RESEARCH PAPER

Rapid FTIR Screening and Solvent-Dependent Phytochemical Characterization of *Cyperus rotundus* L. (Nut Grass) Extracts

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ABSTRACT

Cyperus rotundus L. (commonly known as nut grass or motha) is a medicinally important plant widely recognized for its antimicrobial, antioxidant, antiamoebic and cytotoxic properties. The present study aimed to comparatively characterize the functional groups present in leaf and rhizome extracts of C. *rotundus* obtained using solvents of different polarities, including ethanol, methanol, ethyl acetate, and chloroform, through Fourier Transform Infrared (FTIR) spectroscopy. Dried plant materials were extracted separately using solvent extraction and the resulting extracts were analyzed within the spectral range of 4000–400 cm^{-1}. The FTIR spectra revealed several characteristic absorption bands corresponding to important functional groups such as hydroxyl (O–H), aliphatic C–H, carbonyl (C=O), aromatic C=C and C–O stretching vibrations, indicating the presence of diverse classes of phytochemicals. Extracts obtained with polar solvents exhibited stronger hydroxyl and carbonyl absorption bands, suggesting efficient extraction of phenolic and flavonoid compounds. In contrast, moderately polar and non-polar solvents demonstrated relatively pronounced aliphatic and aromatic bands, indicating the presence of terpenoids and other hydrophobic constituents.

Comparative spectral evaluation between plant parts revealed noticeable qualitative variations in the distribution of functional groups, with rhizome extracts displaying relatively greater functional group diversity than leaf extracts. These observations suggest that rhizomes may possess a richer phytochemical composition compared to aerial tissues. The findings highlight solvent polarity as an important factor influencing phytochemical extraction efficiency and confirm the usefulness of FTIR spectroscopy as a rapid and reliable analytical tool for preliminary phytochemical profiling and functional group identification in *C. rotundus*. The study also provides a basis for further chromatographic and bioactivity-guided investigations aimed at isolating and characterizing bioactive compounds from this medicinal plant.

Keywords: *Cyperus rotundus*, FTIR spectroscopy, phytochemical profiling, solvent extraction, functional groups, medicinal plant.

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INTRODUCTION

Medicinal plants represent a major source of structurally diverse bioactive compounds that continue to play an important role in modern drug discovery and pharmaceutical development. Plant-derived secondary metabolites such as phenolics, flavonoids, alkaloids, terpenoids and glycosides possess a wide range of biological activities including antioxidant, antimicrobial, anti-inflammatory and anticancer effects (Cowan, 1999; Rates, 2001; Atanasov et al., 2021). According to the World Health Organization, nearly 80% of the global population relies on plant-based traditional medicines for primary healthcare (WHO, 2014). Consequently, scientific evaluation of medicinal plants has gained increasing attention for the identification of novel bioactive compounds and therapeutic agents. Among the medicinally important species, *Cyperus rotundus* L. (family Cyperaceae), commonly known as nut grass or purple nutsedge, is widely distributed in tropical and subtropical regions. The plant has been extensively used in traditional systems of medicine for the treatment of gastrointestinal disorders, fever, inflammation, menstrual irregularities and metabolic ailments (Dang et al., 2011; Ghannadi et al., 2012). Several pharmacological studies have demonstrated that extracts of *C. rotundus* exhibit significant antioxidant, antimicrobial, hepatoprotective,

anti-inflammatory and cytotoxic activities (Taheri et al., 2021; Xue et al., 2023).

Phytochemical investigations of *C. rotundus* have revealed the presence of diverse classes of secondary metabolites including flavonoids, phenolic compounds, terpenoids, sesquiterpenes and essential oils (Singh et al., 2014; Xue et al., 2023). Compounds such as α-cyperone, cyperotundone, germacrene D and caryophyllene oxide have been reported as major constituents responsible for many of the plant's pharmacological properties (Dang et al., 2011; Taheri et al., 2021). The extraction of these phytochemicals is strongly influenced by the polarity of the solvent used, as different solvents selectively dissolve specific groups of chemical constituents, thereby affecting the qualitative and quantitative composition of plant extracts (Azwanida, 2015). Spectroscopic techniques are widely used for rapid identification and characterization of phytochemicals present in plant extracts. Among them, Fourier Transform Infrared (FTIR) spectroscopy is considered a reliable and non-destructive analytical technique for the preliminary identification of functional groups in natural products (Stuart, 2004; Socrates, 2001). FTIR spectroscopy enables the detection of characteristic absorption bands corresponding to functional groups such as hydroxyl, carbonyl, carboxyl and aromatic groups, which are commonly associated with phenolics, flavonoids and other bioactive compounds in medicinal plants (Kumar et al., 2017).

