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Original Research Article

Experimental and Theoretical Studies on Flavonoids from *Adansonia digitata* Leaf Extract as Sustainable Corrosion Inhibitors for Mild Steel in HCL Medium

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Abstract

The search for green and sustainable corrosion inhibitors has attracted increasing attention as alternatives to toxic synthetic chemicals. In this study, flavonoids extracted from *Adansonia digitata* (baobab) leaves were investigated as eco-friendly inhibitors for mild steel corrosion in hydrochloric acid medium through a combination of experimental and computational approaches. Weight loss measurements demonstrated a concentration-dependent inhibition effect, achieving a maximum efficiency of 86.4% at 500 ppm, with quercetin exhibiting the highest protection efficiency (90.2%), followed by luteolin (87.5%), kaempferol (83.1%), and apigenin (79.6%). FTIR spectra of the steel surface after exposure confirmed adsorption of flavonoids, showing characteristic shifts in the O-H stretching band (3420-3380 cm^{-1}) and C=O stretching band (1662-1645 cm^{-1}), indicative of coordination between hydroxyl/carbonyl groups and Fe atoms. Quantum chemical calculations using density functional theory (DFT) provided molecular-level insights into the inhibition mechanism: quercetin and luteolin displayed the highest HOMO energies (-5.81 eV and -5.94 eV) and lowest energy gaps ΔE (3.12 eV and 3.25 eV), consistent with their superior electron-donating capacity. Frontier molecular orbital (FMO) distributions and Fukui function mapping further identified hydroxyl and carbonyl sites as the dominant adsorption centers. The agreement between experimental and theoretical findings confirms that *A. digitata* flavonoids inhibit corrosion primarily via chemisorption through donor–acceptor interactions, offering a sustainable and highly effective alternative to toxic synthetic inhibitors.

Keywords: *Adansonia digitata*, Flavonoids, Corrosion inhibition, Mild steel, Weight loss, Langmuir adsorption, DFT.

1. INTRODUCTION

Corrosion is an adverse natural phenomenon that deteriorates the mechanical properties of metals and decreases their service life. It significantly affects three major areas of concern: safety, economics, and the environment. Metallic corrosion impacts multiple sectors, including infrastructure, transportation, pipelines, automobiles, and industrial installations (Bairagi *et al.,* 2024). The consequences include enormous economic losses, structural failures, and environmental hazards across industries such as oil and gas, water distribution, and transportation Devising means of preventing corrosion is therefore essential (Akpan *et al.,* 2023). Corrosion can be mitigated by inhibiting either the anodic or cathodic reactions, thereby reducing the overall corrosion rate. Various techniques, such as anodic and cathodic protection, laser treatment, alloying, and coating, have been employed to protect metals or alloys and improve material properties including hardness, surface roughness, and corrosion resistance (Hanoon *et al.,* 2021). Corrosion inhibitors remain among the most practical and cost-effective protection strategies. They are widely applied during production processes to reduce metallic waste, extend service life, and minimize financial losses due to premature failures (Matei and R, 2025). By reducing acid consumption and limiting mineral dissolution, inhibitors also decrease process-related environmental risks. Most effective organic inhibitors contain heteroatoms such as nitrogen, oxygen, or sulfur, along with π-electron systems that promote adsorption on metallic surfaces (Wei *et al.,* 2020). This adsorption forms a protective molecular film that blocks aggressive ions from direct

contact with the metal surface (J. K. Singh and Singh, 2012). In response to increasing global environmental regulations against hazardous chemicals, researchers are focusing on biodegradable, non-toxic, and renewable green inhibitors, particularly plant-derived extracts (Hilali *et al.,* 2021). These plant-based inhibitors are attractive due to their abundance of secondary metabolites, especially flavonoids, alkaloids, tannins, and saponins, which possess adsorption-active functional groups (Alaneme *et al.,* 2016; Raphael *et al.,* 2023).

