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# Near-infrared spectroscopy as a green technology to monitor coffee roasting

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#### Abstract:

Wet chemistry methods are traditionally used to evaluate the quality of a coffee beverage and its chemical characteristics. These old methods need to be replaced with more rapid, objective, and simple analytical methods for routine analysis. Near-infrared spectroscopy is an increasingly popular technique for nondestructive quality evaluation called a green technology.

Our study aimed to apply near-infrared spectroscopy to evaluate the quality of coffee samples of different origin (Brazil, Guatemala, Peru, and Congo). Particularly, we analyzed the roasting time and its effect on the quality of coffee. The colorimetric method determined a relation between the coffee color and the time of roasting. Partial least squares regression analysis assessed a possibility of predicting the roasting conditions from the near-infrared spectra.

The regression results confirmed the possibility of applying near-infrared spectra to estimate the roasting conditions. The correlation between the spectra and the roasting time had  $R^2$  values of 0.96 and 0.95 for calibration and validation, respectively. The root mean square errors of prediction were low -0.92 and 1.05 for calibration and validation, respectively. We also found a linear relation between the spectra and the roasting power. The quality of the models differed depending on the coffee origin and sub-region. All the coffee samples showed a good correlation between the spectra and the brightness ( $L^*$  parameter), with  $R^2$  values of 0.96 and 0.95 for the calibration and validation curves, respectively.

According to the results, near-infrared spectroscopy can be used together with the chemometric analysis as a green technology to assess the quality of coffee.

Keywords: Spectroscopy, near-infrared spectroscopy, coffee, roasting, partial least squares analysis

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# INTRODUCTION

Near-infrared spectroscopy (NIRS) is an increasingly popular technique used for non-destructive quality evaluation in a variety of industries, including the food, agricultural, pharmaceutical, and wood industries [1–3]. It ensures rapid and easy measurements without the need for multiple chemical reagents. Recent NIRS methods include online measurement, portable measurement, and imaging analysis [4–6]. NIRS is continuously expanding its uses in food analysis and becoming an important tool for food quality control.

The quality of coffee as a beverage is determined by multiple factors such as the production system, geographical origin, chemical composition of roasted beans, and final beverage characteristics. Raw coffee beans contain a wide range of chemical compounds which interact amongst themselves at all stages of coffee roasting, resulting in greatly diverse final products [7–9]. For instance, the caffeine content, which has a significant effect on the final quality of coffee products, needs to be determined fast and reliably by analytical techniques.

Wet chemistry methods are traditionally used to evaluate coffee quality and chemical characteristics, but these methods are destructive and time-consuming. Therefore, it is in scientific interests to find rapid, more objective, and simpler analytical methods for routine coffee analysis to replace the old methods.

Recent research has shown that spectroscopy in nearinfrared (NIR) and mid-infrared (MIR) radiation is useful in coffee analysis [10–20]. Infrared spectroscopy (especially NIRS) coupled with chemometrics has been proposed as an analytical method to determine the degree of coffee roasting, adulterants in ground coffee, and sensory attributes [17, 18, 21]. It is also used to distinguish between robusta and arabica varieties,

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discriminate coffee based on origin, and predict its chemical composition [15, 20, 22–24].

The growing global demand for specialty coffee increases the need for improved coffee quality assessment. For this reason, Tolessa *et al.* proposed NIR spectroscopy to predict specialty coffee quality [13]. They examined the NIR spectra of 86 green Arabica bean samples of various quality. To create a model that correlates spectral data to cupping score data, they applied the partial least squares (PLS) regression method. The high correlation coefficient between the measured and predicted cupping scores ( $R^2$ -values of 90, 90,78, 72 and 72) indicate that NIR spectroscopy coupled with chemometric analysis could be a promising tool for fast and accurate prediction of coffee quality and for classifying green coffee beans into different specialty grades.

The sensory analysis of espresso coffee with the attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR) was proposed by Belchior et al. [10]. The authors evaluated the potential of ATR-FTIR and chemometrics in discriminating espresso coffees with different sensory characteristics reported by a panel of coffee tasters. They performed partial least-squares discriminant analysis (PLS-DA) based on spectroscopic data to classify the coffee their samples according to sensory qualities, demonstrating the potential of FTIR and chemometric analysis in assessing coffee quality.

In another study, Magalhaes *et al.* proposed FT-NIR spectroscopy and PLS regression as a non-destructive and rapid tool to assess the content of three main phenolics (caffeic acid, (+)-catechin, and chlorogenic acid) and methylxanthines (caffeine, theobromine, and theophylline) in spent coffee grounds [11]. The best PLS model was obtained for caffeine content (0.95) followed by caffeic acid (0.92), (+)-catechin (0.88), theophylline (0.84), and chlorogenic acid (0.71), indicating FT-NIR spectroscopy as a suitable technique to screen spent coffee grounds.

Mees *et al.* identified coffee leaves using FT-NIR spectroscopy and soft independent modelling by class analogy (SIMCA) [12]. In particular, they investigated nine taxa of *Coffea* leaves harvested over nine years in a tropical greenhouse of the Meise Botanic Garden (Belgium). The FT-NIR coupled with SIMCA allowed the authors to discriminate the spectral profile by taxon, aging stage, and harvest period with a correct classification rate of 90, 100, and 90%, respectively.

NIRS, PLS, and variable selection were used by Ribeiro *et al.* to predict concentrations of a wide range of compounds in raw coffee beans [15]. The authors proposed NIR spectroscopy coupled with chemometrics as a low-cost, rapid, and eco-friendly method in both off-line and on-line analyses of coffee beans and coffee beverages. The obtained values of root mean square error of prediction (RMSEP) (0.08, 0.07 and 0.27) and  $r_{cy}$  (0.98, 0.96, and 0.96) showed linear relations of PLS models for quantifying caffeine, trigonelline, and 5-caffeoylquinic acid, respectively.

Near-infrared spectroscopy was used by Macedo *et al.* to evaluate the chemical properties of intact green coffee beans based on PLS regression models [25]. The highest determination coefficients obtained for the samples in the validation set were 0.810, 0.516, 0.694, and 0.781 for moisture, soluble solids, total sugar, and reducing sugars, respectively. These results indicate that the NIR technology can be applied routinely to predict the chemical properties of green coffee.

