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GC-MS analysis of Polycarpaea corymbosa (L.) Lam whole plant

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1. Introduction

Natural remedies from medicinal plants are found to be safe and effective. Many plants species have been used in folkloric medicine to treat various ailments. Even today compounds from plants continue to play a major role in primary health care as therapeutic remedies in many developing countries^[1].Standardization of plant materials is the need of the day. Several pharmacopoeia containing monographs of the plant materials describe only the physicochemical parameters. Hence the modern methods describing the identification and quantification of active constituents in the plant material may be useful for proper standardization of herbals and its formulations. Also the WHO has emphasized the need to ensure the quality of medicinal plants products using modern controlled technique and applying suitable standards^[2].GC-MS is the best technique to identify the bioactive constituents of long chain hydrocarbons, alcohols, acids, esters, alkaloids, steroids, amino and nitro compounds etc^[3]

Polycarpaea corymbosa(L.) Lam. belongs to "Caryophyllaceae" is commonly known as "Pallipoondu" in Palliyar tribals of Sirumalai hills, Western Ghats Tamil Nadu. Paste prepared from the leaf is taken once in a day for period of 2–3 weeks to treat jaundice by the palliyars^[4].

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ABSTRACT

Objective: To investigate the phytoconstitutent of ethanol extract of *Polycarpaea corymbosa* (L.) Lam using GC-MS. **Methods :** GC-MS analysis of whole plant extract were performed using a Perkin–Elmer GC Clarus 500 system and Gas Chromotograph interfaced to a Mass Spectrometer (GC-MS) equipped with a Elite – I, fused Silica Capillary Column (30mm× 0.25mm 1D×1 μ Mdf ,composed of 100% Dimethyl polysiloxane). **Results:** The results of the GC-MS analysis confirmed the presence of thirteen compounds. The most prevailing compounds are Furazano [3,4-b] pyrazin–5(4H)–one, 6–(1–pyrrolidinyl)–,1,(2–Acetoxyethyl)–3,6–diazahomoadamantam–9–one oxime, cycloarbital etc. **Conclusions:** From the results, it can be concluded that the plant extract show the presence of 13 phytocompounds. The presence of various bioactive compounds justifies the use of the whole plant for various ailments by traditional practitioners.

> Taking into consideration of the medicinal importance of this plant, the ethanol extract of whole plant of *Polycarpaea corymbosa* were analyzed for the first time using GC-MS. Persual of literature reveals that information on the GC-MS analysis of *Polycarpaea corymbosa* is totally lacking. Hence, the objective of the present study is to identify the phytochemical constitutents with the acid of GC-MS technique.

2. Materials and methods

The whole plant of *Polycarpaea corymbosa*(L.)Lam were collected from the Agasthiarmalai Biosphere Reserve, Western Ghats, Tamil Nadu. The plants were shaded dried and pulverized to powder in a mechanical grinder. Required quantity of powder was weighed and transferred to stoppered flask, and treated with ethanol until the powder is fully immersed. The flask was shaken every hour for the first 6 hours and then it was kept aside and again shaken after 24 hours. This process was repeated for 3 days and then the extract was filtered. The extract was collected and evaporated to dryness by using a vacuum distillation unit. The final residue thus obtained was then subjected to GC–MS analysis.

2.1. GC–MS Analysis

GC-MS analysis of these extracts were performed using a



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Perkin-Elmer GC Clarus 500 system and Gas chromatograph interfaced to a Mass spectrometer (GC-MS) equipped with a Elite-I, fused silica capillary column (30mmX0.25mm 1D X 1 μ Mdf, composed of 100% Dimethyl poly siloxane). For GC-MS detection, an electron ionization system with ionizing energy of 70 eV was used. Helium gas (99.999%) was used as the carrier gas at constant flow rate 1ml/min and an injection volume of $2 \mu l$ was employed (split ratio of 10:1); Injector temperature 250 °C; Ion-source temperature 280 °C. The oven temperature was programmed from 110 $^{\circ}$ (isothermal for 2 min.), with an increase of 10 $^{\circ}$ /min, to 200 $^{\circ}$, then 5 $^{\circ}$ / min to 280 °C, ending with a 9min isothermal at 280 °C. Mass spectra were taken at 70 eV; a scan interval of 0.5 seconds and fragments from 45 to 450 Da. Total GC running time was 36 minutes. The relative % amount of each component was calculated by comparing its average peak area to the total areas, software adopted to handle mass spectra and chromatograms was a Turbomass.