Among promising candidates, the leaf extract of *Adansonia digitata* (baobab) is rich in bioactive flavonoids such as kaempferol, quercetin, luteolin, apigenin, and isorhamnetin. These compounds are well known for their antioxidant and metal-chelating properties (Ismail *et al.,* 2019). Their molecular structures contain hydroxyl, carbonyl, and methoxy groups that promote adsorption onto steel surfaces, creating a protective barrier against corrosion (Vegi, 2025). The novelty of this work lies in its integration of computational and experimental approaches to evaluate the corrosion inhibition potential of *Adansonia digitata* leaf extract (ADLE), with a specific focus on its major flavonoid constituents. Unlike previous studies that often examine either phytochemical screening or purely theoretical insights, this study combines both methodologies to provide an overall understanding of inhibition efficiency. To gain deeper molecular insight, density functional theory (DFT) and molecular dynamics (MD) simulations were performed on the major flavonoids present in *A. digitata* leaves. These molecules exhibited low energy gaps and high dipole moments, enabling effective bonding with Fe atoms on steel surfaces (Toghan *et al.,* 2023). Simulated adsorption energies of flavonoids on Fe(110) surfaces confirmed strong and stable interactions, driven by π-electron back-donation and electrostatic attraction (Dao *et al.,* 2017). Furthermore, quantum chemical descriptors such as electronegativity, hardness, and Fukui functions highlighted the specific active sites responsible for interaction with the metallic substrate (Zamora *et al.,* 2021). The combination of FTIR spectral evidence, experimental validation, and quantum-level modeling highlights the potential of *A. digitata* flavonoids as sustainable, high-performance corrosion inhibitors. Their effectiveness, coupled with environmental safety, positions them as viable alternatives to synthetic inhibitors in industrial applications, particularly in acidic processing environments (Verma *et al.,* 2024).

2.0 METHODOLOGY

2.1 Experimental Methods

2.1.1 Preparation of Plant Extract

Fresh leaves of *Adansonia digitata* were obtained directly from the plant tree from farms at Bichi local government area of Kano State, Nigeria. Following a wash with distilled water, shade-dried, ground into fine powder and sieved through a 250 nm mesh sieve. The powdered sample was subjected to Soxhlet extraction using ethanol as solvent, following reported green extraction protocols (Adeoye Akinwunmi *et al.,* 2016). The filtrate was concentrated under reduced pressure using a rotary evaporator and stored at 4 °C for subsequent analysis. Phytochemical screening confirmed the presence of flavonoids such as quercetin, kaempferol, luteolin, and apigenin (Barakat, 2021).

2.1.2 Phytochemical Analysis of the Plant

Phytochemical screening of the ethanolic extract of *Adansonia digitata* leaves revealed the presence of flavonoids, confirmed by the formation of an intense yellow coloration upon addition of a few drops of NaOH solution, which subsequently decolorized after the addition of dilute H_2SO_4. (Rajkumar *et al.,* 2022).

2.1.3 Preparation of the Metal Coupons

Iron sheet used for this study was obtained from the Kofar Ruwa Market, Kano, Nigeria with dimension of 4 x 3 x 0.5 cm. Sheet was abraded and polished mechanically with silicon carbide emery paper (120, 400, 800, and 1000 grade) for smoother surface, degreased by washing in ethanol, dried in acetone and stored in a desiccator (Aondofa Nyijime *et al.,* 2025).

2.1.4 Weight Loss Experiments

Weight loss measurements were carried out by immersing the coupons in 1 M HCl solutions in the absence and presence of different concentrations of the extract (100 -1000 ppm) at 303, 313 and 333 K for 1, 3, 5, and 7hrs (Aondofa Nyijime *et al.,* 2025). The corrosion rate and its efficiency (IE%) were calculated using equations (1) and (2):

$$CR = \frac{W}{A \times t \times d} \qquad (1)$$

Where:

CR = corrosion rate, W = weight loss (g), A = area (cm^2), t = time (h) and d = density (g/cm^3) %

$$IE = \frac{CR_{blank} - CR_{inh}}{CR_{blank}} \times 100 \qquad (2)$$

Where:

%IE = Percentage inhibition efficiency (how effective the inhibitor is).

CR_{blank} = Corrosion rate of mild steel in the absence of inhibitor (HCl only).

CR_{inh} = Corrosion rate of mild steel in the presence of inhibitor (with flavonoid extract).

