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Effect of the roasting level on the content of bioactive and aromatic compounds in Arabica coffee beans

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Abstract. In the present study, three degrees of roasting (light, medium, and dark), which significantly differentiate the properties of coffee beans, were analyzed. Additionally, the effect of the roasting level on the profile of volatile and biologically active compounds, including chlorogenic acids, tocopherols, and caffeine, was determined. Light-roast coffee beans, referred to as the Cinnamon roast, were obtained at 198°C. In turn, American roast beans were obtained at 212°C before the second crack, and dark beans classified as the Italian roast were obtained in a roasting process carried out at 228-230°C. The content of bioactive compounds in green coffee beans was determined as well. The 'Typica' cultivar of *Arabica* coffee originating from a plantation located at an altitude of 1680 m a.s.l. in Huehuetenango Department, Guatemala, was used in the study. The analyses showed that the different parameters of coffee bean roasting (Cinnamon, American, and Italian roast) resulted in differences in the levels of phenolic compounds, caffeine, and tocopherols. The American roast style was shown to be the most balanced type of roasting in terms of the content of bioactive compounds as well as the chemical groups and profile of volatile compounds. This roasting type also exhibited the highest intensity of emission of volatile compounds, which is expected by the consumer. The study also demonstrated that the coffee bean roasting process generated different levels of phenolic compounds, caffeine, and tocopherols.

Keywords: coffee, volatile organic compounds, antioxidants, bioactive compounds, coffee bean roasting level, electronic nose

1. INTRODUCTION

Coffee is one of the most commercialized food products. It can be prepared with the use of various techniques, depending on consumer preferences. In terms of the chemical composition, the two main species of coffee, *Arabica* and *Canephora* (often called Robusta from the name of the first widespread variety of this species), can be a rich source of biologically active compounds, and their potential impact on human health is associated with physiological differences in caffeine absorption by the organism and the amount of coffee consumed per day (George *et al.*, 2008; Wołosiak *et al.*, 2023). Chlorogenic acids (CGAs) are one of the most important groups of compounds present in coffee. Despite the large variations, the total CGA content may reach 7.0-14.4% of dry matter in green *Robusta* and 4.0-8.4% in green *Arabica* beans (Farah and Donangelo, 2006). Caffeic, ferulic, and p-coumaric acids are the main phenolic compounds in coffee derived from trans-cinnamic acid. They occur naturally as mono- or diesters with quinic acid, forming chlorogenic acids (Farah and Donangelo, 2006), which are known to be the most active antioxidant compounds. CGAs are water-soluble compounds (Farah *et al.*, 2006; Rodrigues and Bragagnolo, 2013). They can be divided

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into caffeoylquinic acids (CQAs) with 3 isomers (3-, 4-, and 5-CQAs), feruloylquinic acids (FQAs) with 3 isomers (3-, 4-, and 5-FQA), dicaffeoylquinic acids (diCQAs) with 3 isomers (3,4-diCQA; 3,5-diCQA; and 4,5-diCQA) and, less abundant p-coumaroylquinic acids (pCoQAs) with 3 isomers (3-, 4-, and 5-pCoQA). CQAs are the most abundant compounds contained in coffee (Crozier *et al.*, 2012; Farah and Donangelo, 2006). Since CGAs contribute to the acidity, astringency, and bitterness of brewed coffee (Farah *et al.*, 2006) they are highly important for assessment of coffee quality, especially for evaluation of the sensory properties of coffee beverages. Additionally, the antioxidant properties of CGAs have been well documented in the literature. These compounds also exert a protective effect against type 2 diabetes and Alzheimer's disease (Kim *et al.*, 2012).

Many steps in the coffee production process may have an impact on the CGA content in the final product; however, the roasting process is described as the most important stage having a substantial impact on the chemical composition of products (Farah *et al.*, 2005; Mills *et al.*, 2013; Moon *et al.*, 2009). Hence, coffee infusions, especially those prepared with pressure methods, can serve as potential sources of such antioxidants as CQAs. The CGA content in brewed coffee may vary, depending on other parameters, *e.g.* the variety or species of coffee, the origin of coffee beans (Campa *et al.*, 2005), harvesting methods, subsequent post-harvest processing, and brewing methods (Fujioka and Shibamoto, 2008; Tfouni *et al.*, 2014). Although the CQA content in coffee beans and the impact of brewing conditions and new procedures have been partially reported (Gloess *et al.*, 2013; Parenti *et al.*, 2014), there are only few studies of the effect of the roasting process and, especially, the level of roasting on the CGA content (Farah *et al.*, 2005; Moon *et al.*, 2009). Coffee can be brewed in many ways (Santanatoglia *et al.*, 2023a,b) depending on consumers' tastes and preferences. The properties of the beverage is also influenced by cultural customs regarding specific methods of brewing, which often have an effect on the content of bioactive compounds or coffee flavor and aroma. In turn, there is no sufficient knowledge of the effects of the methods or levels of roasting.

The process and degree of coffee roasting not only is one of the most important determinants of the aroma, flavor, and volatile organic compounds (VOC) profile in coffee, but also may have a significant impact on the content of active compounds (Hečimović *et al.*, 2011; Marek *et al.*, 2020) exhibiting neuroprotective and anticancer properties. Roasting profiles are described by many terms, depending on the region of coffee origin, consumer preferences, and the specific experience of the coffee roaster. In general, the coffee roasting degrees are defined as light, medium, medium dark, and dark, which is associated with one of the four color categories or lightness degrees (Lu *et al.*, 2023). The light roast is achieved when the internal temperature in the beans reaches a value between 180 and 205°C. A crackling sound is usually heard at this point as the beans enlarge. The light roast is achieved by roasting no longer than until the first crack. Light roast coffee has a sour flavor, and the beans exhibit no oil on the surface. They are the best material for preparation of pour-over beverages. The light brown color of beans is generally preferred in the case of milder coffee varieties. There is no oil on the surface of such beans, as they are roasted for a short time and the oils do not migrate onto the bean surface. The light roast level is referred to as Light City, Half City, and Cinnamon roast. Some coffee roasting plants also use the names New England or White Coffee. The medium level of roasting is usually achieved at a temperature in the range of 210-220°C, *i.e.* at a point of occurrence of the second crack, and which the process should be discontinued. Medium and medium-dark roasting ensures a better aroma and lower acidity. Additionally, the beans contain more caffeine than in the light roast process and tend to have a more balanced flavor profile. This type of coffee has a medium brown color, a stronger flavor, and a non-greasy surface. It is often called the American roast, as it is widely preferred in the United States. These roasting degrees are referred to as City, American, and Breakfast roast. The medium-dark roast, often called Full City, has a richer aroma. The beans have a dark color, some oil on the surface, and a slight bittersweet aftertaste. This roast degree is achieved at high temperatures in the range of 220-240°C, at which oils are released on the surface of coffee beans. They determine the coffee flavor and produce a shiny black bitter surface; then, the beans are classified as the dark roast. Dark roast coffees range from slightly dark to charred, and the following names are often used interchangeably: High, Continental, New Orleans, European, Espresso, Viennese, Italian, and French roast.

