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A CURRENT REVIEW ON THE DEVELOPMENT OF COFFEE AROMA: VOLATILE COMPOUNDS AND ANALYSIS WITH NEW ANALYTICAL APPROACHES

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ABSTRACT

Coffee, widely consumed worldwide with significant agricultural and commercial importance, is rich in bioactive components like tannins, polyphenols, caffeine, while also containing volatile organic compounds (VOCs), responsible for coffee's unique aroma, beneficial to human health. This review summarizes the development of coffee aroma, the VOCs and non-VOCs, their precursors and effects on aroma and current analytical methods. HS-SPME-GC-MS play a critical role in the analysis of VOCs, while HPLC methods are crucial for the analysis of non-VOCs. The obtained data can be combined with modern chemometric methods, PCA, PLS-DA and ANNs, for geographical origin verification and quality grading. According to the study's objective, since there is no single analytical method for determination, researchers may benefit from selecting hybrid models that combine analytical precision with human expertise, processing chromatographic and spectroscopic data with advanced machine-learning algorithms. Integrated approaches aim to provide a more transparent and objective grading system throughout the coffee value chain.

Keywords: Coffee, aroma, volatile compounds, arabica, robusta, HPLC, GC

KAHVE AROMASININ GELİŞİMİ ÜZERİNE GÜNCEL BİR DERLEME: UÇUCU BİLEŞİKLER VE YENİ ANALİTİK YAKLAŞIMLAR İLE ANALİZİ

ÖZ

Dünya çapında çok tüketilen, tarımsal ve ticari öneme sahip olan kahve; taninler, polifenoller ve kafein gibi biyoaktif bileşenlerce zengin olmakla birlikte, kahvenin eşsiz aromasından da sorumlu olan ve insan sağlığına faydalı uçucu bileşikler de içermektedir. Bu inceleme; kahve aromasının gelişimini, içerdiği uçucu ve uçucu olmayan bileşikleri, uçucu bileşiklerin öncüllerini ve girdikleri reaksiyonlar ile aromaya etkilerini güncel analiz yöntemleriyle özetlemeyi amaçlamaktadır. Uçucu bileşiklerin analizinde HS-SPME-GC-MS, uçucu olmayan biyoaktif bileşenlerin analizinde ise HPLC yöntemleri kritik rol oynar. Elde edilen veriler; coğrafi orijin doğrulaması ve kalite derecelendirmesi amacıyla PCA, PLS-DA ve ANNs gibi modern kemometrik yöntemlerle birleştirilebilir. Kahve aromasını ve bileşimini belirlemek için belirli tek bir analitik yöntem bulunmadığından; araştırmacılar, çalışmanın amacına uygun, analitik kesinliği insan uzmanlığıyla birleştiren, kromatografik ve spektroskopik verileri ileri makine öğrenmesi algoritmalarıyla işleyen hibrit modeller seçmelidir. Entegre yaklaşımlar, bilimsel titizliği artırırken; kahve değer zincirinde şeffaf ve objektif bir derecelendirme sistemi oluşturmaktadır.

Anahtar Kelimeler: Kahve, aroma, uçucu bileşikler, arabica, robusta, HPLC, GC

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INTRODUCTION

Coffee is widely recognized as a major beverage consumed globally and represents a primary agricultural commodity in international trade. According to International Coffee Organization (ICO), world coffee consumption was 173.1 million bags in 2022/2023 and the expected world coffee consumption will increase by 2.2% to 177.0 million bags (ICO, 2023). Coffee, a globally recognized product, is a part of the culinary culture of many countries and in terms of monetary value, the world coffee market is the second largest market after the crude oil market (Marek et al., 2020).

The *Coffea* genus, which belongs to the Rubiaceae family, with over 100 species; however, commercial production and trade predominantly focus on two species: *Coffea arabica* L. (Arabica) and *Coffea canephora Pierre* ex A. *Froehner* (Robusta) (Bastian et al., 2021 & Moccand et al., 2023). As shown in Table 1, these two species differ from one another in many respects, including shape, environmental conditions, climate, chemical composition, taste and aroma.

Table 1. Comparative analysis of *Coffea arabica* L. and *Coffea canephor*a P*ierre* ex A. Froehner characteristics

Characteristics	**Coffea arabica L. (Arabica)**	**Coffea canephora Pierre ex A. Froehner (Robusta)**	**References**
Bean Morphology	Characterized by a flatter and longer structure.	Typically, smaller and more spherical in shape.	(National Coffee Association, 2025)
Cultivation Requirements	Thrives at higher altitudes (>1000m); sensitive to environmental stressors.	Resilient at lower altitudes (200–900m); adapted to warmer, tropical climates.	(Konieczka et al., 2020; National Coffee Association, 2025)
Non-VOC Precursors	Richer in trigonelline and lipids; lower levels of chlorogenic acids compared to Robusta.	Contains approximately 50–60% more caffeine and higher concentrations of chlorogenic acids compared to Arabica.	(Gantner et al., 2024; Konieczka et al., 2020)
Green Bean VOC Intensity	Moderate volatile intensity in raw form; characterized by a complex aroma potential.	Absolute intensity of VOCs is higher in green beans compared to Arabica.	(Debona et al., 2025)
Roasting Dynamics	Higher sugar content promotes intense Maillard reactions; pyridine is a more prominent marker.	Contains higher concentration of pyrazines and lower aldehydes; 2-heptanol is a significant marker.	(Caporaso et al., 2022; Debona et al., 2025; Taiti et al., 2025)
VOC Emission Capacity	Higher total VOC emissions, especially in Bourbon and Typica genetic lineages.	Remarkably, lower total VOC emissions (avg. 4500 ppbv) compared to specialty Arabica.	(Taiti et al., 2025)
Organic Acid Profile	Exhibits a more balanced and harmonious acidic profile.	Generally richer in organic acids, especially pentanoic and acetic acids, leading to a sharper aroma.	(Gantner et al., 2024)
Sensory Profile	Distinguished by high acidity, fruity/floral notes (linked to linalool) and a harmonious aroma.	Characterized by a stronger, more bitter profile with woody, earthy or muddy aromatic notes.	(Gantner et al., 2024; Konieczka et al., 2020; Marek et al., 2020)

Table 1. Continued

Economic & Market Value	Commands premium pricing due to superior sensory characteristics and high-value, unique origin demand.	Primarily used in commercial blends and instant coffee for body, crema and cost-efficiency.	(Bordiga et al., 2025; Dippong et al., 2022)
Leaf Bioactive Content	Young leaves contain high levels of alkaloids, polyphenols and unique xanthones like mangiferin.	Bioactive concentrations are highest in early stages of development, similar to Arabica.	(Patil et al., 2023)
Industrial Potential	High trigonelline and low caffeine content in leaves offer strategic value for health-focused products.	High biomass recycling potential thanks to early harvest of bioactive-rich young leaves.	(Patil et al., 2023)

Coffee has a rich composition of carbohydrates, lipids, vitamins, nitrogen compounds, minerals, alkaloids and phenolic compounds that affects its flavor, aroma and the quality (Caporaso et al., 2022; Rusinek et al., 2022; Elefante et al., 2025; Paiva et al., 2025). Ever since the beginning of twentieth century, there have been many studies on the chemical constituents of coffee, especially volatile organic compounds (VOCs), one of the key factors influencing coffee quality and its acceptance by consumers (Wang et al., 2022). In the past decades, about 1000 VOCs have been detected in coffee. However, only 5% of the detected VOCs are known to contribute to the coffee aroma. Except for VOCs, there are phenols, hydrocarbons, acids, anhydrides, esters, alcohols and sulfur compounds. VOCs include about 400 species of heterocyclic compounds, including pyrroles, furans, thiazoles, oxazoles, thiophenes, pyridines, imidazoles and pyrazines (Zakidou et al. 2021; Catão et al., 2022; Wang et al., 2022; Asensio-Ramos and D'Orazio, 2023; Gantner et al., 2024; Wan et al., 2024). Among these, furan derivatives (24–41%) and pyrazines (25–39%) represent the predominant chemical categories that decisively shape the final aromatic profile (Zakidou et al., 2021; Shi et al., 2024). Scientific studies have identified 100 VOCs in coffee beans, including compounds containing sulfur, pyrazine, pyridine, oxazole, pyrrole, furan, aldehyde, higher alcohol, ketone, ester and phenol (Wang et al. 2024; Zhai et al., 2024). These aromatic compounds are primarily formed through the transformation of precursor substances (sugars, amino acids, lipids) in green coffee beans via thermal processes that occur during roasting, such as the Maillard reaction, Strecker degradation, caramelization and pyrolysis (Agnoletti et al. 2022; Pua et al., 2022; Wang et al. 2022; Cao et al., 2023; Debona et al., 2025).

Coffee consumption has been associated with various health benefits and may play a role in the prevention of certain diseases (Cañas et al., 2023; Zhai et al., 2024). Research suggests that the refreshing, antidepressant, antioxidant, antibacterial, DNA-protective, anticancer and neurological modulating activities of coffee are fundamentally linked to specific constituents such as caffeine, chlorogenic acids (CGAs), trigonelline, diterpenes, phenolics and VOCs (Wang et al., 2022; Zhai et al., 2024; Chen at al., 2025). Furthermore, the phenolic compounds found in coffee byproducts have the potential to mitigate oxidative stress-related disorders, such as diabetes mellitus type 2, obesity and inflammation-related disorders (Cañas et al., 2023; Caprioli et al., 2025). Chemical profile undergoes a dynamic transformation during thermal roasting; natural phenolics such as CGAs degrade significantly (often up to 90%), transforming into volatile phenols or contributing to the synthesis of newly formed functional substances such as melanoidins; this can functionally maintain or enhance the overall antioxidant capacity (Heo, J. et al., 2020; Dippong et al., 2022; Wu et al. 2022; Elhalis, H. et al., 2023; Kašpar et al., 2025; Wang et al. 2026). In this context, the key bioactive component categories in the coffee matrix, their associated biological activities and literature-supported health effects are comprehensively summarized in Table 2.

