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Using hyperspectral imaging to characterize consistency of coffee brands and their respective roasting classes

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A B S T R A C T

The uniqueness and consistency of commercial food and beverage brands are critically important for their marketability. Thus, it is important to develop quality control tools and measures, so that both companies and consumers can monitor whether a given food product or beverage meets certain quality expectations and/or is consistent when purchased at different times or at different locations. In this study, we characterized the consistency (levels of extractable protein and reducing sugars) of 15 brands of roasted coffee beans, which were obtained from a supermarket at two dates about six months apart. Coffee brands varied markedly in extractable protein and reducing sugar contents between dates, and also within and among roasting classes (light, medium, medium-dark, and dark roasts). We acquired hyperspectral imaging data (selected bands out of 220 narrow spectral bands from 408 nm to 1008 nm) from ground samples of the roasted coffee beans, and reflectance-based classification of roasting classes was associated with fairly low accuracy. We provide evidence that the combination of hyperspectral imaging and a general quality indicator (such as extractable protein content) can be used to monitor brand consistency and quality control. We demonstrated that a non-destructive method, potentially real-time and automated, and quantitative method can be used to monitor the consistency of a highly complex beverage product. We believe the results from this study of brand consistency are not only of relevance to the coffee industry but to a wide range of commercial food and beverage brands.

1. Introduction

Radiometric data, such as reflectance or vibrational profiles, are used as explanatory variables in two types of classifications: 1) Estimation or prediction of the concentration of particular compounds or physical traits along continuous scales. Such classifications include levels of purity of pharmaceutical samples (Amigo and Ravn, 2009; Gowen et al., 2008, 2011; Ravn et al., 2008), and food products (Huang et al., 2014; Lefcout and Kim, 2006; Park et al., 2006; Vargas et al., 2005). 2) To classify food objects with or without particular defects (Gaston et al., 2011; Heitschmidt et al., 2004; Nansen et al., 2014; Singh et al., 2009, 2010; Wang et al., 2010, 2011; Zhang et al., 2015) or food into specific classes (Barbin et al., 2012; Blasco et al., 2003; Cubero et al., 2011; Kamruzzaman et al., 2012). There are several important and comprehensive reviews of applications of hyperspectral imaging in studies of both food quality and food safety (Elmasry et al., 2012; Feng and Sun, 2012; Huang et al., 2014). Thus, there is a widespread appreciation for the potential of automated machine vision systems in food safety and quality control of food and beverage products.

Coffee is one of the most popular beverages in the world (Duarte et al., 2005) with consumption per capita of 4 kg in the US and 5 kg per capita in Europe (http://www.worldmapper.org/posters/worldmapper_1038_coffee_consumption_ver2.pdf). Moreover, it has been estimated that American consumers spend about $21 per week on coffee (http://www.statista.com/topics/1248/coffee-

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market/). Due to national and regional variations in growing conditions and cultivation of *arabica* and *robusta* coffee varieties, there is a considerable diversity in potential sources of green coffee beans. Hyperspectral imaging has been used to discriminate 33 samples of green beans of *arabica* and *robusta* with over 97% classification accuracy (Calvini et al., 2015). In addition, RGB imaging (Red, Green and Blue color) of 120 green bean samples from four color classes (whitish, green, cane green, and bluish-green) were classified with over 99% accuracy (de Oliveira et al., 2016). These studies underscore the potential for reflectance-based classification and quality assessment of coffee samples.

As part of the roasting process, green coffee beans are heated to specific temperatures for varying durations depending on the roast level. The organic compounds that result from roasting of coffee beans have been studied for over 50 years (Rhoades, 1960), and more than 850 substances have been identified from volatile fractions of roasted coffee (Franca et al., 2009; Rocha et al., 2004; Yeretzian et al., 2014). The chemical changes during the roasting process are associated with Maillard and Strecker reactions, amino acid and protein degradations, and changes to profiles of polysaccharides and trigonelline and chlorogenic acids (De Maria et al., 1996; Duarte et al., 2005; Montavon et al., 2003; van Boekel, 2006). Yeretzian et al. (2014) studied the chemical changes during 0–30 min after roasting, and it highlighted the complexity of the chemical and biochemical reactions associated with roasting of coffee beans.

