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Metabolic dynamics of secondary metabolites in Arabica coffee (*Coffea arabica*): From biosynthesis to post-harvest transformations

Abstract. Coffee (*Coffea arabica*) is a globally significant beverage whose sensory profile and physiological effects derive from a complex matrix of secondary metabolites. This review presents a comprehensive "lifecycle" perspective of three pivotal classes: the alkaloid caffeine, phenolic chlorogenic acids (CGA), and the diterpenoids cafestol and kahweol. Here, 'lifecycle' defines a metabolite's continuous biochemical trajectory, tracking its genetic origin and ecological function in the plant through structural modifications during fermentation, drying, storage, and roasting. These classes are highlighted because they serve as the primary drivers of bitterness, acidity, and health bioactivities with fundamentally distinct transformational pathways. Following a systematic methodology, this study traces these compounds from biosynthesis to their fate during post-harvest processing. The synthesis reveals that post-harvest interventions cannot create quality but only modulate the bean's inherent chemical potential established by genetics and agronomy. Specifically, fermentation primarily reshapes hydrophilic phenolics (CGA) via hydrolysis to soften astringency, whereas roasting acts as a thermochemical trigger that degrades labile CGA into sensory critical melanoidin precursors and liberates insulated lipophilic diterpenoids. Current literature frequently compartmentalizes pre harvest plant omics and post-harvest food chemistry. This review addresses this gap by integrating these disciplines into a continuous mechanistic model, demonstrating how botanical origins inherently precondition processing outcomes. This holistic perspective offers practical insights for agronomists, processors, and roasters to predict, preserve, and intentionally enhance the sensory and bioactive profile of coffee across the supply chain.

Keywords: Caffeine · Chlorogenic acid · *Coffea arabica* L · Diterpenoids · Post-harvest processing

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Introduction

Arabica coffee (*Coffea arabica*) is a significant agricultural commodity and beverage worldwide, accounting for 60% to 70% of global production and dominating the specialty market segment (Farah, 2009; Bastian et al., 2021; Liu et al., 2025). The global popularity is grounded in the rich sensory attributes of the aroma, flavor, and mouthfeel, as well as the psychoactive and physiological effects, sustaining high consumer demand and premium market value (Farah, 2009; Ludwig et al., 2014; Hu et al., 2019). Beyond the simple label of a caffeine source, coffee beans represent a complex biological matrix rich in a diverse array of secondary metabolites. These compounds act as the fundamental biochemical building blocks that sustain high consumer demand and generate premium market value (Ludwig et al., 2014; Hu et al., 2019).

In the living Arabica plant, the formation of these secondary metabolites is deeply rooted in genetic diversity and environmental adaptation across varied agroecosystems (Maxiselly et al., 2025a). Major metabolite groups, specifically alkaloids, phenolic compounds, and diterpenoids, serve as essential dual actors. In plant, they function as critical defense mechanisms against pathogens and herbivores, while also mediating growth and resilience against environmental stressors. In the harvested bean, however, these exact same protective compounds transition into direct flavor and aroma precursors. They ultimately determine the taste, bioactivity, and sensory profile of the brewed beverage, illustrating a profound functional shift from ecological survival to culinary value (Farah & Donangelo, 2006; Esquivel & Jiménez, 2012).

The initial composition and concentration of these essential precursors are not uniform but are instead highly variable and dependent on the plant's cultivation environment. Agronomic and environmental conditions, such as altitude, microclimate, soil health, and specific shade management practices, interact dynamically with the plant's genetic background to establish a fundamental metabolic baseline (Ludwig et al., 2014; Kim et al., 2025). Furthermore, preharvest agricultural inputs and symbiotic relationships with the soil microbiome significantly influence the plant's physiological capacity to synthesize these target compounds (Bastian et al., 2021). Consequently, the developmental stage at harvest and the ecological health of the plantation dictate the maximum botanical potential of the green bean before any processing begins.

Once harvested, this botanical potential is subjected to the first major phase of chemical and structural transformation through postharvest processing. The transition from a freshly picked cherry to a stable green bean involves depulping, fermentation, drying, and storage. Different processing methodologies, commonly categorized as natural, honey, or fully washed, impose distinct moisture gradients, oxygen availability, and microbial regimes on the beans (De Bruyn et al., 2016; Happyana et al., 2024; Zainal & Cherie, 2025). Microbial communities metabolize sugars and organic acids in the outer fruit layers, indirectly driving changes in the endosperm's primary and secondary metabolites. This stage acts as a crucial intermediate filter, subtly modifying the precursor pool and setting the stage for subsequent thermal reactions.

The peak of the coffee lifecycle occurs during roasting, which represents the most chemically intense stage of transformation. Subjected to high temperature regimes, the preconditioned matrix of secondary metabolites undergoes profound pyrolytic degradation, Maillard reactions, and caramelization (Ludwig et al., 2014; Novaes et al., 2023). Thermally labile compounds are broken down into hundreds of volatile aromatics and nonvolatile gustatory compounds, while other relatively heat stable alkaloids persist into the final brew. Crucially, the trajectory of these complex thermal reactions is entirely dependent on the specific concentration, spatial localization, and conjugation state of the precursors that survived the initial postharvest processing phase.

Despite the extensive body of literature documenting coffee chemistry, a significant conceptual gap remains in synthesizing these distinct developmental stages. Current research is frequently compartmentalized by scientific discipline. Plant physiologists and geneticists emphasize the in-planta regulation, biosynthesis, and ecological roles of secondary metabolites (Liu et al., 2025). Conversely, food scientists and processing technologists focus predominantly on postharvest degradation, microbial fermentation, and the reaction mechanisms of roasting (Moeenfard & Alves, 2020; Martins et al., 2024). This fragmented approach fails to capture the continuous, interdependent nature of coffee chemistry. The chemical behavior of metabolites

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during fermentation and roasting cannot be fully understood without acknowledging how they were initially structured, compartmentalized, and influenced by environmental stressors during the plant's growth (Bi et al., 2023; Martins et al., 2024).

