

GC-MS/MS Study of *Parthenium hysterophorus* Root, Antimicrobial Activity

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ABSTRACT

Parthenium hysterophorus belonging to Asteraceae family is used as a medicinal plant in the treatment of pain, rashes, inflammation, asthma. The plant *Parthenium hysterophorus* possess numerous medicinal properties, so, it was decided to study the phytochemicals in the root of *Parthenium hysterophorus* through analytical technique. 20 compounds were identified in the ethanol extract of *Parthenium hysterophorus*. From the results of GC-MS/MS it was known that highest peaks were observed with 9,12-Octadecadienoic acid, methyl ester, (E,E)-, 9,12-Octadecadienoic acid (Z,Z)-, β -Sitosterol. The peak was lower with L-Valine, N-(3-methylbut-2-enoyl)-, heptyl ester. The phytochemicals present in the root of plant *Parthenium* was found to be a good antifungal agent as it showed higher zone of inhibition with *Aspergillus niger*, *Candida albicans*.

Key words: Bacterial, Chromatogram, Fungal, GC-MS/MS, *Parthenium*.

INTRODUCTION

Root is a branching organ, grow deep into the soil, branches developed from roots are random in nature but not from nodes like stems. Roots play a major role in nutrient, water, oxygen absorption and also helps in protecting the environment by holding the soil in its position thereby preventing soil erosion. Usually roots grow towards the environment required for its existence. But poor soil condition allows the root to become dry. Roots also form as a food which are consumed by human beings. Root decoction is used in the treatment dysentery¹. The root also composed of traces of histamine² parthenin, caffeic, chlorogenic, p- hydroxybenzoic, p-anisic, vanilic, salicylic, gentisic, neo-chlorogenic, proto-catechuic acids. Hence, the present study was planned and phytoconstituents was analysed through GC-MS/MS, antimicrobial activity. Flavones in plant also contribute for its pharmacological properties^{3,4}.

MATERIALS AND METHODS

Sample collection

Fresh *Parthenium hysterophorus* root was collected, shade dried, and powdered. 25grams of powdered root sample was used for ethanol extraction. The extracted sample was used for phytochemical analysis through GC-MS/MS, anti-microbial activity. The plant was authenticated by Dr. A. Balasubramanian. The authentication number was AUT/PUS/069 dated 17/12/2014.

Analytical method

GC-MS/MS was performed on a Scion 436-GC Bruker carrying Triple quadruple mass spectrophotometer with fused silica capillary column BR-5MS (5% Diphenyl/95%

Dimethyl poly siloxane), 30m x 0.25mm ID x 0.25m df. The column oven temperature program was as follows: 80°C hold for 2 min, Up to 160°C at the rate of 20°C/min-No hold, Up to 280°C at the rate of 5°C / min-No hold, Up to 300°C at the rate of 20°C/min-10 min hold, Injector temperature 280°C, Total GC running time was 41 min. The inlet temperature was set at 280°C, source temperature 250°C; ionization mode, ionization at 70-eV ionization energy; For single scan analysis, the scan range was set from m/z 40 to 600; Solvent Delay: 0-3.5 min; and the injection volume was 2 μ l. The GC-MS/MS was performed by Institute of crop processing technology, Tanjavur.

Antimicrobial assay

The antimicrobial activity was assessed by means of Kirby- Bauer technique³.

RESULTS AND DISCUSSION

The results of compounds identified are shown in Table.1.

Phytochemicals assessed

Table.1 shows the results of phytochemicals assessed in the ethanol extract of *Parthenium hysterophorus* root. 20 compounds were identified in *Parthenium hysterophorus* root. Out of 20 compounds, few showed highest peak area percent. The name of the compound, retention time, molecular formulae, molecular weight, peak area percent are shown below: 9,12-Octadecadienoic acid, methyl ester, (E,E)- showing 27.78, C₁₉H₃₄O₂, 294, 21.48. 9,12-Octadecadienoic acid (Z,Z)-, 19.34, 19.34, C₁₈H₃₂O₂, 280, 16.91. β -Sitosterol 35.43, C₂₉H₅₀O, 414, 12.23. Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester, 25.10, C₁₉H₃₈O₄, 330, 10.09. Stigmasterol 34.46,

