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(RESEARCH ARTICLE)

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Functional group profiling of medicinal plants using FTIR spectroscopy

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Abstract

The chemical diversity of plants underpins their extensive use in medicine, cosmetics, and industry. This study utilizes Fourier Transform Infrared (FTIR) spectroscopy to identify and characterize the functional groups present in five medicinal plants: *Curcuma longa* (turmeric), *Mentha piperita* (peppermint), *Aegiceras corniculatum* (mangrove), *Zingiber officinale* (ginger), and *Piper nigrum* (black pepper). FTIR spectroscopy is a non-destructive, rapid technique that identifies molecular vibrations associated with functional groups such as O-H, C-H, C=O, and N-H, facilitating the characterization of both organic and inorganic compounds. The plants analyzed are known for their therapeutic properties, including antioxidant, antimicrobial, anti-inflammatory, and anticancer effects. The FTIR spectra revealed the presence of various functional groups, including hydroxyl, carbonyl, aliphatic C-H, and aromatic groups. The fingerprint region (600–1500 cm^{-1}) exhibited complex absorption bands specific to each plant, reflecting the molecular structure and chemical composition of their bioactive compounds. Unique spectral features such as metal-ligand vibrations in *Aegiceras corniculatum* highlight the diverse phytochemical profile of this plants. This study underscores the potential of FTIR spectroscopy in identifying bioactive compounds, facilitating their applications in pharmaceutical and nutraceutical development, and contributing to the growing database of FTIR spectral signatures for medicinal plants.

Keywords: FTIR spectroscopy; Functional groups; Medicinal plants; Bioactive compounds

1. Introduction

Plants are a rich source of bioactive compounds, which are widely utilized in medicine, cosmetics, and industry. The identification of functional groups in plant extracts provides insight into their bioactive compounds, which play critical roles in therapeutic activities such as antioxidant, antimicrobial, and anti-inflammatory effects (Kumar & Pandey, 2015). Fourier Transform Infrared (FTIR) spectroscopy is a powerful, non-destructive analytical technique that identifies molecular vibrations associated with bonds like O-H, C-H, C=O, and N-H, enabling the characterization of organic and inorganic compounds (Stuart, 2004).

FTIR spectroscopy is particularly useful in plant science for detecting secondary metabolites such as alkaloids, flavonoids, terpenes, and phenols, which are responsible for plants' pharmacological properties (Coates, 2000). For instance, phenolic compounds exhibit strong hydroxyl (O-H) stretching bands, while carbonyl (C=O) stretching is characteristic of esters, aldehydes, and ketones (Smith, 2011). By analyzing the FTIR spectra of plants, researchers can obtain a molecular fingerprint of their chemical composition, facilitating the identification of functional groups that contribute to its biological activities (Selvaraju *et al.,* 2021).

The plants analyzed in this study—*Curcuma longa, Mentha piperita, Aegiceras corniculatum, Zingiber officinale,* and *Piper nigrum*—are known for their medicinal properties. For example, *Curcuma longa* (turmeric) contains curcuminoids, known for their anti-inflammatory and antioxidant activities (Aggarwal *et al.,* 2007). *Mentha piperita* (peppermint) is

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rich in essential oils with antimicrobial and carminative properties (McKay & Blumberg, 2006). *Aegiceras corniculatum* is a mangrove plant with phytochemicals showing anti-inflammatory and antifungal properties (Bandaranayake, 2002). *Zingiber officinale* (ginger) is widely used in traditional medicine for its anti-nausea, anti-inflammatory, and anticancer properties (Ali *et al*., 2008). Lastly, *Piper nigrum* (black pepper) contains piperine, which has antioxidant, anti-inflammatory, and bioavailability-enhancing properties (Srinivasan, 2009).

This study employs FTIR spectroscopy to systematically analyze the functional groups present in these plants. By correlating FTIR peaks to functional groups, the research highlights their chemical diversity and potential applications in pharmaceuticals and nutraceuticals.

2. Materials and Methods

2.1. Plant Materials

Plant materials were collected from Ratnagiri, a coastal city located at 16.9954° N latitude and 73.3120° E longitude in the western part of Maharashtra, India, along the Arabian Sea. The samples included the rhizome of *Zingiber officinale*, leaves of *Curcuma longa, Mentha piperita*, and *Aegiceras corniculatum*, as well as seeds of *Piper nigrum*. After harvesting, the materials were thoroughly washed with water and stored in dry bags. The collected samples were transported to the Department of Zoology laboratory at Gogate Jogalekar College, Ratnagiri, for further processing.

