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FT-IR and Functional Group Characterization of *Aloe barbadensis* and *Cymbopogon citratus* Extracts for Potential Heavy Metal Biosorption

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Abstract

Heavy metal toxicity poses significant health and environmental risks due to the persistent, bioaccumulative, and non-biodegradable nature of the metals cadmium (Cd), chromium (Cr), and lead (Pb). These metals can damage vital organs, disrupt metabolic processes, and induce oxidative stress, inflammation, and tissue injury. Consequently, the search for safe, affordable, and eco-friendly remediation strategies has increased, with growing interest in plant-based biosorbents. This study investigated the FT-IR and classical functional group characterization of *Aloe barbadensis* and *Cymbopogon citratus* extracts for heavy metal biosorption. Classical qualitative tests were used for the identification of functional groups responsible for metal binding, including the sodium hydrogen carbonate test for carboxylic acids, the 2,4-dinitrophenylhydrazine (2,4-DNP) test for ketones, the sodium hydroxide plus heat test for amides, the Hinsberg test for amines, and the Lucas test for alcohols. Fourier Transform Infrared (FT-IR) spectroscopy was employed to confirm the results. The findings revealed the presence of carboxylic acids in both extracts, while ketones and amides were detected only in *C. citratus*. Secondary amines and secondary alcohols were identified in *A. barbadensis*, whereas *C. citratus* contained primary amines and tertiary alcohols. These functional groups serve as active sites for binding metal ions through chelation, ion exchange, and complexation mechanisms. The results suggest that both extracts, particularly *C. citratus* have strong potential as affordable and eco-friendly biosorbents for the removal of heavy metals.

Keywords: Cadmium, Chromium, Lead, *Aloe barbadensis*, *Cymbopogon citratus*

Introduction

Heavy metal contamination has become a major global environmental and public health concern due to the increasing release of toxic metals into ecosystems through industrialization, urbanization, mining activities, agricultural practices, battery manufacturing, electroplating, textile processing, and improper waste disposal. Among the most hazardous heavy metals are cadmium (Cd), chromium (Cr), and lead (Pb), which are non-biodegradable, persistent, and capable of accumulating in biological systems over time. Their presence in water, soil, and food chains poses significant threats to both environmental sustainability and human health [1–3].

Cadmium exposure has been associated with renal dysfunction, hepatic damage, skeletal disorders, and carcinogenic effects, while chromium, particularly hexavalent chromium [Cr(VI)], is known for its mutagenic and carcinogenic properties. Lead toxicity affects multiple organ systems, including the nervous,

hematopoietic, renal, and reproductive systems, even at relatively low concentrations. Due to their bioaccumulative nature, these metals can persist in living organisms and biomagnify across trophic levels, thereby increasing long-term toxicological risks to humans and animals [4–6].

Various physicochemical techniques have been employed for the removal of heavy metals from contaminated environments, including chemical precipitation, membrane filtration, reverse osmosis, coagulation-flocculation, electrochemical treatment, and ion exchange. Although these methods may achieve significant metal removal efficiencies, they are often associated with high operational costs, energy requirements, incomplete metal removal, sludge generation, and secondary environmental pollution [7,8]. Consequently, there has been increasing interest in the development of low-cost, environmentally



friendly, and sustainable alternatives for heavy metal remediation.

Biosorption has emerged as a promising eco-friendly approach for the removal of toxic metals from aqueous and biological systems. Biosorption involves the passive binding of metal ions onto biological materials through physicochemical interactions such as adsorption, ion exchange, complexation, chelation, and microprecipitation. Plant-derived biosorbents are particularly attractive because they are renewable, biodegradable, inexpensive, widely available, and rich in functional groups capable of interacting with metal ions [9–11]. The efficiency of biosorption largely depends on the nature and abundance of active binding sites present in the biosorbent matrix. Functional groups such as hydroxyl (-OH), carboxyl (-COOH), amino (-NH₂), carbonyl (C=O), sulfhydryl (-SH), and phosphate groups play important roles in metal ion binding and sequestration [12,13].

