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Phytochemical Profiling And Spectroscopy Characterization Of Coleus Vettiveroides K.C. Jacob

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Abstract

Coleus vettiveroides (syn. Plectranthus vettiveroides), a member of the Lamiaceae family, is a medicinal plant traditionally used in Siddha medicine for treating various ailments. Its roots, rich in bioactive compounds such as alkaloids, flavonoids and terpenoids are valued for treating allergies, bronchitis, rheumatism and other ailments. Phytochemical and FTIR analyses revealed a diverse chemical profile, with functional groups like alkanes, esters and sulfonates linked to medicinal properties. The FTIR analysis of ethanolic root, stem and leaf extracts from C. vettiveroides revealed diverse functional groups, highlighting the presence of bioactive compounds include N-H stretching (amines and amine salts), C=O stretching (ketones, esters and conjugated carbonyls) and O-H stretching/bending (alcohols and phenols). GC-MS spectra of ethanol leaf extracts of C. vettiveroides revealed several compounds in the extract, with notable richness in n-hexadecanoic acid and γ-sitosterol , n-Hexadecanoic acid a fatty acid, is widely recognized for its antioxidant and anti-inflammatory properties, while γ-sitosterol a phytosterol. The stem extract identified three compounds, underscoring the significance of 4-n-butylthiane, s,s-dioxide as a key contributor to the extract's bioactivity. The rich components are present in root extracts include ferruginol, stigmasterol and aromadendrene (dehydro). This study highlighted the therapeutic potential of C. vettiveroides as a source of valuable bioactive compounds for medicinal applications.

Keywords: *Coleus vettiveroides, FTIR, GC-MS, medicinal properties, phytochemical analysis.*

1. INTRODUCTION:

Coleus vettiveroides K.C.Jacob (syn. Plectranthus vettiveroides (K.C.Jacob) N.P.Singh & B.D.Sharma), belonging to the Lamiaceae family, is a traditional medicinal plant widely used in Siddha medicine for treating various ailments (Murugan et al., 2015; Ravikumar and Ved, 2000). Although this species is considered endemic to southern India, its presence in the wild has not been documented, as it has only been reported under cultivation since its discovery. It is a versatile herb with a wide range of uses across various regions of the world. Belonging to the Lamiaceae (formerly Labiatae) family and the Plectranthus genus, this aromatic perennial herb typically grows to a height of 30–90 cm. It features thick, fleshy stems and leaves and is known for its succulent nature. A highly aromatic, extensively branched, fleshy herb with pubescent stems and leaves that emit a distinctive fragrance (Wadikar and Patki, 2016).Currently, the plant is cultivated on a small scale in selected regions of Tamil Nadu, India, primarily for its valuable aromatic roots. It is classified as an underutilized crop species, along with eight other species of Plectranthus (Sailaja et al., 2021).

The entire plant of C. vettiveroides is known for its aromatic, bitter and cooling properties. It acts as a febrifuge, diaphoretic, stimulant and diuretic and is beneficial in conditions associated with an imbalance of pitta such as burning sensations, leprosy, skin disorders, leukoderma, fever, vomiting, diarrhea, ulcers as well as promoting digestion and menstrual health. The roots are particularly valued for treating allergies, bronchitis, internal bleeding, dizziness, headaches, rheumatism and have carminative properties. They are also used to address conditions like insanity, thirst and promote hair growth. Due to their medicinal benefits, the roots of C. vettiveroides are highly sought after in the market (Velvizhi et al., 2020)

Natural products obtained from plants are biologically active secondary metabolites with significant potential for treating various diseases. These bioactive substances include alkaloids, flavonoids, terpenoids, saponins and others etc.,. (Mohd Zishan, 2024). The root extract of C. vettiveroides was analyzed for its chemical composition using phytochemical screening and Fourier Transform Infrared Spectroscopy (FTIR). Phytochemical screening involves the identification of bioactive compounds such as alkaloids, flavonoids, saponins, terpenoids and phenols which are often associated with medicinal properties. FTIR spectroscopy, on the other hand was used to identify specific functional groups in the extract by measuring the absorption of infrared light at various wavelengths, helping to characterize the molecular structure and identify chemical components present in the root extract (Santhi et al., 2024). This study aims to identify bioactive compounds present in C. vettiveroides using the GC-MS technique, with the potential to discover therapeutically valuable compounds (Momoh Johnson Oshiobugie, et al 2017).

