

HETEROCYCLIC COMPOUNDS IN MEDIUM ROASTED COFFEE HARVESTED FROM VARIOUS GEOGRAPHIC REGIONS

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ABSTRACT

The research is focused on GC-MS identification of heterocyclic compounds (HCCs) in commercially most accepted medium roasted specialty coffee beans from renowned harvesting sites from Africa and America and their precursors in green beans. Obtained GC-MS data showed the most abundant HCCs group in medium roasted coffee was furan derivatives and pyrazine derivatives, reaching an average of 24.17% in African samples, 22.27% in American samples, and 13.41% and 17.62%, respectively. Pyridine derivatives reached similar concentrations, 5.02% in African and 5.27% in American samples. The least abundant group was pyrrole derivatives, reaching only 2.79% in African and 1.91% in American samples. Pearson's correlation proved weak positive correlations between all HCCs (furan derivatives, pyrrole derivatives, pyrazines derivatives, and pyridine derivatives) and volatiles hydrocarbons measured in green samples. Further correlation analysis proved the positive correlation between aldehydes, furanes, and pyrazines. However, Pearson's correlation coefficient proved a weak correlation (0.273 – 0.455). ANOVA pointed out that after the roasting, only pyrazine derivatives showed geographical dependence, suggesting there might be other precursors that need to be studied to better understand safety and quality issues from the perspective of origin and roasting of the commodity.

Keywords: Coffea arabica, heterocyclic compounds, volatiles, origin, safety, GC-MS

INTRODUCTION

Coffee has been the subject of extensive research due to its complex chemical composition and potential health benefits. The primary chemical constituents of coffee include carbohydrates, lipids, amino acids, minerals, and various bioactive compounds, such as alkaloids, diterpenes, and phenolic compounds (Tsiaka *et al.*, 2023). These compounds are responsible for the unique flavor and aroma of coffee, as well as its potential health benefits. On the other hand, some of these compounds are marked as human carcinogens, potential human carcinogens, or probable human carcinogens (da Costa *et al.*, 2023).

The specialty coffee market is a complex chain, at the end of which are consumers who seek high-end products. Cultivation, harvesting, post-harvest processing, and storage are crucial for consistency and quality (Aguilar-Alvarez *et al.*, 2021). This biological material might contain more than 800 volatile compounds responsible for qualitative characteristics, such as taste and aroma (Gao *et al.*, 2023). Various publications, including Gao *et al.*, (2023), Shibamoto *et al.*, (2012), and Stark and Hofmann (2005), reported that heterocyclic compounds (HCCs) are mainly based on the roasting process and are responsible for specific taste and aroma. The same authors reported that among HCCs, compounds derived from furan, pyrazine, and pyrrole are the most abundant. Available results state that around 30% of the bitterness of the final beverage is caused by these compounds.

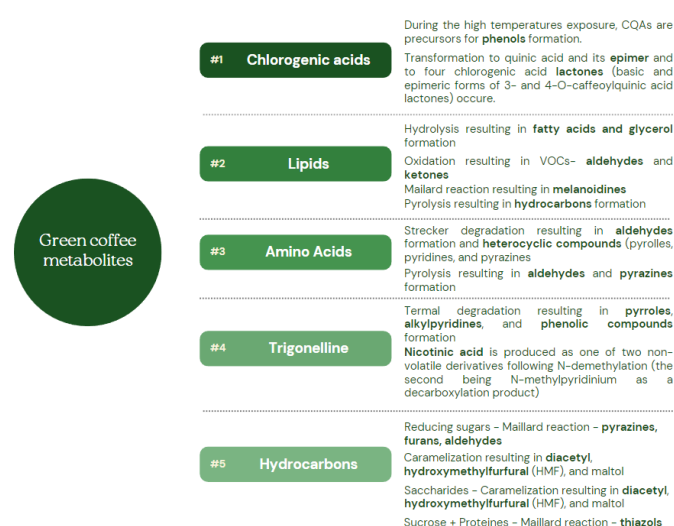


Figure 1 Scheme of coffee metabolites formed from their precursors during the roasting process (Dawidowicz and Typek 2017; Konstantinides *et al.*, 2023; Maksimowski *et al.*, 2022; Yeretian *et al.*, 2002; Shahidi and Hossain 2022; Schenker *et al.*, 2002; Wei and Tanokura, 2015)

Green coffee beans have a wide spectrum of compounds with various physical and chemical characteristics. According to Fadai *et al.*, (2012) and Poisson *et al.*, (2017), the primary sources of aroma are insoluble carbohydrates (cellulose and hemicellulose), soluble carbohydrates (such as arabinose, fructose, galactose, glucose, sucrose, raffinose, and stachyose), lipids, and molecules containing nitrogen.