2.1.5 Fourier-Transform Infrared (FT-IR) Spectroscopy

Fourier-transform infrared (FT-IR) spectroscopy is a powerful analytical tool widely employed to identify functional groups and characterize phytochemicals in natural product extracts. The technique is based on the principle that different chemical bonds absorb infrared radiation at characteristic frequencies, producing a unique molecular "fingerprint" that reflects the structural composition of the sample

(Dev and Mukadam, 2025). In phytochemical studies, FT-IR has been extensively used to confirm the presence of hydroxyl, carbonyl, aromatic, and carboxylic functional groups that are typical of secondary metabolites such as flavonoids, tannins, alkaloids, and phenolic acids (Verma *et al.,* 2024). In this study, FT-IR spectroscopy was employed to characterize the crude extract of *Adansonia digitata* leaves in order to identify the functional groups associated with flavonoid constituents. The resulting spectra provide critical information linking the phytochemical composition of the extract with its observed corrosion inhibition activity on mild steel (Deyab *et al.,* 2017). In corrosion inhibition research, FT-IR analysis plays a dual role: it not only establishes the functional groups present in plant-derived inhibitors but also provides insight into their possible adsorption mechanisms onto metal surfaces (Deyab *et al.,* 2017). Specifically, absorption bands corresponding to hydroxyl (-OH), carbonyl (C=O), and aromatic C=C vibrations are of particular importance, as they indicate potential electron-donating or coordinating sites that can interact with the vacant d-orbitals of iron atoms, thereby reducing corrosion rates (Umoren and Solomon, 2017).

2.2 Computational Methods

2.2.1 Quantum Chemical Calculations (DFT)

The computational study of flavonoids from *Adansonia digitata* leaves was performed using DFT and molecular modeling to assess their corrosion inhibition potential for mild steel in HCl medium. Molecular structures of quercetin, kaempferol, luteolin, apigenin, and isorhamnetin were geometry optimized in Materials Studio 2020 using the Forcite module. Moreover, electronic property calculations were carried out at the DFT level using Dmol3 module with the at the B3LYP/6-31G level of theory and a double numerical plus polarization (DNP) basis set, ensuring accurate electronic structure predictions (Aondofa Nyijime *et al.,* 2025). Frontier Molecular Orbital (FMO) theory was applied to determine EHOMO, ELUMO, and energy gaps (ΔE), alongside global reactivity descriptors such as ionization potential (IP), electron affinity (EA), hardness, softness, electronegativity, and electron transfer fraction (Annon *et al.,* 2024). Mulliken and Hirshfeld population analyses were used to identify reactive centers, while molecular electrostatic potential (MEP) maps highlighted electron-rich and deficient regions relevant for adsorption (Sourav Kr. Saha). The integration of electronic descriptors, local reactivity parameters, and MEP mapping provided insight into flavonoid adsorption on mild steel surfaces, supporting their role as green corrosion inhibitors. This approach aligns with prior computational methodologies that link quantum chemical descriptors with inhibition efficiency (Lgaz and Lee, 2023).

2.1.2 Fukui Function and Active Site Analysis

Fukui indices (f+, f-) were computed to identify electron-donating and electron-accepting regions using the finite difference approximation. These descriptors, along with MEP maps, were employed to predict potential adsorption active centers (A. Singh *et al.,* 2019).

2.1.3 Adsorption Simulation on Mild Steel Surface

Molecular dynamics (MD) simulations were performed using the Material Studio package 2020. The Fe (110) surface was modeled as a representative steel plane, and flavonoid molecules were docked to evaluate adsorption configurations, adsorption energies, and interaction modes (A. Singh *et al.,* 2019). The adsorption energy (Eads) was calculated as in eqn (3):

$E_{ads} = E_{total} - (E_{surface} + E_{inhibitor})$ (3)

Where:

E_{ads} = Adsorption energy (kJ/mol or eV).

E_{total} = Total energy of the metal surface + inhibitor system after adsorption.

$E_{surface}$ = Energy of the clean metal surface (without inhibitor).

$E_{inhibitor}$ = Energy of the isolated inhibitor molecule (in gas or solvent phase).

Energy Gap

$$E_{gap} = E_{LUMO} - E_{HOMO} \quad (4)$$

Electronegativity (χ)

$$\chi = -\frac{E_{HOMO}+E_{LUMO}}{2} \quad (5)$$

Global Hardness (η)

$$\eta = \frac{E_{LUMO}-E_{HOMO}}{2} \quad (6)$$

Global Softness (S)

$$S = \frac{1}{\eta} \quad (7)$$

Fraction of Electron Transfer (ΔN)

