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Identification of Headspace Volatile Compounds of Blended Coffee and Application to Principal Component Analysis

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ABSTRACT: Coffee can be blended to create a variety of products to meet consumer's needs. In order to uncover the blending effect of coffee beans, we performed an experiment using principal component analysis (PCA). Twelve varieties of green beans were tested in 11 experimental groups, and the volatile compounds of the beans were analyzed. A total of 41 volatile compounds were identified. PCA was performed on 13 compounds that had a low odor threshold value or a high concentration among the identified compounds. PCA of total volatile compounds showed that principal component (PC) 1 and PC2 were extracted within 80% cumulative dispersion level. In PC1 and PC2, furfuryl alcohol and formic acid ethyl ester showed the greatest positive correlation coefficients among all the volatile compounds. The largest negative correlation coefficients in PC1 and PC2 were 4-hydroxy-2-butanone and 3-(ethylthio)propanal, respectively. Using PCA of the major volatile compounds in coffee, propanal and 1-methylpyrrole were found to have the largest positive correlation coefficients in PC1 and PC2, respectively. In the score plot of the major volatile components, 4 kinds of blended coffee were closely grouped, therefore showing similar aroma qualities. However, 5 kinds of other blended coffees showed a positive correlation with PC2. This is probably due to 3-(ethylthio)propanal acting as a specific value. The application of statistical methods to blended coffee allows for logical and systematic data analysis of data and may be used as a basis for quality evaluation.

Keywords: blended coffee, espresso, volatile compounds, dynamic headspace analysis, principal component analysis

INTRODUCTION

Coffee is the most consumed beverage every year per capita in Korea. Coffee therefore has a big impact on the domestic beverage industry. Many large, medium, and small coffee shops allow people to enjoy the culture and sensitivity of coffee. In 2017, domestic coffee consumption per capita was determined to be growing at a rate of 400 cups per year. The size of the coffee sales market has surpassed 6 trillion won, indicative of rapid growth (Joung, 2019). However, the domestic coffee market, which has been dominated by large franchise-oriented cafés for the past 10 years, has started to show a preference for cafés that offer high-quality coffee rather than those low-priced and of uniform quality (Kim, 2017). The main taste components of coffee are sourness and bitterness. The sour taste is the first taste that is recognized when the bean is extracted. The following taste is bitterness. These coffee flavors depend on the time taken to extract the blended beans using an espresso machine (Shin et al., 2011). Volatile compounds are involved in various and complex flavors of coffee flavor components, and many studies have been conducted on them. However, little research has been carried out on the volatile compounds of blended coffee (BC) using principal component analysis (PCA).

Coffee blending is the process of mixing different beans before and after roasting to produce a desirable taste and aroma. Mixing two or more types of coffee beans creates a coffee with a new flavor. This reinforces the mixing effect of certain kinds of green beans with other species to create a more harmonious taste and aroma. In coffee processing, roasting time and temperature influence the composition of aroma compounds in the roasted bean. The major chemical reactions in the roasting process are Maillard reactions of non-enzymatic browning, Strecker degradations, and other reactions (Baggensloss et al., 2008; Buffo et al., 2004).

Volatile compounds are important for coffee quality

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through contributing to the coffee quality. More than 800 volatile compounds are present in coffee, which affect the taste and aroma according to the origin and variety of the beans, the modalities and the degree of roasting (Yang, 2016). The volatile compounds of coffee are composed of hydrocarbon, pyrazines, furans, phenols, alcohol, aldehyde, ketones, esters, carboxylic acids, and others. Of these, the sulfur-containing compounds, furans, and pyrazines are most abundant and have a major influence on the coffee aroma (Cecilia et al., 2012). Gonzalez-Rios et al. (2007) reported that ketones, pyrazines, pyridine, and pyrrole make up of the main chemicals in Arabica coffee. Rocha et al. (2004) determined that espresso coffee majorly contains furans, followed by pyrazines, aldehydes, and pyridines.