Interpretation on mass spectrum GC-MS was conducted using the database of National Institute Standard and technology (NIST) having more than 62,000 patterns. The spectrum of the unknown component was compared with the spectrum of the known components stored in the NIST library. The Name, Molecular weight and structure of the components of the test materials were ascertained.

3. Results

The compounds present in the ethanol extract of whole plant of *Polycarpaea corymbosa* were identified by GC-MS analysis (Fig.1). The active principles with their retention time (RT), molecular formula, molecular weight (MW) and concentration % in the ethanol extract of whole plant of *Polycarpaea corymbosa* are presented inTable1. The prevailing compounds in ethanol extract of whole plant were Furazano[3,4-b]pyrazin-5(4H)one, 6-(1-pyrrolidinyl)-(27.18%), 1-(2-Acetoxyethyl)-3,6-diazahomoadamantan-9-one oxime (21.36%), Cyclobarbital (11.65%), 3-[3-[1-Aziridinyl]propoxy]-2,5-dimethylpyrazine(9.71%), Cyclopropylamine, N-isobutylidene- (7.77%), 1-Heptadecanol (5.83%) and 2-Pyrrolidinone, 1-ethenyl-(5.83%).Figure2,3 and 4 shows mass spectrum and structures of dl-Citrulline,Cyclobarbital,2-Pyrrolidineacetic acid and 2-Pyrrolidinone,1-ethenyl respectively. Table 2 listed the major phytocomponents and its biological activities obtained through GC-MS study of *Polycarpaea corymbosa*.

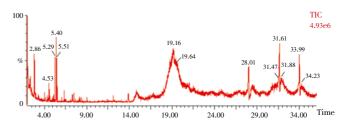


Fig.1 GC-MS Chromotogram of the ethanol extract of whole plant of Polycarpaea corymbosa

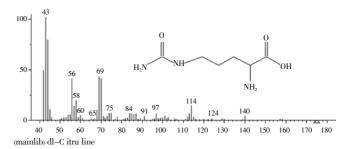


Fig.2 Mass Spectrum of dl-Citrulline

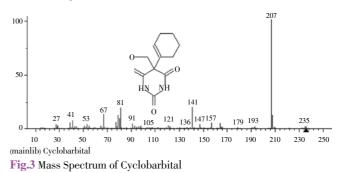


Table 1

Components detected in the whole plant ethanol extract of Polycarpaea corymbosa

No.	RT	Name of the compound	Molecular formula	MW	Peak Area %
1.	2.86	Cyclopropylamine, N–isobutylidene–	C7H13N	111	7.77
2.	4.53	2-Methylcyclohexylamine	C7H15N	113	2.91
3.	5.29	2-Pyrrolidinone, 1-ethenyl-	C6H9NO	111	5.83
4.	5.40	3-[3-[1-Aziridinyl]propoxy]-2,5-dimethylpyrazine	C11H17N3O	207	9.71
5.	5.51	1-Heptadecanol	C17H36O	256	5.83
6.	6.33	Pregna-6,16-diene-11,20-diol, 3,9-epoxy-18-[N-methyl-N-[14-(2'-epoxyethyl)]amino]-	C25H37NO5	431	0.97
7.	7.38	dl–Citrulline	C6H13N3O3	175	0.97
8.	7.50	2-Pyrrolidineacetic acid	C6H11NO2	129	0.97
9.	12.14	9,12-Hexadecadienoic acid, methyl ester	C17H30O2	266	1.94
10.	13.91	Ethaneperoxoic acid, 1-cyano-1-[2-(2-phenyl-1,3-dioxolan-2-yl)ethyl]pentyl ester	C19H25NO5	347	2.91
11.	28.01	Cyclobarbital	C12H16N2O3	236	11.65
12.	31.61	Furazano[3,4-b]pyrazin-5(4H)-one, 6-(1-pyrrolidinyl)-	C8H9N5O2	207	27.18
13.	33.99	1-(2-Acetoxyethyl)-3,6-diazahomoadamantan-9-one oxime	C13H21N3O3	267	21.36

