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A Study of Illicit Cocaine Seizure Classification by Pattern Recognition Techniques Applied to Metal Data

ABSTRACT: Fifteen metallic species, silver (Ag), aluminum (Al), calcium (Ca), cadmium (Cd), chromium (Cr), copper (Cu), iron (Fe), potassium (K), magnesium (Mg), manganese (Mn), sodium (Na), nickel (Ni), lead (Pb), strontium (Sr) and zinc (Zn), were determined in 46 cocaine samples confiscated by the Spanish police in Galicia (northwest Spain). Classification of these cocaine samples according to their geographic origin (Colombia and Venezuela) was achieved by the application of pattern recognition techniques to the metallic content data. Cocaine samples, around 0.5 g, were directly dissolved in 2 mL of 35.0%(v/v) HNO_3, diluted to 10 mL with ultrapure water. The metals were quantified by means of electrothermal atomic absorption spectrometry (Ag, Al, Cd, Cr, Cu, Mn, Ni, Pb and Sr), flame atomic absorption spectrometry (Ca, Fe, Mg and Zn), and flame atomic emission spectrometry (K and Na). Results show that two geographic origins can be established through the presence of trace and major elements.

KEYWORDS: forensic science, cocaine, seizures, metallic species, geographical classification, atomic absorption/emission spectrometry

For legal purposes it is useful to know if an illicit drug sample comes from the same batch as a drug whose origin is already known in order to determine the source of illict drug supply and thus to discover drug trafficking routes (1).

As the cocaine sold in the illegal market is normally a mixture of cocaine with different kinds of cuts, several substances have been used as parameters for determining the origin of illicit cocaine seizures. These substances can be classified into four different groups (2): (*a*) impurities, which are other natural products present in the cocaine; (*b*) additives or dilution agents, which are substances without pharmacologic activity that are added to cocaine to dilute the final product; (*c*) adulterators, which are substances with pharmacologic activity similar to cocaine; and (*d*) contaminants, which are substances that are present in cocaine as a consequence of contamination during the preparation of the final product from the coca leaves. The contaminants are usually classified into two different groups (2), biotic contaminants and abiotic contaminants. Different microorganisms such as fungus and bacteria are englobed in the first group, while species like metals are related to the second one.

Most investigations on organic substances (impurities, additives or adulterants) have been used to establish the origin of illicit cocaine samples (1, 3–22). The analytical techniques employed are infrared spectroscopy (3) and mainly chromatography (4–19). The use of specific biosensors (20) and thermal analysis as differential scanning calorimetry (21) has also been applied to cocaine analysis. Recently, Violante et al. (22) have proposed an analytical pilot study on trace elements (contaminants) in cocaine and heroin. From their conclusions, the quantification of metallic species can contribute to the characterization and traceability of additive drugs.

In this work, the use of the levels of trace elements (Ag, Al, Cd, Cr, Cu, Mn, Ni, Pb and Sr) and major elements (Ca, Fe, K, Mg, Na and Zn) as parameters for determining the origin of illegal cocaine has been proposed. The application of classical pattern recognition techniques such as principal component analysis (PCA), cluster analysis and linear discrimination analysis (LDA), have been used in order to observe groups of samples as a function of their trace metals in order to determine their origin.

Methods

Apparatus

Two Perkin-Elmer model 1100B atomic absorption spectrometers with HGA-400 and HGA-700 graphite furnaces, and AS-40 and AS-70 autosamplers, respectively, were used for Ag, Al, Cr, Cu, Mn, Ni, Pb and Sr determinations. Hollow cathode lamps were used in all cases, with the spectrometer parameters shown in Table 1. A deuterium lamp was used as a background correction for Ag, Al, Mn, Ni and Pb determinations, while background correction based on the Zeeman effect was used for Cd determination. The use of background correction was not considered for Ca, Cr, Cu, Fe, K, Mg, Na, Sr and Zn determinations. Pd was used as a chemical modifier at concentrations of 25 mg L^{-1} for Mn and 30 mg L^{-1} for Ag and Pb (23,24), while $Mg(NO_3)_2$ was selected for Al, Cr and Ni at concentrations of 25, 15 and 5 mg L^{-1}, respectively (25–27). For Cu determination (28), a mixture of Pd-$Mg(NO_3)_2$ was used at concentrations of 10 mg L^{-1}. For Sr (25), concentrations of 25 and 20 mg L^{-1} for Pd and $Mg(NO_3)_2$ were used, respectively.

