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GC-MS Determination of Bioactive Compounds of *Polygonum glabrum* (Wild).

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Summary

In this study, the bioactive compounds of *Polygonum glabrum* have been evaluated using GC-MS. The chemical compositions of the whole plant ethanol extract of *P. glabrum* were investigated using Perkin-Elmer Gas Chromatography-Mass Spectrometry, while the mass spectra of the compounds found in the extract was matched with the National Institute of Standards and Technology (NIST) library. GC-MS analysis of *P. glabrum* whole plant ethanol extract revealed the existence of the ether compound –Propane 1,1-diethoxy- (64.86%), alkane compound -2-Heptane, 5-ethyl-2,4-dimethyl- (13.51%), sulphur compound –Tiophene-2-Carboxamide, N-(2-furfuryl)- (8.!!%), alcoholic compound -1,14-Tetradecanediol (5.41%), and plasticizer compounds -1,2-Benzenedicarboxylic acid, isodecyloctyl ester (5.41%) and 1,2,3-Benzenetriol (2.79%). The results of this study offer a base of using *P. glabrum* as herbal alternative for the synthesis of antimicrobial agents.

Key Words: GC-MS analysis, Bioactive compounds, *Polygonum glabrum*, Ethanol extract

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 properties [1]. 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 they may serve as talented source of bulk antibiotic prototypes [2, 3]. The family Polygonaceae consists of several important medicinal plants with wide range of biological activities and interesting phytochemical constituents. *Polygonum glabrum* (Wild.) was selected for the present study, based on its therapeutic value and the degree of research work which is not done mostly in earlier. In this study, *P. glabrum* whole plant ethanol extract was used for the screening of different phytochemical constituents by GC-MS analysis.

Material and Methods

Plant material

Polygonum glabrum was collected from Srivaikuntam, Thuthukudi District, Tamil Nadu in India and identified by Dr. Chelladurai, Research Officer, at Central Council for Research in Ayurveda and Siddha, Palaymkottai. Herbarium of the plant, *P. glabrum* was prepared and preserved in the Department of Botany, S. T. Hindu College, Nagercoil, Kanyakumari District, Tamil Nadu, India.

Preparation of extract

The whole plant material of *P. glabrum* was collected from wild, shade dried and pulverized to powder in a mechanical grinder. Required quantity of the whole plant powder of *P. glabrum* was weighted, transferred to flask, treated with the ethanol until the powder was fully immersed, incubated over night and filtered through a Whatmann No.-41 filter paper along with sodium sulphate to remove the sediments and traces of water in the filter paper. Before filtering, the filter paper along with sodium sulphate was wetted with absolute alcohol. The filtrate is then concentrated to 1ml by bubbling nitrogen gas into the solution. The extract contains both polar and non-polar components of the plant material and 2µl sample of the solutions was employed in GC-MS for analysis of different compounds.

GC-MS *analysis*

GC-MS analysis of the ethanol extract of *P. glabrum* was performed using a Perkin Elmer GC Clarus 500 system comprising AOC-20i auto-sampler and a Gas Chromatograph interfaced to a Mass Spectrometer (GC-MS) equipped with a Elite-5MS (5% Diphenyl/ 95% Dimethyl poly siloxane) fused capillary column (30 x 0.25µm ID x 0.25µm df). For GC-MS detection, an electron ionization system was operated in electron impact mode with ionization energy of 70eV. Helium gas (99.999%) was used as carrier gas at a constant flow rate of 1ml/min, and an injection volume of 2µl was employed (split ratio of 10: 1). The injector temperature was maintained at 250°C, the ion-source temperature was 200°C, the oven temperature was programmed form 110°C (isothermal for 2min), with an increase of 10°C/min to 200°C, then 5°C/min to 280°C, ending with a 9min isothermal at 280°C. Mass spectra were taken at 70eV; a scan interval of 0.5 seconds and fragments from 45-450Da. The solvent delay was 0 to 2min and the total GC/MS running time was 36min. The relative percentage amount of each component was calculated by comparing its average peak area to the total areas. The Mass-detector used in this analysis was Turbo-Mass Gold-Perkin Elmer and the software adopted to handle mass spectra and chromatograms was a Turbo-Mass ver-5.2.

