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Quantitative assessment of specific defects in roasted ground coffee via infrared-photoacoustic spectroscopy

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ABSTRACT

Chemical analyses and sensory evaluation are the most applied methods for quality control of roasted and ground coffee (RG). However, faster alternatives would be highly valuable. Here, we applied infrared-photoacoustic spectroscopy (FTIR-PAS) on RG powder. Mixtures of specific defective beans were blended with healthy (defect-free) *Coffea arabica* and *Coffea canephora* bases in specific ratios, forming different classes of blends. Principal Component Analysis allowed predicting the amount/fraction and nature of the defects in blends while partial Least Squares Discriminant Analysis revealed similarities between blends (=samples). A successful predictive model was obtained using six classes of blends. The model could classify 100% of the samples into four classes. The specificities were higher than 0.9. Application of FTIR-PAS on RG coffee to characterize and classify blends has shown to be an accurate, easy, quick and "green" alternative to current methods.

1. Introduction

Coffee is a major economic factor for a number of producing as well as consuming countries (see the updated statistics by International Coffee Organization, ICO, 2017). Twenty years ago, coffee was essentially a commodity. Since the 1990th, the rise of the specialty coffee movement has created an important new segment for the coffee market. Consumers are looking for special brands, origins and flavors, and are willing to pay higher prices for these qualities. This has created a fast-growing upmarket segment for which control of coffee quality is increasingly important (ABIC, 2006; ICO, 2017) and which benefits the whole coffee value chain.

Coffea arabica (Arabica) and *Coffea canephora* (Robusta) are the main species of coffee, representing 99% of the world production (ICO, 2017). Besides genetic, chemical and sensory differences, cherries of Arabica and Robusta coffees can also be visually distinguished, based on physical and morphological characteristics (González, Pablos, Martín, León-Camacho, & Valdenebro, 2001; Wermelinger, D'Ambrosio, Klopprogge, & Yeretzian, 2011). Beverages of Arabica produce in general a more intense flavor, with wider body and acidity variations. In contrast, Robusta has in general a lower marketing value (ICO, 2017) and blends of both species are often used in the industries in order to create specific flavor profiles, standardize the quality and adjust the price.

Defining the quality of coffee is by no means a simple endeavor. In this situation, the concept of defects still dominates the assessment of the quality of green coffee. While there are different green coffee beans defect classification standard, the Brazilian classification method is one of the most applied and important. It is possibly superior over some other systems in that it better accounts for the relationship between the defective coffee beans and the cup quality.

Defects occur due to genetic or physiological effects, or from failures in agricultural processes such as fertilization, problems with pests and diseases, drought and frost damages, and inadequate preparation, or from industrial processes, including peeling, drying, storage and processing (Franca, Oliveira, Mendonça, & Silva, 2005; Oliveira, Franca,

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Mendonça, & Barros-Júnior, 2006). The most common defects of coffee, produced by late or early harvest, or by fermentation of beans in contact with the ground, are sour, black and immature beans; particularly the first two are related to a strong reduction in sensory quality. Other types of defects may occur due to the presence of foreign bodies such as woods, skin and stones (Franca et al., 2005; Oliveira et al., 2006).

In the Brazilian productive chain of coffee, the largest worldwide in terms of production and export of green beans, defective beans can reach a considerable proportion of 20% of a crop. After harvesting, defective beans are mechanically separated from healthy beans (e.g. by color sorting). However, given the associated production costs, these defective beans are not discarded but sold both in the internal Brazilian market and on the international trade market. A large proportion of the defective coffee beans can legally be added to healthy beans (beans without defects) in order to obtain a standard blend for particular markets (ABIC, 2006). Considering the importance of such blends of healthy bean with specific proportions of defects for the coffee market, a classification was established for these blends based on the proportion and type of defects, which can be identified and controlled by mechanical and visual assessments prior to roasting and grinding. Yet, once roasted and ground, the traditional classification procedures (by instruments and/or experts) do not allow anymore to identify proportion and types of defects in a particular coffee. In sensory analysis, even trained coffee tasters may have a wide spread and uncertainties in their sensory scores (Wermelinger et al., 2011), and it is not possible to accurately classify coffees according to proportion and types of defects by sensory evaluation. Thus, the development of fast, simple and robust instrumental methodologies that provide sufficient precision and reliability for roast and ground (RG) coffee quality classification according to defects would be highly warranted. An emerging and promising approach is the use of spectroscopic techniques.

Methods based on near (NIR) and mid infrared spectroscopy for the discrimination of coffee species (Esteban-Díez, González-Sáiz, Sáenz-González, & Pizarro, 2007; Scholz et al., 2014), cultivars (Moreira & Scarminio, 2013) and to detect the presence of impurities (Ebrahimi-Najafabadi et al., 2012; Reis, Franca, & Oliveira, 2013), and defects of coffee (Santos, Sarraguça, Rangel, & Lopes, 2012) have been successfully developed. Recently, Fourier Transform Raman Spectroscopy was explored for distinguishing between Arabica and Robusta coffee species (Dias & Yeretzian, 2016; El-Abassy, Donfack, & Materny, 2011; Keidel, von Stetten, Rodrigues, Máguas, & Hildebrandt, 2010; Rubayiza & Meurens, 2005; Wermelinger et al., 2011), and low-field ^{1}H NMR spectroscopy proved to be a promising technique for the same purpose (Defernez et al., 2017). However, no reports using spectroscopy techniques were observed for coffee species differentiation, considering the quality of roasted beans in blends with respect to proportion and type of defects.

