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Effects of roasting on profiles of non-volatile and volatile compounds in Liberica coffee from Jambi, Indonesia

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Abstract

Roasting is an essential stage that helps achieve the desired flavour of coffee while decreasing its bioactivity. Despite the limited studies on its chemical composition, Liberica coffee is a coffee species that has re-emerged in a warmer climate. The present work aimed to examine the effects of the commercial roasting process on the composition of non-volatile and volatile compounds in Liberica coffee collected from different regions (Betara, Bram Itam, Kuala Betara, Pengabuan, and Senyerang) in Jambi Province, Indonesia. Results indicated that 41 and 43 constituents were putative non-volatile compounds identified from green and roasted beans, respectively, with alkaloids, organic acids, and phenolics being predominant. Moreover, targeted analysis of the compounds revealed that green beans obtained from different regions in Jambi Province produced diverse caffeoylquinic acid (CQA) isomers 3, 4, and 5, as well as alkaloids (trigonelline, theobromine, and caffeine). In terms of CQAs and alkaloid contents, Betara green beans exhibited characteristics similar to those of Pengabuan green beans, whereas the rest showed distinct chemical characteristics. Roasting in lightness level L* of 39.05 - 39.48 resulted in similar contents of CQA isomers 3, 4, and 5, as well as alkaloids (theobromine and caffeine), between the different types of Liberica coffee. The commercial roasting process led to the chemical degradation of CQAs, whereas alkaloids remained stable. This process increased the volatile compounds of coffee in relative content of furan and pyrazine compounds.

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Introduction

Coffee is one of the most popular beverages in the world. Its demand has been reported to increase by 1.1% between 2017 and 2021 (ICO, 2021a). Globally, 124 coffee species have been identified; however, only three species (*Coffea arabica* [Arabica], *C. canephora* [Robusta], and *C. liberica* [Liberica]) are commonly traded (Davis *et al*., 2006; Davis, 2011). Arabica and Robusta dominated the coffee business, contributing 59 and 41% of the market share, respectively (ICO, 2021b), whereas Liberica contributed only 1 - 2% of the share (Wingtens, 2004). The limited contribution of Liberica coffee to the global coffee trade indicates its rarity, making it one of the exotic coffees that need to be studied further. Moreover, it demonstrates superior disease resistance and adaptability to peatlands and climate change (Davis *et al*., 2022; Hafif *et al*., 2024). This makes Liberica coffee more promising in a warmer climate.

Liberica coffee is commonly known as "jackfruit coffee" owing to its distinctive flavour and greater antioxidant activity than Arabica and Robusta (Saw *et al*., 2015; Wibowo *et al*., 2024). Indonesia has been recognised as one of the producers of Liberica coffee in Asia, particularly in Tanjung Jabung Barat District, Jambi Province. In that district, there are five main regions of coffee production, namely Betara, Bram Itam, Kuala Betara, Pengabuan, and Senyerang. Studies on the correlation between plantation geography and coffee properties have been conducted. Previous studies have investigated how Liberica coffee's various places of origin influence changes in its antioxidant activity and physical properties (Insanu *et al*., 2021; Hanifah *et al*., 2022).

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However, research has yet to be conducted on its variations in non-volatile components. The different geographic locations for coffee farming exerted remarkable effects on non-volatile compounds (chlorogenic acids and alkaloids) in Arabica green beans (Mehari *et al*., 2016a; 2016b). Interestingly, some studies (di Donfrancesco *et al*., 2019; Badmos *et al*., 2020) reported no correlation between the farming locations and the sensory characteristics and chlorogenic acids in Arabica roasted beans. This raises suspicion regarding the influence of roasting on the diversity of non-volatile compounds in coffee, particularly as certain non-volatile compounds, such as caffeine and chlorogenic acid, significantly influence the sensory quality and antioxidant activity of coffee (Barbosa *et al*., 2019).

Roasting is a crucial phase in coffee production. It determines the development of the desired flavours of coffee while substantially reducing its bioactivity (Turan *et al*., 2021). The commercial roasting of Liberica coffee does not diminish its antioxidant properties (Hanifah *et al*., 2022). Meanwhile, different roasting levels produced different characteristics of volatile compounds in fermented Liberica coffee from Riau (Wibowo *et al*., 2024). However, research on Liberica coffee from different locations in Jambi Province has not yet been conducted. Different types of coffee result in different degradation rates of chemical compounds (Macheiner *et al*., 2021).

The present work performed roasting on Liberica coffee harvested from different farming locations in Jambi Province, Indonesia, to discover the impacts of roasting on the profile of non-volatile, including chlorogenic acid, alkaloid contents, and volatile compounds. Conducting various research on Liberica coffee, particularly those designed to understand their characteristics and diversity, is key to strengthening their coffee trade status. Whenever Liberica coffee from several regions in Jambi Province has similar characteristics, it can be mixed and increased in trading capacity; otherwise, coffee with different characteristics can be used as data to determine its uniqueness.

Materials and methods

Materials

Liberica green beans (var. *Liberica tungkal*) were obtained from five regions (Betara, Bram Itam, Kuala Betara, Pengabuan, and Senyerang) in the Regency of Tanjung Jabung Barat, Jambi Province, Indonesia. Roasted beans were prepared by roasting 1 kg of green beans at an initial temperature of 200°C, and a final temperature of 195°C for 11 - 12 min using a roaster machine (Garuda Roaster, Indonesia) to reach the lightness level (L*) of 39.05 - 39.48, which was measured using a chromameter (CR-400, Konica Minolta, Osaka, Japan).

Chemicals (3-caffeoylquinic acid [3CQA], 4-caffeoylquinic acid [4CQA], 5-caffeoylquinic acid [5CQA], caffeine, theobromine, trigonelline hydrochloride, 3-heptanone, and alkane standard) were purchased from Sigma-Aldrich (St. Louis, MO, USA). LC-grade water, LC-grade methanol, and formic acid were purchased from Merck Millipore International (Darmstadt, Germany).

Extraction of non-volatile compounds

Roasted beans were ground using a grinder (Eureka EMG50 Sesto Fiorentino, Italy). For green beans, liquid nitrogen was added before grinding to facilitate the process. Coffee extraction was performed following a method previously described by Herawati *et al*. (2018). Approximately, 5 g of coffee powder was dissolved in 100 mL of boiling water, and stirred for 1 min. The mixture was then cooled with ice cubes, and stirred for 2 min. The brewed coffee was subsequently filtered using a Whatman no. 1 filter paper. The extraction was performed in triplicates, and the extract was stored at -20°C for further analyses.

Untargeted non-volatile compound analysis

Analysis of non-volatile compounds was conducted using the Vanquish Flex UHPLC Tandem Q Exactive Plus Orbitrap high-resolution mass spectrometer (UHPLC Q Orbitrap HRMS, Thermo Fisher Scientific, Bremen, Germany) with two replications. The procedure was performed following a previously described method (Herawati *et al*., 2019) with modification. Briefly, coffee filtrate was added with methanol (1:9, v/v), and filtered using a 0.22-µm Millipore membrane (Merck, KGaA, Darmstadt, Germany). The aliquot (5 µL) was injected into the UHPLC, and separated using an Accucore Vanquish C18+ column (100 × 2.1 mm, 1.5 µm) (Thermo Fisher Scientific, Bremen, Germany) at 40°C. The mobile phase consisted of methanol (A) and formic acid 0.05% in water (B), ran at a rate of 0.2 mL/min followed by gradient elution as follows: 0 min (5% A), 0 - 17 min (90% A), 17 - 20 min (90% A), 20 - 23

min (5% A), and 23 - 30 min (5% A). Positive and negative ionisation modes of electrospray ionisation (ESI) was applied, followed by Q Orbitrap mass analysis. The analysis was conducted at an *m/z* of 70 - 900; gas (N_2) and nebuliser average desolvation rates of 15 and 1.5 L/min, respectively; scan speed of 883 u/s; ESI voltages of +4.5 and -3.5 kV; capillary temperature of 250°C; DL temperature of 250°C, heated block temperature of 200°C; and detector voltages of -1.1 and -1.0 kV. UV detection was operated at wavelengths of 220, 265, 272, and 320 nm. Raw data from the analysis were processed using Discoverer 3.1 and a Thermo Xcalibur 2.0 mass spectral library (Thermo Fisher Scientific). The identified compounds were estimated by comparison using MS/MS information from databases and published studies.

Targeted non-volatile compound analysis

Chlorogenic acid

The analysis procedure fully conformed to a previous method (Herawati *et al*., 2019) in triplicate. Three standards (3CQA, 4CQA, and 5CQA) were used to quantify chlorogenic acid with a concentration range of 31.25 - 500 mg/mL at a 5-point calibration curve (Limit of Detection [LoD] of 3CQA = 0.79 mg/mL and R^2 = 0.997; LoD of 4CQA = 4.39 mg/mL and R^2 = 0.996; and LoD of 5CQA = 6.41 mg/mL and R^2 = 0.996).

Alkaloid content

The alkaloid content was determined following a previously described method (Caprioli *et al*., 2014), with a modification of 265-nm wavelength. The coffee filtrate was filtered using a 0.45-µm membrane (polytetrafluoroethylene, AVIXA, New Delhi, India). The aliquot (20 µL) was injected into HPLC (Shimadzu, LC20AD, Kyoto, Japan), and separated *via* a Zorbax C18 column (id. 4.6 × 150 mm, 5 µm) (Agilent Technologies, Santa Clara, USA). Quantitative analysis was conducted in triplicates using chemical standards of trigonelline, theobromine, and caffeine with a concentration range of 12.5 - 500 mg/mL at a 5-point calibration curve (LoD of trigonelline = 143 mg/mL and R^2 = 0.999; LoD of theobromine = 1.99 mg/mL and R^2 = 0.999; and LoD of caffeine = 1.70 mg/mL and R^2 = 0.999).

