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Research Article

Survey of Medicinal and Invasive Weeds in Paddy Field – Phytochemical and GC-MS Profiling of *Cyanotis axillaris* R. & S.

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ABSTRACT

This study aims to determine the dominant weed species associated with rice crop fields in the Eppodhumvendran region of Thoothukudi district, Tamil Nadu and to analyze the phytochemicals, identify the bioactive compounds in ethanol extract using gas chromatography–mass spectrometry (GC-MS) and find their bioactivity using prediction of activity spectra for substances (PASS) prediction in *Cyanotis axillaris*. The documentation of medicinal weeds was carried out with the help of traditional local healers in Eppodhumvendran region. Phytochemical screening and GC-MS analysis of *C. axillaris* were performed to evaluate the chemical profiling of the extract. A total of 25 plant species regarded as invasive species/weeds were identified with the help of traditional local healers. The most commonly mentioned plant family was the Poaceae with a total of five species followed by the Euphorbiaceae, Asteraceae and Commelinaceae. Among these, *C. axillaris* is being studied for its potentiality due to its strong therapeutic value. The aerial plant part contains phytoconstituents such as alkaloids, glycosides, quinones, phenolics, steroids and terpenoids. The GC-MS results revealed 30 bioactive compounds, which were predicted using the PASS prediction method. The study highlights the importance of weeds in the paddy field ecosystem. The results reveal that *C. axillaris* contains various phytocomponents and that more research into their phytopharmaceutical relevance is required in the future.

Keywords: Medicinal weeds, Invasive flora, *Cyanotis axillaris*, Gas chromatography mass spectrometry, Prediction of activity spectra for substances.

INTRODUCTION

India has tremendous biodiversity and is endowed with many valuable plants. The diverse climatic conditions in India favour the most adopted weeds to prevail and cause severe crop yield losses. Weeds are one of the undesirable major constraints to crop cultivation that grow where they are not desired. These plant species grow spontaneously in crop ecosystems and also on open land areas finally which can affect crop yield qualitatively and quantitatively based on their species composition and density [1]. Invasive alien weeds are those plant species that are introduced to a geographical area where it does not grow naturally. Once invasive plants are introduced into a new ecosystem, they can become widespread and have direct, adverse impacts on public goods [2]. While the term 'weed' generally has a negative connotation and many plants known as weeds can have beneficial properties. Many of the weeds are used economically as fodder for animals, leafy vegetables by human beings, utilized as ornamental and hedge plants. Even, certain weeds have nematicidal and medicinal properties. Some of the weeds are used for the production of biofertilizer biomass-based energy and also for soil conservation aspects [3]. However, it is a matter of interest that some well-known weeds act as a source of drugs and traditional medicines. Weeds possess non-nutritive plant chemicals that contain protective disease-preventing compounds against various microorganisms. This medicinal importance of plants is especially due to the presence of secondary metabolites which play an important role in different metabolic activities of living organisms such as attracting pollinators and chemical defense against microorganisms, insects and higher predators which are present in each part of the weed plants like leaves, stems, roots, rhizomes and flowers. The present study has been initiated to work with the survey of weeds in paddy fields, screening their phytochemical activity, identification of phytoconstituents and prediction of their activity status. In connection with this, the common weeds are collected and information about medicinal usages was gathered from the local traditional healers of paddy fields in the Eppodhumvendran region of Thoothukudi district, Tamil Nadu. The main objectives of the study are, to document the weed and invasive plant species grown among rice fields (*Oryza sativa* L.) and to analyze the phytochemical screening, Gas chromatography mass spectrometry (GC-MS) studies and to predict the bioactive compounds of *C. axillaris* by using PASS prediction.

MATERIAL AND METHODS

Study Area

The medicinal weeds and invasive flora survey was conducted in the Eppodumvendran village of Ottapidaram Taluk in the Thoothukudi district of Tamil Nadu (Figs 1 and 2). The area of investigation approximately lies between the latitude of 9.02 North and a longitude of 78.05 East at 40.00 m/131.23 ft altitude with a total area of about

1226.38 hectares. The study area has a total population of 3,659 people, out of which the male population is 1,823 while the female population is 1,836. The average annual temperature and rainfall ranges from 26 to 28°C and 12 to 31 mm.

Collection and Identification of Medicinal Weeds

The present study was conducted in the region of rice crop fields in the Eppodhumvendran village. The survey was conducted after the rainy season (October to December – 2022). During the survey, some of the edible, medicinally potent and common weeds were noted in the rice crop field. The medicinally important weeds in the study area which are widely used by local people to treat various ailments were documented and photographs were taken. The discussion was carried out orally to get knowledge about the vernacular names, flowering, fruiting, medicinal and economic usage of weed plants in the study area. The collected medicinal plants were identified with the help of standard floras such as the flora of Presidency of Madras [4] and the flora of Tamil Nadu carnatic [5].

