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COMPARATIVE GC-MS ANALYSIS OF PHYTOCHEMICAL COMPOUNDS IN THE ETHANOLIC EXTRACTS OF *TAGETES ERECTA* AND *TRIDAX PROCUMBENS*

Lalita Kushwah[1]*, Rupali Dutt[2] and D.K. Sharma[1]

[1]Department of Zoology
S.M.S. Govt. Model Science College, Gwalior (M.P.), India
[2]Centre for Ayurvedic Translational Research
Jiwaji University, Gwalior (M.P.), India

**Corresponding author*: lalitakuashwah@gmail.com

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Abstract: This study was aimed to identify the phytochemical compounds present in extracts from *Tagetes erecta* (flower) and *Tridax procumbens* (whole plant). The air-dried plant parts were powdered and extracted using ethanol. The extracts were then analyzed using gas chromatography-mass spectrometry (GC-MS). The analysis revealed the presence of 36 compounds in the ethanolic extract of *Tagetes erecta* and 31 compounds in *Tridax procumbens*. Ten compounds (Stigmasterol, alpha-Amyrin, Tetradecanoic acid (Myristic acid), 9,12,15-Octadecatrienoic acid, Ethyl ester (Z,Z,Z)-(Linolenic acid), Ethyl tridecanoate (Tridecanoic acid), dl-alpha-Tocopherol, 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl (Quercetin) and Phenol, 2,6-dimethoxy were identified commonly in both plant ethanolic extract. Some of these compounds have been reported to be pharmacologically active. Based on these findings, and considering that plants are commonly used to prevent or treat various diseases, it is clear that these plants contain many active compounds. These compounds could be utilized in developing plant-based drugs.

Keywords: GC-MS, Medicinal plants, Phytochemicals, *Tagetes erecta, Tridax procumbens*.

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INTRODUCTION

Plants have a crucial role in the prevention and treatment of diseases, and they can also help to minimize the adverse effects of standard treatments (Bachrach, 2012). They are rich sources of chemical compounds that hold significant biological and pharmacological value. Throughout history, plants have provided successful drugs and will remain vital for discovering new lead compounds (Atanasov *et al.,* 2015; Atul *et al.,* 2021). A key aspect of studying medicinal plants involves identifying the biologically active compounds within them, paving the way for further biological and pharmacological research (Guo *et al.,* 2013; Momin *et al.,* 2014; Farid *et al.,* 2015).

Tagetes erecta, a member of the Asteraceae family, is a versatile plant with both medicinal and ornamental properties (Lal Mohan, 2022). It is

highly valued for its medicinal uses (Priyanka *et al.,* 2013), serving as a source of medicine, nematocide (Pérez *et al.,* 2006), phosphate solubilizer (Abou Aly *et al.,* 2006), cosmetics (Farjana *et al.,* 2009), food additives (Nandita *et al.,* 2012), dye, fodder (Nilani and Saravanan, 2010), essential oil (Richard, 2006), and pest control (Nikkon *et al.,* 2009). The essential oil extracted from *Tagetes erecta* has been found to possess antibiotic, antimicrobial, antiparasitic, antiseptic, wound healing and antispasmodic properties (Huang *et al.,* 2022; Rahman *et al.,* 2022).

Tridax procumbens, also known as coat buttons or *Tridax* daisy, is a flowering plant belonging to the daisy family (Andriana *et al.,* 2019). This plant is widely recognized as a pervasive weed and pest species. It is classified as a noxious weed and is commonly found in fields, meadows, croplands, disturbed areas, lawns, and roadsides in regions with tropical or semi-tropical climates. In India, *Tridax procumbens* has been traditionally used for its wound-healing properties and as an anticoagulant, antifungal, and insect repellent. The juice extracted from its leaves is directly applied to wounds, and its leaf extracts have been utilized in folk medicines to treat infectious skin diseases (Bhagwat *et al.,* 2008; Wani *et al.,* 2010). Additionally, in Ayurvedic medicine, it is employed for liver disorders, hepato-protection, gastritis, and heartburn. Local healers across the India utilize various plants, animals and their parts/ products to treat the boils, blisters and cuts (Sateesh, 2013; Prakash and Verma, 2021). This study was designed to identify the bioactive compounds present in *T. erecta* (flower) and *T. procumbens* (whole plant) through the use of GC-MS analysis.

