

### IDENTIFICATION OF VOLATILES IN GREEN *COFFEA ARABICA* AND DETERMINATION OF CHANGES CAUSED BY THE ROASTING PROCESS

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#### ABSTRACT

This study was aimed to understand and analyze the variability of volatile compounds in green and roasted coffee. We observed the influence and change in the profile of volatiles in samples roasted on medium roasting level, originating from different growing areas. We analyzed 9 samples, which we differentiated into three groups: Africa (Burundi, Uganda, Rwanda), Central America (Guatemala, Costa Rica, Honduras), South America (Colombia, Brazil, Bolivia). Volatiles were analyzed using GC-MS. Approximately 350 volatile compounds have been identified in green coffee. The main compounds identified in coffee samples included furan derivatives, aldehydes, alcohols, organic acids and their esters, hydrocarbons (alkanes, alkenes, alkynes, and aromatic hydrocarbons), terpenoids, heterocyclic compounds, ketones, amines, alkynes, and nitriles. Content of volatiles was expressed as concentration (%). The results show that the roasting process significantly affects the presence and concentration of volatiles, given the formation of new volatile compounds and degradation of several occurred. In our research, aldehydes, alcohols, organic acids and esters, alkanes, terpenoids, alkenes, nitriles, aromatic hydrocarbons decreased due to the roasting process. Nevertheless, only in Central America samples, aromatic hydrocarbons increase due to roasting. Furan derivatives, heterocyclic compounds, ketones, amine, alkynes increased due to the roasting process. However, only in South America samples, alkynes decreased due to roasting. However, alkynes in Central America samples remained unchanged due to the roasting.

**Keywords:** volatile compounds, green coffee, roasted coffee, coffee quality, chromatography (GS-MS)

#### INTRODUCTION

Volatiles are organic compounds that evaporate at room temperature and are directly related to the aroma. The final quality of coffee beverage and the chemical composition of roasted beans is affected by the chemical components of raw green beans and the processing conditions after harvest (storage, roasting). Coffee is one of the most complex beverages, which contain many non-volatile and volatile compounds. The non-volatile compounds of coffee are carbohydrates, lipids, melanoidins, minerals, and alkaloids such as caffeine, trigonelline, and chlorogenic acid. These are degraded, due to the effect of heat treatment, in particular roasting. Chlorogenic acid and trigonelline degrade rapidly during roasting to form phenolic mixtures and pyridines/pyrroles. Together with other volatiles, these newly formed compounds affect the quality or taste of coffee (Heo *et al.*, 2020).

Volatile compounds in coffee are the most valuable part of roasted coffee beans and create a unique taste and aroma. The aroma of coffee is one of the distinctive characteristics of this commodity (Kim *et al.*, 2019).

Seninde and Chambers (2020) stated that the aroma intensity and the profile of the coffee could vary depending on the degree of roasting, origin, and type. Green coffee beans are characterized by unpleasant taste. Thermal reactions achieve further development of requested pleasant and characteristic tastes during the roasting process. Compared to roasted beans, green coffee beans have only a basic chemical composition of volatiles. However, roasted coffee contains significantly more types of volatile substances (Pereira *et al.*, 2019). The concentration of total volatile compounds in roasted coffee can undergo significant changes depending on the heat profile used during the roasting process (Toci *et al.*, 2020).

Medium roasting is a prevalent type of roasting. The green beans are heated to 200-240 °C for 10-15 minutes during the roasting process, depending on the desired degree of roasting. The roasting process leads to fundamental changes in coffee's chemical composition and biological activities due to the development of compounds in the Maillard reaction and the organic reactions caused by pyrolysis. Pereira *et al.*, (2019) confirmed that the most important reactions associated with the volatile profile of coffee beans are Strecker degradation, Maillard reaction, and pyrolysis. Due to the roasting of coffee, taste and aromatic properties are achieved and formed (Somporn *et al.*, 2011). The formed aroma results from exothermic and endothermic reactions when the coffee beans reach a temperature of approx. 190 °C. Several free amino acids and peptides are used in

the Strecker degradation process, while other amino acids and sucrose participate in Maillard reactions, resulting in a change in bean color. From light brown to almost black (Seninde and Chambers, 2020).

