International Journal of
Life Sciences
International Peer Reviewed Open Access Refereed Journal

Int. J. of Life Sciences, 2024; 12 (2): 163-169
ISSN:2320-7817(p) | 2320-964X(o)

Research Article Open Access

Characterization of Phytochemical compounds in *Digitaria ciliaris* (Retz) Koel Leaf Extract Using GC-MS Analysis

Warghat VR*, Ratnaparkhi DM and Pawade PN

Smt. Narsamma Arts, Commerce and Science College, Amravati 444606, Maharashtra, India.
*Corresponding author Email: warghatvishal@gmail.com

Manuscript details:

Received: 26.05.2024
Accepted: 28.06.2024
Published: 31.07.2024

Cite this article as:
Warghat VR, Ratnaparkhi DM and Pawade PN (2024) Characterization of Phytochemical compounds in *Digitaria ciliaris* (Retz) Koel Leaf Extract Using GC-MS Analysis, *Int. J. of Life Sciences*, 12 (2): 163-169.

Available online on http://www.ijlsci.in
ISSN: 2320-964X (Online)
ISSN: 2320-7817 (Print)

ABSTRACT

This study aimed to explain the phytochemical profile of *Digitaria ciliaris* (Retz) Koel leaf ethanol extract using Gas Chromatography-Mass Spectrometry (GC-MS) analysis. *Digitaria ciliaris*, commonly known as Southern crabgrass or summer grass, is traditionally recognized for its medicinal properties, including anti-inflammatory and anti-diabetic effects. Leaves were collected from Borgaon, Amravati, India, and subjected to ethanol extraction. GC-MS analysis identified a complex mixture of sixteen compounds, with hexanoic acid, ethyl ester (36.22%) being the most abundant, followed by 2,2,4-trimethyl-1,3-pentanediol diisobutyrate (15.33%) and 2-myristynoyl pantetheine (9.70%). Other notable compounds included pregna-6,16-diene-11,20-diol, octanoic acid, ethyl ester, and β-N-acetylneuraminic acid derivatives. The identified compounds suggest a range of pharmacological activities, such as antimicrobial, anti-inflammatory, antiviral, and immune-modulating effects. This comprehensive phytochemical characterization underscores the therapeutic potential of *Digitaria ciliaris* leaf extract, warranting further research to isolate these bioactive compounds and evaluate their individual and synergistic effects in various biological models. The findings contribute to a deeper understanding of the medicinal properties of *Digitaria ciliaris* and support its potential use in pharmaceutical and nutraceutical applications.

Keywords: *Digitaria ciliaris*, GC-MS analysis, phytochemical profiling, ethanolic extract, bioactive compounds.

INTRODUCTION

Digitaria ciliaris (Retz) Koel, commonly known as Southern crabgrass or summer grass, is a prevalent annual grass within the Poaceae family. It thrives in tropical and subtropical regions, often found in

diverse habitats such as agricultural fields, roadsides, and disturbed areas. Throughout history, traditional medicine has embraced *Digitaria ciliaris* for its alleged medicinal virtues, ranging from anti-inflammatory to anti-diabetic effects, among others..

The analysis of phytochemical constituents plays a pivotal role in unraveling the bioactive components present in medicinal plants, thereby shedding light on their potential therapeutic applications. Among the various analytical techniques utilized for phytochemical profiling, Gas Chromatography-Mass Spectrometry (GC-MS) emerges as a potent tool for identifying and quantifying diverse chemical compounds within plant extracts.

The medicinal efficacy of *Digitaria ciliaris* is often attributed to its diverse phytochemical composition, which includes alkaloids, flavonoids, phenolic compounds, and terpenoids. These chemical constituents have been associated with a spectrum of pharmacological activities, encompassing antioxidant, anti-inflammatory, antimicrobial, and anticancer properties. While previous studies have explored the phytochemical composition and pharmacological activities of *Digitaria ciliaris* extracts using various extraction solvents and analytical methods, a comprehensive GC-MS investigation focusing on the phytochemical characterization of *Digitaria ciliaris* leaf extract appears to be lacking.