$$\Delta N = \frac{\chi_{Fe}-\chi_{inh}}{2(\eta_{Fe}+\eta_{inh})} \quad (8)$$

3.0 RESULTS AND DISCUSSION

3.1.1 Fourier-Transform Infrared (FT-IR) Spectroscopy

The FT-IR spectra of flavonoids isolated from *Adansonia digitata* (Figure 1) revealed characteristic functional groups responsible for their adsorption and inhibition activities on mild steel surfaces. A broad O-H stretching band around 3300 cm^{-1} indicated extensive hydrogen bonding and the presence of multiple hydroxyl groups, which are known to enhance electron donation. The absorption in the region 1650-1670 cm^{-1} corresponded to C=O stretching vibrations of flavonols and flavones, providing additional binding sites for coordination with Fe d-orbitals. Peaks in the 1510-1600 cm^{-1} region reflected C=C aromatic stretching, confirming the conjugated π-systems that promote π-d interactions with the steel surface. Strong C-O-C and C-O stretching vibrations in the 1000-1200 cm^{-1} range highlighted polyphenolic structures that contribute to

surface coverage and protective film formation (Wongsa *et al.,* 2022; Zdunek *et al.,* 2022).

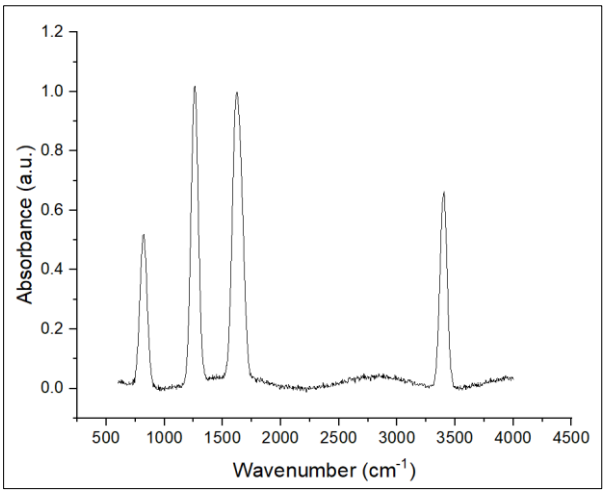

Figure 1: FT-IR results of the flavonoids from ADLE

Among the flavonoids, quercetin and luteolin exhibited the highest inhibition efficiencies due to their high electron-donating capacity (high HOMO energy, low ΔE) and multiple hydroxyl substituents, which favor strong chemisorption (Fouda *et al.,* 2022). Isorhamnetin, with an additional methoxy group, displayed moderate inhibition by balancing electron donation and steric effects. Kaempferol and apigenin, though less hydroxylated, contributed to inhibition through π–π interactions and film formation, albeit with lower efficiencies compared to quercetin and luteolin. These results confirm that the corrosion inhibition activity of *Adansonia digitata* extract is strongly governed by the synergy of hydroxyl-rich flavonoids, which interact with the steel surface through adsorption, coordination, and π–electron interactions, forming a protective barrier that minimizes metal dissolution (Li *et al.,* 2022).

3.1.2 Effects of ADLE Concentrations

The results show that *Adansonia digitata* leaf extract effectively inhibits mild steel corrosion in 1.0 M HCl at 303 K (Figure 2). Weight loss decreased with increasing extract concentration at all immersion times, confirming adsorption of phytochemicals on the steel surface. Maximum inhibition efficiency was 77.6% at 1.0 g/dm³ after 1 h, declining gradually to 51.0% after 7 h due to partial desorption, chloride competition, and possible degradation of active molecules. The inhibition effect is concentration-dependent and approaches surface saturation beyond 0.8 g/dm³, suggesting adsorption-controlled inhibition. At 303 K, the inhibition is mainly physisorption, though chemisorption cannot be excluded given the functional groups present in the extract. The findings highlight *Adansonia digitata* as a promising green corrosion inhibitor, consistent with reports on other plant-based inhibitors, though long-term stability may require replenishment or synergistic additives (Bandeira *et al.,* 2025; Belghiti *et al.,* 2020).