Roasted coffee beans are commercialized under general roasting classes, such as light, medium, medium-dark, and dark roasts. Many supermarkets offer large bins with a wide variety of bulk roasted coffee brands within each of these roasting classes. As described by Franca et al. (2009), industry evaluation of both green and roasted coffee beans is based on reflectance and/or visual inspection. For instance, the National Coffee Association of the USA (http://www.ncausa.org/About-Coffee/Coffee-Roasts-Guide) refers to: 1) light roasts as “light brown in color”, 2) medium roasts as “medium brown in color”, 3) medium dark roasts as “dark in color”, and 4) dark roasts as “shiny black beans”.

The main purpose of this study was to investigate the consistency of samples a highly complex and valuable beverage, coffee, which is commercialized under a wide variety of brands and roasting classes. In particular, we intended to demonstrate the potential of classification of hyperspectral imaging data as a non-destructive, potentially real-time and automated (quantitative) analytical method to determine the consistency of ground coffee. We conducted extractable protein and reducing sugar content analyses of 15 coffee brands, which were acquired at two time points (30 samples). These two chemical traits were chosen as consistency indicators, as they provide broad and fairly non-specific information about the composition of food and beverages. In addition, we acquired hyperspectral imaging data (220 narrow spectral bands from 408 nm to 1008 nm) from all combinations of coffee brand and date of sampling. The specific objectives were: 1) determine the consistency of extractable protein and reducing sugar contents in commercial coffee brands at two time points, 2) compare extractable protein and reducing sugar contents across roasting classes (light, medium, medium-dark, and dark roasts), 3) use hyperspectral imaging data to classify coffee samples into existing roasting classes, and 4) provide evidence that commercial coffee brands can be classified accurately based on hyperspectral imaging data, if a quantifiable variable, such as extractable protein content, is used to divide coffee brands into discrete classes. Due to the importance of consistency of commercial brands, we believe this study is of considerable relevance to a wide range of food and beverage products.

2. Materials and methods

2.1. Coffee samples

On April 7th and October 29th, 2015, we collected samples from 15 commercial brands of coffee from a supermarket in Davis, California (30 samples in total). On both dates, we sampled the same coffees, and they represented the following roasting classes: “light roast” (1 brand), “medium roast” (7 brands), “medium-dark roast” (4 brands), and “dark roast” (3 brands). Although we did not have any means to quantify the relative differences among the blends/roasts, we used this information as a potential classifier of the coffee samples, as roasting class is important in the commercialization of brands of roasted coffee. Subsamples of 10 g roasted coffee beans were ground for 2 min with a coffee grinder (Mr Coffee, www.walmart.com), which was cleaned thoroughly between samples. Immediately after grinding, coffee samples were transferred to sealed bags and placed in a −8 °C freezer. Ground coffee samples were thawed for approximately 20 min before being subjected to hyperspectral imaging and then transferred back to a −8 °C freezer. Hyperspectral imaging was completed in about 60 min. The ground coffee samples were kept in the freezer until being subjected to analyses of extractable protein and reducing sugar content.

