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Chemical composition of *Ocimum sanctum* by GC-MS Analysis

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Abstract

The chemical composition of the n-hexane extract from the aerial parts of *Ocimum sanctum.*, was investigated using gas chromatography-mass spectrometry (GC/MS), identifying 46 different compounds. Terpenoids were the most abundant, with monoterpenes representing 21.82% of the extract. The primary components identified were methyl eugenol (27.24%), squalene (11.84%) α-bergamotene (9.83%), linalool (8.42%), and fenchyl acetate (7.56%). These results indicate that *O. sanctum* could serve as a valuable source of food and medicinal agents.

Keywords: *Ocimum sanctum.*, GC

INTRODUCTION

Medicinal plants are well-known for their diverse range of bioactive compounds, which have long been used to treat chronic and infectious diseases (Periyasamy Ashokkumar et al., 2010). Natural products derived from plant extracts/fractions are potent therapeutic agents for various infectious as well as degenerative diseases. In herbal medicines, various parts of the plant (root, stem, flower, fruit, twig exudates and modified plant organs) are used having diverse therapeutic properties. To utilize these plants, they are collected on the minute scale by local communities and folk healers, while to trade for herbal industries numerous other plants are collected in large amounts as a raw material (Sahreen et al., 2015). In recent years for the management and protection against pathogens, a large number of plants have been examined for their antimicrobial characteristics as an integrative system of medicine (Hosseinzadeh et al., 2015).

For centuries, plant extracts and oils have served various medicinal and practical purposes (EL-

Kamali & EL-Amir, 2010). The genus *Ocimum*, which includes 160 species, is distributed across tropical and subtropical regions, showing considerable morphological variability from herbs to sub-shrubs (Mustafa & El-kamali, 2019). The morphology of *Ocimum* varies from herb to sub-shrubs with large variations in leaf shape, size, glands, hairs and many more morphological peculiarities. Each species produces essential oils with antimicrobial, antioxidant, antifungal, and anti-inflammatory properties, although their taxonomy remains somewhat unclear (Nahak et al., 2011).

Ocimum sanctum., is widely recognized in traditional and modern medicine across Africa, Asia, Europe, and South America (Mustafa & El-kamali, 2020). This study aims to identify the chemical composition of the n-hexane extract from the aerial parts of *O. sanctum*.

MATERIALS AND METHODS

Plant Material

The aerial parts of *Ocimum sanctum.,* were collected from Sinnar State in April, 2018 and identified by Prof. Maha Kordofani from the University of Khartoum, Botany Department, Sudan.

Extraction

Twenty grams (20g) of dried aerial parts were macerated in n-hexane for 72 hours. After filtration, the extract was concentrated, yielding 80 mg of dried material (Omer et al., 2024).

GC-MS Analysis

GC/MS analysis was performed on a Shimadzu GC/MS-QP2010A system in ET mode (70ev) equipped with at a split /splitters injector (250ºC), at split ratio of 5/50 using DB-5MSColumn (30m x 0.25mm id, film thickness: 0002E25 miss J and W scientific, fulsome, CA,WA). Injection volume was 1misarlitre and electronic pressure programming was used to maintain a constant flame (0.67ml/mins) of the Helium carrier gas. The oven temperature was programmed from 150ºC (4mins) to 320ºC at a rate of 2c/mins and held at that temperature 200ºC and interface temperature 250ºC. The relative approach percentage of each compound was determined by area. Components identification was carried out using the NIST 147 and NIST 27 libraries (Mustafa & El-kamali, 2019).

RESULTSAND DISCUSSION

GC-MS analysis of the n-hexane extract from *O. sanctum.,* aerial parts revealed 46 chemical constituents (Table1) The major compound was methyl eugenol (27.24%), followed by squalene (11.84%), α-bergamotene (9.83%), linalool (8.42%), and fenchyl acetate (7.56%). Sesquiterpenes (48.33%) and monoterpenes (21.25%) were the dominant compound groups, with other identified components including triterpenol hydrocarbons, esters, ketones, fatty acids, and alcohols.

