HAYATI
Journal of Biosciences

Vol. 32 No. 6, November 2025 1584-1591
DOI:10.4308/hjb.32.6.1584-1591
ISSN: 1978-3019
EISSN: 2086-4094

Research Article

Check for updates

OPEN ACCESS

FTIR-Fingerprinting Spectra Combined with Chemometrics Analysis for Distinguishing *Strobilanthes phyllostachya* Leaves Extracts and Correlation with Their Antioxidant Activity

Mohamad Rafi[1*], Devanka Aulia Tohib[2], Agus Saputra[3], Zuhelmi Aziz[2], Alfi Hudatul Karomah[4]

[1]*Department of Chemistry, Faculty of Mathematics and Natural Sciences, IPB University, Bogor 16680, Indonesia*
[2]*Faculty of Pharmacy, University of Pancasila, Srengseng Sawah, Jagakarsa, South Jakarta 12640, Indonesia*
[3]*Department of Anatomy, Physiology, Pharmacology, and Biochemistry, Faculty of Medicine and Veterinary Medicine, Universitas Nusa Cendana, Jalan Penfui, Kupang 85228, Indonesia*
[4]*TropBRC IPB University, Bogor 16128, Indonesia*

ARTICLE INFO

Article history:
Received January 14, 2025
Received in revised form June 3, 2025
Accepted June 16, 2025
Available Online August 27, 2025

KEYWORDS:
antioxidant,
chemometrics,
fingerprint analysis,
medicinal plant
S. phyllostachya

ABSTRACT

The leaves of *Strobilanthes phyllostachya* have a long history of use as a herbal medicine, and research has demonstrated that they contain a range of metabolites with antioxidant activity. This study will employ a chemometric approach to analyze the correlation between functional groups from Fourier Transform Infrared Spectroscopy (FTIR) spectra and antioxidant activity. The leaf samples will be extracted with water and ethanol at 30%, 50%, 70%, and ethanol p.a. Moreover, the extracts will be evaluated for their antioxidant activity and analyzed using FTIR spectroscopy. The antioxidant activity measurement results indicate that the 70% ethanol extract of *S. phyllostachya* exhibits the highest antioxidant activity. The IR spectra of the water and ethanol extracts exhibited slight differences in their patterns. While the spectra of the various ethanol extracts exhibited similarities, their absorption values differed. A principal component analysis with absorbance from the FTIR spectra at wavenumber 3400-2800 and 1800-1000 cm^{-1} gave a good cluster of different solvent extractions used in this study. The total variation of principal component-1 (PC-1) and PC-2 is 90%. The partial least square regression (PLSR) analysis results were used to correlate the absorbance value of FTIR spectra of *S. phyllostachya* extract with antioxidant activity. From the PLS-R analysis, we identified a functional group, *i.e.* carbonyl and hydroxyl, which significantly contributed to the antioxidant activity of the *S. phyllostachya* extract. The value of the R2 parameter, which assesses the goodness of fit, was found to be 0.9630, indicating that the PLSR model is good.

1. Introduction

Strobilanthes phyllostachya, or *Strobilanthes crispa*, is indigenous to several countries, including Malaysia, Madagascar, and Indonesia. It is commonly called keji beling in Indonesia. It is a flowering plant species belonging to the Acanthaceae family (Al-Henhena *et al*. 2015; Ban *et al*. 2022; Kladwong & Chantaranothai 2024). *S. phyllostachya* has also been of interest due to its possible therapeutic aspect and traditional usage in herbal medicine (Koay *et al*. 2013). Phytochemical investigations have confirmed

* Corresponding Author
E-mail Address: mra@apps.ipb.ac.id

the existence of several bioactive components in *S. phyllostachya*, including flavonoids, phenolic compounds, and terpenoids, which may contribute to its pharmacological properties. In some cultures, extracts, and decoctions derived from *S. phyllostachya* leaves have been used for their anti-inflammatory, antibacterial, and antioxidant activities (Ramadhani *et al*. 2021).

Antioxidants are a varied group of chemicals that play an essential role in maintaining cellular homeostasis by combating the harmful effects of oxidative stress. Oxidative stress is the excessive production of reactive oxygen species (ROS) caused by metabolic and inflammatory activities (Cockfield & Schafer 2019; Irnawati *et al*. 2021). These ROS, which include superoxide anion, hydroxyl radicals, and hydrogen peroxide, have unpaired electrons, making them highly reactive and capable of destroying biomolecules like proteins, lipids, and nucleic acids. This can impair cellular function and integrity, contributing to the advancement of diseases. Antioxidants serve as ROS scavengers, giving electrons or hydrogen atoms to neutralize and stabilize these reactive species. The antioxidant defense system includes enzymatic antioxidants like superoxide dismutase, catalase, and glutathione peroxidase and non-enzymatic antioxidants like phytochemicals (*e.g*., flavonoids, polyphenols) obtained from plants (Flieger *et al*. 2021).

