WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 5, 697-711. Research Article ISSN 2277–7105

GC–MS ANALYSIS OF BIOACTIVE COMPOUNDS IN THE ETHANOLIC ROOT EXTRACT OF *UNCARIA TOMENTOSA* (WILLD.) DC

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Article Received on 03 Feb. 2026,
Article Revised on 23 Feb. 2026,
Article Published on 01 March 2026,

https://doi.org/10.5281/zenodo.18797999

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How to cite this Article: Khushboo Lokhande*, Arun Kakkar. (2026) Gc–ms analysis of bioactive compounds in the ethanolic root extract of uncaria tomentosa (willd.) Dc. World Journal of Pharmaceutical Research, 15(5), 697–711.

ABSTRACT

Medicinal plants play a vital role in the primary healthcare systems of developing nations, and their therapeutic value is largely determined by the biochemical constituents present in specific plant parts. *Uncaria tomentosa* (Willd.) DC. is an important medicinal plant known for its diverse bioactive compounds used in pharmaceutical applications. The present study aims to identify bioactive constituents present in the ethanolic root extract of *U. tomentosa* using Gas Chromatography–Mass Spectrometry (GC–MS). Fifteen compounds were identified in the ethanolic root extract. The major constituents detected were benzoic acid (68.50%), benzoic acid ethyl ester (6.68%), and 2-(4,5-dihydro-3-methyl-5-oxo-1-phenyl-4-pyrazolyl)-5-nitrobenzoic acid (5.39%). The identified compounds are associated with several biological activities such as anti-inflammatory, antimicrobial, antioxidant, antiviral, anticancer, and hypoglycemic effects. These findings suggest that the roots of *U. tomentosa* are a potential source of pharmacologically important compounds.

KEYWORDS: *Uncaria tomentosa*, phytochemicals, root extract, ethanol, GC–MS analysis.

INTRODUCTION

Medicinal plants have long been used in traditional medicine, and in recent years they have been widely studied for their healing properties. In drug research, they are important as sources of useful chemicals and may provide new medicines with strong therapeutic effects.

It is believed that more than 80% of people in developing countries rely on traditional medicine for their basic healthcare needs. Studying medicinal plants for their active compounds can help in finding new drugs and support further medical research.[1] Secondary metabolites with intriguing biological functions are abundant in plants. With a range of structural arrangements and properties, these secondary metabolites are generally an important source.[2] Plants are primary sources of bioactive components which play a dominant role in the maintenance of human health.[3] Knowledge about the chemical components of plants is important not only for discovering new medicines but also for identifying new plant-based materials that can be used to create complex chemicals and for appreciating the value of traditional herbal remedies.[4] *U. tomentosa* is commonly known as cat's claw which has small, curved-back thorns on the stem at the leaf junction. It is a tropical medicinal vine of the Rubiaceae family that is widely distributed in the Amazon rainforest and other areas of South and Central America[5] and is present throughout India. *U. tomentosa* aired hook-like thorns rising from outstanding peduncles have originated its common name.[6] Bark and root have long been used as a remedy for a wide range of ailments, including infections, cancer, gastric ulcers, arthritis.[7] and inflammations. It has also been shown to be used for blood purifications, wound cleaning following childbirth to promote skin healing, kidney cleansing, asthma, fever[8] inhibition of various diseases, irregular menstruation and hemorrhages and to have a balancing effect on bodily systems.[9] It was discovered that the main alkaloids in the leaves and stems of *U. tomentosa* were rhynchophylline and isorhynchophylline, as well as their N-oxides, mitraphylline, isomitraphylline, dihydrocorynantheine and hirsuteine.[10] The compound epicatechin, which is found in cat's claw, is a potent antioxidant that promotes heart health and may lower the risk of diabetes.[11] In the last three decades GC-MS has become firmly established as a key technological machine for secondary metabolite profiling in both plant and non-plant species.[12-14] The study aims to determine chemical composition of *U. tomentosa* roots in ethanol extract using GC–MS analysis. Ethanol is used due to its low toxicity and polarity in extracting both polar and nonpolar phytochemicals.

MATERIALS AND METHODS

Collection and identification of plant material

The roots of *Uncaria tomentosa* (Willd.) DC. were collected from Kasturi Floriculture, Sadar, Jabalpur, Madhya Pradesh, India, in March 2024. The plant material was authenticated by A.

P. Tiwari, Department of Botany, Jawaharlal Nehru Krishi Vishwavidyalaya, Jabalpur, Madhya Pradesh, India.

Preparation of root extract

Fresh roots were thoroughly washed with distilled water, cut into small pieces, and shade dried at room temperature. The dried material was powdered using a mechanical grinder and stored in an airtight container. About 100 g of powdered root material was extracted with ethanol by refluxing for seven days. The extract was filtered through Whatman filter paper No. 1 and collected in a clean glass container. The filtrate was concentrated at 30°C and stored for GC–MS analysis.

GC–MS analysis

Ethanolic extracts were subjected to chemical analysis by using GC-MS instruments, Perkin Elmer, USA & Model - Auto system XL with Turbo Mass. Compounds were separated on PE-5MS 30m x 0.250mm x 0.250µm column. Oven temp was programmed as follows: isothermal temp of 75°C for min and then increased up to 280°C at rate of 10° C/ min and held for 15 min. Injection temp was 250°C and injection volume was 1 µ1. EI source temp was set as 220°C. Helium was used as carrier gas 1 ml/ min flow rate. MW range was recorded from 22 to 620 amu. Interpretation of the mass spectrum of GC-MS was conducted using a database of NIST. The spectrum of investigated components was compared with the spectrum of known components stored in NIST. Molecular weight, molecular formula and number of hits were used to identify names of compounds from NIST Library.