The results can be justified by the already reported work (Khair-ul-Bariyah, 2013). The work has been reported regarding the chemical constituents of *O. sanctum* (Mondello et al., 2002). Similarly, linalool of up to 71.4% in essential oil from Bulgaria has been reported (Jirovetz et al., 2001). From China, Croatia, Israel, the Republic of Guinea, Nigeria, Egypt, Pakistan and Malaysia, (z)cinnamic acid methyl ester, linalool, eugenol, estragol, bergamotene, 1,8-cineol, α-cadinol, methyl cinnamate and limonene has been listed as major components of the essential oil. Forty seven components comprising 97.99% of total oil have been reported (Hassanpouraghdam et al., 2010).

Generally, the work has been reported monoterpenoids comprise the major fraction of the oil (77.8%) followed by sesquiterpenoids (12.8%). Oxygenated monoterpenes are 75.3% present with estragole (21.5%), menthone (33.1%), menthol (6.1%), isoneomenthol (7.5%) and pulegone (3.7%) being the main compounds. The only monoterpene hydrocarbon is limonene (1.5%). Menthyl acetate was found in trace amounts (5.6%) (Khair-ul-Bariyah, 2013). The presence of bioactive compounds supports the traditional use of *O. sanctum* for medicinal purposes, and it was classified as a methyl eugenol chemotype.

