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# Coffee volatile compounds

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**Abstract**
Coffee is a staple that has been widely consumed all over the world. It is not only well-known for its stimulating effects but also for its desirable and fascinating aroma. Coffee volatile chemicals are created from green coffee beans' precursors, which include lipids, phenolic compounds, proteins, alkaloids, and carbohydrates. By using integrated method for researching, this review was aimed to provide the deep insight into the factors that contribute to coffee aroma variation, as well as the key compounds that indicate the differences. This review was focused on benefiting future studies by providing valuable information about qualitative and quantitative research in terms of coffee aroma and it was also purposed to be the base for further application in the beverage industry, especially in Vietnam.

**Keywords:** Coffee aroma, coffee volatile compounds

## Introduction

Coffee volatile compounds are made from precursors in green coffee, mainly carbohydrates, phenolic compounds, proteins, alkaloids, and lipids. The changes in aroma are well-observed in the roasting step, where the chemicals in the bean go through Maillard reaction [1], Strecker degradation and breakdown of other substances, such as phenolic acids, carotenoid, sulfur amino acids (production of potent aroma compounds despite the small amount), lipids, etc. [2]. Although more than 1,000 volatile compounds are found in studies of coffee VOCs [3], some researchers suggested that only around 20-30 volatile compounds are significant for the perceived characteristics of coffee [4]. This part would mainly cover research about VOCs in roasted coffee since the aroma perception of coffee is the strongest only after they are roasted.

Coffee volatile compounds are divided into many groups, such as Aldehydes, acids, esters, furans, sulfur-containing compounds, thiols, thiophenes, thiazoles, furanones, ketones, noriprenoids, phenolic compounds, pyrazines, pyridines, terpenes [5]. While pyrazines and furans are the most abundant in coffee aroma in terms of quantity, pyrazines, and sulfur-containing compounds have the most contribution to coffee perception [3]. Different groups have their distinctive characteristics, therefore, their contributions to coffee aroma also vary. Studies about coffee aroma, mainly using GC-MS coupled with olfactometry methods have provided insights about the most sensory-contributed groups, which are mainly furan [6], sulfur-containing compounds [7], pyrazine [4, 8], furanone groups [8, 9] and several phenolic compounds [7, 8]. The specific compounds in each group and their perceived sensory characteristics in Arabica coffee aroma as well as their concentration and sensory threshold are presented in Table 1.

A variety of coffee products are often seen on the market, which can vary from low to extremely high prices due to many processing variables, including coffee growing regions, post-harvesting methods, roasting types, cultivars, etc. [51]. Those drivers of flavor differences in coffee were analyzed within the past 50 years, which were listed in Table 2. Since dissimilarities in the flavors of coffee can decide the overall acceptance and affect the buying decision of the customers, researchers have been invested in the findings of indicators of flavors, in other words, volatile compounds in different types of coffee for further application in the beverage industry [11, 12, 13, 14]. Many methods for correlation between VOCs and their perceived sensory characteristics were developed, including the application of odor activity value (OAV) using the Olfactometer coupled with GC-MS, which involves the ratio of VOCs concentration by their sensory threshold [6] or the application of E-Nose supported by statistical analysis tools (PCA, ML, etc). By the application of those methods, many essential compounds have recently been characterized as indicators of quality in different types of coffee. It is worth noticing that the findings are not perfect due to the variables of methods that have been used, which can alter the results of VOCs during operation, as well as the variables from panelists during sensory analysis. This part would review the aroma markers based on the most important factors that characterized the quality of the coffee.