The mode of heat transfer and the applied temperature profile are the most critical processing parameters that affect roasted coffee beans' physical and chemical properties, coffee quality, and biological activities (Somporn *et al.*, 2011).

Scientific analyzes of the volatile composition of coffee have so far revealed approximately 1,000 volatile ingredients, including aromatic active and non-aromatic active ingredients from both green and roasted coffee. Approximately 0.1% by weight of roasted coffee is volatile (Mahmud *et al.*, 2020).

The main aim of this research was a complex overview on volatiles contained in green *Coffea arabica* from various well-known growing areas from Africa, Central America, and South America. And a statistical comparison of profile of volatiles in green coffee beans and their roasted form. For this purpose, we used Medium roasting level, given the vast popularity among consumers.

#### MATERIAL AND METHODS

##### Material

Samples of green *Coffea arabica* were purchased from Barzzuz Ltd. (Banská Bystrica, Slovakia). This company imports and processes coffee. We analyzed samples from Africa, Central America, and South America from various well-known regions. Table 1 contains a detailed list of green samples. Furthermore, green samples were then roasted to Medium roasting level Full City++ (232 °C) using a roasting machine (Behmor 1600, model TO9500T). During the roasting, the first crack occurred at 205 °C, end of the first crack at 215 °C. The second crack started at 225-230 °C (level Full City +). After five seconds, the temperature gets to 232 °C, thus Full City ++ (approx. time of roasting 10 minutes). Analyzed were both green samples and their roasted forms.

**Table 1** List of analyzed samples

Continent	Country	Variety	Processing	Region	Altitude (mamsl)
Africa	Burundi	B	W	Kayanza	1700 - 1800
Africa	Uganda	B	W	Buigsu	1300 - 2600
Africa	Rwanda	K, B	W	Gasetza	1500 - 1700
South America	Brazil	B	PN	São Sebastião da Grama,	1150 - 1350
South America	Columbia	C1, B, T	W	Multiple	1200 - 2000
South America	Bolivia	C1, C2, P1	W	Altiplano-Hochebene	1500 - 1700
Central America	Guatemala	B	W	Rainforest Coban	1300 - 1500
Central America	Costa Rica	C1	W	San Rafael Tarrazu	1200 - 2000
Central America	Honduras	B, T, C2, L	N	La Paz, Marcala	1200 -1800

Note: Variety: B – Bourbon, C1 – Caturra, C2 – Catuai, K – Kent, L- Lempira, P1 – Poca, T – Typica, W - washed, wet processed, PN - pulped natural, N – dry process, natural; mamsl – meters above mean sea level

**Methodology**

**Identification of volatiles using gas chromatography (GC-MS)**

For GC-MS, 10 g of homogenized green coffee beans were put into 40 mL glass vials with septum Archon caps ptf/sil. The samples was warmed up to 35 °C for 15 minutes in Metalthermblock Liebisch Labortechnik. Self-sorption was performed with Fiber: Carboxen® / PDMS (CAR/PDMS) 2 cm, time 30 minutes at 35 °C, followed by GC-MS analysis. Volatiles were determined according to method previously described in *Sádecká et al., (2014)* with modifications. The Agilent Technologies 6890 gas chromatograph (Agilent Technology, Palo Alto, USA) equipped with an Agilent Technologies 5973 selective inertial detector (MSD). Volatiles were separated using a J&W 122-7333 DB-WAXetr 30m x 0.25mm x 0.5µm capillary column. The carrier gas was helium, and the injector temperature was 250 °C. The oven temperature was programmed to be isothermal at 50 °C for 1 minute, then heated to 250 °C at a rate of 5 °C.min<sup>-1</sup>. Input parameters were as follows: splitless mode (green coffee), split mode (roasted coffee), initial temperature: 250 °C, pressure: 88.9 kPa, flow rate: 20.0 mL.min<sup>-1</sup>, cleaning time: 1.00 min, total flow rate: 24.6 mL.min<sup>-1</sup>. Electron ionization (EI) was set to 70 eV. The transfer line temperature and ion source temperature were 280 °C. The mass spectrometer collected data in full scan mode. Identification was performed by

