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Bioactive Compound Profiling of *Theriophonum minutam* (Willd.) Baill. using GC–MS: Implications for Pharmaceutical and Therapeutic Application

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ABSTRACT

The present investigation aimed to characterise the bioactive compounds present in the leaf extract of Theriophonum minutum(Willd.) Baill. Using Gas Chromatography-Mass Spectrometry (GC-MS). This plant, known locally as undirkani in the Vidarbha region, belongs to the Araceae family and is typically collected from natural forest habitat in Gadchiroli district between July to September. It is widely consumed as a wild leafy vegetable, and traditional healers use it for treating ulcers, skin& wound problems, and Relief from body pain. In vitro, it exhibits antimitotic and antiproliferative activity against Human prostate & colon cancer. They have gained significance for their potential health benefits, including disease resistance and overall health improvement. The GC-MS analysis revealed the presence of 57 Bioactive compounds, each with distinct therapeutic properties. Major phytocompounds identified include 7,9-Di-tert-butyl-1- oxaspiro(4,5)deca-6,9- diene-2,8-dione(92.9%),2-Pentadecanone, 6,10,14-trimethyl(86%) 6-Hydroxy-4,4,7a- trimethyl-5,6,7,7a- tetrahydrobenzofuran-2(82.45), Tetradecanoic acid(63.15%),1,3-Diazacyclooctane-2- thione (40.55%),1-Propanamine,2-methyl-N-(2-methylpropylidene)26.89%, & Guanidineacetic acid, Deoxyspergualin, β Cyclocostunolide Identified first time from this plants. These compounds were identified based on their retention times and peak areas using the NIST library. The pharmacognostic activities of these compounds suggest that the leaves of Theriophonum minutam contain a variety of phytoconstituents with potential medicinal and nutraceutical properties. Given these findings, the plant is recommended for further exploration as a wild leafy vegetable with promising health benefits.

Keywords: *Bioactive compound, Theriophonum minutam, GC-MS, Wild leafy vegetable.*

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Introduction

Medicinal plants are crucial in both the pharmaceutical and food sectors. Phytochemical substances derived from these plants have been converted into commercial medications and continue to be a source for discovering new drugs. [1] Numerous plant species contain a variety of chemical components traditionally utilised for managing illnesses. Many drug formulations are rooted in the use of these substances in customary medicine.[2]

The genus *Theriophonum* (Araceae), consisting of seasonally tuberous perennials, is commonly found in India and Sri Lanka. *Theriophonum minutum* is a wild edible plant exhibiting natural diversity and offering higher nutritional values than standard food sources. Several studies indicate that Theriophonum minutum has been analysed regarding its phytochemical composition and pharmacological effects, although it is primarily noted for its exceptional nutritional benefits.[3]

Ethnomedical practices show that the tubers of *Theriophonum minutum* (Willd.) Baill. are prepared by boiling with tamarind leaves, rinsed, and then cooked as a vegetable by the Konda reddis and Koyas from the East Godavari district of Andhra Pradesh, as well as by the Koyas of the Lankapalli Forest Reserve in Khammam district, Telangana. Tuber powder mixed with honey is used to treat gastrointestinal issues, small intestinal injuries, and stomach pain.[4]

In Maharashtra, the Indian vernacular names for this species are Doda and Tangya. In the Vidarbha region, it is called undirkani; the Koyas of Andhra Pradesh refer to it as "adavi champak." The leaves of T. fischeri Sivad. They are blended with turmeric and applied externally to address skin conditions and wounds, as well as to alleviate rheumatic pain. [5] The boiled tubers are consumed for two weeks to treat piles and ease body aches.[6]

Indigenous people of Gadchiroli District, Maharashtra, use the leaves of *Theriophonum minutum* to prepare chille (leaves chopped finely and made into chapati). This is often complemented by additional wild foods. Different communities consume these species based on local availability. Various preparations of plant species are created and marketed in tribal markets.[7]

Modern pharmacology highlights the significance of natural products in the development of new medications. Numerous natural compounds have served as the basis for creating drugs and are still employed today to treat a range of illnesses. Nevertheless, using contemporary medications presents various challenges, such as significant side effects and resistance to antibiotics or even cancer treatments, necessitating the development of new drugs.[8] A thorough literature review indicates that *Theriophonum minutum* has not yet been examined for GC-MS analysis or the identification of bioactive compounds. This study represents the initial effort to identify different bioactive compounds using GC-MS and explore their pharmaceutical and therapeutic applications.