## Volatile compounds in different coffee species and origins

Analysis of VOCs is important as they can act as indicators to identify different types of coffee, which are coffee species, which are commonly known as Robusta and Arabica. While Arabica is popularly grown at high altitudes with either seasonal or frequent rainfall, which is characterized by a sweeter flavor with more chocolate and sugar notes, Robusta is grown at much lower altitudes with high tolerance to warm temperature, which is characterized by stronger, harsher, and bitter flavor with more roasty and buttery notes. Many researchers have been working on detection of distinctive VOCs in roasted beans of the 2 species. It was in the study of A.M.C. Freitas and others (2001), application of HS-SPME-GC-MS was carried out for differentiation of VOCs between Robusta and Arabica coffee [15]. As the result, Robusta coffee from different origins had similar VOCs: pyridine, methyl-ethyl-pyrazine, and methyl-pyrrole carboxaldehyde, while Arabica coffee shared the same VOCs including acetyl-pyrrole, 2-propanone 1-acetyl, and furane-methanol. Furthermore, the study of Caporaso and others (2018), who used HS-SPME-GC-MS method for the analysis of VOCs from single roasted coffee, was able to differentiate roasted Arabica and Robusta coffee by pointing out the noticeable amount of 2,3-butaniedione, 2,3-pentandione, furfural, 1-(acetyloxy)-2-propanone, 2-acetylfuran, ethyl propanoate, furaneol, acetoin and 1- hydroxy-2-butanone in roasted Arabica coffee, while Robusta was found with high amount of pyrazine derivatives including 2-methyl-pyrazine, 2,6-dimethylpyrazine, 2,5-dimethylpyrazine, ethylpyrazine, 2-ethyl-6-methylpyrazine, and 2-ethyl-5-methylpyrazine [17]. Although much research about the differentiation of coffee species has been made, key differences in VOCs between roasted coffee cultivars are not well-understood [17]. On the other hand, D.R. Seninde (2020) pointed out that coffee origins can contribute to the differences in the aroma of coffee [10]. Akiyama M. *et al*., suggested the DHS-SPME-GC-MS with Olfactometry method to study the differences of VOCs, both quantitatively and qualitatively, in roasted Indonesian and Vietnamese coffee [17]. While Robusta coffee in Vietnam was characterized by smoke and nutty roast odor (2-5-dimethylpyrazine, 3-methyl-2-butene-1-thiol, 4-hydroxyl-2,5-dimethyl-3(2H) furanone), Indonesian Robusta had stronger sweet-fruity and sweet-caramel aroma ((E)-beta-damascenone, 2-hydroxyl-3-methyl-2-cyclopentene-1-one, 2-ethyl-4-hydroxy-5-methyl-3(2H)-furanone) in different roasting degrees. Another study also supported the correlation of growing origins and species that can affect the VOCs of roasted Robusta and Arabica coffee is from Freista (1999). Roasted Arabica coffee in Brazil was characterized by high contents of 5-methyl-1H-pyrrole-2-carbaldehyde and 3-pentylfuran and Arabica coffee in Costa Rica was observed with γ - butyrolactone, 2-furanomethanol acetate, and methylpyrazine. In roasted Robusta coffee, 3-ethyl- 2, 5-dimethylpyrazine was found in Ivory Coast's coffee, 2-furanomethanol acetate found in Indian coffee, and 4-ethyl-2methyl-pyrrole was detected in Cameroon, Uganda, and Angola coffee. It is also believed that the VOCs of Arabica are related to the growing altitude, who made the hypothesis of the higher the altitude, the more distinct the flavor with notable acid and desirable aroma. However, the effects of the growing climate on VOCs should be further analyzed [18].