In another study, Baqueta *et al.* investigated the use of NIR spectroscopy in conjunction with the PLS approach to identify the sensory properties of coffee [21]. The coffee samples varied in species, production region, variety, drying conditions, transit, postharvest procedure, storage times, coffee blend, coffee composition, and roasting process. The performance of PLS models was verified with the following merit parameters: sensitivity, accuracy, linearity, residual prediction deviation, fit, quantification, and detection limits. Since all the sensory qualities were predicted with acceptable values compatible with the merit criteria, the created models were suitable for quantifying, detecting, differentiating, and predicting the sensory features of coffee samples.

Kyaw *et al.* reported encouraging findings about utilizing NIR spectroscopy to forecast the moisture content of ground unroasted coffee beans [26]. The spectral data processed with second derivative and Kubelka-Munk (K/S) data yielded good accuracy for moisture prediction (r = 0.87 and accuracy = 99%).

In view of the above, we aimed to develop a simple, rapid, and accurate method for evaluating the quality of coffee samples by NIR spectroscopy, especially to investigate changes in the coffee spectra during roasting.

# STUDY OBJECTS AND METHODS

**Samples.** Our study objects were arabica coffee samples roasted by the Cafe Creator in Poznań, Poland. The coffee samples were divided into four groups based on their origin, namely Brazil, Guatemala, Peru, and Congo. Their roasting parameters included the roaster power and roasting time (Table 1).

**Color measurements.** The color of 41 samples of coffee beans was measured by the  $L^* a^* b^*$  method using a Konica Minolta Chroma Meter CR-310 trichromatic colorimeter. Each sample was measured 10 times. Before the measurements, the device was calibrated against a white standard with the following parameters: Y = 93.00, x = 0.3170, y = 0.3330. The entire analysis was carried out using a D65 light source, i.e. the daylight phase and the CIE  $L^* a^* b^*$  color system.

**Near-infrared (NIR) measurements.** NIR spectra were performed on a MPA/FT-NIR spectrometer (Bruker). Single beam spectra of the coffee samples were collected and rationed against the background of air. For each sample, the NIR spectra were recorded from 12500 to 400 cm<sup>-1</sup> by co-adding 16 interferograms at a resolution of 4 cm<sup>-1</sup>. Each sample was measured five

Table 1	1 Roasting	parameters	of coffee	samples
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Origin	Power of the roaster, %	Roasting time, min
Brazil	Green	-
	75	8, 10, 12, 13
	80	8, 10, 12
	95	8, 10, 12
Guatemala	Green	-
	75	8, 10, 12, 15
	80	8, 10, 12, 14
	95	8, 10, 12, 13
Peru	Green	-
	75	8, 10, 12, 14
	80	8, 10, 12, 14
	95	8, 10, 12, 14
Congo	Green	-
	80	8, 10, 12



**Figure 1** Absorption spectra of ground coffee in near-infrared region (12500–4000 cm<sup>-1</sup>)

times. The coffee was ground in an electric grinder for measurements. Between the measurements, the samples were mixed in order to obtain reliable results. The measurements were registered in the OPUS software (Bruker, USA).

**Partial Least Squares (PLS) regression.** The PLS regression method was used to determine relations between the spectra and the roasting time. Independent variables (X) were the NIR spectra and dependent variables (Y) were the color parameter or the roasting time. Full cross-validation was applied to the regression model. The regression models were evaluated using the adjusted  $R^2$  and the root mean-square error of cross-validation. The quality models were evaluated by the ratio of the standard deviation of reference data to the root mean-square error of prediction, or the ratio of performance to deviation. The PLS analysis was carried out using the Unscrambler X software (CAMO, Oslo, Norway).

#### **RESULTS AND DISCUSSION**

**Color measurements.** Table 2 shows the color measurements of coffee beans in the  $L^*$ ,  $a^*$ ,  $b^*$  system.

The  $L^*$  parameter is responsible for the brightness of color in the tristimulus model. The higher it is, the greater the brightness of the tested sample. Among the coffees under study, the green coffee beans from Peru had the highest  $L^*$  value, i.e., the highest brightness. The Congo coffee, which was roasted at the power of 80% for 12 min, had the lowest  $L^*$  parameter, i.e., the lowest brightness. All the samples had positive  $a^*$  and  $b^*$  values, with their shades varying between red and yellow.

As we can see in Table 2, the green coffee beans showed the greatest brightness, followed by the samples roasted for 8 min. With the increasing degree of roasting, the color of coffee beans became darker, which is consistent with literature [27, 28].

Spectral characteristics of coffee samples. Figure 1 shows the absorption spectra of the coffees from Brazil, Congo, Guatemala, and Peru roasted for 12 min (80% roasting power). The spectral range was recorded throughout the region of 12 500-4000 cm<sup>-1</sup>. The most intense absorption bands were recorded in the range of 8230-4440 cm<sup>-1</sup>. The spectra were characterized by seven bands with maximum absorption at 8238, 6819, 5800, 5700, 5100, 4700, and 4440 cm<sup>-1</sup>. These bands corresponded to the C-H, N-H, and O-H vibrations [29]. The spectral range of 4545–4000 cm<sup>-1</sup> corresponded to the C-H stretching vibrations. The bands in the region of 5000-4545 cm<sup>-1</sup> were assigned to the combination of the N-H and O-H stretching vibrations. The range of 6060–5555 cm<sup>-1</sup> corresponded to the first tone of the C-H stretching vibration. In the 7142–6666 cm<sup>-1</sup> region, it was associated with the first shade of the N-H and O-H stretching vibrations, while the absorption band in the 7692-7142 cm<sup>-1</sup> range was derived from the C-H stretching vibrations. The band in the region of 9090-8163 cm<sup>-1</sup> originated from the second tone of the C-H stretching vibrations [30]. Specific chemical compounds can be described with the following wavenumbers: caffeine (8865, 7704, 5981, 5794, and 5171 cm<sup>-1</sup>), trigonelline (8865 cm<sup>-1</sup>), chlorogenic acid (6770, 5794, 5171, and 4699 cm<sup>-1</sup>), lipids (6770, 5794, 5171, and 4699 cm<sup>-1</sup>), hydrocarbons (6770, 5171, and 4699 cm<sup>-1</sup>), sucrose (5794, 5405, and 5171 cm<sup>-1</sup>), proteins and amino acids (5171 cm<sup>-1</sup>), and water (5171 cm<sup>-1</sup>) [9, 14, 31]. Table 3 presents the origin of the bonds occurring at the given wavenumbers for the tested coffee beans.

