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Extraction and characterization of phytoconstituents of *Cleome chelidonii* by GC/MS

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ABSTRACT

The aim of the present study was to determine the pet ether extract of the entire parts of *C. chelidonii* for its phytochemical compound using GC-MS. Compounds were identified by various methods, the major compounds being 9,12,15-Octadecadienoic acid (Z,Z,Z)-, methyl ester (20.61%), 9,12-Octadecenoic acid (Z,Z)-, methyl ester (3.10%), n – decamoic acid (0.69%), Hexadecanoic acid and Squalene (0.55%). More than 35 compounds have been identified. The sesquiterpenes (0.66%) are mainly represented by Caryophyllene (0.04%), phytol (1.99%) and Ledene oxide-(II) (0.58%).

Keywords: GC-MS, *C. Chelidonii*, 9,12-Octadecadienoic acid (Z,Z)-, methyl ester, n-decanoic acid, Squalene, Caryophyllene, Ledene oxide-(II).

1. INTRODUCTION

Cleome chelidonii (L.) Linn var. (CC) Synonyms / other Latin name are *Polanisia chelidonii* DC, [family: Capparaceae] most places throughout the India and Tropical and warm temperate regions. It is grown as perennials throughout dry seasons. [1] The leaves of *C. chelidonii* are used as the stimulant in Indo China; the roots *C. chelidonii* are used as the stimulant, antiscorbutic, and anthelmintic; the seeds *C. chelidonii* are used as the rubefacient, vesicant, anthlemintic and carminative. An infusion of the plant is commonly used in gingivitis and in the treatment of skin diseases. [2] The objective of the present study is to determine the phytochemical composition from the entire plants of *Cleome chelidonii* L.

2. MATERIALS AND METHODS

2.1. Collection and identification of plant materials

The samples (entire plant) of *Cleome chelidonii* were collected from Sengottai of Tamilnadu, India in October 2008. The plant material was taxonomically identified and authenticated by the Department of Botany, Annamalai University, Annamalai nagar, India. A voucher specimen was deposited at the Herbarium of the Department of Pharmacy.

2.2. Preparation of extracts

Shade dried entire plants (500g) were subjected to solvent extraction using soxhlet apparatus for 24hrs continuously which was yielded (2.78%). The solvent used for extraction was petroleum ether. To the best of our knowledge, which is based on the available literature, this is the first report on this plant using GC and GC/MS from this *C. chelidonii* species has not been investigated.

2.3. Gas chromatography

2.3.1. Operating parameters

For quantitation (area %), the GC analyses were carried out by using JEOL JMS-700 by the electron impact method where an electronic accelerating voltage of 75eV and an ion accelerating voltage of 8 - 10kV. The reservoir inlet systems were used. The capillary columns were: nonpolar column DB-5MS (J&W Scientific; 30 m x 0.25 mm, film thickness 0.25 µm) and polar column TC-Wax (60 m x 0.25 mm, film thickness 0.25 µm). The dynamic range for the peak intensities was 3 digits, and the accuracy of the mass number was 0.5. The oven temperature was programmed from 40°-240°C at a rate of 4°C/min and held at 240°C for 5 min. The injector and detector temperatures were 240°C and 280°C. The flow rates of the carrier gas (He) were 1.8

mL/min. GLC data reported are given as area percentage. He at 49.9 KPa was used as carrier gas and the FID detector was maintained at 250°C. The oil constituents were identified on the basis of their retention data and by using GC/M S analytical conditions similar to that of GC/FID. The mass spectra were recorded on a mass spectrometer coupled to a JEOL JMS-700 gas chromatograph (EI mode 70 eV, source temperature 230°C, scanned mass ranged 35 - 350 amu). The characteristic fragmentation patterns have been analyzed and compared to those of Wiley 275.L database.

2.3.2. Identification of compounds

The identification of the compounds was based on comparison with the library spectra (NIST-I, NIST-2, Wiley 275 and Adams libraries) of their relative retention indices with literature values. [3,4] The relative percentage amount of each component was calculated by comparing its average peak area to the total areas. The name, molecular weight, molecular formula and structure of the component of the test material were determined and the data are presented in table 1.

