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VOLATILE COMPOUNDS OF *COFFEA ARABICA* L. GREEN AND ROASTED BEANS *

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ABSTRACT

Volatile compounds of green and roasted beans of *Coffea arabica* L. (Rubiaceae) were investigated by this study. Volatile compounds were trapped with Headspace Solid-Phase Microextraction (HS-SPME) technique and analyzed by Gas Chromatography-Mass Spectrometry (GC/MS). The main components of the green coffee were identified as isoamylalcohol (10.4%), hexanal (10.4%) and hexacosane (8.2%) while furfurylalcohol (13.6%), furfurylacetate (10.7%) and 5-methyl furfural (9.27%) were identified as the main components of the roasted coffee. In conclusion, using HP-SPME-GC-MS, it was possible to quantify different volatile compouns like as alcohols, aldehydes, ketones, pyrazines, pyridines, and furans in green and roasted coffee beans which belong to different chemical classes.

Keywords: *Coffea arabica* L., Green coffee, Roasted coffee, Volatile compounds

COFFEA ARABICA L.'NIN YEŞİL VE KAVRULMUŞ ÇEKİRDEKLERİNİN UÇUCU BİLEŞENLERİ

ÖZET

Bu çalışmada *Coffea arabica* L. (Rubiaceae)'nın yeşil ve kavrulmuş çekirdeklerinin uçucu bileşikleri incelenmiştir. Uçucu bileşenler, Headspace Katı Faz Mikroekstraksiyon (HS-SPME) tekniği ile elde edilmiş ve Gaz Kromatografisi-Kütle Spektrometresi (GC/MS) ile analiz edilmiştir. Yeşil kahve çekirdeklerinin ana bileşenleri izoamilalkol (% 10.4), hekzanal (% 10.4) ve hekzakosan (% 8.2) iken, kavrulmuş çekirdeklerin ana bileşenleri förfurilalkol (% 13.6), förfurilasetat (% 10.7) ve 5-metil förfural (% 9.27) olarak belirlenmiştir. Sonuç olarak, HS-SPME-GC-MS kullanılarak yeşil ve kavrulmuş kahve çekirdeklerinde alkol, aldehit, keton, pirazin, piridin ve furan gibi değişik kimyasal gruplara ait farklı uçucu bileşenlerin belirlenmesi mümkün olmuştur." şeklinde olmalıdır.

Anahtar Kelimeler: *Coffea arabica* L., Yeşil kahve, Kavrulmuş kahve, Uçucu bileşikler

1. INTRODUCTION

Coffee is one of the most popular beverages around the world, constituting a significant portion of daily beverage intake in many Western countries. With the advancement of the research on antioxidants and health, coffee has been recognized as a rich source of dietary antioxidants with potential to improve health [1]. Green coffee beans are a major source of chlorogenic acid in nature and consumption of them produced antihypertensive effect, improvement in human vasoreactivity, inhibitory effect on fat accumulation and body weight in mice and humans [2]. The roasting process of green coffee beans reduces amounts of some chlorogenic acid isomers [3, 4]. The basic chemical composition of green coffee depends primarily on genetic aspects, especially species, and on physiologic aspects such as degree of maturation. The poor volatile fraction of unroasted coffee seeds gives them a weak but characteristic aroma. Approximately 100 different volatile compounds have been identified in green coffee seeds. The variety and concentrations of volatile compounds in roasted coffee depend on the composition of nonvolatile compounds in the raw seeds and on roasting conditions. Therefore, the factors such as genetics, soil,

agricultural practices, climate, and degree of maturation influence the final composition of the volatile fraction of roasted coffee. More than 950 compounds have been identified after roasting in different types of coffee, depending on their origin, degree of roasting, and analytical methods used [5].

Determination of the HS-SPME volatile profile of the green and roasted beans of *Coffea arabica* L. obtained commercially was aimed in this study.

2. MATERIAL and METHODS

Coffea arabica L. (Rubiaceae) green and roasted beans were obtained from a local market in Eskişehir, Turkey in 2014 (Temiz-İş Kurukahveci, Eskişehir).

2.1. Headspace-SPME

The manual SPME device (Supelco, Bellafonte, PA, USA) with a fiber precoated of a 65 μm thick layer of polydimethylsiloxane/divinylbenzene (PDMS/DVB-blue) was used for extraction of the volatiles. The vial containing the sample was sealed with parafilm. The fiber was pushed through the film layer for exposure to the headspace of the coffee beans for 15 min at 50°C. The fiber was then inserted immediately into the injection port of the GC/MS for desorption of the adsorbed volatile compounds for analysis.

