Communication in Physical Sciences 2020, 6(1): 635-648

Theoretical and Biochemical Information studies on Compounds Detected in GCMS of Ethanol Extract of *Chromolaena odorate* Leaf

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Received 25 June 2020/Accepted 25 August 2020/Published online: 01 September 2020

Abstract *In order to investigate the presence of chemical and biological active molecules in Chromolaena odorate leaf, ethanol extract of the was subjected to GCMS analysis. The results obtained indicated that most abundant phytochemicals detected in the GCMS analysis of ethanol extract of Chromolaena odorate leaf were octadecanoic acid (11.35%), methyl elaidate(19.02%) and erucic acid (20.55%). Others were 6-methyl-1-heptanol, 3-tetradecene, phenol 3,5-bis(1,1-dimethyl)- (3,5-di-tert-butylphenol), 1-methyl-2-(3-methylpentyl)-cyclopropane, 9-methyl-5-undecene, iminodiacetonitrile, metholene, 2-ethyl-heptanoic acid, 1-nitrododecane, 4,4-dimethyl-cyclohex-2-en-1-ol, cyclohexylpropanamide, nobilinem6-hydroxy, decamethylene glycol, 3,3,5-trimethyl-1,4-hexadiene and 1,1,3,3-tetramethylcyclopentane. Application of physicochemical and molecular descriptors analysis indicated that nobiline, 6-hydroxy is leaf the most reactive component of the phytochemical while 1,1,3,3-tetramethylcyclopentane is the least reactive. Chemical and biological activities of the compounds in ethanol extract of Chromolaena odorate leaf have been documented in this work. Docking of some of the biological active component is recommended for further study.*

Key Word: *Biochemical active molecules, Chromolaena odorate leaf, GCMS study, computational chemistry simulation*

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1.0 Introduction

Plant extract are useful in pharmaceutical and medicinal sciences (Onyeije & Okop, 2020).), in the food industries (ref) in the corrosion industries (Eddy and Odiongeny, 2010; Eddy *et al*., 2011a) and in some green synthesis (Pirtarigha, *et al*., 2019). The choice of any plant extract for a given purpose depends on its chemical composition which may include proximate, antinutritional factors, elemental, vitamins and phytochemical constituents (Okwunodulu *et al*., 2020). However, phytochemical constituents of most plant extract are bioactive against several microorganism while some may also contain useful industrial intermediates (Eddy *et al*., 2010). Therefore, knowledge of phytochemical constituents of plant is essential in understanding their useful applications. Phytochemical screening can provide information on the class of phytochemicals in a given plant extract but cannot reveal information on their chemical structures. The use of GCMS has been found to be one of the best option available for analysing phytochemical constituents of plant extract (Eddy *et al*., 2011b). Therefore, the present study is aimed at investigating the phytochemical constituents of ethanol extract of *Chromolaena odorate* leaf using GCMS instrument and to present information on their chemical applications as well as biological activities. Also, based on the structures of the identified compounds, computational chemistry shall be used to assessed the contribution of each constituents to the activity of the extract (Eddy *et al*., 2018).

2.0 Materials and Methods

2.1 Sample preparation

The leaf samples were obtained from Akwa Ibom State University botanical garden and transported to the Chemistry laboratory of the same university. They were thoroughly washed with distilled water and allowed to dry. The leaves were sun dried for a week until the moisture content was reduced to minimum. The dried leaves were grounded to a powder form and soaked in a solution containing equal volume of ethanol and acetone solution. (Eddy *et al*., 2011a; Eddy and Odiongenyi, 2010). The

mixed solvent was recovered using cold extractor, leaving behind, acetone/ethanol extract of *Chromolaena odorate* leaves.

2.2 GCMS analysis

The produced extract was used for GCMS analysis using spectroscopically pure acetone solvent (Eddy *et al*., 2011b). The GCMS-QP2010 PLUS Schimadzu (made in Japan) instrument was used for the analysis. The analytical steps taken were plugger speed (high), syringe injection speed (high), viscosity/compression time (0.2 second), injection mode (normal), pumping time (5), injection port dwell time (0.3 second), terminated air cap (No), plugger washing speed (high), washing volume (8µl), syring suction position (0), syringe injection position (0) and used three solvent vial (3). The operational setting of the GCMS instrument were column oven temperature (60°C), injection temperature (200°C), injection mode (split), flow control mode (linear velocity), pressure (100.2 kPa), total flow (6.2 ml/minute), linear velocity (46.3 cm/sec), purge flow (3.0ml/min) and split ratio (1.0). The high-pressure injection, carrier gas server and splitter hold functions were switch off. The initial rate of oven temperature program was 5 °C/min and was gradually increased to 140°C after which the temperature was increased to 280 °C at a rate of 10 °C/minute. Some heat unit and detector functions were checked in order to ensure consistency. These included column oven, SPL2, MS, SPL2 carrier, SPL2 purge and were ensured to be on. However, the APC setting was turned off.

Other setting functions of the machine were ion source temperature (200 °C), interface temperature (250 °C), solvent cut time ((2.50 minutes), detector gain mode (relative), detector gain (0.00kV), threshold (1000). The analytical start time was 3 minutes and the machine run for 45 minutes using ACQ scan mode at a scan speed of 769. However, mass/charge started at 50 and ended with 400 units. Gas chromatogram and mass spectrum were automatically plotted and suggested chemical structures were obtained using the National Science Technology library installed in the machine. Percentage concentrations of each identified component was calculated using area normalization.

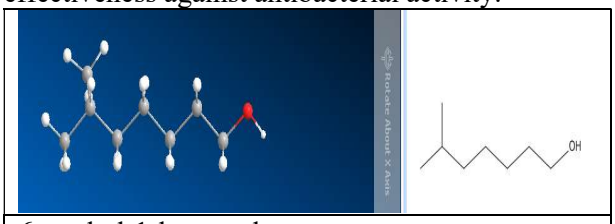
2.3 Computational chemistry calculation

All computational chemistry softwares used in this study were provided by Prof. Nnabuk Okon Eddy of the Department of Pure and Industrial Chemistry, University of Nigeria, Nsukka. These included ChemBio programme (used for drawing structure), hyperchem(used for geometry optimization through molecular mechanics setting and for the calculation of physicochemical; descriptors; logP, surface area, polarizability, refractivity and hydration energy), MOPAC (used for calculation of frontier molecular orbital energies, electronic, core-core and total molecular energies).

