IDENTIFICATION AND COMPARISON OF FUNCTIONAL GROUPS IN MEDICINAL PLANTS USING ATTENUATED TOTAL REFLECTANCE-FOURIER TRANSFORM INFRARED (ATR-FTIR) SPECTROSCOPY

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Abstract. The biochemical profiles of five chosen medicinal plant leaves in both fresh and shade-dried forms were analyzed using attenuated total reflectance–Fourier transform infrared (ATR-FTIR) spectroscopy. Major functional groups were identified, spectral variations between the medicinal plants were assessed, and the impact of drying on functional groups was analyzed. Samples were scanned in the mid-infrared range (4000–400 cm^{-1}), and spectra were processed using baseline correction, normalization, and averaging among repeats. Prominent absorption bands corresponding to hydroxyl, aliphatic, carbonyl, amide, and carbohydrate functional groups were consistently observed across the analyzed medicinal plants. Fresh samples displayed wide and powerful O–H bands due to greater moisture content, which concealed underlying biomolecular characteristics. Shade-drying considerably decreased water-associated absorptions, increasing the resolution of protein (amide I and amide II), lipid, and polysaccharide bands. The study shows that ATR-FTIR is a quick, non-destructive analytical method that can produce repeatable biochemical fingerprints for therapeutic plants. Furthermore, shade-dried leaves were shown to provide sharper spectral fingerprints than fresh material, indicating their applicability for spectroscopic authentication and phytochemical screening. These findings provide baseline FTIR spectral assignments for the investigated species and show the potential of vibrational spectroscopy for quality control.

Key words: ATR-FTIR, functional groups, medicinal plants, biomolecules, phytochemicals.

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INTRODUCTION

Medicinal plants have long been central to traditional folk medicine, forming a key component of traditional ecological knowledge. For centuries, ancient civilizations have relied on these plants for their therapeutic properties and healing effects, and this knowledge has been preserved and passed down through generations [56]. Medicinal plants continue to play a vital role in the management of numerous diseases, largely due to the diverse secondary metabolites they produce. These metabolites commonly referred to as bioactive compounds are responsible for the plants curative potential and are of significant interest in modern drug discovery [37, 70].

Bioactive compounds exhibit a broad spectrum of pharmacological activities, including antimicrobial, antioxidant, anti-inflammatory, and anticancer effects, making them valuable candidates for therapeutic development [63]. Identifying and characterizing these compounds is essential for understanding the medicinal potential of plant species, as they offer promising avenues for the treatment of chronic, acute, and infectious diseases [23].

Increasing attention has been directed toward medicinal plants that contain exceptionally high levels of antioxidants, phenolics, diterpenoids, and alkaloids. These classes of compounds are widely recognized for their diverse pharmacological properties, particularly their cardiovascular and general health benefits. Several of these plants hold significant potential for human use, either as medicinal resources or as functional foods due to their bioactive profiles [41].

Beyond their direct therapeutic value, many medicinal plants are utilized in a variety of applications. They serve as traditional medicines [52, 55, 72], as sources of animal fodder [7], as natural food additives that delay oxidative processes [15, 35], and as reducing agents in the synthesis of nanomaterials [65]. Their richness in natural antioxidants further enhances their utility across multiple fields, underscoring their importance as versatile biological resources with broad scientific and industrial relevance [4, 5].

Understanding the molecular fingerprint of medicinal plants is essential for identifying the bioactive compounds responsible for their therapeutic effects. These plants contain diverse phytochemicals, many of which can be targeted for the treatment of specific diseases. Therefore, dissecting and characterizing the biochemical signatures of medicinal plants is a critical step in advancing their pharmacological applications [57].

Among the various analytical tools available, Fourier transform infrared (FTIR) spectroscopy is one of the most widely used and powerful techniques for profiling functional groups. FTIR provides valuable insight into the functional groups and chemical constituents present in plant tissues, making it a crucial method for elucidating the biochemical composition of medicinal species [39, 66].

