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GCMS Profiling Analysis of Five Different Solvent Leaf Extracts of *Eupatorium Triplinerve Vahl*

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Abstract:- Medicinal plants are more crucial in the field of pharmacology as most pharmaceutical industries; it may depend on medicinal plants for their raw materials. *Eupatorium Triplinerve Vahl* belongs to Asteraceae family, it is also known as "Ayapana" used for various medicinal properties. The present study was carried out to identify the phytoconstituents in the different solvents of the plant leaf extract. In this investigation, Gas Chromatography-Mass Spectrometry GC-MS) screening was performed to evaluate the phytocompounds and their biological activity. The GC-MS analysis provided peaks area 20.4% of 1-ISOPROPYL-2,5-DIMETHOXY-4-METHYLBENZENE in ethanol leaf extract, 2H-1-BENZOPYRAN-2-ONE, 7-METHOXY (peak area 7.07%) in methanol leaf extract, 3-Oxabicyclo[4.2.0]oct-5-ene (peak area 19.47%) in acetone leaf extract respectively. The GC-MS profiling of different leaf extracts revealed the presence of bioactive compounds. There are 90 chemical compounds that have new potential sources of medicines for the treatment of various diseases and are responsible for their therapeutic effects. The results show that *Eupatorium Triplinerve* contains various bioactive compounds and is recommended as a plant of phytopharmaceutical importance.

Keywords:- *Pharmacology, Phytoconstituents, Ayapana, Phytocompounds.*

I. INTRODUCTION

Plants are commonly used as medicines for various illnesses and they may serve as a source of potent drugs due to the presence of certain bioactive compounds (Gopalakrishnan & Udayakumar, 2014). Plants contain different phytochemicals or secondary metabolites, to use for various disorders to improve human health conditions (Mahomoodally, 2013; Patel, 2022). Secondary metabolites are plays a vital role in the pharmaceutical industry for the development of new drugs and to preparation of new therapeutic agents. The development of new drugs begins with the identification of active components from natural sources in various plant species (Nisha et al., 2011). Plants provide us with rich sources of natural antioxidants used in folk medicines and remedies. All medicinal plants contain various primary metabolites whereas; secondary metabolites enable interaction with environmental conditions. GC-MS methods are used to analysis of leaf extracts as a tool for testing the active compounds in herbs that are used in cosmetics, drugs, pharmaceuticals, and the food industry (Gomathi et al., 2015). Phytochemicals such as alkaloids, flavonoids, phenol, coumarin, and terpenoids have plenty of biological properties like anti-oxidant, anti-ulcer, anti-cancer, anti-inflammatory, and so on (Starlin et al., 2012). According to the World Health Organization, the traditional medicinal system plays an essential role in the health care sector for the purpose of scientific validation or discovery of new lead compounds for use as therapeutic drugs (Vuorela et al., 2004).

Eupatorium triplinerve vahl is locally known as Ayapana in Tamil, Mrithasanjeevani in Malayalam, and Ayaparna in Hindi. The plant is an ornamental erect perennial and slender herb with a semi-woody base growing up to 1m in height (Gauvin-bialecki & Marodon, 2009). Traditionally, the leaf extracts are consumed orally to reduce hemorrhage and they also heal induced ulceration in any place within or inside gout(Cheriyan et al., 2019). It helps in ailments like gastric and duodenal ulcers, Crohn's disease, and hemorrhoids (Cheriyan et al., 2019; Garg & Nakhare, 1993; Garg & Nigam, 1970). The leaves are very useful in reducing pain and inflammation. The plant serves as a natural therapeutic agent for neurodegenerative and hepatotoxic disorders due to the presence of unique bioactive components like coumarin, thymohydroquinone, umbelliferone, herniarin, stigmasterol, and sabinene. Coumarin is present in other plants as well as (7-methoxy coumarin) is used as an anti-tumor agent and is considered to be a component of the general defense response to abiotic and biotic stresses which exhibit anti-inflammatory activity (Biswas & Bhattacharya, 2012; Vahl, 2016). Several research reports state that the plant has various medicinal properties like antimicrobial, antioxidant, antineoplastic, sedatives, analgesic, antiseptic, and anti-hemorrhoid activity (Canales-Martínez et al., 2005; Yadava & Saini, 1990). The ethanol leaf extract results showed analgesic, antibacterial, antifungal, and antiseptic activity when used to treat hemorrhage, (Ghani, 1998; Matos Lopes et al., 2015). The methanolic leaf extracts produced hepatoprotective and antioxidant effects. Additionally, the plant has significant antinociceptive and anti-inflammatory activity (Sugumar et al., 2015; Varghese et al., 2017).

The combined analytical method known as GC-MS is used to determine and identify the compounds that appear in a plant sample. GC-MS plays a vital role in the phytochemical analysis and chemotaxonomic studies of the medicinal plant properties that contain biologically active

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compounds. This technique has superior separation potency that can lead to producing a high accuracy and precision of biochemical fingerprints. However, quantitative data with the coupled mass spectral database can be described by GC-MS which can have tremendous value for the correlation of bioactive compounds and their applications.

II. MATERIALS AND METHODS

➢ *Collection and Authentication of Plant Material*

Eupatorium Triplinerve Vahl, a member of the Asteraceae family, was obtained at the Institute of Forest Genetics and Tree Breeding (IFGTB) in Coimbatore, India, in December 2017. The plant's authenticity was confirmed by the Botanical Survey of India (BSI), also located in Coimbatore, Tamil Nadu, India. The identified and reported plant specimen's voucher number is BSI/SRC/5/23/2019/TECH/250.

➢ *Preparation of Plant Leaf Extract:*

Weighing and thoroughly washing the *Eupatorium triplinerve Vahl* leaves (270 g wet leaf), they was then fully rinsed with sterile distilled watered. The leaf was then shade-dried in ordered to prevent the loss of volatile components for about 8 days. Using a crusher and pestle, the dried leaves was ground into a coarse powder and stored at room temperature until required.

Based on the polarity index units, different solvents, including petroleum ether (0.1), hexane (0.1), acetone (5.1), methanol (5.1), and ethanol (5.2), was used to dissolve the powdered leaf (20g). For approximately 16 to 24 hours, the leaf extract was collected in a round-bottom flask. The solvent was then allowed to evaporate at room temperature before being filtered through Whatmann No. 1 filter paper. Additionally, the undiluted extract was gathered and kept at 4º C. The extracted sample's percentage yield (%) was calculated and presented in Table 1. (Redfern *et al.*,2014).

➢ *Characterization of Phytochemicals:*

- *Gas Chromatography-Mass Spectrum (GC-MS) of Five Solvent Leaf Extracts of Eupatorium Triplinerve Vahl*

The phytocompounds present in all five solvent leaf extracts was analyzed using GC-MS (Clarus 500 GC Perkin Elmer system). The columns was used in a condition of comprising an AOC-20i autosampler and equipped with a mass detector Turbo mass Gold-Perkin Elmer Tubromass 5.2 spectrometer with a fused silica capillary column packed with Elite –5MS (5% diphenyl/ 95% dimethyl polysiloxane) 30m× 0.25µm DF which was operating in an electron impact mode at 70eV. Components have been separated by using Helium as carrier gas at the constant flow of 1ml/min and injection volume of 0.5 EI (Split ratio 10:1 injector temperature 250°C; ion source temperature 280°C). The Oven temperature was programmed from 110°C (isothermal to maintain for 2 min) with an increase of 10ºC/min, to 200°C then 5°C /min to 280°C, ending with a 9 min isothermal at 280°C. Mass spectra was taken at 70eV; a scanning interval of 0.5s and fragments from 40 to 550 Da. The spectrum obtained was compared and validated by using NIST, MS data library version year 2011(Selvamangai & Bhaskar, 2012).