3.0 Results and Discussion

Fig. 1 shows the GCMS spectrum of ethanol extract of *Chromolaena odorate* leaf. Analytical parameters deduced from the spectrum are recorded in Table 1. Eighteen peaks were identified in the spectrum. The retention time for the detected compounds ranged from 13.992 to 50.753 minutes while the molecular mass of identified compounds ranged from 95 to 309 g/mol. Detected compounds with significant concentrations were octadecanoic acid (11.35%), methyl elaidate(19.02%) and erucic acid (20.55%). Others were 6-methyl-1-heptanol, 3-tetradecene, phenol 3,5-bis(1,1-dimethyl)- (3,5-di-tert-butylphenol), 1-methyl-2-(3-methylpentyl)-cyclopropane, 9-methyl-5-undecene, iminodiacetonitrile, metholene, 2-ethyl-heptanoic acid, 1-nitrododecane, 4,4-dimethyl-cyclohex-2-en-1-ol, cyclohexylpropanamide, nobilinem6-hydroxy, decamethylene glycol, 3,3,5-trimethyl-1,4-hexadiene and 1,1,3,3-tetramethylcyclopentane.

6-methyl-1-heptanol was identified in ethanol extract of *Chromolaena odorate* leaf. It is a primary alcohol and a volatile organic compound The compound is a known solvent, in the making of cutting and lubricating oils, in hydraulic fluids, and in the production of other chemicals. 6-methylhep-1-ol is a primary alcohol in which the heptane is substituted by a methyl group at position 6 and a hydroxy group at position 1. It has a role as a mammalian metabolite. Okwu and Ighodaro, (2009) has also identified this compound in the stem bark of *Dacryodes edulis G.* and reported its effectiveness against antibacterial activity.



6-methyl-1-heptanol

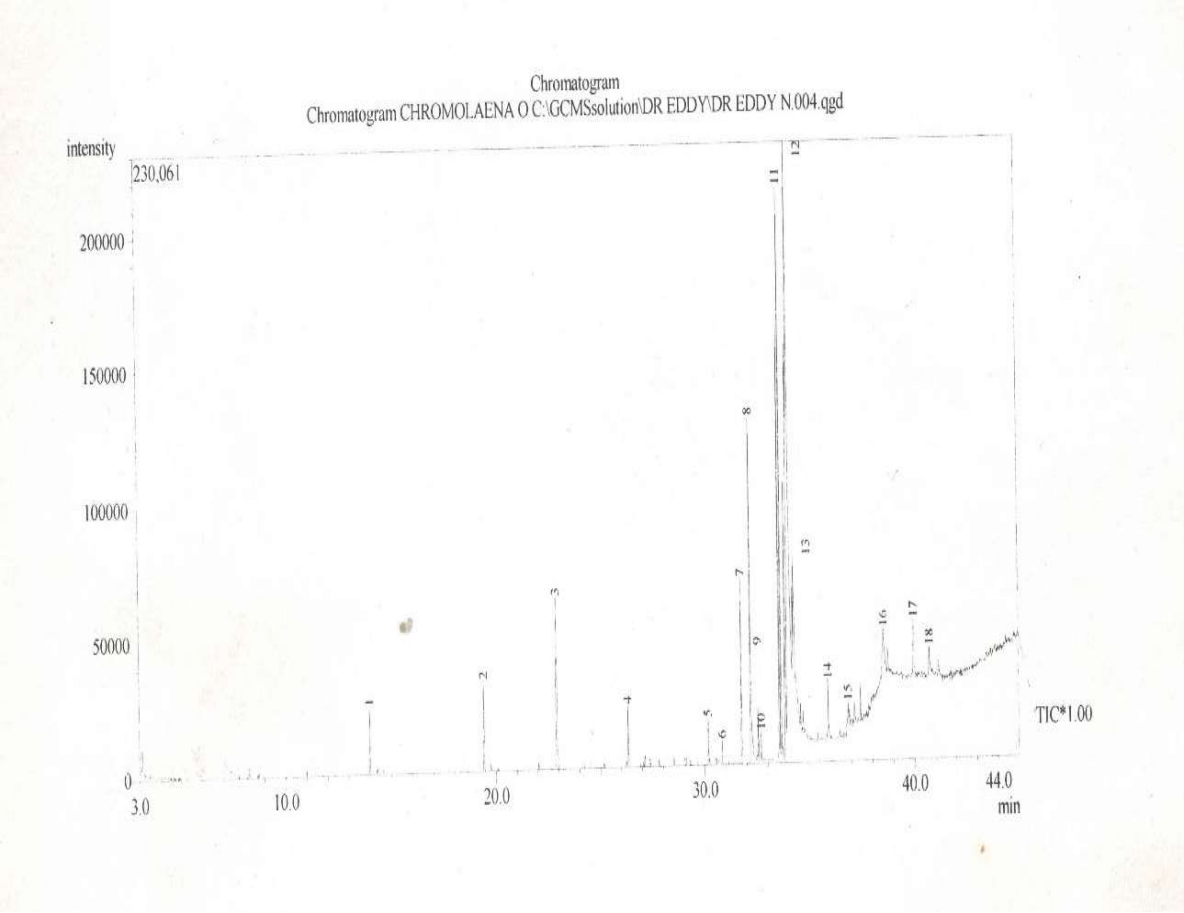


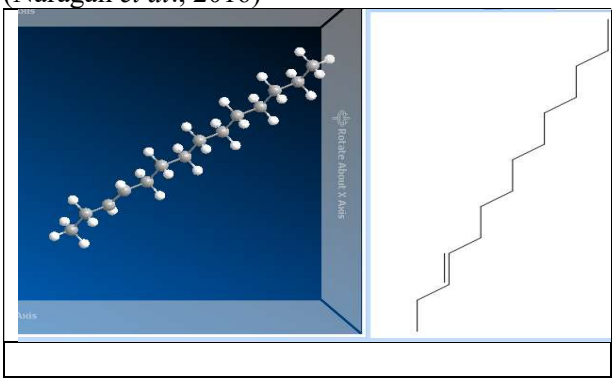
Fig. 1: GCMS spectrum of ethanol extract of *Chromolaena odorate*