3. RESULTS AND DISCUSSIONS

The phytoconstituents was found to contain sesquiterpenes hydrocarbons (2.61%), mainly represented by Caryophyllene (0.04%), phytol (1.99%) and Ledene oxide-(II) (0.58%). The phytoconstituents was analyzed on GC and GC/MS; the gas chromatogram was shown in figure 1. The percentage composition and modes of identification of the oil components were listed in table 1. The extract was found to contain 65 components, representing 86.6% of the total phytoconstituents. It was determined to be rich in hydrocarbons -containing compounds. The main components in the extracts 9,12,15-Octadecadienoic acid (Z,Z,Z)-, methyl ester (20.61%), 9,12-Octadecenoic acid (Z,Z)-, methyl ester (3.10%), n-decanoic acid (0.69%), Hexadecanoic acid (0.21%), Squalene (0.55%), Caryophyllene (0.04%), phytol (1.99%) and Ledene oxide-(II) (0.58%). Further studies are needed for comparison with the extracts from other *Cleome* species.

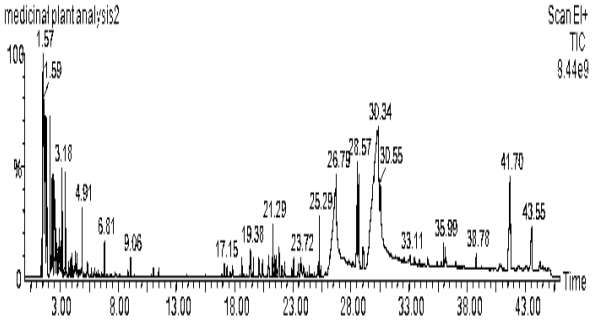

Figure - 1: GC-MS chromatogram of phytoconstituents of petroleum ether extract of the entire plant of *C. Chelidonii* 9,12,15-Octadecadienoic acid (Z,Z,Z)-, methyl ester.

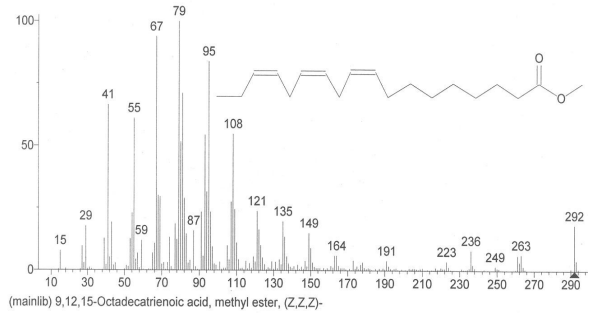

Figure - 2: GC-MS spectrum of phytoconstituents of petroleum ether extract of the entire plant of *C. Chelidonii* 9,12,15-Octadecadienoic acid (Z,Z,Z)-, methyl ester.

Table - 1: Mass spectral data of components identified in the petroleum ether extract of *C. Chelidonii 9,12-Octadecenoic acid (Z)-, methyl ester*

RT	Name	Formula	MW	Peak Area (%)	Compound nature	Activity reported
3.18	p-Xylene	C_8H_{10}	106	1.85	Aromatic	No activity reported
3.47	Nonane	C_9H_{20}	128	2.22	Alkane	No activity reported
3.75	Cyclohexane, 1-ethyl-2-methyl-	C_9H_{18}	126	0.24	Aromatic	No activity reported
3.93	2-Nonen-1-ol, (E)-	$C_9H_{18}O$	142	0.34	Alcohol	Antimicrobial
4.03	Cyclohexane, propyl-	C_9H_{18}	126	0.46	Aromatic	No activity reported
4.34	Benzene, 1-ethyl-3-methyl-	C_9H_{12}	120	0.48	Aromatic	No activity reported
4.45	Benzene, 1,2,4-trimethyl-	C_9H_{12}	120	0.42	Aromatic	No activity reported
4.91	Decane	$C_{10}H_{22}$	142	1.48	Alkane	No activity reported

