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Metabolite Profiling of Kintamani and Preanger Arabica Roasted Coffees Using ^{1}H NMR-Based Metabolomics

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Abstract

Kintamani and Preanger Arabica coffees are two of Indonesian popular coffees having unique flavors. This study focused on comparing the metabolite profiles of roasted Arabica coffees from Kintamani-Bali and Preanger-West Java using ^{1}H NMR-based metabolomics. A total of 24 metabolites were identified, including chlorogenic acids, trigonelline, acetic acid, caffeine, and various organic acids. Evaluation using PLSDA technique successfully separated metabolite profiles of Kintamani and Preanger coffees. The PLSDA model identified trigonelline, caffeoylquinic acids (CQAs), and arabinose as key differentiating metabolites for Preanger coffees, while mannose, quinic acid, lipids, citric acid, and malic acid were dominant in Kintamani coffees. These findings highlight the influence of regional factors on the metabolite composition of Indonesian Arabica coffees and can contribute to quality control and authentication efforts in the coffee industry.

Keywords: Kintamani coffee, Preanger coffee, Arabica roasted coffee, metabolomics, NMR.

INTRODUCTION

Coffee is one of the most globally consumed beverages and well known for its interesting flavor profile, stimulating effects, and health benefits. Coffee quality is influenced by various factors, including cultivation condition, geographical origin, climate, genetics, and post-harvest processing [1]. Arabica (*Coffea arabica* L.) and Robusta (*Coffea canephora* P.) are the two most popular types of coffee globally. Arabica is often regarded as superior to Robusta due to its enhanced flavor, richer aroma, and lower caffeine levels [2].

Indonesia, as one of the leading coffee producers, is home to several distinctive coffee-growing regions, including Sumatra, Java, Bali, Flores and Sulawesi. Preanger coffee is one of famous Indonesian coffee cultivated in the volcanic highlands of West Java. In our previous report [3], Preanger coffee was reported to have a more pronounced acidity compared to coffees from Gayo-Sumatera, Toraja-Sulawesi, and Bajawa Flores. As a continuation of that research, in this study, we compared this Preanger coffee with another Indonesian coffee recognized for its distinctive acidity flavor as well, namely Kintamani coffee. Grown in the high-altitude Kintamani region of Bali, this coffee benefits from the volcanic soil, and is characterized by its fruity and bright acidity flavor [4].

Metabolomics, the comprehensive study of small molecules within biological systems, offers a powerful approach to understanding the metabolic profiles that contribute to the distinctive qualities of coffee. Among the various analytical techniques available, proton nuclear magnetic resonance (^{1}H NMR) spectroscopy has proven particularly useful for profiling complex mixtures such as coffee [5–7] ^{1}H NMR-based metabolomics allows for the simultaneous detection of a wide range of metabolites, providing a holistic view of the biochemical differences that may arise due to geographical origin [8–10], processing methods [11], or roasting conditions [12].

This study aimed to differentiate the metabolite profiles of Preanger Arabica and Kintamani Arabica roasted coffees using ^{1}H NMR-based metabolomics. Through this non-targeted analytical approach, we sought

to identify key metabolites that distinguish these two prominent coffees having distinctive acidity flavors, offering insights into the regional influences on coffee chemical composition.

EXPERIMENTAL SECTION

Material and Instrumental

Deuterated water, used for coffee extraction and in the buffer solution, was sourced from Merck (Darmstadt, Germany). Sodium-3-(trimethylsilyl)-2,2,3,3-tetradeuteriopropionate (TSP), serving as the chemical shift standard for the ^{1}H NMR measurements, was also acquired from Merck (Darmstadt, Germany). KH_2PO_4 and K_2HPO_4, which were used in the buffer solution, were purchased from Merck (Darmstadt, Germany).

An Encore grinder (Baratza, USA) was used to grind the roasted coffee beans. A Krisbow ultrasonic bath (Indonesia) was employed to sonicate the samples. An MC-12 High Speed Microcentrifuge (Benchmark Scientific, USA) was employed to centrifuge the samples. A 500 MHz Varian Unity INOVA spectrometer (Agilent Technologies, USA) recorded the ^{1}H NMR spectra of the roasted coffee samples.

