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Research Note

Profiling of the Volatile Compounds of the Different Local Coffee Cultivars through Headspace – Gas Chromatography – Mass Spectrometry

Kevinilo P. Marquez[1,*] and Ruel M. Mojica[2]

[1]Institute of Chemistry, College of Arts and Sciences, University of the Philippines Los Baños, College, Laguna, Philippines
[2]National Coffee Research Development and Extension Center, Cavite State University, Indang, Cavite, Philippines

[*]Author for correspondence; e-mail: kgperez3@up.edu.ph; Tel.: +639173055227 Research project proposed by the authors and funded by the University of the Philippines Natural Sciences Research Institute

The study sought to provide the data necessary for the identification, authentication, and quality analysis of coffee products cultivated locally. Four varieties of locally cultivated coffee beans (Arabica, Robusta, Excelsa, and Liberica) were analyzed for their respective aroma profiles using Headspace - Gas Chromatography - Mass Spectrometry. For the aroma profiles, a total of 66 compounds were detected across varieties and roasting degrees based on the National Institute of Standards and Technology (NIST) Library Search Engine. An 85% mass spectral profile match percentage served as the main criteria. The aroma profiles were analyzed to differentiate the varieties and their respective roasting degrees quantitatively through the varying amounts of the volatile compounds emitted as aroma, and to determine the effects of roasting on the resulting composition of such components.

Key Words: aroma, coffee, fatty acid, gas chromatography, mass spectrometry, headspace

Abbreviations: AD – Arabica Dark Roast, AL – Arabica Light Roast, AM – Arabica Medium Roast, AVD – Arabica Very Dark Roast, ED – Excelsa Dark Roast, EL – Excelsa Light Roast, EM – Excelsa Medium Roast, EVD – Excelsa Very Dark Roast, HS - GC - MS – Headspace - Gas Chromatography - Mass Spectrometry, LD – Liberica Dark Roast, LL – Liberica Light Roast, LM – Liberica Medium Roast, LVD – Liberica Very Dark Roast, NIST – National Institute of Standards and Technology, RL – Robusta Light Roast, RM – Robusta Medium Roast, RD – Robusta Dark Roast, RVD – Robusta Very Dark Roast

INTRODUCTION

The study of coffee and its composition has been of interest in many industries around the world due to the popularity of coffee as a routine and social beverage. Caffeine, the main ingredient in coffee, is a substance that boosts mental function and alters mood temporarily (Evatt and Griffiths 2013). Coffee is predominant in many countries, especially in Brazil and other South American countries, and many regions in Africa and Asia, particularly the Philippines.

One of the most popular studies on coffee is its aroma, together with its fatty acid content (Oliveira et al. 2006). The aroma of coffee is composed of many volatile compounds such as aldehydes, terpenoids, pyrroles, some alkanes, esters, furans, sulfur-containing compounds, and others (Mondello et al. 2005). Studies on the way these volatile compounds and fatty acids differ across some major coffee cultivars, namely, Arabica, Robusta, Liberica, and Excelsa, and how they vary according to geographical source (Freitas and Mosca 1999), roasting process (De Maria et al. 1994) and storage conditions (Kallio et al. 1990) would help to assess the overall quality of the coffee product. The volatile compounds of coffee were the subject of several comparative and discriminatory studies using tandem Gas Chromatography-Mass Spectrometry (GC-MS) (Hovell et al. 2010). Headspace is usually done for the preparation of coffee samples prior to aroma compound analysis in GC-MS (Sanz et al. 2001). This technique is predominantly applied to aroma compound analysis in coffee because it represents a realistic aroma correlation with those perceived by coffee users (Mondello et al. 2005).

Aroma compound analysis in coffee was found to be very challenging because of the immediate volatility of the compounds and their presence in trace amounts (Freitas and Mosca 1999). Gas chromatography coupled with mass spectroscopy proved to be a reliable technique in determining and characterizing aroma compounds in coffee (Grob and Barry 2004). The four coffee cultivars used in this study were grown and harvested in the Philippines. This study is one of the pioneering efforts in the characterization and identification of volatile and aroma compounds from Philippine-grown coffee cultivars. An earlier study was done on the use of GC-MS to analyze the aroma components of Philippine civet coffee (Ongo et al. 2012). Variations in the composition of coffee volatiles from different Philippine-grown coffee cultivars and different roasting degrees were assessed and analyzed using headspace GC-MS.

MATERIALS AND METHODS

Four locally grown coffee cultivars (Arabica, Robusta, Liberica, and Excelsa) were obtained from the National Coffee Research Development and Extension Center, Cavite State University (NCRDE-CavSU), Indang, Cavite, Philippines.

The coffee samples were roasted at 230°C using a laboratory scale roaster (Roure Roaster Mod. E-1.A, Barcelona, Spain) at 7, 9, 12, and 15 min, and were then classified as Light (L), Medium (M), Dark (D), and Very Dark (VD) roasts, respectively, based on the classification of NCRDE-CavSU. The samples were then left to cool for 24 h to develop their natural aroma. The samples were vacuum sealed in foil plastic bags and stored at 18°C prior to analysis.

