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Classification using FTIR and UV-Vis spectra combined with chemometrics and GC-MS profiles of *Brucea javanica* fruit extracts with different extracting solvents

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Abstract

Brucea javanica L. Merr. has long been used for its antimalarial, anti-diabetic, antibacterial, and antioxidant effects. Its bioactivity depends on both its chemical constituents and the type of solvent employed during extraction. Integrating FTIR and UV-Vis spectral data with chemometric approaches enables classification of fruit extracts based on the solvent used, while GC-MS analysis provides detailed compound identification. Using sonication, extraction with methanol, ethyl acetate, and n-hexane produced yields of 30.61% ± 0.80, 19.20% ± 0.75, and 18.12% ± 0.89, respectively. FTIR spectra were recorded over 600–4000 cm^{-1}, and UV-Vis spectra were measured across 200–800 nm. Analysis showed that ethyl acetate and n-hexane extracts exhibited similar profiles, which differed from that of the methanol extract. PCA successfully distinguished all three extracts, with cumulative PC1 and PC2 values above 70%. FTIR-based PCA provided better separation due to its broader fingerprint region compared to UV-Vis spectra. GC-MS results revealed that the compound profiles were largely similar across the extracts, although more compounds were detected in the methanol extract than in the ethyl acetate or n-hexane extracts.

Keywords: *B. javanica; chemometric; FTIR; GC-MS; spectroscopy; UV-Vis*.

Introduction

As medicinal ingredients, plants have been widely used by humans since ancient times based on inheritance from generation to generation in the form of traditional medicines and herbal medicine. In traditional medicine, various parts of plants such as roots, stems, leaves, flowers, and fruits can be utilized[1]. Their therapeutic potential arises from the presence of bioactive secondary metabolites[2]. Indonesia's rich biodiversity offers vast potential as a source of medicinal plants, one of which is *B. javanica* L. Merr.

B. javanica is an Asian plant found in Indonesia, Thailand, and Malaysia, belonging to the genus *Brucea* (Simaroubaceae) and growing up to 3 meters[3]. Nearly all parts, including leaves, fruit, and seeds, have medicinal uses. Traditionally, its fruit is used as an antimalarial and, in some regions, as an anti-diabetic. Studies have shown it possesses antimalarial[4],[5], anti-diabetic[6], anti-microbial, anti-oxidant[3],[7],[8], and anti-tumor[9] activities. Its bioactive compounds include quassinoids (bruceine A–I, brusatol A, dihydrobrusatol B), bruceosides (A–S), brusatol amarissima E2-glucosidase, brusatol ketoacid, and bruceen[10].

The concentration of bioactive compounds and the quality of medicinal plants are strongly influenced by genetic factors, cultivation

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conditions[11], plant age, harvest time[12],[13], nd the choice of extraction solvent[14],[15]. Solvent selection is critical, as it affects the composition, concentration, and biological activity of the extracted compounds[16],[17]. In *B. javanica*, polar solvents such as ethanol and methanol efficiently extract quassinoids, flavonoids, and phenolics, which contribute to antitumor and antidiabetic effects[3],[18]. Conversely, non-polar solvents like n-hexane or petroleum ether primarily yield *B. javanica* oil (BJO), rich in fatty acids, often used in pharmaceutical formulations[19],[20]. Using solvents of different polarities produces distinct extract fractions with varying bioactivities, as evidenced in herbicidal studies[21].

Analytical methods are used in the identification and classification of natural products to determine the levels of one or more active compounds, following the characteristic compound approach[22]. Current identification, discrimination, and authentication techniques focus on the chemical constituents of natural materials. Common laboratory methods include high-performance liquid chromatography (HPLC), gas chromatography (GC)[23], thin-layer chromatography (TLC)[24],[25], nd spectroscopic techniques such as UV-Vis, FTIR, and NMR[11],[13],[26]–[31], often combined with chemometric analysis for enhanced.

FTIR and UV-Vis spectroscopy are efficient, rapid, and cost-effective methods for distinguishing metabolite profiles based on solvent polarity[22],[32]. Previous research on *B. javanica* has mainly focused on compound-specific analysis using HPLC, GC, or NMR, which, although accurate, are costly, time-consuming, and dependent on pure reference standards. These methods provide limited information on the overall metabolite composition of extracts obtained with different solvents. In contrast, FTIR and UV-Vis spectroscopy combined with chemometrics offer a rapid, low-cost, and holistic approach to discriminate extracts based on solvent polarity and chemical fingerprint. To date, this strategy has rarely been applied to *B. javanica*, creating a research gap that this study seeks to address.