Methods

Sample preparations

The roasted Arabica coffee beans used in this study included 5 samples each from Kintamani (Bali) and Preanger (West Java), sourced from various local coffee companies as described in Table 1. The roasted beans were ground into powders smaller than 1 mm using an Encore mill (Baratza, Bellevue, United States). For each sample, 200 mg of the ground coffee was placed in a plastic tube, combined with 1 mL of deuterated water containing 1.00 mM TSP, and sonicated for 20 minutes. The samples were then incubated at 90°C for 30 minutes, cooled in water for 10 minutes, and centrifuged at 12,000 rpm for 5 minutes. A 400 µL aliquot of the supernatant was then transferred to a new tube, mixed with 100 µL of phosphate buffer (pH 5), and placed in 5 mm NMR tubes.

^{1}H NMR spectra measurements

The measurements of ^{1}H NMR spectra of the roasted coffee samples were carried out using a Varian Unity INOVA-500 spectrometer (Agilent Technologies, Santa Clara, United States), operating at a frequency of 500 MHz. The spectra were measured with a presaturation pulse sequence, utilizing the following parameters: an acquisition time of 2.72 seconds, a relaxation delay of 2 seconds, 64,000 data points, a spectral width of 8012 Hz, and 128 scans.

^{1}H NMR spectra processing

The processing of the ^{1}H NMR spectra was carried out with ACD/Labs 12.0 software (ACD/Labs, Toronto, Canada). This process involved the Fourier transformation of free-induction decay (FID) data, baseline correction, chemical shift scaling, alignment, and bucketing. The chemical shifts of ^{1}H NMR spectra were calibrated to the TSP signal and then aligned. The spectra were divided into integrated buckets with an equal width of 0.04 ppm within the range of δ 0.50 - 10.00 ppm using the intelligent bucketing mode. Signals from residual water (δ 4.73 - 5.22 ppm) were excluded from the analysis. Additionally, the caffeine signals at δ 3.22 - 3.49 ppm and δ 3.82 - 3.88 ppm were removed to avoid spurious principal components (PCs) due to their shifting signals. The resulting data were normalized to the total integral to mitigate dilution effects across samples.

Multivariate data analysis

The data sets were subsequently imported into SIMCA-P version 12.0 (Umetrics, Umeå, Sweden) for multivariate statistical analysis. Pareto scaling was applied to the data. Initially, principal component analysis (PCA) was performed to explore inherent variation within the data. Partial least squares discriminant analysis (PLSDA) and orthogonal projections to latent structures-discriminant analysis (OPLSDA) were employed to achieve optimal separation among the samples. The roasted coffee data were grouped into two classes based on geographical origins and analysed using PLSDA and OPLSDA models. Model performance metrics, including the explained variation (R2X and R2Y) and predictive ability (Q2) from cross-validation, were calculated. Validation of the PLSDA model was conducted through a permutation test with 200 iterations.

RESULTS AND DISCUSSION

Identified Metabolites in the roasted Arabica coffee samples

In this study, metabolites present in the roasted Arabica coffee samples were identified by detecting their fingerprint signals in the ^{1}H NMR spectra. The detailed elucidation of metabolite identification could be seen on our previous work.[3] As the result, a total of 24 metabolites were identified putatively. Major metabolites, such as acetic acid, caffeine, chlorogenic acids [3-caffeoyl quinic acid (3-CQA), 4-caffeoyl quinic acid (4-CQA), and 5-caffeoyl quinic acid (5-CQA)], formic acid, and trigonelline were clearly visible in the spectra, as illustrated in Figure 1, confirming their prominence in the roasted coffee samples. Other detected acidic compounds included lactic acid, malic acid, citric acid, and quinic acid. Additionally, γ-quinide, an ester cyclic of quinic acid, along with myo-inositol, and lipids were also detected in aliphatic region of the ^{1}H NMR spectra. Some carbohydrate compounds, including α-(1-3)-L-arabino-furanose unit (3-arabinose), α-(1-5)-L-arabino-furanose unit (5-arabinose), β-(1-4)-D-manno-pyranose unit (mannose), β-(1-3)-D-galacto-pyranose unit (3-galactose), β-(1-6)-D-galacto-pyranose unit (6-galactose) were successfully recorded as well. Investigation in the aromatic region of the 1H NMR spectra successfully detected N-methyl-pyridine, 2-furyl-methanol and 5-(hydroxymethyl)-furfural. The detailed characteristic signals of annotated metabolites are depicted in Table 1 and Figure 1. The characteristic signals of the identified metabolites were further verified by comparison with reference spectra and further confirmed using NMR data from roasted coffee beans reported in the literature [10,12,13]. The molecular structures of some annotated metabolites are described in Figure 2.