Moon and Shibamoto (2009) described heterocyclic compounds as a result of the Maillard reaction, a crucial chemical pathway during roasting. Other processes such as Strecker degradation, oxidative, or direct degradation also contribute

significantly to sensory quality perception. During roasting, low-molecular-weight carbohydrates like fructose, glucose, and sucrose help to generate volatile chemicals and acids. Furthermore, according to **Bufo and Cardelli-Freire (2004)**, polysaccharides are crucial components for the retention of volatiles and, as a result, flavor development. Green coffee beans also contain high concentrations of nitrogen-containing substances, such as proteins and alkaloids (such as caffeine and trigonelline), as well as nonvolatile aliphatic acids (such as citric, malic, and quinic acids) and volatile acids (such as acetic, butanoic, decanoic, formic, hexanoic, isovaleric, and propanoic acids). As a result of these chemicals' breakdown during roasting, significant flavor attributes metabolites such pyridines and pyrroles are produced (**Sunarharum et al., 2014**, **Poisson et al., 2017**, **Maksimowski et al., 2019**). Caffeoylquinic acid (CQA), feruloylquinic acid (FQA), and dicaffeoylquinic acid (diCQA) are the three most significant phenolic compounds found in coffee. It is well known that these substances not only contribute to the rich flavor of coffee but also have several positive effects on human health, including antioxidant activity (**Ogawa, 2014**). Altitude, humidity, temperature, and shade during the coffee fruit's creation are some of the environmental aspects that affect the metabolites abundance in green coffee beans. Given that the concentration of HCCs depends on technological processes such as roasting and precursor concentrations, which might be affected by the origin of beans, this study focuses primarily on the qualitative and quantitative determination of selected precursors and heterocyclic compounds in the commercially most accepted type of roasted coffee—medium roast—regarding the origin of coffee beans. The preliminary findings of this research could significantly contribute to our understanding of the chemical composition of coffee beans and their impact on flavor and health.

MATERIAL AND METHODS

Material

Specialty coffee beans samples were obtained from the Café ORO Zvolen (Zvolen, Slovakia). For the purpose of this study, we analyzed samples from America (n=5) and Africa (n=5). All samples were harvested in 2023. According to the International Coffee Organisation, specialty coffee is defined as high-grade coffee scoring 80 points or above on a 100-point scale, rated by certified Q Graders or the Specialty Coffee Association (SCA). It signifies excellence throughout the supply chain, from specialized farming and hand-picking to careful roasting, characterized by distinct flavors, traceability, and minimal defects. Detailed description of green samples is shown Table 1.

Table 1 Samples description

ID green/ID roasted	Origin	Country	Altitude	Variety	post-harvest processing
1G/1R	Africa	Ethiopia	Highlands	B,H	W
2G/2R	Africa	Ethiopia	Highlands	H	W
3G/3R	Africa	Ethiopia	Highlands	H	N
4G/4R	Africa	Ethiopia	Highlands	H	W
5G/5R	Africa	Burundi	Midlands	B	N
6G/6R	America	Brazil	Midlands	B	PN
7G/7R	America	Brazil	Lowlands	B	PN
8G/8R	America	Brazil	Lowlands	B	W
9G/9R	America	Brazil	Midlands	B	PN
10G/10R	America	Brazil	Lowlands	B	PN

Note: G=green; R=roasted; B=Bourbon; H=Heirloom; W=wet processing; PN=pulped natural (semi-washed); N=natural; highlands = harvested above 1500 meters above mean sea level (mamsl); midlands = 1200-1500 mamsl; lowlands harvested below 1200 mamsl

Batches of green coffee were roasted using laboratory roaster Sample PRO 100 Series roaster (Coffee PRO Direct, Hong Kong). To monitor the roasting time and temperature, we used the NI – TC01 (National Instruments Corp., USA). Roasting was conducted under controlled conditions with a total duration of 6 min and an initial drum temperature of 180 °C. During the process, the minimum recorded temperature reached 135.4 °C, while the maximum temperature attained was 225.8 °C. The onset of the first crack was observed at 3 min 30 s, corresponding to a bean temperature of 175.4 °C. The second crack occurred at 5 min 40 s, at a temperature of approximately 220 °C.

