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Identification of the Phytocomponents in *Cymbopogon citratus* Methanol Extract by Gas Chromatography-Mass Spectrometry

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Abstract-*Phytocomponents in methanolic extract of Cymbopogon citratus leaf was studied using GC MS analysis. 5 compounds were identified from the extract. The most abundant compounds were, Dimercaprolwith[RT: 22.727, Peak area: 44.88 % and Molecular formula: $C_3H_8OS_2$]. Pentafluoropropanoyl with [RT: 21.942, Peak area: 34.16% and Molecular formula: $C_{14}H_8F_{10}O_4$] with an unknown bioactivity and Palmitic acid with [RT: 19.950, Peak area: 14.14 % and Molecular formula: $C_{16}H_{32}O_2$] which presented an antioxidant property. Other phytocompounds identified by GCMS but at different lower concentrations were 5-Chloropyrimidin-2-amin with [RT: 19.331, Peak area: 5.02 % and Molecular formula: $C_4H_4ClN_3$]and 3-Chloropyridin-2-ol with [RT: 18.375, Peak area: 1.80% and Molecular formula C_5H_4ClNO]. The bioactive compounds in the methanol leaf extract of Cymbopogon citratus leaf demonstrated phytopharmacological action and hence could be of clinical use against some ailments.*

Keywords: Dimercaprol, GCMS, *Cymbopogon citratus*, Antioxidant.

1. INTRODUCTION

Plant is a major source of drug and research has shown that they are safe and therefore have little or no adverse effects and less development of drug resistance observed in synthetic drugs. Hence there is need to rely more on plants as source for treatment. The use of plants for the treatment of various diseases and the major phyto-components responsible for these therapeutic activities should be identified and documented. *Cymbopogon citratus* popularly known as lemon grass belongs to the family of Poaceae. It is a perennial grass having slender edge with pointed apex. It is mostly found in the tropical region [1]. *Cymbopogon citratus* oil has demonstrated both antibacterial and antifungal agents[2] and its extracts also reported to have antifungal, antibacterial and antiviral activities [3]. Most people in Nigeria use it to solve stomach problems and typhoid fever[4].

The essential oil from *Cymbopogon citratus* has the strength to inhibit microbial growth in food such as *Staphylococcus aureus* and *Escherichia coli*. The antioxidant activity of its oil can be compared with alpha-tocopherol which is known to demonstrate strong antioxidant activity[5]. Previous researches conducted on the essential oil of *Cymbopogon citratus* showed that its antimicrobial compound to the citronel and geranoil acetate [6][7]. In Ohafia town in Nigeria, it is popularly consumed as an aromatic drink for making tea. *Cymbopogon citratus* has also been found to be effective in the treatment of feverish condition and as a relaxant and sleep aid, and an antidepressant [8].

This study is therefore designed to find out the phytochemicals in methanol extract of *Cymbopogon citratus* by GC-SM analysis and to determine the phytochemicals responsible for the claimed effect on the inhibition microbial growth.

2. MATERIAL AND METHODS

2.1 Plant Materials

Fresh leaves of *Cymbopogon citratus* was harvested at Owerri town in Imo State, Nigeria. The plant leaves were identified by Prof M C Dike at the Taxonomy section of College of Natural Resources and Environmental Management, Michael Okpara University of Agriculture, Umudike, Nigeria.

Figure 1 shows picture of *Cymbopogon citratus* harvested in Owerri town in Nigeria

2.2 Preparation of Plant Extract

The plant material of *Cymbopogon citratus* was collected from wild, shade dried for 10 days and pulverized to powder using mechanical grinder. The plant extract was prepared using Soxhlet method described by [9]. Thirty five grams (35 g) of powdered sample was introduced into the extraction chamber of the Soxhlet extractor using methanol as solvent. Temperature was maintained at 70° C throughout the extraction period of 48 hrs. At the end of the extraction period, the extract was concentrated using oven at 35° C to obtain dried extract which was sent for GCMS analysis.

