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FTIR-BASED PROFILING OF FUNCTIONAL GROUPS IN FOUR INDIGENOUS AFRICAN MEDICINAL TREES FOR NATURAL PRODUCT DISCOVERY

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ABSTRACT

The rising global demand for natural and sustainable products has prompted more targeted research on indigenous African medicinal tree species. This research presents the findings of an investigation on extracts from four native medicinal tree species; *Calophyllum inophyllum*, *Cola nitida, Kigelia africana*, and *Pleioceras barteri*. These trees were selected based on their traditional medicinal uses, availability and scanty information on their bioactive compounds. The dataset identified and characterized the bioactive compounds in the plant extracts, providing valuable insights into their potential medicinal and therapeutic properties. The plant extracts were prepared from leaves and stem barks using ethanol as solvent. Attenuated Total Reflectance Fourier-Transform Infrared (ATR-FTIR) spectroscopy was employed to obtain the infrared spectra of the extracts, which provided information about the functional groups present in the molecules. The result of the spectroscopy revealed the presence of major classes of metabolites including alkaloids, terpenoids, phenolic compounds, glycosides, steroids, organic acids and quinones. This dataset provides a valuable resource for researchers studying the medicinal properties of indigenous plants, drug discovery, and natural product chemistry. The information can be utilized to identify potential bioactive compounds, guide further chemical analysis, and inform the development of new natural products.

Keywords: Bioactive compounds; drug discovery, sustainable health; spectroscopy; african tree; medicinal plant

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INTRODUCTION

Africa house a vast variety of indigenous medicinal trees that have been utilized for generations by traditional healers to treat various ailments [1]. These trees contain a richness of bioactive chemicals that have been demonstrated to possess a range of pharmacological characteristics that confers health benefits [2]. Bowen University, located in Iwo, Osun State, Nigeria is wonderfully constructed and naturally endowed with untapped indigenous medicinal tree species of tremendous potentials for food, nutrition, nutraceutical and therapeutic characteristics. Some of the tree species include *Calophyllum inophyllum* L., *Cola nitida* Schott & Endl., *Kigelia africana* (Lam.) Benth., and *Pleoiceras barteri* Baill. These four trees species were selected based on their traditional medicinal uses, availability and scanty information on their bioactive compounds. *Calophyllum inophyllum* is commonly called oil-nut in English, "odogbo" in Yoruba and belongs to the family Calophyllaceae. The leaves, stem barks and seeds of *C. inophyllum* are used to treat skin infections, wounds, and respiratory disorders [3].

Cola nitida is commonly called bitter kola in English, "igi obi" in Yoruba and belongs to the family Malvaceae. The fruit is used as a stimulant, appetite suppressant, and to treat various digestive ailments. The stem barks of *Cola* are used to treat fever, headaches, and body aches while its leaves are known to contain chemicals with antibacterial activity, making them effective for treating infections [4].

Kigelia africana common called the sausage tree in English and "pandoro" in Yoruba language, belongs to the family Bignoniaceae. It is traditionally used as a cure for multiple diseases, such as its use for wounds healing, ulcers, rheumatism, psoriasis, diarrhoea and stomach disorders [5].

Pleioceras barteri is called Barter's pleioceras in English, 'dàgbá ọmọde' in Yoruba language and belongs to the family Apocynaceae. is used to cure fever, malaria, and skin problems [6].

To our knowledge, these tree species have not been properly characterized and investigated based on their chemical compounds to enhance their sustainable utilization as a veritable source of bioactive ingredients.

As research continues to find the bioactive compounds and pharmacological capabilities of these plants, they hold immense promise for the generation of new natural pharmaceuticals. This research identified the functional groups present in the leaves and stem barks of *Calophyllum inophyllum, Cola nitida, Kigelia africana*, and *Pleioceras barteri*, which are African indigenous medicinal tree species using the Attenuated Total Reflectance Fourier-Transform Infrared (ATR-FTIR) spectroscopy.

MATERIALS AND METHODS

Plant Collection: The leaves and stem barks of the four indigenous medicinal tree species *Calophyllum inophyllum, Cola nitida, Kigelia africana*, and *Pleioceras barteri* were collected from the open field of Bowen University, Iwo, Osun State, Nigeria (7.60^{o} N, 4.42^{o} E). The leaves and stem barks were spread on the laboratory benches and air-dried at room temperature (28°C - 30°C) for 14 days and 28 days respectively. The dried leaves and stem bark samples were separately milled into powdered forms using a commercial milling machine. The samples were then packaged into labelled envelopes for Fourier-Transformed Infrared Spectroscopy analysis.

