



Research article

Electrochemical assessment and DFT/DFTB insights of *Melastoma candidum* leaf extract as a corrosion inhibitor for carbon steel

Nurdin Ali ^{a,*}, Syarizal Fonna ^a, Husni Usman ^b, Yumaidi Saputra ^{c,d}, Muhibul Jamal ^e, Ali Imran ^a, Lala Adetia Marlina ^f

^a Department of Mechanical and Industrial Engineering, Universitas Syiah Kuala, Banda Aceh 23111, Indonesia

^b Department of Mining Engineering, School of Earth Engineering, Faculty of Engineering, Universitas Syiah Kuala, Banda Aceh 23111, Indonesia

^c Department of Mechanical Engineering, Sekolah Tinggi Teknik Iskandar Thani, Banda Aceh 23114, Indonesia

^d Doctoral Program, School of Engineering, Universitas Syiah Kuala, Banda Aceh 23111, Indonesia

^e Department of Electrical Engineering, Universitas Cipta Mandiri, Peunaga Cut Ujong, Aceh Barat 23681, Indonesia

^f Research Center for Computing National Research and Innovation Agency (BRIN), Cibinong, Bogor 16911, Indonesia

ARTICLE INFO

Keywords:

Adsorption mechanism

Corrosion inhibitor

Carbon steel

Electrochemical analysis

Melastoma candidum leaf extract

3.5% NaCl

ABSTRACT

The superior mechanical properties contribute to the use of carbon steel for various purposes. However, the weak corrosion resistance presents a challenge for users, showing the need for appropriate prevention methods such as natural corrosion inhibitors from *Melastoma candidum* leaf extract (MCLE). Therefore, this study aimed to investigate the role of MCLE inhibitors in protecting carbon steel in 3.5% NaCl solution. Potentiodynamic polarization (PDP) and electrochemical impedance spectroscopy (EIS) tests were applied to examine the role of inhibitor molecules by mixing at concentrations of 0, 200, 400, 600, 800, and 1000 ppm. The results showed that the highest inhibition efficiency of 83.89% (PDP) and 85.07% (EIS) was achieved at the maximum concentration (1000 ppm), with MCLE classified as mixed inhibitors. To analyze the inhibition mechanism, adsorption isotherm theories were applied, with the Frumkin isotherm providing the best fit. This suggested that the molecules of the organic inhibitor were adsorbed on the steel surface based on physisorption. DFT calculations revealed favorable electronic properties of MCLE phytochemicals, with oxygen-containing groups serving as active adsorption sites. SCC-DFTB simulations confirmed strong adsorption on the Fe(110) surface, with adsorption energies of -39.54 to -206.83 kcal/mol, indicating the formation of a stable protective film. Surface characterization further validated the corrosion protection ability of MCLE, highlighting its potential as a sustainable inhibitor for carbon steel in chloride environments.

1. Introduction

Low-carbon steel is a metal material often used in various industrial sectors, such as building construction, storage tanks, piping systems, and materials in the production process [1–3]. The advantages of this material are supported by excellent mechanical properties, including high strength, flexibility, ease of treatment, good durability, and a relatively lower price [4,5]. However, during application, metal corrosion is a major problem that is difficult to avoid, causing adverse effects in the form of loss of aesthetics, financial losses to consumers, and damage to the environment [6].

Corrosion is the process of metal returning to original form, namely iron ore (Fe_2O_3), after interacting with the surrounding environment [7,

8]. Generally, corrosion reactions often occur when the metal interacts with anions contained in water, causing an increase in the electrochemical reaction. Corrosive media, such as a salty environment (NaCl), are characterized by a fairly bad level of corrosivity [9]. As a strong electrolyte, NaCl dissolves in water to form Na^+ and Cl^- ions [10]. Increasing the content of Cl^- ions in water affects the electrochemical reaction, causing a corresponding rise in current density to accelerate the rate of corrosion in metals [11,12].

Preventive measures can be implemented through the application of corrosion inhibitors by mixing with corrosive solutions at low concentrations [13]. These inhibitors are often derived from organic and inorganic materials. However, the continuous use of inorganic materials poses a significant environmental risk, which limits their application,

* Corresponding author.

E-mail address: nurdin.ali@usk.ac.id (N. Ali).

<https://doi.org/10.1016/j.nxmte.2026.102975>

Received 27 February 2026; Received in revised form 11 June 2026; Accepted 28 July 2026

Available online 31 July 2026

2949-8228/© 2026 The Author(s). Published by Elsevier Ltd. This is an open access article under the CC BY-NC license (<http://creativecommons.org/licenses/by-nc/4.0/>).

particularly at high intensities [14]. Therefore, the use of natural materials is a necessary measure due to their abundant availability, affordable price, and environmental friendliness. Organic materials from plants can address all of these challenges [8,15–18], as the presence of heteroatom compounds such as N, S, O, and P facilitates attachment to metal surfaces [19].