- *Prediction of Activity Spectra for Substance (PASS) Analysis*

The Predicted Biological Activity Spectrum (BAS) program software was used to analyze the data from the NIST library that was representative of various physiological functions, biochemical mechanisms of action, and pharmacological effects. The Prediction of Activity Spectra for Substance (PASS) program software was used to analyze particular toxicities based on their structural formula obtained from the GC-MS. The spectrum of a compound was assigned to represent the list of activities by Probable activity (Pa) and Probable inactivity (Pi), it was considered in the order of Probable Pa > Pi.

- *Pharma Expert:*

PharmaExpert software analyzes the relationship between biological activities to identify drug interactions and search for a compound action on multiple targets (Benaamane *et al.*,2008).

III. RESULTS AND DISCUSSION

➢ *Gas Chromatography-Mass Spectrum (GC-MS) by Spectrophotometric Analysis*

The % peak area and spectrum profile was obtained based on their retention time (RT). The chemical compound present in five different solvent leaf extracts *Eupatorium Triplinerve Vahl* was obtained by performing a GC-MS analysis. The identified and characterized chemical compounds with the chemical structure, and activities predicted by NIST and MS library were tabulated (Table: 1). The percentage composition and molecular weight was predicted based on Dr.Duke's (published 1994) phytochemical and ethno botanical databases and added.

The GCMS Chromatogram of the five different solvent leaf extracts shows the retention time (RT) in the column and detects peaks that correspond to the bioactive compounds present in the leaf extracts. Stigmasterol was present both in petroleum ether and acetone extracts in different quantities, 1-ISOPROPYL-2,5-DIMETHOXY-4-METHYLBENZENE was presented in different peak areas and retention time quantities both in ethanol and methanol extracts. However, further studies on determining the biological function of the bioactive compounds in the treatment of hemorrhoids and to cure inflammation and rectal bleeding in the anus and elucidation of their pharmacological activities were necessary to confirm their potential benefits.

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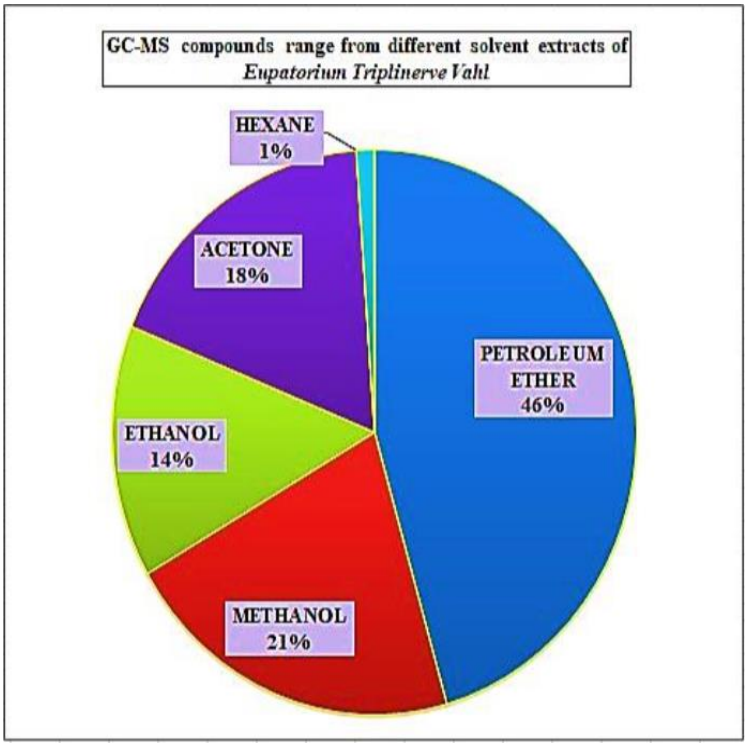

Fig 1 GC-MS Compounds Ranges of *Eupatorium Triplinerve Vahl* Leaf Extracts

- *PASS Prediction:*

The biological activity and inhibitory properties (Pa and Pi) values are described in the form of a bar graph representation as prediction results. PASS analysis, the compounds found in the various solvent leaf extracts varies in their different biological activities ranging from cytotoxicity, anti-bleeding, inflammation, itching, and intra-abdominal pressure. The analysis estimates anti-inflammatory, astringent, anti-hemorrhagic, antinephritic, antifibrinolytic, antispasmodic activity, and other biological activities to express structural predicted target site for drug design and serves as a beneficial tool to assess the compounds, their side effects, and toxicity.

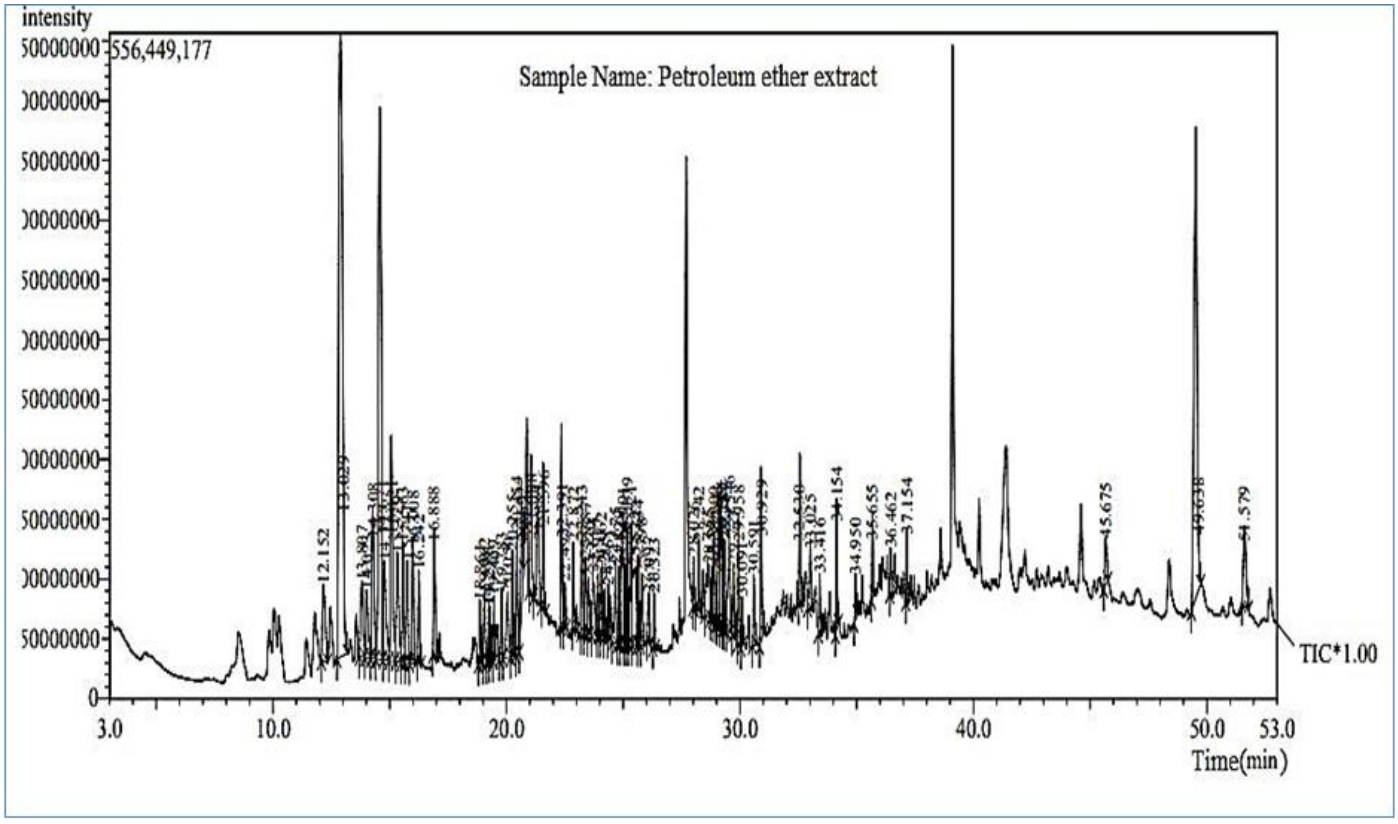

Fig 2 GC-MS Analysis of Phytocompoenets in the PETROLEUM ETHER of *Eupatorium Triplinerve Vahl*