Methods

Dry matter (DM) determination

The DM was determined by laboratory analyzer KERN DAB 100-3 (KERN and SOHN GmbH, Balingen, Germany). The drying program was set to go on continuously at 110 °C to reach the constant weight of the sample.

Determination of volatile compounds using gas chromatography (GC-MS)

Ten grams of homogenized green coffee beans were put into 40 mL glass vials with ptfe/sil septum Archon caps (Agilent Technology, Palo Alto, USA). The samples were warmed to 35 °C for 15 min in Metalttermoblock (Liebisch Labortechnik GmbH & Co., Bielefeld, Germany). Volatiles were collected with a 2 cm Carboxen®/PDMS (CAR/PDMS) SPME fiber (Sigma-Aldrich GmbH, Steinheim, Germany), exposed for 30 min at 35 °C, followed by GC-MS analysis. Volatiles were determined according to the method described in **Demianová et al., (2022)** and **Sádecká et al. (2014)** with modifications, using an Agilent Technologies 6890 gas chromatograph (Agilent Technology, Palo Alto, USA) equipped with an Agilent Technologies 5973 selective inertial detector (MSD) and a J&W 122-7333 DB-WAXetr 30 m × 0.25 mm × 0.5 µm capillary column (Agilent Technology, Palo Alto, USA). The carrier gas was helium, and the injector temperature was 250 °C, used splitless mode with initial temperature 250 °C. Pressure was 88.9 kPa, flow rate was 20.0 mL min⁻¹, cleaning time was 1.00 min, and total flow rate was 24.6 mL min⁻¹. The oven temperature was programmed to be isothermal at 50 °C for 1 min, then heated to 250 °C at 5 °C.min⁻¹. The transfer line temperature and ion source temperature were 280 °C. Electron ionization (EI) was set to 70 eV and the mass spectrometer collected data in full scan mode. Identification was performed by comparing the collected mass spectra and chromatography data with reference materials and the NIST 14 library. The GC-MS analysis was performed as a semi-quantitative approach, where the relative abundances of volatile compounds were expressed as percentages of the total VOC peak area. Each sample was analyzed once under strictly controlled and identical analytical conditions. This approach is considered appropriate for comparative profiling of volatile composition, as it enables the evaluation of relative differences between samples rather than absolute quantification.

Statistical analysis

Statistical analysis was done using Microsoft Office Excel 365 for Windows with the XLSTAT Addinsoft (2021) and Microsoft Office Excel 365 for iOS with the XLSTAT (2022). To describe statistically significant differences we used ANOVA Duncan, Dunn, and REGWQ test with $\alpha = 0.05$. To observe correlations between precursors in green coffee and HCC metabolites in medium roasted coffee, Pearson's correlation was employed.

RESULTS AND DISCUSSION

Specialty Coffee Association of America (SCAA) in Annex 7 and FAO provide a list of requirements and exporting standards that must be met to grade coffee beans as specialty. Authorities stated that for Specialty Grade (1): 5 full defects in 300 grams of coffee or less. No primary defects are allowed. A maximum of 5% above or below the screen size indicated is tolerated. Must possess at least one distinctive attribute in the body, flavor, aroma, or acidity. It must be free of faults and taints. No quakers are permitted. Moisture content is between 9-13%. However, exporting standards even lower this interval to 8-12.5% of moisture content (**ICC Resolution No. 407/02**).

Based on Figure 2, the analyzed samples met all producing and exporting standards. ANOVA proved no significant difference in DM regarding the post-harvest processing of specialty beans or their geographical origin. These results emphasized that producers could produce specialty beans of uniform quality and meet all necessary requirements. Results align with various publications, including **Bobková et al., (2022)**. The average dry matter content reached 91.12%. Very similar results are described in **Dong et al., (2023)** and **Therdtatha et al., (2023)**.