Volatile compound analysis

The volatile compounds were extracted and analysed following a method previously described by Caporaso *et al*. (2018) with modification. Approximately, 7 g of coffee powder was dropped in a 22-mL-vial for solid-phase microextraction, followed by 3 µL of 0.01% 3-heptanone in LC-MS-grade methanol (w/v) for green beans and 5 µL of 0.01% 3-heptanone for roasted beans. In the extraction of volatile compounds, 2-cm fibre DBV/Carbonex/PDMS was used for 30 min at 50°C. Furthermore, the coffee extract was injected into GC Agilent 7890 A (Agilent Technologies, Santa Clara, USA) equipped with a mass spectrophotometer detector (Agilent 597C XL EI/CI MSD, Agilent Technologies, Santa Clara, USA). The samples were eluted in column DB-Wax (30 m, 250 µm, 0.25 µm). The flow rate of carrier gas (helium) was 1 mL/min at an injection temperature of 250°C. The gradient mode for elusion was set as follows: 40°C for 5 min, 3°C/min to 180°C for 0 min, and then 10°C/min to 240°C for 0 min.

Volatile compounds were identified *via* computer matching by comparing the mass spectra patterns of the sample components with those of the same components in the NIST 12 (National Institute of Standard Technology) mass spectra library. Moreover, the linear retention index (LRI) of the compound from the sample was compared with that of the same compound with the same column from published references. The LRI of each component in the sample was determined based on the retention time of the *n*-alkane standard injected under the same conditions as the sample injection. Meanwhile, the relative content of the volatile compounds in the sample was calculated by comparing the area of the sample compound with that of the internal standard (3-heptanone 0.01%).

Statistical analysis

One-way analysis of variance with the Duncan's test ($p < 0.05$) was conducted to assess the impact of regional variations on the content of chlorogenic acids and alkaloids in green and roasted beans. The independent samples *t*-test ($\alpha = 5\%$) was conducted to verify the effect of the roasting process on non-volatile compounds, chlorogenic acids, and alkaloids, whereas the Mann-Whitney U test ($\alpha = 5\%$) was conducted to verify its impact on volatile compounds. The SPSS software (trial version, IBM Corporation, Austin, TX, USA) was used in the analysis. Furthermore, principal component analysis (PCA) was applied to group the coffee based on its non-volatile composition through untargeted and

targeted settings in the XLSTAT software version 2021 (Addinsoft, Paris, France).

Results and discussion

Profile of non-volatile compounds in Liberica coffee identified via untargeted analysis

The identification of non-volatile compounds was performed using UHPLC Q Orbitrap HRMS analysis with positive and negative ionisation modes and UV spectrum. Table 1 presents the total numbers of non-volatile compounds identified in green and roasted beans, which were 41 and 43, respectively. The compounds greatly varied, including alkaloids, organic acids, phenolics, phenolic derivatives, amino acids, fatty acids, and other constituents.

Alkaloids

Table 1 presents four alkaloid compounds in Liberica coffee. These compounds were identified using the positive ion mode (Alonso-Salces *et al*., 2009; Rodrigues and Bragagnolo, 2013); choline (1), trigonelline (4), theophylline (25), and caffeine (31) were detected in the sample. Alkaloid contains a nitrogen atom other than amide and peptide linkage. Purine alkaloid (*e.g.*, caffeine and theophylline) and pyridine alkaloid (*e.g*., trigonelline) are two alkaloid compounds commonly found in coffee, and choline is also commonly detected in Arabica and Robusta coffee (Wei *et al*., 2012; Hu *et al*., 2020). Caffeine, trigonelline, and choline were detected in green and roasted beans, whereas theophylline was only detected in Pengabuan green beans (GB4) and Senyerang green beans (GB5) (Table 1). As reported by Jeszka-Skowron *et al*. (2020), the difference in coffee origin correlated with the theophylline content in Arabica and Robusta green beans. However, the alkaloids present in Arabica and Robusta reported in many previous studies are not different from those present in Liberica assessed in the present work.

Roasting increased the relative area percentage of alkaloids ($p < 0.05$) in Liberica coffee (Table 2). Some alkaloid groups, such as caffeine, trigonelline, and choline in Arabica and Robusta coffee tended to be stable during a light-medium roasting stage (Herawati *et al*., 2018; Hu *et al*., 2020; Mehaya and Mohammad, 2020). Furthermore, roasting decreased bean mass due to the loss of chemicals, such as water, CO_2, and volatile compounds, but facilitated their extraction (Wei, 2015; Schouten *et al*., 2021). This presumably contributed to the increase in the relative area percentage of alkaloids in roasted beans.

Organic acids

The present work identified five organic acids in Liberica coffee through untargeted analysis (Table 1), which have also been previously detected in Arabica and Robusta coffee. Furthermore, the three acid compounds (citric acid (9), malic acid (10), and succinic acid (17)) found in all samples of the green and roasted beans of Liberica coffee are also the major organic acids in Arabica green beans (Yeager *et al*., 2021). Gluconic acid (2) was detected only in Bram Itam green beans (GB2). Based on a former study, gluconic acid was found in the green beans of Arabica and Robusta (De Bruyn *et al*., 2017). Meanwhile, mesaconic acid (18) was the only organic acid detected in roasted beans (Table 1). The compound was also found in Arabica and Robusta roasted beans (Gamboa-Becerra *et al*., 2017). Results showed that the composition of organic acids in Liberica coffee was comparable with those of Arabica and Robusta coffee.

The degree of commercial roasting did not affect the relative area percentage of organic acids ($p > 0.05$) in Liberica coffee (Table 2). This could have been due to the formation of organic acid compounds, whereas some compounds are degraded during roasting. For example, mesaconic acid was formed due to degradation of citric acid during roasting (Feldman *et al*., 1969).

Phenolic compounds

The present work identified 20 phenolic compounds using negative and positive ion modes (Table 1). Many studies also previously identified phenolics using the positive and negative ion modes (Alonso-Salces *et al*., 2009; Rodrigues and Bragagnolo, 2013; Asamenew *et al*., 2019).

A total of ten phenolic compounds, including quinic acid (6), 3-caffeoyquinic acid (22), 5CQA (26, 32), 3-O-feruloylquinic acid (27), 7-hydroxycoumarine (28), 4CQA (29), 5-O-feruloylquinic acid (35), and 4-O-feruloylquinic acid (41) were identified in the green and roasted beans. Furthermore, six phenolic compounds, namely caffeic acid (30), 5-*p*-coumaroylquinic acid (33), 3,4-O-dicaffeoylquinic acid (46), 3,5-O-dicaffeoylquinic acid (47), 4-O-caffeoyl-5-O-feruloylquinic acid (50), and 4,5-O-dicaffeoylquinic acid (51) were identified

Table 1. Profile of non-volatile compounds in Liberica coffee harvested from different locations in Jambi, Indonesia.

No.	Compound	RT (min)	MW	*m/z*	MS^2 (*m/z*)	Formula	Error (ppm)	Sample
				Alkaloids				
1	Choline	1.08	103.09974	104.10690 [M+H]+	104, 60	$C_5H_{13}NO$	-0.29	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
4	Trigonelline	1.12	137.04733	138.05467 [M+H]+	138	$C_7H_7NO_2$	2.48	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
25	Theophylline	6.04	180.06444	181.07164 [M+H]+	181, 84, 121, 124	$C_7H_8N_4O_2$	1.44	GB: 4, 5
31	Caffeine	7.30	194.07961	195.08690 [M+H]+	195, 138	$C_8H_{10}N_4O_2$	3.92	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
				Organic acids				
2	Gluconic acid	1.10	196.05758	195.05026 [M-H]-	195, 129, 75	$C_6H_{12}O_7$	-3.67	GB: 2
9	Citric acid	1.15	192.02631	191.01891 [M-H]-	111, 87	$C_6H_8O_7$	-3.59	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
10	DL-Malic acid	1.17	134.02100	133.01331 [M-H]-	115, 71, 133	$C_4H_6O_5$	-5.08	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
17	Succinic acid	1,90	118.02600	117.01826 [M-H]-	73, 117	$C_4H_6O_4$	-5.08	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
18	Mesaconic acid	2,36	130.02600	129.01834[M-H]-	85, 61, 87, 128	$C_5H_6O_5$	-4.61	RB: 1, 2, 3, 4, 5
				Phenolic compounds				
6	Quinic acid	1.13	192.06252	191.05528 [M-H]-	191	$C_7H_{12}O_6$	4.48	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
21	3-O-Caffeoylquinic acid (1)	4.97	354.09479	353.08765 [M-H]-	191, 135, 179	$C_{16}H_{18}O_9$	0.82	RB: 3
22	3-O-Caffeoylquinic acid (2)	5.20	354.09433	353.08768 [M-H]-	191, 135, 179	$C_{16}H_{18}O_9$	2.12	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
24	4-Hydroxybenzoic acid	5.54	138.03100	137.02346 [M-H]-	137	$C_7H_6O_3$	5.00	RB: 1, 2, 3, 4, 5
26	5-O-Caffeoylquinic acid (1)	6.64	354.09434	353.08740[M-H]-	191	$C_{16}H_{18}O_9$	2.09	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
27	3-O-Feruloylquinic acid	6.85	368.11035	367.10345 [M-H]-	193, 134, 191 173	$C_{17}H_{20}O_9$	1.03	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
28	7-Hydroxycoumarine	5.18	162.03114	163.03854 [M+H]+	163, 145, 117	$C_9H_6O_3$	3.39	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
29	4-O-Caffeoylquinic acid	7.03	354.09434	353.08768 [M-H]-	191, 173, 135, 179	$C_{16}H_{18}O_9$	1.64	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
30	Caffeic acid	7.20	180.04158	179.03430 [M-H]-	135	$C_9H_8O_4$	3.72	GB: 1, 2, 3, 4, 5
32	5-O-Caffeoylquinic acid (2)	7.80	354.09458	353.08750 [M-H]-	191	$C_{16}H_{18}O_9$	1.41	GB: 1, 2, 3, 4, 5, RB: 1, 2, 3, 4, 5
33	5-*p*-Coumaroylquinic acid	7.85	338.10006	337.09344 [M-H]-	191, 163	$C_{16}H_{18}O_8$	0.30	GB: 1, 2, 3, 4, 5
35	5-O-Feruloylquinic acid	8.03	368.11062	367.10345 [M-H]-	191, 173	$C_{17}H_{20}O_9$	0.30	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
40	Ferulic acid	8.91	194.05734	193.04999 [M-H]-	193	$C_{10}H_{10}O_4$	2.89	RB: 1, 2, 3, 4, 5
41	4-O-Feruloylquinic acid	9.27	368.11030	367.10345 [M-H]-	173, 191	$C_{17}H_{20}O_9$	1.17	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
46	3,4-O-Dicaffeoylquinic acid	10.00	516.12670	515.11969 [M-H]-	353, 191, 179, 173, 135	$C_{25}H_{24}O_{12}$	1.17	GB: 1, 2, 3, 4, 5
47	3,5-O-Dicaffeoylquinic acid	10.84	516.12670	515.11975 [M-H]-	353, 179	$C_{25}H_{24}O_{12}$	0.14	GB: 1, 2, 3, 4, 5
48	3,4-Dimethoxycinnamic acid	11.20	208.07343	209.08060 [M+H]+	191, 163	$C_{11}H_{12}O_4$	0.58	RB: 1, 2, 3, 4, 5

