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(RESEARCH ARTICLE)

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Density functional theory study, extraction and characterization of lemon grass oil (*Cymbopogon citratus*) as antimalaria repellant

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Abstract

Malaria is a life threatening disease, it is caused by female Anopheles Mosquitoes and it is a problem in several areas of the world especially Africa. Control of mosquitoes is something of utmost importance in the present day with rising number of mosquito borne illnesses. Thus, specialty products like mosquito repellent used to combat mosquitoes are required.The main objective of the work was to extract, characterize and take theoretical study of the active ingredient in *Cymbopogon citratus* leave and to formulate a mosquito repellent cream naturally obtained from medicinal plants.. The formulation of cream have smooth texture with a pH 7.20 which is non-irritant and suitable for the skin. The efficacy of the extract of Lemon grass (*Cymbopogon citratus*) was investigated on mosquito in this research using different concentrations of the oil extract. The cream with the highest concentration of the active ingredient extracted was found to be most effective in repelling mosquitoes.The oil samples extracted were analyzed to evaluate its quality by determined its chemical constituents through GC-MS. The main components detected in the Lemongrass (*Cymbopogon citratus*) essential oil were Citral, β-mycrene and β-Thujene. And Fourier transform infrared spectroscopy (FTIR) analysis (functional group determination) were also performed for the samples. Computational techniques using DFT at the B3LYP/6-31G* basis level was used to compare their reactivity and stability based on some theoretically calculated parameters. Quantum chemical calculations reveal total energy, dipole moment,large energy gap between the LUMO and HOMO of the constituent lemon grass oil indicating a theoretically significant interaction.It was proved that lemongrass oil cream provide good resistance against mosquito bites and also concluded that this process is one of eco-friendly.

Keywords: Density Functional Theory (DFT); Lemon Grass Oil; Extraction; Malaria; Oleic Acid; Palmitic Acid; Mosquito Repellant

1. Introduction

Malaria is a life threatening disease, it is caused by female Anopheles Mosquitoes and it is a problem in several areas of the world especially Africa. Mosquitoes are a serious threat to public health transmitting several dangerous diseases for over two million people in the tropics.. Deforestation and industrialized farming are also two of the factors causing an alarming increase in the range mosquitoes [1]. Mosquitoes need to be eradicated using the right tools and with a little bit of effort.The mosquitoes are horrific they're highly aggressive, you can be bitten hundreds of times without protection, its torture, impossible to bear. Many species in the plant kingdom synthesize a variety of secondary metabolites which play a vital role in defense of plants against insects/mosquitoes. Plants may be alternative source for mosquito repellent agents since they constitute a rich source of bioactive chemicals [2, 3] .Plant products can be used,

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either as an insecticide for killing larvae or adult mosquitoes or as repellents for protection against mosquito bites, depending on the type of activity they possess [4] . At present, the personal protective measures are taken from mosquito bites through applying mosquito repellant as skins lotions, coils, creams, and liquidators are providing limited support [5]. Coating of suitable mosquito repellant over the clothing is an innovative method to avoid mosquito bites as the large portion of human body is coved [6].The plant lemon grass oil (*Cymbopon citratus* oil) can be used to exterminated mosquitoes.

Lemon grass *(Cymbopogon citratus*) is an aromatic plant belonging to the *Gramineae* family [7]. it is tall, clumped perennial grass growing to a height of 1m. The leaf-blade is linear, tapered at both ends and can grow to a length of 50 cm and width of 1.5 m [8]. The leaf-sheath is tabular in shape and acts as a pseudostem. They also produces flowers at matured stages of growth [9]. The lemon grass Essential oil comes from the leaves of the lemon grass plant (*Cymbopogon citratus* plant). The oil has a light and fresh lemony smell with earthy undertones. They were formed by varied and complex volatile mixtures of chemical compounds, with predominance of terpene associated to aldehyde, alcohols and ketone which were deposited in various structure of plant [10]. lemon grass contains mainly citral [11] and 1 to 2 % essential oil on a dry basis [12]. They are used medicinally and others as insect repellant (citronella). This research work is to extract, characterize and take theoretical study of lemon grass oil as antimalaria repellant. This Lemon grass oil can be incorporated into cream and fabrics like night wear, bed sheet and bed net as a repellant.

2. Material and methods

2.1. Quantum Chemical Calculation

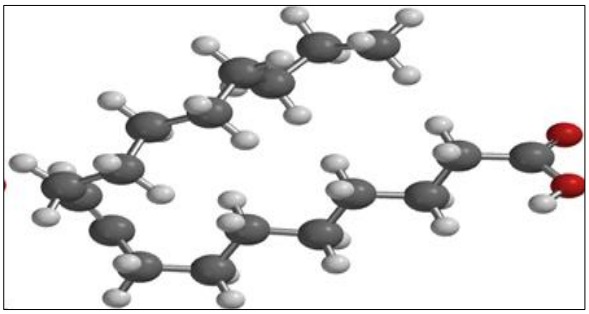

Figure 1 (i) Optimized structure of oleic acid using DFT at the B3LYP/6-31G* basis set level

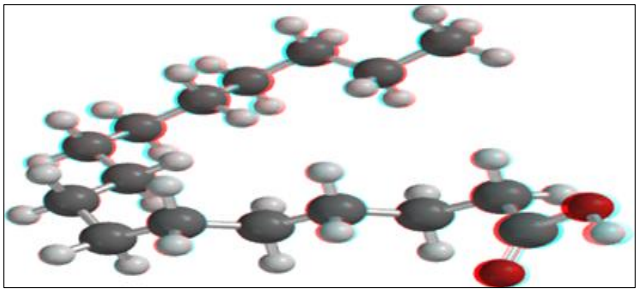

Figure 1 (ii) Optimized structure of palmitic acid using DFT at the B3LYP/6-31G* basis set level

Quantum chemical calculation methods are now extensively utilized to help explain trends in experimental results. The conceptual density functional theory (DFT) is one of the important tool in quantum chemistry that has been accurately used to understand the reactivity and selectivity of molecules [13].All the computations were performed with Spartan 20 programs by wave function Inc. DFT calculation was carried out on Lemon grass oil constituent (trans13-octadecenoic acid or oleic acid and n- hexadecanoic acid or palmitic acid) structure and optimized with the Becke's three parameter exchange functional along with the Lee– Yang–Parr non-local correlation functional (B3LYP) and 6-31G*

basis set in vaccum [14,15]. The molecular properties of the descriptors estimated include Homo-Lumo energy gap, total energy, dipole moment, electronegativity (χ), hardness (η), softness(S), etc were calculated.

