



Determination of aromatic profiles of coffee beans according to different roasting times by SPME/GC-MS analysis

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ABSTRACT

Coffee is the most widely consumed beverage around the globe. The flavor and fragrance of coffee are directly associated with its volatile compositions. This research aimed to determine the effect of roasting times on the aromatic compositions of coffee beans. For this purpose, Brazilian, Ethiopian, Colombia Supremo, Ethiopia 210, and Indonesia Mandheling coffee beans were purchased in South Korea. To determine the adequate roasting time for Brazilian and Ethiopian coffee varieties, coffee beans were roasted at 210°C with different time durations such as 11, 12, 13, and 14 minutes, and the remaining coffee cultivars were roasted at 210°C for 13 minutes. The color parameters and the aromatic composition of roasted coffee beans were determined. The SPME/GC-MS analyses revealed the identification of 234 aromatic components from the eight coffee beans of Brazilian and Ethiopian varieties based on different roasting times. 2-Furanmethanol was a predominant component in all the roasted coffee beans (13.65%–19.30%). The amount of pyridine and 2-furanmethanol, acetate was markedly decreased when increasing roasting times from 11 to 14 minutes in both coffee beans. In contrast, the concentration of 5-methyl-2-furancarboxaldehyde was increased when increasing roasting time. The results indicated that the aromatic profiles of these coffee beans varied both qualitatively and quantitatively according to different roasting times. The data of this study may be used as a standard to identify better aroma quality of different coffee bean varieties.

INTRODUCTION

Coffee is an important traded agricultural commodity and has entered the daily routine of many people around the world for its unique sensory properties (Lopes *et al.*, 2021). The species of the genus *Coffea* (Rubiaceae) have been extensively used as medicines for centuries owing to the presence of various bioactive substances. Among various *Coffea* species, commercially and economically significant species are *C. arabica* L. (Arabica coffee) and *C. canephora* Pierre ex A. Froehner (Robusta coffee). The third important commercialized coffee species is *C. liberica* Hiern (Angeloni *et al.*, 2021; Craig *et al.*, 2018). Coffee is chiefly

cultivated in equatorial or subtropical regions. In particular, *C. arabica* cultivars are cultivated in the high mountains above 1,000 m with temperatures between 5°C and 15°C, whereas *C. canephora* species are cultivated in the low plains (Folmer, 2017).

In Korea, coffee is one of the most consumed beverages next to the water. The coffee industry is rapidly increasing, and as of 2018, the number of coffee shops in Korea reached 66,000, and it is known that the sales amount reached around 4.8 trillion Korean won (Kim, 2019). The average coffee consumption per adult is 353 cups per year, which is about 2.7 times higher than the world's average consumption (Korea Coffee Association, 2022; Song, 2020). In the rapidly changing coffee market environment, the coffee industry is continuously developing new high-quality products to satisfy the intense competition in the coffee market and the changing needs of consumers. Therefore, the necessity for improving the flavor and fragrance of coffee beans has been increased to produce high-quality coffee (Angeloni *et al.*, 2021).

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The complexity of the aroma of coffee is directly associated with its volatile composition. In general, coffee beans produce different aromas under identical roasting or brewing conditions due to coffee bean cultivars, geographical origins, and postharvest treatments (Lopez-Galilea *et al.*, 2006; Pereira *et al.*, 2019; Rao *et al.*, 2020). Roasting and brewing coffee beans produce the characteristic aroma of the coffee, and these methods play a major role in the price and quality of coffee (Lopes *et al.*, 2021). Further, coffee is known to contain >1,000 chemical components that contribute to the flavor and fragrance of coffee. These chemical components affect the sensorial perceptions of the oral and nasal mucosa (Angeloni *et al.*, 2021; Kreuml *et al.*, 2013).

In coffee beans, the roasting process is highly responsible for the development of flavor. The development of the aroma of coffee is a complex and time-temperature-dependent process (Farah *et al.*, 2006). Numerous chemical reactions and modifications occur during the coffee roasting process (Giacalone *et al.*, 2019; Yang *et al.*, 2016). Maillard reaction and Strecker reaction and protein degradation are important chemical modifications in roasted coffee beans (Kreuml *et al.*, 2013). The gas chromatography and mass spectrometry (GC-MS) technique is an excellent approach for detecting complex mixtures of aroma components in different cultivars of coffee (Lopes *et al.*, 2021). The GC-MS-based analyzes allow the identification of different chemical families in roasted coffee bean cultivars, mainly pyrazines, pyridines, pyrroles, furans, and others (Ongo *et al.*, 2020; Marek *et al.*, 2020; Ryan *et al.*, 2004). There are numerous coffee cultivars in the domestic market, but the appearance of different cultivars of roasted coffee beans is similar. Hence, the determination of the aromatic profile of roasted coffee beans is an appropriate way to clarify the cultivars of coffee. With this background, this study aimed to compare the aromatic profiles of coffee beans of Brazilian and Ethiopian varieties according to different roasting times by solid-phase microextraction (SPME)/GC-MS analysis. In addition, the aromatic profiles of three popular coffee bean cultivars in Korea, such as Colombia Supremo, Ethiopia 210, and Indonesia Mandheling, were studied.

MATERIALS AND METHODS

Collection of plant samples

Green coffee beans of different cultivars such as Brazilian, Ethiopian, Colombia Supremo, Ethiopia 210, and Indonesia Mandheling coffee beans were purchased in the local markets in Korea. Ten batches of each cultivar were purchased from the market. In these, 20 green coffee beans, identical in size, were randomly selected for each roasting condition. The green coffee beans were pale green with a milky smell. The coffee roasting process was carried out in triplicate.

Coffee roasting

The roasting process for the Brazilian and Ethiopian coffee beans was set at 210°C with different roasting times such as 11, 12, 13, and 14 minutes. In the case of Colombia Supremo, Ethiopia 210, and Indonesia Mandheling cultivars, coffee beans were roasted at 210°C for 13 minutes. The coffee beans were roasted using a fluidized bed roaster. Each coffee bean cultivar was roasted separately and powdered. The ground coffee beans were kept at -20°C prior to SPME-GC-MS analysis.

Color determination

The pulverized roasted bean samples were measured using a spectrophotometer (CM-3600A, Konica Minolta, Japan) and were expressed as Hunter's values, L* (lightness), a* (redness), and b* (yellowness). The color determination was carried out according to the procedure of Dong *et al.* (2017).

Determination of aromatic profile by SPME/GC-MS analysis

Aromatic components of roasted coffee cultivars were analyzed using SPME-GC-MS based on the method of Caporaso *et al.* (2018). Ground roasted coffee samples, exactly 100 mg, were placed in 5 ml vials. These samples were allowed to equilibrate for 10 minutes at the constant temperature of 40°C, followed by 20 minutes of fiber exposure using a 50/30 µm divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) SPME fiber (Supelco, Bellefonte, PA, USA). Volatile components were desorbed by inserting the fiber for 10 minutes into the injection port of the gas chromatograph (GC), kept at 250°C. A Bruker CP-3800 model GC with Varian 1200 Mass spectrometry was used to analyze volatile components. GC/MS column used was VF-5MS (low polarity; 30 m * 0.25 mm * 0.25 µm), and helium was used as a carrier gas at a 1.2 ml/minute flow rate. For GC conditions, the injection volume was 1 µl, the split ratio was 10:1, the inlet temperature was 250°C, and the oven temperature was programmed from 50°C to 250°C at 3°C/minute. The ion source (detector) and interface temperatures were 270°C and 250°C, respectively. For MS analysis, the spectrum was taken at 70 eV with a mass scan range of 50–400 m/z. The detection of volatile components in different coffee bean cultivars was done by mass spectra data (NIST library version 3.0). The results of volatile compositions were expressed as the relative percentage of each compound peak area to the total GC-MS peak area. Each analysis was carried out in triplicate.

RESULTS

Color parameters, such as L* (lightness), a* (redness), and b* (yellowness), were determined to observe the effect of different roasting times on coffee beans (Table 1). The results indicated that the roasting time significantly affected the color parameters of coffee beans. The L*, a*, and b* values of Ethiopian coffee beans (40.86 ± 0.02–36.53 ± 0.04, 6.53 ± 0.04–2.12 ± 0.05, 7.03 ± 0.06–1.13 ± 0.07, respectively) were markedly decreased when increasing roasting time from 11 to 14 minutes. In contrast, the L*, a*, and b* values of Brazilian coffee beans increased during 12 minutes of roasting time and decreased afterward.

The SPME/GC-MS analyses revealed the identification of 234 aromatic components in Brazilian and Ethiopian coffee beans in relation to different roasting times (Table 2). In particular, 2-furanmethanol was the predominant component in all the roasted coffee beans (13.65%–19.30%), followed by pyridine (3.69%–18.7%), 2-furanmethanol, acetate (2.89%–12.00%), 5-methyl-2-furancarboxaldehyde (2.30%–11.60%), methylpyrazine (4.53%–9.42%), and ethylpyrazine (2.06%–3.73%).

It was observed that roasting times significantly affect the aromatic profiles of Brazilian and Ethiopian coffee beans. The concentration of pyridine and 2-furanmethanol, acetate was markedly decreased when increasing roasting times from 11 to 14 minutes in both Brazilian (18.70%–4.01% and 12.00%–2.89%,

Table 1. Color analysis of different roasted coffee cultivars.

