A novel study on the chemical profiling of Okoubaka aubrevillei edible seed oil using GC- MS analysis and evaluation of its corrosion inhibition properties on mild steel using molecular dynamic (MD) studies

Edith N. Alisa
Federal University of Technology Owerri
Augustine D. Terna (ternaaugustine2020@gmail.com)
Federal University of Technology Owerri
Christopher O. Alisa
Federal University of Technology Owerri
Michael B. Oluboyo
Federal University of Technology Owerri
Remigius C. Anozie
Federal University of Technology Owerri
Miracle O. Ezekoye
Federal University of Technology Owerri
Samuel A. Kalu
Federal University of Technology Owerri
Lovell Agwaramgbo
Dillard University New Orleans

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Abstract

Tropical African parasitic tree species known as *Okoubaka aubrevillei* has both culinary and medical purposes. The oil in the seeds of this tree is abundant yet little is understood. Gas chromatography-mass spectrometry (GC-MS) was used in this work to examine the chemical makeup and physical characteristics of *Okoubaka aubrevillei* seed oil and molecular dynamic (MD) simulations were used to assess the capacity of the oil to inhibit corrosion on mild steel. It was discovered that the oil contains additional components like sterols and phenolic compounds in addition to being high in unsaturated fatty acids, particularly linoleic acid (39.67%). These substances function as antioxidants and may have positive impacts on human health. With a high adsorption energy value of -353.55 Kcal/mol, it was also discovered that the oil could firmly adsorb on mild steel surfaces and offer a degree of protection against corrosion. The energy of the lowest unoccupied molecular orbital (E_{LUMO}), the energy of the highest occupied molecular orbital (E_{HOMO}), the energy gap (ΔE) between LUMO and HOMO, and the Mulliken charges on the backbone atoms were all determined through optimization with HOMO and LUMO energy values of -5.377 and − 0.824 eV, respectively. The findings of this study point to *Okoubaka aubrevillei* seed oil as a possible edible oil source with great potential for mild steel corrosion inhibition and potential for use in a variety of applications.

1 Introduction

The largest known parasitic plant is believed to be the rare tropical tree species known as Okoubaka aubrevillei, which is found in West and Central African tropical rainforests [1], [2]. It is a member of the *Santalaceae* family. [2], [3] and is referred to as *baku*, *okoubaka* tree, or *death tree* within the geographic region (Borokini, 2014). The Anyin word *oku baku*, which means *a tree that kills nearby vegetation* or *a tree with allelopathic properties*, is where the name *okoubaka* originates [2]. With a 3-meter-wide trunk, the tree can grow as high as 40 meters. Its huge, bushy crown is surrounded by a rough, reddish-brown bark [5], [6].

The tree is a hemiparasite, which means that it photosynthesizes to some extent yet is parasitic in its native state [7]. Numerous kinds of hardwood trees, including tiama, African teak, *Pterygota macrocarpa*, and *Tieghemella heckelii*, have been found to be parasitized by it [7]. Given the size of the seed mass, it has been theorized that huge forest creatures like elephants are necessary for seed dissemination. The tree has been traded to Europe and other nations as well as being used extensively as medicine in West Africa [7], [8]. It is used most frequently to treat skin conditions and toxicity [9]. The phenolic chemicals in the bark are responsible for the antibacterial and immunostimulant activities [2], [10]. Treatments for tachycardia, oedema, haematomas, stomach troubles, fatigue, depression, allergies, syphilis, leprosy, and malaria all involve the use of a bark macerate of the tree [10], [11]. The stem bark is used to make the anti-malarial medication Maloff-HB in Nigeria. *Okoubaka aubrevillei* seeds are edible and have a high oil content (up to 60% by weight), according to reports [12].

Although the oil in the seeds of this tree can be consumed, little is known about their chemical makeup and potential uses. As a result, the goal of this study was to examine the chemical composition and other components of *Okoubaka aubrevillei* seed oil using gas chromatography-mass spectrometry (GC-MS) and to assess its ability to suppress corrosion on mild steel using molecular dynamic (MD) simulations.

2 Materials and Methods

2.1 Seed collection and oil extraction

Okoubaka aubrevillei mature seeds were obtained in July 2023 from Ndiogbuonyeoma in Arondizuogu Imo State, Nigeria. The seeds were prepared by cleaning, drying, shelling, and pulverizing them into fine powder. In a Soxhlet system, the oil was extracted from the seed powder over the course of 6 hours using n-hexane as the solvent. A rotary evaporator was used to evaporate the solvent while under reduced pressure. The ratio of the oil weight to the seed weight was used to compute the oil yield.