**Volatile compounds in coffee processing**

Post-harvest processing is one of the most important steps that is responsible for the unique aroma of coffee. This part of the review would focus on the indicators of popular post-harvest processing methods in roasted coffee, such as wet-processing (fermentation of de-pulped, underwater, fresh coffee), dry processing (drying of whole coffee cherries until reaching 11% moisture content), semi-washed coffee (drying of de-pulped cherries until reaching 11% moisture content) and bio- digested coffee (coffee products harvested after the consumption, digestion, and excretion of animals). These methods are the main reason for the polarization of coffee prices in the market by having different distinct tastes and aromas; therefore, research on this topic is undeniably important to discover. The majority of analysis focused on the differentiation of post-harvest coffee processing types based on their major flavor precursors in green coffee, physio-chemical analysis of green and roasted coffee as well as sensory characterization of those coffee [19, 20, 21]; however, only a few researches used VOCs to characterize different post-harvest methods of roasted coffee. This part would discuss the relevant papers to provide an overview about the topic. Studies about volatile compounds in both green and roasted coffee with different types of processing were carried out in a study of O. Gonzalez-Rios and others (2007a, 2007b) [20, 22]. The processing methods involved 2 different de-pulping conditions and 4 treatments of Arabica coffee. Applying HS-SPME-GC-MS method with Olfactometry, treatment 1 (treatment that resembled the wet-processing method) had the least ketones, furans, and pyrazines while the other "drier" methods, had a much higher concentration of those substances. The differences were also displayed in the perceived aroma of VOCs that included the variability in almond notes, fruity, floral, and spicy notes, such as guaiacols, furfurals, etc [22]. In Arruda *et al*. study, the effects of dry-washed, and semi-washed methods on roasted Arabica coffee VOCs profile were measured. Wet processing had the most volatile phenols such as 4-methoxyphenol, 4-ethylguaiacol, while Guaiacols are responsible for being burnt and roasted with spicy notes [22], which were also significant during the detection of volatile phenolic compounds in "drier" methods. Wet processing was also reported with high unsaturated alicyclic ketones, especially 2-hydroxyl-3-methyl-cyclopentene-1-one, which relates to the sweet-caramel character in roasted Arabica coffee. In P. Soonthomkamol (2004), a study of coffee post-harvest processing between dry and wet method, which applied the DHS-GC-MS method for the analysis with medium roasted coffee as samples, showed that the differences in VOCs of roasted coffee from different post-harvest processing methods were quite significant [23]. Volatile groups of furans and pyridines were higher in wet processing than dry processing. Moreover, 3-ethyl- 2-methyl-1, 3-hexadiene and 1-(2-furanylmethyl)-1-H-pyrrole were exclusively found in wet processing. Pyrazines and acetic acid, on the other hand, were the most abundant in dry-processing coffee while alkanes were most found in wet processing. Moreover, analysis from M. Haile *et al*. (2020), also showed the comparison of VOCs among dry, wet processing, and biological processing coffee (Elephant dung) by using GC-MS, the result suggested that the different types of coffee shared the similarities of VOCs, including 2-furanmethanol, acetic acid, 2-methylpyrazine, 2,6-dimethylpyrazine, pyridine, and 5-methylfurfural. Furthermore, they were also able to identify the VOCs that only found in 2 types of Black Ivory coffee, including 2-hydroxymethylpyrrole, 3- methylfuran, 2-methylfuran, 2-ethyl-3-methylpyrazine and 2-hexanol in black ivory coffee with completely digested pulp; propionic acid, 4-ethylguaiacol, 1-furfurylpyrrole, and 2-methylphenol in black ivory coffee with undigested pulp.

Further research focusing on indicators from different aspects that might affect the VOCs profile in roasted beans during the processing of green coffee is also paid attention to, which namely includes the application of starter culture in coffee fermentation and coffee defects. The effects of using selective strains in starter culture for post-harvest processing were a topic of interest in the present time as it is claimed to enhance the overall coffee quality. The individual effect of *Saccharomyces cerevisiae* and *Pichia kluyveri* on coffee fermentation has been documented [11, 12]. By using HS-SPME-GC-MS methods, they were able to identify the aroma production from the individual yeast. Distinctive aromatic substances from yeast metabolism can exist in the roasted coffee that can affect the overall perception of the coffee, in particular, fruity-smelling acetate ester: isoamyl acetate produced from *P. Kluyveri* and buttery note of 2,3-butanedione (diacetyl) from *S. cerevisiae.* Similar results were observed in the later research from C. Wang and others (2020) about the coculture of *Saccharomyces cerevisiae* and *Pichia kluyveri* with the addition of LAB, *Lc. lactic subsp. cremoris.* The coffee not only resulted in the winey and fruity acetate in the roasted coffee but also the formation of caramel-smelling furfurals during roasting [11, 12]. Contrary to good coffee quality indicators, the VOCs profile of defective coffee is also paid attention to, and it has been researched in the past years to identify and solve the problems, as D. L. Kalschne and others (2018) mentioned [24]. The VOCs characterized as a defect or undesirable smell (rancid, cabbage, cheese, ammonia, moldy, etc) was reported in Toci (2008), supported by the detection of 2,3,5,6-tetra-methylpyrazine, which was responsible for black and sour bean defect in roasted coffee. VOCs such as 2, 3-butanedione, 2-methylbutanal, 3-methylbutanal, 4-ethylguaiacol, 4-methylthiazole were found in roasted PVA mixture- commercial mixture of non-defective and defective seeds. And finally, volatiles as 2, 5-dimethylpyrazine, 2, 6-dimethylpyrazine, 2-acetyl-3,5-dimethylpyrazine, 2,3-dimethylpyrazine and pyridine were correlated with the black, sour, immature and off-flavor from defective coffee [25, 26, 27].