A similar pattern of no significant differences between samples was observed even in roasted samples. In this case, the average DM value reached 97.59% (Figure 3). **Seninde and Chambers (2020)** stated that DM in coffee depends on various factors, and the roasting intensity can range between 1.5 – 5%.

Various authors, including **Dong et al., (2023)**, pointed out that it is crucial to constantly study precursors in green coffee to understand pathways of roasted coffee metabolite development. It is essential to emphasize that the concentration of these precursors might relate to the samples' origin. Therefore, we applied a correlation test to observe the relationships between aldehydes and VOCs hydrocarbons quantified in green coffee with HCCs in medium roasted coffee (Figure 4). According to Pearson's correlation, neither a positive nor negative relationship was observed between aldehydes in green coffee beans and pyrroles in medium-roasted coffee. This might be explained given free amino acids, particularly proline, can undergo reactions with sugars to form pyrroles further sugars like glucose and fructose are crucial in the Maillard reaction, leading to the formation of various heterocyclic compounds, including pyrroles (**Zakidou et al., 2021**).

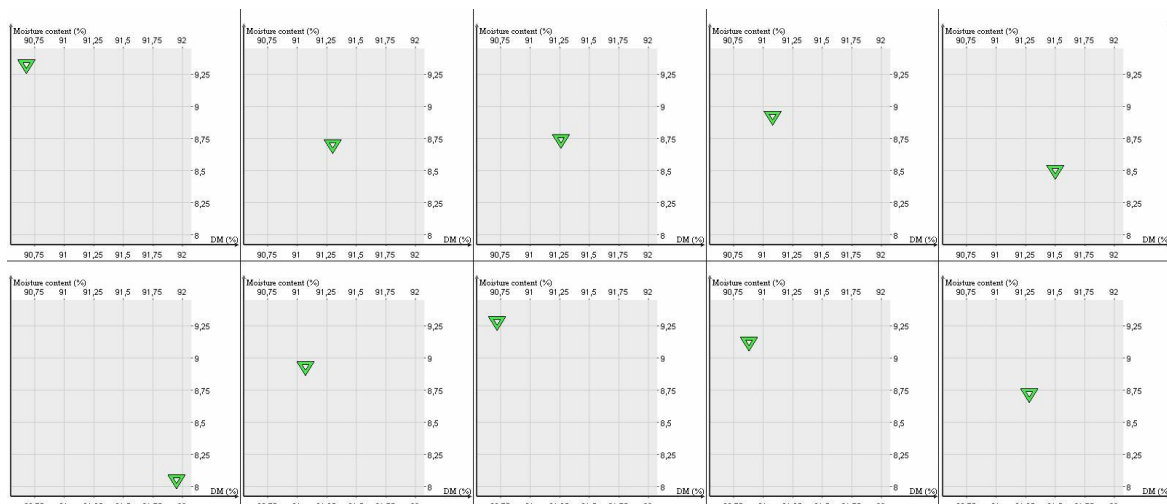


Figure 2 Dry matter content and moisture content of green specialty coffee.