Identification of phytocomponents

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 components was compared with the spectrum of known components stored in the NIST library. The name, molecular weight and structure of the components of the test materials were ascertained.

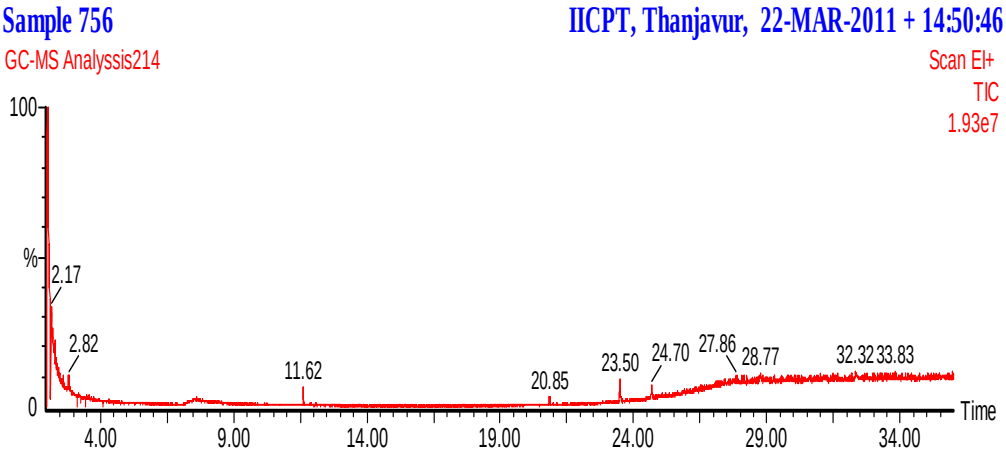

Fig.-1. GC-MS Chromatogram of *Polygonum glabrum* ethanolic extracts.

Result and Discussion

The studies on the active principles in the *P. glabrum* whole plant ethanolic extract by GC-MS analysis clearly showed the presence of six compounds (Tabl.-1). The active principles with their retention time (RT), molecular formula, molecular weight (MW), and concentration (peak area %) are presented in Table-1. The GC-MS chromatogram of the five peaks of the compounds detected was shown in Figure-1. The mass spectrum and structure of the compounds identified were shown in Figure-2.

Tab.-1. Phytocomponents* identified in the ethanolic extract of *Polygonum glabrum* by GC-MS study.

No.	RT	Name of the compound	Molecular Formula	MW	Peak Area %
1.	2.82	Propane, 1,1-diethoxy-	$C_7H_{16}O_2$	132	64.86
2.	7.62	1,2,3-Benzenetriol	$C_6H_6O_3$	126	2.70
3.	11.62	1,14-Tetradecanediol	$C_{14}H_{30}O_2$	230	5.41
4.	20.85	1,2-Benzenedicarboxylic acid, isodecyl octyl ester	$C_{26}H_{42}O_4$	418	5.41
5.	23.50	2-Heptene, 5-ethyl-2,4-dimethyl-	$C_{11}H_{22}$	154	13.51
6.	24.70	Thiophene-2-carboxamide, N-(2-furfuryl)-	$C_{10}H_9NO_2S$	207	8.11

*Parameters tested are not covered under the scope of NABL accreditation

Tab.-2. Bioactivity of phytocomponents identified in the ethanolic extracts of *Polygonum glabrum* by GC-MS study

No.	RT	Name of the compound	Nature of compound	**Activity
1	2.83	Propane, 1,1diethoxy-	Ether compound	No activity reported
2	7.62	1,2,3 Benzene triol-	Poly Phenol compound-Pyrogallol	Antioxidant, Antiseptic, Antibacterial, Antidermatitic Fungicide, Pesticide, Antimutaginic Dye, Candidicide
3	11.62	1, 14 Tetradecanediol	Alcoholic compound	Antimicrobial
4	20.85	1,2-Benzenedicarboxylic acid, isodecyl octyl ester	Plasticizer compound	Antimicrobial, Antifouling
5	23.50	2-Heptane, 5-ethyl-2,4-dimethyl-	Alkane compound	No activity reported
6	24.70	Thiophene-2-Carboxamide, N-(2-furfuryl)-	Sulfur compound	Antimicrobial

