



# IJPPR

INTERNATIONAL JOURNAL OF PHARMACY & PHARMACEUTICAL RESEARCH  
An official Publication of Human Journals

ISSN 2349-7203




Human Journals

Research Article

February 2021 Vol.:20, Issue:3


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## GCMS Profile of Phyto-Compounds in *Cymbopogon martinii*



**IJPPR**  
INTERNATIONAL JOURNAL OF PHARMACY & PHARMACEUTICAL RESEARCH  
An official Publication of Human Journals

ISSN 2349-7203



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**Submitted:** 10 January 2021  
**Revised:** 30 January 2021  
**Accepted:** 19 February 2021



HUMAN JOURNALS

[www.ijppr.humanjournals.com](http://www.ijppr.humanjournals.com)

**Keywords:** *Cymbopogon martinii* Essential Oil (CMEO); Bioactive Compounds; GCMS

### ABSTRACT

Plant-Based Natural Products (PBNPs) have contributed significantly to the development of plant-based drugs. Studies indicate that *Cymbopogon martinii* essential oil (CMEO) extracts exhibit a wide range of biological activities. It is well known that the biological properties in palmarosa essential oil may be due to the presence of compounds like 4-Decent-6-yne, (Z), 2-Ethylimino-4-methyl-pent-3-enenitrile, Dihydrocarvyl acetate, 2-Methylbenzaldehyde, Geranyl butyrate, 1,5,9,9-Tetramethyl-1,4,7-cycloundecatriene. However, its application is limited because of the odor, color, and taste. Owing to widespread applications of Phyto-compounds in CMEO - GCMS analysis was performed and 20 bioactive compounds were detected. **Rational of the work:** *Cymbopogon martinii* essential oil (CMEO) extract is well known for a wide range of biological activity. To ascertain the functional role of the compounds we must understand the physio-chemical nature of the individual compounds. GCMS is expected to elucidate the composition, abundance, structure and function of components of CMEO.

## INTRODUCTION:

The genus *Cymbopogon* is widely distributed in the tropical and subtropical regions of Africa, Asia, and America. Comprised of 144 species, this genus is famous for its high content of essential oils (Avoseh et al., 2015). Studies have led to the isolation of alkaloids, volatile and non-volatile terpenoids, flavonoids, carotenoids, and tannins from every part of the *Cymbopogon* species. *Cymbopogon martinii* is a species of grass in the genus *Cymbopogon* (lemongrasses) native to India and Indochina but widely cultivated in many places for its aromatic oil. Generally known as Palmarosa, the plant has other common names include Indian geranium, ginger grass, rosha, and rosha grass. Besides, therapeutic application, it is commonly used as a condiment and food preservative. Palmarosa contains many bioactive molecules, Phyto-compounds, endowed with pharmacological activities, such as antimicrobial (Prashar et al., 2003). The essential oil of Palmarosa contains geraniol, which is valued for its scent and several traditional medicinal and household uses. Palmarosa oil is of commercial importance, being extensively used in perfumes, soaps, cosmetics, toiletry, and tobacco products (Raina et al., 2003). Palmarosa essential oil is an effective insect repellent when applied to stored grain and beans (Kumar et al., 2007) an antihelmintic against nematodes (Katiki et al., 2011), and an antifungal (Kalagatur et al., 2018) and mosquito repellent (Caballero-Gallardo et al., 2012). CMEO has been used in aromatherapy as a skin tonic due to its antimicrobial properties. It has also used in Ayurvedic medicine for skin problems and to relieve nerve pain. Immunomodulatory action CMEO (geraniol) was evaluated towards the production of pro-and anti-inflammatory cytokines (TNF- $\alpha$  and IL-10) by human monocytes in vitro. Data indicated that TNF- $\alpha$  production was not affected by CMEO and geraniol, at a concentration of 5  $\mu\text{g/ml}$  of CMEO stimulated its production. On the other hand, all concentrations of CMEO and geraniol tested, increased IL-10 production by human monocytes (Murbach Teles Andrade et al., 2014).