Although there are literature reports showing that coffee infusions provide varying levels of CQAs (26.1-295.6 mg 100 mL^{-1}), there are limited data on the effect of the roasting degree on CQA levels, especially since most coffees on the market are often blends of *Arabica* beans from the Santos region in Brazil with *Canephora* coffees, *i.e*. *Robusta* beans from Vietnam, which are often of low quality. Taking into account the high consumption of espresso-based beverages in Poland, Europe, and other world countries, it should be concluded that the amount of CQAs in human nutrition is high, and the most important CGA group is relevant for human health. Therefore, this comprehensive study was aimed at assessment of the effect of the degree of coffee bean roasting on the content of CQAs (3-CQA, 5-CQA, and 4-CQA) and the impact of the process on the profile of aromatic compounds.

2. MATERIALS AND METHODS

2.1. Materials

The study was carried out on Arabica coffee beans *cv*. 'Typica' from a plantation located at an altitude of 1680 m a.s.l. in Huehuetenango, Guatemala. Typica is a variety of Arabica species, which is grown in many regions of the world, hence the diversity in its physicochemical traits, as in the case of other crops (Rybiński *et al.*, 2008). It is believed that the best 'Typica' beans come from Central America. The best quality is ascribed to coffee beans from bushes growing at altitudes above 1600 m a.s.l. in the mountainous regions of Huehuetenango and Coban facing the Caribbean Sea or in the San Marcos area facing the Pacific Ocean, where coffee beans have a fruitier flavor and higher acidity. It was the reason that we decided take reach in flavor variety in present study. As mentioned in the Introduction, there are several levels of roasting that differentiate the aroma or physical and chemical properties of coffee beans, but adjacent levels often only slightly differentiate these properties. Three degrees of roasting (light, medium, and dark), which are expected to differentiate coffee bean properties substantially, were used in the present study. These included the Cinnamon roast (light), the American roast (medium), and the Italian roast (dark) classified in color categories or rather brightness levels (Supplementary Materials, Photograph S1). Light beans classified as the Cinnamon roast were obtained at a temperature of 198°C, and the medium degree referred to as the American roast was achieved at a temperature of 212°C before the second crack. The process of roasting at a higher temperature in the range of 228-230°C until the second crack yielded dark beans classified as the Italian roast. The coffee beans were roasted at Rovigo Caffee using a Coffed SR 5 roaster equipped with a double-walled drum with sensors of the coffee bean and exhaust temperature. The computer-aided control and monitoring of the temperature in the roaster, the temperature of the coffee beans during the process, and the increase in the temperature of the beans referred to as the rate of rise (ROR) helped to achieve the expected roasting level.

2.2. Preparation of samples for determination of the bioactive compound content

Coffee beans (150 g) were ground in a Russell Hobbs grinder to achieve a grind size of 250-380 μm, with the largest proportion (75%) of particles with a maximum size of 320 μm (obtained using the sieve method). The ground samples were stored at a temperature of approximately 4°C in tightly closed polyethylene bags.

2.3. Preparation of phenolic compound extracts

Phenolic compounds contained in the samples were extracted three times with an 80% aqueous methanol solution in a ratio of 1:3 (v/v), each time shaking the samples for 30 min. The extracts were combined and the solvent was evaporated using a rotary vacuum evaporator (Rotavapor-EL, Büchi Labortechnik AG, Flawil, Switzerland). The residue was quantitatively transferred with an 80% aqueous methanol solution into 50 cm^3 volumetric flasks.

2.4. Determination of the total phenolic content

The content of phenolic compounds in methanol extracts and infusions was determined with the colorimetric method using the Folin-Ciocalteu reagent (Sigma-Aldrich, St. Louis, MO, USA) (Fig. S1 Supplementary Materials). 5 cm^3 of distilled water and 0.5 cm^3 of Folin-Ciocalteu reagent were placed in a 10 cm^3 volumetric flask. Next, 0.2 cm^3 of the extract was added and thoroughly mixed. The solution was left for three minutes at room temperature: then, 1 cm^3 of a saturated Na_2CO_3 solution was added and the flask was filled with distilled water to the mark. Absorbance was measured at λ_{max} 725 nm exactly after 1 h. Based on the standard curve, the total phenolic content in the coffee extracts and infusions was determined and expressed as gallic acid equivalents ($y = 0.0109x$; $R^2 = 0.996$).

2.5. Separation of phenolic compounds from extracts

The Chromabond® System (Macherey – Nagle, Germany) with SPE Bakerbond spe™ columns filled with quaternary amine (500 mg) was used for the separation of the phenolic acid fraction. The process consisted of four stages: I° – conditioning the columns (10 cm^3 of methanol, 10 cm^3 of distilled water, and 10 cm^3 of a 0.15% $NaHCO_3$ solution); II° – application of the sample (5 cm^3); III° – washing the column (15 cm^3 of a 0.15% $NaHCO_3$ solution); IV° – elution of phenolic acids with a mixture of 0.2 M H_3PO_4 and methanol (2:1 v/v) (10 cm^3). The eluate pH value was adjusted to approx. 3 by addition of 1 M NaOH.

2.6. Determination of the CGA content

The separation and identification of phenolic compounds was performed using high performance liquid chromatography (HPLC – Waters Milford, MA, USA) (Hečimović *et al.*, 2011; Rodrigues and Bragagnolo, 2013) (Fig. S2 Supplementary Materials). An XBridge C-18 column (4.6 x 100 mm; 3.5 μm) was used for the separation process carried out in the reversed phase system. The mobile phase comprised a mixture of a 50% aqueous acetonitrile solution (v/v) [A] with H_2O at pH 2.7 (acidified with ortho-phosphoric acid) [B]. The process was performed in a gradient mode. The concentration of phase [A] increased to 50% within 50 min; next, its concentration returned to 1% over the next 10 min. The mobile phase flow rate was 1 ml min^{-1}. The measurements were made with the use of a UV-Vis photodiode detector (Waters 2998) at a wavelength of 320 nm. The content of each CGA was calculated from the peak areas and standard curves and converted into chlorogenic acid equivalents.

