Food Chemistry 255 (2018) 132–138

Contents lists available at ScienceDirect

Food Chemistry

journal homepage: www.elsevier.com/locate/foodchem

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

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ARTICLE INFO

Keywords:
FTIR-PAS
Chemometric methods
Coffee defects
Species of coffee
Blends of coffee

Chemical compounds studied in this article:
Pyruvic acid (PubChem CID: 1060)
Pyridine (PubChem CID: 1049)
Quinic acid (PubChem CID: 6508)
Trigonelline (PubChem CID: 5570)
Caffeine (PubChem CID: 2519)
Chlorogenic acid (PubChem CID: 1794427)
Fructose (PubChem CID: 5984)

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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https://doi.org/10.1016/j.foodchem.2018.02.076
Received 8 November 2017; Received in revised form 8 February 2018; Accepted 13 February 2018
Available online 14 February 2018

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.

In addition to the healthy and whole beans already included into each selection, as listed in the second column of in Table 1 (Dias et al., 2018), each selection was further blended into a base of healthy coffee beans in the proportions of 20% and 40% (w/w) of selection. Three such bases were used: (i) 100% of Arabica coffee, (ii) a mix of Arabica to Robusta in the proportions of 80:20 and (iii) a mix of Arabica to Robusta in the proportions 50:50 (w/w). These blend ratios were chosen based on information provided by coffee producers and roaster technicians, and represents the range most applied in the coffee industry. More than 50% of selections in a blend with a basis is very uncommon. Thus, considering that each of the three bases were blended with each selection at 20% and 40% selection in the final sample, this amounted thus to 150 samples composed of selections and bases. Adding to the analysis the three pure bases and a sample of healthy Robusta coffee, 154 samples were analyzed. Table 2 (see in Dias et al., 2018) provides a detailed description of the final composition of all 154 samples, after combining each section at 20 and 40% with the three bases.

All samples were roasted to a medium degree (Probat Emmerich am Rhein, Germany, model PRG1Z, ERD Gas), corresponding to 17% of weight loss, and between 22 and 26 of luminosity, L^* (Konica Minolta portable colorimeter BC-10). The coffee was ground on a Ditting grinder (Bachenbülach, Switzerland), model KR805, on level/setting 2.

2.2. FTIR-PAS spectroscopy analysis

A Bruker FTIR spectrometer (Billerica, USA), model Tensor 37 coupled to a Gasera photoacoustic detector (Turku, Finland), model PA 301, interfaced with a DSP Module was used to obtain the PAS spectra of samples, in triplicate. A circular metal PAS cell of 9 mm diameter and 5 mm in depth containing the sample of RG coffee was hermetically isolated from the room atmosphere and purged with helium for 1 min before the analysis in order to reduce water vapor and carbon dioxide in the sample chamber. Infrared light was focused on the sample and the PAS signal was detected. The PAS spectrum was obtained from the average of 16 scans, with 4 cm^{-1} resolution in a wavenumber region of 600–4000 cm^{-1}. No sample preparation steps were required. Thirty days elapsed between obtaining the classified selections and the analysis by FTIR-PAS. On the other hand, the total measurement time per sample was no more than 2 min. Before analysis, the PAS signal was calibrated with a polyethylene standard sample. As recommended (Gordillo-Delgado et al., 2012), a PAS signal normalization process to a black body coated reference sample, commonly named as *carbon-black*, was performed for eliminating the influence of the non-uniform intensity of the light source spectrum. Thus, the FTIR-PAS normalized signal was the ratio between the sample PAS signal amplitude and the carbon-black PAS signal amplitude. The resulting signal, which generates the PAS spectrum, is dependent on the composition of the sample because it is directly proportional to the amount of light energy absorbed by the sample at each wavenumber.

2.3. Data analysis

The average (triplicate) of FTIR-PAS measurements was used for multivariate analysis. The 154 spectra (each spectrum is an average from three replicates) and their intensity values at 1763 wavelength values were organized as a 154 × 1763 matrix and processed with MATLAB R2007b. PCA (Principal Component Analysis) and PLS-DA (Partial Least Squares with Discriminant Analysis) were performed by the PLS Toolbox 5.2 from Eigenvector Research.