## 1. Volatile compounds in roasted coffee and preservation

Roasting is an important stage for the overall development of coffee flavor. This is a process that uses the heat of around 300ºC to change the biochemical precursors in the green coffee (lipids, proteins, carbohydrates, phenolic compounds, and alkaloids) into a unique fragrant aroma and distinctive taste. During the roasting stage, thermal degradations and Maillard reaction coupled with Strecker degradation and pyrolysis would be the most common reactions causing the transformation. Thermal degradations not only contribute to the caramel flavors and release of other N and O containing aliphatic compounds, but also contribute to the breakdown of chlorogenic acids and other phenolics to provide precursors of phenolic volatile compounds such as guaiacol, p- vinylguaiacol, and others**.** An increase of pyrrols and pyridines in roasted coffee from alkaloids in green coffee is also observed in this stage [28]. On the other hand, Maillard reactions give rises to pyrazines, pyrroles, pyridines (which are responsible for the nutty and roasty aroma in coffee brew) thiols, thiophenes, furanones [28] by the interaction of reducing sugars with free amino acids, along with Strecker degradation and pyrolysis.

It was reported that 31 furans, 31 carbonyl compounds, 25 pyrazines, 18 benzene derivatives, 11 sulfur-containing compounds, 5 pyridines, 11 alcohols, 3 hydrocarbons, 4 esters, 6 pyrrols and single pyranes, oxazols, and lactones were found in the headspaces of roasted coffee using 3 different methods of roasting, including convectively roasted (CR), microwaved (MR), and roasted by the coupled convective–microwave method [29, 30]; however, only a few of them contributed to the roasted coffee, such as 2,3-pentanedione, 2,5- dimethylpyrazine, 2-ethylpyrazine, 2,3-dimethylpyrazine, 3-ethyl-2,5-dimethylpyrazine, 2-methylbutanal, 2-ethylguaiacol, and 4- vinylguaiacol [63]. Studies about VOCs during the differences of roasting degrees were also carried out. It was reported that light roasted Arabica coffee had notable furfural (swe*et al*mond roast) and 2-methylbutanal (buttery note) [31, 32]. It was also found in a study by Moon (2009) that furfuryl alcohol, 5-hydroxymethylfurfural, and γ-butyrolactone in medium-roasted beans; furfuryl alcohol, γ-butyro- lactone, and 2-acetylpyrrole in city-roasted beans; and γ-butyrolactone, furfuryl alcohol, and catechol in French-roasted beans using GC-MS and GC-FID methods [32]. The conclusion was drawn from the study that the most volatile substances had a less significant role in the roasted coffee aroma as VOCs groups such as furfurals, volatile acids, and furanones (fruity, floral aroma notes) were decreased in darker roast while the pyridines and pyrroles, as well as phenols and lactones (spicy, roasty, nutty notes), increased in a dark roast. Furthermore, studies about VOCs with different coffee roasting rates also suggested a new approach for the coffee industry as mentioned in To ci and others (2014) [33], medium roasting of coffee achieved by slow rate (15 min, 190°C, intermediate (8 min, 210°C) and fast rate roasting (5 min, 230°C) resulted in the variation of quality in terms of aroma in coffee. The indicators for quality in different roasting rates were 2, 5-dimethylpyrazine, 2-ethylpyrazine, 2,3-dimethylpyrazine, 2,5-dimethyl-3-ethylpyrazine, guaicol, 2-ethylguaicol, and 4-vinyl-guaiacol [26]. Guaicol was reported as an indicator for slow roast with the highest amount whereas 4-ethylguaiacol was identified in fast roasting. However, the study contained several variables such as the un-uniform of bean quality and differences in roasting equipment; therefore, this topic needs to be studied more carefully in the future before having a final conclusion of the effect of roasting rate on overall roasted coffee VOCs.