2.2. Sample Preparation

The plant parts were chopped into small pieces and air-dried in the shade within the laboratory premises. Once completely dried, the materials were ground into a fine powder using a grinder. The resulting powder was stored in clean, airtight polythene bags to preserve its quality. For FTIR analysis, 10 mg of the dried powder was mixed with 100 mg of potassium bromide (KBr) to form pellets.

2.3. FTIR Spectroscopy

FTIR spectra were recorded in the range of 500-4000 cm^{-1} using a spectrometer. Transmittance was measured to identify the absorption peaks corresponding to various molecular vibrations.

3. Results and Discussion

The FTIR spectra of the plant samples revealed diverse functional groups associated with their chemical composition. Key results included the identification of hydroxyl (-OH), carbonyl (C=O), aliphatic C-H, and aromatic groups, among others. Each plant sample exhibited unique spectral characteristics that correlate with its phytochemical composition and potential bioactive compounds.

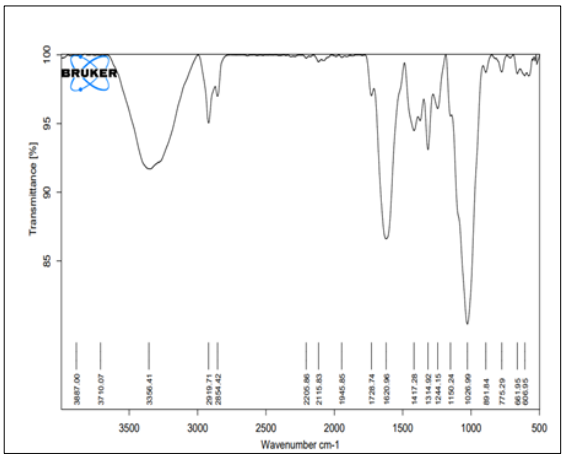

Figure 1 FTIR Spectrum of *Curcuma longa*

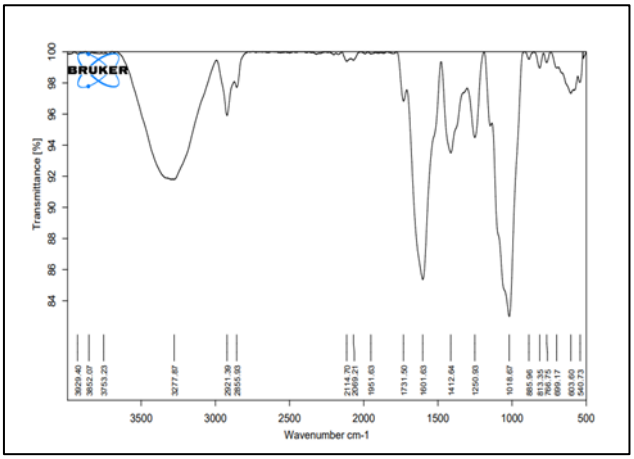

Figure 2 FTIR Spectrum of *Mentha piperita*

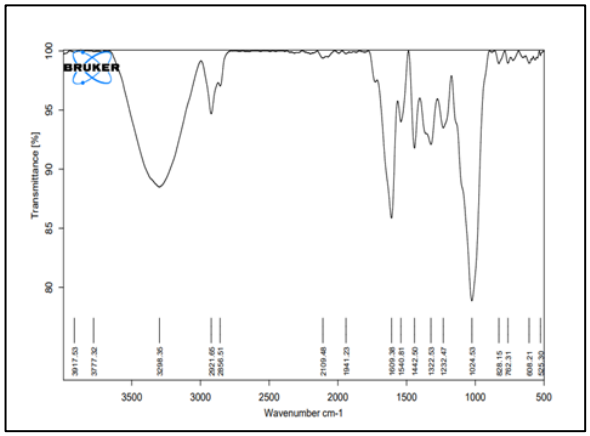

Figure 3 FTIR Spectrum of *Aegiceras corniculatum*

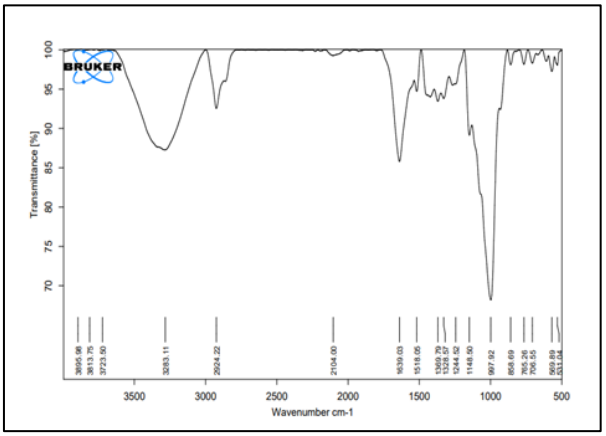

Figure 4 FTIR Spectrum of *Zingiber officinale*

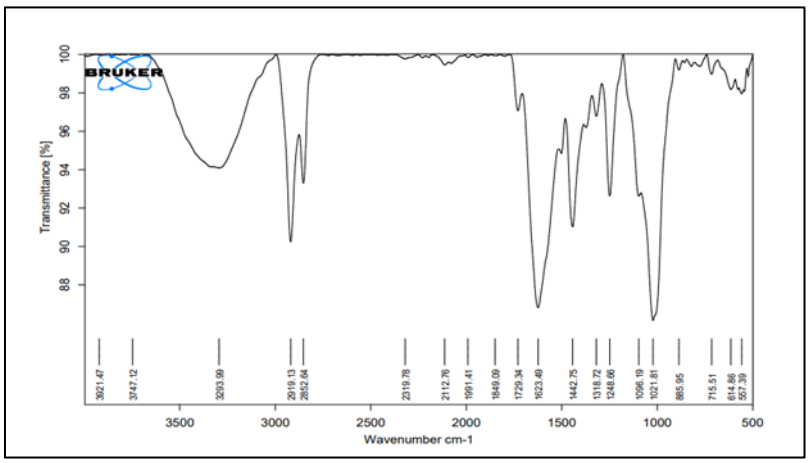

Figure 5 FTIR Spectrum of *Piper nigrum*

Table 1 FTIR Peaks with Functional Group: *Curcuma longa*

Peak (cm^{-1})	**Functional Group**	**Interpretation**
3710.07	Strong O-H stretching (hydroxyl groups)	Presence of alcohols or water
3356.41	O-H stretching	Hydrogen bonding, typical in alcohols or phenols
2919.71	C-H stretching (aliphatic hydrocarbons)	Presence of alkanes or fatty acids
2854.42	C-H stretching (methyl and methylene groups)	Further supports aliphatic compounds