A Perkin-Elmer model 4100ZL atomic absorption spectrometer with THGA transversal graphite furnace and AS-71 autosampler were used for Cd determination. Spectrometer operating conditions are also shown in Table 1. $(NH_4)_2HPO_4$ was used as a chemical modifier at a concentration of 0.2%(m/v) (29).

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TABLE 1—*Spectrometer operating conditions and techniques.*

	Wavelength, nm	Spectral Bandwidth, nm	Lamp Current, mA	Background Correction	Technique
Ag	328.1	0.7	10	Deuterium	ETAAS*
Al	309.3	0.7	20	Deuterium	ETAAS
Ca	422.7	0.7	10	. . .	FAAS†
Cd	228.8	0.7	4	Zeeman	ETAAS
Cr	357.9	0.7	25	. . .	ETAAS
Cu	324.8	0.7	15	. . .	ETAAS
Fe	248.2	0.2	15	. . .	FAAS
K	766.5	0.4	. . .	. . .	FAES‡
Mg	285.2	0.7	10	. . .	FAAS
Mn	279.5	0.2	30	Deuterium	ETAAS
Na	589.0	0.2	. . .	. . .	FAES
Ni	232.0	0.2	25	Deuterium	ETAAS
Pb	283.3	0.7	10	Deuterium	ETAAS
Sr	460.7	0.2	20	. . .	ETAAS
Zn	213.8	0.7	10	. . .	FAAS

* Electrothermal atomic absorption spectrometry.
† Flame atomic absorption spectrometry.
‡ Flame atomic emission spectrometry.

TABLE 2—*Optimum charring and atomization temperatures corresponding to the determination of Ag, Al, Cd, Cr, Cu, Mn, Ni, Pb y Sr by ETAAS.*

	Charring Temperature, °C	Atomization Temperature, °C	Reference
Ag	1000	1800	24
Al	1400	2300	25
Cd	800	1400	29
Cr	1600	2500	26
Cu	1300	2400	28
Mn	1300	2200	24
Ni	1600	2500	27
Pb	1000	2400	23
Sr	1800	2300	25

The optimum charring and atomization temperatures found for the determinations by electrothermal atomic absorption spectrometry (23–29) have been summarized Table 2.

A Perkin-Elmer model 2280 atomic absorption spectrometer with a Pt impact bead nebulizer was used for Ca, Fe, Mg and Zn determinations. In all cases, a reduced air/acetylene flame was used. The determinations of K and Na were carried out by atomic emission spectrometry using a Perkin-Elmer model 5000 atomic absorption/emission spectrometer with a Pt impact bead nebulizer. A reduced air/acetylene flame was also used throughout. Spectrometer operating conditions are also given in Table 1.

Determinations were carried out using aqueous calibration for Ag, Al, Ca, Cr, Cu, Mg, Mn, Na, Ni, Pb, Sr and Zn, while the standard addition method was needed for Cd, Fe and K measurements.

Cocaine Seizures and Pretreatment

Cocaine samples were supplied by the External Health Office from A Coruña. The samples corresponded to a confiscation carried out in Galicia (northwest Spain) over the period of October 1994 to March of 1996. Due to the fact that Galicia is one of the main entrances of cocaine into Europe, a large number of the cocaine samples used in this study were of high purity, around 90%. The possible origin of some cocaine samples was established on the basis of information from the External Health Office in A Coruña, which implied Venezuela or Colombia as possible sources.

The cocaine sample pretreatment was the dissolution of the sample (0.5 g) in 2 mL of 35.0%(v/v) HNO_3, diluting to 10 mL with ultrapure water.

Chemicals

All chemicals used were of ultrapure grade, using ultrapure water, with a resistance of 18 MΩ cm^{-1}, which was obtained from a Milli-Q purification device (Millipore Co., Bedford, MA).

Data Manipulation and Pattem Recognition Analysis

All statistical analyses have been performed by means of the SPSS 5.0.1 Professional Statistics 1992 and STATISTICA 4.5 Stat-Soft 1993, run on IBM-compatible hardware.