Herbarium Deposition and Voucher Number: Plant parts including leaves, stems, flowers and fruits were collected as

herbarium samples for proper identification and authentication. The plants were identified by plant taxonomists and samples deposited at Bowen University Herbarium. The plant specimens were assigned voucher numbers as recorded in Table 1 below.

Table 1: Plant authentication and voucher numbers

S/N	Plant	Herbarium Identification Number
1	*Calophyllum inophyllum*	BUH047
2	*Cola nitida*	BUH048
3	*Kigelia africana*	BUH051
4	*Pleoiceras barteri*	BUH054

Detection of functional groups from plant samples using Attenuated Total Reflectance Fourier-Transform Infrared (ATR-FTIR)

One hundred grams (100 g) each of the powered leaves and stem bark of the four plants were used for the detection of functional groups as previously described by [7]. The powdered samples were soaked in 100 mL of ethanol for 48 hours in glass jars with intermittent shaking, while dissolved compounds were extracted with Whatman No.1 filter paper. Bibby rotary evaporator (Bibby Scientific, UK) was used to concentrate the sieved plant extracts. Extracted solvents (100 mL) were concentrated at 20 rpm for 30 minutes in the rotary evaporator machine. The concentrated plant extracts were taken to Bowen University Central Laboratory for the ATR-FTIR analysis. The Agilent Cary 630 FTIR spectrometer (Agilent Technologies, Germany) with resolution and scan range of 4000 to 600 cm^{-1}.was used to analyze the extracts. One gram (1g) of various plants extracts was used for the analysis following standard procedure [8]. Interpretation of the infrared spectra was done using [9] after the graph were displayed by the ATR-FTIR out-put device.

RESULTS

The result of the FTIR analysis from the leaf and stem extracts were as presented in spectra in Figures 1 to 4 below. Showing the peaks and bends of the functional groups present in the plant extracts.

The commonly detected compounds from the stem extracts and the leaves extracts giving information about the presence or absence of the names of functional groups were highlighted in Tables 2 to 5 below.

Alcohols such as phenols, amine group, carboxylate and quinones were detected in both the stem and leaf extracts of *C. inophyllum*. Functional groups such as aromatic amine, methylene and methyne when found to be present only in the stem extract. While, compounds such as cyanate, esters, diakyl, aromatic amine, and vinylidene are only present in the leaf extract (Table 2).

The stem and leaf extracts of *C. nitida* both contains methyne, tertiary alcohol (phenol),

primary alcohol, vinylidene, amines, aromatic tertiary amine, diakyl, cyanate, carboxylate, and isothiocyanate groups. Aromatic ethers, aromatic phosphate and methyl are present in only in the stem extract. While quinone, aldehyde, organic sulfates and ester are found only in the leaf extract of *C. nitida* (Table 3).

The functional groups found both in the stem and leaf extracts of *K. africana* were tertiary alcohol (phenol), carboxylate, vinyl, isothiocyanate, open-chain imino and open-chain azo. Primary and secondary alcohol, aromatic ethers, aromatic primary and tertiary amine, vinylidene, quinone, diakyl, cyanide ion, and cyanate were found only in the stem extract. Organic sulphates group are peculiar to the leaf extract of *K. Africana* (Table 4).

Primary and tertiary alcohol (phenol), organic siloxane, aromatic ethers, primary and secondary amine, quinone, methylene, open-chain imino and open-chain azo were functional groups found in both stem and leaf extracts of *P. barteri*. Vinylidene, aromatic tertiary amine, diakyl, vinyl, aldehyde, ester, and aliphatic secondary amine were detected only in the stem extract. While, organic sulfates group are peculiar to *P. barteri* leaf extract (Table 5).