The relationship between antioxidants and their possible anticancer effects has been the focus of extensive scientific research, fueled by the rising identification of oxidative stress as a contributor to carcinogenesis and tumor growth (Cockfield & Schafer 2019). In this regard, identifying antioxidants in plants using simple approaches and producing precise results is critical nowadays. Chromatographic-based techniques combined with MS detectors are commonly used to detect and identify antioxidant compounds despite their high cost, reliance on sophisticated apparatus, and the requirement for qualified analysts. A simple and dependable vibrational spectroscopy technique is proposed to address this issue. Vibrational spectroscopy (infrared spectroscopy) is one of the most extensively used fingerprinting techniques for identification, authentication, and evaluation of biological activity, such as antioxidant activity in medicinal when combined with chemometrics analysis (Christou *et al*. 2018; Rohaeti *et al*. 2020). Chemometrics uses mathematical and statistical approaches to convert chemical responses into more intelligible data, such as pattern detection and discrimination (Ahmad *et al*. 2022; Sharma *et al*. 2024). Spectroscopy and chemometrics for pattern recognition provide a dependable and straightforward method (Elhamdaoui *et al*. 2021; Rohman *et al*. 2021; Shiyan *et al*. 2022; Umar *et al*. 2022)

In this study, we used a chemometric analysis to examine Fourier Transform Infrared Spectroscopy (FTIR) spectroscopy data from *S. phyllostachya* extract with water and different concentrations of ethanol. There is no reported paper regarding applying FTIR spectroscopy combined with chemometrics to predict a compound functional group as an antioxidant in *S. phyllostachya*. This study used fingerprint analysis using FTIR combined with chemometrics to differentiate extracts with various extracting solvents. The PCA technique in this study was used to differentiate extracts based on their extraction solvents, while PLS-R was used to correlate FTIR spectra and the antioxidant activity to find important functional groups from the active compound that exhibit an antioxidant. The results of this study can be used as a reference for selecting effective extraction solvents to optimally extract bioactive compounds in *S. phyllostachya*, because different extraction solvents will produce extracts with varying contents of metabolite.

2. Materials and Methods

Plant samples were collected from The Spice, Medicinal and Aromatic Plant Instrument Standard Testing Center (BPSI TROA), Bogor, West Java, Indonesia. The plant has been identified at the Department of Biology, Faculty of Mathematics and Natural Sciences, Universitas Indonesia (No. 159/UN2.F3.11/PDP.02.00/2021) as *Strobilanthes phyllostachya* from the Acanthaceae family. Methanol and ethanol were purchased from Merck (Darmstadt, Germany). Ascorbic acid, 2,2-diphenyl-1-picrylhydrazyl (DPPH), and potassium bromide (KBr) FTIR spectroscopy grade were obtained from Sigma-Aldrich (St. Louis, USA).

2.1. Sample Preparation and Extraction

The sample was powdered at room temperature. Approximately 20 grams of dry powder were fully extracted three times with 300 ml, 100 ml, and 50 ml of solvent for 30 minutes each using ultrasonication

procedures. The solvents used are ethanol p.a., 30%, 50%, 70% ethanol, and water. The filtrate extracts were dried with a rotary evaporator and then freeze-dried. The sample extract is then ready to be used for further analysis.

2.2. Antioxidant Activity

The antioxidant activity of the extract was measured using the DPPH method described by Rafi *et al*. (2018). The extract was dissolved in methanol and a series of concentrations were made. Each 1.0 ml solution was mixed with 1.0 ml of 0.4 mM DPPH and 5 ml of methanol. The mixture was incubated in the dark at room temperature for 30 minutes. The solution's absorbance was measured using a visible light spectrophotometer at a wavelength of 516 nm. The negative and positive controls were created by mixing 1.0 ml of ethanol or ascorbic acid with 1.0 ml of 0.4 mM DPPH, respectively.

2.3. Measurement of FTIR Spectra

A Tensor 37 FTIR spectrophotometer (Bruker, Ettlingen, Germany) with a deuterated triglycerine sulfate detector was used to obtain FTIR spectra. The sample was made by mixing 2 mg of extract and 200 mg of KBr until homogenous, and then the pellet was manually compressed at 8 tons for 15 minutes. The pellet was inserted into the sample chamber. The FTIR spectra were measured in the 4000-400 cm^{-1} range with a resolution of 4 cm^{-1} and a scan rate of 32 scans per minute using OPUS 4.2 software (Bruker, Ettlingen, Germany). The FTIR spectra were saved in a data point table.

2.4. Chemometrics Analysis

The extraction yield data and antioxidant activity obtained in triplicate measurements were analyzed using analysis of variance (ANOVA) and the Tukey test to determine the significance of the difference and reported as mean ± standard deviation. A significant difference was defined at the 95% confidence level ($p<0.05$). PCA was performed to differentiate the sample extracts according to the extracting solvents using absorbance value from the FTIR spectra as the variable. Before PCA analysis, preprocessing such as normalization is carried out to avoid problems due to baseline shifts and to increase the resolution of overlapping spectra. PLS-R analysis was used to identify functional groups that contributed significantly to antioxidant activity by examining the correlation between absorbance from FTIR spectra (variable X) and IC_{50} values (variable Y). We used the Unscrambler X version 10.1We used the Unscrambler X version 10.1 (CAMO, Oslo, Norway) for PCA and PLSR analysis.