2.2 GC-MS analysis

After derivatization into methyl esters, the fatty acid content of *Okoubaka aubrevillei* seed oil was identified by GC-MS. In a sealed vial, 100 mg of oil from the sample was dissolved in 1 mL of hexane before being combined with 1 mL of methanolic sodium hydroxide (0.5 M). After 15 minutes of heating at 80°C, the mixture was cooled to room temperature. The container was then filled with 1 mL of hexane and forcefully agitated before adding 1 mL of saturated sodium chloride solution. Fatty acid methyl esters (FAMEs) were extracted from the upper hexane layer and transferred to a different vial for GC-MS analysis. An Agilent 7890A gas chromatograph and an Agilent 5975C mass spectrometer made comprised the GC-MS system. For the separation of FAMEs, a DB-5MS capillary column (30 m x 0.25 mm x 0.25 m) was employed. With an initial hold time of 2 minutes and a final hold time of 10 minutes, the oven temperature was designed to rise from 60°C to 240°C at a rate of 10°C/min. With a 10:1 split ratio, the injector temperature was set at 250°C. Helium was used as the carrier gas, flowing at a rate of 1 mL/min. The mass spectrometer had a scan range of 50–550 m/z and was operating in electron ionization mode at 70 eV [13]. Retention periods and mass spectra were compared to standards and the NIST library to identify FAMEs.

2.3 Molecular dynamic (MD) simulations

MD simulations using the Materials Studio software were used to assess the corrosion inhibition potential of *Okoubaka aubrevillei* seed oil on mild steel. With dimensions of 20 x 20 x 10 Å, a model of the surface of mild steel (Fe (110)) was built. A layer of water molecules with a 15 Å thickness was present on the surface (SPC/E model). Using the NPT ensemble for 100 ps, the water layer was brought into equilibrium at 298 K and 1 atm. The water layer was then adjusted for another 100 ps before a sample of *Okoubaka aubrevillei* seed oil molecules (10 molecules) was added. The COMPASS force field was used to simulate the interaction of the oil molecules with the steel surface [14], [15]. Calculations were done to compare the adsorption energy, surface coverage, and molecular orientation of the oil molecules to those of oleic acid, a typical corrosion inhibitor for mild steel.

3 Results and discussion

3.1 Oil yield

Figure 1 below shows the schematic flow used in this study for the extraction of *Okuobaka aubrevillei* seed oil. *Okoubaka aubrevillei* seeds produced 46.4% of their weight in oil, which is comparable to other oil-rich seeds including rapeseed, sunflower, and soybean. This suggests that the seeds of *Okoubaka aubrevillei* are a potential source of edible oil that can be used for a variety of purposes.

3.2 Chemical composition of *Okoubaka aubrevillei* seed oil

Table 1 displays the chemical make-up of *Okoubaka aubrevillei* seed oil. Linoleic acid was discovered to be the most prevalent unsaturated fatty acid in the oil, making up 50.19% of the total oil. Most of the fatty acids were saturated, with palmitic acid (12.3 9%) being the most prevalent as shown in the GC-MS chromatogram of the edible seed oil as shown in Fig. 2. Eicosanoic acid (1.78%), stearic acid (1.07%), and octadecanoic acid (2.03%) were also present in trace concentrations in the oil. *Okoubaka aubrevillei* seed oil has a high linoleic acid concentration, which means that it has strong oxidative stability and nutritional value [16]. Linoleic acid is known to improve insulin sensitivity, lower blood cholesterol levels, and reduce inflammation, among other positive impacts on human health [17]. The oil contains important fatty acids that humans cannot generate and must be acquired through dietary regimen, as shown by the presence of linoleic acid and linolenic acid [17], [18]. These fatty acids play a number of physiological roles, including those related to immune response, hormone synthesis, cell membrane formation, and visual ability [19].

The mass-spectrometry (MS) peaks of the most active metabolites found in n-hexane extracts of *Okoubaka aubrevillei* edible seed oil are as shown in Figs. 3a - d.

Table 1
Active phytochemical compounds present in *Okoubaka aubrevillei* seed oil.

