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ORIGINAL ARTICLE

Fourier Transform Infrared Spectroscopy combined with chemometrics for quality control of *Curcuma aeruginosa* rhizomes: An essential oil analysis

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ABSTRACT

Rhizome of *Curcuma aeruginosa* is a traditional herb utilized in many nations. The compound content in *C. aeruginosa* rhizomes can vary depending on their geographical origin. This study aims to determine the chemical fingerprints for quality control and identify the active ingredients in *C. aeruginosa* essential oil (CAEO) based on multiple geographic origins. Chemical fingerprints of CAEO from five different geographic origins have been determined using Fourier Transform Infrared Spectroscopy (FTIR). Principal component analysis and partial least squares discriminant analysis were utilized to examine the chemical data of CAEO utilizing pattern recognition techniques. A total of 52 fluctuating compounds were identified in gas chromatography-mass spectra instrumentation, and the highest essential oil result was the 1,8-cineole compound content. According to the results from the FTIR analysis, CAEO samples were successfully grouped based on their geographical origins. The experimental results showed that the wave numbers 1489.0715, 1475.3892, 1520.7538, and 1653.0743 per cm were used as markers to identify compounds in the CAEO based on the differences in the place of growth and quality control. This study showed that chemometric methods combined with FTIR-based fingerprinting could offer a dependable platform for verifying quality control and authentication.

Key words: *Curcuma aeruginosa*, chemometric, essential oil, Fourier Transform Infrared Spectroscopy, gas chromatography-mass spectra

INTRODUCTION

Central Java is the largest traditional medicine business center in Indonesia, and it produces many medicinal plants from the Zingiberaceae family,^[1] one of which is *Curcuma*

aeruginosa. *C. aeruginosa* essential oil (CAEO) has potent antioxidant activity^[2,3] and antimicrobial properties, and it is used in food preservation, pharmaceuticals, and natural therapy.^[4,5] The essential oil content is influenced by several factors, namely genetics, environmental conditions, climate, geographic origin, and others.^[6] Several studies from various regions state that the CAEO content in Malaysia is dominated by camphor (29.39%) and germacrone (21.21%) and in Thailand is dominated by curcumenol (38.70%) and β -pinene (27.50%). In India, it is dominated by curzerenone (32.21%) and 1,8-cineole (15.35%),^[7] while

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in Nepal, it is dominated by curzerenone (59.60%) and germacrone (5.3%).^[8] Therefore, it is very important to assess the differences in the quality and examine the chemical composition of CAEO based on geographic origin.

Currently, a number of chromatographic and spectroscopic methods have been widely used to control herbal medication quality. The chemical components in CAEO can be determined effectively using Fourier Transform Infrared Spectroscopy (FTIR) fingerprint technology combined with chemometrics.^[9,10] The fingerprint method uses pattern recognition technology to identify chemical components in sample fingerprints. It may also be used as a quality criterion for herbs based on similarity values. Several studies on the chemical diversity of medicinal plants used a chemometric approach.^[11-13] Therefore, to overcome this, principal component analysis (PCA) and partial least squares discriminant analysis (PLS-DA) are used to reduce the dimensions of the extensive data, grouping samples more accurately, but PLS-DA is more effective and relevant for multicollinearity problems.^[14]

In chemometric data processing, samples from different origins can be classified efficiently, and the characteristic factors leading to this classification can be determined. This study uses FTIR applications combined with chemometrics to classify and analyze the CAEO using gas chromatography-mass spectra (GC-MS).

MATERIALS AND METHODS

Materials

The samples used in this research were rhizomes of *C. aeruginosa* from five regions, harvested in October 2022: Kaloran Temanggung; Kalibakung, Tegal; Jumantono, Karanganyar; Bayat, Klaten; and Trucuk, Klaten, while Na₂SO₄ was obtained from SmartLab.

Methods

Preparation of essential oils

Fresh rhizomes of *C. aeruginosa* were sliced with a thickness of approximately 1-2 mm, and then steamed and distilled for 4 hours over medium heat. The resulting distillate was separated from water by adding anhydrous Na₂SO₄. Then, they were centrifuged at 4000 rpm for 5 min.^[15]

Analysis of essential oil profiles using gas chromatography-mass spectra

Fourier Transform Infrared Spectroscopy analysis

FTIR spectra were obtained using a Cary 630 Agilent FTIR spectrophotometer (USA) equipped with an attenuated total reflectance (ATR) accessory crystal with a resolution of 8/cm at 32 scans. Spectra were scanned in the absorbance mode from 4000 to 650/cm, and the data were handled with MicroLab Expert (Bio-Rad Laboratories, headquartered in

Hercules, California, USA). Analyses were carried out at room temperature.^[16,17]

