

Electrochemical and Computational study of the Ocimum Americanum Extract for steel in Acidic medium: A Green Pathway to reduce the corrosion of steel

Abhishek Sharma

Chandigarh University

Raghvi Jande

Chandigarh University

Akhil Saxena

akhil.uis@cumail.in

Chandigarh University

Jasdeep Kaur

Chandigarh University

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Abstract

This study explores the potential of *Ocimum Americanum* as an environmentally friendly steel corrosion inhibitor in an acidic medium, as many industrial applications suffer from corrosion. The study aims to reduce corrosion by utilizing *Ocimum Americanum*'s inherent benefits as an eco-friendly alternative to traditional inhibitors. The capacity of *Ocimum Americanum* to regulate corrosion was evaluated using various surface analytical and electrochemical techniques. Steel was tested for corrosion using PDP and EIS in an acidic medium containing extract from *Ocimum Americanum* at varying concentrations. *Ocimum Americanum*'s efficiency as a green corrosion inhibitor was demonstrated through surface examination techniques like SEM and UV, revealing a significant reduction in corrosion rate. The study found that *Ocimum Americanum* extracts form a protective layer on mild steel surfaces, limiting corrosive attack in acidic media due to morphological changes and functional groups. The study evaluated the environmental friendliness of *Ocimum Americanum* as a corrosion inhibitor, focusing on its biodegradability and toxicity compared to conventional chemical inhibitors. *Ocimum Americanum*'s sustained quality provides a strong argument for its use in economic sectors to mitigate environmental harm.

1. INTRODUCTION

Steel is a strong, fracture-resistant iron and carbon alloy used in several sectors because of its tensile strength and inexpensive. Along with iron, manganese, and carbon steel comprises various other metal elements in it. Due to the presence of different types of elements in steel, it comes into four types which are Carbon, alloy, mild, and stainless steel. Steel's evolution began 4,000 years ago during the Iron Age, replacing bronze in tools and weapons due to its strength and durability. Initially, steel was produced in bloomery furnaces but Henry Bessemer's discovery of oxygen-based methods in 1856 to lower iron carbon content marked the greatest innovation in steel history, establishing the modern steel industry. Steel consumption is expected to continue growing globally in 2024, with a global increase of 20–30 million tons.[1] The building and infrastructure industry is the primary steel user, accounting for 41% of global demand, with other industries like energy, automotive, and machinery also contributing significantly [2][3]. The building and infrastructure industry is the primary steel user, accounting for 41% of global demand, with other industries like energy, automotive, and machinery also contributing significantly [4]. Steel is extensively utilized in the automotive industry for automobile production and in the agriculture sector for farming equipment like tractors, barns, and silos [5]. Steel is a crucial material in packing materials and transportation due to its exceptional toughness [6]. Steel is a crucial material in transportation due to its high durability and is also utilized in packing materials. Steel buildings are constructed faster due to prefabrication methods, which in turn reduce project timelines. Steel buildings are environmentally friendly and sustainable due to their indefinite recycling capabilities.

Corrosion is a natural process where metals, when combined with atmospheric moisture and oxygen, create metal oxides [7]. This slow, harmful process can deteriorate the material's physical and

mechanical properties, with factors like temperature, humidity, and corrosive materials influencing its development [8].

Acid corrosion is the corrosive action of acids, causing material deterioration or disintegration. Common acids include sulfuric, hydrochloric, and nitric acids. It can lead to material loss, pits or fissures, and structural deterioration [9]. Industries must use corrosion-resistant materials or protective coatings to mitigate its harmful effects [10].

Some of the methods applied for corrosion mitigation are summarized as follows,

- Alloying – Corrosion susceptibility can be greatly decreased by using corrosion-resistant alloys when fabricating metal components. Aluminum and stainless steel are two examples [11].
- Hot-dip galvanization - Dipping steel in molten zinc creates a strong, bonded alloy layer, a method used for over 250 years to prevent corrosion on playground equipment and creative sculptures [12]. Galvanization requires immediate removal of equipment, potentially due to equipment size, zinc peeling or chipping, prolonged exposure to elements, and the release of poisonous fumes, necessitating further care [13].
- Covers for barriers - Paint, plastic, or powder are examples of barrier coatings that are easy to use and economical methods to prevent corrosion, using powdered like urethane and epoxy to adhere to metallic surfaces [14]. The paint works as a preventing layer that keeps the electrochemical charge off the metal's surface generated by corrosive substances [15].
- Protective cathodic layer - The protective cathodic layer uses electrochemical methods, with galvanic anodes providing electrons to change active sites on metal surfaces into passive ones, preventing corrosion [16]. Although anodes require regular inspections, wear down over time, and can raise maintenance costs, cathodic protection is an effective method. High-resistivity situations may not always be effective, adding weight to the structure.

A chemical compound known as a corrosion inhibitor lowers the rate of corrosion in a liquid or gas, depending on the fluid's composition, water content, and flow pattern [17]. They are commonly used in industry and over-the-counter items to prevent leaks in pipes [18]. Naturally occurring and synthetic corrosion inhibitors are the two main categories of corrosion inhibitors (Fig. 1).

Natural occurring inhibitors control corrosion rates by applying a natural ingredient into pickling or cleaning solutions, inhibiting oxidation or reduction, and creating a layer of protection at the metal's surface through material or chemisorption [19].

Synthetic inhibitors, such as phosphates, nitrites, and amine salts, are highly effective and reliable in corrosive conditions. They react with corrosive chemicals, creating a protective coating on metal surfaces [20]. Synthetic inhibitors are ideal for maintenance-intensive applications like offshore platforms, pipelines, and nuclear power facilities, but require careful selection and dosage to avoid environmental harm and system interference [21].

Other names for *Ocimum Americanum* include lime, American, and hoary basil. It belongs to the Lamiaceae family of annual herbs. Africa, the Indian Subcontinent, China, and Southeast Asia are its original home regions [22]. Additionally, this herb has therapeutic qualities. The literature research indicates that luteolin, quinic acid, and jasmonic acid are the three main phytochemicals found in *Ocimum Americanum* [23] as shown in Fig. 2. A brief summary of the natural corrosion inhibitors is reported in the Table 1.