2205.86, 2115.83	C≡C stretching (alkynes) or C≡N stretching (nitriles)	Unsaturated hydrocarbons or nitriles
1945.85	May correspond to C=O stretching in ketones/aldehydes	Potential carbonyl compounds
1728.74	Strong C=O stretching (carbonyl group)	Esters, ketones, or aldehydes
1620.96	C=C stretching (aromatic compounds)	Presence of aromatic rings
1417.28, 1314.92	C-H bending vibrations	Aliphatic or aromatic hydrocarbons
1244.15, 1150.24	C-O stretching (alcohols, ethers, esters)	Alcohols or esters
1026.99	C-O stretching	Further indicates alcohols or ethers
891.84 and below (775.29, 661.95, 606.95, 500)	Out-of-plane bending vibrations	Varies based on sample context

Table 2 FTIR Peaks with Functional Group: *Mentha piperita*

Peak (cm^{-1})	Functional Group	Interpretation
3852.07	O-H stretching (free hydroxyl groups)	Presence of alcohols or phenols
3753.23	O-H stretching (hydrogen-bonded)	Hydrogen-bonded hydroxyl groups, typical in alcohols or carboxylic acids
3277.87	N-H stretching	Presence of amines or amides
2921.39	C-H stretching (aliphatic)	Common in alkanes
2855.93	C-H stretching (aliphatic)	Confirms the presence of aliphatic hydrocarbons
2114.70, 2069.21	C≡C stretching (alkyne)	Suggests the presence of terminal alkynes
1951.63	C=O stretching (carbonyl)	Indicates ketones or aldehydes
1731.50	C=O stretching (ester or carbonyl)	Typical for esters or saturated carbonyl compounds
1601.63	C=C stretching (aromatic)	Presence of aromatic compounds
1412.64	C-H bending (in-plane)	Associated with aliphatic compounds
1250.93	C-O stretching	Common in alcohols, ethers, and esters
1018.67	C-O stretching	Confirms the presence of alcohols or ethers
885.96, 813.35	Out-of-plane C-H bending	Typically associated with aromatic compounds
766.75, 699.17	Out-of-plane C-H bending	Further confirms the presence of aromatic structures
603.60, 540.73	Skeletal vibrations or out-of-plane bending modes	Related to structural features in complex organic compounds