Material & Methods

Plant Collection and Extraction

The fresh plant specimen was collected from the area of Ghot, District Gadchiroli, Maharashtra (Fig. A & B) with latitude 19.81247^{0}& Longitude 79.991825$^{0.}$A voucher specimen was deposited atthe Department of Botany, Bhawabhuti Mahavidyalaya, Amgaon. (voucher numberBMV 731). The plant specimen was verified by a field botanist of the same institute uponcollection from the wild. The mature leaves (500gm) were cleaned, air-dried for 5 days,homogenized using a heavy-duty blender, and subjected to Cold Maceration & Extracted with Methanol after extraction Sample was allowed to dry in room temperature for 5-6 days until semisolid crud drugs were from after that 1mg sample was dissolve in 10 ml of methanol & sample was send for GC-MS analysis.

GC-MS Analysis

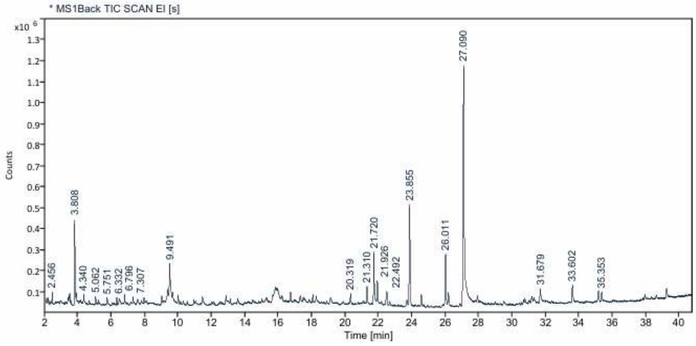
The Crude drug of *Theriophonum minutam* was diluted in methanol and subsequently sent to the Sophisticated Analytical Instrument Facility at IIT Madras. The sample was injected (1 µL) into a GC-MS system consisting of a gas chromatography system (Agilent 8890) coupled with a mass spectrometry detector (Agilent 5977B). An HP-5MSultrainert (30 m × 250 µm ×0.25 µm) capillary column was used with 0.25 µm film thickness of coated material. The injector temperature was set to 350 ∘C, and the temperature program followed was as follows: it started at 60 ∘C and held for 0.5 minutes, then ramped from 60 ∘C to 350 ∘C at a rate of 0.5 ∘C/min, followed by a 0.5-minute hold. A post-run phase at 50 ∘C for 3 minutes was conducted to prepare for the subsequent injection.Gas chromatography was conducted in splitless mode, utilising helium gas as the carrier at a consistent flow rate of 1 mL/min. Compounds were identified by referencing the NIST database, and their compositions were calculated based on the peak abundances observed in the chromatogram. The entire analysis was completed in triplicate.