2.2. Measurement of extractable protein and reducing sugar content

To obtain quantitative data on the consistency, we quantified the total extractable protein and reducing sugar contents of all coffee samples. It is important to highlight that these two indicators are unlikely valid indicators of the actual quality of the coffee samples, but they provide fairly broad and non-specific information and were therefore considered valid indicators of consistency of the coffee samples. It is also important to highlight that analytical chemistry can be time consuming, expensive, and require special equipment and highly trained personnel. Thus, it is highly desirable to rely on analytical methods that are both well-described, easy and inexpensive. Even if such analytical methods are not directly linked to quality of a food or beverage product, they may be highly preferable due time constraints in large scale manufacturing, repeatability, and cost concerns. Ground roasted coffee was extracted using a hydrothermal method described previously (Conde and Mussatto, 2016). For each coffee sample, 2 g of ground roasted coffee beans were combined with 40 mL of DI water in a pressure tube (Ace Glass, Vineland, NJ). Mixtures were heated at 121 °C for 20 min in an autoclave. Mixtures were then transferred to centrifuge tubes and separated via centrifugation at 2500 × g for 10 min. Supernatants were filtered through PTFE syringe filters (0.2 μm pore size, Thermo Fisher Scientific, Waltham, MA) and stored at −20 °C until further use. The protein content in extracts was determined using the Bradford technique (Bradford, 1976). Reducing sugar content in extracts was measured using a reducing sugar assay described previously (Allison et al., 2016). Bovine serum albumin (BSA) (Thermo Fisher Scientific) and glucose were used as standards for the Bradford and reducing sugar assays, respectively. Triplicate extractable protein and reducing sugar content measurements were made on each extract. The measured extractable protein and reducing sugar concentrations in each extract were used in conjunction with the dry weight of the extracted coffee sample and the total extract volume to calculate the mass of extractable compounds per unit of dry roasted coffee mass.

Using PC-SAS 9.3 (SAS Institute, NC), we conducted pairwise *t*-test (proc ttest) of extractable protein and reducing sugar contents in coffee samples from the two sampling days, and tukey analysis of variance (proc anova with option = tukey) was used to compare average extractable protein and reducing sugar contents among roasting classes.

2.3. Hyperspectral imaging

We used a hyperspectral spectral camera (PIKA II, Resonon Inc., Bozeman, MT) with the lens mounted 15 cm above coffee samples placed in a small glass Petri dish (Fig. 2a). Hyperspectral reflectance data were acquired with a spatial resolution of 15 by 10 pixels per mm^2. The main specifications of the spectral camera are as follows: interface, IEEE 1394b Firewire connection; 12 bit digital output, and angular field of view of 7°. The objective lens had a 35 mm focal length with maximum aperture of F1.4, optimized for the near-infrared and visible near-infrared spectra. Hyperspectral images were collected with artificial lighting from 15 W, 12 V LEDs mounted on either side of the lens. A piece of white teflon (K-Mac Plastics, MI, USA) was used for white calibration, and "relative reflectance" was determined as the proportional reflectance compared to reflectance obtained from teflon (relative reflectance values ranged between 0 and 1).

2.4. Preprocessing of hyperspectral imaging data

A total of six replicated images were acquired from each combination of coffee brand (15 brands) and sampling dates (two dates), so that a total of 180 hyperspectral images were acquired. Regarding spectral data processing, the original spectral data consisted of 240 spectral bands from 383 nm to 1036 nm (spectral resolution = 2.1 nm), but we discarded the 10 spectral bands at either end of the examined spectrum due to high levels of noise, so that only 220 narrow spectral bands from 408 nm to 1008 nm were included. *A priori* analyses of spectral binning was performed, in which we, similar to Zhang et al. (2015), performed the following binnings of spectral bands: 1) (averaging the original 220 spectral bands into 110 bands), 2) (averaging the original 220 spectral bands into 73 bands), 3) (averaging the original 220 spectral bands into 54 bands), 4) (averaging the original 220 spectral bands into 44 bands), and 5) (averaging the original 220 spectral bands into 36 bands). However, all binnings of spectral bands yielded lower classification accuracies than when using the original spectral bands, so we decided to use the original spectral bands as explanatory variables. Similar to published studies (Nansen et al., 2013; Zhang et al., 2015), a radiometric filter was used to only include pixels that had relative reflectance values within certain ranges in two specific spectral bands [599 nm (R599) and 880 nm (R880)]: if R599 < 0.09 and R880 > 0.20.