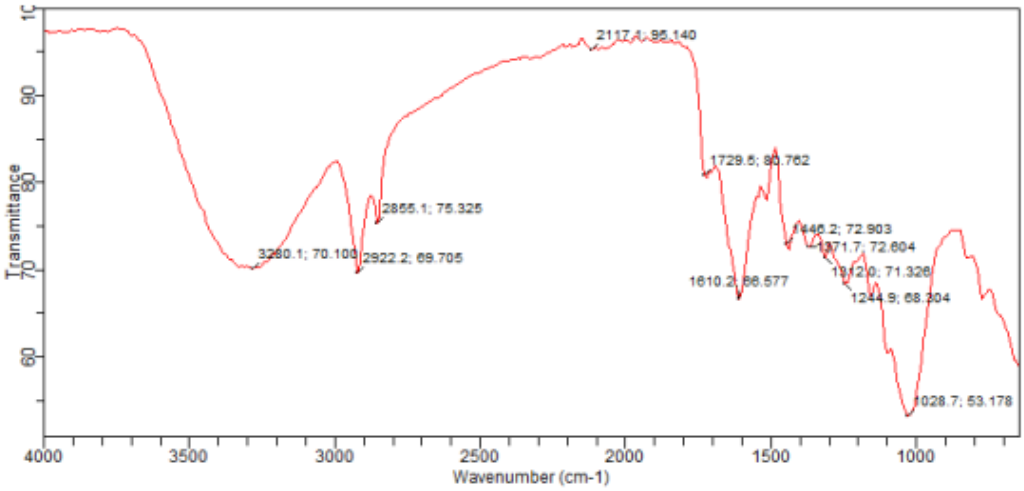

Figure 1a: FTIR spectrum of *Calophyllum inophyllum* leaf extract

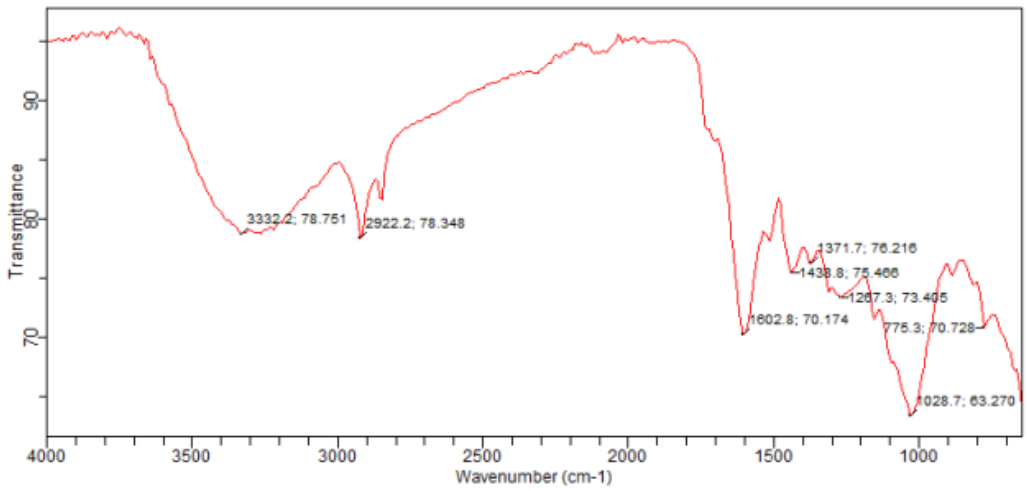

Figure 1b: FTIR spectrum of *Calophyllum inophyllum* stem extracts

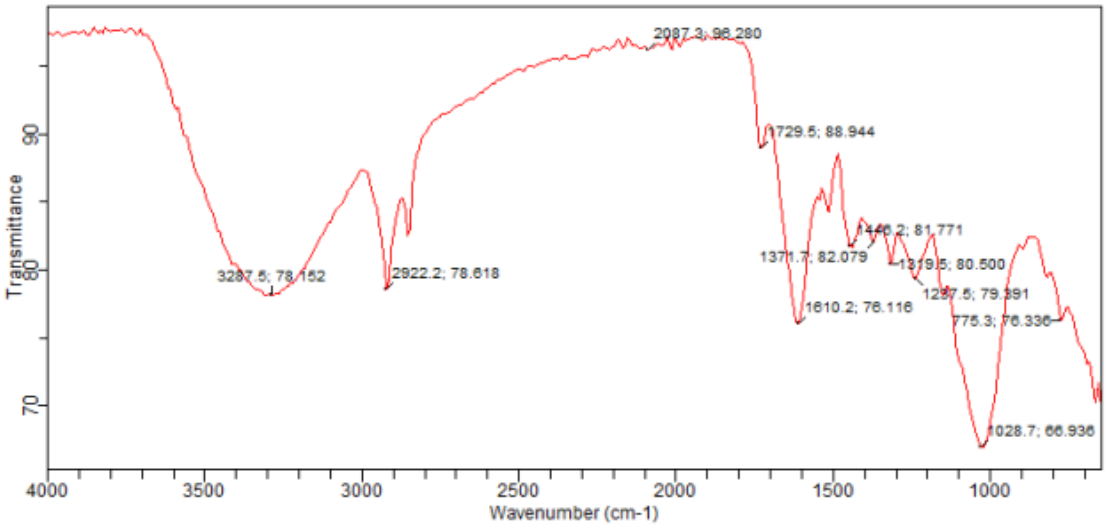

Figure 2a: FTIR spectrum of *Cola nitida* leaf extracts

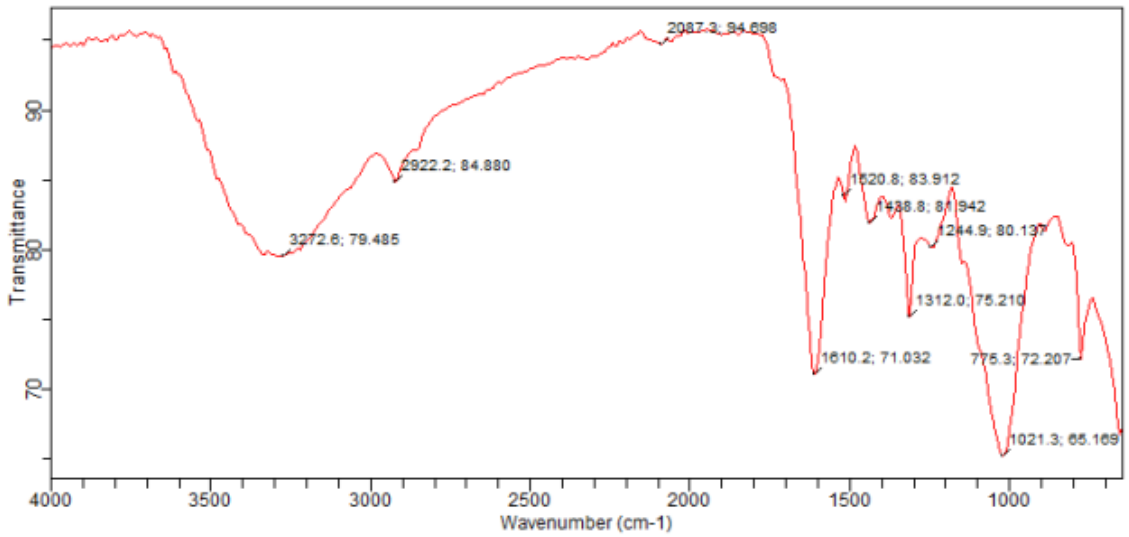

Figure 2b: FTIR spectrum of *Cola nitida* stem extracts