Fig.A Whole plant

Fig.B. Inflorescence

Results & Discussion

GC-MS Results of *Theriophonum Minutum* vegetative leaf Methanol extract. Identified 57 unique compounds, as shown in Graph1 & table 1. The chromatograms, peak, Real time, Area, Area Percentage, Name of compound, Probability of compound, CAS number,Molecular formula & Molecular weight are represented in table No.1. Major phytocompounds identified include 7,9-Di-tert-butyl-1- oxaspiro(4,5)deca-6,9- diene-2,8-dione(92.9%),2-Pentadecanone, 6,10,14trimethyl (86%), 6Hydroxy4,4,7atrimethyl5,6,7,7tetrahydrobenzofuran2(82.45),Tetradecanoicacid(63.15%),1,3Diazacyclooctane2thione(40. 55%),Pyrimidine2,4,6trione,l(+)Ascorbicacid2,6dihe xadecano ate(37.54%),1cyclohexyl5[(2piperazin1yl(36.02%),1Propana mine,2methylN(2methylpropylidene)26.89%,cyclohexanespir o-5-(2,4,4-trimethyl-2-oxazoline (23.62%) These are the major compounds having a probability rate of more than 20%. Other 49 compounds have been found in *Theriophonum minutum* with a probability rate between 1 and 20%. A variety of compounds have been found in different classes.A few important classes of bioactive compounds, such as fatty acids, branched alkenes, saturated hydrocarbons, terpenoids, esters, aldehydes, flavonoids, and vitamin C, were detected in the extract of TM. Out of the 57 compounds, 9 fatty acids, 4 heterocycliccompounds, 4 Organic nitrogen compounds, 6 esters, 4 amines, 4 ketones, 3 terpenoids, 2 saturated hydrocarbons, 2 aldehydes, 2branched alkenes, 2 steroids,1 flavonoid,and 1 pyrimidinewere detected as major contributors to thePharmaceutical&Therapeutic application of TM. Several Compound has different pharmaceutical & biological role reported by other researches & these compound also found in *Theriophonum minutam*such as 2-Cyclohexylpiperidine has used full for synthesizing novel medicine, particularly those used as analgesic, anaesthetics, antiparasitic, anti-inflammatory& antibacterial[9], 3,3,3-Trifluro-1-piperidin-1-yl-2-Trifluromethyl-propane-1 used for novel drug discovery, 1,3-Dicyclohexylurea shows Potent inhibitory action against soluble epoxide hydroxylase and also antihypertensive effect, vasodilation & anti-inflammatory activity studied in the study on Pharmacokinetic evaluation of a 1,3-dicyclohexylurea[10].Role in creatine biosynthesis, reduces blood glucose, hormonal regulation,& Neuromodulation activity shows by Guanidineacetic acid.[11] Deoxyspergualine compound isolated from TM shows Immunosuppressive agent & used in Organ transplantation, autoimmune diseases& cancer treatment. [12]β-Cyclocostunolide compound shows antioxidative, anti-inflammatory, and antiallergic bone remodelling, Neuroprotective activity.[13] Most of the compounds reported to have Antibacterial, Antioxidant, Anti-inflammatory, Anticancerous, Neuroprotective, and hepatoprotective activity are listed & summarized in Table No.2