RESULT

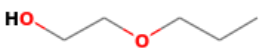
Results obtained from GC-MS analysis lead to identification of compounds from GC fractions in ethanolic extract of *uncaria tomentosa*. They were identified through mass spectroscopy attached with GC. Results of the GC-MS analysis identified various compounds present in root extract (Table 1 and Figure 1) and compared through NIST Library, Gas chromatography showed presence of fifteen major peaks and components corresponding to the peaks were determined as follows. Ethanol,2-propoxy-[3.13%], 7-Dehydrocholestrol isocaproate [1.54%], Diacetamide [2.41%], Biphenyl[1.57%], Benzoic acid, ethyl ester [6.68%], n-hexadecanoic acid [0.75%], Benzoic acid [68.50%], 5-Chloro-2h-1,2,4-triazole-3-carboxylic acid[0.42%], 2,3-Epoxyhexanol[1.64%], 2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-4-pyrazoyl)-5-nitrobenoic acid [5.39%], 1,2-Benzenedicarboxylic acid bis (2-methylpropyl) ester [0.42%], 1'-Biphenyl, 4-methyl- [0.40%], Diphenylmethane[2.08%],

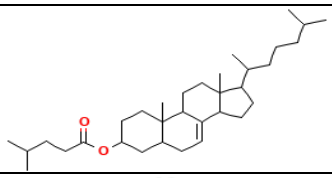
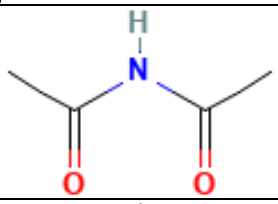
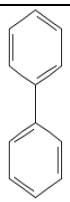
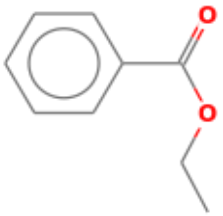
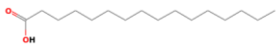
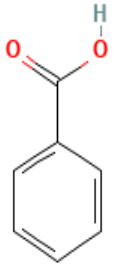
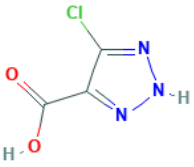
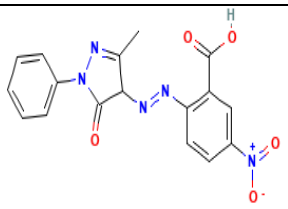
Acetic acid, phenyl methyl ester [1.26%], Guanidine(4-aminobutyl) [2.46%]. The chemical constituents with their retention time. Molecular weight, molecular formula and concentration (peak area %) are given in Table-1. The identified compounds with their retention time, structure and activities related with medicinal uses are given in Tables 2. Mass fragmentation spectra of identified compounds from *uncaria tomentosa* are given in Fig.[2-16]

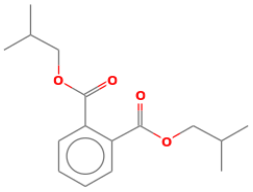
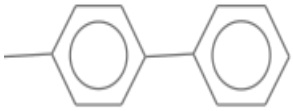
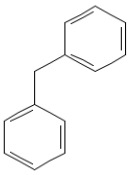
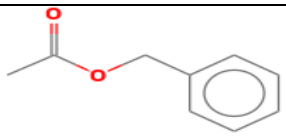
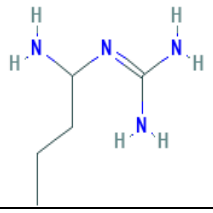
Table 1: Phytochemicals identified in the ethanolic root extract of *uncaria tomentosa* by GC-MS analysis.

S. No.	Name of the compound	Molecular formula	Molecular weight (amu)	Retention time (min)	Peak area%	Nature of compound
1	Ethanol, 2- Propoxy	$C_5H_{12}O_2$	104	3.314	3.13	Glycol ether
2	7-Dehydrocholestrolisocaproate	$C_{33}H_{54}O_2$	482	41.204	1.54	Steroids
3	Diacetamide	$C_4H_7NO_2$	101	2.749	2.41	Amide
4	Biphenyl	$C_{12}H_{10}$	154	12.327	1.57	aromatic compound
5	Benzoic acid,ethyl ester	$C_9H_{10}O_2$	150	8.246	6.68	Ester
6	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	256	21.581	0.75	Palmitic acid
7	Benzoic Acid	$C_7H_6O_2$	122	8.631	68.30	Aromatic acid
8	5-Chloro-2h-1,2,4-triazole-3-carboxylic acid	$C_3H_2O_2N_3Cl$	147	5.66	0.42	Heterocyclic
9	2,3-Epoxyhexanol	$C_6H_{12}O_2$	116	7.175	1.64	Alcoholic
10	2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-4-pyrazoyl)-5-nitrobenoic acid	$C_{17}H_{13}N_5O_5$	367	13.623	5.39	Heterocyclic
11	1,2-Benzenedicarboxylic acid bis (2-methylpropyl) ester	$C_{16}H_{22}O_4$	278	20.095	0.42	Phthalic ester
12	1,1'-Biphenyl, 4-methyl-	$C_{13}H_{12}$	168	14.218	0.40	Biphenyl
13	Diphenylmethane	$C_{13}H_{12}$	168	12.632	2.08	Aromatic hydrocarbon
14	Acetic acid, phenylmethyl ester	$C_9H_{10}O_2$	150	8.071	1.26	Ester
15	Guanidine,(4-aminobutyl)	$C_5H_{14}N_4$	130	4.249	2.46	Amino compound

Table 2: Therapeutic Activityand uses of the Phytochemical constituents identified from the ethanol root by GC-MS.

