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Rapid and Non-Destructive Analysis of Plant Material Using FTIR and Chemometric Methods

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Abstract
Plant material analysis requires efficient, reliable, and sustainable methods for characterization, authentication, and quality control. Fourier Transform Infrared Spectroscopy (FTIR), combined with chemometrics, has emerged as a non-destructive approach that requires minimal sample preparation. This review summarizes developments and applications of FTIR chemometrics in plant analysis from 2015 to 2025, based on more than 32 published studies. The evolution of data analysis is described from classical techniques, including Principal Component Analysis and Partial Least Squares, to machine learning methods such as Support Vector Machines and Random Forests. Various FTIR modes, namely ATR FTIR, DRIFTS, and FTIR PAS, are discussed for analyses of leaves, roots, rhizomes, flowers, fruits, and fossilized plant materials. Reported applications include species identification with accuracies approaching 100%, geographic origin authentication with 77-94% accuracy, detection of adulteration in high-value commodities such as saffron, quantification of bioactive constituents with determination coefficients of 0.96-0.99, and assessment of environmental or agronomic influences on plant composition. Although challenges remain, particularly matrix complexity and calibration transfer, FTIR chemometrics represents a sustainable, rapid, and cost-effective tool for research and industrial quality control. Future directions emphasize the global integration of artificial intelligence and instrument miniaturization.

Keywords: authentication, chemometrics, FTIR spectroscopy, machine learning, plant analysis, quality control

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Pendekatan Cepat dan Non-Destruktif Bahan Tanaman Menggunakan Metode FTIR dan Kemometrik

Abstrak
Analisis bahan tanaman memerlukan metode yang efisien, andal, dan berkelanjutan untuk karakterisasi, autentikasi, serta pengendalian mutu. Fourier Transform Infrared Spectroscopy (FTIR) yang dikombinasikan dengan kemometrika telah berkembang sebagai pendekatan non-destruktif yang memerlukan persiapan sampel minimal. Tinjauan ini merangkum perkembangan dan aplikasi kemometrika FTIR dalam analisis tanaman pada periode 2015 hingga 2025, berdasarkan lebih dari tiga puluh dua studi yang telah dipublikasikan. Perkembangan metode analisis data dibahas mulai dari teknik klasik, termasuk Principal Component Analysis dan Partial Least Squares, hingga metode pembelajaran mesin seperti Support Vector Machines dan Random Forests. Berbagai mode FTIR, yaitu ATR-FTIR, DRIFTS, dan FTIR-PAS, dibahas untuk analisis daun, akar, rimpang, bunga, buah, serta material tanaman terfosilkan. Aplikasi yang dilaporkan meliputi identifikasi spesies dengan tingkat akurasi mendekati seratus persen, autentikasi asal geografis dengan akurasi 77-94%, deteksi pemalsuan pada komoditas bernilai tinggi seperti saffron, kuantifikasi senyawa bioaktif dengan koefisien determinasi 0,96 hingga 0,99, serta evaluasi pengaruh faktor lingkungan atau agronomis terhadap komposisi tanaman. Meskipun masih terdapat tantangan, khususnya kompleksitas matriks dan transfer kalibrasi, kemometrika FTIR merupakan alat yang berkelanjutan, cepat, dan hemat biaya untuk penelitian dan pengendalian mutu industri. Arah pengembangan ke depan menekankan integrasi kecerdasan buatan dan miniaturisasi instrumen secara global.

Kata Kunci: analisis tanaman, autentikasi, kemometrik, kontrol kualitas, pembelajaran mesin, spektroskopi FTIR

1. Introduction

Herbal plants remain integral to global healthcare systems, with the World Health Organization estimating that 80% of the world's population relies on traditional plant-based medicines for primary healthcare.[1] The global herbal products market, projected to reach USD 411 billion by 2026, reflects a growing interest in natural therapeutics, especially across developed nations.[2,3] However, this rapid expansion also raises major concerns regarding product authenticity, quality consistency, and clinical reliability. Inadequate quality control has led to cases of adulteration, misidentification, and variability in bioactive constituents, compromising both safety and therapeutic efficacy.

The complexity of plant matrices, which contain hundreds to thousands of metabolites at varying concentrations, presents significant analytical challenges.[4,5] Phytochemical composition varies substantially due to genetic, environmental, and post-harvest factors, while supply chain risks include substitution, adulteration, and contamination.[6,7] Conventional chromatographic approaches, despite their specificity, face limitations including high costs, extensive sample preparation, and an inability to capture synergistic effects in complex formulations.[8,9]