2.7. Determination of the tocochromanol content in coffee beans

2 g (± 0.0001 g) of ground coffee beans and 0.5 g of pyrogallol were placed in a round-bottom flask. Next, 20 cm^3 of ethyl alcohol (96%) and 2.5 cm^3 of a 60% KOH aqueous solution were added. The sample was subjected to a 30-min saponification process under reflux at the solvent boiling point (78.4°C). Then, 50 cm^3 of a 1% NaCl solution was added to the saponified sample and cooled under running water; afterwards, 50 cm^3 of n-hexane with 10% ethyl acetate were added. The mixture was shaken at 300 rpm in a sealed flask for 30 min. Next, the sample was treated with 2 cm^3 of a saturated NaCl solution for thorough separation of the organic fraction containing unsaponifiable substances. After 15 min, an appropriate amount was taken from the upper organic layer into which unsaponifiable substances were extracted for chromatographic analyses. The content of tocochromanols was determined using high-performance liquid chromatography HPLC (Waters 600 Asc. Milord) (Gawrysiak-Witulska *et al.*, 2016; Górnaś *et al.*, 2014). A LiChrosorb Si 60 column (250 x 4.6 mm, 5 µm) and a fluorimetric detector (Waters 474) were used in the analysis. n-Hexane and 1.4-dioxane (96:4 v/v) were used as the mobile phase at a flow rate of 1.0 cm^3 min^{-1}. The measurements were carried out at the excitation wavelength $\lambda = 295$ nm and the emission wavelength $\lambda = 330$ nm. The compounds were identified through comparison of the retention times of individual peaks in the chromatograms of the analyzed samples and standard solutions.

2.8. Determination of the caffeine content

The caffeine content in the coffee extracts and infusions was determined using the same chromatographic system as for the determination of phenolic compounds (Hečimović *et al.*, 2011) (Fig. S3 Supplementary Materials). The measurements were made using a UV-Vis photodiode detector (Waters 2998) at a wavelength of 270 nm. The caffeine content was calculated from the peak area and the standard curve ($y = 2374885.56x$; $R^2 = 1.00$).

2.9. An electronic nose

An Agrinose electronic nose constructed at the Institute of Agrophysics, Polish Academy of Sciences (Lublin, Poland) in Lublin, was used in the analyses (Gancarz *et al.*, 2022; Rusinek *et al.*, 2022; Wilson, 2023). It consists of eight MOS gas sensors (AS-MLV-P2-CO, butane, methane, ethanol, hydrogen, specifically designed for volatile organic compounds; TGS2602-ammonia, hydrogen sulfide, high sensitivity to VOCs, and odorous gases; TGS2603-odors generated from spoiled foods; TGS2612-methane, propane, and butane; TGS2610-LP gas, butane; TGS2611-natural gas, methane; TGS2620-solvent vapors, volatile vapors, alcohol; TGS2600-general air contaminants, hydrogen, and carbon monoxide). Maximum responses of the sensors to emission of VOCs (volatile organic compounds) were analyzed in the study (Rasekh *et al.*, 2022). Each sample of coffee was placed into a special Gas Test Box (Figaro, Japan) The measurement cycle and the sampling protocol consisted of a baseline purge for 10 s, a sample draw-in for 60 s, and a sample purge for 140 s. DasyLab software was used to convert analog signals to digital signals. The graph obtained was converted to the *.xls format and analyzed using statistical software.

2.10. GC-MS Analysis

The intensity of the signals of volatile organic compounds contained in the coffee was determined with the use of a Trace GC Ultra gas chromatograph (ThermoFisher Scientific, Waltham, MA, USA) integrated with an ITQ 1100 mass spectrometer (ThermoFisher Scientific, Waltham, MA, USA). An SPME (solid-phase micro-extraction) fiber with an absorbent (50/30 µm Divinylbenzene/Carboxene/Polydimethylsiloxane (DVB/CAR/PDMS), Stableflex (2 cm) 24 Ga (Sigma Aldrich, Poznań, Poland)) was placed in the measuring chamber for 30 min together with the material emitting volatile compounds. Next, it was transferred to a GC injector for 5 min to desorb VOCs. A Zebron ZB-5Msplus Capillary GC 30 m x 0.25 mm x 0.25 µm column was used for the analysis. The injection temperature was 60°C for 5 min, and then increased from 60 to 250°C at a rate of 5°C min^{-1} and from 250 to 270°C at 10°C min^{-1}. The final temperature was maintained for 5 min. The helium flow rate was kept constant at 2.2 mL min^{-1}. The compounds were identified with the use of the Wiley library (Żytek *et al.*, 2023).

2.11. Statistical analysis

Statistica software (version 12.0, StatSoft Inc., Tulsa, OK, USA) was used for statistical analyses. Principal component analysis (PCA), analysis of variance, and determination of correlations were performed at a significance level of $\alpha = 0.05$. The PCA data matrix for the statistical analysis of the results of the tests had 28 columns (volatile compounds, tocopherols, caffeine contents, volatile emission intensity, and bioactive compounds) and 9 rows (Cinnamon, American, and Italian roast). The input matrix was scaled automatically. The optimal number of principal components obtained in the analysis was determined based on the Cattel criterion.

