GC-MS analysis of Bioactive compounds from ethanolic extract of aerial parts of *Mollugo pentaphylla* L. and their pharmacological activities

Nagannawar Anju G.* and Jayaraj M.

Department of Botany, Karnatak University, Dharwad – 580003, Karnataka INDIA *2016anju@gmail.com

Abstract

Plant secondary metabolites are rich sources of bioactive compounds and are used in pharmaceutical industries and production of nutrient-rich food materials. These bioactive compounds are used to treat various diseases and to improve the health of people both by traditional and conventional ways of administrations. Therefore, Mollugo pentaphylla L., is a traditional medicinal herb, indicated for a number of medicinal properties. The present investigation was undertaken to identify the bioactive compounds present in the aerial parts powder of Mollugo pentaphylla L., by Gas chromatography- Mass spectrometry (GC-MS) Gas chromatography analysis- Mass analysis. spectrometer (GC-MS) was carried out at Karnatak University, Dharwad, Karnataka, India.

It is one of the key techniques, generally used for identification of different groups of plant bioactive compounds. Quantification of the Mollugo pentaphylla L., showed 28 bioactive compounds and among these 7 major compounds identified are Pentadecanoic acid, 9-Octadecenoic acid. 2-Dodecenoic acid. Hexadecanoic acid, Oleic acid, Nonadecane and Octadecane. In the mass spectrum, each compound was identified based on their retention time and peak area. Pharmacological activities of these bioactive compounds indicated that the plant can be used as a crude drug and can also be used to develop a new drug and these bioactive compounds are indicated based on available pharmacological literature.

Keywords: Bioactive compounds, Ethanoic extract, GC-MS, *Mollugo pentaphylla* L., Pharmacological activity.

Introduction

Plants are the richest sources of secondary metabolites with varying biological activities. These secondary metabolites are the important source with a variety of structural arrangements and functions. Plants have the capacity of synthesizing the organic compounds and are called secondary metabolites, they have unique and complex structures^{8,21}. Volatile compounds play an important role in health care systems. Volatile compounds are identified by the GC-MS analysis⁷. Recently GC-MS analysis is progressively applied for the analysis of secondary metabolites present in the medicinal plants and this

technique proved to be a valuable method for analysis and identification of potentially bioactive compounds.

Mollugo pentaphylla L. is a traditional medicinal herb belonging to Molluginaceae. It is commonly known as slender carpetweed (English). It is a highly valued medicinal plant and possesses antimicrobial, anticancerous, antiinflammatory, antiseptic properties and it is antidiabetic²². Traditionally it is also used to treat stomachache, wound, earache, cough, aperients, skin diseases²⁴. In the last few years, the GC-MS has become the key tool for analysis of secondary metabolites investigation in plants. The present study is undertaken to know the bioactive compounds by GC-MS profile of ethanolic extract of aerial parts powder of *Mollugo pentaphylla* L. and their pharmacological activities.

Material and Methods

Material: *Mollugo pentaphylla* L. belongs to family Molluginaceae⁹. It is herb growing in subtropical and tropical regions in India. It is commonly called as carpetweed. The *Mollugo pentaphylla* L. (Voucher specimen no: KUD/BOT/AN/JM/002), the plant was collected from Karnatak University Campus, Dharwad, Karnataka. The plant was washed with running tap water and later dried at room temperature. The shade dried plant was powdered using an electric blender. Thus obtained powder was sieved and stored in an airtight container at room temperature for further analysis¹⁰.

Aerial Parts of Plant Extract: About 15gms of powder was subjected for extraction with ethanol (250 ml) using Soxhlet apparatus. This extract was subjected to GC-MS analysis to identify the bioactive compounds.

GC-MS Analysis: The analysis was performed using a GC-MS Shimadzu, Japan: QP2010S fitted with a 1.4 μ m column Rxi-5si1MS 30-meter length, 0.25 mm inner diameter and 0.25 μ m film thickness. Carrier gas helium was used with a flow rate of 0.98 ml/min; column temperature 80 °C; initial temperature 70 °C, injector temperature 260 °C and detector temperature 300 °C followed by a linear programmed temperature from 70- 280 °C at a rate of 10 °C/min, operating in electron impact mode. The samples were injected in splitless mode and interface temperature was kept at 280 °C. The pressure of the carrier gas was kept at 63.6 kPa. The constituents were determined based on the retention time of a series and identification of each compound was confirmed by comparison of its retention index with data available in the literature³.