5.34	Decane, 4-methyl-	$C_{11}H_{24}$	156	0.30	Hydrocarbon	No activity reported
5.41	Benzene, 1,2,3-trimethyl-	C_9H_{12}	120	0.26	Aromatic	No activity reported
6.81	Undecane	$C_{11}H_{24}$	156	0.62	Alkane	No activity reported
7.34	Benzene, 1,2,3,4-tetramethyl-	$C_{10}H_{14}$	134	trace	Aromatic	No activity reported
7.45	trans-Decalin, 2-methyl-	$C_{11}H_{20}$	152	trace	Hydrocarbon	No activity reported
7.77	5-Isopropenyl-1,2-dimethylcyclohex-2-enol	$C_{11}H_{18}O$	166	trace	Alcohol	No activity reported
7.83	trans-4a-Methyl-decahydronaphthalene	$C_{11}H_{20}$	152	trace	Aromatic	Insecticide
8.84	Naphthalene	$C_{10}H_8$	128	trace	Aromatic	Insecticide [5]
9.06	Dodecane	$C_{12}H_{26}$	170	0.40	Alkane	No activity
9.23	Curlone	$C_{15}H_{22}O$	218	trace	Hydrocarbon	Antioxidant Antimutagenic [6]
9.43	Undecane, 2,6-dimethyl-	$C_{13}H_{28}$	184	trace	Hydrocarbon	No activity reported
10.47	Nonanoic acid	$C_9H_{18}O_2$	158	0.04	Acid	No activity reported
10.85	Octane, 2,3,7-trimethyl-	$C_{11}H_{24}$	156	0.05	Hydrocarbon	No activity reported
11.06	Thymol	$C_{10}H_{14}O$	150	0.21	Essential oil	Antibacterial [7]
11.46	Tridecane	$C_{13}H_{28}$	184	0.23	Alkane	No activity reported
11.89	1H-Indene, 1-ethylidene-	$C_{11}H_{10}$	142	0.05	Hydrocarbon	No activity reported
12.87	n-Decanoic acid	$_{10}H_{20}O_2$	172	trace	Acid	Antimicrobial [8]
13.40	Naphthalene, 2-ethenyl-	$C_{12}H_{10}$	154	trace	Aromatic	N0 activity reported
13.89	Tetradecane	$C_{14}H_{30}$	198	0.07	Alkane	No activity reported
14.89	Caryophyllene	$C_{15}H_{24}$	204	0.04	Sesquiterpene	Antiinflammatory, [9], Sedative [10]
15.07	1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [s-(E,E)]-	$C_{15}H_{24}$	204	0.04	Sesquiterpene	No activity reported
15.50	1-Dodecanol	$C_{12}H_{26}O$	186	0.06	Alcohol	No activity reported
16.49	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	$_{11}H_{16}O_2$	180	trace	Aromatic	Antioxidant, Cell protective [11]
17.15	Benzene, (1-butylhexyl)-	$C_{16}H_{26}$	218	0.31	Aromatic	No activity reported
17.36	Benzene, (1-propylheptyl)-	$C_{16}H_{26}$	218	0.24	Aromatic compound	No activity reported
17.65	Dodecanoic acid	$C_{12}H_{24}O_2$	200	0.15	Lauric acid	Antibacterial [12]
17.82	Benzene, (1-ethyloctyl)-	$C_{16}H_{26}$	218	0.23	Aromatic	No activity reported
18.48	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1aà,4aà,7á,7aá,7bà)]-	$C_{15}H_{24}O$	220	trace	Terpenoids	No activity reported
18.63	Benzene, (1-	$C_{16}H_{26}$	218	0.07	Aromatic	No activity reported