S. No	Name of compounds	Structure of phytochemical	Therapeutic Activity/Uses
1	Ethanol, 2- propoxy		As Solvent[15]

2	7-Dehydrocholestrol isocaproate		Its used to produce vitamin D3 by UV exposure.[16]
3	Diacetamide		Alkali metal chelation[17] complexation[18]
4	Biphenyl		Antibacterial[19]
5	Benzoic acid, ethyl ester		flavouring agent, fragrance and volatile oil component[20]
6	n-Hexadecanoic acid		Antifungal, Antioxidant, hypocholesterolemic, nematicide, anti-androgenic flavour, haemolytic, 5-Alpha reductase inhibitor, potent antimicrobial agent, antimalarial and antifungal[21-23]
7	Benzoic Acid		Antifungal[24] food, cosmetics, and drugs[25]
8	5-Chloro-2h-1,2,4-triazole-3-carboxylic acid		Antimicrobial[26]
9	2,3-Epoxyhexanol		Antibacterial, Antioxidants[27]
10	2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-4-pyrazolyl)-5-nitrobenzoic acid		as pesticide, miticide, and weed killers, it also possess good antibacterial[28]

11	1,2-Benzenedicarboxylic acid bis (2-methylpropyl) ester		Used in preparation of perfumes and cosmetics, plasticized vinyl seats on furniture, cars, and clothing including jackets, raincoats, and boots and used in textiles, as dyestuffs, cosmetics, and glass making[29]
12	1,1'-Biphenyl, 4-methyl-		As Solvent[30]
13	Diphenylmethane		used in the fragrance industry[31]
14	Acetic Acid, Phenylmethyl ester		Flavoring compound in Perfumes and soaps[32]
15	Guanidine, (4-aminobutyl)-		Antidepressive and anxiolytic, Neuroprotective properties,[33] hypoglycemic effects,[34] oxidative stress, apoptosis, inflammation[35]

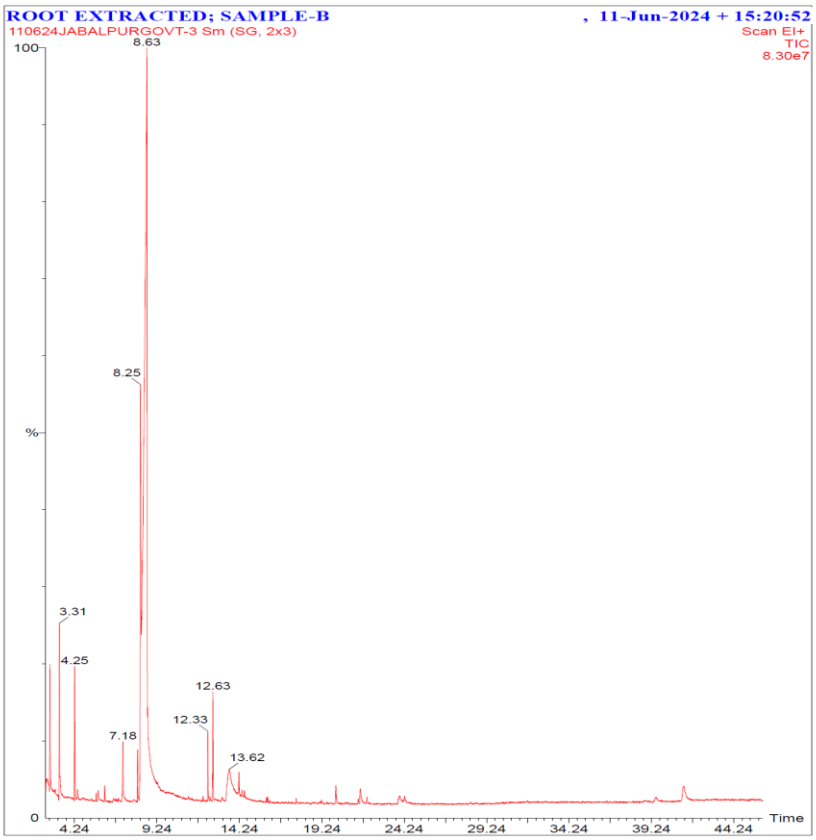


Fig. 1: Chromatogram of phytochemicals in ethanol roots extract.

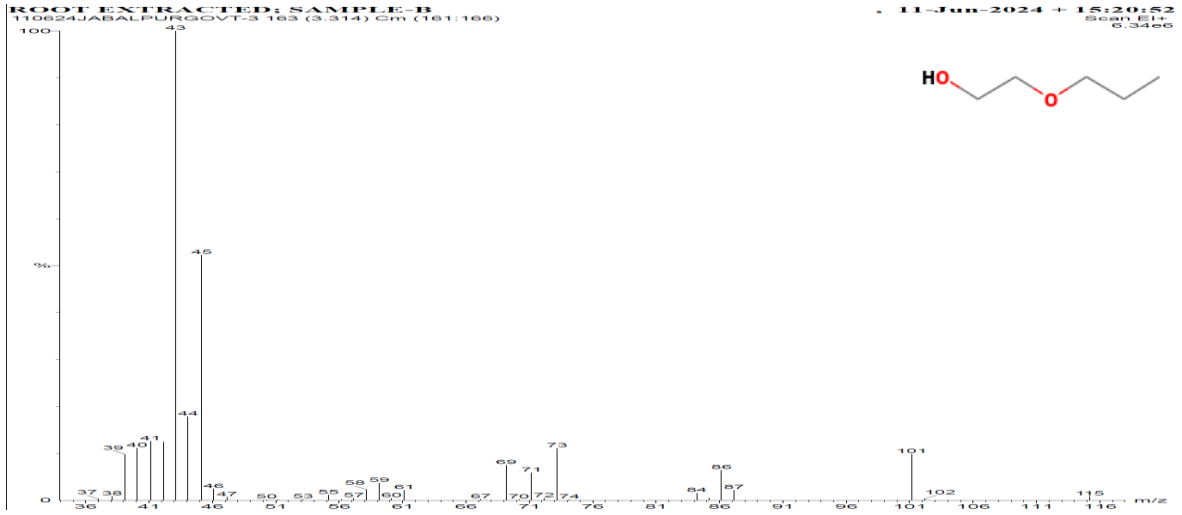


Fig. 2: Mass spectrum fragmentation of Ethanol, 2- Propoxy.

Fig. 3: Mass spectrum fragmentation of 7-Dehydrocholestrol isocaproate.

