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Research Article

Application of FTIR spectroscopy and chemometrics for discrimination of *Kleinhovia hospita* L. in South Sulawesi

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Abstract: Paliasa (*Kleinhovia hospita* L.) is a plant that has been used in traditional medicine for various diseases by several ethnicities in South Sulawesi, including hepatitis and liver cancer (Makassarese, Buginese, and Torajanese). The discrimination and classification of *K. hospita* from various regions in South Sulawesi is important to ensure the consistency of the quality of raw materials for traditional medicine using Fourier Transform Infrared (FTIR) spectroscopy combined with a chemometric approach. The leaves of *K. hospita* from each region were measured using Fourier-transform infrared (FTIR) spectroscopy in the middle region (4000-400 cm^{-1}). Subsequently, principal component analysis (PCA) was performed to identify the similarity of compound content in plants. The results showed that *K. hospita* can be differentiated through visual analysis of the FTIR spectra using marker bands, where the score plot from FTIR spectroscopy revealed four groups based on regions that have similar compound contents with the following intensity ranges: group 1 from the Maros area (26.907-98.505); group 2 (Barru, Takalar, Soppeng, Pare-Pare and Toraja) (12.875-99.994); group 3 (Pangkep, Bulukumba, Pinrang, Bantaeng, and Malino) (9.771-99.404); and group 4 (Sidrap and Bone) (4.825-99.513). This study concludes that FTIR spectroscopy combined with a chemometric approach can be used as a rapid analytical method for the discrimination and classification of *K. hospita* based on its growing location from various regions.

INTRODUCTION

K. hospita is a member of the Malvaceae family, which has a long history of use by various tribes in Indonesia for the treatment of a range of ailments, including hepatitis, kidney disease, malaria, hypertension, stomach disorders, and cholesterol imbalance (USDA, 2024; Muhammad *et al.*, 2022; KEMKES, 2024). *K. hospita* has been found to contain a number of different chemical compounds, including alkaloids, terpenoids, triterpenoids, coumarins, steroids, and fatty acids (Muhammad, *et al.*, 2022). Additionally, Rahim *et al.* (2018) have identified the presence of new compounds in the leaf extract of *K. hospita*, namely Kleinhospitin E and cycloartan triterpenoid alkaloids.

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The quantity and quality of compounds found in plants typically exhibit variability. The influence of environmental conditions, including light, temperature, humidity, pH, soil nutrient content, and altitude, on plant growth and development are a crucial factor in understanding the variability observed in plant chemical composition. Altitude is one of the factors that affects plant growth (Sholekah, 2017). Altitude differences can impact light intensity, temperature, humidity, and soil type. Additionally, it impacts the chemical composition of plants (Rachmawati *et al.*, 2023). Consequently, it is hypothesized that varying altitudes in the southern Sulawesi region will influence the growth and development of *K. hospita* plants. This, in turn, may disrupt a series of metabolic processes in these plants, consequently affecting the compounds produced from these processes at each altitude (Laily *et al.*, 2012).

The pharmacological activity of *K. hospita* may be attributed to the similarity of its chemical compounds (Rohaeti *et al.*, 2015). The inconsistency of raw materials that make up a herbal product from various regions based on the place of growth can have significant implications for efficacy. This is because the effectiveness of the product may be compromised due to the variability in the quality and composition of the raw materials (Purwakusumah *et al.*, 2014). Therefore, it is crucial to discrimination the *K. hospita* plants from various regions in South Sulawesi to ensure the quality, safety, and efficacy of traditional medicinal raw materials. This can be achieved through the use of a rapid, straightforward, and precise analytical method.

A variety of analytical techniques have been employed to identify and differentiate the chemical composition of medicinal plants. These include spectroscopy (ultraviolet-visible, Fourier transform infrared, nuclear magnetic resonance, and mass spectrometry) and chromatography (thin-layer chromatography, high-performance liquid chromatography, and gas chromatography). Fourier transform infrared (FTIR) spectroscopy is an attractive option for meeting the criteria of efficient, easy-to-use, fast, inexpensive, and non-destructive analysis. Moreover, this technique is frequently employed on a multitude of materials under a plethora of conditions. It is not uncommon for FTIR spectra to differ even within the same species, given the vast array of chemical compounds present in medicinal plants. In numerous herbal medicine industries, FTIR has been extensively employed for the quality control of simplisia (Amit & Jamwal, 2023; Arrout *et al.*, 2024; Rohaeti *et al.*, 2015; Umar *et al.*, 2016; Wang *et al.*, 2024).