Table 1: Components identified in *Parthenium hysterophorus* root

S.No	RT	Name of the compound	Molecular Formulae	MW	Peak area %
1.	6.84	4-Acetoxy-3-methoxystyrene	C ₁₁ H ₁₂ O ₃	192	1.11
2.	9.95	L-Valine, N-(3-methylbut-2-enoyl)-, heptyl ester	C ₁₇ H ₃₁ NO ₃	297	0.23
3.	13.50	N-(1,1-Dimethyl-2-propynyl)-N-tert.-butylamine	C ₉ H ₁₇ N	139	0.38
4.	15.19	Tetradecanoic acid, 10,13-dimethyl-, methyl ester	C ₁₇ H ₃₄ O ₂	270	0.92
5.	16.25	n-Hexadecanoic acid	C ₁₆ H ₃₂ O ₂	256	7.82
6.	18.22	1,4-Cyclohexanedimethanol	C ₈ H ₁₆ O ₂	144	3.80
7.	19.34	9,12-Octadecadienoic acid (Z,Z)-	C ₁₈ H ₃₂ O ₂	280	16.91
8.	21.37	Carbonic acid, 2-dimethylaminoethyl ethyl ester	C ₇ H ₁₅ NO ₃	161	1.40
9.	21.93	3-Octene-2,5-dione, 6,6,7-trimethyl-, (E)-	C ₁₁ H ₁₈ O ₂	182	2.52
10.	24.17	Cyclobutanecarboxylic acid, 2-dimethylaminoethyl ester	C ₉ H ₁₇ NO ₂	171	2.32
11.	25.10	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	C ₁₉ H ₃₈ O ₄	330	10.09
12.	27.78	9,12-Octadecadienoic acid, methyl ester, (E,E)-	C ₁₉ H ₃₄ O ₂	294	21.48
13.	29.35	Cyclopropanecarboxylic acid, oct-3-en-2-yl ester	C ₁₂ H ₂₀ O ₂	196	0.94
14.	31.94	γ-Tocopherol	C ₂₈ H ₄₈ O ₂	416	2.83
15.	34.00	Campesterol	C ₂₈ H ₄₈ O	400	1.89
16.	34.46	Stigmasterol	C ₂₉ H ₄₈ O	412	9.26
17.	35.43	β-Sitosterol	C ₂₉ H ₅₀ O	414	12.23
18.	35.87	Cholane-5,20(22)-diene-3b-phenoxy	C ₃₀ H ₄₂ O	418	1.88
19.	36.66	Solavetivone	C ₁₅ H ₂₂ O	218	1.13
20.	37.48	1,2-Pentanediol, 5-(6-bromodecahydro-2-hydroxy-2,5,5a,8a-tetramethyl-1-naphthalenyl)-3-methylene-	C ₂₀ H ₃₅ BrO ₃	402	0.87