Experimental

Materials

The materials utilized were *B. javanica* fruits, methanol, ethyl acetate, n-hexane, acetone, and distilled water (Brataco Lab). All solvents were obtained from Merck.

Instruments

The equipment employed in this study included an ATR Alpha FTIR Spectrophotometer (Bruker, Germany), a UV-Vis spectrophotometer (Agilent Technologies Cary 60), an oven, a rotary evaporator (Buchi, Flawil, Switzerland), a Power Dry LL1500 freeze dryer (Thermo Fisher Scientific, USA), a GC-MS system (Thermo Fisher Scientific, USA), a 50-mesh sieve, and standard laboratory glassware.

Methods

Sample Collection and Preparation

B. javanica fruit samples were taken from Agroecotechnology Laboratory, University of Bengkulu (X = 3° 45' 24.71" S; Y = 102° 16' 22.10" E). The fruit that has been taken is then dried on paper under normal air-drying (room temperature) for 7 days. The dried *B. javanica* fruit samples were then mashed and sieved with a 50 mesh sieve to obtain *B. javanica* fruit simplicia.

Extraction process

A total of 7 g of *B. javanica* simplicia was extracted with 75 mL of methanol using sonication in an ultrasonic bath at 35 kHz and 30 °C.. The same simplicia was then re-sonicated with an additional 75 mL of methanol, resulting in a total of 150 mL methanol extract. The same procedure was applied using ethyl acetate and n-hexane as solvents. Each extraction with the different solvents was replicated 10 times, yielding a total of 30 extracts. Fresh extracts were measured by UV-Vis, then concentrated and freeze-dried for FTIR analysis.

UV-Vis Spectrum and FTIR Spectrum Measurement

UV-Vis spectra were recorded by diluting 15 µL of extract in 3 mL of solvent and scanning from 200–800 nm, with data exported to Excel. FTIR spectra were obtained by placing ~100 mg of extract on the ATR crystal, scanning from 4000–600 cm^{-1} at 32 scans per spectrum and 16 cm^{-1} resolution, and saving the data in .dpt format.

Chemical Composition Analysis with GC-MS

Compound analysis of *B. javanica* extract was performed using GC-MS with Chromeleon 7 software (Version 7.2.10.24543). The MS was operated with hydrogen as the carrier gas, employing an HP-5MS UI column (30 m length, 0.250 mm ID, 0.25 µm film thickness). The front inlet was set to splitless mode with an initial temperature of 305 °C and a split flow of 50 mL/min. Mass spectrometry was carried out in electron-ionization (EI) mode, with spectra recorded over an m/z range of 40–500.

Chemometrics Analysis

FTIR and UV-Vis spectra were processed using multivariate analysis, specifically principal component analysis (PCA), to classify *B. javanica* fruit extracts according to the different extraction solvents. Prior to PCA, spectral pre-treatment steps, including baseline correction and area normalization, were applied. The multivariate analysis was performed with the aid of Orange software (version 3.29.3).

Results and Discussion

Extraction of *B. javanica* Fruit by Different Solvents

The extraction of *B. javanica* fruit was performed using the sonication method in an ultrasonic bath at 30 °C for 30 minutes with three different solvents: methanol, ethyl acetate, and n-hexane. As shown in Figure 1 and Table 1, the methanol (MeOH) extract produced a yellowish-brown color with a yield of 30.61% ± 0.80, the ethyl acetate (EtOAc) extract was also yellowish-brown with a yield of 19.20% ± 0.75, while the n-hexane extract appeared yellow with a yield of 18.12% ± 0.89.

The variation in extract color and yield reflects differences in metabolite composition, as solvent polarity strongly influences the types of compounds extracted. Polar solvents such as methanol generally provide higher yields by solubilizing a wider range of polar and semi-polar metabolites, although higher yield does not necessarily equate to higher concentrations of bioactive compounds[33].