Preservation of Plant Specimen

Fresh aerial plant parts of *C. axillaris* R & S. were collected with the help of traditional local healers who inhabited this region. The plants were collected in the flowering and fruiting after the rainy season from the natural habitat from October to December. The collected plant specimens were pressed properly following the method [6]. All the preserved specimens were deposited for future reference at the Department of Botany, Vellalar College for Women (Autonomous), Thindal, Erode. The voucher specimen was deposited in the Vellalar College herbarium, Erode with a valid accession number (VCW/BH/Acc.No.37) for further use.

Pharmacognostical Studies

Macroscopical and physico-chemical studies

The macroscopic observation of *C. axillaris* was examined as per the methodology [7,8]. The organoleptic evaluation of whole aerial plant powder and extracts was carried out as per the methodology of Trease and Evans (1983).

Soxhlet extraction and their yield percentage

The air-dried and powdered whole aerial plant powder of *Cyanotis axillaris* was filled in the thimble and extracted successively with petroleum ether (60–80°C) and ethanol (64.7°C) (20 g/200 mL) using a soxhlet extractor for 6 to 8 hours. Finally, the material was macerated using hot water (99.98°C) with occasional stirring for 5 hours and the water extract was filtered. The percentage of yields was calculated as well as color and consistency of the extracts were also observed. The prepared extracts were subjected to further phytochemical and GC-MS analysis.

Qualitative phytochemical analysis

Phytochemical screening of different successive solvent extracts of *C. axillaris* was followed as per the methods adopted by Harborne (1984), Kokate *et al*. (1995) and Prabhakaran (1996).

GC/MS studies

The crude ethanol (1 μL) extract containing different compounds of *C. axillaris* was subjected to GC-MS analysis on the instrument -

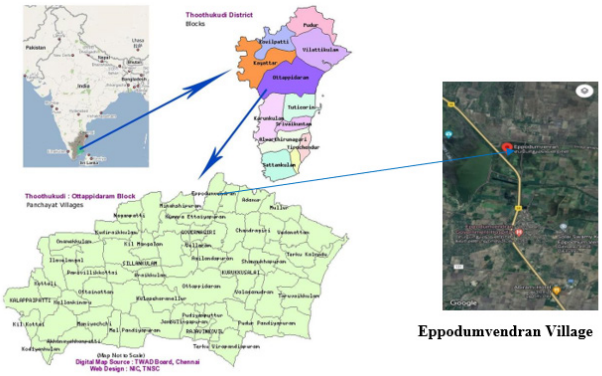

Fig. 1: The Eppodumvendran region in Thoothukudi District, Tamil Nadu, India

Field image during plowing time

Field image during the seedling time

Fig. 2: Paddy crop field of Eppodumvendran region, Thoothukudi district, Tamil Nadu, India.

Agilent GC 7890A/Gas Chromatograph Mass Spectrometer Detector MS5975C, equipped with a fused silica capillary column Agilent DB5MS of length: 30 mm, internal diameter: 0.25 mm and 0.25-micron film thickness. The mass spectrum of individual unknown compounds was compared with the known compounds stored in the software database libraries. The name, molecular weight and structure of components of the test materials were ascertained.

PASS prediction

The prediction of activity spectra for substances (PASS) prediction of the screened bioactive compounds was carried out by the PASS-Way2Drug server (http://www.way2drug.com/PASSOnline/predict.php), using the canonical SMILES from the PubChem server (https://pubchem.ncbi.nlm.nih.gov/) [12].

RESULTS AND DISCUSSION

Data Analysis of Medicinal Weeds

In the present investigation, about 25 medicinal weeds and invasive flora were recorded. Out of this, 1 was pteridophyte, 13 were dicotyledons and 11 were monocotyledons in the paddy field ecosystem. The weed surveys were done in September, October and November months, during the end of the rainy season. The present weed diversity observation of this study provides the plant species across the 16 families and 23 genera in the paddy field. During the survey, weeds were identified using a random method. Some of the major weeds are shown in Fig. 3. Likewise, Panda *et al*. (2014) demonstrated the medicinal weed diversity and ethnomedicinal weeds screening used by the tribal's of Koraput, India and recorded the presence of 33 plant species belonging to 32 genera and 20 families, being used as 36 ailment categories. Similarly, Mohamed *et al.* (2018) carried out a weed flora survey in garlic (*Allium sativum*) and onion (*Allium cepa*) crop fields in Dongola area, Northern state, Sudan revealed the presence of 26 species of annual and perennial weeds belonging to 15 families in garlic and 28 species belonging to 15 families in onion.