Researchers have utilized FTIR spectroscopy to examine the biomolecular composition of several medicinal plant species, including *Atylosia albicans*, *Tephrosia tinctoria*, *Humboldtia brunonis*, *Kingiodendron pinnatum*, *Derris*

scandens, and *Caesalpinia mimosoides* [69]. These analyses demonstrate that FTIR spectroscopy effectively discriminates and identifies a wide range of functional groups, including C=O, C–H, C=C, C–O, and C–C vibrations. These spectral features correspond to key biochemical constituents such as alkyl and methyl groups, alcohols, ethers, esters, carboxylic acids, anhydrides, and carbohydrate-related moieties such as deoxyribose. Such assignments are consistent with established infrared absorption characteristics of plant biomolecules. Furthermore, the FTIR results revealed clear variations in functional group distribution among the taxa investigated, indicating compositional heterogeneity. Notably, the relative spectral contributions of major biomolecular groups varied across the different plant parts analysed, reflecting tissue-specific biochemical organization and metabolic specialization [34, 38].

In this context, we aimed to characterize and compare the functional groups present in five medicinal plant leaves such as guava (*Psidium guajava*), amla (*Phyllanthus emblica*), papaya (*Carica papaya*), neem (*Azadirachta indica*), and ashanti blood (*Mussaenda erythrophylla*) before and after drying using ATR-FTIR spectroscopy.

MATERIALS AND METHODS

COLLECTION AND IDENTIFICATION OF PLANT MATERIAL

Leaves from five medicinal plants: guava (*Psidium guajava*), amla (*Phyllanthus emblica*), papaya (*Carica papaya*), neem (*Azadirachta indica*), and Ashanti blood (*Mussaenda erythrophylla)* were collected from the Herbal Garden of JSS College of Pharmacy, Mysuru District, Karnataka, India. Fresh, healthy leaves were excised, cleaned thoroughly, and powdered using a sterile pestle and mortar.

PREPARATION OF PLANT MATERIAL POWDER

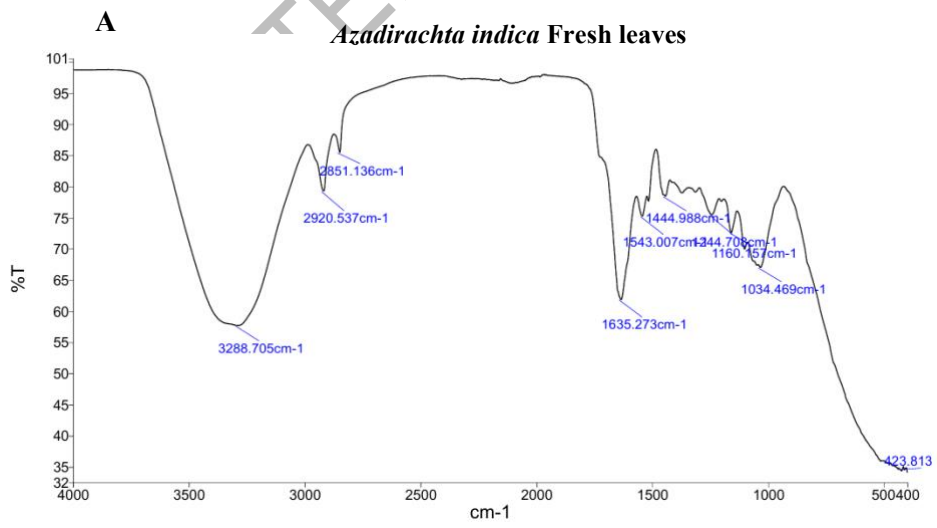
To compare the functional group profiles of fresh and dried samples, the collected leaves were divided into two sets. Fresh leaves were powdered immediately after cleaning. For dried samples, leaves were shade dried at room temperature in a clean environment for seven days to prevent contamination, and then finely powdered using a pestle and mortar. All powdered samples were stored in airtight containers and analysed immediately using ATR-FTIR to avoid moisture interference.