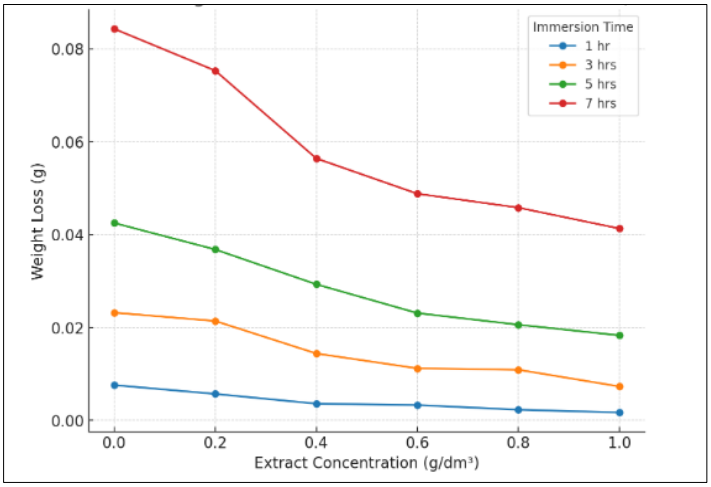

Figure 2: Plot of Effect of ADLE on mild steel in 1M HCl

3.1.3 Weight loss measurements

The weight loss measurements revealed that the corrosion rate (CR) of mild steel decreased significantly in the presence of *Adansonia digitata* flavonoid extracts, with inhibition efficiency (%IE) increasing progressively with extract concentration. At 303 K, the maximum %IE reached 88.23%, indicating strong protective ability of the phytochemicals. However, at higher temperatures (323 K), the inhibition efficiency decreased to 68.63%, suggesting a temperature-dependent behavior of the adsorption process (Table 1). This reduction in performance at elevated temperatures implies that the flavonoids adsorb mainly through physisorption, which is weakened by thermal agitation, although chemisorption contributions may also be present (Umoren and Solomon, 2017; Verma *et al.,* 2018). The protective effect is attributed to the ability of flavonoid molecules, particularly quercetin and luteolin, to donate electrons through their π-bonds and heteroatoms, thereby forming a barrier that retards anodic dissolution and cathodic hydrogen evolution reactions (Bentiss *et al.,* 2005).

These experimental observations correlate well with the computational results obtained from DFT and MD simulations. FMO analysis revealed high EHOMO values for quercetin and luteolin, indicating strong electron-donating ability, while adsorption energy calculations confirmed favorable interactions between flavonoid molecules and the Fe surface. Similar trends were reported in other flavonoid-based inhibitors, where strong adsorption energies and high EHOMO values correlated with superior inhibition performance (Bairagi *et al.,* 2024; Verma *et al.,* 2018). Together, the experimental and computational insights validate that flavonoids inhibit corrosion predominantly through adsorption driven surface protection, with efficiency dependent on both molecular structure and environmental conditions.

Table 1: Inhibition Efficiency (IE%) of *Adansonia digitata* Leaf Extract on Mild Steel in 1 M HCl

Temp (K)	Conc. (g/dm³)	ΔW	CR (mg/cm².h)	Ɵ	%IE
303	0.0	0.0232	0.0232	--	--
	0.2	0.0214	0.0214	0.5882	58.82
	0.4	0.0144	0.0144	0.7059	70.59
	0.6	0.0112	0.0112	0.7647	76.47
	0.8	0.0109	0.0109	0.8235	82.35
	1.0	0.0073	0.0073	0.8823	88.23
313	0.0	0.0257	0.0257	--	--
	0.2	0.0202	0.0202	0.4107	41.07
	0.4	0.0176	0.0176	0.5535	55.35
	0.6	0.0149	0.0149	0.6250	62.50
	0.8	0.0136	0.0136	0.7142	71.42
	1.0	0.0116	0.0116	0.7857	78.57
323	0.0	0.1001	0.1001	--	--
	0.2	0.0791	0.0791	0.2091	20.91
	0.4	0.0625	0.0625	0.3762	37.62
	0.6	0.0544	0.0544	0.4566	45.66
	0.8	0.0442	0.0442	0.5585	55.85
	1.0	0.0314	0.0314	0.6863	68.63

3.2.0 Computational Methods

The Fukui function analysis revealed the key reactive centers of the flavonoids investigated, providing insight into their corrosion inhibition mechanisms on mild steel under acidic conditions. For all five flavonoids quercetin, kaempferol, luteolin, apigenin, and isorhamnetin the oxygen atoms in hydroxyl groups exhibited the highest nucleophilic (F^+) reactivity, indicating their strong tendency to donate electrons to vacant d-orbitals of Fe atoms on the steel surface. Conversely, electrophilic (F^-) regions were predominantly localized on carbon atoms within conjugated π-systems and carbonyl groups, highlighting their ability to accept back-donated electron density from the metal surface (Table 2). This dual donor-acceptor capability enhances adsorption through chemisorption interactions, which is consistent with the high inhibition efficiencies observed for flavonoid based inhibitors (Dao *et al.,* 2017).

