



GC-MS Determination of Bioactive components of *Polycarphaea corymbosa* Lam. (*Caryophyllaceae*)

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Abstract

Plan: The investigation was carried out to determine the possible chemical components from *Polycarphaea corymbosa* Lam. root and aerial parts.

Methodology: GC-MS was analysed using Agilent (Model 5975C) Gas Chromatography–Mass Spectrometry.

Outcome: GC-MS analysis of methanolic extract of root and aerial part led to identification of 30 and 24 compounds respectively. The components were identified by comparing their retention indices and mass spectra fragmentation patterns with those stored in the National Institute of Standards and Technology (NIST) library. The major constituents reported are *n*-Hexadecanoic acid in methanolic aerial extract and 5-Hydroxymethylfurfural in methanolic root extract.

Keywords: *Polycarphaea corymbosa*, *n*-Hexadecanoic acid, 5-Hydroxymethylfurfural.

1. Introduction

Plants are rich source of secondary metabolites with interesting biological activities. In general, these secondary metabolites are an important source with a variety of structural arrangements and properties¹. Distinguished examples of these compounds include flavonoids, phenols and phenolic glycosides, saponins and cyanogenic glycosides^{2, 3}. Natural products from microbial sources have been the primary source of antibiotics, but with the increasing recognition of herbal medicine as an alternative form of health care, the screening of medicinal plants for active compounds has become very significant because these may serve as talented sources of novel antibiotic prototypes^{4,5}. It has been shown that *in vitro* screening methods could provide the needed preliminary observations necessary to select crude plant extracts with potentially useful properties for further chemical and pharmacological investigations⁶.

Polycarphaea corymbosa Lam. belongs to the family “Caryophyllaceae”. It is commonly known as Oldman’s cap, Pallipoondu or Nilaisedachi in Tamil. Mostly found on open, often moist, sandy soils, less often in grassy places on mountain slopes above 1200 m sea level.

It is an annual herb or short lived perennial with erect stem, 15-35 cm tall, mostly branching above middle, occasionally branched at base⁷.



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The leaves of the plant *P.corymbosa* are used in Indian traditional medicinal system in inflammatory swellings and in treatment of jaundice⁸.

2. Materials and Methods

2.1. Plant material

Polycarpaea corymbosa Lam. was collected in Erode District of Tamilnadu. The plant was confirmed by Botanical Survey of India, Coimbatore circle. A voucher specimen (89/Nov/2011) was submitted in the Herbarium of Botany Department of Kongunadu Arts and Science College, Coimbatore.

2.2. Plant Extraction

The collected plant materials were air dried and ground into uniform powder. Dry powder of plant sample was extracted with methanol using soxhlet apparatus for 6 hours. The extract concentrated using rotary evaporator. The concentrated extract (3.1g) was subjected to freeze drying in a lyophilizer till dry powder was obtained. Finally the extracted powder was resuspended with the methanol at the concentration of 100mg/ml (w/v). 1µl of this solution was employed for GC-MS analysis.

2.3. GC-MS Analysis

The essential oils were analysed on a Agilent gas chromatograph Model 5975C, equipped with a DB5 MS Agilent column (30m X 0.25mm, 0.25µm), programming from 70°C (2 min) to 300°C at 9 min, 5 min hold. ; helium (99.999%) was used as carrier gas at a constant flow of 1 ml /min and an injection volume of 0.5 µl was employed (split ratio of 10:1) injector temperature 240 °C; ion-source temperature 200 °C. The oven temperature was programmed from 70 °C (isothermal for 2 min), with an increase of 10 °C/min, to 300°C, ending with a 9min isothermal at 280°C. Mass spectra were taken at 70eV; a scan range of 40 – 1000 m/z .Total GC running time is 35min.

2.4. Identification of Components

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 of the components of the test materials was ascertained.

3. Results and Discussion

GC-MS data indicated the presence of 30 compounds in the root and 24 compounds in the aerial parts of *P.corymbosa*. The active principles with their retention time (RT) and Peak area (%) are presented in Tables 1 and 2 and Figs 1 and 2.