Medicinal plants have received considerable attention as potential biosorbents due to their rich phytochemical composition and diverse biological properties. Aloe barbadensis (Aloe vera) is widely recognized for its medicinal, antioxidant, anti-inflammatory, antimicrobial, and detoxifying properties. The plant contains numerous bioactive constituents, including polysaccharides, flavonoids, tannins, saponins, anthraquinones, glycoproteins, vitamins, and phenolic compounds, many of which possess functional groups capable of interacting with heavy metal ions [14–16]. The mucilaginous gel of Aloe vera is particularly rich in polysaccharides such as acemannan, which may contribute significantly to metal adsorption through hydroxyl and carboxyl functionalities.

Similarly, *Cymbopogon citratus* (lemongrass), a perennial aromatic herb belonging to the Poaceae family, possesses a wide range of phytochemicals, including citral, flavonoids, terpenoids, tannins, alkaloids, and phenolic acids [17,18]. These compounds contain multiple reactive functional groups that may facilitate the binding and immobilization of toxic metal ions. In addition to its medicinal and antioxidant properties, *C. citratus* has attracted scientific interest for its potential applications in environmental remediation and wastewater treatment.

Characterization of the functional groups present in plant extracts is essential for understanding the mechanisms underlying biosorption processes. Qualitative phytochemical screening provides preliminary information regarding the classes of bioactive compounds present, while Fourier-transform infrared (FTIR) spectroscopy enables the identification of specific functional groups involved in metal binding interactions. FTIR analysis has been widely employed in biosorption studies to determine the chemical moieties responsible for adsorption and to elucidate possible mechanisms of metal uptake by biosorbent materials [19,20].

Despite increasing interest in plant-based biosorbents, limited studies have comparatively evaluated the functional group composition and biosorptive potential of *A. barbadensis* and *C. citratus* extracts specifically in relation to cadmium, chromium, and lead interactions. Therefore, this study aimed to qualitatively identify phytochemical constituents and characterize the functional groups present in *A. barbadensis* and *C. citratus* extracts using phytochemical screening and Fourier-transform infrared spectroscopy. The findings of this study may contribute to the development of inexpensive, natural, and sustainable biosorbent materials for heavy metal remediation and detoxification applications.

Materials and Methods

Reagents

Every chemical and reagent used was of analytical grade from JHD Chemicals; this included cadmium (II) chloride, potassium dichromate, lead (II) nitrate, sulfuric acid, sodium hydrogen phosphate, sodium dihydrogen phosphate, perchloric acid, chloroform, xylene, ethanol, formalin, sodium hydroxide, hydrochloric acid, nitric acid, distilled water, hematoxylin stain, eosin stain, etc.

Collection, drying, and preparation of plant materials

Plant sample authentication

The leaves of *Aloe barbadensis* and *Cymbopogon citratus* were collected from a farm in Sabongari-Zaria, Kaduna State, Nigeria. These were taken for authentication at the Botany Department's Herbarium at Ahmadu Bello University Zaria, Kaduna State, where voucher numbers (ABU02890 and ABU017430, respectively) were deposited.

Preparation of plant samples

A. barbadensis and *C. citratus* leaves were washed, air-dried, ground into coarse powder, and sieved (350 mm mesh). The powders were oven-dried at 80°C for 24 hours and stored in polyethylene containers for further use [11].

Extraction of Plant Materials

The powdered plant material was extracted with methanol (1:5 w/v) by cold maceration for 48 hours with periodic shaking. The mixture was filtered, and the filtrate was concentrated using a rotary evaporator, dried to constant weight, and stored in a refrigerator until use.

Functional Group Analysis

Qualitative test tube functional group analyses were carried out on *A. barbadensis* and *C. citratus* extracts to determine the presence of carboxylic acids, ketones, amides, amines, phenols, and alcohols. This was carried out in the Main Teaching Laboratory, Department of Chemistry, Ahmadu Bello University, Zaria. The tests were selected based on classical organic qualitative analysis and are summarized in Table I.

