



Identification of adulteration in ground roasted coffees using UV–Vis spectroscopy and SPA-LDA



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ABSTRACT

The pleasant taste and flavor of coffee are responsible for making it one of the most preferred and consumed beverages around the world. Industrial coffee plants usually roast both coffee and adulterants together, which affects directly the quality of the product, specially the sensorial characteristics of the drink. Therefore, this work aims the identification of adulterations in ground roasted coffees (due to the presence of husks and sticks) using ultraviolet–visible spectroscopy and the Successive Projections Algorithm for variable selection in association with Linear Discriminant Analysis (SPA-LDA). For this purpose, extracts of ground roasted coffees prepared in hot water alone (representing the final product as ingested by the consumers) were then analyzed. The proposed methodology obtained a 100% classification in both training and test sets, providing a simple and fast analysis of the aqueous extracts of ground roasted coffees. Moreover, it can also afford security to coffee consumers and regulatory agencies, preventing the fraudulent labeling.

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1. Introduction

Coffee is one of the most preferred and consumed beverages around the world due to its pleasant taste and flavor. In order to stimulate the growth in demand for coffee through the establishment of a better overall standard of quality to the global market, the International Coffee Organization (ICO) implemented in 2002 the Coffee Quality Improvement Programme (CQP), subsequently modified by Resolution No. 420 of May 2004. This Programme consists of target standards for exportable coffee, restricting exports of coffee below a minimum accepted quality level and diverting low-grade coffee to alternative uses. This improvement of coffee quality and the consequent increase in its demand took the coffee to be one of the world's top commodities, being Brazil the largest coffee-producing country (more than a third of the total world production in the crop year of 2012/2013 (Nebesny & Budryn, 2006; Van der Vossen, 2009, Souto et al., 2014; ICO, 2014)).

As the largest exporting member of ICO, the Brazilian Coffee Industry Association (ABIC) also implemented the CQP, aiming supply the highest standard of quality to its ground roasted coffees. Moreover, in 2010 the Brazilian Ministry of Agriculture, Livestock, and Food Supply (MAPA) issued the Normative Instruction No. 16, establishing a maximum limit of 1 g/100 g for a set of impurities (husks and sticks), sediments (stones, clods and sand), and foreign matter (corn, rye, sugar, barley, *açaí* seeds, etc.) in ground roasted coffees in order to avoid an illegal practice of adulteration by coffee producers (MAPA, 2010).

Nevertheless, there is an intentional or unintentional character of defrauding the ground roasted coffee by some sectors of the coffee production chain, encompassing some cooperatives and industries roasting. Industrial coffee plants usually roast both coffee and adulterants together, in increasing degrees of roasting levels (whether light, medium, medium-dark, or dark), favoring the adhesion of fine roasted coffee particles onto the surface of the adulterants due to oil absorption. Thus, the presence of these impurities affects directly the quality of the ground roasted coffee, specially the sensorial characteristics of the drink (Sano, Assad,

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Cunha, Correa, & Rodrigues, 2003; Toledo, Hantao, Ho, Augusto, & Anderson, 2014).

Quality control of the drink depends on its basic attributes (aroma, flavor, body and acidity), which are traditionally evaluated by skillful tasters. However, this human sensory assessment is markedly impartial and unreliable (Murray, Delahunty, & Baxter, 2001; Sano et al., 2003; Tavares et al., 2012). To overcome these drawbacks, several analytical techniques have been applied to detect and/or quantify coffee adulteration, such as gas chromatography/mass spectrometry (Toledo et al., 2014), and high performance liquid chromatography (Pauli et al., 2014; Domingues et al., 2014), Fourier transform infrared spectroscopy (Reis, Franca, & Oliveira, 2013), near infrared spectroscopy (Ebrahimi-Najafabadi et al., 2012), mid-infrared spectroscopy (Tavares et al., 2012), and digital image processing (Sano et al., 2003; Souto et al., 2014).

A simple alternative is to develop an analytical methodology using ultraviolet–visible (UV–Vis) spectroscopy, which is one of the most common and inexpensive techniques used in routine analysis. Therefore, this work aims the identification of adulterations in ground roasted coffees (due to the presence of husks and sticks) using UV–Vis spectroscopy and the Successive Projections Algorithm for variable selection in association with Linear Discriminant Analysis (SPA-LDA). For this purpose, extracts of ground roasted coffees prepared in hot water alone (representing the final product as ingested by the consumers) were then analyzed. For comparison, others supervised pattern recognition techniques such as Soft Independent Modelling by Class Analogy (SIMCA) and Partial Least Squares Discriminant Analysis (PLS-DA) were also used. It is worth to highlight that UV–Vis spectroscopy and pattern recognition techniques were already successfully used to classify aqueous extracts of Brazilian ground roast coffee according to its type (caffeinated/decaffeinated) and conservation state (expired and non-expired shelf-life) (Souto et al., 2010).