2. MATERIALS AND METHODS

2.1 Preparation of Plant extracts

The Coleus vettiveroides plant was collected from Kollidam in the Mayiladuthurai District of Tamil Nadu which shown in Figure 1 (a and b). Its identification and authentication were carried out by the Department of Botany at Annamalai University, where it was assigned the accession number AUBOT#606. The collected plant material was thoroughly washed to eliminate any debris and then shade-dried. After drying, the roots, stem and leaf were ground into a coarse powder using a mechanical pulverizer. A total of 100 g of the powder was subjected to repeated extractions with Ethanol solvent was used in a 500 mL round-bottom flask with 250 mL of solvent and the extraction was carried out in a Soxhlet apparatus. After extraction, the solution was filtered and the filtrate was allowed to dry at room temperature. The concentrated extract was then collected and further concentrated using a rotary evaporator (Heidolph) under controlled temperature and pressure conditions (Nie et al., 2013).

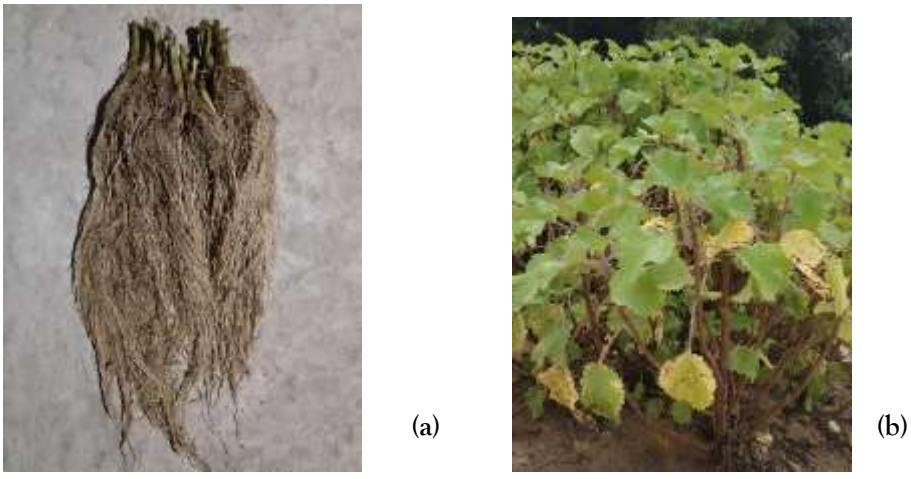

Figure 1 (a and b) Morphology of collected plant C. vettiveroides root (a) and shoot (b)

2.2 Preliminary phytochemical analysis

The qualitative phytochemical screening of the extracts was conducted following the methodologies described below.

2.2.1 Alkaloids:
Three drops of Wagner's reagent (a solution of iodine in potassium iodide were added to three drops of methanolic and plant extracts. The appearance of a reddish-brown precipitate indicated the presence of alkaloids (Mussa et al., 2024).

2.2.2 Tannins:
Gelatin Test: A 1% gelatin solution with sodium chloride is added to the plant extract. The appearance of a white precipitate confirms the presence of tannins
(Nishi Yadav, 2020).

2.2.3 Flavonoids:
The plant extract was placed in a test tube, followed by the addition of 5 ml of dilute ammonia and concentrated sulfuric acid. The formation of yellow precipitates indicates the presence of flavonoids (Sujamol et al., 2020).

2.2.4 Glycosides:
The plant extract was mixed with 5 ml of Molisch's reagent and concentrated sulfuric acid in a test tube. The appearance of a violet color confirms the presence of glycosides (Mohd Zishan, 2024).

2.2.5 Saponins:
A small quantity of the plant extract is placed in a test tube, and approximately 5 ml of distilled water is added. The mixture is shaken vigorously for a few minutes. The formation of stable and lasting froth indicates the presence of saponins (Devi and Battu, 2019).

2.2.6 Phenols:
To a small amount of the plant extract, a few drops of ferric chloride solution are added. The appearance of a blue, green, or purple coloration confirms the presence of phenols (Misganaw Gedlu Agidew, 2022).

2.2.7 Sterols:
Add 2 mL of acetic anhydride to the plant extract, followed by the addition of concentrated sulfuric acid. The development of a blue or green coloration indicates the presence of sterols (Mohamed Azar et al., 2022).

2.2.8 Terpenoids:
In a test tube, 2 mL of chloroform is mixed with 0.5 mL of the plant extract. Then, 3 mL of concentrated sulfuric acid is carefully added to form a distinct layer. The presence of terpenoids is indicated by a reddish-brown coloration at the interface (Rao, 2016).