MATERIALS AND METHODS

Plant materials

The plants *T. erecta* and *T. procumbens* were collected from 'Charak Udyan' of Jiwaji University (JU) Gwalior, India. These were authenticated by JU's Institute of Ethnobiology and assigned the codes as *Tagetes erecta* (IOE-438) and *Tridax procumbens* (IOE-440).

Preparation of extracts

The flowers of *Tagetes erecta* and whole plant of *Tridax procumbens* were washed and shade-dried for 7 to 10 days and made a fine powder. The extract was prepared using the Soxhlet method with 95% ethanol solvent, and was dried in a hot air oven at 45°C for 2-3 days. The extracts were collected and stored in an airtight bottle at 4°C.

GC-MS analysis ethanolic extracts

The Gas Chromatography- Mass Spectrometry (GC-MS) analysis of ethanolic extracts of *Tagetes erecta* and *Tridax procumbens* were performed using a GC-MS triple quadrupole (GC-MS TQ8030), Shimadzu Corp. Japan. GC-MS equipped with a capillary column (30 × 0.25 mm) and RXI-5MS. Helium gas (99.999%) was used as a carrier gas at a constant flow rate of 1 ml/min and 2 μl filtered extract sample was injected. The injector temperature was maintained at 300 °C, and the ion-source temperature at 200 °C. The MS was taken at 70 eV. The total GC-MS running time was 71 min. The identification of compounds was done by comparing the spectrum of unknown compounds with the spectrum of known compounds in the NIST spectral library store in the computer software of the GC-MS and the name, molecular weight and structure were worked out.

RESULTS AND DISCUSSION

The Gas Chromatography-Mass Spectrometry (GC-MS) analysis revealed the presence of a variety of components in the ethanolic extract of both plants. Figures 1 and 2 illustrate the different retention times of these components. Detailed information about the identified compounds, including their retention time (RT), molecular formula, molecular weight (MW) and abundance (peak area %) are shown in Tables 1 and 2. As the larger compounds fragmented into smaller ones, peaks at different m/z ratios were observed.

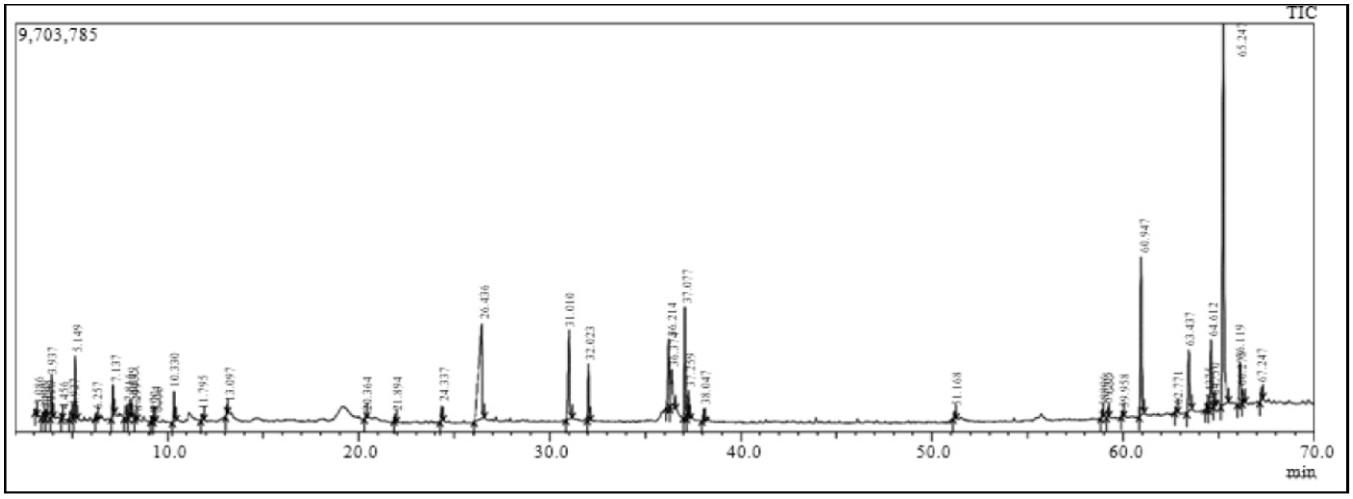

Fig. 1: GC-MS chromatogram of ethanolic extract of *Tagetes erecta*.