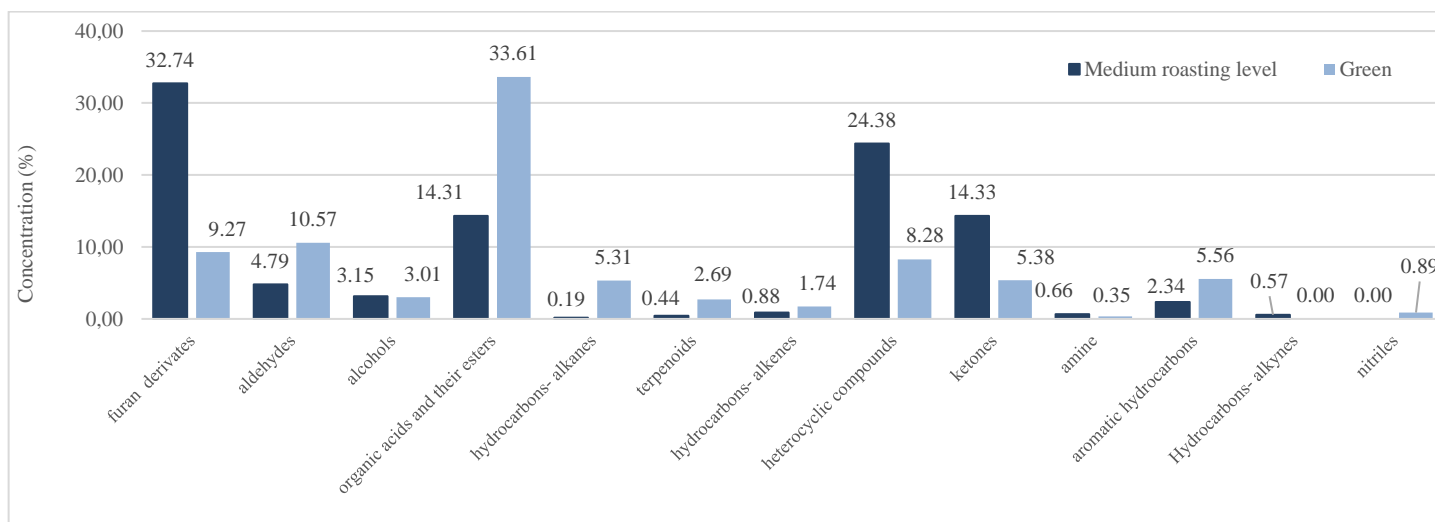
comparing the target compounds' mass spectra and chromatography data with reference materials and the NIST 14 library.