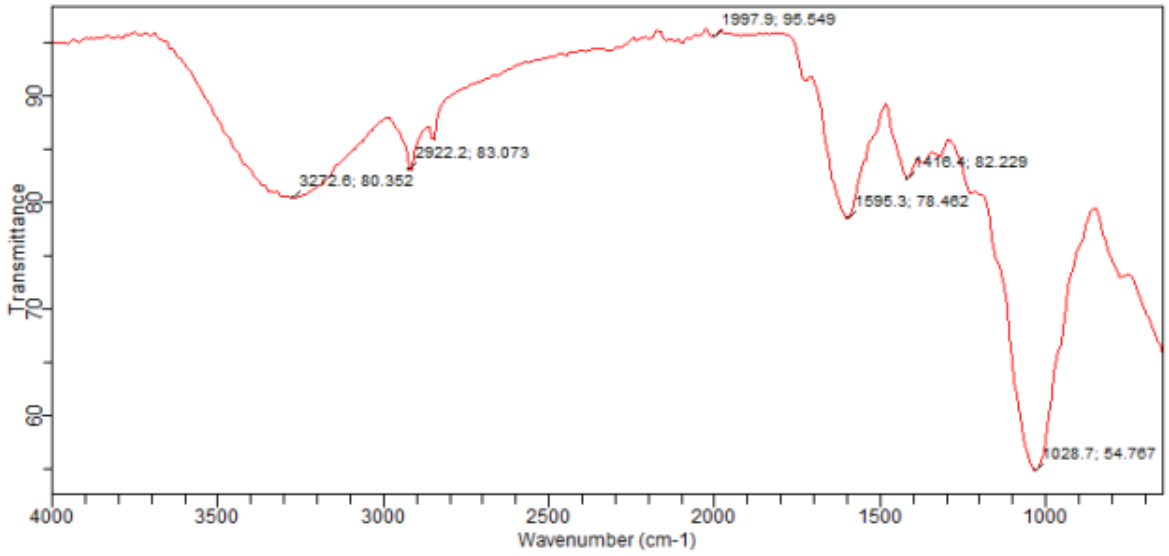

Figure 3a: FTIR spectrum of *Kigelia africana* leaf extracts

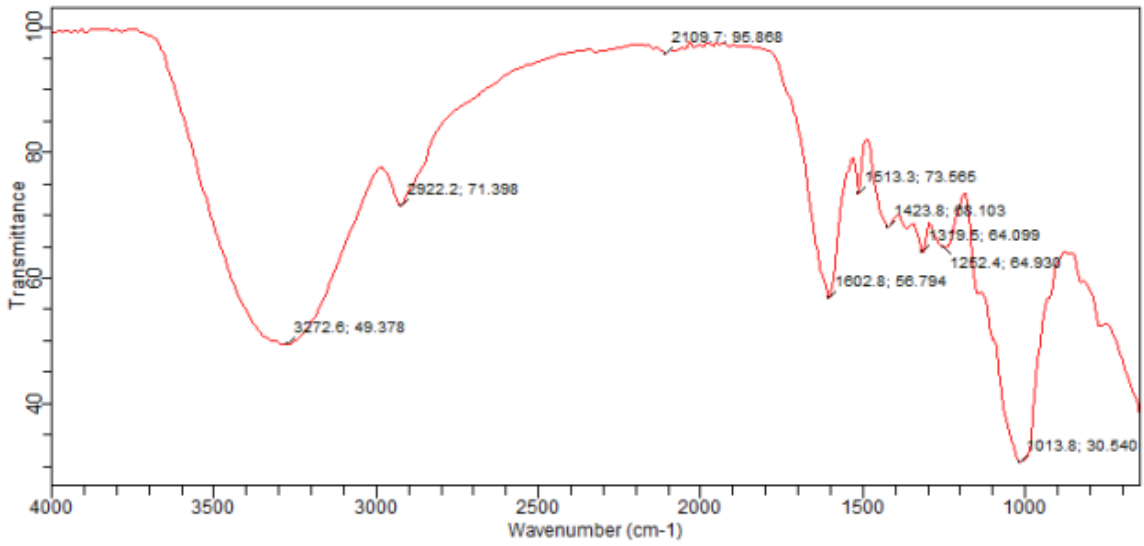

Figure 3b: FTIR spectrum of *Kigelia africana* stem extracts

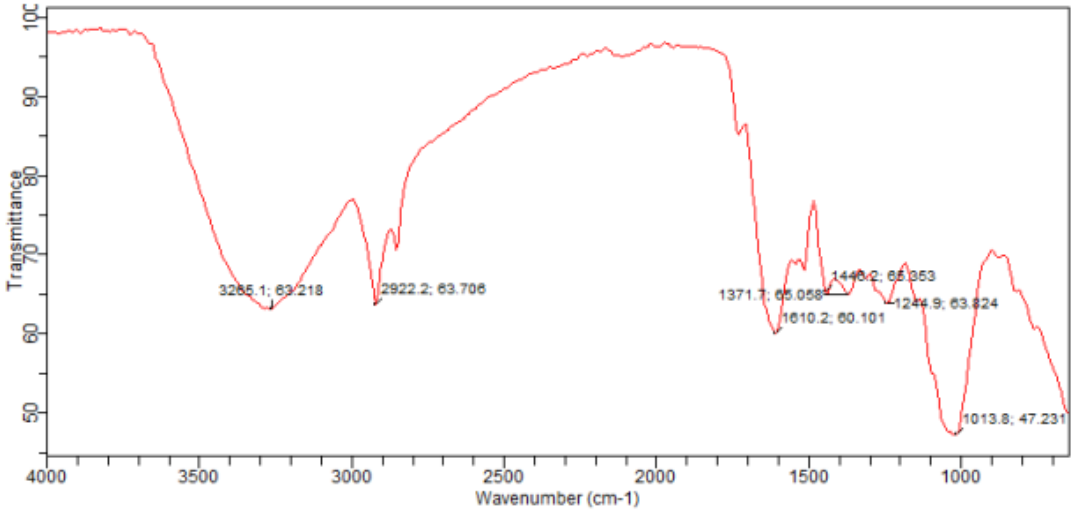

Figure 4a: FTIR spectrum of *Pleoiceras barteri* leaf extracts

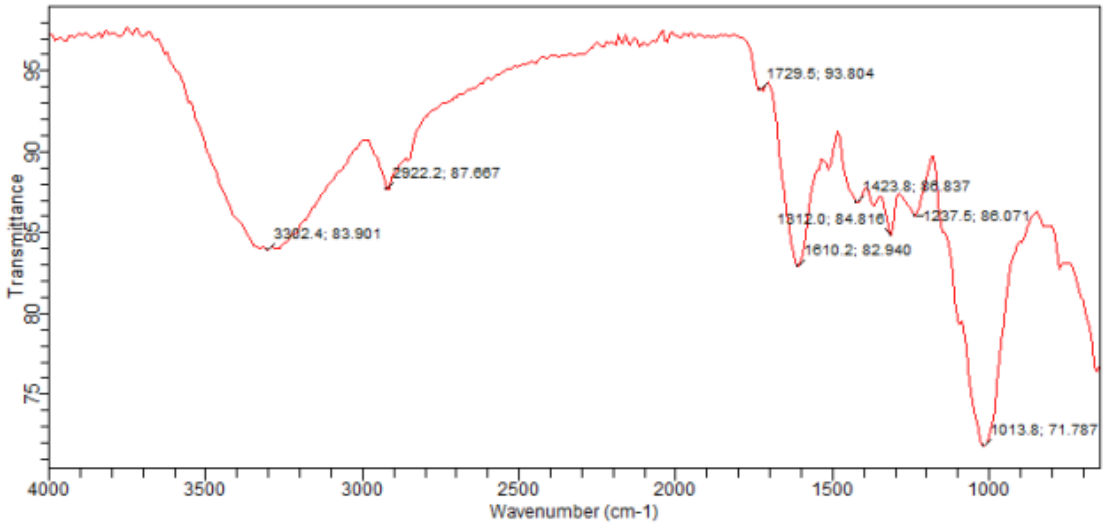

Figure 4b: FTIR spectrum of *Pleoiceras barteri* stem extracts