**Table 1: Functional group qualitative tests employed [12]**

Test	Expected observation	Inference
HCl + Extract	Insoluble	No phenol or carboxylic acid confirm
5% NaHCO ₃ solution + Extract	Effervescence (CO ₂ bubble)	Carboxylic acid (-COOH), confirm
Brady's solution + Extract	Yellow/Orange/Red precipitates.	Ketone is present (C=O).
NaOH + Extract	Ammonia evolved (pungent smell) turns moist red litmus paper blue.	Amide is present (CONH ₂).
Benzene-sulfonyl chloride + NaOH + extract, shaken	The primary amine is soluble and reprecipitates in acid; the secondary amine is insoluble and precipitates; the tertiary amine has no reaction.	Amine present (NH ₂)
Con HCl + ZnCl + Extract, shaken.	Tertiary alcohol is cloudy immediately, secondary alcohol is cloudy in 5-10 minutes, and primary alcohol shows no change.	Alcohol present (OH)

Fourier transform infrared analysis of *Aloe barbadensis* and *Cymbopogon citratus*

The *A. barbadensis* and the *C. citratus* extracts were prepared in the forms of potassium bromide (KBr) disks (the extracts were blended with potassium bromide), and the IR spectra were taken at a frequency range of 4000-400 cm⁻¹. The distinctive absorption bands were examined to determine the active functional groups.

Results and Discussion

Functional Group Analyses (classical test) Results

The qualitative functional group tests provided insight into the chemical nature of *A. barbadensis* and *C. citratus* extracts. The observed reactions and their interpretations were summarized in Table 2. The presence of carboxyl (-COOH), hydroxyl (-OH), amine (-NH₂), and carbonyl (C=O) functional groups suggests potential chelation binding sites and adsorption of heavy metals [13-14].

The results showed that both extracts contain carboxylic acid and hydroxyl groups that play significant roles in metal ion binding through ion-exchange mechanisms and hydrogen bonding interactions [15-16]. The existence of amine groups provides more coordination sites for metal complexation, while the carbonyl functional groups detected in *C. citratus* further enhance its metal-binding capacity [17-18].

Carboxyl groups are widely reported as dominant metal-binding sites because of their ability to donate electrons and participate in ion-exchange reactions [19]. There have been

reports of similar findings for plant-based adsorbents such as *Moringa oleifera*, *Azadirachta indica*, and *C. citratus*, where carboxyl groups significantly contributed to cadmium, lead, and chromium adsorption [16, 14].

Hydroxyl groups detected via the Lucas test in both extracts further enhance metal binding through hydrogen bonding and surface complexation mechanisms. Hydroxyl-rich biosorbents have been shown to exhibit high affinity for divalent and trivalent metal ions, particularly Pb²⁺ and Cd²⁺ [15]. The immediate cloudiness observed in *C. citratus* suggests the presence of tertiary alcohols, which may offer greater steric stability and stronger surface interactions in contrast to the secondary alcohols identified in *A. barbadensis*. This agrees with earlier studies reporting superior adsorption efficiencies for *C. citratus* extracts compared to other medicinal plants [19].

The Hinsberg test indicated the presence of secondary amines in *A. barbadensis* and primary amines in *C. citratus*. Amine groups are renowned for their role in chelation, as the single pair of electrons on nitrogen is capable of forming coordinate bonds with metal ions [20]. Primary amines, in particular, have been demonstrated to exhibit stronger metal coordination ability than secondary amines due to reduced steric hindrance, which could account for the increased adsorption capacity seen for *C. citratus* in this study.

The presence of carbonyl (C=O) and amide functional groups exclusively in *C. citratus*, as confirmed by the 2, 4-DNP and NaOH heating tests, further strengthens its adsorption potential. Carbonyl groups act as electron donors and are



involved in complexation reactions with heavy metals, particularly chromium and lead [19].

These qualitative results align with FTIR results reported in related studies, where shifts in O–H, C=O, and N–H stretching vibrations after metal exposure confirmed the direct involvement of these functional groups in adsorption processes [15,18]. The combined presence of multiple functional groups in *C. citratus* likely provides synergistic binding sites, resulting in higher adsorption efficiency compared to *A. barbadensis*.