	methylnonyl)-					
19.04	Ledene oxide-(II)	$C_{15}H_{24}O$	220	0.58	Sesquiterpenoid	Antibacterial, Antioxidant [13]
19.31	Benzene, (1-pentylhexyl)-	$C_{17}H_{28}$	232	0.08	Aromatic	No activity reported
19.38	Benzene, (1-butylheptyl)-	$C_{17}H_{28}$	232	0.27	Aromatic	No activity reported
19.63	Benzene, (1-propyloctyl)-	$C_{17}H_{28}$	232	0.64	Aromatic	No activity reported
20.12	Benzene, (1-ethylnonyl)-	$C_{17}H_{28}$	232	0.47	Aromatic	No activity reported
20.43	Dodecyl acrylate	$C_{15}H_{28}O_2$	240	0.53	Plasticizer	No activity reported
20.93	Benzene, (1-methyldecyl)-	$C_{17}H_{28}$	232	0.37	Aromatic	No activity reported
21.29	9H-Fluorene, 9-diazo-	$C_{13}H_8N_2$	192	0.46	Nitrogen	No activity reported
21.44	Benzene, (1-pentylheptyl)-	$C_{18}H_{30}$	246	1.59	Aromatic	No activity reported
21.55	Benzene, (1-butyloctyl)-	$C_{18}H_{30}$	246	0.45	Aromatic	No activity reported
21.82	Benzene, (1-propylnonyl)-	$C_{18}H_{30}$	246	0.46	Aromatic	No activity reported
22.08	Tetradecanoic acid	$C_{14}H_{28}O_2$	228	0.69	Myristic acid	No activity reported
22.31	Benzene, (1-ethyldecyl)-	$C_{18}H_{30}$	246	0.31	Aromatic	No activity reported
22.94	Octadecane	$C_{18}H_{38}$	254	0.39	Alkane	No activity reported
23.10	1-Hexene, 3-methyl-6-phenyl-4-(1-phenylethoxy)-	$C_{21}H_{26}O$	294	0.18	Ether	No activity reported
23.50	Benzene, (1-pentyloctyl)-	$C_{19}H_{32}$	260	0.39	Aromatic	No activity reported
23.64	; Benzene, (1-butylnonyl)-	$C_{19}H_{32}$	260	0.39	Aromatic	No activity reported
23.72	2-Pentadecanone, 6,10,14-trimethyl-	$C_{18}H_{36}O$	268	0.22	Ketone	No activity reported
23.91	Benzene, (1-propyldecyl)-	$C_{19}H_{32}$	260	0.52	Aromatic	No activity reported
24.42	Benzene, (1-ethylundecyl)-	$C_{19}H_{32}$	260	0.19	Aromatic	No activity reported
25.18	Benzene, (1-methyldodecyl)-	$C_{19}H_{32}$	260	0.20	Aromatic	No activity reported
25.29	Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	270	0.21	Palmitic acid ester	Antifungal, Antioxidant, Hypocholesterolemic Nematicide, Pesticide, Antiandrogenic Flavour, Haemolytic, 5-Alpha Reductase Inhibitor,Potent Antimicrobial Activity [14]
25.42	Unknown	-	-	1.46	***	* * * * * *

26.79	n-Hexadecanoic acid	$C_{16}H_{32}O_2$	256	0.18	Palmitic acid	Antifungal, Antioxidant, Hypocholesterolemic Nematicide, Anti-Androgenic Flavour, Haemolytic 5-Alphareductase Inhibitor, Potent Antimicrobial Agent, Antimalarial And Antifungal [15]
28.57	9,12-Octadecadienoic acid (Z,Z)-, methyl ester	$C_{19}H_{34}O_2$	294	20.61	*trans* Linoleic acid	No Activity Reported
28.67	9-Octadecenoic acid (Z)-, methyl ester	$C_{19}H_{36}O_2$	296	3.10	Oleic acid ester	Antioxidant Activity, Anticarcinogenic, Human Blood And Urine And Serve As Endogenous Peroxisome Proliferator Activated Receptor Ligand, Dermatitigenic Flavour [16]
29.03	Phytol	$C_{20}H_{40}O$	296	1.99	Diterpene	Antimicrobial, Anticancer, Cancer Preventive, Diuretic Antiinflammatory [17]
29.09	Octadecanoic acid, methyl ester	$C_{19}H_{38}O_2$	298	0.53	Stearic acid ester	No Activity Reported
30.34	9,12-Octadecadienoic acid (Z,Z)-	$C_{18}H_{32}O_2$	280	0.43	*trans* Linoleic acid	Antiinflammatory, Hypocholesterolemic, Cancer Preventive, Hepatoprotective, Nematicide, Insectifuge, Antihistaminic, Antieczemic, Antiacne, 5-Alpha Reductase Inhibitor Antiandrogenic, Antiarthritic, Anticoronary, Insectifuge [18]
30.55	Octadecanoic acid	$C_{18}H_{36}O_2$	284	35.18	Stearic acid	No activity
35.99	1,2-Benzenedicarboxylic acid, diisooctyl ester	$C_{24}H_{38}O_4$	390	6.72	Plasticizer	No activity
41.70	Squalene	$C_{30}H_{50}$	410	0.55	Triterpene	Antioxidant Antitumor [19]
43.55	Nonacosane	$C_{29}H_{60}$	408	6.19	Alkane	No activity reported