2.5. Classification and analyses of hyperspectral imaging data

All spectral data were processed and analyzed in PC-SAS 9.3 (SAS Institute, NC) and were based on an average reflectance profile derived from each hyperspectral image cube. Linear Discriminant Analyses (LDA) (Fisher, 1936) was used to classify coffee samples into discrete classes (either the four roasting classes or three classes identified based on extractable protein content). Initially, we conducted a forward stepwise LDA (proc stepwise) to only include spectral bands that contributed significantly to each classification. Classification accuracy of each LDA was based on independent validation, as the original average reflectance profiles had been divided randomly into three groups and using 67% as training data and 33% independent validation data, and each third was used as validation data set. This validation procedure was repeated three times (nine validations). We conducted partial least square (PLS) (Wold, 1966) to predict extractable protein or reducing sugar contents in coffee samples based on reflectance values in spectral bands from 408 nm to 1008 nm as explanatory variables.

3. Results and discussion

3.1. Brand consistency based on extractable protein and reducing sugar contents

As broad and non-specific measurements of brand consistency, we quantified total average levels of extractable protein and reducing sugar. Regarding total extractable protein content, we found that (Fig. 1a): 1) across all 15 brands, extractable protein content was consistently higher in samples from October 29 compared to samples from the same coffee brands sampled about six months earlier ($df = 14$, t-value = 8.07, P-value < 0.001), 2) there was no significant difference in average total extractable protein content among roasting classes ($df = 3{,}29$, F-value = 0.29, P-value = 0.83). We conducted a correlation analysis (Fig. 1c) between the two sampling dates, and there was no significant association ($P > 0.05$). In other words, coffee brands did not show consistently high or low extractable protein contents for both sampling dates. Regarding reducing sugar content, we found (Fig. 1b): 1) there was no significant difference between sampling dates ($df = 14$, t-value = 1.34, P-value = 0.201), 2) marked variation both within and among roasting classes, and 3) there was no significant difference in average total extractable reducing sugar content among roasting classes ($df = 3{,}29$, F-value = 1.92, P-value = 0.15). We conducted a correlation analysis (Fig. 1c) between the two sampling dates, and coffee brands did not show consistently high or low reducing sugar contents for both sampling dates ($P > 0.05$).

3.2. Brand consistency based on reflectance profiles

Plotting average reflectance profiles of the 15 coffee brands showed that (Fig. 2a): the brands had almost identical reflectance in spectral bands from 407 to 500 nm, 2) all averages followed the same overall profile with a maximum reflectance value near 950 nm, 3) as expected, dark roasted brands had lower average reflectance, and 4) light roasted samples were not associated with the highest average reflectance. We also examined the relative consistency of average reflectance profiles of each of the 15 coffee brands, and a 5% "difference" (either below 0.95 or above 1.05) may be used as a threshold of consistency between sampling dates (dashed lines in Fig. 2b). Only five of the 15 coffee brands had difference values below 5% for the entire range of the examined spectrum from 407 to 1010 nm. In other words, there was considerable inconsistency in average reflectance profiles for the various coffee brands, and the inconsistency varied among brands in terms of which portion of the spectrum was most pronounced and whether there was an increase or decrease in average reflectance between sampling dates. Overall, it appeared that all roasting classes showed similar levels of inconsistency.

3.3. Reflectance based classification of coffee samples

We used partial least square (PLS) analysis to predict extractable protein and reducing sugar contents based on average reflectance profiles. Reducing sugar content was poorly predicted, but we found a strongly significant correlation between observed and