49	3-Methylsalicylic acid	11.54	152.04655	151.03932 [M-H]-	107, 151	$C_8H_8O_3$	5.20	GB: 1, 4, 5 RB: 1, 2, 3, 4, 5
50	4-O-Caffeoyl-5-O-feruloylquinic acid	11.81	530.14245	529.13684 [M-H]-	353, 367, 173, 191	$C_{26}H_{26}O_{12}$	-0.06	GB: 4
51	4,5-O-Dicaffeoylquinic acid	12.02	516.12690	515.11938 [M-H]-	353, 173	$C_{25}H_{24}O_{12}$	-0.25	GB: 1, 2, 3, 4, 5
	Phenolic derivatives							
36	3-Caffeoylquinic acid lactone	8.12	336.08450	335.07761 [M-H]-	161, 135	$C_{16}H_{16}O_8$	0.03	RB: 1, 2, 3, 4, 5
39	4-Caffeoylquinic acid lactone	8.66	336.08450	335.07761 [M-H]-	161, 135	$C_{16}H_{16}O_8$	0.00	RB: 1, 2, 3, 4, 5
44	3-Feruloylquinic acid lactone	9.54	350.09999	349.09280 [M-H]-	175, 160, 149, 193	$C_{17}H_{18}O_8$	0.49	RB: 1, 2, 3, 4, 5
45	4-Feruloylquinic acid lactone	9.94	350.10022	349.09286 [M-H]-	175, 160, 149, 193	$C_{17}H_{18}O_8$	-0.17	RB: 1, 2, 3, 4, 5
	Amino acids and derivatives							
5	DL-Arginine	1.12	174.11142	175.11864 [M+H]+	70, 60, 160	$C_6H_{14}H_4O_2$	1.44	GB: 1, 2, 3, 4, 5
7	L-Tyrosine	1.14	181.07363	182.08130 [M+H]+	136, 123, 165	$C_9H_{11}NO_3$	1.44	RB: 1, 2, 3, 4, 5
8	L-Glutamic acid	1.15	147.05285	148.06015 [M+H]+	84, 130, 102	$C_5H_9NO_4$	2.04	GB: 1, 2, 3, 4, 5
11	L-Histidine	1.17	155.06933	156.07657 [M+H]+	110, 156, 85	$C_6H_9N_3O_2$	0.90	GB: 3
12	Valine	1.17	117.07891	118.08626 [M+H]+	72, 70	$C_5H_{11}NO_2$	0.51	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
13	L-Aspartic acid	1.20	133.03738	134.04468 [M+H]+	86, 74, 69, 88	$C_4H_7NO_4$	0.90	GB: 1, 3, 4, 5
14	L-Norleucine	1.26	131.09439	132.10164 [M+H]+	86	$C_6H_{13}NO_2$	1.75	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
16	L-Pyroglutamic acid	1.62	129.04210	130.04962 [M+H]+	84, 130	$C_5H_7NO_3$	3.80	GB: 5 RB: 1, 2, 3, 4, 5
20	L-Phenylalanine	3.64	165.07848	166.08572 [M+H]+	120, 85	$C_9H_{11}NO_2$	2.97	GB: 1, 2, 3, 4, 5
23	DL-Tryptophan	5.34	204.08932	205.09665 [M+H]+	146, 188, 118	$C_{11}H_{12}N_2O_2$	2.69	GB: 1, 2, 3, 4, 5
37	N-Acetyl-L-leucine	8,55	173.10472	172.09732 [M-H]-	130, 170, 172	$C_8H_{15}NO_3$	2.72	RB: 1, 2, 3, 4, 5
38	N-Acetyl-L-phenylalanine	8.59	207.08905	206.08177 [M-H]-	164, 147, 296	$C_{11}H_{13}NO_3$	2.37	GB: 1, 2, 3, 4, 5
43	N-Acetyl-DL-tryptophan	9.36	246.10009	247.10739 [M+H]+	159, 188, 201	$C_{13}H_{14}N_2O_3$	1.42	RB: 1, 2, 3, 4, 5
	Fatty acids							
42	Suberic acid	9.32	173.08118	174.08850 [M-H]-	111, 173, 83	$C_8H_{14}O_4$	4.02	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
52	Dodecanedioic acid	15.52	230.15153	229.14426 [M-H]-	229, 167, 211	$C_{12}H_{22}O_4$	1.17	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
53	Hexadecanedioic acid	18.73	286.21446	285.20718 [M-H]-	285, 223, 267	$C_{16}H_{30}O_4$	-0.21	GB: 1, 2, 3, 4
54	Palmitoleic acid	18.89	254.22448	255.23116 [M+H]+	219	$C_{16}H_{30}O_2$	0.39	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
55	16-Hydroxyhexadecanoic acid	18.90	271.22794	272.23512 [M-H]-	271, 273, 272	$C_{16}H_{32}O_3$	0.07	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
56	Stearic acid	19.95	284.27146	283.26416 [M-H]-	283, 284	$C_{18}H_{36}O_2$	0.25	RB: 1, 2, 3, 4, 5
57	Linoleic acid	22.56	280.24020	279.23279 [M-H]-	279	$C_{18}H_{32}O_2$	0,11	GB: 1, 2, 3, 4, 5
57	1-Stearoylglycerol	28.95	358.30715	359.31433 [M+H]+	57, 341, 95	$C_{21}H_{42}O_4$	3.21	GB: 1, 2, 3, 4, 5 RB: 1, 2, 3, 4, 5
	Other components							
3	D-(-)-Fructose	1.11	180.06266	179.05536 [M-H]-	161, 179, 85	$C_6H_{12}O_6$	4.00	RB: 1, 2, 3, 4, 5
15	Nicotinic acid	1.36	123.03195	124.03925 [M+H]+	124, 126	$C_6H_5NO_2$	0.57	RB: 1, 2, 3, 5
19	5-Hydroxymethyl furfural	3.63	126.03149	127.03874 [M+H]+	109, 81	$C_6H_6O_3$	1.59	RB: 1, 2, 3, 4, 5
34	3-Hydroxy-2-methylpyridine	8.00	109.05275	110.06010 [M+H]+	82, 110, 67	C_6H_7NO	0.09	RB: 1, 2, 3, 4, 5

Green beans (GB) and roasted beans (RB) were collected from five different locations in Jambi, Indonesia: (1) Betara, (2) Bram Itam, (3) Kuala Betara, (4) Pengabuan, and (5) Senyerang.

Table 2. Effects of roasting on non-volatile compounds.

Compound group	% Area relative					
	1	2	3	4	5	Mean
Green bean						
Alkaloids*	56.05	56.73	53.36	52.12	54.33	54.52 ± 1.90[a]
Phenolics**	25.29	24.04	23.30	27.08	28.18	25.58 ± 2.04[b]
Organic acids	9.83	9.78	11.39	11.09	8.17	10.05 ± 1.28[a]
Amino acids**	6.61	5.40	9.28	7.24	6.32	6.97 ± 1.45[b]
Phenolic derivatives	nd	nd	nd	nd	nd	-
Furan	nd	nd	nd	nd	nd	-
Pyridine	nd	nd	nd	nd	nd	-
Fatty acids*	2.21	2.31	2.66	2.26	2.28	2.34 ± 0.18[a]
Fructose	nd	nd	nd	nd	nd	-
Roasted bean						
Alkaloids*	60.56	60.49	59.29	61.35	60.65	60.47 ± 0.74[b]
Phenolics**	19.01	18.25	18.92	19.22	18.86	18.77 ± 0.35[a]
Organic acids	11.16	13.23	11.32	11.09	11.32	11.62 ± 0.90[a]
Amino acids**	1.67	1.89	1.69	1.57	1.65	1.69 ± 0.12[a]
Phenolic derivatives	3.30	2.04	3.61	2.74	3.50	3.04 ± 0.65
Furan	0.41	0.51	0.45	0.45	0.45	0.45 ± 0.04
Pyridine	0.53	0.51	0.51	0.36	0.35	0.45 ± 0.09
Fatty acids*	3.01	2.71	3.87	2.83	2.83	3.05 ± 0.47[b]
Fructose	0.05	0.10	0.04	0.06	0.06	0.06 ± 0.02

Green beans (GB) and roasted beans (RB) were collected from five different locations in Jambi, Indonesia: (1) Betara, (2) Bram Itam, (3) Kuala Betara, (4) Pengabuan, and (5) Senyerang. Values are mean ± standard deviation of duplicate (n = 2). nd: not identified. Means with similar lowercase superscript within coffee group are not significantly different (p > 0.05). (*) Indicates increase in relative area percentage upon roasting. (**) Indicates decrease in relative area percentage upon roasting.

in green beans, whereas two compounds, ferulic acid (40) and 3,4-dimethoxycinnamic acid (48) were identified in roasted beans.

