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Research Article

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NIR analysis of hair samples as a possible forensic chemistry tool: identifying smoker and nonsmoker persons

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Abstract In the present report it is shown that a chemometric analysis of near infrared spectroscopy (NIR) data obtained for hair samplescan be successfully employed to differentiate between smoker and nonsmoker persons. It is worth noting that only NIR data are enough to such identification, with no kind of classical chemical analysis been necessary. Such achievement demonstrates that a chemometric analysis of hair based on NIR spectra has possible applications in forensic chemistry.

Keywords NIR spectroscopy, Chemometrics, Hair, Smoker, Forensics

Introduction

Frequently, crimes involve direct physical contact between victim and suspect, with the transfer of hairs and fibers. Hence, hair examination may be used to provide information for crime scene reconstruction and suspects identification, as well as toxicological analysis [1-2]. By macroscopic analysis of hair (a single head hair, for example) information such as race, sex and age of its owner can be obtained.

The importance of hair analysis in criminal investigation is well established since the early studies in the middle XIX century, and have been shown [3] that smoking and nosmoking persons can exhibits very different hair chemical compositions. Such chemical analysis are traditionally performed by atomic absorption spectrometry of some related technique.

Traditionally, forensic analysis of hair samples are performed by optical microscopy, for example. Hence, from a forensic point of view, have been investigated the use of some "non-traditional" techniques such as thermogravimetry [4] to the study of head and pubic hair samples.

Near infrared spectroscopy (NIR), have been successfully applied to to evaluate the friction, twist, and gloss of human hair [5], hair interior and surface damage [6], and as a method of analysing eumelanin in hair samples[7].

In this connection, in the present work it is shown that a chemometric analysis of near infrared spectroscopy (NIR) data obtained for hair samples, can be successfully employed to differentiate between smoker and nonsmoker persons. It is worth noting that only NIR data are enough for such identification, with no kind of classical chemical analysis been necessary.

Experimental

A total of 20 hair samples were analyzed (10 from smoker and 10 from nonsmoker persons) from both, males and females of different ages. The smoker persons are in the 26-74 years old range. The nonsmoker persons in the 3-41 years old range.

Among the population of the smoker persons, there is one that has been a smoker for 8 years and another one that is a smoker for 63 years. The sample data are summarized in Table 1. The hair samples were collected form the nape region.

Table 1: Summary of the investigated hair samples

Sample	Sex[1]	Age/years	Years as smoker
1	M	49	20
2	F	54	38
3	M	43	22
4	F	50	37
5	F	68	53
6	M	26	8
7	F	50	35
8	F	73	63
9	F	74	60
10	M	49	27
11	F	11	NS
12	F	27	NS
13	F	33	NS
14	F	24	NS
15	F	15	NS
16	F	41	NS
17	F	40	NS
18	F	11	NS
19	M	3	NS
20	F	30	NS

[1]M = male; F = female; [2]NS = not smoker

NIR reflectance spectra were obtained using a Bomem apparatus model MB 160 coupled to a diffuse reflectance accessory. Each measured spectrum (in triplicate) was the average of 50 scans obtained with a resolution of 8 cm^{-1} in the 1100–2500 nm range. The spectrum of a polytetrafluoroethylene (PTFE) sample was used as background. In the present study, the analyzed spectral data were in the 1800-2500 nm range, and the spectral data were analyzed after treatment (smoothing and Savitzky-Golay first order derivative) as shown in Figure 1.