The beans were then ground using a Krups 100-g capacity home grinder until the samples became fine. Then, 1.50 g of each sample were placed in a Perkin-Elmer 17-mL gas chromatography sample vial, tightly sealed in a metal cap with a Teflon septum. The samples were then placed in the Perkin Elmer Turbomass Headspace Autosampler for one-by-one pre-incubation.

The headspace conditions were as follows: initial sample heating at 90°C for 15 min, followed by injection of the sample headspace, where the desorption and injector temperatures were set at 220°C.

The Gas Chromatograph (GC) is a Perkin-Elmer GC, in tandem with a Perkin-Elmer Turbomass Quadrupole Mass Spectrometer (MS). The temperature program was set initially at 40°C for 5 min, then an increase up to 220°C at 4°C/min, followed by another increase to 280°C at 50°C/min. The total GC run time was 51.2 min. The ion source and trap parameters for the mass spectrometer were set at 220°C and 150°C, respectively, where the scan time was 1.00 s. The following data for the Gas Chromatography - Mass Spectrometry (GC-MS) analysis were then obtained and tabulated: retention time, total peak area, and the candidate compound identity, which is based on the comparison between the mass spectral data and the list of mass spectra in the National Institute of Standards and Technology (NIST) Database, which contains thousands of mass spectra for different compounds. The method used the software NIST MS Search, which is included in the Perkin Elmer Turbomass Software of the GC-MS.

RESULTS AND DISCUSSION

Comparison of the Peaks Detected across Different Varieties and Roasting Degrees

A total of 66 unique compounds were detected for all samples (Tables 1 and 2). The detected peaks were then identified based on the detected retention times and mass spectra (Fig. 1–4). Analysis of the observed retention time and the similarities in the mass spectrum of the peaks across each variety and roasting degrees showed consistent results. This observation strongly suggests that the compounds located in such peaks were identical, regardless of the variety and degree of roasting.

Identification of Aroma Compounds in Light, Medium, Dark, and Very Dark Roasted Arabica Coffee Samples

Qualitative analysis of the four different roasts of Arabica yielded chromatograms with different numbers of peaks. Twenty-four (24) compounds were identified in Arabica Light roast (AL), 25 compounds in Arabica Medium roast (AM), 28 in Arabica Dark roast (AD), and 22 in Arabica Very Dark roast (AVD). Figure 1 shows the total ion chromatogram for the four different roasts of Arabica coffee samples.

Based on the GC-MS results, Arabica roasts produced mostly pyridine and furan analogs in their headspace. The three most abundant compounds based on the % composition (calculated from peak area) found in AL were 2-furanmethanol (24.7%), 3-methyl-2-butanone (13.9%), and 2-methoxyphenol (8.0%). In AM, pyridine was the most abundant at 31.5%, followed by 2-furanmethanol at 28.3% and 3-methylbutanal at 6.7%. For AD, pyridine (34.2%), pentanedial (23.9%), and 2-furanmethanol (10.9%) were the most abundant constituents. For AVD, an unidentified compound was detected at 44.3%, followed by pyridine (31.8%) and 2-furanmethanol (8.4%).

Table 1. Retention time data for volatiles and aroma compounds in Arabica and Robusta cultivars under different roasting degrees.