3. Results

3.1. Extraction Yield

In this study, *S. phyllostachya* metabolites were extracted using water and ethanol solvents individually and with various concentrations using the ultrasonication method. Water solvent provided the highest yield (8.27%±0.58). For ethanol solvent, increasing the concentration reduced the yield. The yield of ethanol solvent varied from 3.55% to 7.35% (Table 1). The result of ANOVA showed that extraction solvent concentration significantly affected the extraction yield at the 5% significance level (p-value <0.05). Furthermore, based on Tukey's post hoc test, the yields of 70% ethanol and 96% ethanol p.a. were not significantly different.

3.2 Antioxidant Activity

DPPH is one of the techniques used to assess antioxidant activity. According to the result obtained, the 70% ethanol extract exhibited the strongest antioxidant activity, with an IC_{50} of 45.30 µg/ml. An increase in initial ethanol concentration was associated with increased antioxidant activity, except for ethanol p.a, which decreased activity compared to 50% ethanol. IC_{50} of antioxidant activity of all extracts is shown in Table 1. The IC_{50} of *S. phyllostachya* extracts ranged from 45.30±1.09 to 245.50±25.00 µg/ml and was significantly different at the 95% significance level (p-value <0.05). All extracts had lower antioxidant activity than the positive control, with an IC_{50} value of 3.64 µg/ml.

3.3. FTIR Spectra

Representative FTIR absorption spectra of the ethanol and extract water of *S. phyllostachya* leaves in

Table 1. Antioxidant activity of *S. phyllostachya* leaves extract

Solvent	Yield (%)	IC_{50} (µg/ml)
Water	$8.26±0.58^{a}$	$70.46±2.20^{b}$
Ethanol 30%	$7.35±0.24^{b}$	$245.50±25.00^{a}$
Ethanol 50%	$5.72±0.33^{c}$	$50.01±3.82^{bc}$
Ethanol 70%	$4.43±0.22^{d}$	$45.30±1.09^{c}$
Ethanol p.a	$3.55±0.11^{d}$	$58.27±9.64^{bc}$
Ascorbic acid		3.64

The reported values are mean ± SD of the triplicate assay for each sample. The mean ± SD within each extract in the same column followed with different superscript letters represent significant differences at $p < 0.05$.

the 400–4000 cm^{-1} range are shown in Figure 1. The IR spectra of water and ethanol extracts show slightly distinct patterns. While the spectra of the various ethanol extract concentrations were similar, the absorption values differed. The FTIR spectrum revealed several typical absorption peaks. The absorption peak at wavenumbers approximately 1700 cm^{-1}, indicating carbonyl groups (C=O stretching), was observed in all extracts, particularly the ethanol p.a extract. The absorbance peak at wavenumbers 3370-3404 cm^{-1} is broad, indicating carboxylic groups. This is supported by absorption peaks in the 1300-1000 cm^{-1} region, indicating the presence of C–O stretching groups. Aliphatic and aromatic C-H stretching functional groups were also observed, with absorption peaks at around 2900 cm^{-1} and 3000 cm^{-1}, respectively.

3.4. Chemometric Analysis

The chemometric analysis of the FTIR spectral data set matrix was performed using the Unscrambler X application version 10.1 First, PCA generated a data model (pattern) for extract grouping based on solvent variation. Before subjected to PCA, signal preprocessing was applied to eliminate shifting of the baseline, increase the resolution of the overlapping spectrum, and correction of light scattering by using normalization, baseline correction, and standard normal variate, respectively. The PC-1 and PC-2 values were 71% and 15%, respectively, according to the score plot in Figure 2, which is the outcome of spectrum data analysis over the complete range of wavenumbers (4000-400 cm^{-1}). The PC-1 and PC-2 values increased by 73% and 17%, respectively, when the data were analyzed using a segmentation approach at wavenumbers 3400-2800 and 1800-1000 cm^{-1}. This shows that the use of absorbance values at these wavelengths produces a clearer grouping pattern than using all wavelengths.

The correlation of FTIR spectra absorbance data with antioxidant activity will be investigated using PLS-R. Figure 3 shows the spectrum pattern from the PLS-R analysis. The downward-pointing spectrum pattern indicates peaks positively associated with antioxidant activity, whereas the upward-pointing ones are not because we used IC_{50} as the antioxidant activity value. Positively correlated absorption peaks in the 4000-400 cm^{-1} range include 3330-3116 (O–H stretching), 3000-2900 (C–H stretching), 1700 (C=O stretching), 1384 (C–O stretching), 1270-1260 (C–O stretching), and 1050 cm^{-1} (C–O stretching). While segmenting wavenumbers 3400-2800 cm^{-1} and 1800-1000 cm^{-1}, the absorption with a positive correlation is obtained in the range of wavenumbers 3270-3100, 3000-2900, 1384, 1290-1250, and 1050-1029 cm^{-1}.