Samples	Roasting time (at 210°C)	<i>L</i> * Lightness (White-Black)	<i>a</i> * Redness (Red-Green)	<i>b</i> * Yellowness (Yellow-Blue)
Brazilian coffee	11 minutes	40.76 ± 0.03	6.13 ± 0.02	6.91 ± 0.06
	12 minutes	41.12 ± 0.09	6.24 ± 0.10	7.22 ± 0.17
	13 minutes	38.75 ± 0.03	4.18 ± 0.01	3.68 ± 0.07
	14 minutes	37.36 ± 0.03	2.74 ± 0.05	1.82 ± 0.07
Ethiopian coffee	11 minutes	40.86 ± 0.02	6.53 ± 0.04	7.03 ± 0.06
	12 minutes	38.28 ± 0.01	4.20 ± 0.01	3.65 ± 0.01
	13 minutes	37.31 ± 0.01	3.00 ± 0.03	2.11 ± 0.01
	14 minutes	36.53 ± 0.04	2.12 ± 0.05	1.13 ± 0.07
Colombia Supremo	13 minutes	39.77 ± 0.17	5.18 ± 0.19	5.22 ± 0.19
Ethiopia 210	13 minutes	39.17 ± 0.09	4.91 ± 0.06	4.39 ± 0.11
Indonesia Mandeling	13 minutes	39.09 ± 0.07	4.99 ± 0.098	4.59 ± 0.20

Table 2. Aromatic profile of roasted coffee beans of Brazilian and Ethiopian varieties according to different roasting times at 210°C.

S.No.	Retention Time	Compounds	Brazilian coffee beans (Area %)				Ethiopian coffee beans (Area %)			
			11 minutes	12 minutes	13 minutes	14 minutes	11 minutes	12 minutes	13 minutes	14 minutes
1	1.621	trimethylamine	0.13 ± 0.04	-	-	-	-	-	-	-
2	1.704	2-p-bromo- α -methylethylamine	-	-	-	-	-	-	0.09 ± 0.01	-
3	1.726	1,3-pentadiene	-	-	-	0.22 ± 0.01	-	-	-	-
4	1.888	carbon disulfide	-	0.03 ± 0.00	-	0.06 ± 0.00	-	-	-	-
5	2.113	amino-1-hexanol	-	-	0.25 ± 0.01	0.42 ± 0.01	-	0.15 ± 0.01	-	0.21 ± 0.14
6	2.127	(S)-(+)-isoleucinol	-	-	-	-	-	-	0.17 ± 0.03	-
7	2.200	3-methylfuran	1.17 ± 0.18	1.01 ± 0.13	1.23 ± 0.16	1.38 ± 0.17	1.73 ± 0.03	1.25 ± 0.16	0.84 ± 0.07	1.13 ± 0.16
8	2.275	methyl formate	-	-	0.50 ± 0.04	1.18 ± 0.06	-	-	0.60 ± 0.09	0.96 ± 0.07
9	2.749	etilefrin-propionyl	-	-	-	-	-	-	-	0.10 ± 0.01
10	2.843	N-tert-butylhydroxylamine	-	-	0.76 ± 0.04	1.67 ± 0.03	-	-	0.66 ± 0.03	1.30 ± 0.18
11	2.866	propionaldehyde	-	0.15 ± 0.01	-	0.12 ± 0.00	0.40 ± 0.00	0.48 ± 0.17	-	-
12	3.268	dimethylsilanediol	-	-	-	0.39 ± 0.19	-	-	-	-
13	3.471	2,5-dimethylfuran)	-	-	-	-	0.17 ± 0.00	0.12 ± 0.02	-	0.14 ± 0.01
14	3.849	vinylfuran	0.06 ± 0.01	-	0.11 ± 0.09	-	0.12 ± 0.01	-	-	-
15	4.053	3-methyl-3-buten-1-ol	-	-	0.04 ± 0.00	0.05 ± 0.00	-	-	-	0.10 ± 0.02
16	4.136	pyrazine	0.41 ± 0.03	-	-	-	0.37 ± 0.01	0.27 ± 0.03	0.36 ± 0.05	-
17	4.223	N-methylpyrrole	-	-	-	-	-	0.34 ± 0.02	0.27 ± 0.03	-
18	4.225	3-methyl-1H-pyrrole	-	0.45 ± 0.00	-	0.45 ± 0.04	-	-	-	0.38 ± 0.06
19	4.231	1-methyl-1H-pyrrole	-	-	-	-	0.57 ± 0.04	-	-	-
20	4.411	pyridine	18.7 ± 0.62	15.6 ± 0.80	8.19 ± 0.06	4.01 ± 0.04	15.3 ± 0.10	10.30 ± 0.03	6.90 ± 0.13	3.69 ± 0.18
21	5.051	toluene	-	-	-	0.04 ± 0.01	0.13 ± 0.01	-	-	-
22	5.415	3-(hydroxymethyl)-2,2-1-pyrrolidinyl	-	-	-	-	0.14 ± 0.02	-	-	-
23	5.921	1,2,3,6-tetrahydro-1-methyl- pyridine	0.43 ± 0.04	-	-	-	0.21 ± 0.06	-	-	-
24	5.967	1-penten-3-one	-	-	-	-	-	0.07 ± 0.03	-	-
25	6.303	4-hydroxy-3-hexanone	-	0.39 ± 0.01	0.5 ± 0.04	0.5 ± 0.01	-	-	-	-
26	6.307	8-methyl-1,8-nonanediol	-	-	-	-	0.41 ± 0.01	0.45 ± 0.05	-	-
27	6.317	3,3-dimethylbutanamide,	-	-	-	-	-	-	0.52 ± 0.08	0.51 ± 0.03
28	6.396	3-pentanone	0.12 ± 0.00	0.42 ± 0.04	0.9 ± 0.11	1.07 ± 0.04	0.46 ± 0.04	0.5 ± 0.03	0.75 ± 0.15	1.07 ± 0.03

Continued

S.No.	Retention Time	Compounds	Brazilian coffee beans (Area %)				Ethiopian coffee beans (Area %)			
			11 minutes	12 minutes	13 minutes	14 minutes	11 minutes	12 minutes	13 minutes	14 minutes
29	6.398	di-tert-butyl dicarbonate	-	0.17 ± 0.01	-	0.81 ± 0.04	0.19 ± 0.00	0.29 ± 0.02	-	-
30	6.400	3,4-bis(1,1-dimethylethyl)-2,2,5-hexane	-	-	-	-	0.26 ± 0.03	-	-	0.17 ± 0.16
31	6.408	di-t-butyl trisulfide	-	-	-	-	-	-	0.25 ± 0.06	-
32	6.622	2,7-dioxabicyclo[4.1.0]heptan-3-one, 5,5	0.54 ± 0.04	1.04 ± 0.03	1.47 ± 0.05	1.51 ± 0.03	0.83 ± 0.01	-	1.30 ± 0.19	1.60 ± 0.27
33	6.632	diethyl carbamoyl t-butoxy sulfide	-	-	-	-	-	1.06 ± 0.03	-	-
34	6.713	2-ethyl-1H-pyrrole	-	-	-	-	0.08 ± 0.01	-	-	-
35	6.810	hexamethyl-cyclotrisiloxane	-	-	-	0.06 ± 0.00	-	-	-	0.04 ± 0.01
36	6.981	2-methyl-pyridine	0.09 ± 0.04	-	-	-	0.18 ± 0.07	-	-	-
37	7.295	methylpyrazine	6.13 ± 0.64	9.42 ± 0.13	7.76 ± 0.02	7.46 ± 0.03	4.53 ± 0.04	4.49 ± 0.12	5.9 ± 0.27	5.34 ± 0.08
38	7.394	4-methyl-pyrimidine	0.43 ± 0.01	-	-	-	-	-	-	-
39	7.397	2-(methoxymethyl)-furan	-	-	-	-	0.54 ± 0.10	0.48 ± 0.06	-	-
40	7.472	N-carbobenzyloxy-l-tyrosyl-l-valine	0.53 ± 0.04	-	0.62 ± 0.06	0.64 ± 0.00	-	-	0.41 ± 0.02	0.55 ± 0.03
41	7.474	cresol	-	-	-	-	0.33 ± 0.04	0.58 ± 0.03	-	-
42	7.676	3-furaldehyde	1.36 ± 0.04	2.50 ± 0.02	6.60 ± 0.33	10.90 ± 0.03	2.12 ± 0.10	3.78 ± 0.12	-	0.30 ± 0.00
43	7.801	furfural	-	-	-	-	-	-	9.9 ± 0.08	16.9 ± 0.35
44	7.919	2,2-dimethyl-propanoic acid	-	-	-	-	0.17 ± 0.01	-	-	-
45	7.943	aniline	-	-	-	0.50 ± 0.03	-	-	-	-
46	8.027	(E)-3-hexene-2,2-dimethyl	-	-	-	-	0.17 ± 0.02	-	-	-
47	8.587	2-(2-propenyl)-furan	0.07 ± 0.01	-	-	-	0.13 ± 0.05	-	-	-
48	9.083	2,4-dimethyl-1H-pyrrole	-	-	-	-	-	-	-	0.12 ± 0.13
49	9.165	2-furanmethanol	18.40 ± 0.06	17.00 ± 0.06	17.90 ± 0.29	19.30 ± 0.38	17.10 ± 0.23	17.70 ± 0.37	14.00 ± 0.08	14.90 ± 0.31
50	9.306	1-bromo-4-chloro-butane	-	-	-	-	-	-	-	0.29 ± 0.00
51	9.341	3-methyl-pyridine	0.05 ± 0.00	-	-	-	-	-	-	-
52	9.525	dibucaine	-	-	1.65 ± 0.09	1.01 ± 0.25	-	-	-	-
53	9.629	nadolol tri-TMS derivative	1.65 ± 0.08	1.81 ± 0.09	-	-	1.97 ± 0.14	3.1 ± 0.27	2.09 ± 0.08	1.74 ± 0.00
54	9.979	bicyclo[3.1.0]hexan-2-one	-	-	-	0.13 ± 0.02	-	-	-	-
55	10.059	4-cyclohexene-1,2-diol	-	-	-	-	-	-	0.19 ± 0.03	0.37 ± 0.02
56	10.133	2,4-dimethyl-thietane	0.13 ± 0.12	-	-	-	0.52 ± 0.18	0.39 ± 0.11	0.35 ± 0.04	0.22 ± 0.09
57	10.215	methyl-β-D-ribosepyranoside	-	-	-	-	-	0.27 ± 0.02	-	-
58	10.219	2,6-octadiene-4,5-diol	0.11 ± 0.00	-	-	-	-	-	-	-
59	10.224	methyl 6-de-α-L-galactopyranoside	-	-	-	-	0.44 ± 0.17	-	-	-
60	10.503	propionic anhydride	-	-	-	-	-	-	0.20 ± 0.1	-
61	10.510	3-methyl-pentanoic acid	-	-	-	-	0.32 ± 0.12	0.41 ± 0.11	-	-
62	10.721	2-methyl-butanoic acid	-	-	-	-	-	0.35 ± 0.01	-	0.34 ± 0.16
63	10.800	2,2,3-trimethyl-decane	-	-	-	0.29 ± 0.18	-	-	-	-
64	11.125	2-methyl-2-cyclopenten-1-one	0.20 ± 0.01	0.20 ± 0.01	0.18 ± 0.01	-	0.24 ± 0.03	0.21 ± 0.02	0.14 ± 0.01	0.18 ± 0.02
65	11.241	furfuryl formate	1.16 ± 0.05	1.19 ± 0.02	1.1 ± 0.05	0.94 ± 0.04	1.14 ± 0.03	1.21 ± 0.05	1.25 ± 0.06	0.98 ± 0.11
66	11.402	2-furyl methyl ketone	1.06 ± 0.04	1.28 ± 0.11	1.45 ± 0.05	1.49 ± 0.03	1.76 ± 0.05	1.87 ± 0.07	1.91 ± 0.06	1.76 ± 0.03
67	11.580	4-methylphenol	3.86 ± 0.19	-	5.76 ± 0.37	6.28 ± 0.06	2.76 ± 0.15	3.4 ± 0.12	4.29 ± 0.27	4.25 ± 0.11
68	11.757	ethylpyrazine	3.73 ± 0.04	2.96 ± 0.03	2.11 ± 0.09	2.5 ± 0.14	2.63 ± 0.09	2.55 ± 0.05	2.28 ± 0.06	2.06 ± 0.03