Photoacoustic spectroscopy (PAS) is a little explored technique for RG coffee assessments. It was successfully applied to investigate adulterated coffee samples with corn, barley and parchment (inner peel of coffee) (Cesar, Vargas, Lima, Mendes Filho, & Miranda, 1984). Another study demonstrated that it is possible to discriminate organic from non-organic coffees comparing the PAS spectra of the samples (Gordillo-Delgado, Marín, Cortés-Hernández, Mejía-Morales, & García-Salcedo, 2012).

PAS is based on the photoacoustic effect measured when electromagnetic radiation (usually in the infrared wave-range), with a periodic modulation of intensity, is focused on a sample. As a result, light absorption with subsequent periodic heating of the sample is observed. The modulated temperature changes are dependent on the variation of the intensity of the focused light. This periodic heat generation produces acoustic waves in the atmosphere within an enclosed cell containing the sample. In this environment, an ultrasensitive microphone detects these waves and generates the PAS signal, which represents the sample spectrum (Gordillo-Delgado et al., 2012; Michaelian, 2010).

A current limitation of spectroscopic techniques in general is the scattering of light. But such interferences do not occur in PAS since only the light absorbed by the sample is converted into a signal. From an operational point of view, PAS does not require a rigorous sample preparation, and it is a non-destructive analysis (Kinney & Staley, 1982; Michaelian, 2010). PAS provides optical absorption spectra of solids, semi-solids, liquids and gases, and offers the great advantage for analysis of optically opaque samples, which is a limitation of others methods, e.g. for Raman Spectroscopy (Kinney & Staley, 1982). Another positive characteristic is that the photoacoustic signal contains information of surface and inner layers of the samples, which allows the evaluation of materials with compositional gradient, e.g., samples of coffee, since commercial products may contain different species, defects, and even contaminants.

Spectroscopic techniques associated to chemometric methods for multivariate analysis such, as PCA (Principal Component Analysis) and PLS (Partial Least Squares Regression), and variations of this, such as PLS-DA (PLS Discriminant Analysis), have been successfully applied in the past for the analysis of spectral data. The methodologies provided interesting information for monitoring the quality of coffee, assisting in the discrimination of species, cultivars, production lots of coffee, and geographical origin (de Toledo et al., 2017; Ebrahimi-Najafabadi et al., 2012; El-Abassy et al., 2011; Keidel et al., 2010; Moreira & Scarminio, 2013; Reis et al., 2013; Rubayiza & Meurens, 2005; Santos et al., 2012; Wermelinger et al., 2011).

In extension to former FTIR-PAS studies, it is pertinent to consider that slight variations in the Fourier Transform Infrared Photoacoustic spectra profiles probably result from variations in the composition of samples under investigation. With the aim of developing a fast, robust and simple technology and associated tool for quality control of RG coffee, this study investigated the possibility of using FTIR-PAS to the discrimination of blends of coffee considering different coffee species, type and amount of defects, in combination with data analysis using PCA and PLS-DA.

2. Material and methods

2.1. Samples of coffee

Samples of healthy beans of *Coffea arabica* (Arabica) and *Coffea canephora* (Robusta), and 25 blends of defective and healthy beans of Arabica, namely *selections*, were supplied by Instituto Agronômico do Paraná – IAPAR. The coffee beans were harvested in Londrina – Paraná – Brazil: Latitude −23.29, Longitude −51.17; 23° 17′ 34″ S, 51° 10′ 24″ W, humid subtropical climate.

The selections (see Table 1 and Fig. 2 in Dias et al., 2018) differ in the proportion of specific defects and healthy coffee beans. Roasting companies acquire the selections and blend them with healthy beans (namely *basis*) in a specific proportion dependent on the composition of the selection. For example, a selection with large proportion of sour beans, e.g., #15 (see Table 1 in Dias et al., 2018), will be blended with a basis of healthy beans in a low ratio, since sour beans severely depreciates the quality of coffee beverage. It is important to highlight that both Arabica and Robusta coffees can be used as basis in the final blend. Normally the basis is composed by only Arabica coffee or a blend of Arabica and Robusta, and the ratio of species are dependent on the desired standard of quality.

Trained coffee selectors from IAPAR manually classified each selection bean by bean. The selections may contain broken, sour, black and healthy beans, skin and coffee woods (see Table 1 in Dias et al., 2018). The use of these selections, to obtain the sample blends, is an important advantage of this research because the method practiced in the industry was exactly reproduced, making the study authentic and highly relevant to industrial operations. To the best of our knowledge, there is no report describing analysis of such *real* coffee blends, but only essays using samples produced in laboratory, with specific manipulated proportions.