Principal components analysis (PCA) was used to achieved a reduction of dimension, i.e., to fit a K-dimensional subspace to the original *p*-variate objects ($p > K$) and to observe a primary evaluation of the between-class similarity (30).

Cluster analysis was used to observe possible different classes. This clustering technique is an unsupervised classification procedure that involves a measurement of the similarity between objects to be clustered. Objects will group in clusters in terms of their nearness or similarity (31).

Linear discriminant analysis (LDA) was used, after the evidence of different classes obtained by means of cluster analysis, to classify the samples according to different categories. This classification procedure (32) maximizes the variance between categories and minimizes the variance within categories. This method renders a number of orthogonal linear discriminant functions equal to the number of categories minus 1.

Results

First, and due to the fact that the concentration ranges for the metals are very different among them, it is necessary to standardize the concentrations of each element for each cocaine sample. This operation, named autoscale, was introduced by Kowalski and Bender (33) and the procedure standardizes an *m* variable according to the equation

$$Y_{mj} = \frac{(x_{mj} - \bar{x}_{mj})}{S_m}$$

where Y_{mj} is the *j* value (*j* cocaine sample) for the *m* variable after scaling, x_{mj} is the *j* value before scaling, $\bar{x}_m$ is the mean of the variable, and S_m is the standard deviation of the variable. This operation was carried out using the SPSS and STATISTICA routines.

Principal Component Analysis (PCA)

The correlation matrix **R** (15 variables and 46 observations) is displayed in Table 3. Strong positive correlations are observed between the pairs K/Na (0.971), Fe/Zn (0.734) and Mg/Sr (0.755). Therefore, the application of the principal component analysis can be considered suitable to extract information due to the observed correlations between variables. Mathematically, each principal component or eigenvector is orthogonal and is a linear combination of the original variables. Six principal components (with eigenvalues ≥ 1) were chosen from fifteen components. They account for

TABLE 3—*Correlation matrix between pairs of elements* (n = 46).

	Ag	Al	Ca	Cd	Cr	Cu	Fe	K	Mg	Mn	Na	Ni	Pb	Sr	Zn
Ag	1.00														
Al	0.14	1.00													
Ca	−0.13	−0.05	1.00												
Cd	0.15	−0.10	−0.19	1.00											
Cr	0.24	0.40	0.15	0.12	1.00										
Cu	0.04	0.24	0.37	−0.13	0.29	1.00									
Fe	0.04	0.51	0.12	−0.15	0.58	0.28	1.00								
K	0.11	0.00	0.02	0.22	0.51	−0.03	−0.03	1.00							
Mg	0.05	0.39	0.10	−0.15	0.11	0.52	0.19	0.00	1.00						
Mn	−0.05	−0.10	0.05	−0.09	0.11	0.06	0.49	−0.10	−0.06	1.00					
Na	0.08	0.02	0.05	0.19	0.49	0.03	−0.03	0.97	0.20	−0.11	1.00				
Ni	0.23	0.52	−0.10	0.06	0.58	0.21	0.41	0.25	0.12	0.23	0.23	1.00			
Pb	0.12	0.49	0.23	−0.16	0.34	0.68	0.34	−0.06	0.10	−0.06	−0.06	0.37	1.00		
Sr	−0.07	0.04	0.36	−0.09	0.16	0.34	0.12	−0.02	0.75	0.16	0.16	−0.02	0.32	1.00	
Zn	0.27	0.68	0.30	−0.24	0.55	0.56	0.73	−0.03	0.24	−0.04	−0.04	0.47	0.51	0.09	1.00

TABLE 4—*Communalities after principal component extraction (unrotated solution).*

	Principal Component					
Variables	1	2	3	4	5	6
Ag	0.23	0.24	−0.30	−0.27	−0.19	**−0.71**
Al	**0.71**	−0.04	−0.25	−0.45	0.03	0.01
Ca	0.29	−0.24	0.50	0.41	−0.26	0.35
Cd	−0.16	0.48	−0.14	−0.01	−0.09	**−0.72**
Cr	**0.74**	0.46	−0.08	0.19	0.07	−0.16
Cu	0.61	−0.28	0.15	0.24	−0.50	−0.03
Fe	**0.74**	−0.16	−0.25	0.20	0.45	0.10
K	0.19	**0.89**	0.19	0.23	−0.03	−0.06
Mg	0.40	−0.05	0.59	−0.58	0.36	0.05
Mn	0.19	−0.25	−0.12	0.56	0.59	0.01
Na	0.22	**0.86**	0.36	0.13	0.06	−0.03
Ni	0.64	0.31	−0.34	−0.18	−0.02	−0.02
Pb	0.69	−0.27	0.01	0.05	−0.38	−0.10
Sr	0.37	−0.16	**0.81**	−0.15	0.12	0.01
Zn	**0.86**	−0.20	−0.22	0.00	−0.03	0.04