Table 1: Chemical compounds in ethanol extract of *Chromolaena odorate* leaf

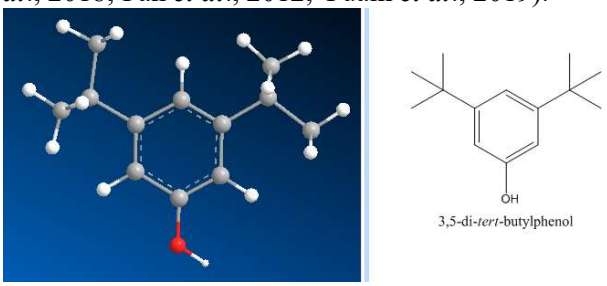
Line number	Name	Retention time	Molecular mass	Base peak	C (%)
1	6-methyl-1-heptanol	13.992	130	56.05	1.99
2	3-tetradecene	19.425	196	55.00	2.76
3	phenol 3,5-bis(1,1-dimethyl)- (3,5-di-tert-butylphenol)	22.917	206	57.06	5.83
4	1-methyl-2-(3-methylpentyl)-cyclopropane	26.333	140	57.05	1.84
5	9-methyl-5-undecene	30.175	168	57.05	1.53
6	2,2-iminobis-acetonitrile (iminodiacetonitrile)	30.820	95	68.05	0.77
7	n-hexadecanoic acid methyl ester (metholene)	31.758	270	74.05	6.13
8	Octadecanoic acid (stearic acid)	32.200	284	60.00	11.35
9	2-ethyl-heptanoic acid	32.558	158	88.10	3.68
10	1-nitrododecane	32.692	215	69.05	0.61
11	9-octadecenoic acid, methyl ester (methyl elaidate)	33.650	296	55.00	19.02
12	Erucic acid (prifrac 299)	34.042	338	55.00	20.55
13	4,4-dimethyl-cyclohex-2-en-1-ol	34.283	126	55.00	6.75

14	3-cyclohexylproponamide (cyclohexylpropanamide)	35.892	155	59.00	2.76
15	1,4-Methano-2H-cyclopent[d]oxepin-2,5(4H)-dione, 6-[(dimethylamino)methyl]hexahydro-8a-hydroxy-5a-methyl-9-(1-methylethyl)-, [1R-(1.alpha.,4.alpha.,5a.alpha.,6.beta.,8a.alpha.,9S*)]-(Nobiine, 6-hydroxy)	36.842	309	58.05	1.84
16	1,10-decanediol (decamethylene glycol)	38.550	174	55.00	4.29
17	3,3,5-trimethyl-1,4-hexadiene	39.983	124	69.05	4.60
18	1,1,3,3-tetramethylcyclopentane	40.753	126	70.10	3.68

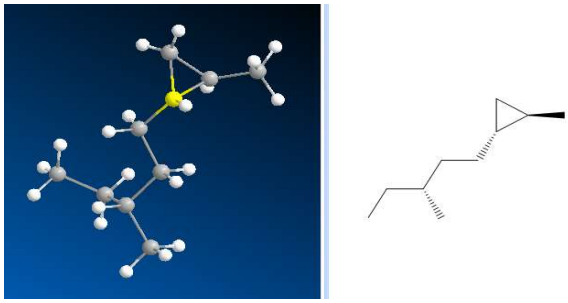
Tetradecene was identified in acetone extract of *C.babylonica (L.) L*. The extract showed significant antibacterial activity against *Bacillus cereus*, *P. aeruginosa* and *C. albicans* (MIC: 1.6 mg/mL) (Guvensen *et al.*, 2019). Also, 1-tetradecene, 1-Hexadecene and cyclo tetracosanethat were identified in *Gynura segetum*'s leaf extracts showed potent antimicrobial activities (Naragan *et al*., 2016)



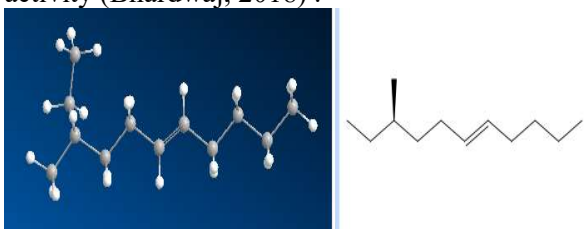
3,5-bis(1,1-dimethyl)-phenol is an antioxidant and reportedly has some anticancer property (Mohd *et al*., 2014). The compound has also been reported to be presence in flowers of *Aesculus chinensis*, *fungal Coriolus versicolor*, *Aquilaria sinensis (Lour*.) *Gilg* , whole plants of *Hedyotis lancea Thunb*., and seeds of *Plukenetia volubilis* (Chen *et al*., 2018; Gao *et al*., 2018; Pan *et al*., 2012; Yuain *et al*., 2019).



Bhardwaj, (2018) reported the presence of 1-methyl-2-(3-methylpentyl)-cyclopropane as a contributor to the antimicrobial activity of *Tecomella undulata* extract. Studies conducted by Naz *et al*. (2020) also identified this compound as one of the bioactive components that contributed to the antioxidant, anti-inflammatory and anti-cancer properties of *Jacaranda mimosifolia* leaf. They also predicted the potential of this plant for therapeutic, nutraceutical and functional food applications. 1-methyl-2-(3-methylpentyl)-cyclopropane (chemical structure is shown below) has also been identified by El-Shanawany *et al*. (2014) in the methanol extract *Anisotes trisulcus* aerial plant at a retention time of 13.573 minutes.

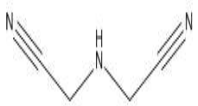


. In peak five, 9-methyl-5-undecene (see chemical structure below) was identified at a retention time of 30.175 minutes and the base peak was 57.05. Literature is scanty on the biological activity of this compounds but some of its isomers including 6-methyl-2-undecene and 7-methyl-3-undecene have been found in plants that exhibit good antimicrobial activity (Bhardwaj, 2018) .