The identified compound such as 5-Hydroxymethylfurfural (26.68), 2-Chlorophenyl isothiocyanate (11.10) in root and n-Hexadecanoic acid (14.28) and Oleic Acid (12.94) in aerial parts were determined to be the compounds of high peak areas which mainly indulge in the anti-inflammatory properties.

Ten compounds, having high percentage peak areas in root with their individual uses are 5-Hydroxymethylfurfural, 2-Chlorophenyl isothiocyanate, 1-Isobutyl-7, 7-dimethyl-octahydro isobenzofuran-3a-ol, 4-Methylurazole (antitode)⁹, 1,2,3-Benzenetriol (Antiseptic, Antioxidant, Antidermatitic, Fungicide, Insecticide)¹⁰, 2-Aminopyrimidine-1-oxide, Gamma-Sitosterol, 2,5-Furandicarboxaldehyde, Propanedioic acid, oxo-, dimethyl ester and Oleic Acid. Ten compounds having high percentage peak areas in aerial parts with individual use of *P.corymbosa* are as follows: n-Hexadecanoic acid (Antioxidant)¹¹, Oleic Acid (Anti-inflammatory)¹², 5-Hydroxymethylfurfural, 1,3,5-Triazine-2,4,6-triamine, Hentriacontane, Eicosane, Octadecane, Heneicosane, Heptadecane and Octadecanoic (acid antibacterial and antifungal activity)^{13,14}.

The compounds of very lower peak area include Undecane and 2H-Pyran-2,6(3H)-dione in methanolic root extract and Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl- in aerial methanolic extract are also identified.

4. Conclusion

It has been widely observed and accepted that the medicinal value of a plant lies in the bioactive compounds present in it. In the present study, the aerial parts and root of *P.corymbosa* have been subjected to GC-MS analysis. It is the first report in this plant which revealed the presence of bio active compounds (alkaloids, terpenoids, saturated and unsaturated fatty acids) and hence to prove the therapeutic values of *P.corymbosa*.

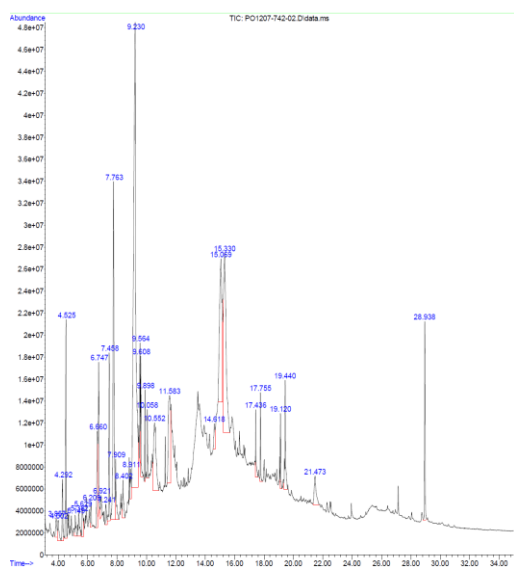


Figure 1. GC-MS Chromatogram of *P.corymbosa* root

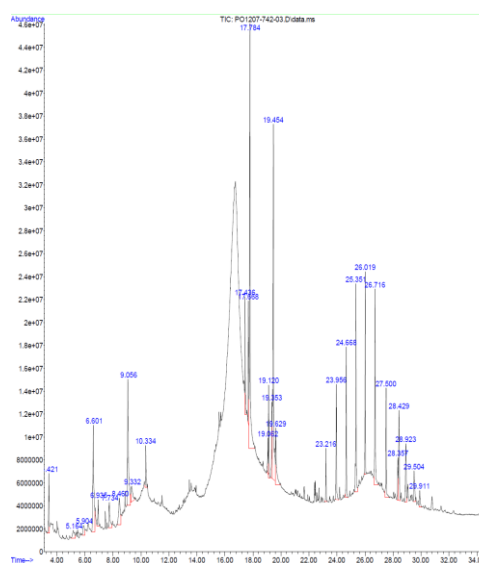


Figure 2. GC-MS Chromatogram of *P.corymbosa* aerial part

Table 1- Compounds identified in the root extract of *P.corymbosa* by GC-MS.