Principal Component Analysis (PCA) is an unsupervised pattern recognition method that should be employed only for exploratory analysis and is not suited to make predictions (Alves & Valderrama, 2015). In this method, the spectra set was organized in a matrix (**X**), which was decomposed by principal components (PCs) into scores (**T**) and loadings (**P**) matrices (Valderrama, Paiva, Março, & Valderrama, 2016), according to Eq. (1).

$$\mathbf{X} = \mathbf{TP^T} \quad (1)$$

The scores matrix carries information about the samples (lines of **X** matrix), whereas the loadings provide information about variables (columns of **X** matrix). The results of scores and loadings can be graphically interpreted (Valderrama et al., 2016).

Partial Least Squares – Discriminant Analysis (PLS-DA) is a supervised pattern recognition method. In PLS-DA the matrix **X** is related to another matrix, **Y** that contains information about the sample class in binary code 'zero' and 'one' (Barker & Rayens, 2003). For example, consider three classes and, a sample in the second class, the **y** value for this sample is y = 0 1 0. The **X** and **Y** matrices are decomposed simultaneously into scores and loadings. The PCs, orthogonal in PCA, suffer from modifications in PLS-DA method. These modifications take place in order to find the maximum covariance between **X** and **Y** and then the PCs receive the terminology of Latent Variables (LVs) (Geladi & Kowalski, 1986). A regression model is determined based on the scores and loadings from **X** matrix and based on scores from **Y** matrix.

Due to the supervised characteristic of the PLS-DA method, it is possible to make predictions of future samples on the modeled classes. The predicted results from PLS-DA must be 'zero' or 'one'. However, experimentally these values are close to this. A threshold value is calculated between the predicted values while values above this threshold indicate that the sample belongs to the modeled class. On the other hand, predicted values below the threshold limit indicate that the sample does not belong to the modeled class. For threshold estimation, the distribution of the predicted values obtained from a PLS-DA model in the calibration samples is needed to find a threshold value which will best split those classes with the least probability of false classifications of future predictions (Alves & Valderrama, 2015). It is assumed that the predicted values for each class are approximately normally distributed and the calculation is performed by using Bayesian statistics (Pastore et al., 2011).

The optimum PLS-DA model dimension is determined by the minimum root mean square error of cross-validation (RMSECV) for the calibration samples, obtained by the leave one-out or contiguous block procedure.

3. Results and discussion

The PAS spectrum profiles of the samples were similar to the results found in the literature (Gordillo-Delgado et al., 2012). On the other hand, the great similarity among the spectra of samples makes impracticable the interpretation of results without detailed statistical data analysis (see Fig. 1 in Dias et al., 2018).

Based on the PAS spectra acquired, a data matrix of 154 lines (samples) and 850 columns (each normalized PA signal at wavenumber between 600 and 4000 cm^{-1}, with 4 cm^{-1} resolution) was generated. On this matrix, an exploratory analysis was performed by PCA. The first two principal components, PC1 and PC2, accounted for approximately 95% of the variability (Fig. 1).

The scores plot from PC1 *vs.* PC2 revealed similar features of the coffee samples, such as the group of the samples 52 to 64 (highlighted in red, Fig. 1), which are blends composed by 20% of the selection and 80% of the basis 80:20 (Arabica:Robusta). The samples between 126 and 150 (marked in green in Fig. 1) have the percentage of selection (40%) and the basis (50:50, Arabica:Robusta) in common. The three bases, 100% Arabica (151), 80:20 Arabica:Robusta (152), and 50:50 Arabica:Robusta (153), and the sample 100% Robusta (154) were plotted in the same group (green dashed line circle in Fig. 1), but they were vertically discriminated, indicating the significant contribution of PC2 in the differentiation of coffee species.

The more pronounced discrimination among the samples was observed in the scores plot of PC1 against PC4 (Fig. 2), where the variability of both PCs was around 70%.

