JOURNAL OF LIFE SCIENCE AND ENVIRONMENTAL PROTECTION
https://www.worldlinkpub.com/journals/journal-of-life-science-and-environmental-protecti/

ISSN: 3141-5989

GC–MS AND FTIR PROFILING OF SELECTED NIGERIAN BOTANICALS WITH POTENTIAL BIOACTIVE PROPERTIES

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Received: 24 May 2026
Accepted for publication: 20 June 2026
Published: 01 July 2026

ABSTRACT

The search for environmentally friendly alternatives to synthetic fungicides has increased interest in plant-derived bioactive compounds with potential antifungal applications. This study characterized the phytochemical constituents, functional groups, and physicochemical properties of oils extracted from lemon peels (*Citrus limon*), banana peels (*Musa* spp.), turmeric rhizomes (*Curcuma longa*), neem leaves (*Azadirachta indica*), and lemongrass (*Cymbopogon citratus)*. Plant materials were collected, air-dried, pulverized, and subjected to hydrodistillation using a Clevenger-type apparatus. The extracted oils were analysed using Gas Chromatography–Mass Spectrometry (GC–MS), Fourier Transform Infrared (FTIR) spectroscopy, and physicochemical characterization techniques. GC–MS analysis revealed diverse phytochemical constituents including n-hexadecanoic acid, cis-vaccenic acid, phytol, turmerone, curlone, β-sitosterol, pentadecanoic acid, and other bioactive compounds. Lemon peel extract contained notable levels of n-hexadecanoic acid (17.27%) and 9,12,15-octadecatrienoic acid (15.66%), while banana peel extract was dominated by cis-vaccenic acid (25.35%) and n-hexadecanoic acid (23.30%). Turmeric rhizome extract was characterized by high concentrations of turmerone (29.93%) and curlone (12.28%). FTIR analysis confirmed the presence of hydroxyl (O–H), carbonyl (C=O), aliphatic (C–H), alkene (C=C), and ether (C–O) functional groups associated with phenolics, fatty acids, terpenoids, alcohols, and related phytochemicals. Physicochemical analyses revealed variations in saponification, acid, peroxide, iodine, and viscosity values among the extracts. The findings demonstrate the phytochemical richness and chemical diversity of the investigated botanicals and provide scientific evidence supporting their potential as natural sources of bioactive compounds for food preservation, postharvest protection, and sustainable fungal management.

Keywords: Antifungal activity, Botanical extracts, FTIR spectroscopy, GC–MS analysis, Phytochemical characterization, Sustainable fungal management.

1.0 INTRODUCTION

Fungal contamination remains a major challenge affecting food quality, food safety, agricultural productivity, and public health worldwide. Many fungal species are capable of colonizing agricultural commodities during cultivation, harvest, processing, transportation, and storage, resulting in deterioration of food products and significant economic losses. Among these fungi, *Aspergillus flavus* is particularly important because of its ability to produce aflatoxins, a group of highly toxic secondary metabolites associated with hepatotoxicity, immunosuppression, mutagenicity, carcinogenicity, and reduced livestock productivity (Amaike and Keller, 2011; Abbas *et al*., 2011). The widespread occurrence of aflatoxin-producing fungi in food and feed systems continues to pose serious challenges to food security and public health, particularly in tropical and subtropical regions where environmental conditions favour fungal growth and toxin production (Atehnkeng *et al*., 2008; Kumar *et al*., 2021).

The management of fungal pathogens has traditionally relied on synthetic fungicides and chemical preservatives. Although these agents have contributed significantly to disease control and postharvest preservation, their prolonged use has raised concerns regarding environmental pollution, chemical residues, toxicity to non-target organisms, and the emergence of resistant fungal strains (Tripathi and Dubey, 2004; Kim *et al*., 2017). Growing awareness of these limitations has

Cite this article: Ilebode-Sam, M.O., Oluma, H.O.A., Ogbonna, I.O. and Ilebode-Sam, B.I. (2026). GC–MS and FTIR profiling of selected Nigerian botanicals with potential bioactive properties. Journal of Life Science and Environmental Protection, 1(1): 83-88

stimulated research into safer, eco-friendly, and sustainable alternatives for fungal control. Recent studies have further highlighted the potential of essential oils as natural antifungal agents for the protection of organic materials and agricultural products (Taha *et al.*, 2024). Consequently, plant-derived products have attracted considerable scientific interest as potential sources of natural antifungal compounds with reduced environmental impact (Bakkali *et al.*, 2008; Hyldgaard *et al.*, 2012; Gonçalves *et al.*, 2025).