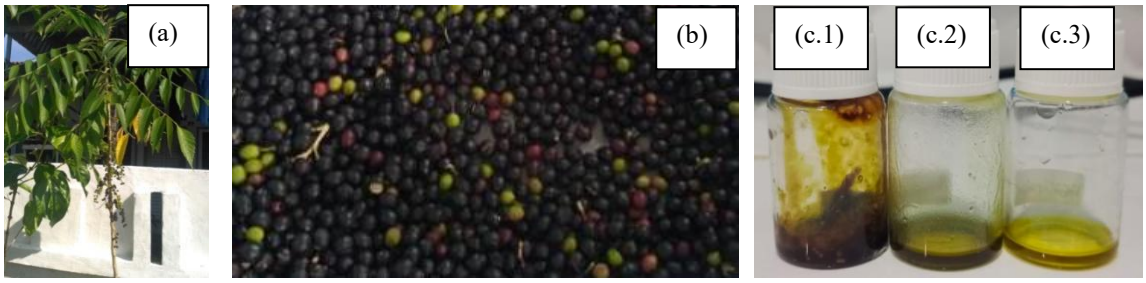

Figure 1. *Brucea* (a) plant; (b) fruits; (c) fruits extracts (c.1. MeOH extract; c.2. EtOAc extract; c.3. n-hexane extract).

Table 1. Extraction yield of *B. javanica* fruit.

Solvent extraction	yield (%) ± SD*
MeOH	30.61 ± 0.80
EtOAc	19.20 ± 0.75
n-hexane	18.12 ± 0.89

Note: SD based on 10 replications

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UV-Vis Spectra of *B. javanica* Fruit Extract

The differences in absorption bands observed among the methanol, ethyl acetate, and n-hexane extracts are attributed to the distinct metabolite classes solubilized by each solvent according to their polarity. Methanol, as a polar solvent, predominantly extracts phenolics, flavonoids, and quassinoids, which show strong $\pi \rightarrow \pi^*$ transitions in the UV region around 200–300 nm[34]. Ethyl acetate, with intermediate polarity, recovers both flavonoid aglycones and chlorophyll derivatives, resulting in characteristic absorption between 280–330 nm and extended bands near 410 and 667 nm. Apart from that, the methanol extract also appears at an absorption peak at a wavelength of 205.9 nm, which is thought to be an absorption peak from quassinoid[35]. In contrast, the non-polar n-hexane extract is rich in lipids, carotenoids, and chlorophylls, producing broader absorption features at 269, 329, 409, and 686 nm. These results highlight that solvent polarity governs the type of metabolites extracted and, consequently, the spectral profile observed.

FTIR Spectrum of *B. javanica* Fruit Extract

Based on the representative FTIR spectrum of *B. javanica* fruit extracts, it can be seen that there are similar patterns between the ethyl acetate extract and the n-hexane extract, both of which are significantly different from the methanol extract (Figure 3). It is suspected that there are similarities in the metabolite profile components between the ethyl acetate extract and the n-hexane extract, and it is also suspected that there are differences in the metabolite profile components in these two extracts compared to the methanol extract.

Analysis of the FTIR spectrum can be seen that the same absorption peaks (ethyl acetate extract and n-hexane extract) are seen at wave numbers 2852 cm^{-1} and 2922 cm^{-1} which are C-H stretching vibrations, wave number 1744 cm^{-1} which is δ stretching vibrations -lactone, wave number 1463 cm^{-1} which is the C-H bending vibration, wave number 1159 cm^{-1} which is the C-O stretching vibration, and at wave number 722 cm^{-1} which is the vibration of rocking vibration of long-chain $–(CH_2)–$ groups (Figure 3). Apart from that, in the methanol extract, O-H stretching vibrations were also seen in the 3369 - 3012 cm^{-1} area and C-O-C bending vibrations in the 1026 cm^{-1} area, where these two vibrations were not visible in the ethyl acetate extract and n-hexane extract.

Classification of *B. javanica* Fruit Extracts

Classification of *B. javanica* fruit extracts was carried out based on differences in the polarity of the extracting solvent used. This classification is intended to identify variations in metabolite levels across the different extracts. FTIR spectral measurements provide information limited to functional groups. The FTIR spectra reveal distinct profile differences among methanol, ethyl acetate, and n-hexane extracts, although the profiles of ethyl acetate and n-hexane appear relatively similar and challenging to distinguish. A comparable pattern is observed in the UV-Vis spectra, where the ethyl acetate and n-hexane extracts of *B. javanica* fruit also show notable similarities. Therefore, a chemometric approach is needed to classify *B. javanica* fruit extracts, namely using Principal Component Analysis (PCA) based on differences in the polarity of the extracting solvent used.