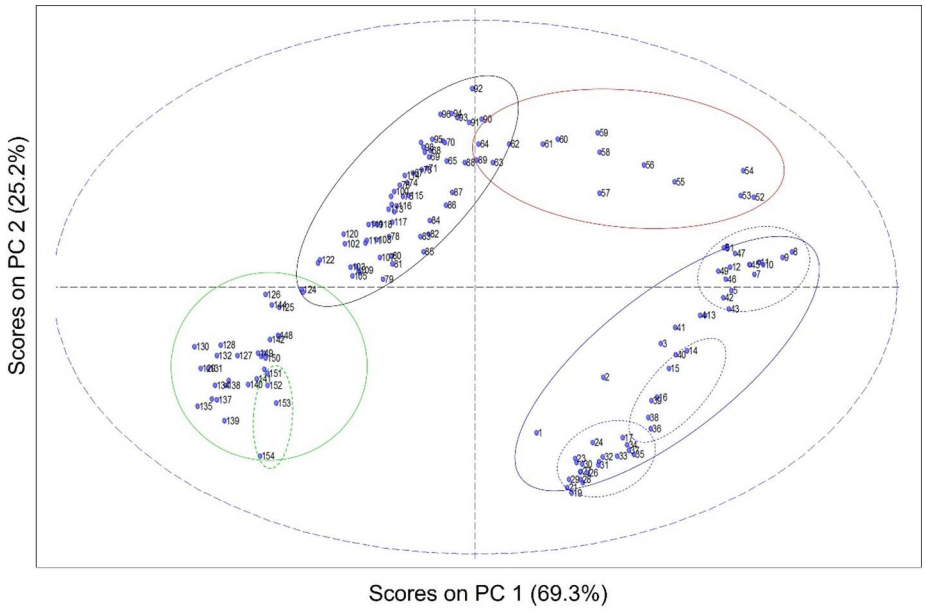

Fig. 1. PCA-scores of normalized PAS signal spectra of coffee samples (PC1 *versus* PC2). Numbers refer to the 154 samples described in Table 2 (Dias et al., 2018).

The samples located in the positive quadrant of PC4 and PC1 (Fig. 2-a) have more intense PAS bands between 3200 and 3450 cm^{-1} (Fig. 2-b and c). The samples in the negative PC1 (Fig. 2-a) have more intense bands between 800 and 1800 cm^{-1}, since the loadings are negative in this region (Fig. 2-b).

The loading plots of PCs 1 and 4 (Fig. 2-b and c) indicate the great contribution of the bands located between 3000 and 3600 cm^{-1} for the discrimination of samples, with similar contribution of each PC. The band at 1067 cm^{-1} is attributed to structures of pyruvic acid, pyridine, and quinic acid, while the band at 3356 cm^{-1} is specific for chlorogenic acids (CQA) (Gordillo-Delgado, et al., 2012). Oscillations in the spectral intensity between 1000 and 1750 cm^{-1} usually involve trigonelline and caffeine alkaloids. The region between 600 and 1000 cm^{-1} was used to discriminate organic from conventional coffees using PCA data analysis (Gordillo-Delgado, et al., 2012). It is important to emphasize that levels of trigonelline, caffeine, CQA, quinic acid, fructose and lipids are dependent on the proportions of coffee species (Alves, Casal, Alves, & Oliveira, 2009; Alves, Dias, Benassi, & Scholz, 2006; Andrade, Leitão, Seabra, Oliveira, & Ferreira, 1998; Campanha, Dias, & Benassi, 2010; Dias et al., 2010; Martín, 1998; Nicolau de Souza, Canuto, Dias, & Benassi, 2010; Speer & Kölling-Speer, 2006) and coffee defects (Franca et al., 2005; Mazzafera, 1999; Oliveira et al., 2006; Vasconcelos, Franca, Glória, & Mendonça, 2007) in a blend.

In addition to the PCA assessments considering all samples, the distribution within each class was also observed, where only the percentage of selection was varied. It allowed evaluating the correlation