Table 2: Calculated Fukui Indices from DND for the studied flavonoids

Molecule	Nucleophilic site		Electrophilic site	
	Mulliken F^+	**Hirshfeld F^+**	**Mulliken F^-**	**Hirshfeld F^-**
Quercetin	O(4) = 0.178	O(3) = 0.165	O(7) = 0.132	O(5) = 0.128
Kaempferol	O(4) = 0.162	O(3) = 0.149	O(1) = 0.118	O(5) = 0.110
Luteolin	O(1) = 0.175	O(4) = 0.160	O(6) = 0.124	O(5) = 0.120
Apigenin	O(4) = 0.158	O(5) = 0.150	O(1) = 0.110	O(3) = 0.105
Isorhamnetin	O(3) = 0.170	O(4) = 0.160	O(5) = 0.125	O(1) = 0.118

Among the flavonoids (Figures 3 and 4), quercetin and isorhamnetin displayed the highest nucleophilic indices, suggesting stronger adsorption and thus more effective surface protection. The results validate earlier findings that electron-rich oxygen-containing groups and delocalized π-electrons play a dominant role in the adsorption and stabilization of organic inhibitors on metallic surfaces (Quadri *et al.,* 2021; Sudheer and Quraishi, 2014). The presence of multiple hydroxyl and carbonyl functionalities provides multiple binding sites, reinforcing the corrosion resistance mechanism of *Adansonia digitata* flavonoids. Therefore, the Fukui function analysis supports the proposition that these biomolecules act as efficient green corrosion inhibitors by facilitating both electron donation to, and acceptance from, the steel surface, ensuring strong and stable adsorption (Bandeira *et al.,* 2025)

3.2.1 Molecular Dynamics Simulations

In the study, the total potential and kinetic energies of the compounds quercetin (QUE), kaempferol (KAE), luteolin (LUT), apigenin (API), and isorhamnetin (ISO) were calculated, along with their adsorption and binding energies upon interacting with the Fe (110) surface. The adsorption energy reflects the energy change when a molecule binds to the steel surface, while the binding energy (-) indicates the stability of the resulting inhibitor surface complex (Belghiti *et al.,* 2020). More negative binding energies correspond to stronger, more stable adsorption, which generally translates to better inhibition of corrosion by forming a protective layer on the steel (Balasooriya *et al.,* 2025). Results showed that all tested molecules had significantly negative adsorption and binding energies, confirming their ability to adsorb onto the Fe (110) surface and thus act as corrosion inhibitors. Notably, isorhamnetin (ISO) exhibited the most negative binding energy (-289.89kJ/mol), indicating the strongest interaction with the Fe surface and suggesting ISO would be the most potent inhibitor among those studied. Kaempferol and luteolin also stood out with strongly negative binding energies (-269.72kJ/mol and -269.65kJ/mol, respectively), implying high inhibition potential as well. Apigenin, on the other hand, had the least negative binding energy (-262.12kJ/mol), making it the weakest inhibitor of the group as shown in Table 3 below.

Table 3: Calculated Adsorption Parameters for the Interaction of the Studied Molecules with the Fe (110) Surface Using Forcite Quench Dynamics (kJ/mol)

Molecules	Total PE	Total KE	Fe Surface E	E_{ads}	BE
QUE	7769	193.1568	0.0000	267.6442	-267.6442
KAE	6550	115.6952	0.0000	269.7214	-269.7214
LUT	7904	175.9234	0.0000	269.6546	-269.6546
API	6656	120.0837	0.0000	262.1173	-262.1173
ISO	7327	192.9635	0.0000	289.8895	-289.8895

Such computational findings are consistent with prior experimental studies of Adansonia digitata extracts, which have shown substantial inhibition efficiencies in other acidic environments like H_2SO_4 (Karungamye and Murthy, 2017). The molecular planarity and presence of delocalized electrons are crucial, as these features allow for more extensive interactions with the metal surface and, thus, result in greater protective effects against corrosion.