**Coffee roasting.** Many physical and chemical changes take place during coffee roasting. The method of roasting depends on the origin of coffee beans and consumer preferences. Heavily roasted coffee has a lower nutritional value than light coffee [32].

Numerous efforts have already been made to use NIR spectroscopy as an alternative technique to determine coffee quality during roasting and analyze its chemical composition. According to Ribeiro *et al.*, NIR spectroscopy can be used to determine the relationship

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Tabl	le 2	Col	or	measur	rements	s of	green	and	roasted	coffee	beans
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Guatemala (green beans)         -         -         51.670.40.200         0.870.1.20         11.700.40.141           Guatemala (roasted beans)         95         8         45.440.40.163         5.980.40.057         12.650.40.013           12         38.050.40.099         3.520.40.0040         9.810.40.177         12.650.40.013           12         38.050.40.0318         3.210.40.0042         4.760.40.086           80         45.4580.40.255         6.000.40.22         4.760.40.086           10         42.460.40.283         5.300.40.106         9.980.40.131           12         39.720.40.191         4.150.40077         7.380.40.025           14         36.770.40.282         3.230.40.077         4.550.40.085           75         8         48.120.40.184         6.280.40.163         14.470.40.134           10         43.210.40.269         5.600.40.106         10.490.40.185           12         40.620.40.184         4.570.40.0064         4.160.40.012           15         36.460.40.141         3.300.40.064         4.160.40.014           12         38.060.40.014         3.700.40.014         4.160.40.0234           14         13.660.40.0157         1.800.40.064         5.270.40.049           15         3.440	Origin	Power of the roaster, %	Roasting time, min	L* average	<i>b</i> * average	a* average
Guatemala (roasted beans)         95         8         45 440 + 0.163         5 980 + 0.077         12.650 + 0.013           10         42 410 + 0.233         5 240 + 0.064         9.810 + 0.177           12         38.005 ± 0.099         3.550 ± 0.099         6.250 ± 0.085           13         36.390 ± 0.318         3.210 ± 0.042         4.760 ± 0.086           10         42.460 ± 0.283         5.300 ± 0.109         9.80 ± 0.163           12         39.720 ± 0.191         4.150 ± 0.042         4.500 ± 0.085           12         39.720 ± 0.191         4.150 ± 0.077         7.380 ± 0.055           14         36.770 ± 0.283         3.230 ± 0.077         4.550 ± 0.085           75         8         48.120 ± 0.184         6.280 ± 0.163         14.470 ± 0.134           10         43.210 ± 0.269         5.600 ± 0.165         12.840 ± 0.078           75         8         48.120 ± 0.184         6.280 ± 0.163         14.400 ± 0.141           10         3.240 ± 0.025         5.600 ± 0.064         12.840 ± 0.078         12.840 ± 0.078         12.840 ± 0.078           Peru (green beans)         -         -         5.3440 ± 0.042         0.880 ± 0.057         12.840 ± 0.071           Peru (roasted beans)         95         8	Guatemala (green beans)	_	_	$51.670 \pm 0.200$	$0.870 \pm 0.120$	$11.700 \pm 0.141$
Image: Provide the set of the se	Guatemala (roasted beans)	95	8	$45.440 \pm 0.163$	$5.980 \pm 0.057$	$12.650 \pm 0.013$
12         38.050 ± 0.099         3.550 ± 0.099         6.250 ± 0.085           13         36.390 ± 0.318         3.210 ± 0.042         4.760 ± 0.086           10         42.460 ± 0.233         5.300 ± 0.106         9.980 ± 0.163           12         39.720 ± 0.191         4.150 ± 0.077         7.380 ± 0.205           14         35.670 ± 0.282         3.230 ± 0.016         9.980 ± 0.163           12         39.720 ± 0.191         4.150 ± 0.077         7.380 ± 0.205           75         8         48.120 ± 0.184         6.280 ± 0.163         14.470 ± 0.134           10         43.210 ± 0.265         5.600 ± 0.106         10.490 ± 0.185           12         40.620 ± 0.184         6.280 ± 0.163         14.470 ± 0.134           10         43.210 ± 0.265         5.600 ± 0.064         1.600 ± 0.185           Peru (green beans)         -         -         53.440 ± 0.042         0.880 ± 0.049         12.840 ± 0.078           Peru (roasted beans)         95         8         42.540 ± 0.102         5.560 ± 0.085         10.430 ± 0.148           10         38.940 ± 0.099         4.330 ± 0.064         7.280 ± 0.057         12.380 ± 0.057         12.040 ± 0.057           12         39.010 ± 0.156         4.160 ± 0.020         7.510 ± 0.10			10	$42.410 \pm 0.233$	$5.240 \pm 0.064$	$9.810 \pm 0.177$
Image: space			12	$38.050 \pm 0.099$	$3.550 \pm 0.099$	$6.250 \pm 0.085$
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Image: Problem State         Image: Imag			10	$42.460 \pm 0.283$	$5.300 \pm 0.106$	$9.980 \pm 0.163$
Internal state         Interna			12	$39.720 \pm 0.191$	$4.150\pm0.077$	$7.380\pm0.205$