**Statistical analysis**

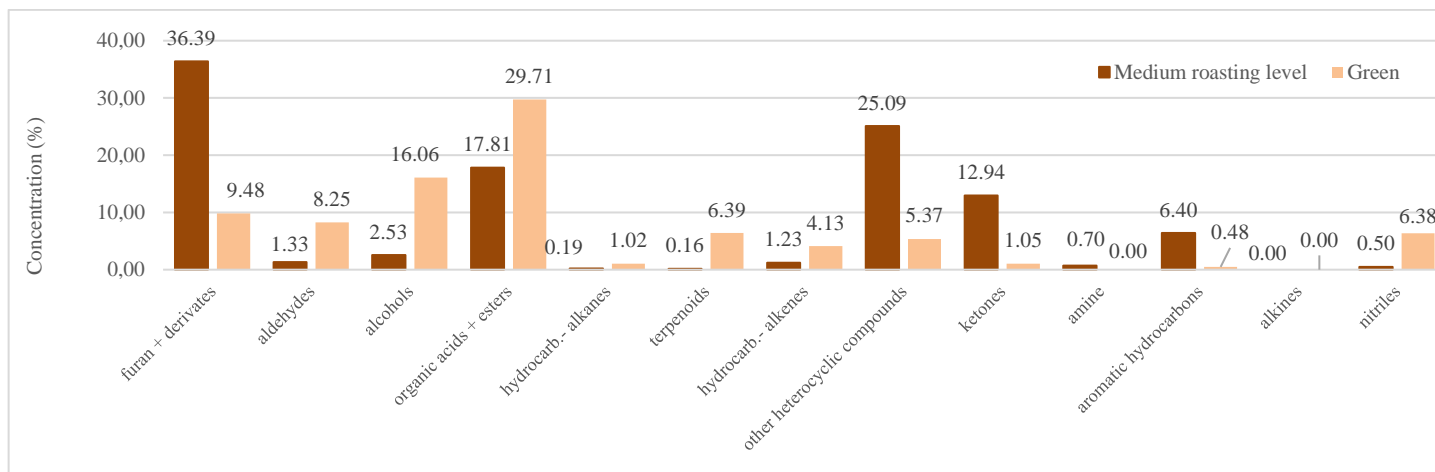
Descriptive statistic was used for the summarizing of our results. To evaluate any possible differences within green and roasted coffee, ANOVA Duncan test and REGWQ was used. For the visualization of differences between roasted and green samples, PCA was used. All statistical analysis were performed using Microsoft Office Excel 365 for Windows (XLStat, Addinsoft).

**RESULTS AND DISCUSSION**

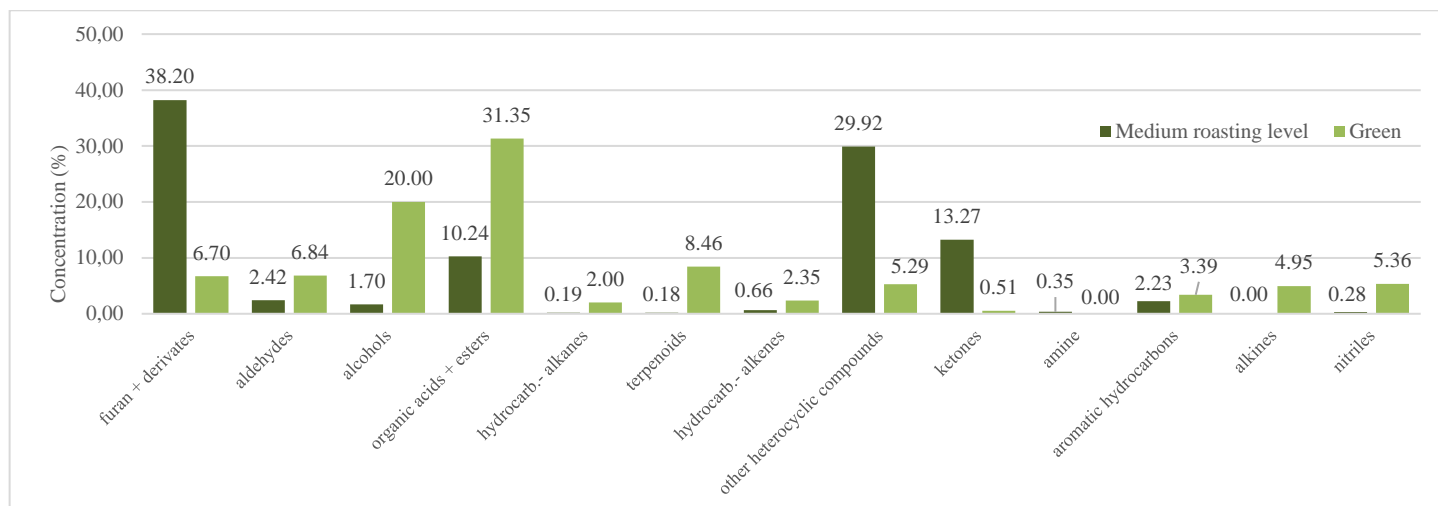
Based on the chemical structure, identified volatiles were divided into furan derivatives, aldehydes, alcohols, organic acids, their esters, and hydrocarbons (alkanes, alkenes, alkynes, and alkynes aromatic hydrocarbons), terpenoids, heterocyclic components, ketones, amines, and nitriles. These groups of volatiles are the main compounds identified in coffee samples. A comparison of average concentration values regarding geographical origin and roasting is shown in Figure 1, 2, 3.