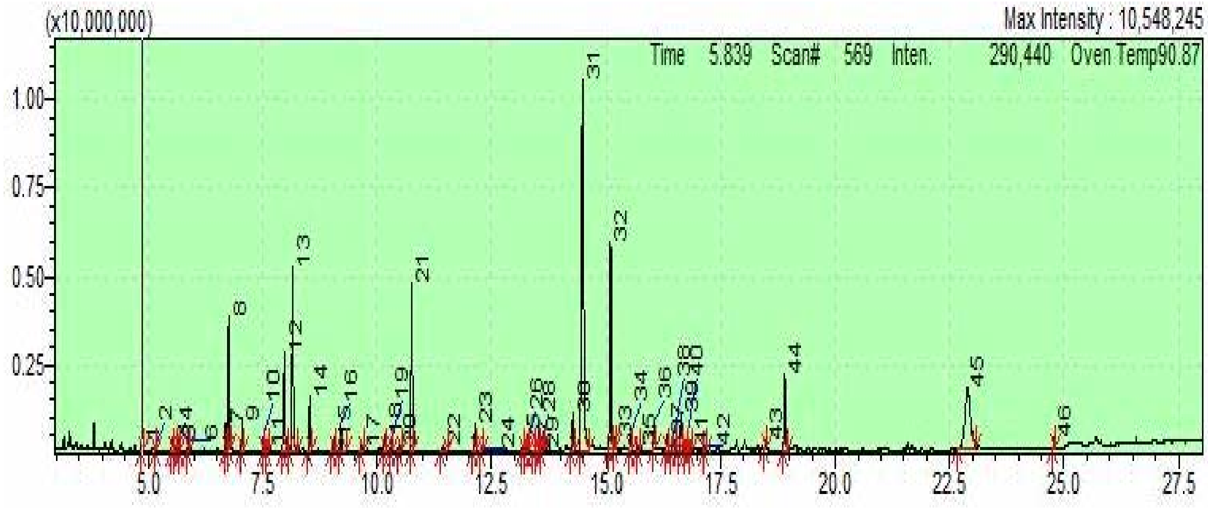

Figure (1). GC/MC chromatogram of *Ocimum sanctum.,* n-hexan extract

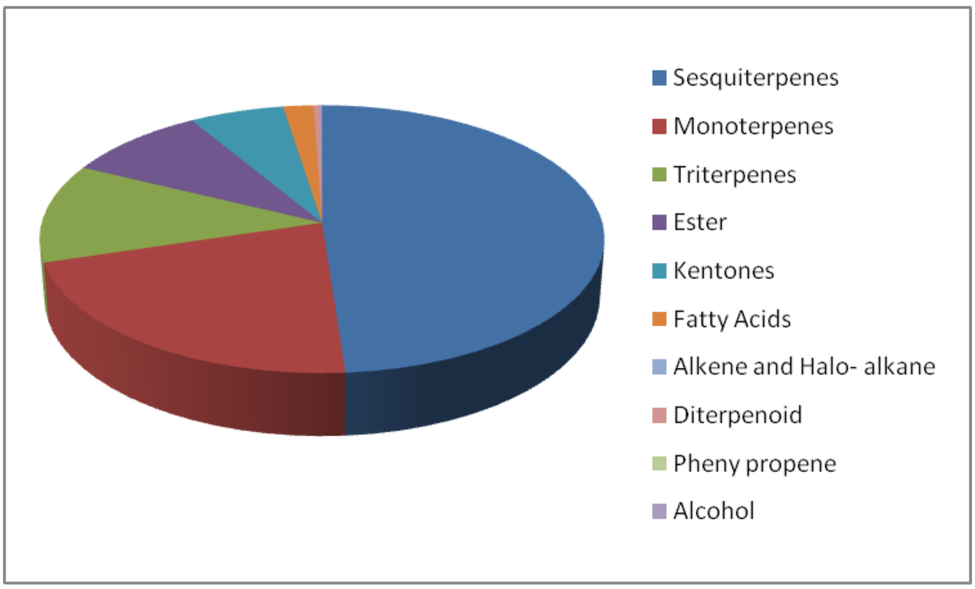

Figure (2). Percentage of compounds

Table(1). Chemical composition of n-hexane extract of aerial parts of *Ocimum sanctum.,:*