2.2. Experimental Methods

2.2.1. Extraction of Lemongrass Oil

Fresh leaves of lemon grass (*Cymbopogon Citratus*) were collected in Ado-Ekiti, Nigeria, sliced and grinded into fine powder. Two hundred grams (200 g) of grinded leaves were placed in a porous thimble, for oil extraction using the Soxhlet extraction method, with n-Hexane solvent.About 17.60 ml of oil, weighing 9.76 g, was extracted and stored in the refrigerator for 4^{o}C.

2.3. Cream production

Cream production involve two phases:

- Water soluble phase
- Oil soluble phase

In water soluble phase, distilled water of 30 ml was put in a beaker and heated to the boiling point and stirred in 0.5 ml of Borax for about 5 mins.

For the oil soluble phase, 20 ml of mineral oil, 10ml vitamin E oil, 8 g Beeswax, 10 g petroleum jelly, and 10 ml lanolin were mixed together in beaker and heated gently on water bath for about 5 mins with continuously stirring to avoid.

The mixtures of water soluble phase was added gently into the beaker that contained the oil soluble phase and stirring continuously, the oil soluble phase turned white immediately to show the emulsification reaction, and it cooled to solidified in a ice water bath.

2.4. Mosquitoes Repellency Test

The prepared cream was portioned into six containers with lids with different concentration of the lemon grass oil extract. Container A,B, C,D, E consist of 0.5,1.0,1.5,2.0, 2.5ml of the lemon grass oil extract and the F container served as the control experiment. The experiment was done in the night to ensure availability of mosquitoes.

2.5. Fourier Transform Infrared Spectroscopy (FTIR) Analysis

Fourier transform infrared spectroscopy spectrum of *Cymbopogon citratus* extract (oil) was obtained using FTIR spectrophotometer (Perkin Elmer). FTIR used for chemical identification as each molecule and chemical structure creates a unique spectra. The IR spectra were accounted in % transmittance. The wave number region for analysis was 4000–400 cm-1 (mid-infrared range.) with resolution of 0.15 cm-1.

2.6. Gas chromatography-mass spectrometry (GC-MS) analysis

The extract of *Cymbopogon citratus* (Lemon grass oil) was analyze using GC-MS (Agilent 5975C) equipped with DB-WAX capillary column. Helium was used as carrier gas. Temperature ranges between 230 and 325°C. Initially, column temperature was set at 70°C and further increased to 325°C. Dilute sample (1/50 in methanol) of 0.1 µl was used. The components were identified on the basis of their mass spectra using National Institute for Standards and Technology [NIST] Mass Spectrometry Data Center (2018) library data of GC-MS system.

3. Results and discussion

3.1. Dipole Moment

An important parameter that helps in the understanding of interaction between atoms in the same or different molecules is the dipole moment. It is a measure of the net molecular polarity, which is the magnitude of charge (/Q/) at the either ends of the molecular dipole time the distance between the charges (equation 1). Dipole moment increases with increase in electronegativity of atoms [16]. Chemical reactivity usually increases with increase in dipole moment.

The use of dipole moment to probe chemical reactivity according to our theoretical study suggests that Oleic acid (μ=1.40 Debye) would be more reactive than Palmitic acid (μ=1.28 Debye), which would imply that palmitic acid would be more stable than Oleic acid.

$$\mu = /Q/r \text{ ---------- (1)}$$

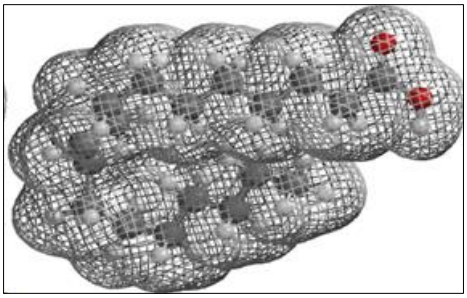

Figure 2(i) The density of mesh Palmitic acid using DFT at the B3LYP/6-31G*basis set level

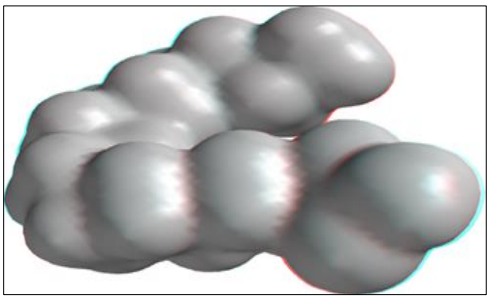

Figure 2(ii) The density of Oleic acid using DFT at the B3LYP/6-31G*basis set level

3.2. Total Energy

The minimum value of the total energy functional is the ground state energy of a system [17]. The electronic charge density which yields this minimum is then the exact single particle ground state energy. This makes the total energy calculated by quantum mechanical method a beneficial parameter. The total energy determines the occurrence or non-occurrence of chemical reactions and stereospecific paths in intra- and intermolecular processes.The total energy of a system is composed of the internal, potential, and kinetic energy. Hohenberg and Kohn [18] proved that the total energy of a system including that of the many body effects of electrons (exchange and correlation) in the presence of static external potential (for example, the atomic nuclei) is a unique functional of the charge density. The minimum value of the total energy functional is the ground state energy of the system. The electronic charge density which yields this minimum is then the exact single particle ground state energy. From our study, the total energy (absolute values) of oleic acid is higher than that of palmitic acid.