8         48.120±0.184         6.280±0.163         14.470±0.134           10         43.210±0.269         5.600±0.166         10.490±0.185           12         40.620±0.184         4.570±0.099         7.860±0.120           15         36.460±0.141         3.300±0.064         4.160±0.141           Peru (roasted beans)         -         -         53.440±0.042         0.880±0.049         12.840±0.078           Peru (roasted beans)         95         8         42.540±0.120         5.560±0.085         10.430±0.148           10         38.940±0.099         4.330±0.064         7.280±0.057         12         38.060±0.110         3.710±0.121         6.440±0.234           14         36.860±0.155         3.390±0.064         5.270±0.049         12         10         42.240±0.078         5.510±0.020         7.510±0.106           14         37.350±0.120         3.200±0.045         5.360±0.099         1.260±0.014         3.260±0.014         3.260±0.014         3.260±0.014         3.260±0.014         3.260±0.014         12.230±0.011         14         3.30±0.021         5.440±0.071         12.930±0.106         14         3.30±0.014         4.260±0.014         3.20±0.014         12.930±0.106         12.930±0.106         12.930±0.106         10.10±0.057         1.30±0.071 </td <td></td> <td></td> <td>14</td> <td><math>36.770 \pm 0.282</math></td> <td><math display="block">3.230\pm0.071</math></td> <td><math display="block">4.550\pm0.085</math></td>			14	$36.770 \pm 0.282$	$3.230\pm0.071$	$4.550\pm0.085$
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Peru (green beans)         -         -         53.440 ± 0.042         0.880 ± 0.049         12.840 ± 0.078           Peru (roasted beans)         95         8         42.540 ± 0.120         5.560 ± 0.085         10.430 ± 0.044           10         38.940 ± 0.099         4.330 ± 0.064         7.280 ± 0.057           12         38.060 ± 0.155         3.390 ± 0.064         5.270 ± 0.049           14         36.860 ± 0.155         3.390 ± 0.064         5.270 ± 0.049           10         42.240 ± 0.078         5.360 ± 0.052         10.420 ± 0.127           12         39.910 ± 0.156         4.160 ± 0.020         7.510 ± 0.106           14         37.350 ± 0.120         3.200 ± 0.049         5.360 ± 0.099           75         8         45.350 ± 0.092         6.440 ± 0.057         12.930 ± 0.106           10         40.240 ± 0.157         4.850 ± 0.049         7.130 ± 0.071           12         39.270 ± 0.0120         5.440 ± 0.057         12.930 ± 0.106           10         40.240 ± 0.157         4.850 ± 0.049         7.130 ± 0.071           12         39.270 ± 0.0194         4.120 ± 0.049         7.130 ± 0.071           12         39.270 ± 0.0156         2.670 ± 0.085         3.950 ± 0.041           12         36.			15	$36.460 \pm 0.141$	$3.300\pm0.064$	$4.160\pm0.141$
Peru (roasted beans)         95         8         42.540 ± 0.120         5.560 ± 0.085         10.430 ± 0.148           10         38.940 ± 0.099         4.330 ± 0.064         7.280 ± 0.057           12         38.060 ± 0.155         3.390 ± 0.064         5.270 ± 0.049           80         8         45.010 ± 0.057         6.360 ± 0.054         5.270 ± 0.049           10         42.240 ± 0.078         5.510 ± 0.092         10.420 ± 0.127           12         39.910 ± 0.156         4.160 ± 0.020         7.510 ± 0.106           14         37.350 ± 0.049         5.360 ± 0.049         5.360 ± 0.042           10         42.240 ± 0.078         5.510 ± 0.022         7.510 ± 0.106           14         37.350 ± 0.029         6.440 ± 0.057         12.930 ± 0.106           10         40.240 ± 0.157         4.850 ± 0.085         8.290 ± 0.142           12         39.270 ± 0.099         4.120 ± 0.049         7.130 ± 0.071           14         37.610 ± 0.134         3.610 ± 0.025         1.140 ± 0.071           Congo (green beans)         -         -         51.440 ± 0.134         0.610 ± 0.085         11.050 ± 0.071           Congo (roasted beans)         80         -         52.360 ± 0.141         4.620 ± 0.041         9.270 ± 0.078	Peru (green beans)	-	-	$53.440 \pm 0.042$	$0.880\pm0.049$	$12.840 \pm 0.078$
$ \begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	Peru (roasted beans)	95	8	$42.540 \pm 0.120$	$5.560\pm0.085$	$10.430\pm0.148$
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$			10	$38.940 \pm 0.099$	$4.330\pm0.064$	$7.280\pm0.057$
$ \begin{tabular}{ c c c c c c } \hline $14$ & $36.860 \pm 0.155$ & $3.390 \pm 0.064$ & $5.270 \pm 0.049$ \\ \hline $80$ & $8$ & $45.010 \pm 0.057$ & $6.360 \pm 0.064$ & $12.620 \pm 0.042$ \\ \hline $10$ & $42.240 \pm 0.078$ & $5.510 \pm 0.092$ & $10.420 \pm 0.127$ \\ \hline $12$ & $39.910 \pm 0.156$ & $4.160 \pm 0.020$ & $7.510 \pm 0.106$ \\ \hline $14$ & $37.350 \pm 0.120$ & $3.200 \pm 0.049$ & $5.360 \pm 0.099$ \\ \hline $14$ & $37.550 \pm 0.120$ & $3.200 \pm 0.049$ & $5.360 \pm 0.099$ \\ \hline $12$ & $39.270 \pm 0.092$ & $6.440 \pm 0.057$ & $12.930 \pm 0.106$ \\ \hline $10$ & $40.240 \pm 0.157$ & $4.850 \pm 0.085$ & $8.290 \pm 0.142$ \\ \hline $12$ & $39.270 \pm 0.099$ & $4.120 \pm 0.049$ & $7.130 \pm 0.071$ \\ \hline $14$ & $37.610 \pm 0.134$ & $0.610 \pm 0.085$ & $11.050 \pm 0.071$ \\ \hline $14$ & $37.610 \pm 0.134$ & $0.610 \pm 0.085$ & $11.050 \pm 0.071$ \\ \hline $14$ & $37.610 \pm 0.134$ & $0.610 \pm 0.085$ & $11.050 \pm 0.071$ \\ \hline $10$ & $39.240 \pm 0.141$ & $4.620 \pm 0.041$ & $9.270 \pm 0.078$ \\ \hline $10$ & $39.240 \pm 0.141$ & $3.810 \pm 0.078$ & $6.680 \pm 0.078$ \\ \hline $12$ & $36.120 \pm 0.156$ & $2.670 \pm 0.085$ & $3.950 \pm 0.041$ \\ \hline $12$ & $36.120 \pm 0.156$ & $2.670 \pm 0.085$ & $3.950 \pm 0.041$ \\ \hline $12$ & $36.99 \pm 0.085$ & $3.460 \pm 0.057$ & $13.080 \pm 0.058$ \\ \hline $10$ & $41.650 \pm 0.128$ & $5.360 \pm 0.044$ & $13.910 \pm 0.099$ \\ \hline $10$ & $41.650 \pm 0.128$ & $5.360 \pm 0.044$ & $9.310 \pm 0.064$ \\ \hline $12$ & $36.99 \pm 0.085$ & $3.460 \pm 0.085$ & $4.780 \pm 0.064$ \\ \hline $12$ & $36.99 \pm 0.085$ & $3.460 \pm 0.085$ & $4.780 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.092$ & $0.140 \pm 0.071$ & $5.860 \pm 0.042$ \\ \hline $12$ & $37.930 \pm 0.025$ & $1.140 \pm 0.057$ & $11.300 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.025$ & $1.140 \pm 0.057$ & $11.300 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.025$ & $3.460 \pm 0.085$ & $4.780 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.025$ & $1.140 \pm 0.057$ & $11.300 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.025$ & $3.460 \pm 0.085$ & $4.780 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.025$ & $1.140 \pm 0.057$ & $11.300 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.025$ & $1.140 \pm 0.057$ & $11.300 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.025$ & $1.140 \pm 0.057$ & $11.300 \pm 0.064$ \\ \hline $12$ & $37.930 \pm 0.025$ & $1.140 \pm 0.057$ & $11.300 \pm 0.064$ \\ \hline $12$ & $$			12	$38.060\pm0.410$	$3.710\pm0.121$	$6.440\pm0.234$