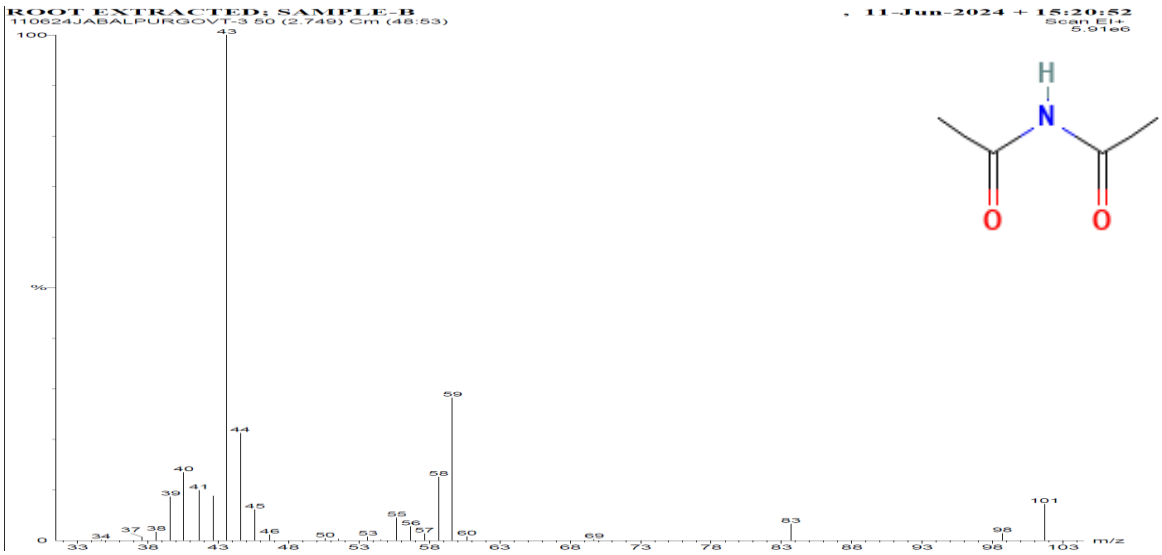


Fig. 4: Mass spectrum fragmentation of Diacetamide.

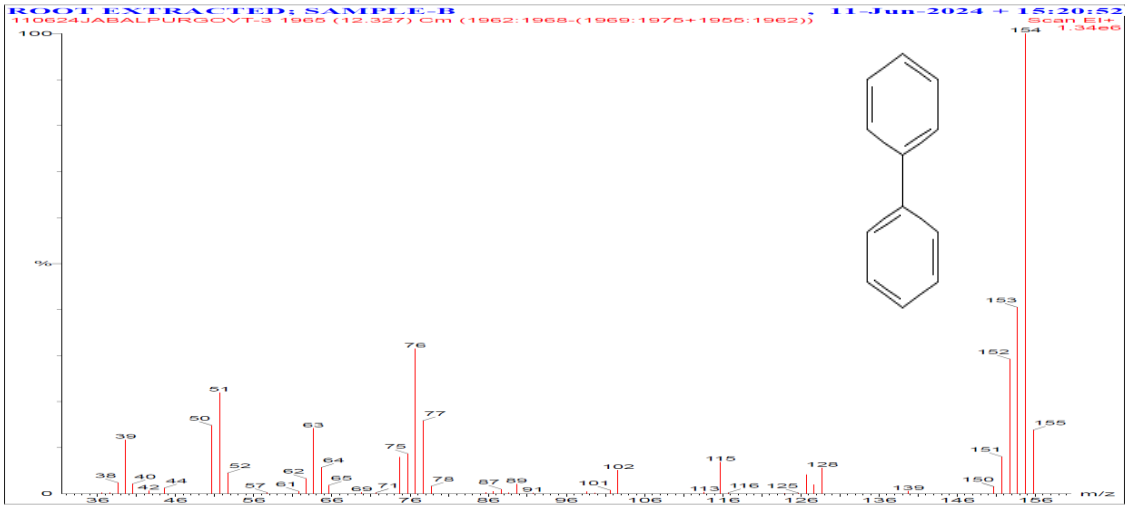


Fig. 5: Mass spectrum fragmentation of Biphenyl.

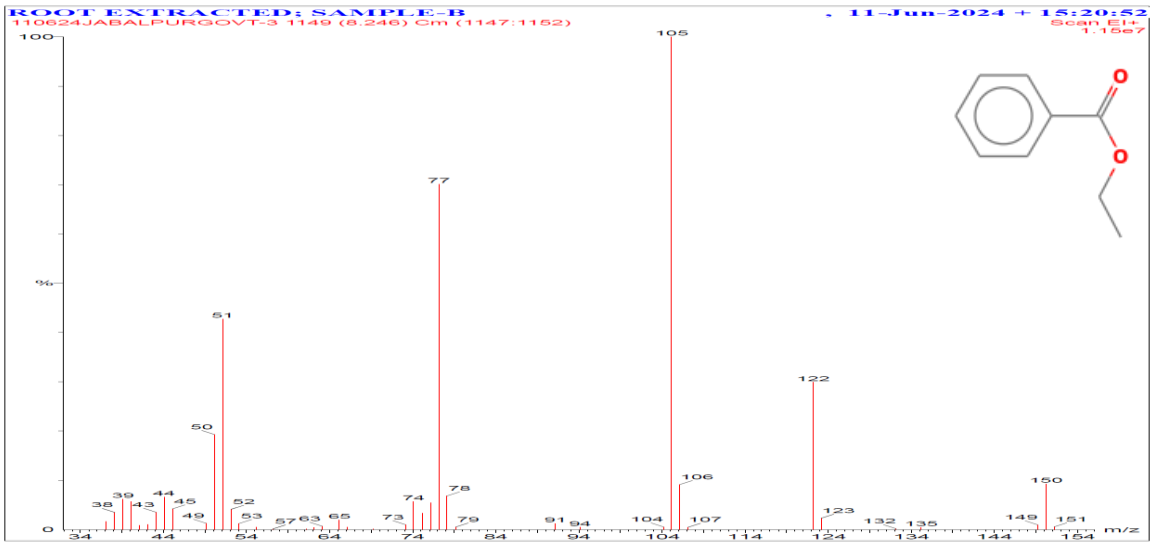


Fig. 6: Mass spectrum fragmentation of Benzoic acid, ethyl ester.

