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Research Article

Volatile compounds of don severino's aguinaldo blend coffee from indang cavite philippines by gas chromatography mass spectrometry

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Abstract

Coffee blending technology refers to the process of incorporating coffee varieties for the improvement of sensory attributes. Don Severino's Aguinaldo Blend Coffee consists of Arabica, Robusta and Liberica beans. The study investigated volatile compounds using Static Headspace Gas Chromatography Mass Spectrometry (SH-GC/MS) and a total of 27 volatile compounds were tentatively identified based on the National Institute of Standards and Technology (NIST) Library following an 85% mass spectral profile match percentage. The results revealed the presence of 2-Methylfuran, 2-Methylbutanal, 2,6-Dimethylpyrazine, and 2-Furanmethanol as distinct volatile compounds. Moreover, chemical groups such as furans, pyrazines, pyridines, pyrroles, aldehydes, ketones, alcohol, and esters dominated among other groups. The study gives baseline information regarding aroma profile present in Don Severino's Aguinaldo Blend Coffee.

Keywords: Blended coffee, Volatile compounds, SH/GC-MS

INTRODUCTION

The study of coffee and its composition has piqued the interest of various industries around the world and Philippines has an ideal soil and climate for the cultivation of Arabica, Robusta,Excelsa and Liberica coffee **(Santos et al., 2018).**

Coffee blending refers to the process of incorporating different beans before and after roasting to produce a desirable taste and aroma. Combining two or more coffee varieties creates a coffee with a distinct flavor since it enhances the mixing effect of green beans with other varieties to produce a more balanced taste and aroma. In coffee processing, roasting time and temperature generally influences the composition of volatile compounds in the roasted beans through formations from Pyrolysis, Maillard reactions of non-enzymatic browning, Strecker degradation, and other reactions **(Kim et al., 2019)**

Volatile compounds are involved in differentiation of roasted coffee based on their geographical origins or authenticity purposes related to species **(Caporaso et al., 2018)**. However, few researches have been carried out on the volatile compounds of blended coffee. Thus, this study aims to identify, characterize, and quantify the volatile compounds and their chemical groups in Don Severino's Aguinaldo Blend Coffee.

MATERIALS AND METHODS

Sample collection and preparation

Don Severino's Aguinaldo Blend Coffee was purchased from

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Cavite State University located in Indang Cavite, Philippines. The sample was packed in vacuum sealed black plastic bags and was immediately stored at 15° C to 25°C prior to analysis.

Optimization of SH/GC-MS analysis

Two (2) grams of the sample was introduced to a 20 mL vial which was sealed with silicone rubber Teflon cap. The vial was equilibrated at 70 °C for 30 minutes in the static headspace sampler and 1 mL of the coffee headspace sample was injected to the HP-5MS column (30m x 0.250mm, 0.25-micron film thickness). The volatile compounds were separated on an HP-5MS capillary column (30m x 0.250 mm, 0.25-micron film thickness) which showed a good compromise between resolution and speed of volatile compound separation. The method was also based in the previous studies of **(Sarghini et al. 2019)** with appropriate modification **(Table 1).**

Analysis of the volatile compound profile

The injector temperature was set at 220 °C with split injection mode and the follow of the helium carrier gas was 1mL/min. The oven temperature was set at an initial 40 °C, followed by an increase of 2 °C/min to 80 °C, and 20 °C/ min to 220 °C (held for 5 minutes). Mass spectrometry was carried out using the 5977B Mass Selective Detector (MSD) coupled to the GC system. The mass spectrometer operated in the electron impact ionization mode of 70 eV, with a scan range of 27 to 400 amu.