3.3. HOMO-LUMO Energy Gap

It is common knowledge that similar to the way electrons occupy the atomic orbitals, electrons occupy the molecular orbitals surrounding the molecule. The formations of molecular orbitals are from the linear combination of atomic orbitals or more specific, from the wave interaction of atomic orbitals. The study of energies of pairs of frontier orbitals, namely HOMO and LUMO of molecules provide reliable and quantitative data for straightforward prediction and comparative study of stabilities of molecules both from chemical and thermodynamic viewpoints. It has been reported earlier that HOMO-LUMO energy gap (ΔE) is an important stability index [19]. A large energy gap implies higher stability and lower chemical reactivity and vice versa. From the calculations made using DFT at the B3LYP/6-31G* basis set level, EHOMO of palmitic acid (-7.46 eV) is greater than that of oleic acid (-6.30 eV). Also, the ELUMO of oleic acid (0.24 eV) is less than that of palmitic acid (0.30 eV). This suggests than oleic acid would be of higher reactivity than palmitic acid. The higher reactivity of oleic acid would indicate a lower stability relative to palmitic acid. It could further be seen from the calculated amount of ΔE values (table 1) that palmitic acid has higher band gap energy than oleic acid.

Thermodynamically, a lower energy is representative of higher stability of molecules and low reactivity. However, a molecule may be thermodynamically stable but kinetically unstable. Therefore, the proposed higher stability of palmitic acid may be ascribed to kinetic stability due to saturation of the hydrophobic moiety compared to the unsaturation of that of oleic acid. The two double bonds at positions 9 and 12 from the hydrophobic component in addition to the hydrophilic carboxylic group of oleic acid would probably convey enhanced reactivity on the molecule. An experimental verification would probably help to provide more explanations these discrepancies.

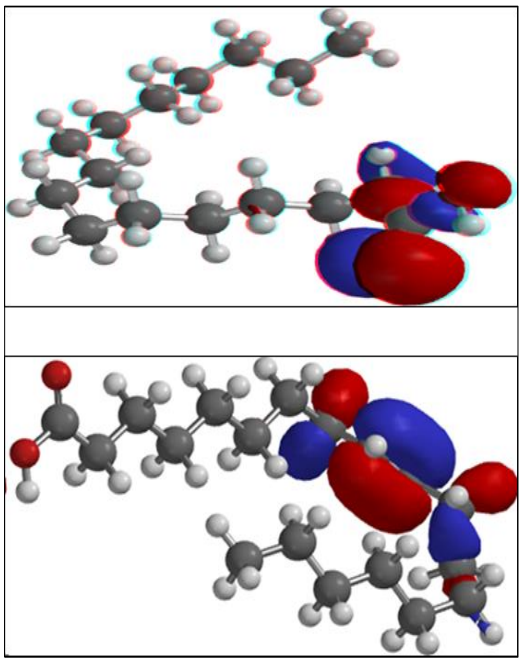

Figure 3 The highest occupied molecular orbital (HOMO) density of (i) palmitic acid and (ii) oleic acid using DFT at the B3LYP/6-31G*basis set level

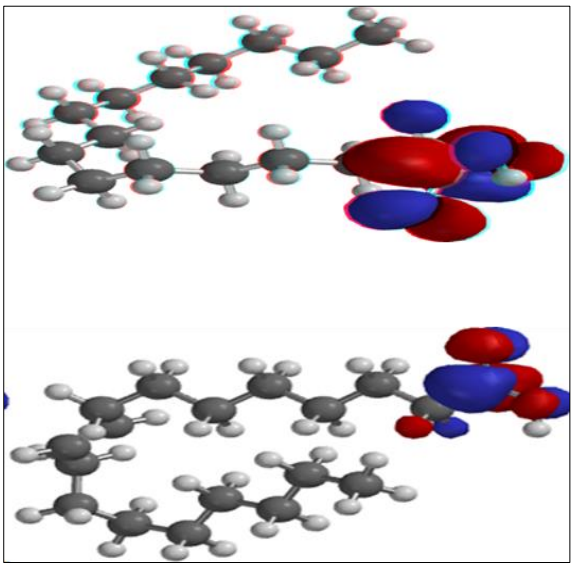

Figure 4 The Lowest unoccupied molecular orbital (LUMO) density of (i) palmitic acid and (ii) oleic acid using DFT at the B3LYP/6-31G*basis set level

3.4. Global Hardness and Global Softness

Table 1 Some molecular properties of palmitic acid and oleic acid calculated using DFT at the B3LYP/6-31G* basis set level

Parameter	Palmitic acid	oleic acid
EHOMO(eV)	-7.46	-6.43
ELUMO (eV)	0.30	0.24
ΔE (eV)	7.76	6.67
Total energy	-21209.30	-23316.64
Dipole moment(Debye)	1.28	1.40
Global hardness	3.88	3.88
Global softness	0.2577	0.2577

Table 2 (a) Mullikan charge distribution of palmitic acid calculated using DFT at the B3LYP/6-31G* basis set level

ATOM	C1	O1	O2	H2	C2	H1	H4	C3	H5	H6
CHARGE	+0.579	-0.464	-0.568	+0.407	-0.354	+0.170	+0.177	-0.252	+0.155	+0.131
ATOM	C4	H3	H7	C5	H9	H10	C6	H8	H11	C7
CHARGE	-0.261	+0.122	+0.151	-0.261	+0.133	+0.133	-0.255	+0.126	+0.132	-0.260
ATOM	H12	H13	C8	H14	H15	C9	H16	H18	C10	H17
CHARGE	+0.129	+0.128	-0.255	+0.126	+0.126	-0.255	+0.141	+0.125	-0.255	+0.126
ATOM	H19	C11	H21	H22	C12	H20	H24	C13	H25	H26
CHARGE	+0.127	-0.254	+0.126	+0.126	-0.256	+0.124	+0.137	-0.255	+0.127	+0.126
ATOM	C14	H23	H27	C15	H28	H30	C16	H29	H31	H32
CHARGE	-0.247	+0.125	+0.126	-0.247	+0.133	+0.129	-0.441	+0.141	+0.142	+0.139

Table 2 (b) Mullikan charge distribution of oleic acid calculated using DFT at the B3LYP/6-31G * basis set level