Table 2. A summary of bioactive compounds in coffee, associated health effects and evidence-based context

Compound Category	Key Bioactive Components	Associated Biological Activities & Potential Health Benefits	Evidence-Based Context& References
Alkaloids	Caffeine; Trigonelline	Functions as a strong neurological and respiratory modulator; exhibits diuretic properties and enhances cognitive performance and memory retention.	Caffeine is a globally recognized stimulant, while trigonelline plays a dual role as a bioactive agent and a critical chemical precursor that degrades into pyridines and pyrroles during roasting (Heo et al., 2020; Bastian et al., 2021; Wu et al., 2022; Gantner et al., 2024; Zhai et al., 2024; Qiu et al. 2026).
Phenolic Acids	Chlorogenic Acids (CGAs) (e.g., 5-CQA); Caffeic acid; Ferulic acid	Evidenced antioxidant, antimicrobial and anti-inflammatory activities; potential role in DNA protection and reducing the risk of metabolic syndromes such as type 2 diabetes.	CGAs are the main determinants of antioxidant potential; however, they undergo up to 90% thermal degradation during roasting, transforming into volatile phenols such as guaiacol (Heo et al., 2020; Caporaso et al., 2022; Dippong et al., 2022; Wang et al., 2022; Chen at al., 2025; Kašpar et al., 2025).
Polyphenols & Flavonoids	Quercetin; Rutin; Tannins	Alleviates cellular oxidative stress; associated with managing obesity-related inflammatory pathways.	Concentrated intensely in coffee pulp and leaves, these compounds act as protective barriers against chronic diseases associated with oxidative stress (Rusinek et al., 2022; Wang et al., 2022; Cañas et al., 2023; Patil et al., 2023; Zhai et al., 2024).
Xanthones	Mangiferin; Iso-mangiferin	Remarkable antioxidant capacity; exhibits xanthine oxidase (XO) inhibitory potential; promising for high-value functional beverages.	Identified only in C. arabica leaves, offering significant biomass recycling opportunities; interacts with L-Cysteine during roasting to regulate quality (Rusinek et al., 2022; Patil et al., 2023; Wang et al., 2026).
Diterpenes	Cafestol (Kahweol); Kahweol	Linked to complex biological activities, including potential anticancer and chemopreventive effects.	As integral parts of the lipid fraction, these diterpenes represent a complex non-volatile matrix that impacts both health potential and final cup quality (Wang et al., 2022; Cao et al., 2023; Chen et al., 2025; Paiva et al., 2025).
Volatile Organic Compounds (VOCs)	Sulfur compounds; Pyrazines; Aldehydes; Pyridines; Furans	Catalysts for the comprehensive sensory experience; proven sedative and calming effects through the regulation of stress biomarkers.	VOCs activate the olfactory system and have been shown to reduce salivary α-amylase and cortisol levels, indicating anxiolytic properties (M. Chen et al., 2022; Shi et al., 2024; Zhai et al., 2024; Taiti et al., 2025).

Table 2. Continued

Maillard Reaction Products	Melanoidins	High-molecular-weight nitrogenous pigments with outstanding antioxidant activity; responsible for the characteristic brown color and roasted notes.	The formation of these neo-formed substances during roasting can practically compensate for the loss of natural phenolics in terms of overall antioxidant stability (Caporaso et al., 2022; Wu et al., 2022; Cao et al., 2023; Elhalis, H. et al., 2023; Shi et al., 2024; Debona et al., 2025).
Thermally Induced Risk Compounds	Acrylamide; 5-Hydroxymethylfurfural (5-HMF)	Identified as potentially harmful intermediates with	These are undesired by-products of Maillard and caramelization reactions; acrylamide levels peak in light roasts, while 5-HMF accumulates significantly in darker roasted profiles (Cascos et al., 2024; Park et al., 2024; Wang et al., 2026).

Although the diverse chemical profiles of VOCs in coffee and the standard instruments used for their extraction have been successfully documented in numerous comprehensive review studies, there remains a significant knowledge gap regarding a systematic synthesis of how raw analytical datasets are transformed into predictive quality models. The current literature primarily focuses on standard chromatographic outputs or isolated biological mechanisms and generally evaluates analytical instrumentation and data calculation independently. This study aims to evaluate the effects of volatile compounds on coffee aroma and the analytical approaches used to identify them. It examines current applications and new approaches that incorporate hybrid models combining chromatographic and spectroscopic techniques. This review covers advanced analytical platforms ranging from high-performance multidimensional separation systems (e.g., GC×GC-MS) to real-time scanning sensors (e.g., PTR-MS, e-nose) and clearly links them to modern computational intelligence, including chemometrics (PCA, PLS-DA) and Artificial Neural Networks (ANN), thereby addressing this critical gap. Furthermore, unlike traditional overviews, this article evaluates these methodologies within a unified data processing workflow and identifies future analytical methods to enable high-precision origin tracking throughout the coffee supply chain.

REVIEW METHODOLOGY AND LITERATURE SEARCH STRATEGY

The methodology used in preparing this review, including the literature search strategy, which covers the databases consulted, the keywords used, the inclusion and exclusion criteria and the time frame of the studies examined, is available in Table 3.

Table 3. Systematic review methodology and literature search strategy

Methodology Component	Details and Implementation Criteria
Databases	Web of Science, Scopus, ScienceDirect, Google Scholar and PubMed.
Keywords	Coffee, aroma, volatile organic compounds (VOCs), Arabica, Robusta, HPLC, GC-MS, chemometrics, machine learning and sensory analysis.
Time Frame	Primary focus on recent literature published between 2020 and 2026 to ensure the inclusion of cutting-edge analytical and AI developments.

Inclusion Criteria	•	Peer-reviewed journal articles and book chapters focusing on coffee aroma and quality.
	•	Studies exploring advanced analytical techniques (e.g., GC×GC-MS, PTR-MS, MSI).
	•	Research integrating chemometric or machine learning models for coffee authentication.
Exclusion Criteria	•	Non-peer-reviewed sources, reports or conference abstracts without complete technical data.
	•	Studies not published in English.
	•	Outdated sources (typically those prior to 2020).
Quality Assessment		Technical rigor of the analytical methods used, the validity of the chemometric models (e.g., cross-validation, R^2 values) and the relevance to current industry challenges (e.g., fraud detection).

VOLATILE ORGANIC COMPOUNDS (VOCs) IN COFFEE: THEIR FORMATION AND ANALYSIS

Volatile Organic Compounds (VOCs) in Coffee

The aroma profile of coffee is directly related to VOCs. Non-VOCs contribute to the body, bitterness, astringency and acidic flavor of the coffee bean. VOCs of various chemical classes such as alcohols, aldehydes, esters, furans, ketones, phenols, pyrazines, pyridines, pyrroles and sulfur compounds in roasted coffee determine the sensory properties of coffee. Some of them, such as furans, can be harmful to human health (Cao et al., 2023; Cascos et al.,2024; Zhai et al., 2024). VOCs with low odor threshold contribute significantly to the coffee aroma (Zakidou et al., 2021; Shi et al., 2024). Volatile thiols are among the compounds that highly affect coffee quality and aroma, even at very low concentrations (Heo et al., 2020; Zakidou et al., 2021). Polyphenols are an essential source of dietary antioxidants and are abundant in vegetables, fruits, cereals and plant-derived beverages such as red wine, tea, cocoa and coffee (Zakidou et al., 2021; Dippong et al., 2022; Cao et al., 2023).

Genetic lines are a determining factor in total VOC emission capacity; pure Arabica varieties such as Bourbon and Typica exhibit higher total VOC emissions than Robusta hybrids (Taiti et al., 2025). The growing altitude of coffee beans directly influences the development of VOCs; higher altitudes allow for a more concentrated development of hexanoic acid and furans, thereby enhancing aromatic quality (Bordiga et al., 2025). Specific VOC markers (e.g., pyridine and 2-methylpyrazine) provide a geographical fingerprint with over 90% accuracy in distinguishing coffees from different regions such as Brazil, Ethiopia, Colombia, etc. (Bordiga et al., 2025; Elefante et al., 2025).

The VOC profile of coffee beans is formed as a result of the gradual reactions that precursors-such as non-volatile carbohydrates, lipids, proteins and amino acids in green beans-undergo during processing, storage and especially roasting (Elefante et al., 2025). The fermentation method and the resulting microbial ecology significantly alter the composition of both volatile and non-volatile compounds in coffee. The post-harvest drying and fermentation stages are critical for the formation of volatile compounds, while non-volatile components derived from carbohydrates, carboxylic acids and alkaloids are significantly reshaped as a result of these processes. For example, while traditional spontaneous fermentation typically results in inconsistent and unpredictable quality due to environmental variability; controlled anaerobic methods such as carbonic maceration or self-induced anaerobic fermentation (SIAF) enhance the volatility of specific aroma compounds (Suaib et al, 2024; Zhai et al., 2024; Shen et al. 2025).

The roasting temperature of coffee beans visibly affects the polyphenolic profile through the Maillard reaction, giving coffee a pleasant aroma and flavor. Coffee is also a major source of essential elements and micronutrients such as K, Ca, P, Fe, Mn, Zn and Cu (Dippong et al., 2022). The degree of roasting plays a more dominant role in the formation of aroma compounds than the influence of geographical origin, making it the primary factor determining the coffee's final volatile composition (Zakidou et al., 2021; Vezzulli et al., 2023). Table 4 illustrates an integrative synthesis of the literature, highlighting the correlations between VOC classes, precursors, formation pathways and their resultant odor thresholds and sensory contributions.

Table 4. Integral synthesis of VOC classes, formation mechanisms, Odor thresholds and Odor Activity Values (OAVs)