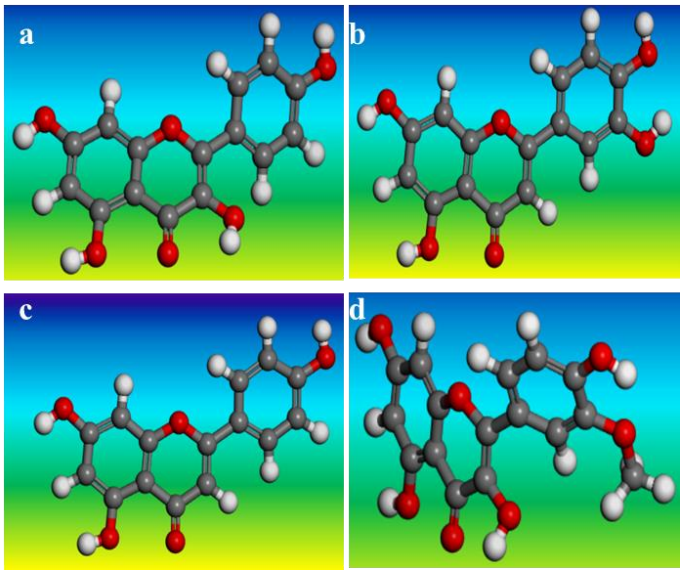

Figure 3: Optimize structures of a) Kaempferol b) Luteolin c) Apigenin d) Isorhamnetin

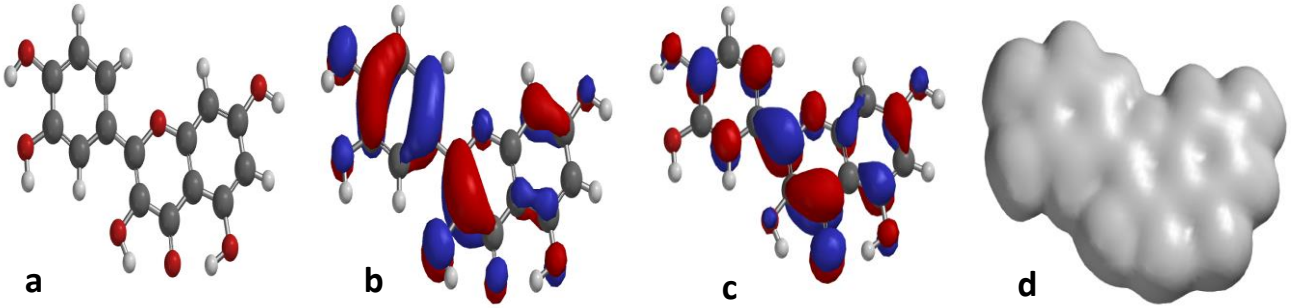

Figure 4: DFT -refined Electronic and Structural Properties of the Quercetin molecule a) Geometry optimize b) HOMO c) LUMO d) Total electron density

In the present computational study, the FMO analysis and global reactivity descriptors provided key insights into their inhibition efficiencies. The HOMO energy levels, which reflect the electron-donating ability of the molecules, were found to be relatively high for quercetin and kaempferol, suggesting strong adsorption potential on the mild steel surface via electron donation to vacant d-orbitals of Fe atoms. Equally, the LUMO energy levels indicated their capacity to accept electrons from the metal surface, thereby facilitating back-donation interactions that further stabilize the adsorption process (Obot and Gasem, 2014). The calculated energy gaps (ΔE) revealed that luteolin and apigenin possess relatively lower ΔE values compared to other flavonoids, implying higher chemical reactivity and greater adsorption tendencies (Gece, 2008). IP and electron affinity (EA) values were consistent with the observed FMO energies, where lower IP values correlate with easier electron donation, and higher EA values favor electron acceptance during metal-inhibitor interactions (Dao *et al.,* 2017).Quercetin > Luteolin > Isorhamnetin > Kaempferol > Apigenin.

The FMO analysis shows that flavonoids such as Quercetin and Luteolin, with higher (less negative) EHOMO values, possess strong electron-donating ability to Fe atoms on the mild steel surface, while their lower ELUMO values favour back-donation, stabilizing adsorption. The small energy gap (ΔE) observed for Quercetin, followed by Luteolin, highlights their higher chemical reactivity and stronger adsorption tendency, consistent with their conjugated structures and hydroxyl groups that promote electron delocalization. Additionally, IP and EA further confirm Quercetin's strong donating ability and Luteolin's ability to accept electrons from Fe, facilitating donor-acceptor interactions (Belghiti *et al.,* 2020). Their low global hardness and high softness reinforce reactivity, while moderate electronegativity supports strong but reversible adsorption. Fraction of electron transfer (ΔN) values indicate Quercetin and Isorhamnetin as the most effective electron donors, enhancing film stability and inhibition efficiency. Additionally, larger molecular size and multiple adsorption centers in flavonoids like Quercetin contribute to greater surface coverage, leading to superior corrosion inhibition performance (Table 4).