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Table 1 GC-MS Analysis of Phytocompoenets in the PETROLEUM ETHER of *Eupatorium Triplinerve Vahl*

S.NO	Retention Time (RT)	Name of the Compound	Molecular Formula	Molecular Weight	Peak Area (%)
1	12.152	CYCLOHEXANE, 1-ETHENYL-1-METH	C15H24	204	1.97
2	13.029	BICYCLO[7.2.0]UNDEC-4-ENE, 4,11,11-	C15H24	204	6.27
3	13.807	TETRADECANE	C14H30	198	1.65
4	14.023	OCTADECANE	C18H38	254	1.39
5	14.308	1H-Cycloprop[e]azulen-4-ol, decahydro-1,	C15H26O	222	2.77
6	14.671	NAPHTHALENE	C15H24	204	4.82
7	14.777	Longifolene-(V4)	C15H24	204	2.34
8	15.121	Phenol, 3,5-bis(1,1-dimethylethyl)-	C14H22O	206	3.34
9	15.329	Nonadecyl trifluoroacetate	C21H39F3O2	380	2.37
10	15.563	1-Nonadecene	C19H38	266	1.73
11	15.747	Nonadecyl trifluoroacetate	C21H39F3O2	380	1.83
12	16.888	(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE,,12-TRIMETHYL-9-METHYLENE-,	C15H24O	220	1.91
13	18.861	PENTADECANE	C19H40	268	0.77
14	19.062	OCTADECANE	C18H38	254	0.86
15	19.236	Eicosane	C20H42	282	0.54
16	20.05	cis-1-Chloro-9-octadecene	C18H35C1	286	
17	20.692	Carbonic acid, dodecyl 2,2,2-trichloroethyl ester	C15H27C13O3	360	1.6
18	22.391	2-HEXADECEN-1-OL, 3,7,11,15-TETRAMETHYL	C20H40O	296	1.38
19	22.497	2-PENTADECANON	C18H36O	268	0.46
20	22.872	2,6,10-TRIMETHYL,14-ETHYLENE-14-PENTADECNE	C20H38	278	0.77
21	23.213	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	C20H40O	296	1.24
22	23.387	3-(Hydroxy-phenyl-methyl)-2,3-dimethyl-octan-4-one	C17H26O2	262	1.12
23	23.917	1,54-DIBROMOTETRAPENTACONTANE	C54H10Br2	914	0.66
24	24.829	Docosyl heptafluorobutyrate	C26H45F7O2	522	0.88
25	24.991	Nonadecyl pentafluoropropionate	C22H39F5O2	430	2.27
26	25.067	1,2-Tetradecanediol	C14H30O2	230	1.2
27	25.179	Nonadecyl heptafluorobutyrate	C23H39F7O2	480	1.62
28	25.321	Ditetradecyl ether	C28H58O	410	2.41
29	25.798	Hexatriacontyl trifluoroacetate	C38H73F3O2	618	0.9
30	28.026	1H-PURIN-6-AMINE, [(2-FLUOROPHENYL)METHYL]-	C12H10FN5	243	0.49
31	28.242	14-.BETA.-H-PREGNA	C21H36	288	0.76
32	28.786	Tetratriacontyl heptafluorobutyrate	C38H69F7O2	690	0.61
33	29.017	Heptacosyl heptafluorobutyrate	C31H55F7O2	592	0.43
34	29.221	Eicosyl heptafluorobutyrate	C24H41F7O2	494	1.46
35	30.591	Octatriacontyl pentafluoropropionate	C41H77F5O2	696	0.95
36	33.416	Dotriacontyl pentafluoropropionate	C35H65F5O2	612	0.61
37	34.95	DIOCTYL PHTHALATE	C24H38O4	390	0.48
38	45.675	dl-.alpha.-Tocopherol	C29H50O2	430	0.83
39	49.638	Stigmasterol	C29H48O	412	3.29
40	51.579	STIGMAST-5-EN-3-OL, (3.BETA.)-	C29H50O	414	1.83

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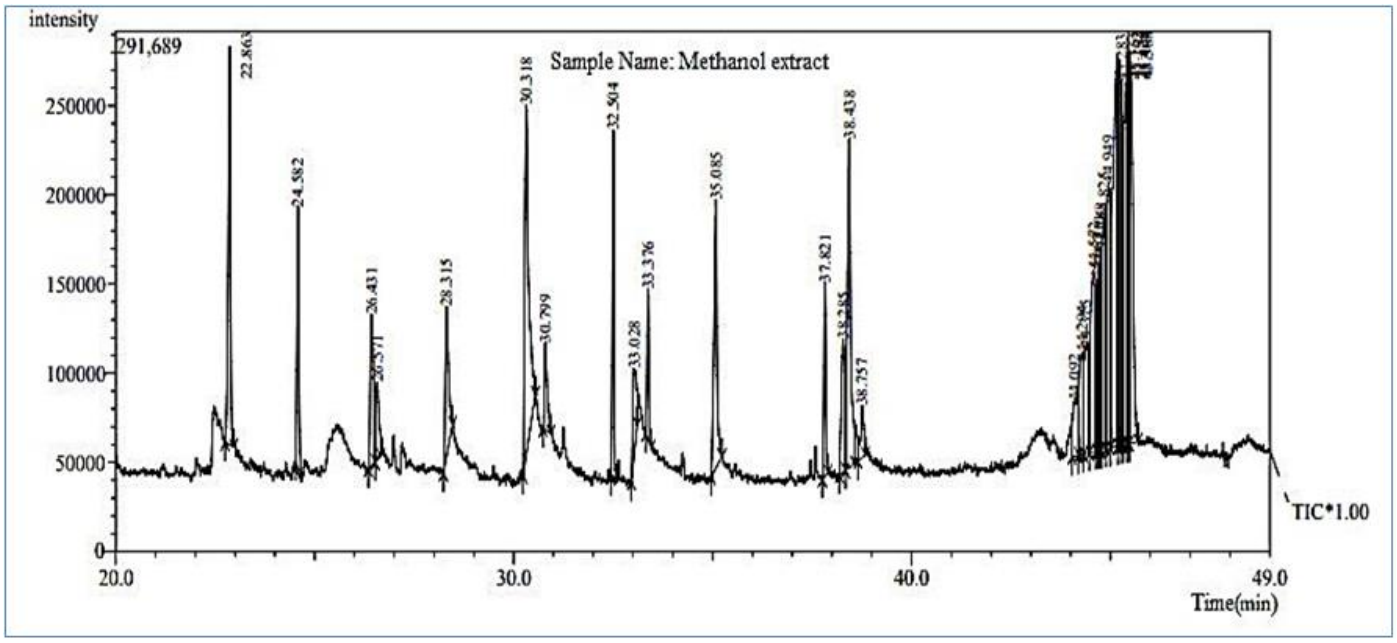

Fig 3 GC-MS Analysis of Phytocompoenets in the METHANOL of *Eupatorium Triplinerve Vahl*

Table 2 GC-MS Analysis of Phytocompoenets in the METHANOL of *Eupatorium Triplinerve Vahl*