Essential oils (EOs) a major group of photogenic bioactive compounds (PBAC) has been used for a variety of purposes over thousands of years. Due to their strong aromatic properties and bioactive nature, EOs has been used in aromatherapy, as flavor and fragrances in cosmetics, foods, and more recently as pharmaceuticals, natural preservatives, additives, and biopesticides (Al-Shalah et al., 2020). EOs are a concentrated form of liquid mixtures of volatile compounds of plant origin with unique structural chemistry including terpenoid and non-terpenoid hydrocarbons and their oxygenated derivatives, with natural color, odor, and flavor, or “essence” of their source - volatile/ odoriferous oil. Essential oils are isolated from

various plant components such as leaves, fruit, bark, root, wood, heartwood, gum, balsam, berries, seeds, flowers, twigs, and buds (Chávez-González *et al.*, 2016). However, validating and using plants as phytopharmaceutical chemistry requires a great deal of basic and applied research, to set this resource at the same level of importance.

## **MATERIALS AND METHODS:**

### **Preparation and extraction of sample**

Protocol for preparation of sample was according to the methods previously described by Eleyinmi (2007), but with modifications wrt temperature and duration of drying the sample. A 100 g leaf was weighed and dried in an oven at 60°C. The dried sample was ground into powder using a Thomas-Willey milling machine and sieved on a wire mesh screen (3 × 3 mm<sup>2</sup>). The sample was stored at 4°C in an air-tight container with screw caps. The sample was prepared according to the methods previously described by Rašković *et al.*, (2015). 25 g of sample was suspended in 250 mL of distilled water in stoppered flasks and allowed to stand for 24 h, filtered with Whatman No 24 filter paper, concentrated in a rotary evaporator for 12 h at 50°C, and dried in a vacuum desiccator. The yield was calculated to be 6.06% w/w. The extract was suspended in ethyl acetate and subjected to GC-MS analysis.

### **GC-MS Analysis**

*Cymbopogon martini* (Palmarosa) Essential Oil was purchased commercially from the local market in Palani, Dindigul District, Tamil Nadu, India. Phyto-components were identified using GC-MS detection system as previously described Rašković *et al.*, (2015) but with minor modification, whereby a portion of the extract was analyzed directly by headspace sampling. GC-MS analysis was accomplished using an Agilent 7890A GC system set up with 5975C VL MSD (Agilent Technologies, CA, and the USA). The capillary column used was DB-5MS (30 m × 0.25 mm, film thickness of 0.25 µm; J&W Scientific, CA, USA). The temperature program was set as follows: initial temperature 50°C held for 1 min, 5°C per min to 100°C, 9°C per min to 200°C held for 7.89 min, and the total run time was 30 min. The flow rate of helium as a carrier gas was 0.811851 mL/min. MS system was performed in electron ionization (EI) mode with Selected Ion Monitoring (SIM). The ion source temperature and quadrupole temperature were set at 230°C and 150°C, respectively. Identification of phyto-components was performed by comparison of their retention times

and mass with those of authentic standards spectra using computer searches in NIST 08.L and Wiley 7n.l libraries.

## RESULTS AND DISCUSSION:

### GCMS analysis of *Cymbopogon martini* (Palmarosa) essential oil

The chemical composition of EOs depends on plant genetics, growth conditions, development stage at harvest, and processes of extracting active compounds. Different parts of the plant (bark, leaf, fruit and seed) have been extensively investigated for their bioactive phytochemical constituents in various plants (Ramya *et al.*, 2012). GC-MS analysis revealed that the extract of *Cymbopogon martini* contained different volatile oils (Fig. 1). 4-Decen-6-yne, (Z)- ( $C_{10}H_{16}$ ), 3.568 min, 10 hits; 2-Ethylimino-4-methyl-pent-3-enenitrile ( $C_8H_{12}N_2$ ), 3.913 min, 10 hits; Cyanogen bromide (CBrN), 4.024, 1 hits; Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1.alpha.,2.beta.,5.alpha.) - ( $C_{10}H_{18}O$ ), 4.503 min, 10 hits; Cyclohexa-1,3-diene, 5,6-diethyl- ( $C_{10}H_{16}$ ), 4.915 min, 10 hits; Benzaldehyde, 2-methyl- ( $C_8H_8O$ ), 8.154 min, 10 hits; Pyrazine ( $C_4H_4N_2$ ), 9.32, 5 hits; 2-Norbornaneacetic acid ( $C_9H_{14}O_2$ ), 9.378, 8 hits; cis-syn-trans-Tricyclo[7.3.0.0(2,6)]dodec-7-ene ( $C_{12}H_{18}$ ), 9.509 min, 10 hits; 1,2,4-Metheno-1H-indene, octahydro-1,7a-dimethyl -5-(1-methylethyl)-, [1S (1.alpha.,2.alpha.,3A. beta.,4.alpha.,5.alpha.,7A. be tA.,8S\*)]- ( $C_{15}H_{24}$ ), 9.913 min, 10 hits; 1,4,7-Cycloun-decatriene, 1,5,9,9-tetramethyl-Z,Z,Z- ( $C_{15}H_{24}$ ), 10.343 min, 10 hits; Naphthalene, decahydro-4a-methyl-1-methylene- 7-(1-methylethylidene)-, (4aR-trans)- ( $C_{15}H_{24}$ ), 10.738 min, 10 hits; Butanoic acid, 3,7-dimethyl-2,6-octadienyl ester,(E)- ( $C_{14}H_{24}O_2$ ), 11.772 min, 10 hits; Nerolidol 2 ( $C_{15}H_{26}O$ ), 11.948 min, 10 hits; Caryophyllene oxide ( $C_{15}H_{24}O$ ), 12.525 min, 10 hits; 2-Azidomethyl-1,3,3-trimethyl-cyclohexene ( $C_{10}H_{17}N_3$ ), 15.152 min, 10 hits; Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)- ( $C_{16}H_{28}O_2$ ), 15.423 min, 10 hits; Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)- ( $C_{16}H_{28}O_2$ ), 15.701 min, 10 hits; Farnesol, acetate ( $C_{17}H_{28}O_2$ ), 17.258 min, 10 hits; 2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (Z)- ( $C_{13}H_{22}O_2$ ), 20.158, 10 hits respectively (Table 1).