In response to the current lack of a unified perspective, this review introduces an integrative cradle to cup lifecycle model to track the metabolic fate of coffee's primary secondary metabolites. By systematically connecting the biosynthetic origins and ecological functions in the plant with their subsequent chemical trajectories during postharvest processing and roasting, this work bridges the divide between agricultural science and food chemistry. Moving beyond a disjointed stage by stage account, this review provides a mechanistic synthesis of the holistic sculpting process, demonstrating how botanical potential is progressively transformed through biochemical and thermochemical interventions to determine the ultimate sensory and functional profile of specialty coffee.

Materials and Methods

This review adopted a systematic literature search strategy by querying major academic databases, including Scopus, Web of Science, ScienceDirect, Springer, PubMed, and Google Scholar. The search utilized a defined set of Boolean operators, specifically ("Coffea arabica" OR "Arabica coffee") AND ("secondary metabolites" OR "caffeine" OR "chlorogenic acid" OR "diterpenoids") AND ("biosynthesis" OR "metabolomics" OR "fermentation" OR "roasting"). To capture recent advances in systems biology, including transcriptomics and metabolomics, as well as modern processing technologies, the selection prioritized original peer reviewed research articles and authoritative reviews published between 2005 and 2026.

During the initial search phase, a total of 205 records were identified across the databases. The distribution of records retrieved was as follows: Scopus (65), ScienceDirect (55), Web of Science (40), Google Scholar (25), Springer (12), and PubMed (8). After removing 34 duplicate records, the remaining 171 articles underwent title and abstract screening. At this stage, no articles were excluded as they initially appeared to meet the broad criteria. Consequently, 171 full text articles were assessed for eligibility. Of these, 85 full text articles were excluded because they lacked robust analytical methodologies, such as purely descriptive sensory papers without chemical validation, or did not provide empirical data linking metabolomic profiles to specific genetic, environmental, or processing variables. Ultimately, a final selection of 86 references was critically evaluated to extract pertinent data.

The screening and data extraction processes were rigorously guided by the "Coffee Metabolite Lifecycle Framework." This framework is a systematic model that tracks the continuous biochemical trajectory of secondary metabolites through four sequential stages: (1) pre harvest factors, encompassing genetic regulation, fruit development, and environmental modulation in the plantation; (2) primary processing, highlighting harvesting and microbial interactions during fermentation; (3) stabilization, covering drying kinetics and green bean storage; and (4) thermochemical transformation, detailing the intense degradation and synthesis reactions during roasting. Articles were deemed suitable for inclusion only if they offered direct analytical insights into at least one of these interconnected lifecycle stages.

Results and Discussion

The Alkaloid Fraction: Biosynthesis and Regulation in Caffeine. The alkaloid fraction of coffee, and caffeine in particular, represents one of the best characterized examples of a specialized plant defense system that has been intensively shaped at the biochemical, genetic, and regulatory levels. Caffeine (1,3,7 trimethylxanthine) is the most prominent and pharmacologically significant purine alkaloid in *Coffea arabica* L., and its ecological functions as a natural insecticide, fungitoxic agent, and allelopathic compound are now well supported by both in planta and transgenic studies (Perrois et al., 2015; Antoine et al., 2022). In its native environment, caffeine deters herbivores and pathogens and suppresses germination and growth of competing plant species, thereby conferring a measurable fitness advantage (Perrois et al., 2015; Lin et al., 2023; Montis et al., 2024). These defensive roles are mirrored in the spatial and temporal patterns of caffeine biosynthesis, which are highly specialized and tightly regulated across organs, developmental stages, and environmental conditions (Perrois et al., 2015; Djerrab et al., 2021; Combes et al., 2022).

Caffeine biosynthesis in *C. arabica* occurs predominantly in the cytoplasm of specialized parenchyma cells, with the highest flux in young, metabolically active tissues, expanding leaves, flower buds, developing pericarp, and immature seeds rather than in mature organs (Perrois et al., 2015). While the canonical pathway involving sequential N methylations (via XMT, MXMT, and DXMT) is well established, recent genomic mapping has provided new critical insights. High-quality genome assemblies demonstrate that these N methyltransferase (NMT) gene families evolved independently via tandem duplication. Modern transcriptomic analyses reveal that caffeine accumulation is not static; it is heavily regulated by hormonal signaling, such as jasmonic acid (JA) pathways, which balance plant growth with chemical defense mechanisms. From a critical perspective, these transcriptomic findings suggest that agronomic interventions targeting JA pathways could theoretically modulate baseline caffeine levels prior to harvest, offering an alternative to mechanical decaffeination.

The regulation of caffeine biosynthesis is strongly integrated with plant hormone signaling and environmental cues. JA, a central regulator of induced defense, has emerged as a key upstream signal modulating caffeine production. In *C. canephora*, methyl jasmonate (MeJA) and salicylic acid treatments can restore or enhance transcription of NMT genes in leaves and in maturing endosperm, which are otherwise transcriptionally repressed, resulting in higher theobromine and caffeine levels (Kumar & Giridhar, 2015; Kumar et al., 2017). In coffee seedlings, MeJA also promotes the expression of caffeine pathway genes, as well as those for proanthocyanidins and linalool, under simulated stress (Shen et al., 2025). Comparative work in tea shows that JA regulated MYB184 directly activates a caffeine synthase gene (TCS1), with CsDELLA JAZ MYC2 MYB184 TCS1 modules balancing growth and defense; many of these transcriptional mechanisms appear at least partly conserved between tea and coffee (Zhang et al., 2022; Ye et al., 2025; Li et al., 2022).