3. RESULTS AND DISCUSSION

3.1. Determination of the content of bioactive compounds and caffeine

The results of the analysis of the effect of the Cinnamon, American, and Italian roast processes on the content of bioactive compounds are presented in Tables 1-3. The highest total phenolic content was detected in the green coffee (32.30 mg g^{-1}). Grzelczyk *et al.* (2023) indicated potential pro-health effects of enzymes contained in coffee extracts

Table 1. Content of phenolic compounds of Guatemalan coffee

Roasting level	Total phenolic content	3-caffeoylquinic acid; 3-CQ	5-caffeoylquinic acid; 5-CQA	4-caffeoylquinic acid; 4-CQA	4-feruloylquinic acid; 4-FQA	5-feruloylquinic acid; 5-FQA	3,4-dicaffeoylquinic acid; 3,4-diCQA	3,5-dicaffeoylquinic acid; 3,5-diCQA	4,5-dicaffeoylquinic acid; 4,5-diCQA	Content of phenolic compounds
	(mg GA g^{-1})	(mg g^{-1})								
Green coffee	29.81±0.34	2.02±0.02	21.06±0.08	2.80±0.02	0.41±0.01	1.56±0.01	0.96±0.01	2.11±0.01	1.37±0.01	32.30±0.13
Cinnamon roast	23.76±1.34	2.06±0.03	5.24±0.03	2.82±0.02	0.31±0.01	0.55±0.01	0.25±0.01	0.20±0.01	0.34±0.02	11.8±0.07
American roast	24.08±1.13	1.67±0.01	4.24±0.01	2.34±0.01	0.27±0.01	0.48±0.01	0.19±0.01	0.15±0.01	0.27±0.01	9.62±0.02
Italian roast	26.34±1.86	1.36±0.01	3.55±0.02	2.07±0.01	0.23±0.01	0.41±0.01	0.17±0.01	0.13±0.01	0.22±0.01	8.25±0.05

Table 2. Content of tocopherol of Guatemalan coffee

Roasting level	α-T	β-T	Total
	(mg 100 g^{-1})		
Green coffee	2.29±0.06	5.89±0.06	8.18±0.12
Cinnamon roast	2.35±0.04	7.08±0.04	9.42±0.01
American roast	2.46±0.08	8.04±0.03	10.50±0.04
Italian roast	2.43±0.05	8.19±0.04	10.62±0.01

Table 3. Content of caffeine compounds of Guatemalan coffee

Roasting level	Caffeine content (mg g^{-1})
Green coffee	15.22±0.07
Cinnamon roast	12.79±0.17
American roast	12.55±0.05
Italian roast	12.02±0.04

on the human organism, with the greatest potential exhibited by isolates of dichlorogenic acids from green Arabica coffee (Grzelczyk *et al.*, 2023). Each subsequent coffee roasting at increasing temperatures reduced the content of phenolic compounds as follows: from 11.8 mg g^{-1} in Cinnamon roast coffee and 9.26 mg g^{-1} in American roast to 8.25 mg g^{-1} in Italian roast. The decrease was caused by the increasing roasting temperature and time (Socała *et al.*, 2021). In the group of polyphenols, the largest reduction was exhibited by 5-caffeoylquinic acid (5-CQA): from 21.06 mg g^{-1} in the green coffee beans to 5.24, 4.24, and 3.55 mg g^{-1} in the subsequent roasting level, respectively. In addition to their positive effects on health, phenolic compounds present in coffee beans have an impact on the sensory quality of coffee beverages. They are responsible for their astringency (dryness, roughness, and smoky sensation in the mouth) and bitterness. However, the detailed biochemical mechanisms (interactions of chemical compounds with other components or interactions of compounds with saliva) have not been fully elucidated to date (Dinnella *et al.*, 2009; Ong *et al.*, 2018). During the roasting process, CGAs can isomerize and hydrolyze to form quinic and cinnamic acids. They can also form chlorogenic lactones responsible for the bitterness of coffee (Farah *et al.*, 2005). At the high coffee roasting temperature, CGAs can also be incorporated into melanoidins (products of the Maillard reaction), which are responsible for coffee bitterness together with other bitter flavor compounds, *e.g.* caffeine and trigonelline. The thermal degradation of CGAs leads to generation of volatile phenols, *e.g.* guaiacol, 4-ethylguaiacol, and 4-vinylguaiacol, which are responsible for the spicy and smoky aroma of coffee (Toci and Farah, 2014).

Two homologues of tocopherols α-T and β-T were detected in the analyzed coffee beans. The lowest content of tocopherols and their sum, *i.e.* 8.18 mg 100 g^{-1}, was

determined in the green coffee beans, which is consistent with literature data (Socała *et al.*, 2021). A slight increase in total tocopherols was noted in the subsequent roasting levels, *i.e.* the content of these compounds was 9.42 mg 100 g^{-1} in the Cinnamon roast beans, 10.50 mg 100 g^{-1} in the American roast coffee, and 10.62 mg 100 g^{-1} in the Italian roast variant. Tocochromanols are lipophilic vitamin E active compounds with antioxidant properties protecting polyene fatty acids from oxidation. The coffee bean roasting process is accompanied by changes in the fat fraction. Autooxidation of fats leads to generation of volatile aldehydes and other compounds, *i.e.* 2,3-methylbutanone and hydroxyacetone. Aldehydes derived from the oxidation of polyene fatty acids, *e.g.* hexanal formed from linoleic acid, may be responsible for coffee rancidity. Terpenoids may disintegrate into monoterpenoids as well (Makri *et al.*, 2011).

The highest caffeine content, *i.e.* 15.22 mg g^{-1}, was determined in the green coffee. A slight decrease in its content was observed in each subsequent roasting level and reached 12.79 mg g^{-1} in the Cinnamon roast beans, 12.55 mg g^{-1} in the American roast coffee, and 12.02 mg g^{-1} in the Italian roast. These results and trends are in agreement with results reported by other researchers (Górecki and Hallmann, 2020). Caffeine, which is an odorless and bitter substance, is very stable during the roasting procedure and may contribute to the sensory bitterness of coffee beverages.

3.2. Determination of volatile compounds by GC-MS

Tables showing the volatile compounds detected in the green coffee and in the Cinnamon, American, and Italian roast level are presented in the Tables 4 and 5. Table 4 shows 18 major volatile compounds that were identified and compared with library data (Gancarz *et al.*, 2022). The largest percentage in the VOC profile was represented by propane, 2-methyl-1-nitro- (34.04%), 4,5-difluoroctane isomer (11.55%), and 2-furanmethanol, acetate (6.25%). These three compounds accounted for 51.75% of the total VOC profile. All the three main volatile compounds had a low carbon index, which proves their high volatility. In the next step, the individual compounds were classified into chemical groups: alcohols, acids, ketones, azines, esters, amines, terpenes, and others (unidentified).

Coffee bean of each roasting level had approximately two-fold higher contents of the main volatile compounds, likewise in previous studies on coffee roasting defects (Rusinek *et al.*, 2022). The present results are qualitatively and quantitatively consistent with findings reported in previous studies. The slight differences in the range of several percent may be associated with the biological differences between both the research material batches and the roasting modes.