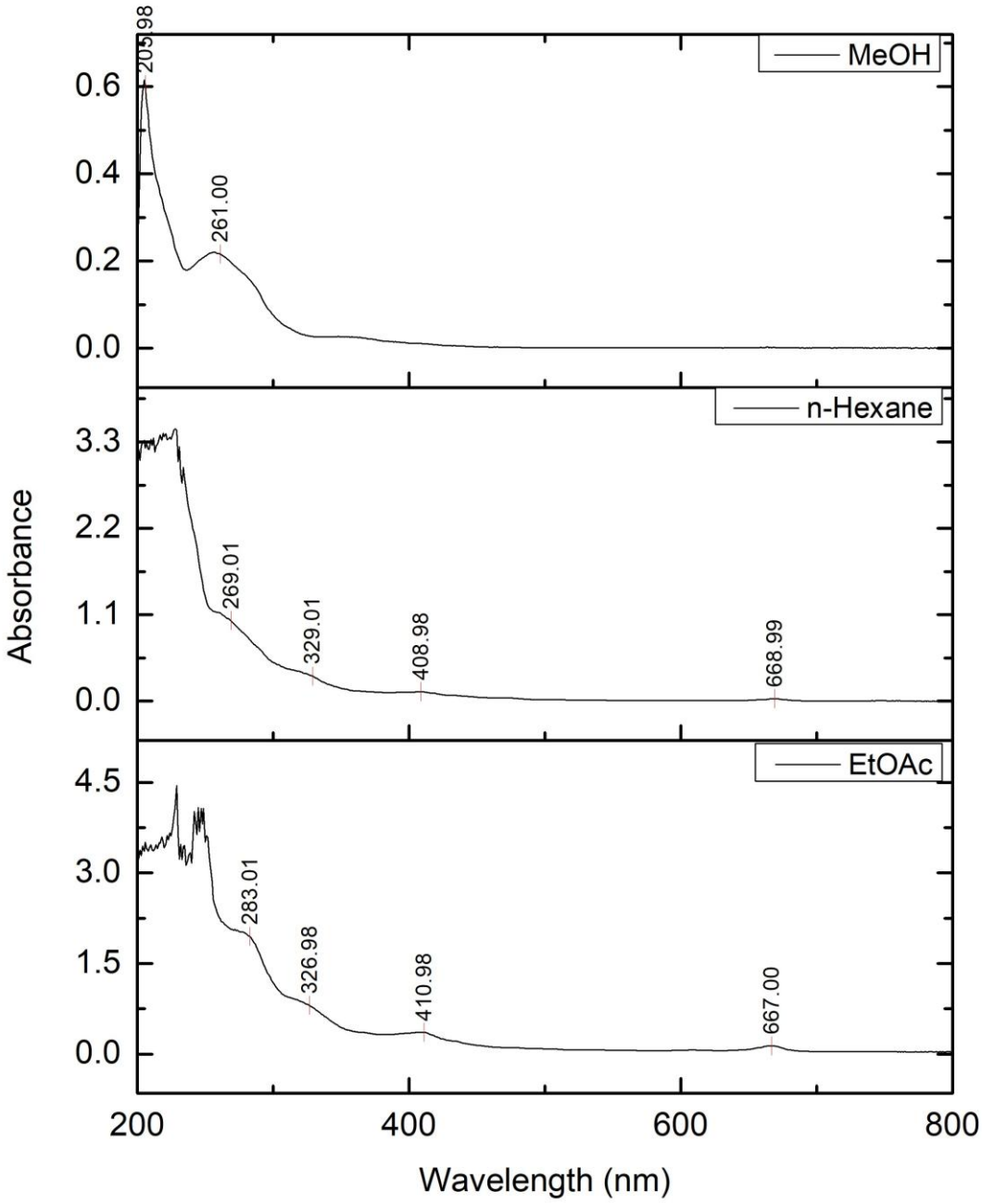

Figure 2. Representative UV-Vis spectrum of *B. javanica* fruit extracts based on different solvent extraction.