Graph No.1 Chromatograms of Theriophonum Minutam

Table No. 1: GC-MS Observation Table of T.minutam

Sr. No	Real Time	Area	Area %	Compound name	Prob. %	CAS#	MF	MW (g/mol)	Class of Compound
1	2.456	74148.83	0.53	1-Propanamine,2-methyl-N-(2-methylpropylidene	26.89	6898-82-4	$C_8H_{19}N$	129.2432	Organic Nitrogen Comp.
				2-Cyclohexylpiperidine	7.62	56528-77-9	$C_{11}H_{21}N$	167.2911	Cyclic Amine
				3,3,3-Trifluro-1-piperidin-1-yl-2-Trifluromethyl-propane-1	6.73		$C_9H_{11}F_6NO$	277.208	Amide
2	3.808	889065.037	6.3	Glycerin	19.59	56-81-5	$C_3H_8O_3$	92.0938	Polyol compound
				1,3-Dicyclohexylurea	4.76	2387-23-7	$C_{13}H_{24}N_2O$	224.34	Organic Compound
				Tetramethyl phosphonium cation	4.76	32589-80-3	$C_4H_{12}P+$	91.11	Organophosphorus Compound
3	4.34	74327.437	0.53	cyclohexanespiro-5-(2,4,4-trimethyl-2-oxazoline)	23.62	91875-85-3	$C_{11}H_{21}NO$	113.16	Oxazoline
				Decenyl tiglate,2E-	5.03		$C_{15}H_{26}O_2$	238.37	Ester
				Buta ne-1,1-dicarbonitrile,1-cyclohexyl-3-methyl-	4.44		$C_{13}H_{20}N_2$	204.31	Nitrite
4	5.062	66674.39	0.47	1-Butanamine, 2- methyl-N-(2-methylbutylidene)-	14.06	54518-97-7	$C_{10}H_{21}N$	155.2804	Amines
				N-Ethyl-Hexahydro-1H-azepine	10.49	6763-91-3	$C_8H_{17}N$	127.2273	Heterocyclic Comp.
				1,3-Dicyclohexylurea	9.27	62220-14-8	$C_{11}H_{25}N_2O_3PS$	280.37	Thiophosphate
5	5.751	85134.271	0.6	1H-Azonine, octahydro-1- nitroso-	13.91	20917-50-4	$C_8H_{16}N_2$	156.23	Nitrosamine
				1-Methyl-trans- decahydroquinol-4(axial)- ol	7.17		$C_{10}H_{19}NO$	169.26	Amino-Alcohol
				1,3-Cyclopentanedione, 2,4-dimethyl	5.49	34598-80-6	$C_7H_{10}O_2$	126.15	Cyclic diketones
6	6.332	69780.63	0.49	Octadecane, 6-methyl-	10.71	10544-96-4	$C_{19}H_{40}$	268.5209	Saturated Hydrocarbon
				Tetradecane, 2,6,10- trimethyl-	7.78	14905-56-7	$C_{17}H_{36}$	240.4677	Branched alkanes
				2-Azido-2,4,4,6,6-pentamethylheptane	5.96		$C_{12}H_{25}N_3$	211.35	Branched Alkanes
7	6.796	131395.21	0.93	Pyrimidine-2,4,6-trione, 1-cyclohexyl-5-[(2- piperazin-1-yl-	36.02		$C_{17}H_{27}N_5O_3$	349.4	Nitrogen Compound
				Guanidineacetic acid	6.86	352-97-6	$C_3H_7N_3O_2$	117.11	Amino-acid
				2-Thioxo- dihydropyrimidine-4,6- dione, 1-phenyl-5-[(2-pipera	6.33		$C_{16}H_{10}N_4O_4S_2$	386.4	Pyrimidines
8	7.307	83166.062	0.59	1,3-Diazacyclooctane-2- thione	40.55	5269-85-2	$C_6H_{12}N_2S$	144.24	Heterocyclic Compound
				Cyclohexane carboxylic acid, 2-hydroxy-, ethyl ester	9.56	3444-72-2	$C_9H_{16}O_3$	172.22	Carboxylic acid esters
				Deoxyspergualin	6.17		$C_{17}H_{37}N_7O_3$	387.52	Polyamines
9	9.491	1029860.765	7.3	1,3,6-Trioxa-2- Sila cyclooctane, 2,2,-dimethyl silyl-	8.45		$C_6H_{14}O_3Si$	162.26	Cyclic Organic Compound
				10-Chlorotricyclo [4.2.1.1(2, 5)]deca-3,7-dien-9-ol	7.47		$C_{10}H_{11}ClO$	182	Haloalkenols
				3-Hydroxymethyl-2-trimethylsilyloxypentane	5.57		$C_9H_{22}O_2Si$	190.36	Ethers
10	20.319	135705.477	0.96	9-Hexadecenoic acid	5.82	2091-29-4	$C_6H_{30}O$	254.4	Fatty acid