Table.2 Activity of Phyto-components identified in the ethanol extract of whole plant of Polycarpaea corymbosa

Name of the compound	Molecular formula Compound nature		**Activity		
Cyclopropylamine, N–isobutylidene–	C7H13N	Nitrogen compound	Antimicrobial		
2-Methylcyclohexylamine	C7H15N	Amino compound	Antimicrobial		
2-Pyrrolidinone, 1-ethenyl-	C6H9NO	Alkaloid	Antimicrobial, Anti-inflammatory		
3–[3–[1–Aziridinyl]propoxy]–2,5– dimethylpyrazine	C11H17N3O	Nitrogen compound	Antimicrobial		
1–Heptadecanol	C17H36O	Aliphatic alcohol	Antimicrobial		
Pregna-6,16-diene-11,20-diol, 3,9-epoxy-18-[N-methy]-N-[14- (2´-epoxyethyl)]amino]-	C25H37NO5	Nitrogen compound	Antimicrobial		
dl–Citrulline	C6H13N3O3	Amino acid compound	Alzheimer's disease cure Antidiabetic, vasodilator		
2–Pyrrolidineacetic acid	C6H11NO2	Alkaloid	Antimicrobial, Anti-inflammatory		
9,12–Hexadecadienoic acid, methyl ester	C17H30O2	Linoleic acid ester	Antiinflammatory, Hypocholesterolemic, Cancer preventive, Hepatoprotective, Nematicide, Insectifuge, Antihistaminic, Antieczemic, Antiacne, Alpha reductase inhibitorAntiandrogenic, Antiarthritic, Anticoronary, Insectifuge		
Cyclobarbital	C12H16N2O3	Nitrogen compound	Sedative		
Furazano[3,4-b]pyrazin-5(4H)-one, 6-(1-pyrrolidinyl)-	C8H9N5O2	Nitrogen compound	Antimicrobial		
1–(2–Acetoxyethyl)–3,6– diazahomoadamantan–9–one oxime	C13H21N3O3	Nitrogen compound	Antimicrobial		

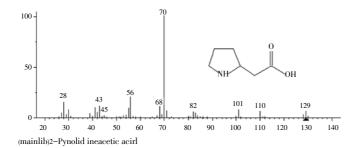


Fig.4 Mass Spectrum of 2-Pyrrolidineacetic acid

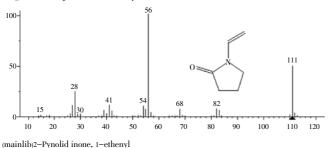


Fig.5 Mass Spectrum of 2-Pyrrolidinone,1-ethenyl

4. Discussion

Authentication of medicinal plants as genetic and chemical level is a critical step in the use of these botanical materials for both research purposes and commercial preparations. For any living organism, identity is very important in order to distinguish itself from other organisms within the population and other populations. In plant taxonomy, during this molecular era, the morphological characters also play a vital role in plant systematic study and used as a tool for the classification of a taxon. In recent times, in addition morphological markers, anatomical, cytological, biochemical, and molecular markers are also being used to classify the organisms. Gas Chromatography-Mass Spectrometry (GC-MS) is a valuable for tool for reliable identification of phytocompounds^[5,6]. In the present study, 13 compounds have been identified from the ethanol extract of the whole plant of Polycarpaea corymbosa by Gas Chromatogra aphy-Mass Spectrometry analysis. Among the identified phytochemicals, dL-citrulline is used for Alzheimer's disease, dementia, fatigue, muscle weakness, sickle cell disease, erectile dysfunction, high blood pressure, and diabetes. It is used for heart disease, body building, increasing energy, and for improving athletic performance. L-citrulline supplementation reduces pulmonary hypertension [7]. Thus this type of GC-MS analyses is the first step towards understanding the nature of active principles in this medicinal plant and this type of study will be helpful for further detailed study. Further investigation into the pharmacological of Polycarpaea corymbosa and their diversity and detailed phytochemistry may add new knowledge to the information in the traditional medical systems.

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