Plants synthesize a wide range of secondary metabolites that contribute to their defense against microbial attack and environmental stress. These bioactive compounds include terpenoids, phenolics, flavonoids, alkaloids, saponins, tannins, fatty acids, and various volatile organic compounds that have been reported to possess antimicrobial, antioxidant, anti-inflammatory, and antifungal activities (Prasad and Aggarwal, 2011; Ravindran *et al*., 2007). Numerous studies have demonstrated that plant extracts and essential oils can inhibit fungal growth through multiple mechanisms, including disruption of cell membrane integrity, inhibition of spore germination, interference with cellular metabolism, and induction of oxidative stress within fungal cells (Burt, 2004; Hyldgaard *et al*., 2012; Sawadogo *et al*., 2022).

Among the botanicals commonly investigated for antimicrobial applications are turmeric (*Curcuma longa*), neem (*Azadirachta indica*), lemongrass (*Cymbopogon citratus*), lemon peel (*Citrus limon*), and banana peel (*Musa* spp.). These plant materials contain diverse phytochemical constituents that have been associated with broad-spectrum biological activities, including antifungal effects against several economically important fungal pathogens (Prasad and Aggarwal, 2011; Ravindran *et al*., 2007; Freitas and Cattelan, 2018). In addition to their medicinal significance, some of these materials, particularly fruit peels, represent agricultural by-products whose valorization may contribute to sustainable waste management and the development of natural bioactive products.

The biological activity of plant extracts is largely influenced by their phytochemical composition and the functional groups present within their constituent compounds. Therefore, characterization of these constituents is essential for understanding the mechanisms underlying their antimicrobial and antifungal properties. Modern analytical techniques such as Gas Chromatography–Mass Spectrometry (GC–MS) and Fourier Transform Infrared (FTIR) spectroscopy have become valuable tools for the identification of phytochemical constituents and functional groups in plant-derived extracts. GC–MS enables the separation and tentative identification of volatile and semi-volatile compounds, while FTIR spectroscopy provides information on the major functional groups associated with biological activity (Silverstein *et al*., 2014; Singh *et al*., 2022). The combined application of these techniques provides a more comprehensive understanding of the chemical constituents responsible for the observed biological effects of botanical extracts.

Despite the increasing interest in plant-derived antifungal agents, comparative information on the phytochemical composition, functional-group profiles, and physicochemical characteristics of oils obtained from selected botanicals remains limited. Furthermore, establishing relationships between phytochemical constituents and reported biological activities is important for supporting the development of natural products for food preservation, postharvest protection, and environmentally sustainable fungal management strategies (Gonçalves *et al*., 2025). This knowledge gap necessitates further characterization of botanically derived oils using complementary analytical approaches. Improved understanding of their chemical composition and functional-group profiles may provide valuable insights into the biological activities associated with these botanicals and support their potential application in sustainable antifungal management strategies.

Therefore, this study aimed to determine the physicochemical properties, phytochemical constituents and functional-group profiles of selected botanical oils using GC-MS and FTIR analyses and to relate the identified compounds to their reported biological and antifungal activities.

2.0 MATERIALS AND METHODS

2.1 Study Area

The study was conducted in Makurdi, Benue State, Nigeria. Plant materials used in the study were obtained from local markets within Makurdi and processed at the Department of Biological Sciences Laboratory, Joseph Sarwuan Tarka University, Makurdi.

2.2 Sample Collection

Fresh lemon fruits (*Citrus limon*), turmeric rhizomes (*Curcuma longa*), neem leaves (*Azadirachta indica*), banana peels (*Musa* spp.) and lemongrass (*Cymbopogon citratus*) were obtained from local markets and farms in Makurdi, Benue State, Nigeria.

2.3 Sample Identification

The collected plant materials were identified and authenticated in the Department of Plant Science and Biotechnology, College of Biological Sciences, Joseph Sarwuan Tarka University, Makurdi.