Table 3 FTIR Peaks with Functional Group: *Aegiceras corniculatum*

Peak (cm^{-1})	Functional Group	Interpretation
500	Metal-ligand or skeletal vibrations	Indicates metal-ligand interactions or structural features in organic compounds
800 - 1000	Out-of-plane C-H bending vibrations	Associated with aromatic compounds
1000 - 1300	C-O stretching vibrations	Common in alcohols, ethers, and esters
1400 - 1500	C-H bending vibrations	Typical in aliphatic compounds
1600 - 1700	C=C stretching or C=O stretching	Found in alkenes or carbonyl compounds (ketones, aldehydes)
1700 - 1750	Carbonyl (C=O) stretches	Common in ketones and carboxylic acids
2100	C≡C stretching vibrations	Indicates alkynes
2800 - 3000	C-H stretching vibrations (sp^3, sp^2, or aromatic)	Found in alkanes, alkenes, or aromatic compounds
3200 - 3500	O-H or N-H stretching	Found in alcohols, carboxylic acids, amines, or amides

Table 4 FTIR Peaks with Functional Group: *Zingiber officinale*

Peak (cm^{-1})	Functional Group	Interpretation
Around 3283	O-H stretching	Typical of alcohols or phenols
2924	C-H stretching	Found in alkanes
1639	C=C stretching	Indicates alkenes or aromatic compounds
3813.75, 3723.50	O-H stretching	Suggests the presence of hydroxyl groups in alcohols or phenols
3283.11	N-H stretching	May indicate amino groups, suggesting the presence of amines
2104.00	C≡C stretching	Indicates the presence of alkynes
1639.03, 1518.05	C=C stretching	Suggests double bonds typical of alkenes or aromatic systems
1244.52, 1148.50	C-O stretching	Indicates ether or alcohol functionalities
997.92, 858.69, 765.26, 706.55	C-H bending vibrations	Confirms the presence of aromatic compounds

Table 5 FTIR Peaks with Functional Group: *Piper nigrum*

Peak (cm^{-1})	Functional Group	Interpretation
3747.12	O-H Stretch (Alcohols, Phenols)	Broad peak indicates the presence of hydroxyl groups
3293.99	N-H Stretch (Amines, Amides)	Suggests amine or amide functional groups
2919.13, 2852.64	C-H Stretch (Alkanes)	Symmetric and asymmetric stretching of C-H bonds in aliphatic hydrocarbons
2319.78	C≡C Stretch (Alkynes)	Indicates terminal alkynes
2112.76	C≡N Stretch (Nitriles)	Suggests the presence of nitrile groups
1991.41	C=O Stretch (Carbonyls)	Indicates carbonyl compounds like ketones or aldehydes
1729.34	C=O Stretch (Esters, Lactones)	Strong peak typical of ester or lactone functional groups
1623.49	C=C Stretch (Alkenes)	Suggests double bonds in alkenes
1442.75, 1318.72	CH_2 Bending	Indicative of methylene bending vibrations in aliphatic compounds
1248.66, 1096.19	C-O Stretch (Alcohols, Ethers)	Suggests the presence of alcohols or ethers
1021.81, 885.95	C-O-C Stretch (Ethers)	Characteristic of ether linkages
715.51, 614.86	Out-of-plane C-H Bending	Indicates substituted aromatic rings
557.39, 500	Metal-ligand vibrations or complex interactions	Less commonly associated with organic functional groups

3.1. *Curcuma longa*

The FTIR analysis of *Curcuma longa* identified significant peaks at 3710 cm^{-1} and 1728 cm^{-1}, corresponding to O-H and C=O stretching vibrations, respectively. This is consistent with previous studies, where curcumin, a major bioactive compound in turmeric, was shown to exhibit strong carbonyl and hydroxyl absorption bands (Aggarwal *et al.,* 2007).