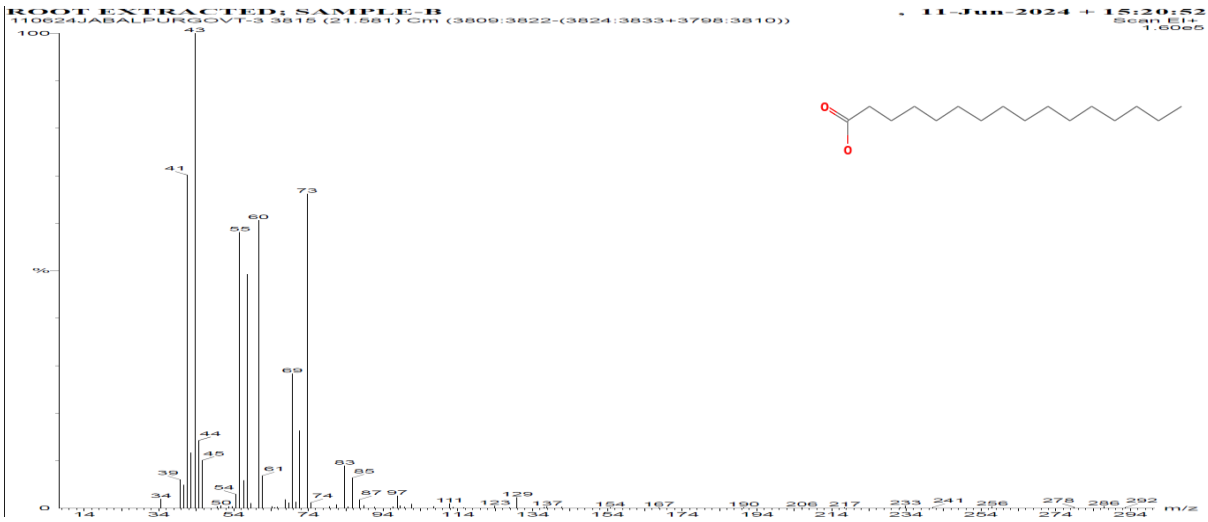


Fig. 7: Mass spectrum fragmentation of n-Hexadecanoic acid.

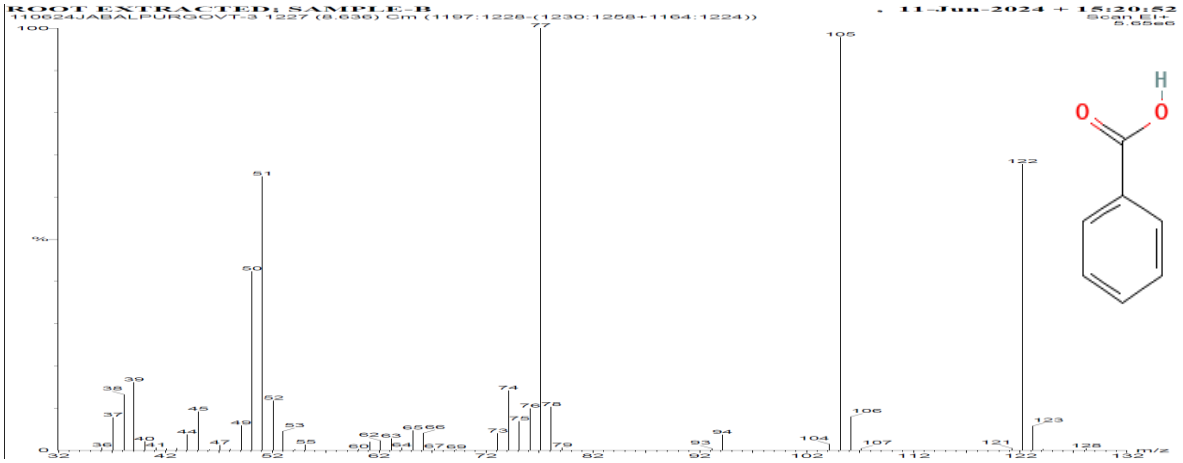


Fig. 8: Mass spectrum fragmentation of Benzoic Acid.

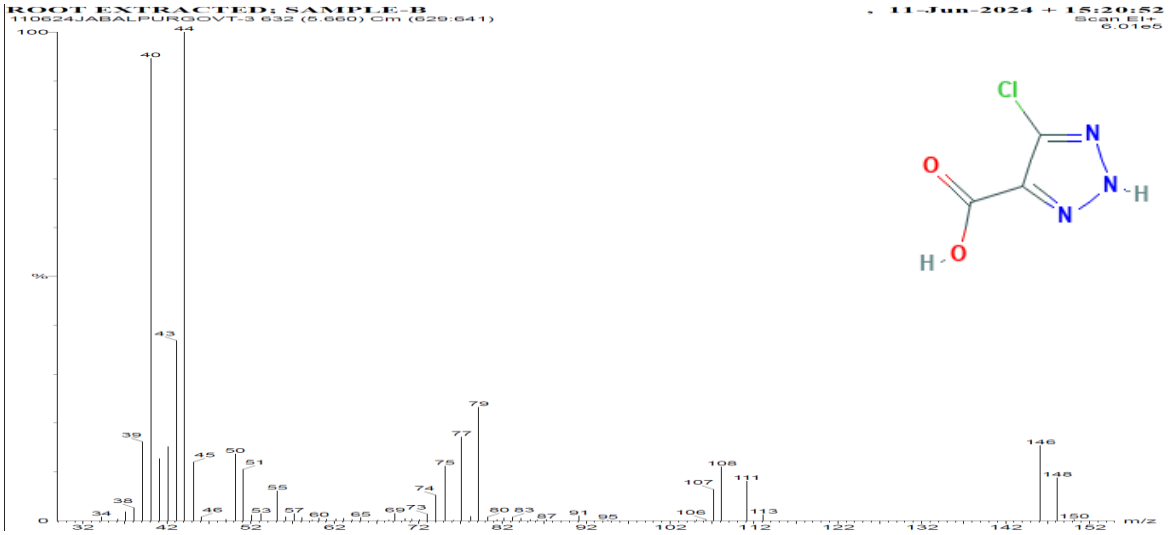


Fig. 9: Mass spectrum fragmentation of 5-Chloro-2h-1,2,4-triazole-3-carboxylic acid.