VOC Class	Key Aroma Compounds	Formation Mechanism & Precursors	Odor Threshold & Impact	OAV & Sensory Contribution	Sensory Descriptors & Quality Impact	Notes & References
Pyrazines	2,5-Dimethylpyrazine; 2-Ethyl-3,5-dimethylpyrazine; Hazelnut pyrazine	Formed via Maillard reactions between reducing sugars and amino acids.	Moderate to high threshold.	Significant OAV; fundamental for defining the intensity of the "roasted" character.	Nutty, roasted, earthy and chocolate-like notes.	Pyrazine levels correlate with the degree of roasting and are key quality markers (Zakidou et al., 2021; Caporaso et al., 2022; Wu et al., 2022; Elhalis et al., 2023; Shi et al., 2024; Chen et al., 2025; Jeon et al., 2026).
Pyridines	Pyridine; 3-Ethylpyridine	Formed through the degradation of trigonelline.	Moderate threshold.	Variable OAV; contributes to "body" but can lead to off-notes if too high.	Sour, roasted, bitter and tobacco-like notes.	Pyridine provides a roasted character but can develop "fishy" off-notes at excessive levels (Bastian et al., 2021; Wu et al., 2022; Cao et al., 2023; Elhalis et al., 2023; Chen et al., 2025).
Thiols	2-Furfurylthiol; 2-Methyl-3-furanthiol; Methanethiol	Sulfur-containing precursors; highly sensitive to thermal and storage conditions.	Extremely low threshold.	Very High OAV; even trace amounts dominate the "fresh coffee" perception.	Roasty, meaty and coffee-freshness attributes.	2-Furfurylthiol is the primary factor in aroma loss, losing over 50% during storage (Elhalis et al., 2023; Sun et al., 2024).
Aldehydes	2-Methylbutanal; 3-Methylbutanal; Hexanal	Produced via Strecker degradation and lipid oxidation.	Low threshold.	High OAV; 3-methylbutanal is a main contributor to malty and fruity nuances.	Malty, fruity, pungent and green/grassy notes.	Hexanal indicates lipid oxidation (off-flavors), while methylbutanals are key roasting markers (Cao et al., 2023; Elhalis et al., 2023; Gantner et al., 2024; Shi et al., 2024; Debona et al., 2025; Qiu et al., 2026).
Ketones	β-Damascenone; Butan-2,3-dione (Diacetyl)	Thermal degradation of carotenoids and sugars.	Very low threshold.	Significant OAV; diacetyl provides essential "buttery" notes even in complex matrices.	Fruity, honey-like, buttery and creamy nuances.	β-Damascenone provides complex honey nuances at trace concentrations (Caporaso et al., 2022; Cao et al., 2023; Elhalis et al., 2023; Shi et al., 2024; Wu et al., 2024; Chen et al., 2025).
Esters & Terpenes	Ethyl acetate; Ethyl-2-methylbutyrate; Linalool	Produced during fermentation and enzymatic activities.	Low threshold.	High OAV; linalool is a representative compound for high-quality "floral" notes.	Fruity, floral, sweet and ethereal notes.	Linalool and ethyl acetate are markers for fruity-floral nuances in fermented African Arabica (Cao et al., 2023; Vezzulli et al., 2023; Shi et al., 2024; de Melo Pereira et al., 2025).
Furans & Furanones	Furfural; 2-Furanmethanol; 4-Hydroxy-2,5-dimethyl-3(2H)-furanone	Derived from caramelization and Maillard reactions.	High Threshold.	Moderate OAV; very high concentrations reaching impact levels.	Sweet, caramel, burnt and almond-like; forms the sweet backbone.	2-Furanmethanol acetate serves as a specific marker for coffee adulteration with additives (Cao et al., 2023; Elhalis et al., 2023; Cascos et al., 2024; de Souza et al., 2024; Park et al., 2024; Chen et al., 2025; Jeon et al., 2026).

Acids	Acetic acid; 3-Methylbutanoic acid; Propionic acid	Byproducts of fermentation metabolites and sugar degradation.	High threshold.	High OAV in light roasts/fermented beans; defines the sharp profile.	Vinegar, pungent, sweaty and sharp acidity.	Propionic acid is a specific marker for monitored fermentation and maceration conditions (Wu et al., 2022; Elhalis et al., 2023; Gantner et al., 2024; Chen et al., 2025; Dos Santos Gomes et al., 2025).
Hydrocarbons	1-Nonadecene; Anethole	Naturally occurring bioactive lipids within the coffee matrix.	Variable threshold.	Predictive OAV; 1-nonadecene is a key predictor of fragrance, body and balance.	Contributes to the overall fragrance, body and aftertaste.	1-Nonadecene is identified as a significant bioactive determinant of Arabica specialty coffee quality (Zakidou et al., 2021; Agnoletti et al., 2022; Wu et al., 2022; Cascos et al., 2024).
Phenolic Com-	Guaiacol; 4-Ethylguaiacol; p-Vinylguaiacol	Thermal degradation of CGAs during roasting.	Low to moderate threshold.	Significant OAV in dark roasts; contributes to the "spicy/smoky" depth.	Spicy, smoky, phenolic and clove-like descriptors.	Concentrations increase continuously with roasting as CGAs decompose into volatile phenols (Elhalis et al., 2023; Urugo et al., 2024; Chen et al., 2025; Kašpar et al., 2025).

Sensory analysis is generally performed according to guidelines set by the Specialty Coffee Association (SCA), where a group of trained professionals conducts a sensory evaluation of coffee samples in a specially designed room that meets specific requirements (SCA, 2021). Research indicates that the sensory-significant classes of VOCs in roasted coffee are frequently furans/furanones, pyrazines, aldehydes, ketones, esters, alcohols, acids, pyrroles, pyridines, phenols and volatile thiols. These classes contribute to the nutty-chocolate, caramel-sweet, fruity/floral and off-note (burnt, cabbage, sulfurous) aroma profiles of roasted coffee.

Aroma Development and Formation Mechanisms of Coffee

Coffee quality begins with the careful selection of fruits with uniform ripeness to reduce the proportion of defective beans and achieve optimal aromatic potential. Post-harvest primary processing and the drying process dynamically modulate aroma precursors in the bean through physical and physiological changes (Wang et al., 2022; Cao et al., 2023). The complex post-harvest processes applied before roasting, such as harvesting and progressing through fermentation, drying and roasting, culminating in brewing and storage, shape the aroma due to its volatile compounds. The different primary treatments applied alter the caffeine, trigonelline, lipid, chlorogenic acid, oligosaccharide and polysaccharide content of green coffee beans. Post-harvest approaches also significantly influence the content of these compounds (Zhai et al., 2024). During this process, various physical and chemical changes occur. The fermentation period increases the volatile compounds of acids and decreases the concentration of volatile compounds in general, because the synthesis of volatile compounds is reduced by the restriction of enzymatic activity during long fermentation, reducing aroma precursors such as pyrazines and furfurans (Galarza and Figueroa, 2022). These biochemical transformations occurring in the bean tissue are the key factors that directly determine VOCs formation during roasting and the sensory profile of the final cup (Bastian et al., 2021; Zakidou et al., 2021; Zhai et al., 2024; Debona et al., 2025).

During the coffee processing process, more than 90% of the biomass of coffee beans is converted into coffee processing waste, mostly in the form of coffee grounds, mucilage, husk or pulp, depending on the chosen processing method (Figure 1) (Miron-Merida et al., 2021). All processes, shown in Figure 1, to some extent activate aroma components through fermentation: on the one hand, under the influence of microorganisms and enzymes, sugars and other substances are transferred to alcohols and other acid components; on the other hand, precursor compounds formed in coffee husks can diffuse into the beans, which can then be involved in the Maillard reaction, especially in the coffee roasting process (Wan et al., 2024; Messias et al., 2025; Shen et al., 2025).

Figure 1. Different primary processes applied to coffee fruits (Wan et al., 2024). (Figure was recreated by authors).

Post-harvest primary processing methods manipulate the VOC profile by altering the pool of precursors in coffee beans (Zhai et al., 2024). Wet processing offers a cleaner aroma profile while promoting the formation of green notes such as hexanal (Cao et al., 2023; Vezzulli et al., 2023). Anaerobic fermentation increases the volatility of aroma compounds; dry processing is characterized by high alcohol and ester concentrations associated with fruity and sweet notes (Arenas et al., 2022; Zhai et al., 2024). During spontaneous fermentation, the metabolic activities of microorganisms (carbon and nitrogen metabolism) shape the key aroma precursors (reducing sugars, amino acids) released after roasting (Bressani et al., 2020; Wu et al., 2024).

During the fermentation stage, lactic acid bacteria play a critical role in aroma development by breaking down the coffee mucilage and facilitating the separation of the fruit layers. Additionally, by converting fermentable sugars into metabolites such as lactic acid, they directly shape the final acidity and support the formation of volatile aroma compounds. Inoculation with selected microorganisms can shorten the fermentation time, suppress unwanted microorganisms and ultimately provide a more controlled and reproducible sensory profile. Therefore, the use of defined starter cultures is becoming increasingly important for standardization at an industrial scale (Wu et al. 2024; Zhai et al. 2024; Shen et al., 2025).

The final aroma is developed during thermal roasting (Bastian et al., 2021; Zhai et al., 2024). The temperature used during the coffee roasting process changes the concentration of VOCs and degrades non-volatiles (Heo et al., 2020; Rusinek et al., 2022). Caffeine is moderately heat-resistant during coffee roasting. Chlorogenic acid and trigonelline rapidly degrade, forming phenolic compounds and pyridines/pyrroles, respectively. Chlorogenic acid breaks down into feruloylquinic acid lactones, caffeoylquinic acid lactones and p-coumaroylquinic acid lactones; these newly formed compounds, along with other volatile compounds, create the flavor and affect the quality (Heo et al., 2020; Bastian et al., 2021). The chemical components of raw coffee beans undergo reactions during and after roasting to create the unique and pleasant aroma of coffee. These reactions involve the production of more than 840 VOCs, which can be classified as furans, pyrroles, pyrazines, pyridines, indoles, phenolic compounds, acids, aldehydes, esters, alcohols and ketones (Wang et al., 2022). The VOC profile undergoes a dynamic evolution throughout the roasting process; while aldehydes, anhydrides and furans show a positive correlation with desired sensory characteristics, alcohols and xanthines exhibit a negative relationship (Debona et al., 2025).

Some of the processes that take place during coffee roasting directly affect VOCs. The longer the time after the bean breaks, the more the VOC profile changes negatively. In particular, exceeding 30 seconds reduces the aromatic quality of the coffee and lowers its sensory score groups (Catão et al., 2022). VOCs begin to form at 190°C (7th minute) and begin to decrease due to thermal degradation after reaching a peak at 221°C (11th minute) in Arabica coffees (Debona et al., 2025). During the roasting process, the majority of volatile compounds are furans (24–41%) and pyrazines (25–39%), which are the source of sweet and nutty notes (Zakidou et al., 2021). At the medium roast level, where total aroma content is highest, aldehydes serve as a key indicator for determining the ideal roasting point (Caporaso et al., 2022; Debona et al., 2025). However, in dark roasts, due to intense heat and pyrolysis, desired levels of furans and furfural decrease, while the concentration of pyridines, associated with bitter, smoky and burnt notes, increases (Cao et al., 2023; Debona et al., 2025). In contrast, there is an inverse relationship between roast intensity and the levels of potentially harmful compounds in coffee. While acrylamide concentrations reach their highest levels during low-temperature roasting (light roast), 5-HMF (5-hydroxymethylfurfural) levels rise significantly as roasting time and temperature increase (dark roast). This demonstrates that balancing the roasting profile is critical not only for aroma but also for food safety (Cascos et al., 2024; Wang et al., 2026).