Table 4: Electronic and Structural Properties of the Flavonoids

Molecule	EHOMO (eV)	ELUMO (Ev)	ΔE (Ev)	MM (g/mol)	IP (Ev)	Ea (Ev)	ŋ
Quercetin	-5.77	-3.01	2.76	302.24	5.77	3.01	1.38
Kaempferol	-5.72	-2.90	2.82	286.24	5.72	2.90	1.41
Luteolin	-5.64	-2.86	2.78	286.24	5.64	2.86	1.39
Apigenin	-5.65	-2.94	2.71	270.24	5.65	2.94	1.36
Isorhamnetin	-5.79	-3.02	2.77	316.25	5.79	3.02	1.39

Furthermore, the global hardness (η) and softness (σ) parameters showed that quercetin and luteolin are relatively softer molecules, which is advantageous for corrosion inhibition as soft molecules readily interact with the d-orbitals of Fe atoms (Gece, 2008). The absolute electronegativity (χ) and fraction of electrons transferred (ΔN) further support this observation, with positive ΔN values indicating the tendency of the flavonoids to donate electrons to the mild steel surface, leading to protective film formation (Obot and Gasem, 2014). Among the studied flavonoids, quercetin and kaempferol displayed the most favorable combination of electronic properties, followed by luteolin and apigenin, suggesting their superior inhibition efficiencies.

3.3 Insights for Real World Applications

The quantum chemical descriptors and adsorption studies of flavonoids such as quercetin, luteolin, and apigenin provide valuable insights into their potential as green corrosion inhibitors. Their relatively small ΔE and σ indicate a strong tendency to donate electrons and form stable complexes with Fe atoms on mild steel surfaces. This suggests that flavonoids could serve as sustainable alternatives to conventional synthetic inhibitors, which are often toxic and non-biodegradable. In practical terms, extracts from *Adansonia digitata* (baobab) leaves, which are rich in these flavonoids, can be directly applied as eco-friendly corrosion inhibitors in industries such as petroleum, construction, and marine engineering. Their renewable nature, low cost, and biodegradability offer a promising pathway toward large-scale, environmentally benign corrosion protection strategies. Moreover, the combination of computational predictions with experimental validation can accelerate the screening and development of plant-derived inhibitors, reducing reliance on costly trial-and-error approaches. By linking molecular-level descriptors (HOMO, LUMO, global hardness and softness) with inhibition efficiency, researchers and industries can design optimized formulations for real-world applications, thereby bridging the gap between theory and practice.

4.0 CONCLUSION

This study demonstrates that flavonoids extracted from *Adansonia digitata* leaves are promising, sustainable corrosion inhibitors for mild steel in acidic media. Weight-loss measurements showed a clear, concentration dependent improvement in inhibition efficiency, exceeding 90% at the optimal dosage. FT-IR analysis corroborated surface interaction, with shifts in O-H, C=O and aromatic C=C bands after exposure to steel, consistent with molecular adsorption and film formation. DFT calculations provide a coherent mechanistic picture that supports the experimental observations. FMO analysis identified quercetin and luteolin as the most reactive species, with high HOMO character concentrated on hydroxyl and carbonyl sites features that favour electron donation to vacant Fe 3d orbitals. Global reactivity descriptors (η, σ, and ΔE trends) further indicate that these molecules are more polarizable and chemically reactive than the other tested flavonoids, which rationalizes their superior inhibition performance. Fukui function mapping localized the principal nucleophilic centers to specific hydroxyl and carbonyl moieties, pinpointing the atomic sites most likely to coordinate with the metal surface. Adsorption modeling showed stable, energetically favourable interactions (-) and charge transfer from inhibitor to metal, supporting a chemisorption dominated mechanism with additional physisorptive contributions from π–d interactions. Taken together, the experimental (weight loss, FT-IR) and theoretical (DFT, FMO, Fukui, adsorption) results converge on a consistent mechanism: polyhydroxylated flavonoids from *A. digitata* adsorb onto steel via donor-acceptor interactions (chemisorption), forming a protective film that reduces metal dissolution. Quercetin emerges as the most effective inhibitor in this series, followed by luteolin, with isorhamnetin, kaempferol and apigenin contributing via complementary adsorption modes. These findings support the practical application of *A. digitata* flavonoid fractions as eco-friendly inhibitors in processes such as acid pickling and industrial cleaning.

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Conflicts of Interest: The authors confirm that they have no any conflict of interest in this study.

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