ATOM	C1	O1	O2	H2	C2	H3	H4	C3	H1	H5
CHARGE	+0.587	-0.463	-0.572	+0.408	-0.384	+0.175	+0.182	-0.251	+0.151	+0.150
ATOM	C4	H7	H8	C5	H6	H9	C6	H10	H11	C7
CHARGE	-0.270	+0.126	+0.148	-0.258	+0.131	+0.130	+0.263	+0.132	+0.131	-0.263
ATOM	H12	H14	C8	H13	H15	C9	H16	C10	H20	C11
CHARGE	+0.133	+0.140	-0.261	+0.130	+0.127	-0.256	+0.139	+0.126	-0.259	+0.127
ATOM	H28	C15	H26	H29	C16	H31	H32	C17	H33	H34
CHARGE	+0.132	-0.254	+0.130	+0.126	-0.251	+0.125	+0.122	-0.248	+0.127	+0.127
ATOM	C18	H30	H35	H36						
CHARGE	-0.454	+0.143	+0.139	+0.158						

On the basis of the assumptions of the HSAB principle of Pearson, [20], within the framework of density functional theory, chemical reactivity and stability of a molecule may be associated with its global hardness (α) and global softness (β) calculated according to equation 2 and 3. Increase in hardness increases movement of the system towards a more stable configuration-equilibrium configuration. When a molecule moves away from its equilibrium configuration its hardness value decreases. Greater hardness therefore implies high stability and low reactivity. Global softness has an inverse relationship with hardness: soft molecules undergo changes in electron density more easily than the hard molecules and are more reactive than the hard molecules [21]. Values of global hardness and global softness calculated for palmitic acid and oleic acid show that palmitic acid would be harder than oleic acid. In other words, oleic acid would be a softer molecule than palmitic acid. This is in agreement with the higher reactivity and lower stability earlier predicted for oleic acid than palmitic acid.

$$\alpha = \Delta / 2 \quad \text{---------- (1)}$$

$$\beta = 1 / \alpha \quad \text{---------- (2)}$$

Table 3 (a) Bond order of palmitic acid calculated using DFT at the B3LYP/6-31G* basis set level

BOND ORDER	**C1O1**	**C1O2**	**C1C2**	**O1O2**	**O1H2**	**O2H2**	**C2H1**	**C2H4**	**C2C3**	**C3H5**
MULLIKAN	1.865	1.070	0.967	0.065	0.037	0.760	0.921	0.920	0.993	0.931
BOND ORDER	C3H6	C3C4	C4H3	C4H7	C4C5	C5H9	C5H10	C5C6	C6H8	C6H11
MULLIKAN	0.936	1.010	0.938	0.930	1.009	0.938	0.931	1.012	0.939	0.942
BOND ORDER	C6C7	C7H12	C7H13	C7C8	C8H14	C8H15	C8C9	C9H16	C9H18	C9C10
MULLIKAN	0.990	0.943	0.938	1.013	0.938	0.939	1.012	0.927	0.938	1.006
BOND ORDER	C10H17	C10H19	C10C11	C11H21	C11H22	C11C12	C12H20	C12H24	C12C13	C13H25
MULLIKAN	0.938	0.939	1.003	0.939	0.938	1.009	0.939	0.930	1.009	0.940
BOND ORDER	C13H26	C13C14	C14H23	C14H27	C14C15	C15H28	C15H30	C15C16	C15H29	C16H31
MULLIKAN	0.938	1.004	0.938	0.940	1.015	0.939	0.943	1.015	0.952	0.952

Table 3 (b) Bond order of oleic acid calculated using DFT at the B3LYP/6-31G* basis set level

BOND ORDER	**C1O1**	**C1O2**	**C1C2**	**O1O2**	**O1H2**	**O2H2**	**C2H3**	**C2H4**	**C2C3**	**C3H1**
MULLIKAN	1.856	1.056	0.965	0.066	0.037	0.758	0.919	0.915	0.993	0.936
BOND ORDER	C3H5	C3C4	C4H7	C4H8	C4C5	C5H6	C5H9	C5C6	C6H10	C6H11
MULLIKAN	0.938	0.995	0.937	0.924	1.012	0.937	0.939	1.013	0.943	0.939
BOND ORDER	C6C7	C7H12	C7H14	C7C8	C8H13	C8H15	C8C9	C9H16	C9C10	C10H20
MULLIKAN	0.987	0.945	0.941	0.978	0.931	0.936	1.004	0.927	1.930	0.924
BOND ORDER	C10C11	C11H18	C11H21	C11C12	C12H23	C12H24	C12C13	C13H22	C13H25	C13C14
MULLIKAN	1.014	0.937	0.929	0.985	0.940	0.938	1.009	0.927	0.939	1.006
BOND ORDER	C14H27	C14H28	C14C15	C15H26	C15H29	C15C16	C16H31	C16H32	C16C17	C17H33
MULLIKAN	0.939	0.935	1.005	0.935	0.939	1.010	0.941	0.934	1.008	0.942
BOND ORDER	C17H34	C17C18	C18H30	C18H35	C18H36					
MULLIKAN	0.944	1.017	0.950	0.952	0.940					

3.5. Determination of functional using fourier transform infrared spectroscopy (FTIR)

The functional groups present were determined by comparing the vibration frequencies in wave numbers of the sample spectrograph obtained from an FTIR spectrophotometer with those of an IR correlation chart. The vibration frequencies of the solvent was also obtained to aid in the determination of sample vibration frequencies.The IR spectra of lemon grass oil having strong characteristic peaks at 3408 show the presence of OH and peaks at 2918, 2851, and 1461 cm^{-1} show the C–H stretching, a peak at 1710 shows the unsaturated conjugated C=O group present in the oil.

The main component of the *Cymbopogon citratus* oil is citral. In the IR spectrum of the oil of *Cymbopogon citratus*, some functional groups were observed. In the vibrations at 2918 cm^{-1}, a predominant asymmetric stretching of $-CH_3$ is observed corresponding to an alkyl saturated aliphatic group and at 2851, symmetric stretching of $-CH_2$ was observed. The band observed at 1730 cm^{-1} is due to vibrations of C=O, confirming the presence of conjugated double bonds in the oil indicates the aldehyde group. At the 1461 cm^{-1} peak, bending of the -CH group is observed.