The roasting process converts the non-volatile carbohydrates, lipids and proteins in green coffee beans into VOCs through a complex series of reactions; the Maillard reaction, Strecker degradation, caramelization, pyrolysis and the thermal-oxidative breakdown of lipids (Lopes et al., 2021; Zakidou et al., 2021; Pua et al., 2022; Cao et al., 2023; Debona et al., 2025; Paiva et al., 2025). During this process, the beans develop a brown, dry, brittle and porous structure; while caffeine is heat-resistant, trigonelline and chlorogenic acids degrade, converting into pyridines and volatile phenols, respectively (Bastian et al., 2021).

Throughout roasting, varieties of chemical reactions happen, including the Maillard reaction, caramelization and Strecker degradation. These reactions change the color of coffee as well as its flavor and aroma. The volatile aroma compounds in coffee are produced from a variety of compounds in green coffee beans, including reducing sugars, amino acids, lipids, chlorogenic acid and trigonelline (Yu et al., 2021).

Like roasting, grinding and brewing are among the traditional coffee processing methods. Grinding is one of the main steps in coffee brewing. The particle size of ground coffee beans has a crucial role in controlling the degree of extraction (Yu et al., 2021). The journey of coffee cherries turning into a cup of coffee is shown in Figure 2.

Figure 2. The journey of coffee cherries into a cup of coffee (Figure was created by authors).

Nowadays, as the popularity of coffee has increased, coffee consumption has also increased along with the growing demand for coffee. The level and concentration of aroma precursors found in green coffee beans have a significant impact on the aromas of roasted beans and the final coffee beverages (Lopes et al., 2021; Pua et al., 2022). Due to the chemical composition of coffee, non-enzymatic browning reaction occurs during the roasting process, as the green coffee bean is mainly composed of carbohydrates, lipids and proteins. Caramelization and Maillard reaction are the main reaction of non-enzymatic browning and affects chemical changes during the roasting process, including volatile compounds, brown color and unpleasant toxic compounds. These chemical changes in various coffees can be examined to control the quality and safety of the coffee (Park et al., 2024). Figure 3 shows the volatile organic compounds formed during the coffee roasting process.

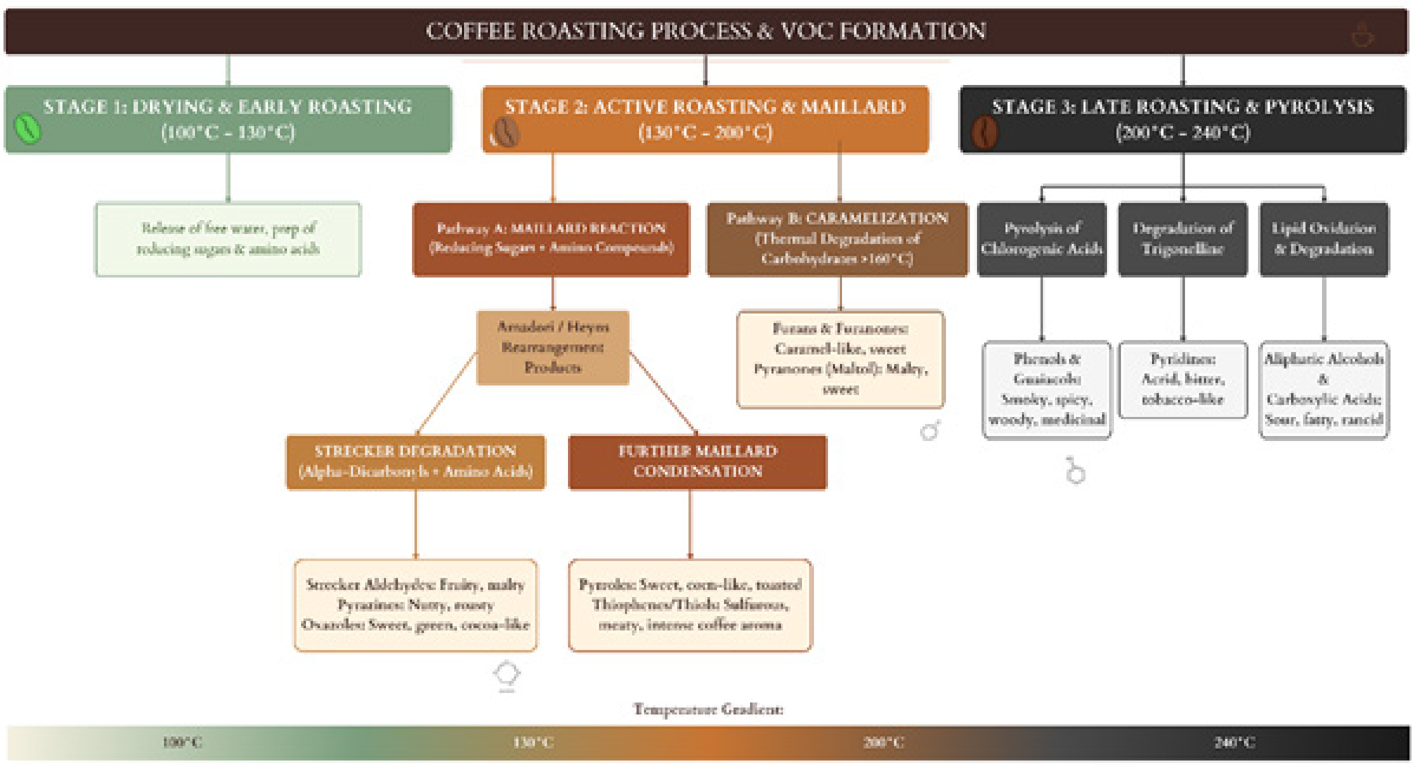

Figure 3. Coffee roasting process and VOC formation (Figure was created by authors).

The Maillard reaction (MR) is a non-enzymatic browning reaction that begins when the temperature reaches approximately 140 °C during roasting; it results from the interaction between reducing sugars and amino acids (Cao et al., 2023). In the intermediate stage the Amadori/Heyns product initiates the formation of sugar breakdown products and the release of the amine group. Then, in the final stage, dehydration, fragmentation, cyclization and polymerization with the reintroduction of the amino group take place and a large number of aromatic compounds, such as furans, pyrazines and pyrroles, are formed (Cao et al., 2023; Park et al., 2024). Pyrazines and pyrroles are also produced another way during roasting through the pyrolysis of hydroxyl amino acids such as serine and threonine. Trigonelline is an alkaloid compound found in green coffee beans that undergoes degradation during heat treatment to produce pyridine and pyrrole compounds. Proteins, amino acids, lipids, polysaccharides, simple sugars, phenolic and chlorogenic compounds are the main aroma precursors found in green beans. In particular, furanones and pyrroles are the primary products of sugar-amino acid interactions in the Maillard reaction and are responsible for the characteristic roasted aroma notes in coffee (Elhalis, et al., 2023; Debona et al., 2025). Approximately 30–40% of the total volatile compounds in coffee are formed directly through this mechanism (Zakidou ve ark., 2021).

Strecker degradation, considered a sub-stage of the Maillard reaction, involves the reaction of dicarbonyl compounds with free amino acids. This process leads to the release of aldehydes, ketones, furanones, furans, sulfur compounds, pyrazines and CO2, which form the basis of coffee aroma (Cao et al., 2023; Caprioli et al., 2025). While the aldehydes produced by Strecker degradation contribute fruity and chocolatey aromas to coffee, they also play a critical role in the formation of pyrazines, which are responsible for nutty and earthy notes (Taiti et al., 2025). Additionally, variables such as the water temperature and pressure used in preparation, and the size of the coffee particles, can affect the aromatic profile and therefore the quality of the beverage (Caprioli et al., 2025).

Caramelization is another browning mechanism that occurs in the absence of amino acids, resulting solely from the thermal degradation of carbohydrates, particularly sucrose, at high temperatures (approximately 170 °C) and is affected by pH and sugar concentrations (Cao et al., 2023; Park et al., 2024). Sugar isomerization and sugar degradation reactions are involved in caramelization. During this process, the breakdown of sucrose produces smaller sugar molecules such as glucose and fructose, and the subsequent concentration step yields maltol (caramel flavor), furans (nutty notes) and acetic acid (sourness) (Cao et al., 2023). Phenols, strong phenolic volatiles such as guaiacol and vinyl guaiacol, are obtained from a series of thermal reactions involving chlorogenic acids and phenolics (Elhalis, et al., 2023). The furans formed as a result of caramelization are among the primary aroma sources that enhance the perceived sweetness of coffee (Cao et al., 2023).

When coffee beans reach temperatures of 190°C or higher, pyrolysis reactions become dominant (Cao et al., 2023). At this stage, while the pyrolysis of sucrose darkens the bean color, the pyrolysis and auto-oxidation of lipids produce alcohols and ketones that give coffee body and antioxidant capacity (Cao et al., 2023). Pyridines, which are important components of coffee aroma, are formed through the degradation of the trigonelline alkaloid via pyrolysis; phenolic compounds such as guaiacol arise from the thermal decomposition of chlorogenic acids (Debona et al., 2025). In particular, esters formed by lipid pyrolysis play a central role in the preservation and development of floral and fruity aromas in coffee (Cao et al., 2023). The formation of the volatile compounds of coffee from the main reactions between precursors is given in Figure 4.

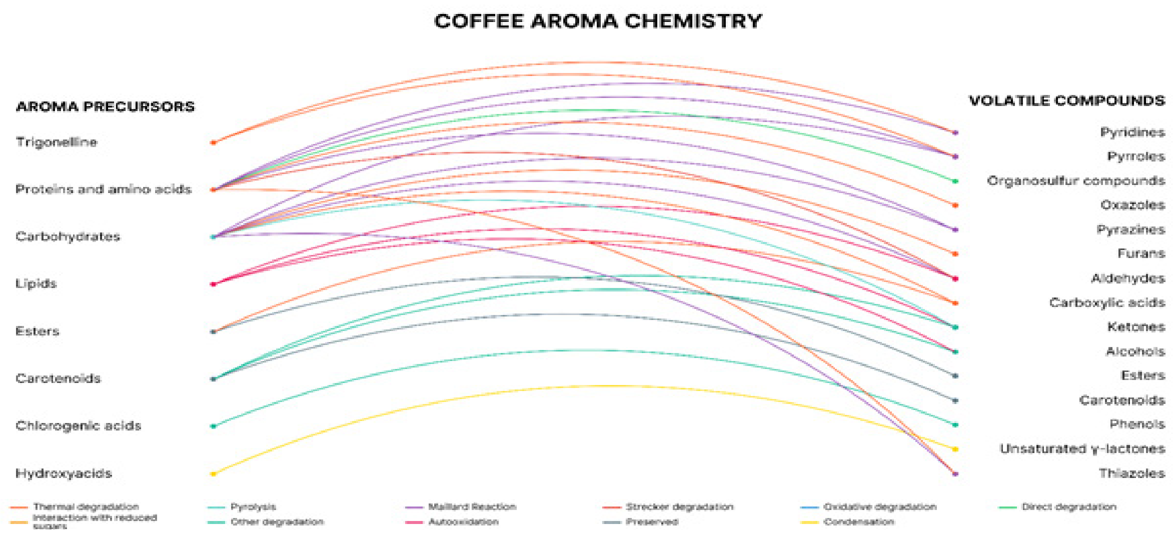

Figure 4. Diagram of the formation of the volatile compounds of coffee from the main reactions between precursors (Pua et al., 2022). (Figure was recreated by authors).