NO	Compounds	R.T	%	Formula	Class type
1	α –pinene	4.866	0.38	$C_{10}H_{16}$	MH
2	Camphene	5.152	0.13	$C_{10}H_{16}$	MH
3	Hexen-2-one	5.523	0.42	$C_6H_{10}O$	OH
4	β – phellandrene	5.598	0.20	$C_{10}H_{16}$	MH
5	β- (-)pinene	5.680	0.40	$C_{10}H_{16}$	MH
6	β – myrcene	5.888	0.41	$C_{10}H_{16}$	MH
7	D- Linanene	6.689	1.06	$C_{10}H_{16}$	MH
8	Eucalyptol	6.762	5.25	$C_{10}H_{18}O$	OM
9	B- Ocimene	7.048	1.09	$C_{10}H_{16}$	MH
10	Cyclohexanol,1-methyl-4-(1-methylethenyl	7.516	0.41	$C_{10}H_{18}O$	OM
11	α-methyl-alpha-(4-mehyl-3pentenyl)	7.609	0.17	$C_{10}H_{18}O_2$	FA
12	L-fenchone	7.976	4.48	$C_{10}H_{16}O$	Ketone
13	Linalool	8.159	8.42	$C_{10}H_{18}O$	OM
14	Bicyclo (2.2.1) hepta-2-ol ,1,3,3-trimethyl-	8.530	2.16	$C_{10}H_{18}O$	OM
15	3-cyclohexene-1-methanol	9.047	0.59	$C_7H_{12}O$	Alkene
16	(+)-2-bornanone	9.207	1.14	$C_{10}H_{16}O$	Ketone
17	L-α- terpineol	9.667	0.29	$C_{10}H_{18}O$	OM
18	α – terpineol	10.167	0.67	$C_{10}H_{18}O$	OM
19	Estragole	10.308	0.33	$C_{10}H_{12}O$	OM
20	Octyl acetate	10.480	0.25	$C_{10}H_{20}O_2$	FA
21	Fenchyl acetate	10.755	7.56	$C_{12}H_{20}O_2$	FA
22	Geraniol	11.440	0.38	$C_{10}H_{18}O$	OM
23	Bornyl acetate	12.136	1.18	$C_{12}H_{20}O_2$	FA
24	Hexadecane,1-chloro	12.280	0.12	$C_{16}H_{33}CL$	Halo-alkane
25	-β elemene	13.181	0.28	$C_{15}H_{24}$	SH
26	2-hydroxycineol	13.253	0.14	$C_{12}H_{20}O_3$	Ether
27	α – culenene	13.423	0.04	$C_{15}H_{24}$	SH
28	6-isopropenyl-3-(methoxy meth-oxy)-3-methyl	13.528	0.07	$C_{12}H_{20}O_2$	FA
29	Hydroxycineol	13.586	0.13	$C_{10}H_{18}O_2$	FA
30	Elemene	14.275	1.64	$C_{11}H_{14}O_2$	FA
31	Methyl eugenol	14.491	27.24	$C_{15}H_{24}$	SH
32	α- Bergamotenol	15.096	9.83	$C_{15}H_{24}$	SH
33	α- Guaiene	15.188	0.45	$C_{15}H_{24}$	SH
34	Humulene	15.537	0.64	$C_{15}H_{24}$	SH
35	β- cubebene	15.700	0.25	$C_{15}H_{24}$	SH
36	β -Ylangene	16.047	1.50	$C_{15}H_{24}$	SH
37	Germcrene B	16.338	0.63	$C_{15}H_{24}$	SH
38	α-bulnesene	16.477	0.71	$C_{15}H_{24}$	SH
39	γ-maurolene	16.636	1.76	$C_{15}H_{24}$	SH
40	β-Sesquiphella-ndrene	16.737	0.34	$C_{15}H_{24}$	SH
41	2-α-trans-bergamolol	16.832	0.20	$C_{15}H_{24}O$	OS
42	Trans –α-begamotol	17.156	0.30	$C_{15}H_{24}O$	OS
43	Cubenol	18.476	0.38	$C_{15}H_{26}O$	OS
44	Cadinol	18.903	3.78	$C_{15}H_{26}O$	OS
45	Squalene	22.884	11.84	$C_{30}H_{50}$	Triterpenoids
46	Phytol	24.788	0.38	$C_{20}H_{40}O$	Diterpene

MH=monoterpene hydrocarbon; OM=oxygenated monoterpene ; FA=fatty acid;
SH=sesquiterpene hydrocarbon; OS=oxygenated sesquiterpene; OH: Oxgenated hydrocarbon.

Table (2). The high compounds in *Ocimum sanctum.*, with biological activity:

Compounds	%	Medicinal uses and biological activity	References
Methyl eugenol	27.24	anti-inflammatory, Nematodes, Antifeedant and Insects.	(Desai et al., 1996; Park et al., 2007)
Squalene	11.42	Antioxidant and Antitumor activities.	(Saint-Leger et al., 1986; Yano, 1987)
α-bergamotene	9.83	Antiepileptic and anti-inflammatory activity.	(Kohno et al., 1995)
Linalool	8.42	Antibacterial, antifungal and Anti-inflammatory.	(Desai et al., 1996)
Fenchyl acetate	7.56	Food flavour (chewing gum, toothpaste).	(Sabogal-Guáqueta et al., 2016)
Eucalyptol	5.25	Insecticidal, flavorings, fragrances, and cosmetics.	(Sfara et al., 2009)

CONCLUSIONS

A higher percentage of sesquiterpenes was found in the *O. sanctum* n-hexane extract which might be used in the pharmaceutic industry, some compounds found in *O. sanctum.*, aerial parts are toxic such as phytol, which requires caution. To establish therapeutic uses of *O. sanctum* in modern medicine, scientists and researchers must study the pharmacological effects of different extracts on different body systems.

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