The result of the fourier transform infrared spectroscopy (FTIR) was shows in table below

Table 4 The result of FTIR Analysis of lemon grass oil.

Peaks	Absorption wave number (cm-1)	Functional group	Inference
3408	3500-3400	N-H	Amine,primary amide
2918	3300-2900	-C-H	Alkene, aromatic ring
2851	3000-2500	O-H	Carboxylic acid
1730	2000-1700	C=O	Aldeyde,Ketone, ester
1710	1700-1600	C-N	Amine
1461	1400-1200	C-O	Alcohol, ether, ester
1379	1300-1000	C-H	Akene
1025	1000-700	C-H	Aromatic ring

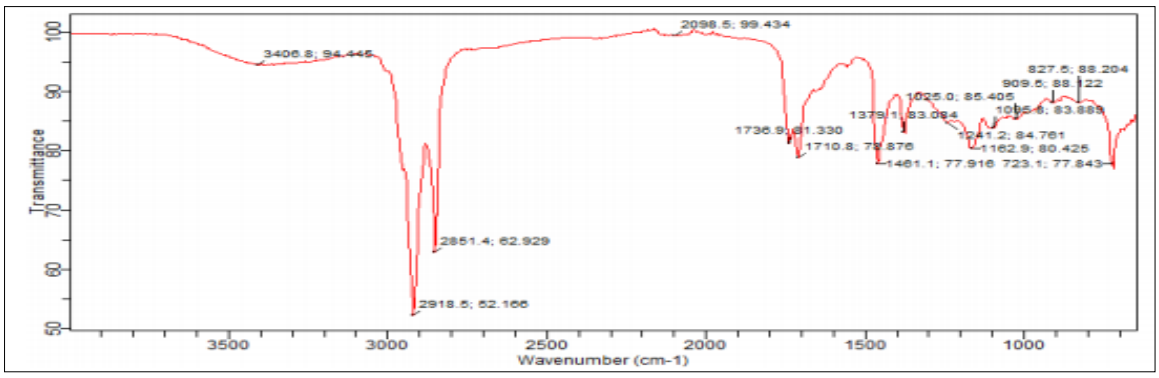

Figure 5 Result of IR spectrophotometer of Lemon grass oil

3.6. GC-MS Chromatogram

The GC Column eluted sixteen components, with different retention times as indicated by the chromatogram (table 5) and were further analyzed with an electron impact MS voyager detector. Identification of constituents was done on the basis of their retention time and mass spectra library search. The mass spectrographs of the identified constituents are given in figure 6 to 13. The relative amount of individual components was calculated based on GC peak areas

The chemical component identification of *Cymbopogon citratus* (lemongrass) leave extract was performed by GC-MS analysis, and the spectra data of these identified compound were interpreted that the major component were trans-1,3-octadecenoic acid (38.91 %), n-hexadecanoic acid (14.65 %), and Linoelaidic acid (3.17 %), 2-benzoic acid (3.13 %), carbonic acid (2.20 %) and methyl Stearate (1.42 %) were minor but significant component (Table 5), the quality of *Cymbopogon citratus* is generally determines by citral content, the cis-isomer and trans-isomer neral.

Table 5 The result of GC-MS analysis of lemon grass oil

	Compound Name	**Relative Peak Area**
1.	Methyl Stearate	1.42
2.	Trans -1,3-Octadecenoic Acid	38.91
3.	9,12 Octadecadienoic acid	3.42
4.	n-hexadecanoic acid	14.65
5.	Hexadecanoic acid, methyl ester	4.26
6.	Tetradecanoic acid	2.30
7.	Dodecanoic acid	4.81
8.	1,6- Octadien-3-ol	1.75
9.	11-Octadecenoic acid, methyl ester	6.18
10.	Carbonic acid, Octadecyl vinyl ester	2.20
11.	Octadecanoic acid	7.72
12.	Linoelaidic acid	3.17
13.	Tritetracontane	1.80
14.	Tetracosane	2.30
15.	2-(heptyloxycarbonyl) Benzoic acid	3.13
16.	Nonahexacontanoc acid	2.00