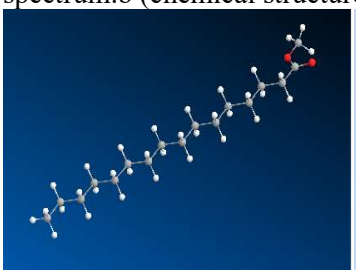


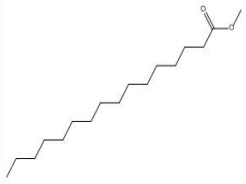
2,2-iminobis-acetonitrile is an alkaloid also called iminodiacetonitrile was identified in peak six at a retention time of 30.820 minutes and the recorded base peak was 68.05. 2,2-iminobis-acetonitrile is a

secondary amino compound in which two of the ammonia hydrogens are substituted by cyanomethyl groups. It is a dinitrile and an aliphatic nitrile. It is a derivative of acetonitrile and is soluble in water, acetone and hot methanol. It is a useful chemical intermediate, in the preparation of iminodiacetic acid and to study the interference of nitriles in cyanide determination.(See chemical structure below)



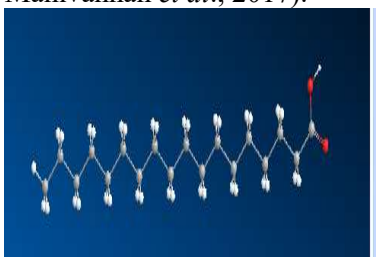
At a retention time of 31.758 minutes, n-hexadecanoic acid methyl ester (metholene) was observed as the seventh peak in the GCMS spectrum.b (chemical structure shown below)



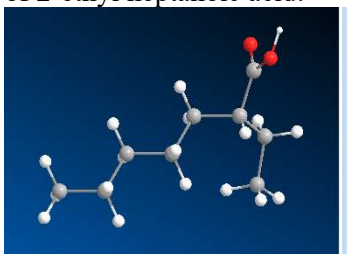


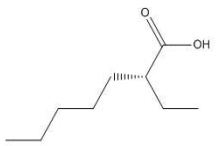
The compound is also known as methyl hexadecanoic acid or palmitic acid methyl ester (PAME). It belongs to class of organic compound called fatty acid methyl esters because they contain fatty acid that is esterified with a methyl group. Palmitic acid methyl ester (PAME) is a known transferable perivascular relaxing factor in rat aorta. However, the role of PAME for similar mechanism in human isyet to be ascertained (Wang, *et al*., 2018). In a study to investigate the antibacterial and antifungal efficacy of fatty acid methyl esters from *Sesuvium portulacastrum L.* leaf extract. it was found that fatty acid methyl esters demonstrated the highest antibacterial and antifungal property (Chandrasekaran *et al.*, 2011, 2008). According to Lima *et al*. (2011) and Canales *et al*. (2011), the methyl esters of fatty acids are endowed with antibacterial and antifungal capacity. Suresh *et al*. (2014) also confirmed that palmitic acid methyl ester (C16:0) represents the main constituent of fatty acids that is responsible for the antibacterial activity observed in the target algal species and that in other reported studies, palmitic acid has been reported to be the major antibacterial compound in a mixture of fatty acids from other algal species.

At a retention time of 32.220 minutes and base peak value of 60.00, octadecanoic acid was observed as the eighth peak in the spectrum (chemical structure shown below). According to Chibuzo and Okop (2020) octadecanoic acid has a strong binding affinity to MMP-2 and can enhance its role as a proapoptotic factor in emancipation of inflammation apart from inducing apoptosis. The acid (stearic acid) were also found to exhibit antibacterial and antifungal activities (Agoramoorthy *et al*., 2007; Manivannan *et al*., 2017).



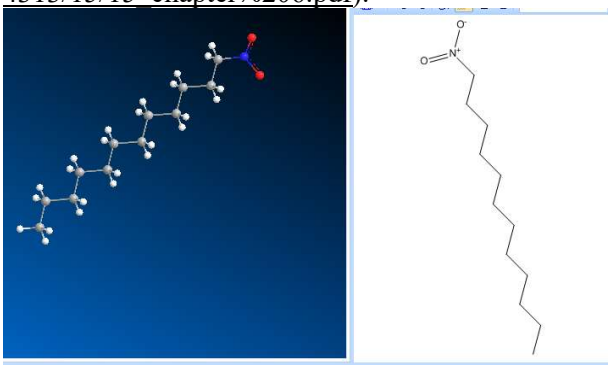
2-ethyl-heptanoic acid was the ninth fraction in the GCMS analysis of ethanol extract of *Chromolaena odorate* leaf (chemical structure shown below). The retention time was 32.558 minutes while the base peak was 88.10. Literature is scanty on the uses and biological activity of this compound but several reports have indicated that most carboxylic acid derivatives have strong antimicrobial activities, which suggest that 2-ethylheptanoic acid might likely have good biological activity (Popiolek *et al*., 2015). Consequently, there is a knowledge gap that must be fill through a research on biological activity of 2-ethyl heptanoic acid.



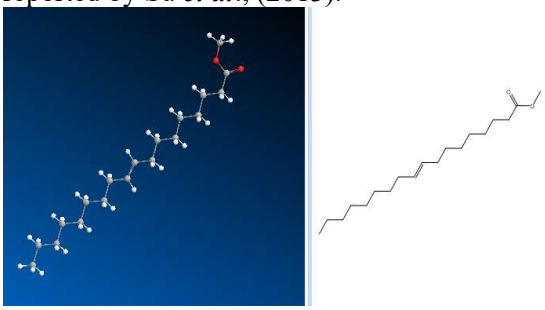


1-nitrododecane was identified in the tenth peak. Similarly. Literature is scanty on the bioactivity of 1-nitrododecane but uncited reference indicated that this compound was identified through GC-MS of the TLC fraction of *P. canescens* extract.