Table 1
Summary of some recently worked natural corrosion inhibitors

S.NO	PLANT NAME	BOTANICAL NAME	METHODS USED	MEDIUM USED	EFFICIENCY
1	Flannel weed	<i>Sida cardifolia</i>	Weight loss, EC Studies, UV-Vis, FTIR	0.5M H ₂ SO ₄	98.96%
2	Blood bananas	<i>Musa acuminata</i>	UV- VIS, FTIR, Adsorption Isotherm	0.5M H ₂ SO ₄	85.69%
3	Orange	<i>Citrus sinensis</i>	Weight loss, EIS, EFM	0.5M H ₂ SO ₄	80.00%
4	Giant dodder	<i>Cuscuta reflexa</i>	Weight loss, UV, FTIR, EIS, SEM	0.5M H ₂ SO ₄	95.47%
5	Nutmeg	<i>Myristica fragrans</i>	Weight loss, UV, IR, EIS, SEM	0.5M H ₂ SO ₄	87.81%
6	Ashoka tree	<i>Saracha ashoka</i>	Weight loss, UV, FTIR,	0.5M H ₂ SO ₄	95.48%
7	Holy Basil	<i>Ocimum Sanctum</i>	Weight loss, Thermometric studies	0.5N HCl	98.67%
8	Chebulic Myrobalan	<i>Terminalia chebula</i>	UV-VIS, FTIR, Adsorption isotherm, EIS	0.5M H ₂ SO ₄	93.23%
9	Hairy basil	<i>Ocimum americanum</i>	Weight loss, UV, IR, EC Studies	0.5M H ₂ SO ₄	85.15%
10	Neem	<i>Azadirachta indica</i>	EC Studies, Adsorption studies	0.5M H ₂ SO ₄	85.05%
11	Tulsi	<i>Ocimum tenuiflorum</i>	Weight loss,	0.5N HCl 2N HNO ₃	98.67% IN HCl, 71.62% in 2N HNO ₃
12	Sandalwood	<i>Santalum album</i>	FTIR, SEM	1N HCl	93.12%
13	Onion peels	<i>Allium Cepa</i>	Weight loss, EC Studies	1M HCl	94.055

The primary goal of all this work is to use *Ocimum Americanum* extract as a novel pickling agent for steel in an acidic environment.

2. EXPERIMENTAL WORK

2.1 PREPARATION OF CORROSIVE MEDIUM

The 0.5M H₂SO₄ was prepared by dissolving Conc. H₂SO₄ in double-distilled water after purchasing concentrated H₂SO₄ from Loba Chemie AR grade [24]. The specific portions of the extract of *Ocimum Americanum* were dissolved in 0.5 M H₂SO₄ preparing different concentrations (1000ppm, 1500ppm, 2000 ppm) of the plant extract [25]. The plant extract's highest solubility was shown in 0.5M sulphuric acid, with 2000 ppm being the highest solubility.

2.2 PREPARATION OF STEEL STRIPS

The metal (mild steel) utilized in the study has the following composition: iron makes up 99.2%, with phosphorous, sulfur, carbon, silicon, and manganese present in the following proportions: 0.120%, 0.105%, 0.378%, 0.079%, and 0.0795%, respectively [26]. The surface area of steel samples is 1cm². Multiple sandpapers of different grades were used to clean the steel coupon's surface before examining the corrosion on them.

2.3 PREPARATION OF PLANT EXTRACT

The *Ocimum Americanum* was purchased from the local fields of Kharar, Punjab, India. During the cleaning process, sand and dust were removed, after which it was washed in double-distilled water and let to air dry for three days. After drying, the sample was roughly crushed and then refluxed with the mixture of ethanol and distilled water having a ratio (50:50) ml, at 343K for around 30 hours with the help of a Soxhlet instrument. Then, to remove contaminants, the finished solution was filtered. Following the extraction process, the extract was dried in a hot water bath.

2.4 WEIGHT LOSS STUDIES

Here, we used a 100 ml volume of the corrosive solution for the weight loss trials. Therefore, we immersed mild steels with 1 cm² size in the corrosive media for 24 hours to perform weight reduction studies [27]. The coupons made of mild steel were precisely weighed both before and after being immersed in the corrosive solution. For each mild steel sample, three tests were carried out [28]. The following equations were used to determine the weight loss data are-

$$\% = \frac{W_0 - W_i}{W_0} \times 100$$

1

$$\theta = \frac{W_0 - W_i}{W_0}$$

2

w₀ and w_i → the decrease in weight when inhibitors are absent and present.

2.5 UV – VISIBLE SPECTRA ANALYSIS

A UV-visible spectrophotometer was also used to examine an extract of *Ocimum Americanum* in 0.5M H₂SO₄. We conducted UV/visible experiments on solutions in which steel specimens were dipped for 24 hours as well as on solutions in which steel specimens were not dipped, in order to examine the adsorption and desorption of the *Ocimum Americanum* extract [29]. Both spectra were analyzed to completely understand the inhibitory mechanism.

2.6 SURFACE ANALYSIS

SEM Of steel was also used to estimate the corrosion-protection procedure. SEM images were utilized to analyze specimens that had been cleansed and immersed in an acidic solution for a day, both with and without an inhibitor [30].

2.7 ELECTROCHEMICAL STUDIES

Steel coupons were subjected to electrochemical investigation using a PGSTAT-204 Metrohm Auto lab electrochemical analyzer. Three electrodes were attached to the corrosion cell: the counter electrode (platinum), the working electrode (steel), and the reference electrode (calomel) [31]. After coating the steel surface with araldite resin, 1 cm² was left uncovered for reaction. The Tafel curves were measured between - 0.1 V and 0.1 V in potential and between 100 nA and 1 mA in current. The PDP analysis, 0.001 V/s as the scan rate, determined the Tafel slope, corrosion potential, and current for anodic and cathodic reactions, with experiments conducted triplicately for reproducibility [32].

The following Eq. (3) is used to compute efficiency:

$$\eta\% = \frac{I_{0corr} - I_{icorr}}{I_{0corr}} \times 100$$

3

I_{icorr} and I_{0corr} are the corrosion current density values with and without *Ocimum Americanum* extract.

An electrochemical workstation similar to the one used for PDP analysis was used for EIS.

The EIS investigations were carried out using an amplitude of 0.01 V and 10 frequencies per decade, covering the 100000 Hz to 0.1 Hz frequency range. An acidic liquid had to be soaked for 45 minutes to set up the OCP electrode [33].

Equation 4 was utilized to evaluate the efficiency of the inhibitor.

$$\eta\% = \frac{R_{ct} - R_{ct}^0}{R_{ct}} \times 100$$

4

The charge transfer resistance is denoted by R_{ct}^0 and R_{ct} , respectively, when *Ocimum Americanum* extract is absent and present.

2.8 QUANTUM CHEMICAL STUDIES

Using the Hyperchem 8.0 programming, molecular structure optimization has been performed. Density functional theory (DFT) was used for theoretical computations. Important variables, such as the energy gaps (ΔE) and LUMO and HOMO energies (E_{LUMO} and E_{HOMO} , respectively) between LUMO and HOMO were computed [34].

3. RESULTS AND DISCUSSION

3.1 weight loss studies

When *Ocimum Americanum* is applied to mild steel in the presence of 0.5 M H_2SO_4 , Table 2 shows the corrosion inhibition efficiency ($\eta\%$), weight loss values, and surface coverage (θ) at different concentrations. The data on weight loss was obtained with the help of the equations (1) and (2) mentioned in the experimental section. The maximum corrosion inhibition efficiency 88.80% was obtained at 2000 ppm. The data in Table 2 indicates that weight loss values drop and inhibition efficacy rises with increasing extract concentration. This occurs when atoms carrying lone pairs are adsorbed onto the metal surface, slowing down the rate at which metal corrodes in the abrasive media. This may be achieved by either blocking anodic and cathodic reaction sites or by changing the mechanisms underlying cathodic and anodic processes.