Table 1. The origins of Arabica roasted coffees.

Sample code	Coffee origin	Company/Supplier
KB1	Kintamani, Bali	JPW Coffee
KB2	Kintamani, Bali	Infokopi
KB3	Kintamani, Bali	Fulcaf Coffee
KB4	Kintamani, Bali	Mr. O Coffee
KB5	Kintamani, Bali	Eastindischekoffie
PJ1	Bandung, West Java, Java	Coffindo
PJ2	Bandung, West Java, Java	Kopi Florist
PJ3	Bandung, West Java, Java	Eastindischekoffie
PJ4	Bandung, West Java, Java	Eastindischekoffie
PJ5	Bandung, West Java, Java	Eastindischekoffie

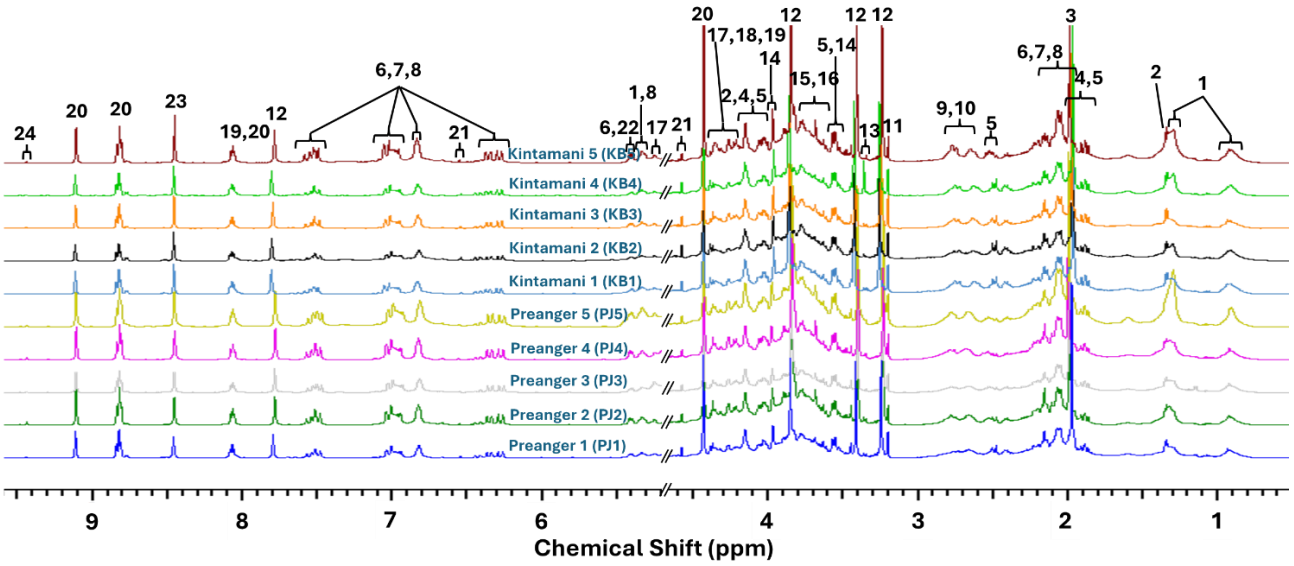

Figure 1. Characteristic signals of the identified metabolites in the ^{1}H NMR spectra of Kintamani and Preanger Arabica roasted coffees. 1: lipids; 2: lactic acid; 3: acetic acid; 4:quinic acid; 5: γ-quinide; 6: 3-caffeoylquinic acid (3-CQA); 7: 4-caffeoylquinic acid (3-CQA); 8: 5-caffeoylquinic acid (3-CQA); 9: citric acid; 10: malic acid; 11: choline; 12: caffeine; 13: inositol; 14: mannose unit; 15: 3-galactose unit; 16: 6-galactose unit; 17: 3-arabinose unit; 18: 5-arabinose unit; 19: N-methyl-pyridinium; 20: trigonelline; 21: 2-furyl-methanol; 22: sucrose, 23: formic acid; 24: 5-(hydroxymethyl) furfural.