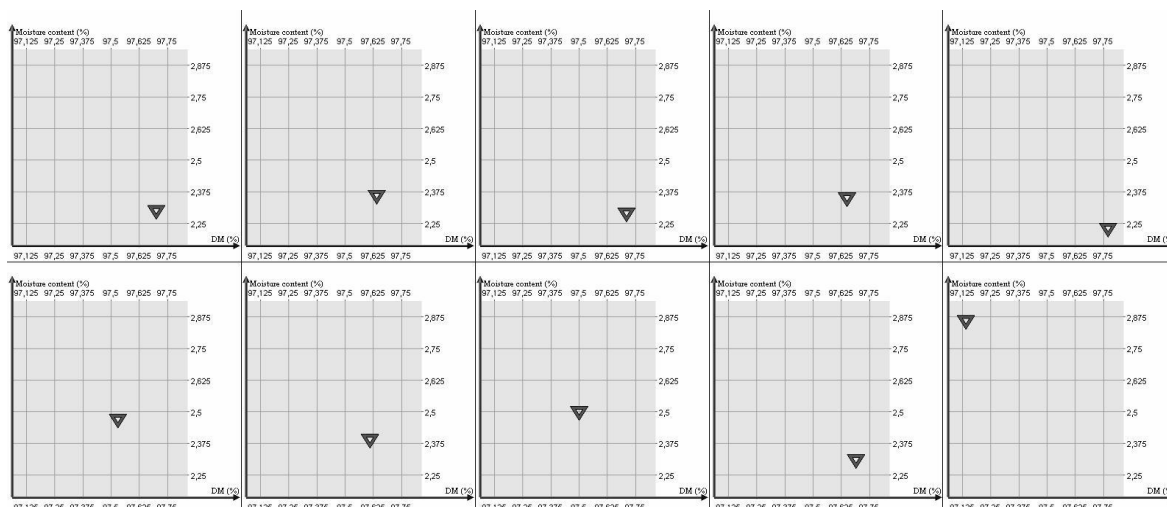


Figure 3 Increase of DM and MC in medium roasted specialty coffee.

We observed a weak positive correlation (0.273 - 0.455) between aldehydes and pyrazine derivatives. Aldehydes such as hexanal and furfural, both identified in the analyzed samples, contribute to the aroma and are precursors to various flavor compounds formed during roasting. This underscores the significant role of aldehydes in the development of flavor in roasted coffee.

Volatile hydrocarbons in green coffee, though present in smaller amounts, also contribute to the overall flavor profile. These include compounds like alkanes and alkenes, which are relatively less reactive but can undergo transformations during roasting. The high temperatures during roasting cause the degradation of these metabolites, which can contribute to the formation of more complex compounds. The Maillard reaction is the most significant reaction during roasting. Aldehydes, particularly those formed from the degradation of sugars, amino acids, and lipids, react with other compounds to form a variety of heterocyclic compounds, including furans, pyridines, and pyrazines. Strecker Degradation is another important pathway where aldehydes react with amino acids to form heterocyclic compounds. Furans are often formed from the thermal degradation of carbohydrates and the breakdown of aldehydes. Pyrroles and pyridines can arise from the interaction of aldehydes with amino acids or from the breakdown of sugars. Pyrazines are formed primarily through the Maillard reaction, where aldehydes play a key role as intermediates (Herdt et al., 2024; Jaiswal et al., 2012; Thammarat et al., 2018). The correlation analysis (Figure 4) showed no statistically meaningful relationship between aldehydes in green coffee and pyrrole derivatives in roasted samples. This suggests that, under the applied roasting conditions, aldehydes quantified in green beans are unlikely to be the dominant precursors contributing to pyrrole formation. Instead, this finding points toward the involvement of other nitrogen-containing precursors not quantified in this study, such as free amino acids. In contrast, weak positive correlations ($r = 0.273-0.455$) were observed between aldehydes and pyrazine derivatives. Specifically, aldehydes identified in the samples, including hexanal and furfural, may act as intermediate compounds during roasting, contributing indirectly to the formation of pyrazines. However, the low correlation coefficients indicate that aldehydes alone do not sufficiently explain the variability

in pyrazine formation across samples. A similarly weak relationship was observed between volatile hydrocarbons and all classes of HCCs. Given their relatively low reactivity, hydrocarbons likely play only a minor or indirect role in HCC formation under the studied conditions. Overall, the weak correlations suggest that the formation of furans, pyrazines, pyridines, and pyrroles is governed by a more complex network of precursors and reactions than captured in this dataset. Therefore, the presented relationships should be interpreted as indicative trends rather than evidence of direct precursor-product dependencies. These findings highlight the need to include additional precursor groups, particularly amino acids and saccharides, in future studies to better resolve the mechanisms of HCC formation. Further research incorporating a broader range of chemical compounds and more robust statistical evaluation is needed to better elucidate these mechanisms. This highlights the need for further research to understand the pathways of HCCs development in roasted coffee and to study the possible correlations with the origin, both botanic and geographical.

From a sensory perspective heterocyclic compound, or their precursors in green coffee, are fundamental for developing the typical coffee aroma and flavor. As stated by Várady et al., (2022) certain heterocyclic compounds, such as 3(2H)-furanone, dihydro-2-methyl-, are characteristic constituents of coffee and contribute to desirable sensory attributes, including sweet, nutty, and bread-like aromas. In contrast, nitrogen-containing heterocycles, particularly pyridine and pyrazine derivatives, are typically associated with more intense sensory notes described as burnt, roasted, and pungent. Despite their relevance to flavor formation, the occurrence and concentration of these compounds in food matrices warrant careful monitoring, as some members of these chemical classes have been classified within carcinogenic risk groups by the International Agency for Research on Cancer (IARC). Consequently, their quantitative assessment is essential to ensure both product quality and food safety. Dong et al., (2023) focused on exploring correlations between green beans components and thermal contaminants in roasted coffee beans. Authors proved presence of furan derivatives in green coffee beans, which is in line with our findings (Figure 5).