Biological activities of these secondary metabolites of *Cymbopogon martini* (Palmarosa) have been reported for its antitumor, antioxidant, anti-infectious, anti-inflammatory, and analgesic activities and effects on the central nervous system, endocrine system, disorders such as cardiac remodeling after myocardial infarction, body weight changes, dyslipidemia, cerebral ischemia, hepato-nephrotoxicity, stress, and anxiety. The anti-inflammatory activity of CMEO has been attributed to the presence and synergistic activity of carnosol and

carnosic, rosmarinic, ursolic, oleanolic, and micrometric acids (A). Specifically, anti-inflammatory activity has been attributed to synergic effects of ursolic and micrometric acids present in CMEO. These natural drugs can be proposed for preclinical and clinical studies in different diseases and pathological conditions.

## CONCLUSION:

*Cymbopogon* species have been used as a traditional medicine in many countries since antiquity. CMEO has been used in traditional and conventional medicine due to the pharmacological potential of their phytochemicals. *C. martini* (Palmarosa) contains a large variety of bioactive molecules with great therapeutic potential and biological activities such as insecticidal, anti-protozoan, anticancer, anti-HIV, anti-inflammatory, and anti-diabetes effects. CMEO has remarkable anti-inflammatory, antimicrobial, and antioxidant properties, which have been extensively reported in several formulations. However, the development of new formulations containing other less common CMEO extracts is warranted through trials to evaluate and establish the credentials of pharmacologically active Phyto-compounds towards safety and efficacy, in treating various pathological conditions.

## ACKNOWLEDGMENT

The author is grateful to the Management, Arulmigu Palaniandavar College of Arts and Culture, Palani - 624601, Dindigul District, Tamil Nadu, India for their support by providing the required facilities to carry out the research work.