The analysis showed the presence of 29 different compounds in the American roast beans, 25 in the Cinnamon roast variant, and 24 in the Italian roast coffee (Table 5).

Table 4. Percentage of chemical compounds for green beans with standard deviations (±)

R_{time}	Name of compounds	Chemical formula	Green beans (%)
1.87	4,5-difluoroctane isomer	C8H10F2	11.55±0.32
3.09	8,11,14-eicosatrienoic acid, methyl ester	C21H36O2	5.61±0.33
4.05	2-furanmethanol	C5H6O2	5.66±0.23
5.82	2-methyl-3-(2-methylpropyl) pyrazine	C9H14N2	4.4±0.18
6.47	1,3,7-octatriene, 3,7-dimethyl-, E-	C10H16	4.88±0.24
7.44	5-amino-1-benzoyl-1H-pyrazole-3,4-dicarbonitrile	C12H7N5O	5.01±0.35
8.35	Propane, 2-methyl-1-nitro-	C4H9NO2	34.04±0.98
8.47	2-furanmethanol, acetate	C7H8O3	6.25±0.46
9.61	Oxiranecarboxamide, 2-ethyl-3-propyl-	C8H15NO2	1.59±0.11
9.70	6,6-dimethyl-2-methylene-bicyclo[3.1.1] heptane	C10H16	5.31±0.42
9.86	2-cyclopropyl-2-methylspiro[2.2]pentane-1-carboxylic acid	C10H14O2	4.01±0.22
15.22	4-hydroxy-4-methyl-hex-5-enoic acid tert-butyl ester	C11H20O3	2.61±0.11
15.42	9,12,15-octadecatrienoic acid, methyl ester	C19H32O2	1.02±0.09
18.15	16-methylene-1,20-dioxopregn-4-en-17-yl acetate	C24H32O4	1.02±0.07
21.06	1,4-methanoazulene,decahydro-4,8,8-trimethyl-9-methylene-,[1S-(1α,3Aβ,4α,8Aβ)]-	C15H24	1.12±0.10
23.37	Ethanone, 1-(5,6,7,8-tetrahydro-2,8,8-trimethyl-4H-cyclohepta[B]furan-5-yl)-	C14H20O2	1.55±0.20
31.28	Alanine, 3-(benzyloxy)-, L-	C10H13NO3	1.11±0.07
32.19	Hexadecadienoic acid, methyl ester	C17H30O2	3.26±0.22

Table 5. Volatile compounds determined in the chromatographic analysis. %-percentage share of the compound in the tested sample immediately after roasting of Cinnamon roast, American roast and Italian roast with standard deviations (±)

No.	R_{time}	Name of compounds	Chemical formula	Cinnamon roast	American roast	Italian roast
				(%)		
1	1.29	2-acetonyl-3-cyano-2,3-dimethylcyclobutane-1-carboxylic acid	C11H15NO3	0	9.52±0.99	0
2	1.61	Furan, 2-methyl-	C5H6O	5.12±0.22	4.23±0.55	6.55±0.34
3	1.85	Butanal, 2-methyl-	C5H10O	2.88±0.12	2.7±0.16	2.57±0.11
4	2.01	(2E)-2-(hydroxyimino)etyl acetate	C4H7NO3	1.33±0.09	0	0
5	2.42	Pyridine	C5H5N	9.41±0.55	6.25±0.78	10.99±078
6	3.14	Pregnane-3,11,20,21-tetrol, cyclic 20,21-(butyl boronate), (3α,5β,11β,20R)-	C25H43BO4	0.89±0.07	0	0
7	3.17	2-butanone	C4H8O	3.26±0.12	2.7±0.22	2.70±0.23
8	3.20	2-thiopheneethanol,5-(4,5-dihydro-4,4-dimethyl-2-oxazolyl)-	C11H15NO2S	0	0	2.28±0.11
9	3.48	Pyrimidine, 2-methyl-	C5H6N2	8.69±0.40	8.22±0.44	8.89±0.41
10	3.60	2-furancarboxaldehyde	C5H4O2	6.22±0.31	6.44±0.34	0
11	4.01	2-furanmethanol	C5H6O2	9.71±0.22	8.19±0.55	13.88±0.76
12	4.31	1,5-dimethyl-2,3-dihydro-1H-pyrrole	C6H11N	0	3.02±0.21	5.10±0.28
13	5.50	Ethyl 2,3-pentadienoate	C7H10O2	1.6±0.07	0	1.78±0.09
14	5.63	2-amino-4-methyl-2-pentennitrile	C6H10N2	3.02±0.11	2.33±0.12	2.90±0.11
15	5.75	Pyrimidine, 4,6-dimethyl-	C6H8N2	13.01±0.37	10.12±0.22	10.99±0.40
16	5.86	Pyridine-2-D, 6-ethyl-	C7H8DN	4.06±0.09	3.22±0.12	3.48±0.22
17	7.35	2-furancarboxaldehyde, 5-methyl-	C6H6O2	7.14±0.39	5.96±0.21	6.20±0.24
18	8.45	2-furanmethanol, acetate	C7H8O3	10.49±0.99	6.56±0.23	10.70±0.333
19	8.60	2-pyridinecarbonitrile, 1,2,5,6-tetrahydro-1-methyl-	C7H10N2	4.78±0.32	3.39±0.27	3.90±0.11
20	8.79	Pyrazine, 2-ethyl-5-methyl-	C7H10N2	3.29±0.11	2.33±0.11	2.60±0.09
21	11.28	Pyrazine, 3-ethyl-2,5-dimethyl-	C8H12N2	2.01±0.07	1.32±0.09	1.53±0.06
22	11.42	Furan, 2,2'-methylenebis-	C9H8O2	0.96±0.05	0.6±0.04	0
23	11.69	2-cyclopenten-1-one, 3-ethyl-2-hydroxy-	C7H10O2	0	0	0.83±0.04
24	14.51	1,1-dimethyl-1,3-dihydroisobenzofuran-3-one	C10H10O2	0.48±0.03	0	0.70±0.02
25	14.79	2-hydroxymethylene-6-isopropyl-3-methyl-cyclohexanone	C11H18O2	0	0.40±0.05	0
26	18.34	3,5-heptadienal, 2-ethylidene-6-methyl-	C10H14O	0.33±0.01	0.30±0.03	0.41±0.01
27	19.50	Ethyl (2E,4E,6E)-9-formyl-10-oxo-2,4,6,8-decatetraenoate	C13H14O4	0	0	0.11±0.01
28	22.48	1H-2-benzopyran, 3-(3,4-dimethoxyphenyl) -6,7-dimethoxy-1-methyl-	C20H22O5	0.19±0.01	0.29±0.05	0.29±0.01
29	26.08	2,7-diphenyl-1,6-dioxopyridazino[4,5-2',3'] pyrrolo[4',5'-D]pyridazine	C20H13N5O2	0.21±0.01	0.28±0.03	0
30	26.18	4H-1-benzopyran-4-one, 2-(3,4-dimethoxyphenyl)-3,5-dihydroxy-7-methoxy-	C18H16O7	0	0.23±0.05	0
31	28.39	Cholan-24-oic acid, 3,7,12-trihydroxy-, (3α,5β,7α,12α)-	C24H40O5	0	0.53±0.06	0
32	28.44	Tridecanoic acid, 12-methyl-, methyl ester	C15H30O2	0	0.33±0.02	0
33	31.28	1-isothiocyanato-3-methyladamantane	C12H17NS	0.14±0.01	0.11±0.01	0.14±0.01
34	32.19	Methyl (7E)-7-hexadecenoate	C17H32O2	0.78±0.03	7.09±0.48	0.48±0.02
35	32.64	Hexadecanoic acid, methyl ester	C17H34O2	0	3.00±0.13	0
36	34.60	Heptadecanoic acid, methyl ester	C18H36O2	0	0.34±0.05	0

