Int.J.Curr.Microbiol.App.Sci (2021) *10*(10): 283-290

International Journal of Current Microbiology and Applied Sciences
***ISSN: 2319-7706* Volume 10 Number 10 (2021)**
Journal homepage: http://www.ijcmas.com

Original Research Article https://doi.org/10.20546/ijcmas.2021.1010.034

GC-MS Analysis of Bioactive Compounds in Lemongrass (*Cymbopogon citratus*) Powder

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Keywords

Bioactive compound, Chromatography, GC/MS, Lemongrass, Phytocompound

Article Info

Accepted:
10 September 2021
Available Online:
10 October 2021

A B S T R A C T

The bioactive components of lemongrass powder have been evaluated using GC-MS. The GC-MS analysis was performed on GC-MS comprising an automatic liquid sampler and agilent gas chromatograph interfaced to mass spectrometer (GC-MS). Interpretation of the mass spectrum GC-MS was conducted using the database of National Institute Standard and Technology (NIST). The compound bioactivity prediction is based on Dr. Duke's phytochemical and ethnobotanical Database. GC/MS analysis of methanolic extract of lemongrass leaves revealed the existence of Pentane, 2,4-Dimethyl, Dodecanoic acid tert-butyl ester, 2,6 Bis (1,1-dimethylethyl)-4-[(4-chloro-6-(3,5, bis (1,1-dimethylethyl)-4- hydroxyanilino)-1,3,5-triazin-2-yl)amino]phenol and 3-Formyl-4,5-dimethyl-pyrrole. The presence of these compounds in the plant extract may at least be responsible for the pharmacological properties of *Cymbopogon citratus* and thus recommended as plant of phytopharmaceutical importance.

Introduction

Medicinal plants are source of a great economic value. Plant herbs are naturally gifted at the synthesis of medicinal compounds. Medicinal plants are used in herbalism and known for their medicinal properties. Medical Plant constitutes an important therapeutic aid in alleviating ailments. The traditional medicine or medicinal plants are used at normative basis for maintenance of good health in developing countries (UNESCO, 1996). The extraction and characterization of bioactive compounds

from medicinal plants have resulted in the discovery of new drugs with high therapeutic value. Treatment using medicines of natural origin is gaining momentum nowadays on account of increasing concern about potentially harmful synthetic additives (Reische, 1998). *Cymbopogan citratus* is a great interest due to its commercially valuable essential oils and widely used in food technology as well as in traditional medicine. Due to increased demand of natural products from medicinal plants in healthcare serves worldwide, herbal plant producers have commenced the use of different extraction methods in order to see and detach the chemical compounds present in them (Achi and Ohaeri, 2015). The main intent of detection of phytocompound in plants is to arrive at the therapeutically desired active portion/fraction and to purge superfluous materials (Waldesch *et al.*, 2003). An exceptional facet of advanced plants is their competence to manufacture various organic chemicals of high structural density (Achi and Ohaeri, 2015). The awareness of the chemical constituents of plants is not only advantageous for discovery of curative agents but also for disclosing new sources of important economic phytocompounds for the synthesis of complex chemical substances and for discovering the actual significance of folklorica (Uraku *et al.*, 2015).

The aim of this study is to determine the organic compounds present in the *cymbopogon citratus* powder with the aid of GC-MS technique, which may provide an insight in its use in traditional medicine.

Materials and Methods

Collection and identification of plant material

Fresh leaves of *Cymbopogon citratus* were collected and authenticated from Department of Botany, Vasantrao Naik Marathwada Krishi Vidyapeeth, Parbhani (India).

Preparation of plant material

The leaves of *Cymbopogon citratus* were sorted, washed thoroughly with distilled water to remove dirt and debris, cut into smaller pieces before these was cabinet dried for 5 hrs at 45^0C temperature. The dried leaves were pulverized into fine powder. The powdered materials were stored in air tight polyethene bags protected from direct sunlight until required for use.

Preparation of lemongrass leaves extract

The extraction of leaves was carried out with slight modification in method given by Uraku, (2015). Forty grams of the powdered leaves were extracted with 100 mL of 40% methanol overnight in a stopped bottle and with occasional stirring at room temperature (28 ± 3^0C). The sample was first sieved using muslin cloth and then filtered using Whatman No. 1 filter paper. This process was repeated three times. The filtrate was concentrated under reduced pressure at 40^0C for 45 min in a rotary vacuum evaporator and then lyophilized to get a brown aromatic solid extract. The dry extract obtained was kept in a refrigerator at 4°C until required for use.