Environmental conditions at the plantation scale further modulate caffeine content. Shade and reduced light intensity generally correlate with lower caffeine levels in leaves and beans, likely through altered carbon allocation and downregulation of NMT expression, whereas full sun or stress exposed plants tend to accumulate more caffeine as part of a generalized defense response (Tolessa et al., 2017; Djerrab et al., 2021). Water stress and nutrient limitation have more variable, genotype dependent effects, sometimes enhancing caffeine as a protective solute and sometimes reducing it due to global metabolic slowdown (Tran et al., 2018; Perrois et al., 2015).

The specific anatomical localization of caffeine across different plant tissues reinforces its interpretation as an allelochemical and defense metabolite. Quantitative analyses show that concentrations are highest in young leaves, flower buds, and especially the outer pericarp and pulp of developing cherries, with somewhat lower levels in mature seeds, implying that the endosperm is shielded by a chemically fortified pulp barrier (Perrois et al., 2015; Montis et al., 2024). From a technological perspective, a significant fraction of the caffeine produced by plants is removed with the pulp during wet processing, an aspect relevant to both waste valorization and the caffeine load of the final green bean. Overall, caffeine in *C. arabica* exemplifies how a specialized purine alkaloid can link plant defense ecology, genome evolution, and agronomic traits, with its biosynthesis controlled by a dedicated enzymatic pathway, complex regulatory networks, and environmental modulation.

Phenolic Compounds: Chlorogenic Acids (CGA). Chlorogenic acids represent the single largest group of soluble phenolic compounds in green coffee beans, constituting from 6% to 12% of the dry weight depending on genetic and environmental factors (Farah & Donangelo, 2006). They are a diverse family of esters formed between quinic acid and residues of trans cinnamic acids, primarily caffeic acid, ferulic acid, and para coumaric acid. The monoesters, particularly 5 O caffeoylquinic acid, dominate the profile in *C. arabica*.

The biosynthesis of these acids is routed through the phenylpropanoid pathway, a major secondary metabolic network that channels carbon from primary metabolism into phenolic compounds essential for plant structure and defense (Vogt, 2010). The predominant route for synthesis in coffee involves the enzyme hydroxycinnamoyl coenzyme A quinate hydroxycinnamoyl transferase. This enzyme directly transfers the cinnamoyl moiety to the hydroxyl group of quinic acid. A remarkable evolutionary adaptation in coffee involves a genetic diversion. Coffee possesses a

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nonfunctional duplicated copy of the chalcone synthase gene. This pseudo enzyme sequesters transcription factors that would normally activate the entire flavonoid pathway. This genetic diversion effectively acts as a metabolic sink, shunting the vast majority of phenylpropanoid flux directly toward the massive accumulation of chlorogenic acids, making coffee a unique phenolic powerhouse.

The ecological rationale for this immense investment is robust. In the plant, these acids serve as potent antioxidants, scavenging reactive oxygen species generated during normal metabolism or under stress conditions such as high ultraviolet radiation. They also exhibit antimicrobial properties contributing to defense against pathogens. Their accumulation is highly sensitive to environmental cues. High altitude cultivation naturally elevates these acid levels as a protective response (Avelino et al., 2005). The interaction between genotype and environment creates a specific chemical potential that dictates the baseline quality of the harvested cherry.

Postharvest processing initiates the transformation of these compounds. During fermentation, endogenous polyphenol oxidases can catalyze the oxidation of these acids to quinones, leading to undesirable browning if the process is uncontrolled. Concurrently, microbial metabolism plays a significant role. Selected strains of lactic acid bacteria and yeasts possess esterase activity that hydrolyzes the ester bond, releasing free caffeic acid and quinic acid (De Bruyn et al., 2016). Studies document reductions in total chlorogenic acid content of 5% to 15% during well managed fermentations. Drying continues this stabilization phase. Optimal slow drying preserves the complex phenolic profile, while improper rapid drying can lead to premature nonenzymatic browning or oxidation.

Roasting represents the final and most dramatic stage of postharvest processing. Chlorogenic acids are thermally unstable and undergo a cascade of reactions that fundamentally shape the sensory character of the brew. Total content plummets with increasing roast degree. Light roasts may retain up to 80% of the original green bean content, whereas dark roasts retain less than 20% (Ludwig et al., 2014). During heating, the ester bond is susceptible to transesterification, forming other isomers that subtly alter the acid profile. A critical degradation pathway is the formation of lactones through intramolecular dehydration. These lactones are major contributors to the characteristic citric acidity in light and medium roasts, though they can introduce harsh bitterness in darker roasts (Farah & de Paula Lima, 2019). Finally, the breakdown fragments readily participate in Maillard reactions and caramelization, becoming incorporated into melanoidins. These high molecular weight polymers are responsible for the color, body, and post roast antioxidant activity of the beverage.

Diterpenoids: Cafestol and Kahweol. Cafestol and its dehydrogenated analog kahweol are unique pentacyclic furan diterpenoids of the ent kaurane family that occur almost exclusively in *Coffea* species and represent up to 2 to 3.5% of the bean dry mass, or about 20% of the oil fraction (Novaes, 2018). These compounds are synthesized and stored as fatty acid esters in lipid bodies of the endosperm, but free dialcohols and ether forms are also distributed in roots, stems, leaves, flowers, and fruits (Ivamoto et al., 2017; Novaes, 2018). Ecologically, cafestol and kahweol are interpreted as defensive phytochemicals, with roles as antifeedants, antimicrobial agents, membrane stabilizers under temperature stress, and possibly signaling molecules within plant defense networks (Ivamoto et al., 2017; Martins et al., 2024). Their significance extends to human nutrition and health, where they exhibit a dual physiological profile, hypercholesterolemic on one hand and anti-inflammatory, hepatoprotective, and chemopreventive on the other (Ren et al., 2019; Silva et al., 2023).