S.NO	Retention Time (RT)	Name of the Compound	Molecular Formula	Molecular Weight	Peak Area (%)
1	22.863	1-ISOPROPYL-2,5-DIMETHOXY-4-METHYLBENZENE	C12H18O2	194	4.49
2	24.582	7-ISOPROPENYL-4A-METHYL-1-METHYLENEDECAHYDRONAPHTHALENE	C15H24	204	2.55
3	26.431	2-METHOXY-4-ETHYL-6-METHYLPHENOL	C10H14O2	166	2.72
4	26.574	4-METHYL-2,5-DIMETHOXYBENZALDEHYDE	C10H12O3	180	1.24
5	28.315	2H-1,4-Benzoxazin-3(4H)-one, 6-amino-7-methyl	C9H10N2O2	178	2.4
6	30.318	2H-1-BENZOPYRAN-2-ONE, 7-METHOXY-	C10H8O3	176	7.07
7	30.799	3,4-Dihydrocoumarin, 4,4-dimethyl-6-hydroxy-	C11H12O3	192	1.13
8	32.504	2,6,10-TRIMETHYL,14-ETHYLENE-14-PENTADECNE	C20H38	278	2.82
9	33.028	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	C20H40O	296	1.47
10	33.376	2,6,10-TRIMETHYL,14-ETHYLENE-14-PENTADECNE	C20H38	278	1.28
11	35.085	l-(+)-Ascorbic acid 2,6-dihexadecanoate	C38H68O8	652	4.01
12	37.821	PHYTOL ISOMER	C20H40O	296	1.71
13	38.285	9,12-Octadecadienoic acid (Z,Z)-	C18H32O	280	2.33
14	38.438	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	C18H32O2	278	5.62
15	38.757	Octadecanoic acid	C18H36O2	284	0.89
16	44.092	4-Isopropylcyclohexanone	C9H16O	140	1.55
17	44.294	Lup-20(29)-en-3-ol, acetate, (3.beta.)-	C32H52O2	468	1.87
18	44.375	1-NAPHTHALENEPROPANOL	C20H36O2	308	2.62
19	44.825	Betulin	C30H50O2	442	4.44
20	45.408	9,19-Cyclolanost-23-ene-3,25-diol, (3.beta.,23E)-	C30H50O2	442	6.03
21	45.447	LUP-20(29)-EN-3-YL ACETATE	C32H52O2	468	3.43

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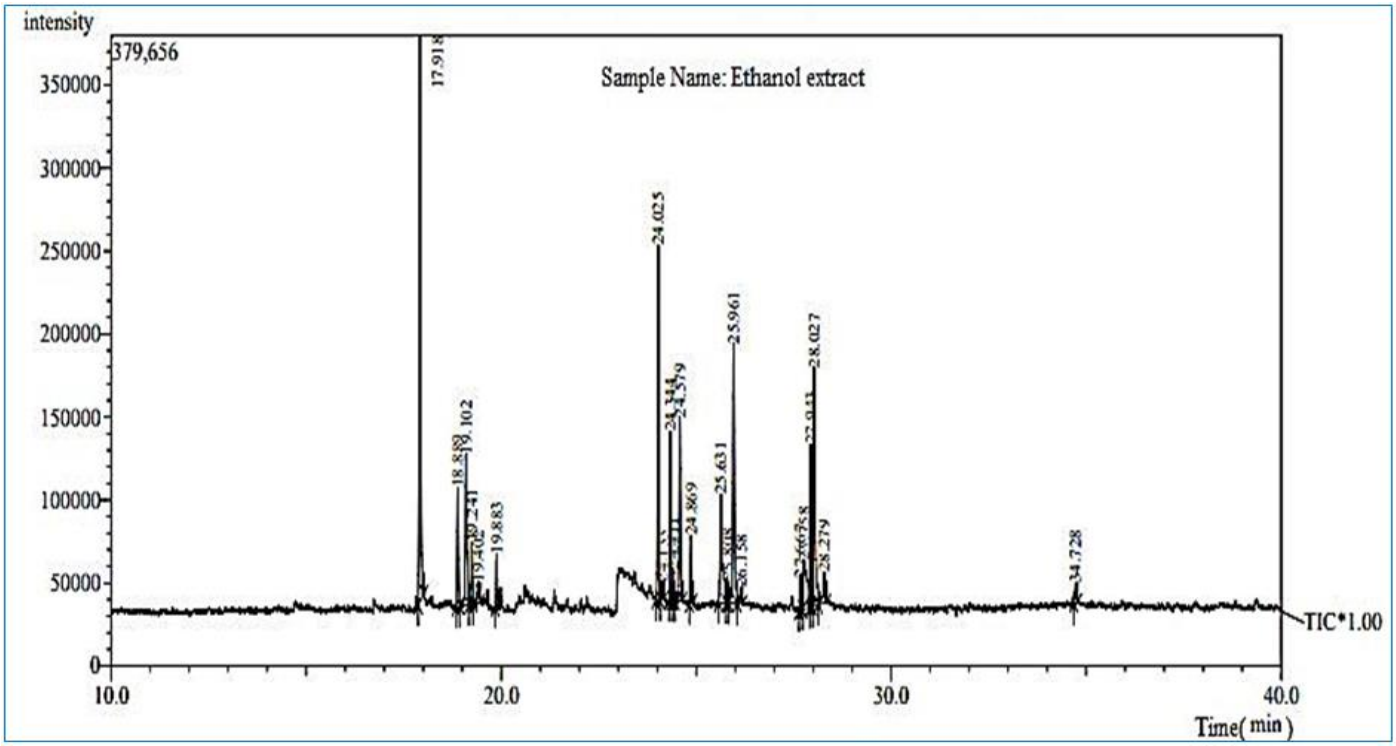

Fig 4 GC-MS Analysis of Phytocompoenets in the ETHANOL of *Eupatorium Triplinerve Vahl*

Table 3 GC-MS Analysis of Phytocompoenets in the ETHANOL of *Eupatorium Triplinerve Vahl*

S.NO	Retention Time (RT)	Name of the Compound	Molecular Formula	Molecular Weight	Peak Area (%)
1	17.918	1-ISOPROPYL-2,5-DIMETHOXY-4-METHYLBENZENE	C12H18O2	194	20.4
2	18.889	2-Isopropenyl-4a,8-dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalene	C15H24	204	3.48
3	19.102	NAPHTHALENE	C15H24	204	6.01
4	19.241	ALPHA.-SELINENE	C15H24	204	2.21
5	19.402	Phenol, 3,5-bis(1,1-dimethylethyl)-	C14H22O	206	0.83
6	19.883	1H-CYCLOPROP[E]AZULENE, 1A,2,3,4,4A,5,6,7B-OCTAHYDRO-1,1,4,7-TETRAMETHYL-	C15H24	204	1.59
7	24.025	2,6,10-TRIMETHYL,14-ETHYLENE-14-PENTADECNE	C20H38	278	9.92
8	24.133	2-CYCLOHEXENE-1-CARBOXALDEHYDE, 2,6,6-TRIMETHYL-	C10H15O	152	0.74
9	24.344	2,6,10-TRIMETHYL,14-ETHYLENE-14-PENTADECNE	C20H38	278	4.77
10	34.411	3-METHYL-5-(1,4,4-TRIMETHYL-2-CYCLOHEXEN-1-YL)-1-PENTANOL	C15H28O	224	0.88
11	24.869	CYCLOHEXANE, 1-METHYLENE-3-(1-METHYLETHYL)-	C10H18	138	1.83
12	25.631	n-Hexadecanoic acid	C16H32O2	256	5.84
13	25.808	Heptanoic acid, anhydride	C14H26O3	242	0.96
14	25.961	HEXADECANOIC ACID, ETHYL ESTER	C18H36O2	284	9.52
15	26.158	Furan, tetrahydro-2-isopentyl-5-propyl-	C12H24O	184	0.82
16	27.667	9,12-Octadecadienoic acid (Z,Z)-	C18H32O2	280	1.89
17	27.758	9,12,15-Octadecatrienoic acid,	C18H30O2	278	4.89
18	27.943	ETHYL (9Z,12Z)-9,12-OCTADECADIENOATE	C20H36O2	308	5.47
19	28.027	9,12,15-Octadecatrienoic acid, ethyl ester	C20H34O2	306	9.79
20	28.279	OCTADECANOIC ACID, ETHYL ESTER	C20H40O2	312	1.8
21	34.728	Squalene	C30H50	410	0.81