Chemometric

MetaboAnalyst 6.0 software performed chemometry techniques such as PCA and PLS-DA. PCA is an unsupervised technique that uses class labels as a point of reference to find the most explanatory direction variance in a dataset. The PLS-DA technique is a regression extension of PCA, utilizing class information to maximize separation between observation groups.^[14]

RESULTS AND DISCUSSION

The distillation process was carried out to obtain the essential oils contained in the rhizomes of *C. aeruginosa*. The distillation was carried out using the steam-water distillation method because it can yield a lot of essential oils. According to the Indonesian Herbal Pharmacopoeia 2nd edition, the CAEO must contain not less than 1.89%.^[18] The *C. aeruginosa* rhizomes from the five areas had essential oil levels below 1.89%. This is because different soil types and heights of growing *C. aeruginosa* plants can affect oil yield. The results of the % essential oil yield of *C. aeruginosa* rhizome are shown in Table 1.

Essential oil content of *Curcuma aeruginosa* rhizome

The GC-MS method [Table 2] was used to analyze the content of the CAEO. The essential oils in *C. aeruginosa* rhizomes

Table 1: Percentage yield *Curcuma aeruginosa* rhizome essential oil

Number	Area	Yield (%)
1	Kaloran - Temanggung	0.108
2	Kalibakung - Tegal	0.104
3	Jumantono - Karanganyar	0.105
4	Bayat - Klaten	0.079
5	Trucuk - Klaten	0.120

Table 2: Gas chromatography-mass spectra chromatography conditions

Condition	Setting value
GC instrument	GC-MS-QP 2010 SE (Shimadzu, Japan)
Column/oven temp	Agilent® capillary column/75°C
Injection temperature (°C)	175
Flow rate of carrier gas (mL/min)	He at 0.8
Pressure (kPa)	45.9
Total flow (mL/min)	83.8
Linier velocity (cm/s)	32.9
Purge flow (mL/min)	3.0
Split ratio	100.0
Ion source temperature (°C)	200
Interface temperature (°C)	225