The regulation of diterpenoid biosynthesis in coffee is influenced by both genetic background and environmental conditions. Genotype is a primary determinant: Arabica coffee typically contains substantial amounts of both cafestol and kahweol, with kahweol:cafestol ratios often between 1:2 and 2:1, whereas *C. canephora* (robusta) is nearly devoid of kahweol but accumulates significant cafestol and 16 O methylcafestol (Mori et al., 2016; Francisco et al., 2021). Genome wide association analysis in Arabica has identified SNPs associated with total lipids, cafestol, kahweol, and their ratio, which are located near candidate genes in isoprenoid and diterpene pathways, confirming strong genetic control and suggesting directional selection on diterpene traits (Sant'Ana et al., 2018). Within Arabica, both traditional and introgressed cultivars show wide quantitative variation, with cafestol ranging from 414 to 742 mg/100 g and kahweol from 439 to 1068 mg/100

g in roasted beans under uniform conditions (Kitzberger et al., 2014).

Environmental factors modulate this genetic baseline. Light incidence and cropping system affect expression of MVA/MEP genes (CaHMGR, CaMVD, CaDXR, CaIDS) and P450s (CaCYP82C2, CaCYP71A25, CaCYP74A1, CaCYP701A3), with full sun plants showing higher transcript levels in developing fruits than shade grown plants (de Oliveira et al., 2021). Diterpene accumulation in fruits peaks during mid late development (around 120 to 210 days after flowering), paralleling increased expression of these genes (Ivamoto et al., 2017; de Oliveira et al., 2021). Altitude and temperature further shape cafestol and kahweol contents: across an altitudinal gradient, warmer conditions were positively correlated with lipids and volatiles, and genotype specific responses in cafestol/kahweol were observed, underlining complex genotype environment interactions (Sarzynski et al., 2023).

Post harvest and technological steps add another regulatory layer. While cafestol and kahweol are relatively stable in green beans, they are thermolabile during roasting. Classical studies indicated that their total content is only modestly affected by light medium roasting, whereas dark roasting promotes dehydration of the tertiary hydroxyl at C 15/16 and oxidation of the furan ring, generating 15,16 dehydrocafestol, 15,16 dehydrokahweol, cafestal, kahweal, iso kahweol, seco kahweol, and other derivatives (Novaes et al., 2023; Martins et al., 2024). A recent kinetic study identified sixteen main degradation products, ten from kahweol and six from cafestol, and showed that the degree of roast (time temperature profile) is the dominant determinant of thermodegradation, whereas green bean composition primarily sets the starting pool of diterpenes (Novaes et al., 2023). Some oxidation products may retain or even gain biological activities, but their pharmacology is far less characterized than that of the parent compounds (Martins et al., 2024; Silva et al., 2023).

The brewing method plays a crucial role in determining how much cafestol and kahweol reach the final beverage. Because these diterpenes are fat-soluble, they are naturally trapped within the oils of the coffee grounds. When coffee is passed through a paper filter, the filter effectively blocks these oils, removing almost all diterpenes from the drink. In contrast, unfiltered brewing techniques, such as French press, Moka, Turkish, or boiled coffee, allow the oil droplets to pass freely into the cup, significantly increasing the amount of cafestol and kahweol consumed (Ren et al., 2019; Novaes et al., 2023). Typical unfiltered coffee contains approximately 3 to 6 mg/cup of cafestol plus kahweol, while paper filtered brews contain only trace amounts (Ren et al., 2019). Migration of oil to the bean surface during roasting enhances extractability in such methods, increasing the consumer's daily intake of these diterpenoids (Novaes et al., 2023).

In humans, cafestol and kahweol are efficiently absorbed (70%), extensively metabolized, and undergo enterohepatic cycling, accumulating primarily in the liver and gastrointestinal tissues (Ren et al., 2019). Repeated consumption can raise serum LDL cholesterol and liver enzymes, particularly when drinking unfiltered coffee (Ren et al., 2019). At the same time, a large body of in vitro and in vivo work shows antitumor, anti-inflammatory, and hepatoprotective activities, driven by induction of glutathione S transferase, modulation of NF κB and Nrf2 pathways, inhibition of angiogenesis, and pro apoptotic effects in cancer cells (Ren et al., 2019; Silva et al., 2023). Structure activity comparisons suggest that kahweol's extra double bond confers subtle differences in potency and target selectivity, but this relationship is not yet fully resolved (Ren et al., 2019; Silva et al., 2023; Heise et al., 2025).

Overall, cafestol and kahweol exemplify how a single specialized metabolic pathway from GGPP through ent kaurene, P450 mediated oxidation, and esterification, connects plant defense, bean chemistry, processing technology, and human health. Their levels are co shaped by coffee genetics, environment, fruit development, roasting, and brewing method, making them central markers at the interface of plant physiology, coffee quality, and nutritional risk benefit assessment.

Post-Harvest Transformations: Fermentation. Following harvest, coffee beans remain metabolically active, and post-harvest operations such as fermentation, drying, and storage trigger extensive biochemical transformations that remodel the secondary metabolite profile established during seed development (Haile & Kang, 2019). In wet processing, fermentation is not merely a logistical step for mucilage removal; it is a biochemical reprogramming phase in which microbial ecology intersects with seed physiology to shape the bean's final chemical and

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sensory identity (Haile & Kang, 2019; Shen et al., 2024).