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$			14	$36.860 \pm 0.155$	$3.390\pm0.064$	$5.270\pm0.049$
$ \begin{tabular}{ c c c c c c c } \hline 10 & 42.240 \pm 0.078 & 5.510 \pm 0.092 & 10.420 \pm 0.127 \\ \hline 12 & 39.910 \pm 0.156 & 4.160 \pm 0.020 & 7.510 \pm 0.106 \\ \hline 14 & 37.350 \pm 0.120 & 3.200 \pm 0.049 & 5.360 \pm 0.099 \\ \hline 75 & 8 & 45.350 \pm 0.092 & 6.440 \pm 0.057 & 12.930 \pm 0.106 \\ \hline 10 & 40.240 \pm 0.157 & 4.850 \pm 0.085 & 8.290 \pm 0.142 \\ \hline 12 & 39.270 \pm 0.099 & 4.120 \pm 0.049 & 7.130 \pm 0.071 \\ \hline 14 & 37.610 \pm 0.134 & 3.530 \pm 0.021 & 5.440 \pm 0.071 \\ \hline Congo (green beans) & - & - & 51.440 \pm 0.134 & 0.610 \pm 0.085 & 11.050 \pm 0.071 \\ \hline Congo (roasted beans) & 80 & 8 & 42.150 \pm 0.141 & 3.810 \pm 0.078 & 6.680 \pm 0.078 \\ \hline 10 & 39.240 \pm 0.141 & 3.810 \pm 0.078 & 6.680 \pm 0.078 \\ \hline 12 & 36.120 \pm 0.156 & 2.670 \pm 0.085 & 3.950 \pm 0.041 \\ \hline Brazil (green beans) & - & - & 52.360 \pm 0.205 & 1.140 \pm 0.057 & 13.080 \pm 0.058 \\ \hline 10 & 41.650 \pm 0.128 & 5.360 \pm 0.041 & 3.910 \pm 0.099 \\ \hline 10 & 41.650 \pm 0.128 & 5.360 \pm 0.640 & 9.310 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 13 & 39.340 \pm 0.128 & 4.600 \pm 0.057 & 7.340 \pm 0.014 \\ \hline 12 & 37.440 \pm 0.170 & 3.710 \pm 0.058 & 5.160 \pm 0.085 \\ \hline 13 & 36.690 \pm 0.134 & 3.080 \pm 0.057 & 4.210 \pm 0.071 \\ \hline 14 & 37.440 \pm 0.170 & 3.710 \pm 0.058 & 5.160 \pm 0.085 \\ \hline 13 & 36.690 \pm 0.1$		80	8	$45.010 \pm 0.057$	$6.360\pm0.064$	$12.620 \pm 0.042$
$ \begin{tabular}{ c c c c c c c c c c c c c c c c c c c$			10	$42.240 \pm 0.078$	$5.510\pm0.092$	$10.420 \pm 0.127$
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$			12	$39.910 \pm 0.156$	$4.160\pm0.020$	$7.510\pm0.106$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			14	$37.350\pm0.120$	$3.200\pm0.049$	$5.360\pm0.099$
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		75	8	$45.350 \pm 0.092$	$6.440\pm0.057$	$12.930 \pm 0.106$
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $			10	$40.240 \pm 0.157$	$4.850\pm0.085$	$8.290\pm0.142$
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$			12	$39.270 \pm 0.099$	$4.120\pm0.049$	$7.130\pm0.071$
$ \begin{array}{c cccc} Congo (green beans) & - & - & 51.440 \pm 0.134 & 0.610 \pm 0.085 & 11.050 \pm 0.071 \\ \hline Congo (roasted beans) & 80 & 8 & 42.150 \pm 0.141 & 4.620 \pm 0.041 & 9.270 \pm 0.078 \\ \hline 10 & 39.240 \pm 0.141 & 3.810 \pm 0.078 & 6.680 \pm 0.078 \\ \hline 12 & 36.120 \pm 0.156 & 2.670 \pm 0.085 & 3.950 \pm 0.041 \\ \hline Brazil (green beans) & - & - & 52.360 \pm 0.205 & 1.140 \pm 0.057 & 13.080 \pm 0.058 \\ \hline & & & & & & & & & & & & & & & & & &$			14	$37.610 \pm 0.134$	$3.530\pm0.021$	$5.440\pm0.071$
$ \begin{array}{c} \text{Congo (roasted beans)} & 80 \\ & 8 \\ \hline 10 \\ \hline 10 \\ \hline 39.240 \pm 0.141 \\ \hline 3.810 \pm 0.078 \\ \hline 6.680 \pm 0.078 \\ \hline 12 \\ \hline 36.120 \pm 0.156 \\ \hline 2.670 \pm 0.085 \\ \hline 3.950 \pm 0.041 \\ \hline 12 \\ \hline 36.120 \pm 0.156 \\ \hline 2.670 \pm 0.085 \\ \hline 3.950 \pm 0.041 \\ \hline 13.080 \pm 0.058 \\ \hline 10 \\ \hline 41.650 \pm 0.128 \\ \hline 5.360 \pm 0.640 \\ \hline 9.310 \pm 0.064 \\ \hline 12 \\ \hline 36.980 \pm 0.085 \\ \hline 3.460 \pm 0.085 \\ \hline 4.780 \pm 0.064 \\ \hline 12 \\ \hline 36.980 \pm 0.085 \\ \hline 3.460 \pm 0.085 \\ \hline 4.780 \pm 0.064 \\ \hline 13.110 \pm 0.099 \\ \hline 10 \\ \hline 42.290 \pm 0.134 \\ \hline 5.800 \pm 0.099 \\ \hline 10.290 \pm 0.065 \\ \hline 12 \\ \hline 37.930 \pm 0.092 \\ \hline 3.910 \pm 0.071 \\ \hline 5.860 \pm 0.042 \\ \hline 12 \\ \hline 37.930 \pm 0.092 \\ \hline 3.910 \pm 0.071 \\ \hline 5.860 \pm 0.042 \\ \hline 12 \\ \hline 37.930 \pm 0.092 \\ \hline 3.910 \pm 0.057 \\ \hline 11.300 \pm 0.064 \\ \hline 12 \\ \hline 37.440 \pm 0.170 \\ \hline 3.710 \pm 0.058 \\ \hline 5.160 \pm 0.085 \\ \hline 13 \\ \hline 36.690 \pm 0.134 \\ \hline 3.080 \pm 0.057 \\ \hline 4.210 \pm 0.071 \\ \hline \end{array} $	Congo (green beans)	-	-	$51.440 \pm 0.134$	$0.610\pm0.085$	$11.050 \pm 0.071$
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Congo (roasted beans)	80	8	$42.150\pm0.141$	$4.620\pm0.041$	$9.270\pm0.078$
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $			10	$39.240 \pm 0.141$	$3.810\pm0.078$	$6.680\pm0.078$
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $			12	$36.120 \pm 0.156$	$2.670\pm0.085$	$3.950\pm0.041$