PCA was proposed by Pearson (1901), and transforms high dimensional data into low dimensional data, allowing data to be grouped and trends to be determined. PCA is mostly used to create tools or predictive models of exploratory data analysis, after standardizing the data matrix for each attribute. When converted from data to one axis, except for non-significant properties, distribution is the first main component. The data is then converted linearly onto the new coordinates so that the second largest axis is placed as the second main component. Petisca et al. (2013) performed PCA of volatile compounds according to the roasting speed of three kinds of beans in espresso coffee. Maeztu et al. (2001) classified volatile compounds and fractions in espresso coffee by PCA analysis. The objectives of the present study are to identify the headspace volatile compounds from 11 kinds of BC bean, to investigate the major aroma compounds among the headspace volatile compounds, and to analyze the blending types of 12 varieties of coffee bean by using PCA.

MATERIALS AND METHODS

Sample preparation

The 12 varieties of green beans used in this experiment are shown in Table 1.

The beans were obtained from a local coffee company: 3 kinds of natural and pulped natural, 6 kinds of washed, 2 kinds of honey, and a kind of glazed green. The blending process varied depending on the number of products randomly blended with green beans. Eleven kinds of BC were prepared after mixing 6 or 7 kinds of green beans. The blended green beans were freeze-dried in a freeze dryer (FD8518, Ilshin Biobase Co., Ltd., Dongducheon, Korea) at a temperature of −30°C and a pressure of 0.8 mmHg for 36 h. The dried samples were roasted at 225°C for 15 min and crushed. The crushed sample was used for further analyses.

Analysis of headspace volatile compounds using purge & trap and gas chromatography (GC)-mass spectrometry (MS)

Blended, freeze-dried, and crushed coffee (3 mL) was added to a 250 mL serum bottle (Wheaton, Millville, NJ, USA) and incubated at 50°C for 30 min. Volatile compounds in the headspace were adsorbed by a Tenax TA tube (Sigma-Aldrich Co., St. Louis, MO, USA). The absorbed volatile compounds were desorbed into ATD400 (Perkin Elmer, Waltham, MA, USA), isolated and identified by GC-MS. The HP-5MSVI column (30 m×0.25 mm ×0.25 μm) was used for experimentation. Helium gas (99.9999%) was used as the carrier gas and the flow rate was set at 7.5 mL/min. The temperature of the inlet was set at 230°C. The conditions for the ATD400 were as follows. The first desorption was carried out at 350°C for 4 min. The cryogenic temperature was set at −30°C and the second desorption carried out at 350°C for 1 min. The flow of the desorb was set at 50.2 mL/min and that of the outlet split at 11.5 mL/min. The inlet split was not given. For GC, the column pressure was set to 15.9 psi

Table 1. Basic information of 12 varieties of green beans used in 11 blended coffee experiments

No.	Country	Farm	Kind	Processing
1	Panama	Hartman	Geisha	Natural
2	El Salvador	Siberia	bourbon	Glazed
3	Nicaragua	Bella Aurora	Maracatula	Washed
4	Honduras	Las Moras	Lempira	Washed
5	Kenya	Gatugi	SL28, SL34	Washed
6	Brazil	Casamub	Acaia	Pulped natural
7	Guatemala	Inherto	Geisha	Washed
8	Guatemala	Isnul	Parkamara	Washed
9	Ethiopia	Sakiso	Ethiopian	Natural
10	Ethiopia	Bunna	Ethiopian	Washed
11	Costa Rica	Hellas−Magdarena Vega	Caturra	White honey
12	Costa Rica	Vista Alvarez−Zapoté	Billa sarchi	Red honey

SL, stands for Scott laboratory.

and the oven temperature was maintained at 35°C for 10 min, increased by 8°C/min, and then maintained at 120°C for 10 min. It was then maintained at 35°C for 10 min, elevated at a rate of 12°C for 8 min and, when the temperature reached 80°C, maintained for 7 min. Finally, the temperature was increased up to 230°C by rate of 15°C for 10 min. For mass selective detector (MSD), the interface temperature was set to 230°C and quadruple mass filters were used. The detector temperature was 250°C and the ionization voltage was 70 eV. The mass range was set to 20 to 350 m/z.

PCA

PCA was performed to examine the effect of the volatile compounds in 11 types of BC beans. PCA of the major volatile compounds, which have the greatest effect on the coffee aroma among the total volatile compounds, was additionally carried out. The principal components (PCs) of the total volatile compounds and the major volatile compounds for which data variability is not greater than 80% among the PCs of eigenvalue 1 were removed using SPSS (ver. 25, SPSS Inc., Chicago, IL, USA). PC score plot represents the correlation between PC1, PC2, and reduced data variance.