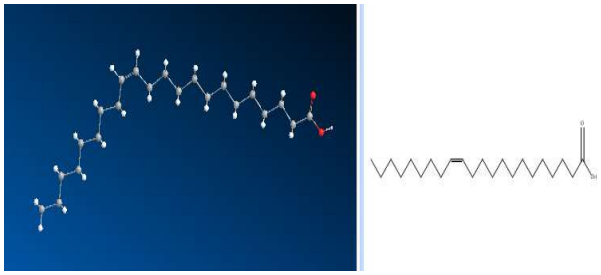
(http://14.139.13.47:8080/jspui/bitstream/10603/214313/15/15_chapter%206.pdf).



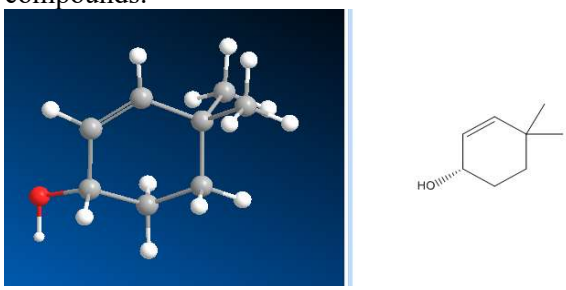
The eleventh peak in the spectrum reveal the presence of 9-octadecenoic acid, methyl ester (methyl elaidate) in ethanol extract of *Chromolaena odorate* leaf (chemical structure shown below). As stated earlier, most fatty acid methyl esters have been confirmed to exhibit good biological activities. In addition, cytotoxic activity of methyl elaidiate extracted from fruits of *Brucea javanica* has been reported by Su *et al*., (2013).



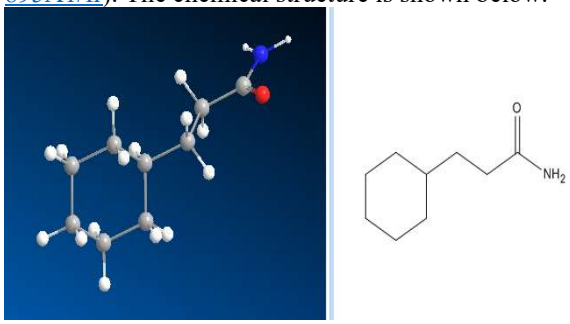
Erucic acid was identified in the twelfth peak of the spectrum at a retention time and base peak values of 34.650 minutes and 55.00 respectively. Erucic acid is a monounsaturated omega-9 fatty acid, whose health risk has been confirmed for highly exposed children. Erucic acid (chemical structure shown below) can cause a reversible heart condition called myocardial lipidosis and other potential effects including changes in the weight of the liver, kidney and skeletal muscle (at slightly higher doses). Based on this information, experts on EFSA's Panel on Contaminants in the Food Chain (CONTAM Panel) established a tolerable daily intake of 7 milligrams per kilogram of body weight (mg/kg bw) per day. However, erucic acid has some industrial applications. According to Aukema, and Campbell (2011), the major industrial application of erucic acid is the use of its primary derivative, erucamide, as a slip agent for plastic film, such as in bread wrappers and garbage bags. They are also usefull in the polymer industry and in the detergent, photographic, cosmetic, pharmaceutical, ink, paper, textile, lubricant, food, and fuel industries. The chemical structure of this compound is shown below.



4,4-dimethyl-cyclohex-2-en-1-ol was found in peak 13 at a retention time of 34.283 minutes and base peak of 55.00 which its chemical structure is shown below. Literature is scanty on the biological activity of this plant extract but Kurahove *et al*. (2016) has identified the compound in freshwater *macrophytes* and attributed anti-inflammatory and antineoplastic activities of freshwater *macrophytes* to the presence of 4,4-dimethyl-cyclohex-2-en-1-ol and other compounds.

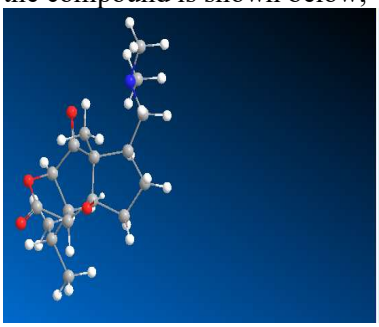


Cyclohexylpropanamide was observed in peak 14 at retention time of 35.892 minutes and mass peak value of 59.00. Literature is scanty on the application or biological activities of this compound but there are scanty information that suggest that it could have some herbicidal and insecticidal potentials (https://patents.google.com/patent/ EP3264 -895A1/fr). The chemical structure is shown below.



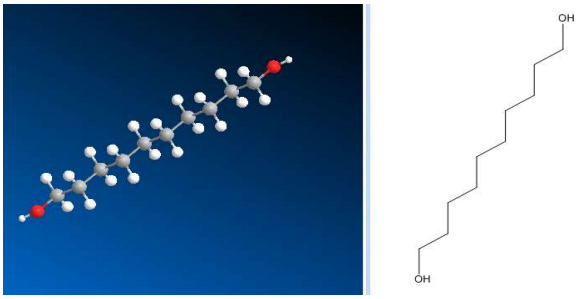
1,4-methano-2H-cyclopent[d]oxepin-2,5(4H)-dione, 6-[(dimethylamino)methyl]hexahydro-8a-

hydroxy-5a-methyl-9-(1-methylethyl)l- (see chemical structure below), which is also called noviline, 6-hydroxy was detected with a characteristics retention time of 36.842 minutes and base peak value of 58.05. The chemical structure of the compound is shown below,



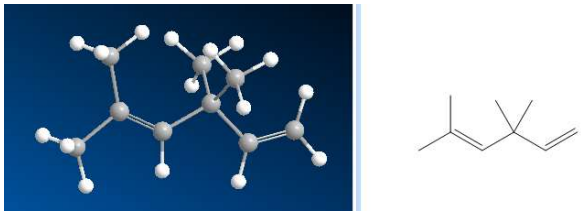
Available literature reveal that there is no plant with detectable concentration of nobiline except *Dendrobium nobile* (Yamarura and Hirata, 1964). However, this alkaloid (nobiline, 6-hydroxy) is reported in this plant at concentration of 1.84%, Much has not been reported on the biological activity of nobiline, 6-hydroxy but its derivatives has been found to exhibit higher antioxidant activity than Vitamin C and stronger inhibitory effects on the production of nitrogen (II) oxide than resveratrol (Zhang *et al*., 2007a,b). Strong antimutagenic properties including anticarcinogenic effects against lung carcinoma, ovary adenocarcinoma, and promyelocytic leukemia have also been attributed to the presence of nobiline **(**Miyazawa *et al*., 1997; Suzuki *et al*., 1973; Zhao *et al*., 2001). Nobiline has also been reported as the source of numerous drugs in China and Japan (http://14.139.116.20:8080/jspui/bitstream/10603/136205/6/06_chapter2.pdf). The chemical structure of nobiline is shown in the next figure.