Compounds	Arabica				Robusta			
	Light	Medium	Dark	Very Dark	Light	Medium	Dark	Very Dark
1-acetoxy-2-butanone	ND	ND	ND	ND	ND	ND	ND	ND
1-acetoxy-2-propanone	9.85	9.88	8.99	ND	ND	7.26	9.86	9.86
1-butyl-1H-pyrrole	5.35	ND	ND	ND	ND	ND	ND	ND
1-furfurylpyrrole	22.83	22.84	22.83	22.83	22.83	22.84	22.85	22.86
1-methyl-1H-pyrrole	ND	ND	ND	5.28	ND	ND	ND	ND
1-methyl-1H-pyrrole-2 carboxaldehyde	ND	ND	15.6	ND	ND	ND	ND	ND
1-methyl-pyrazole-4-carboxaldehyde	ND	ND	ND	13.81	ND	ND	ND	ND
1-pentyl-1H-pyrrole	16.43	ND	ND	ND	ND	ND	ND	ND
2,3-butanedione	ND	ND	ND	ND	ND	3.05	ND	ND
2,3-dimethylpyrazine	ND	ND	ND	ND	ND	ND	11.88	ND
2,3-pentadione	ND	ND	ND	ND	ND	ND	ND	ND
2,5-dimethylpyrazine	ND	ND	ND	ND	11.71	ND	ND	ND
2,6-dimethylpyrazine	ND	ND	ND	9.08	10.44	11.68	ND	ND
2,6-dimethylpyridinamine	ND	15.61	ND	ND	ND	15.59	ND	ND
2-acetyl-1-methylpyrrole	ND	18.6	18.59	ND	ND	ND	ND	ND
2-acetylpyrrole	ND	18.19	18.17	ND	ND	17.7	17.61	17.68
2-ethyl-3,5-dimethylpyrazine	18.72	ND	ND	ND	ND	ND	18.13	ND
2-ethyl-3-methylpyrazine	ND	ND	ND	15.6	15.6	14.37	15.54	15.55
2-ethyl-5-methylpyrazine	ND	ND	ND	ND	ND	15.38	ND	15.39
2-ethyl-6-methylpyrazine	ND	15.41	15.4	15.4	15.43	14.18	15.38	ND
2-formylpyrrole	ND	ND	ND	ND	ND	15.3	ND	ND
2-furanmethanol	9.28	9.26	9.26	9.26	9.24	9.28	9.39	9.39
2-furanmethanoyl acetate	15.19	15.2	15.2	15.2	ND	15.21	15.21	15.21
2-furfuryl-5-methylfuran	20.63	ND	ND	ND	ND	ND	ND	ND
2-furfurylfuran	ND	18.91	18.89	18.89	ND	ND	ND	18.92
2-methoxy-4-vinylphenol	ND	27.81	27.81	ND	27.81	ND	ND	27.83
2-methoxybenzamine	ND	ND	ND	18.59	ND	ND	ND	ND
2-methoxyphenol	12.83	19.1	19.1	19.1	ND	19.11	19.12	19.13
2-methyl-1H-pyrrole	ND	ND	5.24	ND	ND	ND	ND	ND
2-methylfuran	ND	ND	ND	ND	ND	ND	ND	ND
2-methylpropanal	ND	ND	ND	ND	2.87	ND	ND	ND
2-methylundecane	ND	ND	ND	ND	26.5	ND	ND	ND
3,5-diethyl-2-methylpyrazine	ND	21.9	21.9	ND	ND	21.9	21.9	21.9
3,6-dimethyl-2-pyridinamine	15.58	ND	ND	ND	ND	ND	ND	ND
3-acetyl-1H-pyrroline	ND	ND	ND	ND	ND	ND	18.61	ND
3-ethenyl-3-methylcyclopentanone	ND	ND	ND	19.61	ND	ND	ND	ND
3-ethyl-2,5-dimethylpyrazine	11.96	18.74	18.73	18.73	ND	18.72	18.73	18.73
3-ethylpyridine	ND	ND	ND	ND	ND	ND	ND	ND
3-furanmethanol	ND	ND	ND	ND	ND	6.39	5.53	ND
3-methyl-2-butanone	3.06	3.08	ND	ND	ND	ND	ND	ND
3-methylbutanal	3.83	3.86	3.81	ND	3.85	3.83	ND	ND
4-ethyl-2-methoxyphenol	25.52	26.5	ND	26.47	ND	26.5	26.49	26.38
4-ethyl-2-methylphenol	ND	ND	26.47	ND	ND	ND	ND	ND
4-methyl-2-ethoxyphenol	ND	ND	ND	ND	ND	ND	ND	26.49
4-methylpyrimidine	ND	ND	8.08	ND	ND	8.07	ND	8.03
5-methyl-2-furancarboxaldehyde	13.78	13.82	ND	ND	ND	ND	ND	ND
5-methylfurfural	ND	ND	ND	ND	13.83	13.8	13.81	ND
acetaldehyde	2.24	2.25	2.24	2.25	2.25	2.24	ND	ND
acetic acid	ND	ND	ND	ND	ND	ND	ND	3.04
acetone	2.48	ND	ND	ND	ND	ND	ND	ND
acetylfuran	ND	ND	ND	ND	ND	11.53	ND	ND
butyrolactone	11.59	11.6	11.57	11.57	ND	9.62	11.63	11.66
difurfuryl ether	ND	27.35	27.34	27.34	ND	ND	27.36	27.37
dihydro-2-methyl-3(2H)-furanone	7.48	7.48	7.47	ND	ND	ND	ND	ND
dihydro-2-methylfuranone	ND	ND	ND	ND	ND	ND	ND	ND
formylpyridine	ND	ND	ND	ND	ND	ND	ND	5.46
furfuryl ether	26.63	ND	ND	ND	ND	ND	ND	ND
furfurylpentanoate	ND	ND	ND	ND	ND	ND	ND	ND
N-acetyl-4H-pyridine	ND	ND	16.28	ND	ND	ND	ND	ND
nonanal	ND	ND	4.73	ND	ND	ND	ND	ND
pentanal	4.41	4.43	4.41	4.38	4.4	ND	ND	ND
pentanedial	ND	ND	3.12	ND	ND	ND	ND	ND
phenol	ND	14.71	14.71	14.72	ND	ND	14.77	14.79
pyridine	5.62	5.54	5.45	5.44	ND	0.61	2.45	0.28
pyridinecarboxylic acid	1.37	ND	ND	ND	ND	ND	ND	ND
tetrahydropyrrole-3-amino-2,5-dione	ND	ND	ND	ND	ND	9.87	ND	ND

ND – not detected

Table 2. Retention time data for volatiles and aroma compounds in Excelsa and Liberica cultivars under different roasting degrees.