2. Materials and methods

2.1. Sample preparation

A total of 102 ground roasted coffee samples were collected from 14 different regions of Brazil (State producers) along 6 months. They were then, certified by the Brazilian Coffee Industry Association (ABIC), and were provided by the Brazilian research laboratories *Global Center for Analysis and Research* (NUGAP), and *National Service for Industrial Training* (SENAI). The samples were distributed into two classes, being 45 non-adulterated and 57 adulterated with husks and sticks. Non-adulterated coffees are exclusively composed of ground roasted coffee beans without adulterations by husks and sticks. The adulterations in the ground roasted coffee samples were in the range of 1.04–7.63 g/100 g (4.05 ± 1.66 g/100 g) by following the Normative Instruction No. 16 of Brazilian Ministry of Agriculture, Livestock, and Food Supply (MAPA, 2010), which is based on gravimetry and optical microscopy.

An aqueous extraction procedure of the coffee samples was performed as described by Souto et al. (2010). Initially, 1.0 g of each sample was weighed and placed in a filter funnel containing a 25 μ m pore-sized quantitative filter paper (J. Prolab® white ribbon filter) coupled with an erlenmeyer. The extractions were performed by using distilled water at 90–98 °C during 25 min for each sample. After cooling process to room temperature (for 30 min), all extracts were then diluted in the proportion of 1:20 (mL:mL) with distilled water. UV–Vis spectra from the aqueous extracts were acquired according to procedure described as follows.

2.2. Instrumentation and data acquisition

UV–Vis spectra (239–405 nm) were acquired in triplicate by using a Hewlett Packard model HP 8453 UV–Vis spectrophotometer equipped with a quartz cell with optical path of 10 mm, and spectral resolution of 1 nm at a 23 ± 1 °C room temperature. Before the measurements step, blank (the same water used in extraction step) was placed inside of the sample cell to adjust the 100% transmittance signal.

2.3. Chemometric procedures and software

The obtained data set was divided into training (63 samples, being 26 non-adulterated and 37 adulterated coffees) and test (39 samples, being 19 non-adulterated and 20 adulterated coffees) sets by applying the Kennard–Stone (KS) uniform sampling algorithm (Kennard & Stone, 1969). Unsupervised (Principal Component Analysis – PCA) and supervised (SIMCA, PLS-DA and SPA-LDA) pattern recognition techniques were employed. The validation step for each of the algorithms was performed using full cross-validation. The test samples were used for the final data evaluation, and for comparison of the classification models only (Soares, Gomes, Galvão Filho, Araújo, & Galvão, 2013). The classification performance of the models was evaluated for accuracy, sensitivity and specificity (Massart, Vandeginste, Buydens, Lewi, & Smeyers-Verbeke, 1998; Lavine, 2009).

The KS and SPA-LDA algorithms were performed with Matlab® 2009b (Mathworks Inc.) software. SIMCA and PLS-DA were calculated by using the Classification toolbox for Matlab® (version 2.0) released by Milano Chemometrics, and QSAR Research Group (Ballabio & Consonni, 2013).

3. Results and discussion

The quality of the coffee beans is affected by several factors coming from the stages of harvesting, processing and storage. In fact, there is a direct influence of the quality of the ground roasted coffee powder on its aqueous extracts in terms of flavor and aroma. In this sense, the main contribution is given by changes during the roasting process, in which occur relevant physicochemical reactions (such as Maillard reaction, Strecker degradation, sugars caramelizing, chlorogenic acids degradation, proteins and polysaccharides degradation) due to interactions between the various chemical compounds present in the coffee beans (proteins, carbohydrates, chlorogenic acids, caffeine, trigonelline, lipids etc.) when subjected to heat (Nicoli, Anese, Manzocco, & Lerici, 1997; Baggenstoss, Poisson, Kaegi, Perren, & Escher, 2008; Vignoli, Viegas, Bassoli, & Benassi, 2014). These differential characteristics

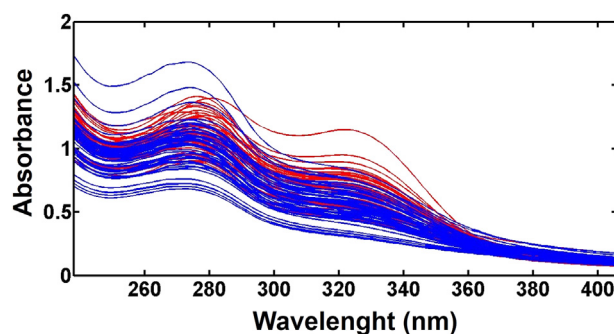


Fig. 1. UV–Vis spectra of the 102 studied roasted coffee samples: non-adulterated (in red) and adulterated (in blue) coffee samples. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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