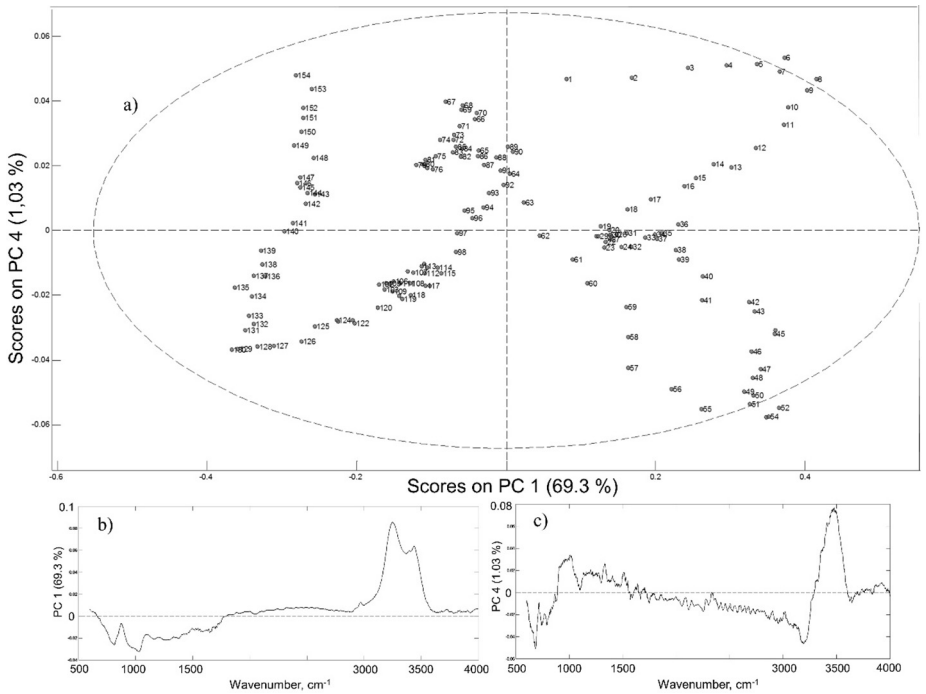

Fig. 2. Score-plot of PCA model (PC1 *vs.* PC4) with normalized FTIR-PAS spectra (a). Numbers refer to 154 samples listed in Table 2 of Dias et al. (2018). Loading-plots of PC1 (b) and PC4 (c).

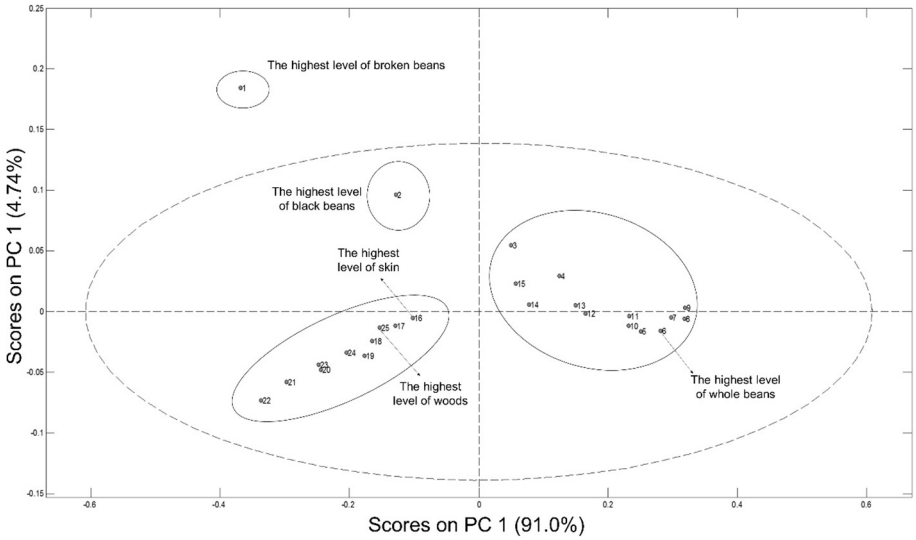

Fig. 3. Scores plots of PCA model (PC1 *vs.* PC2) for class 20A (20% of selection and 80% of basis 100% Arabica). Numbers refer to the coffee blends (Table 2, Dias et al., 2018).

between the composition of selection and the groups found in the score plots, as shown in Fig. 3 for class 20A.

PCA analysis for the 20A group is presented to demonstrate that individual class evaluation is applicable for assessing the behavior of samples when the proportion of selection (defects) varies within a basis. In this case, PC1 and PC2 explained more than 95% of variability (Fig. 3). The sample containing the larger number of broken beans (#1) was distinguished from two other groups and from the sample with the highest ratio of black beans (#2), which was also plotted separately. Other interesting behaviors were observed. The samples with more broken beans (#1) and more whole beans (#6) were plotted on a transverse axis, in different groups. The blends #16 and #25 were classified in the same group. They are samples with the highest level of skin and woods, respectively (Fig. 3). In order to observe the best overview of the influence of each defect in the sample discrimination, the results within each group will be discussed in a forthcoming report as an extension of this work.

In order to build a prediction model, a PLS-DA was developed with six classes, composed by the sample types 20A (samples 1-25), 40A (26-50), 20AR20 (51-75), 40AR40 (76-100), 20AR50 (101-125), 40AR50 (126-150) (Table 2, Dias et al., 2018).