The volatile fraction was found to contain several compounds that are often found in thermally treated products (Nooshkam *et al.*, 2019). These were *e.g.* furans formed as by-products of sucrose degradation, pyrazine derived from protein degradation, and pyridines generated through trigonelline degradation. Heat-induced volatile compounds (furans, pyrazines, and pyridines) are more closely related to the aroma of roasted coffee than esters, which are abundant in green coffee (Chrostowska-Siwek, 2011).

Pyrimidine, 4,6-dimethyl- was one of the most abundant volatile substances accounting for 13.01% in beans of the Cinnamon roast coffee, 10.12% in the American roast, and 10.99% in the Italian roast (Yuwono *et al.*, 2019). Another compound constituting a high percentage was 2-furanmethanol (furfuryl alcohol) (Tang *et al.*, 2022). This furan is a product of the Maillard reaction. Large amounts of 2-furancarboxaldehyde, 5-methyl, known as 5-methylfurfural, were detected as well. These Maillard reaction products impart the flavor of almonds, burnt sugar, and caramel to foodstuffs. Pyridine was present in a high amount (approx. 9-10%) in the beans of Cinnamon and Italian roast, but constituted only 6.25% in the American roast variant. The content of 2-furanmethanol, *i.e.* furfuryl acetate responsible for a sweet and fruity flavor, was 9.71% in the beans of Cinnamon roast, 8.19% in the American roast, and 13.88% in the Italian roast. High content of 2-acetonyl-3-cyano-2,3-dimethylcyclobutane-1-carboxylic acid (9.52%) was detected only in the American roast coffee.

The volatile substances determined in the study were assigned to chemical groups, and the percentage content of the groups in the entire aroma composition was calculated (Table 6). Azines were the largest group accounting for 35.13% in the American roast beans, 45.46% in the Cinnamon roast, and 42.38% in the Italian roast. Alcohols were the other abundant group of compounds; their content was estimated at 15.15% in the beans of American roast, 20.20% in the Cinnamon roast, and 26.86% in the Italian roast. Aldehydes and furans were abundant groups as well (Table 6). The presence of acids was only detected in the American roast; hence, this type of roasting procedure ensures the widest composition of various groups of compounds (Rusinek *et al.*, 2022). Therefore, it can be assumed that this roasting level results in the largest composition of aromas.

3.3. Electronic Nose response to the intensity of VOC emission

The results of the VOC emission intensity analyses are presented in Table 7. The intensity of the emission of volatile substances varied, depending on the roasting method (Lu *et al.*, 2023; Radi *et al.*, 2016). The highest ΔR/Rmax values were recorded in the beans of American roast, *i.e.* the most popular roasting mode. This indicates the high aromatic potential and the varied aroma of this of roasting level. Sensors detecting volatile orga-nic compounds and food aroma, *i.e.* TGS 2602, TGS 2603, and AMS-MLV-P2, exhibited the lowest responses in the case of the Italian roast. This may be related to the loss of some of the coffee aroma during the intensive roasting process in comparison with the other roasting levels, *i.e.* the Cinnamon and American roasts.

3.4. Principal component analysis

All roasted coffee parameters, *i.e.* the content of CGAs, tocopherols, caffeine, groups of volatile compounds, and VOC emission intensity, were analyzed to correlate these variables with the three roasting level of coffee bean.

Figure 1a shows the projection of the variables onto the PC1 and PC2 planes. The first and second principal components describe 84.64 and 8.36% of the correlations,

Table 6. Groups of chemical compounds

Roasting level	Acids	Furanes	Aldehydes	Esters	Azines	Ketones	Alcohols	Amines	Pyranes	Others
	(%)									
Cinnamon roast	n.d.	6.08±0.05	16.57±0.25	3.71±0.08	45.46±0.85	3.74±0.06	20.20±0.88	3.16±0.04	0.19±0.01	0.89±0.02
American roast	10.05	7.85±0.11	15.4±0.16	10.76±0.22	35.13±0.96	2.7±0.07	15.15±0.57	2.44±0.08	0.52±0.01	n.d.
Italian roast	n.d.	11.65±0.10	9.18±0.09	2.37±0.05	42.38±0.89	4.23±0.04	26.86±0.75	3.04±0.07	0.29±0.01	n.d.

n.d. - not detected.