Therefore, this study endeavours to address this gap by employing GC-MS analysis to characterize the phytochemical compounds present in *Digitaria ciliaris* (Retz) Koel leaf ethanol extract. Through elucidating the chemical profile of the extract, we aim to identify and quantify the bioactive constituents responsible for its medicinal properties. This endeavour holds promise for enhancing our understanding of the therapeutic potential of *Digitaria ciliaris* leaf extract and may contribute to its utilization in pharmaceutical and nutraceutical applications.

MATERIALS AND METHODS

Collection of Plant Material

Digitaria ciliaris (Retz) Koel leaves were collected from Borgaon, District Amravati, Maharashtra, India. Healthy and mature leaves were carefully handpicked to minimize contamination and damage.

Preparation of Leaf Extract

The collected *Digitaria ciliaris* leaves were thoroughly washed with distilled water to remove any adhering dirt or debris. After drying at room temperature, the leaves were finely ground into powder using a mechanical grinder. The powdered plant material was then subjected to ethanol extraction using a Soxhlet extractor. Ethanol was chosen as the solvent due to its ability to extract a wide range of phytochemicals. The extraction process was carried out to ensure efficient extraction of bioactive compounds. The resulting ethanol extract was filtered, and the solvent was evaporated under reduced pressure using a rotary evaporator to obtain a concentrated extract.

GC-MS Analysis

In this study, Gas Chromatography-Mass Spectrometry (GC-MS) was employed as the analytical tool to characterize the phytochemical Compounds within the *Digitaria ciliaris* leaf ethanol extract. Before analysis, the extract was dissolved in an appropriate solvent, typically methanol, to achieve an optimal concentration for analysis. A GC-MS instrument, tailored with specific specifications including column type, temperature program, and detector details, was meticulously chosen to ensure efficient separation and detection of compounds present in the extract. Chromatographic separation was meticulously optimized to ensure the clear resolution of individual compounds. Mass spectra were generated using electron ionization (EI) mode, and compound identification was facilitated by comparing retention times and mass spectra with those of reference standards accessible in the NIST Mass Spectral Library. This approach ensured accurate and reliable identification of phytochemical constituents within the *Digitaria ciliaris* leaf ethanol extract.

RESULTS AND DISCUSSION

The GC-MS analysis of the ethanolic extract of *Digitaria ciliaris* leaf revealed a complex mixture of compounds. A total of sixteen distinct compounds were identified, each characterized by its retention time (RT), molecular weight, molecular formula, and peak area percentage. The identified compounds and their corresponding data are presented in Table 1 and Fig.1. The most abundant compound in the extract was Hexanoic acid, ethyl ester, which accounted for 36.22% of the total peak area. This was followed by

2,2,4-Trimethyl-1,3-pentanediol diisobutyrate, with a peak area percentage of 15.33%, and 2-Myristynoyl pantetheine, which represented 9.70% of the extract. Other notable compounds included Pregna-6,16-diene-11,20-diol, 3,9-epoxy-18-[N-methyl-N-[14-(2'-epoxy ethyl)]amino]- (8.79%), and Octanoic acid, ethyl ester (6.58%). Several compounds were present in smaller quantities, such as N-Acetylneuraminic acid, methyl ester-2-methyl-7,9-methyl-boronate-3,8-di (trimethylsilyl)- (0.38%), α-D-Glucofuranose, 6-O-(trimethylsilyl)-, cyclic 1,2:3,5-bis(butylboronate) (0.69%), and Borinic acid, diphenyl-, methyl ester (0.99%).