2.3 GCMS analysis of *Cymbopogon citratus*

The characterization of the Phytochemicals in *Cymbopogon citratus* was done using GC-MS QP2010 Plus (Shimadzu, Japan). The identification of the phytochemicals in the sample was carried out using a QP2010 gas chromatography with Thermal Desorption System, TD 20 coupled with Mass Spectroscopy (Shimadzu). The ionization voltage was 70eV. Gas Chromatography was conducted in the temperature programming mode with a Restek column (0.25 mm, 60 m, XTI-5).The initial column temperature was 80°Cfor 1min, and then increased linearly at 70°C min^{-1} to 220°C, held for 3 min followed by linear increased temperature 10°C min^{-1} to 290°C for 10 min. The temperature of the injection port was 290°Cand the GC-MS interface was maintained at 290°C .The sample was introduced via an all-glass injector working in the split mode, with helium carrier gas low rate of 1.2 ml min^{-1}. The identification of compounds was accomplished by comparison of retention time and fragmentation pattern, as well as with mass spectra of the GC-MS.

2.4 Identification of Phytocomponents in Cymbopogoncitratus

GC-MS Chromatogram of *Cymbopogon citratus* revealed five peaks showing that five different compounds were present.

Identity of the active components in the extractwas done by comparison of their retention indices, peak area percentage and mass spectra fragmentation pattern with those stored in the database of National Institute of Standards and Technology (NIST) and also with published literature, NIST08.LIB[10], WILEY8.LIB[11], PESTEI-3.LIB and FA-ME.LIB library sources were used for matching the identified components from the plant material. The name, molecular weight, formula, structure and bioactivities of the compounds were ascertained.

3. RESULTS AND DISCUSSION

3.1 Results

GCMS chromatogram of the ethanolic extract of *Cymbopogon citratus* Figure 2 showed five peaks which indicated the presence of five phytochemicals constituents.