RESULTS AND DISCUSSION

Flavor compounds

Dynamic headspace volatile compounds of 11 BC bean products were isolated, separated and identified by using Purge & Trap, GC-MS, and MSD. The identified headspace volatile compounds were grouped by main functional groups, shown in Table 2. A total of 41 volatile compounds were identified and classified into 6 aldehydes, 4 esters, 10 furans, 11 ketones, 8 nitrogen-containing compounds, and 2 others.

The identified aldehydes were acetaldehyde (cabbage aroma), propanal (solvent and pungent aroma), 2-methylpropanal (smoke and fatty aroma), 3-methylbutanal (cocoa and almond aroma), and 2-methylbutanal; the most prevalent were 2-methylpropanal and 2-methylbutanal. Miyake et al. (1993) carried out GC analysis of aldehydes in food and beverages, and reported acetaldehydes at 1.09 ppm. Maeztu et al. (2001) identified volatile compounds extracted from espressos comprised from three different kinds of beans; analysis of the volatile compounds of Arabica through headspace GC-MS revealed aldehydes were present in the following quantities: 0.36% acetaldehyde, 0.52% propanal, 1.80% 2-methylpropanal, 1.25% 2-methylbutanal, 2.61% 3-methylbutanal, and 0.05% hexanal. In both studies, 3-methylbutanal was the most frequently detected, followed by both 2-methylpropanal and 2-methylbutanal.

The esters, formic acid methyl ester, formic acid ethyl ester, acetic acid methyl ester, and acetic acid ethyl ester were detected in this study. Among these, the most abundant esters were methyl ester formic acid and methyl ester acetic acid. In the study by Dryahina et al. (2018), the beans of seven Arabica species were blended and quantified by GC-MS; however, only small amounts of methyl formate, methyl acetate, methyl propionate, C5 and C6 esters were detected. More diverse types of methyl esters were detected in the present study, possibly due to differences between coffee varieties and processing conditions.

The furans detected in this study were 2-methylfuran, furfural (bread, almond, and sweet), dihydro-2-methyl-3 (2H)-furanone, 2-(methoxymethyl)furan, furfuryl alcohol (burnt), 1-(2-furyl)-2-propanone, 5-methyl-2-furancarboxaldehyde, 2-furanmethanol,acetate, and 1-(2-furanyl)-ethanone. Furfural and 2-methoxyfuran were present at the highest abundances. Arisseto et al. (2011) did not find furans in green beans, but recorded quantities of up to 6,000 μg/kg in roasted beans. Becalski et al. (2016) recorded volatile compounds in espresso from roasted beans; headspace analysis showed highest average concentrations of 2-methylfuran (172 ng/g), furan (38.7 ng/g), and 3-methylfuran (6.4 ng/g).

The ketones detected in this study were 2,3-butanedione, 2-butanone (camphor aroma), 4-hydroxy-2-butanone, 2-pentanone (ether aroma), 2,3-pentadione (cream and butter aroma), 3-pentanone, 2,3-hexanedione, 3-hexanone (ether and grape aroma), 3,4-hexadione, 3-hexanone, and 1-(acetyloxy)-2-propanone. Of these, the most abundant ketone was 2,3-pentanedione. Caporaso et al. (2018) analyzed 25 types of beans using headspace analysis to find that the average concentration of ketones was approximately 5% in both Arabica and Robusta species. However, in the present study we showed ketones make up 17% of the total volatile compounds.

The nitrogen-containing compounds detected in this study were 1-methyl-1H-pyrrole, 1-methyl-1H-pyrrole-2-carboxaldehyde, pyridine, 2-methylpyrazine, methylpyrazine, 2,5-dimethyl-pyrazine, ethylpyrazine, and cyclopentapyrazole. Among these, 2 kinds of pyrrole, 4 kinds of pyrazine, a pyridine, and a pyrazole were classified, and 1-methyl-1H-pyrrole was detected at the highest abundance. Toci et al. (2008) detected no or only small amounts of nitrogen-containing compounds in three samples of green beans, but identified 31 nitrogen-containing compounds in roasted beans. Lim et al. (2017) reported the amounts of volatile compounds isolated from Brazilian Santos beans extracted using solvents. They concluded that the nitrogen-containing compounds, methyl and ethyl pyrazines were low or undetectable in uncrushed beans. However, with a medium strength crushing force, the concentrations of these esters were much higher; lower crushing forces subsequently lead to