Overall, the functional group composition revealed by qualitative analysis provides a mechanistic reason for the superior metal adsorption performance of *C. citratus*. These findings are in line with previous reports on plant-based biosorbents and support the application of *C. citratus* and *A. barbadensis* extracts as effective, low-cost, and environmentally friendly materials for heavy metal remediation.

Table 2: Results of Functional Group Tests on *A. barbadensis* and *C. citratus* extracts

Functional Group	Test	Observation in <i>Aloe barbadensis</i> Extracts	Observation in <i>Cymbopogon citratus</i> extract	Inference
Carboxylic acid	NaHCO test	Effervescence observed.	Effervescence was observed.	Carboxylic acids are present in both extracts.
Ketone	2,4-DNP test	No precipitate formed.	Yellow precipitate formed.	Ketone is absent in <i>A. barbadensis</i> , present in <i>Cymbopogon citratus</i> extract.
Amide	NaOH + Heat:	No ammonia detected.	Ammonia-evolved	amide present in <i>C. citratus</i> extract only.
Amine	Hinsberg test	insoluble precipitate is formed.	Soluble product precipitated on acidification.	<i>Aloe barbadensis</i> contains secondary amines; <i>Cymbopogon citratus</i> contains primary amines.
Alcohol	Lucas test	cloudiness after 10 minutes.	Immediate cloudiness:	<i>Aloe barbadensis</i> contains secondary alcohol; <i>Cymbopogon citratus</i> contains tertiary alcohol.

Fourier Transform Infrared (FTIR) Spectrum Results of *Aloe barbadensis* Extract

The Fourier Transform Infrared (FTIR) spectrum of *A. barbadensis* extract (Figure 1) showed the presence of several characteristic absorption bands that indicate functional groups involved in metal binding and adsorption. Prominent peaks were observed at 1058.6 cm^{-1} , 1707.1 cm^{-1} , 2922.2 cm^{-1} , and a broad absorption band around 3373.2 cm^{-1} .

The sharp absorption peak at 1707.1 cm^{-1} is attributed to the C=O stretching vibration of carbonyl groups, commonly associated with carboxylic acids, aldehydes, ketones, or esters. Similar FTIR features have been reported for *Aloe vera* extracts by [21-22], who identified carbonyl groups as major contributors to metal chelation because of their ability to donate electron pairs to metal ions. The presence of this functional group enhances the affinity of the plant extract toward divalent heavy metals such as Cd^{2+} , Pb^{2+} , and Cr^{3+} through coordination bonding.

The broad absorption band at 3373.2 cm^{-1} corresponds to O–H stretching vibrations of hydroxyl groups from alcohols and phenolic compounds and possibly N–H stretching from amine groups. The broad nature of this peak indicates extensive hydrogen bonding, which is typical of plant-based biomaterials. Recent studies have shown that hydroxyl and amine groups play an important role in metal adsorption by facilitating hydrogen bonding, electrostatic attraction, and surface complexation [23, 15]. These interactions significantly improve the biosorption efficiency of plant extracts.

The absorption band observed at 1058.6 cm^{-1} is characteristic of C–O stretching vibrations in alcohols, phenols, and ether groups. This finding is in line with reports by [24-25], who noted that oxygen-containing functional groups like C–O and O–H increase adsorption capacity by acting as metal ion binding sites. These groups enhance chelation through ion-exchange mechanisms and surface adsorption.

Additionally, the moderate band around 2922.2 cm^{-1} is associated with C–H stretching vibrations of aliphatic chains,



indicating the existence of organic constituents like polysaccharides and lipophilic compounds commonly found in *A. barbadensis*. Such biomolecules contribute to surface heterogeneity, which has been reported to favor multilayer adsorption processes [26]. The FTIR analysis confirms that *A. barbadensis* extract is rich in carbonyl (C=O), hydroxyl (O-H),

and ether/alcohol (C-O) functional groups, which are well-documented in literature as effective metal-binding moieties. The presence of these functional groups supports the suitability of *A. barbadensis* as a natural, low-cost, and efficient biosorbent for the adsorption of ions of heavy metals in biological and environmental systems.