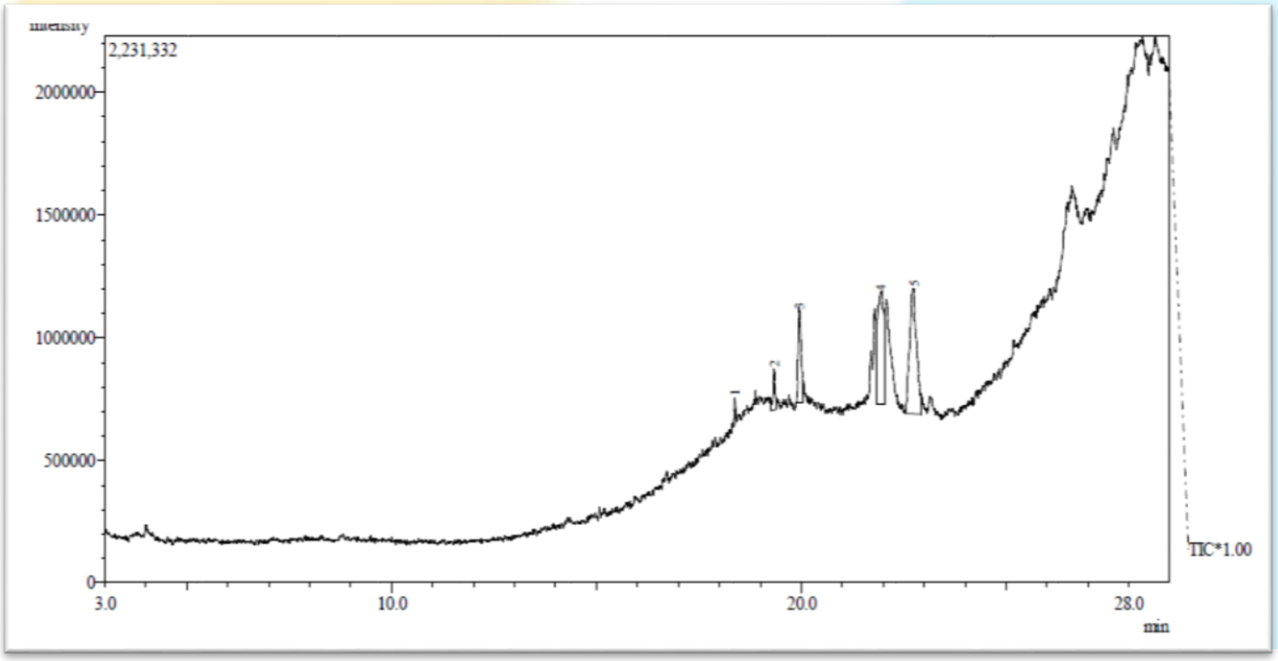


Figure 2 Shows the chromatogram of *Cymbopogoncitratus*

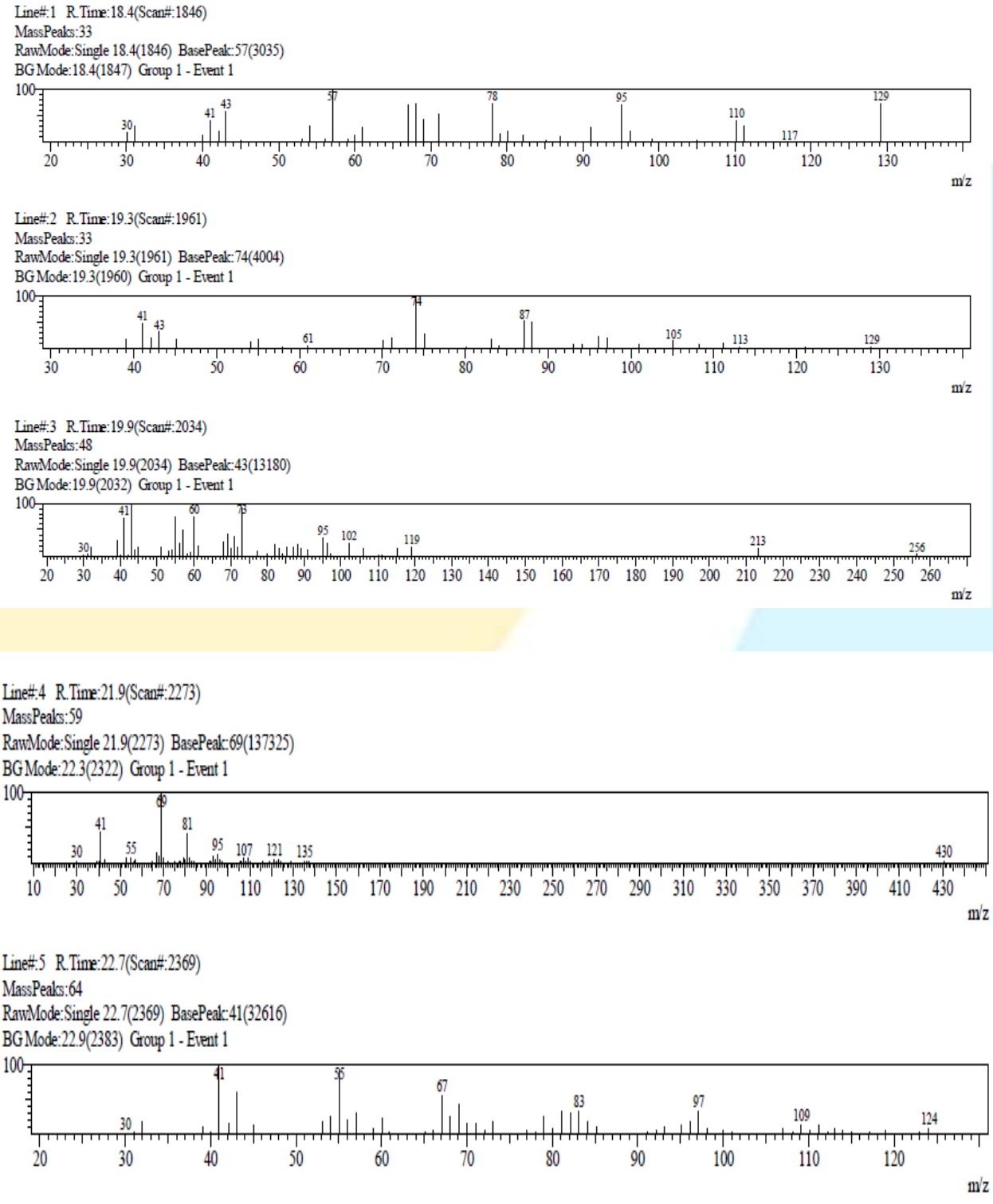
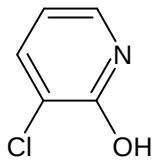
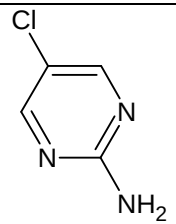
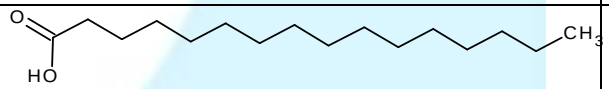
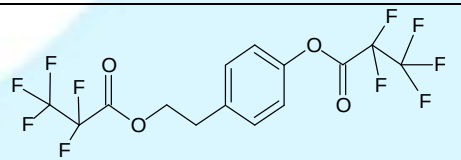
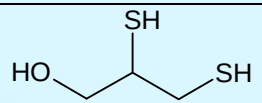