GC: Gas chromatography, GC-MS: GC-mass spectra

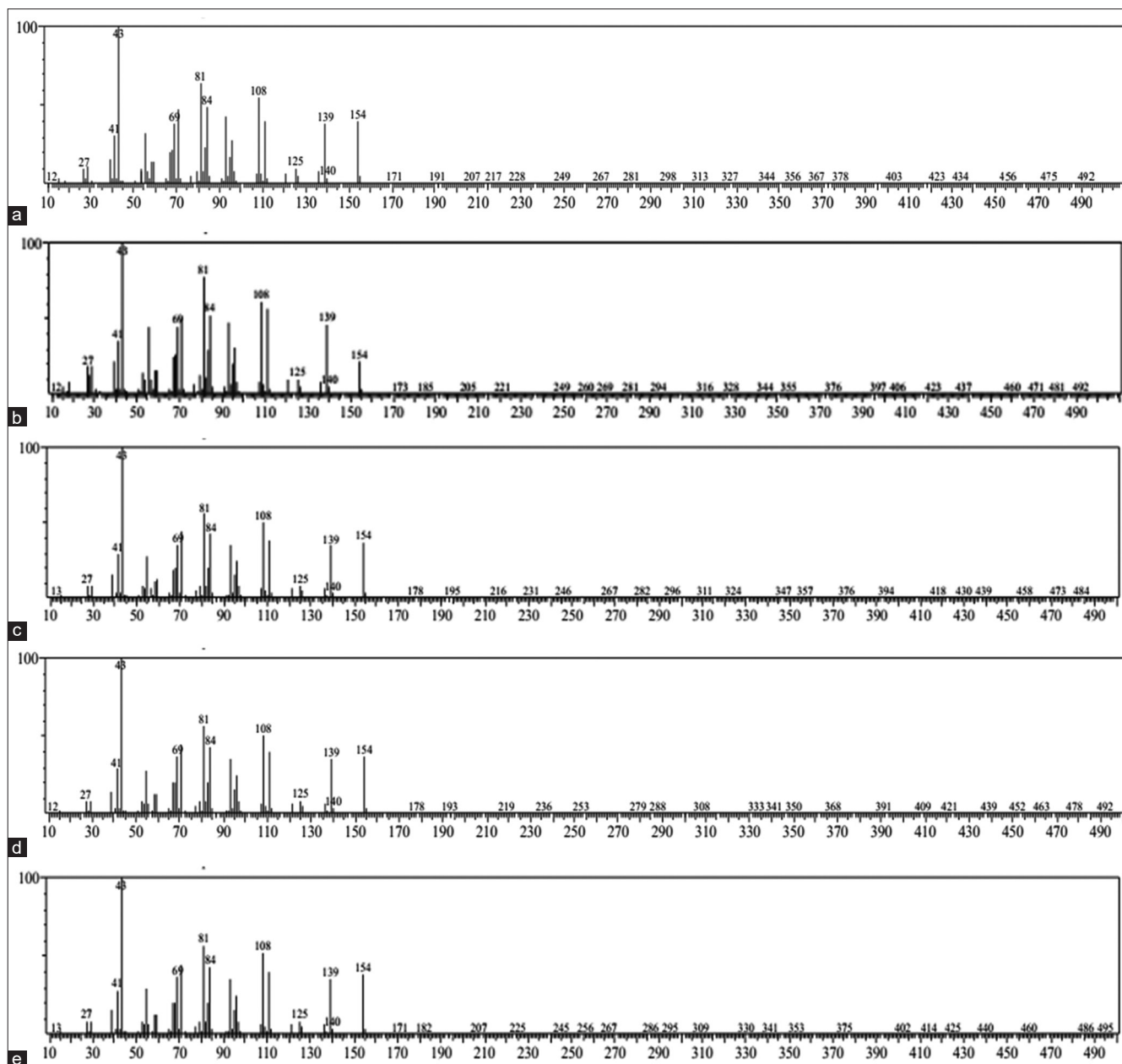


Figure 1: Representative chromatogram of *Curcuma aeruginosa* rhizome essential oil from different origins: (a) Kaloran, (b) Kalibakung, (c) Jumantono, (d) Bayat, (e) Trucuk

originating from the five regions contained similar contents but with different levels. Such differences were influenced by the geographical conditions where the plants grew, such as weather, soil height, soil type, soil pH, temperature, and humidity, thus influencing the levels of plant metabolite content.^[19] The essential oil content of *C. aeruginosa* rhizomes is shown in Table 3. Table 3 displays the 52 peaks that accounted for 98.04%–99.76% of the volatile compounds. However, only 8–12 major compounds were identified, with a more than 2% peak area. The 1,8-cineole compound was found to have the highest level in the essential oils from the five regions. The camphor and isocurcumenol compounds had different essential oil compositions among

the five regions. Variations in the chemical composition of essential oils may be caused by differences in geographical origins and environmental conditions, leading to differences in the quality of *C. aeruginosa* rhizome [Figure 1].

The compound 1,8-cineole is a compound contained in CAEO that is thought to inhibitor of Wnt/ β -catenin activity in HNSCC through decreased GSK-3 inhibition, which leads to decreased levels of WNT11^[20] and inhibiting the growth of MCF-7 cancer cells,^[21] likewise as an antibacterial^[22] and anti-inflammatory.^[23] Another compound also identified in the CAEO is camphor, capable of inhibiting the cell cycle and inducing apoptosis through the mitochondrial pathway in HCT-116 cells

Table 3: Essential oil content of *Curcuma aeruginosa* rhizomes (2 replications)