A number of studies have employed FTIR for the purpose of verifying the authenticity of foodstuffs. One such study, conducted by Zotte *et al* (2013), concerned the authentication of freeze-dried raw and cooked rainbow trout (Oncorhynchus mykiss) fillets. The authentication of freeze-dried fresh fish samples (Ottavian *et al.*, 2013), the classification and rapid quantification of omega-3 marine oil supplements (Karunathilaka *et al.*, 2023), the authentication analysis of milkfish oil (Mustafidah *et al.*, 2021), and the discrimination of different species and classification of fish surimi (Zhang *et al.*, 2017) have all been successfully achieved using FTIR.

It is imperative to conduct research on the discrimination of chemical compounds present in different species of *K. hospita* plants in order to advance traditional medicine and improve public health. *K. hospita* plants have been utilized as traditional medicine in various regions for generations. However, there is still a lack of understanding regarding the diversity of chemical compounds present in different species. Consequently, this study was conducted to investigate the differences in chemical compound content among various species of *K. hospita* plants in South Sulawesi.

METHOD

K. hospita leaves were obtained from 13 regions in South Sulawesi, including Takalar district, Soppeng district, Pare-pare city, Bulukumba district, Bantaeng district, Pangkep district, Bone district, Maros district, Sidrap district, Gowa district, Pinrang district, Barru district, and Toraja district. All samples were sorted, dried at 35^{o}C for 48 hours in an oven. This temperature was chosen to prevent enzymatic and non-enzymatic denaturation, which could lead to degradation

of bioactive compound (Borowska *et al.*, 2009; Mahardani *et al.*, 2021), The dried samples were then pulverized using a Philips blender. They were then sieved with a 100-mesh sieve.

FTIR Spectrum Measurement

Measurements of all *K. hospita* leaf samples were carried out based on those described by Rohaeti et al. Measurement of the FTIR spectrum of all samples us an FTIR Spectrophotometer (Shimadzu). Measurements were made in the mid-infrared wavenumber region 4000-400 cm^{-1} with a scan number of 26 and a resolution of 4 cm^{-1}.

Chemometric Analysis

Chemometric analysis was performed in this study using the *Minitab 18* application. Unsupervised pattern recognition analysis techniques such as Principal Component Analysis (PCA) were also used.

RESULTS

FTIR Profile of *K. hospita* Leaves

This study utilizes botanical *simplisia* in the form of *paliasa* leaves collected from various regions, as presented in the Table 1 below. FTIR spectroscopy provided specific fingerprint spectra for *K. hospita* leaf samples from different regions. *K. hospita* leaf samples were measured at wavenumbers of 4000-400 cm^{-1} which can be seen in Figure 1. Medicinal plants have a complex mixture of chemicals, so the FTIR spectrum will show the overlap of several functional group band absorption characteristics (Rohaeti *et al.*, 2015).

Table 1. Source of sample and climatological data of sample source.

No.	Source	Climatology			
		RH (%)	Temperature (°C)	Altitude (masl)	Rainfall (mm/Years)
1	Bangkai village, Watangpulu sub-district, Sidrap district	70 - 90	24 - 33	32	1.200
2	Binuang village, Balusu sub-district, Barru district	53 - 96	27 - 32	500	3.341
3	Bonto Matene village, Segeri sub-district, Pangkep district	77 - 81	22 - 30	6	2.300 - 3.500
4	Bulukunyi village, Polombangkeng sub-district, Takakar district	81	21 -33	50	2.300 - 3.100
5	Garanta village, Ujung Loe sub-district, Bulukumba district	60 - 80	23 - 27	70	800 - 2.000
6	Lompoe village, Bacukiki sub-district, Pare-pare district	80 - 90	28 - 31	48.45	1.738
7	Lonrong village, Eremerasa sub-district, Bantaeng district	71 - 71	25 - 27	1.000	4.751
8	Parigi village, Tinggimoncong sub-district, Gowa district	54 - 98	22 - 33	528	4.234
9	Rompegading village, Cenrana sub-district, Maros district	60 - 82	29 - 32	374	2.400 - 4.488
10	Tellulimpoe village, Marioriawa sub-district, Soppeng district	80 - 90	30 - 32	31	400
11	Watangpulu village, Suppa sub-district, Pinrang district	64 - 98	28 - 31	15	2.099
12	Kamali Pentalluan village, Makale sub-district, Toraja district	82 - 86	15 - 28	744	1.500 - 3.500
13	Majang village, West Tanete Riattang sub-district, Bone district	77 - 86	24 - 27	41	2.415 - 7.656

Source: District Goverments of Sidrap, Barru, Pangkep, Takalar, Bulukumba, Pare-pare, Bantaeng, Gowa, Maros, Soppeng, Pinrang, Toraja, Bone.