The calibration and validation datasets were composed of 108 samples (18 samples of each sample type) and 48 samples (8 samples of each sample type, respectively). These samples were selected by a specific algorithm in order to obtain representative samples for all classes (Kennard & Stone, 1969).

The optimum PLS-DA model dimensions were determined by the minimum RMSECV for the calibration samples, obtained by the leave-one-out procedure with 108 samples. This procedure results in the choice of six latent variables for mean-centered model development.

The next step was dedicated to outlier identification. Outliers, defined as observations showing some type of difference from the bulk of the data, may occur due to many different reasons as laboratory error, objects from another population or instrument error. In this work, the outliers were identified based on leverage and Q residuals analyses on the calibration and validation samples. Leverage represents how much one sample is distant from the center of the data, and Q residuals represent the unmodeled residuals in spectra (Alves & Valderrama, 2015). According to Fig. 4-a, two calibration samples from type 20A present a high Q residual (on the top). However, these samples present a low leverage. Samples can be considered certainly outliers when they have both high leverage and high Q residuals; the calibration and validation datasets have no outliers since no sample presents simultaneously high leverage and Q residuals values.

The distribution of the estimated class values for both calibration and validation datasets are presented in the Fig. 4 from 'b' until 'g'. For all types of samples, a clear separation between the estimated class values can be observed. The upper dashed line in each plot represents the threshold.

The discrimination of all classes of samples (20A, 40A, 20AR20, 40AR20, 20AR50, and 40AR50) according to the bases used in the blends was achieved by using the PLS-DA models. The agreement between RMSEC, RMSEP and RMSECV values, for all classes, confirms that the number of latent variables was suited, and the model presented neither lack of adjustment nor superposition effect. Root Mean Square Errors, sensitivity and specificity for the classes of PLS-DA model can be found in Table 3 of Dias et al. (2018).

Sensitivity is defined as the model ability to classify the validation samples belonging to a particular class. In this sense, if the model classifies all samples in a given class correctly, then the sensitivity to this class is equal to 1. For the model developed in this study, the sensitivities were 0.857 for the classes 40AR20 and 20AR50. For the classes 20A, 40A, 20AR20 and 40AR50 the sensitivities were 1.000. Based on these results, the model was able to correctly classify 100% of the samples in the classes 20A, 40A, 20AR20 and 40AR50.

The specificity is related to the incorrect prediction of validation samples of other classes in a particular class. Thus, if the model does not present error in predicting any sample, its specificity will be equal to 1. The 20AR20 class presented specificity equal to 1, which means that not a single sample of another classes was classified in the 20AR20 class. The 40A, 40AR20, and 40AR50 classes presented specificity 0.971 due to the prediction of one sample of the other class in their class. The 20A and 20AR50 classes presented specificity 0.941 and 0.912, respectively. This result is due to the prediction of two samples of the other class in the 20A class, and the prediction of three samples of the other class in the 20AR50 class. The 20AR50 class have the lowest specificity parameter, but it is still considered a high value (higher than 0.900) (Table 3, Dias et al., 2018). This class comprises the samples with a basis of 50% of Arabica and 50% of Robusta in blends of 80% of this basis and 20% of each selection, being very similar to the samples with the same basis and different proportion of selection (samples of class 40AR50). Indeed, one sample from the class 40AR50 was predicted as belonging to 20AR50 class (Fig. 4-f).

The PLS-DA model was considered excellent, since only a few samples were misclassified (Fig. 4 b-g), even with the great similarity observed among the spectra (see Fig. 1 in Dias et al., 2018). Moreover, the model was developed in order to simultaneously evaluate the different classes. According to the literature (da Silva, et al., 2014), PLS-