Table 1: Phytochemical compounds identified in ethanolic extract of *Tagetes erecta* by GC-MS.

Sl. No.	RT (min)	Area	Peak area%	Molecular weight	Structure	Name of Compounds
1.	3.086	382352	0.19	112.8	$C_5H_4O_3$	2H-Pyran-2,6 (3H)-dione
2.	3.648	524913	0.27	174.1	$C_8H_{14}O_4$	Butyl 2-acetoxyacetate
3.	3.937	3014379	1.53	126.1	$C_3H_6N_6$	1,3,5-Triazine-2,4,6-triamine
4.	4.456	255357	0.13	115.1	$C_5H_9NO_2$	dl-Proline
5.	4.927	917753	0.47	102.3	$C_5H_{10}O_2$	Pentanoic acid, 3-hydroxy-4 methyl-, methyl ester
6.	5.149	4163961	2.11	144.12	$C_6H_8O_4$	4H-Pyran-4-one, 2,3-dihydro-3,5 dihydroxy-6-methyl (Quercetin)
7.	6.257	527953	0.27	711	C_4H_9N	Pyrrolidine, N-(3-methyl-3-butenyl)-
8.	7.137	2606720	1.32	134.1	$C_5H_{10}O_4$	1,2,3-Propanetriol, 1-acetate
9.	7.816	1688764	0.86	110.1	$C_6H_6O_2$	1,2-Benzenediol, 3-methoxy-
10.	8.299	325044	0.16	148.6	$C_6H_{12}O_4$	(S)-(-)-1,2,4-Butanetriol, 2-acetate
11.	9.170	491777	0.25	156.1	$C_8H_{12}O_4$	1-Carbmethoxy-3,3 dimethyldiaziridine
12.	9.264	582249	0.30	150.1	$C_9H_{10}O_2$	2-Methoxy-4-vinylphenol
13.	10.330	2904140	1.47	94.1	$C_9H_{12}O_3$	Phenol, 2,6-dimethoxy
14.	11.795	835068	0.42	161.3	$C_7H_{19}NOSI$	Dimethyl{bis[(2Z)-pent-2-en-1 yloxy]}silane
15.	13.097	753480	0.38	157.1	$C_7H_{11}NO_3$	2-Pyrrolidinecarboxylic acid-5-oxo-, ethyl ester
16.	20.364	246597	0.13	179.1	$C_{11}H_{22}BN$	Propylamine, N-[9-borabicyclo] 3.3.1[non-9yl]-
17.	21.894	675200	0.34	213.4	$C_{14}H_{31}N$	N-Ethyl-4-propyl-4-nonanamine
18.	24.337	1279656	0.65	228.3	$C_{14}H_{28}O_2$	Tetradecanoic acid (Myristic acid)
19.	26.436	28202800	14.32	122.1	$C_7H_6O_2$	Benzoic acid, 4-hydroxy-3,5 dimethoxy-
20.	31.010	11512272	5.84	242.3	$C_{15}H_{30}O_2$	Pentadecanoic acid, Ethyl tridecanoate