Compounds	Excelsa				Liberica			
	Light	Medium	Dark	Very Dark	Light	Medium	Dark	Very Dark
1-acetoxy-2-butanone	14.05	ND	ND	ND	14.03	ND	14.02	ND
1-acetoxy-2-propanone	9.88	9.87	9.9	ND	9.86	9.84	9.84	ND
1-butyl-1H-pyrrole	ND	ND	ND	ND	ND	ND	ND	ND
1-furfurylpyrrole	22.86	22.85	22.86	22.83	22.84	22.84	22.84	22.84
1-methyl-1H-pyrrole	ND	ND	ND	ND	ND	ND	ND	ND
1-methyl-1H-pyrrole-2 carboxaldehyde	ND	ND	ND	ND	ND	ND	ND	ND
1-methyl-pyrazole-4-carboxaldehyde	ND	ND	ND	ND	ND	ND	ND	ND
1-pentyl-1H-pyrrole	ND	ND	ND	ND	ND	ND	ND	ND
2,3-butanedione	ND	ND	ND	ND	ND	ND	ND	ND
2,3-dimethylpyrazine	11.91	11.9	11.93	ND	11.91	ND	ND	ND
2,3-pentadione	ND	ND	ND	ND	ND	ND	ND	ND
2,5-dimethylpyrazine	11.66	11.66	11.73	ND	11.65	ND	ND	ND
2,6-dimethylpyrazine	ND	ND	ND	ND	ND	11.65	ND	ND
2,6-dimethylpyridinamine	ND	ND	ND	ND	ND	ND	ND	ND
2-acetyl-1-methylpyrrole	ND	ND	ND	ND	ND	ND	ND	ND
2-acetylpyrrole	18.24	18.25	18.16	ND	18.22	17.6	18.2	18.19
2-ethyl-3,5-dimethylpyrazine	19.01	ND	ND	ND	ND	ND	ND	ND
2-ethyl-3-methylpyrazine	15.55	15.56	15.58	15.54	15.55	15.54	15.54	15.59
2-ethyl-5-methylpyrazine	ND	ND	ND	ND	ND	ND	ND	ND
2-ethyl-6-methylpyrazine	15.38	15.38	15.41	15.38	15.38	15.37	15.37	15.4
2-formylpyrrole	16.14	16.12	ND	ND	ND	ND	ND	ND
2-furanmethanol	9.47	9.47	9.5	9.29	9.43	9.35	9.37	9.27
2-furanmethanoyl acetate	15.22	15.21	15.22	15.2	15.21	15.19	15.2	15.21
2-furfuryl-5-methylfuran	ND	ND	22.8	ND	ND	ND	ND	ND
2-furfurylfuran	ND	18.91	18.91	18.9	ND	ND	ND	ND
2-methoxy-4-vinylphenol	ND	ND	ND	27.82	ND	ND	ND	ND
2-methoxybenzamine	ND	ND	ND	ND	ND	ND	ND	ND
2-methoxyphenol	19.12	19.12	19.14	19.09	19.11	19.09	19.11	19.1
2-methyl-1H-pyrrole	ND	ND	ND	ND	ND	ND	ND	ND
2-methylfuran	ND	ND	ND	3.11	ND	ND	ND	3.1
2-methylpropanal	ND	ND	ND	ND	ND	ND	ND	ND
2-methylundecane	ND	ND	ND	ND	ND	ND	ND	ND
3,5-diethyl-2-methylpyrazine	ND	21.9	ND	21.89	ND	ND	ND	ND
3,6-dimethyl-2-pyridinamine	ND	ND	ND	14.4	ND	ND	ND	ND
3-acetyl-1H-pyrroline	ND	ND	ND	ND	ND	18.2	17.53	ND
3-ethenyl-3-methylcyclopentanone	ND	ND	ND	ND	ND	ND	ND	ND
3-ethyl-2,5-dimethylpyrazine	18.74	18.74	18.75	18.72	18.73	18.73	18.72	ND
3-ethylpyridine	ND	13.69	13.41	ND	13.69	ND	ND	12.21
3-furanmethanol	ND	ND	8.8	ND	ND	5.16	5.69	ND
3-methyl-2-butanone	ND	ND	ND	ND	ND	ND	9.84	ND
3-methylbutanal	ND	3.83	ND	3.83	ND	3.81	3.85	3.34
4-ethyl-2-methoxyphenol	26.34	26.48	26.5	26.46	26.49	ND	26.49	ND
4-ethyl-2-methylphenol	ND	ND	ND	ND	ND	ND	ND	ND
4-methyl-2-ethoxyphenol	ND	ND	ND	ND	ND	ND	ND	ND
4-methylpyrimidine	8.02	ND	ND	8.07	ND	ND	ND	ND
5-methyl-2-furancarboxaldehyde	ND	ND	ND	ND	13.79	13.78	ND	ND
5-methylfurfural	13.8	13.81	13.81	13.81	ND	ND	13.8	ND
acetaldehyde	2.25	2.24	ND	2.24	2.24	2.24	2.25	2.24
acetic acid	3.09	3.06	3.18	ND	3.1	3.02	3.01	ND
acetone	ND	ND	ND	ND	ND	ND	ND	2.49
acetylfuran	ND	11.53	ND	ND	11.52	11.52	11.52	ND
butyrolactone	ND	ND	11.3	11.58	ND	ND	ND	11.57
difurfuryl ether	ND	27.36	27.37	27.34	ND	ND	ND	27.35
dihydro-2-methyl-3(2H)-furanone	7.44	ND	ND	7.48	ND	ND	ND	ND
dihydro-2-methylfuranone	ND	ND	ND	ND	ND	ND	ND	ND
formylpyridine	ND	ND	ND	ND	ND	ND	ND	ND
furfuryl ether	ND	27.36	27.37	27.34	ND	ND	ND	27.35
furfurylpentanoate	ND	ND	ND	ND	24.47	24.46	24.46	24.47
N-acetyl-4H-pyridine	ND	ND	ND	ND	ND	ND	ND	ND
nonanal	ND	ND	ND	ND	ND	ND	ND	ND
pentanal	4.42	4.42	ND	ND	ND	4.41	ND	3.84
pentanedial	ND	ND	ND	ND	ND	ND	ND	ND
phenol	ND	ND	ND	14.73	ND	ND	14.76	14.73
pyridine	5.47	5.46	5.49	5.48	5.41	ND	5.45	5.44
pyridinecarboxylic acid	ND	ND	ND	ND	ND	ND	ND	ND
tetrahydropyrrole-3-amino-2,5-dione	ND	ND	ND	ND	ND	ND	ND	ND