In peak 16, 1,10-decanediol (also called decamethylene glycol) was identified at a retention time of 38.550 minutes and mass peak value of 55.00. The optimized structure of the compound is shown below



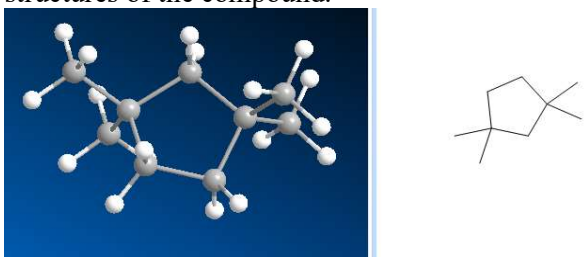
Decamethylene glycol is useful in trace concentration as an intermediate for the production of polyesters. Decamethylene glycol is a useful intermediate in the formulation of perfume, essence, and some pharmaceuticals (Tan *et* al., 1995).

Peak 17 indicated the presence of 3,3,5-trimethyl-1,4-hexadiene under a retention time of 39.983 minutes and mass peak value of 69.05. The chemical and optimized structure of this compound is as shown below



The compound has 24 bonds (consisting of eight non bonded hydrogen bond, two rotatable bonds, two multiple bond and two double bond which implies that it is an unsaturated compound. This compound has also been detected in the root of *Panax japonicas C.A. Mayer* by Zhang *et al*. (2011). Pthman *et al*. (2020) also identified 3,3,5-trimethyl-1,4-hexadiene in essential oil of some plant extracts that demonstrated good antifungal properties.

Peak 18 indicated the presence of 1,1,3,3-tetramethylcyclopentane at a retention time of 40.753 minutes and mass peak value of 70.10. The figure below shows the skeletal and optimized structures of the compound.



1, 1, 3, 3-tetramethylcyclopentane has been reportedly used by Sauders *et al*. (2007) to study reaction mechanism. Investigation of antioxidant activity using the DPPH radical scavenging assay on *Prunus dulcis* nut indicated that the n-butanol extract (which contained 1,1,3,3-tetramethylcycopentane) showed mild activity against the gramnegative *E. coli* with inhibition zone diameter 8 mm

3.2 Theoretical study

3.2.1 Physicochemical Parameters

Some structure related physicochemical parameters

of the compounds identified in the GCMS of ethanol extract of *Chromolaena odorate* are presented in Table 2. The parameters include logP, hydration energy, surface area, polarizability and refractivity. The results indicate that erucic acid has the least value of logP and highest values of hydration energy, surface area, polarizability and refractivity. This acid also has the highest value of molecular mass (i.e 388 g/mol) among all the compounds detected in the spectrum

Table 2: Calculated physicochemical parameters of compound identified in GCMS spectrum of ethanol extract of *Chromolaena odorate*

	logP	Hydration Energy	Surface area	Polarizability	Refractivity
6-methyl-1-heptanol	2.46	-3.16	421.40	16.09	40.49
3-tetradecene	5.79	5.27	620.44	26.27	67.22
3,5-di-tert-butylphenol	3.20	-3.19	469.58	25.75	68.37
1-methyl-2-(3-methylpentyl)-cyclopropane	3.77	3.94	398.22	18.35	45.85
9-methyl-5-undecene	4.93	4.41	538.54	22.60	58.08
2,2-iminobis-acetonitrile (iminodiacetonitrile)	0.05	-12.93	340.10	9.50	25.12
n-hexadecanoic acid methyl ester (metholene)	5.64	4.05	609.82	32.69	81.85
octadecanoic acid	6.40	1.26	774.16	34.53	36.29
2-ethyl-heptanoic acid	3.00	-3.41	424.91	18.01	44.85
1-nitrododecane	2.74	-0.27	604.91	24.63	62.77
9-octadecenoic acid, methyl ester	6.18	4.70	813.74	36.17	92.17
Erucic acid	7.73	-0.12	899.48	41.68	105.81
4,4-dimethyl-cyclohex-2-en-1-ol	1.97	-3.62	311.13	15.13	39.26
3-Cyclohexylpropanamide	1.40	-3.82	338.42	17.95	44.84
1,4-methano-2H-cyclopent(d}pxepin-2,5(4H)=dione,6,9-[(dimethylamino)methyl]hexahydro-8a-hydoxy-5a-methyl-9-(1-methylethyl)-	1.89	-2.19	456.28	22.44	82.03
1,10-decanediol (decamethylene glycol)	2.17	-9.53	523.80	20.40	51.67
3,3,5-trimethyl-1,4-hexadiene	3.32	1.59	387.01	16.91	43.87
1,1,3,3-tetramethylcyclopentane	3.51	3.35	367.25	16.52	41.05

The partition coefficient (P) describes the propensity of a neutral (uncharged) compound to dissolve in an immiscible biphasic system octan-1-ol and water. Negative values of logP indicates that the compound has higher affinity for water than octan-1-ol. Therefore, all the compound identified in the GCMS of ethanol extract of *Chromolaena odorate* seems to have strong affinity for octan-1-ol than water. Therefore, these compounds are more lipophilic than hydrophilic. The highest lipophilicity is displayed by erucic acid while the least is displayed by n-hexadecanoic acid methyl ester (metholene).

Hydration is the energy released when one mole of an ion dissolve. Therefore, positive value of hydration energy indicates that heat is absorbed while negative indicate that heat is released. The hydration energy was positive for 3,3,5-trimethyl-1,4-hexadiene,3,3,5-trimethyl-1,4-hexadiene, 9-octadecenoic acid, methyl ester, octadecanoic acid, n-hexadecanoic acid methyl ester (metholene), 3-, tetradecane,1-methyl-2-(3-methylpentyl)-cyclopro - pane and 9-methyl-5-undecene but negative for other nine components of the extract. The least negative value of hydration energy was recorded for

the molecule that had the highest molecular mass and highest logP.