In the present study, 25 weed species have been enumerated (Table 1). Some of the weeds are consumed as cooked leaf, stem and seed (10 plants), sap (1 plant), juice (3 plants), extract (10 plants) and powder (1 plant) in paddy fields. Similar work was carried out by Reena and David Samuel (2019) who investigated the occurrence of edible weeds and their traditional use in human nutrition in Thuckalay Block, Kanyakumari district and reported 55 weed food plants belonging to 32 families.

Pharmacognostical Studies of Selected Plant

Macroscopical studies

The present macroscopical examinations of the whole aerial plant of *C. axillaris* showed that the species is a prostate herb and it grows up to

Fig. 3: The image represents the major weeds of the paddy field

Table 1: List of surveyed species and their therapeutic potential in the paddy crop field of Eppodumvendran region, Thoothukudi district, Tamil Nadu, India.

S. No.	*Botanical name of the plant*	*Family*	*Vernacular name*	*Part used*	*Edible parts*	*Utilization method*	*Medicinal uses*	*Flowering period*
Weed Flora in Paddy Field								
1.	*Ageratum conyzoides* L.	Asteraceae	Billygoat weed	Leaves, roots and flowers	Young leaves	Leaf and stem extract	Dysentry and diarrhoea	May - June
2.	*Ammannia baccifera* L.	Lythraceae	Nellicheera	Leaves	Young leaves	Boiling the leaf	Antibacterial and rheumatic pain	August - December
3.	*Asteracantha longifolia* Nees.	Acanthaceae	Gokulakantha	Seeds and roots	Seeds	Extract of roots and seed	Sedative blood diseases and Aphrodisiac tonic	September - March
4.	*Celosia argentea* L.	Amaranthaceae	Cock's comb	Leaves, roots and seeds	Young leaves	Boiled or cooked leaves and roots	Painful menstruation, skin eruption, ulcers and sores	April – June
5.	*Centella asiatica* Urb.	Apiaceae	Indian pennywort	Leaves	Leaves	Boiled or cooked leaves and stem	Minor wounds, improve mental clarity and treat skin diseases	May - October
6.	*Commelina benghalensis* L.	Commelinaceae	Dayflower	Leaves	Leaves and Stem	Cooked stem	Laxative, diuretic and Febri fungal	March-August
7.	*Cyanotis axillaris* (L.) R. & S.	Commelinaceae	Spreading dayflower	Whole plant	Leaves	Raw material used in food for pigs	Rheumatism and joint pains	August - October
8.	*Cynodon dactylon* (L.) Pers.	Poaceae	Bermuda grass	Rhizomes and Grass juice	Young leaves	Extract or powder root	Diuretic, astringent, snakebite,diarrhoea, stones and tumours	August
9.	*Cyperus alternifolius* L.	Cyperaceae	Umbrella plant	Whole plant	Inner base of the young stem	Raw tuber	Digestive, fever and wounds	June - July
10.	*Cyperus rotundus* L.	Cyperaceae	Purple nut sedge	Whole plant	Tuber Seed	Raw tuber or powder of tuber	Diarrhoea and bowel disorders	September - March
11.	*Dactyloctenium aegyptium* (L.) Willd.	Poaceae	Cow foot grass	Whole plant	Seeds	Fresh juice	Smallpox, wounds, ulcers, Antipyretic and anti-cancer	All the year
12.	*Echinochloa colona* (L.) Link.	Poaceae	Jungle rice	Seeds	Young plants, shoots and seeds	Cooked seeds	Forage eaten by humans	All year
13.	*Echinochola crus-galli* (L.) P. Beauv.	Poaceae	Barnyard grass	Shoot and root extraction	Young shoots, stem tips and seeds	Plant extract and cooked young shoots	Indigestion, spleen cancer and Wounds	January - March