4. Discussion

It has been demonstrated that *S. phyllostachya* contains a range of bioactive metabolites crucial for maintaining

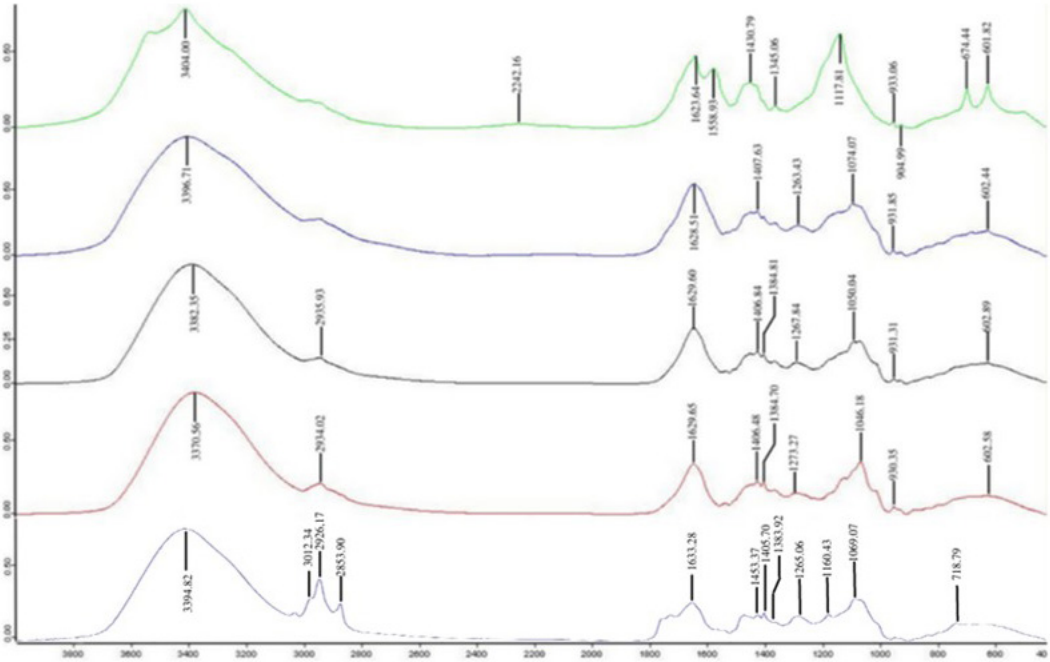
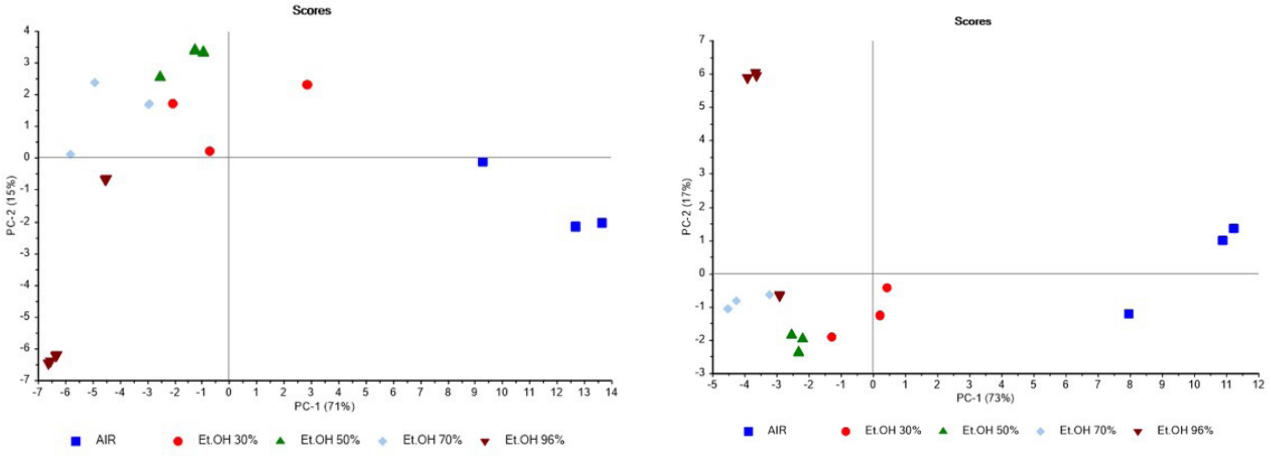
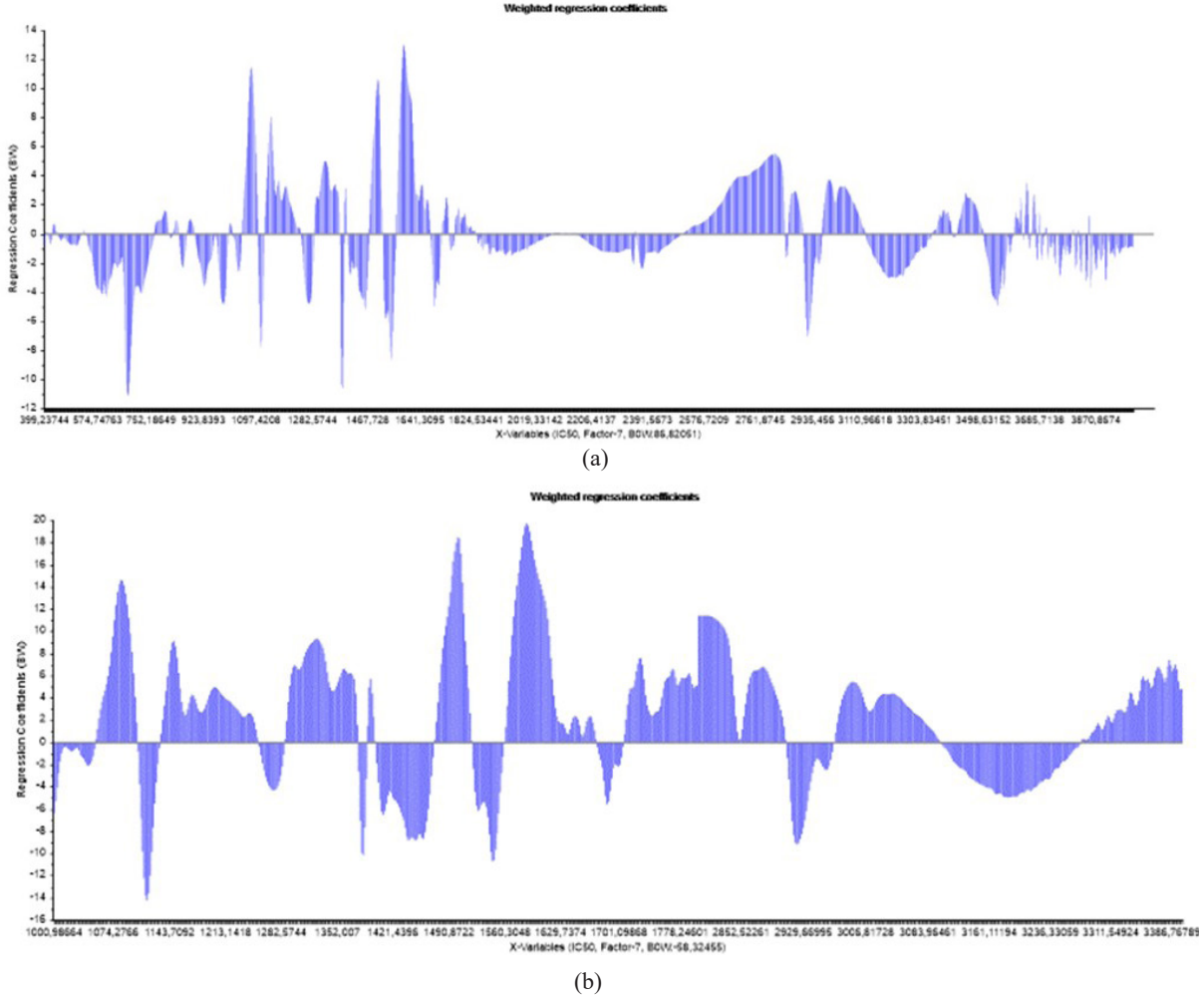