Fourier Transform Infrared (FTIR) spectroscopy offers a compelling alternative, providing unique spectral fingerprints of chemical composition through molecular bond vibrations.[10] It has been successfully applied to various plant-derived materials, including edible oils.[11] Modern developments in Attenuated Total Reflectance (ATR) modules enable direct analysis with minimal sample preparation.[12] Key advantages include rapid analysis (under one minute), minimal sample preparation, low operational costs, non-destructive testing, environmental compatibility, and alignment with holistic medicinal philosophies, making FTIR an attractive approach for routine herbal authentication.[13,14] However, the intrinsic complexity of spectral data necessitates robust multivariate analysis. Chemometric analysis, encompassing both unsupervised methods (Principal Component Analysis, Hierarchical Cluster Analysis) and supervised methods (Partial Least Squares-Discriminant Analysis, Support Vector Machines), is crucial for extracting meaningful information from high-dimensional spectral datasets.[15]

Similar chemometric approaches have been applied beyond FTIR, such as Partial Least Squares Regression (PLS-R) on Raman spectral data to quantify curcumin in turmeric rhizomes[16] and Principal Component Analysis (PCA) on GC-MS data to authenticate lemongrass oil,[17] highlighting the versatility of multivariate techniques in herbal quality control. Furthermore, emerging machine learning approaches, such as Random Forests and Artificial Neural Networks, enhance the ability to model complex, non-linear relationships.[18,19] The integration of FTIR with chemometrics has demonstrated significant potential in taxonomic authentication, geographic origin tracing, adulteration detection, and even preliminary bioactive profiling across various plant species.[20,21]Because phytochemical profiles often vary markedly across plant parts, and specific organs frequently correlate with therapeutic effects in traditional medicine, focusing on plant-part-specific analysis is essential for accurate characterization and reliable standardization.[1,22]

Despite these advances, however, a comprehensive evaluation of how FTIR combined with chemometrics has been applied to different plant parts and its potential for predicting biological activity, especially for medicinal plants, remains scarce. This review addresses that gap by providing a structured synthesis of FTIR spectroscopy, integrated with chemometric analysis, for herbal plant characterization, organized by plant part. Covering studies from 2015-2025, we critically evaluate methodological advances, assess current capabilities and limitations for authentication and standardization, and identify research directions essential to establish reliable, rapid, and cost-effective quality control strategies for modern herbal medicine

2. Materials and Method

Literature Search Strategy

2.1. Database Search and Selection Criteria

A comprehensive literature search was conducted across multiple electronic databases, including Web of Science, Scopus, PubMed/MEDLINE, ScienceDirect, and Google Scholar, to identify relevant studies published between January 2015 and May 2025. This timeframe was selected to capture recent developments and technological advances in FTIR-chemometric applications for plant analysis.The search strategy employed a combination of keywords using Boolean operators: ("FTIR" OR "Fourier Transform Infrared" OR "infrared spectroscopy") AND ("chemometrics" OR "multivariate analysis" OR "PCA" OR "PLS") AND ("medicinal plant*" OR "herbal medicine" OR "plant*") AND ("root*" OR "leaf" OR "leaves" OR "stem*" OR "bark" OR "flower*" OR "seed*" OR "fruit*").

2.2. Inclusion and Exclusion Criteria

2.2.1. Inclusion criteria

- Original research articles applying FTIR spectroscopy combined with at least one

chemometric method
- Studies focusing on plant material analysis with clearly defined plant parts
- Articles providing sufficient methodological details for FTIR techniques and chemometric analysis
- Publications with quantitative results and statistical validation
- Studies published in peer-reviewed journals

2.2.2. Exclusion criteria

- Review articles, book chapters, and conference abstracts without original data
- Studies using only conventional infrared spectroscopy without Fourier transform
- Articles lacking chemometric analysis or using only basic statistical methods
- Studies with insufficient methodological information
- Publications focusing solely on synthetic compounds or non-plant materials

2.3. Literature Selection Process

The literature selection followed a two-stage screening process. Initial screening involved reviewing titles and abstracts to identify potentially relevant studies. Full-text screening was then conducted to assess methodological quality and relevance to the research objectives. Additional relevant articles were identified by reviewing the reference list and consulting experts. While English-language publications were prioritized, articles in other languages with comprehensive English abstracts were included when they provided significant methodological or technical contributions.The PRISMA flowchart process can be seen in Figure 1.

3. Result

3.1. FTIR-Chemometric Application Based On Plant Part

3.1.1. Leaf Analysis

Twenty-three studies focused on leaf analysis, making leaves the most analyzed plant part using FTIR-Chemometrics. For species identification, a study on *Camellia japonica* cultivar identification[23] achieved 100% accuracy using spectral-based machine learning with FTIR. Similarly, Passiflora studies[24] distinguished six species using ATR-FTIR and PCA. Studies of *Vitis*