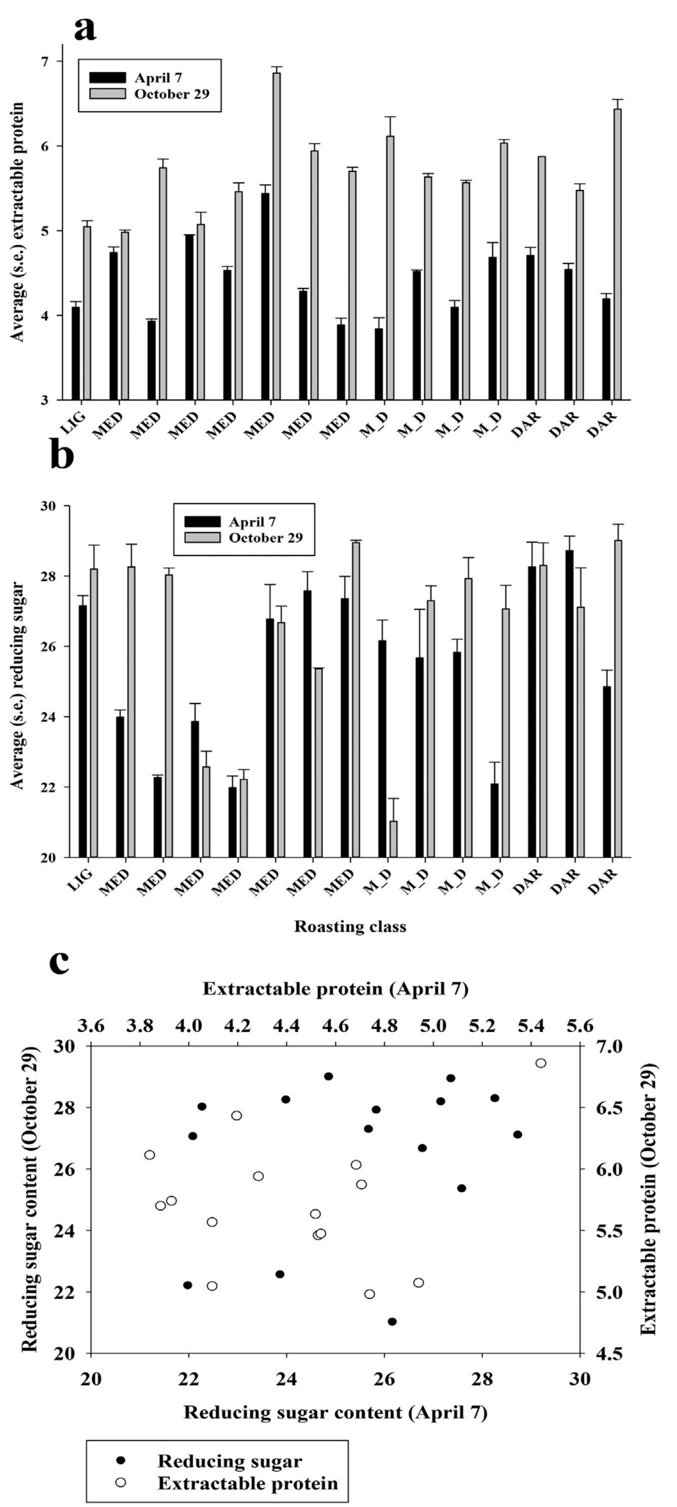

Fig. 1. Average total extractable protein (mg BSA equivalent/g dry weight) (**a**) and reducing sugar (mg glucose equivalent/g dry weight) (**b**) contents of 15 coffee brands collected at two sampling dates. The coffee brands belonged to the following roasting classes: "light roast" (1 brand), "medium roast" (7 brands), "medium-dark roast" (4 brands), and "dark roast" (3 brands). Correlations between total extractable protein and reducing sugar on the two sampling dates (**c**).

predicted (based on reflectance) extractable protein content (adjusted $R^2 = 0.76$, df $= 2,29 =$ F-value $= 91.85$, P-value < 0.001) (Fig. 3a). This result suggested that, although coffee samples appeared to show considerable inconsistency between sampling dates, quantitative variables, such as extractable protein content of coffee samples, can be determined fairly accurately based on reflectance values in selected spectral bands.

We developed classifications of coffee samples based on linear discriminant analysis (LDA), and classification accuracies were based on using a third of the data set as independent validation. In separate analyses, we classified the 180 coffee samples based on roasting class (four classes) and coffee brand for each sampling date (30 classes) and obtained classification accuracies which varied considerably among roasting classes (Fig. 4a). Specifically, brands in the dark roasting class were classified with about 98% accuracy, light roast classification was associated with about 45% accuracy, and medium and medium-dark coffee brands were associated with about 65% accuracy.

Based on extractable protein content, we divided the 30 coffee samples into three discrete classes: low, medium, and high (Fig. 3b). This grouping was used as classifier in a LDA of the coffee samples and yielded classification accuracies between 77% and 90% for the three groups (Fig. 4b).