Continued

S.No.	Retention Time	Compounds	Brazilian coffee beans (Area %)				Ethiopian coffee beans (Area %)			
			11 minutes	12 minutes	13 minutes	14 minutes	11 minutes	12 minutes	13 minutes	14 minutes
69	11.860	2,3-dimethyl-pyrazine	0.73 ± 0.01	0.75 ± 0.01	0.92 ± 0.08	1.12 ± 0.02	0.87 ± 0.01	0.57 ± 0.02	0.76 ± 0.09	0.69 ± 0.01
70	11.986	1,4-benzenediamine	0.19 ± 0.10	5.74 ± 0.15	-	0.17 ± 0.16	-	0.11 ± 0.01	-	-
71	12.086	trans-2-chlorocyclohexanol	-	0.08 ± 0.04	-	-	-	-	-	-
72	12.091	1,2,3,3a,4,7a-hexahydro-5H-inden-5-one	-	-	-	-	-	-	-	0.10 ± 0.03
73	12.115	hexahydro-4,7-di-1,3-isobenzofurandione	-	-	-	-	-	0.15 ± 0.03	-	-
74	12.224	2-oxo-cyclohexanepropanenitrile	-	-	-	-	-	-	-	0.06 ± 0.01
75	12.335	tetrahydro-6-pentyl-2H-pyran-2-one	-	0.18 ± 0.03	-	-	-	-	0.29 ± 0.06	-
76	12.373	1-methylcyclohexanol	0.24 ± 0.06	-	0.26 ± 0.01	0.23 ± 0.00	0.38 ± 0.04	0.32 ± 0.03	-	0.21 ± 0.03
77	12.441	β-[3-[N-aziridyl]propyl]aminopropio	-	-	-	0.35 ± 0.01	-	-	-	-
78	12.456	thiocyanic acid, [1-(4-amino-1,2,5-oxadi	-	-	0.34 ± 0.01	-	-	-	-	-
79	12.488	trans-2-cyano-1-cyclohexanol	-	-	-	-	-	-	-	0.30 ± 0.06
80	12.512	ethenylpyrazine	0.25 ± 0.01	-	-	-	-	-	-	-
81	12.536	pyrazine diazohydroxide	-	-	-	-	0.26 ± 0.01	0.29 ± 0.02	0.35 ± 0.07	-
82	12.767	4-cyclobutyl-4-oxo-2-butynoic acid	-	-	-	0.17 ± 0.01	0.14 ± 0.00	-	0.16 ± 0.05	0.14 ± 0.02
83	12.794	4-octyne	-	-	-	-	0.09 ± 0.03	-	-	-
84	13.186	1-butyl-1H-pyrrole	-	-	-	-	0.06 ± 0.02	-	-	-
85	13.326	2-(1-hydroxy-1-methyl-2-3(2H)-furanone	-	-	-	0.33 ± 0.01	0.26 ± 0.01	0.33 ± 0.01	0.37 ± 0.02	0.34 ± 0.01
86	13.335	uracil	-	-	0.34 ± 0.01	-	-	-	-	-
87	13.638	2-n-butyl furan	0.45 ± 0.01	0.48 ± 0.00	0.29 ± 0.01	0.2 ± 0.01	0.62 ± 0.06	0.58 ± 0.01	0.48 ± 0.02	0.26 ± 0.01
88	13.649	5-methyl-2-furanmethanol	-	-	-	0.19 ± 0.01	-	-	-	-
89	13.718	1-cyclohexyl-4,4-diethoxy-2-butyne-1-one,	-	-	-	-	-	-	-	0.14 ± 0.01
90	13.869	3-ethylpyridine	0.12 ± 0.01	-	-	-	-	0.26 ± 0.00	-	-
91	13.929	4-methylphenylhydrazine	-	-	0.1 ± 0.01	-	0.36 ± 0.01	-	-	-
92	14.147	5-methyl-2-furancarboxaldehyde	2.3 ± 0.01	5.97 ± 0.14	8.47 ± 0.7	9.4 ± 0.03	3.8 ± 0.14	6.66 ± 0.08	11.5 ± 0.17	11.6 ± 0.4
93	14.262	2,2,4,4-tetramethyl-pentane	-	2.68 ± 0.4	3.21 ± 0.02	-	-	2.16 ± 0.11	2 ± 0.13	-
94	14.299	vinyl propionate	1.69 ± 0.08	1.8 ± 0.12	2.78 ± 0.03	4.43 ± 0.00	1.54 ± 0.06	0.6 ± 0.06	3.27 ± 0.08	-
95	14.448	ethane-1,1-diol dipropoate	0.75 ± 0.63	-	-	-	-	-	-	-
96	14.476	phosphinothioic fluoride	-	-	-	-	-	1.78 ± 0.06	-	1.4 ± 0.00
97	14.732	2-acetyl-5-methylfuran	-	0.05 ± 0.01	-	-	-	-	-	0.06 ± 0.01
98	14.896	4-acetyl-heptanenitrile	-	-	-	-	-	-	-	0.38 ± 0.04
99	14.975	3-mercapto-3-methylbutanol	-	-	-	-	0.32 ± 0.01	0.3 ± 0.01	0.22 ± 0.15	-
100	15.219	2,6-dimethyl-2,6-octadiene	-	-	-	-	0.17 ± 0.01	-	-	-
101	15.227	octamethyl-cyclotetrasiloxane	-	-	-	0.24 ± 0.05	-	-	0.22 ± 0.15	0.27 ± 0.04
102	15.432	phenol	-	-	-	-	-	0.25 ± 0.12	-	-
103	15.454	p-hydroxyphenyl-phosphonic acid	0.35 ± 0.01	-	-	-	-	0.13 ± 0.01	-	-
104	15.509	β-pinene	-	-	-	-	0.39 ± 0.05	-	-	-