SPECTROSCOPIC ANALYSIS

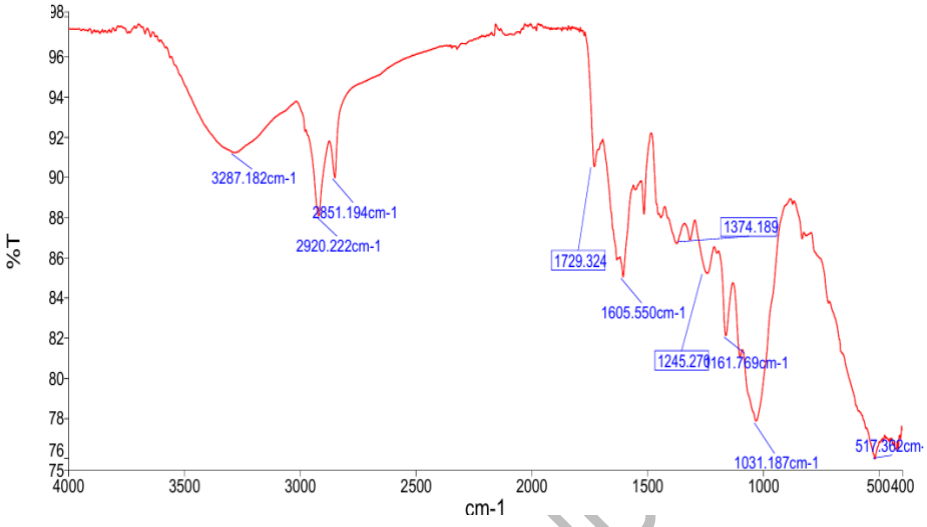
ATR-FTIR spectra were recorded using a PerkinElmer Spectrum Two™ (Shelton, CT, USA) spectrometer. Both fresh and shade-dried powdered samples were scanned at room temperature (25±2 °C) over a spectral range of 4000–400 cm^{-1} with 16 scans per sample. To enhance the signal-to-noise ratio, 100 interferograms were averaged at a spectral resolution of ±4 cm^{-1}. Background spectra, obtained under identical conditions, were automatically subtracted from the sample spectra. Each sample was analysed in five replicate powder preparations, with careful attention to consistency in powdering. This standardized approach improved spectral reproducibility and enabled reliable relative comparisons of absorption band intensities associated with major functional groups across samples [37].

RESULTS AND DISCUSSION

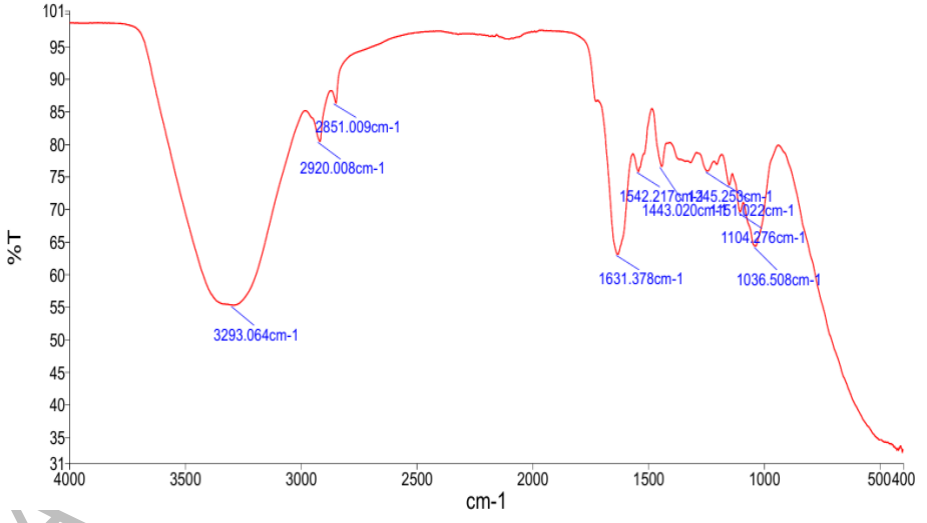
The basic tenet of FT-IR relies on vibration of chemical bonds in the IR region. In this study, ATR-FTIR profiling of both fresh and dried leaves from 5 different medicinal plants was performed to compare the changes before and after drying at the functional groups level. All the samples were scanned across the 400–4000 cm^{-1} spectral range [44]. The representative ATR-FTIR spectra of leaves from five medicinal plants guava (*Psidium guajava*), amla (*Phyllanthus emblica*), papaya (*Carica papaya*), neem (*Azadirachta indica*), and Ashanti blood (*Mussaenda erythrophylla*) are shown in Figure 1. Spectra are analysed in the most informative region 1800–600 cm^{-1} and 3000–2500 cm^{-1} [16].