ND – not detected

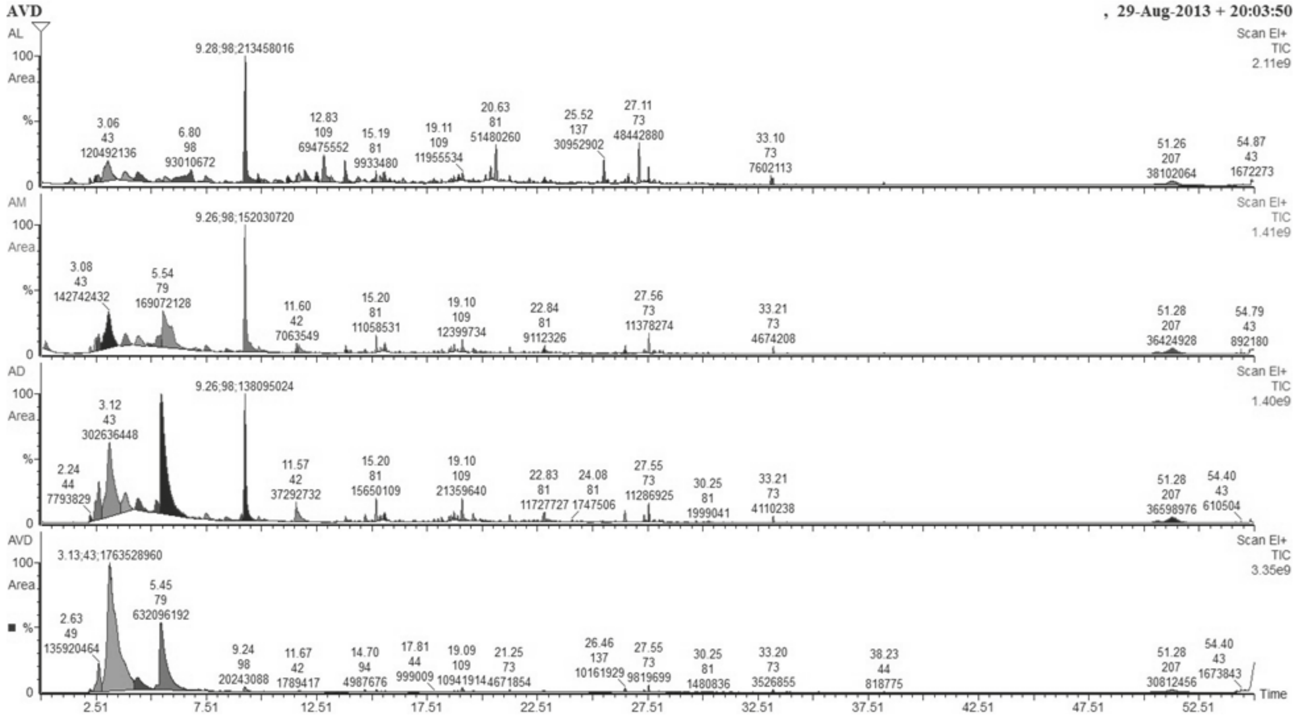

Fig. 1. Gas chromatograms of Arabica Light (AL), Medium (AM), Dark (AD) and Very Dark (AVD) roasts.