The present work identified two *cis-trans* isomers for compounds 5CQA and 3CQA. Compound 26 was *trans*-5CQA, whereas compound 32 possibly corresponded to *cis*-5CQA. Compound 21 was *cis*-3CQA, whereas compound 22 was *trans*-3CQA. In a previous study (Clifford *et al*., 2008), *cis*-5CQA was reported to be more hydrophobic, causing it to elute more slowly than its *trans*-compounds, as analysed in reversed-phase chromatography with UV detection at 320 nm. In addition, the present work showed the similarity of fragmentation between *cis*-3CQA and *trans*-3CQA, but their retention time differed, as observed in reversed-phase chromatography with UV detection at UV 320 nm. *Trans*-3CQA was more hydrophobic; thus, it eluted more slowly than *cis*-3CQA (Clifford *et al*., 2008). The biosynthetic pathway of CQAs in plants produced CQAs at *trans* isomers. *Cis*-CQA isomers can be formed during processing treatments, including UV exposure, sun-drying, and roasting (Clifford, 2000; Asamenew *et al*., 2019).

Quinic acid was detected in green and roasted beans, caffeic acid only in green beans, and ferulic acid only in roasted beans (Table 1). Quinic, caffeic, and ferulic acids are common free cinnamic acids in green beans (Asamenew *et al*., 2019). However, as Somporn *et al*. (2011) reported, ferulic acid was not detected in Arabica green beans, but its content increased with the increase in roasting degree. Free cinnamic acid was naturally detected in green beans, and it can also form through hydrolysis and decomposition of CQA and feruloylquinic acid (FQA) during roasting (Dawidowicz and Typek, 2016). However, previous studies reported the degradation of caffeic acid compounds in Arabica coffee in light roasting levels, but the level of the compound was increased at medium roasting levels (Somporn *et al*., 2011). CQA, FQA, and diCQA (dicaffeoylquinic acid) are three major chlorogenic acids in green beans (Bicho *et al*., 2012; Rodrigues and Bragagnolo, 2013). Meanwhile, *p*-

coumaroylquinic acid (pCoQA) was assigned as a minor chlorogenic acid in green beans, whereas 5-pCoQA was assigned as a major pCoQA in Arabica, Robusta, and some Liberica coffee. Interestingly, several Liberica coffee were reported to have pCoQA compounds, dominated by the 3-isomer (Ortiz *et al*., 2019). The putative compound of 4-O-caffeoyl-5-O-feruloylquinic acid (4C,5FQA) was only detected in Pengabuan green beans (GB4). The compound 4C,5FQA belonged to minor CQAs in Arabica and Robusta coffee, and only detected in particular areas (Mullen *et al*., 2013).

The present work demonstrated the presence of two phenolic compounds (24 and 48), particularly in Arabica and Robusta coffee, similar to previous studies (Bicho *et al*., 2012; Somporn *et al*., 2012). Both phenolics were only detected in roasted beans of Liberica; a previous study (Somporn *et al*., 2011) also reported that roasting increased the content of 4-hydroxybenzoic acid in Arabica coffee.

Phenolics are among the secondary metabolites synthesised by plants in response to environmental stress. The presence of CQA, FQA, diCQA, ferulic acid, and 3,4-dimethoxycinnamic acid confer coffee beans with distinct characteristics based on their genotypes, namely, Arabica, Robusta, and Excelsa (Bicho *et al*., 2012). However, 3-methylsalysilate was only detected in Liberica coffee in the present work. 3-methylsalysilate is often found in fruits (Aresta and Zambonin, 2016), and yet to be reported in Arabica and Robusta coffee. Notably, the phenolic compounds in Liberica coffee tested in the present work were comparable with those in Arabica and Robusta reported in previous studies. The degree of commercial roasting decreased the relative area of phenolics in Liberica coffee (Table 2). Phenolic compounds are thermolabile, and roasting was also found responsible for the decrease in total phenolics in Arabica and Robusta coffee (Herawati *et al*., 2018; Mehaya and Mohammad, 2020).

Phenolic derivatives

Phenolic derivatives were identified, including quinic acid lactone (Table 1), based on the negative ion mode. CQA lactones (CQL) included 3CQL and 4CQL, whereas feruloyl quinic acid lactones (FQL) included 3FQL and 4FQL. CQL and FQL were results of lactonisation after the loss of water molecules in the quinic acid ring, and only occurred in isomers 3 and 4, induced by the roasting of Arabica and Robusta (Farah *et al*., 2005).

Amino acids and derivatives

The amino acid groups were identified using the positive and negative ion modes (Table 1) which yielded 13 compounds and their derivatives in coffee samples. Six compounds (DL-arginine, L-glutamic acid, L-aspartic acid, L-phenylalanine, DL-tryptophan, and N-acetyl-L-phenylalanine) were detected in green beans. L-histidine was also detected and was only found in Bram Itam green beans (GB2).

Several amino acids and their derivatives were also detected in roasted beans, namely, L-tyrosine, L-pyroglutamic acid, N-acetyl-L-leucine, and N-acetyl-DL-tryptophan. Furthermore, valine and L-norleucine were found in green and roasted beans. Several amino acids, such as histidine, were not detected in roasted beans, which was possibly due to their instability against heat exposure. The high-temperature roasting treatment also triggered the Maillard reaction between the amino acids and reducing sugars, thereby yielding other compounds, such as arginine, glutamic acid, and aspartic acid. These amino acids were important constituents for the synthesis of melanoidin (Hofmann, 1998; Wei *et al*., 2012). This resulted in a decrease in the relative area percentage for the amino acid group ($p < 0.05$) in the roasting stage (Table 2). However, some amino acids in Arabica and Robusta coffee were heat-stable, such as tyrosine and valine (Casal *et al*., 2005).

Amino acids are minor non-volatile compounds in coffee beans, and their compositions in Arabica and Robusta coffee (Casal *et al*., 2005) are similar to those in Liberica coffee observed in the present work. The derivatives (N-acetyl-amino acid), including N-acetyl phenylalanine in coffee beans, as well as N-acetyl-DL-tryptophan and N-acetyl-L-leucine, were detected in roasted beans. Previous studies (Raza *et al*., 2021; Zhao *et al*., 2021) reported that these three compounds were the results of stress conditions during the growth of rapeseed. In the case of coffee beans, the derivatives were only detected in the Liberica coffee tested in the present work.

Fatty acids and their conjugates

Fatty acid analysis was conducted in the positive and negative ion modes (Table 1), which detected seven fatty acids in Liberica coffee, including hexadecanedioic and linoleic acids in green beans, as well as stearic acid in roasted beans. Meanwhile, suberic, dodecanedioic, palmitoleic, and 16-hydroxydecanoic acids, as well as 1-stearoylglycerol, were detected in green and roasted

beans. Linoleic and stearic acids are two major fatty acids in Arabica coffee. Linoleic acid is abundant in green beans; however, palmitoleic acid is a minor component in green beans (Fitri *et al*., 2021).

Table 2 shows that commercial roasting increased the relative area percentage for fatty acid groups ($p < 0.05$) in Liberica coffee. The increase in total fatty acid induced by roasting was also reported in Luwak Arabica coffee (Fitri *et al*., 2021). The increasing relative area percentage for fatty acids upon roasting may be associated with the movement of oil droplets to the surface as the structure of coffee beans degrades (Hu *et al*., 2020), leading to the rising extractability of fatty acids in roasted beans.

Other components

Fructose was detected in the negative ion mode, whereas nicotinic acid, 5-hydroxymethyl furfural (HMF), and 3-hydroxy-2-methylpyridine were detected in the positive ion mode (Table 1). All of these compounds were identified only in roasted beans.

Fructose is a natural sugar in green beans (Bicho *et al*., 2012; Somporn *et al*., 2012). However, fructose in roasted beans is formed due to the hydrolysis of sucrose during roasting (Diviš *et al*., 2019), whereas nicotinic acid is a result of trigonelline degradation due to pyrolysis during roasting (Taguchi *et al*., 1985; Viani and Petracco, 2012). HMF and 3-hydroxy-2-methylpyridine were also detected. HMF belongs to the furan group, acting as an intermediate compound of the Maillard reaction induced by roasting (Mehaya and Mohammad, 2020), whereas 3-hydroxy-2-methylpyridine can be formed through the reaction between amino acids (phenylalanine) and glucose present at high temperature (Baltes and Mevissen, 1988).

Targeted analysis of non-volatile compounds

We conducted a targeted analysis of non-volatile compounds in samples, focusing on chlorogenic acids (3CQA, 4CQA, and 5CQA) and alkaloids (trigonelline, theobromine, and caffeine). The results indicated that the most abundant chlorogenic acid in five coffee brew samples was 5CQA, ranging from 3.91 to 5.20 g/100 g db (dry basis), whereas 4CQA and 3CQA reached 0.87 - 1.32 and 0.60 - 0.93 g/100 g db, respectively. From Table 3, it can be seen that the contents of chlorogenic acids (3CQA, 4CQA, and 5CQA) in Liberica green beans were higher than those in Arabica and Robusta reported in previous studies. Arabica green beans contained 0.15 - 0.14 g/100 g db (3CQA), 0.21 - 0.48 g/100 g db (4CQA), and 2.23 - 4.53 g/100 g db (5CQA); and Robusta green beans contained 0.27 - 0.57 g/100 g db (3CQA), 0.37 - 0.68 g/100 g db (4CQA), and 2.16 - 4.29 g/100 g db (5CQA) (Alonso-Salces *et al*., 2009).