Table 2: Functional groups detected from the stems and leaves of *Calophyllum inophyllum*

S/N	Functional group	STEM	LEAVES
1	Aromatic ethers	+	+
2	Organic phosphates	+	+
3	Dimethyl or “iso” -doublet	+	+
4	Phenol or tertiary alcohol	+	+
5	Carboxylate	+	+
6	Aliphatic nitro compounds	+	+
7	Organic sulfates	+	+
8	Primary amine, secondary amine	+	+
9	Quinone or conjugated ketone	+	+
10	Open-chain imino	+	+
11	Open-chain azo	+	+
12	Aliphatic fluoro compounds	+	+
13	Primary alcohol	+	+
14	Aliphatic phosphate	+	+
15	Organic siloxane	+	+
16	Methylene	+	-
17	Aliphatic chloro compounds	+	-
18	Methyne	+	-
19	Aromatic primary amine	+	-
20	Aromatic phosphate	-	+
21	Vinylidene	-	+
22	Aromatic tertiary amine	-	+

23	Diakyl	-	+
24	Ester	-	+
25	Aldehyde	-	+
26	Terminal alkyne	-	+
27	Thiocyanate	-	+
28	Isothiocyanate	-	+
29	Methoxy	-	+
30	Methyl ether	-	+

Key (+ Present; - Absent)