Table 7. Results (with standard deviation ±) of measuring the intensity of the impact of volatile substances by Agrinose (ΔR/Rmax)

Roasting level	TGS 2602	AMS-MLV-P2	TGS 2603	TGS 2612	TGS 2610	TGS 2611	TGS 2620	TGS 2600
Cinnamon roast	3.03±0.07	1.01±0.04	0.40±0.04	0.20±0.03	0.54±0.03	0.43±0.02	1.26±0.09	1.19±0.08
American roast	3.06±0.01	1.77±0.18	0.75±0.07	0.89±0.12	0.93±0.03	0.72±0.05	1.87±0.06	1.83±0.03
Italian roast	2.36±0.37	0.65±0.10	0.34±0.05	0.37±0.05	0.70±0.10	0.70±0.07	1.58±0.24	1.47±0.23

respectively. All phenolic compounds and caffeine content are strongly positively correlated with each other (Febrianto and Zhu, 2023; Jiang *et al.*, 2023), strongly negatively correlated with β-T, and less strongly correlated with α-T. The presence and levels of all phenolic compounds as well as the caffeine content are positively correlated with the Cinnamon roast mode. In turn, α-T and β-T tocopherols are correlated with the Italian and American roast modes. Generally, the first principal component PC1 describes the level of coffee roast (Fig. 1b). The light Cinnamon roast coffee is located on the positive side of PC1. The American roast are located closer to the PC1 axis on the negative side, whereas the Italian roast are located farther from the axis.

Figure 2a shows the projection of the variables onto the PC1 (74.52%) and PC2 (22.84%) planes. Figure 2b presents the projection of the cases on the PC1 and PC2 planes. The two principal components explain 97.36% of the relationship between the variables (chemical groups of volatile compounds and sensor responses – intensity of volatile compound emission) and the cases (three types of coffee roast). It can be concluded from Fig. 2a that the intensity of VOC emission reflected by the e-nose sensor responses is positively strongly correlated with the presence of pyranes, esters, and acids and negatively correlated with the content of ketones, amines, and azines (Lu *et al.*, 2023; Rusinek *et al.*, 2022). The emission intensity determined by the sensors

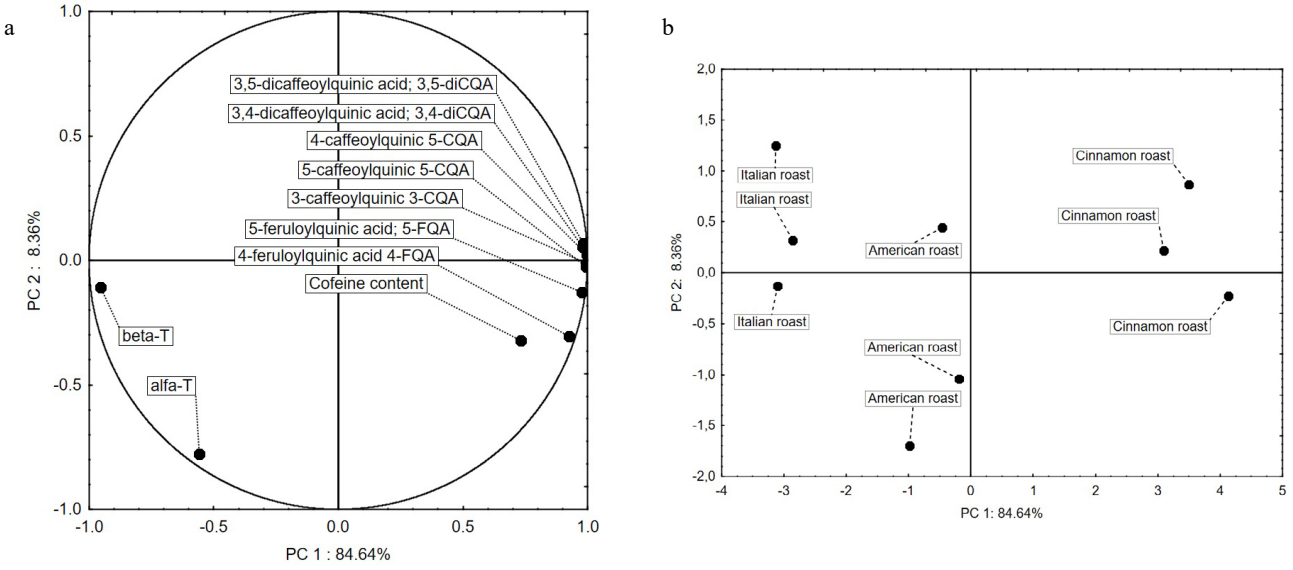

Fig. 1. Projection of variables: bioactive compounds, tocopherols, and caffeine characterizing the types of roasting on the PC1 and PC2 loadings plot (a), projection of cases characterizing the roasting level on the PC1 and PC2 scores plot (b).

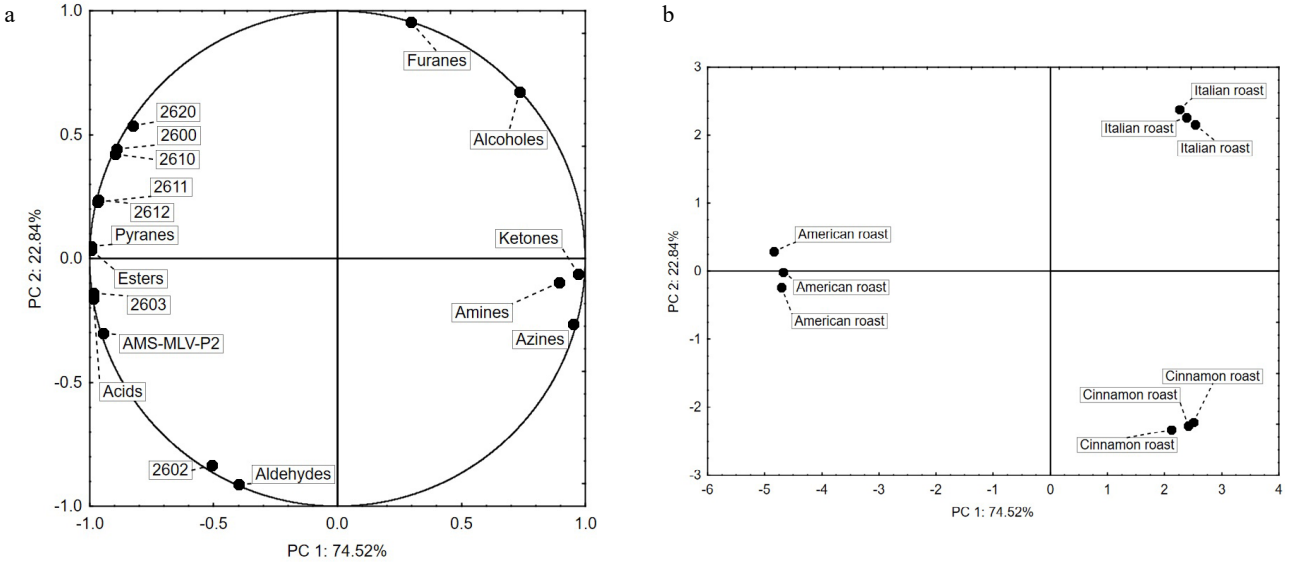

Fig. 2. Projection of variables: chemical groups of volatile compounds and sensor responses (volatile emission intensity) characterizing the roasting level on the PC1 and PC2 loadings plot (a), projection of cases characterizing the roasting level on the PC1 and PC2 scores plot (b).