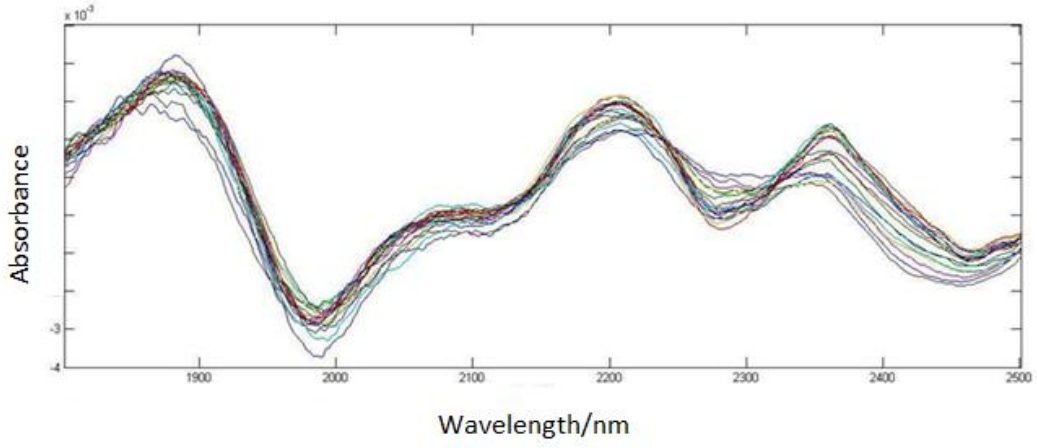

Figure 1: NIR spectra for the investigated hair samples after treatment

The chemometrics were performed as follows: A data set with many variable scan be simplified by performing data reduction which makes the system more easily interpretable. Principal Component Analysis (PCA) [8] is a well-known method to reduce the number of variables, in which the spectral matrix X is decomposed as: $X = TP^t + E$**(**where X is the *I x J* data matrix, T is the *I x A* matrix of score vectors); the score vectors t_a are orthogonal (i.e., $T^tT = diag(l_a)$ and l_a are eigenvalues of the matrix X^tX), P is the *J x A* matrix of loadings vectors, E is the *I x J* residual matrix, *I* is the number of objects, *J* is the number of variables, and *A* is the number of components calculated.

Data analysis was performed using MATLABversion6.5 (The Math-Works, Natick, USA) employing the PLS-toolbox (Eigenvector Research, Inc., Wenatchee, WA, USA, version 6.01). Different preprocessing methods were used, including the derivative and smoothing Savitzky-Golay methods, with variable number of window points

Results and Discussion

The obtained results can be summarized in Figure 2.

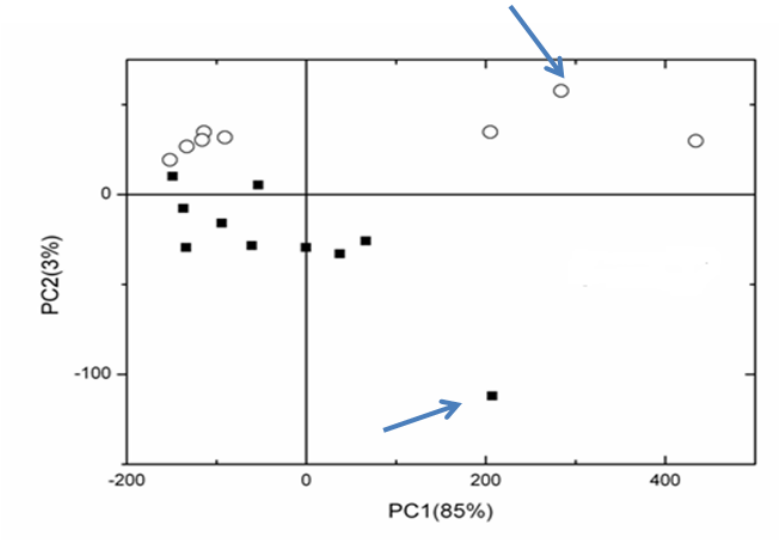

Figure 2: Chemometrics results (based on NIR spectra for hair samples) to smoker (○) and nonsmoker (■) persons.

The results summarized in Figure 2 were obtained based on Figure 1 data. As can be verified, after chemometric analysis, samples from smoker and nonsmoker persons are positioned in different graphic regions, that is, both "populations" are clearly separated. So, it is shown that by using NIR infrared spectra of hair sample, it is possible to differentiate (identify) if that hair sample came from a smoker or a nonsmoker person. So easy and straightforward differentiation it is, of course, of very interesting possible applications, such as a preliminary screening for forensic identification.

Despite the fact that certainly the different chemical composition of smoker and nonsmoker hair samples are the main reason beneath such separation data, it is worth noting that no classical chemical analysis was necessary in this case, and that the separation between smoker and nonsmoker persons can be easily made only by using NIR spectra.

It is also worth noting that among the samples from smoker persons, the circles (Figure 2) in the upper right part of the curve are related with the hair samples that came from persons with a larger number of years as smokers. So, such results could be employed, also, as a preliminary screening for possible lung cancer cases. In such interpretation, as lower the point it is in the graphic, the lower is the probability of develop a lung cancer.

In Figure 2, the highlighted points in the lower and upper parts of the graphic are related with a three years old child (nonsmoker, of course) and an adult that has been a smoker for 63 years.

It is worth noting that considering only not smoker persons, the ones that are "passive" smokers, that is, persons that lives or works closer to smoker persons, have their results located progressively closer to the upper part of the graphic. So, it is possible to establish a relationship between the position of the point in the graphic and the time of exposition to a smoking environment.

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