Table 2. Total volatile compounds identified from 11 kinds of blended coffee bean and their eigenvectors as determined by principal component analysis

Name	Experimental no. (peak area×10^6)											Eigenvector	
	1	2	3	4	5	6	7	8	9	10	11	PC1	PC2
Aldehyde (6)													
Acetaldehyde	138.9	133.5	152.9	105.9	124.9	92.8	139.4	104.6	126.7	104.6	103.9	0.144	0.345
Propanal	256.5	236.3	194.5	197.7	197.4	170.9	247.0	193.2	188.0	216.2	216.2	0.870	0.220
2-Methylpropanal	287.4	225.7	267.8	208.1	211.5	213.2	260.8	245.9	201.3	254.3	244.4	0.600	0.491
3-Methylbutanal	227.3	152.4	161.3	138.8	134.4	141.1	196.9	176.2	139.9	162.6	183.2	0.672	0.625
2-Methylbutanal	350.3	257.1	288.9	237.4	244.5	255.6	308.6	300.1	255.2	303.5	305.5	0.583	0.580
Butanal	15.4	11.4	7.5	–	–	–	15.1	10.7	–	–	12.8	0.616	0.428
Sub total	1,275.8	1,016.4	1,072.9	887.9	912.7	873.6	1,167.8	1,030.7	911.1	941.2	1,066.0		
Ester (4)													
Formic acid, methyl ester	109.6	92.7	125.7	92.5	97.7	92.0	126.2	93.5	107.5	104.7	98.8	0.164	0.416
Formic acid, ethyl ester	74.4	–	–	–	60.6	78.7	101.3	89.1	–	–	–	−0.165	0.856
Acetic acid, methyl ester	99.3	96.6	66.3	95.8	100.3	90.4	115.8	94.6	77.0	108.3	129.3	0.294	0.003
Acetic acid, ethyl ester	103.4	19.8	–	–	–	–	46.5	36.7	–	–	–	0.659	0.699
Sub total	386.7	209.1	192.0	188.3	258.6	261.1	389.8	313.9	184.5	213.0	228.1		
Furan (10)													
Furan	46.1	29.0	40.2	23.9	21.1	21.3	35.7	27.4	28.9	36.2	36.6	0.712	0.305
2-Methylfuran	130.5	101.9	99.4	102.2	73.7	72.7	97.1	80.5	75.4	103.5	110.3	0.921	0.006
Furfural	123.4	93.5	87.4	77.2	76.7	69.2	84.7	90.3	80.8	91.6	88.1	0.877	0.339
Dihydro-2-methyl-3(2H)-furanone	52.5	32.0	26.8	24.7	23.5	19.7	30.8	25.8	23.5	27.7	28.8	0.904	0.412
2-(Methoxymethyl)furan	18.2	–	–	–	–	–	12.3	–	–	–	–	0.617	0.716
Furfuryl alcohol	68.7	54.5	39.8	38.8	33.0	19.1	49.5	35.7	32.0	34.7	42.1	0.937	0.220
1-(2-Furyl)-2-propanone	11.9	–	–	–	–	–	5.5	–	–	–	4.3	0.708	0.621
5-Methyl-2-furancarboxaldehyde	64.0	39.3	31.4	28.4	28.5	21.8	33.4	26.8	27.0	30.3	30.5	0.901	0.364
2-Furanmethanol,acetate	55.4	27.5	18.7	18.7	18.5	15.2	27.4	16.6	15.9	22.0	22.4	0.875	0.436
1-(2-Furanyl)-ethanone	15.6	8.9	6.0	6.6	5.4	–	6.9	5.3	5.0	5.8	6.1	0.935	0.228
Sub total	586.3	386.6	349.7	320.5	280.4	239	383.3	308.4	288.5	351.8	369.2		
Ketone (11)													
2,3-Butanedione	85.3	64.8	55.3	52.8	50.4	45.8	59.4	55.6	51.0	56.9	58.8	0.932	0.337
2-Butanone	102.8	66.0	59.1	54.4	56.2	48.7	78.9	56.1	53.5	62.9	71.0	0.851	0.483
4-Hydroxy-2-butanone	–	–	–	–	–	29.7	–	–	–	37.3	–	−0.264	−0.141
2-Pentanone	9.2	–	–	–	–	–	–	–	–	–	–	0.915	0.340
2,3-Pentanedione	229.1	161.0	140.1	119.2	110.5	101.3	137.5	126.4	112.5	129.9	134.1	0.664	0.697
3-Pentanone	15.7	–	–	–	–	–	7.7	–	–	–	–	0.905	0.285
2,3-Hexanedione	14.8	6.7	4.8	–	–	–	5.7	–	–	5.3	5.7	0.905	0.285
3-Hexanone	8.6	5.3	–	–	–	–	5.0	–	–	–	4.9	0.831	0.311
3,4-Hexanedione	17.0	8.4	6.6	5.6	4.9	4.3	6.1	4.7	4.3	5.5	6.1	0.872	0.373
3-Hexanone	9.5	5.4	–	–	–	–	4.1	–	–	–	–	0.818	0.398
1-(Acetyloxy)-2-propanone	11.5	6.0	–	–	4.3	–	7.1	–	5.9	–	–	0.592	0.469
Sub total	503.5	323.6	265.9	232.0	226.3	229.8	311.5	242.8	227.2	297.8	280.6		