Therefore, the present study aims to comparatively evaluate the functional group profiles of leaf and rhizome extracts of *Cyperus rotundus* obtained using solvents of varying polarity through FTIR spectroscopy, in order to identify major functional groups associated with phytoconstituents and to understand solvent-dependent variations in the phytochemical composition of the plant extracts.

MATERIALS AND METHODS

2.1 Plant Material Collection and Authentication

Fresh leaves and rhizomes of *Cyperus rotundus* L. were collected from the Nanded district, Maharashtra, India. The collected plant materials were carefully cleaned to remove adhering soil and debris. Taxonomic identification and authentication were carried out (Ref. No.: BOT/2024-25) by a taxonomist Sr. Prof. and Dr. A. S. Dhabe (Herbarium In-charge), Dr. Babasaheb Ambedkar Marathwada University, Chhatrapati Sambhajinagar (MS) and a voucher specimen (Accession No.: 01139) was deposited in the departmental herbarium for future reference. A valid botanical authentication is essential to ensure the reliability and reproducibility of phytochemical investigations (Heinrich et al., 2020; Xue et al., 2023).

2.2 Preparation of Extracts

The collected plant materials (leaves and rhizomes) were washed thoroughly with distilled water and air-dried at room temperature under shade to prevent degradation of thermolabile phytoconstituents. The dried samples were then ground into a fine powder using a mechanical grinder and stored in airtight containers until further analysis. Approximately 20 g of powdered plant material was extracted separately with different organic solvents including ethanol, methanol, ethyl acetate and chloroform using a Soxhlet extraction apparatus. Each extraction was carried out for 6–8 hours until the solvent in the siphon tube became colorless. The obtained extracts were filtered and concentrated under reduced pressure using a rotary evaporator to remove excess solvent and obtain crude extracts. The use of solvents with different polarities facilitates the extraction of a broad spectrum of phytochemicals, as solvent polarity significantly influences the solubility and recovery of secondary metabolites from plant materials (Azwanida, 2015; Sasidharan et al., 2011).

2.3 FTIR Analysis

Fourier Transform Infrared (FTIR) spectroscopy was employed to identify the functional groups present in the plant extracts. FTIR spectra of the dried extracts were recorded using a Bruker ALPHA II FTIR spectrophotometer in the spectral range of 4000–400 cm^{-1} with a resolution of 2 cm^{-1}. The samples were prepared using the potassium bromide (KBr) pellet method, where a small amount of dried extract was finely mixed with spectroscopic-grade KBr and compressed into a transparent pellet for spectral analysis. Prior to sample measurement, background correction was performed to eliminate atmospheric interference and instrumental noise. FTIR spectroscopy is widely used for rapid and non-destructive characterization of phytochemicals, as it enables the identification of major functional groups such as hydroxyl, carbonyl, alkyl and aromatic groups present in plant-derived compounds (Stuart, 2004; Kumar et al., 2017; Coates, 2022). The obtained spectra were interpreted based on characteristic absorption bands corresponding to specific functional groups reported in standard FTIR reference literature.

RESULTS AND DISCUSSION

The Fourier Transform Infrared (FTIR) spectra of leaf and rhizome extracts of *Cyperus rotundus* obtained using solvents of varying polarity are presented in Figures 1–2, while the major absorption bands and their functional group assignments are summarized in Table 1. FTIR spectroscopy is widely recognized as a rapid and reliable analytical technique for identifying functional groups in plant extracts through characteristic vibrational frequencies, thereby providing preliminary insights into the chemical composition of phytoconstituents (Stuart, 2004; Coates, 2022).