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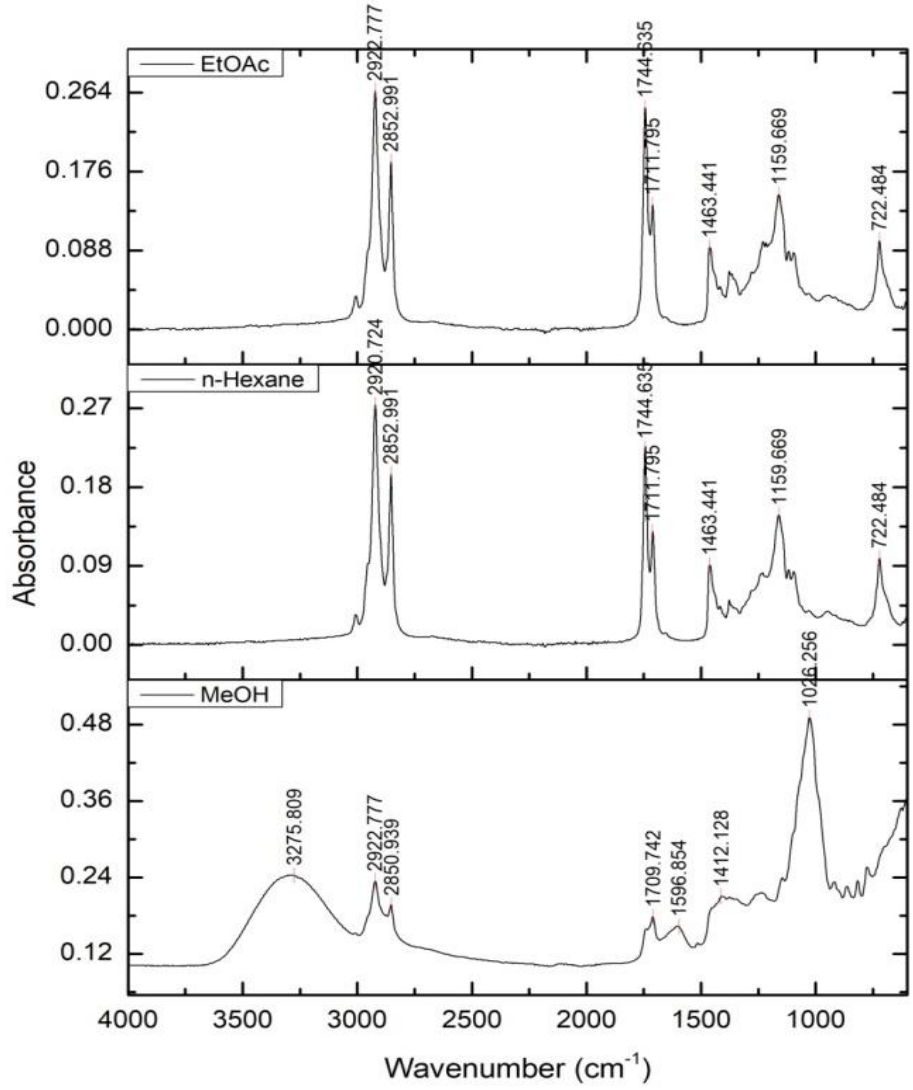

Figure 3. Representative FTIR spectrum of *B. javanica* fruit extracts based on different solvent extraction.