In submerged wet fermentation, the immersion of depulped beans in water creates a specific microaerophilic environment that selectively enriches fermentative microbiota over time. Early stages often see a rapid consumption of available sugars, which gradually lowers the pH and allows yeasts and lactic acid bacteria to dominate the ecosystem (Todhanakasem et al., 2024). These thriving microbial communities profoundly modify the physicochemical conditions surrounding the seed. They secrete a diverse suite of extracellular enzymes, including pectinases, cellulases, proteases, lipases, and esterases. While pectinases primarily drive the physical degradation and removal of the mucilage, the enzymatic actions of esterases and glycosidases extend much deeper. They begin to interact with the outer seed tissues to generate vital flavor precursors, including phenolic derivatives, organic acids, and bound aroma compounds (Ran et al., 2025).

Through these metabolic activities, yeasts and lactic acid bacteria act as fundamental flavor architects for the final beverage. They contribute a wide array of desirable fruity and floral attributes by producing higher alcohols, volatile organic acids, and complex esters via their central carbon and amino acid metabolism. For instance, the generation of lactic and acetic acids alongside ester linked volatiles significantly enhances perceived acidity and cup complexity. Concurrently, the dominance of these beneficial microbes naturally suppresses spoilage organisms, thereby preventing the formation of undesirable sensory defects and correlating strongly with elevated cupping scores (Vale et al., 2024).

The transition from spontaneous fermentation to controlled inoculation has further strengthened the causal link between microbial composition and bean chemistry. The application of mixed starter cultures significantly increases sensory balance, fragrance, and acidity scores, frequently outperforming traditional spontaneous methods (Duque Buitrago et al., 2025). Inoculated Arabica beans display a highly distinct metabolomic signature, characterized by higher concentrations of sucrose, mannitol, and malic, citric, and quinic acids. Furthermore, guided fermentations help reduce the levels of aminophenol and free phenols that are typically associated with phenolic cup defects, proving that microbial interventions can precisely modulate the precursor pool (Madrid Restrepo et al., 2025).

However, this microbially driven reprogramming is simultaneously constrained by the initial metabolic matrix of the bean and its ongoing endogenous stress responses. Crucially, the coffee seed itself remains metabolically active during early fermentation and drying. Environmental pressures such as anoxia, low pH, and severe osmotic stress trigger internal respiratory shifts and stress response pathways within the seed. These biological reactions lead to the mobilization and endogenous degradation of internal carbohydrate, amino acid, and phenolic reserves before the seed is entirely inactivated by desiccation (De Bruyn et al., 2016). This internal biological activity complicates attempts to entirely separate plant driven chemistry from microbially driven chemistry.

The fate of key secondary metabolites varies significantly during this active processing phase. Caffeine is chemically stable under typical fermentation conditions but remains subject to solubility driven migration. The prolonged immersion of depulped beans in water during wet fermentation significantly impacts both the physical and chemical traits of the seed. Recent multivariate analyses demonstrate that specific combinations of harvesting techniques and soaking times directly influence the morphological characteristics and quality baseline of Arabica beans (Maxiselly et al., 2025b). Furthermore, this extended soaking allows a minor leaching of water-soluble caffeine into the fermentation liquor, typically resulting in a roughly 2 to 8% reduction in seed caffeine during standard wet processing (Sunarharum et al., 2023). In sharp contrast, chlorogenic acids are highly labile and follow a complex dual pathway transformation. Mechanical damage during pulping exposes chlorogenic acids to endogenous polyphenol oxidases, leading to oxidation and potential browning. In parallel, microbial esterases hydrolyze these acids to produce caffeic and quinic acids, often reducing total chlorogenic acid content by 5% to 15% (Lee et al., 2015). Subsequent microbial metabolism can transform the released caffeic acid into volatile phenols. While moderate amounts of these volatile phenols contribute pleasant spicy or clove like notes, higher concentrations rapidly cause noticeable phenolic defects in the cup.

Unlike the hydrophilic metabolites, the lipophilic diterpenoids cafestol and kahweol are

safely sequestered as fatty acid esters within the endosperm oil bodies. This unique cellular compartmentation largely insulates them from the aqueous fermentation environment and associated microbial enzymes. Consequently, studies tracking the lipid and diterpene fractions report no significant losses or structural transformations during typical wet fermentation; their primary chemical modifications only occur later through dehydration and oxidation during roasting (Novaes et al., 2023). Ultimately, specialty coffee production increasingly treats fermentation as a tunable interface. When managed carefully, targeted microbial consortia protect the inherent botanical potential of the bean while selectively augmenting it through biochemical conversions of sugars and phenolics, purposefully leaving recalcitrant metabolites intact.

Post-Harvest Transformation: Drying and Storage. Drying marks the decisive transition from a metabolically active seed to a stable, storable commodity. The central technological goal during this phase is to systematically reduce the initial moisture content from approximately 45% to 60% at harvest down to a safe threshold of 10% to 12%. Achieving a water activity below 0.60 is critical, as it effectively halts microbial proliferation and minimizes undesirable biochemical deterioration (Abreu et al., 2025). During this progressive moisture reduction, nonvolatile constituents such as caffeine, trigonelline, chlorogenic acids, and lipids naturally increase in concentration on a dry matter basis, establishing the foundational matrix for the green bean (Moon et al., 2025).