Table 2
The data on weight loss, surface coverage, and inhibitory efficiency with and without *Ocimum Americanum* in 0.5M H_2SO_4 .

Corrosive medium	Concentration of inhibitor (ppm)	Weight loss in gm. (ΔW)	Surface Coverage (ϑ)	$\eta\%$
0.5M H_2SO_4	0	0.554	-	-
	1000	0.105	0.810	81.04
	1500	0.085	0.846	84.65
	2000	0.062	0.888	88.80

3.2 electrochemical results

3.2.1 Potentiodynamic polarization study (PDP)

The specific details of the particular inhibition efficiencies and corrosion tests are given in Table 3, and Fig. 3 displays the cathodic and anodic polarization investigations of mild steel coupons in the aggressive solvent with different extract concentrations. PDP studies are used to determine the corrosion potential (E_{corr}) and corrosion current density (I_{corr}) by extrapolating linear portions of cathodic and anodic curves. The Tafel curves indicate that the presence of *Ocimum Americanum* extract results in a decrease in the cathodic and anodic portions of current density. The inhibitor demonstrated the ability to halt the metal oxidation process and the production of cathodic H_2 gas. *Ocimum Americanum* extracts altered Tafel graphs of anodic and cathodic reactions, indicating its inhibitory effect on cathode H_2 gas evolution and obstructing Fe dissolution. *Ocimum Americanum* extract, when mixed with 0.5M H_2SO_4 , effectively prevents cathodic and anodic corrosion reactions. The study suggests that increasing the extract from *Ocimum Americanum* may help prevent mild steel corrosion, suggesting that increased extract activity may reduce corrosion activity.

Table 3

Polarization parameters of steel in 0.5M H_2SO_4 without and with different concentrations of *Ocimum Americanum* extract.

Concentration of Plant Extract(ppm)	E_{corr} (V/SCE)	β_a (V/dec)	β_c (V/dec)	I_{corr} (A cm^2)	Corrosion rate(mm/y)	Inhibition Efficiency (%)
0	-0.521	0.091	0.087	65×10^{-5}	75.79	0
1000	-0.506	0.060	0.090	34×10^{-5}	39.51	47.69%
1500	-0.485	0.048	0.098	15×10^{-5}	18.59	76.92%
2000	-0.486	0.059	0.086	11×10^{-5}	13.4	83.07%

Table 3 shows that the corrosion current density is lowered by the concentration of *Ocimum Americanum* extract. For the blank solution (0 ppm), the calculated corrosion current density values are $65 \times 10^{-5} A/cm^2$. This value rose with each increase in inhibitor concentration, reaching $11 \times 10^{-5} A/cm^2$ at a higher concentration at 2000 ppm. As the inhibitor concentration increases, so do the inhibition efficiency values. The measured maximum inhibition efficiency was 83.07%. The extract adsorbs onto the metal's surface and inhibits its dissolution, acting as a protective layer.

3.2.2 ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY (EIS) STUDY

The Nyquist and Bode diagrams are shown in Fig. 4(a) and Fig. 4(b) results from the findings are depicted in Table 3. In Fig. 4(a), the breadth of the capacitive loops increased when the extract was present, indicating that the presence of an inhibitor considerably inhibited the dissolving of mild steel. The working electrode's (steel) roughness and corrosion-induced inhomogeneity are the causes of the semicircle divergence from the Nyquist plot. Charge transfer resistance (R_{ct}), constant phase element (CPE), and solution resistance (R_s) are the circuit's elements that are formed by fitting EIS data. CPE can be added to the working electrode to decrease its surface roughness and inhomogeneity. Table 4 shows that increasing the inhibitor's concentration enhances its inhibition efficiency and R_{ct} value.

Table 4

EIS results for the steel in 0.5M H₂SO₄ without and with different concentrations of *Ocimum Americanum* extract

Corrosive medium	Concentration of Plant Extract (ppm)	$R_s(\Omega)$	$R_{ct}(\Omega)$	CPE (μFcm^{-2})	N	Inhibition efficiency (%)
0.5M H ₂ SO ₄	0	3.43	18.34	5.7×10^{-5}	0.86	0
	1000	2.58	33.16	5.17×10^{-5}	0.85	44.69
	1500	2.17	55.32	6.5×10^{-5}	0.84	66.84
	2000	1.97	80.95	8.1×10^{-5}	0.81	77.34

The Bode angle diagram demonstrates how the curves enlarge and move to the left following the formation of a protective layer on the surface following the introduction of an inhibitor. Specifically, this study has shown that R_{ct} values climb as inhibitor concentrations do. This suggests that the *Ocimum Americanum* extract is readily absorbed on the mild steel surface, with a maximum effectiveness of 77.34% at 2000 ppm. Flattened semi-circles indicate imperfect capacitors due to surface reactions or electrode defects.

3.3 UV – VISIBLE SPECTRA

Two separate experimental setups were used to capture the UV spectra of the 0.5M H₂SO₄ corrosive solutions at 2000ppm inhibitor concentration. Firstly, we measured the UV spectra at 2000 ppm for 0.5M H₂SO₄ without dipping the mild steel coupons. Secondly, we submerged the steel coupon in the same solution for a whole day. After that, the absorbance values of these two UV spectra were compared. As seen in Fig. 5, the mild steel coupons exposed to the corrosive solution (after the corrosion test) had a lower absorbance value in comparison to the unrestricted solution before the corrosion test.

3.4 SURFACE INVESTIGATION USING SEM

The surface morphology of mild steel in 0.5M H₂SO₄ solution in the absence and presence of *Ocimum Americanum* inhibitor has been shown in Fig. 6. The SEM images of polished mild steel are shown in Fig. 6(a), the SEM image of a mild steel sample after a 24-hour immersion in 0.5M H₂SO₄ in Fig. 6(b), and the SEM image of a mild steel specimen immersed in 0.5M H₂SO₄ with *Ocimum Americanum* extract present in Fig. 6[c]. Without an inhibitor, a mild steel specimen submerged in a 0.5M H₂SO₄ solution, its morphology becomes extremely rough, causing the mild steel's corrosion to cause surface damage, although when *Ocimum Americanum* extract is present, the mild steel's surface exhibits less surface damage than in Fig. 6[b], indicating the development of an inhibitory coating for protection at the mild steel surface in Fig. 6(c). When *Ocimum Americanum* extract is present, the mild steel specimen's morphology is smoother than when the inhibitor is not present.