14.	*Eclipta alba* L.	Asteraceae	False daisy	Whole plant, Leaves, Stem, roots and flowers	Leaves and young shoots	Leaf juice	Antiseptic	February - May
15.	*Eleusine indica* (L.) Gaertn	Poaceae	Goose grass	Whole plant and Leaves	Seeds,young seedlings and Root	Root juice	Diuretic, laxative, malaria, Stop bleeding and post childbirth cleansing	All year
16.	*Euphorbia hirta* L.	Euphorbiaceae	Garden spang or asthma weed	Whole plant, stem, leaves and latex	Leaves, flowers and Shoots	Raw fruit extract and cooked leaf	Asthma, fever and malaria	March - August
17.	*Ipomoea aquatic* Forssk.	Convolvulaceae	Water spinach or swamp morning glory	Leaves, Young shoots and roots	Leaves and Young shoots	Cooked tender shoots and leaves	Piles, jaundice and hypertension	June - August
18.	*Ludwigia adscendens* (L.) H. Hara	Onagraceae	Water primrose	Whole plant and aerial parts,	Leaves and Young shoots	Leaf sap	Antiseptic and ulcers	April - November
19.	*Marsilea quadrifolia* L.	Marsileaceae	Marsilea	Whole plant	Leaves and Young stems	Cooked leaf and extract of leaf	Snake bite and diuretic	-
20.	*Phylo nodiflora* (L.) Greene	Verbenaceae	Frog fruit	Whole plant and Root	Leaves	Plant powder	Diuretic and antiseptic	December - February
21.	*Phyllanthus niruri* L.	Euphorbiaceae	Niruri	Whole plants, Roots, fruits and seeds	-	Leaf extract and plant extract	Urinary stones	July - September
22.	*Portulaca oleracea* L.	Portulacaceae	Purslane	Whole plant, Leaves and Seeds	Young plants, leaves and stems	Raw or cooked leaf, shoots and flower	Antibacterial and inflammation	June - August
23.	*Setaria viridis*(L.) P. Beauv.	Poaceae	Green bristle grass	Seeds	Seeds	Plant extract mixed with water	Diuretic	November - December
24.	*Trianthema portulacastrum* L.	Aizoaceae	Horse purslane	Leaves, roots and seeds	Leaves	Cooked vegetables, root extract	Anaemia, laxative, inflammation and night blindness	December - April
Invasive Weed Flora in Paddy Field								
25.	*Monochoria vaginalis* Presl.	Pontendariaceae	Oval-leafed pondweed	Leaves and roots	Leaves, young inflorescence and rhizomes	Leaf juice and boiled leaf	Liver problems and antipyretic	April - October

Table 2: Qualitative phytochemical screening of different solvent extracts of *C. axillaris*

S. No.	*Phyto constituents*	*Test/Reagent*	*Petroleum ether extract*	*Ethanol extract*	*Aqueous extract*
1.	Proteins	Biuret test	_	+	_
2.	Amino acids	Ninhydrin test	-	+	-
3.	Carbohydrates	Barfoed's test	+	+	_
4.	Alkaloids	Wagner's reagent	–	+	+
5.	Flavonoids	Lead acetate test	+	–	+
6.	Glycosides	Borntrager's test	+	+	_
7.	Quinones	Sulphuric acid test	+	+	_
8.	Anthraquinone	Borntrager's test	_	+	+
9.	Coumarin	NaOH test	–	+	_
10.	Saponins	Frothing test	+	+	+
11.	Tannins	Braymer's test	+	+	_
12.	Phenolics	Lead acetate test	+	+	_
13.	Steroids	Libermann and Burchard's test	–	+	–
14.	Terpenoids	Libermann test	+	+	+
15.	Fixed oil	Stain test	_	+	_

Note: (+) Presence of chemical compound; (-) Absence of chemical compounds

the height of 60 cm. The leaves are simple, alternate and are arranged in spiral phyllotaxy. The size of the leaves approximately ranged from 1.5 to 8 in long and about 1 to 4 in wide. Bothsurfaces of the leaves are glabrous and it is sessile with a sheathing leaf base. The herbaceous, green-colored stem shows a bitter taste and characteristic odor. The inflorescence is solitary and axillary in position. The flower is purple with a characteristic arrangement of floral parts with three sepals and three petals. The androecium is composed of densely bearded filiform stamen which is six in number. The gynoecium consists of the 3-celled ovary with two ovules in each cell. The fruit is a beaked capsule with a glabrous surface.

Organoleptic characteristics of whole aerial plant powder and their extracts

The organoleptic characteristics such as color, texture, taste and odor of the whole aerial plant powder are presented. The coarse greenish study powder expressed a characteristic odor and bitter taste. The extractive yield of petroleum ether, ethanolic and aqueous extracts of whole aerial plant powder of *C. axillaris* was also noted.

Successive solvent extraction and phytochemical screening

The percent yield was maximum in ethanol extract (8.5%) followed by petroleum ether extract (6.5%) and aqueous (5.5%). To investigate the chemical constituents of *C. axillaris* whole aerial plant powder, the successive solvent extracts were subjected to qualitative phytochemical screening. The results of preliminary phytochemical screening showed the presence of various phytochemicals (Table 2). The ethanolic extract contains maximum of phytoconstituents

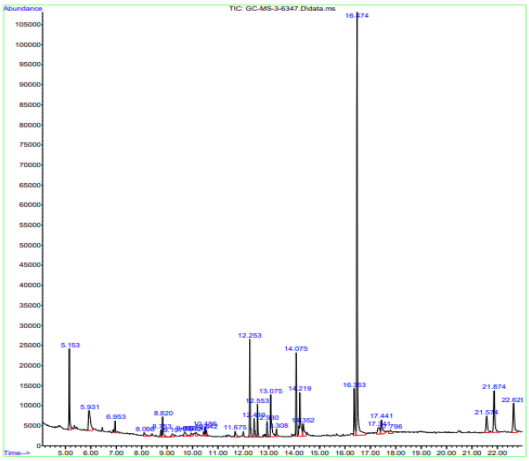

Fig. 4: GC-MS spectra of ethanolic leaf extract of *Cyanotis axillaris* R. & S.