No	RT	Name of the component	Peak area (%)
1	3.857	1H-Imidazole, 4,5-dihydro-2-methyl-	0.60
2	4.002	1-Piperidin-1-ylpropan-2-yl acetate	0.65
3	4.292	1H-Imidazole	1.14
4	4.525	2-Aminopyrimidine-1-oxide	3.49
5	5.149	2H-Pyran-2,6(3H)-dione	0.54
6	5.382	1,3-Dioxane, 2-methyl-	0.78
7	5.629	Isobutyl (2-methoxyethyl) carbonate	0.88
8	6.209	Silanol, tris(1-methylethyl)-	0.56
9	6.747	2,5-Furandicarboxaldehyde	2.83
10	6.921	Undecane	0.54
11	7.241	1,2-Ethanediol, 1-(2-phenyl-1,3,2-dioxaborolan-4-yl)-,	0.55
12	7.458	Propanedioic acid, oxo-, dimethyl ester	2.27
13	7.763	4-Methylurazole	9.00
14	7.909	Thiophene, 2-methyl-5-propyl-	1.19
15	8.402	4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-	0.90
16	9.230	5-Hydroxymethylfurfural	26.68
17	9.564	Piperidin-2-one-5-carboxylic acid,5,6-didehydro-, ethyl(ester)	1.37
18	9.608	4-Chlorobenzoic acid, pent-2-en-4-ynyl ester	1.33
19	9.898	Butanoic acid, di(isopropyl)silyl ester	0.87
20	10.058	2,5-Difluorobenzoic acid, 4-dodecyl ester	0.90
21	11.583	1,2,3-Benzenetriol	4.76
22	14.618	alpha.-D-Glucopyranoside	0.79
23	15.069	1-Isobutyl-7,7-dimethyl-octahydro isobenzofuran-3a-ol	9.26
24	15.330	2-Chlorophenyl isothiocyanate	11.10
25	17.436	Hexadecanoic acid, methyl ester	0.88
26	17.755	n-Hexadecanoic acid	0.88
27	19.120	8-Octadecenoic acid, methyl ester	0.77
28	19.440	Oleic Acid	2.02
29	21.473	5-Aminoimidazole-4-carboxylic acid, methyl ester	1.45
30	28.938	gamma.-Sitosterol	3.31

Table 2- Compounds identified in the Aerial extract of *P.corymbosa* by GC-MS.

No	RT	Name of the component	Peak area (%)
1	3.421	4-Cyclopentene-1,3-dione	1.74
2	5.164	2-Vinyl-9-[.beta.-d-ribofuranosyl]hypoxanthine	0.80
3	5.904	Piperazine, 1,4-dimethyl-	0.87
4	6.601	1,3,5-Triazine-2,4,6-triamine	6.48
5	6.935	Undecane	0.79
6	7.734	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	1.43
7	8.460	2-Furanmethanol, tetrahydro-5-methyl-, trans-	2.28
8	9.056	5-Hydroxymethylfurfural	6.68
9	9.332	d-Mannitol, 1,4-anhydro-	1.34
10	10.334	2-Methoxy-4-vinylphenol	1.29
11	17.436	Pentadecanoic acid, 14-methyl-, methyl ester	2.32
12	17.784	n-Hexadecanoic acid	14.28
13	19.062	Z,E-2,13-Octadecadien-1-ol	0.91
14	19.120	7-Octadecenoic acid, methyl ester	1.79
15	19.454	Oleic Acid	12.94
16	19.629	Octadecanoic acid	2.70
17	23.956	Heptadecane	3.36
18	25.351	Eicosane	5.39
19	26.019	Octadecane	4.12
20	26.716	Hentriacontane	5.77
21	27.500	Heneicosane	3.73
22	28.357	Stigmasterol	1.54
23	28.923	Stigmasta-7,16-dien-3-ol, (3.beta.,.5.alpha.)-	2.30
24	29.911	Octasiloxane,1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	0.71

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