Compound	Molecular weight	Concentration (%)				
		Kaloran, Temanggung	Kalibakung, Tegal	Jumantono, Karanganyar	Bayat, Klaten	Trucuk, Klaten
Alpha-pinene	C ₁₀ H ₁₆	0.35	0.24	0.55	0.53	0.65
Camphene	C ₁₀ H ₁₆	0.93	0.73	1.21	-	1.58
Beta-pinene	C ₁₀ H ₁₆	1.28	-	1.64	1.52	1.52
Beta-myrcene	C ₁₀ H ₁₇	-	-	0.21	0.16	0.19
1.8-cineole	C ₁₀ H ₁₈ O	26.66	28.38	34.01	29.35	30.93
Camphor	C ₁₀ H ₁₆ O	11.47	19.05	3.24	18.37	18.86
2-undecanol	C ₁₁ H ₂₄ O	-	0.47	0.46	-	-
Endo-borneol	C ₁₀ H ₁₈ O	0.70	1.09	0.91	0.92	1.00
4-terpineol	C ₁₀ H ₁₈ O	0.46	1.00	0.89	0.82	0.90
Alpha-terpinyl acetate	C ₁₂ H ₂₀ O ₂	0.74	1.75	0.16	1.41	1.50
Beta-elements	C ₁₅ H ₂₄	0.56	0.49	0.48	0.85	0.58
Trans-caryophyllene	C ₁₅ H ₂₄	0.24	0.18	0.48	0.20	0.18
Beta-farnesene	C ₁₅ H ₂₄	-	-	0.28	0.27	0.20
Alpha-humulene	C ₁₀ H ₁₆	1.83	-	-	0.21	-
Germacrene D	C ₁₅ H ₂₄	0.22	0.18	0.21	0.19	0.26
Beta-selinene	C ₁₅ H ₂₄	-	0.15	-	0.14	0.17
Curzerene	C ₁₅ H ₂₀ O	0.43	0.41	0.35	0.41	0.41
Germacrene A	C ₁₅ H ₂₄	0.17	0.15	0.16	0.15	0.19
Germacrene B	C ₁₅ H ₂₄	0.17	-	0.15	-	0.18
Epiglobulol	C ₁₅ H ₂₆ O	0.40	0.46	0.40	0.41	0.39
Elemol	C ₁₅ H ₂₆ O	0.29	0.26	0.22	0.24	0.30
Boldenone	C ₁₉ H ₂₆ O ₂	19.06	-	14.97	14.53	13.90
Isocurcumenol	C ₁₅ H ₂₂ O ₂	2.86	8.89	5.97	5.55	4.68
Juniper camphor	C ₁₅ H ₂₆ O	-	-	1.47	1.58	1.94
1 (10), 4-aromedenradiene	C ₁₅ H ₂₂	-	-	0.51	0.55	0.54
Spathulenol	C ₁₅ H ₂₄ O	-	-	1.08	1.44	0.15
Germacrene	C ₁₅ H ₂₂ O	-	3.38	3.14	3.62	3.45
Aromadendrene epoxide	C ₁₅ H ₂₄ O	-	-	1.84	0.48	0.50
Trans-longipinocarveol	C ₁₅ H ₂₄ O	-	0.41	0.57	-	-
Germacrol	C ₁₅ H ₂₂ O	-	-	3.42	-	-
3-methyl-5-(2,6,6-trimethyl-1-cyclohexene-1-yl)-1-pentyl-3-ol	C ₁₅ H ₂₄ O	1.44	1.73	-	-	0.45
(E)-2,3,3-Trimethyl-2-(3'-methyl-1'-3'-butadiene-1'-yl)-6-methylidencyclohexanone	C ₂₆ H ₃₈ O	3.27	2.97	-	-	2.48
Tricyclo[5.1.0.0 (3.5)]octane-2,6-dione. 1.3.5.7-tetramethyl-	C ₁₆ H ₂₈ O ₂	-	-	3.69	3.49	-
Cyclohexane. 1.1-dimethyl-2,4-bis (1-methyl ethenyl)-, cis-	C ₁₅ H ₂₆	5.16	-	3.84	-	-
2-cyclohexen-1-one, 4-ethynyl-4-hydroxy-3,5,5-trimethyl-	C ₁₀ H ₁₄ O	-	15.95	-	-	-
3,7-cyclodecadien-1-one, 10-(1-methyl ethenyl)-, (E,E)	C ₁₅ H ₂₂ O	3.15	-	-	-	-

Contd...

Table 3: Contd...

Compound	Molecular weight	Concentration (%)				
		Kaloran, Temanggung	Kalibakung, Tegal	Jumantono, Karanganyar	Bayat, Klaten	Trucuk, Klaten
Dihydrocarvone	C ₁₀ H ₁₆ O	-	4.01	-	4.47	4.33
Calarene	C ₁₅ H ₂₄	5.39	-	3.33	3.93	4.12
Bicyclo[2.2.2]Octa-2,5-Diene. 1.2.3.6-tetramethyl	C ₁₂ H ₁₈	-	4.70	-	-	-
Ledenoxide-(II)	C ₁₅ H ₂₄ O	0.96	0.86	0.72	1.11	0.86
Curdione	C ₁₅ H ₂₄ O ₂	2.76	-	-	-	-
Ledane	C ₁₅ H ₂₆	-	-	2.84	-	-
1H-cyclopropa(a)naphthalene, 1A,2,4,5,6,7,7A,7B-octahydro-1,1,7,7A-	C ₁₅ H ₂₄	-	-	3.59	-	-
(E)-2,3,3-trimethyl-2-(3'-methyl-1'-3'-butadien-1'-yl)-6-methylidencyclohexanone	C ₁₄ H ₂₂ O	-	-	2.32	2.75	-
Tricyclo[5.2.2.0 (1,6)]undecan-3-ol, 2-methylene-6,8,8-trimethyl-	C ₁₅ H ₂₄ O	0.66	-	-	-	-
(3E)-5-isopropyliden-6-methyl-3,6,9-decatrien-2-one	C ₁₄ H ₂₀ O	5.04	-	-	-	-
Trans-p-mentha-1 (7),8-dien-2-ol	C ₁₀ H ₁₆ O	0.89	-	-	-	-
Hexadecane, 2,6,10,14-tetramethyl-	C ₂₀ H ₄₂	0.42	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-2,6-dimethyl-7-octyl-	C ₂₀ H ₃₂	0.60	-	-	-	-
Tetradecane, 1-chloro-	C ₁₄ H ₂₉ Cl	0.90	-	-	-	-
Phenanthrene. 1.2.3.4.5.6.7.8-Octahydro-	C ₁₅ H ₁₇ NO	-	0.22	0.17	0.15	0.69
Total identified (%)		99.46	98.11	99.45	99.76	98.04
Monoterpene hydrocarbons (%)		4.39	0.97	3.61	2.42	3.93
Oxygenated monoterpenes (%)		40.92	71.70	39.66	55.32	57.51
Sesquiterpene hydrocarbons (%)		11.91	1.15	18.19	6.28	6.41
Oxygenated sesquiterpenes (%)		37.05	16.40	34.14	32.10	27.15
Oxygenated diterpenes (%)		1.02	-	-	-	-
Others (%)		4.17	7.89	3.86	3.64	3.17