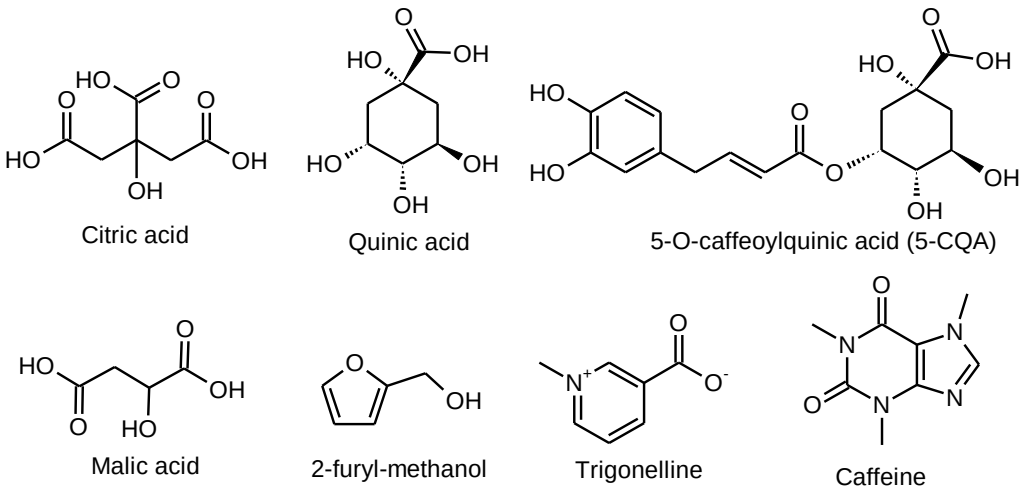

Figure 2. Some molecular structures of annotated compounds in the ^{1}H NMR spectra of Kintamani and Preanger Arabica roasted coffees.

Table 2. Signals of the annotated compounds in the ^{1}H NMR spectra of Kintamani and Preanger roasted Arabica coffees. + : detected.

No.	Compound	Chemical shift (ppm)	Kintamani	Preanger
1.	Lipids	0.92 (m), 1.30 (m), 1.61 (m), 5.32 (m)	+	+
2.	Lactic acid	1.35 (d)	+	+
3.	Acetic acid	1.98 (s)	+	+
4.	Quinic acid	1.89 (m), 1.96 (m), 2.06 (m), 3.56 (m), 4.03 (m), 4.16 (m)	+	+
5.	γ-quinide	1.95 (m), 2.14 (m), 2.41 (m), 2.49 (m), 3.89 (m), 4.06 (m), 4.91 (m)	+	+
6..	3-caffeoyl quinic acid	2.04 (m), 2.16 (m), 5.40 (m), 6.35 (d), 6.82 (br s), 6.96 (m), 7.02 (m), 7. 51 (m)	+	+
7.	4-caffeoyl quinic acid	2.04 (m), 2.16 (m), 4.92 (m), 6.35 (d), 6.82 (br s), 6.96 (m), 7.02 (m), 7.53 (m)	+	+
8.	5-caffeoyl quinic acid	2.04 (m), 2.16 (m), 5.33 (m), 6.27 (d), 6.82 (br s), 6.96 (m), 7.02 (m), 7.48 (m)	+	+
9.	Citric acid	2.61 (d), 2.74 (d)	+	+
10.	Malic acid	2.44 (m), 2.68 (m)	+	+
11.	Choline	3.20 (s)	+	+
12.	Caffeine	3.26 (s), 3.45 (s), 3.88 (s), 7.83(s)	+	+
13.	Myo-inositol	3.27 (t), 3.52 (m), 3.62 (m), 4.06 (m)	+	+
14.	Mannose unit	3.55 (m), 3.82 (m), 3.93 (m), 5.17 (br s)	+	+
15.	3-galactose unit	3. 65 (m), 4.62 (d)	+	+
16.	6-galactose unit	3.73 (m), 4.44 (br s)	+	+
17.	3-arabinose unit	4.27 (br s), 5.25 (br s)	+	+
18.	5-arabinose unit	4.21 (br s), 5.10 (br s)	+	+
19.	N-methyl-pyridine	4.37 (s), 8.02 (m), 8.52 (t) and 8.77 (d)	+	+
20.	Trigonelline	4.43 (s), 8.09 (t), 8.82 (m), 8.84 (m), 9.12 (s)	+	+
21.	2-furyl-methanol	4.58 (s), 6.43 (m), 7.57 (br s)	+	+
22.	Sucrose	5.42 (d)	+	+
23.	Formic acid	8.46 (s)	+	+
24.	5-(hydroxymethyl)-furfural	9.49 (s)	+	+