Storage of coffee is also categorized as an influential factor in the overall coffee aroma since coffee VOCs are susceptible to extrinsic factors such as temperature, humidity, exposing the condition of coffee, and packaging types. The loss of aroma can be due to the diffusion of VOCs along with $CO_2$ and water, which are stored in the coffee beans or absorbed in the active site right after being roasted or they can be oxidized, causing rancid flavor in coffee. During the storage of roasted coffee, the VOCs will be affected by the level of oxygen, including sulfur-containing volatile compounds and aldehydes, in which hexanal (rancid aroma) was reported to have the indicative role of coffee exposed to oxygen during storage [34]. Another factor that affects the VOCs of roasted coffee is water activity as this can speed up the oxidation rate [34], this was best observed in sulfur-containing compounds such as dimethyl trisulfide and dimethyl sulfide, they were found to be increased in coffee stored at higher water activities. Furthermore, storage temperature is also a reason for the degradation of roasted coffee quality as Perez-Martinez and others (2008) detected the increase of oxidative products, including hexanal, butanal, dimethyl disulfide, and dimethyl trisulfide, which were mainly responsible for rancidity and other off-flavor [35]. On the other end of the spectrum, studies of the freshness indicators in roasted coffee are carried out to determine the coffee shelf-life. Information about the shelf-life of roasted coffee can be proposed in ratio or specific chemicals. In ratios, P. Poltronieri (2016) suggested the ratio of 2-butanone/2-methylfuran and 2,3-butanedione/2-methylfuran is the indicator for whole beans, which is inversely related to 2-methylfuran and 2,3-butanedione, and dimethyl disulfide/methanethiol and 2-butanone/methanethiol are the indicator of roasted and ground coffee [36]. On the other hand, 2-furfurylthiol and dihydroxybenzenes or trihydroxybenzenes were identified as indicators of freshness in roasted coffee in terms of individual indicators [37].

## 2. Volatile compounds in Vietnamese Robusta coffee

While Vietnam and Indonesia are the two countries with the most dominant production and selling of Robusta coffee, Vietnamese Robusta coffee is more well-known for its strong and robust flavor, with higher caffeine content compared to other origins [38]. This coffee subject has been involved in many aroma-related studies, in which roasted Vietnamese coffee is usually correlated with a nutty, buttery, roasty, and spicy aroma. In specific, it was found with an increasing amount of pyridine (sweet, brown, woody, bready, caramellic), 1-(1H1pyrrol-2-yl)-ethanone, 2- ((methylthio)methyl) furan (Smoke, roast, onion, garlic, sulfuraceous, pungent, vegetable, horseradish), furfuryl propanoate (green banana) and 2,2'-methylenebisfuran (rich-roasted) in dark roasting [17]. Furthermore, when compared to Indonesian Robusta, Vietnamese coffee showed its superiority in quality, which had notably higher intensity of sweet caramel, phenolic, buttery-oily, smoke-roast, and acidic in medium-roast condition, using the GC-O method for characterization. Robusta coffee, however, in general, is usually characterized by an earthy odor and another undesirable aroma, which is relatively unappealing to the majority of the population. Therefore, many efforts were made to improve the aroma profile of Robusta coffee, especially involving with Vietnamese type, namely in T.N.H. Nguyen (2013) study, optimization of roasting temperature, time (230ºC in 18 min) and espresso extracting temperature (110ºC) were concluded based on the highest concentration of Robusta quality indicators, including 4-ethylguaiacol (clove-like profile complemented by interesting woody and sweet vanilla); 2-ethyl-3,5-dimethylpyrazine (toasty, chocolaty); 2,3- diethyl-5-methylpyrazine (nutty, roasted, vegetable); and 2-furfuryl (roasty, dominant in freshly roasted coffee)[39]. Furthermore, several studies attempted to modify Vietnamese Robusta coffee VOCs by altering the flavor precursors in green coffee by using different individual carbohydrates (glucose, fructose, and sucrose). As the result, the aroma profile of fructose treated Vietnamese Robusta coffee was improved, in which, most furans, ketones, and organic acids significantly increase 2-3 times compared to the non-treated Robusta beans, which relatively resembled the sensory attributes of Arabica coffee [40]. Another study about the enhancement of coffee aroma involved the application of acetic acid-treated Vietnamese Robusta samples, which showed an increase of furanic compounds (sweet, caramel) and a decreased number of pyrazines, which correlate to 14% of coffee volatile compounds and indicate the roasted, earthy and somewhat bitter aroma in Vietnamese Robusta [40]. Similarly, efforts for aroma improvement of Vietnamese Robusta coffee were also made using L-leucine Powder and this resulted in the decrease of bitter aroma including pyrazines, pyrroles, phenols, and their derivatives [41]. In the future, further research needs to be carried out to understand how Vietnamese Robusta coffee has its unique aroma and understand how to strengthen its distinctive profiles. These research types can be applied not only in coffee products but also in many other industries; furthermore, their application may make Vietnamese Robusta coffee one of the best coffees in the world.