				cis-13-Eicosenoic acid	4.58	17735-94-3	$C_{20}H_{38}O$	310.51	Fatty acid
				Cyclopentadecanone, 2- hydroxy-	3.6	4727-18-8	$C_{15}H_{28}O_2$	240.38	Hydroxy ketones
11	21.31	201641.03	1.43	6-Hydroxy-4,4,7a- trimethyl-5,6,7,7a- tetrahydrobenzofuran-2	82.45	73410-02-3	$C_{11}H_{16}O$	196.24	Organo-Heterocyclic
				Propiolic acid, 3-(1- hydroxy-2-isopropyl-5- methyl cyclohexyl	1.82		$C_{13}H_{20}O_3$	224	Acetylenic Carboxylic acid
12	21.72	902653.46	6.4	Tetra decanoic acid	63.15	544-63-8	$C_{14}H_{28}O_2$	228.37	Fatty acid
				Pentadecanoic acid	9.18	1002-84-2	$C_{15}H_{30}O_2$	242.4	Fatty acid
				Tridecanoic acid	5.75	638-53-9	$C_{13}H_{26}O_2$	214.34	Fatty Acid
13	21.926	503360.156	3.57	Acetic acid, 2-(2,2,6- trimethyl-7-oxa- bicyclo [4.1.0] hept-1-	3.54	90165-14-3	$C_{14}H_{22}O_3$	238.32	Ester Epoxy Compound.
14	22.492	189789.89	1.35	4-Octadecenal	5.23	56554-98-4	$C_{18}H_{34}O$	266.46	Fatty aldehyde
				Acetic acid, chloro-, octadecyl ester	3.8	5348-82-3	$C_{20}H_{39}ClO_2$	347	Saturated Organic Compound
				5-Octadecenal	3.21	56554-88-2	$C_{18}H_{34}O$	266.46	Fatty aldehyde
15	23.855	1856876.198	13.16	2-Pentadecanone, 6,10,14-trimethyl-	86	502-69-2	$C_{18}H_{36}O$	268.47	Sesquiterpenoids
				2-Undecanone, 6,10-dimethyl-	2.09	1604-34-8	$C_{13}H_{26}O$	198.34	Dialkyl ketone
				E-8-Octadecacen-1-ol acetate	1.27	2195-90-6	$C_{20}H_{38}O$	310.51	Fatty alcohol ester
16	26.011	1021543.754	7.24	7,9-Di-tert-butyl-1- oxaspiro (4,5) deca-6,9- diene-2,8-dione	92.9	82304-66-3	$C_{17}H_{24}O$	276.37	Flavonoids
				β-Cyclocostunolide	0.92	2221-82-1	$C_{15}H_{20}O$	232.31	Sesquiterpene
				1,3-Dithiolane, 2- (1,3,4,4a,5,6,7-hexahydro-2,5,5-trimethyl	0.85	32388-57-1	$C_3H_6S_2$	106.21	Heterocyclic compound
17	27.09	6137425.27	43.5	n-Hexadecenoic acid	46.34	57-10-3	$C_{16}H_{32}O_2$	256.42	Fatty acid
				l-(+)-Ascorbic acid 2,6- dihexadecanoate	37.35	28474-90-0	$C_{38}H_{68}O_8$	652.49	Fatty acid ester
				Palmitic anhydride	9.77	623-65-4	$C_{32}H_{62}O_3$	494.84	Fatty acid
18	31.679	233170.595	1.65	Octadecanoic acid	53.74	57-11-4	$C_{18}H_{36}O_2$	284.47	Fatty acid
				L-Ascorbic acid, 6- octadecenoate	14.94	10605-09-1	$C_{24}H_{42}O_7$	442.59	Fatty acid ester
				Octadecanoic acid, 2-(2- hydroxy ethoxy) ethyl ester	7.7	106-11-6	$C_{22}H_{44}O_4$	372.58	Ester
19	33.602	283282.933	2.01	Ethanol, 2-(9- octadecenyloxy)-, (Z)-	8.67	5353-25-3	$C_{20}H_{40}O_2$	312.538	Organooxygen compound
				Undec-10-ynoic acid, heptadecyl ester	5.25		$C_{28}H_{52}O$	420.71	Fatty acid ester
				cis-10-Nonadecenoic acid	4.44	73033-09-7	$C_{19}H_{36}O_2$	296.271	Fatty acid
20	35.353	141240.62	1	Cholestan-3-one, cyclic 1,2-ethanediyl acetal, (5α)-	6.19	1858-14-6	$C_{2950}O_2$	430.71	Steroids
				4,8,12,16-tetramethylheptadecane-4-olide	3.75	96168-15-9	$C_{21}H_{40}O_2$	324.54	Terpenoids
				Cholestan-3-one, cyclic 1,2-ethanediyl aetal, (5β)-	3.75	25328-53-4	$C_{2950}O_2$	430.71	Steroids