$ Brazil (roasted beans) \begin{cases} 8 & 46.240 \pm 0.092 & 6.810 \pm 0.064 & 13.910 \pm 0.099 \\ \hline 10 & 41.650 \pm 0.128 & 5.360 \pm 0.640 & 9.310 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.084 & 13.110 \pm 0.099 \\ \hline 10 & 42.290 \pm 0.134 & 5.800 \pm 0.099 & 10.290 \pm 0.065 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 10 & 39.340 \pm 0.128 & 4.600 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 10 & 39.340 \pm 0.128 & 4.600 \pm 0.057 & 7.340 \pm 0.014 \\ \hline 12 & 37.440 \pm 0.170 & 3.710 \pm 0.058 & 5.160 \pm 0.085 \\ \hline 13 & 36.690 \pm 0.134 & 3.080 \pm 0.057 & 4.210 \pm 0.071 \\ \hline \end{cases} $	Brazil (green beans)	-	-	$52.360 \pm 0.205$	$1.140\pm0.057$	$13.080 \pm 0.058$
$ Brazil (roasted beans) \begin{cases} 95 & 10 & 41.650 \pm 0.128 & 5.360 \pm 0.640 & 9.310 \pm 0.064 \\ 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 12 & 36.980 \pm 0.085 & 3.460 \pm 0.084 & 13.110 \pm 0.099 \\ \hline 10 & 42.290 \pm 0.134 & 5.800 \pm 0.099 & 10.290 \pm 0.065 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 10 & 39.340 \pm 0.128 & 4.600 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 10 & 39.340 \pm 0.128 & 4.600 \pm 0.057 & 7.340 \pm 0.014 \\ \hline 12 & 37.440 \pm 0.170 & 3.710 \pm 0.058 & 5.160 \pm 0.085 \\ \hline 13 & 36.690 \pm 0.134 & 3.080 \pm 0.057 & 4.210 \pm 0.071 \end{cases}$			8	$46.240 \pm 0.092$	$6.810\pm0.064$	$13.910 \pm 0.099$
$Brazil (roasted beans) = \begin{bmatrix} 12 & 36.980 \pm 0.085 & 3.460 \pm 0.085 & 4.780 \pm 0.064 \\ \hline 8 & 45.600 \pm 0.071 & 6.040 \pm 0.084 & 13.110 \pm 0.099 \\ \hline 10 & 42.290 \pm 0.134 & 5.800 \pm 0.099 & 10.290 \pm 0.065 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 12 & 37.930 \pm 0.128 & 4.600 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 10 & 39.340 \pm 0.128 & 4.600 \pm 0.057 & 7.340 \pm 0.014 \\ \hline 12 & 37.440 \pm 0.170 & 3.710 \pm 0.058 & 5.160 \pm 0.085 \\ \hline 13 & 36.690 \pm 0.134 & 3.080 \pm 0.057 & 4.210 \pm 0.071 \end{bmatrix}$		95	10	$41.650 \pm 0.128$	$5.360\pm0.640$	$9.310\pm0.064$
$ Brazil (roasted beans) \begin{cases} 80 & \frac{8}{10} & \frac{45.600 \pm 0.071}{42.290 \pm 0.134} & \frac{6.040 \pm 0.084}{5.800 \pm 0.099} & \frac{13.110 \pm 0.099}{10.290 \pm 0.065} \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 12 & 37.930 \pm 0.092 & 3.910 \pm 0.071 & 5.860 \pm 0.042 \\ \hline 10 & 39.340 \pm 0.128 & 4.600 \pm 0.057 & 11.300 \pm 0.064 \\ \hline 12 & 37.440 \pm 0.170 & 3.710 \pm 0.058 & 5.160 \pm 0.085 \\ \hline 13 & 36.690 \pm 0.134 & 3.080 \pm 0.057 & 4.210 \pm 0.071 \\ \hline \end{cases} $			12	$36.980 \pm 0.085$	$3.460\pm0.085$	$4.780\pm0.064$
$ \begin{array}{c} \text{Brazil (roasted beans)} \\ \end{array} \begin{array}{c} 80 \\ \hline 10 \\ 12 \\ 75 \end{array} \begin{array}{c} 10 \\ 12 \\ 75 \end{array} \begin{array}{c} 42.290 \pm 0.134 \\ 37.930 \pm 0.092 \\ 3.910 \pm 0.071 \\ 37.930 \pm 0.092 \\ 3.910 \pm 0.071 \\ 5.860 \pm 0.042 \\ 11.300 \pm 0.064 \\ 10 \\ 39.340 \pm 0.128 \\ 4.600 \pm 0.057 \\ 7.340 \pm 0.014 \\ 12 \\ 37.440 \pm 0.170 \\ 3.710 \pm 0.058 \\ 5.160 \pm 0.085 \\ 13 \\ 36.690 \pm 0.134 \\ 3.080 \pm 0.057 \\ 4.210 \pm 0.071 \end{array} $			8	$45.600 \pm 0.071$	$6.040\pm0.084$	$13.110 \pm 0.099$
$\frac{12}{75} \qquad \frac{37.930 \pm 0.092}{10} \qquad \frac{3.910 \pm 0.071}{5.860 \pm 0.042} \qquad \frac{5.860 \pm 0.042}{11.300 \pm 0.064} \\ \frac{8}{39.340 \pm 0.128} \qquad \frac{4.600 \pm 0.057}{4.600 \pm 0.057} \qquad \frac{7.340 \pm 0.014}{7.340 \pm 0.014} \\ \frac{12}{12} \qquad \frac{37.440 \pm 0.170}{3.6.690 \pm 0.134} \qquad \frac{3.080 \pm 0.057}{3.080 \pm 0.057} \qquad \frac{4.210 \pm 0.071}{4.210 \pm 0.071} \\ \frac{37.440 \pm 0.170}{12} \qquad \frac{3.080 \pm 0.057}{11} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{37.440 \pm 0.170}{12} \qquad \frac{3.080 \pm 0.057}{11} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{37.440 \pm 0.170}{10} \qquad \frac{3.080 \pm 0.057}{11} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{37.440 \pm 0.170}{10} \qquad \frac{3.080 \pm 0.057}{11} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{37.440 \pm 0.170}{10} \qquad \frac{3.080 \pm 0.057}{11} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{37.440 \pm 0.170}{10} \qquad \frac{3.080 \pm 0.057}{11} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{37.440 \pm 0.170}{10} \qquad \frac{3.080 \pm 0.057}{11} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{37.440 \pm 0.170}{10} \qquad \frac{3.080 \pm 0.057}{10} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{3.080 \pm 0.057}{10} \qquad \frac{4.210 \pm 0.057}{10} \\ \frac{3.080 \pm 0.057}{10} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{3.080 \pm 0.057}{10} \qquad \frac{4.210 \pm 0.071}{10} \\ \frac{3.080 \pm 0.057}{10} \qquad \frac{4.210 \pm 0.057}{10} \\ \frac{3.080 \pm 0.057}{10} \qquad \frac{4.210 \pm 0.057}{10} \\ \frac{3.080 \pm 0.057}{10} $	Prozil (reasted beens)	80	10	$42.290\pm0.134$	$5.800\pm0.099$	$10.290 \pm 0.065$
$\frac{8}{10} \qquad \frac{43.570 \pm 0.184}{39.340 \pm 0.128} \qquad \frac{6.190 \pm 0.057}{4.600 \pm 0.057} \qquad \frac{11.300 \pm 0.064}{7.340 \pm 0.014}$ $\frac{12}{12} \qquad \frac{37.440 \pm 0.170}{3.710 \pm 0.058} \qquad \frac{5.160 \pm 0.085}{5.160 \pm 0.085}$ $\frac{13}{36.690 \pm 0.134} \qquad \frac{3.080 \pm 0.057}{3.080 \pm 0.057} \qquad \frac{4.210 \pm 0.071}{4.210 \pm 0.071}$	Diazii (loasteu bealis)		12	$37.930 \pm 0.092$	$3.910\pm0.071$	$5.860\pm0.042$
$10$ $39.340 \pm 0.128$ $4.600 \pm 0.057$ $7.340 \pm 0.014$ $12$ $37.440 \pm 0.170$ $3.710 \pm 0.058$ $5.160 \pm 0.085$ $13$ $36.690 \pm 0.134$ $3.080 \pm 0.057$ $4.210 \pm 0.071$			8	$43.570\pm0.184$	$6.190\pm0.057$	$11.300 \pm 0.064$
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		75	10	$39.340 \pm 0.128$	$4.600 \pm 0.057$	$7.340 \pm 0.014$
13 $36.690 \pm 0.134$ $3.080 \pm 0.057$ $4.210 \pm 0.071$		15	12	$37.440 \pm 0.170$	$3.710 \pm 0.058$	$5.160 \pm 0.085$
			13	$36.690 \pm 0.134$	$3.080 \pm 0.057$	$4.210 \pm 0.071$