## Conclusion

Throughout the past, the coffee aroma has been an interesting topic due to the non-stop increasing consumption all over the world. Many researchers have attempted to study the coffee volatile compounds in order to comprehensively understand the nature behind the aroma of roasted coffee and apply it to related industries. In nearly 100 years of studying coffee aroma, researchers have been focusing on the detection of volatile substances and identification of their concentration as well as volatility to predict the contribution of VOCs to the aroma of coffee; thus, resulting in the development of a database (WILEY, NIST, etc.) for the identification of VOCs, which benefits the future research of coffee VOCs. Along with this solid base for analysis, the development of artificial intelligence (artificial neural network, machine learning programs, etc.) in the present day has efficiently been applied for qualitative studies of coffee VOCs and this approach has a lot of potential for the whole picture of coffee aroma as well as its application the food industry.

**Table 1:** Roasted coffee VOCs and their perceived aroma

| Roasted Coffee VOCs | Perceived sensory attributes | References |
|---|---|---|
| **Aldehyde** | | |
| 2-Methylbutanal | Rancid, almond-like, toasty | [5] |
| 2-Methylpropanal | Toasty, caprylic, cheesy, dark chocolate, ethereal, fruity, malty, pungent | |
| 3-Methylbutanal | Fruity, almond-like, toasty, ethereal, chocolaty, peachy, fatty | |
| (E)-2-nonenal | Fatty, green, cucumber, citrus | |
| Acetaldehyde | Pungent, ethereal, fresh, lifting, penetrating, fruity, musty | |
| 4- Methoxybenzaldehyde | Sweet, powdery, vanilla, anise, woody, coumarin, creamy | |
| Phenylacetaldehyde | Sweet, fruity, honey, floral, fermented | |
| Propanal | Ethereal, pungent, earthy, alcoholic | |
| 5- Methylfurfural | Sweet-spicy, warm, caramel | [40] |
| **Acid** | | |
| 2-Methylbutyric acid | Acidic, fruity, dirty, cheese | [5] |
| 3-Methylbutyric acid | Cheesy, dairy, acidic, sour, pungent, fruity | |