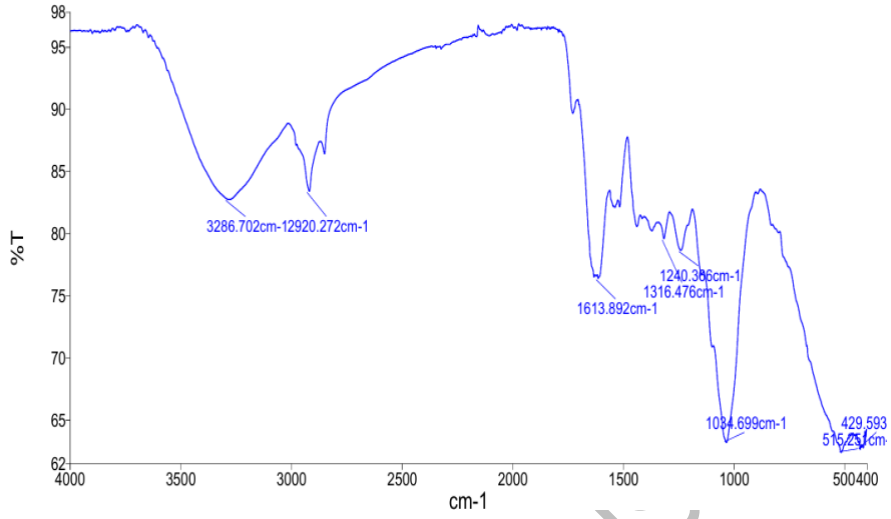
B ***Azadirachta indica* Dried leaves**



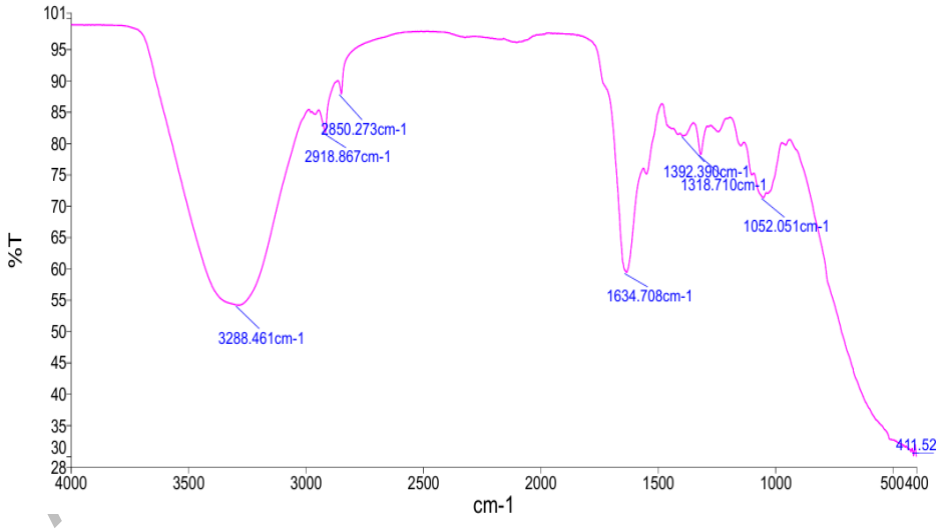
C ***Phyllanthus emblica* Fresh leaves**