**Figure 1** Comparison of volatiles profile in green and roasted beans C.arabica for African Samples



**Figure 2** Comparison of volatiles profile in green and roasted beans *C.arabica* for Central American Samples



**Figure 3** Comparison of volatiles profile in green and roasted beans *C.arabica* for South American Samples

Among African coffees, the highest concentration had furan derivatives 32.74% (specifically 2-Furanmethanol, acetate, and 2-furanmethanol), heterocyclic compounds 24.38% in a roasted form, while the most abundant was pyridine at a concentration level of 4.7%. However, organic acids and their esters (33.61%) were prevalent in the green form of African samples. The main representatives of organic acid were butanoic acid, 3-methyl, and acetic acid. These three groups had the most observable differences between green and roasted samples. Galilea et al. (2007) defined pyridine as the main member belonging to the group of heterocyclic compounds in roasted coffee. On the other hand, in one African sample (from Burundi) the most abundant groups were aldehydes. Significant representatives were hexanal, and butanoic acid, 3-methyl. The nitrile content decreased due to roasting, on the contrary, the values of alkynes increased as a result of roasting. Volatiles profile is shown in Figure 1a.

The most representative groups of volatile compounds among Central American coffees were furan derivatives, average 36.39% and heterocyclic compounds 25.09% in the roasted form. High concentration reached compounds such as pyridine 4.0-4.3%. The highest concentration in green form had organic acids derivatives 29.71% averagely, and the main representatives were butanoic acid, 3-methyl 7.7 %-10.9%, and acetic acid 4.1%-7.29 %. Also, alcohols reached an average of 16.06% of the profile of volatiles measured in Central American samples. Caporaso et al. (2018) also analyzed acetic acid and pyridine as the main volatile compounds in coffee. We further observed that the roasting process produces a small amount of amines. Samples originating in Central America did not contain alkynes in either green or roasted form. The profile of volatiles for Central America is shown in Figure 1b.

In the samples from South America, the most abundant groups of volatile substances were the same as those from Africa and Central America, but the concentrations were different. Similarly, Colombian samples contained mostly organic acids and their esters in their green form (Figure 1c). Moreover, among South American samples, Colombia also reached the highest concentration of this group in the roasted form. The Brazilian and Bolivian samples in their roasted form contained the highest concentration of heterocyclic compounds. Mostly pyridine (6.2%) was observed. The high concentrations in the green form reached the group of alcohols, the most abundant compounds belonging to this group were 2,3-

butanediol with 6.5% and ethanol 4.9%. Organic acids were another abundant group in the green form, and their esters, 31.35%, had the largest concentration share. In highest concentrations reached ethyl acetate 17.5% and acetic acid 7.3%. These results showed that the major components of volatile compounds found in coffee were organic acids and their esters, specifically acetic acid, butanoic acid, 3-methyl- and organic acid (Lee et al., 2017). Moreover, the same was concluded by other research by Tsegay et al. (2019), and Cheong et al. (2013) also pointed out similar conclusions.

Haile et al. (2020) confirmed that the most significant part of volatile substances had the heterocyclic character in roasted coffee. Furthermore, they proved that pyridine was one of the most abundant substances.