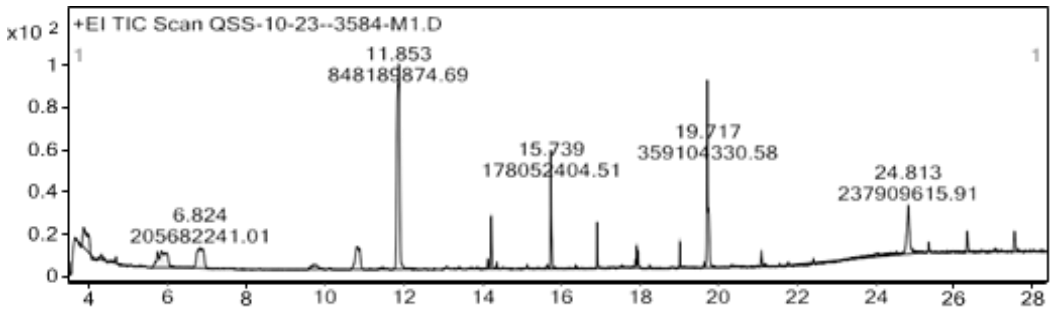
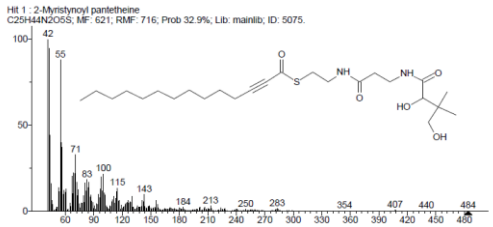
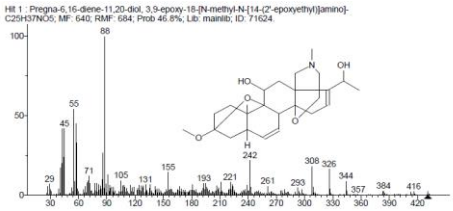
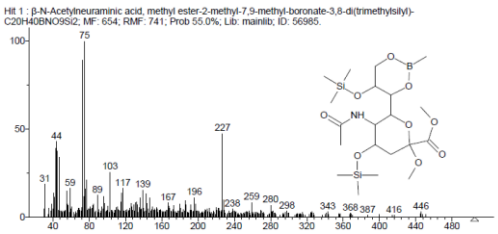
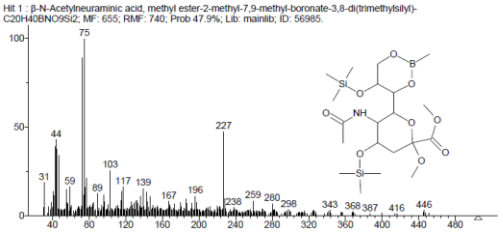
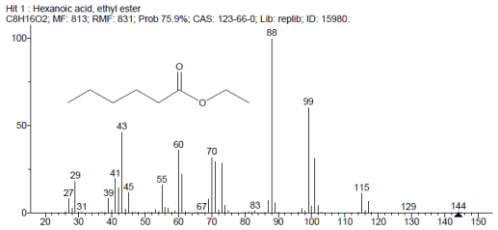
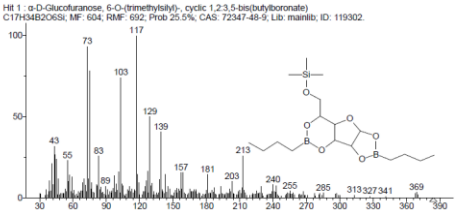
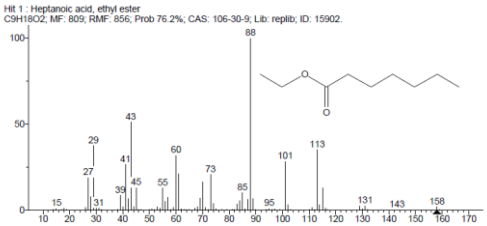
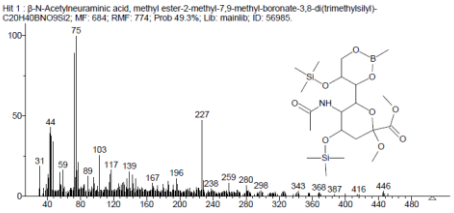
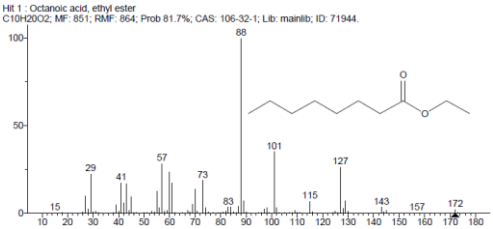
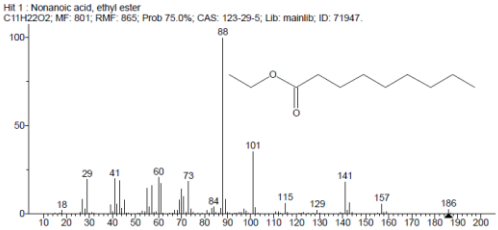


Fig.1. GC-MS chromatogram for ethanolic extract of *Digitaria ciliaris* leaf.