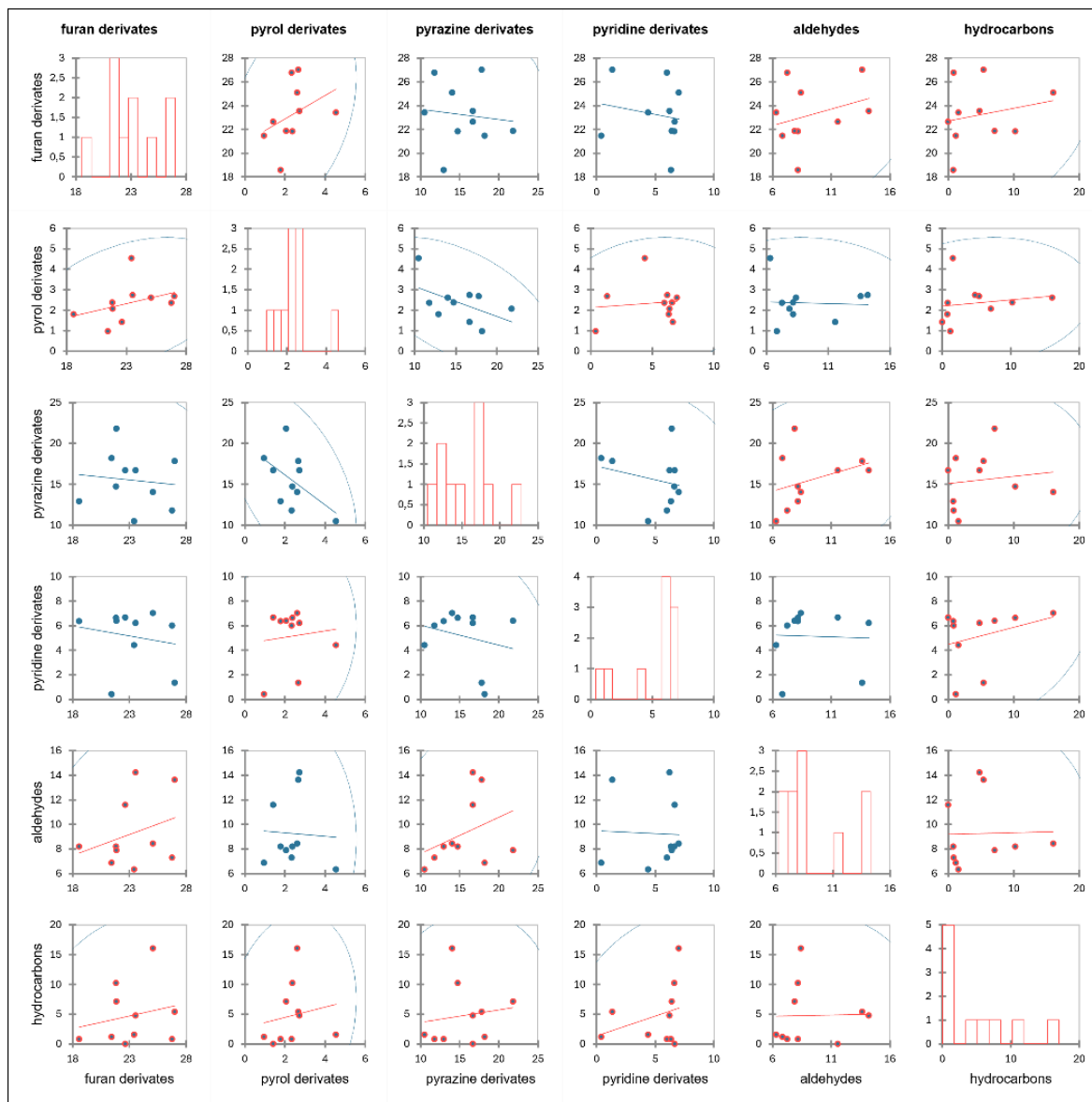


Figure 4 Pearson's correlation between HCCs precursors in green coffee (aldehydes, hydrocarbons) and HCCs in medium roasted coffee