**Source: Dr. Duke's: Phytochemical and Ethnobotanical Databases.

Most of identified compounds reported to have antimicrobial property (Tab.-2) were polyphenol compound –pyrogallol (1,2,3 Benzene triol-), alcoholic compound (1, 14 Tetradecanediol), plasticizer compound (1,2-Benzenedicarboxylic acid, isodecyl octyl ester), and sulphur compound (Thiophene-2-Carboxamide, N-(2-furfuryl)-). Besides antimicrobial activity, the polyphenol (pyrogallol) compound reported to have antioxidant, antiseptic, antidermatitic, fungicide, pesticide, antimutagenic, candidicide and dye properties. The plasticizer compound showed antifouling activity also. The most prevailing compound identified in the whole plant ethanol extract of *P. glabrum* was an ether compound –Propane,1,1-diethoxy (64.86%) in which no activity was reported. Similarly, the alkane compound (2-Heptane, 5-ethyl-2,4-dimethyl-) was also reported to have no activity (Tab.-2). The results of this study offer a base of using *P. glabrum* as herbal alternative for the synthesis of antimicrobial agents.

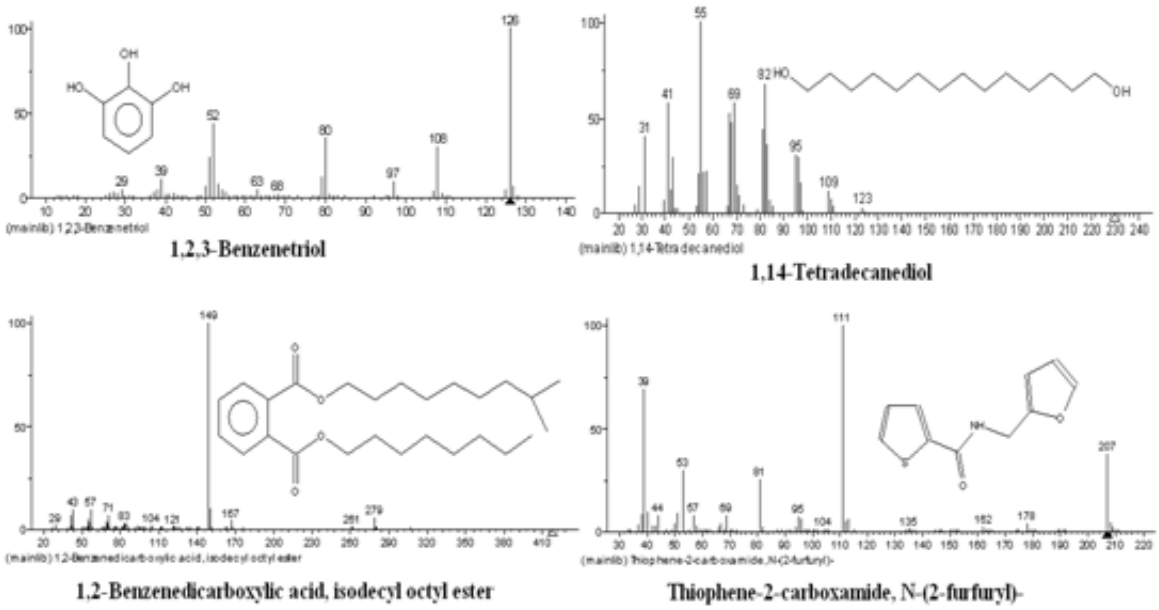

Fig.-2. Mass spectrum and structure of phytocomponent identified by GCMS in the ethanolic extracts of *Polygonum glabrum.*

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