Table 2. Continued

Name	Experimental no. (peak area×10^6)											Eigenvector	
	1	2	3	4	5	6	7	8	9	10	11	PC1	PC2
N-containing compound (8)													
1-Methyl-1H-pyrrole	45.4	25.6	16.4	17.8	17.2	–	22.2	13.4	12.7	15.2	21.3	0.937	0.251
1-Methyl-1H-pyrrole-2-carboxaldehyde	11.7	–	–	–	–	–	7.8	5.7	–	–	–	0.501	0.810
Pyridine	20.5	–	–	–	–	–	5.4	–	–	4.0	6.8	0.762	0.524
2-Methylpyrazine	33.2	18.3	13.6	10.4	11.9	6.5	14.3	11.6	10.0	11.2	12.6	0.886	0.394
Methylpyrazine	–	6.7	6.3	6.9	–	5.3	6.2	6.4	6.0	6.4	7.4	−0.236	−0.518
2,5-Dimethyl-pyrazine	18.1	11.1	9.0	7.7	7.9	–	8.7	7.9	6.9	7.8	8.2	0.905	0.221
Ethylpyrazine	9.6	5.7	–	4.9	5.1	–	5.1	5.0	–	4.5	4.6	0.763	0.201
Cyclopentapyrazole	6.3	–	–	–	–	–	–	4.8	–	–	–	0.437	0.629
Sub total	144.8	67.4	45.3	47.7	42.1	11.8	69.7	54.8	35.6	49.1	60.9		
Others (2)													
Ethanol	57.5	–	14.3	5.9	7.6	12.8	38	28.6	8.5	24.2	7.1	0.447	0.802
3-(Ethylthio)propanal	–	76.7	–	75.7	–	–	–	–	–	61.2	–	0.308	−0.777
Total	2,954.6	2,079.8	1,940.1	1,758.0	1,727.7	1,628.1	2,360.1	1,979.2	1,655.4	1,938.3	2,011.9		

lower concentrations. Other compounds that were identified included ethanol and 3-(ethylthio)propanal. Small amounts of carbonyl compounds, such as aldehydes and ketones, may have been converted to ethanol (Park et al., 1994).

PCA

The correlations between the 11 kinds of BC and the volatile compounds were analyzed using PCA. PCA of 41 total volatile compounds isolated from the BC samples and PCA of 17 volatile compounds known as major flavor compounds of coffee were compared. Analysis of total flavor compounds was carried out using eigenvalue confirmation, with data variability that did not exceed 80% after component extraction.

Table 2 shows the eigenvectors correlations between the flavor compounds with PC1 and PC2. PC1 and PC2 showed total variance of 66.7% and 8.2%, respectively. In PC1, positive correlation coefficients were found for 4-hydroxy-2-butanone and methyl-pyrazine but not formic acid ethyl ester; however, the greatest positive correlation was shown for furfuryl alcohol. In PC2, formic acid ethyl ester showed the greatest positive correlation coefficient, and except 4-hydroxy-2-butanone, methlypyrazine, and 3-(ethylthio)propanal, all showed positive correlation coefficients. The score plot of the samples is shown in Fig. 1.