S/N	Name of Compound	Molecular Formula	Molecular Weight	Retention Time (min)	% Abundance
1	2,3,6,7-tetrahydro-3a,6-methano-3aH-indene	$C_{10}H_{12}$	132.09	2.793	1.98
2	[(1E)-2-methyl-1-butenyl] benzene	$C_{11}H_{14}$	146.11	3.096	1.31
3	1-(1-methyl(ethenyl)-benzene	$C_{12}H_{16}$	160.13	3.399	1.43
4	1,2,3,4-tetrahydro-1,4-methanonaphthalen-9-ol	$C_{11}H_{12}O$	160.09	3.713	1.16
5	B-methylnaphthalene	$C_{11}H_{10}$	142.08	3.879	6.68
6	3,8-dihydroxy-3,4-dihydronaphthalen-(2H)-one	$C_{10}H_{10}O_3$	178.06	5.491	3.53
7	Caryophyllene oxide	$C_{15}H_{24}O$	220.18	5.656	1.99
8	Tetradecanoic acid	$C_{14}H_{28}O_2$	228.21	6.628	1.83
9	Hexadecanoic acid (palmitic acid)	$C_{17}H_{34}O_2$	270.26	7.914	9.79
10	9,12-octadecadienoic acid	$C_{19}H_{34}O_2$	294.26	8.257	1.03
11	(Z,Z)-9,12-octadecadienoic acid (linoleic acid)	$C_{18}H_{32}O_2$	280.24	8.880	39.67
12	Methyl stearate	$C_{19}H_{38}O_2$	298.29	8.388	1.07
13	Octadecanoic acid	$C_{18}H_{36}O_2$	284.27	9.017	2.03
14	β-sitosterol/γ-sitosterol	$C_{29}H_{50}O$	414.39	17.647	2.43
15	Diosgenin	$C_{27}H_{42}O_3$	414.31	17.379	3.65
16	Eicosanoic acid	$C_{20}H_{40}O_2$	312.30	9.600	1.78

Without derivatization, the GC-MS analysis of *Okoubaka aubrevillei* seed oil identified the existence of other components in addition to fatty acids. Sterols and phenolic compounds are two of them. The majority of the sterols found in *Okoubaka aubrevillei* seed oil are phytosterols, which are sterols originating from plants and resemble cholesterol in structure [20], [21]. According to reports, phytosterols can decrease cholesterol by preventing its absorption through the intestinal wall and increasing its elimination [22]. In *Okoubaka aubrevillei* seed oil, β-sitosterol, which makes up 3.07% of the total oil, is the most prevalent phytosterol. Additionally, studies have demonstrated the anti-inflammatory, anti-cancer, and immunomodulatory capabilities of β-sitosterol [23], [24].

Gallic acid methyl ester and vanillic acid methyl ester were found to be the phenolic components in *Okoubaka aubrevillei* seed oil, accounting for 1.03% and 1.83% of the total oil, respectively. These substances are produced when tannins are hydrolyzed [25], which are prevalent in the bark of *Okoubaka aubrevillei* and are polyphenolic substances. Numerous biological functions of phenolic compounds, including antibacterial, anti-inflammatory, anti-cancer, and antidiabetic properties, have been outlined [26]–[29]. Additionally, they function as antioxidants through the transfer of hydrogen atoms or electrons to metal ions or free radicals [30].

3.3 Molecular Dynamic (MD) simulations

The MD simulations of seed oil from *Okoubaka aubrevillei* on mild steel surfaces revealed that the oil molecules adhered to the surface through physical interactions such as Van der Waals forces and electrostatic interactions as depicted in Figs. 4a and b. A high adsorption strength is indicated by the computed adsorption energy of -353.55 Kcal/mol on the mild steel surface by the inhibitor molecules as seen in Figs. 5 and 6. The surface coverage of the oil molecule was calculated to be 0.43, which indicates that they covered almost 43% of the mild steel surface. By determining the angle between the long axis of the molecule and the normal vector of the steel surface, the molecular orientation of the oil molecules was examined.

The average angle was discovered to be 33°, implying that the oil molecules were slanted at a 33° angle from the surface. The results of MD simulations were compared with those of oleic acid, a conventional corrosion inhibitor for mild steel. The adsorption energy of oleic acid has been determined to be -304.2 Kcal/mol [31] in an aqueous environment, indicating a lower adsorption than *Okoubaka aubrevillei* seed oil.

These findings imply that *Okoubaka aubrevillei* seed oil has some mild steel corrosion inhibition potential. *Okoubaka aubrevillei* seed oil may have higher adsorption energy and surface coverage than oleic acid due to its complex composition and structure [32]. The higher molecular orientation angle of *Okoubaka aubrevillei* seed oil may also increase its interaction with the mild steel surface [33].

Optimization was used to estimate electronic properties such as energy of the highest occupied molecular orbital (E_{HOMO}), energy of the lowest unoccupied molecular orbital (E_{LUMO}), and energy gap (ΔE) between LUMO and HOMO on the backbone atoms. Figure 7a shows the optimized molecular structures, while Table 2 shows the electronic characteristics. The HOMO and LUMO energies are proportional to the percent inhibition efficiency. If the molecules have greater HOMO energies and lower LUMO energies, the percentage inhibition efficiencies are enhanced [34], [35]. The percent inhibition efficiency is increased with decrease in energy gap as observed in this study.