Continued

S.No.	Retention Time	Compounds	Brazilian coffee beans (Area %)				Ethiopian coffee beans (Area %)			
			11 minutes	12 minutes	13 minutes	14 minutes	11 minutes	12 minutes	13 minutes	14 minutes
105	15.515	bicyclo[3.1.1]heptane, 6,6-dimethyl-2-me	-	-	-	-	-	0.61 ± 0.16	0.47 ± 0.03	0.49 ± 0.01
106	15.608	dihydro-2-methyl-3(2H)-thiophenone	-	0.24 ± 0.04	0.22 ± 0.05	0.17 ± 0.02	-	-	0.21 ± 0.03	0.18 ± 0.00
107	15.638	diethylpentamide	-	-	-	-	0.38 ± 0.01	-	-	-
108	15.642	1-(ethenylthio)-butane	-	-	-	-	-	0.34 ± 0.04	-	-
109	15.957	2-furanmethanol, acetate	12.00 ± 0.6	8.49 ± 0.54	5.26 ± 0.00	2.89 ± 0.18	10.7 ± 0.07	9.20 ± 0.14	6.38 ± 0.36	3.38 ± 0.26
110	15.983	2-ethyl-6-methylpyrazine	-	2.01 ± 0.05	1.89 ± 0.07	1.87 ± 0.06	0.88 ± 0.03	2.57 ± 0.03	1.67 ± 0.06	1.58 ± 0.04
111	16.120	2-ethyl-3-methyl-pyrazine	-	-	0.99 ± 0.05	1.05 ± 0.03	-	-	-	0.73 ± 0.09
112	16.214	2-ethyl-5-methylpyrazine	-	1.30 ± 0.03	0.80 ± 0.10	1.01 ± 0.06	-	-	1.48 ± 0.09	0.81 ± 0.02
113	16.228	2,6-dimethyl-3-pyridinamine	1.44 ± 0.07	-	-	-	1.21 ± 0.08	-	-	-
114	16.356	1-methyl-1H-pyrrole-2-carboxaldehyde	0.67 ± 0.04	0.81 ± 0.03	0.81 ± 0.01	0.72 ± 0.07	0.8 ± 0.04	0.89 ± 0.02	0.93 ± 0.05	0.79 ± 0.06
115	16.443	bicyclo[3.2.1]oct-2-ene, 3-(1,1-dimethyl	-	-	-	0.15 ± 0.02	-	-	-	-
116	16.448	4-methyl-2-propyl-furan	-	-	0.17 ± 0.02	-	-	-	-	-
117	16.499	1-(2-furanyl)-1-propanone	0.16 ± 0.00	0.18 ± 0.02	-	-	0.20 ± 0.00	0.22 ± 0.01	0.19 ± 0.01	0.16 ± 0.00
118	16.572	2-(n-propyl)-pyrazine	0.11 ± 0.01	0.11 ± 0.02	0.11 ± 0.03	-	0.09 ± 0.01	-	-	-
119	16.842	2,2-dimethyl-propyl 2,2-dimethyl-propane	0.14 ± 0.04	-	-	0.05 ± 0.00	0.14 ± 0.00	0.14 ± 0.01	-	-
120	16.962	2-ethenyl-6-methyl-pyrazine	-	0.18 ± 0.02	0.17 ± 0.02	-	-	-	0.18 ± 0.06	-
121	16.984	1-methyl-1H-pyrrole-2-acetonitrile	0.25 ± 0.01	-	-	0.16 ± 0.01	0.34 ± 0.1	0.28 ± 0.02	-	-
122	17.157	pyrazinamide	0.73 ± 0.13	0.61 ± 0.05	0.61 ± 0.02	0.64 ± 0.05	0.73 ± 0.03	0.8 ± 0.01	0.58 ± 0.03	0.47 ± 0.01
123	17.240	acetylpyrazine	-	0.15 ± 0.01	0.16 ± 0.01	-	-	-	0.15 ± 0.06	0.15 ± 0.01
124	17.323	2-hydroxy-3-methyl-2-cyclopenten-1-one	-	-	-	0.14 ± 0.02	-	-	-	-
125	17.376	2-azido-2,4,4,6,6-pentamethylheptane	-	-	-	0.22 ± 0.06	-	-	0.18 ± 0.05	0.15 ± 0.01
126	17.378	7-oxabicyclo[4.1.0]heptan-2-one	-	-	-	-	-	-	-	0.31 ± 0.00
127	17.388	7,8-dioxabicyclo[3.2.1]oct-2-ene	-	0.33 ± 0.04	-	-	-	-	-	-
128	17.436	methylphosphonic acid, fluoroanhydride,	0.4 ± 0.01	-	-	-	0.51 ± 0.01	0.49 ± 0.02	-	-
129	17.507	D-limonene	-	0.09 ± 0.01	0.11 ± 0.02	0.14 ± 0.05	0.45 ± 0.04	0.45 ± 0.02	0.73 ± 0.18	0.51 ± 0.03
130	17.644	1-fluoro-dodecane	-	-	-	0.11 ± 0.01	-	-	-	-
131	17.746	1-(2-pyridinyl)-ethanone	-	-	-	0.10 ± 0.02	-	-	-	-
132	17.834	1,2-butadiene	0.37 ± 0.02	0.31 ± 0.03	0.22 ± 0.04	-	0.75 ± 0.00	0.45 ± 0.01	0.31 ± 0.03	0.13 ± 0.00
133	17.897	2,3-dimethyl-2-cyclopenten-1-one	0.31 ± 0.04	0.17 ± 0.01	-	-	-	0.19 ± 0.03	0.12 ± 0.01	-
134	17.966	imidazo[1,2-a]pyridin-2(3H)-one	-	0.06 ± 0.01	-	-	-	-	-	-
135	17.985	3,3'-Bi-1H-pyrazole	-	-	-	-	-	0.11 ± 0.01	-	-
136	18.149	1-cyclobutene-1,2-dicarboxylic acid	-	-	-	-	-	-	0.15 ± 0.06	-
137	18.150	dihydro-3-methylene-2(3H)-furanone	0.08 ± 0.00	-	-	-	0.12 ± 0.01	-	-	-
138	18.154	1-(3,3,3-trifluoro-2-hydroxypropyl)piper	-	-	-	-	-	0.13 ± 0.01	-	-

Continued

S.No.	Retention Time	Compounds	Brazilian coffee beans (Area %)				Ethiopian coffee beans (Area %)			
			11 minutes	12 minutes	13 minutes	14 minutes	11 minutes	12 minutes	13 minutes	14 minutes
139	18.156	2,3-dihydro-6-hydroxy-3-oxo-2-(piperidin	-	-	-	-	-	-	-	0.10 ± 0.01
140	18.241	2-methyl-1,4-benzenediol	-	-	-	-	-	-	-	0.05 ± 0.01
141	18.262	3,5-dihydroxytoluene	-	-	-	-	0.05 ± 0.01	-	-	-
142	18.349	2-butyne	-	-	-	-	0.05 ± 0.01	-	-	-
143	18.397	1-benzyloxy-2,4-difluorobenzene	-	-	-	0.11 ± 0.01	-	-	-	-
144	18.423	benzeneacetaldehyde	-	-	-	-	-	-	-	0.08 ± 0.01
145	18.427	phenylacetaldehyde	-	-	-	-	-	0.09 ± 0.01	-	-
146	18.464	1-(1,2-dimethyl-cyclopent-2-enyl)-ethano	-	0.14 ± 0.01	-	-	-	-	-	-
147	18.498	1-methyl-3-vinyloxy-cyclohexene	-	-	-	-	-	0.26 ± 0.01	-	-
148	18.500	santolina triene	-	-	-	-	0.30 ± 0.05	-	0.24 ± 0.05	-
149	18.509	ocimene	-	-	-	-	-	-	-	0.29 ± 0.1
150	18.606	hexahydroindole	-	-	0.07 ± 0.02	-	-	-	-	-
151	18.753	1-pentyl-1H-pyrrole	-	-	-	-	0.09 ± 0.08	-	-	-
152	18.789	aziridine, 2-methyl-2-(2,2,4,4-tetrameth	-	-	-	0.11 ± 0.12	0.1 ± 0.09	0.1 ± 0.03	-	0.14 ± 0.01
153	18.879	2,4-dimethyl-1,3-cyclopentanedione	0.44 ± 0.21	-	0.16 ± 0.09	-	0.34 ± 0.00	0.3 ± 0.01	0.23 ± 0.07	-
154	19.010	3-methyl-phenol	-	-	-	-	0.33 ± 0.06	-	-	-
155	19.160	2,3,4-trimethyl-2-cyclopenten-1-one	-	-	-	-	0.09 ± 0.01	0.07 ± 0.00	-	-
156	19.186	isocyanato-methane	-	-	0.85 ± 0.02	-	1.22 ± 0.18	-	0.25 ± 0.03	4.19 ± 0.01
157	19.228	sulfurous acid, butyl isobutyl ester	-	-	-	-	-	0.23 ± 0.03	-	-
158	19.433	1H-pyrrole-2-carboxaldehyde	-	-	0.37 ± 0.11	0.31 ± 0.11	-	-	-	-
159	19.457	4-pyridinol	-	-	-	-	-	-	0.18 ± 0.05	0.25 ± 0.09
160	19.586	1-(1H-pyrrol-2-yl)-ethanone	0.32 ± 0.01	0.19 ± 0.02	-	-	0.28 ± 0.01	0.24 ± 0.01	-	-
161	19.729	5-ethenyltetrahydro-2-furanmethanol	-	0.14 ± 0.01	-	0.15 ± 0.03	-	-	-	-
162	19.760	α-methyl-α-4-methyl-3-pente	-	-	-	-	0.36 ± 0.02	0.41 ± 0.01	0.37 ± 0.03	0.38 ± 0.02
163	19.941	1-(1-methyl-1H-pyrrol-2-yl)-ethanone	0.41 ± 0.00	0.33 ± 0.01	0.21 ± 0.03	0.15 ± 0.02	0.42 ± 0.02	0.41 ± 0.01	0.20 ± 0.02	0.24 ± 0.16
164	20.059	3-ethyl-2,5-dimethyl-pyrazine	0.55 ± 0.04	0.68 ± 0.01	0.67 ± 0.03	0.85 ± 0.19	-	-	0.52 ± 0.02	0.55 ± 0.11
165	20.071	2,6-diethyl-pyrazine	-	-	-	-	0.43 ± 0.00	0.49 ± 0.01	-	-
166	20.290	2,2'-methylenebis-furan	0.41 ± 0.03	0.24 ± 0.01	0.13 ± 0.03	-	0.48 ± 0.02	0.38 ± 0.01	0.19 ± 0.01	0.11 ± 0.01
167	20.367	2-ethyl-3,5-dimethyl-pyrazine	-	0.15 ± 0.03	0.12 ± 0.01	0.13 ± 0.02	0.19 ± 0.08	0.10 ± 0.01	-	0.32 ± 0.28
168	20.491	2,5-dipropionylpyrazine	-	-	-	0.33 ± 0.01	-	-	-	-
169	20.514	3,5-dimethyl-4-allylpyrazole	-	-	-	-	-	-	-	0.35 ± 0.05
170	20.545	2-methoxy-phenol	0.53 ± 0.01	0.40 ± 0.00	-	-	-	-	0.40 ± 0.03	-
171	20.564	1-chlorosulfonyl-3-methyl-1-azaspiro[3.5	-	-	0.29 ± 0.06	0.14 ± 0.00	1.11 ± 0.08	-	-	-
172	20.592	furfuryl propionate	0.42 ± 0.02	0.32 ± 0.01	0.25 ± 0.06	-	0.13 ± 0.05	0.49 ± 0.01	-	-