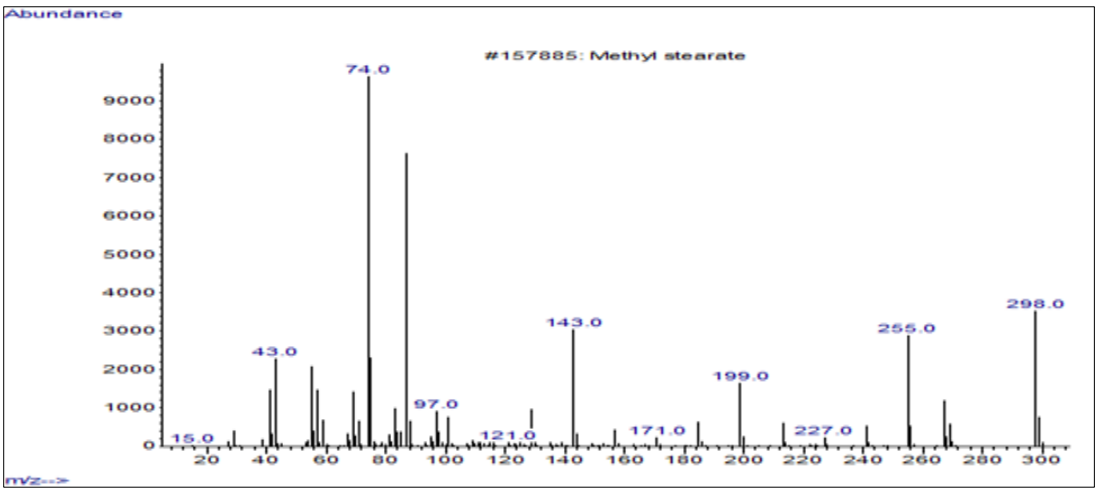

Figure 6 Fragmentation Pattern of Methyl Stearate Content of Essential Oil

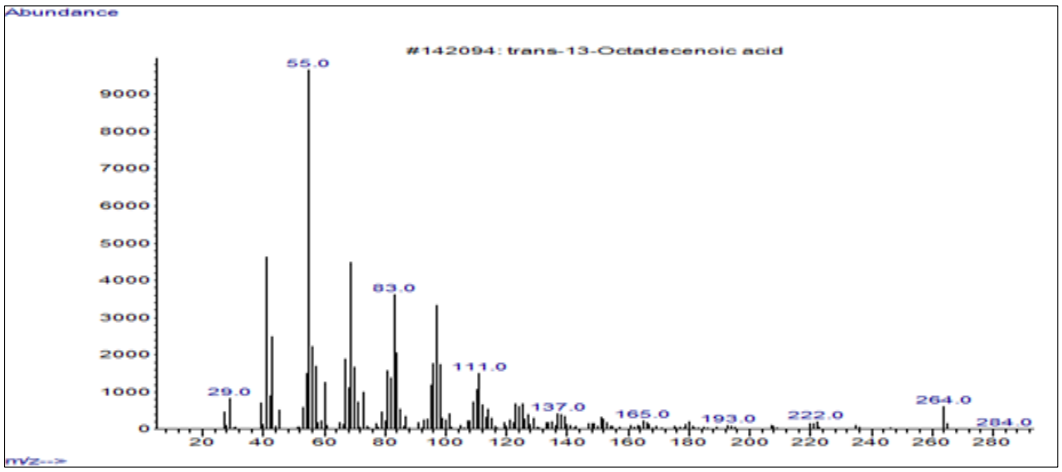

Figure 7 Fragmentation Pattern of Octadecanoic Acid Content of Essential Oil

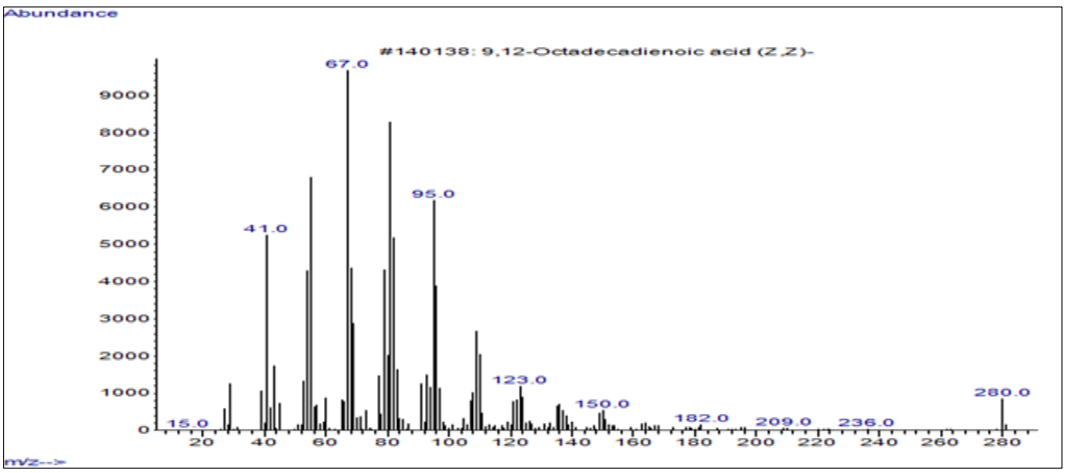

Figure 8 Fragmentation Pattern of Octadecadienoic Acid Content of Essential Oil

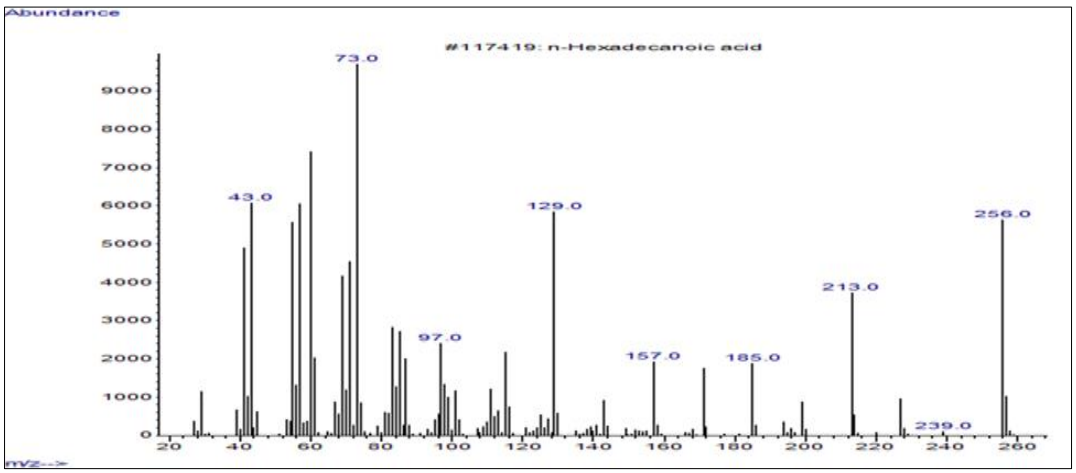

Figure 9 Fragmentation Pattern of Hexadecanoic Acid Content of Essential Oil