The kinetics and method of drying determine the chemical integrity of the bean. In the early phase, the seed is physiologically active, and endogenous enzymes such as polyphenol oxidase (PPO), peroxidase, esterases, and lipases may remain functional when moisture remains above about 30% (Pazmiño Arteaga et al., 2022). The choice of drying method, ranging from traditional sun and shade drying to modern solar and mechanical systems, profoundly influences metabolite preservation. Traditional sun drying, while economical, exposes beans to fluctuating temperatures and direct UV radiation, which can prolong PPO activity and accelerate the oxidation of CGA into brown polymeric pigments, thereby reducing antioxidant capacity (Tripetch & Borompichaichartkul, 2019; Kulapichitr et al., 2021). Conversely, shade drying offers a slower, gentler moisture reduction that better preserves cellular integrity, hydrophilic antioxidants, and organic acids. Modern mechanical and controlled solar drying systems allow for precise temperature regulation, which, when optimized, effectively retains sucrose, free amino acids, and total phenolics (Abreu et al., 2025; Moon et al., 2024). Recent metabolomic studies highlight specific markers associated with these drying stresses; for example, elevated levels of free fatty acids and volatile aldehydes serve as markers for lipid damage in aggressively dried beans, whereas the retention of specific organic acids marks a successfully preserved metabolic baseline (Abreu et al., 2025).

Conversely, excessively rapid drying driven by high thermal stress introduces a different set of risks. The literature indicates a practical upper temperature limit of approximately 40 °C for drying green coffee. When bean temperatures exceed this threshold for extended periods, the cellular membranes and oil body structures begin to rupture (Dong et al., 2017; Coelho et al., 2024). This structural disruption exposes the lipid fraction to oxygen, promoting rapid primary and secondary lipid oxidation. Furthermore, extreme heat can cause case hardening, a condition where a desiccated outer layer traps moisture within the bean interior, creating microenvironments prone to mold growth and musty flavors (Pazmiño Arteaga et al., 2022). Therefore, gentle drying under controlled environments around 25 to 30 °C and 50% to 55% RH is highly recommended to preserve cellular integrity and sensory clarity (Abreu et al., 2025).

Once optimally dried, green coffee enters a variable storage period. It is a misconception that dried green beans are entirely inert; rather, they remain biologically semi alive. Residual cellular respiration, along with slow oxidation and hydrolysis reactions, continues to modify the complex carbohydrate, protein, and phenolic matrix over time. While caffeine remains highly stable both thermally and oxidatively throughout this entire postharvest lifecycle, chlorogenic acids are vulnerable to slow degradation. Over 12 to 15 months of storage, particularly under conditions of elevated temperature and humidity, chlorogenic acids undergo progressive ester hydrolysis and oxidation. This chemical breakdown correlates directly with the attenuation of desirable acidity and the emergence of flat, woody, or paper like sensory notes (Zarębska et al., 2021; Badmos & Kuhnert, 2025).

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Alongside phenolic degradation, the lipid fraction and volatile precursors are primary drivers of quality loss during long term storage. Triglycerides are highly susceptible to hydrolysis, releasing free fatty acids that subsequently undergo peroxidation. Metabolomic and volatile analyses reveal that extended storage leads to a marked loss of positive aroma precursors (such as specific free amino acids and reducing sugars) and the volatilization of endogenous esters and beneficial aldehydes. Simultaneously, there is an accumulation of lipid oxidation products, particularly hexanal and nonanal, which serve as direct chemical markers for sensory deterioration, correlating with the emergence of flat, woody, or "past-crop" sensory notes (Cong et al., 2020; Moon et al., 2022; Pazmiño Arteaga et al., 2022).

Crucially, these metabolite changes during drying and storage directly precondition subsequent roasting chemistry and final cup quality. The premature degradation of CGA means fewer intact precursors are available for thermal conversion into desirable chlorogenic acid lactones and antioxidant melanoidins during roasting, resulting in a flatter acidity profile. Similarly, the loss of sucrose and amino acids attenuates the Maillard and Strecker degradation pathways, leading to a noticeable loss of complex caramel and nutty aromatics. Furthermore, oxidized lipids cannot be "roasted out"; rancid precursors and lipid degradation markers often survive thermal treatment, directly imparting harsh, stale, or cardboard-like notes to the brewed beverage (Pazmiño Arteaga et al., 2022; Błaszkiewicz et al., 2023). To mitigate these cumulative deteriorative processes, careful environmental management is imperative. By restricting oxygen ingress and preventing moisture fluctuations, controlled storage preserves the vital phenolic profile and lipid stability required to maintain specialty grade scores until the coffee is finally roasted (Matias et al., 2025).

Comparative storage trials suggest that:

- Beans stored at 20 °C age fastest, with pronounced increases in FFAs and loss of aroma volatiles.
- Storage at 10 °C or 10 °C slows quality decline, but research reports complex effects on CGA retention depending on processing (washed vs natural) and packaging (Zarębska et al., 2021; Błaszkiewicz et al., 2023).
- Impermeable, high barrier packaging improves the stability of fatty acids and better preserves specialty grade scores over 6 to 12 months than jute or other permeable materials at 30 to 35 °C, 50% RH storage (Borém et al., 2019; Matias et al., 2025).

Overall, cool, dry, dark storage with minimal oxygen exchange, typically achieved through high barrier bags, sometimes with refrigeration is recommended to maintain the physical integrity, phenolic profile, and lipid stability of green coffee until roasting (Tripetch & Borompichaichartkul, 2019; Moon et al., 2022; Pazmiño Arteaga et al., 2022). While caffeine remains chemically stable, the gradual hardening of the seed matrix and cumulative oxidative changes in phenolics and lipids ultimately limit the "freshness window" of green coffee, even under ideal conditions.