3.5 COMPUTATIONAL STUDIES

The border molecular orbital density distributions (HOMO and LUMO) and the geometry of the main components found in the *Ocimum Americanum* extract are depicted in Fig. 7. The computed values of the quantum chemical parameters, which include E_{HOMO}, E_{LUMO}, ΔE (energy gap between LUMO and HOMO), absolute electronegativity (χ), global hardness (γ), and softness (σ) are present in Table 5. Using the following equations, quantum chemical parameters were calculated:

Table 5
Quantum chemical parameters of Luteolin, Quinic Acid, and Jasmonic Acid calculated with the DFT method.

Molecule	E _{HOMO} (eV)	E _{LUMO} (eV)	ΔE (Ev)	χ (eV)	σ (eV ⁻¹)	X (eV)
Luteolin	-9.12	-1.07	8.05	4.025	0.248	5.095
Quinic Acid	-11.02	-0.56	10.46	5.23	0.191	5.79
Jasmonic Acid	-9.69	-0.77	8.92	4.46	0.224	5.23

$$\Delta E = E_{LUMO} - E_{HOMO} \text{ (5)}$$

6

$$\chi = -\frac{(E_{LUMO} + E_{HOMO})}{2}$$

$$\gamma = \frac{(E_{LUMO} + E_{HOMO})}{2}$$

7

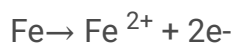
$$\sigma = 1/\gamma \text{ (8)}$$

The inhibition efficiency is linked to the HOMO and LUMO energies, with higher E_{HOMO} values resulting in stronger chemisorption and higher metal inhibition efficiency. Additionally,

A smaller ΔE ($E_{\text{LUMO}} - E_{\text{HOMO}}$) may result in a higher inhibitor's chemisorption on the metal surface.

3.6 Corrosion Inhibition Mechanism by the Phytochemicals Present in the Ocimum Americanum Extract

Corrosion occurs when the anode undergoes oxidation, while the cathode undergoes reduction.



The Ocimum Americanum extract's ability to inhibit mild steel corrosion in a 0.5 M H₂SO₄ solution is attributed to the absorption of molecules. The inhibitor being examined would have been adsorbent on a mild steel surface in one or more of the following ways-

- (a) The interactions between the π electrons of the aromatic ring and the unoccupied d-orbitals of surface iron atoms.
- (b) The interaction between the surface's unoccupied orbital and the unshared electron pair of the inhibitor's heteroatoms.

Generally, it is possible to examine two adsorption modes. Chemisorption is a method of inhibitor adsorption on steel surfaces, where water molecules are removed and electrons are shared between the inhibitor and iron atoms. The inhibitor molecule may be adsorbed on the steel surface through donor-acceptor interactions between the surface iron's d-orbital and the heterocyclic ring's π electrons, as illustrated in Fig. 8.

4. CONCLUSION

Numerous studies have been conducted to ascertain the anti-corrosive properties of *Ocimum Americanum* extract. Electrochemical experiments and weight loss are utilized to assess the effectiveness of *Ocimum Americanum* extract in inhibiting corrosion. The EIS experiments show that the highest inhibition efficiency 77.34% was achieved at a concentration of 2000ppm of inhibitor. The observed inhibition effectiveness at different doses supports the idea that increasing inhibitor concentration leads to increased inhibition efficiency and decreased corrosion rate. Surface morphology studies suggest that a protective layer should form on the metal surface. Based on the computational analysis of all three compounds, relatively high ΔE values were found, suggesting that the inhibitors are highly stable and less likely to degrade. Compared to Luteolin, Quinic Acid and Jasmonic Acid have

greater ΔE values, indicating that they might be more stable and have a protective effect that lasts longer.

Declarations

Competing Interest:

There is no conflict of interest regarding the submission of this manuscript. All authors are agreeing for its submission.

Author Contribution

Abhishek Sharma: Writing original draft, formal analysis
Raghvi: Raghvi original draft
Akhil Saxena: Supervision, validation
Jasdeep Kaur: Validation, formal analysis, supervision

Data Availability:

No data is made available for anyone. No part of the manuscript is published in full or partially.

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Figures

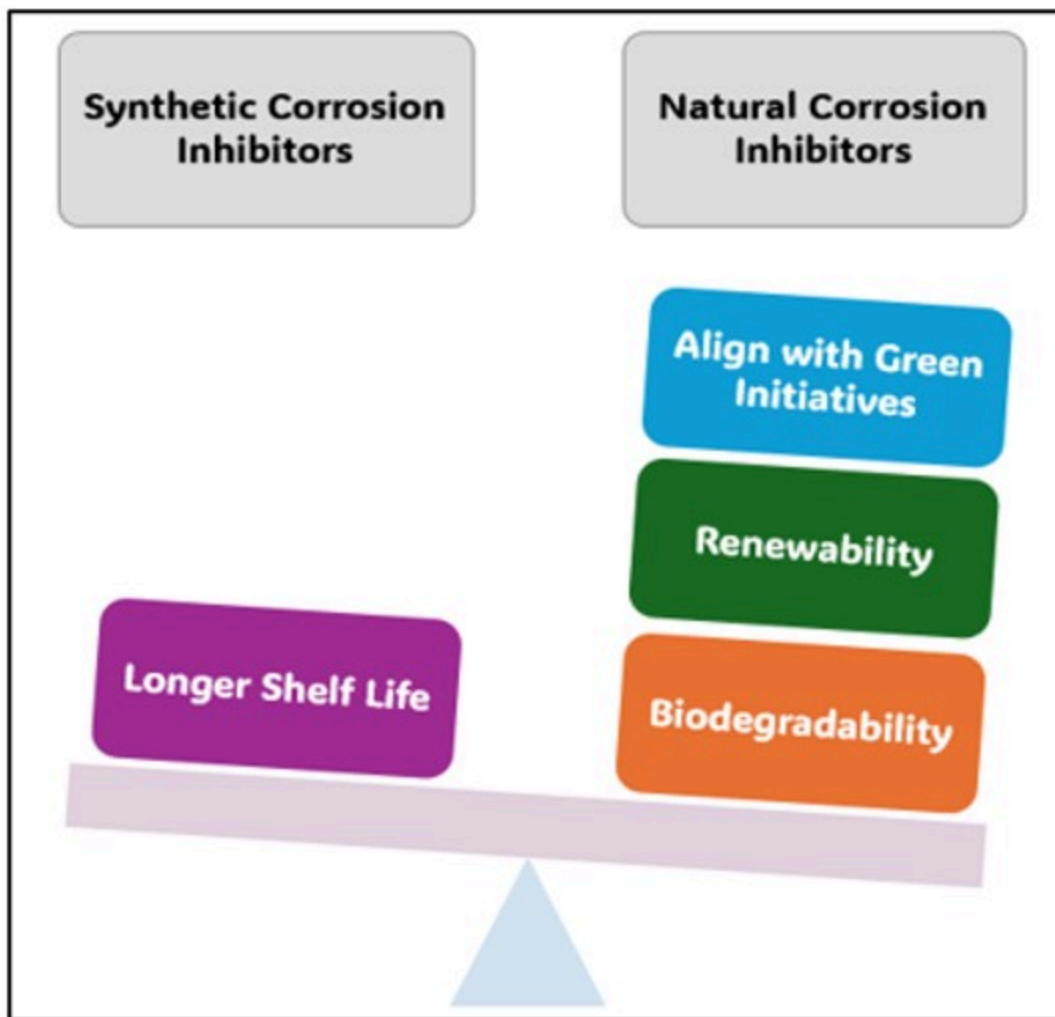


Figure 1

Profitability of Natural corrosion inhibitors over Synthetic corrosion inhibitors