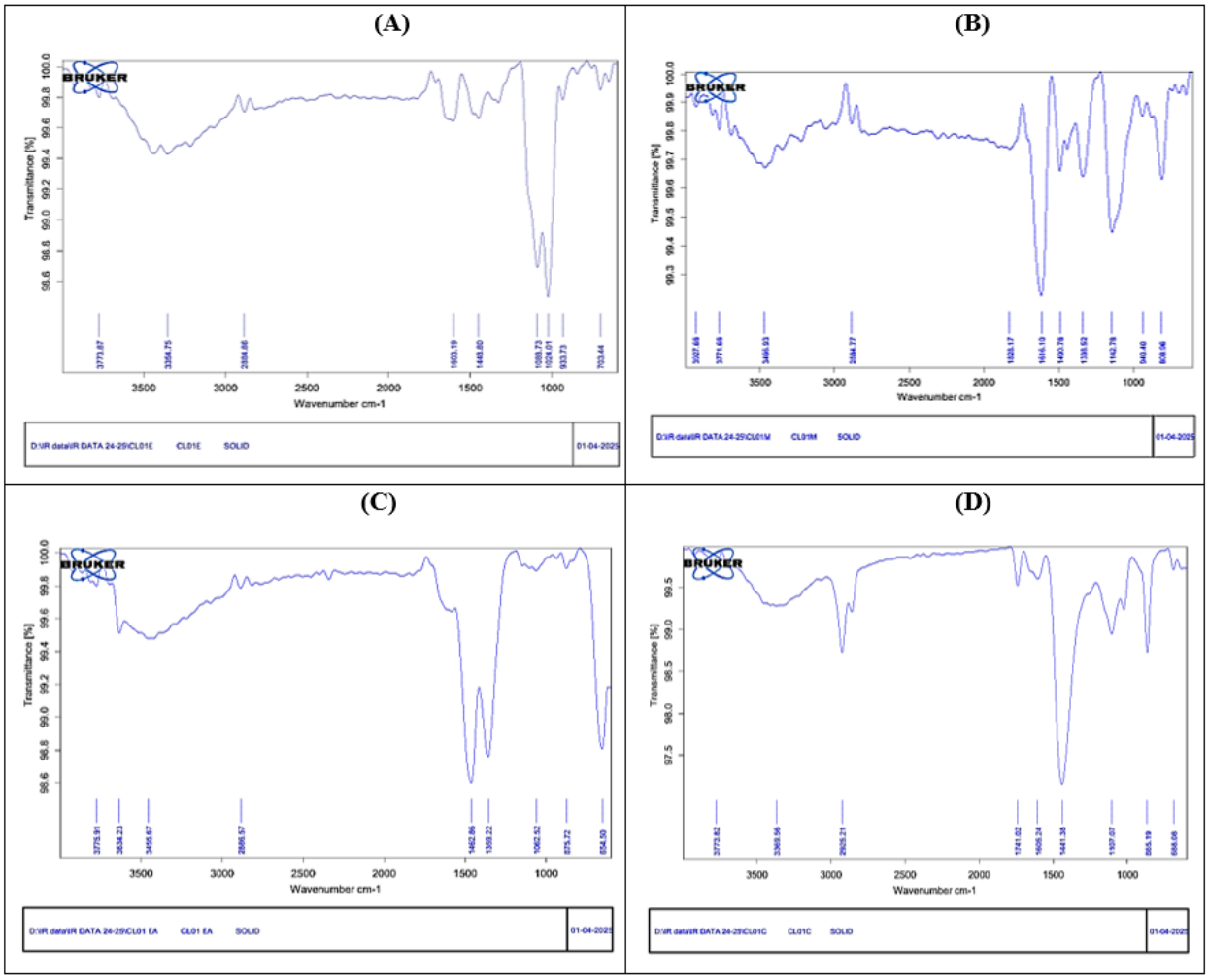

Figure 1. FTIR spectra of *Cyperus rotundus* L. leaf extracts obtained using different solvents. (A-Ethanol, B-Methanol, C-Ethyl Acetate D-Chloroform)