(proteins, amino acids, carbohydrates, alkaloids, glycosides, quinones, anthraquinone, coumarin, saponins, tannins, phenolics, steroids, terpenoids and fixed oil) compare to other extracts (petroleum ether and aqueous extract). Similar phytochemical screening was carried out by several scientist in various plants like *Commelina bengalensis* (Ghosh and Chatterjee, 2011), *Cyperus rotundus* tuber (Ghannadi *et al.,* 2012), some weeds like *Alternanthera sessilis*, *Amaranthus spinosa*, *Lantana camera* and *Xanthium strumarium* (Chavan *et al.,* 2013), *C. esculentus* tuber (Imam *et al*., 2013), *Cyanotis axillaris* and *C. cerifolia* (Nikam *et al.,* 2013) and *Enicostemma littorale* (Sanmugarajah*et al.,* 2013).

GC-MS studies

In the present study, the components present in the ethanolic extract of *C. axillaris* were identified by GC-MS screening and are depicted in Table 3. The present study was undertaken to find out the bioactive compounds present in the ethanolic extract of *C. axillaris* which revealed the presence of thirty active constituents with an intensity of different peaks at various RT were recorded and given in chromatogram (Fig. 4). A compound like 1,2-benzenedicarboxylic acid expressed the highest peak area percentage (29.53) followed by stigmasterol (6.10) and oleyl alcohol, heptafluorobutyrate (5.74) with a retention time of 16.474, 21.874 and 14.219 minutes, respectively.

PASS prediction

Prediction of activity spectra for substances (PASS) was used to predict the biological activities of 29 phytoconstituents that are screened from ethanolic extract of *C. axillaris* plant by using GC-MS analysis. In the present work, the Pa values for predicted bioactivities of compounds lie between 0.970 to 0.017, which are listed in Table 4.

Among the 29 compounds screened, 13 compounds were predicted to have high antineoplastic activity (0.670–0.285), eleven constituents have the antiseborrheic property (0.907–0.844) and ten compounds are responsible for the antieczematic property (0.806–0.707). These three compounds are major predicted compounds in the plant extract. The plant extract contains many predicted compounds holding many therapeutic properties. Similar PASS prediction was carried out by Mojumda *et al.* (2016) who assessed molecular docking and PASS prediction for the analgesic activity of some isolated compounds screened from *Acalypha indica* and the results highlighted that PASS prediction property for the analgesic activity of the isolated

Table 3: GC-MS analysis of bioactive compounds in ethanolic leaf extract of *C. axillaris*