Table 1. GC-MS spectral analysis of ethanolic extract of *Digitaria ciliaris* leaf

No.	RT(Min)	Name of the compound	Peak Area %	Molecular Weight	Molecular Formula
1	5.888	2-Myristynoyl pantetheine	9.70	484	$C_{25}H_{44}N_2O_5S$
2	6.824	Pregna-6,16-diene-11,20-diol, 3,9- epoxy-18-[N-methyl-N-[14-(2'- epoxy ethyl)]amino]-	8.79	640	$C_{25}H_{37}NO_3$
3	9.727	β-N-Acetylneuraminic acid, methyl ester-2-methyl-7,9-methyl- boronate-3,8-di(trimethylsilyl)-	1.88	505	$C_{13}H_{23}NO_8$
4	10.796	N-Acetylneuraminic acid, methyl ester-2-methyl-7,9-methyl- boronate-3,8-di(trimethylsilyl	6.89	505	$C_{13}H_{23}NO_8$
5	11.853	Hexanoic acid, ethyl ester	36.22	144	$C_8H_{16}O_2$
6	14.131	α-D-Glucofuranose, 6-O- (trimethylsilyl)-, cyclic 1,2:3,5-bis(butylboronate)	0.69	384	$C_{17}H_{34}B_2O_6Si$
7	14.215	Heptanoic acid, ethyl ester	3.38	158	$C_9H_{18}O_2$
8	14.355	β-N-Acetylneuraminic acid, methyl ester-2-methyl-7,9-methyl- boronate-3,8-di(trimethylsilyl)-	0.38	505	$C_{13}H_{23}NO_8$
9	15.732	Octanoic acid, ethyl ester	6.58	172	$C_{10}H_{20}O_2$
10	16.913	Nonanoic acid, ethyl ester	2.27	186	$C_{11}H_{22}O_2$
11	17.91	Decanoic acid, ethyl ester	1.80	200	$C_{12}H_{24}O_2$
12	19.01	Phenol, 2,5-bis(1,1-dimethylethyl)-	1.06	206	$C_{14}H_{22}O$
13	19.717	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	15.33	286	$C_{16}H_{30}O_4$
14	21.081	Borinic acid, diphenyl-, methyl ester	0.99	196	$C_{13}H_{13}BO$
15	26.319	Octadecane, 3-ethyl-5-(2-ethylbutyl)-	1.84	366	$C_{26}H_{54}$
16	27.52	4a,7b-Dihydroxy-3- (hydroxymethyl)-1,1,6,8-tetramethyl-9a-((2- methylpropanoyl)oxy)-5-oxo-1a,1b,4	2.19	590	$C_{28}H_{38}Cl_2O_8$

2-Myristynoyl pantetheine	Pregna-6,16-diene-11,20-diol, 3,9-epoxy-18-[N-methyl-N-[14-(2'-epoxyethyl)]amino]-
	
β-N-Acetylneuraminic acid, methyl ester-2-methyl-7,9-methyl-boronate-3,8-di(trimethylsilyl)-	β-N-Acetylneuraminic acid, methyl ester-2-methyl-7,9-methyl-boronate-3,8-di(trimethylsilyl)-
	
Hexanoic acid, ethyl ester	α-D-Glucofuranose, 6-O-(trimethylsilyl)-, cyclic 1,2:3,5-bis(butylboronate)
	
Heptanoic acid, ethyl ester	β-N-Acetylneuraminic acid, methyl ester-2-methyl-7,9-methyl-boronate-3,8-di(trimethylsilyl)-
	