Continued

S.No.	Retention Time	Compounds	Brazilian coffee beans (Area %)				Ethiopian coffee beans (Area %)			
			11 minutes	12 minutes	13 minutes	14 minutes	11 minutes	12 minutes	13 minutes	14 minutes
173	20.596	4-methyl-2,7-dioxatricyclo[4.4.0.0(3,8)]	-	-	-	-	-	0.68 ± 0.03	-	-
174	20.599	linalool oxide	-	-	-	-	-	-	0.40 ± 0.04	-
175	20.804	2,5-diethyl-pyrazine	-	-	-	0.08 ± 0.01	-	-	-	-
176	20.845	1-10,10-dimethyl-3,3-dioxo-3-thia-4-aza	-	-	-	-	-	0.11 ± 0.01	-	-
177	20.854	2,4,4,6,6,8,8-Heptamethyl-2-nonene	-	-	-	-	0.12 ± 0.01	-	-	-
178	20.995	3-cyclohex-3-enyl-propionic acid	-	-	-	0.15 ± 0.03	-	-	-	-
179	20.999	dimethyl(chloromethyl)silyloxycyclohexan	-	-	0.22 ± 0.01	-	-	-	0.20 ± 0.02	-
180	21.003	9-thiabicyclo[3.3.1]non-2-en-6-amine, 9,	-	-	-	-	-	0.14 ± 0.01	-	-
181	21.029	2,2,4,10,12,12-hexamethyl-7-tridecane	-	-	-	-	0.35 ± 0.20	-	-	0.18 ± 0.02
182	21.107	methyl 11,12-tetradecadienoate	-	0.26 ± 0.06	0.19 ± 0.01	-	-	-	-	-
183	21.117	1-Methyl-3,4-dihydropyrrolo[1,2-a]pyrazine	-	-	-	0.04 ± 0.01	-	-	-	-
184	21.120	6-[(3,5-dinitrosalicylidene)amino]benzimidazole	-	-	-	0.12 ± 0.02	-	-	-	-
185	21.133	octahydro-1,4-divinyl-pentalene	-	-	-	-	-	-	-	0.12 ± 0.01
186	21.134	1-(1'-propenyl)-2-hydroxym-cyclopropane	-	-	-	-	-	-	0.23 ± 0.02	-
187	21.139	3-heptyn-1-ol	0.47 ± 0.00	-	-	-	0.37 ± 0.04	0.52 ± 0.01	-	-
188	21.286	2H-imidazole-2-thione, 1,3-dihydro-1-met	-	-	-	0.15 ± 0.01	-	-	-	-
189	21.292	3-pentenoic acid, methyl ester	-	0.15 ± 0.01	-	-	-	-	-	-
190	21.316	3,7-dimethyl-1,6-octadien-3-ol	-	-	-	-	0.17 ± 0.06	0.27 ± 0.01	0.28 ± 0.02	0.31 ± 0.01
191	21.324	methimazole	0.14 ± 0.00	-	-	-	-	-	-	-
192	21.466	N-[2-[[2-pyridylmethyl]amino]ethyl]	0.09 ± 0.01	-	-	-	-	-	-	-
193	21.537	nonanal	-	-	-	0.12 ± 0.04	-	-	-	-
194	21.541	2-nonen-1-ol	-	-	0.15 ± 0.02	-	-	-	-	-
195	21.595	1-methylethenyl-pyrazine	-	0.14 ± 0.01	-	-	-	-	-	0.22 ± 0.11
196	21.715	o-(2-butenylthio)-phenol	-	0.24 ± 0.02	-	-	-	-	-	-
197	21.762	maltol	0.39 ± 0.03	-	0.17 ± 0.02	0.12 ± 0.01	0.49 ± 0.00	0.41 ± 0.02	0.24 ± 0.05	0.19 ± 0.06
198	21.865	cyclopentanepropanoic acid, 2-oxo-, meth	-	-	-	-	-	-	0.19 ± 0.02	-
199	21.870	cyclodecene	0.24 ± 0.01	-	-	0.12 ± 0.01	0.24 ± 0.01	0.27 ± 0.01	-	0.12 ± 0.01
200	21.989	1-(5-methyl-2-pyrazinyl)-1-ethanone	-	-	-	-	-	-	-	0.23 ± 0.04
201	22.081	3-ethyl-2-hydroxy-2-cyclopenten-1-one	0.34 ± 0.26	0.46 ± 0.05	0.18 ± 0.01	0.20 ± 0.03	0.60 ± 0.04	0.63 ± 0.01	0.46 ± 0.07	0.31 ± 0.01
202	22.191	1,3-diazine	0.11 ± 0.00	0.45 ± 0.00	0.43 ± 0.00	0.41 ± 0.00	-	0.12 ± 0.01	-	0.29 ± 0.00
203	22.201	3-oxabicyclo[3.3.0]oct-6-en-2-one, 4-met	-	-	-	-	0.12 ± 0.01	-	-	-