Figure 3 Shows the mass spectra of the five phytocompounds identified by GCMS analysis in *Cymbopogon citratus*

Table 1 Shows results of GCMS phytocompound analysis of *Cymbopogoncitratus*

S.No	Name of Compound	Retention time	Peak area %	Molecular weight	Molecular formular	Molecular structure	Bioactivity
1	3-Chloropyridin-2-ol	18.375	1.80	129.54	C_5H_4ClNO		EGFr, epidermal growth factor receptor
2	5-Chlorpyrimidin-2-amin	19.331	5.02	129.54	$C_4H_4ClN_3$		PDGFrb, platelet derived growth factor receptor kinase
3	n-Hexadecanoic acid or Palmitic acid	19.950	14.14	256.42	$C_{16}H_{32}O_2$		Mild antioxidant and anti-atherosclerotic activity [12]
4	4-{2-[(2,2,3,3,3-Pentafluoropropanoyl)oxy]ethyl}phenyl pentafluoropropanoate	21.942	34.16	430.19	$C_{14}H_8F_{10}O_4$		Unknown
5	Dimercaprol2,3-(disulfanylpropan-1-ol)	22.727	44.88	124.22	$C_3H_8OS_2$		Antidote

3.2 Discussion

From the gas chromatography-mass spectrometry (GCMS) analysis of *Cymbopogon citratus* methanolic extract, 5 phytocomponents were identified. The chromatogram of *Cymbopogon citratus* shown in Figure 1 had five peaks indicating the presence of five phytocomponents in the extract. Table 1 shows the name, retention time, peak area percentage, molecular weight, molecular structure and bioactivity of the phytocomponents. The most abundant compounds were, Dimercaprol with Retention time 22.727, Peak area44.88 % and Molecular formula $C_3H_8OS_2$ which had antidote activity. Dimercaprol is used as a chelating therapy in metal toxicity which is associated with heavy metal poisoning for example, poisoning by Arsenic, mercury, gold, lead and antimony [13]. In psychosis associated with lead poisoning, dimercaprol a phytocompound in *Cymbopogon citratus* could be a pharmaceutical remedy for its control. Furthermore, in Wilson disease which is a genetic disorder in which the body retains copper, dimercaprol has been used as an antidote [14]. Pentafluoropropanoyl with [RT:21.942, Peak area: 34.16% and Molecular formula $C_{14}H_8F_{10}O_4$] with an unknown bioactivity but had a similar compound named Pentafluoropropionic acid (PFPA) which is a metal free catalyst that efficiently catalyzes a three-component reaction of aromatic aldehyde, malononitrile, and dimedone to yield tetrahydrobenzo[b]pyran derivatives in high yields which is known to have a wide variety of biological actions such as anticancer, anticoagulant, diuretic and spasmolytic actions [15]. Moreover, this phytocompound Pentafluoropropanoyl we identified with GCMS in our extract had fluorine in its substituent R^1 and R^2 branches indicating that it may have some antibacterial action since most halogens have antibacterial activity. Palmitic acid which was also identified by GCMS analysis in our extract with Retention time 19.950, Peak area: 14.14 % and Molecular formula $C_{16}H_{32}O_2$ presented an antioxidant property especially when combined with retinol to form retinylpalmitate which has an antioxidant activity and could serve as a source of vitamin A [16]. The compound 5-Chloropyrimidin-2-amin was also identified by GCMS with Retention time 19.331, Peak area 5.02 % and Molecular formula $C_4H_4ClN_3$ as one of the phytocompounds in the extract with a bioactivity as a Platelet Derived Growth Factor receptor kinase (PDGFrb). A related compound 2-Amino-5-Chloropyridine was found to be used to produce herbicides and the drug Zopiclone, therefore 5-Chloropyrimidin-2-amin may have such action. 3-Chloropyridin-2-ol also identified by GCMS with [RT: 18.375, Peak area: 1.80% and Molecular formula C_5H_4ClNO] as one of the phytocompounds in the extract with a bioactivity as Epidermal Growth Factor receptor (PGFr).

4. CONCLUSION

From GCMS analysis *Cymbopogon citratus* methanol leaf extract contain five major bioactive compounds in their various concentrations. The major components were, Dimercaprol with peak area of 44.88 % which had antidote activity followed by Pentafluoropropanoyl with peak area 34.16 % but with an unknown bioactivity and Palmitic acid with peak area of 14.14 %.

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