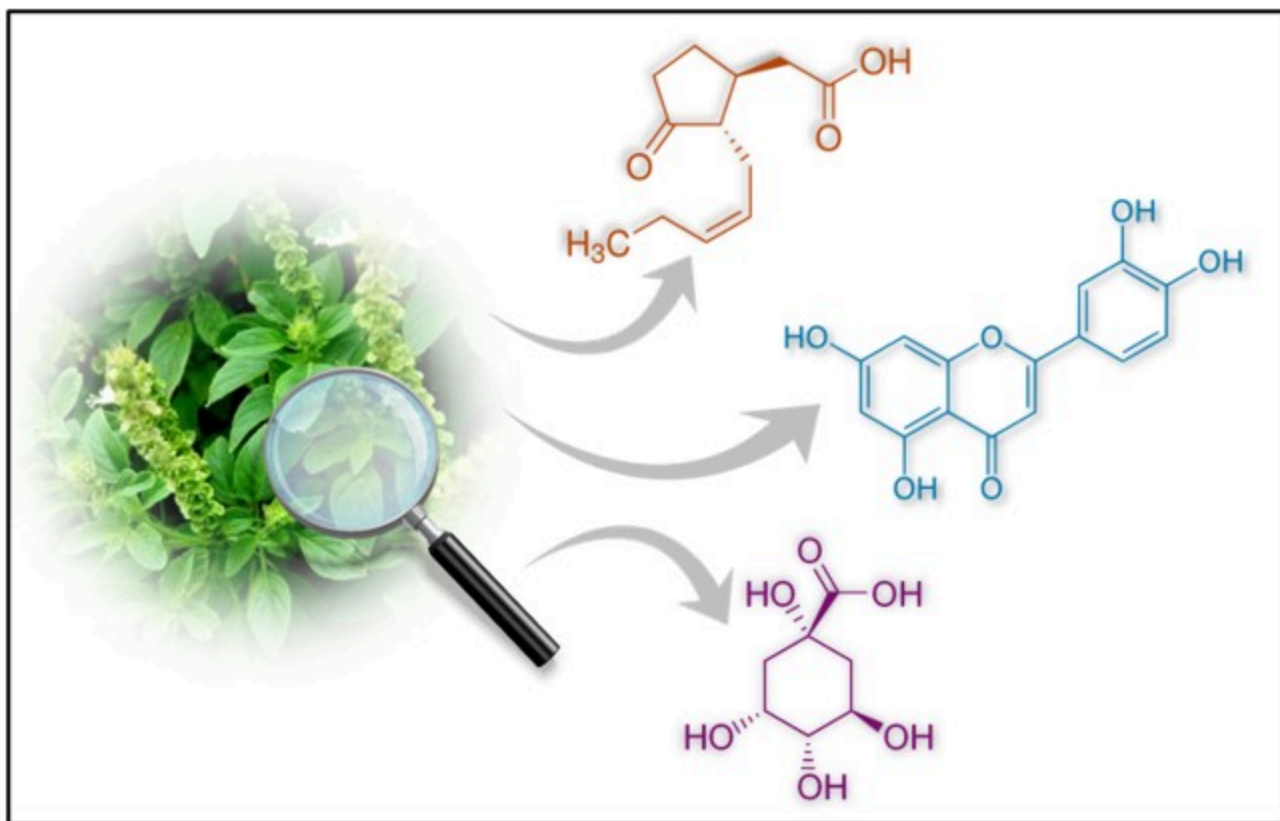


Figure 2

Major phytochemicals are present in *Ocimum Americanum* extract.