Storage conditions are important not only for preventing the loss of primary aroma compounds but also for preventing the formation of undesirable new volatile profiles resulting from lipid oxidation and the transformation of thermal processing byproducts (M. Chen et al., 2022; Gantner et al., 2024). While keeping the moisture content of coffee below 5% ensures long-term storage stability from a food safety perspective, this level is not suitable for freshly roasted coffee due to CO loss and aroma degradation. In this regard, low-temperature applications and modified atmosphere packaging play a critical role by slowing down the rate of chemical reactions and extending shelf life by preserving the stability of key odorants such as 2-furfurylthiol. Because thiols such as 2-furfurylthiol, rapidly polymerize in the presence of oxygen even just one day after roasting, leading to a stale taste (Cascos et al., 2024; Gantner et al., 2024; Sun et al., 2024).

This study provides a comprehensive overview of the mechanisms by which precursor compounds in coffee beans are converted into aromatic volatile organic compounds through fundamental thermal reactions such as the Maillard reaction and caramelization (Figures 3 and 4), their decisive roles in the final sensory perception as determined by odor activity values (OAV) and their roles in coffee aroma from a holistic perspective (Table 4).

Analytical Techniques for Determination of Coffee Aroma

Determining the aroma of coffee requires the characterization of a complex biological matrix composed of thousands of volatile compounds. Therefore, it is necessary to use advanced techniques that offer high separation efficiency and analytical sensitivity. These techniques primarily proceed along two main lines: the profiling of volatile compounds and the analysis of non-volatile components that serve as precursors to these aromas. Gas chromatography (GC) is used to identify the characteristic “fingerprint” of the volatile compounds responsible for coffee aroma, while liquid chromatography (LC) is used to analyze the non-volatile components that influence the aroma and shape the flavor profile.

Among these instrumental techniques using for coffee research, HS-SPME-GC-MS is widely recognized as a robust and highly effective method for the detection, separation and identification of VOCs with its much higher peak capacity; HPLC is considered one of the most appropriate techniques for analyzing the non-volatile compounds responsible for the highly complex aroma profile of coffee (Catão et al., 2022; Asensio-Ramos and D’Orazio, 2023; Urugo et al., 2024; Kirtil, 2025; Quintanilla-Casas et al., 2025; Resende et al., 2025; Urugo et al., 2025; Xie et al. 2025). Comprehensive Two-Dimensional Gas Chromatography (GC×GC-MS) offers much higher resolution (peak capacity), providing fingerprint analysis in complex matrices containing over a thousand components, such as coffee (Kirtil, 2025; Resende et al., 2025). In this technique, which uses two different columns, compounds are spread out in a plane and since compounds cannot be hidden under a single peak as in one-dimensional analysis, thousands of compounds become distinguishable (Courregelongue et al., 2025). Gas Chromatography-Olfactometry (GC-O) matches chemical data with the human nose to determine which compound is responsible for which odor (Kirtil, 2025). Electronic noses (e-noses) create fast and non-destructive "odor traces" using sensor arrays that mimic the human olfactory system (Mohammadian et al., 2024; Urugo et al., 2025; Melikoglu, 2026). The aroma profile is not limited to VOCs; measuring non-volatile components such as acidity, body and bitterness using the electronic tongue (e-tongue) offers a much faster and more cost-effective industrial solution compared to chromatographic methods like HPLC (Cao et al.,2023; Shi et al., 2024). Spectroscopic methods (NIR, FTIR) provide rapid, fingerprint-based quality estimation using chemical bond vibrations (Urugo et al., 2025).

Processing the massive and high-dimensional data obtained from these instrumental devices necessitates the use of chemometric tools. To understand natural groupings, origin differences, or roasting degrees in a dataset, unsupervised learning methods such as Principal Component Analysis (PCA) and Hierarchical Clustering Analysis (HCA) are initially used; these methods visualize similarities between samples by reducing the dimensionality of the data (Catão et al., 2022; de León-Solis et al., 2023; Mohammadian et al., 2024; Chen at al., 2025; Resende et al., 2025). For classification problems such as geographical origin verification and the identification of specific quality markers, supervised models such as Partial Least Squares Discriminant Analysis (PLS-DA) and Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA), which offer higher interpretability, come to the forefront (de León-Solis et al., 2023; Quintanilla-Casas et al., 2025; Urugo et al., 2025). An integrated approach with HS-GC-IMS and GC-MS techniques to characterize the aroma profile of coffee; VOCs are detected by GC-MS and identified by the high sensitivity of GC-IMS to low molecular weight and low boiling point compounds, especially alcohols (Zhai et al.,2024). The PCA and PLS-DA models reveal the effects of different primary processing methods on aroma; it is determined that anaerobic fermentation significantly increases fruity and floral notes, while honey processing significantly increases caramel and roasted aroma characteristics as a result of PLS-DA analysis, confirming the superiority of HS-GC-IMS in creating a fast and sensitive "volatile fingerprint" for coffee samples. To capture more complex and nonlinear aroma interactions such as synergy or masking, advanced machine learning algorithms such as ANNs, Support Vector Machines (SVM) and RF can predict sensory SCA scores from chemical profiles with over 90% accuracy (Mohammadian et al., 2024; Urugo et al., 2025). While these techniques offer notable advantages, including high sensitivity, analytical precision and increased objectivity, they are also associated with certain challenges, such as high instrumentation costs, the requirement for specialized technical expertise and the potential risk of overfitting when processing small datasets (Kirtil, 2025; Urugo et al., 2025; Melikoglu, 2026).

When determining the ideal method, the primary objective of the analysis must be taken into account. If the goal is to accurately determine trace amounts of compounds, leveraging the technical capabilities of chromatographic systems may be a sound approach. However, if speed and non-destructive analysis are the objectives, the use of hybrid models and sensor arrays can strike a balance between scientific rigor and industrial practicality (Mohammadian et al., 2024; Kirtil, 2025; Urugo et al., 2025). Furthermore, analyzing not only volatile compounds but also non-volatile bioactive components such as caffeine and chlorogenic acids responsible for taste and bitterness via HPLC and including them in the data offers a holistic approach to creating a complete quality map of coffee (Asensio-Ramos and D'Orazio, 2023; Urugo et al., 2024). In order to provide a comprehensive assessment of the current analytical environment in coffee research, a systematic classification and comparative evaluation of various chromatographic and non-chromatographic techniques, their technical advantages, methodological limitations and basic applications are given in Table 5 and illustrated in Figure 5.

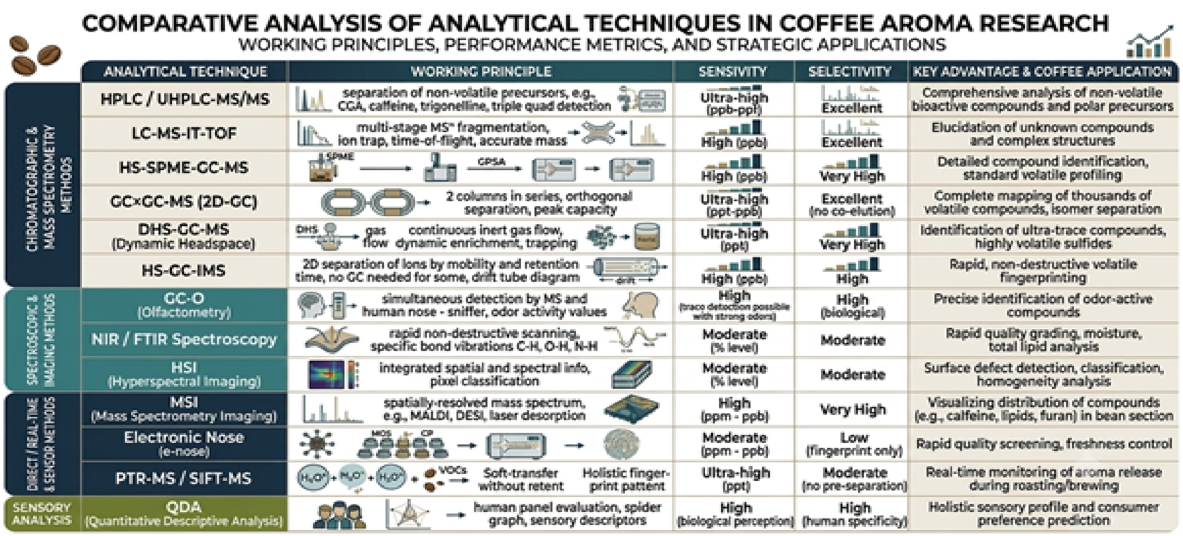

Figure 5. Comparative analysis of analytical techniques in coffee aroma research: working principles, performance metrics and strategic applications (Figure was created by authors).

Table 5. Systematic classification and comparative evaluation of analytical methods for coffee analysis

I. CHROMATOGRAPHIC METHODS - Liquid Chromatography (LC)				
Analytical Technique	Technical Advantages & Analytical Superiorities	Methodological & Operational Limitations	Primary Analytical Applications	References
HPLC-MS	o Superior sensitivity and selectivity Complex biological matrices o Preserves chemical structure o No need complex derivatization for non-VOC profiling	o Significant consumption of organic solvents o Limited to non-VOCs o Requires integration with GC-MS to create a comprehensive quality map o High operating costs o Needs advanced technical expertise for data interpretation o Performs in a laboratory setting o Difficult to implement for real-time industrial monitoring compared to sensor technologies	o Precise quantification of taste and bitterness markers: caffeine, trigonelline and chlorogenic acids o Analysis of thermal process intermediates and contaminants such as acrylamide and 5-HMF o Phytochemical fingerprinting for verification of geographical origin and variety identification	(Asensio-Ramos and D'Orazio, 2023; Urugo et al., 2024, 2025; Kašpar et al., 2025; Zhao et al., 2025)
UHPLC-MS	o Ultra-high separation efficiency o Ideal for phytochemical purity and purity control o Significantly higher resolution, speed and sensitivity compared to conventional HPLC-DAD systems	o Unsuitable for the direct analysis of VOCs o Requires solvent-based preparation	o Caffeine, chlorogenic acids and trigonelline content	(Bressani et al., 2020; Heo et al., 2020; Urugo et al., 2025; Zhao et al., 2025).
HPLC-DAD (Diode-Array Detector)	o Multiple key components in a single analysis o Simultaneous detection and quantification o Extremely robust o Reliable for the quantitative determination of high-concentration analytes o No need to alter the molecular structure o No need for complex derivatization o Creates a comprehensive aroma profile by mapping non-volatile markers	o Lower sensitivity and selectivity for trace-level components compared to MS systems o A destructive method; significant consumption of organic solvents o Risk of peak overlap in highly complex matrices when relying solely on UV/Vis spectra o Limited to the non-volatile fraction o Provides only a partial view of the total aroma profile	o Quantitative analysis of caffeine and trigonelline o Determination of the profile of major chlorogenic acids and hydroxycinnamic acids o Quality assessment of brewed coffee and commercial extracts	(Urugo et al., 2024, 2025; Kašpar et al., 2025; Heo et al., 2020; Zhao et al., 2025; Melikoglu, 2026).