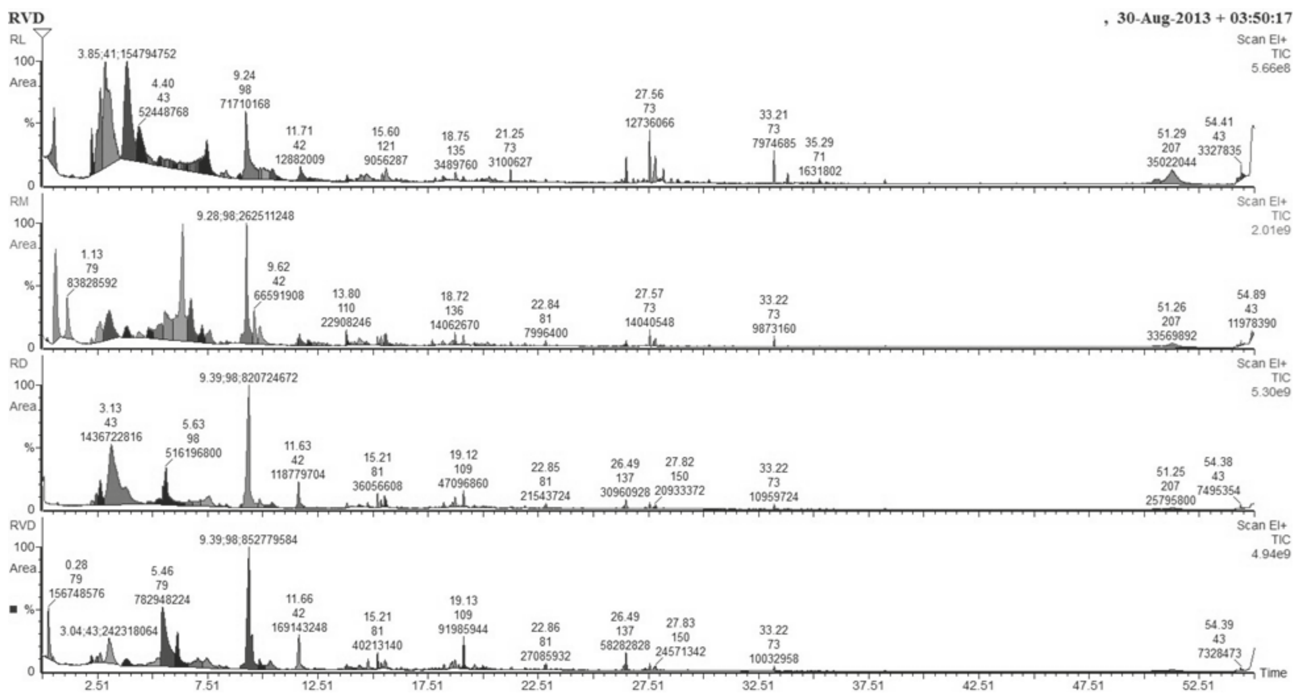

Fig. 2. Gas chromatograms of Robusta Light (RL), Medium (RM), Dark (RD) and Very Dark (RVD) roasts.

Identification of Aroma Compounds in Light, Medium, Dark, and Very Dark Roasted Robusta Coffee Samples

Qualitative analysis of the four Robusta roasts yielded chromatograms with different numbers of peaks. A total of 14 compounds were identified in Robusta Light roast (RL), 26 compounds in Robusta Medium roast (RM), 22 compounds in Robusta Dark roast (RD), and 22 compounds in Robusta Very Dark roast (RVD). Figure 2 shows the total ion chromatograms for the Robusta roasts.