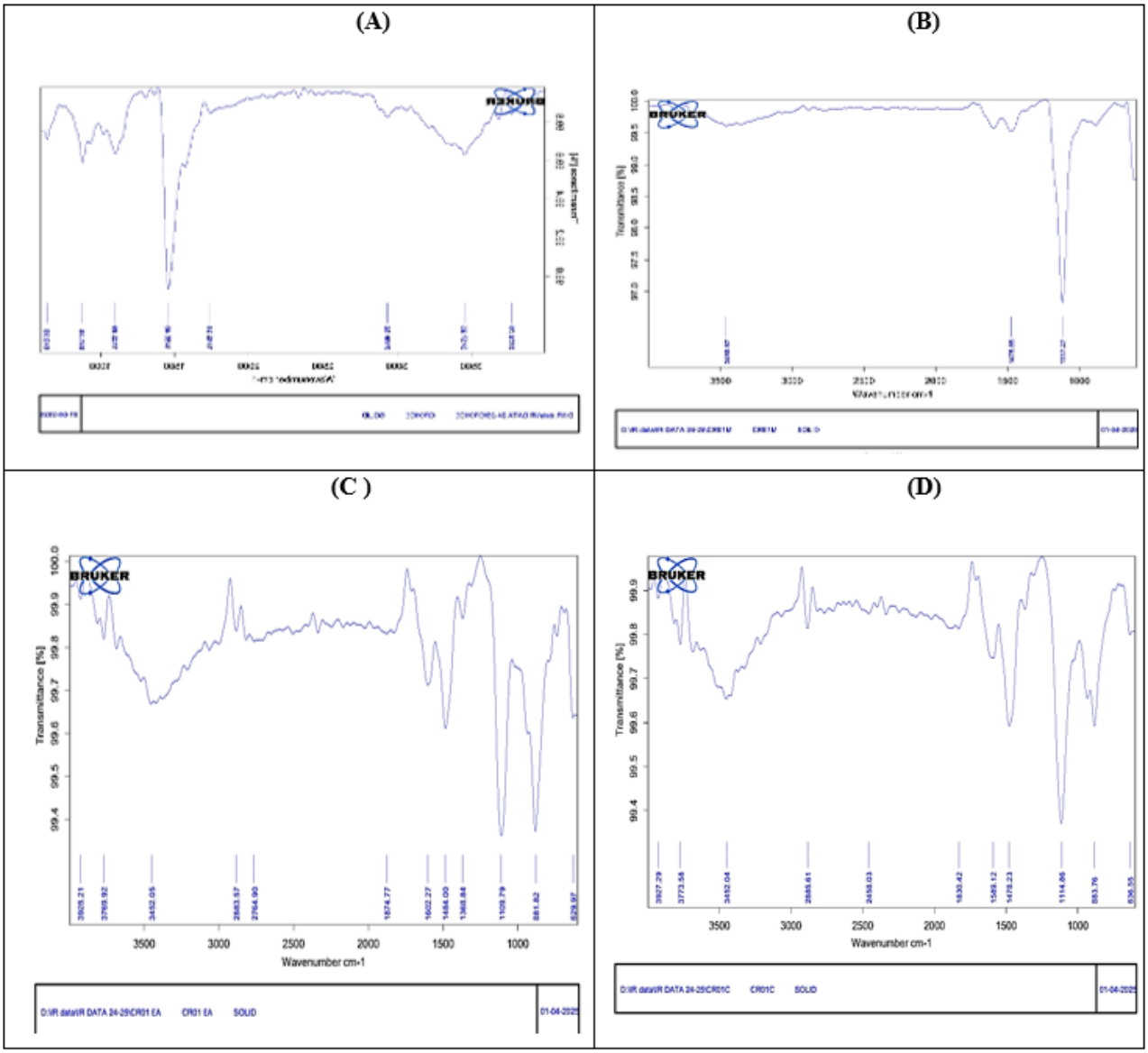

Figure 2. FTIR spectra of *Cyperus rotundus* L. rhizome extracts obtained using different solvents. (A-Ethanol, B-Methanol, C-Ethyl Acetate D-Chloroform)

Table 1. Comparative FTIR peak assignment of *Cyperus rotundus* leaf and rhizome extracts obtained using different solvents.