2.3 Fourier Transform Infrared Spectroscopy (FTIR) Analysis
Infrared (IR) spectroscopy is a highly effective analytical method employed for chemical identification, relying on the specific absorption of infrared radiation by different substances. When molecules absorb infrared radiation, they vibrate, producing unique absorption patterns that are captured in the form of an absorption spectrum. For the FTIR analysis, a small quantity of plant extract was directly placed onto the germanium crystal of the infrared spectrometer. Consistent pressure was applied to achieve uniform distribution of the sample. The infrared absorbance data was recorded over a wavenumber range from 4000 cm^{-1} to 650 cm^{-1}, and the results were subsequently analyzed using Agilent technologies software The reference spectra were obtained from the cleaned blank crystal before analyzing each sample replicate. All spectra were recorded with a resolution of 4 cm^{-1} (Nivetha & Prasanna, 2016).

2.4 GC-MS Analysis

The Clarus 680 GC was used in the analysis employed a fused silica column, packed with Elite-5MS (5% biphenyl 95% dimethylpolysiloxane, 30 m × 0.25 mm ID × 250μm df) and the components were separated using Helium as carrier gas at a constant flow of 1 ml/min. The injector temperature was set at 260°C during the chromatographic run. The 1μL of plant extract sample was injected into the instrument the oven temperature was as follows: 60 °C (2 min); followed by 300 °C at the rate of 10 °C min^{-1}; and 300 °C, where it was held for 6 min. The mass detector conditions were: transfer line temperature of 240 °C; ion source temperature of 240 °C; and ionization mode electron impact at 70 eV, a scan time of 0.2 sec and scan of 0.1 sec. The fragments from 40 to 600 Da. The spectrum of the components were compared with the database of a spectrum of known components stored in the GC-MS NIST (2008) library.

3. RESULTS

3.1 Phytochemical analysis of C. vettiveroides extracts

The examination of bioactive compounds in the root, stem and leaf extracts of C. vettiveroides revealed the presence, absence or lack of detection of various phytochemicals. Ethanol extracts from the root, stem and leaf of C. vettiveroides were shown to contain alkaloids, flavonoids, glycosides, tannins, saponins, sterols and terpenoids, with phenolic compounds notably absent (Table 1).

Table 1: Preliminary phytochemical screening of active constituents in C. vettiveroides extracts

S. No	Phytochemical tests	Ethanolic root extract	Ethanolic stem extract	Ethanolic leaf Extract
1	Alkaloids	+	+	-
2	Tannins	-	-	-
3	Saponins	+	+	+
4	Flavonoids	+	-	+
5	Phenols	+	+	+
6	Glycosides	-	-	-
7	Sterols	+	+	-
8	Terpenoids	+	+	+

(+) Present; (-) Absent

3.2 FTIR analysis of C. vettiveroides extracts

FT-IR analysis of C. vettiveroides leaf, stem and root extracts revealed diverse functional groups, indicating a rich chemical composition and bioactive potential are presented in (Figure 2, 3 and 4) and (Table 2, 3 and 4). The leaf extract showed groups like N-H (amines), C-H (alkanes), N=C=S (isothiocyanates), C=C (alkenes), S=O (sulfonates), and CO-O-CO (anhydrides), suggesting proteins, lipids, glucosinolates, flavonoids, and esters. The stem extract highlighted N-H (amines), C=O (conjugated ketones), O-H (phenols), C-O (ethers/alcohols), and N-O (nitro compounds), emphasizing its complex profile. Root extract analysis identified O-H (alcohols/phenols), C-H (alkanes/alkenes), C=O (α, β-unsaturated esters), C=C (alkenes), and S=O (sulfoxides).

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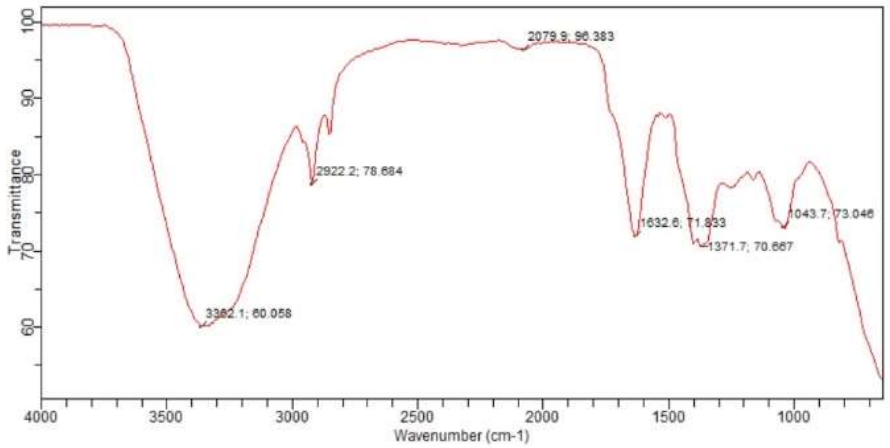