Data interpretation

The following data produced from Gas Chromatography - Mass Spectrometry (GC-MS) analysis was obtained and tabulated. The tentative identified compound was compared to the peaks from the library's mass spectra in the National Institute of Standards and Technology (NIST). The Agilent mass hunter qualitative analysis 10.00.was utilized to process the data, while the NIST MS Search 2.3 database was utilized for the identification of the peaks present in the chromatogram **(Figure 1)**. An 85% mass spectral profile match percentage was considered as the main criteria. Furthermore, the relative percentages of individual compounds were calculated from the total contents of volatiles on the chromatograms.

$$\% \text{ Relative Peak Area} = \frac{\text{Area of an individual compound}}{\text{Total Area}} \text{x } 100$$

RESULTS AND DISCUSSION

GC Chromatograms **(Figure 2)** showed that Don Severino's Aguinaldo Blend contained similar volatile compound profiles with that of Arabica, Robusta and Liberica coffee, however, unique volatile compounds were also formed

Table 1. SH/GC-MS Parameters.

Column	Incubation Temperature	Incubation Time	Injection Volume	Split less injection	Carrier Gas Flow	Oven Temperature	Electron Ionization	Mass Range
HP5-MS	70°C	30 min	1mL	1:10	1mL/min	220 for 5 minutes	70 eV	27 to 400 amu

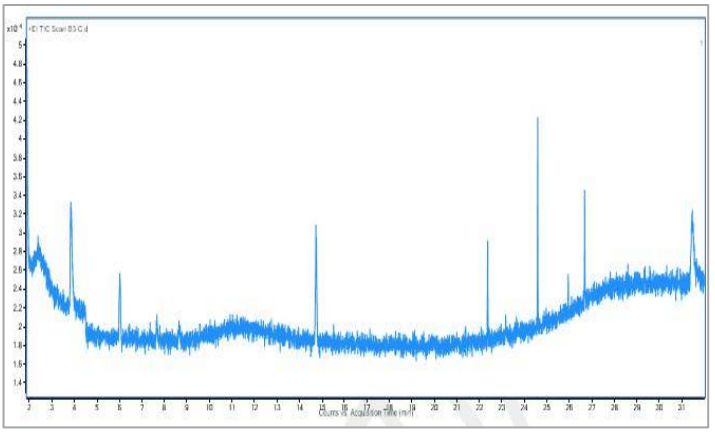

Figure 1. GC-MS Total Ion Chromatogram of the Blank.

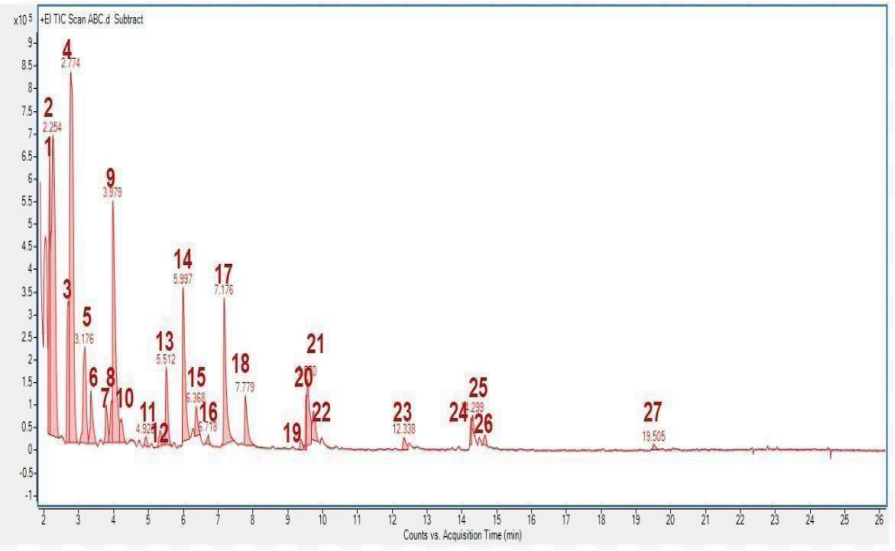

Figure 2. GC-MS Total Ion Chromatogram of Don Severino's Aguinaldo Blend Coffee.

Table 2. Don Severino's Aguinaldo Blend Coffee.