D ***Phyllanthus emblica*** **Dried leaves**



E ***Carica papaya*** **Fresh leaves**



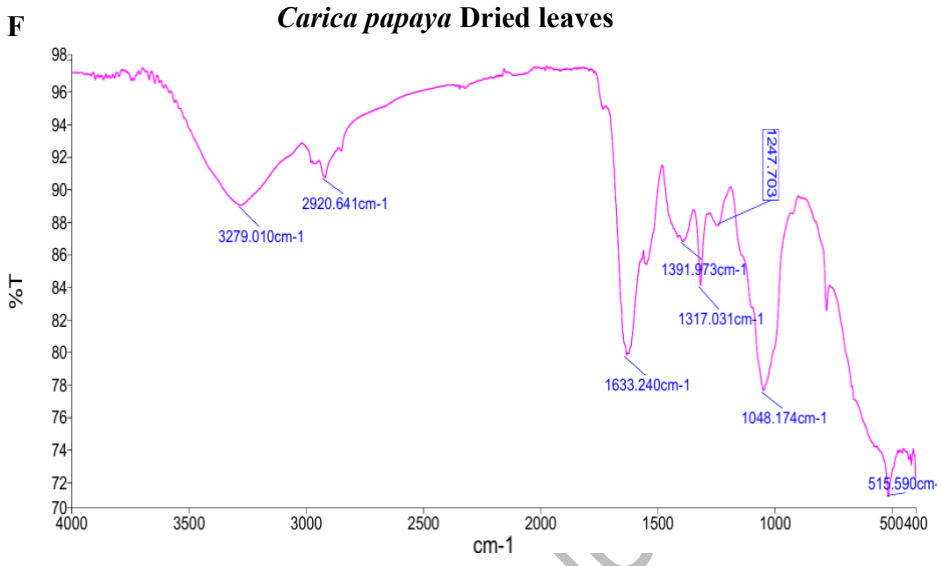
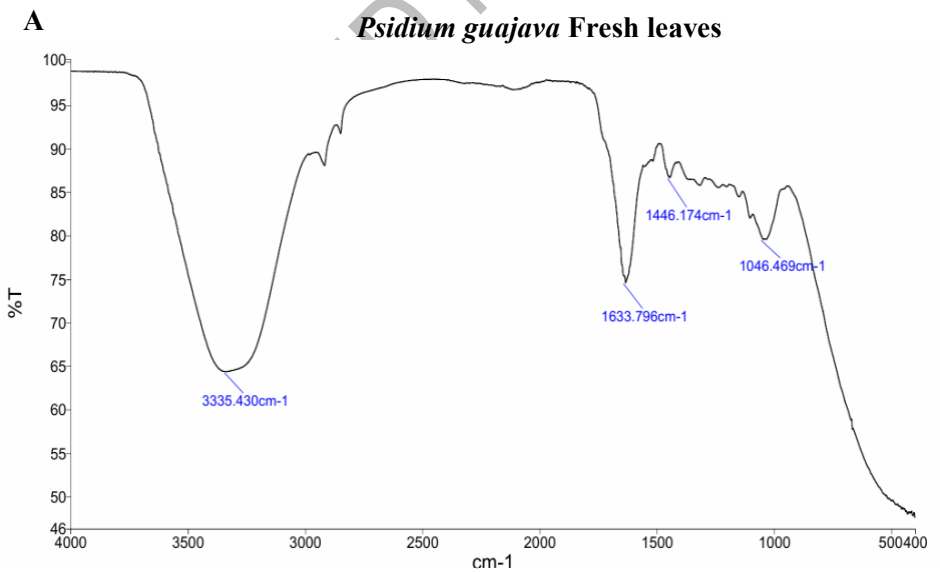
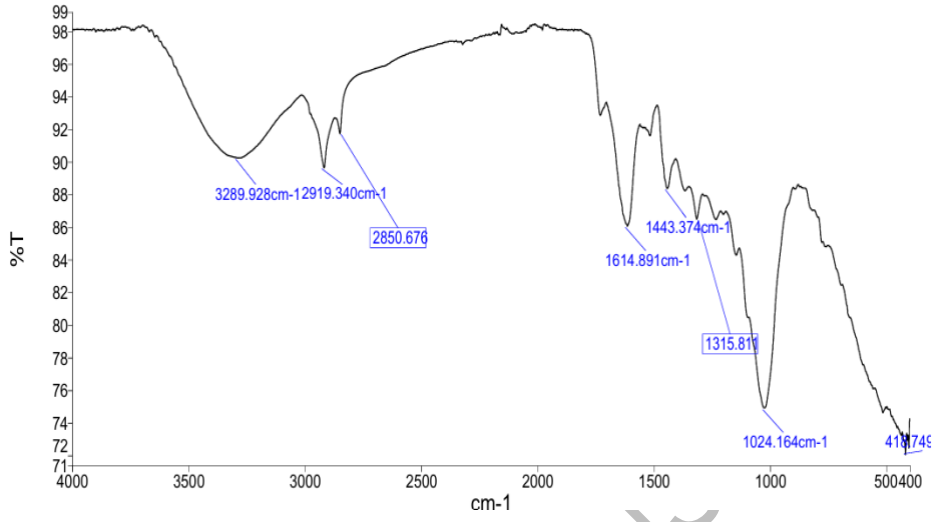


Fig. 1. ATR-FTIR spectra of fresh and dried leaves of *Azadirachta indica*, *Phyllanthus emblica*, and *Carica papaya* (A–F). Spectra were recorded across the 4000–400 cm^{-1} range, and comparative analysis highlights distinct differences in functional group profiles between fresh and dried samples.