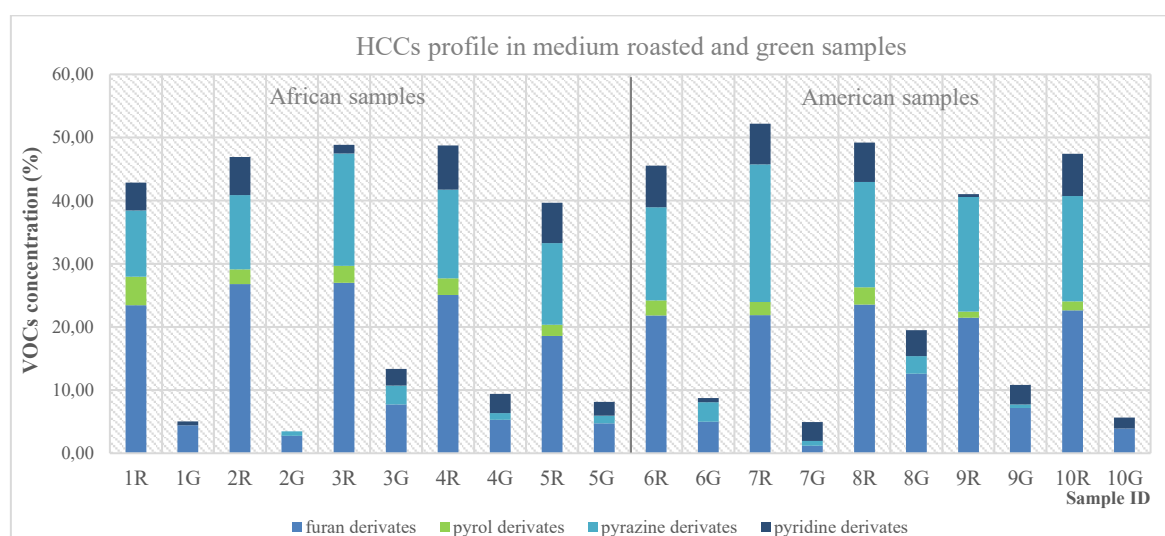


Figure 5 HCCs profile in medium roasted and green samples. **Note:** Results are expressed as concentration (%) from total concentration of VOCs, G=green, R=roasted coffee

Furan itself was not proved in either of the analyzed samples. However, its methyl- and ethyl-derivates were abundant. Concentrations of furan derivatives ranged averagely from 2.76% to 11.71% in African green beans. Not significantly higher concentration range was measured in American samples, 1.39% to 12.87%. Among green African samples, the most abundant were furan, 2-methyl, furan, 3-

methyl, furfural, 2-furanmethanol, and furan, 2-penthyll. Comparing green and roasted African beans, we observed a significant increase from an average of 4.99% to 22.26%. In roasted samples, the most abundant were furan, 2-methyl-; furanmethanol; 2-furanmethanol; 2-furanmethanol, 5-methyl, and 2,5-furandione, 3,4-dimethyl-. The same compounds were observed in American samples, too.

ANOVA proved no significant difference between American and African samples in this group. **Da Costa et al., (2023)** described contaminants in roasted coffee induced by roasting. They proved the occurrence of furan derivatives in roasted African samples. Furan and its derivatives, such as 2-furfural (furfuraldehyde), 2-methylfuran, and 5-hydroxymethylfurfural (HMF), are generated during the roasting process of coffee beans. These compounds result from the thermal degradation of carbohydrates (Maillard reaction) and the breakdown of sugars and other organic matter. The concentration of furan derivatives can vary depending on the degree of roasting, with light roast having lower levels and dark roast having higher levels. Medium roasting typically produces a moderate amount of these compounds, contributing to the flavor profile and aroma of the coffee (**Gruczyńska et al., 2018, Da Costa et al., 2023**), however, geographical origin dependence was not described for these groups of HCCs.