LC-MS-IT-ToF (Ion Trap Time-of-Fight)	o High-resolution MS with ion-trap capabilities for structural elucidation of new analogs o Crucial for identifying unknown compounds not found in standard libraries o Uses precise elemental composition data o Effective separation of isobaric species and trace metabolites in complex biological matrices such as coffee beans	o Very high investment cost o Limited to specific safety and toxicological applications	o Toxicological risk assessment and identification of Maillard intermediates o Identification of biomarkers for geographical origin and coffee variety classification o Structural characterization of novel phenolic derivatives and reaction intermediates formed during roasting o Advanced metabolomic fingerprinting and spatial metabolomic studies	(Chen et al., 2022; Urugo et al., 2025; Zhao et al., 2025; Wang et al., 2026).
I. CHROMATOGRAPHIC METHODS - Gas Chromatography (GC)				
Analytical Technique	Technical Advantages & Analytical Superiorities	Methodological & Operational Limitations	Primary Analytical Applications	References
HS-SPME-GC-MS	o Gold standard for VOC profiling o Ability to detect even trace amounts of aromatic compounds in the upper space of green and roasted coffee beans o Minimum sample quantity (solid or liquid) Simple sample preparation method o HS-SPME; solvent-free extraction, low chemical waste, minimal environmental impact	o Struggling in fully resolving peaks in highly complex coffee matrices o Lower quantitative accuracy and enrichment capacity compared to DHS methods as a balance-based extraction method o Risk of deviation in quantitative accuracy due to matrix effects and fiber region competition o Requires high equipment investment and time-intensive work cycles	o Standard protocol for VOC profiling and molecular marker identification o Monitoring changes in aroma profiles during roasting, fermentation and storage o Reliable differentiation of coffee samples according to geographic origin and botanical variety o Identification of additives and detection of adulteration in commercial samples	(Bressani et al., 2020; Zakidou et al., 2021; Agnoletti et al., 2022; Arenas et al., 2022; Wu et al., 2022; Vezzulli et al., 2023; Cascos et al., 2024; de Souza et al., 2024; Urugo et al., 2024, 2025; Zhai et al., 2024; Debona et al., 2025; Rovelli et al., 2026; Xu et al., 2026).

GC×GC-MS (2D-GC)	o An accurate and precise "aroma fingerprint" for in-depth molecular profiling o Unparalleled resolution and peak capacity o Ability to distinguish over 1000 different components in highly complex matrices o Superior sensitivity and enrichment for detecting trace and ultra-trace amounts of VOCs o Eliminating peak co-elution risks by spreading VOCs in a two-dimensional plane	o Generating large, high-dimensional datasets o Requires advanced chemometric tools, sophisticated data mining strategies, deep technical expertise and specialized training o Due to the enormous volume of information generated, manual analysis of individual peaks is inefficient o Significant investment and maintenance costs compared to conventional one-dimensional GC systems	o Comprehensive molecular-level mapping of aroma development and Maillard reaction products o Identification of key bioactive fragrance compounds and previously unidentified volatile markers o High-precision geographic origin verification and botanical identification through region-specific pattern recognition	(Bordiga et al., 2025; Courregelongue et al., 2025; Kirtil, 2025; Paiva et al., 2025; Resende et al., 2025; Urugo et al., 2025).
DHS-GC-MS (Dynamic Headspace)	– Ideal for monitoring the evolutionary profiles of VOCs during roasting – Effectively captures a wide range of both VOCs and semi-VOCs (SVOCs) – Significantly higher extraction capacity and sensitivity compared to static HS-SPME by continuously capturing volatile substances in sorbent tubes – Better quantitative accuracy and enrichment for trace components thanks to its non-equilibrium structure	– Requires the application of chemometric tools (e.g., PLS-DA) for robust data interpretation – Requires specialized hardware, including sorbent-filled thermal desorption (TD) tubes and automated desorption modules – Requires a higher initial investment and operating costs compared to routine passive clearance methods	– Real-time monitoring of aroma formation kinetics and chemical transformations at various roasting stages – Strategic optimization of roasting profiles to enhance the quality of specialty coffees – In-depth characterization of the volatile matter cloud released during post-harvest processing and thermal treatments	(Paiva et al., 2025; Resende et al., 2025; Urugo et al., 2025).

HS-GC-IMS (Ion Mobility Spectrometry)	o Ideal for industrial quality control o Provides rapid analysis and high-throughput screening o Operates at lower temperatures and preserves heat-sensitive natural VOCs; reflects the original state of samples o No need for complex sample pretreatment o Ability to detect trace amounts of VOCs (ng/L or ppbv) o Improves the separation of isomeric and isobaric compounds (e.g., different C6 aldehydes and ketones) through secondary separation in the drift tube o Solvent-free operation and low nitrogen gas consumption; environmentally friendly method	o Difficult to precise compound identification o Depends on the availability of comprehensive IMS spectral libraries o Highly sensitive to instrumental deviations and environmental changes o Requires consistent normalization via reaction ion peak (RIP) o Lower chemical resolution and compound identification power compared to high-resolution MS platforms o Difficulty in deconvolution of highly complex coffee matrices without MS connectivity	o Detection of counterfeit Arabica/Robusta blends in commercial samples with 100% accuracy in approximately 25 minutes o Rapid geographic origin verification and variety identification using 2D molecular fingerprinting o Differentiation between different post-harvest primary processing methods based on unique VOC patterns o Monitoring storage aging and freshness by tracking key biomarkers such as acrolein and butanoic acid	(Konieczka et al., 2020; M. Chen et al., 2022; Y. Chen et al., 2022; Zhai et al., 2024; Bordiga et al., 2025; Shi et al., 2024; Urugo et al., 2025).
CHROMATOGRAPHIC METHODS – Gas Chromatography (GC)				
Analytical Technique	– Technical Advantages & Analytical Superiorities	Methodological & Operational Limitations	– Primary Analytical Applications	References

MSI **(Mass Spectrometry Imaging)**	– Unique ability to visualize the spatial distribution of aroma and bioactive components directly within the bean tissue – Overcomes the lack of spatial resolution inherent in conventional chromatographic methods – Enables for the mapping of components in their natural state without the need for bulk extraction, preserving context – Capable of mapping hundreds of metabolites and precursors in a single imaging run	– Requires highly specialized equipment and significant technical expertise to operate and interpret the results – Requires very high initial investment and maintenance costs compared to standard MS systems – Necessitates precise sectioning and preparation of the bean to maintain chemical localization and integrity – Generates massive datasets that require advanced chemometric and spatial-spectral processing tools	– Visualizing the distribution of aroma precursors and bioactive compounds within the core tissue – Advanced phytochemical fingerprinting to identify variety-specific distribution patterns – Studying the internal chemical transformations that occur throughout bean development and roasting stages	(Urugo et al., 2025; Zhao et al., 2025).
II. NON-CHROMATOGRAPHIC & SENSORY METHODOLOGIES - Biomimetic & Real-Time Monitoring				
Analytical Technique	**Technical Advantages & Analytical Superiorities**	**Methodological & Operational Limitations**	**Primary Analytical Applications**	**References**
Electronic Nose **(e-nose)**	o Uses gas sensor arrays (e.g., metal oxide semiconductors) to mimic the human olfactory system o Creates a “holistic chemical signature” or “odor trace” of the sample o Enables highly efficient screening without altering the sample’s integrity or requiring complex chemical pretreatment o Achieves high predictive accuracy (often >90%) for sensory scores and volatile peak areas when coupled with Machine Learning (ANNs, RF, SVM) o A portable and affordable solution for small producers and field applications, especially where GC-MS is inaccessible	o Unlike GC-MS, cannot identify specific individual volatile molecules; only responds to the overall pattern across the sensor array o Highly dependent on the stability of the sensors o Requires robust chemometric modeling to interpret high-dimensional data o Necessitates baseline normalization since o fluctuations in ambient temperature and humidity can affect sensor performance, o Success depends on pre-established reference datasets for effective pattern recognition	– Rapid classification of roasting intensity and monitoring of roasting kinetics – Differentiates coffee varieties (Arabica vs. Robusta) and verifying geographical origin – Estimates levels of toxic compounds like acrylamide and 5-HMF through sensory defect correlations – Provides objective quality grading to minimize the impact of human panelist fatigue	(Marek et al., 2020; Y. Chen et al., 2022; Cascos et al., 2024; Gantner et al., 2024; Mohammadian et al., 2024; Urugo et al., 2025; Melikoglu, 2026; Qiu et al. 2026).