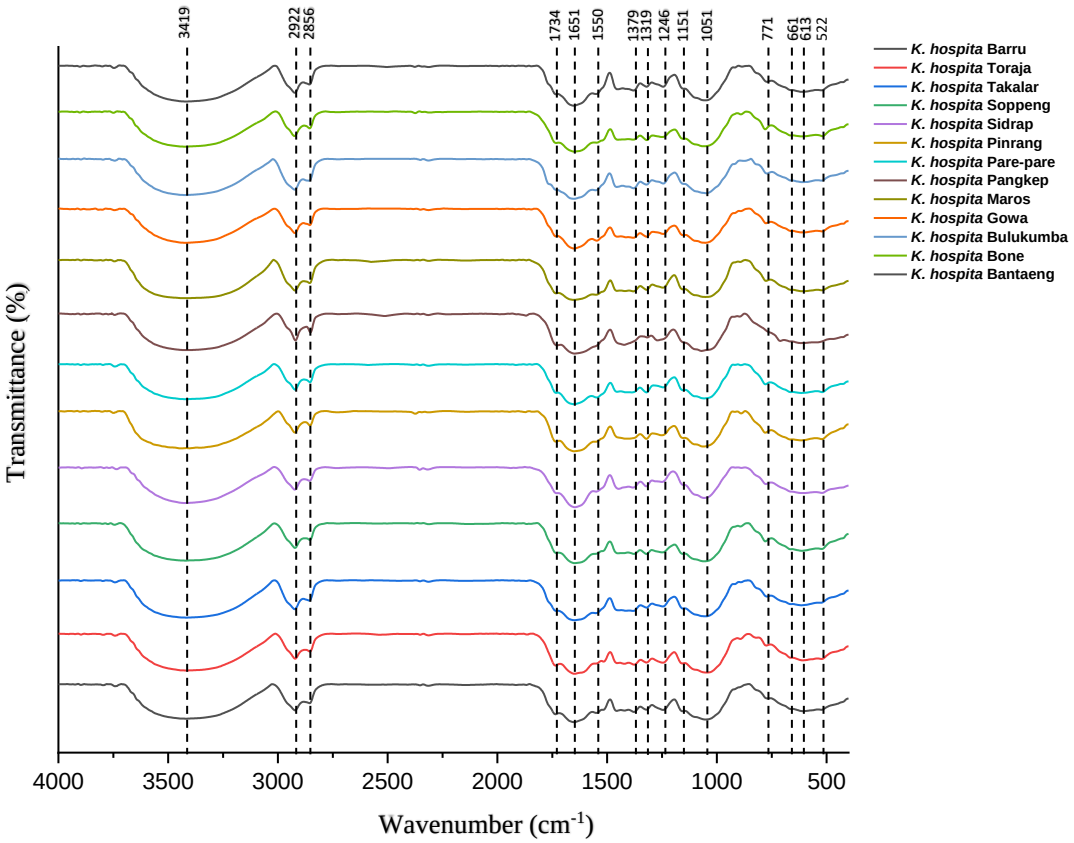


Figure 1. FTIR measurement result of *K. hospita* leaves from 13 region.

Table 2 presents the characteristic FTIR bands identified in *K. hospita* leaves, together with their chemical assignments. The 3446-3415 cm^{-1} peaks indicate the absorption of -OH (hydroxyl), and NH (amine) functional groups. All *K. hospita* showed high intensity peaks at these wavenumbers, indicating the presence of protein or alkaloid compounds. This is in accordance with the literature which states that wavenumbers of 4000-3000 cm^{-1} are areas of hydroxyl and amine functional groups. Potential phenolic and flavonoid compounds were detected, shown at peaks of 3400 cm^{-1} (O-H) and 1650 cm^{-1} (C=C). Lipids and fatty acids were shown at peaks of 2920-2850 cm^{-1} (C-H) and 1734 cm^{-1} (C=O). Symmetric and asymmetric stretching vibrations of methyl (-CH3) and methylene (-CH2) groups appear at 2920-2850 cm^{-1}, which indicate C-H groups in aliphatic compounds (saturated carbon chains). (Hikma *et al.*, 2023; Pavia *et al.*, 2001; Stuart, 2005). Ester or Ether compounds are shown in the fingerprint wavenumber peak of 1500-400 cm^{-1} (Auha & Alauhdin, 2021; Cano-Trujillo *et al.*, 2023; Pavia *et al.*, 2001; Puspitasari *et al.*, 2021; Saji *et al.*, 2024; Stuart, 2005; Tastekin *et al.*, 2024).