The different growing locations of Liberica green beans in Jambi Province resulted in different contents of 5CQA, 4CQA, 3CQA, and total CQA ($p < 0.05$). The highest contents of 3CQA, 4CQA, and 5CQA were detected in Kuala Betara green beans (GB3), whereas the lowest contents were detected in Bram Itam green beans (GB2), as shown in Table 3. Similarly, Mehari *et al*. (2016b) reported the difference in chlorogenic acid contents in Arabica green beans due to the different locations. However, these chemicals did not differ between roasted beans (Table 3). As reported by Badmos *et al*. (2020), the growing locations did not affect the chlorogenic acid content of Arabica roasted beans, but their quantity in the beans was not mentioned. Moreover, our experiment showed that the roasting process decreased the contents of 3CQA, 4CQA, 5CQA, and total CQA ($p < 0.05$). The process accounted for a significant drop of up to 49% for 5CQA, 22% for 4CQA, and 29% for 3CQA, which resulted in a 42% decrease in the total CQA in Liberica coffee. Previous research demonstrated that the degradation of 5CQA compounds during commercial roasting was more pronounced in Arabica coffee (37.9 to 5.54 mg/g or 85% loss) than in Robusta coffee (34.1 to 10.7 mg/g or 68.6% loss) (Macheiner *et al*., 2021). In addition, Arabica coffee exhibited a 71.0 - 86.4% loss of phenolic acids, whereas Robusta coffee showed a 84.4 - 85.6% loss (Asamenew *et al*., 2019). The highest decrease was detected in 5CQA, which was reported as the most susceptible to heat, followed by 3CQA and 4CQA in Arabica coffee (Asamenew *et al*., 2019). Another study reported that species variations are associated with the degradation rate of CQAs, with Robusta exhibiting a more accelerated degradation of 5CQA than Arabica (Yeager *et al*., 2021). However, the degradation resulting from CQA isomerisation in Robusta is slower than that in Arabica during the initial cracking phase of the roasting process (Macheiner *et al*., 2021). This indicated that the various species exhibited a diminished response to roasting.

During roasting, 5CQA initially turned into 4CQA, and finally into 3CQA, which contributed to

Table 3. Contents of chlorogenic acids and alkaloids in coffee samples.

Sample	Chlorogenic acid (g/100 g dry basis)				Alkaloid (g/100 g dry basis)			
	3CQA	4CQA	5CQA	Total CQA	Trigonelline	Theobromine	Caffeine	Chlorogenic acids Alkaloids
Green bean								
GB 1	0.70 ± 0.07^{b}	1.09 ± 0.12^{b}	5.18 ± 0.49^{c}	6.97 ± 0.68^{bc}	0.89 ± 0.04^{b}	0.77 ± 0.01^{b}	4.12 ± 0.21^{c}	5.78 ± 0.17^{c}
GB 2	0.60 ± 0.05^{a}	0.87 ± 0.09^{a}	3.91 ± 0.32^{a}	5.37 ± 0.46^{a}	0.69 ± 0.01^{a}	0.64 ± 0.05^{a}	3.04 ± 0.12^{a}	4.36 ± 0.16^{a}
GB 3	0.93 ± 0.07^{c}	1.32 ± 0.13^{c}	5.20 ± 0.41^{c}	7.45 ± 0.61^{c}	0.75 ± 0.02^{a}	0.95 ± 0.02^{d}	4.07 ± 0.09^{c}	5.78 ± 0.12^{c}
GB 4	0.73 ± 0.02^{b}	0.98 ± 0.06^{ab}	4.92 ± 0.20^{bc}	6.63 ± 0.27^{bc}	0.84 ± 0.06^{b}	0.81 ± 0.01^{b}	3.65 ± 0.14^{b}	5.30 ± 0.09^{b}
GB 5	0.79 ± 0.05^{b}	1.10 ± 0.12^{b}	4.43 ± 0.38^{ab}	6.32 ± 0.55^{ab}	0.69 ± 0.02^{a}	0.89 ± 0.01^{c}	3.75 ± 0.03^{b}	5.33 ± 0.06^{b}
Range	0.60 - 0.93	0.87 - 1.32	3.91 - 5.20	5.37 - 7.45	0.69 - 0.89	0.64 - 0.95	3.04 - 4.12	4.36 - 5.78
Mean*	0.75 ± 0.12^{b}	1.07 ± 0.17^{b}	4.73 ± 0.55^{b}	6.55 ± 0.78^{b}	0.77 ± 0.09^{a}	0.81 ± 0.12^{a}	3.77 ± 0.43^{a}	5.31 ± 0.58^{a}
Roasted bean								
RB 1	0.48 ± 0.05^{a}	0.76 ± 0.08^{a}	2.25 ± 0.19^{a}	3.49 ± 0.33^{a}	0.72 ± 0.04^{a}	0.62 ± 0.04^{a}	4.17 ± 0.23^{a}	5.51 ± 0.31^{a}
RB 2	0.53 ± 0.04^{a}	0.83 ± 0.07^{a}	2.38 ± 0.17^{a}	3.74 ± 0.28^{a}	0.89 ± 0.03^{b}	0.69 ± 0.04^{a}	4.11 ± 0.21^{a}	5.69 ± 0.18^{a}
RB 3	0.56 ± 0.04^{a}	0.89 ± 0.08^{a}	2.62 ± 0.20^{a}	4.06 ± 0.32^{a}	0.72 ± 0.06^{a}	0.68 ± 0.08^{a}	4.28 ± 0.22^{a}	5.67 ± 0.35^{a}
RB 4	0.53 ± 0.04^{a}	0.83 ± 0.07^{a}	2.42 ± 0.14^{a}	3.78 ± 0.24^{a}	0.83 ± 0.06^{b}	0.72 ± 0.02^{a}	4.47 ± 0.54^{a}	6.02 ± 0.57^{a}
RB 5	0.55 ± 0.00^{a}	0.85 ± 0.03^{a}	2.44 ± 0.09^{a}	3.84 ± 0.12^{a}	0.69 ± 0.03^{a}	0.74 ± 0.08^{a}	4.10 ± 0.07^{a}	5.52 ± 0.03^{a}
Range	0.48 - 0.56	0.76 - 0.89	2.25 - 2.62	3.49 - 4.06	0.69 - 0.89	0.62 - 0.74	4.10 - 4.47	5.51 - 6.02
Mean*	0.53 ± 0.03^{a}	0.83 ± 0.47^{a}	2.42 ± 0.13^{a}	3.78 ± 0.20^{a}	0.77 ± 0.09^{a}	0.69 ± 0.05^{a}	4.23 ± 0.16^{a}	5.68 ± 0.21^{a}

Values are mean ± standard deviation of triplicate (n = 3) and expressed in g/100 g db. (dry basis) of coffee samples. The means with the same lowercase superscript within the same column per region are not significantly different (p > 0.05) based on Duncan's test. *Mean represents the average value of green bean (GB) or roasted bean (RB) from five regions. Same superscripts following the values in each GB and RB column indicate no significant difference (p > 0.05) based on the t-test.

the increase in the 3CQA and 4CQA contents in Arabica and Robusta coffee (Deshpande *et al*., 2014; Schouten *et al*., 2021). Notably, in some cases, 3CQA is not the final form as it can be hydrolysed to caffeic and quinic acids. This means that the contents of 3CQA and 4CQA in the final product might be lower after roasting (Asamenew *et al*., 2019). In the present work, commercial roasting was responsible for the decrease in the 3CQA, 4CQA, and 5CQA contents in Liberica coffee.

The contents of caffeine, trigonelline, and theobromine in Liberica green beans from the five different regions were 3.04 - 4.12, 0.69 - 0.89, and 0.64 - 0.95 g/100 g db, respectively. The special feature of Liberica green beans investigated in the present work was the higher contents of theobromine and caffeine, but lower content of trigonelline than those of Arabica and Robusta previously reported. Arabica green beans may contain 0.02 - 0.03 g/100 g db (theobromine), 1.01 - 1.39 g/100 g db (caffeine), and 0.92 - 1.78 g/100 g db (trigonelline), whereas Robusta green beans may contain 0.02 - 0.05 g/100 g db (theobromine), 1.37 - 2.56 g/100 g db (caffeine), and 1.15 - 1.59 g/100 g db (trigonelline) (Jeszka-Skowron *et al*., 2020).

The lowest contents of alkaloids (trigonelline, theobromine, and caffeine) were found in Bram Itam green beans (GB2). In this case, the locations of coffee origin substantially affected the contents of caffeine, trigonelline, and theobromine (p < 0.05) in Liberica green beans. The effect of the variability in the growing sites was also reported in Arabica green beans (Mehari *et al*., 2016a), indicating that the contents of caffeine, trigonelline, and theobromine also substantially varied. Furthermore, no significant difference was observed in the theobromine and caffeine contents in roasted beans from the five regions studied (p > 0.05).

Based on previous studies (Herawati *et al*., 2018; Jeszka-Skowron *et al*., 2020), the contents of trigonelline, theobromine, and caffeine in Arabica and Robusta coffee markedly decreased due to roasting. Meanwhile, Hu *et al*. (2020) reported that light and medium roasting did not change the trigonelline and caffeine contents in Arabica coffee. The variations in Arabica and Robusta coffee species correlated with the decrease in alkaloid contents after roasting (Schouten *et al*., 2021). In the present work, commercial roasting did not alter the contents of trigonelline, theobromine, caffeine, and total

alkaloids (p > 0.05) in Liberica coffee. Caffeine, which belongs to alkaloids, is more thermostable than chlorogenic acids (Mehaya and Mohammad, 2020). Alkaloids exhibit better stability during roasting, which is likely attributed to their aromatic ring structure, whereas chlorogenic acid, an ester formed from caffeic and quinic acids, possesses a more unstable ester link and a hydroxyl group that is believed to be more susceptible to heat degradation.