Continued

S.No.	Retention Time	Compounds	Brazilian coffee beans (Area %)				Ethiopian coffee beans (Area %)			
			11 minutes	12 minutes	13 minutes	14 minutes	11 minutes	12 minutes	13 minutes	14 minutes
204	22.296	1-(6-methyl-2-pyrazinyl)-1-ethanone	0.16 ± 0.02	0.23 ± 0.01	0.23 ± 0.04	0.35 ± 0.06	0.10 ± 0.01	0.18 ± 0.02	0.22 ± 0.12	
205	22.388	2-ethyl-hexanoic acid	-	0.08 ± 0.03	-	-	-	-	-	-
206	22.645	1-(5-methyl-2-furanyl)-1-propanone	-	0.13 ± 0.01	-	-	-	-	-	-
207	22.668	α-dehydro-elsholtzine	-	-	-	-	-	0.14 ± 0.04	-	-
208	22.684	3-hydroxy-6-methylpyridine	0.06 ± 0.03	-	-	-	0.15 ± 0.01	-	-	-
209	23.033	decamethyl-cyclopentasiloxane	0.13 ± 0.04	0.13 ± 0.02	0.17 ± 0.03	0.32 ± 0.00	0.06 ± 0.01	0.17 ± 0.02	-	0.13 ± 0.01
210	23.224	5H-5-methyl-6,7-dihydrocyclopentapyrazin	0.13 ± 0.01	0.11 ± 0.01	-	-	-	-	-	-
211	23.234	3-methoxy-2-nitrobenzaldehyde	-	-	-	-	0.14 ± 0.01	0.12 ± 0.01	-	-
212	23.792	2,3-diethyl-5-methyl-pyrazine	-	-	0.02 ± 0.01	-	-	-	-	-
213	23.953	3,5-diethyl-2-methyl-pyrazine	0.09 ± 0.01	0.09 ± 0.01	0.07 ± 0.01	-	-	-	-	-
214	24.553	4-[5-(2-furfurylthio)-2-nitromorpholine	-	0.07 ± 0.04	-	-	-	-	-	-
215	24.757	5-methyl-2-(1-methylethyl-cyclohexanone	-	0.05 ± 0.01	-	-	-	-	-	-
216	25.083	2-(2-furanylmethyl)-5-methyl-furan	0.15 ± 0.04	0.12 ± 0.01	-	-	0.21 ± 0.01	0.20 ± 0.01	0.09 ± 0.01	-
217	25.169	1-(2-furanylmethyl)-1H-pyrrole	0.24 ± 0.04	0.25 ± 0.02	0.17 ± 0.02	0.10 ± 0.03	0.31 ± 0.00	0.28 ± 0.03	0.25 ± 0.03	0.17 ± 0.01
218	25.400	5-(4-nitrophenyl)-2-furancarboxyaldehyde	-	-	0.1 ± 0.02	0.12 ± 0.07	0.14 ± 0.01	0.15 ± 0.02	-	0.11 ± 0.01
219	25.430	allo-xanthine	-	-	-	-	-	-	0.16 ± 0.02	-
220	25.554	meta-methoxybenzenethiol	-	0.19 ± 0.02	0.18 ± 0.02	0.17 ± 0.03	-	0.15 ± 0.03	0.17 ± 0.02	-
221	25.569	2-ethyl-3-methoxy-2-cyclopentenone	-	-	-	-	-	-	-	0.16 ± 0.01
222	25.572	5a-methoxy-9a-methyl-3,4,5a,6,7,8,9a,10-methyl	-	-	-	-	0.15 ± 0.01	-	-	-
223	25.752	4,5-tetradecadienoate	-	0.05 ± 0.01	-	-	-	-	-	-
224	25.760	4-propyl-3-heptene	0.07 ± 0.02	-	-	-	-	-	-	-
225	29.495	nonanoic acid	-	0.1 ± 0.01	0.12 ± 0.08	0.23 ± 0.01	-	-	0.17 ± 0.03	0.12 ± 0.06
226	29.615	4-ethyl-2-methoxy-phenol	0.08 ± 0.02	0.05 ± 0.00	-	-	-	-	-	-
227	30.769	2,2'-[oxybis(methylene)]bis-furan	0.09 ± 0.01	0.05 ± 0.00	-	-	-	0.09 ± 0.00	-	-
228	30.850	dodecamethyl-cyclohexasiloxane	-	0.06 ± 0.01	0.09 ± 0.02	0.13 ± 0.02	-	-	-	-
229	31.309	2-methoxy-4-vinylphenol	0.12 ± 0.01	0.17 ± 0.01	0.16 ± 0.01	0.17 ± 0.03	0.28 ± 0.03	0.19 ± 0.08	0.12 ± 0.01	0.10 ± 0.03
230	35.185	2,6,8-trimethyl-decane	0.11 ± 0.02	-	-	-	-	-	-	-
231	39.396	butylated hydroxytoluene	-	-	-	0.12 ± 0.01	-	-	-	-
232	55.156	n-hexadecanoic acid	-	0.04 ± 0.01	-	-	-	-	-	-
233	58.253	octadecanoic acid	-	0.05 ± 0.01	-	-	-	-	-	-
234	61.550	hexadecamethyl-heptasiloxane	2.51 ± 0.08	-	-	-	-	-	-	-
		Total	93.05 ± 2.69	94.70 ± 3.87	93.08 ± 3.99	97.13 ± 3.89	95 ± 4.25	95.82 ± 3.79	94.83 ± 4.95	97.2 ± 5.49

Area values are mean of three replicate determinations ($n = 3$) ± standard deviation.

respectively) and Ethiopian coffee beans (15.30%–3.69% and 10.70%–3.38%, respectively). On the other hand, the concentration of 5-methyl-2-furancarboxaldehyde was increased when increasing roasting time (2.30%–9.40% in Brazilian beans and 3.80%–11.60% in Ethiopian beans). Moreover, some aromatic components were detected during 11 minutes of roasting time, and these components were not detected with subsequent increments of roasting time. For example, trimethylamine, 1,2,3,6-tetrahydro-1-methyl- pyridine, ethane-1,1-diol dipropanoate, 2,6-dimethyl-3-pyridinamine, 3-heptyn-1-ol, and hexadecamethylheptasiloxane were detected only during 11 minutes of roasting time in Brazilian coffee beans. In the case of Ethiopian coffee beans, diethylpentamide, β -pinene, 4-methylphenylhydrazine, 1,2,3,6-tetrahydro-1-methyl- pyridine, 1-methyl-1H-pyrrole, and vinylfuran were detected only during 11 minutes of roasting time.

Conversely, some aromatic components were detected only during the highest roasting time (14 minutes) for coffee to caramelize. For example, 5-methyl-2-furanmethanol, 2-(1-hydroxy-1-methyl-2-(2H)-furanone, 4-cyclobutyl-4-oxo-2-butynoic acid, 2,2,3-trimethyl-decane, octamethyl-cyclotetrasiloxane, 2-azido-2,4,4,6,6-pentamethylheptane, and butylated hydroxytoluene were detected in Brazilian coffee beans. In contrast, 2-ethyl-3-methoxy-2-cyclopentenone, 1-methylethenyl-pyrazine, 3,5-dimethyl-4-allylpyrazole, ocimene, 7-oxabicyclo[4.1.0]heptan-2-one, trans-2-cyano-1-cyclohexanol, 1-bromo-4-chlorobutane, and 3-methyl-1H-pyrrole were detected in Ethiopian coffee beans. In the case of Colombia Supremo, Ethiopia 210, and Indonesia Mandheling coffee beans, 105 aromatic components were identified (Table 3). The SPME/GC-MS results revealed that Colombia Supremo, Ethiopia 210, and Indonesia Mandheling cultivars registered almost identical aromatic profiles with similar major components. Of 105 aromatic components, 60 were detected in these three coffee cultivars of roasted coffee beans. However, there was a significant variation in the composition of minutes or

components. In particular, 16 components were identified only in Ethiopia 210, and five components in each Colombia Supremo and Indonesia Mandheling.

Similar to Brazilian and Ethiopian roasted coffee beans, 2-furanmethanol was the most abundant component in Colombia Supremo (15.70%), Ethiopia 210 (14.73%), and Indonesia Mandheling (13.65%) coffee beans roasted at 210°C for 13 minutes. In addition, 5-methyl-2-furancarboxaldehyde (10.89%), furfural (9.16%), methylpyrazine (7.55%), 2-furanmethanol, acetate (6.23%), 4-methylphenol (6.08%), and pyridine (4.43%) were major components in the Colombia Supremo cultivar. 5-Methyl-2-furancarboxaldehyde (10.87%), furfural (10.08%), methylpyrazine (8.09%), pyridine (5.50%), 2,4-methylphenol (5.27%), and 2-furanmethanol, acetate (4.77%) were major components in the Ethiopia 210 cultivar. In the case of Indonesia Mandheling cultivar, 5-methyl-2-furancarboxaldehyde, (10.08%), methylpyrazine, (9.12%), 4-methylphenol (7.18%), furfural (6.69%), 2-furanmethanol, acetate (6.40%), pyridine (5.55%), and 2,2,4,4-tetramethylpentane (4.76%) were major components in this cultivar.

DISCUSSION

In the coffee roasting process, the type of roaster, temperature, and roasting time play a crucial role in the taste of brewed coffee (Angeloni *et al.*, 2018). Further, there is a correlation between coffee quality and chemical constituents (Gancarz *et al.*, 2021). The Brazilian and Ethiopian coffee beans were roasted at 210°C for different roasting times, such as 11, 12, 13, and 14 minutes. Further, Colombia Supremo, Ethiopia 210, and Indonesia Mandheling coffee beans were roasted at 210°C for 13 minutes before SPME/GC-MS analysis. The roasting time markedly affected the color parameters of coffee beans. The darker shade of coffee beans is specified by the lower values of lightness (L^*) and higher values of redness

Table 3. Aromatic profile of different coffee cultivars.

S. No.	Retention Time	Compounds	Area (%)		
			Colombia Supremo	Ethiopia 210	Indonesia Mandheling
1	1.718	propionaldehyde	0.06 ± 0.01	0.06 ± 0.02	0.62 ± 0.01
2	2.111	2-amino-1-hexanol	-	0.16 ± 0.02	0.15 ± 0.03
3	2.159	methyl formate	0.85 ± 0.05	0.79 ± 0.22	0.50 ± 0.07
4	2.194	3-methylfuran,	0.70 ± 0.05	0.59 ± 0.15	0.68 ± 0.20
5	2.841	N-tert-butylhydroxylamine	0.62 ± 0.03	0.66 ± 0.08	-
6	3.319	vinyl propionate	3.48 ± 0.03	0.91 ± 0.04	0.78 ± 0.03
7	4.131	1,3-diazine	0.38 ± 0.04	0.44 ± 0.08	0.40 ± 0.02
8	4.205	3-methyl-1H-pyrrole	0.26 ± 0.03	0.28 ± 0.06	0.26 ± 0.05
9	4.600	pyridine	4.43 ± 0.16	5.50 ± 0.52	5.55 ± 0.23
10	5.124	3-pentanone	0.70 ± 0.01	0.79 ± 0.04	0.58 ± 0.12
11	6.136	methyl isocyanate	0.25 ± 0.01	0.22 ± 0.01	0.19 ± 0.13
12	6.292	3,3-dimethyl-butanamide	0.34 ± 0.01	0.42 ± 0.11	0.37 ± 0.06
13	6.378	di-tert-butyl dicarbonate	0.20 ± 0.01	0.24 ± 0.02	0.19 ± 0.04
14	6.610	2,7-dioxabicyclo[4.1.0]heptan-3-one, 5,5	1.09 ± 0.01	1.06 ± 0.18	0.97 ± 0.14
15	7.270	methylpyrazine	7.55 ± 0.32	8.09 ± 0.69	9.12 ± 0.70