The wavenumbers of 1556-1548 cm^{-1} indicate the presence of asymmetric stretching vibrations of the nitro functional group (-NO2) or deformation vibrations of the amide II bond, which are characteristic of protein or peptide compounds. These wavenumbers indicate the presence of aromatic compounds that have certain substituents. Sample groups that showed vibrations at this wavenumber included group 1, group 2 and group 4, while group 3 did not show peaks at this wavenumber. The difference in peak position possessed by group 1, 2, and 4 samples may be absent or less in group 3 (Alauhdin *et al.*, 2021; Cano-Trujillo *et al.*, 2023; Puspitasari *et al.*, 2021; Tastekin *et al.*, 2024).

Wavenumbers of 1448-1377 cm^{-1}, groups 1-4 show vibrations, which indicate the presence of methyl (-CH3) and methylene (-CH2) groups commonly found in aliphatic compounds such as lipids, saturated fatty acids and alkanes. In addition, at this wavenumber, vibrations of carboxylic functional groups (-COO-) are also often detected, especially in compounds such as fatty acid salts and other organic acid salts. (Alauhdin *et al.*, 2021; Pavia *et al.*, 2001; Saji *et*

al., 2024; Tastekin *et al.*, 2024). Wavenumbers of 1382-1310 cm^{-1} groups that show vibrations are groups 1, 3 and 4 which indicate the presence of C-H bending groups which are generally found in aliphatic or aromatic hydrocarbon compounds but are not detected in group 2. It is possible that chemical compounds in groups 1, 3 and 4 are not possessed or there are fewer in group 2 (Alauhdin *et al.*, 2021; Auha & Alauhdin, 2021; Stuart, 2005). The wavenumber range of 1300–1000 cm^{-1} indicates C-O stretching vibrations associated with esters, alcohols, or polysaccharides. The spectra in this range confirm their presence in all samples (Hikma *et al.*, 2023).

Table 2. Characteristic FTIR bands and peaks of analysed *K. hospita* samples compared with literature.

Wavenumber (cm^{-1})	Chemical Assignment	Source of	References
3419	O-H stretching vibration	Phenol and flavonoid	Alauhdin *et al*., 2021; Auha & Alauhdin, 2021; Puspitasari, 2021
2922	C-H stretching vibrations	Lipids and fatty acid	Pavia, 2001; Stuart, 2005; Alauhdin *et al*., 2021
2856	C-H stretching vibration	Lipids dan fatty acid	Pavia, 2001; Stuart, 2005; Alauhdin *et al*., 2021
1734	C=O stretching vibration	Carboxylic acid, ester, or ketone	Pavia, 2001; Saji, 2024; Stuart, 2005
1651	C=C stretching vibration	Carboxylic acid, ester, ketone, or flavonoid	Auha & Alauhdin, 2021; Puspitasari, 2021; Stuart, 2005; Alauhdin *et al*., 2021
1550	asymmetric stretching vibrations	Nitro functional groups ($-NO_2$)	Cano, 2023; Puspitasari, 2021; Stuart, 2005
1379	Aliphatic vibration bending $-CH_3$ and $-CH_2$ deformation. Vibration of carboxylic functional groups (-COO-)	Lipids, saturated fatty acids and alkanes	Pavia, 2001; Puspitasari, 2021; Stuart, 2005
1319	Stretching vibration (C-H) of methyl ($-CH_3$) and methylene ($-CH_2$) groups	Aliphatic or aromatic hydrocarbon compounds	Pavia, 2001; Saji, 2024; Tastekin, 2024; Alauhdin *et al*. 2021
1246	C-O stretching vibration	Ester, alcohol, or carbohydrate	Hikma *et al*., 2023
1151	C-O stretching vibration	Ester, alcohol, or carbohydrate	Hikma *et al*., 2023
1051	C-O stretching vibration	Ester, alcohol, or carbohydrate	Hikma *et al*., 2023
771	Out-of-plane deformation vibration of the aromatic ring	Phenolic or flavonoid	Stuart, 2005
660-400	C-Cl or C-Br vibration	Organohalide compounds	Stuart, 2005