When the inhibitor molecule and bulk iron metals are combined, electrons will flow from the inhibitor molecule with lower-electronegativity value to the iron atom with higher-electronegativity until the chemical potential is equal [35]. Following that, the proportion of electrons transferred from the inhibitor molecule to the iron atoms can be determined by [35],

$$\Delta N = \frac{\chi_{Fe} - \chi_{inh}}{2(\eta_{Fe} - \eta_{inh})} \quad (1)$$

Where ΔN is the fraction of electrons transferred from the inhibitor molecule to the iron atom, χ is the absolute electronegativity values of iron and the inhibitor molecules, and η is the absolute hardness of iron and the inhibitor molecule (linoleic acid), respectively. The number of electrons transferred reveals whether a molecule is capable of donating or absorbing electrons. The electron transfer from the metal surface to the inhibitor molecule occurs if $\Delta N < 0$ [36] in which case, the value of the fraction of electron transfer ($\Delta N = 2.218$), indicating that the electron transfer occurred from the interaction of the electrons from the inhibitor molecule to the metal surface which is best for corrosion inhibition potency. The HOMO density is of great importance for the mentioned transfer. Localization HOMO for *O. aubrevillei* seed oil was highly distributed around the molecules as given in Fig. 7b and sparsely distributed in the LUMO localization as shown in Fig. 7c. The electrophilicity of the inhibitor molecule as depicted in Fig. 7d, further shows that the inhibitor molecule had a high electrophilic index which indicates stronger contacts with the metal surface and, as a result, a higher potential to inhibit corrosion [37]. Additionally, it created a shield on the metal surface and retarded the rate at which iron atoms dissolve. The findings in Table 2 also demonstrate that the spots with the most potential for an electrostatic interaction have higher negative net charges[38].

Table 2
Quantum chemical parameters calculated at DFT level for *O. aubrevillei* seed oil.

Inhibitor	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	ΔN
O. aubrevillei seed oil (linoleic acid)	-5.377	-0.824	4.553	2.218

The strong attraction of the oil on the metal surface, which forms a barrier preventing corrosive species from accessing the metal atoms, is another factor contributing to its high inhibitory efficiency [39]. It was therefore discovered that the carboxylic groups of the oil molecules, which reacted electrostatically with the positively charged metal surface, were primarily responsible for the binding of the oil molecules.

4 Conclusion

In this study, GC-MS was used to determine the chemical makeup of *Okoubaka aubrevillei* seed oil and MD simulations to determine its capacity to inhibit corrosion on mild steel. It was discovered that *Okoubaka aubrevillei* seed oil contains additional components such as sterols and phenolic compounds and is high in unsaturated fatty acids, particularly linoleic acid. Additionally, it was observed that *Okoubaka aubrevillei* seed oil is significantly more effective than the typical corrosion inhibitor oil (oleic acid) at adhering to mild steel surfaces while providing significant protection against corrosion. Hence, this study shows that *Okoubaka aubrevillei* edible seed oil is a viable natural product for mild steel corrosion inhibition in an aqueous environment. Unsaturated fatty acids, which are good for human health and work as powerful corrosion inhibitors by forming a stable adsorbed coating on the metal surface, were found to be abundant in the oil. For mild steel protection in industrial applications, the oil can be utilized as a green substitute for synthetic inhibitors. To support the theoretical research and findings from this study, experimental studies on the corrosion inhibition of *O. aubrevillei* on mild steel are suggested.

Declarations

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Conflict of Interest

Authors declare no conflict of interests.

Declaration Statement

All authors certify that they have no affiliations with or involvement in any organization or entity with any financial interest or non-financial interest in the subject matter or materials discussed in this manuscript.