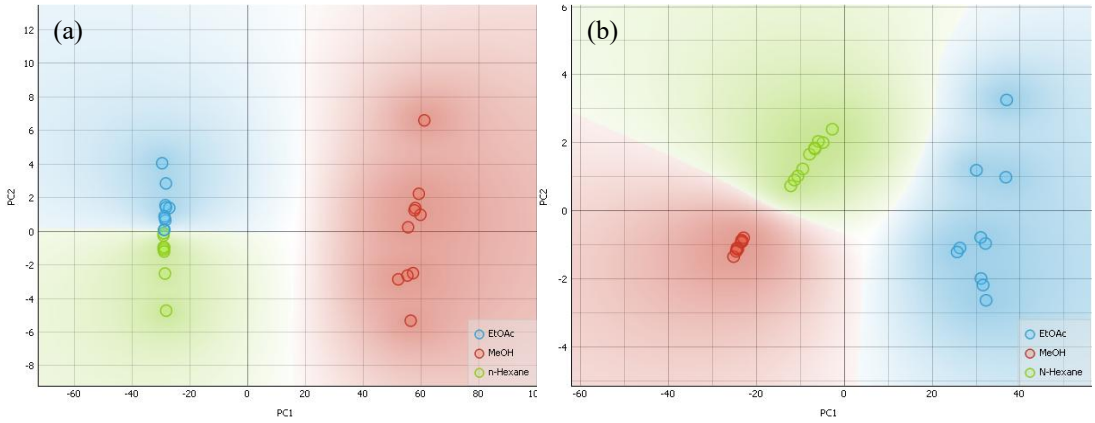

Figure 4. PCA score plots of *B. javanica* fruit extracts based on solvent polarity (a. FTIR spectra, b. UV-Vis spectra).

Figure 4 presents the PCA score plots of the FTIR and UV-Vis spectra of *B. javanica* fruit extracts, grouped according to solvent polarity. The plot shows clear clustering for the FTIR spectra, where PC1 and PC2 together account for 90% of the total variance. In comparison, the PCA plot of the UV-Vis spectra explains 93% of the total variance, indicating strong component representation. A higher cumulative PC value reflects better variance explanation, and total PCs exceeding 70% are considered to provide good clustering and clear visualization[36]. Further evaluation using the confusion matrix (Figure 5) demonstrates that PCA of the FTIR spectra accurately identified all 10 methanol extract samples. For the n-hexane extracts, 9 samples were correctly classified, with 1 sample misclassified as ethyl acetate. Similarly, 8 ethyl acetate extract samples were correctly predicted, while 2 were misclassified as n-hexane. In contrast, the confusion matrix evaluation of PCA from UV-Vis spectra showed perfect prediction, where all extracts were correctly classified. The variation in clustering patterns between FTIR- and UV-Vis-based PCA may be attributed to differences in the spectral fingerprint regions, with FTIR spectra providing more complex profiles compared to the relatively simpler UV-Vis spectra.

The PCA confusion matrix evaluation of FTIR and UV-Vis spectra revealed similarities between the n-hexane and ethyl acetate extracts of *B. javanica* fruit, indicating that both solvents likely extract overlapping chemical components. This observation was further validated by the AUC values, where the PCA FTIR spectra reached 0.96 and the PCA UV-Vis spectra 0.97. Such values reflect excellent classification performance, as models with AUC scores between 0.9 and 1.0 are regarded as highly accurate and reliable[37].

Chemical Composition of *B. javanica* Fruit Extract

Based on the GC–MS analysis, the metabolite composition of *Brucea javanica* fruit extracts was strongly influenced by solvent polarity. The methanol extract, owing to its high polarity, was dominated by sugars (e.g., arabinose, melibiose, mannose, melezitose), sugar alcohols, and glycosidic compounds, along with smaller amounts of fatty acids and sterols, reflecting its affinity for hydrophilic metabolites. In contrast, the ethyl acetate extract contained mainly fatty acid esters, including cis-vaccenic acid, methyl oleate, and methyl linoleate, together with sterols and terpenoid derivatives, which represent compounds of intermediate polarity. The n-hexane extract was highly enriched in lipophilic metabolites such as long-chain fatty acids, hydrocarbons, and sterols, with trans-13-octadecenoic acid and oleic acid as major constituents. These results are consistent with previous findings that polar solvents efficiently extract phenolics, flavonoids, and quassinoids with strong pharmacological potential[3],[18], while non-polar solvents preferentially yield *B. javanica* oil rich in fatty acids for pharmaceutical formulations[19],[20], and semi-polar solvents provide intermediate fractions with distinct bioactivities, including herbicidal effects[21]. Collectively, these data confirm that solvent selection governs the chemical profiles of *B. javanica* extracts, enabling targeted recovery of specific metabolite classes for both pharmacological and analytical applications.