Continued

S. No.	Retention Time	Compounds	Area (%)		
			Colombia Supremo	Ethiopia 210	Indonesia Mandheling
16	7.446	N-carbobenzyloxy-L-tyrosyl-L-valine	0.40 ± 0.29	0.19 ± 0.03	0.28 ± 0.03
17	7.763	furfural	9.16 ± 0.40	10.08 ± 0.34	6.69 ± 0.66
18	8.252	3-methyl-pentanoic acid	-	0.32 ± 0.02	-
19	8.670	2,4-dimethylthietane	-	0.14 ± 0.04	0.28 ± 0.03
20	9.022	2-furanmethanol	15.70 ± 0.99	14.73 ± 1.06	13.65 ± 1.22
21	9.263	N-benzyl-2-ethoxy-5-benzenesulfonamide	0.11 ± 0.01	-	-
22	9.566	nadolol	1.50 ± 0.06	1.81 ± 0.20	1.80 ± 0.23
23	10.037	bicyclo[3.1.0]hexan-3-one	-	0.27 ± 0.06	-
24	10.189	2,6-dimethylpyridine	-	0.19 ± 0.04	-
25	10.395	chloroacetylene	-	0.29 ± 0.08	0.11 ± 0.08
26	10.467	propionic anhydride	0.27 ± 0.03	-	-
27	10.872	2-methyl-butanoic acid	-	0.23 ± 0.06	-
28	11.101	2-methyl-2-cyclopenten-1-one	0.12 ± 0.02	-	0.10 ± 0.01
29	11.201	furfuryl formate	1.40 ± 0.04	1.16 ± 0.03	1.17 ± 0.13
30	11.375	2-furyl methyl ketone	1.97 ± 0.01	1.73 ± 0.04	1.65 ± 0.16
31	11.546	4-methylphenol	6.08 ± 0.08	5.27 ± 0.42	7.18 ± 0.58
32	11.713	ethylpyrazine	2.36 ± 0.11	2.38 ± 0.30	3.11 ± 0.14
33	11.823	2,3-dimethylpyrazine	0.81 ± 0.06	0.79 ± 0.14	0.96 ± 0.10
34	12.063	hexahydro-4,7-di-1,3-isobenzofurandione	0.12 ± 0.03	-	-
35	12.326	1-methylcyclohexanol	0.28 ± 0.01	0.26 ± 0.03	0.23 ± 0.02
36	12.492	ethenylpyrazine	-	0.32 ± 0.02	0.28 ± 0.05
37	12.796	diethylmethylborane	0.16 ± 0.03	-	0.13 ± 0.03
38	12.828	4,4-dimethyl-2-pentene	-	0.13 ± 0.03	-
39	13.341	uracil	0.37 ± 0.01	0.36 ± 0.02	0.33 ± 0.04
40	13.605	2-n-butyl furan	0.36 ± 0.05	0.34 ± 0.02	0.34 ± 0.03
41	13.786	3-pentadecen-2-ol	-	0.10 ± 0.02	-
42	13.924	anisole	0.13 ± 0.02	-	0.14 ± 0.02
43	14.173	5-methyl-2-furancarboxaldehyde	10.89 ± 0.09	10.87 ± 0.92	10.08 ± 0.39
44	14.425	1,1-dimethyle-phosphinothioic fluoride	2.20 ± 0.07	-	-
45	14.452	2,2,4,4-tetramethyl-pentane	-	3.88 ± 0.08	4.76 ± 0.22
46	14.479	2-azido-2,4,4,6,6-pentamethylheptane	0.16 ± 0.01	0.19 ± 0.01	0.33 ± 0.10
47	14.913	4-acetyl-heptanenitrile	-	0.30 ± 0.01	-
48	15.192	2,6-dimethyl-2,6-octadiene	-	0.17 ± 0.02	-
49	15.350	carbamic acid, methyl-, phenyl ester	0.10 ± 0.01	0.18 ± 0.02	-
50	15.492	β -myrcene	-	0.61 ± 0.02	-
51	15.524	6-methyl-bicyclo[4.1.0]heptan-2-one	0.24 ± 0.06	-	0.31 ± 0.01
52	15.596	dihydro-2-methyl-3(2H)-thiophenone,	0.17 ± 0.03	0.19 ± 0.03	0.24 ± 0.01
53	15.860	2-furanmethanol, acetate	6.23 ± 0.08	4.77 ± 0.13	6.40 ± 0.48
54	15.971	2-ethyl-6-methyl-pyrazine	1.95 ± 0.01	1.79 ± 0.05	2.41 ± 0.12
55	16.153	2,6-dimethyl-3-pyridinamine	1.06 ± 0.08	-	1.88 ± 0.28
56	16.194	2-ethyl-5-methyl-pyrazine	0.79 ± 0.13	1.48 ± 0.08	1.06 ± 0.17
57	16.293	1-methyl-1H-pyrrole-2-carboxaldehyde	0.76 ± 0.01	0.83 ± 0.01	0.59 ± 0.04
58	16.455	1-(2-furanyl)-1-propanone	0.22 ± 0.03	0.19 ± 0.04	0.14 ± 0.02
59	16.856	5-methylene-1,3a,4,5,6,6a-hexahydropenta	-	0.11 ± 0.02	-
60	16.948	2-ethenyl-6-methyl-pyrazine	0.19 ± 0.03	0.24 ± 0.03	-
61	17.105	pyrazinamide	0.68 ± 0.01	0.67 ± 0.02	0.57 ± 0.04
62	17.227	acetylpyrazine	0.20 ± 0.01	0.23 ± 0.02	0.39 ± 0.08

Continued

S. No.	Retention Time	Compounds	Area (%)		
			Colombia Supremo	Ethiopia 210	Indonesia Mandheling
63	17.368	methylphosphonic acid, fluoroanhydride,	0.44 ± 0.02	-	-
64	17.400	2-propyl-1-pentyl methylphosphonofluorid	-	0.42 ± 0.03	-
65	17.486	limonene	0.16 ± 0.00	0.52 ± 0.02	0.25 ± 0.16
66	17.628	1-methyl-3,2'-spiro-benzo-1-pyrrolidine	-	-	0.14 ± 0.02
67	17.773	1,2-Butadiene	0.24 ± 0.09	0.33 ± 0.01	0.20 ± 0.13
68	17.863	2-Cyclopenten-1-one, 2,3-dimethyl-	0.14 ± 0.02	-	0.12 ± 0.01
69	17.950	2,2'-bifuran	0.13 ± 0.01	0.15 ± 0.01	0.10 ± 0.01
70	18.111	dihydro-3-methylene-2(3H)-furanone	0.11 ± 0.01	0.11 ± 0.01	0.11 ± 0.01
71	18.394	3-benzyloxy-2-fluoro-4-met-benzaldehyde	0.18 ± 0.02	0.13 ± 0.01	0.12 ± 0.01
72	18.457	1-(1,2-dimethyl-cyclopent-2-enyl)-ethano	-	-	0.10 ± 0.01
73	18.480	ocimene	-	0.25 ± 0.01	-
74	18.639	2,2,4,10,12,12-hexamethyl-7-tridecane	0.15 ± 0.01	0.17 ± 0.02	0.19 ± 0.02-
75	18.794	2-ethyl-1,1-dimethyl-cyclopentane	0.22 ± 0.01	0.16 ± 0.01	0.19 ± 0.02
76	18.944	5-ethyl-2-furaldehyde	0.11 ± 0.02	-	0.11 ± 0.01
77	19.275	2,2,5-trimethyl-decane	-	-	0.13 ± 0.11
78	19.439	1H-pyrrole-2-carboxaldehyde	0.25 ± 0.01	0.20 ± 0.05	0.14 ± 0.10
79	19.699	5-ethenyltetrahydro-al-2-furanmethanol,	-	-	0.16 ± 0.06
80	19.718	α -methyl- α -[4-methyl-3-pente	0.19 ± 0.00	0.44 ± 0.01	-
81	19.904	1-(1-methyl-1H-pyrrol-2-yl)-ethanone	0.24 ± 0.01	0.21 ± 0.02	0.32 ± 0.04
82	20.019	3-ethyl-2,5-dimethylpyrazine	0.65 ± 0.01	0.55 ± 0.02	1.26 ± 0.15
83	20.259	furan, 2,2'-methylenebis-	0.22 ± 0.01	0.16 ± 0.02	0.20 ± 0.01
84	20.488	P-methoxyphenol	0.41 ± 0.00	0.48 ± 0.03	0.51 ± 0.01
85	20.543	1-fluoro-dodecane,	-	0.10 ± 0.00	-
86	20.560	furfuryl propionate	0.30 ± 0.00	0.39 ± 0.03	0.31 ± 0.02
87	20.695	3-ethyl-2-hydroxy-2-cyclopenten-1-one	0.44 ± 0.01	0.38 ± 0.02	0.40 ± 0.02
88	20.800	2,5-diethylpyrazine	0.11 ± 0.01	-	0.10 ± 0.01
89	21.020	2-propenylcyclopropanecarboxylic acid	-	0.17 ± 0.01	0.18 ± 0.01
90	21.097	methyl 12,13-tetradecadienoate	0.26 ± 0.01	0.22 ± 0.02	0.25 ± 0.02
91	21.276	methimazole	0.19 ± 0.01	0.34 ± 0.01	0.16 ± 0.01
92	21.552	2-decen-1-ol	0.11 ± 0.05	0.10 ± 0.01	0.13 ± 0.02
93	21.695	maltol	0.20 ± 0.02	0.21 ± 0.03	0.20 ± 0.01
94	21.831	cyclodecene	0.23 ± 0.01	0.18 ± 0.02	0.21 ± 0.01
95	21.957	1-(5-methyl-2-pyrazinyl)-1-ethanone	-	-	0.10 ± 0.02
96	22.158	3-oxabicyclo[3.3.0]oct-6-en-2-one, 4-met	-	0.10 ± 0.02	-
97	22.253	2-ethyl-hexanoic acid	-	0.12 ± 0.01	-
98	22.258	1-(6-methyl-2-pyrazinyl)-1-ethanone	0.23 ± 0.03	0.25 ± 0.08	0.25 ± 0.05
99	22.640	1,5,5,6-tetramethyl-1,3-cyclohexadiene	-	0.11 ± 0.04	-
100	23.033	decamethyl-cyclopentasiloxane	0.12 ± 0.01		0.20 ± 0.08
101	25.137	1-(2-furanylmethyl)-1H-pyrrole,	0.25 ± 0.00	0.23 ± 0.01	0.29 ± 0.03
102	25.390	1-propanone, 1-(5-methyl-2-furanyl)-	0.17 ± 0.00	0.16 ± 0.01	0.17 ± 0.01
103	25.537	meta-methoxybenzenethiol	0.21 ± 0.01	0.20 ± 0.01	0.23 ± 0.01
104	29.398	nonanoic acid	0.14 ± 0.11	0.20 ± 0.03	0.14 ± 0.10
105	31.278	2-methoxy-4-vinylphenol	0.17 ± 0.01	0.13 ± 0.01	0.16 ± 0.10
		Total	94.81 ± 0.25	95.85 ± 0.58	95.76 ± 0.52