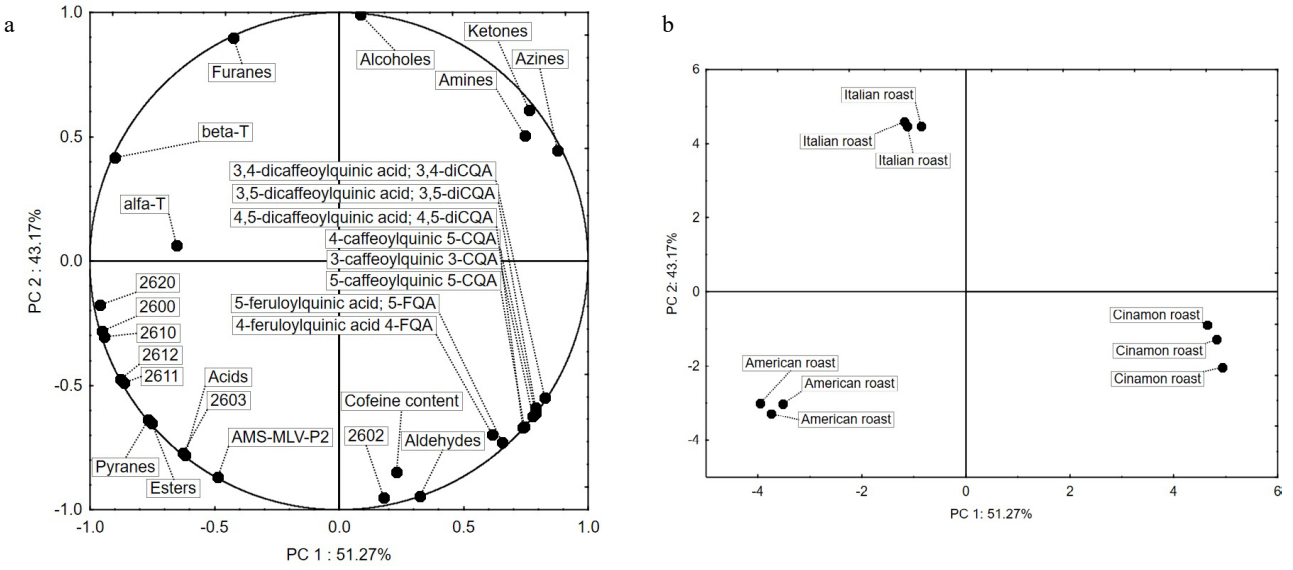

Fig. 3. Cumulative analysis. Projection of variables: chemical groups of volatile compounds, sensor responses (volatile emission intensity), bioactive compounds, tocopherols, and caffeine characterizing the roasting level on the PC1 and PC2 loadings plot (a), projection of cases characterizing the type of roasting on the PC1 and PC2 scores plot (b).

characterizes especially the American roast (Fig. 2b). In this case, the second principal component PC2 reflects the roasting level. The Cinnamon roast (light) are located on the negative side of PC2, the American roast (medium) are located on the PC2 axis, while the Italian roast (dark) are located on the positive side of PC2. Similar correlations were obtained in previous studies of three defective roasting modes (Rusinek *et al.*, 2022).

Figures 3a and 3b present a pooled analysis of all variables characterizing the three level of coffee roast. This analysis fulfils to the main objective of the study, *i.e.* the determination of correlations of bioactive compounds, VOC emission intensity, groups of volatile compounds, tocopherols, and caffeine content with the coffee roasting degree.

The two principal components PC1 (51.27%) and PC2 (43.17%) explain 94.44% of the relationships between the variables (chemical groups of volatile compounds, sensor responses – VOC emission intensity, content of caffeine, tocopherols, and phenolic compounds) and the cases (three coffee roast types). The Cinnamon roast (Fig. 3b) is positively correlated with the content of phenolic compounds, caffeine, and aldehydes. This mild roast leaves the greatest amounts of phenolic compounds and caffeine in the coffee (Lu *et al.*, 2023). In turn, the American roast is positively correlated with the content of acids, esters, and pyranes. The dark Italian roast coffee is characterized by increased amounts of furanes and β-T and α-T tocopherols. The increased content of tocopherols in the Italian roast is associated with the presence of oils on the coffee beans, which is a natural phenomenon in the case of dark roasting. Tocopherols are a class of organic compounds comprising various methyl phenols, many of which exhibit vitamin E activity. They are derived from fats (Gawrysiak-Witulska *et al.*, 2016, 2022).

The intensity of the aroma determined by the electronic nose positively correlates with the American roast mode. This indicates that this type of roasting yields the most intense aroma.

4. CONCLUSIONS

The highest content of total phenolic compounds was detected in the green coffee. Their content was reduced, starting from the Cinnamon roast through the American roast to the Italian roast. The highest caffeine content was detected in the green coffee. A slight decrease in its content was observed in coffee beans subjected to each subsequent roasting level, *i.e.* the Cinnamon, American, and Italian roasts.

Each coffee roasting level (Cinnamon, American, and Italian roasts) generated different content of phenolic compounds, caffeine, tocopherols, and volatile compounds and were responsible for the varied intensity of VOC emission. The American roast proved to be the most balanced type of roasting in terms of the content of bioactive compounds as well as the chemical groups and profile of volatile compounds. This roasting level was also characterized by the highest intensity of VOC emissions, which is expected by the consumer.

The highest content of tocopherols was detected in samples subjected to the Italian roast, which causes the release of oils, and it is well known that fats are a source of tocopherols.

The use of an electronic nose to evaluate the coffee roasting process as an instrumental tool supporting the work of a barista can be an invaluable and objective tool for determination of the intensity of the coffee blend aroma in real time.

Conflicts of interest: The authors declare no conflict of interest.

Declaration of competing interest. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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