Octanoic acid, ethyl ester	Nonanoic acid, ethyl ester
	

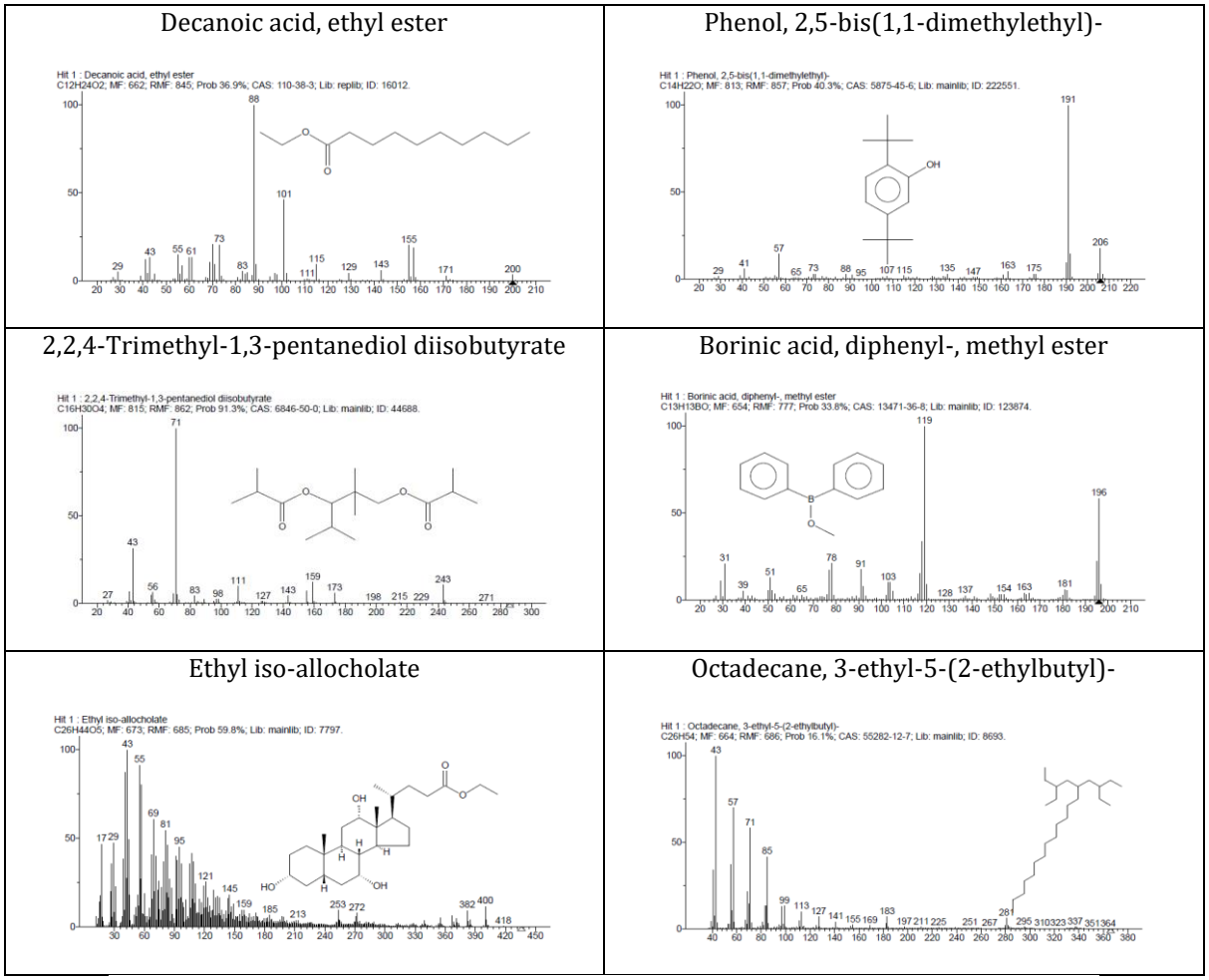


Fig. 2. Mass spectra of identified compound from ethanolic extract of *Digitaria ciliaris* leaf