Amongst the identified volatile compounds, 3-(ethylthio)propanal was only detected in BC2, BC4, and BC10. In PC2, 3-(ethylthio)propanal also showed the largest negative correlation, consistent with the samples score plot. The coffee blends used to produce BC1 and BC6 were 1, 5, 7, 8, 10, 11, and 12, and 1, 2, 4, 5, 6, 10, and 12, respectively. For BC2 and BC4, the coffee blends used were 2, 3, 5, 6, 7, and 11, and 3, 5, 6, 8, 9, and 10. BC1 and BC6 showed a positive correlation coefficient in PC2, whereas BC2 and BC4 had negative coefficients. Maeztu et al. (2001) carried out PCA analysis of different coffees

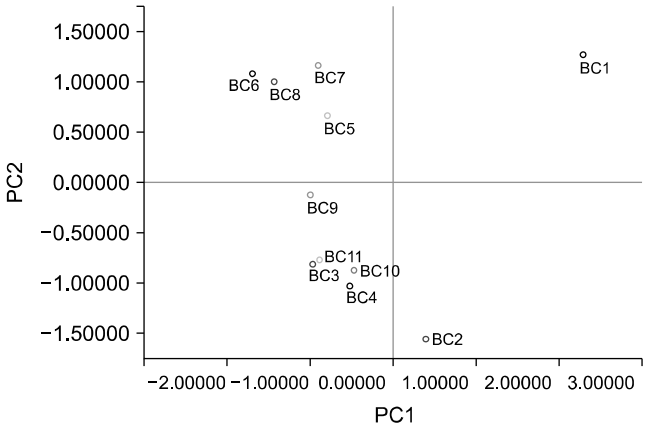

Fig. 1. Score plot of 11 blended coffee by principal components (PC1 and PC2) with total volatile compounds. BC, blended coffee.

Table 3. Odor description of major volatile compounds determined from total volatile compounds of blended coffee bean and their eigenvectors by principal component (PC) analysis

Compounds	Odor description	References	Eigenvector	
			PC1	PC2
Aldehyde (5)				
Acetaldehyde	Pungent, fruity	Cz, G, M	0.640	0.132
Propanal	Ethereal pungent, earthy	Cz, G	0.927	0.200
2-Methyl propanal	Aldehydic floral	H	0.894	0.195
3-Methyl butanal	Ethereal aldehydic	Ak, Cz, G, M, R, S	0.868	0.287
2-Methyl butanal	Musty, chocolate	Ak, Cz, G, M	0.815	0.218
Ketone (2)				
2,3-Butanedione	Sweet, creamy, buttery	Ak, H, M	0.758	0.641
2,3-Pentanedione	Buttery, nutty, toasted	Ak, H, M, R	0.721	0.675
Furan (6)				
Furfural	Sweet, brown, bready	Ch, R	0.292	0.901
2-Furanmethanol acetate	Sweet fruity banana	R	0.446	0.862
2-Metylfuran	Ethereal acetone chocolate	R	0.165	0.893
5-Methyl-2-furancarboxyaldehyde	Sweet, caramellic, bready, brown	Ak, R	0.374	0.902
Dihydro-2-methyl-3(2H)-furanone	Sweet, bread buttery, nutty	F	0.749	0.648
Furfuryl alcohol	Musty, sweet, caramellic, bready	Al	0.784	0.524
Pyrazine (3)				
2-Methyl pyrazine	Nutty, brown, musty	O	0.676	0.719
2,5-Dimethyl-pyrazine	Nutty, peanut, roasted cocoa	Ch	0.686	0.640
Ethyl pyrazine	Nutty, musty fermented, coffee	R	0.642	0.552
Pyrrole (1)				
1-Methyl pyrrole	Smoky woody herbal	R	0.104	0.970

Ak, Akiyama et al., 2003; Al, Albouchi and Murkovic, 2019; Ch, Cheong et al., 2013; Cz, Czerny et al., 1999; F, Farah and Donangelo, 2006; G, Grosch and Mayer, 2000; H, Holscher and Steinhart, 1992; M, Mayer and Grosch, 2001; O, Oliveira et al., 2009; R, Ribeiro et al., 2012; S, Semmelroch and Grosch, 1996.

to show that sulfur compounds have a positive correlation with PC2, similar to those observed in the current study. Species of aldehyde and furan show similar tendencies; however, these vary due to different roasting temperatures and time, storage time, and types of beans blended as a resulting from the differing ketones and nitrogen-containing compounds.