The present work reported that roasted coffee with a similar colour (shown by the L* value) produced a uniform profile of non-volatile compounds (chlorogenic acid, alkaloids) in Liberica coffee (Table 3). During roasting, complex chemical reactions variably occurred, including the degradation of pigment (chlorophyll) and the formation of brown pigment (melanoidin), as a result of the Maillard reaction; hence, colour was one of the critical parameters for the degree of coffee roasting. As previously mentioned (Münchow *et al*., 2020), lightness representing the sample colour of Arabica roasted coffee can determine the sensory profile of a coffee brew.

PCA mapping of green and roasted beans

Untargeted analysis

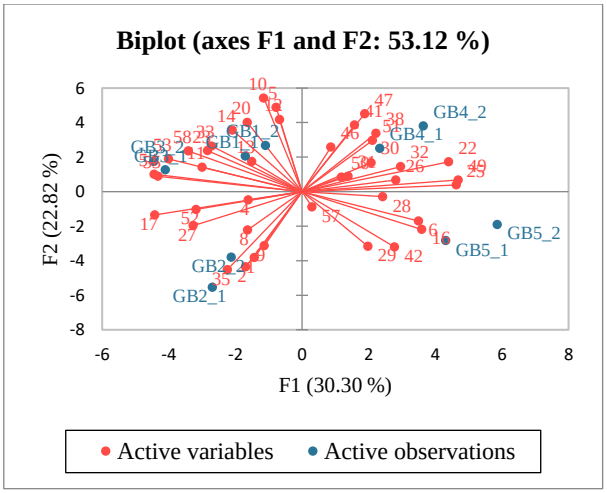
The results indicated that the non-volatile compounds in Liberica green and roasted beans greatly differed between the growing regions in Jambi Province. The mapping for untargeted analysis of non-volatile compounds in green and roasted beans was prepared based on the relative area percentage of the identified non-volatile compounds.

Non-volatile compounds in Liberica green bean samples tended to scatter over the area. As illustrated in Figure 1a, the PCA revealed a total PC of 53.12% (30.30% PC1; 22.82% PC2) of total diversity. The position of GB1 was in proximity to GB3, whereas the remaining was not. The value of total PC was low, suggesting that the grouping of green beans based on their growing locations remained unsatisfied.

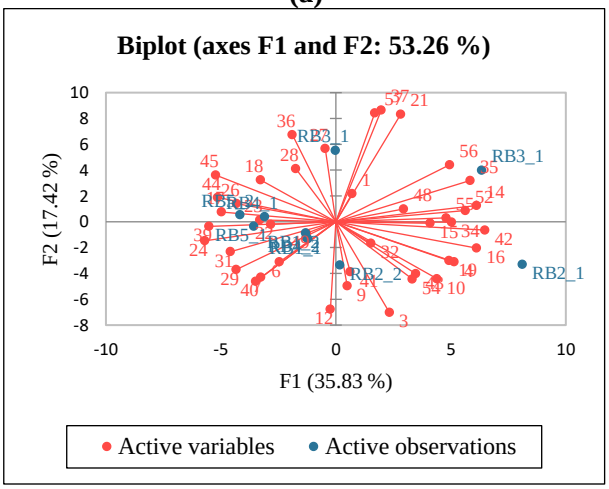
As revealed in Figure 1b, the total PC of roasted bean samples was 53.26% (35.83% PC1; 17.42% PC2), and the position of the roasted beans was scattered. Therefore, there was no specific group based on non-volatile compounds (untargeted).

Targeted analysis

The results indicated that the non-volatile



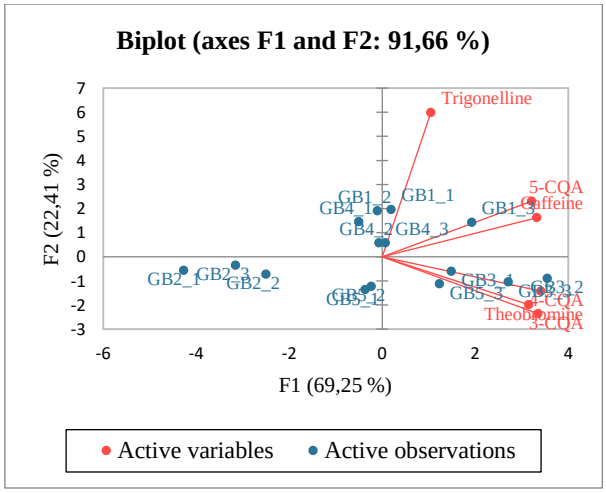
(a)



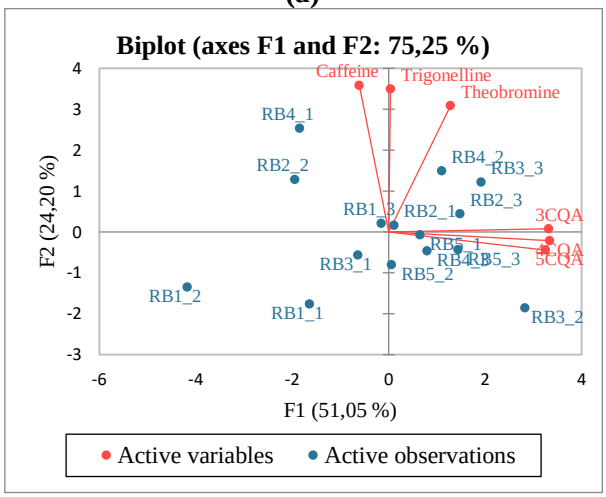
(b)

Figure 1. Biplot PCA for untargeted non-volatile compounds in **(a)** green bean (GB) samples, and **(b)** roasted bean (RB) samples from (1) Betara, (2) Bram Itam, (3) Kuala Betara, (4) Pengabuan, and (5) Senyerang.

compounds in Liberica green beans greatly differed between the growing regions in Jambi Province, but not in roasted beans. The PCA for green beans (Figure 2a) shows a total PC 91.66% (69.25% PC1; 22.41% PC2) of total diversity. The results indicated that the GB1 position existed in adjacent GB4, which was not detected in the remaining samples. The characteristics of Betara green beans were similar to those of Pengabuan green beans in terms of their chlorogenic acid and alkaloid contents. Meanwhile, the position of the remaining green bean samples was scattered. GB3 existed at the positive PC1 associated with the abundance of 3CQA, 4CQA, and theobromine, whereas GB2 existed at the centre of PC1 and GB5 at the negative PC1, representing the low contents of chlorogenic acid and alkaloids.



(a)



(b)

Figure 2. Biplot PCA for targeted non-volatile compounds in **(a)** green bean (GB) samples, and **(b)** roasted bean (RB) samples from (1) Betara, (2) Bram Itam, (3) Kuala Betara, (4) Pengabuan, and (5) Senyerang.

The PCA for roasted beans (Figure 2b) shows a total PC 75.25% (51.05% PC1; 24.20% PC2) of total diversity. The position of Liberica roasted bean was not specifically grouped based on targeted analysis. This is in line with the results of the PCA from untargeted analysis, indicating that the grouping of roasted beans based on non-volatile compounds *via* untargeted analysis was not formed. Considering the contents of chlorogenic acids and alkaloids, the roasted beans from five regions were not different (Table 3).

Profile of volatile compounds in Liberica coffee

The present work compared volatile compounds between green and roasted Liberica coffee beans to evaluate the general trends of roasting effect on volatile compounds. Table 4 shows 84 and 174 volatile compounds of Liberica green beans and roasted beans, respectively. The dominant volatile compounds in green beans were esters (nine compounds) and acids (three compounds), although the relative content of the compounds was lower than that in a roasted sample. Contrarily, the dominant volatile compounds in roasted beans were pyrazine (37 compounds) and furan (25 compounds).

Methyl salicylate, ethyl salicylate (ester group), and isovaleric acid (acid group) were the dominant volatile compounds detected in Liberica green beans. Methyl salicylate was also detected in Arabica green beans with ripe coffee cherries, which had wintergreen, mint-like aroma (Kulapichitr *et al*., 2017). In contrast, ethyl salicylate was predominantly detected in Robusta coffee (Suaib *et al*., 2024). Isovaleric acid was identified as a potent aroma of Excelsa coffee and an indicator of roasted coffee's excellent quality (Caporaso *et al*., 2018; Herawati *et al*., 2022; Cao *et al*., 2023).

The roasting process increased the relative content of volatile compounds in the coffee, and produced volatile compounds that were not present in the green beans (Table 4). During roasting, caramelisation, Maillard reaction, and other chemical reactions, including the breakdown of non-volatile substances, such as amino acids, fatty acids, sugars, and chlorogenic acid, typically occur. Consequently, substantial changes in volatile chemicals and flavour quality may transpire during and after roasting, thereby increasing the contents of some volatile compounds, such as pyrazines, furans, and pyridines (Caporaso *et al*., 2018; Hong *et al*., 2024).

2-Methylpyrazine, 3-ethyl-2,5-dimethylpyrazine, 2-ethyl-6-methyl-pyrazine, 2,6-dimethylpyrazine, 2,5-dimethylpyrazine (pyrazine group), 2-furanmethanol, 5-methylfurfural, furfural (furan group), and pyridine were the predominant compounds detected in Liberica roasted beans (Table 4). Among them, 2-methylpyrazine, 3-ethyl-2,5-dimethylpyrazine, 2-ethyl-6-methyl-pyrazine, 2,6-dimethylpyrazine, and 2,5-dimethylhydrazine were the predominant volatile compounds detected in Robusta coffee, whereas furfural was the dominant volatile compound detected in Arabica coffee (Caporaso *et al*., 2018). In addition, 2-methylpyrazine, 2,6-dimethylpyrazine, 2,5-dimethylpyrazine, furfural, 5-methylfurfural, and pyridine were the identified potent aromas in Excelsa

Table 4. Effects of roasting on volatile compounds of Liberica coffee beans.