4. Concluding remarks

The uniqueness and consistency of commercial brands of food products and beverages are critically important for their marketability. Thus, it is important to develop quality control tools and measures, so that companies and consumers can monitor whether a given food product or beverage meets certain quality expectations. The use of hyperspectral imaging technologies in the food industry provides opportunities for improving food safety and quality control (Feng and Sun, 2012; Gowen et al., 2007; Huang et al., 2014; Van Loo et al., 2012; Wang and Paliwal, 2007). However, there has been much less research into how the same technology can be used to characterize and quantify the consistency of commercial food and beverage brands.

If it is considered reasonable to assume that reflectance features can be used to accurately classify coffee brands (this hypothesis would be supported by the many applications of reflectance based classification of food products), then the findings in this study suggest that the obtained samples were associated with considerable inconsistency between sample dates and within roasting classes. Thus, this study was designed to propose an alternative classification of coffee brands. Despite the inconsistency in extractable protein and reducing sugar levels within and between brands, coffee samples may still be classified reliably according to reflectance based features. We found coffee samples from commercial brands to vary considerably between dates of sampling and also within established roasting classes. This variation is likely attributed to a complex of factors, including: 1) many and highly variable sources of green coffee beans, 2) the complex chemical processes occurring in response to roasting, and 3) the fact that there is acknowledged levels of subjectivity involved in the evaluation process of roasting classes and in quality of green beans. Due to the many factors affecting the quality of roasted coffee beans, it was considered a challenging model system for the development of a reflectance-based classification. Despite the inherent stochastic variation among coffee samples, we demonstrated that: 1) extractable protein content can be predicted based on reflectance data, and 2) division of coffee samples based on extractable protein content (low, medium, or high) enabled development of an accurate classification of coffee samples. We are not necessarily suggesting that extractable protein is the most suitable variable for grouping of coffee samples (as other quantifiable variables may be more related to the quality of roasted coffee beans). In addition, we are not aware of any published studies showing clear relationships

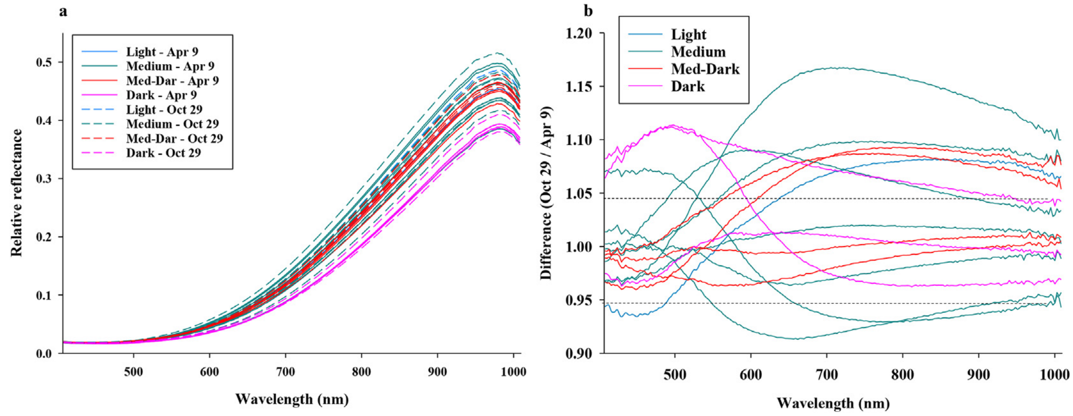

Fig. 2. Average reflectance profiles (407–1008 nm) of roasting classes at two sampling dates, visualized either as relative reflectance (**a**) or as difference between sampling dates (**b**).