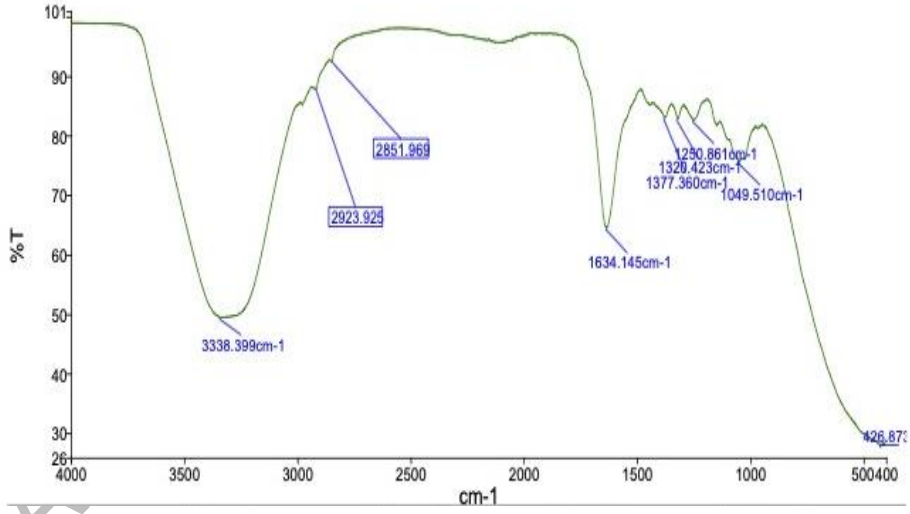


B

***Psidium guajava* Dried leaves**



C ***Mussaenda erythrophylla* Fresh leaves**



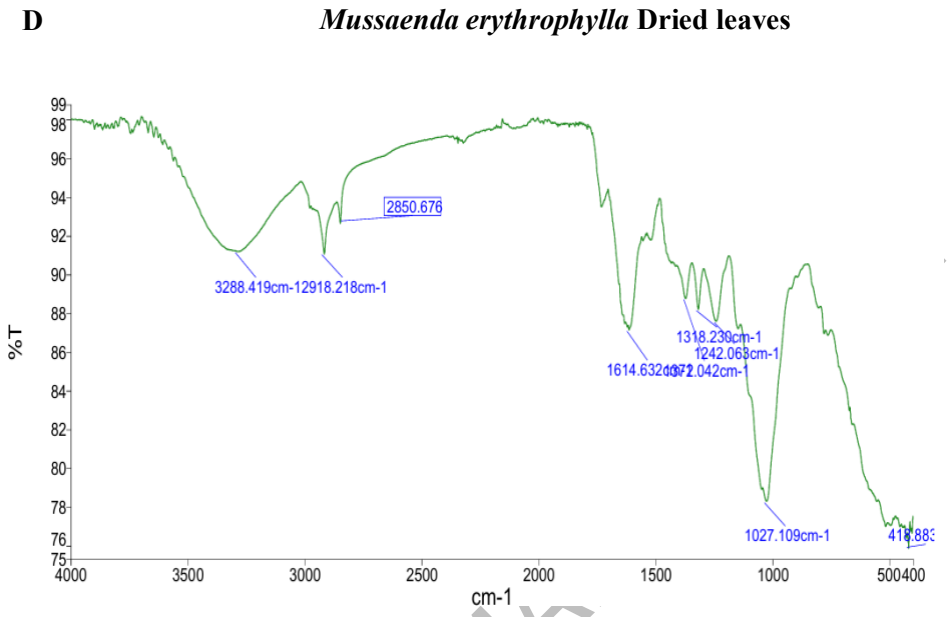


Fig. 2. ATR-FTIR spectra of fresh and dried leaves of *Psidium guajava* and *Mussaenda erythrophylla* (A–D). Spectra were recorded across the 4000–400 cm^{-1} range, and comparative analysis shows clear differences in the functional group profiles between fresh and dried samples.