Additionally, peaks at 2854 cm^{-1} and 2919 cm^{-1} (C-H stretching) were indicative of aliphatic hydrocarbons, supporting reports of sesquiterpenes in turmeric oil (Jayaprakasha *et al*., 2005).

3.2. *Mentha piperita*

The spectrum of *Mentha piperita* revealed peaks at 3852 cm^{-1} (free O-H stretching) and 3277 cm^{-1} (N-H stretching), indicative of hydroxyl and amino groups. Previous studies (McKay & Blumberg, 2006) also reported similar peaks, attributing them to menthol and menthone, key constituents of peppermint essential oil. Peaks at 1731 cm^{-1} and 1601 cm^{-1} were attributed to C=O and C=C stretching, corroborating the presence of esters and aromatic compounds, which are characteristic of this plant's bioactive profile.

3.3. *Aegiceras corniculatum*

Distinct features of *Aegiceras corniculatum* included significant metal-ligand vibrations at lower wavenumbers (500-1000 cm^{-1}), suggesting the presence of coordination compounds, as reported earlier (Bandaranayake, 2002). The peak at 1600-1700 cm^{-1} was indicative of C=C stretching, aligning with findings of polyphenolic compounds in mangrove plants. The clear C-O stretching peaks at 1000-1300 cm^{-1} suggested the presence of simple alcohols or ethers, consistent with secondary metabolite analysis in mangroves.

3.4. *Zingiber officinale*

The spectrum of *Zingiber officinale* exhibited a peak at 3283 cm^{-1} corresponding to O-H stretching, indicative of alcohols and phenols. Peaks at 2924 cm^{-1} and 1639 cm^{-1} (C-H and C=C stretching) further pointed to the presence of alkanes and aromatic compounds, in agreement with studies highlighting gingerol and shogaol as major constituents (Ali *et al.,* 2008). Additional peaks at 2104 cm^{-1} and 1244 cm^{-1} (C≡C and C-O stretching) indicated alkynes and ethers, which have also been reported in ginger essential oils (Singh, 2008).

3.5. *Piper nigrum*

The FTIR spectrum of *Piper nigrum* revealed strong O-H and N-H stretching vibrations at 3747 cm^{-1} and 3293 cm^{-1}, corresponding to hydroxyl and amino groups. These findings align with the presence of piperine, an alkaloid known for its antioxidant and anti-inflammatory properties (Srinivasan, 2007). Peaks at 2919 cm^{-1} and 1729 cm^{-1} (C-H and C=O stretching) further supported the presence of aliphatic hydrocarbons and carbonyl groups, consistent with earlier studies (Ravindran *et al.,* 2000).

The results demonstrated significant overlap with existing literature, confirming the validity of the FTIR analysis. The presence of hydroxyl group was almost common feature across all samples, highlighting their potential as antioxidants or reactive intermediates in biochemical pathways.

The fingerprint region was observed to span the wavenumber range between 600 cm^{-1} and 1500 cm^{-1} in all plant samples. This region is distinct for each molecule, providing a unique "fingerprint" that aids in the identification of specific compounds. Unlike the functional group region (above 1500 cm^{-1}), the fingerprint region exhibited a complex array of absorption bands, which arise from various bending, stretching, and vibrational modes of the atoms within the molecule. The peaks in this region are influenced by the overall molecular structure, including the arrangement of atoms and bonds, contributing to the characteristic pattern observed in the FTIR spectrum.

4. Conclusion

FTIR spectroscopy demonstrated its effectiveness in identifying diverse functional groups within the analyzed plant samples. Notable differences in spectral features were observed among the samples, such as unique metal-ligand vibrations in *Aegiceras corniculatum*. The unique "fingerprint" for each molecule was also noted in all plant samples. These findings provide insights into the chemical composition of the plants, which could inform their potential applications in pharmaceuticals and nutraceuticals. Furthermore, these findings contribute to the growing database of FTIR spectral signatures for medicinal plants, aiding in rapid screening and quality control of phytochemicals.

Compliance with ethical standards

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Disclosure of conflict of interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

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