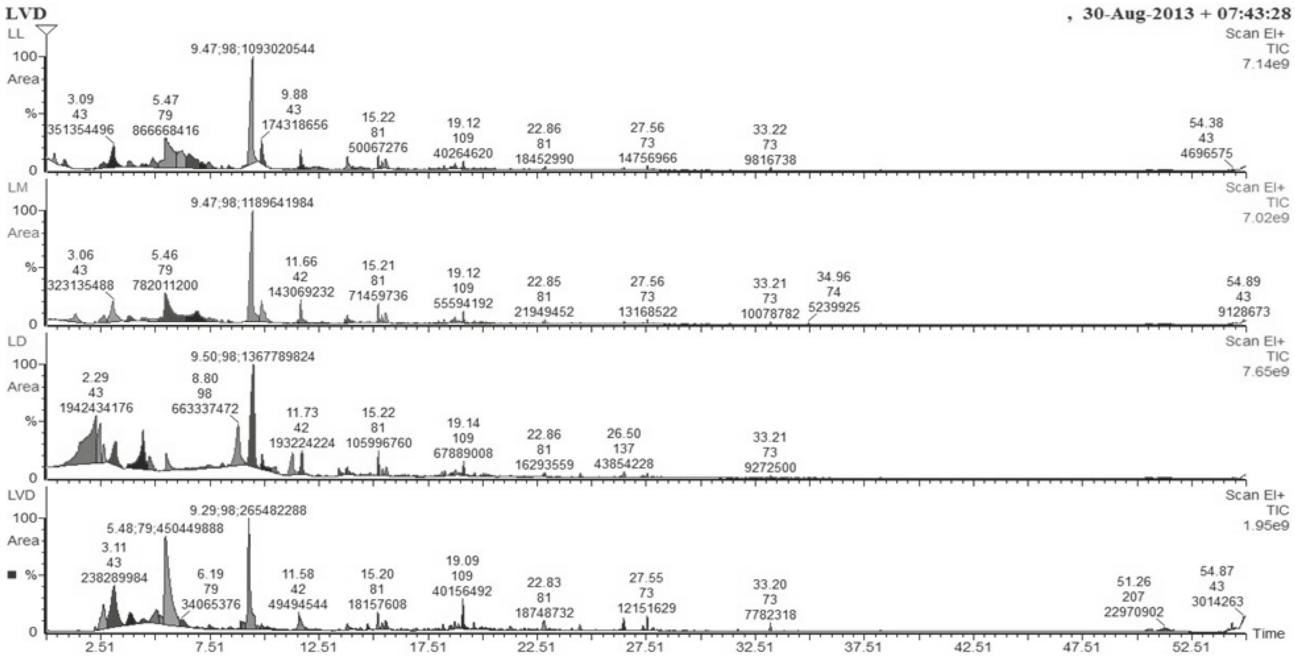

Fig. 3. Gas chromatograms of Liberica Light (LL), Medium (LM), Dark (LD) and Very Dark (LVD) roasts.

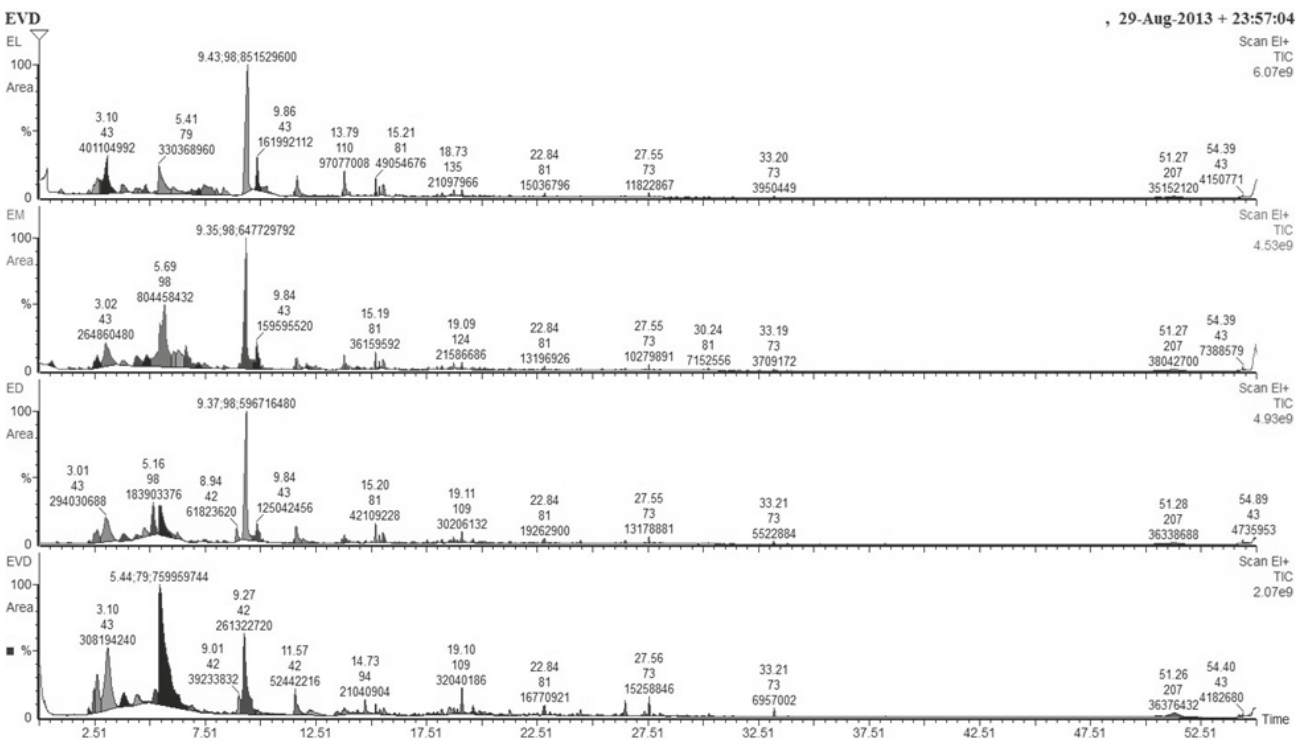

Fig. 4. Gas chromatograms of Excelsa Light (EL), Medium (EM), Dark (ED) and Very Dark (EVD) roasts.