Figure 1. Representative of FTIR spectra of *S. phyllostachya* extract: water (a) and ethanol 30% (b), 50% (c), 70% (d), ethanol p.a. (e)



(a) (b)

Figure 2. PCA score plot of *S. phyllostachya* extracts at wavenumbers 4000-400 cm^{-1} (a) and 3400-2800, 1800-1000 cm^{-1} (b)



(a)

(b)

Figure 3. Regression coefficient plot of PLSR at wavenumber 4000-400 cm^{-1} (a) and 3400-2800, 1800-1000 cm^{-1} (b)

overall human health. This metabolite is associated with their pharmacological action. Prior research has indicated that environmental factors considerably influence phytochemical content and composition. *S. phyllostachya* contains a variety of phytochemical groups and components, including flavonoids, phenolic acids, alkaloids, and ester glycosides. The pharmacological advantages of flavonoids and phenols are well-documented (Rafi *et al*. 2021). A substantial body of evidence from numerous studies has demonstrated that phenols and flavonoids are potent antioxidants (de Oliveira *et al.* 2025). This is because the functional groups of those molecules contain oxygen and nitrogen atom, which have activities to neutralize free radicals. In this investigation, ethanol solvent at a concentration of 70% produced extract with the highest antioxidant activity and belongs to the group of very strong antioxidants (less than 50 ppm). This is because bioactive compounds such as phenolics and flavonoids which have the potential as antioxidants can be optimally extracted using 70% ethanol (Bitwell *et al*. 2023).

The functional groups in a compound are closely related to the vibrational pattern of the molecule. In IR spectroscopy, both phenols and flavonoids exhibit characteristic absorption bands primarily due to their O-HO-H, C-O, C=O, and aromatic functional groups (Kusumadewi *et al*. 2022; Umar *et al*. 2022; Nurani *et al*. 2024). These bands allow for the identification and study of these compounds. These bands' specific positions and intensities can vary depending on the molecular structure, substitution pattern, and presence of hydrogen bonding, providing valuable information about the chemical nature of the analyzed sample (Campanella *et al*. 2021).

All extracts showed absorbance at two regions of the wavenumber range 3400-2800 cm^{-1} and 1800-1000 cm^{-1}. The absorbance intensity alone makes the most noticeable change in the entire FTIR spectrum, and the abundance of absorption peaks indicates that the ethanol p.a. extract contains an enormous number of metabolites. The large number of metabolites contained in the ethanol p.a extract is thought to contribute to the high antioxidant activity produced. However, at several wave numbers, the FTIR spectrum of 70% ethanol extract has a higher absorption peak than other extracts, especially at wave number 1050 cm^{-1}. High absorbance values in the FTIR spectrum are directly proportional to the concentration of a metabolite. Therefore, it is thought that the functional groups at wave number 1050 cm^{-1} contribute greatly to the high antioxidant activity of the 70% ethanol extract. Each plant metabolite has an essential role because it is believed to correlate with the bioactivity of the plant extract.