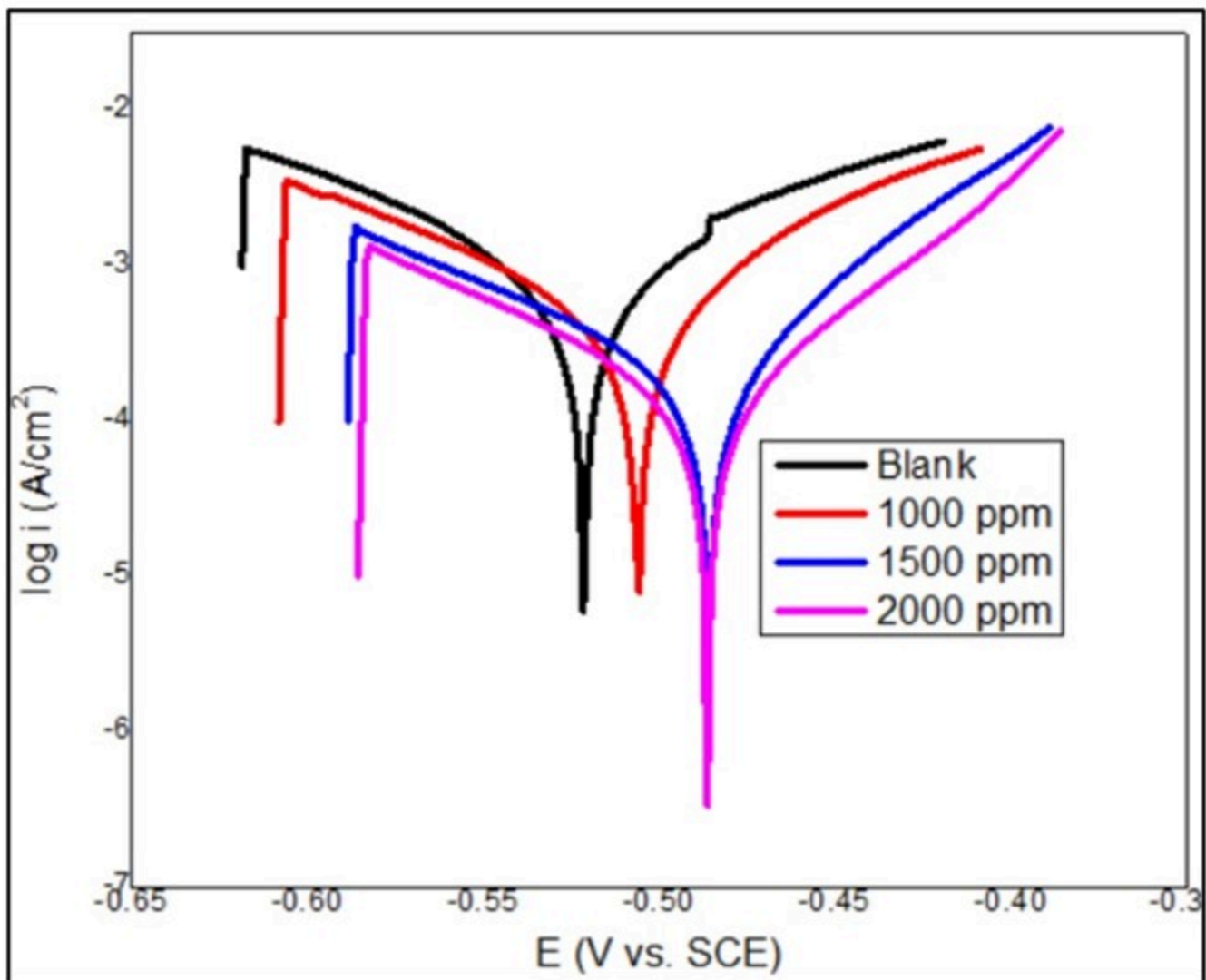
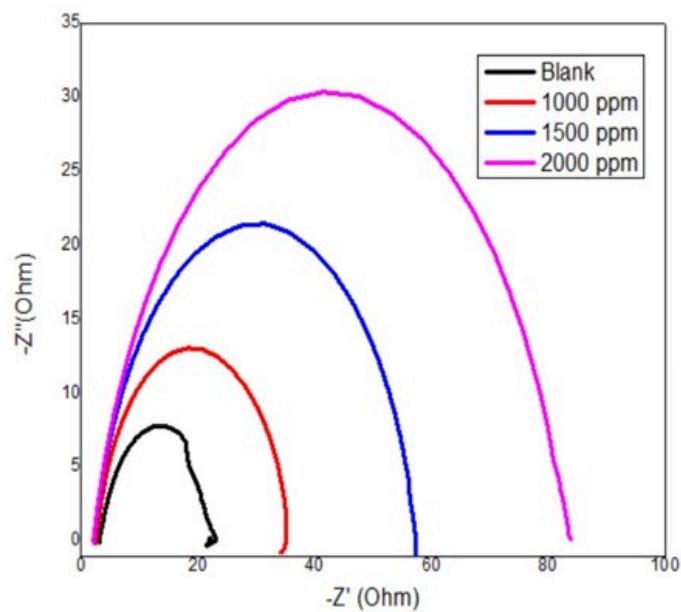
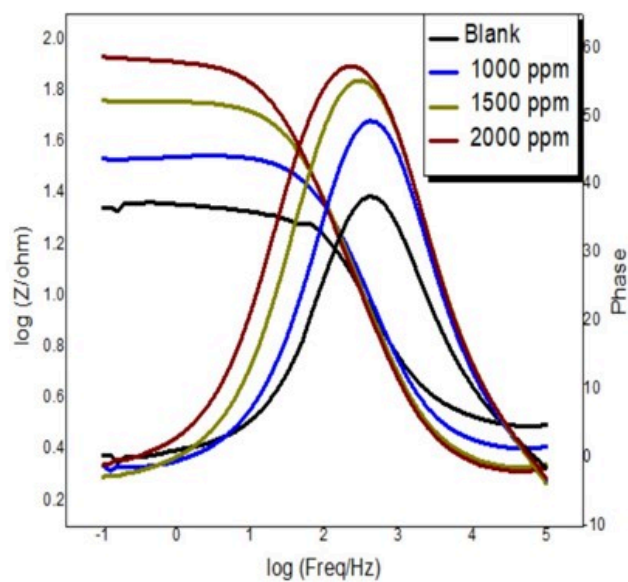


Figure 3

Tafel polarization data in 0.5M H_2SO_4 with and without various *Ocimum Americanum* extract concentrations



(a)



(b)

Figure 4

Nyquist 4(a) and Bode plots 4(b) for steel in 0.5M H_2SO_4 without and with different concentrations of *Ocimum Americanum* extract