in vitro by 30% and then stopping cell proliferation.^[24] The use of camphor relieves pain, itchiness, and irritation in the affected area by activating particular transient receptor potential (TRP) channels, such as TRPV1, TRPV3, and TRPM8, and by inhibiting TRPA1. Camphor also produces a warm sensation and desensitizes sensory nerve endings.^[25] Many pharmacological uses for camphor include expectorant, cough

suppressant, rubefacient, antiseptic, antipruritic, anti-infective, anti-spasmodic, nasal decongestant, and cough suppression.^[26]

Fourier Transform Infrared Spectroscopy analysis

Data for each *C. aeruginosa* rhizome essential oil sample were obtained by scanning the results with an FTIR using ATR. Scanning was performed in five replications

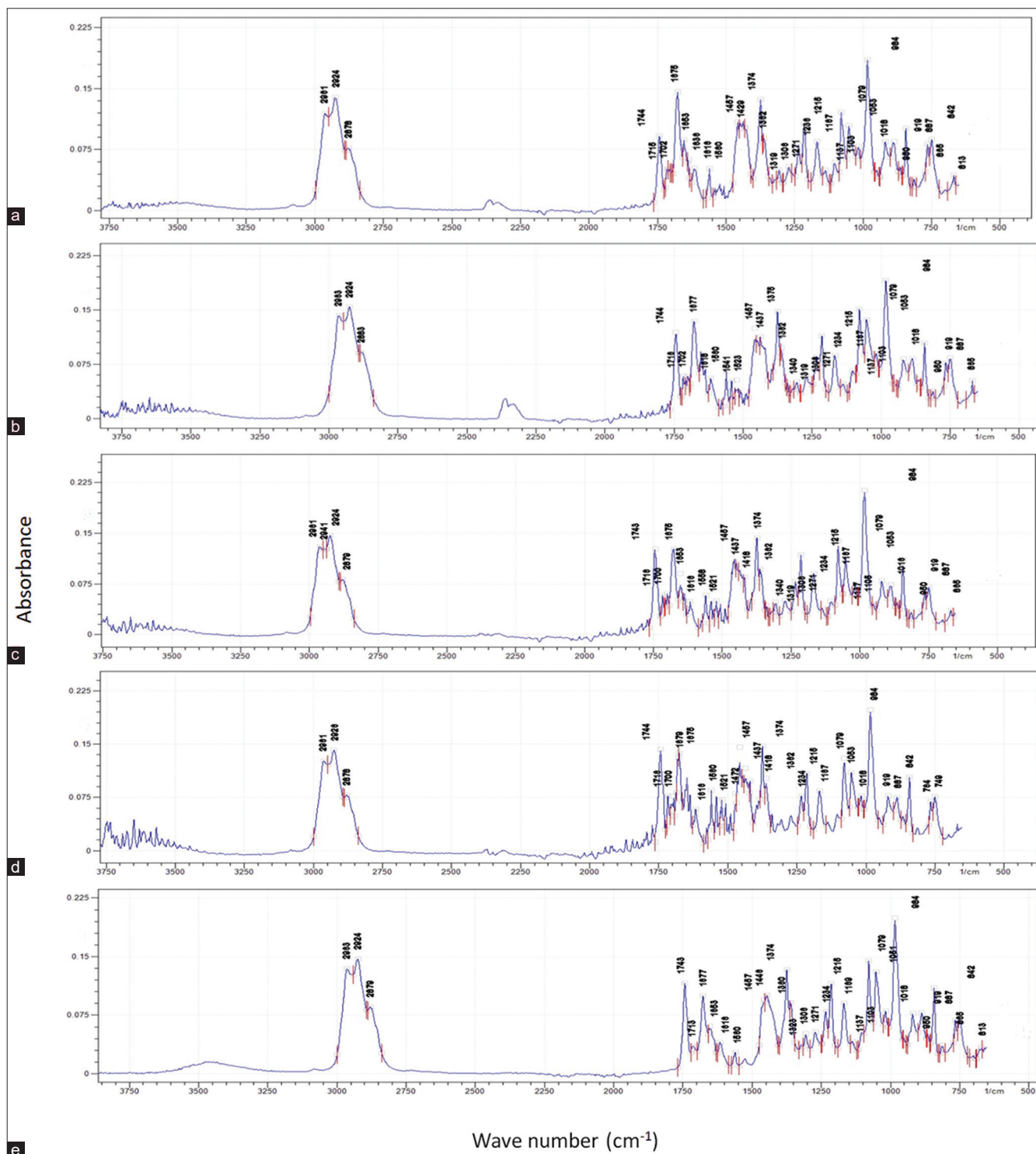


Figure 2: *Curcuma aeruginosa* rhizome essential oil from different regions: (a) Caloran, (b) Kalibakung, (c) Jumantono, (d) Bayat, (e) Trucuk

in waves ranging from 4000 to 650 per cm. Wave number 1750–700 per cm was a fingerprint area with a resolution of 8/cm.

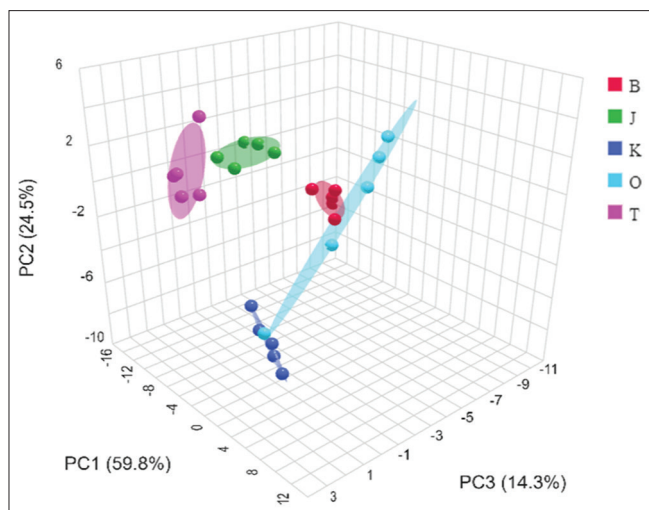


Figure 3: Results principal component analysis