80.9% of the total variability. From the loading of features in the first, second and third eigenvectors (Table 4), Al, Cr, Fe and Zn are the dominating features in the first principal component (28.0% of the total variability), K and Na dominate in the second principal component (16.7% of the total variability), and Sr dominates in the third principal component (12.4%). The variables present low correlations with the fourth, fifth and sixth principal components considered (Table 4). The fourth, fifth and sixth principal components (eigenvalues between 1.376 and 0.968) explain 9.2, 8.2 and 6.4% of the total variablity, respectively. Examining a two-dimensional plot of the cocaine samples in the space defined by the first two principal components, Fig. 1, we can say that a natural separation between samples can be observed.

Cluster Analysis

Due to the fact that the possible origin is known only for a few cocaine samples, it is not possible to use them as a training or learning set. Therefore, cluster analysis was applied in order to observe groups of samples. For this study, the squared Euclidean distance between objects (cocaine samples) and the Ward's method as glomerate procedure were used. This clustering method at each step considers the heterogeneity or deviation (sum squares of the distance of an object from the barycentre of the cluster) of every possible cluster that can be created by linking two existing clusters

(34). The results of cluster analysis are shown as a dendrogram in Fig. 2. They showed the presence of cocaine sample clusters and thus, it can be said that the metal data contained significant information to achieve different category classification between cocaine seizures. As it can be seen, at a linkage distance of 5 (dashed line), there are four principal clusters, the first cluster containing 15 objects, the second cluster with 5 objects, the third with 3 objects and the fourth one containing 11 objects. Then 13 objects are more or less in separate clusters. All these clusters can be formed by cocaine samples from different geographical origins. Information about the origin of some cocaine samples was given by the External Health Office from A Coruña based upon cocaine seizures confiscated in flights from Colombia and Venezuela. Therefore, cocaine samples noted by C32 and C21 were assumed as samples coming from Venezuela. These two samples are in the first cluster, Fig. 2 (at a linkage distance of 5). Therefore, the other cocaine samples that are in these clusters, C36, C39, C37, et., could be assumed as coming from Venezuela. In a similar way, cocaine samples noted by C1, C2, C4, C6, C7, C8, C9, C10, C17, C24, C28, C29 and C30, confiscated in flights from Colombia, were assumed as coming from Colombia. These cocaine samples, except C8, C9, C17 and C30, are in the second, third and fourth clusters (linkage distance of 5 in Fig. 2). Therefore, it can be assumed that the other cocaine samples which are in the second, third and fourth clusters (Fig. 2) come from Colombia. Cocaine samples denoted as C8, C9, C17 and C30 fell in different small clusters (bottom of Fig. 2).

Linear Discriminant Analysis (LDA)

The results from the cluster analysis allow us to establish a learning set: the cocaine samples from the first cluster (starting from the top in Fig. 2) were assumed as cocaine samples from Venezuela (category 1); the cocaine samples from clusters 2, 3 and 4 (starting from the top in Fig. 2) as cocaine samples from Colombia (category 2); and the cocaine samples from the other clusters as unclassified cocaine samples (category 3). This latter category is formed with cocaine samples which were not grouped as cocaine from Colombia or Venezuela after the cluster analysis.