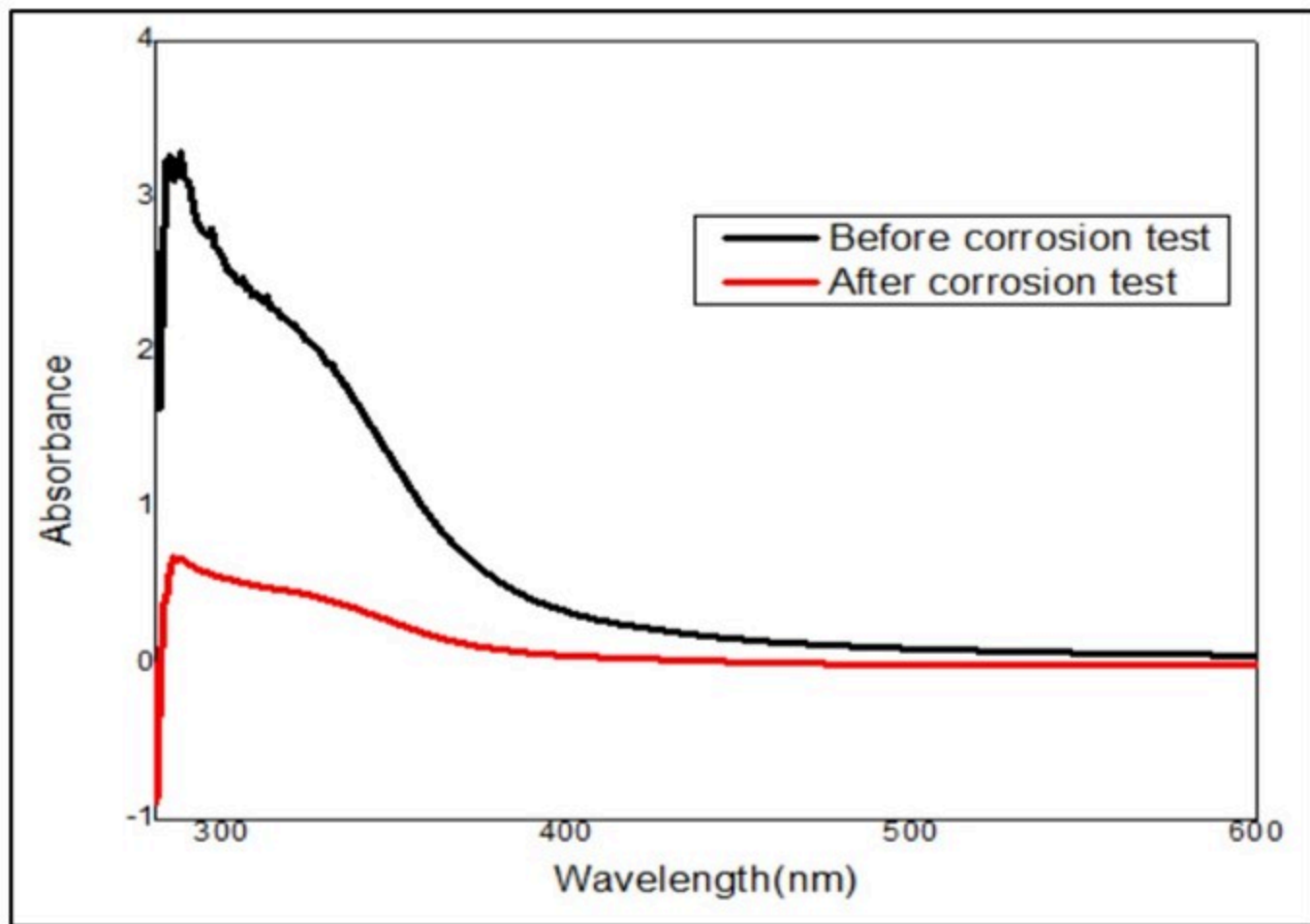


Figure 5

UV Spectra of *Ocimum Americanum* extract before and after immersion of mild steel strips.

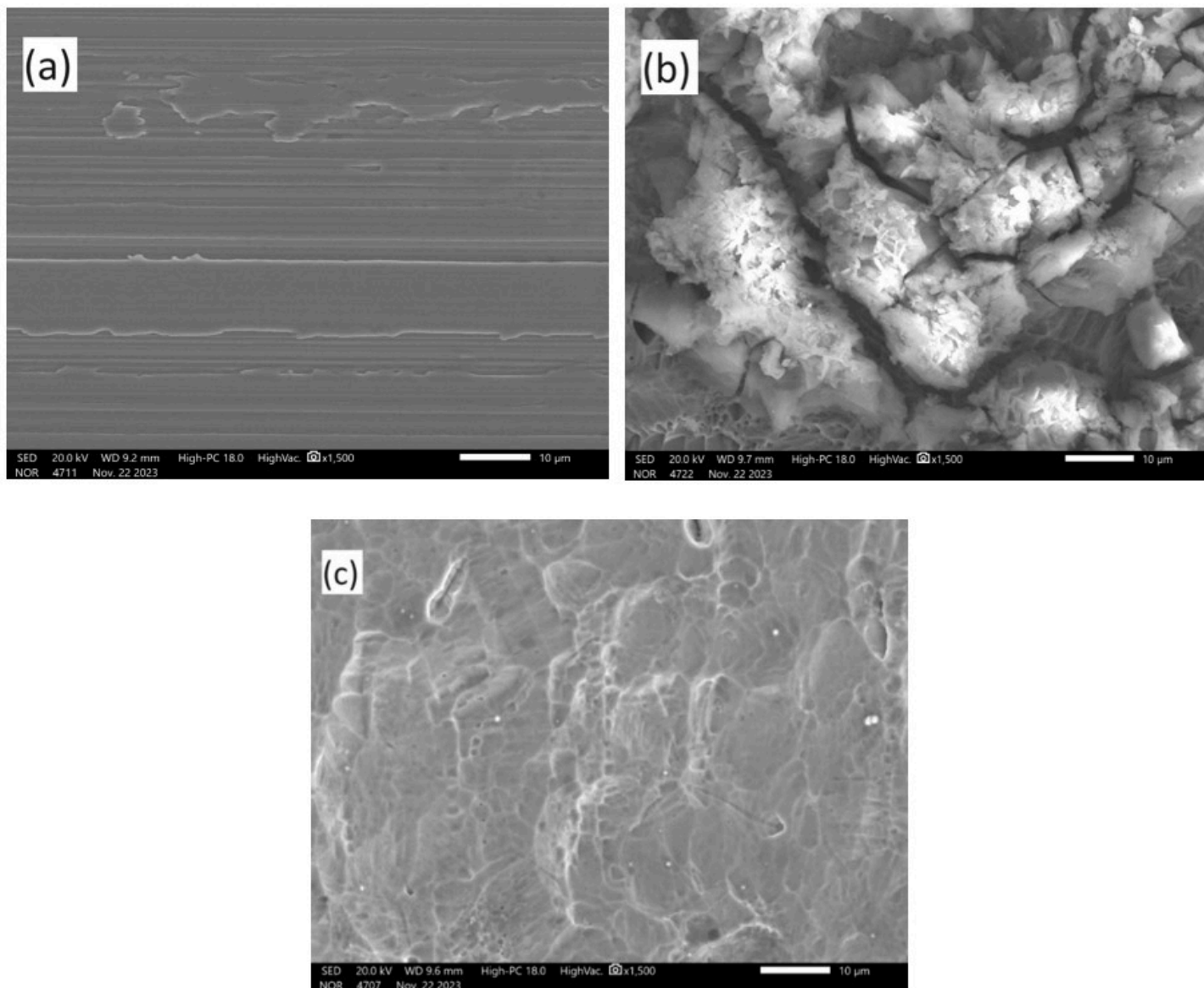


Figure 6

SEM Images of mild steel (a), mild steel immersed in 0.5M H₂SO₄ without inhibitor (b), and mild steel immersed in 0.5 M H₂SO₄ in the presence of *Ocimum Americanum* extract (c).