2.4 Sample Preparation

The collected plant materials were washed thoroughly with clean water to remove adhering dirt and impurities and were subsequently air-dried at room temperature for approximately two weeks. The dried samples were separately ground into fine powder using a clean mortar and pestle and stored in airtight containers until extraction. The preparation procedure was carried out following standard methods for botanical sample processing (Karne *et al*., 2023).

2.5 Experimental Design

The study employed a laboratory-based experimental design involving extraction of oils from five selected botanicals followed by physicochemical characterization, GC–MS analysis and FTIR spectroscopy.

2.6 Data Collection

Botanical oils were extracted from the prepared plant materials by hydrodistillation using a Clevenger-type apparatus following the method of Karne *et al*. (2023) with slight modifications. The extracted oils were collected in sterile vials and stored until analysis.

Gas Chromatography–Mass Spectrometry (GC–MS) analysis was conducted to determine the phytochemical constituents of the extracted oils. Compound identification was achieved by comparing retention times and mass spectra with standard library databases, while relative abundance was estimated from percentage peak areas obtained from the chromatograms (Singh *et al*., 2022).

Fourier Transform Infrared (FTIR) spectroscopy was employed to identify the major functional groups present in the extracted oils. Functional groups were assigned based on characteristic absorption bands and standard reference spectra (Silverstein *et al*., 2014).

Physicochemical properties including acid value, peroxide value, iodine value, saponification value and viscosity were determined using standard analytical procedures for essential oil characterization (Popa *et al*., 2015).

2.7 Data Analysis

GC–MS data were expressed as percentage peak areas of identified compounds, while FTIR spectra were interpreted based on characteristic absorption bands and corresponding functional groups reported in the literature (Silverstein *et al*., 2014). Physicochemical properties were summarized using descriptive statistics and presented in tables and figures.

3.0 RESULTS

3.1 GC–MS Profiles of the Extracted Oils

GC–MS analysis revealed variations in the phytochemical composition of the botanical extracts (Table 1). Lemon peel extract was characterized by relatively high proportions of n-hexadecanoic acid (17.27%) and 9,12,15-octadecatrienoic acid (15.66%), while banana peel extract was dominated by cis-vaccenic acid (25.35%) and n-hexadecanoic acid (23.30%). Turmeric rhizome extract contained predominantly turmerone (29.93%) and curlone (12.28%). Neem leaf extract was overwhelmingly dominated by Bis(2-ethylhexyl) phthalate (92.35%), whereas lemongrass extract contained Bis(2-ethylhexyl) phthalate (18.09%) and n-hexadecanoic acid (13.34%) as the major constituents. The identified compounds comprised fatty acids, terpenoids, sterols, hydrocarbons and related phytochemicals.

Table 1: Major Phytochemical Constituents Identified in Selected Botanical Extracts by GC–MS

Botanical Extract	Major Compounds Identified (Relative Abundance, %)
Lemon peel	n-Hexadecanoic acid (17.27), 9,12,15-Octadecatrienoic acid (15.66), Phytol (8.47), cis-Vaccenic acid (7.14), β-Sitosterol (3.45)
Banana peel	cis-Vaccenic acid (25.35), n-Hexadecanoic acid (23.30), Naphthalene (8.06), Palmitoleic acid (5.86), Octadecanoic acid (4.53)
Turmeric rhizome	Turmerone (29.93), Curlone (12.28), n-Hexadecanoic acid (0.76), cis-Vaccenic acid (0.66), Octadecanoic acid (0.16)
Neem leaf	Bis(2-ethylhexyl) phthalate (92.35), Ar-turmerone (1.04), Cyclopentane, 1-methyl-1-(2-methyl-2-propenyl)- (0.95), n-Hexadecanoic acid (0.59), D:A-Friedoursan-3-one (0.54)
Lemongrass	Bis(2-ethylhexyl) phthalate (18.09), n-Hexadecanoic acid (13.34), N-Methyl-2-(propionylmethylene)pyrrolidine (8.19), Oxazole, 5-hexyl-2,4-dimethyl- (6.69), Pentadecanoic acid (6.37)

Only the five most abundant compounds detected in each extract are presented.