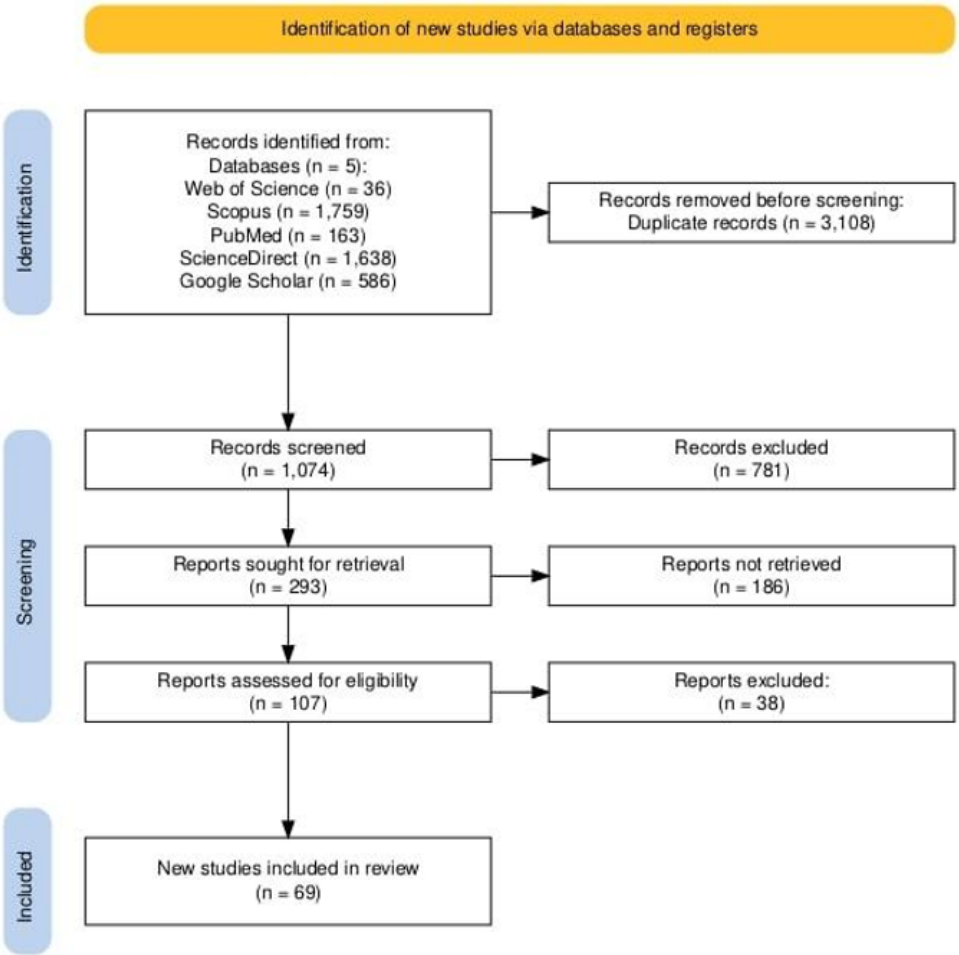

Figure 1. The workflow for the selection of articles according to PRISMA guideline

vinifera L.[25] demonstrated that ATR-FTIR combined with SIMCA and PLS-DA could distinguish grape genotypes with an error rate of only 0.08, including discrimination between clones of the same variety.

Environmental factor analysis revealed significant results in several studies. Japanese knotweed studies[26] used PLSR to predict root water potential with an R^2 of 0.8. Coffee leaf studies[27] successfully distinguished between irrigated and non-irrigated plants using FTIR with OSC-PLS-DA based on differences in carbohydrates, amino acids, and lipids. Soursop leaf studies[28] demonstrated that NIR and FTIR could accurately predict total phenolic content across different growing altitudes.

Geographical authentication studies showed promising results. *Laurus nobilis* L. studies[29] achieved 77.8% correct classification from different Turkish geographical origins using FTIR-ATR with discriminant analysis. *Melastoma malabathricum* studies[30] reported 93.9% classification accuracy for geographic authentication across seven Malaysian locations using ATR-FTIR with PCA, RF, and GA.

3.1.2. Root and Rhizome Analysis

Root and rhizome studies focused primarily on medicinal plant identification and authentication. Studies on *Gentianae macrophyllae*[31] reported 97-100% identification accuracy using FTIR-PAS. *Gastrodia elata* Blume studies[32] successfully and accurately distinguished species and origins using ATR-FTIR combined with OPLS-DA and SVM. Bioactive compound quantification showed excellent results. Curcumin quantification in Curcuma extracts studies[33] developed an FTIR method with PLS, achieving correlation coefficients of R^2 0.96-0.99 compared to HPLC values in Curcuma extracts.

3.1.3. Fruit Analysis

Fruit quality evaluation studies demonstrated practical applications. Fresh-cut jackfruit studies [34] Using PLS-R and ANN predictive models, achieved high correlation ($R^2 > 0.85$) between FTIR data and microbial counts. In Fig cultivar studies,[35] cultivars were successfully distinguished using ATR-FTIR, with PCA revealing two main groups for fruit flesh and five for fruit skin.

3.1.4. Flower and Stigma Analysis

Saffron authentication studies showed exceptional results. Saffron studies36 achieved 99% correct classification for pure saffron samples and detected 5-20% adulterated samples using DRIFTS with PLS-DA, with detection limits of 1.0-3.1% for adulterants.