Compounds	ID	Relative content of compound (µg/g db)	
		Green bean	Roasted bean
Aldehyde			
Butyraldehyde	RI, MS	0.65 ± 0.45	7.54 ± 0.44
Hexanal	RI, MS	1.26 ± 0.53	nd
Benzaldehyde	RI, MS	0.56 ± 0.52	0.34 ± 0.07
3,4-Dimethylbenzaldehyde	MS	nd	1.85 ± 1.47
1,5-Dimethyl-1H-pyrazole-4-carbaldehyde	MS	0.05 ± 0.05	1.84 ± 0.04
2-Methyl-5,6,7,8-tetrahydroquinoxaline	MS	nd	0.83 ± 0.08
Benzeneacetaldehyde	RI, MS	0.02 ± 0.01	nd
4-Methylbenzaldehyde	RI, MS	nd	1.08 ± 0.24
2-Phenyl-2-butenal	RI, MS	nd	0.41 ± 0.04
Total		**2.54 ± 1.22[a]**	**13.90 ± 1.41[b]**
Alcohol			
Isobutyl alcohol	RI, MS	0.11 ± 0.03	nd
2-Hexen-1-ol, (E)-	MS	nd	0.35 ± 0.05
2-Methylbutanol	RI, MS	0.70 ± 0.34	nd
3-Buten-1-ol, 3-methyl-	RI, MS	nd	1.60 ± 0.30
2,3-Butanediol	RI, MS	0.19 ± 0.07	0.87 ± 0.50
Benzylalcohol	RI, MS	0.68 ± 0.45	1.42 ± 0.67
Phenylethyl alcohol	RI, MS	0.43 ± 0.21	1.50 ± 0.34
Anise alcohol	MS	nd	0.27 ± 0.03
Maltol	RI, MS	nd	5.19 ± 2.29
5-Hydroxy maltol	RI, MS	nd	0.15 ± 0.02
Total		**2.06 ± 0.93[a]**	**11.34 ± 2.89[b]**
Benzene			
Ethylbenzene	RI, MS	0.04 ± 0.03	nd
1,3-Diazine	RI, MS	nd	2.14 ± 0.44
3-Methylanisole	RI, MS	0.15 ± 0.11	nd
1,2,3,4-Tetrahydro-1,6,8-trimethyl naphthalene	MS	nd	0.64 ± 0.05
1,2-Dimethoxybenzene	RI, MS	0.02 ± 0.02	nd
4-Ethyl-2-methoxyanisole	RI, MS	0.06 ± 0.06	0.40 ± 0.19
p-Aminotoluene	MS	nd	0.41 ± 0.04
Total		**0.22 ± 0.19[a]**	**3.58 ± 0.62[b]**
Pyrrole			
1-Methylpyrrole	RI, MS	0.05 ± 0.02	0.27 ± 0.04
1-Ethylpyrrole	RI, MS	0.03 ± 0.01	0.12 ± 0.06
1H-Pyrrole	RI, MS	nd	0.93 ± 0.05
1-Methyl-2-formylpyrrole	RI, MS	nd	0.70 ± 0.14
2-Acetyl-1-methylpyrrole	RI, MS	0.01 ± 0.01	1.17 ± 0.03
1-Furfurylpyrrole	RI, MS	0.01 ± 0.00	2.03 ± 0.09
2-Formyl-1-methylpyrrole	RI, MS	0.04 ± 0.03	2.23 ± 0.14
3-Acetyl-1-methylpyrrole	MS	nd	0.62 ± 0.02
Pyrrole-3-butyronitrile	MS	0.30 ± 0.39	1.41 ± 0.08
Propyl 2-furoate	MS	nd	0.13 ± 0.03
2-Acetylpyrrole	RI, MS	0.03 ± 0.02	3.26 ± 0.18
2-Formylpyrrole	MS	nd	1.90 ± 0.11
2-Formyl-5-methylpyrrole	RI, MS	nd	0.92 ± 0.09

2,3,4-Trimethylpyrrole	MS	0.02 ± 0.00	0.37 ± 0.05
Total		**0.43 ± 0.41[a]**	**16.06 ± 0.53[b]**
Pyridine			
Pyridine	RI, MS	0.66 ± 0.74	28.71 ± 1.11
2-Methylpyridine	RI, MS	nd	0.76 ± 0.63
3-Methylpyridine	RI, MS	0.05 ± 0.05	2.77 ± 0.18
2,3-Dimethylpyridine	RI, MS	0.09 ± 0.05	0.41 ± 0.07
3-Ethylpyridine	RI, MS	0.11 ± 0.12	7.13 ± 0.64
3-Propylpyridine	RI, MS	0.02 ± 0.01	0.95 ± 0.10
3-Vinylpyridine	MS	nd	2.60 ± 0.06
2-Acetylpyridine	RI, MS	0.01 ± 0.01	0.99 ± 0.04
2-Acetyl-4-methylpyridine	MS	nd	1.20 ± 0.08
4-Pentylpyridine	MS	nd	0.50 ± 0.15
3-Butylpyridine	MS	0.01 ± 0.01	1.03 ± 0.23
1-Acetyl-1,2,3,4-tetrahydropyridine	MS	nd	0.53 ± 0.09
5-Acetyl-2-methylpyridine	MS	0.02 ± 0.00	0.77 ± 0.04
6-Methyl-3-pyridinol	MS	nd	0.33 ± 0.02
2-Acetyl-1,4,5,6-tetrahydropyridine	MS	nd	0.23 ± 0.03
2,6-Dimethyl pyridin-4-ol	MS	nd	0.45 ± 0.07
4-Ethylpyridine	MS	nd	0.21 ± 0.02
3-Isobutylpyridine	MS	nd	1.19 ± 0.59
4-Methylpyridine	MS	nd	0.28 ± 0.06
Nicotinyl alcohol	MS	0.02	0.28 ± 0.05
2-Methyl-3-hydroxypyridine	MS	nd	0.05 ± 0.01
Total		**0.98 ± 0.95[a]**	**51.36 ± 1.08[b]**
Furan			
2-Pentyl-furane	RI, MS	0.18 ± 0.15	0.24 ± 0.08
2-Furfuryl methyl ether	RI, MS	nd	0.21 ± 0.07
2-Methyltetrahydrofuran-3-one	RI, MS	0.14 ± 0.10	8.24 ± 13.83
Furfural	RI, MS	0.56 ± 0.56	18.10 ± 1.65
Menthofuran	RI, MS	nd	0.27 ± 0.09
2-Acetylfuran	RI, MS	0.11 ± 0.09	8.14 ± 0.80
Furfuryl formate	RI, MS	nd	2.12 ± 0.44
Furfuryl acetate	RI, MS	0.02 ± 0.01	6.17 ± 3.96
5-Methylfurfural	RI, MS	0.07 ± 0.04	20.25 ± 1.60
2-Propanoylfuran	RI, MS	0.01 ± 0.01	0.66 ± 0.06
2,2'-Bifuran	MS	0.02 ± 0.00	0.46 ± 0.36
2-Furfurylfuran	RI, MS	nd	0.69 ± 0.06
2-Furanmethanol	RI, MS	0.07 ± 0.06	38.99 ± 2.40
2-Furylmethyl 3-methylbutanoate	MS	nd	0.74 ± 0.09
3,4-Dimethyl-2,5-furandione	RI, MS	0.03 ± 0.03	0.88 ± 0.02
2(5H)-Furanone	RI, MS	0.02 ± 0.02	1.20 ± 0.24
2-Acetyl-5-methylfuran	MS	nd	1.34 ± 0.10
4-Methyl-2(5H)-furanone	MS	nd	0.44 ± 0.05
2-*n*-Propylfuran	MS	nd	0.57 ± 0.25
Furfural acetone	RI, MS	nd	0.26 ± 0.02
Furfuryl ether	RI, MS	0.01 ± 0.01	0.75 ± 0.32
1-(2-Furanyl)-2-hydroxyethanone	MS	nd	0.48 ± 0.07
Furfuryl methyl ether	MS	nd	0.43 ± 0.04
Furaneol	RI, MS	nd	3.66 ± 0.79
2-Butylfuran	MS	0.01 ± 0.01	0.42 ± 0.04