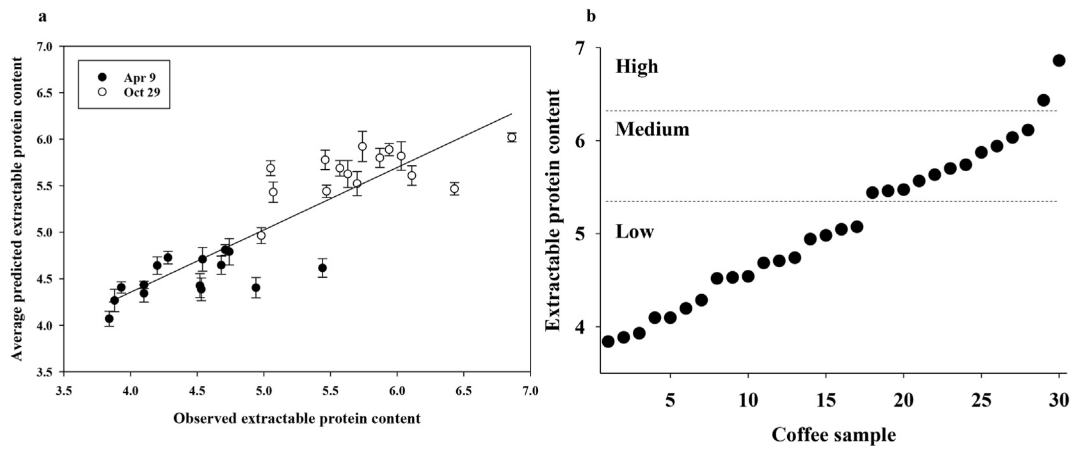

Fig. 3. Partial least square analysis of reflectance values in selected spectral bands to predict extractable protein content (mg BSA equivalent/g dry weight) in coffee brands collected at two sampling dates (**a**). Ascending ranking of coffee samples and subsequent division into three classes (low, medium, and high) based on total extractable protein content (**b**).

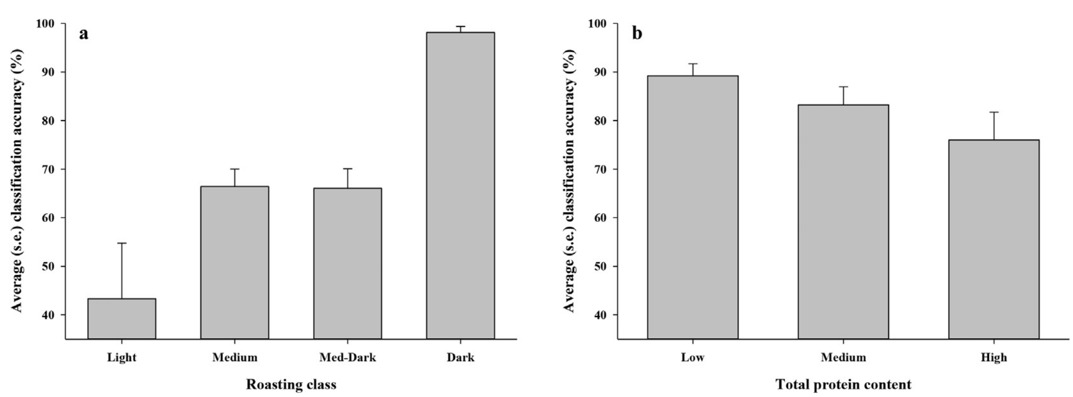

Fig. 4. Classification accuracies of linear discriminant analyses (LDA) with reflectance values in selected spectral bands to classify coffee samples into roasting classes (**a**) and according to three classes based on total extractable protein content (see Fig. 3b) (**b**).

between either reducing sugar or extractable protein contents and actual quality of coffee samples. However, we argue that it seems unlikely that the quality of coffee samples was indeed consistent between sampling days, when both reducing sugar or extractable protein contents (and also reflectance data) varied markedly. The results emphasize the potential of developing a classification system for roasted coffee beans, if it is based on dividing coffee samples into discrete classes according to a quantifiable variable. Furthermore, we demonstrated that such quantifiable variables may be predicted accurately based on reflectance features, and that enables deployment of automated machine vision technologies. As a follow-up to this study, it would be important to screen different quality traits to examine not only their relationship with reflectance data but also their possible association with coffee quality.

We believe that the results from this study are not only of relevance to the coffee industry but to a wide range of commercial food and beverage brands.

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