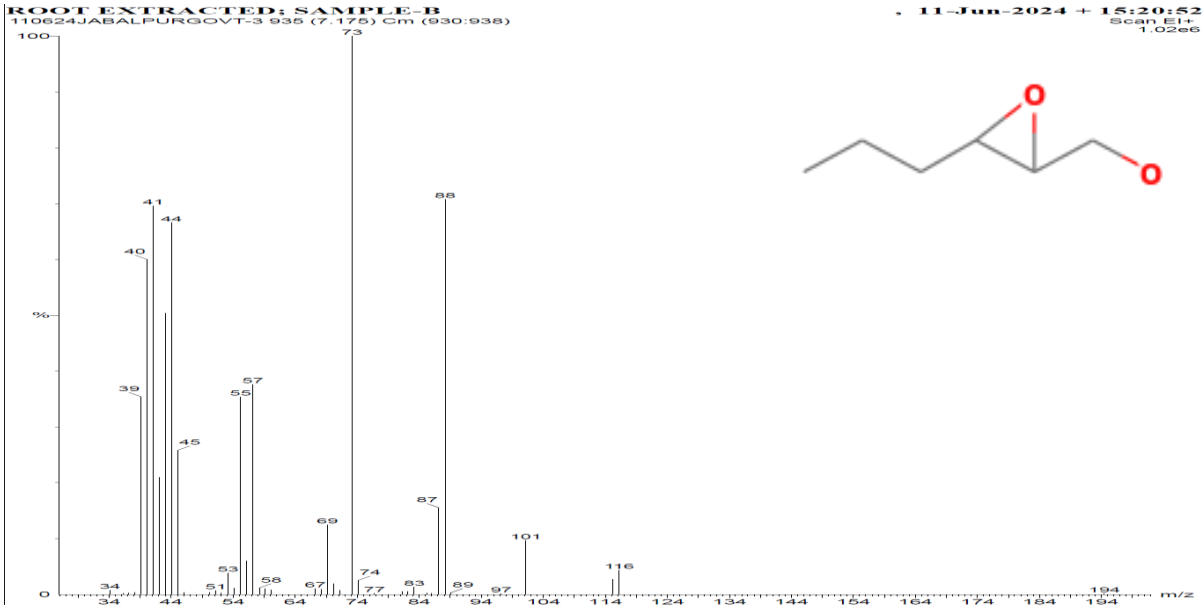


Fig. 10: Mass spectrum fragmentation of 2,3-Epoxyhexanol.

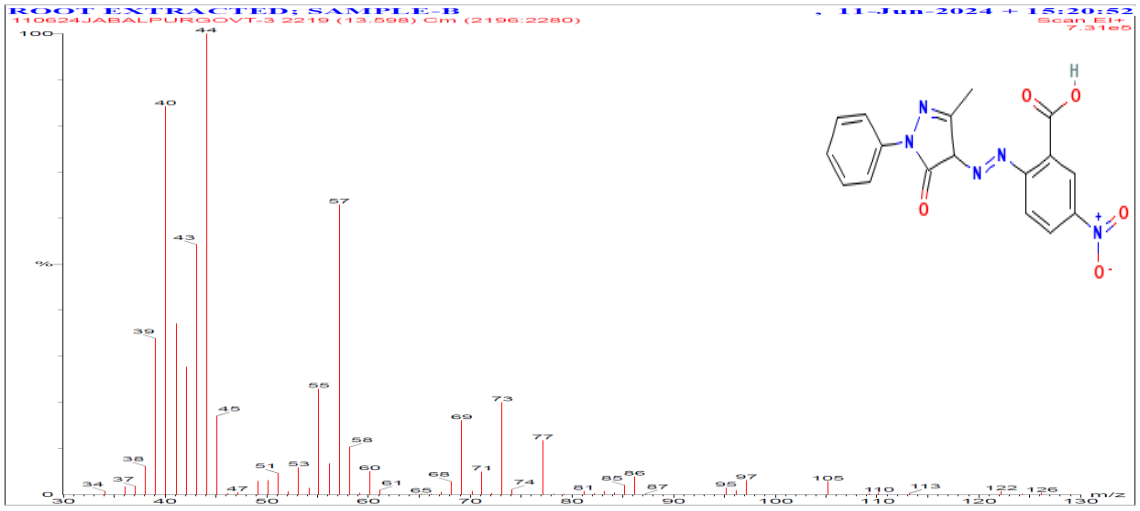


Fig. 11: Mass spectrum fragmentation of 2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-4-pyrazoyl)-5-nitrobenoic acid.

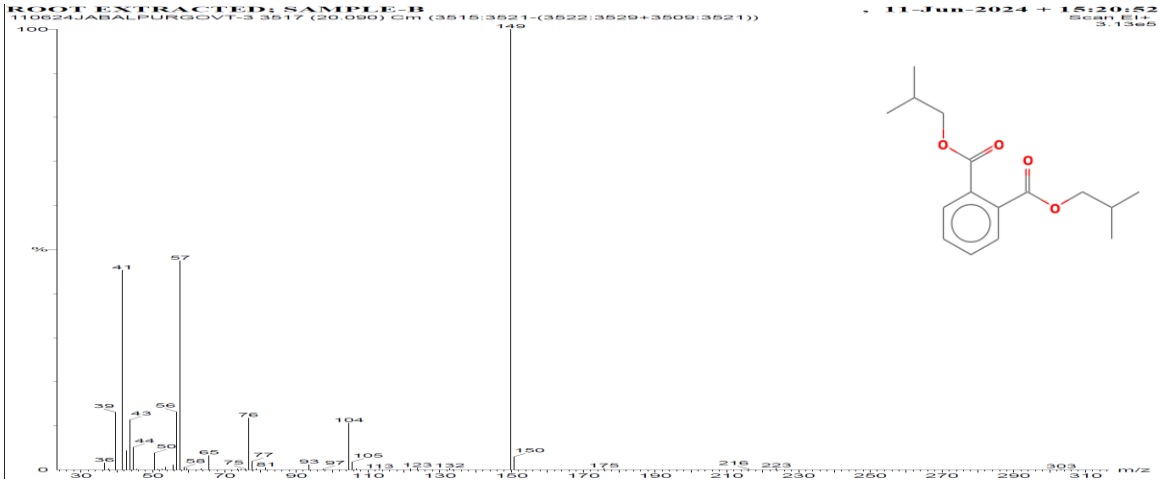


Fig. 12: Mass spectrum fragmentation of 1,2-Benzenedicarboxylic acid bis (2-methylpropyl) ester.