Table No. 2: Pharmaceutical and Therapeutic Application

Sr.No	Name of Compound	Pharmaceutical & Biological Activity	Reference
1	2-Cyclohexylpiperidine	Synthesisingnew drugs, pain relievers, anaesthetics, compounds with antiparasitic effects, and demonstrating anti-inflammatory and antibacterial properties.	[14]
2	3,3,3-Trifluro-1-piperidin-1-yl-2-Trifluromethyl-propane-1	Novel Drug Discovery	NA
3	1,3-Dicyclohexylurea	Antihypertensive effect, Vasodilation &anti-inflammatory activity	[15]
4	Guanidineacetic acid	Function in the production of creatine, lowers blood sugar levels, maintains arginine levels, regulates hormones, promotes protein synthesis, acts as a neuromodulator, and has antioxidant properties.	[16]
5	Decenyl tiglate,2E-	Anticancerousagent,Wound healing, Clinical Trial,	[17]
6	Deoxyspergualin	An immunosuppressive agent used in Organ transplantation,Autoimmunedisease,& Cancer treatment	[18]
7	1H-Azonine, octahydro-1- nitroso-	Carcinogenic	[19]
8	n-Hexadecenoic acid	Anti-inflammatory, Antioxidant, hypocholesterolaemia, nematicide, pesticide, anti-androgenic	[20]
9	E-8-Octadecacen-1-ol acetate	Anticancer, antibacterial, antioxidant, antipyretic, cardioprotective	[21]
10	Pyrimidine-2,4,6-trione, 1-cyclohexyl-5-[(2-piperazin-1-yl-	Novel drug synthesis	[22]
11	β-Cyclocostunolide	Used against dermatitis, antioxidants, anti-inflammatories, stimulates hair growth, cancer-fighting, and has anti-diabetic benefits	[23]
12	l-(+)-Ascorbic acid 2,6- dihexadecanoate	Antinociceptive, antioxidant, anti-inflammatory, anti-mutagenic, and wound healing properties	[24]
13	Undec-10-ynoic acid, heptadecyl ester	Antioxidant	[25]
14	Cholestan-3-one, cyclic 1,2-ethanediyl acetal, (5α)-	Anti-inflammatory agents	[26]
15	Palmitic anhydride	Nutraceutical, Role in Physiological & Metabolism Process	[27]
16	1,3-Dithiolane, 2- (1,3,4,4a,5,6,7-hexahydro-2,5,5-trimethyl	Novel Drug Design	[28]
17	tetramethylheptadecane-4-olide	Potential indicator of VitaminE, Anticancerous activity	[29]
18	cis-10-Nonadecenoic acid	Anti-inflammatory activity	[30]
19	7,9-Di-tert-butyl-1- oxaspiro (4,5) deca-6,9- diene-2,8-dione	Natural antioxidant, cytotoxic activity	[31]
20	Propiolic acid, 3-(1- hydroxy-2-isopropyl-5-methylcyclohexyl	Antiangiogenic & Insecticidal activity	[32]
21	Cyclopentadecanone, 2-hydroxy	Anti-inflammatory &Anticancerous properties	NA
22	1,3-Diazacyclooctane-2- thione	Antimicrobial and antioxidant activity	NA
23	E-8-Octadecacen-1-ol acetate	Pheromone	NA
24	2-Pentadecanone, 6,10,14-trimethyl	antibacterial, anti-inflammatory, anticancer, antioxidant, and antidiabetic activities	[33]

Conclusion

In the current research focusing on the GC-MS analysis of the methanolic extract of *Theriophonum Minutum*(Willd.)Baill leaves, we explore a commonly used ethnobotanical herb found in peninsular India and Sri Lanka during the monsoon season. The review of existing literature indicated a lack of comprehensive studies regarding its phytochemical components, especially in terms of GC-MS analysis. This marks the first GC-MS report on *Theriophonum Minutum*, where we identified 57 bioactive compounds, highlighting the presence of various bioactive constituents in the plant we examined. TM contains a wide range of secondary metabolites, which are extensively utilised in traditional medicine to address numerous health issues, as well as in contemporary medical practices. The identified secondary metabolites, including fatty acids, hydrocarbons, terpenoids, steroids, esters, phenols, tannins, and flavonoids, play a role in alleviating various biological challenges, supporting the use of these plants by traditional healers. Leaves of Theriophonum Minutum are prepared in a specific manner to eliminate their irritating substances. This method of food preparation is a novel contribution to both science and society. Therefore, it is recommended for pharmaceutical and therapeutic uses. Additional research is necessary to determine its bioactivity.

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