Caporaso et al. (2018) confirmed that considering the complexity of coffee aroma, its volatile composition might vary according to genetics, soil composition, climate, agricultural practices, and roasting conditions, a larger number of samples need to be investigated to confirm the present results and identify new potential markers.

When comparing green and roasted coffee, roasting caused a significant change in levels of volatile compounds. The results Yu et al. (2021) prove that the majority groups of volatile compounds in green beans decrease due to roasting. However, the concentration of several specific groups increased. In our research, aldehydes, alcohols, organic acids and esters, alkanes, terpenoids, alkenes, nitriles, aromatic hydrocarbons decreased due to the roasting process. But only in Central America samples, aromatic hydrocarbons increase due to roasting. The concentration of furan derivatives and heterocyclic compounds increased during the roasting process. An exception was the group of alkynes, given their concentration increased in African samples due to the roasting but decreased in South America samples, and in Central America, they remained unchanged due to the roasting.

When comparing volatiles analyzed in green and roasted coffee, we can observe significant differences and decreased concentration values, mainly in furan and derivatives, aldehydes, alcohols, organic acids and esters, alkanes, terpenoids, alkenes, heterocyclic compounds, ketones, and amine. However, aromatic hydrocarbons, alkynes, and nitriles are three groups when we cannot observe significant differences. The results are shown in Table 2.

**Table 2** Statistical analysis ANOVA.

	furan derivatives	aldehydes	alcohols	organic acids + esters	hydrocarbons- alkanes	terpenoids	hydrocarbons- alkenes	heterocyclic compounds	ketones	amine	aromatic hydrocarbons	hydrocarbons- alkynes	nitriles
Green	8.60 <sup>b</sup>	8.55 <sup>a</sup>	16.65 <sup>a</sup>	31.55 <sup>a</sup>	2.77 <sup>a</sup>	5.84 <sup>a</sup>	2.73 <sup>a</sup>	6.31 <sup>b</sup>	2.46 <sup>b</sup>	0.11 <sup>b</sup>	3.14 <sup>a</sup>	1.65 <sup>a</sup>	4.20 <sup>a</sup>
Medium RL	35.78 <sup>a</sup>	2.84 <sup>b</sup>	2.46 <sup>b</sup>	14.12 <sup>b</sup>	0.19 <sup>b</sup>	0.26 <sup>b</sup>	0.92 <sup>b</sup>	26.46 <sup>a</sup>	13.51 <sup>a</sup>	0.57 <sup>a</sup>	3.65 <sup>a</sup>	0.19 <sup>a</sup>	0.26 <sup>a</sup>
Pr > F(Model)	<0.0001	0.015	0.001	0.001	0.045	0.001	0.049	<0.0001	<0.0001	0.009	0.727	0.391	0.053
Significant	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	No	No

Notes: a,b = groups within a column with different superscripts differ significantly at p≤0.05, ANOVA Duncan test, RL- roasting level

The specific changes in concentration of volatile compounds occurred during the roasting, and significant differences were observed. We used PCA statistics for the

visualization of differences between roasted and green samples. These results are shown in Figure 2.