Subsequently, important volatile compounds were chosen from the identified volatile compounds in this study and the numbers of PCs were chosen using a cumulative dispersion level of less than 80%. Linearity started to appear from component 2, and PC1 and PC2 were extracted. The eigenvectors for the extracted principal components of PC1 and PC2 are shown in Table 3.

Of the major components analyzed, PC1 and PC2 accounted for 74.1% and 12.2%, respectively. The volatile compounds showing the largest positive correlation coefficients in PC1 and PC2 were propanal and 1-metylpyrrole, respectively. Score plots of major volatile compounds in the samples are shown in Fig. 2.

BC1, BC2, BC4, and BC6 are consistent with the score plots of major volatile compounds. BC10 showed a negative correlation coefficient for PC2 for all volatile compounds, but a positive correlation coefficient for PC2 for major volatile compounds. This is probably due to the 3-(ethylthio)propanal that was detected in BC10. BC2

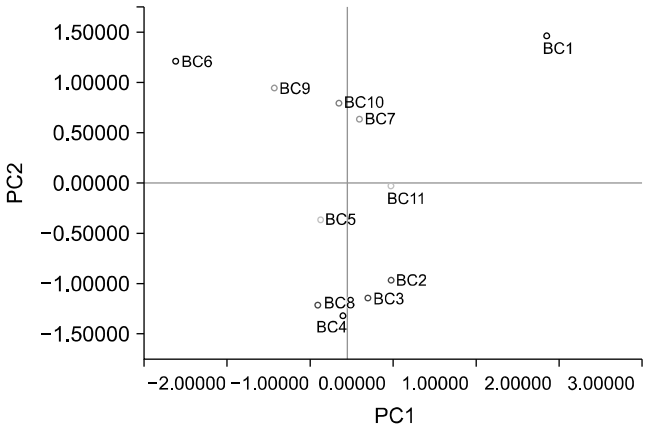

Fig. 2. Score plot of 11 blended coffee by principal components (PC1 and PC2) with 17 major volatile compounds. BC, blended coffee.

and BC4 showed negative correlations for PC2 in major volatile compounds, suggesting that BC1, BC10, and BC12 blending components are positively correlated with PC2.

The volatile flavor components of coffee beans were analyzed by GC-MS. A total of 41 kinds of main flavor components were detected in the coffee. PCA was carried out to investigate the effect of volatile compounds on the BC. By blending various green beans under specific conditions depending on individual characteristics, high quality coffee can be produced. This study therefore provides

insight into developing specialty coffee of high quality, determined through blending and roasting conditions used in the study design and chemical composition analysis carried out by PCA.

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AUTHOR DISCLOSURE STATEMENT

The authors declare no conflict of interest.

REFERENCES

Akiyama M, Murakami K, Ohtani N, Iwatsuki K, Sotoyama K, Wada A, et al. Analysis of volatile compounds released during the grinding of roasted coffee beans using solid-phase microextraction. J Agric Food Chem. 2003. 51:1961-1969.

Albouchi A, Murkovic M. LC method for the direct and simultaneous determination of four major furan derivatives in coffee grounds and brews. J Sep Sci. 2019. 42:1695-1701.

Arisseto AP, Vicente E, Ueno MS, Tfouni SA, Toledo MC. Furan levels in coffee as influenced by species, roast degree, and brewing procedures. J Agric Food Chem. 2011. 59:3118-3124.

Baggensloss J, Poisson L, Kaegi R, Perren R. Coffee roasting and aroma formation: application of different time-temperature conditions. J Agric Food Chem. 2008. 56:5836-5846.

Becalski A, Halldorson T, Hayward S, Roscoe V. Furan, 2-methylfuran and 3-methylfuran in coffee on the Canadian market. J Food Compos Anal. 2016. 47:113-119.

Buffo RA, Freire CC. Coffee flavour: an overview. Flavour Fragr J. 2004. 19:99-104.

Caporasoa N, Whitworth MB, Cui C, Fisk ID. Variability of single bean coffee volatile compounds of Arabica and robusta roasted coffees analysed by SPME-GC-MS. Food Res Intl. 2018. 108: 628-640.

Cecilia K, Glaston K, Simon M, Renaud B, Fredrick N. Volatile organic compounds in brewed Kenyan Arabica coffee genotypes by solid phase extraction gas chromatography mass spectrometry. Food Sci Qual Manage. 2012. 8:18-26.