3.2. FTIR Techniques In Plant Analysis

3.2.1. ATR-FTIR (Attenuated Total Reflectance)

ATR-FTIR is the most widely used FTIR technique for plant material analysis due to its ease of sample preparation.[37,38] This technique uses total internal reflection when an infrared beam enters a crystal with a high refractive index (such as diamond or ZnSe) and interacts with a sample placed on the crystal surface.

In the research table, ATR-FTIR was used in various studies, including *Laurus nobilis* L. leaves,[29] *Gastrodia elata* Blume,[32] and Japanese knotweed.[26] This technique is highly effective for solid and powder samples without complex preparation, making it ideal for routine analysis and rapid screening

3.2.2. DRIFTS (Diffuse Reflectance Infrared Fourier Transform Spectroscopy)

DRIFTS measures infrared radiation diffusely scattered from the surface of a powder or fine-particle sample. This technique is particularly suitable for powdered plant samples and is very effective in authentication studies and counterfeit detection.[38,39]

A significant example of DRIFTS use was in study[36] which detected adulteration of saffron with other plant materials. The study used DRIFTS with PLS-DA and achieved 99% correct classification for pure saffron and adulterated 5-20% (w/w).

3.2.3. FTIR-PAS (Photoacoustic)

FTIR-PAS is a relatively new technique in plant analysis. It measures the acoustic signal generated when a sample absorbs infrared radiation. This technique offers deeper analysis and can be used for opaque samples or complex surface morphologies.40

In reports of *Gentianae Macrophyllae* (Qinjiao),[31] studies used FTIR-PAS to assess quality and verify species origin. The results showed that FTIR-PAS could effectively distinguish Qinjiao samples by species, achieving 97.09-100% accuracy.

3.3. Chemometric Method

Analysis of multivariate methods employed in plant FTIR studies from 2015-2025 reveals distinct developmental phases reflecting both technological advancement and analytical complexity requirements. Early studies (2015-2017) predominantly utilized established chemometric approaches, including PCA, HCA, and PLS, which provided reliable baseline performance with straightforward implementation

(Table 1). The intermediate period (2018-2020) saw the integration of advanced classification techniques, including SIMCA, SVM, and LDA, to address the increasing demand for improved discrimination. Recent studies (2021-2025) demonstrate widespread adoption of machine learning algorithms, including Random Forest, Genetic Algorithms, and deep learning approaches, corresponding to enhanced computational accessibility and automated analysis requirements.

Table 1. FTIR-Chemometric Application Based on Plant Part

Ref	Plants	Plant Parts	Country	Sample Type	FTIR Technique	Chemometric Method	Model Validation	Research Objectives	Key Results
Plant Parts: Roots									
[31]	*Gentianae Macrophyllae* (Qinjiao)	Roots	China	Dry roots	FTIR-PAS (photoacoustic)	OPLS-DA, SVM	Accuracy 97.09-100% with Mcc value 0.80-1.00	Quality assessment and origin verification of Qinjiao species	FTIR-PAS can distinguish Qinjiao samples by species effectively
[32]	*Gastrodia elata Blume*	Roots	China	Roots	ATR-FTIR	OPLS-DA, SVM	Accuracy 97.09-100% and Mcc value 0.80-1.00	Authentication of *G. elata* identity under the influence of biological variability	ATR-FTIR, integrated with chemometric methods, effectively distinguished *G. elata* samples by species
[41]	*Securidaca longipenduculata*	Roots	South Africa	Roots	FTIR	PCA, OPLS-DA, HCA	HCA successfully identified two clusters	Developed HPTLC fingerprinting and FTIR analysis for quality control	HCA analysis of the data identified two clusters, and additional analysis verified quantitative differences between the samples
Plant Parts: Root, stem, leaf									
[42]	*Berberis* spp.	Root, stem, leaf	India	Extract	FTIR-ATR	PCA	PCA model with HPLC successfully classified Berberis species and plant parts	Comparative analysis of TLC, HPLC, and FTIR-ATR for Berberis quality control	The PCA model obtained by the HPLC fingerprinting method successfully classified Berberis species and plant parts.
Plant Parts: Leaves									
[43]	*Monteverdia ilicifolia*	Leaves	Brazil	Leaf, powder, extract	MIR-FTIR	PCA, PLS-DA	94% sensitivity, 100% specificity, and 99% accuracy for extract samples	Developed a method based on chemometrics and machine learning to identify *M. ilicifolia*	PLS-DA achieves superior performance with sample extracts and machine learning algorithms, demonstrating robustness and flexibility
[29]	*Laurus nobilis* L.	Leaves	Turkey	Leaves	FTIR-ATR	PCA, Discriminant Analysis	56 out of 72 samples were classified correctly (77.8%)	Investigating the effects of geographical origin and altitude of the leaves of *Laurus nobilis* L.	PCA analysis explained 88.7% of the variance in the model, and there were differences in the response of the same plant species to their presence in different places of origin.
[44]	*Impatiens balsamina* L.	Leaves	Indonesia	Extract	FTIR, UV-Vis	PCA	Total PC value from UV-Vis spectra is 90%, and the total PC	Classifying *I. balsamina* leaf extracts from different solvent extraction	Combining FTIR and UV-Vis with chemometric techniques successfully classified