The infrared spectrum of CAEO was taken from five geographically different regions [Figure 2], namely Kaloran, Kalibakung, Jumanthoro, Bayat, and Trucuk. The fingerprint area at wave numbers 1750–700 per cm showed a similar spectrum pattern, but there were differences in each absorption value due to the content or concentration of compounds in each CAEO. The CAEO had varying absorption bands: band 1 (3000–2750 per cm) showing the CH group (methyl or methylene) in the aliphatic chain in the essential oil; band 2 (around 1725–1675 per cm) showing the C = O (ketone) group; band 3 (1650–1475 per cm) showing C = C (alkene); and band 4 (1300–1000 per cm), indicating the presence of stretching vibrations of CO in compounds containing ether or alcohol. These bands [Figure 2] showed that they contained the exact contents of chemical compounds but with different levels.

The PCA method was applied using software *metaboanalysis* 6.0 which is freely available at <https://www.metaboanalyst.ca/MetaboAnalyst/ModuleView.xhtml>, resulting in a number of data in the form of score plots and biplots.

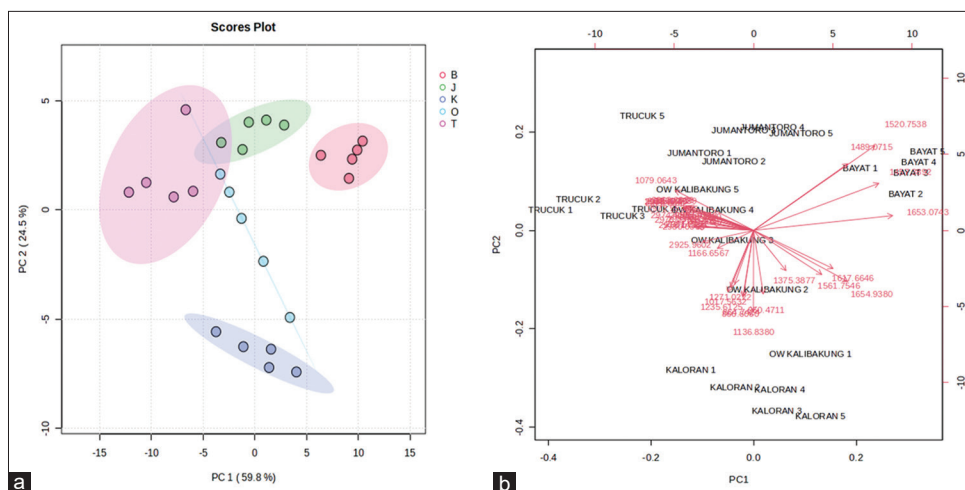


Figure 4: Principal component analysis results: (a) score plot; (b) biplot on Fourier Transform Infrared Spectroscopy