S. No.	*RT*	*Name of the compound*	*Molecular formula*	*Molecular weight*	*Peak area%*	*Nature of compound*	*Activity*
1.	5.153	Benzene, 1,3-dichloro	$C_6H_4Cl_2$	147	5.42	Meta-dichlorobenzen	Fumigant, insecticide and antidiabetic
2.	5.931	2-Cyclohexen-1-ol	$C_6H_{10}O$	98.14	4.73	Hydrocarbon	Carminative and alopecia treatment
3.	6.953	Decane, 2-methyl-	$C_{11}H_{24}$	156.31	0.78	Acyclic branched hydrocarbons	Antieczematic
4.	8.098	Imidazo[5, 1-f] [1,2,4] triazine-2,7-diamine	$C_5H_6N_6$	150.14	0.76	*Crystalline solid*	Antineoplastic, autoimmune disorders treatment and tumour necrosis factor
5.	8.753	21-Norpicrasane-20-carboselenoic acid, 1,2,3-tris(acetyloxy)-13,16-dioxo-, se-phenyl ester, (1. alpha., 2. beta.,3. beta.)-	$C_{32}H_{38}O_{10}Se$	661.6	0.60	*Carboxylic acids*	Antifungal, polarisation stimulant and anti-inflammatory
6.	8.820	Decane, 2-methyl-	$C_{11}H_{24}$	156.31	1.70	Acyclic branched hydrocarbons	Antieczematic
7.	9.197	2,2-Dibromo cholestanone	$C_{27}H_{44}Br_2O$	544.4	0.70	Propylene bromide	Antimetastatic and anti-infertility
8.	9.967	.beta.-D-Glucopyranose,1,6-anhydro-	$C_{12}H_{16}O_8$	288.25	1.00	Anhydrohexose	Respiratory analeptic and antiseborrheic
9.	9.942	Benzoic acid,2-hydroxy-, phenyl ester	$C_{14}H_{12}O_4$	244.24	0.59	Aromatic carboxylic acid	Antipyreticand Anti-infective
10.	10.142	D-(+)-Ribonic acid .gamma.-lactone	$C_5H_8O_5$	148.11	0.68	Ribonic lactone	Antiviral and antihelmintic
11.	10.486	Octatriacontane, 3,5-dimethyl-	$C_{40}H_{82}$	563.1	0.68	Pentafluoro propionate	Antiallergic and anticonvulsant
12.	10.542	2,6,10-Dodecatrien-1-ol,3,7,11-trimethyl-, (E,E)-	$C_{18}H_{30}O_2$	278.4	0.58	-	Antibacterial and antioxidant
13.	11.675	Tetradecanoic acid	$C_{14}H_{28}O_2$	228.37	0.94	Myristic acid	Antioxidant and antiseborrheic
14.	12.253	1,9-Nonanediol, dimethanesulfonate	$C_{11}H_{24}O_6S_2$	316.4	5.60	Nonasulphan, solid	Antiviral and anticancer
15.	12.419	1-Ethynylcyclopentanol	$C_7H_{10}O$	110.15	1.63	Cyclic ether	Antisecretory and antitumor
16.	12.553	6,11-Undecadiene,1-acetoxy-3,7-dimethyl-	$C_{16}H_{28}O_2$	252.39	1.98	-	Antiulcerative and anti-leishmania
17.	12.930	Benzenepropanoic acid,3-5-bis(1,1-dimethylethyl)-4-hydroxy-, methylester	$C_{18}H_{28}O_3$	292.4	0.96	Phenylpropanes	Anti-cholesterol and anti-inflammatory
18.	13.075	Tetradecanoic acid	$C_{14}H_{28}O_2$	228.37	4.52	Myristic acid	Antianemic and anti-protozoal
19.	13.308	.pi.-Cyclopentadienyl-dicarbonyl-ethylisonitril-trichlorgermyl-tungsten	$C_9H_5O_9N_3Cl_3$	662.078	0.66	*Dark* purple crystals	Antibacterial
20.	14.075	Oxirane, decyl-	$C_{12}H_{24}O$	184.32	5.68	Methylmetal compounds	Antipruritic and antihypoxic
21.	14.219	Oleyl alcohol, hetafluorobutyrate	$C_{18}H_{36}O$	268.5	5.74	Unsaturated fatty alcohol	Antiallergic and antiviral

22.	14.352	Heptadecanoic acid	$C_{17}H_{34}O_2$	270.5	2.07	Saturated fatty acid	Antimutagenic and anti-inflammatory
23.	16.363	15-Hydroxypentadecanoic acid	$C_{15}H_{30}O_3$	258.40	4.15	Hydroxylated fatty acid	Antiseborrheic and antisecretory
24.	16.474	1,2-Benzenedicarboxylic acid, diisooctyl ester	$C_8H_6O_4$	166.13	29.53	Phthalate esters	Antioxidant activity, antifungal activity
25.	17.341	Ethane, 1-(4,4,4-trifluoro-1,3-dithiobutyl)-2-(3,3,3-trifluoro-1,2-dithiopropyl)-	$C_5H_6F_6S_4$	308.4	1.79	-	Phobic disorders treatment
26.	17.441	22 beta. -Acetoxy-3.beta.,16 alpha-dihydroxy-13,28-epoxyolean-29-al	$C_{32}H_{50}O_6$	530.7	2.18	-	Hypolipemic and Hepatic disorders treatment
27.	17.796	Silicic acid, diethyl bis(trimethylsilyl)ester	$C_{10}H_{28}O_4Si_3$	296.58	0.88	Silicic acid	Antibacterial, antioxidant and antimicrobial activity
28.	21.574	Barbituric acid, 5-allyl-5-(cyclohex-2-en-1-yl)-	$C_{13}H_{16}N_2O_3$	248.28	2.68	Pheterocyclic	Antibacterial, hypotensive and antisclerotics
29.	21.874	Stigmasterol	$C_{29}H_{48}O$	412.7	6.10	Unsaturated phytosterol	Antiinflammatory and immunomodulatory
30.	22.629	beta-Sitosterol	$C_{29}H_{50}O$	414.7	4.66	Stigmastane sterol	Antioxidant, anticancer, anti-diabetic, antimicrobial and immunomodulatory activities