Cheong MW, Tong KH, Ong JJM, Liu SQ, Curran P, Yu B. Volatile composition and antioxidant capacity of Arabica coffee. Food Res Int. 2013. 51:388-396.

Czerny M, Mayer F, Grosh W. Sensory study on the character impact odorants of roasted Arabica coffee. J Agric Food Chem. 1999. 47:695-699.

Dryahina K, Smith D, Španěl P. Quantification of volatile compounds released by roasted coffee by selected ion flow tube mass spectrometry. Rapid Commun Mass Spectrom. 2018. 32:739-750.

Farah A, Donangelo CM. Phenolic compounds in coffee. Braz J Plant Physiol. 2006. 18:23-36.

Gonzalez-Rios O, Suarez-Quiroz ML, Boulanger R, Barel M, Guyot B, Guiraud JP, et al. Impact of "ecological" post-harvest processing on the volatile fraction of coffee beans: I. Green coffee. J Food Comps Anal. 2007. 20:289-296.

Grosch W, Mayer F. Release of odorants from roasted coffee. In: Roberts DD, Taylor AJ, editors. Flavor Release. ACS Symposium Series, Washington, DC, USA. 2000. Vol 763, p 430-438.

Holscher W, Steinhart H. Investigation of roasted coffee freshness with an improved headspace technique. Z Lebensm Unters Forch. 1992. 195:33-38.

Joung YS. A comparative study of service quality between franchise coffee stores and local coffee stores. Culi Sci Hos Res. 2019. 25:105-112.

Kim DK. World coffee industry trend. World Agric. 2017. 199:45-60.

Lim HB, Jang KI, Kim DH. Physicochemical characteristics and volatile compounds analysis of coffee brews according to coffee bean grinding grade. J Korean Soc Food Sci Nutr. 2017. 46: 730-738.

Maeztu L, Sanz C, Andueza S, De Peña MP, Bello J, Cid C. Characterization of espresso coffee aroma by static headspace GC-MS and sensory flavor profile. J Agric Food Chem. 2001. 49:5437-5444.

Mayer F, Grosch W. Aroma simulation on the basis of the odourant composition of roasted coffee headspace. Flavour Fragrance J. 2001. 16:180-190.

Miyake T, Shibamoto T. Quantitative analysis of acetaldehyde in foods and beverages. J Agric Food Chem. 1993. 41:1968-1970.

Oliveira RCS, Oliveira LS, Franca AS, Augusti R. Evaluation of the potential of SPME-GC-MS and chemometrics to detect adulteration of ground roasted coffee with roasted barley. J Food Compos Anal. 2009. 22:257-261.

Park JS, Lee MY, Kim KS, Lee TS. Volatile flavor components of soybean paste (*Doenjang*) prepared from different types of strains. Korean J Food Sci Technol. 1994. 26:255-260.

Pearson K. On lines and planes of closest fit to systems of points in space. Philos Mag. 1901. 2:559-572.

Petisca C, Pérez-Palacios T, Farah A, Pinho O, Ferreira I. Furans and other volatile compounds in ground roasted and espresso coffee using headspace solid-phase microextraction: effect of roasting speed. Food Bioprod Process. 2013. 91:233-241.

Ribeiro JS, Augusto F, Salva TJG, Ferreira MMC. Prediction models for Arabica coffee beverage quality based on aroma analyses and chemometrics. Talanta. 2012. 101:253-260.

Rocha S, Maeztu L, Barros A, Cid C, Coimbra MA. Screening and distinction of coffee brews based on headspace solid phase microextraction/gas chromatography/principal component analysis. J Sci Food Agric. 2004. 84:43-51.

Semmelroch P, Grosch W. Studies on character impact odorants of coffee brews. J Agric Food Chem. 1996. 44:537-543.

Shin WR, Choi YM, Yoon HH. The sensory characteristics of espresso according to grinding grades of coffee beans. Korean J Food Cook Sci. 2011. 27:85-99.

Toci AT, Farah A. Volatile compounds as potential defective coffee beans' markers. Food Chem. 2008. 108:1133-1141.

Yang N, Liu C, Lic X, Degn TK, Munchow M, Fisk I. Determination of volatile marker compounds of common coffee roast defects. Food Chem. 2016. 211:206-214.