II. NON-CHROMATOGRAPHIC & SENSORY METHODOLOGIES - Biomimetic & Real-Time Monitoring				
Analytical Technique	– **Technical Advantages & Analytical Superiorities**	**Methodological & Operational Limitations**	– **Primary Analytical Applications**	**References**
Electronic Tongue **(e-tongue)**	– Mimics the human taste system by using electrochemical sensors to measure non-volatile taste characteristics (bitterness, acidity and sweetness) – By eliminating the subjective assessments of human panelists, offers a highly reliable way to measure the intense bitterness and body of Robusta beans and the acidity of Arabica beans – Enables near real-time analysis of liquid coffee extracts with minimal sample preparation compared to HPLC. – Creates a complete digital cupping profile that covers both VOCs and non-VOCs, when combined with e-nose data	– Identifies taste fingerprints rather than specific chemical concentrations of molecules like caffeine or CGAs – The high lipid and protein content in some coffee brews can interfere with the electrochemical response of the electrodes – Chemical sensors require frequent cleaning and calibration due to prone to drift over time and can be contaminated by dense coffee matrices	– Predicting SCA scores for acidity and body with high accuracy using machine learning models – Distinguishing between Arabica and Robusta blends based on soluble solid patterns – Monitoring changes in the taste profile during fermentation and storage	(Mohammadian et al., 2024; Wu et al., 2024; Urugo et al., 2025)
PTR-ToF-MS **(Proton Transfer Reaction)**	o Enables the continuous, online monitoring of volatile release during roasting or brewing without chromatographic pre-separation o Provides detection limits for low-molecular-weight compounds, often reaching ppbv or even ppbv levels o Ideal for high-speed screening of large sample sets results (analysis in <1 min), o that requires almost no sample pretreatment and preserves the integrity of the sample headspace	o Higher initial equipment and maintenance costs compared to standard GC-MS systems o Because it lacks a chromatographic column, precise identification of compounds in complex mixtures can be challenging without further validation o High-resolution mass spectra provide sum formulas but struggle to distinguish between isomeric and isobaric compounds	– Optimizing roasting profiles by monitoring roasting kinetics and aroma development dynamics in real time – Industrial online process control to ensure consistency across batches – Objective monitoring of genetic lineage and quality levels in specialty Arabica coffees – Fingerprinting for geographical origin verification and authentication	(Beccaria et al., 2022; Wan et al., 2024; Taiti et al., 2025; Melikoglu, 2026).
SIFT- MS **(Selected Ion Flow Tube)**	o Overcomes the static limitations of conventional chromatography by enabling continuous monitoring of aroma release during roasting or brewing o Provides immediate results without requiring chromatographic pre-separation, thus enabling rapid processing of large sample sets o A non-destructive technique that does not require sample pretreatment and effectively preserves the integrity of highly volatile compounds o Ability to perform absolute quantitative analysis of trace (ppbv) volatile substances using multiple reactive ions for enhanced selectivity	o Struggle to resolve complex isobaric and isomeric mixtures where different molecules share the same mass, without a GC column o Requires a significant capital investment and high maintenance costs compared to routine analytical equipment o Accurate data interpretation and system calibration require advanced technical knowledge in the fields of mass spectrometry and ion chemistry	o Continuous monitoring of volatile substance release and aroma formation kinetics during roasting o Real-time characterization of the aroma plume released during brewing and grinding o High-speed industrial quality control and consistency testing for specialty coffee production	(Beccaria et al., 2022; Melikoglu, 2026).

SIFT- MS **(Selected Ion Flow Tube)**	o Overcomes the static limitations of conventional chromatography by enabling continuous monitoring of aroma release during roasting or brewing o Provides immediate results without requiring chromatographic pre-separation, thus enabling rapid processing of large sample sets o A non-destructive technique that does not require sample pretreatment and effectively preserves the integrity of highly volatile compounds o Ability to perform absolute quantitative analysis of trace (ppbv) volatile substances using multiple reactive ions for enhanced selectivity	o Struggle to resolve complex isobaric and isomeric mixtures where different molecules share the same mass, without a GC column o Requires a significant capital investment and high maintenance costs compared to routine analytical equipment o Accurate data interpretation and system calibration require advanced technical knowledge in the fields of mass spectrometry and ion chemistry	o Continuous monitoring of volatile substance release and aroma formation kinetics during roasting o Real-time characterization of the aroma plume released during brewing and grinding o High-speed industrial quality control and consistency testing for specialty coffee production	(Beccaria et al., 2022; Melikoglu, 2026).
II. NON-CHROMATOGRAPHIC & SENSORY METHODOLOGIES – Sensory Analysis				
Analytical Technique	**Technical Advantages & Analytical Superiorities**	**Methodological & Operational** **Limitations**	**Primary Analytical Applications**	**References**
QDA **(Quantitative Descriptive Analysis)**	– Provides a biological filter that captures the entire sensory experience, including taste, aroma, and mouthfeel; a feature that instrumental methods have not yet fully replicated – Results directly reflect consumer preferences and established industry quality standards, such as SCA cupping scores – Uses trained experts (e.g., Q-graders) to build the relevant set of characteristics through structured discussion to provide a comprehensive description of the product	– Susceptible to human error, individual odor thresholds and psychological biases, leading to potential inter-panel inconsistencies – Accuracy is limited due to panelist fatigue, olfactory adaptation and fluctuations in mood – Extremely time-consuming and expensive due to the need for ongoing professional training and specialized sensory facilities – Inadequate for evaluating samples that may contain irritating or potentially hazardous volatile compounds	– Generating basic accuracy data to calibrate machine learning models and rapid scanning tools such as electronic noses – Mapping the impact of roasting degrees and post-harvest fermentation on final cup quality – Evaluating specialty coffee batches for commercial pricing and geographical origin verification	(Heo et al., 2020; Cao et al., 2023; de León-Solis et al., 2023; Shi et al., 2024; Wu et al., 2024; Urugo et al., 2024, 2025).

Table 5 synthesizes a wide range of methods, from high-resolution chromatography to spectroscopic, imaging techniques and biomimetic sensors (e-nose and e-tongue), comparing them for the first time in terms of analytical advantages and operational limitations, with the aim of closing methodological gaps in the literature. The results synthesized from the literature review show that HS-SPME-GC-MS is still considered the gold standard and a green technique for the detailed identification of individual VOCs; DHS-GC-MS provides in-depth VOC identification, because DHS gives real-time and highly accurate information about aromatic changes, especially during processes such as roasting. For determining and verifying geographical origin and for fingerprinting of coffee VOCs; GCxGC-MS, GC-IMS, NIR-HSI and PTR-ToF-MS methods could be useful for researches. Advanced 2D systems (GC×GC-MS) can be used to identify aroma fingerprints as they excel in deep molecular profiling. Especially PTR-MS and IMS-based tools offer rapid and often online fingerprinting. GC-IMS, PTR-ToF-MS and SIFT provide industry-useful rapid outputs facilitating industrial quality control. HS-GC-IMS provides a practical, fast and cost-effective solution for real-time industrial applications by detecting counterfeit products and verifying their origin. NIR-HSI method's ability to predict volatile component profiles from simple spectral fingerprints allows for the identification of specific coffee beans that may damage aroma profiles or indicate adulteration. PTR-ToF-MS is a method that can be used to understand the aroma formation kinetics, compound formation rate and time during roasting; while SIFT-MS, which has the ability to use multiple precursor ions to distinguish specific chemical interferences, is a method that can be used to monitor how coffee aroma develops during thermal processing beyond static snapshots and to understand its dynamic kinetic processes. Sensory evaluation/QDA could be essential for correlating instrument-based VOC measurements with what consumers actually perceive. Modern research now uses ANNs to predict QDA results with over 90% accuracy. Combining e-nose with machine learning techniques such as ANNs, RF and SVM gives high predictive accuracy for sensory scores and volatile peak areas and minimizes the impact of human panelist fatigue. GC-O, viewed as a sensory filter in coffee studies, can overcome human subjectivity by being integrated with machine learning models. FTIR, faster alternative to GC-MS, can be combined with advanced chemometric tools (such as MLR and PLSR) or upstream GC columns to resolve temporal and spectral overlaps in complex coffee matrices.

In addition to all these techniques used for VOCs; the methods used for the identification, fingerprinting and quantification of non-VOCs such as caffeine, chlorogenic acids and trigonelline that affect taste, bitterness and acidity of coffee are HPLC-MS, UHPLC-MS, HPLC-DAD and LC-MS-IT-ToF. HPLC-MS is considered the gold standard for the characterization of non-volatile precursors and bioactive metabolites that fundamentally shape the taste and physiological effects of coffee. HPLC-DAD is a practical method for routine industrial quantification of key flavor additives such as caffeine and CGAs. UHPLC-MS indicates the concentration of caffeine, trigonelline and chlorogenic acid compounds with higher resolution, speed and sensitivity compared to HPLC-DAD. Researchers seeking a comprehensive quality map often combine HPLC-DAD data with GC-MS results to bridge the gap between taste precursors and final aromatic volatile compounds. LC-MS-IT-ToF is useful for researchers who want to map the hundreds of volatile and non-volatile compounds of the coffee metabolome. Rather than these LC-based techniques, e-tongue provides real-time analysis with minimal sample preparation. HPLC-MS and LC-MS-IT-ToF could be useful for identification and fingerprinting of non-VOCs. By revealing these compounds' location, how roasting penetrates the core and how aroma precursors are localized can be discovered with MSI. Future directions include integrating results with spatial metabolomics (MSI) to map the distribution of these components directly within the core fabric.

Methods that can be used to detect coffee aroma formation during roasting are HS-SPME-GC-MS, DHS-GC-MS, GC-O, PTR-ToF-MS, SIFT-MS, NIR, HSI, FTIR, MSI, LC-MS-IT-ToF, e-nose and QDA. Aroma formation kinetics and chemical transformation during roasting can be analyzed with DHS-GC-MS, GC-O, PTR-ToF-MS, SIFT-MS, MSI and LC-MS-IT-ToF. DHS-GC-MS gives roasting kinetics, chemical transformation at various roasting stages and real-time monitoring of aroma formation. PTR-ToF-MS provides tracking roasting kinetics and dynamics in real-time to optimize roast profiles. LC-MS-IT-ToF can be used for characterization of phenolic derivates and reaction intermediates formed during roasting. MSI can be used for chemical transformations that occurs roasting stages. For monitoring changes in aroma profile during roasting, HS-

SPME-GC-MS can be used. NIR is used for classification of rapid roasting degree; HSI for rapid identification roasting defects; FTIR for quantitively evaluation of specific roasting; QDA for mapping the impact of roasting degrees. Real-time monitoring of aroma formation during roasting can be obtained via DHS-GC-MS, PTR-ToF-MS, NIR, SIFT-MS and e-nose methods.