Wavenumbers around 800-400 cm^{-1}, indicate the presence of C-Cl and C-Br groups which generally indicate the bonding of halogen containing organic compounds. The peak wavenumber 775 cm^{-1} was detected in groups 1, 2, and 4, while group 3 did not show vibrations at this wavenumber. Wavenumber 663 cm^{-1} was detected in groups 2, 3, and 4, but not detected in group 1. Wavenumber of 613-609 cm^{-1}, vibrations were shown by groups 1, 2 and 3 at wavenumber 613 cm^{-1}, while group 4 was shown at wavenumber 609 cm^{-1}. Small differences in peak positions betwAshfieen groups 1-3 and group 4 may indicate variations in the chemical structure of the functional groups of compounds in the *K. hospita* plant. (Alauhdin *et al.*, 2021; Cano-Trujillo *et al.*, 2023; Pavia *et al.*, 2001; Saji *et al.*, 2024; Stuart, 2005).

Chemometrics Analysis

The chemometric analysis process of samples from 13 regions in South Sulawesi was conducted using the Principal Component Analysis (PCA) approach on FTIR spectra. The PCA results, visualized in the form of a scores plot, reveal distinct clustering of samples based on their region of origin. Four main groups were identified based on similarities in FTIR wavenumber data, as shown in Figure 2. This study used the Principal Component Analysis (PCA) approach to classify *K. hospita* samples from various regions based on FTIR spectra at wavenumbers of 2000-400 cm^{-1}. These wavenumbers were chosen because they are rich in information, with many vibrations bound to chemical components in the sample. The analyzed dataset consists of 13 samples with a data matrix of 312 FTIR intensity variables for each specific wavenumber. Figure 2 shows the clustering result of *K. hospita* using the PCA approach based on FTIR data.

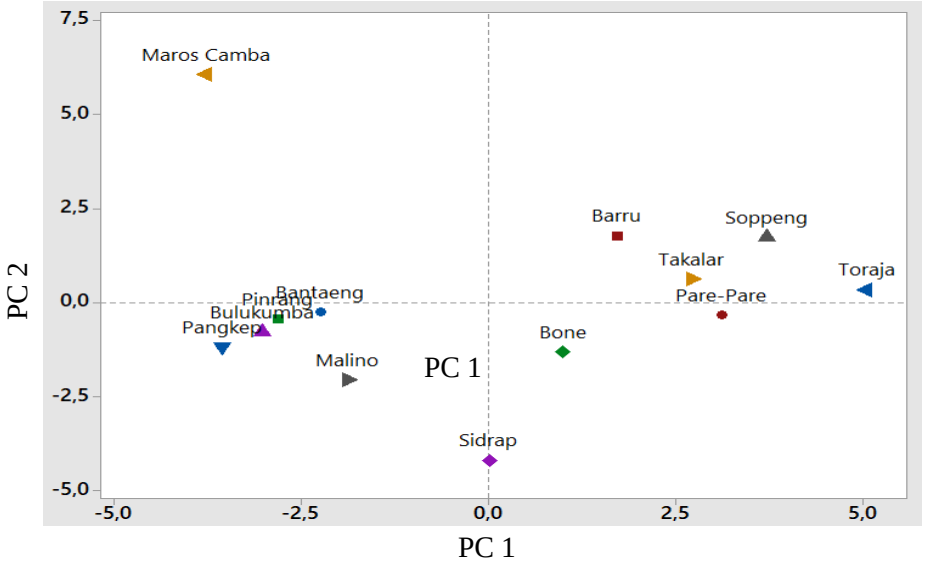


Figure 2. Principal component analysis score plot of *K. hospita.*

Table 3 provides information on the eigenvalues and cumulative percentage of total variance. The eigenvalue shows the amount of variation explained by one particular principal component (PC), while the cumulative percentage of total variance shows how much total information has been covered by several PCs. The eigenvalues and cumulative percentage of total variance of the first 10 PCs in Table 3 show the linear combination of the original variables in the form of intensities at wavenumbers that explain the maximum variation in the data. The cumulative percentage obtained is 99% of the total variation explained by the first 10 PCs of the total variation in the dataset. The PCA plots used and most influential in the clustering analysis are the first two PCs as these two PCs contain the most variation in the data. Figure 2 shows the PCA score plot based on the first two PCs. PC1 and PC2 are the two principal components that represent some of the variation in the data. PC1 shows the main difference in concentration or presence of certain significant functional groups related to the wavenumbers of the variables in the chemical composition between regions, While PC2 shows the secondary variation in the FTIR intensity pattern that is not explained by PC1. The combination of these two axes gives an idea of discrimination or grouping between samples based on spectral characteristics by grouping samples based on similar FTIR patterns and showing the most important variables to distinguish samples. The closer the PC value, the greater the similarity between other samples (Purwakusumah *et al.*, 2014; Rohaeti *et al.*, 2015). The eigenvalue data from the PCA plot for the classification of *K. hospita* plant groupings in South Sulawesi based on PC is 58% of the total variation (PC 1 = 36% and PC 2 = 22%).