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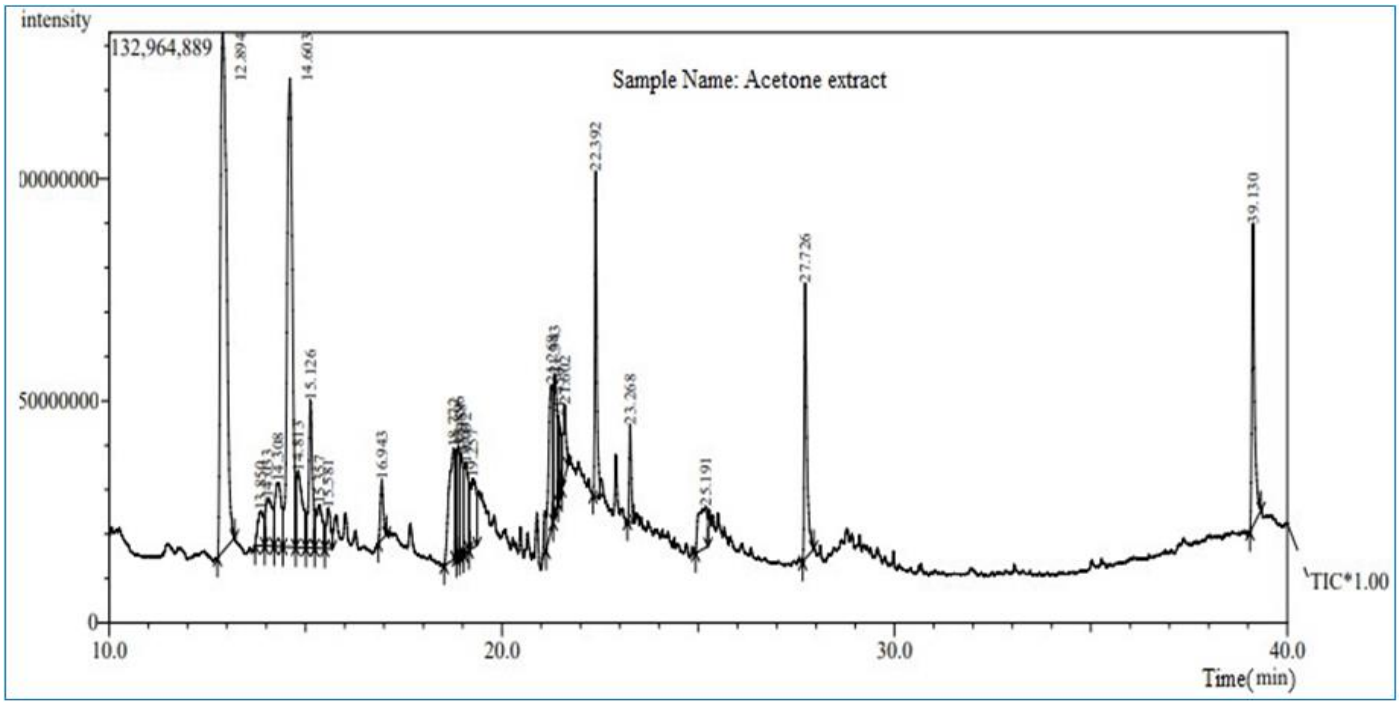

Fig 5 GC-MS Analysis of Phytocompoenets in the ACETONE of *Eupatorium Triplinerve Vahl*

Table 4 GC-MS Analysis of Phytocompoenets in the ACETONE of *Eupatorium Triplinerve Vahl*

S.NO	Retention Time (RT)	Name of the Compound	Molecular Formula	Molecular Weight	Peak Area (%)
1	3.029	2-PROPANOL, 1-AMINO-	C3H9NO	75	3.28
2	12.894	3-Oxabicyclo[4.2.0]oct-5-ene	C11H16O	164	19.47
3	13.85	Nonane, 1-iodo-	C9H19I	254	1.27
4	14.033	Dodecane, 2,6,11-trimethyl	C15H32	212	2.08
5	14.308	Octadecane, 1-chloro-	C18H37CI	288	2.43
6	14.603	"KW3 AUS EPIGLOBULOL" $$ AZULENE	C15H24	204	15.18
7	14.813	Cyclopropane	C12H20O	180	2.97
8	15.126	Phenol, 3,5-bis(1,1-dimethylethyl)-	C14H20O	206	3.47
9	15.357	1-TRIDECANOL	C13H28O	200	1.81
10	16.943	(-)-5-OXATRICYCLO[8.2.0.0(4,6)]DODECANE	C15H24O	220	1.11
11	18.772	3,9-Epoxytricyclo[4.2.1.1(2,4)]decan-10-one, 9-methyl	C11H14O2	178	1.84
12	18.958	2H-Benzocyclohepten-2-one	C12H18O	178	1.96
13	19.092	Eicosane	C20H42	282	2.37
14	19.257	Oxalic acid, 6-ethyloct-3-yl heptyl ester	C19H36O4	328	2.59
15	21.268	BENZOIC ACID, 2-HYDROXY-4-METHOXY-3,5,6-TRIMETHYL-	C11H14O4	210	3.93
16	21.45	2H-1-BENZOPYRAN-2-ONE, 7-METHOXY-	C10H8O3	176	1.3
17	21.602	Octacosyl trifluoroacetate	C30H57F3O2	506	1.42
18	22.392	2-HEXADECEN-1-OL, 3,7,11,15-TETRAMETHYL	C20H40O	296	3.84
19	23.268	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	C20H40O	296	1.22
20	27.726	Phytol	C20H40O	296	4.4
21	39.13	2,6,10,14,18,22-TETRACOSAHEXAENE, 2,6,10,15,19,23-HEXAMETHYL-	C30H50	410	5.13
22	45.705	dl-.alpha.-TocopherоL	C29H50O2	430	1.18
23	49.53	Stigamasterol	C29H48O	412	5.55