between the quality of a coffee cup and the chemical composition of roasted coffee beans [9]. In addition, the authors created a model from roasted beans to predict the quality attributes of a coffee cup (e.g. acidity, body, and flavor).

The relationship between some coffee roasting variables (weight loss, density, and moisture) and near-infrared spectra of original green and differently roasted coffee samples was investigated by Alessandrini *et al.* [14]. They developed separate calibration and validation models based on partial least square (PLS) regression, correlating NIR spectral data of 168 representatives and suitable green and roasted coffee samples with each roasting variable.

As a result, the authors constructed robust and reliable models to predict roasting variables for unknown roasted coffee samples, considering that measured vs. predicted values showed high correlation coefficients (0.92–0.98).

Pires *et al.* used multivariate calibration and NIR spectroscopy to correctly predict roasting degrees in ground coffee and coffee beans as a substitute for the Agtron method [18]. The mathematical models for predicting Agtron values of new coffee samples using the PLS approach were based on the association between NIR spectra data and Agtron reference results. All Agtron roasting characteristics were investigated in order to create representative models. With RMSEP

**Table 3** The origin of bonds occurring at given wavenumbersfor tested coffee beans [31]

Bond type	Wavenumber, cm <sup>-1</sup>
CH <sub>3</sub> ; second overtone; stretching symmetric	8545-8042
СН	7020-6562
CH <sub>3</sub> ; first overtone; stretching asymmetric	5841-5751
CH <sub>2</sub> ; first overtone; stretching asymmetric	5725–5654
OH; stretching	5234-5000
CH; stretching	4954-4509
CH <sub>3</sub> ; stretching	4358-4302

values of 4.48 and 3.67, respectively, the proposed models showed promising results in predicting roasting characteristics in roasted whole coffee beans and ground coffees.

Yergenson and Aston investigated the use of in situ NIR spectroscopy in the prediction of cracking events (start and end) during coffee roasting in order to develop a more robust method of roasting based on cracks [33]. Two sets of popping sounds (first and second cracks) that occur during coffee roasting are essential indicators for establishing the roasting endpoint. The coffee samples were roasted using various time-temperature profiles. In situ NIR spectroscopy proved to be a reliable tool in forecasting the start and finish times of first and second crack occurrences based on the PLS regression (PLSR) with audio recordings from coffee roasting.