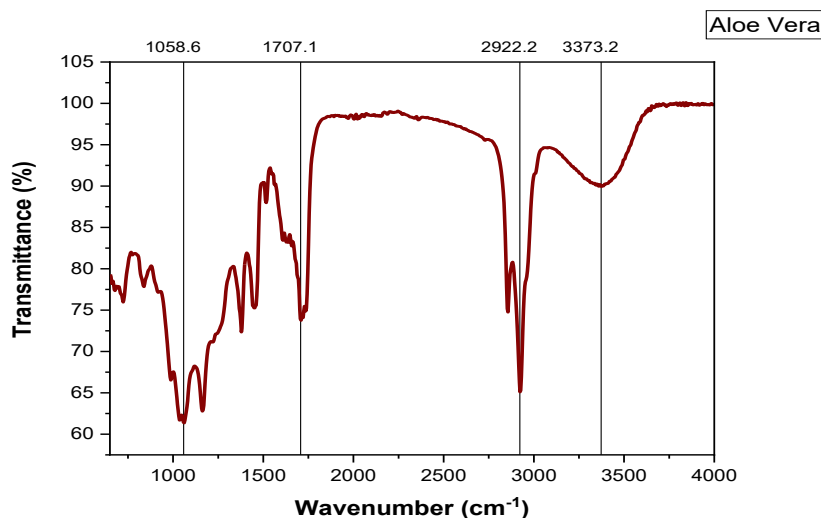


Figure 1: Fourier transform infrared spectrum of *Aloe barbadensis* untreated extract showing sharp peaks at 2922.2 cm^{-1} , 1707.1 cm^{-1} , and 1058.6 cm^{-1} with a broad peak at 3373.2 cm^{-1} .

The Fourier Transform Infrared (FTIR) Spectrum results of *Cymbopogon citratus* extract

The Fourier Transform Infrared (FTIR) spectrum of *Cymbopogon citratus* extract (Figure 2) showed several characteristic absorption bands indicating the presence of functional groups capable of interacting with heavy metal ions. Prominent peaks were observed at 1062.3 cm^{-1} , 1707.1 cm^{-1} , and 2922.2 cm^{-1} , alongside a broad absorption band at 3350.9 cm^{-1} .

The absorption band at 2922.2 cm^{-1} is in line with C-H stretching vibrations of aliphatic (alkyl) groups, which are frequently connected to long-chain hydrocarbons present in plant-derived biomaterials (Silverstein et al., 2014). Alkyl groups, however, are not primary metal-binding sites; they contribute to the hydrophobic backbone that stabilizes the adsorption matrix.

A strong and well-defined peak at 1707.1 cm^{-1} is attributed to the C=O stretching vibration of carbonyl groups, particularly those found in carboxylic acids, aldehydes, or esters. This result is in line with earlier FTIR research on *Cymbopogon citratus*

extracts, which reported carbonyl groups as major contributors to metal chelation due to their electron-donating oxygen atoms [27, 21]. Carbonyl groups play an important role in metal binding through coordination interactions with divalent and trivalent metal ions like Pb^{2+} , Cd^{2+} , and Cr^{3+} .

The broad absorption band observed at 3350.9 cm^{-1} is characteristic of O-H stretching vibrations, indicative of carboxylic acids, phenols, or alcohols' hydroxyl groups. Broad O-H peaks typically signify hydrogen bonding, which enhances surface reactivity and facilitates ion exchange mechanisms during metal adsorption [28, 17]. The coexistence of O-H and C=O bands strongly confirm the existence of carboxylic acid functional groups in the plant extract.

Additional bands at 1457.4 cm^{-1} correspond to C-H bending vibrations of alkanes, while the peak at 916.9 cm^{-1} may be associated with O-H bending or C-O stretching vibrations. The band at 1062.3 cm^{-1} is attributed to C-O stretching vibrations of alcohols or carboxylic acids, further supporting the abundance of oxygen-containing functional groups in the plant extract which have been reported in enhancing metal uptake through surface complexation and coordination bonding [29, 18].

