100	97	100	92	95
Aged (9)	100	100	100	100	100	89	78	100

3.3.3. Analysis of fake samples

Three bottles, labeled as A, B and C, of rested tequilas were purchased in a popular street market of Mexico City for the third

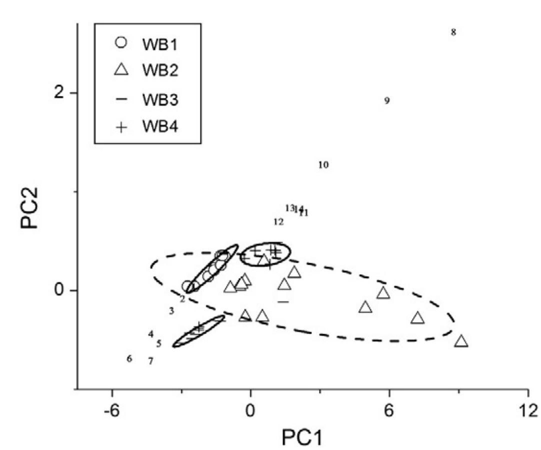

Fig. 8. The 14 adulterated samples obtained from two new bottles of tequila corresponding to sets WB1 and RB1 and plotted in the PC subspace after modeling for white tequilas.

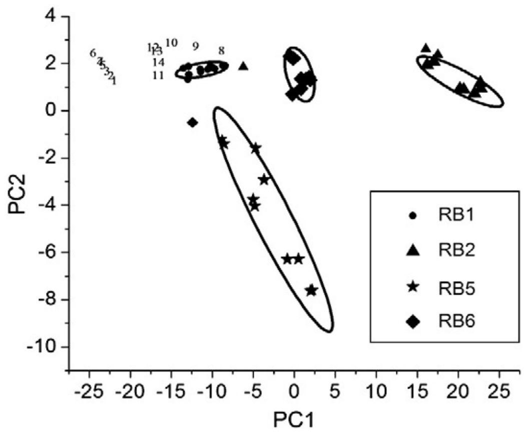

Fig. 9. The 14 adulterated samples obtained from two new bottles of tequila corresponding to sets WB1 and RB1 and plotted in the PC subspace after modeling for rested tequilas.

experiment; these additional samples corresponded, respectively, to brands of the sets RB1, RB5 and RB6. We did not expect that these bottles were genuine brands since the price of each bottle was much lower than the price we paid at the liquor store. Nevertheless, it is worth to mention that at simple glimpse the appearance of the content of those bottles was no different to those seen in authentic tequilas. In fact, the bottles are identical to those used in the corresponding distilleries. Another 3 new spirit bottles corresponding to RB1, RB5 and RB6 (labeled as a, b and c to match those labels of the A, B and C bottles, respectively) were also purchased at a major liquor store. The spectra data of the A, B and C samples were very different from the measured spectra of the a, b and c samples. The formers had no absorption band centered about 280 nm as shown by tequilas a, b and c; see Fig. 1 to recall how the spectra of rested tequilas look like. Fig. 10 shows the PCA results. When the spectra data of the 6 samples was worked out with spectra data of the 4 sets of rested tequilas, it was found that the spectra data of A, B and C samples were not located within the corresponding ellipse of confidence. Contrary to this result the spectra data of samples a, b and c were located, as expected, within the corresponding ellipse of confidence of RB1, RB5 and RB6, respectively. This result should be of interest for consumers in restaurants and bars if they want to make sure that the tequila they order is what is served; this result could be extended to other spirits such as whiskeys, brandies, cognacs. As mentioned in the introduction, fake and adulterated alcoholic beverages, among others, is a worldwide problem and consumers should be aware of this fact and that some alternative methods, as the reported in here, could help.

3.3.4. Analysis of additional samples

Finally another set of samples was under test by using our modeling. Seven new bottles of tequilas were purchased at the liquor store and each bottle belonged to one of the sets WB1, RB1, RB2, RB5 and RB6. These new test samples were introduced in our model and it was found that each new sample was within the corresponding ellipse of confidence. Therefore, it can be concluded that the reported modeling is robust. Further, 2 bottles of cognac, 1 of brandy and 2 of whisky were at hand; all of them were purchased at the liquor store and were used also as samples for the model concerning rested tequilas. Cognacs and brandy showed much higher absorbance than rested tequilas; therefore, they were diluted 1:10 and 1:20, respectively, with desionized water to match about the reported absorbance of rested tequilas; whiskeys also were diluted 1:1. Results showed that these spirits, as expected, were outside of any of the four ellipses of confidence of the rested tequilas. Fig. 11 shows the PCA results.

4. Conclusions

This work carried out a study of 8 brands of tequila, white and rested, and it is focused on identification of fake and adulterated tequilas. The reported method combines UV–VIS spectroscopy and chemometric techniques to confirm the originality of the product. To apply the method one first builds up a database of the corresponding tequila brand. Each database can be defined by an ellipse of confidence and any adulterated or fake tequila can easily be identified since its spectra data can be within or outside the ellipse. Furthermore, if the sample under test is outside of the corresponding ellipse, and the sample is for sure from the genuine brand, some problems on the reproducibility of production process should be considered. It is worth to note that the method could be extended to other spirits, in particular, cognacs, brandies and whiskeys. Therefore, it could be of help in distilleries for reproducibility of the spectral data along the line of production, so that the producer could easily know how well the product is going. This method can be performed on site, is non-expensive and the result can be obtained in minutes. The reported method might play an important role when a quick, trustworthy and feasible result on site is needed.

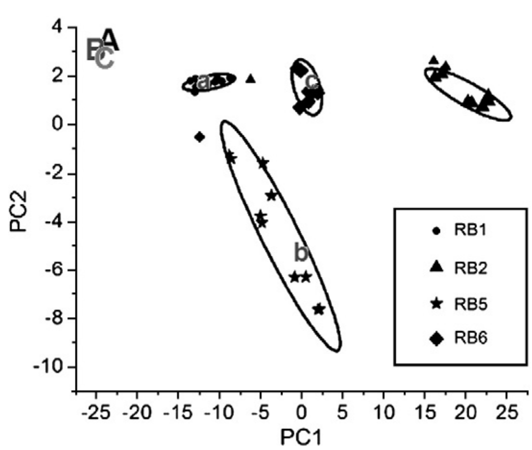

Fig. 10. Fake (A, B and C) and original (a, b and c) rested tequilas corresponding to WR1, WR5, WR6 brands and mapped over the PC1–PC2 subspace with the corresponding spectra data of sets RB1, RB2, RB5 and RB6.

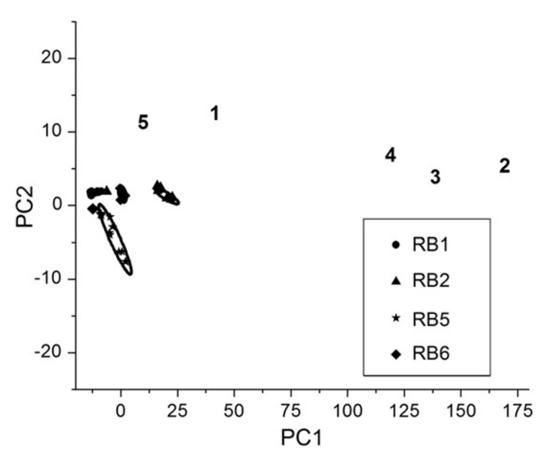

Fig. 11. Two wiskies (1 and 5), two cognacs (3 and 4) and one brandy (2) were mapped over the PC1–PC2 subspace with the corresponding spectra data of sets WB1, WB2, WB3 and WB4.

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