3.2 FTIR Functional Group Analysis

The FTIR spectra of the botanical extracts revealed several characteristic absorption bands corresponding to important phytochemical functional groups (Table 2). Hydroxyl (O–H), aliphatic C–H, carbonyl (C=O), alkene/aromatic (C=C), and C–O functional groups were detected across the extracts. Variations in absorption bands among the botanical oils indicate differences in their chemical compositions; however, the presence of these functional groups confirms the occurrence of diverse phytochemical constituents including phenolics, fatty acids, terpenoids, esters, alcohols, and related oxygenated compounds.

Table 2: Major FTIR Absorption Bands and Functional Groups Identified in Selected Botanical Extracts

Botanical Extract	Major Absorption Bands (cm^{-1})	Functional Groups Identified
Lemon peel	3440, 2918, 2849, 1735, 1597, 1515, 1289–1025	O–H, C–H, C=O, C=C, C–O
Banana peel	3078.8, 2920.4, 2853.3, 1733.2, 1712.7, 1641.9, 1310.2–1039.9	O–H, C–H, C=O, C=C, C–O
Turmeric rhizome	3444, 2924, 2871, 1736, 1626	O–H, C–H, C=O, C=C
Neem leaf	3401, 2918, 2849, 1735, 1031	O–H, C–H, C=O, C–O
Lemongrass	3334, 2916, 2849, 1735, 1641, 1453, 1377, 1056	O–H, C–H, C=O, C=C, C–O

3.3 Physicochemical Properties of the Extracted Oils

The physicochemical properties of the extracted oils are presented in Table 3. Variations were observed among the botanical extracts with respect to saponification, acid, peroxide, iodine, and viscosity values. Turmeric rhizome extract recorded the highest saponification value (323.28 mg/100 g) and peroxide value (109.83 meq/kg), whereas lemon peel extract exhibited the highest viscosity (318.63 mm^2/s cSt). Banana peel extract showed relatively high acid and iodine values, while neem leaf and lemongrass extracts generally recorded lower viscosity and iodine values compared with the other extracts.

Table 3: Physicochemical Properties of the Extracted Oils Obtained from Selected Botanical Materials

Botanical Extract	Saponification value (mg/100 g)	Acid value (KOH/g)	Peroxide value (meq/kg)	Iodine value (g/100 g)	Viscosity (mm^2/s cSt)

Lemon peels	284.71	9.49	102.17	43.26	318.63
Banana peel	201.36	11.17	93.75	43.99	23.34
Turmeric rhizomes	323.28	6.43	109.83	48.72	33.65
Neem leaves	123.69	6.45	77.19	35.18	20.33
Lemongrass	156.83	11.50	81.58	33.16	19.78

Values presented represent analytical measurements obtained from laboratory determinations of the extracted oils.

4.0 DISCUSSION

4.1 Phytochemical Composition of the Botanical Extracts

The present study characterized the phytochemical constituents, functional groups, and physicochemical properties of oils extracted from lemon peels, banana peels, turmeric rhizomes, neem leaves, and lemongrass using GC–MS and FTIR analyses. The findings demonstrated marked variation in chemical composition among the botanical extracts, reflecting differences in their phytochemical profiles and potential biological activities.

GC–MS analysis revealed the presence of diverse classes of compounds including fatty acids, terpenoids, sterols, hydrocarbons, aldehydes, esters, and related phytochemicals. Several of the identified compounds have previously been associated with antimicrobial, antioxidant, and antifungal activities through mechanisms such as disruption of fungal membrane integrity, interference with cellular metabolism, and inhibition of toxin production (Abd Rashed *et al*., 2021; Liang *et al*., 2024). The occurrence and relative abundance of these compounds varied considerably among the botanicals, suggesting differences in metabolic composition and extraction characteristics.

Lemon peel extract was characterized by relatively high proportions of n-hexadecanoic acid, 9,12,15-octadecatrienoic acid, phytol, cis-vaccenic acid, and β-sitosterol. Similar compounds have been reported in citrus-derived extracts and have been associated with antioxidant and antimicrobial properties (Moufida and Marzouk, 2003). Banana peel extract was dominated by cis-vaccenic acid, n-hexadecanoic acid, naphthalene derivatives, and other fatty acid-related compounds, supporting previous reports that banana peels contain bioactive constituents with potential preservative and antimicrobial applications (Adebo *et al*., 2021; Zaini *et al*., 2022).