The FTIR spectrum data of an extract is typically a complex (multivariate) representation of the extract's chemical composition, comprising a multitude of chemical compounds belonging to diverse classes (Rohaeti *et al*. 2020). The interpretation of such data is often challenging due to the resemblance of their spectra (Wakiuchi *et al*. 2023). The PCA method employs a pattern recognition method, forming a control diagram based on the principal component (PC) values obtained. This PC is a linear combination of the spectrum data variables and contains the most relevant information. Ideally, PC-1 and PC-2 add up to explain most of the information in the sample data (García-Pérez *et al*. 2024). This method is an effective approach for identifying similarities or differences between samples (Matwijczuk *et al*. 2019; Rohman *et al*. 2020).

The score plot demonstrates that the degree of similarity between the metabolite profiles of the two samples is directly proportional to their proximity on the plot. The PCs are frequently employed in principal component analysis (PCA). PC1 represents the primary component, encompassing most of the data set's variance. In contrast, PC2 represents residual variations based on the PC1 point of view (Rafi *et al*. 2021; Rohman *et al*. 2021). The clustering of extracts using the segmentation approach of absorbance data in the 3400-2800 cm^{-1} and 1800-1000 cm^{-1} resulted in higher scores than using absorbance data without segmentation in the 4000-400 cm^{-1} range. This plot explains the similarities and differences in the extracts' FTIR spectra. The higher the score, the closer the groups are in terms of similarity.

PCA score plot demonstrates that the degree of similarity between the metabolite profiles of the two samples is directly proportional to their proximity on the plot (Saidi *et al*. 2022). In this study, grouping of extracts using the segmentation approach of absorbance data in the 3400-2800 cm^{-1} and 1800-1000 cm^{-1} resulted in higher scores than using absorbance data without segmentation in the 4000-400 cm^{-1} range. The total value of PC1 and PC2 in this study was 86% for absorbance data without segmentation in the range of 4000-400 cm^{-1}, which indicates that 86% of the variation in the data can be explained by the model. While the PCA model with absorbance segmentation data at 3400-2800 cm^{-1} and 1800-1000 cm^{-1} can explain 90% of the variation in the data. This plot explains the similarities and differences in the extracts' FTIR spectra.

The identification of functional groups that contribute significantly to the level of antioxidant activity of *S. phyllostachya* leaf extract was determined using the method of PLS regression. This method requires two variables, namely data variables and response variables. The antioxidant activity expressed as IC_{50} value obtained by the DPPH method is used as the response variable (Y), while the absorbance of the FTIR spectra is used as the independent variable (X). The quality of the PLS model obtained is determined by the R2 value. A model with a relatively high R2 is usually considered to be wellperformed. The R2 value obtained in this study was 0.9630, indicating model goodness-of-fit (Zheng *et al*. 2024).

The regression coefficient plot illustrates the functional group that contributes most to the antioxidant activity (Rafi *et al*. 2021). The regression coefficients at all wavenumbers and segmented wavenumbers showed similar results. The wave numbers that contribute to antioxidant activity are predicted to be carbonyl (C=O) functional groups (1740-1720 cm^{-1}), -OH (3400-3080 cm^{-1}), C-H sp3 (3012-2831 cm^{-1}) and C-O groups (1300-1000 cm^{-1}). The functional groups identified are characteristic of the phenolic compound group. Five phenolic acids (gallic acid, ferulic acid, cinnamic acid, chlorogenic acid, and caffeic acid) and six flavonoid compounds (quercetin, rutin, kaempferol, catechin, naringenin, and apigenin) were identified from the extracts of *S. phyllostachya* leaves (Koay *et al*. 2013; Ghasemzadeh *et al*. 2015: Aziz *et al*. 2022). Based on the results obtained, it can be predicted that the antioxidant compounds from *S. phyllostachya* leaves extract are phenolics such as phenolic acids and flavonoids.

In Conclusion, The antioxidant activity and compound functional groups of *S. phyllostachya* extracts are closely related. The 70% ethanol extract produced the strongest antioxidant activity compared to ethanol p.a, 96%, 50%, 30%, and water extract. FTIR spectra of ethanol and water extracts showed unique absorption patterns, particularly at wavenumbers 1700 cm^{-1} (C=O) and 3370-3404 cm^{-1} (carboxylic groups). PCA analysis with FTIR spectra absorbance data at wavenumber 3400-2800 and 1800-1000 cm^{-1} has the total variation of PC-1 and PC-2 at 90% compared to only 86% when we used all absorbance data from the FTIR spectrum of the sample. Chemometric analysis using PCA and PLSR linked FTIR spectra with antioxidant activity and identified functional groups such as carbonyl and hydroxyl, which contribute significantly to the antioxidant activity of the *S. phyllostachya* extracts.

The authors have no conflicts of interest regarding this research.