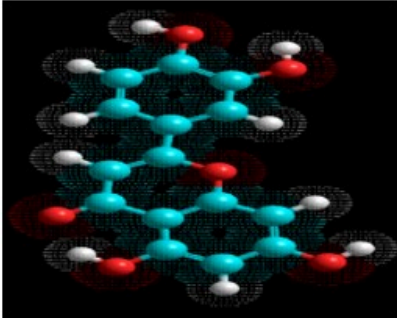
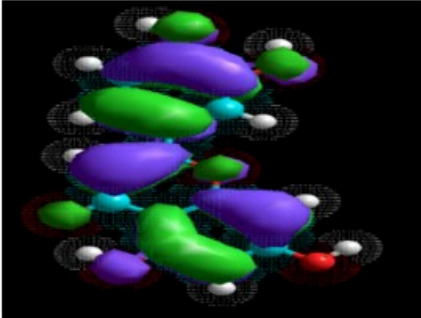
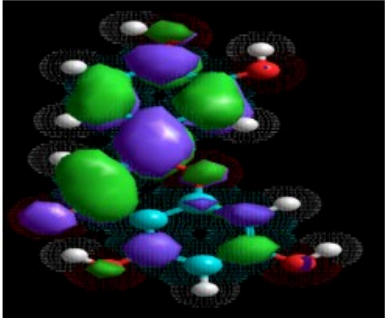
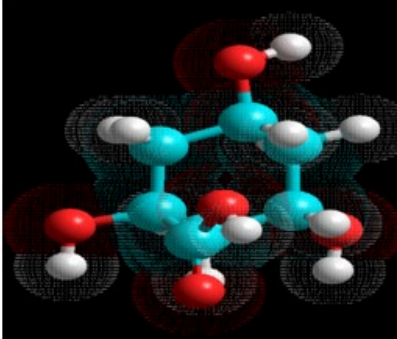
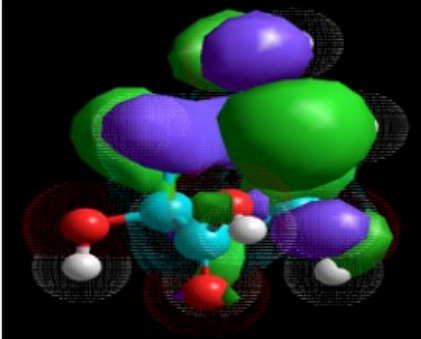
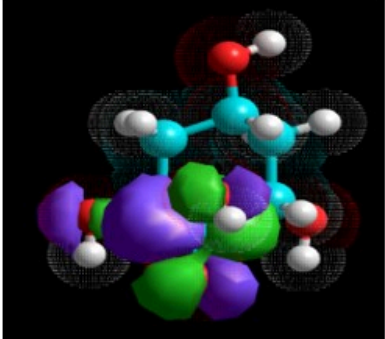
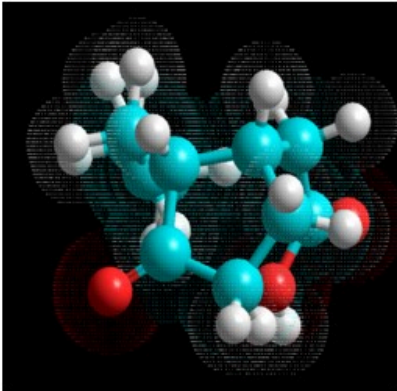
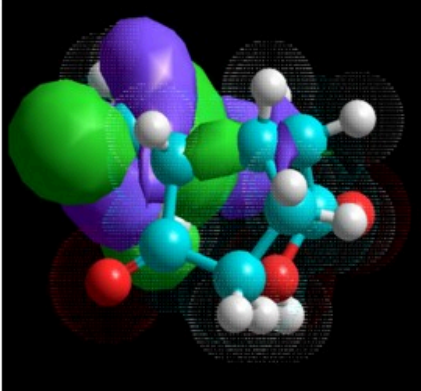
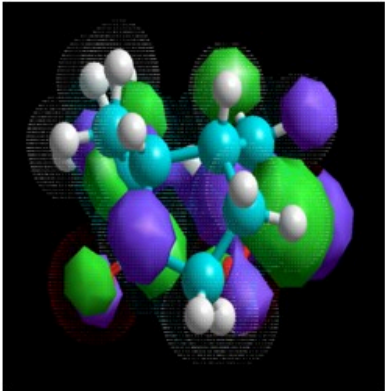
Molecule	Optimized structure	HOMO	LUMO
Luteolin			
Quinic Acid			
Jasmonic Acid			

Figure 7

Optimized structures, HOMO, AND LUMO Of the phytochemicals present in the *Ocimum Americanum*.

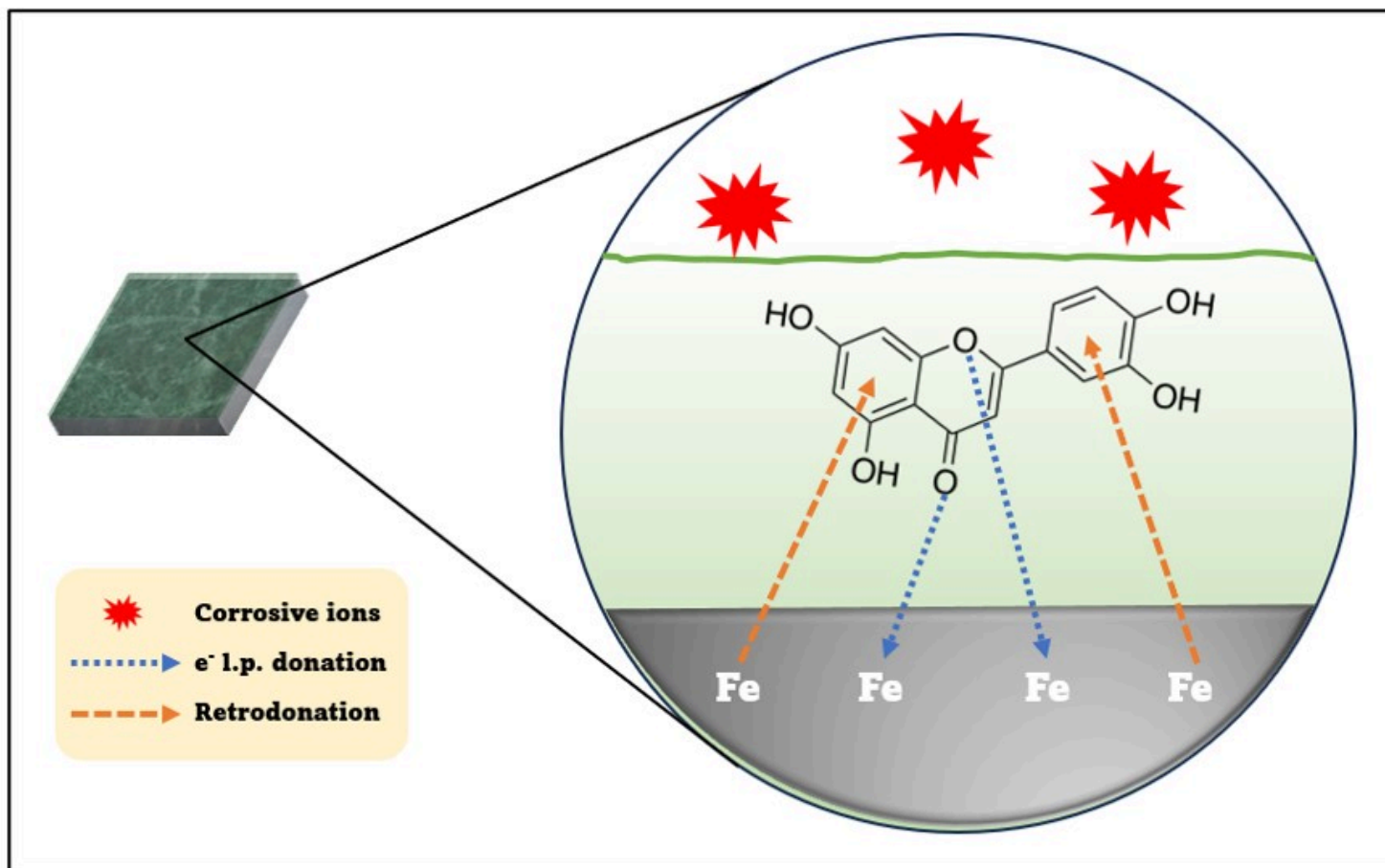


Figure 8

Corrosion inhibition mechanism of the phytochemicals present in the *Ocimum Americanum*.