							value from FTIR spectra is 85%		*I balsamina* leaf extracts from different solvent extractions.
[23]	*Camellia japonica*	Leaves	Portugal	Leaves	NIR, FTIR	PCA, GA-SVM, RF	Approach 2 with FTIR achieved 100% accuracy in cultivar assignment	Testing the impact of two machine learning-based approaches for distinguishing *C. japonica* cultivars	Approach 2 obtained the best results with FTIR spectroscopy data, achieving 100% accuracy in cultivar assignment.
[30]	*Melastoma malabathricum*	Leaves	Malaysia	Extract	ATR-FTIR	PCA, RF, GA	93.9% classification accuracy with RF-selected variables using LDA	Differentiating *M. malabathricum* samples from seven different locations	ATR-FTIR second derivative spectra successfully distinguish *M. malabathricum* samples based on their geographical origin
[45]	Green tea (*Camellia sinensis*)	Leaves	Vietnam	Tea leaves	FTIR	PCA	PC1 and PC2 account for 91.26% of the total variance.	Analyzing elemental profiles and FTIR spectra with chemometric multivariate data analysis	PCA of the FTIR data showed that the first two principal components successfully separated the four green tea varieties into different clusters
[46]	Tea (*Camellia sinensis*)	Leaves	Europe	Tea leaves and brew	ATR-FTIR	PCA	PCA successfully differentiates the spectral profiles of tea leaves and steeping	Investigated 13 differently processed tea leaves and their tea brews	Comparison of spectral profiles of tea leaves and brew emphasizes differences related to different spectral regions
[26]	Japanese knotweed (*Reynoutria japonica*)	Leaves	English	Whole dried leaves	ATR-FTIR	PCA, LDA, SVM, PLSR	PLSR predicts root water potential with an R^2 of 0.8	Investigating the response of Japanese knotweed to varied environmental habitats	Japanese knotweed exhibits an environmentally induced phenotype, indicated by measurable differences in their ATR-FTIR spectra
[47]	*Azadirachta excelsa*	Leaves	Indonesia	Extract	FTIR	PCA	PCA successfully differentiates samples based on the extraction solvent	Examine differences in metabolite fingerprinting and antibacterial activity	The polarity of the extraction solvent has an important effect on the metabolite profile and antibacterial activity of A. excelsa
[48]	Brussels sprout (*Brassica oleracea*)	Leaves	Greece	Leaf layer	ATR-FTIR	Discriminant Analysis	Discriminant analysis effectively classifies leaf layers based on spectral data with high accuracy	Investigating the molecular composition of Brussels sprout leaf layers	ATR-FTIR analysis identified different molecular constituents, including glucosinolates, phenolics, lipids, and polysaccharides
[24]	Passion fruit (*Passiflora* spp.)	Leaves	Brazil	Leaf, powder, extract	ATR-FTIR	PCA	PCA successfully differentiated between Passiflora species	Distinguishing Passiflora species	ATR-FTIR can distinguish six Passiflora species based on their spectral fingerprints