Figure 2: FT-IR spectrum of ethanol leaf extract of C. vettiveroides

Table 2: FT-IR absorption peaks and corresponding functional groups of C. vettiveroides ethanol leaf extract

S. No	Wave Number	Molecular Motion	Functional group	Absorption Intensity
1	3362.1;60.058	O-H Stretching	Aliphatic Primary amine	Curve
2	2922.2;78.684	C-H Stretching	Alkane	Sharp
3	2079.9;96.383	N=C=S Stretching	Isothiocyanate	Weak
4	1632.6;71.833	C=C Stretching	Alkene	Sharp medium
5	1371.7;70.667	S=O Stretching	Sulfonate	Medium
6	1043.7;73.046	CO-O-CO Stretching	anhydride	Medium

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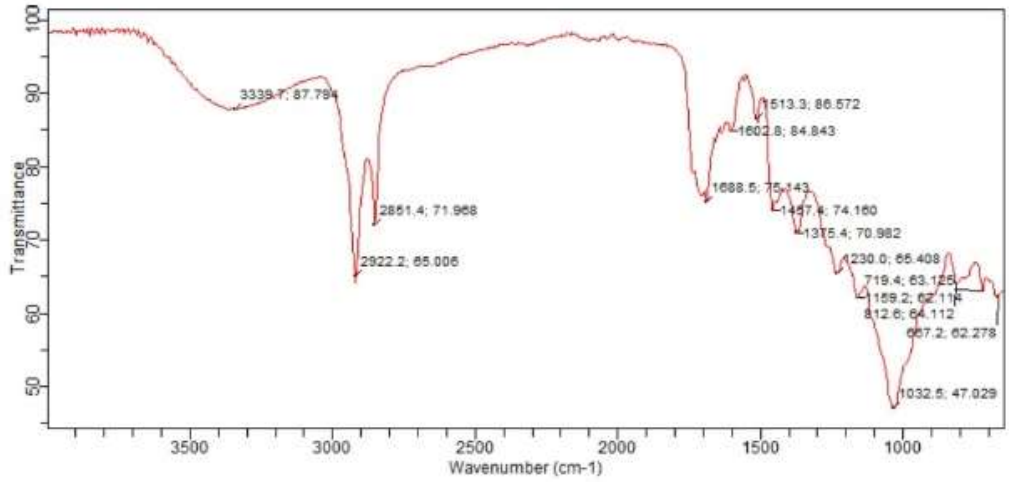

Figure 3: FT-IR spectrum of ethanol stem extract of C. vettiveroides

Table 3: FT-IR absorption peaks and corresponding functional groups of C. vettiveroides ethanol stem extract.

S. No	Wave Number	Molecular Motion	Functional group	Absorption Intensity
1	3339.7;87.794	O-H Stretching	Aliphatic, primary amine	Weak
2	2922.2;65.006	C-H Stretching	Aromatic	Sharp
3	2851.4;71.968	C-H Stretching	Alkane	Medium sharp
4	1688.5;75.143	C=O Stretching	Conjugated ketone	Medium
5	1513.3;86.572	N-O Stretching	Nitro compound	Weak
6	1457.4;74.160	C-H bending	Alkane	Weak
7	1375.4;70.982	O-H bending	Phenol	Medium
8	1230.0;65.408	C-O Stretching	Alkyl aryl ether	Weak sharp
9	1159.2;62.114	C-O Stretching	Tertiary alcohol	Weak

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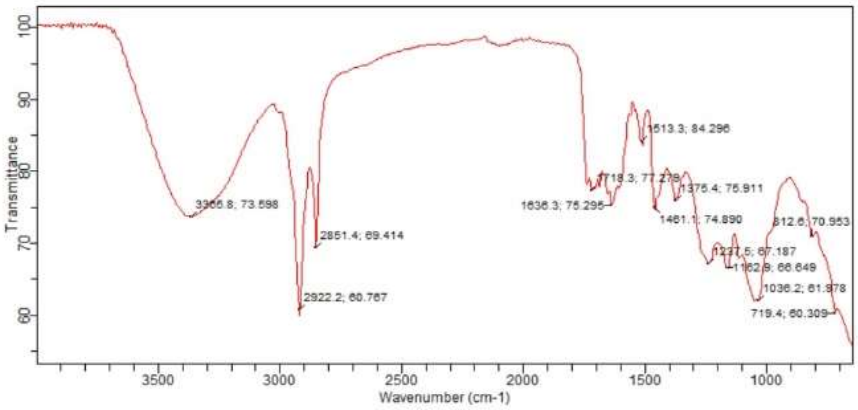

Figure 4: FT-IR spectrum of ethanol root extract of C. vettiveroides.