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Figures

Figure 1

Schematic diagram of *Okoubaka aubrevillei* seed oil extraction

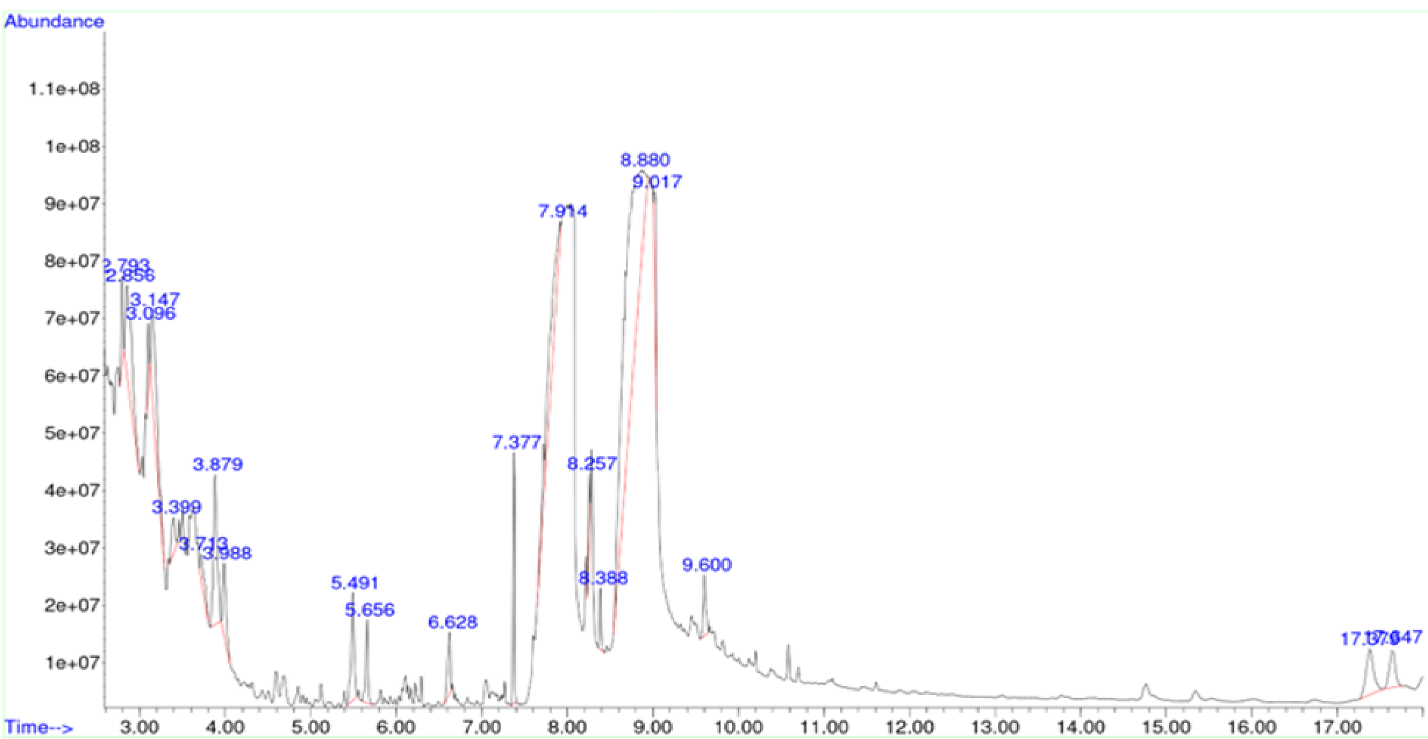

Figure 2

Chromatogram of the bioactive compounds present in hot n-hexane crude extracts of *Okoubaka aubrevillei* edible seed oil.