Identification of Compounds: Bioactive compounds are identified based on the mass spectrum of GC-MS using the database of National Institute Standards and Technology (NIST). The spectrum of the unknown compounds was compared with a spectrum of known compounds with the help of the data present in the NIST library^{8,31}. The name, molecular weight and molecular formula of each compound of the test materials are tabulated.

Results

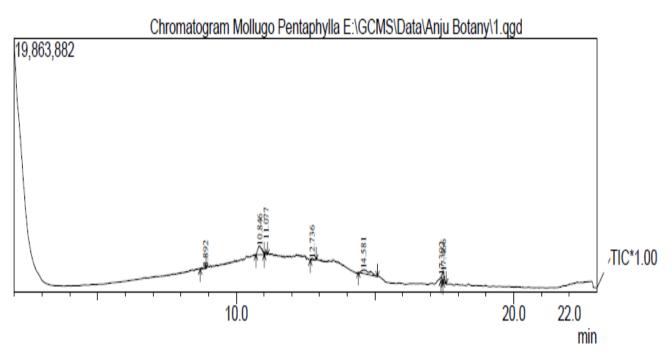
The GC-MS chromatogram of the ethanolic extract of aerial parts powder of *Mollugo pentaphylla* L. showed 7 major peaks indicating the presence of seven bioactive compounds (Fig. 1) and mass spectra of identified compound of the ethanolic extract are recorded (Fig. 2).

The active principles with their peak, retention time (RT), area (%), height (%), molecular formula and molecular

weight are presented (Table 1). The GC-MS analysis showed the presence of seven major bioactive compounds in the ethanol extract of the aerial parts namely Pentadecanoic acid, 9,10- Octadecenoic acid, 2-Dodecenoic acid, Hexadecanoic acid, Oleic acid, Nonadecane, Octadecane (Fig. 2). These compounds have various pharmacological activities and are presented (Table 2).

Discussion

The Gas Chromatography and Mass Spectrometry (**GC-MS**) instrument separates chemical mixtures and identifies the components at a molecular level. In the present study, GC-MS analysis revealed the seven major bioactive compounds. The Octadecane (30.14 %) is the highest chemical compound and Pentadecanoic acid (2.98 %) as the lowest chemical compound.



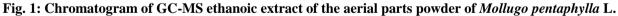


Table 1
GC-MS analysis of bioactive compounds in ethanol extract of aerial parts of Mollugo pentaphylla L.

Peak	R. Time	Area %	Height %	Molecular formula	Molecular Weight	Name of the compound
		, 0	,,,		(g/mol)	
1	8.892	3.49	2.98	$C_{17}H_{30}O_2$	242.3975	Pentadecanoic acid
2	10.846	35.92	25.78	$C_{18}H_{34}O_2$	282.5	9,10-Octadecenoic acid
3	11.077	3.42	6.53	$C_{12}H_{22}O_2$	198.306	2-Dodecenoic acid
4	12.736	3.92	5.59	$C_{16}H_{32}O_2$	256.4	Hexadecanoic acid
5	14.581	32.72	11.68	$C_{18}H_{34}O_2$	282.47	Oleic acid
6	17.392	12.06	17.30	C ₁₉ H ₄₀	268.529	Nonadecane
7	17.466	8.47	30.14	C ₁₈ H ₃₈	254.5	Octadecane

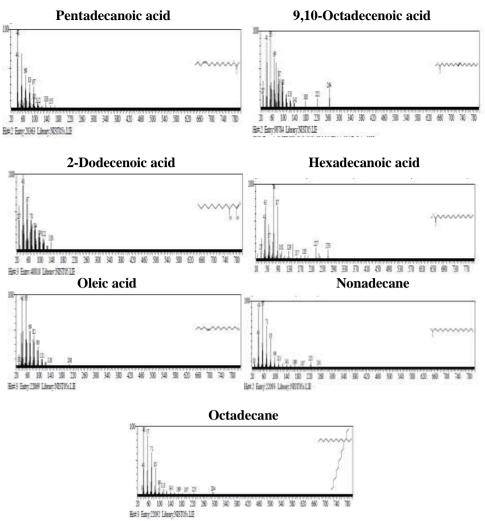


Fig. 2: Mass spectra of identified bioactive compounds of ethanolic extract of aerial parts of Mollugo pentaphylla L.