Table 3: Functional groups detected from the stems and leaves of *Cola nitida*

S/N	Functional group	STEM	LEAVES
1	Aliphatic chloro compounds	+	+
2	Methyne	+	+
3	Aliphatic fluoro compounds	+	+
4	Primary alcohol	+	+
5	Aliphatic phosphate	+	+
6	Organic siloxane	+	+
7	Vinylidene	+	+
8	Phenol or tertiary alcohol	+	+
9	Aromatic tertiary amine	+	+
10	Carboxylate	+	+
11	Diakyl	+	+
12	Organic phosphates	+	+
13	Primary amine, secondary amine	+	+
14	Open-chain imino	+	+
15	Open-chain azo	+	+
16	Isothiocyanate	+	+
17	Methylene	+	+
18	Aromatic ethers	+	-
19	Aromatic phosphate	+	-
20	Methyl	+	-
21	Quinone or conjugated ketone	-	+
22	Secondary alcohol	-	+
23	Dimethyl or “iso” -doublet	-	+
24	Aliphatic nitro compounds	-	+
25	Organic sulfates	-	+
26	Aldehyde	-	+
27	Ester	-	+

Key (+ Present; - Absent)

Table 4: Functional groups detected from the stems and leaves of *Kigelia africana*

S/N	Functional group	STEM	LEAVES
1	Aliphatic fluoro compounds	+	+
2	Primary alcohol	+	+
3	Aliphatic phosphate	+	+
4	Organic siloxane	+	+
5	Phenol or tertiary alcohol	+	+
6	Carboxylate	+	+
7	Vinyl	+	+
8	Primary amine, secondary amine	+	+
9	Open-chain imino	+	+
10	Open-chain azo	+	+
11	Isothiocyanate	+	+
12	Terminal alkyne	+	+
13	Methyne	+	-
14	Primary or secondary alcohol	+	-
15	Aromatic ethers	+	-
16	Aromatic primary amine	+	-
17	Organic phosphates	+	-
18	Vinylidene	+	-
19	Aromatic tertiary amine	+	-
20	Diakyl	+	-
21	Organic phosphates	+	-
22	Aromatic nitro compounds	+	-
23	Quinone or conjugated ketone	+	-
24	Thiocyanate	+	-
25	Cyanide ion	+	-
26	Methylene	+	-
27	Organic sulphates	-	+

Key (+ Present; - Absent)

Table 5: Functional groups detected from the stems and leaves of *Pleoiceras barteri*

S/N	Functional group	STEM	LEAVES
1	Aliphatic fluoro compounds	+	+
2	Primary alcohol	+	+
3	Aliphatic phosphate	+	+
4	Organic siloxane	+	+

5	Aromatic ethers	+	+
6	Aromatic phosphate	+	+
7	Phenol or tertiary alcohol	+	+
8	Carboxylate	+	+
9	Primary amine, secondary amine	+	+
10	Quinone or conjugated ketone	+	+
11	Open-chain imino	+	+
12	Open-chain azo	+	+
13	Methylene	+	+
14	Vinylidene	+	-
15	Aromatic tertiary amine	+	-
16	Diakyl	+	-
17	Organic phosphates	+	-
18	Vinyl	+	-
19	Aldehyde	+	-
20	Ester	+	-
21	Aliphatic secondary amine	+	-
22	Dimethyl or "iso" -doublet	-	+
23	Aliphatic nitro compounds	-	+
24	Organic sulfates	-	+

Key (+ Present; - Absent)

DISCUSSION

Functional groups present in plant molecule confers unique chemical and physical characteristic properties on plant regardless of other compounds attached to them, as they act as the site of chemical reactions. The present study investigated the functional groups and associated secondary metabolites in the leaves and stem bark extracts of *Calophyllum inophyllum*, *Cola nitida*, *Kigelia africana*, and *Pleioceras barteri* using ATR-FTIR spectroscopy. The identification of diverse functional groups indicates the presence of several classes of bioactive compounds including phenolics, alkaloids, terpenoids, glycosides, organic acids, sulfates, ethers, and amines. These finding highlights the chemical richness of African medicinal plants and their potential for pharmacological applications [10, 11]. ATR-FTIR spectroscopy remains an efficient and non-destructive technique for rapid screening of phytochemicals because characteristic peaks correspond to functional groups responsible for biological activity [9, 12]. The detection of hydroxyl, carbonyl, amine, phosphate, and sulfate groups across the extracts further emphasizes the structural diversity of the secondary metabolites within these tree species.

In *C. inophyllum*, functional groups such as quinones, phenols, carboxylates, and amines were present in both leaf and stem extracts, which is consistent with reports describing the species as rich in calophyllolide, coumarins, xanthones, and terpenoids [3, 13].