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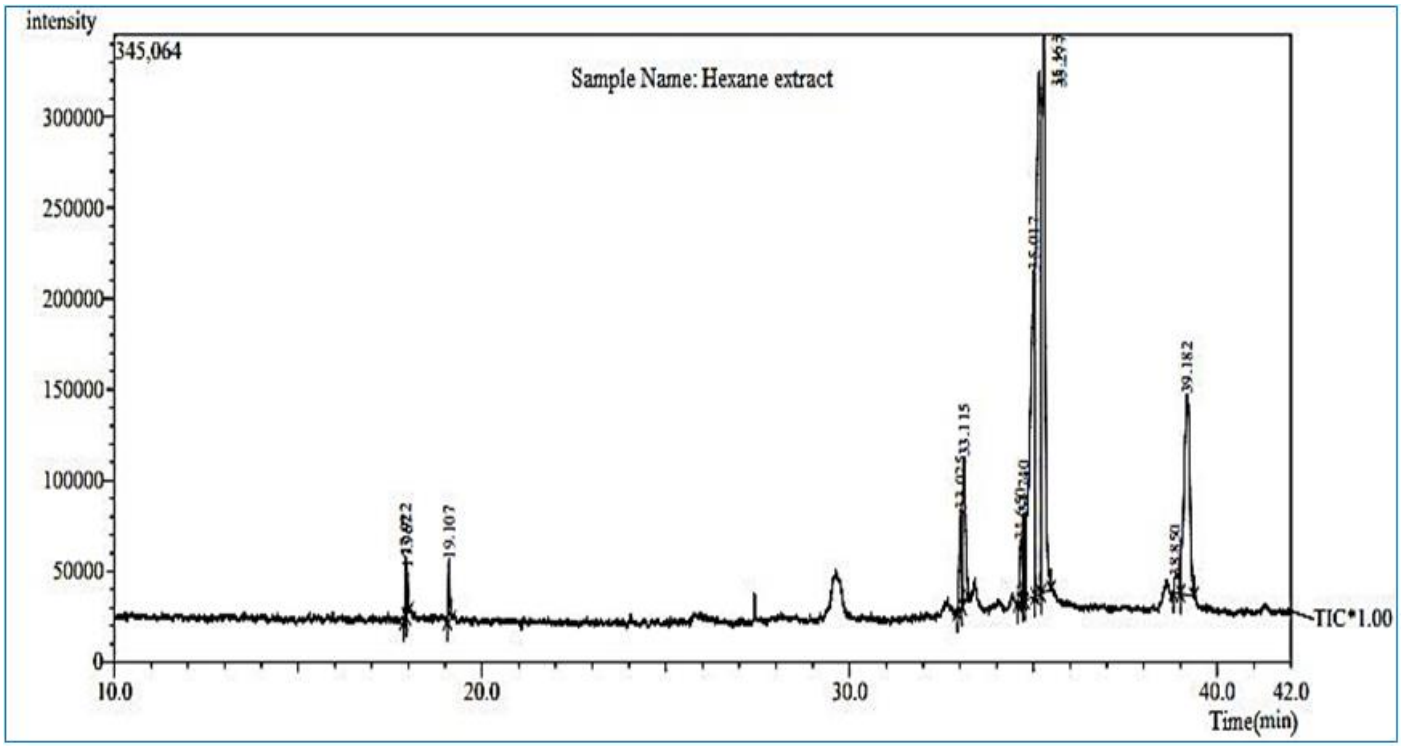

Fig 6 GC-MS Analysis of Phytocompoenets in the HEXANE of *Eupatorium Triplinerve Vahl*

Table 5 GC-MS Analysis of Phytocompoenets in the HEXANE of *Eupatorium Triplinerve Vahl*

S.NO	Retention Time (RT)	Name of the Compound	Molecular Formula	Molecular Weight	Peak Area (%)
1	17.922	1-ISOPROPYL-2,5-DIMETHOXY-4-METHYLBENZENE	C12H18O2	194	0.92
2	17.967	Caryophyllene	C15H24	204	0.74
3	19.107	NAPHTHALENE	C15H24	204	1
4	33.025	NOROLEAN-12-ENE	C29H48	396	2.92
5	34.65	METHYL COMMATE A	C32H52O4	500	2.02
6	34.74	Squalene	C30H50	410	2.17
7	35.017	LUP-20(29)-EN-3-YL ACETATE	C32H52O2	468	19.03
8	38.85	2,6,10-TRIMETHYL,14-ETHYLENE-14-PENTADECNE	C20H38	278	1.25

Leaf extract demonstrated a greater range of plant elements than the other solvents did, possibly as a result of the high polarity of methanol and acetone. These primary and secondary metabolites have a variety of biological and therapeutic qualities, and it is anticipated that they will have a wide range of medical applications.

The technical study of five different solvent leaf extracts of *Eupatorium tripinerve Vahl* was carried out for the GC-MS analysis and PASS prediction to reveal the presence of bioactive compounds. Among the identified bioactive components Stigmasterol, 1-ISOPROPYL-2,5-DIMETHOXY-4-METHYLBENZENE has the highest percent peak area. Stigmasterol (is an unsaturated phytosterol) has the role in antimicrobial, antioxidant, anti-diabetic, anticancer, immunomodulatory, anti-infective, anti-parasitic, neuroprotective, and anti-inflammatory activities and able to reduce plasma cholesterol levels. 1-ISOPROPYL-2,5-DIMETHOXY-4-METHYLBENZENE has various biological functions including antieczematic, fibrinolytic, antineurotic, antifungal, antimicrobial, and antioxidant properties.