GC-MS analysis

The GC-MS analysis was done with modification in the method given by Uraku (2015) and Thenmozhi and Rajan (2015). The analysis was performed at Sophisticated Analytical Instrument Facility (SAIF), Indian Institute of Technology (IIT), Bombay.

The GC-MS analysis was performed on GC-MS (Model: The AccuTof JMS-T100GCV, JEOL ltd., Tokya, Japan) comprising an automatic liquid sampler and agilent gas

chromatograph interfaced to mass spectrometer (GC-MS). The instrument has EI ion source, low acceleration ion-transfer system, reflection type TOF analyser, dual micro channel plate ion detector and the ventilation facility for rotary pump.

The instrument is equipped with capillary column (Rxi-5 ms, manufactured by Restek Corporation, Bellefonte, Pennsylvania, US) of 60 m length, 0.25 mm diameter and 0.25 µm thickness. For GC-MS detection, an electron ionization system was used with ionization energy of 70 eV. Helium was the carrier gas, at a flow rate of 1 ml/min and an injection volume of 0.5 µI was employed (split ratio of 10:1). The injector and MS transfer line temperature were set at 220 and 290^{0}C respectively.

The oven temperature was programmed from 80^{0}C (isothermal for 3 min) with an increase of at 8^{0}C/min to 200^{0}C, increasing at 8^{0}C/min (isothermal for 3 min) reached to 275^{0}C, then 5^{0}C/min to 280^{0}C, ending with 5 min isothermal at 280^{0}C. Mass spectra were taken at 70 eV, a scan interval of 0.5 sec and fragments from 50 to 500 m/z. The total running time of GC-MS was 31 min.

Identification of components

Interpretation of the mass spectrum GC-MS was conducted using the database of National Institute Standard and Technology (NIST) having more than 62,000 patterns. The fragmentation pattern spectra of the unknown components were compared with those of known components stored in the NIST library (NIST, 2010).

The compound bioactivity prediction is based on Dr. Duke's phytochemical and ethnobotanical Database (Duke, 2014). The relative percentage amount of each phyto-component was calculated by comparing its average peak area to the total area. The name, molecular weight and structure of the components of the test materials were ascertained.

Results and Discussion

Four compounds were identified in lemongrass powder by GC-MS analysis. The retention time (RT), retention value, molecular formula and molecular weight were presented in Table 1.

In the present research study, the GC-MS analysis of methanol extract of lemongrass (*Cymbopogon citratus*) revealed that the lemongrass contained a wide range nutraceutical compounds which may be responsible for its therapeutic potential.

The identified phytocompounds comprise mainly hydrocarbons, fatty acids, alcohol, esters and phenols. Among the compounds present in the lemongrass extract include, Pentane 2,4-Dimethyl, Dodecanoic acid tert-butyl ester, 2,6 Bis (1,1-dimethylethyl)-4-[(4-chloro-6-(3,5, bis (1,1-dimethylethyl)-4-hydroxyanilino)-1,3,5-triazin-2-yl)amino] phenol and 3-Formyl-4,5-dimethyl-pyrrole.

The GC-MS method confirms that lemongrass powder contain Pentane, 2,4-Dimethyl, Dodecanoic acid tert-butyl ester, 2,6 Bis (1,1-dimethylethyl)-4-[(4-chloro-6-(3,5, bis (1,1-di methylethyl)-4- hydroxyanilino)-1,3,5-triazin-2-yl) amino]phenol and 3-Formyl-4,5-dimethyl-pyrrole.

The biological activities listed (Table 2) are based on Dr. Duke's Phytochemical and Ethnobotanical Databases by Dr. Jim Duke of the Agricultural Research Service (2013). The pentane, 2,4-Dimethyl were obtained at 6.22 min retention time by GC-MS analysis of lemongrass has retention value 589 iu.