Surface area of a molecular species is a significant factor in guiding adsorption, catalysis, reactivity and other properties. The highest surface area was recorded for erucic acid while least was recorded for 4,4-dimethyl-cyclohex-2-en-1-ol. Increase in surface area can increase adsorption, increase tendency for receptor ligand interaction and can thus affect the mode of adsorption.

Polarizability was also calculated for the detected compounds. Polarizability measures the behaviour of a molecular in the presence of charge and other molecules. Different molecules behave differently when they interact with charged system (Eddy and Essien, 2018; Eddy *et al*., 2020). The polarizability of erucic acid was also found to be the highest while that of 2,2-iminobis-acetonitrile (iminodia - cetonitrile) was the least. The results obtained led to the observation that the different molecules in ethanol extract of *Chromolaena odorate* will interact and behave differently in the presence of a charge system.

Refractivity is a molecular descriptor that represents the real volume of a molecular specie. Molar refractivity is related to the volume and the London dispersive force acting on the molecule. Therefore, higher refractivity points toward higher volume and higher interaction (Padron *et al.*,2002). This explain while erucic acid that has highest molar mass, surface area, polarizability also has the highest value of refractivity

3.2.2 Quantum chemical parameters

Quantum chemical descriptors calculated for molecules in ethanol extract of *Chromolaena odorate* leaf are presented in Table 3. This include the frontier molecular energies, the electronic energy, the core-core repulsion energy and the total molecular energy.

Quantum chemical indices are significant parameters that can be used to predict molecular reactivity, extent of adsorption and other processes (Eddy *et al*., 2020). The frontier molecular energy consist of the energy of the highest occupied molecular orbital (E_{HOMO}), the energy of the lowest unoccupied molecular orbital (E_{LUMO}) and the energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$)(ref). The E_{HOMO} is a quantum chemical descriptor that is associated with reactivity/adsorption of a molecular species. The higher the E_{HOMO}, the better the reactivity and extent of adsorption (ref). Eddy and Essien (2018) has also linked values of E_{HOMO} to toxicity of insecticides. On the other hand, better reactivity or adsorption is favoured by lower value of E_{LUMO} and ΔE (ref). E_{LUMO} is an index for acceptor tendency while E_{HOMO} is an index toward donation (Eddy and Ita, 2011a,b).

Table 3: Quantum chemical descriptors of compound identified in GCMS spectrum of ethanol extract of *Chromolaena odorate* leaf

Name	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	E_{CCR} (eV)	E_T (eV)	E_E (eV)
6-methyl-1-heptanol	-10.525	2.853	13.378	6477.20	-1521.91	-7999.20
3-tetradecene	-9.460	1.272	10.732	11388.73	-2098.84	-13487.57
3,5-di-tert-butylphenol)	-8.904	0.365	9.269	13909.14	-2312.99	-16222.13
1-methyl-2-(3-methyl - pentyl)-cyclopropane	-10.395	2.646	13.041	7603.52	-1498.56	-9100.55
9-methyl-5-undecene	-9.426	1.296	10.722	9456.80	-1798.85	-11255.65
2,2-iminobis-acetonitrile (iminodiacetonitrile)	-10.424	0.252	10.676	2988.06	-1115.84	-4103.90
n-hexadecanoic acid methyl ester (metholene)	-10.701	1.122	11.823	18238.98	-3139.95	-21378.93
Octadecanoic acid (stearic acid)	-10.801	0.933	11.734	19345.66	-3290.37	-22636.03
2-ethyl-heptanoic acid	-10.909	0.956	11.865	8814.55	-1940.62	-10755.17
1-nitrododecane	-10.969	0.018	10.987	12956.21	-2587.08	-15543.29
9-octadecenoic acid, methyl ester	-9.530	1.115	10.645	20275.376	-3412.17	-23687.55

Erucic acid (prifrac 299)	-9.558	0.939	10.497	24522.09	-3862.55	-28384.64
4,4-dimethyl-cyclohex-2-en-1-ol	-9.756	1.054	10.81	6391.88	-1467.27	-7859.145
3-cyclohexylproponamide (cyclohexylpropanamide)	-10.289	1.405	11.694	8532.61	-1817.96	-10350.57
1,4-methano-2H-cyclopent(d}pxepin-2,5(4H)-dione,6—9-[(dimethylamino)methyl] hexahydro-8a-hydoxy-5a-methyl-9-(1-methylethyl)-	-8.850	0.415	9.265	28663.21	-3820.73	-32483.95
1,10-decanediol	-10.553	2.820	13.373	9569.73	-2116.98	-11686.71
3,3,5-trimethyl-1,4-hexadiene	-9.303	1.206	10.509	6153.67	-1321.19	-7474.86
1,1,3,3-tetramethyl cyclopentane	-10.862	3.794	14.656	6904.44	-1349.69	-8254.12

The energy gap provides explanation for softness or hardness of a molecular specie. Hard molecules have higher energy gap while soft molecules have lower energy gap (Eddy *et al.*, 2011). Therefore, according to hard, soft acid base theory (HSAB), soft molecules are more reactive than hard molecules because lower energy is needed to transfer electron from the HOMO to the HOMO and thus facilitate reactivity or adsorption. Levels of variation of the frontier molecular energies of molecules detected in the GCMS of ethanol extract of *Chromolaena odorate* leaf are shown in Fig. 2.