Post-Harvest Transformation: Roasting. Roasting is the non-negotiable, transformative act that converts hard, grassy tasting green beans into the brittle, aromatic roasted product. It is a rapid thermochemical process in which beans are heated from ambient temperature to roughly 200 to 250 °C over 8 to 15 min, losing about 12% to 25% of their mass as water, CO_2, and volatile organic compounds (Mehaya & Mohammad, 2020; Ali et al., 2025). The main drivers of mass loss are moisture evaporation in the early phase and subsequent decomposition of sugars, CGA, amino acids, and trigonelline as roasting severity increases (Mehaya & Mohammad, 2020; Tarigan et al., 2022; Ali et al., 2025). From a thermal and chemical standpoint, the roast can be divided into overlapping phases. The initial endothermic drying phase (up to 160 to 180 °C) is dominated by water evaporation, bean yellowing, and softening of cell walls (Tarigan et al., 2022; Herdt et al., 2024). Sucrose begins to melt and hydrolyze into glucose and fructose, increasing the pool of reducing sugars, while CGA initiate isomerization into 3 CQA and 4 CQA (Ludwig et al., 2014; Macheiner et al., 2021; Honda et al., 2022).

As temperature rises toward 200 °C, internal pressure from steam and accumulating gases leads to the first crack (205 to 210 °C), an audible event associated with rapid expansion, rupture of cell walls, and the onset of vigorous pyrolysis of polysaccharides and hemicellulose (Tarigan et al., 2022; Dippong et al., 2022; Herdt et al., 2024). This turning point marks the explosive acceleration of Maillard reactions between newly formed

reducing sugars and free amino acids released from protein denaturation and proteolysis (Tarigan et al., 2022; Hong et al., 2024). Concomitantly, CGA degradation shifts into a steep decline phase, with major conversion to lactones and smaller phenolic fragments (Dawidowicz & Typek, 2017; Mehaya & Mohammad, 2020; Ali et al., 2025). Through a metabolomics perspective, this phase also triggers the rapid thermal degradation of trigonelline. As heat intensifies, trigonelline undergoes demethylation and cleavage, producing nicotinic acid (niacin), which enhances nutritional value, alongside N methylpyridinium. Importantly, its breakdown generates volatile pyridines and pyrroles that serve as robust chemical biomarkers for roast progression, directly contributing to the roasty, earthy, and characteristic bitter sensory profile of the brew (Ludwig et al., 2014; Hu et al., 2019). The subsequent development phase (205 to 230 °C) is especially critical for flavor, as Maillard and Strecker reactions and advanced sugar degradation generate a dense matrix of volatiles, including Strecker aldehydes, furans, pyrazines, pyridines, and phenols (Hong et al., 2024; Dippong et al., 2022). High molecular melanoidins are formed, governing final color, viscosity, and much of the antioxidant capacity of dark roasts (Moreira et al., 2012; Mehaya & Mohammad, 2020; Freitas et al., 2023). Beyond 230 °C and into the second crack, intense pyrolysis degrades cellulose, lignin, and earlier formed volatiles, shifting the aromatic profile toward pungent roasty, smoky, and burnt characters while destroying most original CGA (Tarigan et al., 2022; Dippong et al., 2022; Ali et al., 2025).

The chemistry of roasting is governed by a set of overlapping thermal reactions, with the transformations of chlorogenic acids (CGA) being among the most studied. Green coffee is rich in 5 CQA and related isomers, which begin to isomerize early in roasting at 140 to 200 °C (Ludwig et al., 2014; Macheiner et al., 2021; Honda et al., 2022). As temperature climbs, CGA progressively degrade into quinic acid, chlorogenic acid lactones (CGLs), smaller phenolic acids, and volatile phenols (Dawidowicz & Typek, 2017; Farah & de Paula Lima, 2019; Rusinek et al., 2023). These lactones contribute to bitterness and perceived acidity in light medium roasts but can impart harsh bitterness at higher concentrations (Farah & de Paula Lima, 2019). With continued heating, CGA fragments are incorporated into melanoidins through Maillard and caramelization pathways, binding phenolics into high molecular structures that strongly affect color, body, and antioxidant activity (Moreira et al., 2012; Mehaya & Mohammad, 2020; Rusinek et al., 2023). Kinetic studies show CGA decreasing from 34 mg/g in green beans to <3 mg/g after severe roasting, while overall antioxidant capacity tends to peak at light city roasts and then decline at darker degrees as CGA are lost faster than antioxidant melanoidins are formed (Freitas et al., 2023; Ali et al., 2025).

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Table 1. Key chemical transformations of major metabolites by roasting temperature phase

Metabolite Class	Key Transformation & Phase	Key Temperature Range	Resulting Products & Impact
Chlorogenic Acids (CGAs)	Isomerization & Initial Degradation (Early to Light Roast)	150 to 205°C	Formation of 3-CQA and 4-CQA isomers; onset of degradation into simpler phenolics, altering the acidic profile (Ludwig et al., 2014).
	Lactonization (CGL Formation) (First Crack & Development)	205 to 225°C	Formation of chlorogenic acid lactones (CGLs/quinides). Primary source of perceived acidity in light-medium roasts; can contribute to harsh bitterness at higher concentrations (Farah & de Paula Lima, 2019).
	Incorporation into Melanoidins (Medium to Dark Roast)	215 to 240°C+	CGA breakdown fragments (e.g., caffeic acid) react in Maillard reactions to form melanoidins, defining color, body, and antioxidant capacity (Moreira et al., 2012).
Trigonelline	Thermal Degradation & Demethylation (Development to Dark Roast)	190 to 230 °C	Cleaves into nicotinic acid (niacin), N methylpyridinium, and volatile pyridines/pyrroles. Acts as a key biomarker for roast degree, reducing original bitterness while contributing to roasty aroma notes and increasing nutritional value (Ludwig et al., 2014; Hu et al., 2019).
Caffeine	Thermal Stability & Physical Concentration (Entire Roast Cycle)	Ambient to >240°C	Minimal chemical degradation (<5%). Relative concentration increases 10-30% due to mass loss, affecting final brew strength (Wang & Lim, 2022).
	Potential Complexation (Mid-Late Roast)	180 to 230°C	Possible formation of chlorogenate-caffeine complexes (CGCs), which may modulate bitterness perception and bioavailability (Farah & de Paula Lima, 2019).
Cafestol & Kahweol	Dehydration & Oxidation (Medium to Dark Roast)	210 to 240°C+	Formation of dehydrocafestol/kahweol and epoxide derivatives, altering the diterpenoid profile (Lindinger et al., 2024); (Lang et al., 2023).
	Increased Extractability (First Crack Onwards)	>205°C	Thermal disruption of cellular and lipid body structures liberates diterpenes, increasing their levels in unfiltered brews and impacting body and physiological effects (Lindinger et al., 2024).