Table 4: FT-IR absorption peaks and corresponding functional groups of C. vettiveroides ethanol root extract

S. No	Wave Number	Molecular Motion	Functional group	Absorption Intensity
1	3365.8;73.598	O-H stretching	Alcohol	Medium
2	2922.2;60.767	C-H stretching	Alkene	Strong sharp
3	2851.4;69.414	C-H stretching	Alkanes	Medium
4	1718.3;77.279	C=O stretching	α, β-unsaturated ester	Medium
5	1636.3;75.295	C=C stretching	Alkene	Medium
6	1513.3;84.296	N-O stretching	Nitro compound	Medium
7	1461.1;74.890	C-H stretching	Alkane	Sharp medium
8	1375.4;75.911	O-H bending	Phenol	Medium
9	1237.5;67.187	C-O bending	Alkyl aryl ether	Weak
10	1162.9;66.649	C-O stretching	Ester	Medium
11	1036.2;61.978	S=O stretching	Sulfoxide	Medium
12	812.6;70.953	C-H bending	1,2,3,4- tetra substitum	Weak

3.3 GC-MS analysis of C. vettiveroides extracts

The bioactive compounds identified in the methanol extracts of the leaf (Figure 5), stem (Figure 6) and root (Figure 7) of Coleus vettiveroides are summarized in (Tables 5, 6, and 7), highlighted their retention times, peak areas, molecular formulas, molecular weights, and biological activities. This study identified 29 compounds, some of which hold notable medicinal significance (Momoh Johnson Oshiobugie and Asoro Iroghama Iyobosa, 2020). Among these, 14 compounds were identified in the leaf. Formic Acid Hydrazide,

1,2,4,5-Tetrazine, Hexahydro-1,2,4,5-Tetramethyl , S-Triazol, 3-Acetamido, 4-Morpholine acetonitrile, Nonamethylene glycol, n-hexadecanoic acid, oxirane, dodecyl, 9,12,15-octadecatrienal, pentadecanoic acid, decane, 5-methyl, 9,12,15-octadecatrienal, 1,4-dimethyl-7-oxo-4,7-dihydro-triazolo(3,4-c)triazine, cholesta-22,24-dien-5-ol, 4,4-dimethyl, gamma.-sitosterol, Formic Acid Hydrazide. GC-MS analysis of the ethanol leaf extract of c. vettiveroides identified 27 compounds, with butylphosphonic acid, pentyl 4-(2-phenylprop-2-yl) phenyl ester, and γ-sitosterol as the major components.

The stem extracts of C. vettiveroides identified three major compounds. The first compound, dimethyl-cyano-phosphine (C_3H_6NP), was detected at a retention time of 1.74 minutes with a peak area contribution of 3.88%. The second compound, tetramethyl ammonium borohydride ($C_4H_{16}NB$), appeared slightly later at 1.88 minutes and accounted for 10.132% of the total peak area. The most prominent compound identified in the extract was 4-n-butylthiane, S,S-dioxide ($C_9H_{18}O_2S$), which was observed at a retention time of 19.26 minutes and contributed the highest peak area of 18.12%. These findings highlight the chemical composition of the ethanol stem extract, with 4-n-butylthiane, S,S-dioxide being the most abundant compound. However, further research is needed to determine the biological significance of these compounds.

Twelve compounds were also identified in the root are acetic acid, 2-methylene-bicyclo[3.2.1]oct-6-en-8-yl ester, benzenemethanamine, 3,4-dimethyl, aromadendrene, dehydro, indapamide,benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl, ferruginol, 2,2,5-trimethyl-cyclohexane-1,4-diol, 7-methoxy-8-oxa-1-azabicyclo(5.1.0)octane, 2-octadecyl-propane-1,3-diol, stigmasterol, 1-octadecyne, octa-decanal. The medicinal uses of the compounds found in the root, stem and leaves of the plant are summarized in (Tables 5, 6, and 7) respectively.