The GC-MS analysis highlights the presence of a diverse array of bioactive compounds in the ethanolic extract of *Digitaria ciliaris* leaf. The high content of ethyl esters of fatty acids such as hexanoic, heptanoic, octanoic, nonanoic, and decanoic acids suggests that these esters may play a significant role in the biological activities of the extract. Ethyl esters of fatty acids are known for their antimicrobial and anti-inflammatory properties, which could contribute to the pharmacological effects observed in traditional uses of the plant. Hexanoic acid, ethyl ester, being the most prominent compound, is particularly noteworthy for its potential therapeutic properties, including antimicrobial and antifungal activities. Similarly, 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate, which was the second most abundant compound, is often used in plasticizers and may influence the extract's biological activity by modulating membrane fluidity and permeability. The presence of complex molecules such as 2-Myristynoyl pantetheine and Pregna-6, 16-diene-11,20-diol,3,9-epoxy-18-[N-methyl-N-[14-(2'-epoxy-ethyl)]amino]- highlights the extract's potential for multifaceted therapeutic applications. 2-Myristynoyl pantetheine, for instance, is a derivative of pantetheine, which is involved in coenzyme A synthesis and may have metabolic regulatory functions. The steroidal structure of Pregna-6,16-diene-11,20-diol suggests potential hormonal or anti-inflammatory activity. N-Acetylneuraminic acid derivatives, although present in lower concentrations, are important as they are related to sialic acids, which play critical roles in cellular communication and microbial pathogenesis. Their presence might indicate potential antiviral or immune-modulating properties of the extract. In conclusion, the ethanolic extract of *Digitaria ciliaris* leaf contains a variety of compounds with significant biological activities. The high proportion of fatty acid ethyl esters suggests strong antimicrobial and anti-inflammatory potentials, while the presence of complex molecules like steroids and sialic acid derivatives points towards a broader spectrum of pharmacological effects. Further studies

are warranted to isolate these compounds and evaluate their individual and synergistic effects in various biological models.

CONCLUSION

The GC-MS analysis of the ethanolic extract of *Digitaria ciliaris* leaf revealed a complex and diverse composition of bioactive compounds, with a total of sixteen identified substances. The extract was predominantly composed of ethyl esters of fatty acids, including hexanoic, heptanoic, octanoic, nonanoic, and decanoic acids, which are known for their antimicrobial and anti-inflammatory properties. The most abundant compound was Hexanoic acid, ethyl ester, representing 36.22% of the total peak area, followed by 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (15.33%) and 2-Myristynoyl pantetheine (9.70%).

The presence of complex molecules such as Pregna-6,16-diene-11,20-diol and β-N-Acetylneuraminic acid derivatives suggests potential hormonal, anti-inflammatory, antiviral, and immune-modulating activities. Compounds like α-D-Glucofuranose and Phenol, 2,5-bis (1,1-dimethylethyl)- add to the therapeutic potential of the extract due to their unique biochemical roles.

The identification of these diverse compounds indicates that the ethanolic extract of *Digitaria ciliaris* leaf could have multifaceted pharmacological effects, supporting its traditional use in herbal medicine. Future research should focus on isolating these individual compounds and investigating their specific biological activities and potential synergistic effects. This could lead to the development of novel therapeutic agents derived from the *Digitaria ciliaris* leaf.

REFERENCES

Adams, RP (2007). Identification of Essential Oil Components by Gas Chromatography/Mass Spectrometry. Allured Publishing Corporation.

Chhetri BK, Ali NAA., Setzer WN (2015) A survey of chemical compositions and biological activities of Yemeni aromatic medicinal plants. Medicines, 2(2), 67-92.

Deng Y & Zhao Y (2011) Investigation of the volatile components of green and black teas by comprehensive two-dimensional gas chromatography/time-of-flight mass spectrometry. Journal of Agricultural and Food Chemistry, 59(12), 6187-6194.

Dudareva N & Pichersky E (2008). Metabolic engineering of plant volatiles. Current Opinion in Biotechnology, 19(2), 181-189.

Edris AE (2007) Pharmaceutical and therapeutic potentials of essential oils and their individual volatile constituents: a review. Phytotherapy Research, 21(4), 308-323.