Total		**1.25 ± 1.03[a]**	**115.69 ± 15.15[b]**
Pyrazine			
2-Methylpyrazine	RI, MS	0.66 ± 0.62	36.15 ± 3.90
2,5-Dimethylpyrazine	RI, MS	0.25 ± 0.23	19.52 ± 3.41
2,6-Dimethylpyrazine	RI, MS	0.32 ± 0.25	22.29 ± 2.59
Ethylpyrazine	RI, MS	0.37 ± 0.31	12.70 ± 1.52
2,3-Dimethylpyrazine	RI, MS	0.08 ± 0.07	5.44 ± 0.77
2-Ethyl-6-methylpyrazine	RI, MS	1.93 ± 1.42	23.76 ± 2.69
2-Ethyl-5-methylpyrazine	RI, MS	0.17 ± 0.12	10.71 ± 1.94
2-Ethyl-3-methylpyrazine	RI, MS	0.03 ± 0.02	2.44 ± 1.18
2,3,5-Trimethylpyrazine	RI, MS	0.18 ± 0.14	11.40 ± 1.05
2-Propylpyrazine	RI, MS	0.05 ± 0.04	0.44 ± 0.07
2,6-Diethylpyrazine	RI, MS	nd	3.42 ± 0.52
3-Ethyl-2,5-dimethylpyrazine	RI, MS	0.27 ± 0.22	24.49 ± 5.53
5-Ethyl-2,3-dimethylpyrazine	RI, MS	nd	4.94 ± 1.19
2-Methyl-6-propylpyrazine	RI, MS	nd	1.01 ± 0.17
2,3,5,6-Tetramethylpyrazine	RI, MS	nd	0.81 ± 0.25
2-Methyl-6-vinylpyrazine	RI, MS	0.01 ± 0.01	1.01 ± 0.50
2-Isobutyl-3-methylpyrazine	MS	nd	0.53 ± 0.27
2-Methyl-5-vinylpyrazine	RI, MS	nd	1.34 ± 1.16
2-Methyl-3,5-diethylpyrazine	RI, MS	0.03 ± 0.03	2.75 ± 0.56
2,3,5-Trimethyl-6-ethylpyrazine	MS	0.06 ± 0.00	1.14 ± 0.36
2-Isobutyl-3-methoxypyrazine	RI, MS	0.17 ± 0.16	0.62 ± 0.14
2,3-Dimethyl-5-isobutylpyrazine	MS	0.07 ± 0.06	0.54 ± 0.09
2-Isoamylpyrazine	MS	nd	0.37 ± 0.04
Isopropenylpyrazine	MS	0.15 ± 0.08	1.35 ± 0.17
5-Methyl-6,7-dihydro-(5H)-cyclopentapyrazine	RI, MS	nd	2.25 ± 0.78
2-Acetylpyrazine	RI, MS	nd	2.32 ± 0.28
2-Methyl-6-[(1E)-1-propenyl] pyrazine	MS	0.01 ± 0.00	0.63 ± 0.05
3,5-Dimethyl-2-butylpyrazine	MS	nd	1.72 ± 0.10
2-Acetyl-5-methylpyrazine	RI, MS	nd	2.95 ± 0.19
2-Acetyl-6-methylpyrazine	RI, MS	nd	8.77 ± 0.63
Pyrazine-2-carboxylic acid, amide	RI, MS	nd	2.88 ± 0.17
Pyrazine-2,5-dimethyl-3-(2-propenyl)-	MS	nd	0.55 ± 0.59
2-Acetyl-3,5-dimethylpyrazine	MS	nd	0.85 ± 0.15
4-Methylpyrrol-1,2-A-pyrazine	MS	nd	0.28 ± 0.02
2-Propylpyrazine	MS	nd	0.07 ± 0.02
2-*n*-Butyl-3-methylpyrazine	MS	nd	0.05 ± 0.01
2-Methyl-3-*n*-propylpyrazine	MS	nd	0.05 ± 0.01
Total		**4.77 ± 3.44[a]**	**212.03 ± 27.20[b]**
Ketone			
2-Pentanone	MS	nd	4.99 ± 0.55
2,3-Pentanedione	MS	nd	4.16 ± 1.65
3-Penten-2-one	RI, MS	nd	0.21 ± 0.05
3-Hydroxy-2-butanone	MS	0.47 ± 0.26	3.53 ± 0.17
1-Hydroxy-2-propanone	RI, MS	0.62 ± 0.49	11.63 ± 0.99
2-Methyl-2-cyclopenten-1-one	RI, MS	0.02 ± 0.02	0.47 ± 0.04
1-Hydroxy-2-butanone	RI, MS	0.02 ± 0.01	0.87 ± 0.07
2-Methyl-3-pentanone	MS	0.01 ± 0.00	3.00 ± 0.95
Acetophenone	RI, MS	0.04 ± 0.03	nd
2,5-Dimethyl-3-hexanone	MS	0.02 ± 0.01	0.28 ± 0.03

2-Methyl-2-pentenal	MS	0.02 ± 0.02	0.65 ± 0.08
2-Cyclohexene-1,4-dione	MS	nd	0.92 ± 0.12
3-Acetylthiophene	MS	nd	0.65 ± 0.06
2,5-Dimethylthiophen-3-yl methyl ketone	MS	nd	0.23 ± 0.01
3-Methyl-1,2-cyclopentanedione	MS	nd	2.76 ± 0.19
3,4-Dimethylcyclopentanone	MS	nd	0.20 ± 0.03
2-Nonanone	MS	nd	0.25 ± 0.05
Fenchone	MS	nd	0.10 ± 0.02
2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one	RI, MS	nd	1.88 ± 0.48
Total		**1.21 ± 0.78[a]**	**36.77 ± 3.07[b]**
Cyclopentene			
2-Hydroxy-3-methyl-2-cyclopenten-1-one	MS	0.02 ± 0.01	0.46 ± 0.03
3-Methyl-2-cyclopenten-1-one	RI, MS	nd	0.34 ± ± 0.02
3-Ethyl-2-hydroxy-2-cyclopentanone	RI, MS	0.02 ± 0.01	1.17 ± 0.36
Total		**0.03 ± 0.02[a]**	**1.97 ± 0.37[b]**
Ester			
Ethylene acetate	RI, MS	0.08 ± 0.06	13.23 ± .07
1-Hydroxy-2-butanone acetate	RI, MS	nd	2.68 ± 2.17
Prenyl acetate	MS	nd	0.32 ± 0.06
Ethyl benzoate	RI, MS	0.01 ± 0.01	nd
Benzyl acetate	RI, MS	0.02 ± 0.01	nd
Methyl salicylate	RI, MS	4.76 ± 2.93	12.71 ± 8.30
Methyl nicotinate	MS	0.03 ± 0.02	3.16 ± 0.14
Ethyl salicylate	RI, MS	3.34 ± 1.70	11.67 ± 1.87
Amyl acetate	MS	0.01 ± 0.00	0.43 ± 0.04
Benzyl isovalerate	RI, MS	0.02 ± 0.01	nd
Methyl 4-methylsalicylate	MS	0.04 ± 0.04	0.33 ± 0.06
Total		**8.27 ± 3.57[a]**	**44.53 ± 8.14[b]**
Acid			
Acetic acid	RI, MS	nd	4.08 ± 1.23
Propanoic acid	RI, MS	0.02 ± 0.00	2.48 ± 3.51
Isovaleric acid	RI, MS	3.19 ± 2.03	21.70 ± 6.02
Nonanoic acid	RI, MS	0.04 ± 0.02	0.54 ± 0.10
Decanoic acid	RI, MS	nd	0.17 ± 0.02
Total		**3.23 ± 2.06[a]**	**28.98 ± 9.76[b]**
Terpene			
Linalool	RI, MS	0.18	1.23
β-Damascenone	RI, MS	0.02	0.25
Total		**0.18 ± 0.16[a]**	**1.48 ± 0.79[b]**
Thiazole			
2,5-Dimethylthiazole	RI, MS	nd	0.06 ± 0.00
2-Acetylthiazole	RI, MS	nd	0.75 ± 0.12
2,4-Dimethyl-5-ethylthiazole	MS	0.01 ± 0.01	0.24 ± 0.03
2-Methyl-2-thiazoline	MS	0.04 ± 0.02	0.32 ± 0.02
Total		**0.04 ± 0.03[a]**	**1.32 ± 0.14[b]**
Phenol			
Anisole	RI, MS	0.26 ± 0.15	nd
p-Cresol acetate	RI, MS	nd	0.42 ± 0.18
4-Amino-m-cresol	MS	nd	0.82 ± 0.04
3,4-Dimethoxyphenol	MS	nd	0.38 ± 0.06
o-Guaiacol	RI, MS	0.02 ± 0.02	5.90 ± 1.34

o-Cresol	MS	0.01 ± 0.00	0.25 ± 0.02
Phenol	RI, MS	0.04 ± 0.03	0.58 ± 0.10
p-Ethylguaiacol	RI, MS	0.02 ± 0.02	1.51 ± 0.17
p-Cresol	RI, MS	0.01 ± 0.01	0.94 ± 0.10
4-Vinylguaicol	MS	0.07 ± 0.08	8.50 ± 0.77
Total		**0.42 ± 0.28[a]**	**19.30 ± 2.03[b]**
Miscellaneous			
Hydrazine	MS	nd	3.98 ± 0.41
δ-Valerolactone	RI, MS	0.06 ± 0.04	nd
γ-Butyrolactone	RI, MS	0.25 ± 0.11	3.18 ± 0.79
2-Isobutyl-4,5-dimethyl-1,3-oxazole	MS	nd	0.46 ± 0.03
2-Furfurylthiol	RI, MS	0.03 ± 0.02	0.27 ± 0.08
Furfuryl methyl sulphide	RI, MS	0.02 ± 0.03	0.52 ± 0.01
2-Formyl-5-methylthiophene	MS	nd	1.07 ± 0.06
2-Hydroxymethylthiophene	RI, MS	nd	0.16 ± 0.06
Styrene	RI, MS	1.02 ± 0.82	0.52 ± 0.47
3,4-Dimethoxystyrene	RI, MS	0.05 ± 0.00	0.29 ± 0.08
Total		**1.35 ± 0.82[a]**	**10.44 ± 1.35[b]**

Mean values of green beans and roasted beans were calculated from five locations in Jambi, Indonesia: (1) Betara, (2) Bram Itam, (3) Kuala Betara, (4) Pengabuan, and (5) Senyerang. nd: not detected. Values are mean ± standard deviation of group compound. Means with similar lowercase superscript within similar row are not significantly different ($p > 0.05$). Identification of compounds were by retention index (RI) and mass spectra (MS).

coffee (Herawati *et al*., 2022). Furan contributes to a sweet aroma, pyrazine to a hazelnut aroma, and pyridine to a chocolate-like aroma (Cao *et al*., 2023).

Conclusion

Untargeted analysis revealed that non-volatile compounds were dominated by alkaloids, organic acids, and phenolics. In response to coffee processing, commercial roasting increased the relative area for alkaloids and fatty acids, but decreased that for phenolics and amino acids. Roasting increased the relative number of volatile compounds, and produced some volatile compounds. In addition, based on targeted analysis, the commercial roasting process decreased the content of chlorogenic acids (3CQA, 4CQA, and 5CQA) in Liberica coffee but did not change the alkaloid contents (trigonelline, theobromine, and caffeine). The present work also demonstrated that the commercial roasting process (with L*: 39.05 - 39.48) resulted in comparable contents of chlorogenic acids (3CQA, 4CQA, and 5CQA) and alkaloids (theobromine and caffeine) between Liberica coffee beans collected from five different locations in Jambi. Furthermore, the commercial roasting process increased the relative contents of volatile compounds, particularly furanes and pyrazines.

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