| | | |
|---|---|---|
| Acetic acid | Vinegary | [40] |
| Propanoic acid | Sour | |
| Ester | | |
| Ethyl-2-methylbutyrate | Fruity, berry | [5] |
| Ethyl-3-methylbutyrate | Fruity | |
| **Furan** | | |
| Furfural | Sweet, brown, woody, bready, caramellic | [5] |
| 2-((Methylthio)methyl) furan/ 2-furfuryl methyl sulfide | Smoke, roast, onion, garlic, sulfuraceous, pungent, vegetable, horseradish | |
| 2-Furfuranmethanol acetate/furfuryl acetate | Onion, garlic, sulfury, pungent, vegetable, horseradish | |
| Furfuryl formate | Ethereal | |
| 5-Methyl-2-furancarboxyalde-hyde/2- methyl furfural | Sweet, caramellic, bready, brown, coffee-like | |
| Furfuryl methyl ether | Roasted coffee | |
| Furfuryl disulfide | Sulfury, coffee, roasted chicken, meaty, onion | |
| 2,2’-methylenebisfuran | Cabbage | |
| Furfuryl propanoate | Rich roasted | [40] |
| 2 acetylfuran | Green banana | |
| 2 furfurylfuran | Caramel, earthy | |
| 2-Methyl furan | Burnt, ethereal (mild), gasoline, acetone, chocolate | |
| 2,5-dimethyl furan | Etheral | |
| 2,3,5-trimethylfuran | Coffee-like | |
| **Sulfur-containing compounds** | | |
| Dimethyl trisulfide | Sulfurous, cooked onion, savory, meaty, cabbage-like | [5] |
| Bis(2-methyl-3-furyl) disulfide | Meaty, roasted scallion, onion, sulfury | |
| Methional | Boiled potato-like, musty, tomato, earthy, vegetable, creamy | |
| Furfuryl methyl sulfide | Coffee-like | [40] |
| 3-methylthiophene | Fatty, winey | |
| **Thiols** | | |
| 3-Mercapto-3-methylbutylformate | Green blackcurrant, herbal, fruity, roasted, sweaty | [5] |
| 2-Furfurylthiol | Roasty (coffee-like), sulfurous | |
| 2-Methyl-3-furanthiol | Sulfury, meaty, fishy, metallic, boiled | |
| 3-Mercapto-3-methylbutylacetace | Roasty, fruity, sulfurous, sweet | |
| 3-Methyl-2-butene-1-thiol | Sulfury, smoky, leeky, onion | |
| Methanethiol | Rotten eggs, meat or fish, cabbage, garlic, cheesy | |
| **Thiophene** | | |
| 3-Methylthiophene | Fatty, winey | [5] |
| **Thiazole** | | |
| 2,4-Dimethyl-5-ethylthiazole | Nutty, roasty, meaty, earthy | [5] |
| 4-methylthiazole | Fruity, nutty, green | [40] |
| **Furanone** | | |
| Dihydro-2-methyl-3(2H)-furanone | Sweet, bread, buttery, nutty | [5] |
| 2-Ethyl-4-hydroxy-5-meth- yl-3(2H)-furanone(homofuraneol) | Sweet, caramel, candy | |
| 3-Hydroxy-4,5-dimethyl-2(5H)-furanone (sotolone | Extremely sweet, strong caramel, maple, burnt sugar, coffee | |
| 4-Hydroxy-2,5-dimethyl-3(2H)-furanone (furaneol) | Sweet, candy, caramel, strawberry, sugar | |
| 5-Ethyl-3-hydroxy-4-methyl-2(5H)- furanone (abhexon | Seasoning-like, caramel-like | |
| 5-Ethyl-4-hydroxy-2-methyl-3(2H)- furanone | Sweet, caramel, bready, maple, brown sugar, burnt | |
| **Ketone** | | |
| 1- Octen-3-one | Herbal, mushroom, earthy, musty, dirty | [5] |
| 2,3-Hexadione | Burnt, buttery, caramel, chocolate cream, creamy, fruity, oily, pear, sweet | |
| 2,3-Butanedione | Buttery, creamy, fatty, oily, sweet, vanilla | |
| 2,3-Pentanedione | Buttery, caramel, creamy, penetrating, sweet | |
| 4-(4′-hydroxyphenyl)-2-butanone | Sweet, fruity, berry, jam, raspberry, ripe, floral (raspberry tone) | |
| 1-(2-Furanyl)-2-butanone | Rummy | |
| **Norisoprenoid** | | |
| (E)-β-damascenone | Honey-like, fruity, apple, rose, honey, tobacco, sweet | [5] |
| **Phenolic compounds** | | |
| Guaiacol | Phenolic, burnt, smoke, spice, vanilla, woody | [5] |
| Vanillin | Sweet, vanilla, creamy | |
| 4-Ethyl guaiacol | Spicy, smoky, bacon, phenolic, clove | [40] |
| 4-Vinyl guaiacol | Spicy, dry woody, fresh amber, cedar, roasted peanut | |
| **Pyrazine** | | |
| 2,3-dimethylpyrazine | Nutty, coffee, peanut butter, walnut, caramel, leather | [5] |