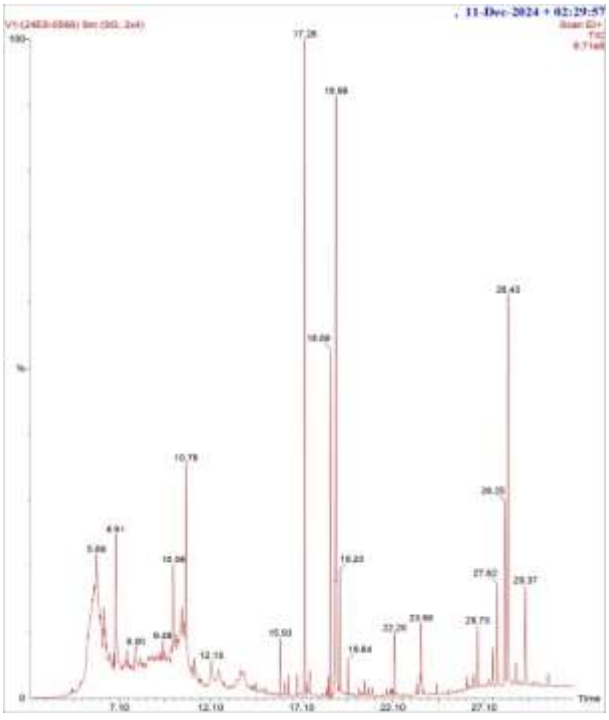

Figure 5: GC-MS spectrum of ethanol leaf extracts of C. vettiveroides.

Table. 5. GC-MS analysis of Ethanol leaf extracts of c. vettiveroides.

1.	Formic Acid Hydrazide	CH_4ON_2	60	5.86	8.755	624-84-0	Antibacterial,
2.	1,2,4,5-Tetrazine, Hexahydro-1,2,4,5-Tetramethyl	$C_6H_{16}N_4$	144	6.91	3.12	20717-38-8	Antifungal, Antibacterial (Nie et al., 2013)
3.	S-Triazol, 3-Acetamido	$C_4H_6ON_4$	126	10.06	3.12	5295-23-8	Antibacterial (Strzelecka & Świątek, 2021)
4.	4-Morpholine acetonitrile	$C_6H_{10}ON_2$	126	10.76	3.51	5807-02-3	NF
5.	Nonamethylene glycol	$C_{11}H_{24}O_3$	204	15.93	0.90	900129-54-8	NF
6.	n-hexadecanoic acid	$C_{16}H_{32}O_2$	256	17.28	15.39	57-10-3	Anti-inflammatory (Aparna et al., 2012). Antioxidant &Antibacterial (Ganesan et al., 2024)
7.	oxirane, dodecyl	$C_{14}H_{28}O$	212	18.69	5.96	3234-28-4	NF
8.	9,12,15-octadecatrienal	$C_{18}H_{30}O$	262	18.99	16.87	26537-71-3	Antimicrobial, Anticancer, Antiarthritic and Antiasthmatic (Kumar, 2021)
9.	pentadecanoic acid	$C_{15}H_{30}O_2$	242	19.20	2.08	1002-84-2	NF
10.	decane, 5-methyl	$C_{11}H_{24}$	156	22.20	1.12	13151-35-4	NF

11.	9,12,15-octadecatrienal	$C_{18}H_{30}O$	262	23.65	1.26	26537-71-3	Antibacterial and Antioxidant activity (Padma et al., 2019)
12.	1,4-dimethyl-7-oxo-4,7-dihydro-triazolo(3,4-c)triazine	$C_6H_7ON_5$	165	26.75	1.36	61402-40-2	NF
13.	cholesta-22,24-dien-5-ol, 4,4-dimethyl	$C_{29}H_{48}O$	412	27.82	2.77	900128-66-1	Trypanocidal Activity and Antibacterial (Venkataravana et al., 2024)
14.	gamma.-sitosterol	$C_{29}H_{50}O$	414	28.43	1.02	83-46-5	Antidiabetic (Tripathi et al., 2013), Anticancer activity (Sundarraj et al., 2012)

Figure 6: GC-MS spectrum of ethanol stem extracts of C. vettiveroides

Table 6. GC-MS analysis of Ethanol stem extracts of C. vettiveroides.