[49]	Black betel (*Piper acre Blume*)	Leaves	Indonesia	Extract	FTIR	PCA, PLS-DA	Discriminant analysis can classify three types of betel nut	Identifying and authenticating piperenamide A compounds in black betel leaf extracts	*Piperenamide A* is only found in black betel (Piper acre) and not in Piper betel and Piper scrotum.
[50]	Tea (*Camellia sinensis*)	Leaves	Iran	Extract	FTIR	GA-SVM	The model showed 100% sensitivity and specificity for training and testing sets.	Distinguishing between eight tea cultivars	The discriminative region of FTIR spectra (1350-1650 cm^{-1}) was selected using GA-SVM, and the model showed 100% sensitivity and specificity.
[51]	Dates (*Phoenix dactylifera*)	Leaves	Oman	Leaves	NIRS, FTIR/ATR, NMR	PCA, PLS-DA	The model successfully distinguishes the gender of dates	Identifying sex differentiation in immature date palm leaves	NIRS/FTIR reflectance and ^{1}H-NMR profiles indicate that monosaccharide (glucose and fructose) and/ or disaccharide (maltose and sucrose) signals play an important role in sex differentiation.
[52]	Pinus nigra (Austrian Pine)	Leaves	United States of America	Whole dried leaves	FT-IR	SIMCA, PLS, SVM	The model can distinguish trees based on their vulnerability	Evaluate Austrian Pine resistance to pathogens	Trees with different susceptibilities can be distinguished based on FT-IR spectra
[53]	Paederia foetida and *Vitis vinifera*	Leaves	Indonesia	Extract	FTIR	PCA, CA	Euclidean distance 0.537 for *P. foetida* and 1.157 for *V. vinifera*	Identifying the similarity of arbutin functional groups in plants	Compounds in *P. foetida* and *V. vinifera* have similarities to arbutin
[25]	Grapes (*Vitis vinifera* L.)	Leaves	Chile	Leaves	ATR-FTIR	SIMCA, PLS-DA	The misclas-sification rate of the spectra of the test set by the two models is 0.08	Differentiating grape genotypes	Direct leaf measurements by ATR-FTIR combined with the chemometric method successfully classified six genotypes
[54]	*Eucalyptus globulus*	Leaves	Portugal	Leaf extract	ATR-FTIR	Cluster Analysis	The chemometric model successfully distinguishes	Enriching the extract with natural bioactive compounds such as triterpenic acids	FTIR-ATR and GC-MS successfully characterized various extracts and provided guidelines for producing triterpenic acid-enriched natural extracts.
[27]	*Coffea arabica* L.	Leaves	Brazil	Leaf extract	FTIR	PCA, OSC-PLS-DA	PCA shows the most suitable ethanol-con-taining extraction solvent	Evaluate the effect of extraction solvents and environmental conditions on metabolites	OSC-PLS-DA suc-cessfully classified leaves from irrigated and non-irrigated plants based on car-bohydrate-, amino acid- and lipid-relat-ed bands
[55]	*Orthosiphon stamineus*	Leaves	Malaysia	Extract	FTIR	PCA, HCA	HPLC and FTIR fingerprints successfully	Profile of selected me-tabolites in *O. stamineus*	Macerated ethanol extract contains high phenolics and flavonoids with high

							categorized the extracts	leaf extract and their correlation with activity	antioxidant activity; aqueous extract shows high polysaccharides
[56]	Hops (*Humulus lupulus* L.)	Leaves	Italy	Dry leaves	ATR-FTIR	PCA	PCA successfully grouped the samples based on the treatment	Investigating the effect of the drying method on the bioactive profile of hop leaves	FD appears to be the most suitable drying method, while OD provides higher carotenoid retention
[57]	*Moringa oleifera Lam.*	Leaves	Came-roon	Leaves	ATR-FTIR	AComDim	The factor "agro-climatic zone" is the most significant	Highlights the impact of climatic and edaphic factors on the chemical composition of Moringa leaves	The diversity of climate and soil in Cameroon must be considered if a certain typicality or constant quality is to be ensured.
Plant Parts: Whole herb									
[58]	*Phyllanthus niruri* L.	Whole herb	Indonesia	Dry crop	FTIR-ATR	PCA	Successfully grouped samples based on harvest time and fertilizer dosage	Determining the effect of fertilizer and harvest age on metabolite profile	Harvest time and fertilizer dose affected *P. niruri* growth parameters, total flavonoid content, and extract yields
Plant Parts: Flower petals									
[59]	Rosela (*Hibiscus sabdariffa* L.)	Flower petals	Indonesia	Extract	FTIR	PCA, Cluster Analysis	Successfully categorized extracts from 12 different regions	Distinguishing roselle extracts from different regions	The FTIR-chemometric method can be used to distinguish roselle extracts from several locations
Plant Parts: Bark									
[60]	*Cinnamomum cassia*	Bark	China	Bark	FTIR	PCA	HPLC and FTIR successfully distinguish different habitats of suitability	Predict the potential distribution of *C. cassia* and evaluate quality in suitable habitats	Trans-sinamaldehyde content (0.85%) was much higher in the high-suitability habitat compared to the medium-low-suitability habitat (0.30%).
Plant Parts: Rhizome									
[33]	*Curcuma longa* and *Curcuma xanthorriza*	Rhi-zome	Indonesia	Ethanol extract	FTIR	PLS	*C. longa* extract: R^2 0.96, RMSEC 0.299; *C. xanthorriza* extract: R^2 0.99, RMSEC 0.089	Develop a quantification method of curcumin in ethanol extracts of *C. longa* and *C. xanthorriza*	FTIR spectroscopy combined with PLS is an alternative technique for determining curcumin in Curcuma species that is rapid, without sample preparation, and does not involve excessive solvents and reagents.
Plant Parts: Flower stigma									
[61]	Saffron (*Crocus sativus* L.)	Flower stigma	Morocco	Saffron powder	ATR-FTIR	PCA	PCA successfully separates samples based on treatment	Determine chemical composition and identify adulterated saffron	ATR-FTIR method can be used to detect saffron adulteration

3.4. Unsupervised Methods

3.4.1. Discovering Hidden Patterns

Unsupervised methods identify inherent data patterns without prior categorical knowledge, serving essential roles in exploratory data analysis and structural assessment of spectral datasets.