References

Ahmad, I., Arifianti, A.E., Fikri, J.A.N., Abdullah, S., Munim, A., 2022. The combination of ATR-FTIR and chemometrics for rapid analysis of essential oil from Myrtaceae plants – a review. *J. Appl. Pharm. Sci*. 12, 30-42. https://doi.org/10.7324/JAPS.2022.120604

Al-Henhena, N., Khalifa, S.A.M., Ying, R.P.Y., Hassandarvish, P., Rouhollahi, E., Al-Wajeeh, N.S., Ali, H.M., Abdulla, M.A., El-Seedi, H.R., 2015. Chemopreventive effects of *Strobilanthes crispus* leaf extract on azoxymethane-induced aberrant crypt foci in rat colon. *Sci. Rep*. 5, 13312. https://doi.org/10.1038/srep13312

Aziz, M., Ahmad, S., Khurshid, U., Pervaiz, I., Lodhi, A.H., Jan, N., Khurshid, S., Arshad, M.A., Ibrahim, M. M., Mersal, G. A.M., Alenazi, F.S., Alamri, A.A.S., Butt, J., Saleem, H., El-Bahy, Z.M., 2022. Comprehensive biological potential, phytochemical profiling using GC-MS and LC-ESI-MS, and in-silico assessment of *Strobilanthes glutinosus* Nees: an important medicinal plant. *Molecules.* 27, 6885. https://doi.org/10.3390/molecules27206885

Ban, W.K., Fong, I.L., Khong, H.Y., Phung, J.H.Y., 2022. Wound healing, antimicrobial and antioxidant properties of *Clinacanthus nutans* (Burm.f.) Lindau and *Strobilanthes crispus* (L.) Blume extracts. *Molecules.* 27, 1722. https://doi.org/10.3390/molecules27051722

Bitwell, C., Indra, S.S., Luke, C., Kakoma, M.K., 2023. A review of modern and conventional extraction techniques and their applications for extracting phytochemicals from plants. *Sci. Afr*. 19, e01585. https://doi.org/10.1016/j.sciaf.2023.e01585

Campanella, B., Palleschi, V., Legnaioli, S., 2021. Introduction to vibrational spectroscopies. *ChemTexts.* 7, 5. https://doi.org/10.1007/s40828-020-00129-4

Christou, C., Agapiou, A., Kokkinofta, R., 2018. Use of FTIR spectroscopy and chemometrics for the classification of carobs origin. *J. Adv. Res*. 10, 1-8. https://doi.org/10.1016/j.jare.2017.12.001

Cockfield, J.A., Schafer, Z.T., 2019. Antioxidant defenses: a context-specific vulnerability of cancer cells. *Cancers.* 11, 1208. https://doi.org/10.3390/cancers11081208

de Oliveira, I., Santos-Buelga, C., Aquino, Y., Barros, L., Heleno, S.A., 2025. New frontiers in the exploration of phenolic compounds and other bioactives as natural preservatives. *Food Biosci*. 68, 106571. https://doi.org/10.1016/j.fbio.2025.106571

Elhamdaoui, O., El Orche, A., Cheikh, A., Karrouchi, K., Laarej, K., Bouatia, M., 2021. Assessment of a nondestructive method for rapid discrimination of Moroccan date palm varieties via mid-infrared spectroscopy combined with chemometric models. *J. AOAC Int*. 104, 1710-1718. https://doi.org/10.1093/jaoacint/qsab068

Flieger, J., Flieger, W., Baj, J., Maciejewski, R., 2021. Antioxidants: classification, natural sources, activity/capacity measurements, and usefulness for the synthesis of nanoparticles. *Materials.* 14, 4135. https://doi.org/10.3390/ma14154135

García-Pérez, P., Becchi, P.P., Zhang, L., Rocchhetti, G., Lucini, L., 2024. Metabolomics and chemometrics: The next-generation analytical toolkit for the evaluation of food quality and authenticity. *Trends Food Sci. Technol*. 147, 104481. https://doi.org/10.1016/j.tifs.2024.104481

Ghasemzadeh, A., Jaafar, H.Z., Rahmat, A., 2015. Phytochemical constituents and biological activities of different extracts of *Strobilanthes crispus* (L.) Bremek leaves grown in different locations of Malaysia. *BMC Complement. Altern. Med*. 15, 422. https://doi.org/10.1186/s12906-015-0873-3

Irnawati, I., Sugeng, R., Sudibyo, M., Rohman, A., 2021. The employment of FTIR spectroscopy and chemometrics for the classification and prediction of antioxidant activities of pumpkin seed oils from different origins. *J. Appl. Pharm. Sci*. 11, 100-107. https://doi.org/10.7324/JAPS.2021.110514

Kladwong, P., Chantaranothai, P., 2024. Notes on Strobilanthes (Acanthaceae) with capitate inflorescences in Thailand. *PhytoKeys.* 244, 89-126. https://doi.org/10.3897/phytokeys.244.124260

Koay, Y.C., Wong, K.C., Osman, H., Asmawi, M.Z., 2013. Chemical constituents and biological activities of *Strobilanthes crispus* L. *Rec. Nat. Prod*. 7, 59-64

Kusumadewi, A.P., Martien, R., Pramono, S., Setyawan, A. A., Windarsih, A., Rohman, A., 2022. Application of FTIR spectroscopy and chemometrics for correlation of antioxidant activities, phenolics and flavonoid contents of Indonesian *Curcuma xanthorrhiza*. *Int. J. Food Prop*. 25, 2364-2372. https://doi.org/10.1080/10942912.2022.2134418