Table 3. Eigenvalues and cumulative percentage of total variance for each PC.

Principal component	Eigenvalue	Cumulative percentage of total variance
1	936.69	36
2	575.89	58.2
3	293.8	69.5
4	215.12	77.7
5	184.05	84.8
6	120.64	89.5
7	93.48	93.1
8	80.61	96.2
9	50.79	98.1
10	24.16	99

Loading plots are necessary in clustering samples based on PC1 and PC2 because they contain information about the variables that contribute most to sample differences. Loading plots provide a direction that shows the variable's relationship with PC1 and PC2, and provide the length of the vector/line that shows the magnitude of the variable's contribution to both components. Variables that have long vectors and move away from the center (0,0) mean that they have a lot of variance in the data and make a large contribution to the PC1 and PC2 patterns. A variable that is close to the center (0,0) means that the variable does not change much or has little variation, therefore it has a small contribution to the main pattern. The greater the variation a variable has (long arrow), the greater its contribution to the main pattern being analyzed. Conversely, if the variable hardly changes (short arrow), then the contribution is small (Abdi & Williams, 2010; Haitao *et al.*, 2011; Jollife and Cadima, 2016; Sitompul *et al.*, 2023). The loading plot in Figure 3 shows the contribution of each variable in this case the FTIR intensity at certain wave numbers, which are labeled as C1, C2, C3, C4 and so on to PC1 and PC2. Loading plot of PCA of *K. hospita* leaves showing variables C22, C23, C24, C25 and these are variables that have a large contribution to the first principal component (PC1) because they are far from the center (0,0) on the X axis of PC1 indicating that the wave numbers associated with these variables are very important in explaining variations in PC1.

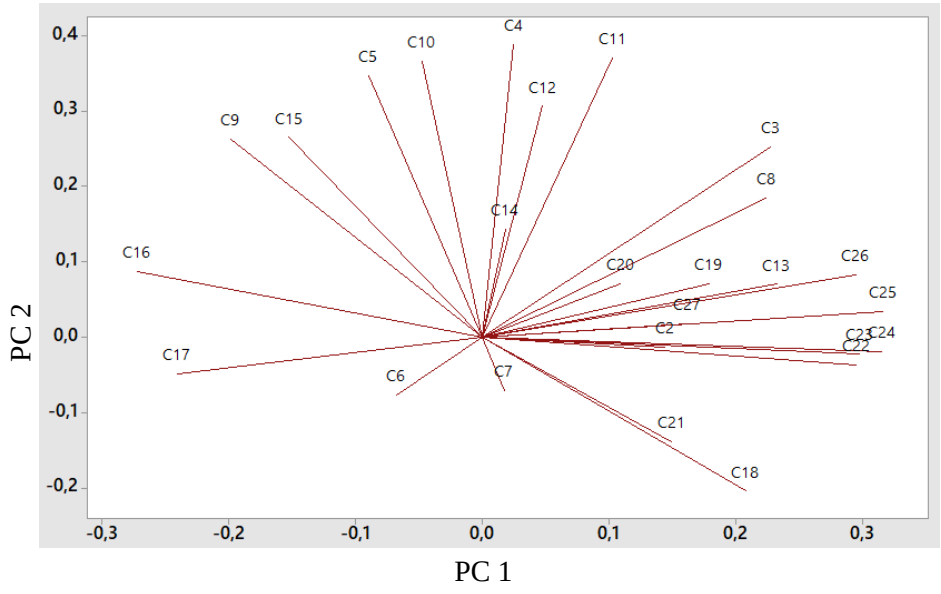


Figure 3. Loading plot PCA of *K. hospita.*

Variables C4, C5, C10, and C11 are variables that have a large contribution to the second principal component (PC2) because they are far from the center (0,0) on the Y-axis of PC2 indicating that the wave numbers associated with these variables are very important in explaining variations in PC2. It generally depends on the direction of the vector shown. The

combination of PC1 and PC2 maps the difference in FTIR intensity, so the sample far from the center has the dominant contribution of the significant variable in the loading plot.