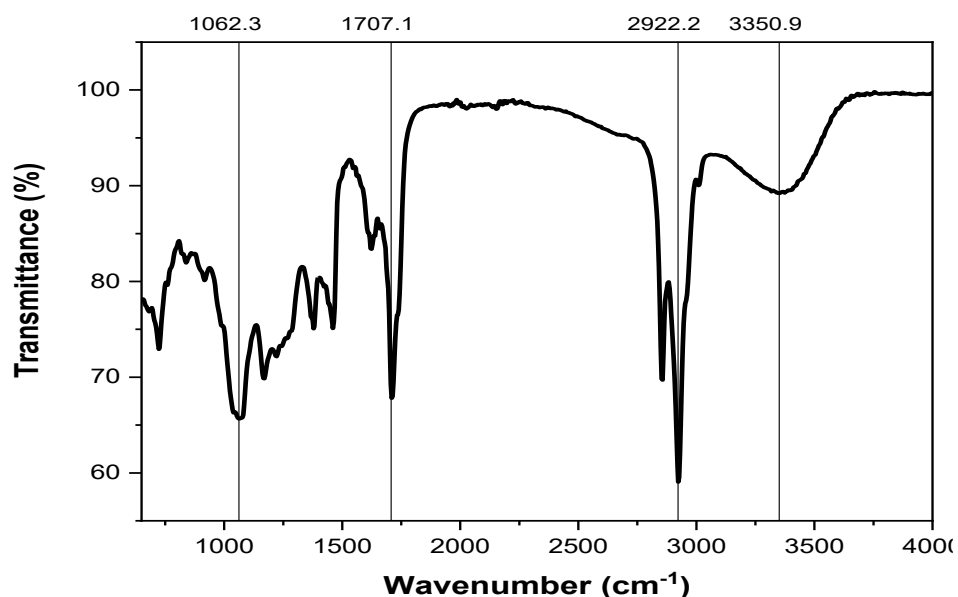


Figure 2: Fourier transform infrared spectrum of *Cymbopogon citratus* extract

Conclusion

This study evaluated the functional group composition and metal-binding potential of extracts from *A. barbadensis* and *C. citratus* using qualitative functional group tests and Fourier transform infrared spectroscopy analysis. The results confirmed several active functional groups capable of interacting with ions of heavy metals, such as carboxyl (-COOH), hydroxyl (-OH), amine (-NH₂), and carbonyl (C=O) groups. Qualitative chemical tests showed that both plant extracts possess carboxylic acid and hydroxyl groups, which are widely recognized as principal sites of adsorption for metal ions through ion-exchange, hydrogen bonding, and surface complexation mechanisms. The detection of amine groups in both extracts further provides coordination sites for metal chelation, enhancing their biosorption capability. However, *C. citratus* exhibited a wider variety of functional groups, including carbonyl and amide functionalities, which were not strongly evident in *A. barbadensis*. These additional groups increase the number of available electron-donating sites, thereby strengthening the interaction between the adsorbent surface and ions of heavy metals. The Fourier transform infrared spectroscopy spectra of both extracts corroborated the qualitative findings by revealing characteristic absorption bands corresponding to O-H, C=O, C-O, and C-H functional groups. These oxygen- and nitrogen-containing groups are known to act as heavy metal binding sites, such as cadmium, lead, and chromium, through coordination and complexation reactions. The strong and well-defined carbonyl and hydroxyl peaks observed in *C. citratus* suggest a higher density of active

adsorption sites compared with *A. barbadensis*. The results showed that both plant extracts possess functional groups capable of facilitating heavy metal adsorption. The study therefore highlights the promising role of plant-based biosorbents in sustainable water purification and environmental detoxification. Future work should further quantify adsorption performance under varying conditions and evaluate the regeneration and reuse potential of these natural biosorbents.

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