The FTIR spectra of fresh leaves exhibited a dominant broad absorption band in the 3000–3500 cm^{-1} region, attributable to O–H stretching vibrations associated with water content. Upon drying, the intensity of this band decreased markedly, indicating substantial moisture loss from the leaf tissues. In contrast, the major absorption features observed in all plant species examined: *Psidium guajava* (guava), *Phyllanthus emblica* (amla), *Mussaenda erythrophylla* (ashanti blood), *Azadirachta indica* (neem), and *Carica papaya* (papaya), were largely conserved.

Prominent peaks in the 3000–2800 cm^{-1} region correspond to C–H stretching vibrations of aliphatic chains, characteristic of lipid constituents. The absorption bands observed in the 1650–1500 cm^{-1} region are assigned to aromatic C=C stretching and protein-related amide vibrations, including Amide I (C=O stretching) and Amide II (N–H bending), reflecting the protein content of the leaves. Additionally, strong absorptions in the 1300–1000 cm^{-1} region are attributed to C–O and C–O–C stretching vibrations, indicative of carbohydrate components. Notably, peaks in the 1000–1100 cm^{-1} range, associated primarily with C–O–C stretching of polysaccharides such as cellulose, became more intense after drying,

suggesting an enhanced relative contribution of structural carbohydrates following water removal [8, 67].

The region between 1500 and 600 cm^{-1} represents the fingerprint region in the spectra of plant leaves, encompassing complex vibrational modes unique to the functional groups of the samples. Overall, the spectral profiles of leaves from all investigated plant species were highly similar, although minor variations in peak intensities were observed, likely reflecting differences in relative biomolecular composition rather than qualitative differences in functional groups [3, 30].

Among the plants examined, aromatic C=C / Amide I, associated to flavonoids, phenolics, proteins, are highest in the Ashanti blood plant, followed by guava, neem, papaya, and amla. Similarly, the 1000–1050 cm^{-1} region is strongly associated with polysaccharides (C–O, C–O–C stretching), especially cellulose and hemicellulose showed stronger signals in neem, papaya, ashanthi blood, guava, and amla. These differences highlight the biochemical diversity and variation in molecular composition in the studied plants. The peaks between 2900-2800 cm^{-1} corresponds to aliphatic CH_2 and CH_3 stretching vibrations, mainly from lipids, waxes, and aliphatic chains [31].

In addition to intensity changes, minor peak shifts observed after drying particularly in the O–H and amide regions indicate alterations in hydrogen bonding environments due to moisture removal and enhanced intermolecular interactions among biomolecules. Weak bands appearing around 1740–1720 cm^{-1} in some dried samples correspond to ester C=O stretching, suggesting increased spectral contribution from lipids, waxes, or cuticular components following drying. As ATR-FTIR primarily probes surface chemistry, drying may also expose cellulose-rich cell wall structures, contributing to enhanced carbohydrate signals. Overall, the preservation of spectral fingerprints confirms that drying maintains the fundamental chemical integrity of the leaves, supporting ATR-FTIR as a rapid, non-destructive tool for assessing post-harvest effects in medicinal plants [47].

Table 1

The table presents the ATR-FTIR spectral regions and their corresponding functional groups in plants

Peak region (cm^{-1})	**Functional group**	**Phytochemicals indicated**	**Reference**
3600–3200	O–H stretching	Water, phenols, polyphenols, flavonoids, tannins	[42]
3300–3200	N–H stretching	Alkaloids, amino compounds	[13]
3000–2800	Aliphatic C–H stretching	Terpenoids, fatty acids, lipids	[49]
1760–1680	C=O stretching	Organic acids, esters, flavonoids	[69]

1650–1600	Aromatic C=C / amide I	Flavonoids, phenolics, proteins	[27]
1580–1500	Amide II (N–H bending)	Protein components	[59]
1500–1450	Aromatic C=C	Flavonoids, tannins	[54]
1450–1370	CH_2 / CH_3 bending	Terpenoids, lipids	[32]
1350–1300	C–N stretching	Alkaloids, proteins	[20]
1300–1000	C–O and C–O–C stretching	Phenols, flavonoids, carbohydrates	[24]
1100–1000	Glycosidic C–O–C	Polysaccharides	[45]
900–690	Aromatic C–H out-of-plane	Aromatic phenolics, flavonoids	[30]
600–400	Fingerprint region	Mixed phytochemicals	[64]