Figure 4 shows the results of grouping the samples into 4 different groups based on regions that have similar compound content. Group 1 consists only of *K. hospita* from Maros which when viewed in Figure 2 is located far from the center (0,0) of the X and Y axes which are influenced by the dominant variables C4, C5, C6, C7, C16 and C17 and indicate that the chemical composition of this *K. hospita* is very different compared to all other *K. hospita* regions which indicates the possibility of unique compounds found only in this sample, making it an isolated group. Group 2 consists of *K. hospita* originating from Barru, Takalar, Soppeng Toraja and Pare-pare which tend to be similar when viewed in Figure 2 located far from the center (0,0) of the X and Y axes influenced by the dominant variables C23, C24 and C25. Although there are slight variations between regions, this group has more uniform chemical composition characteristics. Group 3 consists of *K. hospita* from Pangkep, Bulukumba, Pinrang, Bantaeng and Gowa which are located far from the center (0,0) of the X and Y axes influenced by the dominant variables C6, C7, C16, C17, C18 and C21. Samples from these regions show significant similarities in chemical composition. This could indicate the influence of similar principal chemical components. Group 4 consists of *K. hospita* from Sidrap and Bone which are far from the center (0,0) of the X and Y axes influenced by variables C4, C11, C23, C25 and C26 which show similarities in the FTIR spectral profiles of the secondary components.

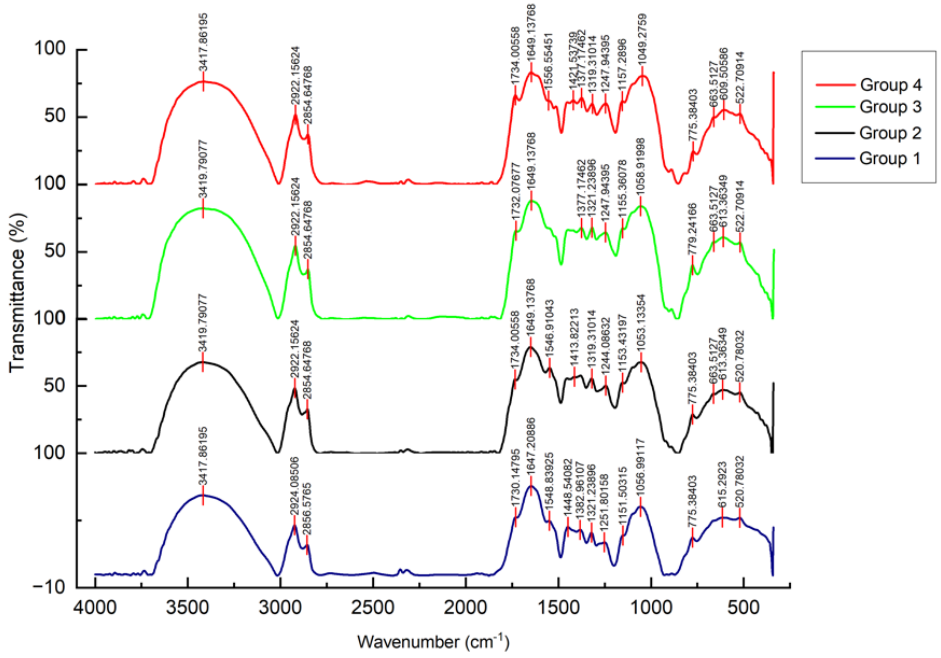


Figure 4. Representative FTIR spectra of *K. hospita* group 1 from Maros; group 2 from Barru, Takalar, Soppeng, and Toraja; group 3 from Pangkep, Bulukumba, Pinrang, Bantaeng, and Malino; and group 4 from Sidrap, Bone, and Pare-pare.

Each sample group clusters into one and it can be explained that of the four groups, the groups that have close response values and almost the same characteristics are groups 2, 3 and 4, while group 1 produces a different response. Grouping in this score plot is a function to determine the similarity of the characteristics of each sample. Based on the results of PCA analysis on *K. hospita* leaf samples, the data showed a grouping of four main groups based on geographical origin which was influenced by differences in chemical profiles detected through FTIR spectra. This is in line with the research of Rohaeti *et al* (2015) who used similar techniques to analyze Curcuma longa, Curcuma xanthorrhiza and Zingiber cassumunar based on geographical origin. The clustering of *K. hospita* plants shows that this PCA method is effective in distinguishing *K. hospita* leaves based on geographical origin. Environmental variations such as soil type,

climate and physiological processes of each plant can affect these results (Laily *et al.*, 2012; Rachmawati *et al.*, 2023; Sholekah, 2017).