Differentiation of metabolite profiles between Kintamani and Preanger Arabica coffees

This study compared the metabolite profiles of roasted Arabica coffees from Kintamani-Bali and Preanger-West Java. The dataset, cleaned and extracted from 1H NMR spectra, underwent multivariate data analysis using SIMCA-P version 12.0 (Umetrics, Umeå, Sweden). Initially, Principal Component Analysis (PCA), an unsupervised method, was employed. PCA is a dimensionality reduction technique that represents

multivariate data in a lower-dimensional space [14]. It helps uncover relationships and variances in the data, provides a model of chemical system behaviour, and distinguishes systematic data from noise [15]. The resulted PCA model had three new principal components (PCs), explaining 67.7% of the cumulative variance (R2X). The PCA score plot, combining PC1 (32.1%) and PC2 (19.9%), almost separated the roasted coffee samples based on their origins as depicted in Figure 3a. However, the cross-validation coefficient (Q2) of this model was below zero, indicating a poor predictive capability.

The evaluation was further pursued using Partial Least Squares Discriminant Analysis (PLSDA), a supervised pattern-recognition approach. This technique incorporates class labels to maximize the separation between predefined groups [16]. PLSDA is effective in reducing the dimensionality of complex datasets by projecting them onto a new set of latent variables that best separate the classes [16]. The resulting PLSDA model effectively separated the roasted Arabica coffee samples according to their geographical origin. This model comprised 3 components, with the first two components accounting for 46.8% of the variation in the spectral data. This PLSDA model had a cross-validation coefficient (Q2) of 86.4%, reflecting strong predictive capability, and explained 60.1% of the total variation in R2X and 99.0% in R2Y. The score plot of the PLSDA model produced by combining the first (29.8%) and the second (16.9%) components, successfully separated Kintamani Arabica roasted coffees from Preanger coffees, as depicted in Figure 3b. It indicated both coffee samples had distinguished metabolite profiles.

To identify the differentiating metabolites in the separation, the corresponding loading plot (Figure 3c) was investigated. The loading plot highlighted several key metabolites contributing significantly to the separation. According to the loading plot, Preanger Arabica roasted coffee were characterized with trigonelline (buckets at δ 4.40-4.46, 8.79-8.45, 9.09-9.15 ppm), caffeoylquinic acids (CQAs, buckets at δ 6.24-6.36, 6.72-6.90 ppm), 3-arabinose unit (bucket at δ 4.25-4.29 ppm), 5-arabinose unit (bucket at 4.20-4.25 ppm), and caffeine (bucket at δ 3.22-3.28, 7.73-7.83 ppm). This result indicated that the concentrations of these compounds were higher in Preanger coffees than in the counterpart samples. Among these metabolites, trigonelline and CQAs were the most important discriminant compounds for Preanger coffees, since their buckets located far from the center. Meanwhile, Kintamani Arabica roasted coffees were distinguished with mannose (bucket at δ 3.93-3.99 ppm), quinic acid (buckets at δ 2.47-2.52, 4.12-4.18 ppm), lipids (buckets at δ 0.94-1.00, 1.62-1.68, 1.48-1.74 ppm), citric acid (buckets at δ 2.70-2.74, 2.74-2.78 ppm), and malic acid (bucket at δ 2.39-2.45 ppm). This result revealed that the amounts of these metabolites were higher in Kintamani coffees than in Preanger coffees. The identification of citric acid as one of the discriminant compounds possibly correlates with the citrus flavor characteristic of Kintamani coffee. Moreover, mannose and quinic acid were the key discriminant compounds for Kintamani coffees, as their bucket locations were significantly distant from the center.