21.	36.214	8683729	4.41	234.4	$C_{17}H_{30}$	1,E-11,Z-13-Heptadecatriene
22.	36.374	6843832	3.47	234.3	$C_{16}H_{26}O$	cis,cis,cis-7,10,13-Hexadecatrienal
23.	37.077	10486962	5.32	280.4	$C_{18}H_{32}O_2$	6,9-Octadecadienoic acid, methyl ester
24.	37.259	2735710	1.39	292.5	$C_{19}H_{32}O_2$	9,12,15-Octadecatrienoic acid, ethyl ester (Linolenic acid)
25.	38.047	1037695	0.53	94.1	$C_{15}H_{30}O_2$	Ethyl tridecanoate
26.	58.896	758037	0.38	416.6	$C_{28}H_{48}O_2$	beta-Tocopherol
27.	59.205	967606	0.49	416.7	$C_{28}H_{48}O_2$	gamma.-Tocopherol
28.	59.958	542590	0.28	116.1	C_9H_8	1H-Inden-1-one, 2,4,5,6,7,7a hexahydro-4,4,7a-trimethyl-
29.	60.947	18379343	9.33	430.7	$C_{29}H50O_2$	dl-.alpha.-Tocopherol (vitamin E)
30.	63.437	7563755	3.84	412.6	$C_{29}H_{48}O$	Stigmasterol
31.	64.612	9040154	4.59	386.7	$C_{27}H_{46}O$	Cholesterol
32.	64.750	658744	0.33	128.1	$C_{10}H_8$	5(1H)-Azulenone,2,4,6,7,8,8a hexahydro-3,8-dimethyl-4 (1-methylethylidene)
33.	65.247	48334846	24.53	118.1	C_9H_{10}	beta-Amyrin
34.	66.119	6080321	3.09	204.3	$C_{15}H_{24}$	(1S,6R,9S)-5,5,9,10 Tetramethyltricyclo [7.3.0.0(1,6)] dodec-10(11)-ene
35.	66.275	1569519	0.80	426.7	$C_{30}H_{50}O$	Obtusifoliol
36.	67.247	1471759	0.75	384.6	$C_{27}H_{44}O$	Cholest-4-en-3-one
		197003930	**100.00**			

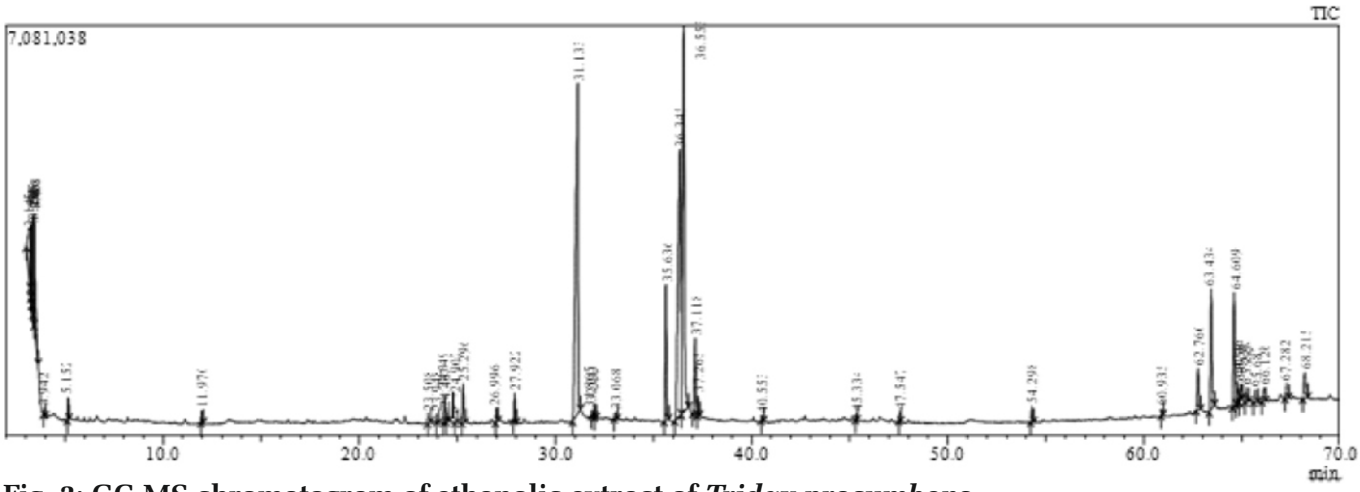

Fig. 2: GC-MS chromatogram of ethanolic extract of *Tridax procumbens*.