Principal Component Analysis (PCA) is the most widely used dimensionality reduction technique in the reviewed studies. The method's fundamental strength lies in orthogonalizing the original spectral variables into uncorrelated principal components while maximizing variance retention. This mathematical approach effectively reduces thousands of wavenumber variables to a manageable number of components without significant loss of information.[62,63] In Vietnamese tea analysis,[21] the first two principal components accounted for 91.26% of total spectral variance, demonstrating PCA's efficiency in capturing essential chemical variability. The orthogonal nature of principal components ensures each component represents independent spectral information, facilitating the interpretation of underlying chemical differences between samples.

Hierarchical Cluster Analysis (HCA) constructs a hierarchical relationship among samples by forming a dendrogram based on spectral similarity measures. The method employs distance metrics, typically Euclidean distance, combined with linkage criteria to progressively merge similar samples or clusters. This approach provides a comprehensive clustering hierarchy visualization, enabling simultaneous assessment of relationships across multiple similarity levels.[64] Application in *Phyllanthus niruri* L. metabolite profiling[58] demonstrated HCA's capability to reveal treatment-specific metabolic groupings related to fertilization and harvest timing effects.

Cluster analysis encompasses various algorithms offering flexibility in handling diverse data structures and cluster characteristics. Unlike hierarchical approaches, methods such as k-means clustering accommodate different cluster shapes and distributions.[65] The *Eucalyptus globulus* leaf extract characterization study[23] utilized cluster analysis to identify solvent-specific extraction patterns, demonstrating the method's adaptability to different analytical objectives.

3.2. Supervised Multivariate Methods

Supervised methods use prior categorical information to develop predictive models for classification and quantification, offering improved accuracy through targeted pattern recognition.

Partial Least Squares (PLS) combines dimensionality reduction with regression analysis to address the multicollinearity inherent in spectral data. The method constructs latent variables that maximize the covariance between the predictor (spectral) and response (concentration) matrices, focusing on spectral regions most relevant to the target analytes.[66] Curcumin quantification in Curcuma extracts[33] achieved R^2 values ranging from 0.96 to 0.99, demonstrating PLS effectiveness for accurate quantitative determinations across varying concentration ranges.

The method's ability to filter spectral noise while maintaining predictive relevance makes it superior to conventional regression approaches for spectroscopic applications.

Partial Least Squares Discriminant Analysis (PLS-DA) for classification tasks while retaining dimensionality reduction advantages. The method constructs discriminant models that emphasize class-discriminating spectral variations while suppressing irrelevant information. A comparative analysis of *Gentiana rigescens* discrimination studies[67] showed that PLS-DA outperformed PCA-based approaches, achieving 100% classification accuracy. Additionally, PLS-DA loading plots provide interpretable identification of discriminative spectral regions, offering valuable chemical insights alongside classification results.

Support Vector Machine (SVM) employs optimization-based classification by identifying optimal hyperplanes that separate classes. The method focuses on support vectors, critical training samples defining class boundaries rather than modeling entire data distributions. This approach is particularly effective for high-dimensional spectral data with complex, nonlinear class boundaries. *Gastrodia elata* Blume classification studies[32] achieved 97-100% accuracy, illustrating SVM's robustness for challenging plant metabolite discrimination tasks. The kernel transformation capability enables modeling nonlinear relationships without requiring explicit data transformations.

Linear Discriminant Analysis (LDA) seeks optimal linear combinations of spectral features maximizing between-class separation while minimizing within-class variation. The method assumes normally distributed classes with equal covariance matrices and performs optimally when these assumptions hold. Local soursop leaf classification[28] achieved 100% accuracy, demonstrating the effectiveness of LDA under appropriate data conditions.

The method provides interpretable discriminant functions revealing which spectral regions contribute most significantly to classification decisions.

3.3. Machine Learning-Based Approaches

Advanced machine learning methods represent recent developments in plant FTIR analysis, offering sophisticated pattern recognition capabilities that exceed traditional chemometric performance in complex analytical scenarios.

Random Forest (RF) uses ensemble learning, combining multiple decision trees trained on different subsets of the data with random feature selection. This approach reduces overfitting while capturing complex, non-linear relationships in spectral data. Each tree contributes to the final predictions through majority voting, while the ensemble provides feature-importance rankings that identify the most discriminative spectral regions. *Camellia japonica* cultivar identification studies[23] achieved 100% classification accuracy while providing insights into spectral regions most relevant for cultivar discrimination. The method's inherent ability to handle missing data and mixed variable types enhances its applicability to diverse analytical challenges.

Genetic Algorithm-Support Vector Machine (GA-SVM) combines evolutionary optimization with machine-learning classification through automated feature selection. The genetic algorithm component evolves optimal spectral feature combinations through selection, crossover, and mutation, while the SVM provides robust classification using optimized feature subsets. This dual optimization ensures utilization of only the most discriminative spectral information, improving both accuracy and computational efficiency. Tea cultivar discrimination studies[68] achieved 100% sensitivity and specificity, demonstrating the method's capability to identify optimal spectral features while maintaining superior classification performance.