2.2. GC/MS Analysis

The GC/MS analysis was carried out with an Agilent 5975 GC-MSD system. Innowax FSC column (60 m x 0.25 mm, 0.25 mm film thickness) was used with helium as carrier gas (0.8 mL/min). GC oven temperature was kept at 60°C for 10 min and programmed to 220°C at a rate of 4°C/min, and kept constant at 220°C for 10 min and then programmed to 240°C at a rate of 1°C/min. The injector temperature was set at 250°C. Mass spectra were recorded at 70 eV. Mass range was from *m/z* 35 to 450. Identification of the volatile components were carried out by comparison of their relative retention times with those of authentic samples or by comparison of their relative retention index (RRI) to series of *n*-alkanes. Computer matching against commercial (Wiley GC/MS Library, MassFinder3 Library) [6, 7] and in-house "Başer Library of Essential Oil Constituents" built up by genuine compounds and components of known oils, as well as MS literature data [8, 9], was used for the identification.

3. RESULTS

The chromatogram of the green/roasted coffee beans is represented in Figure 1. This study aimed the determination of the HS-SPME volatile profile of green and roasted beans of *Coffea arabica* L. The main components for green coffee were identified as hexanal (10.4%), isoamylalcohol (10.4%) and hexacosane (8.2%), while furfurylalcohol (13.6%), furfurylacetate (10.7%) and 5-methyl furfural (9.3%) were identified as the main components of the roasted coffee (Table 1).
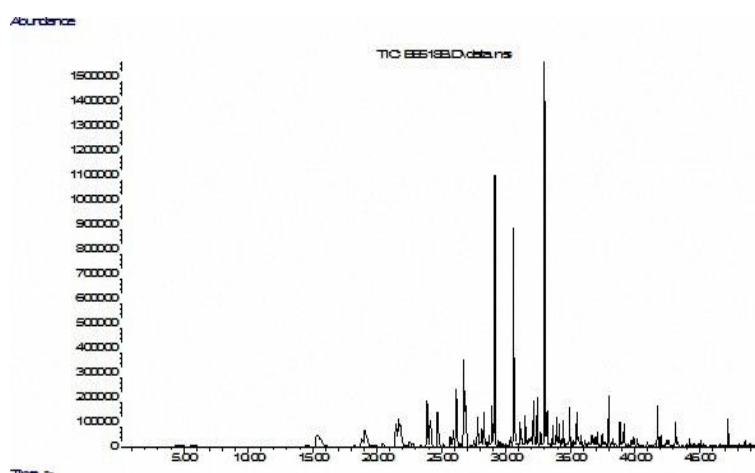
Figure 1. The HS-SPME chromatogram of roasted coffee beans.

Table 1. Volatile compounds of green coffee beans and roasted coffee beans obtained by HS-SPME-GC-MS.

Peak No	RRI*	Volatile Compounds	Green Coffee Beans (%)	Roasted Coffee Beans (%)
1	1093	Hexanal	10.4	-
2	1187	Pyridine	-	3.1
3	1213	Isoamylalcohol	10.4	-
4	1259	1-Pentanol	2.3	-
5	1274	Methylpyrazine	-	2.1
6	1280	*p*-Cymene	1.3	-
7	1322	2-Heptanol	3.6	-
8	1332	2,5-Dimethylpyrazine	-	1.8
9	1335	(E)-2-Heptenal	1.2	-
10	1337	2,6-Dimethylpyrazine	-	2.1
11	1343	2-Ethylpyrazine	-	1.6
12	1360	1-Hexanol	2.8	-
13	1391	2-Ethyl-6-methylpyrazine	-	3.4
14	1395	2-Ethyl-5-methylpyrazine	-	2.3
15	1400	Nonanal	1.5	-
16	1409	Trimethylpyrazine	-	2.8
17	1450	*trans*-Linalool oxide (Furanoid)	-	1.0
18	1452	1-Octen-3 ol	4.1	-
19	1452	2-Ethyl-3,5-dimethylpyrazine	-	3.7
20	1454	1-Acetoxy-2-propanone	-	3.8
21	1479	Furfural	-	2.8
22	1506	Furfurylformate	-	1.6
23	1516	2-Acetyl furan	-	1.6
24	1541	Benzaldehyde	3.8	-
25	1547	Furfuryl acetate	-	10.7
26	1553	Linalool	3.0	-
27	1586	5-Methylfurfural	-	9.3
28	1638	2-Formyl-N-methylpyrrole	-	1.8
29	1648	γ-Butyrolactone	0.9	2.0
30	1671	Furfurylalcohol	-	13.6
31	1684	Isovaleric acid	-	1.4
32	1845	*N*-Furfurylpyrrole	-	1.8
33	1896	Benzylalcohol	0.9	-
34	1937	Phenylethylalcohol	3.2	-
35	1996	2-Acetylpyrrole	-	1.6
36	2218	4-Vinylguaiacol	-	0.9
37	2300	Tricosane	2.5	-
38	2400	Tetracosane	5.0	-
39	2500	Pentacosane	7.6	-
40	2600	Hexacosane	8.2	-
41	2700	Heptacosane	7.6	-
42	2800	Octacosane	6.8	-
43	2900	Nonacosane	6.3	-
		TOTAL	**93.4**	**76.8**

*RRI: Relative retention indices calculated against *n*-alkane % calculated from TIC (Total Ion Chromatogram) data.