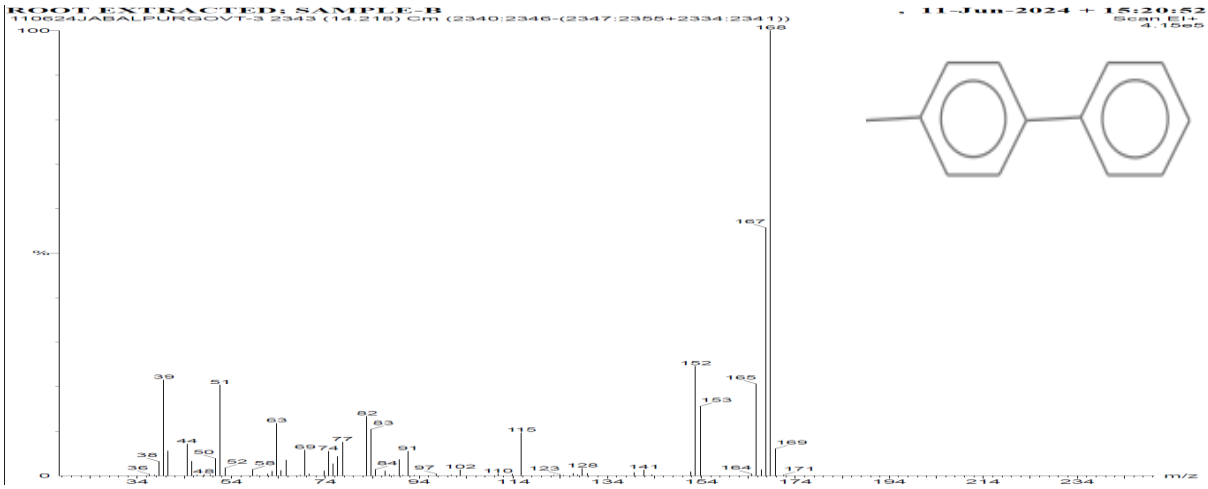


Fig. 13: Mass spectrum fragmentation of 1,1'-Biphenyl, 4-methyl-.

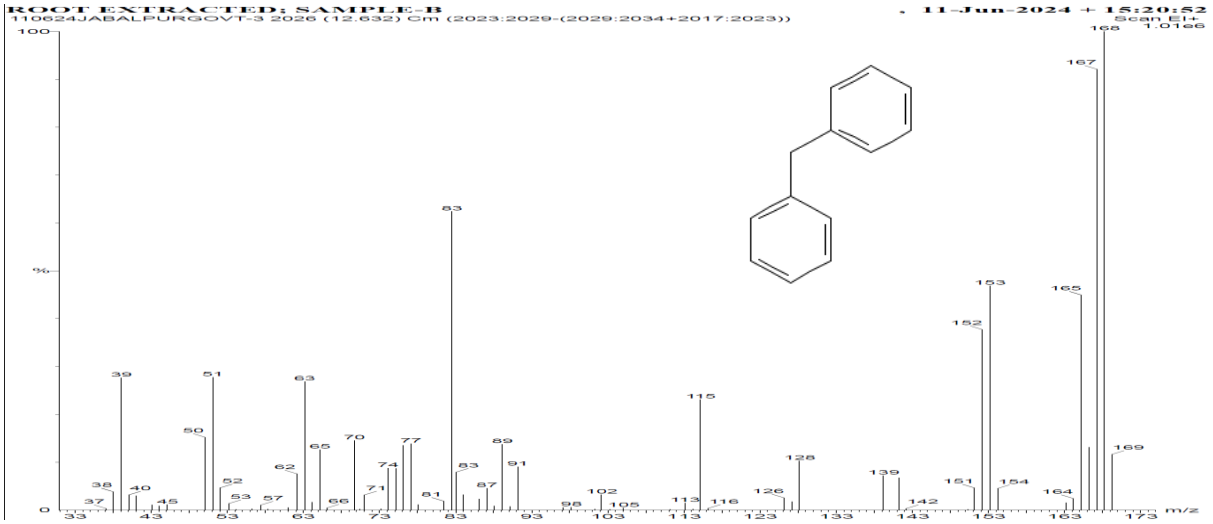


Fig. 14: Mass spectrum fragmentation of Diphenylmethane.