Plant Part	Solvent	Major Absorption Bands (cm^{-1})	Functional Group Assignment	Possible Phytochemical Class
Leaf	Ethanol	3373, 3354	O–H stretching	Phenols, Alcohols
		2884	C–H stretching	Alkanes
		1603	C=C stretching	Aromatic compounds
		1088–1024	C–O stretching	Esters, Ethers

	Methanol	3466	O–H (H-bonded)	Phenols
		1828	C=O stretching	Ketones, Esters
		1616, 1490	Aromatic C=C	Flavonoids
		1142	C–O stretching	Esters
	Ethyl acetate	3455	O–H stretching	Phenols
		2886	C–H stretching	Alkanes
		1462	C=C aromatic	Aromatics
		1359–1062	C–O stretching	Ethers, Esters
	Chloroform	3457	O–H stretching	Phenols
		2936	C–H stretching	Aliphatic chains
		1742	C=O stretching	Esters, Ketones
		1102	C–O stretching	Ethers
Rhizome	Ethanol	3373	O–H stretching	Phenols
		2925	C–H stretching	Alkanes
		1741	C=O stretching	Esters
		1605	C=C aromatic	Aromatics
		1107	C–O stretching	Alcohols
	Methanol	3458	O–H stretching	Alcohols
		1475	C–H bending	Aromatics
		1117	C–O stretching	Esters
	Ethyl acetate	3452	O–H stretching	Phenols
		2883	C–H stretching	Alkanes
		1874	C=O stretching	Anhydrides
		1602	C=C aromatic	Aromatics
	Chloroform	3452	O–H stretching	Phenols
		2885	C–H stretching	Alkanes
		1830	C=O stretching	Ketones

Table 1 presents the comparative FTIR peak assignments of *C. rotundus* leaf and rhizome extracts prepared using ethanol, methanol, ethyl acetate and chloroform. Broad hydroxyl (O–H) stretching bands were observed in all extracts within the range of 3458–3354 cm^{-1}, indicating the presence of hydroxyl-containing compounds such as phenolics and flavonoids. These compounds are commonly associated with antioxidant and anti-inflammatory activities reported in medicinal plants (Taheri et al., 2021; Xue et al., 2023). The occurrence of strong O–H absorption bands in polar solvent extracts suggests efficient extraction of phenolic constituents, particularly in methanol and ethanol fractions, which are known to possess high polarity and strong extraction efficiency for polyphenolic compounds (Azwanida, 2015). Aliphatic C–H stretching vibrations were observed between 2936–2883 cm^{-1} in most extracts, corresponding to the presence of saturated hydrocarbon

chains commonly associated with terpenoids, fatty acids and other lipid-derived phytoconstituents. These compounds are frequently reported in essential oil components and secondary metabolites of *C. rotundus*, particularly within rhizome tissues (Taheri et al., 2021).

Carbonyl (C=O) stretching bands were detected primarily in methanolic and chloroform fractions, especially within the range of 1742–1828 cm^{-1}. The presence of carbonyl functional groups indicates the occurrence of aldehydes, ketones, esters and carboxylic acid derivatives that are commonly found in plant secondary metabolites. Such compounds have been previously reported in phytochemical analyses of *C. rotundus* rhizomes and are associated with various biological activities including antimicrobial and hepatoprotective effects (Xue et al., 2023). Aromatic C=C stretching vibrations were observed between 1605–1462 cm^{-1} across several solvent extracts, suggesting the presence of aromatic compounds such as flavonoids and phenolic derivatives. These compounds contribute significantly to the pharmacological properties of medicinal plants and are widely documented in phytochemical studies of *C. rotundus* (Singh et al., 2014; Taheri et al., 2021). Additionally, absorption peaks recorded in the region of 1117–1024 cm^{-1} correspond to C–O stretching vibrations of alcohols, ethers and ester groups, which are characteristic of glycosides and phenolic compounds present in plant extracts (Coates, 2022).