S.NO	Compound name	Molecular formula	Molecular weight (g/mol)	Retentior Time(minutes)	Peak Area (%)	CAS Number	Biological Activity

1	dimethyl-cyano-phosphine	C_3H_6NP	87	1.74	3.88	6861-61-6	NF
2	tetramethyl ammonium borohydride	$C_4H_{16}NB$	89	1.88	10.132	16883-45-7	NF
3	4-n-butylthiane, s,s-dioxide	$C_9H_{18}O_2S$	190	19.26	18.12	70928-51-7	Antibacterial (Allinson I.B et al 2016)

(NF - Not Found)

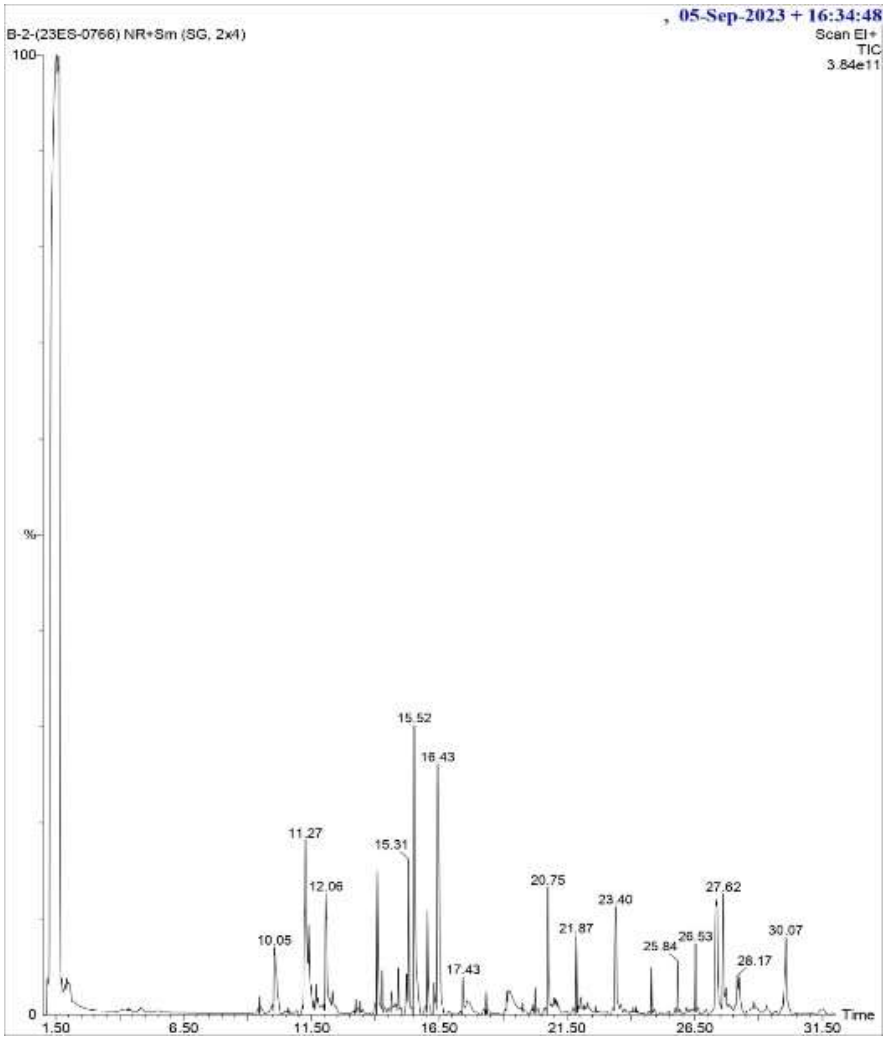

Figure 7: GC-MS spectrum of ethanol root extracts of C. vettiveroides

Table 7. GC-MS analysis of Ethanol root extracts of C. vettiveroides.

S.NO	Compound name	Molecular formula	Molecular weight (g/mol)	Retention Time (minutes)	Peak Area (%)	CAS Number	Biological Activity
1.	acetic acid, 2-methylene-bicyclo[3.2.1]oct-6-en-8-yl ester	$C_{11}H_{14}O_2$	178	10.05	1.67	900190-92-2	NF
2.	benzenemethanamine, 3,4-dimethyl	$C_9H_{13}N$	135	11.27	3.92	102-48-7	NF
3.	aromadendrene, dehydro	$C_{15}H_{22}$	202	15.31	1.63	900156-12-5	Antibacterial (Rural & Pernambuco, 2017)
4.	Indapamide	$C_{16}H_{16}O_3N_3ClS$	365	15.52	1.31	26807-65-8	NF
5.	benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl	$C_{15}H_{22}$	202	16.43	5.24	644-30-4	Anti-inflammatory, antibacterial, and anti-diabetic (Anum et al., 2024)
6.	Ferruginol	$C_{20}H_{30}O$	286	20.75	1.38	514-62-5	NF
7.	2,2,5-trimethyl-cyclohexane-1,4-diol	$C_9H_{18}O_2$	158	21.87	-	900193-39-1	NF
8.	7-methoxy-8-oxa-1-azabicyclo(5.1.0)octane	$C_7H_{13}O_2N$	143	23.40	-	35009-23-5	NF
9.	2-octadecyl-propane-1,3-diol	$C_{21}H_{44}O_2$	328	25.84	-	5337-61-1	NF
10.	Stigmasterol	$C_{29}H_{48}O$	412	27.62	1.30	83-48-7	Antioxidant, anti-inflammatory, anti-cancer, and anti-diabetic (Bakrim et al., 2022)