Table 4: GC-MS bioactive compounds and their PASS prediction activity of *C. axillaris* ethanolic extract

S. No.	*Name of the compound*	*Pub Chem ID*	*Pa*	*Pi*	*Activity*
1.	Benzene, 1,3-dichloro	CID-10943	0.946	0.003	Phobic disorders treatment
			0.907	0.004	Antiseborrheic
			0.837	0.011	Antidiabetic
			0.795	0.014	Anti-inflammatory
			0.707	0.043	Antieczematic
2.	2-Cyclohexen-1-ol	CID-13198	0.663	0.003	Antimetastatic
			0.670	0.031	Antineoplastic
			0.632	0.031	Antidyskinetic
3.	Decane, 2-methyl-	CID-23415	0.837	0.012	Antiseborrheic
			0.717	0.036	Antineurotic
			0.615	0.005	Antiviral (Rhinovirus)
			0.613	0.004	Antimyopathies
4.	Imidazo[5, 1-f][1,2,4]triazine-2,7-diamine	CID-591285	0.835	0.008	Antineoplastic
			0.784	0.009	Antiarthritic
			0.751	0.004	Antiparkinsonian
			0.621	0.014	Antiasthmatic
5.	21-Norpicrasane-20-carboselenoic acid, 1,2,3-tris(acetyloxy)-13,16-dioxo-, se-phenyl ester, (1.alpha.,2.beta.,3.beta.)-	CID-538030	0.939	0.004	Antineoplastic
			0.814	0.004	Antileukemic
			0.720	0.009	Antifungal
			0.578	0.012	Antineoplastic (breast cancer)

			0.837	0.012	Antiseborrheic
			0.744	0.032	Antieczematic
6.	Decane, 2-methyl-	CID-23415	0.717	0.036	Antineurotic
			0.615	0.005	Antiviral (Rhinovirus)
			0.814	0.005	Antihypercholesterolemic
			0.794	0.020	Antieczematic
7.	2,2-Dibromocholestanone	CID-22212696	0.745	0.005	Antipruritic
			0.686	0.006	Antiviral (Influenza)
			0.915	0.005	Antineoplastic
			0.817	0.005	Anti-inflammatory
8.	.beta.-D-Glucopyranose,1,6-anhydro-	CID-91691667	0.640	0.008	Antineoplastic (Lung cancer)
			0.551	0.063	Antiseborrheic
			0.924	0.003	Antiseptic
			0.017	0.009	Antiprotozoal activity enhancer
9.	Benzoic acid,2-hydroxy-, phenyl ester	CID-11436480	0.074	0.067	Antineoplastic antibiotic
			0.038	0.033	Antithrombocytopenic
			0.815	0.015	Antieczematic
			0.787	0.013	Antineoplastic
10.	D-(+)-Ribonic acid .gamma.-lactone	CID-219575	0.728	0.005	Antiviral (Picornavirus)
			0.712	0.004	Antihelmintic (Nematodes)
			0.784	0.022	Antiseborrheic
			0.592	0.020	Anticonvulsant
11.	Octatriacontane, 3,5-dimethyl-	CID-545957	0.566	0.018	Antipruritic, allergic
			0.613	0.067	Antineurotic
			0.797	0.019	Antieczematic
			0.780	0.005	Antisecretory
12.	2,6,10-Dodecatrien-1-ol,3,7,11-trimethyl-, (E,E)-	CID-6431104	0.774	0.004	Antiulcerative
			0.763	0.006	Antihypercholesterolemic
			0.920	0.004	Antieczematic
			0.866	0.008	Antiseborrheic
13.	Tetradecanoic acid	CID-11005	0.798	0.004	Antihypoxic
			0.783	0.004	Antimutagenic
			0.718	0.002	Antineoplastic, alkylator
			0.717	0.023	Antineoplastic
14.	1,9-Nonanediol, di-methanesulfonate	CID-20244	0.467	0.039	Antiviral (Rhinovirus)
			0.405	0.003	Antifibrinolytic
			0.845	0.004	Antiosteoporotic
			0.791	0.021	Antiseborrheic
15.	1-Ethynylcyclopentanol	CID-87074	0.705	0.009	Antisecretory
			0.646	0.028	Antidyskinetic