Both coffees were characterized by distinctive acidity flavors. A previous work reported a positive correlation between the level of CQAs and the sour taste of coffee [13]. Thus, it seems reasonable to suggest that CQAs, the important discriminant compounds of Preanger coffee, play a key role in contributing to its acidity. Meanwhile, the unique sour taste of Kintamani coffee possibly is influenced by their characteristic acidic compounds, including citric acid, quinic acid, and malic acid. These compounds were reported to influence the acidity in brewed coffee [17].

To reveal the most contributing metabolites in the separation, we further assessed the Variable Importance for the Projection (VIP) plot of the PLSDA model, which summarizes the significance of variables in explaining X and their correlation to Y. VIP values greater than 1 denote “important” X-variables, while values below 0.5 indicate “unimportant” X-variables. As described in Figure 4, VIP plot revealed that mannose and trigonelline were the most important compounds distinguishing metabolite profiles of Kintamani Arabica roasted coffee from Preanger coffees, followed by CQAs, quinic acid, 5-arabinose unit, 3-arabinose unit, lipids, and caffeine.

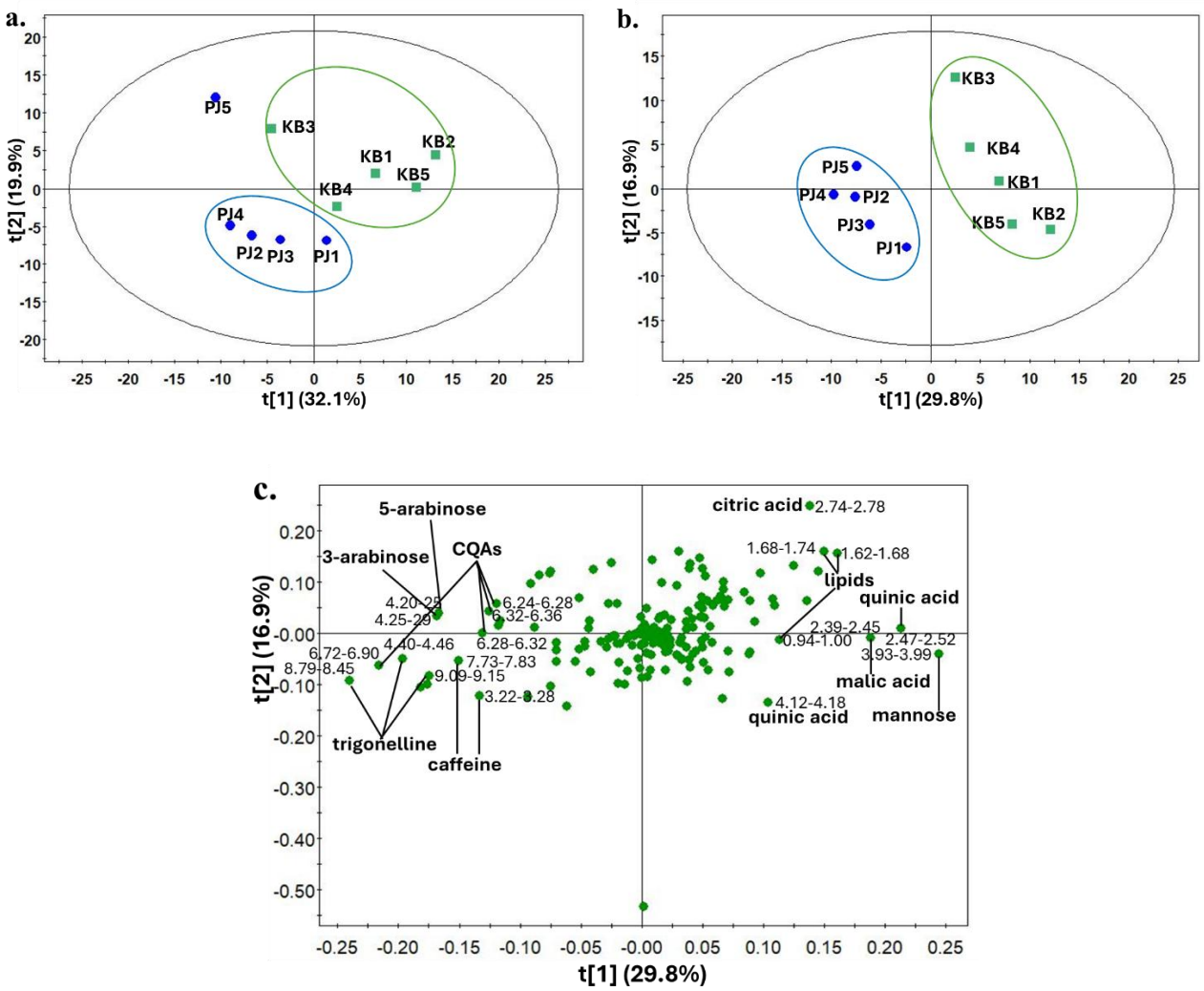

Figure 3. Multivariate data analysis calculated for Kintamani and Preanger Arabica roasted coffees. (a) PCA score plot almost separated Preanger coffees from Kintamani coffees. (b) PLSDA score plot successfully classified the coffee samples based on their origins. (c) PLSDA loading plot revealed the significant buckets contributing to the separation. KB: Kintamani-Bali, PJ: Preanger-Java.

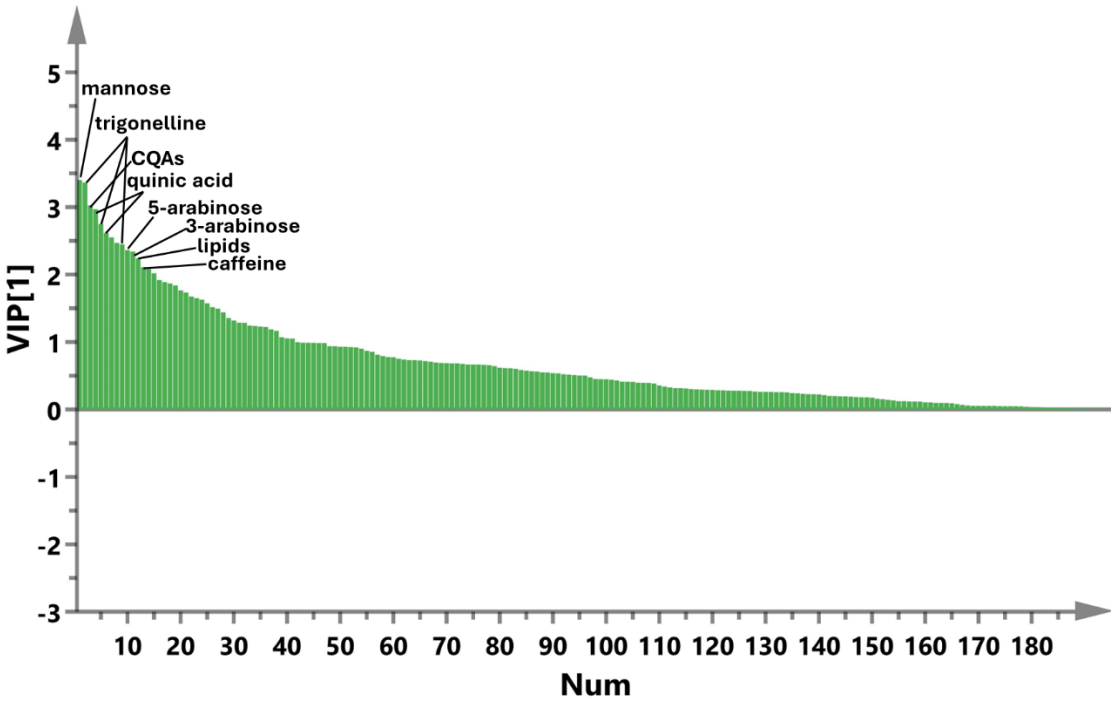

Figure 4. VIP plot of PLSDA model of Kintamani and Preanger Arabica roasted coffees

CONCLUSION

In this work, metabolite profiles of Kintamani and Preanger Arabica roasted coffees were evaluated with ^{1}H NMR-based metabolomics. Preanger Arabica roasted coffees were characterized with trigonelline, caffeoylquinic acids, 3-arabinose unit, 5-arabinose unit, and caffeine. Meanwhile, Kintamani Arabica roasted coffees were distinguished with mannose, quinic acid, lipids, citric acid, and malic acid. This research provides scientific evidence highlighting the unique metabolite compositions of Kintamani and Preanger Arabica roasted coffees, underscoring their distinct regional characteristics.

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