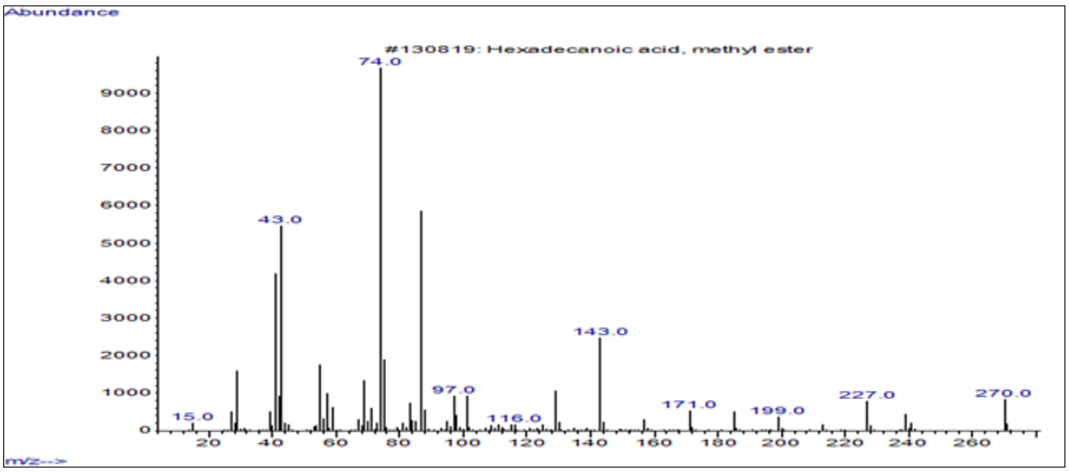

Figure 10 Fragmentation Pattern of Hexadecanoic Acid, Methyl Ester Content of Essential Oil

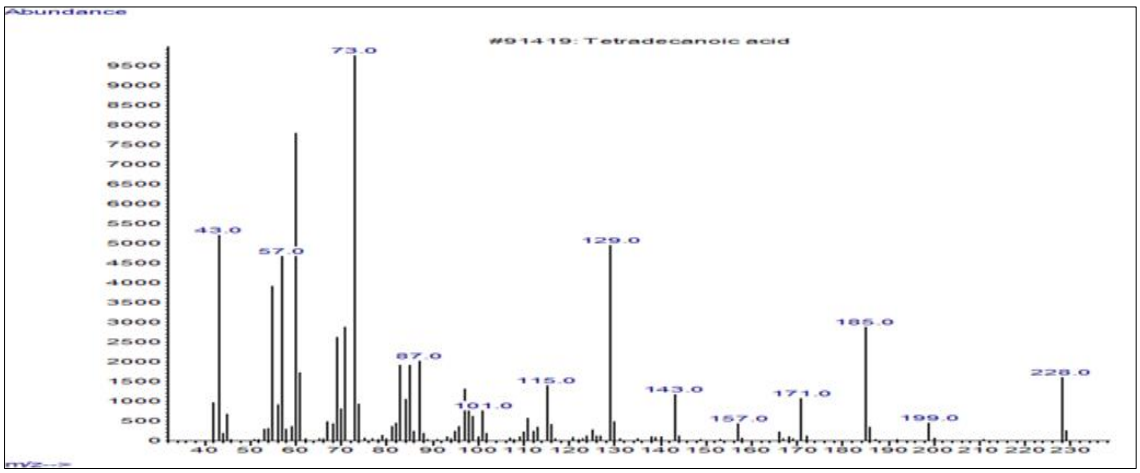

Figure 11 Fragmentation Pattern of Tetradecanoic Acid, Methyl Ester Content of Essential Oil

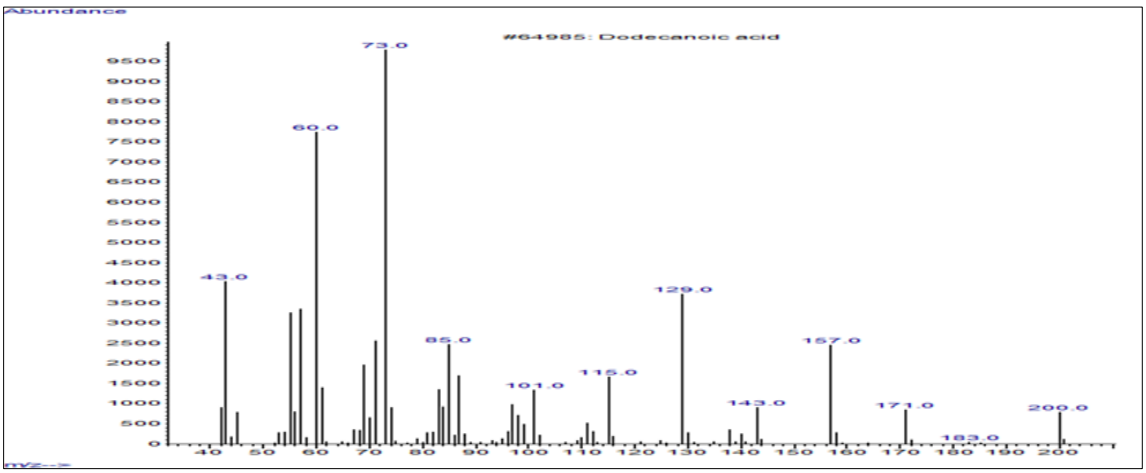

Figure 12 Fragmentation Pattern of Dodecanoic Acid, Methyl Ester Content of Essential Oil