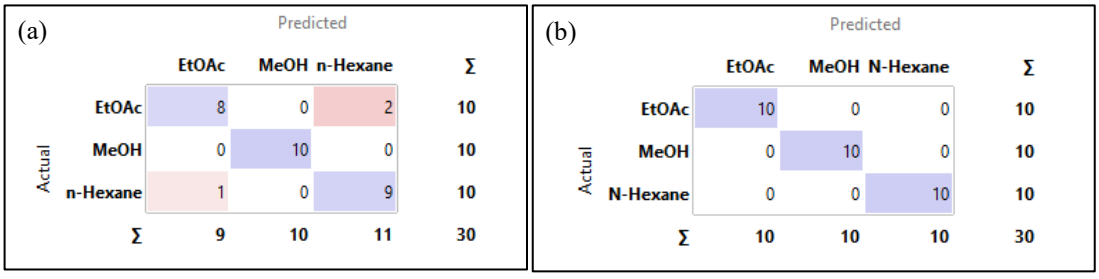

Figure 5. Confusion matrix of PCA classification (a. FTIR spectra, b. UV-Vis spectra).

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Previous studies have reported that *B. javanica* fruit contains various quassinoids, including bruceine derivatives, brusatol A, dihydrobrusatol B, bruceosides L, P, and S, as well as brusatol amarissima E2-glucosidase, brusatol ketoacid, and bruceen[10]. However, in this study, the compounds obtained from GC-MS were quite different, which is thought to be due to differences in analysis methods and optimization of GC-MS so that it was only able to detect organic acids. Another compound that has been isolated from *B. javanica* is another quasinoid group, namely bruceajavanin C-21[9].

Table 2. Tentative chemical compounds of methanol extract of *B. javanica* fruit

Ret.Time (min)	Compound	Peak Area (%)
4.41	9-Hexadecenoic acid	0.08
4.77	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	0.11
4.82	2-Myristynoyl pantetheine	0.08
5.38	l-Gala-l-ido-octose	0.07
5.53	D-Limonene	0.58
6.22	Glycerin	2.49
6.64	2(5H)-Furanone, 3,5,5-trimethyl-	0.65
6.80	Methyl 6-oxoheptanoate	0.14
7.54	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	0.41
8.33	DL-Arabinose	0.51
8.97	Melibiose	0.20
9.10	2-Methyl-oct-2-enedial	1.19
9.97	Ascaridole epoxide	0.91
12.21	Desulphosinigrin	0.26
12.69	2-Myristynoyl pantetheine	0.06
13.51	9-Octadecenoic acid, (2-phenyl-1,3-dioxolan-4-yl)methyl ester, cis-	0.20
14.65	Desulphosinigrin	0.55
14.73	Melezitose	0.92
15.08	3-O-Methyl-d-glucose	1.85
15.24	d-Mannose	0.56
15.31	Desulphosinigrin	0.40
15.55	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	0.06
15.79	7-Methyl-Z-tetradecen-1-ol acetate	0.09
16.04	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	0.08
16.48	Dodecanoic acid, 3-hydroxy-	0.08
16.76	2,4,6-Cycloheptatrien-1-one, 2-hydroxy-5-(3-methyl-2-butenyl)-4-(1-methylethenyl)-	0.49
16.92	Hexadecanoic acid, methyl ester	0.50
17.16	Dodecanoic acid, 3-hydroxy-	0.28
17.39	n-Hexadecanoic acid	9.33
17.57	Estra-1,3,5(10)-trien-17ß-ol	0.06
18.02	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	0.44
18.09	Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester	0.18
18.30	Estra-1,3,5(10)-trien-17ß-ol	0.11

18.45	9-Hexadecenoic acid	0.20
18.54	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	1.03
18.59	trans-13-Octadecenoic acid, methyl ester	2.51
18.82	Heptadecanoic acid, 16-methyl-, methyl ester	0.40
18.97	(Z)-18-Octadec-9-enolide	7.00
19.06	cis-Vaccenic acid	19.64
19.13	cis-13-Octadecenoic acid	18.37
19.20	trans-13-Octadecenoic acid	1.63
19.28	Octadecanoic acid	7.19
20.74	cis-13-Eicosenoic acid	0.16
20.85	trans-13-Octadecenoic acid	0.12
21.47	Ethyl iso-allocholate	0.01
21.80	9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)-	0.19
21.92	9-Hexadecenoic acid	0.26
23.50	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	1.27
28.96	Ethyl iso-allocholate	0.37
29.46	Stigmasterol	1.04
31.90	Ethyl iso-allocholate	0.15

Table 3. Tentative chemical compounds of ethyl acetate extract of *B. javanica* fruit