Comparative observation of FTIR spectra revealed that rhizome extracts exhibited relatively more diverse carbonyl and aromatic peaks than leaf extracts, indicating a higher diversity of phytochemical constituents in the underground plant parts. This observation is consistent with previous phytochemical investigations reporting that rhizomes of *C. rotundus* contain higher concentrations of essential oils, sesquiterpenes and phenolic compounds compared to aerial parts (Xue et al., 2023). The presence of additional functional groups in rhizome extracts may therefore reflect the accumulation of specialized secondary metabolites involved in plant defense and adaptation. Furthermore, variations observed among the different solvent extracts highlight the significant influence of solvent polarity on phytochemical extraction efficiency. Polar solvents such as methanol and ethanol generally facilitate the extraction of phenolics, flavonoids and glycosides, whereas moderately polar and non-polar solvents such as ethyl acetate and chloroform tend to extract terpenoids, lipids and other hydrophobic compounds (Azwanida, 2015). The differences in FTIR spectral profiles among solvent extracts therefore indicate solvent-dependent variations in phytochemical composition. The FTIR analysis confirms the presence of several important functional groups including hydroxyl, aliphatic, carbonyl, aromatic and C–O groups in both leaf and rhizome extracts of *C. rotundus*. These functional groups correspond to various classes of bioactive phytochemicals such as phenolics, flavonoids, terpenoids and glycosides. The comparative FTIR profiling further suggests that rhizome extracts possess relatively greater phytochemical diversity than leaf extracts, highlighting the potential of rhizomes as a richer source of biologically active compounds. The results obtained in the present study are consistent with earlier phytochemical investigations and support the importance of solvent selection in the extraction and characterization of plant-derived bioactive constituents.

CONCLUSION

The present study provides a comparative FTIR spectroscopic evaluation of leaf and rhizome extracts of *Cyperus rotundus* obtained using solvents of varying polarity. The FTIR spectral profiles revealed the presence of several important functional groups including hydroxyl (O–H), aliphatic (C–H), carbonyl (C=O), aromatic (C=C) and C–O stretching vibrations. These functional groups are typically associated with major classes of phytochemicals such as phenolics, flavonoids, terpenoids and glycosides, which are widely reported to contribute to the pharmacological potential of medicinal plants (Taheri et al., 2021; Xue et al., 2023).

The study further highlights the influence of solvent polarity on the extraction efficiency of phytochemicals. Polar solvents such as methanol and ethanol exhibited stronger absorption bands corresponding to hydroxyl and aromatic functional groups, suggesting a greater extraction efficiency for phenolic and flavonoid compounds. Previous investigations have similarly reported that solvent polarity plays a crucial role in determining the qualitative and quantitative recovery of plant secondary metabolites (Azwanida, 2015; Sasidharan et al., 2011).

Comparative spectral interpretation indicated that rhizome extracts of *C. rotundus* demonstrated relatively greater diversity of functional groups compared to leaf extracts. This observation suggests that rhizomes may possess a richer phytochemical composition, which is consistent with earlier phytochemical studies reporting higher concentrations of essential oils, sesquiterpenes and other bioactive metabolites in the underground parts of the plant (Taheri et al., 2021; Xue et al., 2023). Such phytochemical diversity supports the traditional medicinal use of rhizomes and highlights their potential as an important source of biologically active compounds.

Furthermore, the findings of this investigation confirm the applicability of FTIR spectroscopy as a rapid, reliable, and non-destructive analytical technique for preliminary phytochemical screening of medicinal plants. FTIR-based fingerprinting provides valuable

information about functional group composition and serves as an effective preliminary tool prior to detailed phytochemical characterization using advanced chromatographic and spectrometric techniques (Stuart, 2004; Kumar et al., 2017). The study demonstrates that solvent-dependent extraction combined with FTIR analysis provides an efficient approach for the rapid characterization of phytochemical constituents in *C. rotundus*. However, further investigations employing advanced analytical techniques such as gas chromatography–mass spectrometry (GC–MS) or liquid chromatography–mass spectrometry (LC–MS) are recommended for the isolation, identification and structural elucidation of individual bioactive compounds. Additionally, bioactivity-guided fractionation and pharmacological evaluation would provide deeper insights into the therapeutic potential of these phytochemicals and support the development of plant-derived pharmaceutical agents.

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Conflict of Interest: The author declares that there is no conflict of interest.

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