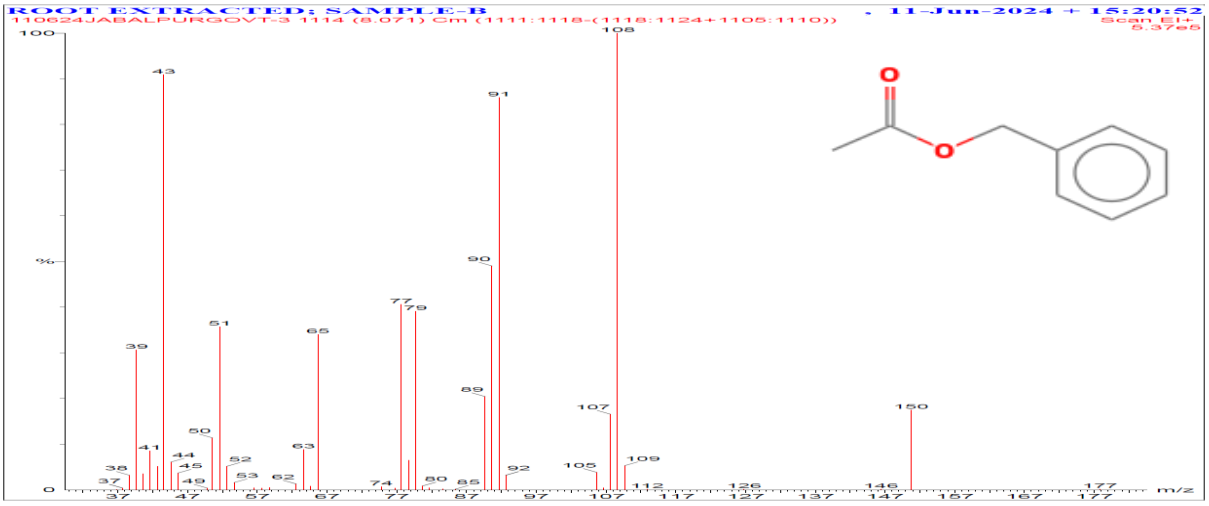


Fig. 15: Mass spectrum fragmentation of Acetic acid, phenylmethyl ester.

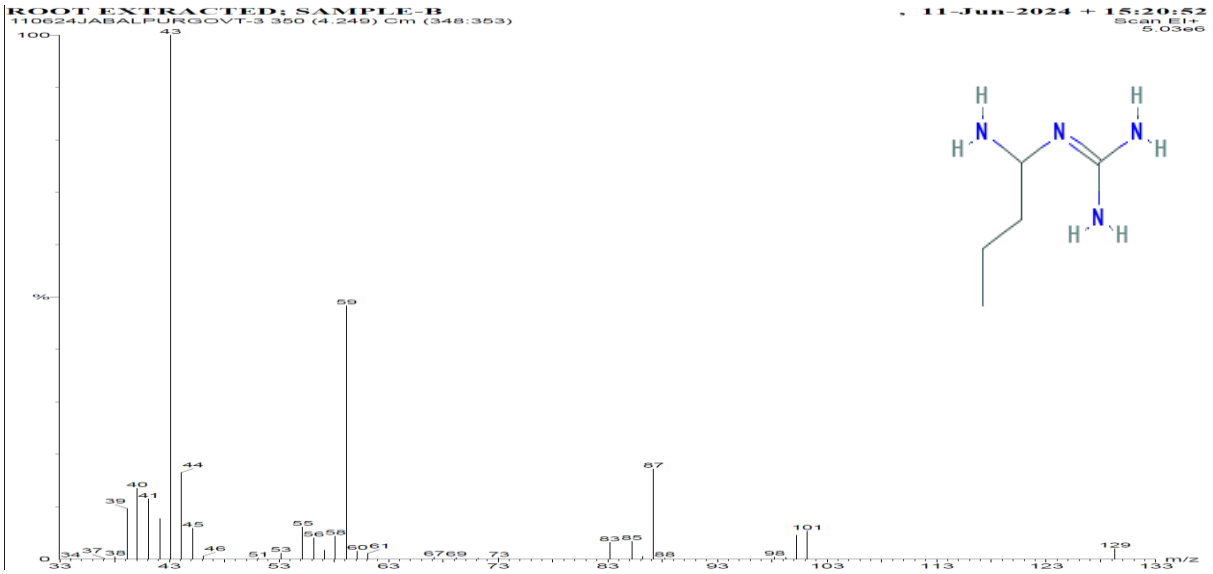


Fig. 16: Mass spectrum fragmentation of Guanidine,(4-aminobutyl).

DISCUSSION

The Gas chromatogram shows that the relative concentration of various compounds are getting eluted as a function of retention time. The height of peaks indicates relative concentration of compounds present in the plants. The mass spectrometer analyzes the compounds eluted at different times by GC and elucidates structure of compounds by fragmentation pattern. These mass spectra are fingerprints of that compounds which can be confirmed from the data library. The reliabilty of medicinal plants for its usage is evaluated by correlating phytochemical compounds with their biological activities. In present study, GC–MS analysis of *Uncaria tomentosa* ethanol extract of root resulted in detection of fifteen compounds that were identified among which Benzoic acid showed highest peak area and 1,1'-Biphenyl, 4-methyl- showed lowest peak area. Benzoic acid, an aromatic acid, has antifungal properties.[24] It is preservative that stops the growth of bacteria, molds, and yeasts mostly used in food, cosmetics, and drugs.[25] The other compounds 1,1'-Biphenyl,4-methyl and Ethanol,2- propoxy used as solvent for pharmaceutical drug preparations.[30,15] Biphenyl compound shown antibacterial, properties[19] and 5-Chloro-2h-1,2,4-triazole-3-carboxylic acid shown Antimicrobial properties.[26] The n-Hexadecanoic acid is palmitic acid compound that possess several medicinal properties such as antifungal, antioxidant, hypocholesterolemic, nematicide, anti-androgenic flavour, haemolytic, 5-Alpha reductase inhibitor, potent antimicrobial agent, antimalarial and antifungal.[21-23] Guanidine, (4-aminobutyl) is effective in treatment of antidepressive and anxiolytic, shows neuroprotective properties.[33] hypoglycemic effects.[34] oxidative stress, apoptosis and inflammation.[35] Acetic acid, phenylmethyl ester and Benzoic acid, ethyl ester is an ester, they have sweet and pleasant aroma and have a role as flavouring agent, Volatile oil component.[32,20] 7-dehydrocholesterol isocaproate is primarily used in research as a stable, deliverable form of 7-DHC for studies related to cholesterol metabolism and vitamin D synthesis.[16]

CONCLUSION

The present GC–MS investigation of the ethanolic root extract of *Uncaria tomentosa* identified fifteen bioactive phytochemical constituents with significant pharmacological potential. The dominance of compounds with antimicrobial, antioxidant, and anti-inflammatory activities suggests that the roots of *U. tomentosa* may serve as an important natural source for drug development. Further pharmacological and clinical studies are recommended to validate the therapeutic applications of these compounds.

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