4. DISCUSSION

It was reported in IARC Monograph the most abundant volatile compounds are alcohols, esters, hydrocarbons and aldehydes in green coffee beans. Ketones, pyrazines, furans and sulfur compounds have also been identified [10]. The maturation stage of the coffee fruits is important for the volatile composition of green coffee. The poor volatile fraction of unroasted coffee seeds gives them a weak but characteristic aroma. Approximately 100 different volatile compounds have been identified in green coffee [5]. In raw coffee, some 200 volatiles have been identified. Some raw coffee volatiles (geosmin, 2,4,6-trichloroanisol/-phenol, 4-heptenal etc.) were identified as characteristic for defects, which are externally caused, maybe by over-fermentation during processing or by insect attacks or immaturity of beans [11]. In another research, the major volatile compounds in green beans were determined as aldehydes (hexanal and benzaldehyde) and alkanes (tetradecane and cyclopentasiloxane, decamethyl-, cyclohexane, 1-methyl-4-(1-methylethenyl)-, *cis-* and cyclotetrasiloxane, octamethyl-), whereas the major volatile compounds in roasted beans were determined furans, pyrazines, and pyridines [12]. Along with green coffee beans HS-SPME results, (E)-2-heptenal and some alkanes (tricosane, tetracosane etc.) were identified.

The variety and concentrations of volatile compounds in roasted coffee depend on the composition of non-volatile compounds in the raw seeds and on roasting conditions. Therefore, the factors such as genetics, soil, agricultural practices, climate, and degree of maturation influence the final composition of the volatile fraction of roasted coffee. More than 950 compounds have been identified after roasting in different types of coffee, depending on their origin, degree of roasting, and analytical methods used. The classes of volatile compounds typically found in roasted coffee are furans and pyrans, pyrazines, pyrroles, ketones and phenols, hydrocarbons, alcohols, aldehydes, acids and anhydrides, esters, lactones, thiophenes, oxazoles, thiazoles, pyridines, amines, and various sulfur and nitrogen compounds. The formation of volatile compounds depends on the stability of their precursors and location within the seed. In addition, different volatile profiles have been observed in coffee samples roasted under different conditions to achieve the same roasting degree. Compounds that may be affected by roasting conditions include pyridine, 2-methylpyrazin, furfural, furfuryl formate, 2-furanomethanol acetate, 5-methyl-furancarbaldehyde, 1-(2-furanylmethyl)-1H-pyrrol, 1-(1H-pyrrol-2-yl)-ethanone, 2-methoxyphenol, and 4-ethyl-2-metoxyphenol. Roasted coffee beans contain odorants as 3-isobutyl-2-methoxypyrazine, 2-methoxy-3-isopropylpyrazine, 2-methoxy-3,5-dimethylpyrazine, 4-vinylguaiacol nearly same concentration or much more than green coffee beans (Oestreich-Janzen 2010). Depend on HS-SPME results of roasted coffee beans, there were determined 2-ethyl-5-methylpyrazine, 2-ethyl-6-methylpyrazine, 2,5-dimethylpyrazine, 2,6-dimethylpyrazine, and 4-vinylguaiacol.

5. CONCLUSION

Using HS-SPME-GC-MS, it was able to quantify different volatile compounds as alcohols, aldehydes, ketones, pyrazines, pyridines, and furans in green and roasted coffee beans belonging to different chemical classes but specific for green or roasted coffee beans obtained commercially. The major volatile contents showed that the percentages of hexanal, *p*-cymene, (E)-2-heptenal, nonanal, benzaldehyde, linalool and alcohols (isoamylalcohol, 1-pentanol, 2-heptanol etc.) and tri- to nonacosanes in green coffee beans, whereas those of pyridine, methylpyrazine and dimethylpyrazine derivatives, trimethylpyrazine, 1-acetoxy-2-propanone, furfuryl and pyrrole derivatives, alcohols (benzylalcohol, phenylethylalcohol) and isovaleric acid were in roasted beans.

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