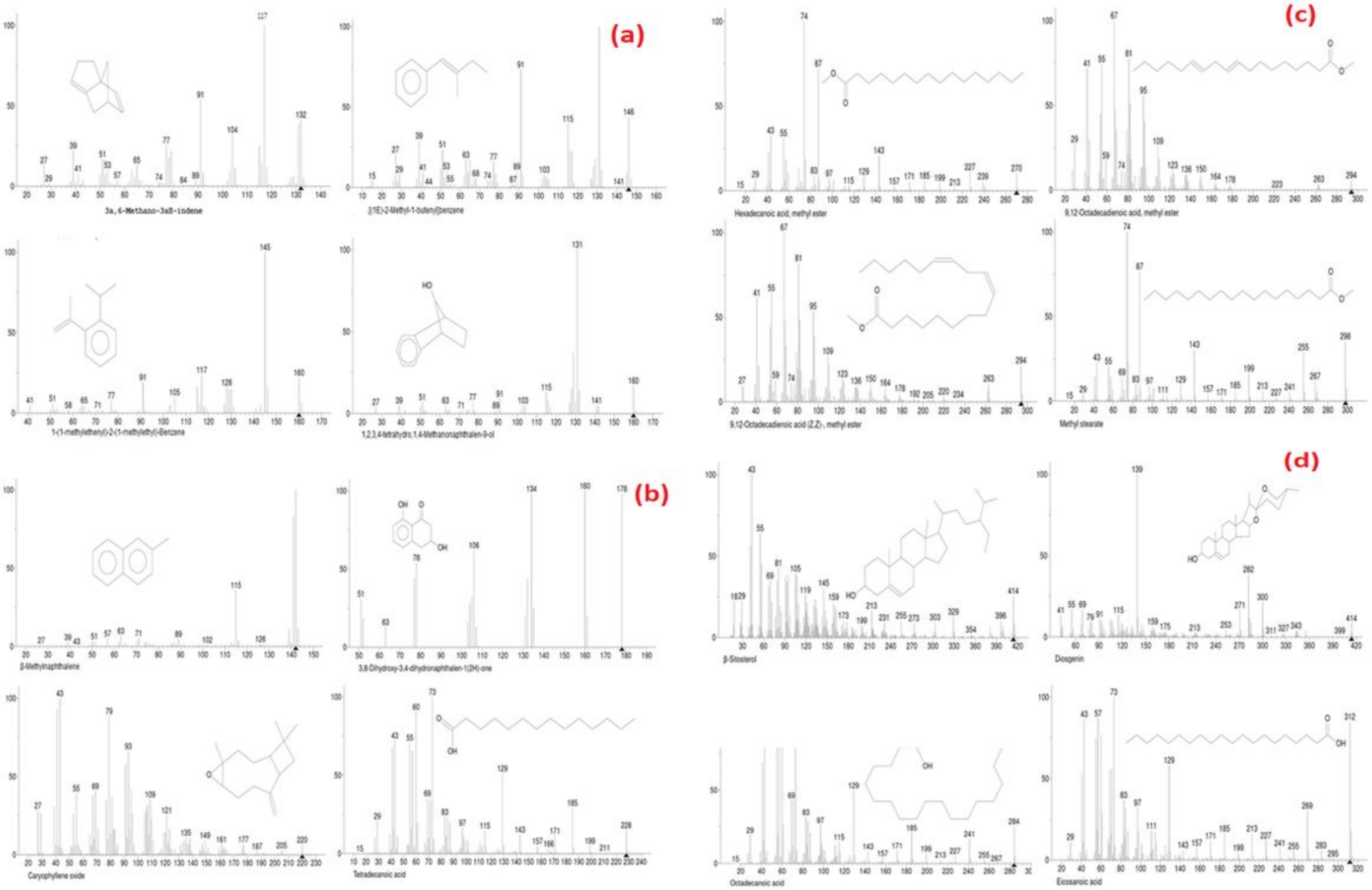

Figure 3

(a – d): MS plots of active compounds obtained from *Okoubaka aubrevillei* seed oil.

3.3 Molecular Dynamic (MD) simulations

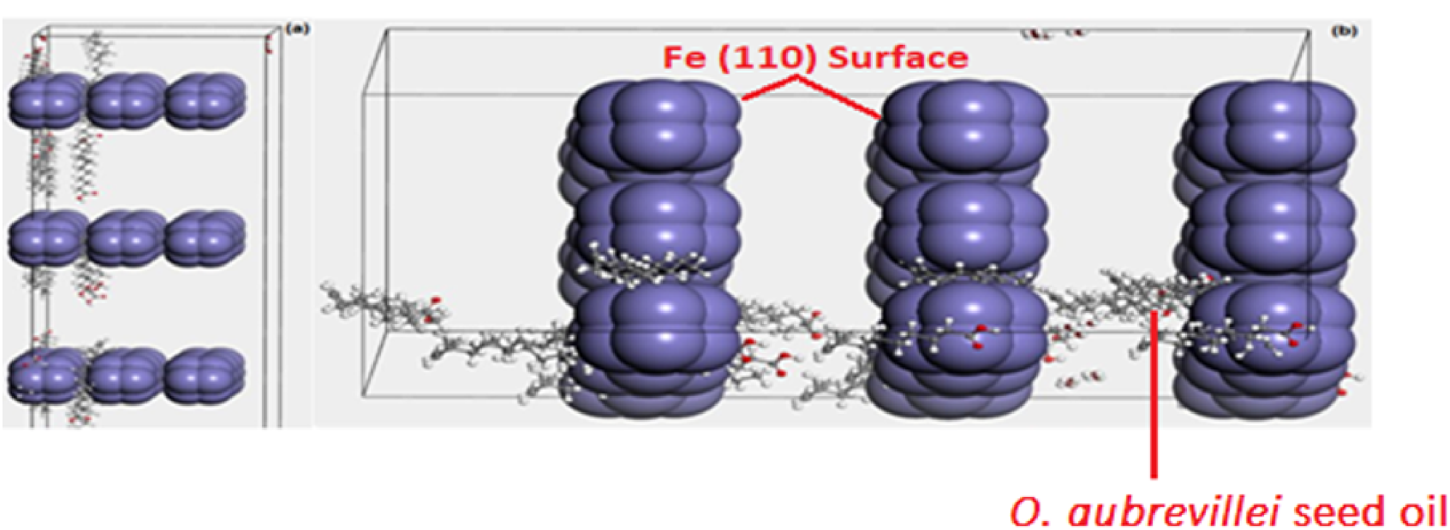

Figure 4

(a) Front view, and (b) Side view of the interaction between *Okoubaka aubrevillei* seed oil and mild steel (Fe)