These mass spectra are unique identifiers for the compounds. Compounds can be identified from the data library (Kanthal *et al.,* 2014). The GC-MS analysis revealed that the ethanolic extract of Tagetes erecta contained a total of 36 different compounds, whereas the extract of Tridax procumbens contained 31 compounds. This difference in compound count can be attributed to the varying composition of natural compounds present in different plant parts and their subsequent recoveries during the extraction process (Iloki-Assanga *et al.,* 2015). Ten compounds (Stigmasterol, beta-Amyrin, Tetradecanoic acid (Myristic acid), 9,12,15-

Table 2: Phytochemical compounds identified in ethanolic extract of *Tridax procumbens* by GC-MS.

Sl. No.	RT (min)	Area	Peak area%	Molecular weight	Structure	Name of Compounds
1.	3.345	4638051	1.89	102.3	$C_5H_{10}O_2$	n-Propyl acetate
2.	3.428	8695608	3.55	92.0	$C_3H_8O_3$	Glycerin
3.	3.942	248136	0.10	126.1	$C_6H_6O_3$	Maltol (Phenol)
4.	5.152	996901	0.41	144.2	$C_6H_8O_4$	4H-Pyran-4-one, 2,3-dihydro-3,5 dihydroxy-6-methyl (Quercetin)
5.	11.970	720562	0.29	206.4	$C_{13}H_{18}O_2$	1-(3,6,6-Trimethyl-1,6,7,7a tetrahydrocyclopenta[c]pyran-1-yl) ethanone
6.	23.948	527840	0.22	172.1	$C_{11}H_8O_2$	3-(5-Hydroxy-2,2,6-trimethyl-7-oxa bicyclo[4.1.0]hept-1-yl)-acrylic acid, methyle
7.	24.349	1757111	0.72	228.3	$C_{14}H_{28}O_2$	Tetradecanoic acid (Myristic acid)
8.	24.467	683844	0.28	60.0	$C_2H_4O_2$	Acetic acid, 2-(2,2,6-trimethyl-7 oxa-bicyclo[4.1.0]hept-1-yl) propenyl ester
9.	24.907	2015864	0.82	324.4	$C_{20}H_{24}O_4$	2,11Dioxatetracyclo [4.3.1.1 (3,10).0(6,9)] undec-4-ene, 3,7,7,10 tetramethyl-
10.	25.296	2783208	1.14	82.1	C_6H_{10}	2-Cyclohexen-1-one, 4-hydroxy3,5,5- trimethyl-4-(3-oxo 1-butenyl)-
11.	26.996	906872	0.37	278.5	$C_{20}H_{38}$	3-Eicosyne
12.	27.922	1731863	0.71	166.1	$C_8H_6O_4$	Phthalic acid, decyl isobutyl ester
13.	31.133	48869106	19.93	176.1	$C_6H_8O_6$	l-(+)-Ascorbic acid 2,6 dihexadecanoate (Vitamin C)
14.	31.865	421456	0.17	94.1	$C_9H_{12}O_3$	Phenol,2,6-dimethoxy
15.	32.016	588435	0.24	242.4	$C_{15}H_{30}O_2$	Ethyl tridecanoate
16.	35.636	10338845	4.22	128.1	$C_{20}H_{40}O$	Phytol (Phenol)
17.	36.345	42043211	17.15	280.4	$C_{15}H_{30}O_2$	Ethyl 9,12-hexadecadienoate
18.	37.118	6318349	2.58	278.4	$C_{18}H_{30}O_2$	Octadecanoic acid
19.	37.265	1385216	0.56	292.5	$C_{19}H_{32}O_2$	9,12,15-Octadecatrienoic acid, methyl ester (Linolenic acid)
20.	40.553	337342	0.14	313.4	$C_4H_4O_4$	Fumaric acid
21.	45.334	309818	0.13	200.2	$C_{10}H_{16}O_4$	3-[(2-Dimethylamino-ethylamino) methyl]-8a-methyl-5-methylene decahydro-naph
22.	47.547	544576	0.22	166.4	$C_8H_6O_4$	Phthalic acid, di (2-propylpentyl) ester
23.	54.298	1063093	0.43	426.7	$C_{30}H_{50}O$	1,6,10,14,18,22-Tetracosahexaen-3 ol, 2,6,10,15,19,23-hexamethyl-, (all-E)-
24.	60.935	362581	0.15	416.6	$C_{28}H_{48}O_2$	dl-.alpha.-Tocopherol (vitamin E)
25.	62.760	4095598	1.67	414.6	$C_{29}H_{50}O$	Ergost-5-en-3-ol, (3.beta.)-