A group of pyrazine derivatives was relatively abundant (Figure 5). Similarly, pyrazine itself was determined only in samples R1 and R3, however, only in minor concentrations, up to 0.4% of total VOCs concentration. Most abundant were pyrazine, methyl-, pyrazine 2,5-dimethyl; pyrazine 2,6-dimethyl; pyrazine, 2-ethyl-6-methyl; pyrazine, trimethyl-, and pyrazine, 2-ethyl-3-5-dimethyl, and pyrazinamide. Pyrazine derivatives are the main precursors of sensory attributes showing a significant mean impact on liking coffee from a consumer's point of view (**Connelly et al., 2022**). The authors also reported that furan derivatives and pyrazine derivatives reached the highest concentration range among HCCs, which aligns with your results. **Caporaso et al., (2018)** described their relevance

regarding sensory perception of HCC. Authors pointed out that these volatiles represent the pleasant aroma, such as nutty, roasted, coffee, cocoa, and peanut butter. Significantly lower concentrations of HCCs were observed in groups of pyridine derivatives (Figure 5). Similarly with other HCCs, the most abundant were methyl- and ethyl- derivatives, especially in position 2,4- and 2,6-, and derivatives with -OH group, such as 3-pyridinol. However, the average concentration was relatively low, up to 0.3% of total VOCs.

Of particular interest is the presence of 1H-pyrrole-2-carboxaldehyde, which was found exclusively in roasted African samples from Ethiopia. **Moon and Shibamoto (2009)** quantified pyrroles in medium roasted samples only in minor concentrations, ranging from 0.11 to 1.18%, and they also identified 1-methyl-1H-pyrrole-2-carboxaldehyde and pyrrole-2-carboxaldehyde in Ethiopian whole beans.

As in all HCCs groups there was a significant difference between roasted and green whole beans regarding the pyridines concentrations. In green beans, the average concentration reached 0 – 4.12%. In African medium roasted samples, the group's concentration reached 0.4% to 7.01%, and in American, from 0.40 – 6.67%. The most abundant from the group was pyridine, pyridine, 3-ethyl-, and pyridine, 2,4-dimethyl.

ANOVA pointed out that after the roasting (Table 2), only pyrazine derivatives showed geographical dependence. However, the precursors in green coffee showed no significant differences. The results suggest that other precursors in green coffee should be focused on.

Table 2 ANOVA comparison of green coffee precursors and HCCs in medium roasted coffee.

Origin	furan derivatives roasted	pyrrol derivatives roasted	pyrazine derivatives roasted	Aldehydes green	Hydrocarbons green
Africa	24.17 ^a	2.79 ^a	13.41 ^a	8.58 ^a	4.91 ^a
America	22.27 ^a	1.91 ^a	17.62 ^a	7.75 ^a	4.66 ^a
Pr > F(Model)	0.92	0.49	0.53	0.76	0.94

Notes: a, b = groups within a column with different superscripts differ significantly at $p \leq 0.05$

CONCLUSION

Heterocyclic compounds are essential from the sensory perspective, given that many are responsible for organoleptic attributes sought by coffee consumers. Methyl and ethyl derivatives of these HCCs are accountable for coffee, roasted, nutty, and other tones that develop an overall impression of coffee beverages. However, some of them are carcinogens. Although certain heterocyclic compounds have been discussed in the literature in relation to toxicological concerns, this study does not perform exposure or risk assessment. Consequently, no conclusions regarding food safety can be drawn, and the results should be considered within a compositional and analytical framework only. Nevertheless, it is necessary to study their concentrations and precursors and the possible impact of external factors on their abundance regarding the possible adjustments in the roasting process. This preliminary study was focused on GC-MS determination of VOC heterocyclic compounds in green and medium roasted specialty beans from African and American production sites. Results showed that after the roasting process, the most abundant groups were furans and pyrazines, mainly their methyl and ethyl derivatives. Further correlation analysis proved only weak positive relationship between aldehydes and VOC hydrocarbons in green beans with furan derivatives, pyrrole derivatives, pyrazines derivatives, and pyridine derivatives. However, Pearson's correlation coefficient proved a weak correlation (0.273 – 0.455). ANOVA pointed out that none of the HCCs groups showed geographical dependence after the roasting. From the perspective of quality and safety, there is a need for further studies to describe correlations with other precursors such as CQAs, saccharides, amino acids, and fatty acids, and to evaluate possible impact and relationships of external factors such as origin, harvesting period, and to possibly adjust the roasting process to obtain safe and high-quality commodity.

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