| | | |
|---|---|---|
| 2,5-dimethylpyrazine | Cocoa, roasted nuts, roast beef, woody, grass, medical | |
| 2,3-diethyl-5-methylpyrazine (hazelnut pyrazine) | Nutty-roast, musty, meaty, vegetable, roasted hazelnut | |
| 2-Ethyl-3,5-dimethylpyrazine | Nutty-roast | |
| 2-Ethyl-3,6-dimethyl-pyrazine(3,6-cocoa pyrazine) | Potato, cocoa, roasty, nutty | |
| 2-Methoxy-3,5-dimethylpyrazine(3,5-cocoa pyrazine) | Earthy, burnt, almonds, roasted nuts, coffee | |
| 2-Methoxy-3,2-methylpropylpyrazine | Green, pea green, bell pepper | |
| 2- Methoxy-3-isopropylpyrazine | Earthy, pea, beany | |
| 3-Ethenyl-2-ethyl-5-methylpyrazine | Earthy | |
| 6,7-dihydro-5-methyl-5H-cyclo- pentapyrazine | Nutty-roast, earthy, baked potato, peanut, roasted | |
| Ethylpyrazine | Peanut butter, musty, nutty, woody, roasted cocoa | |
| Trimethylpyrazines | Nutty | [40] |
| Terpene | | |
| Linalool | Flowery, citrus, orange, terpy, waxy, rose | [5] |
| Limonene | Citrus, herbal, terpene, camphor | |
| Geraniol | Sweet, floral, fruity, rose, waxy, citrus | |
| Pyridines | | |
| Pyridine | Fishy | [5] |
| Pyrrole | Sweet, nutty, ethereal | |
| 1-Methyl pyrrole | Smoky, woody, herbal, negative notes– defective beans | [40] |
| 3-Ethylpyridine | Caramel, roasted, hazelnut | |
| 1-ethylpyrrole | Burnt | |

**Note:** Modified from [5, 40]

**Table 2:** Processing factors affecting coffee's overall flavors.

| Processing step | Effects on sensorial differences | References |
|---|---|---|
| Coffee species | Robusta coffee experienced stronger and more chocolaty, smoky, and bitter flavors, Arabica coffee had a more delicate profile of fruity, floral, and sweet flavors. | [10] |
| Coffee cultivars | Four varieties of Arabica (Catuaí, Caturra, Pache, and Catimor) were assessed by sensory panelists. While Catimor and Catuaí are more balanced than Caturra and Pache, Caturra had higher scores for sensory characteristics. Coffee cultivars affect coffee quality through the shapes and sizes of coffee and biochemical compositions of caffeine and chlorogenic acids were also affected by different cultivars. | [42, 43, 44] |
| Coffee growing environment | Biochemical measurements differences between coffee grown in different altitudes. Higher altitude correlates to higher glucose level. Volatile compounds also change due to difference in temperature, the cooler the temperature, the fruitier and more acidic the aroma. | [45] |
| Coffee post-harvest processing | The flavor from full-washed coffee is more roasty, bitter, and nutty with a more desirable fruity aroma than Turkish natural processing coffee.<br>Washed coffee had better cup quality than unwashed coffee with more desirable body, acidity and aroma.<br>Natural coffee tended to yield stronger body and aroma, sweeter with less acidity.<br>Bio-digestion with civet coffee (*Paradoxurus hermaphroditus*) was described with musty, earthy, smooth, syrupy, and cocoa characteristics.<br>Elephant coffee (*Elephas maximus*) was claimed to have unique flavor characteristics in terms of light roasting. | [46, 47] |
| Coffee secondary drying | Sun-dried and mechanically dried coffee had sweeter and more citrus flavors in the sensory test, but the overall flavor was found to be more intense in the sun-dried samples. | [48] |
| Coffee roasting | Coffee's unique flavor directly corresponds with a roasted aroma and burnt and bitter taste. Changes in volatile and non-volatile compounds in green coffee beans through pyrolysis, Maillard reaction, and Strecker degradation, lead to flavor modification. The darker the roast, the more intense the flavor, other roasting levels correlated to different flavor attributes, specifically in medium roasting level, the beverage provided a more intense cocoa aroma and more balanced body. | [10, 32, 49] |
| Coffee brewing and serving | Ground coffee particle size can affect not only the biochemical extraction yield from roasted coffee but also alter the flavor in cold brewed coffee. Coffee water ratio in preparation of the beverage also correlates to the sensory experience as the higher the ratio, the stronger the flavor of the final cup | [50] |

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