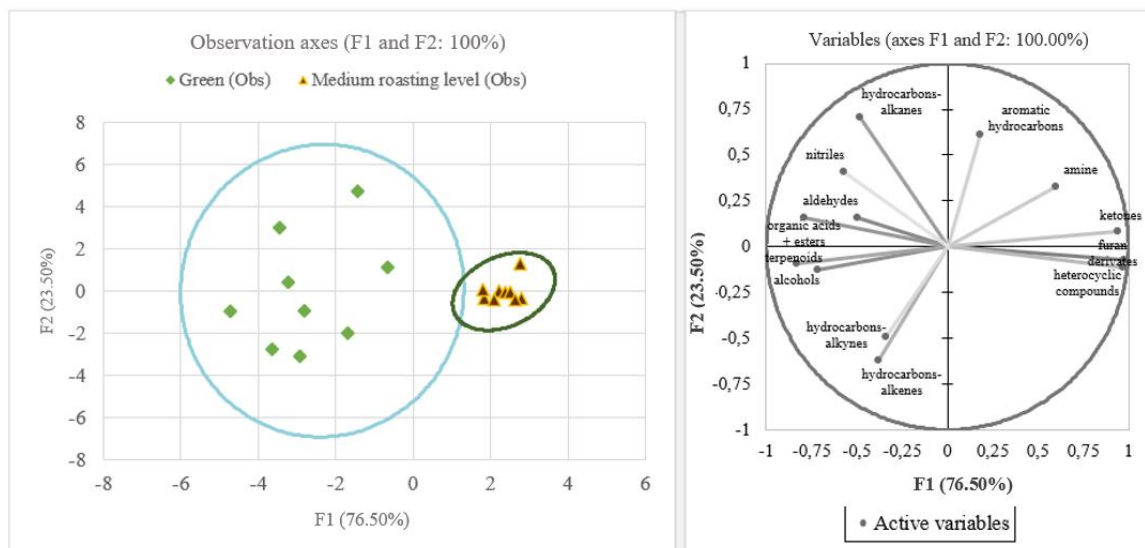


Figure 4 PCA map and variables representation of samples regarding roasting process

As we can see in Figure 4, two factors are needed to explain 100% of the variability of selected samples. Generally, samples of roasted coffee have lower variability, and in the PCA map, they are much more centered around the centroid. Furthermore, green coffee appears to have more variability regarding the concentration of selected volatile compounds. Given the variability of green coffee, we can observe a slight overlap of confidential ellipses.

### CONCLUSION

The volatile compounds were analyzed in coffee beans using gas chromatography (GC-MS). Identified volatiles components were classified into the main groups, namely furan derivatives, aldehydes, alcohols, organic acids and their esters, alkanes, terpenoids, alkenes, heterocyclic compounds, ketones, amines, aromatic hydrocarbons, alkynes, and nitriles. The aim of this study was to analyze the volatile profiles of green and roasted coffee regarding different geographical origins. According to the concentration levels, the most abundant volatiles were organic acids and their esters, the most abundant compounds were: acetic acid, butanoic acid, 3- methyl, ethyl acetate in green coffee. In roasted form, the significant amount of volatiles were identified as heterocyclic compounds for example pyridine, pyrazine. When comparing green and roasted coffee, roasting caused significant changes in levels of volatile compounds. In our research aldehydes, alcohols, organic acids and esters, alkanes, terpenoids, alkenes, nitriles, aromatic hydrocarbons decreased due to the roasting process. However, only in Central America samples, aromatic hydrocarbons increased due to roasting. Furan derivatives, heterocyclic compounds exception were alkynes that increased their concentration in African samples due to the roasting, but decreased in South America samples, and for Central America they remained unchanged due to the roasting. These results suggest that there was an increase in volatile compounds concentration in medium roasted coffee. The most significant changes in the comparison of green and roasted coffee are observed in organic acids and esters, alcohols, furan derivatives, heterocyclic compounds and ketones. When comparing the groups of green and roasted coffee, we cannot observe significant differences and a decrease in the concentration values of volatile substances only in three groups and that aromatic hydrocarbons, alkynes and nitriles.

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### REFERENCES

De Melo Pereira, G. V., de Carvalho Neto, D. P., Magalhães Júnior, A. I., Vásquez, Z. S., Medeiros, A. B. P., Vandenberghe, L. P. S., & Soccol, C. R. (2019). Exploring the impacts of postharvest processing on the aroma formation of coffee beans – A review. *Food Chemistry*, 272, 441–452. doi:10.1016/j.foodchem.2018.08.061

De Melo Pereira, G. V., de Carvalho Neto, D. P., Magalhães Júnior, A. I., Vásquez, Z. S., Medeiros, A. B. P., Vandenberghe, L. P. S., & Soccol, C. R. (2019). Exploring the impacts of postharvest processing on the aroma formation of coffee beans – A review. *Food Chemistry*, 272, 441–452. doi:10.1016/j.foodchem.2018.08.061