El-Sayed AM (2023) The Pherobase: Database of Pheromones and Semiochemicals. Retrieved from http://www.pherobase.com.

Farag MA, Wessjohann LA, Volmer DA (2012) On the interpretation of the trimethylsilyl derivatives of carbohydrates by electron ionization mass spectrometry. Phytochemistry, 81, 113-120.

Fraga BM (2008) Natural sesquiterpenoids. Natural Product Reports, 25(6), 1180-1209.

Gerwick WH & Moore BS (2012) Lessons from the past and charting the future of marine natural products drug discovery and chemical biology. Chemistry & Biology, 19(1), 85-98.

Hall RD (2011) Plant metabolomics: from holistic hope, to hype, to hot topic. New Phytologist, 169(3), 453-468.

Isidorov VA & Jdanova M (2002) Volatile organic compounds from leaves litter. Chemosphere, 48(9), 975-979.

Ji YB, & Liu ZQ (2012) Analysis of volatile organic compounds emitted from indigenous plants: potential application in ecological restoration. International Journal of Environmental Research and Public Health, 9(8), 2789-2803.

Kauffman GB, & Reyes, L (1999). Boranes and heteroboranes. Journal of Chemical Education, 76(10), 1395.

Kim HK, Choi YH & Verpoorte R (2010) NMR-based plant metabolomics: where do we stand, where do we go? Trends in Biotechnology, 28(5), 267-275.

Kulkarni MG & Dalai AK (2006) Waste cooking oil—an economical source for biodiesel: a review. Industrial & Engineering Chemistry Research, 45(9), 2901-2913.

Leffingwell JC & Alford ED (2010) Gas chromatography in essential oil analysis. In Gas Chromatography: Principles, Techniques, and Applications (pp. 89-113). Springer.

Lu X, Zhao X, Bai F (2013) Fermentative production of biofuels from renewable resources. Annual Review of Chemical and Biomolecular Engineering, 4, 99-123.

Milos M & Radonic A (2000) Gas chromatography–mass spectrometry and headspace gas chromatography study of volatile compounds of basil growing in Croatia. Journal of Agricultural and Food Chemistry, 48(10), 4364-4368.

NIST Mass Spectrometry Data Center (2023) NIST Chemistry WebBook, NIST Standard Reference Database Number 69. Retrieved from http://webbook.nist.gov.

Patra JK & Baek KH (2017) Antibacterial activity and action mechanism of silver nanoparticles on Escherichia coli and Staphylococcus aureus. *Applied and Environmental Microbiology*, 83(5), e02900-16.

Raga DD, Tayo LL, Ragasa CY (2001) GC-MS analysis of volatile compounds from the leaves of Vitex negundo L. Journal of Medicinal Plants Research, 5(1), 1-5.

Sangwan NS, Farooqi AHA, Shabih F & Sangwan RS (2001) Regulation of essential oil production in plants. Plant Growth Regulation, 34(1), 3-21.

Šmejkal K, Marek R & Řezanka T (2009) Isolation and identification of 2-myristynoyl pantetheine from the leaves of Aesculus hippocastanum. Phytochemistry Letters, 2(1), 43-46.

Teixeira da Silva, JA, & Dobránszki J (2015) Plant thin cell layers: a 40-year celebration. Journal of Plant Growth Regulation, 34(1), 1-16.

Tholl D (2006) Terpene synthases and the regulation, diversity, and biological roles of terpene metabolism. Current Opinion in Plant Biology, 9(3), 297-304.

Verpoorte R, Choi YH, & Kim HK (2008) Ethnopharmacology and systems biology: a perfect holistic match. Journal of Ethnopharmacology, 113(1), 1-6.

Weckwerth W (2003) Metabolomics in systems biology. Annual Review of Plant Biology, 54(1), 669-689.

Conflict of interest: The authors declare that they have no conflict of interest.

Publisher's Note
IJLSCI remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Correspondence and requests for materials should be addressed to Warghat VR.

Peer review information
IJLSCI thanks the anonymous reviewers for their contribution to the peer review of this work. A peer review file is available.

Reprints and permissions information is available at https://www.ijlsci.in/reprints