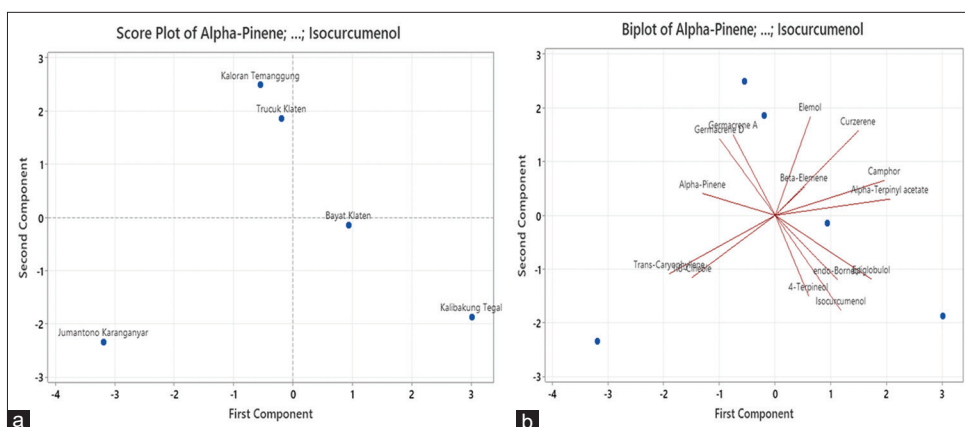


Figure 5: Principal component analysis results: (a) score plot; (b) biplot on gas chromatography-mass spectra

A score plot was used to present a plot of the relationship or similarity between the CAEO from the five regions based on the principal component (PC) values. In this study, two PCs were used, namely PC1 and PC2, marked with points with a certain distance between one point and another. Regarding PC, objects with almost the same or close PC values can be said to have similar physicochemical properties. Therefore, PCA can be used for object grouping purposes.^[27]

A biplot is a combination of a score plot and a loading plot. The loading plot shows how strongly each variable influences the PC by depicting it as a vector. If two vectors form an angle of $<90^\circ$, the two variables correlate positively. If it forms a right angle or around 90° , the two variables cannot correlate. The two variables show a negative correlation if they form an angle $>90^\circ$ – 180° .^[28]

Principal component analysis of *Curcuma aeruginosa* essential oil

In Figure 3, the highest eigenvalue results were shown in PC1 and then PC2, which means that these values

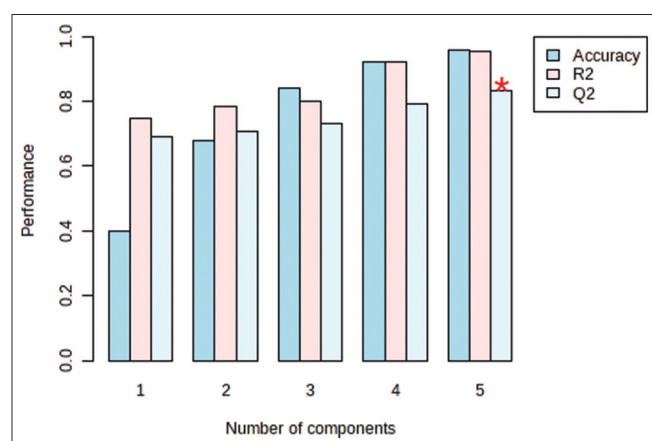


Figure 6: R^2 and Q^2 intercept values from permutations in partial least squares discriminant analysis on Fourier Transform Infrared Spectroscopy. “*” indicates that the model has excellent predictive performance, with $Q^2 \geq 0.7$

contributed to the compound content of 59.8% on PC1 and 24.5% on PC2. In this analysis, PC1 and PC2 can be used to represent 100% of the variables (cumulative).