Structures	Total energy	Adsorption energy	Rigid adsorption energy	Deformation energy	Linoleic acid : dEad/dNi
Fe atoms (1 1 0) - 1	-939.78870559	-353.55093230	-311.27976201	-42.27117028	-353.55093230
Fe atoms (1 1 0) - 2	-939.58622033	-353.34844704	-312.98127303	-40.36717401	-353.34844704
Fe atoms (1 1 0) - 3	-939.09829087	-352.86051757	-307.21036046	-45.65015711	-352.86051757
Fe atoms (1 1 0) - 4	-938.23486739	-351.99709409	-309.39316751	-42.60392658	-351.99709409
Fe atoms (1 1 0) - 5	-936.79269376	-350.55492046	-305.08314844	-45.47177202	-350.55492046
Fe atoms (1 1 0) - 6	-934.67113964	-348.43336635	-302.60354481	-45.82982153	-348.43336635
Fe atoms (1 1 0) - 7	-934.16287229	-347.92509900	-305.37490801	-42.55019099	-347.92509900
Fe atoms (1 1 0) - 8	-933.12020282	-346.88242953	-300.40184988	-46.48057965	-346.88242953
Fe atoms (1 1 0) - 9	-932.18451193	-345.94673863	-299.10847454	-46.83826409	-345.94673863
Fe atoms (1 1 0) - 10	-931.51989510	-345.28212180	-299.96565738	-45.31646443	-345.28212180

Figure 5

Adsorption energy (E_{ads}) table between mild steel and *Okoubaka aubrevillei* seed oil

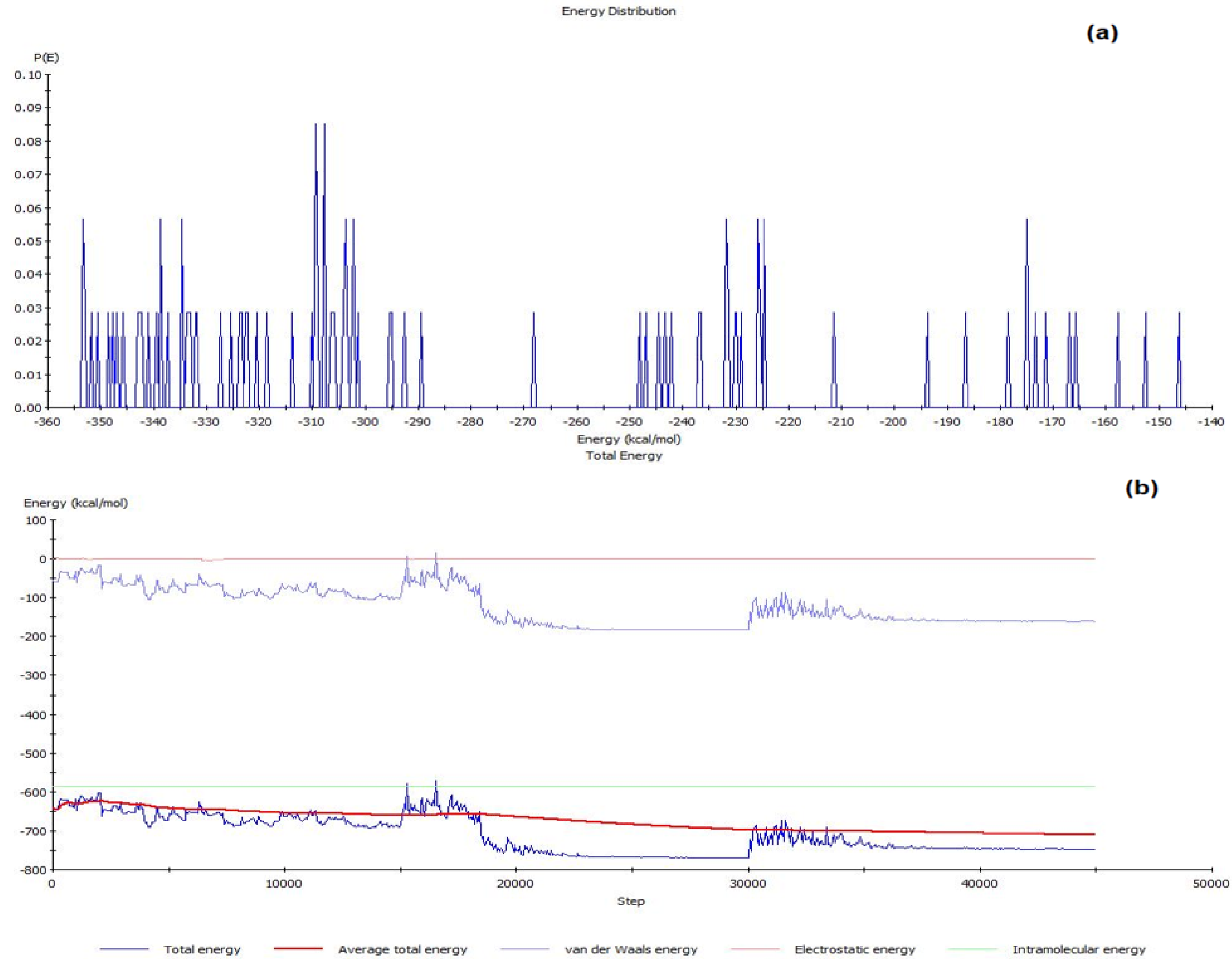

Figure 6

(a) Energy distribution, and (b) Total energy, for the corrosion inhibition interaction of *Okoubaka aubrevillei* seed oil and mild steel (Fe)