26.	63.434	10929602	4.46	412.6	$C_{29}H_{48}O$	Stigmasterol (Steroids)
27.	64.609	10234004	4.17	412.1	$C_{29}H_{50}O$	gamma.-Sitosterol
28.	64.746	1845609	0.75	96.11	$C_8H_{24}O_4si$	4,4,6a,6b,8a,11,11,14b-Octamethyl 1,4,4a,5,6,6a, 6b,7,8,8a,9, 10,11,12,2a,14,14a
29.	64.958	1258646	0.51	426.72	$C_{30}H_{50}O$	Lupeol
30.	65.225	1106381	0.45	118.18	C_9H_{10}	beta-Amyrin
31.	67.282	1493258	0.61	60.0	$C_2H_4O_2$	Acetic acid, 3-hydroxy-7 isopropenyl-1, 4a-dimethyl-2, 3, 4, 4a,5,6,7,8-octahydronap
		245182289	**100.00**			

Octadecatrienoic acid, Ethyl ester (Z,Z,Z) (Linolenic acid), Ethyl tridecanoate (Tridecanoic acid), dl-alpha-Tocopherol (vitamin E), 4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl (Quercetin), Phenol,2,6-dimethoxy) were identified in both the plant extracts.

The major compounds present in the ethanolic extract of *Tagetes erecta* are as follows: beta-Amyrin (24.53%), Benzoic acid, 4-hydroxy-3,5-dimethoxy (14.32%), dl-.alpha-Tocopherol (vitamin E) (9.33%), Pentadecanoic acid, Ethyl tridecanoate (5.34%), 6,9-Octadecadienoic acid, methyl ester (5.32%), Cholesterol (4.59%), 1,E-11,Z-13-Heptadecatriene (4.41%), Stigmasterol (3.84%), Hexadecatrienal (3.47%) and so on are shown in Table 1. The ethanolic extract of *Tridax procumbens* contains Ascorbic acid (Vitamin C) (19.93%), Ethyl 9,12-hexadecadienoate (17.15%), Stigmasterol (4.46%), Phytol (4.22%), gamma-Sitosterol (4.17%), and Glycerin (3.55%) as major compounds, are shown in Table 2.

Some of these major compounds and many others have been identified to possess several biological activities. N-hexadecenoic acid showed anti-inflammatory activity (Aparna *et al.,* 2012), Stigmasterol (Steroids) and beta-Amyrin have anti-hypercholesterolemic, antioxidant, anti-inflammatory and hypoglycemic (Navpreet *et al.,* 2011; Thirupathi *et al.,* 2017). Anti-diabetic activity of gamma-sitosterol has also been reported (Balamurugan *et al.,* 2011). Vitamin E and C (Ascorbic acid) have properties such as anti-oxidant, anti-bacterial, anti-inflammatory and improve skin aging, synthesis of collagen (Verma, 2017; Tarik *et al.,* 2019). Anti-inflammatory, anti-bacterial and anti-cancer properties of beta-Amyrin and Glycerin were demonstrated by Godara *et al.* (2019).

CONCLUSION

The results provide a detailed comparison of bioactive phytochemicals found in the extracts. The ethanolic extracts of *Tagetes erecta* (flower) and *Tridax procumbens* (whole plant) have shown significant biological activities, supporting their traditional medicinal uses. The study identified key bioactive compounds in these extracts, laying the groundwork for further exploration of the potential health benefits of these plants and the need for additional pharmacological research. Future studies need on isolating the active principles of the extracts and elucidating their precise mechanisms of action against various disorders.

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