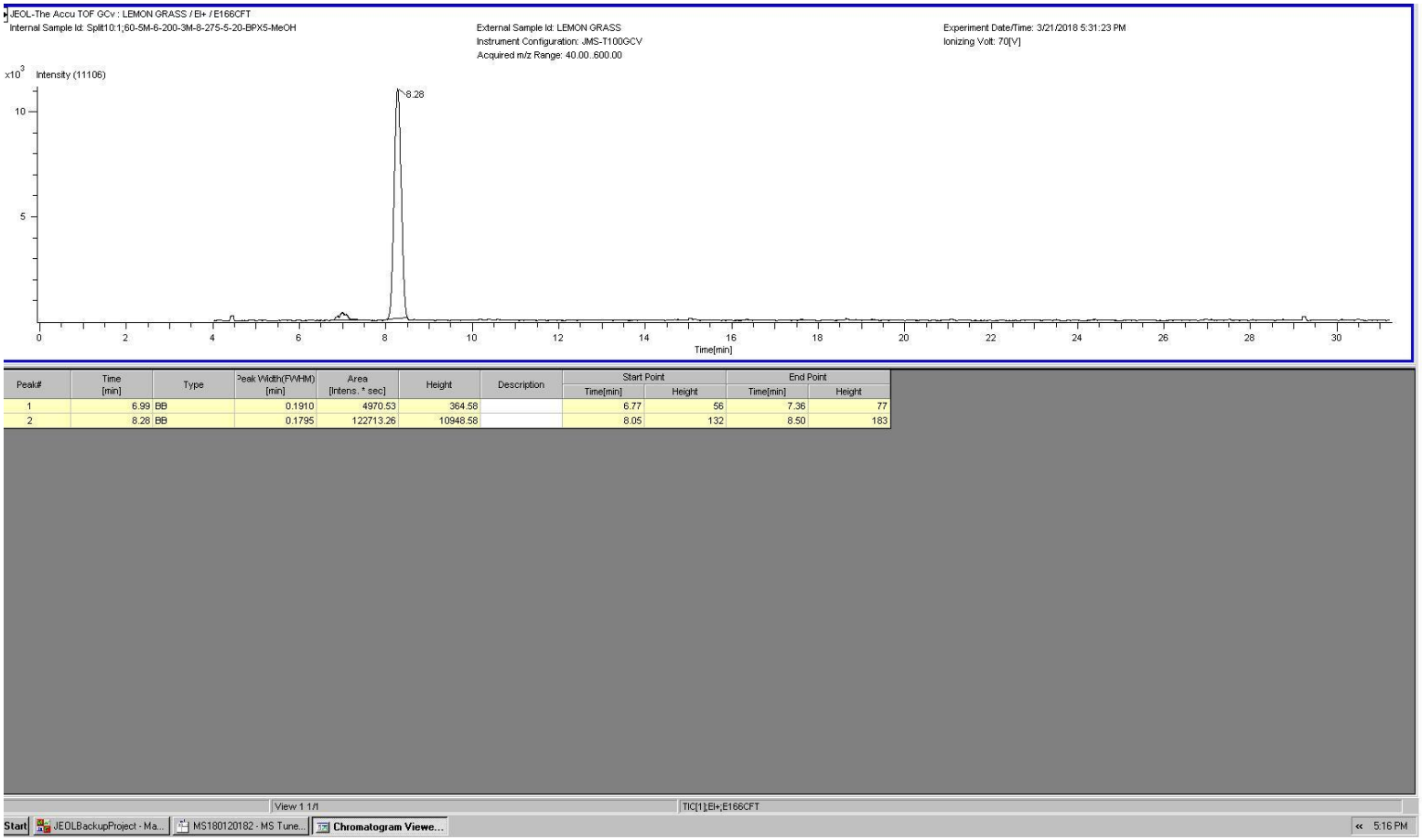
Table.1 GC-MS analysis of lemongrass (*Cymbopogon citratus*) extract

Peak#	Compound Name	Retention time (min)	Retention value (iu)	Molecular formula	Molecular weight (g/mol)
1	Pentane, 2,4-Dimethyl	6.22	589	C_7H_{16}	100.205
2	Dodecanoic acid tert-butyl ester	8.28	1694	$C_{16}H_{32}O_2$	256.43
3	2,6 Bis (1,1-dimethylethyl)-4-[(4-chloro-6-(3,5, bis (1,1-dimethylethyl)-4- hydroxyanilino)-1,3,5-triazin-2-yl)amino]phenol	15.05	4361	$C_{31}H_{44}CIN_5O_2$	553
4	3-Formyl-4,5-dimethyl-pyrrole	29.24	1167	C_7H_9NO	123

Table.2 Biological activity of lemongrass components identified by GC-MS

Name of the Compound	Type of Compound	Biological Activity
Pentane 2,4-Dimethyl	Alkane	Anticancer
Dodecanoic acid tert-butyl ester	Ester	Antiashtmatics, antipruritics, antipsoriatics, flavour
2,6 Bis (1,1-dimethylethyl)-4-[(4-chloro-6-(3,5, bis (1,1-dimethylethyl)-4-hydroxyanilino)-1,3,5-triazin-2-yl)amino]phenol	Phenol	NF
3-Formyl-4,5-dimethyl-pyrrole	Carboxyaldehyde	NF