The linear discriminant analysis was applied to the learning set obtained as indicated above. The recognition ability for the three classes was satisfactory, as it can be seen in Table 5. One cocaine sample, assumed as a cocaine sample from Venezuela (category 1) was misclassified as a sample of category 2 (from Colombia). One cocaine sample from category 2 was also misclassified as cocaine from the first category (Venezuela). This cocaine sample
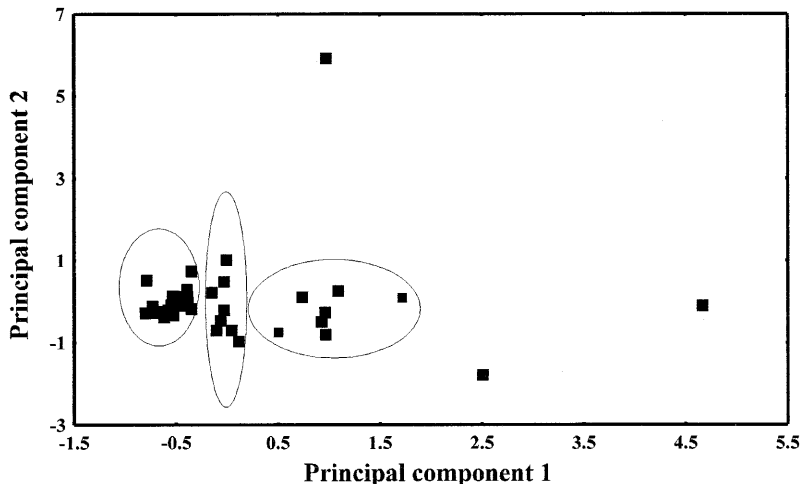
FIG. 1—*Projections of the first and second unrotated principal components of the scores of the 46 cocaine samples.*
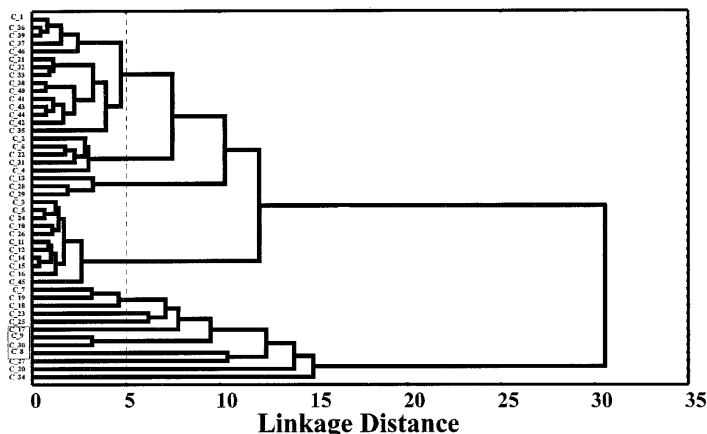

FIG. 2—*Dendrogram of the 46 cocaine samples obtained by the Ward's hierarchical clustering method.*

TABLE 5—*Classification results after lineal discriminant analysis.*

Actual Group	No. of Cases	Predicted Group Membership			
		% Classification	Group 1	Group 2	Group 3
Group 1	14	92.9	13	1	0
Group 2	26	96.2	1	25	0
Group 3	6	50.0	0	3	3
Total	46	89.1	14	29	3

Group 1 = Venezuela; Group 2 = Colombia; Group 3 = unclassified cocaine samples (less pure cocaine samples).

was denoted as C8 and was misclassified as cocaine from category 3 by cluster analysis. It can be clearly seen that cocaine samples denoted as C9, C17 and C30, misclassified by cluster analysis, were correctly classified by linear discriminat analysis. Finally, three cocaine samples from the third category were misclassified as cocaine from Colombia (category 2). From the classification among groups, given in Table 5, it can be said that the percent of ''grouped'' cases correctly classified is 89.1%.

Discussion

The application of pattern recognition techniques to drug monitoring and to forensic purposes can be useful and must be consid-ered for legal medicine and forensic studies. Thus, the determination of the metallic content in illicit cocaine samples can be helpful in obtaining information about their origin. In this work, the information about the origin of some illicit cocaine samples is based upon the confiscation of them in flights from two neighboring South American countries (Colombia and Venezuela) and thus, we cannot speak about a geographical classification of cocaine samples due to the fact that both countries can be used as trans-shipment countries for cocaine exportation and, mainly, because knowledge of the cocaine's origin is not known. Therefore, after the application of classical pattern recognition to metal data, it is only possible to say that cocaine samples which enter Galicia (Northwest Spain) appear to be grouped in three, two of them related to airline flights coming from Colombia and Venezuela.

Due to the complexity of the problem, however, future research on the use of solvents and data on impurities is necessary in order to elucidate the geographical origin of cocaine seizures. In addition, the analyses of known origin standard cocaine will be necessary.

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