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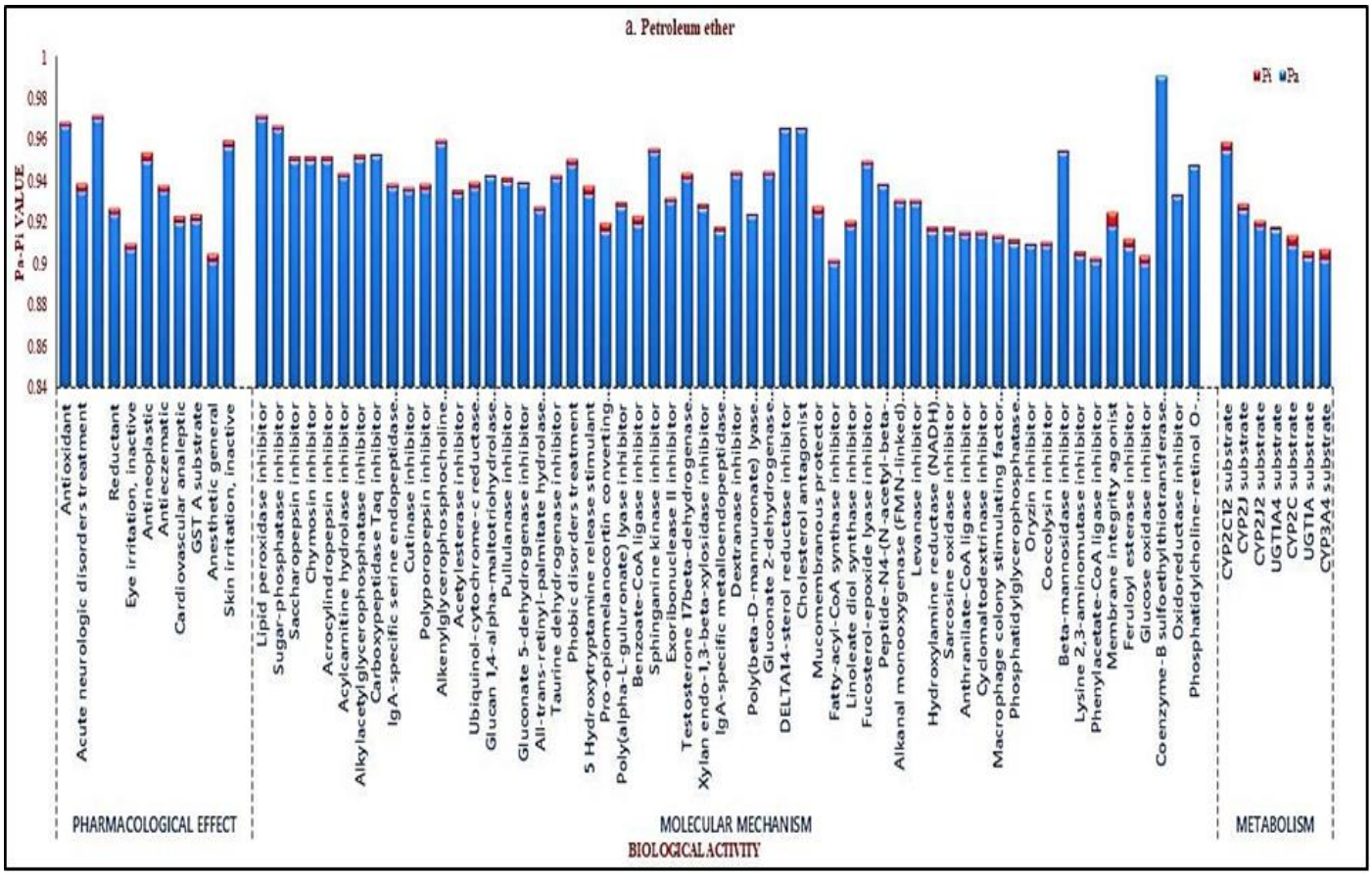
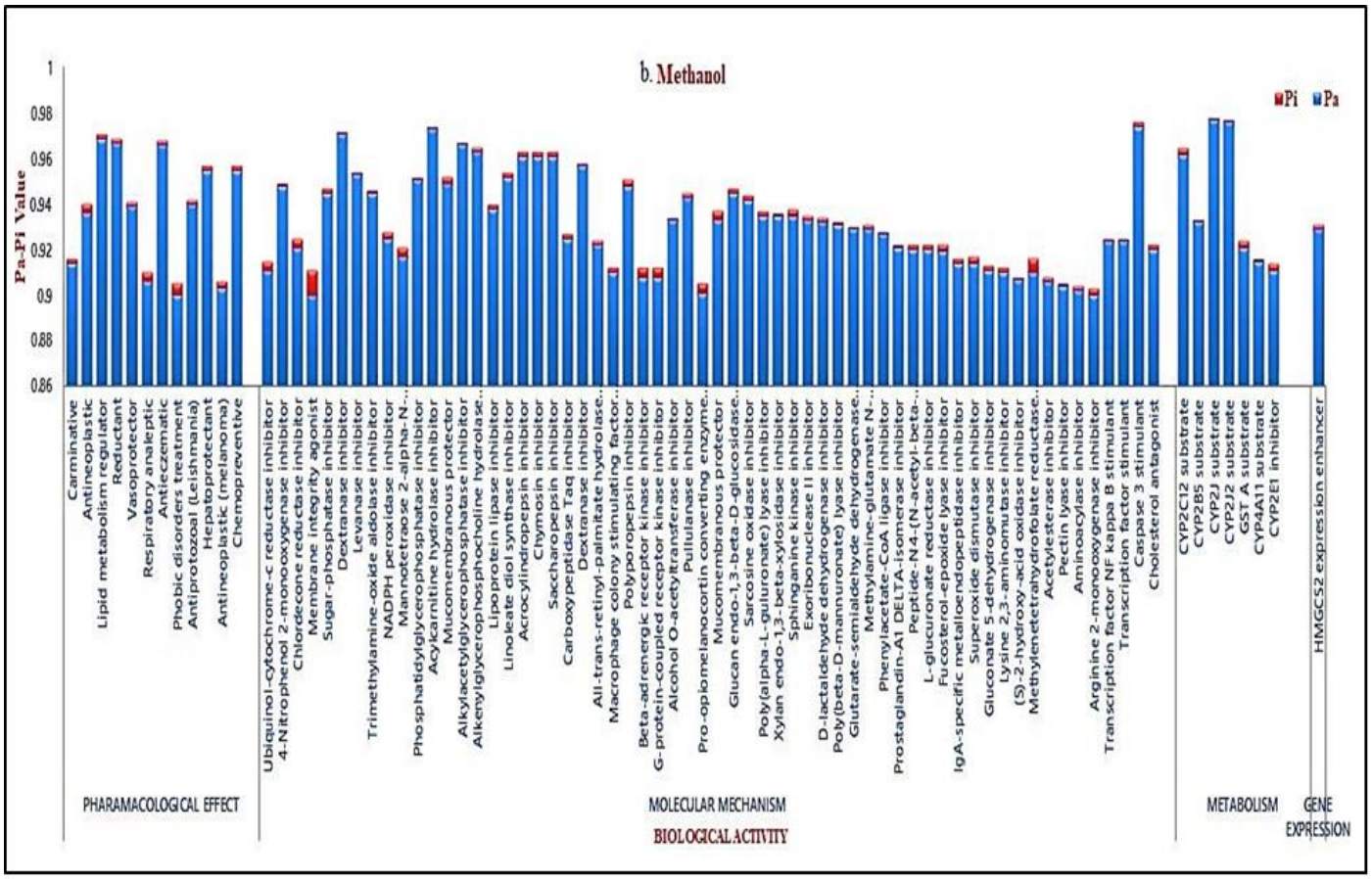
➢ *Prediction of Activity Spectra for Substance (PASS) Analysis*





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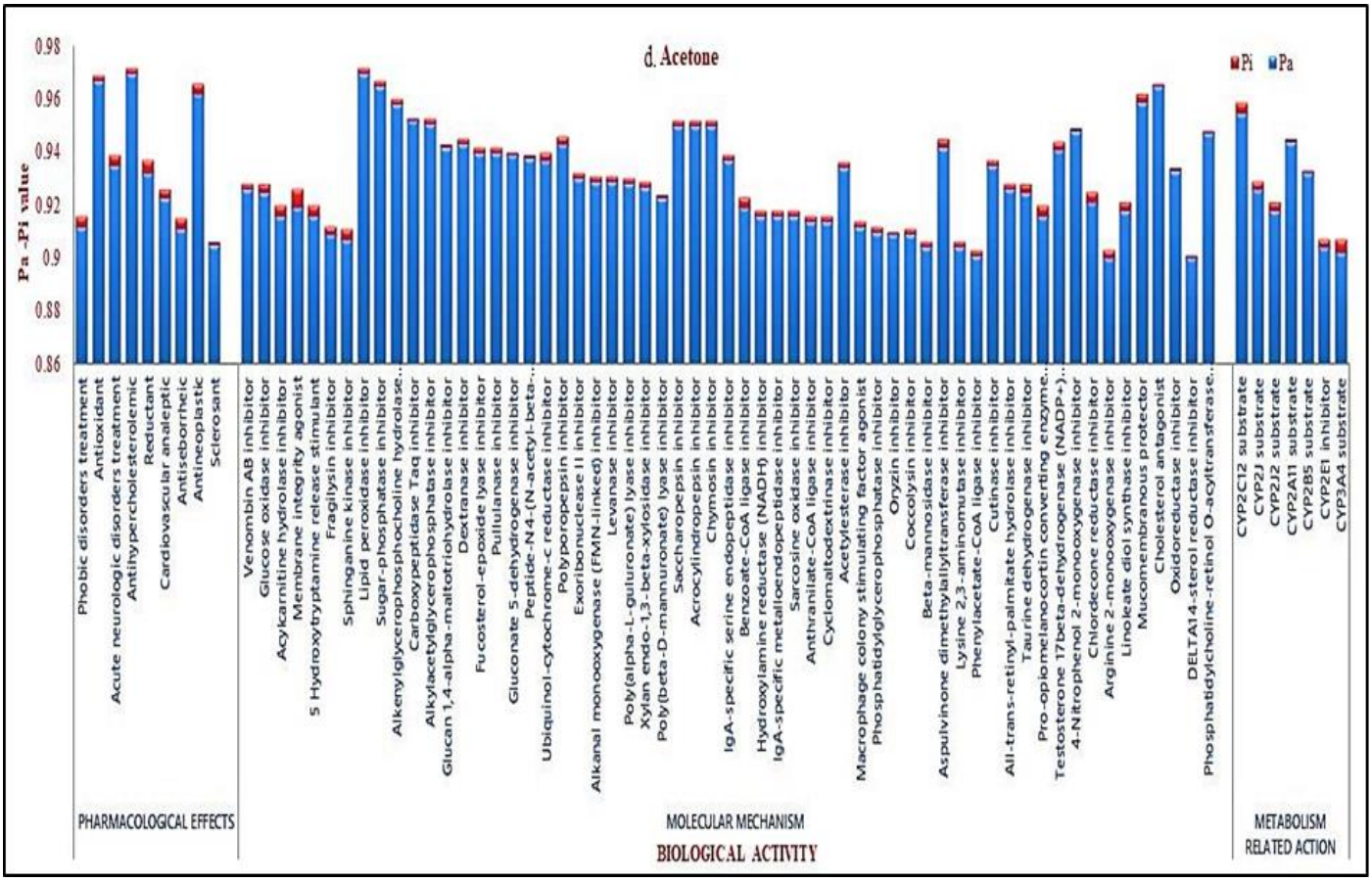