Number	Retention Time (min)	Volatile Compounds	Peak Area %
		Furans	
2	2.254	2-Methylfuran	19.48
15	6.368	Furfural	1.13
24	0.62	Furfuryl acetate	0.62
		Aldehydes	
4	2.774	2-Methylbutanal	20.59
		Pyrazines	
14	5.997	Methylpyrazine	6.04
20	9.570	2,6-Dimethylpyrazine	3.01
22	9.731	Ethylpyrazine	1.42
7	3.791	Pyrazine	1.37
20	9.526	2,5-Dimethylpyrazine	0.84
25	14.299	2-Ethyl-5-methylpyrazine	0.38
26	14.653	2-ethyl-3-methylpyrazine	0.38
27	19.505	2-Ethyl-3,6-dimethylpyrazine	0.24
		Pyridines	
9	3.979	Pyridine	10.90
		Ketones	
5	3.176	Acetylpropionyl	4.94
6	3.342	Acetoin /2-Butanone	2.13
11	4.293	3-n-Propyl-5-methylhexan-2-one	0.34
		Carboxyl	
1	2.162	Acetic Acid	6.01
16	6.718	β-Methylbutyric acid	0.32
		Heteroaromatic	
17	7.176	2-Furanmethanol	5.89
		Alpha Hydrogen Aldehydes	
3	2.708	3-Methyl-1-butanal / Isovaleraldehyde	4.77
		Furanones	
13	5.512	2-Methyl-3-tetrahydrofuranone	2.94

		Alpha-acyloxy Ketones	
18	7.779	Acetol acetate	2.17
		Pyrroles	
8	3.936	N-Methylpyrrole	1.37
10	4.219	Pyrrole	1.09
		n-hydroxycarbamate	
12	5.338	tert-Butyl N-hydroxycarbamate	0.65
		Aryl aldehydes	
23	12.338	2-Formyl-5-methylfuran	0.60
		Ester	
19	9.377	Furfuryl formate	0.38

Which may be due to the blending of these varieties. A total of 27 volatile compounds from different chemical groups were identified as shown in **(Table 2).**

Other chemical groups of volatile compounds that have high relative peak area percentage were Furans specifically 2-Methylfuran (19.48%), Furfural (1.13%) and Furfuryl acetate(0.62%) which imparts fruity and floral notes asstated by Caporaso et al. (2018). Pyrazines include Methylpyrazine (6.04%), 2,6-Dimethylpyrazine (3.01%), Ethylpyrazine (1.42%), Pyrazine (1.37%), 2,5-Dimethylpyrazine (0.84%), 2-Ethyl-5-methylpyrazine (0.38%), 2-ethyl-3-methylpyrazine (0.38%), 2-Ethyl-3,6-dimethylpyrazine (0.24%) that are formed by coffee roasting and imparts earthy/woody notes (**Seninde & Chambers, 2020**). The aldehyde group was considered as one of the important compounds in coffee aroma which also includes 2-Methylbutanal (20.59%).

The presence of 2-Furanmethanol (5.89%) in this sample is primarily due to Robusta Coffee since this compound is generally high in the abovementioned coffee variety as stated in the study of (**Caporaso et al. 2018**). It also contributes to the burnt, sweet, caramel, coffee, and bitter aroma in coffee.

Unique volatile compounds were also detected in this blend such as Isovaleraldehyde, tert-Butyl N-hydroxycarbamate, N-Methylpyrrole, 3-n-Propyl-5-methylhexan-2-one, Acetoin /2-Butanone, 2-Formyl-5-methylfuran, and 3-n-Propyl-5-methylhexan-2-one.

CONCLUSION AND RECOMMENDATION

The sample was analyzed by SH/GC-MS and revealed a total of 27 compounds tentatively identified in Don Severino's Aguinaldo Blend Coffee consisting of Arabica, Robusta, and Liberica beans. Thus, this study provides information regarding the generation of unique volatile compounds, however, standards for confirmation are needed for the confirmation of the tentative identified compounds. Further research could investigate volatile compounds from other variants of Don Severino's Aguinaldo blend such as antioxidant-enriched, naturally sweetened, and liberica based.

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