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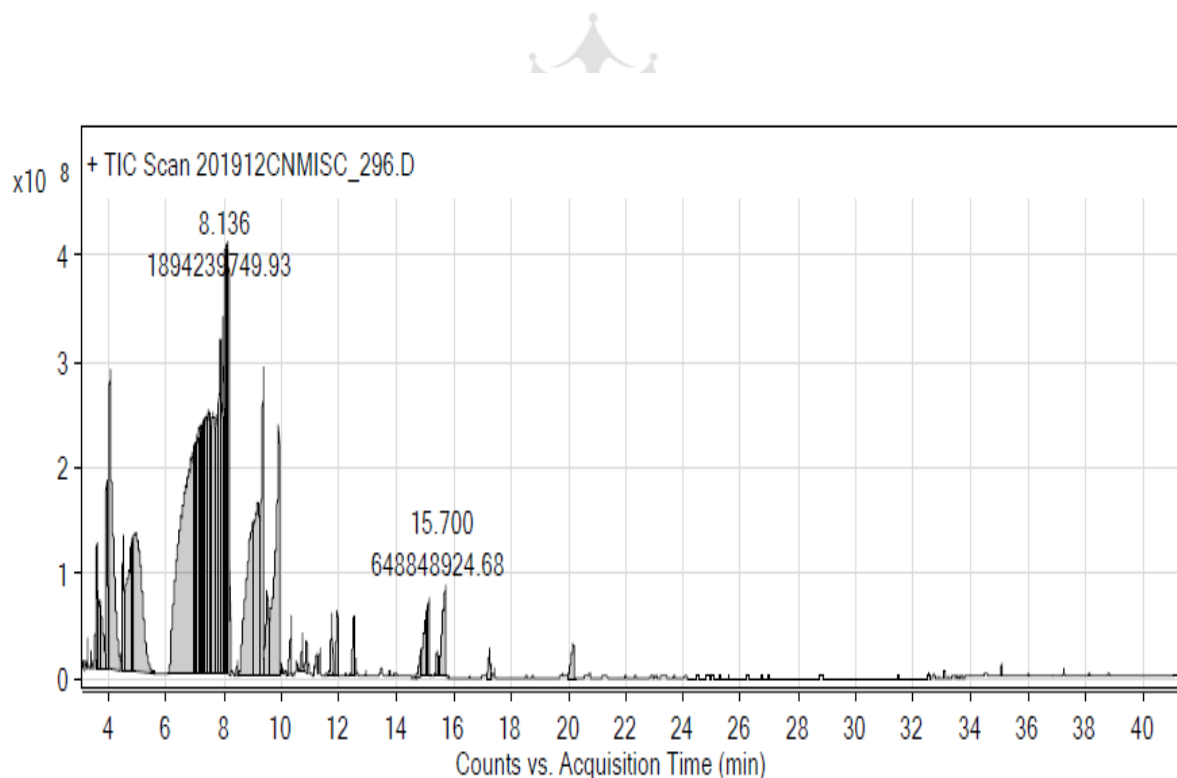


Figure No. 1 GCMS of *Cymbopogon martinii* essential oil

Table no 1: GC-MS based list of bioactive compounds in *C. martini* essential oil

RT	Name of the Compound	Molecular Formula	Hits (DB)
3.568	4-Decen-6-yne, (Z)-	C <sub>10</sub> H <sub>16</sub>	10
3.913	2-Ethylimino-4-methyl-pent-3-enenitrile	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>	10
4.024	Cyanogen bromide	CBrN	1
4.503	Cyclohexanol, 2-methyl-5-(1-methylethenyl)(1.alpha.,2.beta.,5.alpha.)-	C <sub>10</sub> H <sub>18</sub> O	10
4.915	Cyclohexa-1,3-diene, 5,6-diethyl-	C <sub>10</sub> H <sub>16</sub>	10
8.154	Benzaldehyde, 2-methyl-	C <sub>8</sub> H <sub>8</sub> O	10
9.32	Pyrazine	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	5
9.378	2-Norbornaneacetic acid	C <sub>9</sub> H <sub>14</sub> O <sub>2</sub>	8
9.509	cis-syn-trans-Tricyclo[7.3.0.0(2,6)]dodec-7-ene	C <sub>12</sub> H <sub>18</sub>	10
9.913	1,2,4-Metheno-1H-indene, octahydro-1,7a-dimethyl-5-(1-methylethyl)-, [1S-(1.alpha.,2.alpha.,3a.beta.,4.alpha.,5.alpha.,7a.beta.,8S*)]-	C <sub>15</sub> H <sub>24</sub>	10
10.343	1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z-	C <sub>15</sub> H <sub>24</sub>	10
10.738	Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethylidene)-, (4aR-trans)-	C <sub>15</sub> H <sub>24</sub>	10
11.772	Butanoic acid, 3,7-dimethyl-2,6-octadienyl ester,(E)-	C <sub>14</sub> H <sub>24</sub> O <sub>2</sub>	10
11.948	Nerolidol 2	C <sub>15</sub> H <sub>26</sub> O	10
12.525	Caryophyllene oxide	C <sub>15</sub> H <sub>24</sub> O	10
15.152	2-Azidomethyl-1,3,3-trimethyl-cyclohexene	C <sub>10</sub> H <sub>17</sub> N <sub>3</sub>	10
15.423	Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester,(E)-	C <sub>16</sub> H <sub>28</sub> O <sub>2</sub>	10
17.258	Farnesol, acetate	C <sub>16</sub> H <sub>28</sub> O <sub>2</sub>	10
20.158	2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate, (Z)-	C <sub>13</sub> H <sub>22</sub> O <sub>2</sub>	10