The presence of esters, thiocyanates, and aldehydes predominantly in the leaf extract suggests unique biosynthetic variations between plant organs. Phenolic and quinone groups identified in both organs are associated with the plant's well-documented wound-healing and antimicrobial activities [14].

The stem and leaf extracts of *C. nitida* showed widespread detection of phenols, primary and secondary amines, carboxylates, and vinylidene groups, indicating the presence of alkaloids (e.g., caffeine, kolatin) and phenolic compounds reported in earlier research [15,16]. Quinones, aldehydes, and organic sulfates that were identified only in the leaf extract which further supports the role of *C. nitida* leaves in antimicrobial and antioxidant applications [4]. The diversity of functional groups detected specifically in stem extracts, such as aromatic ethers and methyl groups, is also consistent with structural compounds often found in lignified stem bark tissues [17].

K. africana exhibited characteristic phenols, vinyl compounds, carboxylates, imino groups and isothiocyanates in both leaves and stems. These functional groups correspond to known constituents such as iridoids, naphthoquinones, and flavonoids, which contribute to the species' anti-inflammatory, antibacterial, and anticancer properties [18,19]. Organic sulfates detected only in the leaf extract may indicate sulfated flavonoids or glycosides, a group previously associated with enhanced solubility and bioavailability of secondary metabolites [20]. The presence of cyanate and aromatic amines only in the stem supports earlier reports that bark tissues of *K. africana* contain stronger antimicrobial activity than the leaves [21].

The least-studied species among the four, *P. barteri*, showed a wide array of functional groups including phenols, aromatic ethers, quinones, and imino and azo linkages in both plant parts. These findings align with reports that species of the Apocynaceae family are rich in alkaloids and phenolic glycosides with antimalarial and antimicrobial activity [6, 22]. The stem extracts contained more nitrogen-based functional groups (e.g., aromatic tertiary amines, aliphatic secondary amines), potentially indicating higher alkaloid concentration, which supports its traditional use against fever and infections. The presence of sulfates only in leaves may correspond to sulfated polysaccharides or phenolics, which are known for immune-modulating properties [23].

Across the four medicinal species, phenols, carboxylates, amines, and quinones were frequently observed, confirming that these functional groups are common chemical signatures of medicinal plants with antioxidant, antimicrobial, and anti-inflammatory potential [24, 25]. The organ-specific distribution of certain functional groups suggests differences in metabolic allocation within leaves and stems, a phenomenon widely reported in phytochemical studies due to varying physiological roles and exposure to environmental stressors [26]. The presence of organosulfates, aromatic phosphates, and halogenated groups across several samples indicates potential complex derivatives or conjugated metabolites that may contribute to unique pharmacological properties. Studies have shown that sulfate and phosphate conjugation in plants can affect metabolite stability, solubility, and bioactivity.

CONCLUSION

This FTIR-based metabolite profiling provides a foundational dataset for further pharmacological evaluation and compound isolation. The study demonstrates that these

indigenous trees contain broad classes of metabolites relevant to drug discovery and nutraceutical development. Overall, the findings emphasize the chemical potential of these indigenous species and reinforce their significance in traditional medicine, while providing a scientific basis for their future application in natural product research. Therefore, by utilizing FTIR spectroscopy which is one of the affordable spectroscopic method, researchers may effectively assess bioactive chemicals to expedite the discovery and development of innovative therapies, medicines, and industrial goods for application in the allied health sectors.

DATA AVAILABILTY

All data for this study is available and presented within this article. Should any raw data files be needed in another format they are available from the corresponding author upon reasonable request.

CODE AVAILABILITY STATEMENT

No custom code was generated in this study.

CRediT Author Statement

PJO: Conceptualization, Sample collection, Methodology, Supervision, Validation, Writing – review and editing; **IAO**: Conceptualization, Supervision, Sample collection, Methodology, Data interpretation, Writing- original draft; **OEO**: Conceptualization, Sample collection, Methodology; **BOA**: Conceptualization, Sample collection, Methodology; **FDO**: Conceptualization, Sample collection, Methodology; **AEO**: Sample collection, Methodology; **OA:** Sample collection, Methodology; **ASO:** Sample collection, Plant Identification and authentication, Methodology; **AA:** Conceptualization and Writing-review and editing.

Declaration of Competing Interest

The authors declare that there are no competing financial or personal interests that could have influenced the report of this research.

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