 Table 2

 Pharmacological activity of bioactive compounds in the ethanolic extract of aerial parts of *Mollugo pentaphylla* L.

S. N.	Compounds	Pharmacological activity				
1	Pentadecanoic acid	Antibacterial and Antiallergic ²⁹ , Antifungal ² , Antioxidant ^{27,28} , Cyclooxygenase activity ¹⁸ ,				
		Adhesive agent and Lubricants ⁶ .				
2	9,10-Octadecenoic	Antihistaminic, Insectifuge, Anti-eczemic and Anti-acne ¹⁵ , Antimicrobial ^{1,34} , Anti-				
	acid	inflammatory, Cancer preventive and Nematicide ^{5,23,33} , Hepatoprotective, 5-alpha-				
		reductase inhibitor, Antiandrogenic, Antiarthritic and Anticoronary ¹² , Antifibrinolytic and				
		Antioxidant ³⁴ , Antitumor ⁶ .				
3	2-Dodecenoic acid	Antiandrogenic, Anticoronary and 5-Alpha-reductase inhibitor ³⁰ , Signal modulator ¹¹ .				
4	Hexadecanoic acid	Antioxidant and Anti-inflammatory ^{5,16} , Anthelmintic activities ³ , Antibacterial,				
	(Palmitic acid)	Antiallergic ^{25,26} , Hypocholesterolemic, Pesticide, Flavor, Hemolytic and 5-alpha-reductase				
		inhibitor ^{12,20} , Antifibrinolytic ¹⁷ , Antialopecic, Antiandrogenic, Lubricant, Nematicide,				
		Pesticide, Propecic and Soap ²³ .				
5	Oleic acid	Anti-inflammatory, Anticancer, Hypocholesterolemic and Insectifuge ²⁰ , 5-alpha-reductase				
		inhibitor, Anemiagenic, Antiandrogenic, Antialopecic, Dermatitigenic, Flavor,				
		Hypocholesterolemic, Percutaneostimulant, Perfumery, Antileukotriene- cancer-				
		preventive and Choleretic ^{13,23,35} .				
6	Nonadecane	Antioxidant, Antibacterial, Antimicrobial, Anti HIV, Antimalarial, Cytotoxic effects,				
		Unani uses like weakness of the principal organs like heart, brain, liver, general weakness,				
		Haemoptysis, Palpitation, Conjunctivitis, Earache, Stomatitis ⁸ .				
7	Octadecane	Antioxidant, Anti-inflammatory and Antisepsis ^{3,8} , Anticorrosion agent ^{4,20} , Cough, lung				
		diseases and fever detoxification ^{3,25,32} .				

The compound Hexadecanoic acid (5.59 %), 2-Dodecenoic acid (6.53 %) and Oleic acid (11.68 %) showed pharmacological activity as reported in *Mangroves*^{2,23}, *Asclepias curassavica* L.¹² and *Cassia italic*³⁰. Similarly, Nonadecane, 9,10- Octadecenoic acid, Octadecane also showed the various pharmacological activities as reported for *Waltherria indica* Linn.⁸

Conclusion

The ethanolic extract of aerial parts of *Mollugo pentaphylla* L. has seven different bioactive compounds with different pharmacological activities. Secondary metabolites produced by this plant may be of great interest for the pharmaceutical industry and medicinal research and each chemical compound can be extracted individually and used in clinical trials to check the efficacy and to develop a new drug from a crude drug. The GC-MS analysis of *Mollugo pentaphylla* L. will also be a part of a database of bioactive products of natural drugs.

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