Note: Temperature ranges are approximate and represent the primary phase of activity for each transformation. First crack typically occurs at ~205 to 210°C, and second crack at ~225 to 235°C. The precise kinetics depend on the specific roast profile (time-temperature curve).

In contrast to CGA, caffeine is remarkably thermally stable under typical roasting conditions. Across roast degrees, studies report minimal losses (<5 to 10%), with apparent concentration increases largely due to dry mass loss (Ludwig et al., 2014; Mehaya & Mohammad, 2020; Ali et al., 2025; Hong et al., 2024; Ban et al., 2025). Nonetheless, caffeine's sensory contribution interacts with CGA degradation, and evidence for stable chlorogenate caffeine complexes (CGCs) suggests that roasting induced changes in CGA speciation may modulate bitter perception and caffeine bioavailability (Farah

& de Paula Lima, 2019; Ludwig et al., 2014). Conversely, the diterpenes cafestol and kahweol undergo a complex pattern of dehydration, oxidation, and fragmentation. The native diterpenes decrease progressively with increasing roast intensity, accumulating up to 16 dehydro and oxidized derivatives via elimination and oxidation reactions accelerated by higher thermal loads (Novaes et al., 2023; Lang et al., 2023; Lindinger et al., 2024). At the same time, the breakdown of cell matrices and oil bodies during the first crack and beyond increases lipid mobility and extractability of remaining diterpenes into unfiltered brews (Novaes et al., 2023; Lindinger et al., 2024).

The flavour matrix of roasted coffee arises from multiple concurrent thermal reaction networks. The Maillard reaction, initiated above 140 to 150 °C, involves non enzymatic browning between reducing sugars and amino groups, proceeding through Amadori products to generate dicarbonyls, heterocyclic volatiles, and brown melanoidins (Herdt et al., 2024). Within this cascade, Strecker degradation converts amino acids and α dicarbonyls into Strecker aldehydes (e.g., 2 methylpropanal, phenylacetaldehyde), CO_2, and ammonia, which carry essential malty, chocolatey, and floral notes (Hong et al., 2024; Dippong et al., 2022). Concurrently, caramelization above 170 °C consumes virtually all sucrose by medium roast, leading to the formation of caramel like furans, maltol, furanones, and various organic acids (Hong et al., 2024). Pyrolysis becomes dominant above 200 °C, driving the breakdown of polysaccharides, lignin, proteins, and CGA into gases, tars, and phenolic volatiles such as guaiacol, shifting the profile from sweet and nutty to smoky, spicy, and finally burnt (Dawidowicz & Typek, 2017; Tarigan et al., 2022). Throughout these processes, lipid oxidation and thermal degradation proceed in parallel, potentially forming aldehydes and ketones that contribute to fatty or cardboard notes if oxidized excessively, while overlapping with diterpene dehydration to alter both the sensory attributes and health impacts of the brew (Cong et al., 2020; Dippong et al., 2022; Novaes et al., 2023; Lang et al., 2023).

Conclusion

This lifecycle perspective reveals that the coffee bean is not a static repository of flavor precursors, but a dynamic entity whose chemical identity is continuously reshaped from the field to the cup. A key implication is that the 'quality potential' of a bean is not solely determined by genetics or terroir, but is co-created through a cascade of interconnected decisions. For instance, the genetic predisposition for high CGA content, an ecologically beneficial trait, sets the stage for the roaster to develop a specific acidity profile via controlled lactone formation. This framework therefore provides a science-based foundation for intentional quality management across the entire supply chain, from selecting varieties based on their biosynthetic capacity to designing fermentation and roast protocols that leverage rather than simply react to the bean's initial chemical matrix.

This lifecycle perspective reveals that the coffee bean is not a static repository of flavor precursors, but a dynamic entity whose chemical identity is continuously reshaped from the field to the cup. A summary of the main findings highlights fundamentally distinct trajectories for the key secondary metabolites. Caffeine remains chemically stable throughout post harvest processing, primarily concentrating due to moisture and mass loss. In contrast, chlorogenic acids act as highly reactive hydrophilic substrates that undergo microbial and enzymatic hydrolysis during fermentation to soften astringency, followed by extensive thermal degradation during roasting to form sensory critical lactones and melanoidins. Meanwhile, the lipophilic diterpenoids cafestol and kahweol remain heavily insulated within oil bodies until the extreme heat of roasting ruptures the cellular matrix, driving their dehydration and enabling their extraction into the final brew.

Consequently, the quality potential of a coffee bean is not solely determined by genetics or terroir, but is co created through a cascade of interconnected decisions across the supply chain. The genetic predisposition for high CGA content, for instance, sets the stage for the roaster to develop a specific acidity profile via controlled lactone formation.

To advance this field, future research directions must transition from isolated studies of pre harvest or post harvest stages toward integrated, multi omics approaches. Tracking identical coffee batches continuously from the plantation to the brewed cup using combined transcriptomic and metabolomic analyses will allow researchers to definitively map how specific agronomic stresses and microbial interventions cascade into final roasting chemistry. Ultimately,

such predictive modeling will provide a science based foundation for intentional quality management, enabling the coffee industry to proactively leverage rather than simply react to the initial botanical matrix of the bean.

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