The NIR spectra of coffees (beans and ground) roasted under different conditions are shown in Fig. 2. The obtained spectra were similar to each other, although varying in intensity. Longer roasting time lowered the intensity of the bands in all the ranges. This was due to decreased values of coffee components, as well as their volume and weight [34–36]. We found that the samples with the shortest roasting time (8 min) showed the highest absorbance, while those with the longest roasting time (12 min) showed the lowest absorbance at the same wavelength. We also noticed that the intensity of the spectrum bands decreased with increasing roasting time. The NIR spectra obtained during the roasting assays were similar to the spectra reported in other studies [37, 38]. According to the authors, the main changes in the spectra of the roasting process were an absorbance decrease in the water band region (5200-5000 cm<sup>-1</sup>), which was due to moisture loss, and an absorbance increase in the combination band region (5000-4000 cm<sup>-1</sup>). A more detailed discussion of the main wavelength intervals and their relationships to chemical and physical changes in coffee during roasting can be found in the work by Santos et al. [37]. Our results were also consistent with those reported by Catelani et al. [38]. The roasting degraded coffee compounds, process namely chlorogenic acid, coffee sugar, fat, and water. Literature

data shows that the roasting time also affects the caffeine content in coffee [39]. The longer the coffee is roasted, the lower its caffeine content. All the samples showed a lower intensity with an increase in the roasting time. We concluded that regardless of the origin, the roasting time caused a decrease in the coffee components. The most intense bands occurred in the coffees roasted for the shortest time, which means that they lost the least of their components and nutritional value.

The partial least squares (PLS) analysis was performed to determine the time of roasting. The PLS models were obtained for the entire spectral range ( $12500-4000 \text{ cm}^{-1}$ ) and sub-regions without mathematical transformations (Table 4).

We found good correlations between the spectra and the roasting time for all the coffee samples. The  $R^2$  values for the calibration and validation curves were 0.94 and 0.78, respectively. The root mean-square errors (RMSE) were low – 0.39 and 0.76 for calibration and validation, respectively. The obtained models were improved when analyzing each type of coffee samples separately. Also, the sub-regions were used to improve the model quality.

There was a weak correlation between the spectra and the roasting power for all the coffee samples. For this reason, we analyzed the samples separately. The most accurate model for Guatemala coffee was obtained in the spectral region of 6813-5332 cm<sup>-1</sup>. The  $R^2$  was 0.97 for calibration and 0.64 for validation. For Peru coffee, the spectral range of 5374-4954 cm<sup>-1</sup> gave the best quality model, with  $R^2$  values of 0.97 and 0.84 for calibration and validation, respectively. There was no correlation between the spectra and the roasting power for Brazil coffee. The coffee from Congo was not analyzed (only one power condition – 80%).

The degree of coffee roasting can be assessed by the color: the longer the roasting, the darker the beans. We studied a possibility of estimating the roasting time on the basis of the NIR spectra by using the PLS analysis to correlate the NIR spectra (coffee beans) with the  $L^*$  parameter (Table 4). By analyzing the values of the calibration ( $R^2 = 0.96$ ) and validation ( $R^2 = 0.95$ ) curves, as well as the RMSE values (0.92 for calibration and 1.05 for validation), we assumed that the coffee roasting time could be determined based on the PLS regression analysis and the brightness parameter ( $L^*$ ).

Our study indicates the potentiality of NIR spectroscopy in evaluating coffee quality. Based on the changes of spectra, it is possible to monitor changes during roasting. Chemometric analysis also delivered very promising results. The PLS models (for roasting time and power conditions) hold potential as a rapid and reliable method which could be helpful in coffee manufacturing. Our next step will be to determine the chemical composition of the coffee samples and identify the potential of NIR spectroscopy in correlating roasting



**Figure 2** Changes in near-infrared spectra in coffee roasted at different power and time: (a) Guatemala coffee, (b) Peru coffee, (c) Brazil coffee, (d) Congo coffee. Full range spectrum (12500–4000 cm<sup>-1</sup>)

conditions (time and power) with the chemical changes in order to select optimal roasting conditions for the final product.

## CONCLUSION

Our study aimed to apply near-infrared spectroscopy to evaluate the quality of the coffee samples from Brazil, Guatemala, Peru, and Congo. We investigated their composition based on the spectral bands and vibrations.

The regression results confirmed the possibility of applying the NIR spectra to predict the roasting conditions. There was a correlation between the spectra and the roasting time, with the  $R^2$  of 0.94 and 0.78 for calibration and validation, respectively. The RMSEs were low – 0.39 and 0.76 for calibration and validation, respectively. We also obtained a linear relation between the spectra and the roasting power. The quality of the models differed based on the coffee's origin and subregion. All the coffee samples showed a good correlation between the spectra and the brightness ( $L^*$  parameter). The  $R^2$  values were 0.96 and 0.95 for the calibration and validation curves, respectively.

The results proved that NIR spectroscopy coupled with chemometrics could be a promising tool to predict

PLS model	Samples	Spectral region, cm <sup>-1</sup>	Root mean-squ	are error	$R^2$	
			Calibration	Validation	Calibration	Validation
Roasting time	All coffee samples	12500-4000	0.39	0.76	0.94	0.78
	Guatemala	12500-4000	0.09	0.79	0.99	0.83
		6813-5332	0.24	0.48	0.98	0.94
	Peru	12500-4000	0.39	0.70	0.94	0.85
		6030-4000	0.18	0.82	0.99	0.80
	Brazil	12500-4000	0.22	0.30	0.96	0.95
	Congo	-	_	_	_	_
Roasting power	All coffee samples	-	_	-	_	_
	Guatemala	12500-4000	1.15	6.23	0.98	0.57
		6314-5295	1.44	5.72	0.97	0.64
	Peru	12500-4000	1.70	6.16	0.96	0.58
		6314–5295	1.26	4.32	0.98	0.79
		6227-4000	0.84	4.54	0.99	0.77
		5374-4954	1.51	3.84	0.97	0.84
		4416-4090	2.29	4.27	0.93	0.80
	Brazil	_	_	_	_	_
	Congo	-	-	-	-	_
Color ( <i>L</i> * parameter)	All coffee samples	12500-4000	0.92	1.05	0.96	0.95

Table 4 Partial least squares (PLS) regression analysis

the roasting conditions of coffee samples. However, the models developed in this study need to be further tested on independent data sets from other coffee varieties to assess their stability and accuracy. Because of its characteristics, NIR spectroscopy has been applied in different production stages in the coffee industry: from green coffee beans to the end product. The growing interest in NIR spectroscopy is primarily due to the technique's numerous advantages over other analytical techniques. In addition, this technique is nondestructive and noninvasive, with a minimal or non-sample preparation. NIR spectroscopy is also fast, low-cost, and robust, so it can be used in different environments such as laboratories and industrial plants. In the future, the availability of portable instruments will also allow its use in the field. For these reasons, NIR spectroscopy could be named a "green technology".

### **CONFLICT OF INTEREST**

The author declares that there is no conflict of interest.

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