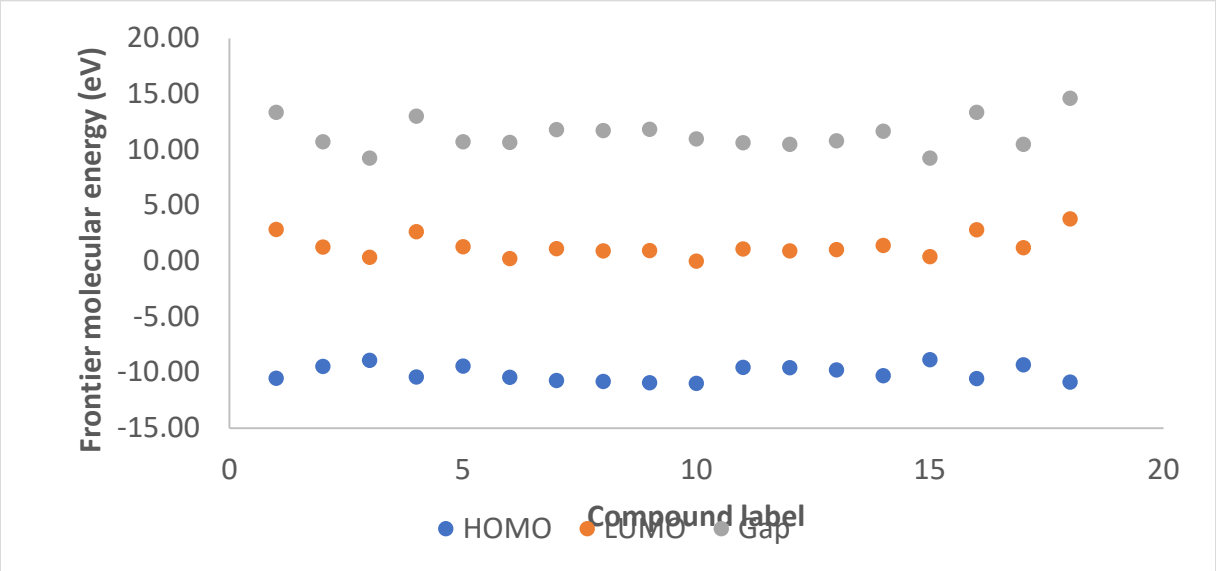


Fig. 2: Levels of frontier molecular energies of compounds in ethanol extract of *Chromolaena odorate* leaf

The independent axis stands for the labelling of the compounds according to their GCMS peak numbers. It is clearly indicated in the diagram that compound 15 (1,4-methano-2H-cyclopent(d}pxepin-2,5(4H)-dione,6—9-[(dimethylamino)methyl]hexahydro-8a-hydoxy-5a-methyl-9-(1-methylethyl)-) is the most reactive molecules in the extract while compound 18 (1,1,3,3-tetramethyl cyclopentane) is the least reactive molecule. Compound 15 is an alkaloid that contains hetero atoms (N and O) in their fussed ring system. The presence of N and O atoms might have conferred better

adsorption/reactivity property on the molecule (Eddy *et al.,*2018). On the other hand, these properties are lacking in 1,1,3,3-tetramethyl cyclopentane compared to other molecules. From the results obtained, frontier molecular orbital energies can be used in conjunction with other indices to predict the reactivity of compounds in ethanol extract of *Chromolaena odorate* leaf.

Other molecular energies that were considered in the study were electronic energy (E_E, which has strong correlation with density function), the core-core repulsion energy (E_{CCR}) and the total molecular energy. The trend for the variation of this energy with each other is shown in Fig. 3. The observed trend indicated no unique disparity with the information deduced from frontier molecular energies. However, reactivity seems to be favoured by decreasing value of electronic energy and increasing value of core-core repulsion energy. This observation does not conflict with findings reported by other with respect to variation of adsorption potential with electronic and core core repulsion energies (Ameh and Eddy, 2018;Eddy *et al*., 2020, 2018)

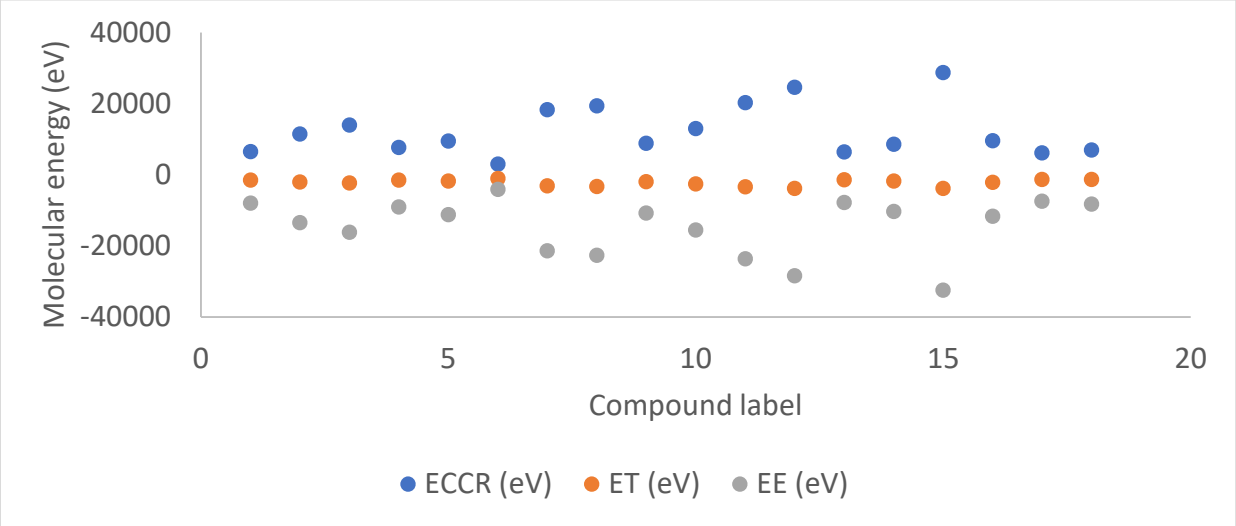


Fig. 3: Levels of electronic, core core and total molecular energies of compounds in ethanol extract of *Chromolaena odorate* leaf

4.0 Conclusion

Ethanol extract of *Chromolaena odorate* leaf contain useful biological molecules that can exhibit various biological activities. Some of the identified molecules are useful industrial intermediate while others like nobiline are major source of some drugs. Erucic acid is predicted to be the most hydrophilic molecules in the plant extract while nobilibe, 6-hydroxy is the most reactive molecule.

5.0 Acknowledgement

The author greatly acknowledges Prof. Nnabuk Okon Eddy of the Department of Pure and Industrial Chemistry for providing all the materials that were used for the study that generated this publication.

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