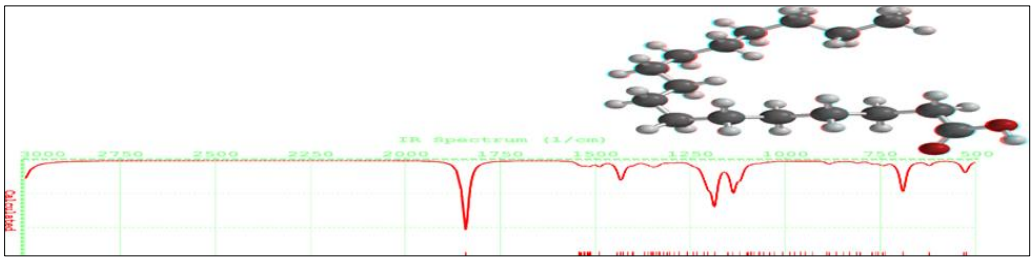

Figure 13 Infra-red spectra of PALMITIC ACID

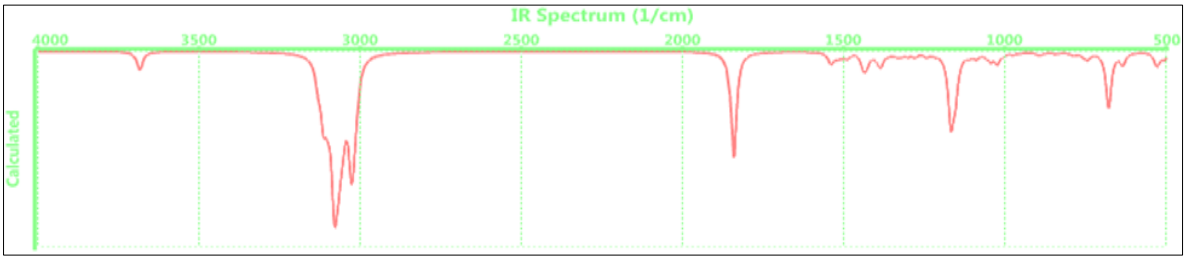

Figure 14 Infra-red spectra of OLEIC ACID

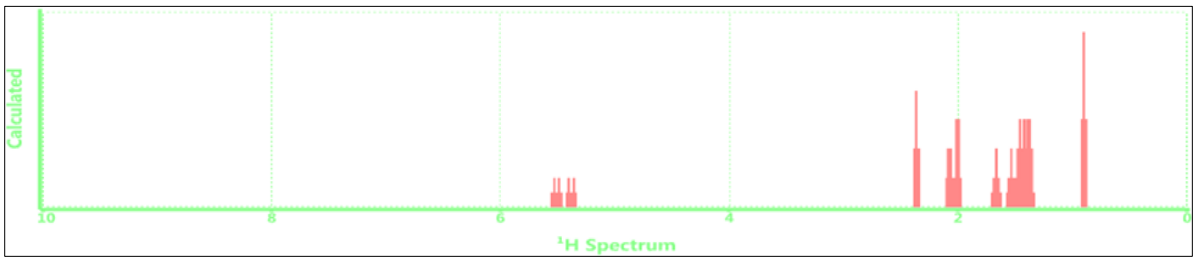

Figure 15 Hydrogen spectrum of OLEIC ACID

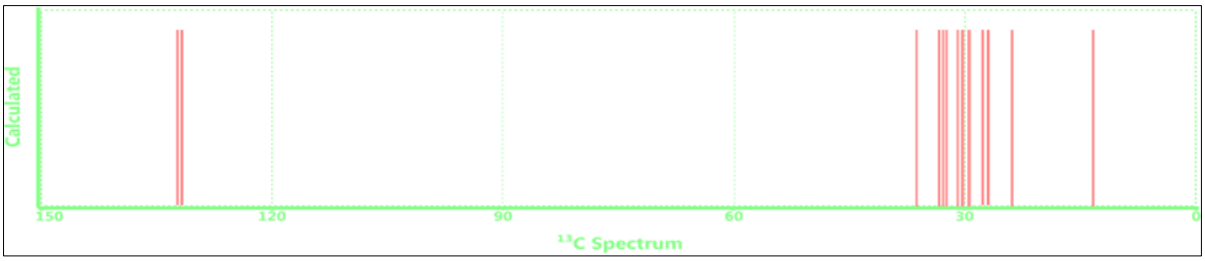

Figure 16 Carbon 13 spectrum of OLEIC ACID

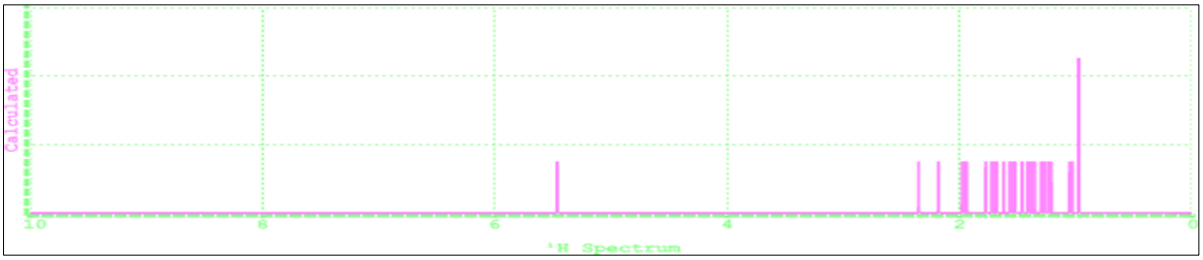

Figure 17 Hydrogen spectrum of PALMITIC ACID

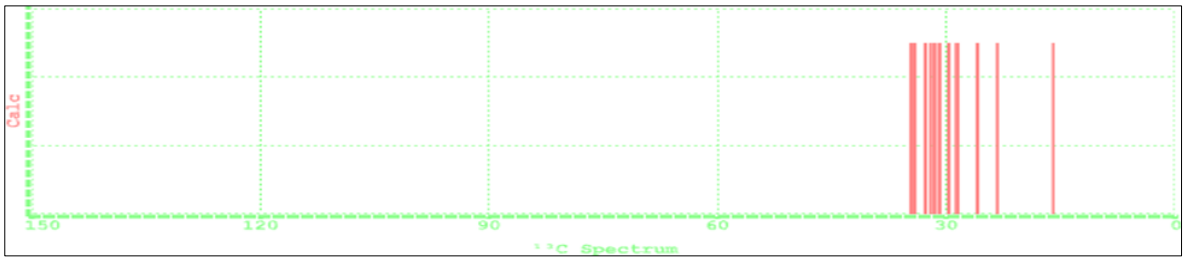

Figure 18 Carbon 13 spectrum of PALMITIC ACID

4. Conclusion

On the basis of this study, it has been concluded that Nigeria *Cymbopogon Citratus* (lemon grass oil) active ingredients has insecticidal properties for the control mosquitoes. The mosquito's repellent cream produced possesses repellence characteristics against mosquitoes. Theoretical study shown that the active constituents, oleic acid and palmitic acid have similar spectral positions, similar global hardness and global softness, and that the oleic acid show higher chemical reactivity than palmitic acid judged from the values of their band gap energy differences, total energies, and dipole moments.

Compliance with ethical standards

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Disclosure of conflict of interest

The authors declare that they have no conflict of interest.

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