The Robusta roasts had mostly furan analogs in their headspace, such as 2-furanmethanol and 3-furanmethanol. In RL, the most abundant compounds were 2-methylpropanal, 3-methylbutanal, and an unknown compound, at 29.6%, 24.7%, and 12.4%, respectively. In RM, the most abundant compounds were 3-furanmethanol, 2-furanmethanol, and pyridine, at 26.15%, 14.9%, and 13.7%, respectively. Furanmethanols (2-furanmethanol and 3-furanmethanol) were identified in RD, with relative compositions of 23.3% and 14.7%, respectively. In RD, the most abundant compound at 40.8 % was unidentified. In RVD, the most abundant compounds were 2-furanmethanol, formylpyridine, and 1 -furfurylpyrrole at 80.0%, 7.3%, and 2.5%, respectively.

Identification of Aroma Compounds in Light, Medium, Dark, and Very Dark Roasted Liberica Coffee Samples

Qualitative analysis of the four Liberica roasts yielded chromatograms with different number of peaks. Exactly 26 compounds were identified in Liberica Light roast (LL), 31 compounds in Liberica Medium roast (LM), 24 compounds in Liberica Dark roast (LD), and 25 compounds in Liberica Very Dark roast (LVD). Figure 3 shows the total ion chromatograms for the four different roasts of Liberica coffee samples.

Some of the volatile compounds found in Liberica roasts were not found in the Robusta and Arabica roasts. In LR, the most abundant compounds found were 2-furanmethanol (35.8%), pyridine (28.4%) and 1-acetoxy-2-propanone (5.7%). In LM, the most abundant compounds were 2-furanmethanol, pyridine, and acetic acid, at 34.6%, 22.7%, and 9.4%, respectively. In LD, the most abundant compounds were 2-furanmethanol, 3-furanmethanol, and acetic acid, at 33.9%, 16.5%, 10.9%, respectively. Pyridine (33.1%) was the top constituent for LVD, followed by 2-furanmethanol (18.8%) and 2-methylfuran (17.5%).

Identification of Aroma Compounds in Light, Medium, Dark, and Very Dark Roasted Excelsa Coffee Samples

Qualitative analysis of the four Excelsa roasts yielded chromatograms with different number of peaks. A total of 24 compounds were identified in Excelsa Light roast (EL), 24 compounds in Excelsa Medium roast (EM), 25 compounds in Excelsa Dark roast (ED), and 21 compounds in Excelsa Very Dark roast (EVD). Figure 4 shows the total ion chromatograms for the four different roasts of Excelsa coffee samples.

The most abundant compounds in EL were 2-furanmethanol (39.5%), followed by pyridine (15.3%), and 1-acetoxy-2-propanone (7.5%). Furanmethanols were also ubiquitous in EM, with 3-furanmethanol and 2-furanmethanol as the most abundant compounds, at 30.8% and 24.8%, respectively. Acetic acid was also found in EM, at 10.5%. In ED, 2-furanmethanol (27.4%), pyridine (14.7%) and acetic acid (13.5%) were the three most abundant compounds. For EVD, the most abundant compounds were pyridine (48.2%), 2-furanmethanol (16.6%), and an unidentified compound (6.5%).

Analysis of Mass Spectral Data and Observed Peaks

The mass spectra of the eluted compounds were analyzed and compared with the mass spectra of compounds found in the NIST library program. The results were screened with respect to factors such as signal-to-noise ratio, comparison against the method blanks, and peak identification through the NIST Library through the NIST MS Search software. An 85% match was chosen as the minimum percentage to ensure that the minor fragments were also considered. This is also the recommended minimum percentage by the software.

Tables 1 and 2 show the retention time data for all the peaks detected and analyzed in the experiment. There were numerous compounds detected which were found in all runs, such as 1-furfurylpyrrole and 2-furanmethanol. Some compounds (4-methylpyridine) were only detected after a significant degree of roasting.

In Arabica and Robusta, as the roast became "darker" due to higher roasting time, the total peak area increased, but the number of peaks tended to increase only in light to medium roast, then declined again in medium to very dark roast in the case of Robusta. For Arabica, the numbers of peaks tended to increase up to the dark roast, and then declined again in dark to very dark roast. This finding suggests that the roasting degree affects the total amount of volatiles produced in the coffee samples.

A similar trend for the number of peaks can be observed for Liberica and Excelsa, but in this case, the total peak area decreased as the roast became darker. In Excelsa, the same number of peaks occurred in light and medium roasts, but the total peak area was greater in the medium than in the light roast.

CONCLUSION

Mostly furan, pyrrole, pyrazine, and pyridine analogs constituted the aroma compounds present in the four Philippine-grown coffee cultivars, regardless of the degree of roasting. Phenols, simple aldehydes and organic acids were also found in the coffee samples. However, there were differences in the number of compounds found in the different coffee cultivars. Roasting affected the number of detected compounds, with optimal detection in medium (Robusta and Liberica) or dark (Arabica and Excelsa) roasts. Prolonged roasting may have depleted some of the volatiles present in the coffee beans, leading to a decrease in the number of compounds detected in dark (Robusta and Liberica) and very dark (Arabica and Excelsa) roasts.

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