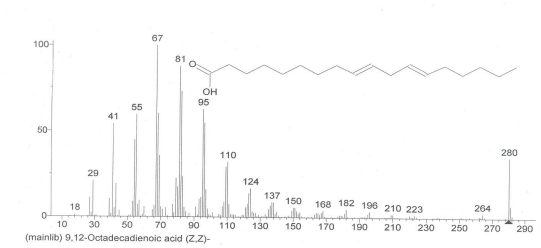

Figure - 3: 9, 12 Octadecadienoic acid

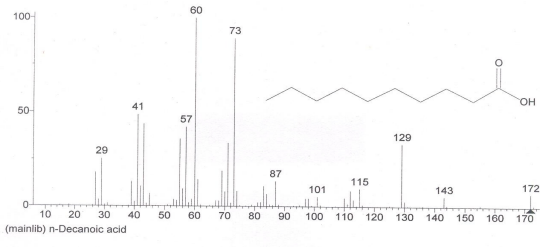

Figure - 4: n-Decanoic acid.

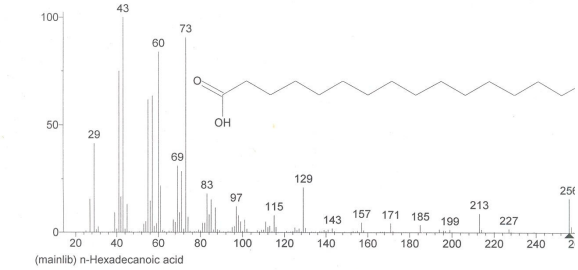

Figure - 5: n- Hexadecanoic acid.

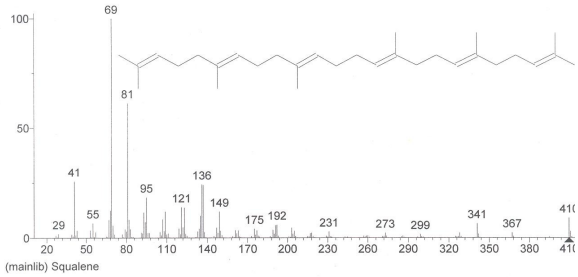

Figure - 6: Squalene.

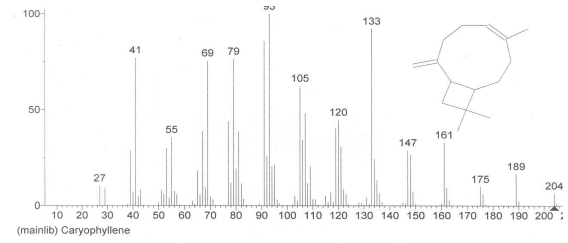

Figure - 7: Caryophyllene.

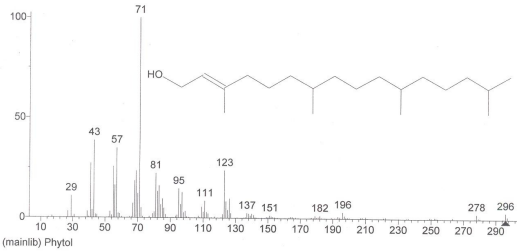

Figure - 8: Phytol.

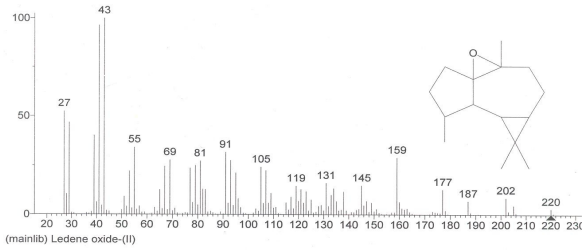

Figure - 9: Ledene oxide-(II).

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