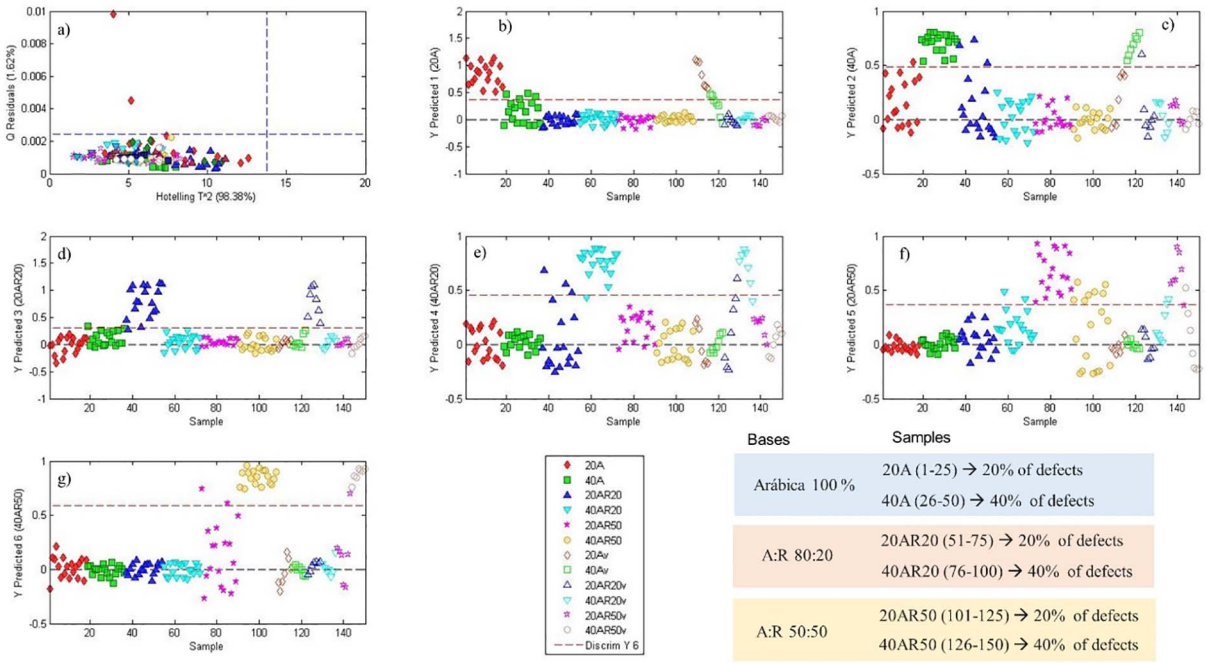

Fig. 4. PLS-DA shows FTIR-PAS spectral analysis of RG coffee blends with different species and defects proportions. Spectral residues (Q) *vs.* leverage (T^2 of Hotelling) for the PLS-DA model (a) and model classes: 20A (b), 40A (c), 20AR20 (d), 40AR20 (e), 20AR50 (f), 40AR50 (g). Sample identification: letter v and empty symbol mean samples of validation. For example, 20Av (empty diamond) is the sample of validation of the class 20A (full diamond). Further information on the samples are in Tables 1 and 2 of Dias et al. (2018).

DA models display more satisfactory results when each class is individually modeled, e.g., the class 20A *versus* another big class containing all samples of the other classes.

The PCA and PLS-DA data analysis demonstrated that the developed methodology based on FTIR-PAS technique provides relevant and sufficient information for a successful discrimination of RG coffee with different proportions of species and different types and ratio of defects. It is important to emphasize that having a large data set is essential to obtaining a statistically reliable PLS-DA model. The sample space must properly cover all characteristics of interest. The PLS-DA model will ensure reliable evaluation of the spectral results only for the previously considered parameters. In this study, the model is ideally valid only for the parameters considered in the samples that originated it, i.e., for the species of coffee and the observed defects, and within the estimated proportion ranges.

4. Conclusion

Optical spectra obtained by infrared spectroscopy with photoacoustic detection (FTIR-PAS) technique proved capable in suppling representative information on the composition of RG coffee with different proportion and type of a series of defects of coffee. The compositional space was chosen such that it covers most of the practical situations, as encountered in the Brazilian market. Successful differentiation was achieved by applying multivariate statistical analysis, here PCA and PLS-DA methods, on FTIR-PAS spectra of all samples. Application of FTIR-PAS for the discrimination of blends with different bases and containing a range of typical defects has shown to be efficient in terms of differentiation, easy and quick to use, and a “green” solution as a quality control tool of roasted and ground coffee.

While the methodology was developed and applied on mixtures of defects as typically encountered in the Brazilian market, it also point at the possibility as developing a more general approach to analyze and quantify the defects in a coffee blend, in general.

Acknowledgement

We acknowledge Science without Borders, a Brazilian government program for students abroad, for the financial support. We also acknowledge the Zurich University of Applied Sciences and the Coffee Excellence Center for financial support and thank Dr. Marco Wellinger, Dr. Samo Smrke, Dr. Christian Adlhart, and Dr. Sebastian Opitz for fruitful discussions.

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