Matwijczuk, A., Oniszczuk, T., Matwijczuk, A., Chruściel, E., Kocira, A., Niemczynowicz, A., Wójtowicz, A., Combrzyński, M., Wiącek, D., 2019. Use of FTIR spectroscopy and chemometrics with respect to storage conditions of Moldavian dragonhead oil. *Sustainability.* 11, 6414. https://doi.org/10.3390/su11226414

Nurani, L.H., Guntarti, A., Lestari, D., Wirnawati, Rohman, A., Windarsih, A., 2024. The Application of FTIR spectra coupled with chemometrics for analysis of lard in food products for halal authentication: a mini review. *Food Res*. 8, 73-83. https://doi.org/10.26656/fr.2017.8(3).489

Rafi, M., Febriany, S., Wulandari, P., Suparto, I.H., Ridwan, T., Rahayu, S., Siswoyo, D.M., 2018. Total phenolics, flavonoids, and anthocyanin contents of six *Vireya rhododendron* from Indonesia and evaluation of their antioxidant activities. *J. Appl. Pharm. Sci*. 8, 49-54. https://doi.org/10.7324/JAPS.2018.8908

Rafi, M., Rismayani, W., Sugiarti, R.M., Syafitri, U.D., Wahyuni, W.T., Rohaeti, E., 2021. FTIR-based fingerprinting combined with chemometrics for discrimination of *Sonchus arvensis* leaf extracts and correlation with their antioxidant activity. *Indones. J. Pharm*. 32, 132-140. https://doi.org/10.22146/ijp.755

Ramadhani, V., Rusdi, R., Azizah, Z., Rivai, H., 2021. Overview of phytochemicals and pharmacological activity of keji beling plant (*Strobilanthes crispus* Bl.). *Int. J. Med. Pharm. Sci.* 6, 25-39. https://doi.org/10.47760/ijpsm.2021.v06i07.003

Rohaeti, E., Karunina, F., Rafi, M., 2020. FTIR-based fingerprinting and chemometrics for rapid investigation of antioxidant activity from *Syzygium polyanthum* extracts. *Indones. J. Chem*. 21, 128-136. https://doi.org/10.22146/ijc.54577

Rohman, A., Ghazali, M.A.B., Windarsih, A., Irnawati, I., Riyanto, S., Yusof, F.M., Mustafa, S., 2020. Comprehensive review on application of FTIR spectroscopy coupled with chemometrics for authentication analysis of fats and oils in the food products. *Molecules.* 25, 5485. https://doi.org/10.3390/molecules25225485

Rohman, A., Ikhtiarini, A.N., Setyanigsih, W., Rafi, M., Aminah, N.S., Insanu, M., Irnawati, I., Santosa, D., 2021. The use of chemometrics for classification of sidaguri (Sida rhombifolia) based on FTIR spectra and antiradical activities. *Indones. J. Chem*. 21, 1568-1576. https://doi.org/10.22146/ijc.64360

Saidi, F., Khetari, S., Yahia, I., Zahran, H. Y., Hidouri, T., Ameur, N., 2022. The use of principal component analysis (pca) and partial least square (pls) for designing new hard inverse perovskites materials. *Comp. Cond. Matter.* 31, e00667. https://doi.org/10.1016/j.cocom.2022.e00667

Sharma, S., Shrestha, B., Bhuyan, N.R., Majumdar, S., Chowdhury, S., Mazumder, R., 2024. Chemometric method development for the determination of naringin and verapamil. *Bull. Natl. Res. Cent*. 48, 13. https://doi.org/10.1186/s42269-024-01169-3

Shiyan, S., Safitri, I.N., Nathasia, J., Fitrotunnisa, L., Fransiska, O. L., Salsabillah, T., Pratiwi, G., 2022. FTIR spectroscopy combined with chemometrics for evaluation of gambir extract–self nano emulsifying formulation from U*ncaria gambir* Roxb. B*iointerface Res. Appl. Chem*. 13, 153. https://doi.org/10.33263/BRIAC132.153

Umar, A.H., Syahruni, R., Ranteta'dung, I., Rafi, M., 2022. FTIR-based fingerprinting combined with chemometrics method for rapid discrimination of *Jatropha* spp. (Euphorbiaceae) from different regions in South Sulawesi. *J. Appl. Pharm. Sci*. 13, 139-149. https://doi.org/10.7324/JAPS.2023.130113

Wakiuchi, A., Jasial, S., Asano, S., Hashizume, R., Hatanaka, M., Ohnishi, Y., Matsubara, T., Ajiro, H., Sugawara, T., Fujii, M., Miyao, T., 2023. Chemometrics approach based on wavelet transforms for the estimation of monomer concentrations from FTIR spectra. *ACS Omega.* 8, 19781-19788. https://doi.org/10.1021/acsomega.3c01515

Zheng, X., Nie, B., Du, J., Rao, Y., Li, H., Chen, J., Du, Y., Zhang, Y., Jin, H., 2024. A non-linear partial least squares based on monotonic inner relation. *Front. Physiol*. 15, 1369165 https://doi.org/10.3389/fphys.2024.1369165