K. hospita Plants Discrimination

This research combined the FTIR spectra method and Chemometric analysis in the classification of *K. hospita* from various regions. This approach was used to confirm the discrimination results obtained through visual FTIR spectra. Chemometrics is widely used to analyze large amounts of data, such as FTIR spectra. The main goal of chemometrics is to summarize the information in the data matrix by reducing its dimensions and finding similarities or differences between samples. In this study, the chemometric technique used is Principal Component Analysis (PCA) to explore and classify samples based on FTIR spectra (Rohaeti *et al.*, 2015).

The discrimination results of *K. hospita* plants with a combination of FTIR and chemometric analysis of the sample groups in this study showed characteristic differences at certain wavenumbers, which indicated differences in the content of chemical compounds between groups. By comparing the FTIR spectra of the four groups of samples, it can be seen that there are variations in the peak positions and intensities at several wavenumbers. For example, group 3 can be distinguished from the other groups because it does not show peaks at 1548-1556 cm^{-1} and 775 cm^{-1}, but has a unique peak at 1377 cm^{-1}. Group 2 can be distinguished from the other groups by the absence of peaks at 1382-1321 cm^{-1}. Group 4 showed a significant difference at 609 cm^{-1} compared to the other groups at 613 cm^{-1}. FTIR spectra can be used for the purpose of identification and discrimination of chemical compounds between sample groups.

The discrimination of *K. hospita* plants was achieved through the application of an FTIR spectrum method in conjunction with a PCA. The PCA clustering method enabled the classification of *K. hospita* plants from diverse geographical origins into four distinct groups, thereby demonstrating the efficacy and non-destructive nature of the developed method for the classification and discrimination of *K. hospita* plants from various regions.

This study successfully applied a combined approach of Fourier Transform Infrared (FTIR) spectroscopy and Principal Component Analysis (PCA) to analyze and differentiate 13 *K. hospita* samples collected from diverse regions in South Sulawesi. The results revealed that the samples could be classified into four distinct groups based on their unique chemical profiles. Group 1 included *K. hospita* from Maros, Group 2 comprised *K. hospita* from Barru, Takalar, Pare-Pare, Soppeng, and Toraja, Group 3 consisted of *K. hospita* from Pangkep, Bulukumba, Pinrang, Bantaeng, and Malino, while Group 4 was represented by *K. hospita* from Sidrap and Bone.

The observed chemical variations among the groups are likely influenced by factors such as geographical location, soil composition, and cultivation practices. The effectiveness of the FTIR-PCA method in distinguishing these samples underscores its potential as a reliable tool for the chemical fingerprinting and classification of *K. hospita* and other plant species. This approach not only provides a deeper understanding of the chemical diversity within *K.hospita* but also highlights the importance of advanced analytical techniques in plant studies.

Furthermore, this research contributes to the broader field of plant taxonomy and chemotaxonomy by demonstrating how chemical data can complement traditional morphological and genetic methods. The identification of distinct chemical groups offers valuable insights into the ecological adaptation and functional properties of *K. hospita*, which could be linked to their potential applications in agriculture, pharmacology, and biotechnology. For instance, the chemical differences observed may correlate with variations in bioactive compounds, such as antioxidants or antimicrobial agents, which could be explored for industrial or medicinal purposes.

In addition to its scientific contributions, this study has practical implications for the conservation and sustainable utilization of paliasa. By providing a clear classification based on

chemical profiles, this research supports efforts to preserve the genetic diversity of *K. hospita* and promotes its sustainable cultivation. The findings also encourage further interdisciplinary studies to explore the relationship between chemical composition, environmental factors, and biological activities in *K. hospita* and other plant species.

CONCLUSION

This study advances our understanding of the chemical diversity of *K. hospita* in South Sulawesi and demonstrates the effectiveness of integrating FTIR and PCA for plant discrimination. The results not only enhance the scientific knowledge of *K. hospita* but also open new avenues for research in plant chemistry, ecology, and biotechnology. By leveraging modern analytical techniques, this work provides a foundation for future studies aimed at unlocking the full potential of paliasa and similar plant species.

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Declaration of Conflicting Interests and Ethics

The authors declare no conflict of interest. This research study complies with research and publishing ethics. The scientific and legal responsibility for manuscripts published in IJSM belongs to the authors.

Data Availability Statement

Research data is available and can be sent with e-maill upon request.

Authorship Contribution Statement

Aderia Angriawan: Investigation, Resources, Visualization, Software, Formal Analysis, and Writing-original draft. **Risfah Yulianty, Muhammad Aswad, Abdul Rahim & Syaharuddin Kasim**: Methodology, Supervision, and Validation. **Muhammad Raihan**: Formal Analysis. & Visualization **Satria Astazaury Awal**: Software.

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