Technological Developments, Innovations and Future Perspective

The analytical focus in coffee research has developed from identifying individual molecules to addressing large, high-dimensional datasets through Flavoromics and Artificial Intelligence (AI) (Catão et al., 2022; Pua et al., 2022; de León-Solis et al., 2023; Mohammadian et al., 2024; Chen at al., 2025; Resende et al., 2025; Qiu et al., 2026). While classic unsupervised chemometric tools like PCA and HCA are used to determine natural groupings, roasting degrees or geographical origin differences; supervised linear models such as PLS-DA and OPLS-DA has start to come to the forefront to prevent fraud in the industry (such as mixing Robusta with Arabica coffee) and to verify origin (Catão et al., 2022; de León-Solis et al., 2023; Mohammadian et al., 2024; Bordiga et al., 2025; Chen at al., 2025; Quintanilla-Casas et al., 2025; Resende et al., 2025; Urugo et al., 2025). However, the fact that compounds in coffee's aromatic matrix often exhibit synergistic or masking effects necessitates the use of advanced machine learning techniques. Algorithms such as Artificial Neural Networks (ANNs), Support Vector Machines (SVM) and Random Forest (RF), which can predict human sensory SCA scores from chemical profiles with over 90% accuracy, can effectively digitize the expert "cupping" process (Mohammadian et al., 2024; Wu et al., 2024; Kirtil, 2025; Urugo et al., 2025). The systematic process of converting complex analytical raw data into validated predictive models via advanced chemometrics and AI architectures is illustrated in Figure 6, which highlights the critical stages of data pre-processing and model validation.

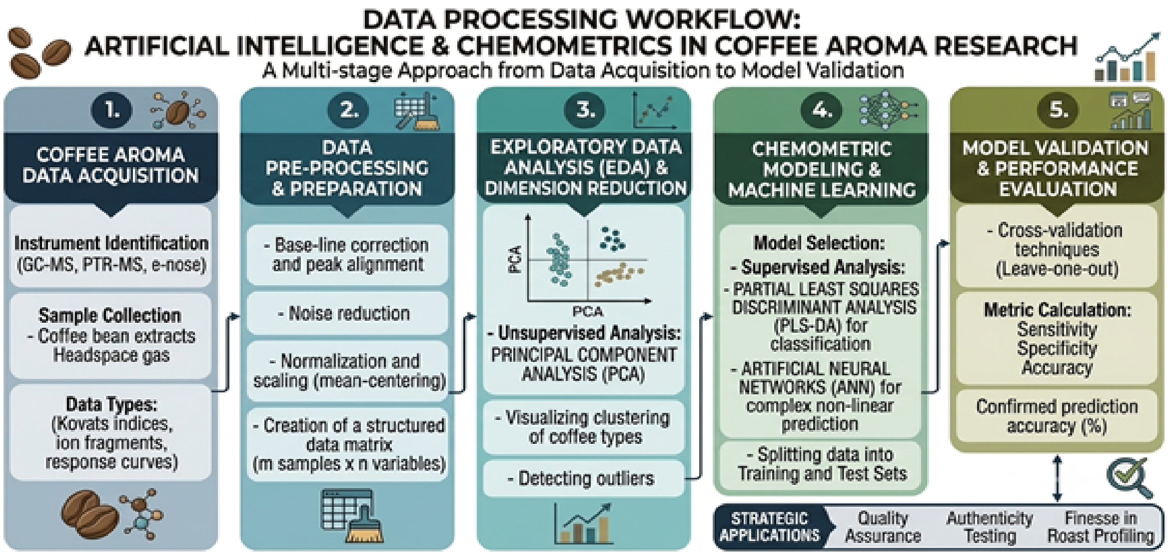

Figure 6. A new approach: artificial intelligence and chemometrics in coffee aroma research (Figure was created by authors).

The integration of MobileNetV4 and deep learning models with portable NIR sensors is seen as a significant industrial milestone; it offers practical solutions by achieving up to 98% accuracy in the non-destructive classification of post-harvest processing methods (Sagita et al., 2026; Sun et al., 2026).

Coffee research can benefit from techniques that allow real-time monitoring and methods that provide spatial resolution. Techniques such as PTR-ToF-MS and SIFT-MS enable continuous monitoring of volatile substance release kinetics during roasting and brewing, providing immediate feedback for process optimization. At the same time, the emergence of MSI technology plays a pioneering role in the field of spatial metabolomics, enabling researchers to visualize the precise distribution of aroma precursors within the bean tissue in situ (Beccaria. et al., 2022; Paiva et al., 2025; Taiti et al. 2025; Melikoglu, 2026). In conclusion, using hybrid analytical models that combine the molecular depth of GC×GC-TOFMS with the speed of biomimetic sensors (e-nose/e-tongue) and the predictive power of artificial intelligence forms the basis of a transparent, objective and standardized quality grading system across the global coffee value chain (Mohammadian et al., 2024; Kirtil, 2025; Urugo et al., 2025; Taiti et al., 2025; Melikoglu, 2026). Table 6 synthesizes emerging technological horizons, such as spatial metabolomics and real-time monitoring, and summarizes their strategic value for next-generation coffee research, guiding future work toward overcoming current analytical hurdles.

Table 6. Future perspectives and new technological horizons in coffee research

Emerging Subject	Technical Implementation & Innovative Approach	Strategic Value for the Industry	Key Research Areas & References
Advanced AI & Deep Learning	The application of lightweight, high-performance architectures such as MobileNetV4 for portable NIR spectral analysis.	Facilitates fraud detection through high-speed, low-cost, real-time quality control.	Achieved 98.33% accuracy in non-destructively identifying coffee processing methods with very low computational requirements (Sun et al., 2026).
Multi-omics Approaches	Integration of microbial-metabolomics analysis to investigate the synergistic effects of fermentation on aroma development.	Enables to precise control over post-harvest processes by identifying specific microbial metabolic pathways that lead to desirable sensory notes.	Specifically used to find out how targeted fermentation (e.g., *Saccharomyces cerevisiae*) contributes to “fruity-floral” notes in specialty Arabica (de Melo Pereira et al., 2025).
Real-time Aroma Monitoring	Usage of direct-injection techniques such as PTR-MS and SIFT-MS for real-time monitoring the aroma release during roasting and brewing.	Enables the observation of dynamic aroma kinetics without the need for pre-separation by eliminating the limitations of static measurements in traditional chromatography.	Enables in-vivo monitoring of volatile compound release, which is critical for optimizing roasting profiles and brewing methods with industrial precision (Beccaria et al., 2022; Melikoglu, 2026).
Smart Roasting Systems	Integration of low-cost, multi-channel spectral sensors (410–940 nm) directly into roasting equipment.	Enables origin-independent, real-time monitoring and automatic control of the roasting degree (Agtron values) via machine learning models.	Ensures consistency in aroma profiles by providing a scalable solution for rapid and accessible quality assessment on the production line (Sagita et al., 2026).
Spatial Metabolomics	Application of MSI to visualize the spatial distribution of metabolites within the core coffee bean tissues.	Provides tissue-specific biomarker analysis, moving beyond traditional bulk screening to understand localized chemical changes.	Presents unprecedented resolution in mapping bioactive components and aroma precursors during different maturation and processing stages (Zhao et al., 2025).
Sustainable & Circular Technologies	Recycling of spent coffee grounds into active zein films using supercritical carbon dioxide ($scCO_2$) impregnation technology.	Encourages a circular economy by transforming massive biomass waste into functional, sustainable and bioactive packaging materials.	Impregnated films show superior light-barrier properties and controlled release of antioxidants, contributing to waste reduction in the value chain (Mottola et al., 2026).

The integration of multi-omics, spatial metabolomics and real-time monitoring systems for next generation coffee research is highlighted in Figure 7. Integrated multi-omics approaches not only enhance scientific rigor but also ensure traceability and sustainability in the specialty coffee industry.

Figure 7. Next generation coffee research (Figure was created by authors).

In future, studies on critical volatile compounds affecting the aroma freshness of coffee during storage could be productive for the coffee industry and for quality control during storage. The recovery of waste through the processing of biomass such as used coffee grounds, fruit pulp, and peels can contribute to sustainability. It is important to conduct studies targeting improved storage and roasting processes; effect of various bacterial and yeast species addition to coffee fermentation on coffee flavor, quality and consumer preferences; techniques on faster and easier detection of adulterated coffee mixtures; increasing increase the flavor-related chemical composition while simultaneously reducing harmful Maillard reaction products; confirming the results obtained from scientific data acquired solely through aroma analysis techniques, along with evidential sensory analysis; integration of high-resolution instrumental devices, biomimetic sensors and artificial intelligence algorithms that interpret complex data obtained from these devices is crucial for filling the gap in the literature.

CONCLUSION

In conclusion, there is no "one-size-fits-all" solution in analytical methods using to determine volatiles of coffee. The criteria for selecting a methodological approach can be determined based on the intended analytical output. According to this review, the integration of chromatographic and spectroscopic techniques within hybrid models is increasingly recognized as a comprehensive solution, especially when coupled with advanced machine learning algorithms for data processing. If comprehensive research on coffee aroma is to be conducted, it is generally recommended to combine a detailed chromatographic method with one or more rapid spectroscopic/IMS techniques, chemometric and sensory analysis.

The results of this study indicate that, by using the two-dimensional GCxGC-MS method as a solution to the peak overlap issue encountered in one-dimensional GC analysis, it is possible to identify VOCs that have not yet been characterized but are already present in coffee. As a new approach, the integration of GC×GC-MS with ToF could enable the creation of molecular signatures to distinguish molecular depth for VOCs and botanical origin of coffee. For the analysis of non-VOCs, affects the coffee aroma as well, HPLC combined with spectrophotometric or MS detectors is still widely accepted as a robust and common technique offering the sensitivity required to characterize critical bioactive components. The use of techniques such as MSI, which enables the mapping of aroma precursors within tissue, or PTR-ToF-MS and SIFT-MS, which provide real-time aroma monitoring; combining operationally fast biomimetic sensors (e-nose/e-tongue) in these hybrid models and integrating them with artificial intelligence algorithms (ANNs, RF, SVM); and then processing the high-dimensional data obtained from all these new techniques using chemometric methods (PCA, HCA, PLS-DA, OPLS-DA) could establish a new framework in coffee science.

This technological transformation can minimize the subjectivity inherent in human senses, thereby achieving extremely high accuracy rates in critical areas such as verifying geographical origin of coffee, detecting counterfeit products and quality grading; it can also establish an objective, transparent and global quality standardization across the entire value chain, from seed to cup. In summary, this integrated approach may significantly improve scientific rigor and enable the transition toward a more transparent and scientifically based grading system for the coffee industry.

AUTHOR CONTRIBUTIONS

This study was written and reviewed by Beyza KURİŞ, Ankara University, Graduate School of Natural and Applied Sciences, Department of Food Engineering, Ankara, Türkiye. Prof. Dr. Rahmi Ertan ANLI is the supervisor and provided contribution to the writing, editing and revision of this review.

CONFLICTS OF INTEREST

The authors have declared that they do not have any conflict of interests.

ARTIFICIAL INTELLIGENCE (AI) USAGE

The authors have used Canva to create the figures. The authors are solely responsible for the content of this publication.

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