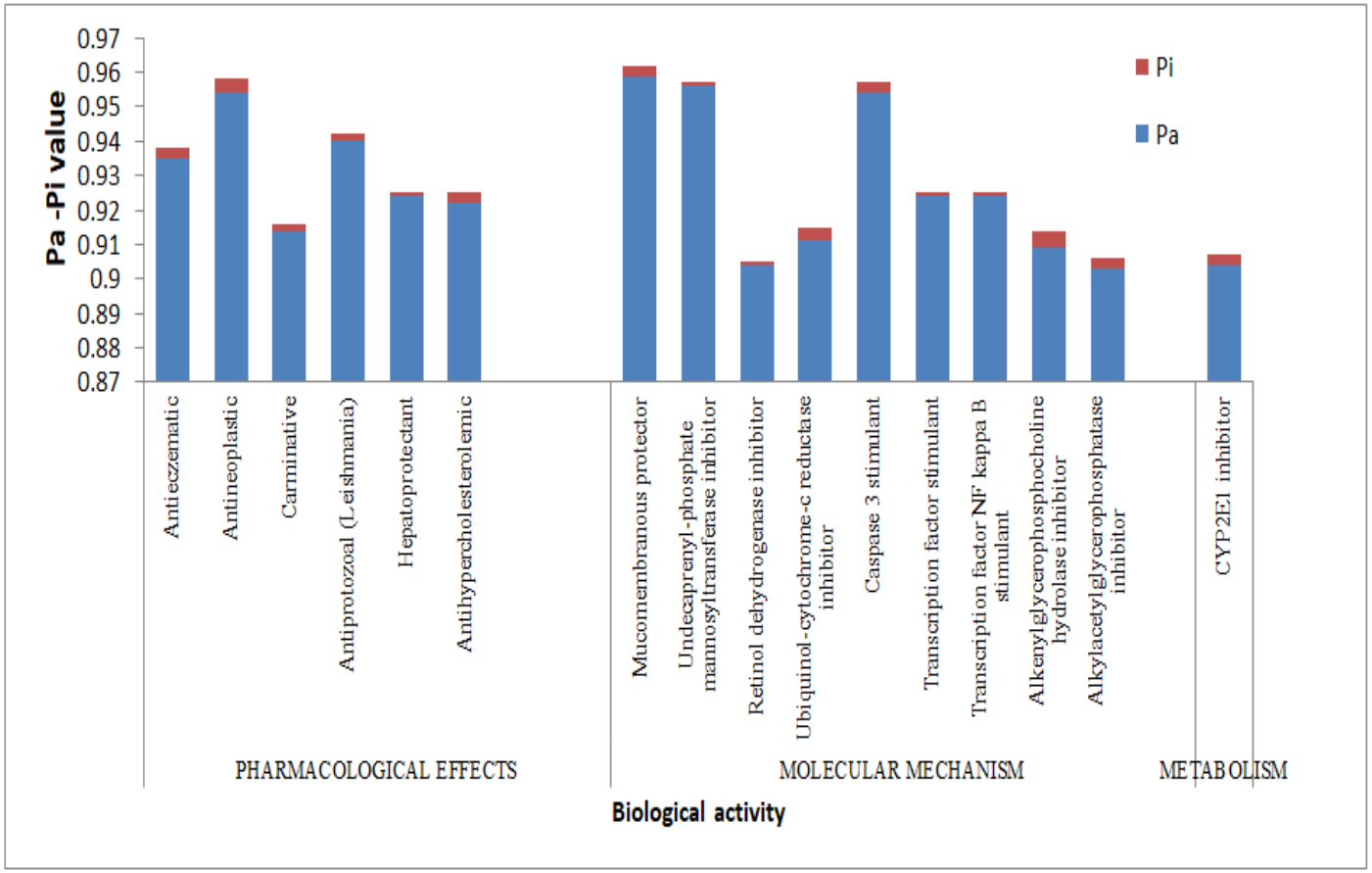

Fig 7 The Prediction of Biological Activity Spectra of the a. Petroleum Ether, b. Methanol, c. Ethanol, d. Acetone Solvent Leaf Extract of *Eupatorium Triplinerve Vahl.*

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The biological activities analyzed with (Pa>850) and bar graph differentiated with pharmacological effects, molecular mechanisms, metabolisms–related action, and gene expression found based on structure-activity relationships.

IV. DISCUSSION

Among the identified phytocompounds, squalene, hexadecanoic acid, and tetradecanoic acid have the properties of antioxidant, antifibrinolytic, antineoplastic, chemopreventive, and antimicrobial activities (Bodoprost & Rosemeyer, 2007; Kala et al., 2011). Octadecadienoic acid (Z, Z) has some properties like anti-inflammatory, antiarthritic activity, antibacterial activity, and hypocholestrolemic activity which was illustrated by the earlier report (Ponnamma & Manjunath, 2012; Uma et al., 2009). Naphthalene is a cytotoxic moiety, extensively explored for an aromatic conjugation application also has good antihypertensive, ant-neurodegenerative, and antidiabetic effects. Squalene (triterpine) is a phenolic compound and are found in latex and resins of some herbal plants and functions as are defense against certain pathogens causing various human and animal diseases (Scortichini & Rossi, 1991). Their properties are a function of the lipophilic activity of the constituent terpines, and for their functional group and aqueous solubility (Ezhilan & Neelamegam, 2012; Mahato & Sen, 1997). It possesses antimicrobial, chemopreventive against colon carcinogenesis, anticancer, pesticide, anti-tumor, gastropreventive, and hepatoprotective effects reported about squalene (Rao et al., 1998; Sunitha et al., 2001; Ukiva, 2002).

Stigmasterol is an unsaturated phytosterol that belongs to the tetracyclic triterpenes, it is one of the common plant sterols found in various natural sources. The findings indicate potent pharmacological effects like anti-osteoarthritis, anti-inflammatory, antiparasitic, antifungal, and neuroprotective properties (Bakrim et al., 2022). The compound is applied in various chemical manufacturing processes to generate various semi-synthetic and synthetic components for the pharmaceutical industry (Cabral & Klein, 2017). Phytol was reported with anti-diuretic, anticancer, anti-inflammatory, and neuroprotective activities (Banjare et al., 2017). 9-12-octadecadienoic acid had anti-arthritic, hepatoprotective and antiandrogenic, antieczemic, ant-acne properties.

In this study, we estimated the accuracy of predicate biological activity profiles and information about quality metrics, and precision in four categories. The best balance accuracy is for about Pa values in the range of 0.4-0.5. For the toxic and adverse effects at Pa = 0.5threshold, the maximum quality of predication was found. In adding the information about metabolites predicted in the activity profile can lead to filtering the potentially harmful drug candidates with probable sites. In this analysis, illustrates by the prediction could not identify toxic and adverse effects for the plant leaf extract which is a relatively narrow therapeutic index that is experimentally determined.

V. CONCLUSION

Medicinal plants are the main purpose is used in traditional medicines, and in the last few decades have been very intensive pharmacological studies. The values of medicinal plants are potential sources of newly identified compounds of therapeutic value and lead compounds in drug development. The identification of bioactive compounds in *Eupatorium Triplinerve Vahl* leaf extract was carried out by GC-MS characterization analysis which displays the presence of 90 compounds such as n-hexadecanoic acid, octadecanoic acid, Squalene have roles in antioxidant, anticancer, antidiabetic and anti-inflammatory effects. From this study, it can be concluded that the plant leaf extract may serve as a new potential source of novel drugs due to the presence of these phytochemicals and bioactive compounds.

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