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
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, aldehydes, 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 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 $-30^\circ C$ 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 $-30^\circ C$ 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.

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**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 quadrupole 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. Maetz 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-furamethanol, 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-hexadiene, 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-pyrole, 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 2-amino(ether and grape aroma), 3,4-hexadiene, 3-hexanone, and 1-(acetyloxy)-2-propanone. Of these, the most abundant ketone was 2,3-pentanedione. 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
| Name                          | Experimental no. (peak area×10^6) | Eigenvector | Eigenvector |
|-------------------------------|-----------------------------------|-------------|-------------|
|                               | 1 2 3 4 5 6 7 8 9 10 11           | 1 2          |             |
| **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 |             |
| Propenal                      | 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**                 | 386.7 209.1 192.0 183.8 256.6 261.1 389.8 313.9 184.5 213.0 228.1 |             |             |
| **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 − − − − − − − − − − − | 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 − − − − − − − − − − − | 0.708 0.621 |             |
| 5-Methyl-2-furanocarboxaldehyde | 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 | 0.951 0.483 |             |
| 4-Hydroxy-2-butanoic          | − − − − − − − − − − − − − − − − − − | −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 − − − − − − − − − − − − − − − − − | 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 − − − − − − − − − − − − − − − − − | 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 − − − − − − − − − − − − − − − − − | 0.818 0.398 |             |
| 1-(Acetyloxy)-2-propanone     | 11.5 6.0 − − − − − − − − − − − − − − − − − | 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 |             |             |
Headspace Analysis of Volatiles in Blended Coffee

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

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 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. 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-pyrole     | 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 1,798.0 1,727.7 1,628.1 2,360.1 1,979.2 1,655.4 1,938.3 2,011.9 |
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 result 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-methylpyrrole, 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 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 compounds 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

**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 |
|--------------------------|---------------------------|-------------------|-------------|
|                          |                           |                   |             |
| Aldehyde (5)             |                           |                   |             |
| Acetaldehyde             | Pungent, fruity           | Cz, G, M          | 0.640       |
| Propanal                 | Ethereal pungent, earthy | Cz, G             | 0.927       |
| 2-Methyl propanal        | Aldehydic                 | H                 | 0.894       |
| 3-Methyl butanal         | Ethereal aldehydic        | Ak, Cz, G, M, R, S| 0.868       |
| 2-Methyl butanal         | Musty, chocolate          | Ak, Cz, G, M      | 0.815       |
| Ketone (2)               |                           |                   |             |
| 2,3-Butanedione          | Sweet, creamy, buttery    | Ak, H, M          | 0.758       |
| 2,3-Pentanedione         | Buttery, nutty, toasted   | Ak, H, M, R       | 0.721       |
| Furan (6)                |                           |                   |             |
| Furfural                 | Sweet, brown, bready      | Ch, R             | 0.292       |
| 2-Furanmethanol acetate  | Sweet fruity banana       | R                 | 0.446       |
| 2-Methylfuran            | Ethereal acetone chocolate| R                 | 0.165       |
| 5-Methyl-2-furancarboxyaldehyde | Sweet, caramellic, bready, brown  | Ak, R | 0.374       |
| Dihydropyrole(3)-3(2H)-furanone | Sweet, bread buttery, nutty  | F            | 0.749       |
| Furfuryl alcohol         | Musty, sweet, caramellic, bready | Al | 0.784       |
| Pyrazine (3)             |                           |                   |             |
| 2-Methyl pyrazine        | Nutty, brown, musty       | O                 | 0.676       |
| 2,5-Dimethyl-pyrazine    | Nutty, peanut, roasted cocoa| Ch          | 0.686       |
| Ethyl pyrazine           | Nutty, musty fermented, coffee | R             | 0.642       |
| Pyrrole (1)              |                           |                   |             |
| 1-Methyl pyrrole         | Smoky woody herbal        | R                 | 0.104       |

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.
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.

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