			0.910	0.003	Antihypercholesterolemic
16.	6,11-Undecadiene,1-acetoxy-3,7-dimethyl-	CID-5367551	0.813	0.004	Antisecretory
			0.801	0.004	Antiulcerative
			0.798	0.005	Antiprotozoal (Leishmania)
			0.753	0.006	Antihypercholesterolemic
17.	Benzenepropanoic acid,3-5-bis(1,1-dimethyl ethyl)-4-hydroxy-,methyl ester	CID-62603	0.689	0.017	Anti-inflammatory
			0.704	0.037	Antiseborrheic
			0.637	0.030	Antidyskinetic
			0.128	0.088	Antianemic
18.	Tetradecanoic acid	CID-11005	0.154	0.115	Antianorexic
			0.167	0.148	Antiprotozoal
			0.177	0.174	Anti-*Helicobacter pylori*
			0.722	0.039	Antieczematic
19.	Oxirane, decyl-	CID-17858	0.549	0.051	Antidyskinetic
			0.521	0.032	Antihypoxic
			0.519	0.031	Antipruritic
			0.851	0.009	Antieczematic
20.	Oleyl alcohol, hetafluorobutyrate	CID-91754008	0.641	0.024	Anti-inflammatory
			0.554	0.011	Antiviral (Rhinovirus)
			0.504	0.038	Antipruritic, allergic
			0.920	0.004	Antieczematic
21.	Heptadecanoic acid	CID-10465	0.866	0.008	Antiseborrheic
			0.798	0.004	Antihypoxic
			0.783	0.004	Antimutagenic
			0.859	0.003	Antihypoxic
22.	15-Hydroxypentadecanoic acid	CID-78360	0.804	0.018	Antiseborrheic
			0.718	0.009	Antisecretory
			0.654	0.011	Antipruritic
			0.844	0.011	Antiseborrheic
23.	1,2-Benzenedicarboxylic acid, diisooctyl ester	CID-33934	0.602	0.006	Antiviral (Rhinovirus)
			0.597	0.013	Antipruritic, allergic
			0.590	0.019	Antihypoxic
			0.362	0.037	Antiprotozoal (Amoeba)
24.	Ethane, 1-(4,4,4-trifluoro-1,3-dithiobutyl)-2-(3,3,3-trifluoro-1,2-dithiopropyl)-	CID-610064	0.289	0.035	Antiprotozoal (Trichomonas)
			0.352	0.156	Antiviral (Picornavirus)
			0.286	0.101	Anti-inflammatory, ophthalmic
			0.937	0.004	Antineoplastic
25.	22.beta.-Acetoxy-3.beta.,16.alpha.-dihydroxy-13,28-epoxyolean-29-al	CID-610201	0.903	0.003	Antineoplastic (lung cancer)
			0.613	0.008	Antileukemic
			0.583	0.006	Antimetastatic

			0.423	0.039	Antimyopathies
			0.400	0.036	Antiviral (Herpes)
26.	Silicic acid, diethyl bis (trimethylsilyl) ester	CID-77092	0.393	0.049	Antiinfective
			0.285	0.017	Antineoplastic (endocrine cancer)
			0.961	0.002	Anesthetic general
			0.698	0.010	Anticonvulsant
27.	Barbituric acid, 5-allyl-5-(cyclohex-2-en-1-yl)-	CID-3032457	0.473	0.028	Antiprotozoal (Leishmania)
			0.414	0.040	Antiulcerative
			0.970	0.002	Antihypercholesterolemic
			0.806	0.017	Antieczematic
28.	Stigmasterol	CID-5280794	0.755	0.004	Antitoxic
			0.751	0.004	Antipsoriatic
			0.960	0.002	Antihypercholesterolemic
			0.762	0.005	Antipruritic
29.	.beta.-Sitosterol	CID-222284	0.706	0.005	Antiosteoporotic
			0.638	0.004	Anti-infertility, female

compounds and showed a wide range of activity and all the compounds showed greater Pa than Pi value.

CONCLUSION

With an emphasis on the above background, the present investigation was undertaken to determine the most prevalent weed species associated with rice crop fields in the Eppodhumvendran region of Thoothukudi district, Tamil Nadu. The Poaceae, Cyperaceae, Euphobiaceae, Commelineaceae and Amaranthaceae were the families with the most members in the study area. The present study was to analyze the whole aerial part of *C. axillaris* which contains alkaloids, glycosides, quinones, anthraquinone, coumarin, saponins, tannins, phenolics, steroids, terpenoids and fixed oils present in the ethanolic extract. Through GC-MS, bioactive compounds of the ethanolic extract of *C. axillaris* were screened and revealed the presence of 30 bioactive constituents. Among the identified compounds, 1,2-benzenedicarboxylic acid, diisooctyl ester showed the highest peak area percentage (29.53%) with phthalate esters and showed antioxidant and antifungal activity. The plant extract contains many predicted compounds with therapeutic properties.The current study was very useful for the weed management of crop fields in the paddy ecosystem. This study may be of great use and interest to researchers, the pharmaceutical industry and medical practitioners. The weed species selected for the study can be used as a potential source of useful antibacterial, antifungal, anti-inflammatory, antileukemic, antineurotic, antiviral and antiseborrheic activity.

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