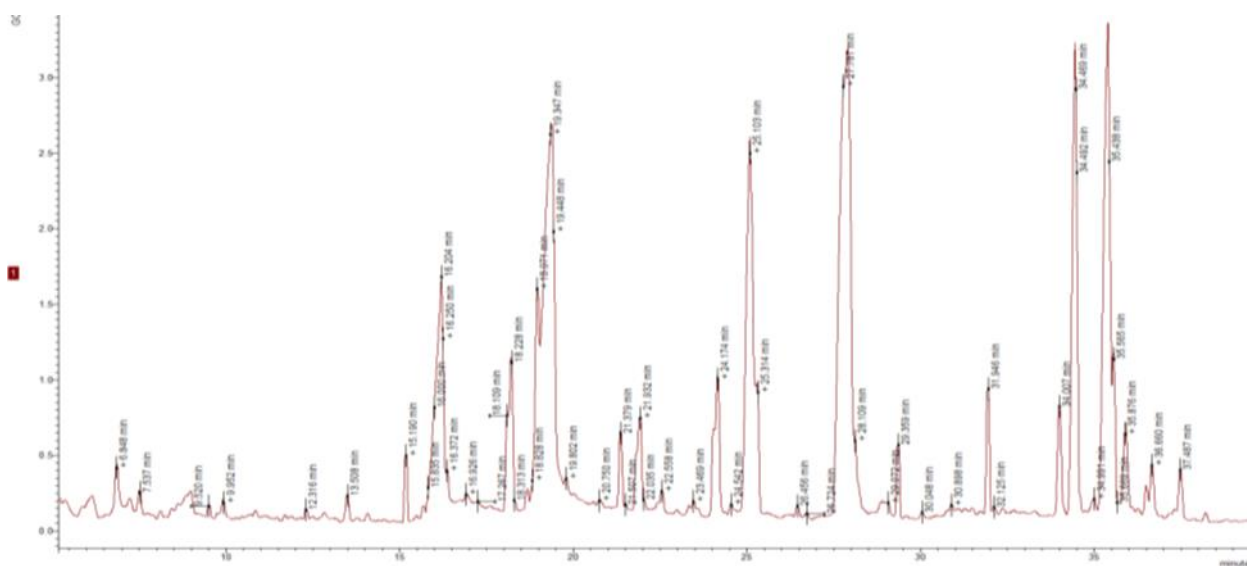


Figure 1: Chromatogram

C₂₉H₄₈O, 412, 9.26. n-Hexadecanoic acid 16.25, C₁₆H₃₂O₂, 256, 7.82. The peak was moderate for 1,4-Cyclohexanedimethanol (18.22, C₈H₁₆O₂, 144, 3.80). γ-Tocopherol (31.94, C₂₈H₄₈O₂, 416, 2.83), 3-Octene-2,5-dione, 6,6,7-trimethyl-, (E)- (21.93, C₁₁H₁₈O₂, 182, 2.52), Cyclobutanecarboxylic acid, 2-dimethylaminoethyl ester (24.17, C₉H₁₇NO₂, 171, 2.32), Campesterol (34.00, C₂₈H₄₈O, 400, 1.89), Cholane-5,20(22)-diene-3b-phenoxy (35.87, C₃₀H₄₂O, 418, 1.88), Carbonic acid, 2-dimethylaminoethyl ethyl ester (21.37, C₇H₁₅NO₃, 161, 1.40), 4-Acetoxy-3-methoxystyrene (6.84, C₁₁H₁₂O₃, 192, 1.11), Solavetivone (36.66, C₁₅H₂₂O,

218, 1.13). The peak area percent was less than one for the following compounds: Cyclopropanecarboxylic acid (29.35, C₁₂H₂₀O₂, 196, 0.94), oct-3-en-2-yl ester, Tetradecanoic acid, 10,13-dimethyl-, methyl ester (15.19, C₁₇H₃₄O₂, 270, 0.92), 1,2-Pentanediol, 5-(6-bromodecahydro-2-hydroxy-2,5,5a,8a-tetramethyl-1-naphthalenyl)-3-methylene- (37.48, C₂₀H₃₅BrO₃, 402, 0.87), N-(1,1-Dimethyl-2-propynyl)-N-tert.-butylamine (13.50, C₉H₁₇N, 139, 0.38), L-Valine, N-(3-methylbut-2-enoyl)-, heptyl ester (9.95, C₁₇H₃₁NO₃, 297, 0.23). The plant *Parthenium hysterophorus* was studied for its air

Table 2: Antimicrobial activity of ethanol extract of *Parthenium hysterophorus* root

Plant /Part used	Microbes tested	Zone of inhibition (mm)
	<i>Escherichia coli</i>	8
Parthenium hysterophorus root	<i>Staphylococcus aureus</i>	-
	<i>Aspergillus niger</i>	10
	<i>Candida albicans</i>	15

Pollution tolerance index, antioxidant activities⁶ phytochemicals⁷ GC-MS/MS^{8,9} by Krishnaveni et.al.

The chromatogram shows the retention time. The peak area percent was calculated using height and width of the peak obtained.

Antimicrobial activity

The results of the antimicrobial activity is shown in Table.2. From the result we can say that the ethanol extract was able to act against fungi in a satisfactory manner when compared to bacteria. Because among the bacteria tested, the extract could act on *E.coli* only showing lesser zone of inhibition i.e 8mm. While, the zone of inhibition was higher for *Aspergillus niger* (10mm), *Candida albicans* (15mm).

CONCLUSION

Antimicrobial agents from natural source is an alternate for synthetic agents. In the present study, ethanol extract of *Parthenium hysterophorus* root showed significant antifungal activity. The compounds like essential oils, secondary metabolites such as phenolics, flavonoids are responsible for the antimicrobial nature of *Parthenium hysterophorus* root extract.

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