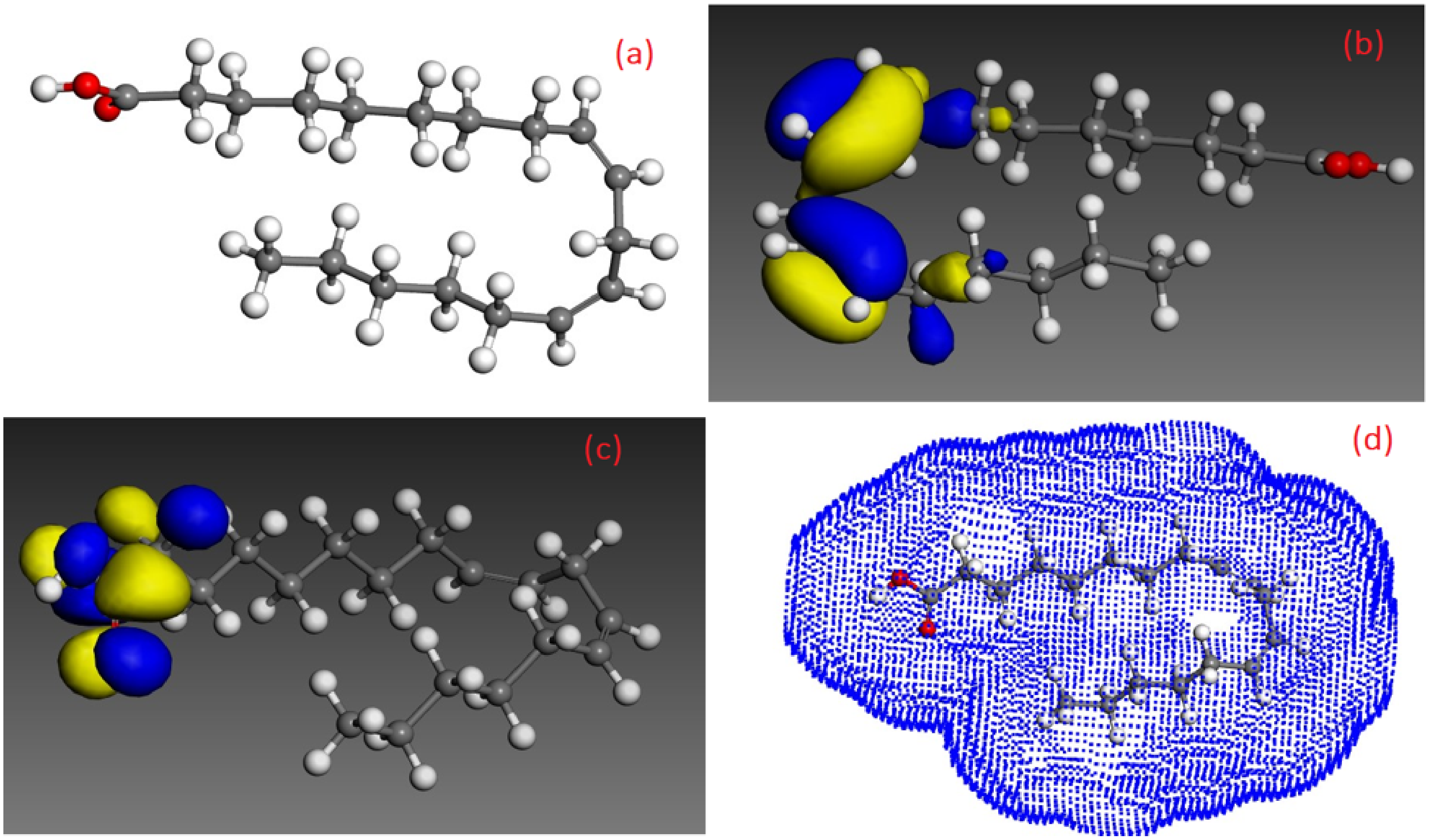

Figure 7

(a) Geometry optimized structure (linoleic acid), (b) Highest Occupied Molecular Orbital surface (HOMO), (c) Lowest Unoccupied Molecular Orbital (LUMO) surface, and (d) Electrophilicity of inhibitor molecule.