The relationship between the five essential oils of *C. aeruginosa* was different, as seen by the score plot and biplot displayed in Figure 4. The score plot displays five points of essential oils from the five locations distant from one another. The conditions of the soil, temperature, and weather at the location of *C. aeruginosa* rhizomes grow are the causes of the dissimilarity. Because of this, the five rhizomes differed in terms of the number of compounds contained, depending on the location in which they grew. The PCA results displayed in Figure 5 demonstrated a favorable association between curzerene and beta element compounds' antibacterial and anti-inflammatory properties when compared to elemol and germacrene. A compound is considered to include essential oil components if its angle is smaller than 90° . The rhizome of *C. aeruginosa*, specifically beta-element, curzerene, elemol, and germacrene D, has antibacterial and antioxidant properties. Curzerene^[29] and germacrene^[30] have been studied for their antioxidant potential. According to Sieniawska et al. (2018), the beta-element in *Nigella damascena* has moderate to strong antibacterial activity against *Mycobacterium tuberculosis*.^[31] The essential oil of *Neomirandea angularis* leaves contains *Bacillus cereus*, which is the target of germacrene D's antibacterial activity.^[32]

Partial least squares discriminant analysis

To obtain a high level of group separation and improve variable recognition for sample classification, the PLS-DA technique was used. 3D PLS-DA obtained on the sample distribution [Figure 6] based on the wave numbers identified in the CAEO showed that all the test samples could be clearly classified into five groups according to their origin.

The main purpose of permutations in PLS-DA is to test the significance of the model that has been built and evaluate

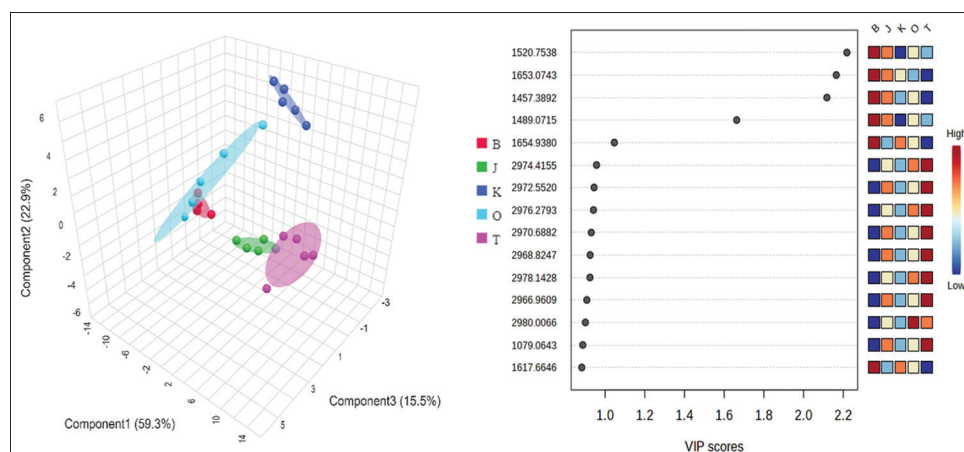


Figure 7: Partial least squares discriminant analysis results and VIP values on Fourier Transform Infrared Spectroscopy

the model. R -squared (R^2) and Q -squared (Q^2) are evaluation parameters often used in the context of discriminant PCA with the PLS-DA method. However, the R^2 and Q^2 values are not obtained directly from permutations but are often used in internal cross-validation of PLS-DA models. R^2 on PC2 was 0.79, where the higher the value, the better the model at explaining variations in response data, while Q^2 on PC2 was 0.70, which was obtained from evaluation through cross-validation; the higher the value, the better the model to predict new data. Some studies use specific significance levels (e.g., $\alpha = 0.05$) to determine whether R^2 and Q^2 values are significant. If the original values are higher or lower than the values resulting from permutation at the selected significance level, the model is considered significant. The above results indicated that the PLS-DA technique would be more suitable than PCA to provide visual differentiation of test samples according to origins regarding quality control.

Based on PLS-DA, the loading plot shows the contribution of each to the sample discrimination variable. Based on Variable Importance Projection (VIP) values in Figure 7, some wave numbers had VIP values >1.5 , so it can be concluded that wave numbers g of 1489.0715; 1475.3892; 1520.7538; and 1653.0743 per cm were the most important wave numbers in showing differences in *C. aeruginosa* rhizome essential oil.

CONCLUSION

C. aeruginosa rhizome is a traditional herb widely used in many countries. This study proposed an efficient strategy for quality control of CAEO as raw materials in the pharmaceutical and natural products industry. Even though there were variations in the chemical contents due to differences in geographical origins, the GC-MS fingerprint profiles of the essential oil samples were similar based on visual inspection, making it difficult to classify the essential oil samples according to their different origins. Therefore, the chemometric technique was applied with the FTIR fingerprint technique to recognize CAEO from various origins. It has shown that some techniques, such as PCA and PLS-DA, could classify the samples objectively. Furthermore, four-wave numbers were the most important variables in differentiating *C. aeruginosa* rhizomes for the quality control of CAEO using quantitative analysis.

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Conflicts of interest

There are no conflicts of interest.

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