11.	1-octadecyne	$C_{18}H_{34}$	250	28.17	-	629-89-0	Anticancer, antibacterial, and antioxidant (Belakhdar et al., 2015)
12.	Octadecanal	$C_{18}H_{36}O$	268	30.07	1.69	638-66-4s	Antibacterial activity(Tripathi et al., 2013)

(NF - Not Found)

4. DISCUSSION:

This suggested that the ethanol extract of C. vettiveroides included all analyzed phytochemicals except for phenols. As per the statement, the ethanol extract of Coleus vettiveroides contains all the tested phytochemicals except phenolic compounds. The findings of the current study and those of (Velvizhi et al. 2019) both highlighted the consistent presence of terpenoids and sterols across various solvents, demonstrating their widespread distribution. Differences are observed in the detection of alkaloids and flavonoids, which vary based on the plant part and solvent used. Both studies reported the absence of tannins and glycosides, while the current study emphasized ethanol's effectiveness in extracting phenols and saponins.

Comparisons with prior studies, such as those by Rosni Sunil et al. (2024), Sasikala et al. (2020), and Manikandan (2017), confirmed the chemical diversity while noting unique findings like isothiocyanates, anhydrides, sulfoxides, and alkyl aryl ethers in the current study. These results underscore the potential of C. vettiveroides extracts for bioactive applications.

The current study reported 12 additional compounds, including sesquiterpenes (aromadendrene), diterpenoids (ferruginol) and sterols (stigmasterol) and the GC-MS analysis of C. vettiveroides root essential oil identified 23 compounds, with Androstan-17-one (24.69%) being most abundant (Saraswathy and Mercy Lavanya, 2013). Both studies highlighted the oil's complex chemical profile, with variations likely due to analytical or environmental differences.

Comparatively, a study by (Wadikar & Patki 2016) on the root extract found different major compounds, such as androstan-17-one and spathulenol, but also detected γ-sitosterol. This suggested that the leaf and root of Coleus vettiveroides contain distinct bioactive compounds, highlighted the plant's potential for diverse therapeutic applications. The stem contains three compounds and it includes: dimethyl-cyano-phosphine, tetramethylammonium borohydride, 4-n-butylthiane, s,s-dioxide.

The comparative analysis of the essential oil composition of Chrysopogon vettiveroides roots conducted by A. (Saraswathy & Mercy Lavanya, 2013) and the present study highlights both commonalities and variations in the chemical constituents. The GC-MS analysis by Saraswathy and Lavanya (2013) identified 36 bioactive

compounds, with Androstan-17-one, 3-ethyl-3-hydroxy-(5α)- being the most abundant at 24.69%, followed by other significant constituents such as 3-Isopropyltricyclo undec-3-en-10-ol, (-)-Spathulenol, and Z-Valerenyl acetate. The study revealed a dominance of sesquiterpenes, alcohols, and hydrocarbons, indicating potential pharmacological and industrial applications. In contrast, the current study identified 12 additional compounds in the root essential oil, including acetic acid, 2-methylene-bicyclo[3.2.1]oct-6-en-8-yl ester, benzenemethanamine, 3,4-dimethyl, aromadendrene, dehydro, and ferruginol, among others. Notably, compounds such as stigmasterol, a known phytosterol with medicinal properties, and 1-octadecyne, a long-chain alkyne, were detected. The presence of these additional compounds suggests a broader chemical diversity in C. vettiveroides roots, which could contribute to enhanced bioactivity and expanded potential applications in medicinal, cosmetic, and industrial fields.

The variations between the two studies may be attributed to differences in environmental conditions, extraction methods, or analytical techniques. The additional compounds identified in the present study suggest that further research may uncover more bioactive molecules with unique therapeutic properties. This highlights the importance of continued phytochemical investigations into C. vettiveroides, as its essential oil holds significant promise for various commercial and medicinal applications.

5. CONCLUSION

This investigation aids in identifying and predicting the structures of bioactive compounds within the plant that may have medicinal potential. Moreover, it strengthens and extends the knowledge of the plant's traditional uses.

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