Area values are mean of three replicate determinations ($n = 3$) ± standard deviation.

(a*) and yellowness (b*) (Kulapichitr *et al.*, 2022). A DVB/Carboxen/PDMS SPME fiber was used to extract volatile components from roasted coffee beans. In previous studies, this type of SPME fiber was reported to be the most efficient one for analyzing coffee bean aroma (Risticvic *et al.*, 2008; Caporaso *et al.*, 2018).

Previous studies stated that the roasting temperature (160°C–200°C) and roasting time (4–12 minutes) play a major role in preparing specialty coffee (Fassio *et al.*, 2017; Tolessa *et al.*, 2016; Tugnolo *et al.*, 2019). Different coffee flavors are developed during roasting by nonenzymatic browning reactions, including the Maillard reaction and caramelization (Münchow *et al.*, 2020). There was a highly positive correlation among pyrazine compounds due to the Maillard reaction during the roasting process. Amino acids and reducing sugars were important flavor precursors in the Maillard reaction (Caporaso *et al.*, 2018). In the roasting process, 2,3-butanedione has been exhibited to be stable at high temperatures. Baggenstoss *et al.* (2008) reported that concentrations of 2,3-butanedione and pentanedione were found to be higher during fast roasts when compared to slower roasts. It is understood that the time-temperature relationship of the roasting process highly influences the aromatic profiles of coffee. Further, regulation of roasting time and temperature is required to obtain a distinctive flavor profile.

Previously, Caporaso *et al.* (2018) determined the volatile composition of different batches of roasted coffees of Arabica and Robusta using SPME/GC-MS. In their study, Arabica and Robusta species (25 batches) were collected from 13 countries. The coffee beans were roasted at 210°C for 3 minutes. A significant variation of 50 volatile components was observed in roasted coffee within batches. The authors found that 2-furanmethanol, acetic acid, and 2-methyl pyrazine were the major components. Further, 2-furanmethanol acetic acid was highly distributed in Arabica coffee beans compared to Robusta coffee beans. Therefore, Brazilian coffee, Ethiopian coffee, Colombia Supremo, Ethiopia 210, and Indonesia Mandheling cultivars may be derived from Arabica species because 2-furanmethanol was the most abundant component in these cultivars. Zou *et al.* (2022) compared the volatile composition of regular and decaffeinated coffee by HS-SPME-GC × GC-ToFMS, and the authors found that the regular coffee chiefly contained pyrazine-derived components, whereas the decaffeinated coffee contained mainly furan-derived components.

A recent study identified 390 aromatic components from 17 chemical families in a single-dose espresso capsule obtained from eight commercial coffee samples. In these, 100 components were detected for the first time in roasted coffee or brews (Lopes *et al.*, 2021). The detected chemical components in the study were also identified in various coffee beans (Akiyama *et al.*, 2008; Mahmud *et al.*, 2020; Toledo *et al.*, 2016). Chemical families such as acids, alcohols, aldehydes, and esters are generally linked with the production of industrial coffee during fermentation (Ruta and Farcasanu, 2021). Furans, ketones, pyrazines, pyridines, and pyrroles are mainly associated with roasting processes. In addition, green coffee beans contain certain types of terpene components (Akiyama *et al.*, 2008; Gonzalez-Rios *et al.*, 2007). These volatile components of coffee are mainly responsible for its final flavor and aroma.

Previous studies reported that the time-temperature profile of the roasting process showed a significant effect on coffee's aromatic composition (Baggenstoss *et al.*, 2008; Franca *et al.*, 2009). In this study, the coffee beans were roasted at 210°C for 11–14 minutes. The roasting of coffee beans highly influences the flavor and aroma of coffee. In addition, the roasting time of coffee beans significantly affects the aromatic profile of coffee cultivars. The flavor and aroma of coffee beans mainly depend on the roasting time and temperature (Kreuml *et al.*, 2013). In particular, the acid types of components in coffee beans were degraded during roasting, thereby forming caffeic acid, lactones, and various phenolic components via the Maillard and Strecker reactions. These chemical changes lead to the development of bitterness, astringency, and aroma of coffee (Pereira *et al.*, 2021).

It is well known that the quality of coffee is determined based on criteria, including size, color, and shape of beans, cupping, and number of defects. In general, roasted beans are susceptible to various physicochemical changes that may significantly influence the sensory characteristics of coffee beverages. Flavor and fragrance play a key role in the sensory analyses of coffee. Ribeiro *et al.* (2009) investigated the correlation between aromatic components from Brazilian Arabica roasted coffees and sensory properties. The authors found that 3-methylpropanal, 2-methylfuran, furfural, furfuryl formate, 2-furanmethanol acetate, and other components were possible markers for the overall quality of the coffee. The aroma components, including pyrroles, pyridines, and pyrazines, are responsible for the aroma characteristics of coffee, such as nutty, roasted, and toasted notes. In these, pyridines and related compounds are associated with the bitterness of coffee (Seninde and Chambers, 2020). Zakidou *et al.* (2021) reported that 2-furanmethanol, acetate exhibited a fruity and sweet aroma and fruity flavor in coffee beans. According to the sensory quality of coffee, the Robusta variety (*Coffea canephora*) has woody and earthy flavors, whereas the Arabica variety (*Coffea arabica*) has fine acidity, better flavor, and more intense aroma (Dippong *et al.*, 2022; Kreuml *et al.*, 2013).

Previous studies found that Arabica varieties possess better sensory characteristics than the Robusta varieties (Olechno *et al.*, 2021; Tugnolo *et al.*, 2019). However, the detection of sensory properties of roasted coffee beans is more complicated due to the initial contents of aromatic precursors in the green beans (Caporaso *et al.*, 2018). It was reported that aromatic components with low odor thresholds significantly affected the coffee flavor. Further, some components, even at very low concentrations, highly influence the sensory properties of roasted coffee (Dong *et al.*, 2019). Bhumiratana *et al.* (2011) reported that light roasting of coffee beans results in less sour and sweeter flavor than that of medium or dark roasted ones (typical characteristics of coffee). Therefore, sensory differences are possibly due to changes in the concentrations of aromatic constituents during excessive roasting. The qualitative and quantitative changes in the aromatic constituents are the main determinants of coffee cup quality.

CONCLUSION

The data of the present study suggest that the roasting time significantly affected the color parameters and aromatic compositions of coffee beans. The results revealed that 2-furanmethanol was a predominant component in all

the roasted coffee beans of Colombia Supremo, Ethiopia 210, and Indonesia Mandheling. Further, 5-methyl-2-furancarboxaldehyde, 2-furanmethanol acetate, methylpyrazine, pyridine, 4-methylphenol, and ethylpyrazine were important components. The variations in the chemical composition of the studied cultivars may be due to the geographical region of the coffee cultivation and chemical reactions during the roasting process. These identified aromatic components, according to different roasting times, can be significant markers for predicting the aromatic quality of particular cultivars. Further studies are warranted about the influence of geographical origin and different roasting temperatures on the aromatic profile of coffee bean cultivars.

AUTHOR CONTRIBUTIONS

All authors made substantial contributions to conception and design, acquisition of data, or analysis and interpretation of data; took part in drafting the article or revising it critically for important intellectual content; agreed to submit to the current journal; gave final approval of the version to be published; and agree to be accountable for all aspects of the work. All the authors are eligible to be an author as per the international committee of medical journal editors (ICMJE) requirements/guidelines.

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