Fig.1 Chromatogram (Major peaks) obtained from GC-MS analysis of lemongrass (*Cymbopogon citratus*) extract

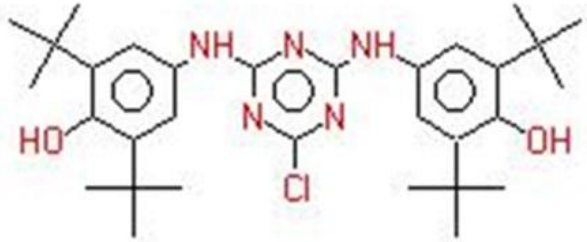


Peak#	Time [min]	Type	Peak Width(FWHM) [min]	Area [Intens. * sec]	Height	Description	Start Point		End Point	
							Time[min]	Height	Time[min]	Height
1	6.99	BB	0.1910	4970.53	364.58		6.77	56	7.36	77
2	8.28	BB	0.1795	122713.26	10948.58		8.05	132	8.50	183

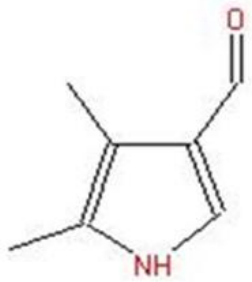
Fig.2 Molecular structure of nutraceutical compounds obtained by GC-MS from lemongrass (Cymbopogon citrates) extract

Pentane, 2,4-Dimethyl

Dodecanoic acid tert-butyl ester



2,6 Bis (1,1-dimethylethyl)-4-[(4-chloro-6-(3,5, bis (1,1-dimethylethyl)-4- hydroxyanilino)-1,3,5-triazin-2-yl)amino]phenol



3-Formyl-4,5-dimethyl-pyrrole

The molecular formula is C_7H_{16} and molecular weight is 100.205 g/mol. It is also known as 2,4-Dimethypentane. It was found that pentane 2,4-penatne has anti-cancerous activity.

The dodecanoic acid tert-butyl ester were obtained by GC-MS analysis of lemongrass extract. The retention time and value for this compound were 8.28 min and 1694 iu. The molecular formula is $C_{16}H_{32}O_2$ with molecular weight 256.43 g/mol. It is also known as dodecanoic acid 1,1-dimethylethylester, lauric acid tert-butyl ester, tert-butyl dodecanoate and tert-butyl laurate. It has antiashtmatics, antipruritics, antipsoriatics and flavour activities.

The phenolic compound 2,6 Bis (1,1-dimethylethyl)-4-[(4-chloro-6-(3,5, bis (1,1-dimethylethyl)-4-hydroxyanilino)-1,3,5-triazin-2-yl)amino]phenol was obtained at retention time 15.05 min has retention value 4361 iu. The molecular formula is $C_{31}H_{44}CIN_5O_2$ with having molecular weight 553 g/mol. There is no synonym were found and also there is no any evidence for its biological activities.

The 3-formyl-4,5-dimethyl-pyrrole was obtained at retention time 29.24 min with retention value 1167 iu from GC-MS analysis of lemongrass extract. The molecular formula is C_7H_9NO with molecular weight 123 g/mol.

The GC-MS analysis of lemongrass (*Cymbopogon citratus*) confirms the presence of enlisted nutraceutical compounds which aid medicinal, nutraceutical and therapeutic value. The presence of these compounds were not identified in the past research studies except n-hexadecanoic acid in lemongrass extract (Uraku, 2015). Most of the studies were conducted on the lemongrass essential oil to isolate and characterize the bioactive compounds.

The GC-MS analysis revealed that the leaf extract of *Cymbopogon citratus* contained Pentane, 2,4-Dimethyl, Dodecanoic acid tert-butyl ester, 2,6 Bis (1,1-dimethylethyl)-4-[(4-chloro-6-(3,5, bis (1,1-dimethylethyl)-4-hydroxyanilino)-1,3,5-triazin-2-yl) amino] phenol and 3-Formyl-4,5-dimethyl-pyrrole. The presence of these phytocompounds may be responsible for its popular use in treatment of numerous diseases by traditional users.

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How to cite this article:

Pradeep P. Thorat, Nikhil D. Solanke and Jayashri D. Ughade. 2021. GC-MS Analysis of Bioactive Compounds in Lemongrass (*Cymbopogon citratus*) Powder. *Int.J.Curr.Microbiol.App.Sci.* 10(10): 283-290. doi: https://doi.org/10.20546/ijcmas.2021.1010.034