Galilea, I. I., Pena, M. P., Cid, C. (2008) Application of multivariate analysis to investigate potential antioxidants in conventional and torrefacto roasted coffee, 227, 141. 147. doi:10.1007/s00217-007-0703-z

Haile, M., Bae, H. M., & Kang, W. H. (2020). Comparison of the Antioxidant Activities and Volatile Compounds of Coffee Beans Obtained Using Digestive

Bio-Processing (Elephant Dung Coffee) and Commonly Known Processing Methods. *Antioxidants*, 9(5), 408. doi:10.3390/antiox9050408

Heo, J., Adhikari, K., Choi, K. S., & Lee, J. (2020). Analysis of Caffeine, Chlorogenic Acid, Trigonelline, and Volatile Compounds in Cold Brew Coffee Using High-Performance Liquid Chromatography and Solid-Phase Microextraction—Gas Chromatography-Mass Spectrometry. *Foods*, 9(12), 1746. doi:10.3390/foods9121746

Cheong, M. W., Tong, K. H., Ong, J. J. M., Liu, S. Q., Curran, P., & Yu, B. (2013). Volatile composition and antioxidant capacity of Arabica coffee. *Food Research International*, 51(1), 388–396. doi:10.1016/j.foodres.2012.12.058

Kim, H.-J., Hong, D.-L., Yu, J.-W., Lee, S.-M., & Lee, Y.-B. (2019). Identification of Headspace Volatile Compounds of Blended Coffee and Application to Principal Component Analysis. *Preventive Nutrition and Food Science*, 24(2), 217–223. doi:10.3746/pnf.2019.24.2.217

Lee, S. J., Kim, M. K., & Lee, K.-G. (2017). Effect of reversed coffee grinding and roasting process on physicochemical properties including volatile compound profiles. *Innovative Food Science & Emerging Technologies*, 44, 97–102. doi:10.1016/j.ifset.2017.07.009

Mahmud, M. M. C., Shellie, R. A., & Keast, R. (2020). Unravelling the relationship between aroma compounds and consumer acceptance: Coffee as an example. *Comprehensive Reviews in Food Science and Food Safety*, 19(5), 2380–2420. doi:10.1111/1541-4337.12595

Sádecká, J., Kolek, E., Pangallo, D., Valík, L., Kuchta, T. (2014) Principal volatile odorants and dynamics of their formation during the production of May bryndza cheese. *Food Chem.*, 150, 301-306. 10.1016/j.foodchem.2013.10.163

Seninde, D. R., & Chambers, E. (2020). Coffee Flavor: A Review. *Beverages*, 6(3), 44. doi:10.3390/beverages6030044

Somporn, C., Kamtuo, A., Theerakulpisut, P., & Siriamornpun, S. (2011). Effects of roasting degree on radical scavenging activity, phenolics and volatile compounds of Arabica coffee beans (*Coffea arabica* L. cv. Catimor). *International Journal of Food Science & Technology*, 46(11), 2287–2296. doi:10.1111/j.1365-2621.2011.02748.x

Toci, A. T., Azevedo, D. A., & Farah, A. (2020). Effect of roasting speed on the volatile composition of coffees with different cup quality. *Food Research International*, 137, 109546. doi:10.1016/j.foodres.2020.109546

Tsegay, G., Redi-Abshiro, M., S. Chandravanshi, B., Ele, E., M. Mohammed, A., & Mamo, H. (2019). Volatile profile of green coffee beans from *Coffea arabica* L. plants grown at different altitudes in Ethiopia. *Bulletin of the Chemical Society of Ethiopia*, 33(3), 401. doi:10.4314/bcse.v33i3.2

Yu, J. M., Chu, M., Park, H., Park, J., Lee, K. G. (2021). Analysis of Volatile Compounds in Coffee Prepared by Various Brewing and Roasting Methods, 10(6), 1347. doi: 10.3390/foods10061347