3.4. Analytical Method Selection Considerations

Method selection depends on multiple factors including analytical objectives, data complexity, sample size constraints, and interpretability requirements. Unsupervised methods provide essential exploratory capabilities and data structure assessment, while traditional supervised methods offer reliable performance with good interpretability for established analytical protocols. Machine learning approaches demonstrate superior accuracy for complex discrimination tasks but may sacrifice interpretability for enhanced performance.

The progression from traditional chemometrics to machine learning reflects the field's evolution toward automated, high-accuracy analytical systems. However, method selection should align with specific research objectives and data characteristics rather than following technological trends alone. Optimal analytical strategies often integrate multiple approaches, utilizing unsupervised methods for initial data exploration followed by supervised techniques for specific quantitative or classification objectives.

4. Discussion

4.1. Analytical Advantages and Plant Part Selection

The predominance of leaf analysis (23 studies) in FTIR-Chemometric applications reflects several practical advantages. Leaves offer easy accessibility, rich secondary-metabolite content, and high plasticity in response to environmental influences, making them ideal analytical targets.69 This finding aligns with the principle that sample accessibility and metabolite density are critical for selecting plant parts for chemometric analysis.

The high success rates in species identification and authentication (94-100% accuracy) demonstrate FTIR-Chemometrics' capability to detect subtle genetic and chemical differences. The ability to distinguish even clones of the same variety, as shown in saffron studies,25 indicates exceptional sensitivity to minor genetic variations. This level of discrimination suggests that FTIR captures comprehensive molecular fingerprints that reflect both primary and secondary metabolite profiles.

4.2. Environmental and Geographic Factors

The successful application of FTIR chemometrics in geographic authentication studies highlights the technique's sensitivity to environmental influences on plant chemistry. The varying accuracy rates (77.8-93.9%) across studies suggest that geographic discrimination success depends on the magnitude of environmental differences between locations and on the plant species' responsiveness to these differences.

The strong correlation between FTIR data and environmental parameters, such as the R^2 of 0.8 for predicting root water potential,26 indicates potential applications in plant physiological monitoring and stress detection. This capability positions FTIR-Chemometrics as a valuable tool for understanding plant-environment interactions and optimizing cultivation practices.

4.3. Methodological Evolution and Performance

The observed evolution from traditional chemometric methods to machine learning approaches reflects the growing sophistication in data analysis capabilities.

The progression from PCA and PLS to Random Forest, Genetic Algorithms, and deep learning indicates recognition that the complexity of plant chemical data requires more advanced analytical approaches.

The consistently high performance across different applications suggests that FTIR-Chemometrics has reached sufficient maturity for practical implementation. However, the variation in accuracy rates between studies (77.8-100%) indicates that method optimization remains crucial for specific applications.

4.4. Limitations and Technical Challenges

Despite the high success rates, several limitations warrant consideration. The complexity of plant matrices, with thousands of overlapping metabolites, can limit the specificity of individual compounds. This challenge explains the trend toward integrating FTIR with complementary techniques like HPLC and GC-MS, as demonstrated in several studies.

Model transferability between instruments and laboratories remains a significant challenge, requiring careful standardization protocols. Dependence on representative calibration datasets limits the immediate applicability of the developed models to new populations or geographic regions.

4.5. Future Implications and Research Directions

The demonstrated success across diverse applications suggests broad potential for the expansion of FTIR-Chemometrics. Integrating IoT and cloud technologies could enable real-time quality monitoring systems, while the development of portable FTIRs opens possibilities for field applications.

The increasing use of deep learning approaches indicates the potential to handle more complex spectral patterns that conventional chemometric methods might miss. However, the interpretability of these advanced models may present challenges for regulatory acceptance.

The trend toward multi-technique integration suggests that future applications will likely combine FTIR's rapid screening capabilities with the specificity of other analytical methods, creating comprehensive analytical platforms for plant quality assessment.

5. Conclusion

FTIR chemometric techniques have emerged as powerful analytical tools for plant material analysis (2015-2025), offering rapid, non-destructive, and environmentally friendly methods for species identification, origin authentication, adulteration detection, and quality evaluation.

The evolution from conventional chemometric methods (PCA, PLS) to advanced machine learning algorithms, combined with FTIR variants (ATR-FTIR, DRIFTS, FTIR-PAS), has significantly enhanced analytical capabilities with high accuracy and reproducibility across various plant parts.

Despite challenges including matrix complexity and calibration requirements, future developments in portable instruments, IoT integration, and AI implementation promise expanded applications. FTIR-Chemometrics represents an optimal balance of speed, convenience, reliability, and accuracy for modern plant analysis, positioning it as a key analytical tool for crop research, quality control, and regulatory applications with proper standardization.

Conflict of Interest

The authors declare no conflicts of interest.

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