Table 2

Identified peaks and functional groups of the studied plant samples

Plant name	Peak (cm^{-1})	Functional group assignment	Reference
Ashanti blood (Fresh)	3338	O–H / N–H stretching	[26]
Ashanti blood (Fresh)	2924	C–H stretching	[19]
Ashanti blood (Fresh)	1634	Amide I / C=C aromatic	[20]
Ashanti blood (Fresh)	1377	CH_2 bending	[48]
Ashanti blood (Fresh)	1049	C–O stretching	[71]
Ashanti blood (Dried)	3288	O–H stretching	[68]
Ashanti blood (Dried)	2918	C–H stretching	[47]
Ashanti blood (Dried)	1615	Amide I / aromatic C=C	[61]
Ashanti blood (Dried)	1318	C–N stretching	[12]
Ashanti blood (Dried)	1027	C–O stretching	[40]
Neem (Fresh)	3289	O–H stretching	[45]
Neem (Fresh)	2921	C–H stretching	[29]
Neem (Fresh)	1635	Amide I	[53]
Neem (Fresh)	1543	Amide II	[49]
Neem (Fresh)	1034	C–O stretching	[51]
Neem (Dried)	3287	O–H stretching	[2]
Neem (Dried)	2920	C–H stretching	[11]
Neem (Dried)	1606	Aromatic C=C	[18]
Neem (Dried)	1245	C–O stretching	[74]
Amla (Fresh)	3293	O–H stretching	[10]
Amla (Fresh)	2920	C–H stretching	[25]
Amla (Fresh)	1631	Amide I	[46]
Amla (Fresh)	1443	CH_2 bending	[62]
Amla (Dried)	1037	C–O stretching	[6]
Amla (Dried)	3287	O–H stretching	[9]
Amla (Dried)	1632	Amide I	[28]
Amla (Dried)	1240	C–O stretching	[74]
Guava (Fresh)	3335	O–H stretching	[60]
Guava (Fresh)	2918	C–H stretching	[58]
Guava (Fresh)	1634	Aromatic C=C	[17]
Guava (Fresh)	1046	C–O stretching	[14]
Guava (Dried)	3289	O–H stretching	[33]
Guava (Dried)	2919	C–H stretching	[22]
Guava (Dried)	1615	Aromatic C=C	[17]
Guava (Dried)	1024	C–O stretching	[3]
Papaya (Fresh)	3288	O–H stretching	[12]
Papaya (Fresh)	2919	C–H stretching	[50]
Papaya (Fresh)	1635	Amide I	[1]
Papaya (Fresh)	1052	C–O stretching	[46]
Papaya (Dried)	3279	O–H stretching	[21]

Papaya (Dried)	2921	C–H stretching	[61]
Papaya (Dried)	1633	Amide I	[30]
Papaya (Dried)	1048	C–O stretching	[22]

CONCLUSION

This study employed ATR-FTIR spectroscopy to characterize and compare the functional group composition of fresh and dried leaves of five plants. The results demonstrate that drying substantially improves spectral clarity and reproducibility by reducing interference from water-associated O–H vibrations. Dried leaf samples consistently exhibited sharper and better-resolved absorption bands, enabling more reliable identification and comparative assessment of key biomolecular constituents such as proteins, lipids, carbohydrates, and phenolic compounds. Although the overall functional group profiles were preserved after drying, variations in band intensities reflected differences in relative biomolecular abundance rather than qualitative chemical changes. The full spectral range of 4000–400 cm^{-1} provided comprehensive molecular fingerprints that allowed effective discrimination among plant species based on their biochemical composition. These findings support the use of dried leaf material as a preferred sample form for FTIR-based phytochemical investigations and highlight ATR-FTIR spectroscopy as a rapid, non-destructive tool for plant biochemical characterization and quality assessment.

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Declaration of generative AI and AI-assisted technologies in the writing process. During the preparation of this work there wasn't any use of AI tools.

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