Turmeric rhizome extract exhibited a distinctive phytochemical profile dominated by turmerone and curlone. These sesquiterpenoids are recognized as characteristic constituents of turmeric and have been widely reported to possess antioxidant, antimicrobial, and anti-inflammatory activities (Li *et al*., 2023; Ferdous *et al*., 2023). The predominance of these compounds confirms the sesquiterpene-rich nature of turmeric rhizomes and supports their biological relevance.

Although neem and lemongrass extracts contained compounds previously associated with biological activity, the chromatographic profiles were notably influenced by the presence of phthalate derivatives, particularly Bis(2-ethylhexyl) phthalate. While phthalate compounds have occasionally been reported from natural sources, their high abundance in certain extracts suggests possible contamination introduced during sample extraction, storage, handling, or instrumental analysis (Net *et al*., 2015; Cheng *et al*., 2019; Javed *et al*., 2022). Consequently, these compounds should be interpreted cautiously when assessing the endogenous phytochemical composition of the investigated botanicals. Nevertheless, minor constituents identified in neem and lemongrass extracts have previously been linked with antimicrobial and antifungal activities (Alzohairy, 2016; García-Díaz *et al*., 2021; Mondall *et al*., 2009).

4.2 Functional Group Characterization by FTIR

The FTIR spectra complemented the GC–MS findings by confirming the presence of important functional groups including hydroxyl (O–H), carbonyl (C=O), aliphatic C–H, alkene/aromatic (C=C), and ether (C–O) groups. These functional groups are commonly associated with phenolics, terpenoids, fatty acids, aldehydes, alcohols, and ester-containing compounds that contribute to the biological activities of plant-derived extracts. Similar FTIR profiles have been reported in phytochemical investigations of botanicals rich in bioactive compounds (Silverstein *et al*., 2014; Singh *et al*., 2022; Yadav *et al*., 2023).

4.3 Physicochemical Properties of the Extracted Oils

The physicochemical properties of the extracts further demonstrated variation among the botanical oils. Differences in saponification, iodine, peroxide, acid, and viscosity values may reflect variations in fatty acid composition, degree of unsaturation, and oxidative stability. The relatively high saponification value observed in turmeric extract suggests the presence of lower molecular weight fatty acid constituents, while iodine values provide an indication of unsaturation within the extracts. Peroxide values are commonly used as indicators of oxidative stability and susceptibility to rancidity during storage (Nounah *et al*., 2021). Such physicochemical characteristics may influence extract stability, preservation potential, and interactions with microbial cell membranes (Freitas and Cattelan, 2018; Abd Rashed *et al*., 2021). Similar variations among plant-derived oils have previously been attributed to differences in fatty acid composition and phytochemical constituents (da Costa *et al*., 2010; Ogunnupebi *et al*., 2020).

4.4 Implications for Antifungal Applications

The utilization of agricultural by-products such as citrus and banana peels as sources of bioactive compounds may additionally support sustainable waste valorization and circular bioeconomy approaches within agro-food systems (Hamam *et al*., 2021).

Overall, the combined GC–MS, FTIR, and physicochemical analyses demonstrated that the investigated botanicals possess chemically diverse phytoconstituents comprising fatty acids, terpenoids, sterols, aldehydes, and related bioactive compounds. These findings provide valuable phytochemical information that may support future investigations into the antifungal, preservative, and industrial applications of plant-derived extracts.

5.0 CONCLUSION

The GC–MS, FTIR, and physicochemical analyses revealed that oils extracted from lemon peels, banana peels, turmeric rhizomes, neem leaves, and lemongrass contain diverse phytochemical constituents and functional groups associated with biological and antifungal relevance. Major compounds identified included fatty acids, terpenoids, sterols, and related phytochemicals, while FTIR analysis confirmed the presence of hydroxyl, carbonyl, aliphatic, alkene, and ether functional groups. These findings provide scientific evidence supporting the potential application of the investigated botanicals as natural sources of bioactive compounds for food preservation, postharvest protection, and environmentally sustainable fungal management.

RECOMMENDATIONS

Further studies should evaluate the antifungal efficacy of the identified phytochemicals against a wider range of fungal pathogens, optimize extraction and characterization procedures, and investigate formulation strategies that could enhance the stability and practical application of these botanical extracts in food preservation and postharvest systems.

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