Ret.Time (min)	**Compound**	**Peak Area (%)**
5.53	D-Limonene	0.28
9.15	2-Decenal, (Z)-	0.66
9.31	Hexadecane, 1,1-bis(dodecyloxy)-	0.12
16.49	trans-13-Octadecenoic acid	0.10
16.91	Hexadecanoic acid, methyl ester	2.47
17.38	n-Hexadecanoic acid	0.16
18.46	trans-13-Octadecenoic acid	0.21
18.54	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	4.36
18.59	9-Octadecenoic acid (Z)-, methyl ester	10.81
18.82	Methyl stearate	2.08
18.89	n-Hexadecanoic acid	0.13
19.19	cis-Vaccenic acid	37.21
21.75	cis-Vaccenic acid	0.23
21.79	Glycidyl oleate	1.49
21.99	cis-13-Octadecenoic acid	0.23
23.16	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.13
24.97	Oleic acid, 3-(octadecyloxy)propyl ester	0.89
27.02	Tritetracontane	3.42
28.94	Ethyl iso-allocholate	0.30
29.44	Stigmasterol	0.92
30.00	(5ß)Pregnane-3,20ß-diol, 14a,18a-[4-methyl-3-oxo-(1-oxa-4-azabutane-1,4-diyl)]-, diacetate	0.22

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Table 4. Tentative chemical compounds of n-hexane extract of *B. javanica* fruit

Ret.Time (min)	Compound	Peak Area (%)
5.52	D-Limonene	0.23
9.15	2-Decenal, (Z)-	0.39
9.31	Hexadecane, 1,1-bis(dodecyloxy)-	0.04
9.66	13-Heptadecyn-1-ol	0.08
14.30	1-Hexadecanol, 2-methyl-	0.05
16.49	9-Hexadecenoic acid	0.04
16.92	Hexadecanoic acid, methyl ester	1.76
17.41	n-Hexadecanoic acid	1.20
17.58	Estra-1,3,5(10)-trien-17ß-ol	0.05
18.54	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	3.24
18.60	9-Octadecenoic acid (Z)-, methyl ester	7.67
18.83	Methyl stearate	1.41
19.15	Oleic Acid	12.55
19.24	trans-13-Octadecenoic acid	39.58
21.76	cis-Vaccenic acid	0.10
21.80	Glycidyl oleate	0.52
23.34	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.16
23.47	cis-11-Eicosenoic acid	0.20
24.98	Octadecane, 3-ethyl-5-(2-ethylbutyl)-	0.82
25.91	Ethyl iso-allocholate	0.19
27.03	Tritetracontane	3.12
29.46	Stigmasterol	0.68
30.03	Ethyl iso-allocholate	0.24

The combined UV-Vis, FTIR, and GC-MS analyses highlight that solvent polarity produces distinct chemical fingerprints of *B. javanica* fruit extracts, which can be directly applied for quality control, authentication, and prediction of biological activity. The clear separation achieved by PCA with high accuracy (AUC 0.96–0.97) demonstrates the reliability of these spectral profiles as rapid tools for ensuring batch consistency and preventing adulteration, in line with recent advances in chemometric-based herbal authentication[38]. Moreover, the methanol extract, enriched in phenolics, flavonoids, and quassinoids, suggests higher potential for antitumor, antioxidant, and antidiabetic activity[3],[18], while ethyl acetate and n-hexane extracts dominated by fatty acids and sterols may be more relevant to anti-inflammatory or immunomodulatory effects[20],[21]. These findings indicate that solvent-dependent metabolite profiles can serve not only as chemical markers for standardization and authentication but also as predictors of pharmacological potential.

Conclusions

FTIR and UV-Vis spectral analysis revealed that the methanol extract of *B. javanica* fruit exhibited clear differences compared to the ethyl acetate and n-hexane extracts. PCA further confirmed that both FTIR and UV-Vis spectra effectively distinguished the extracts based on solvent type, with PC values of 90% and 93%, respectively. However, the confusion matrix indicated some overlap between ethyl acetate and n-hexane extracts in the PCA FTIR spectra, where certain samples were misclassified. Meanwhile, GC-MS

chromatogram analysis showed that *B. javanica* fruit extracts contain organic acids, including carboxylic acid derivatives and other related compounds, with no significant variation observed across different solvents.

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