To reduce reliance on inorganic materials, various plants have been used as corrosion inhibitors. These include leaf extract of cucumber (*Cucumis sativus* L.) [20], *Luffa cylindrica* [21], spinach (*Spinacia oleracea*) [22], ketapang (*Terminalia catappa* L.) [23], cempedak (*Artocarpus integer*) fruit peel extract [24], blackberry [25], *Andrographis paniculata* [26], rubber [27], neem [28], *Desmodium adscendens* [29], and safflower [30]. Overall, the studies conducted show promising potential for protecting metals from corrosion.

Another promising plant candidate is *Melastoma candidum*, a member of the genus *Melastoma* that grows widely in Asia and Oceania [31]. Traditionally, this plant has been used as a medicinal ingredient, such as a treatment for digestive infections. As a unique, innovative feature, and to provide additional benefits, this plant is now used as a corrosion inhibitor. A previous study by Joli et al. showed that *Melastoma candidum* leaf extract (MCLE) was effective in protecting carbon steel in salt solution [32]. The results showed that the inhibitory effectiveness was very high, with an efficiency of 82.89%, leading to a very low corrosion compared to the uninhibited system. However, previous studies have only focused on the weight loss method, showing the need for more comprehensive strategies, such as electrochemical testing, to predict corrosion inhibition mechanisms as a form of deeper innovation related to the benefits of MCLE inhibitors.

Based on the description, this study aims to determine the effectiveness of protection by MCLE inhibitors through electrochemical analysis and evaluate the adsorption mechanism during corrosion control. MCLE is used as a corrosion inhibitor for low-carbon steel contaminated with 3.5% NaCl solution. The results show that the difference in the condition of low-carbon steel with and without protection has a significant influence on the performance of MCLE inhibitors, as indicated by morphological analysis based on various environmental conditions. Furthermore, density functional theory (DFT) calculations were employed to analyze the electronic properties and adsorption activity of major MCLE phytochemicals, while SCC-DFTB simulations were performed to investigate molecular interactions and adsorption configurations on the Fe(110) surface. The results provide insight into the relationship between molecular characteristics, adsorption behavior, and corrosion inhibition performance, supporting the development of MCLE as a sustainable green corrosion inhibitor for carbon steel.

2. Experimental method

2.1. Corrosive materials and solutions

This study used low-carbon steel purchased from a steel shop in Banda Aceh, Indonesia, with the chemical composition shown in Table 1. The steel was cut to dimensions of $1 \times 1 \times 1 \text{ cm}^3$, cleaned using sandpaper, and connected with soldered wire cables. The exposed surface of the specimen measured 1 cm^2 , with the other parts protected with polyester resin. As a corrosive solution, 10 kg of NaCl crystals were prepared, which were purchased from CV. Rudang Jaya, Medan, Indonesia. Subsequently, 35 g of NaCl crystals mixed in 1 L of distilled water were prepared to obtain a 3.5% NaCl solution.

Table 1
Chemical composition of carbon steel.

Element	C	Si	Mn	P	S	Cr	Mo	Ni	Cu	Al	Nb	Fe
wt%	0.18	0.26	1.25	0.03	0.03	0.15	0.03	0.09	0.28	0.01	0.01	Balance

2.2. MCLE inhibitor

A total of 200 g of *Melastoma candidum* leaf was prepared and cleaned with running water to remove impurities. The maceration method was applied by soaking the leaf in 3 L of 96% ethanol solution for 24 h. The macerate was evaporated using an evaporator at 50°C , obtaining 12 g of pure extract. MCLE was used as the primary ingredient for protecting carbon steel in a 3.5% NaCl medium mixed at low concentrations of 200, 400, 600, 800, and 1000 ppm. These concentrations are often used in industrial environments as the most effective method for preventing corrosion [33].

The characterization of MCLE was analyzed using Fourier transform infrared (FTIR) with a Shimadzu IR Prestige-21 and Gas Chromatography-Mass Spectrometry (GC-MS) through Clarus 680 GC with SQ8 MS. The results of FTIR analysis showed functional groups included in the protection process. Meanwhile, GC-MS results showed the presence of several dominant compounds from MCLE extract.

2.3. Corrosion rate testing

Electrochemical corrosion rate measurement was conducted using the potentiodynamic polarization (PDP) and Electrochemical impedance spectroscopy (EIS) method with an Autolab type PGSTAT204 model device (serial number AUT53279), assisted by the Nova 2.1 application, which was produced by Metrohm Autolab B.V. Low-carbon steel, Ag/AgCl, and Ag rings were used as working, reference, and counter electrodes, respectively. Before measurement, the working electrode was immersed in a corrosive solution and a mixture of inhibitors to achieve a steady state condition. The PDP test was carried out with a potential range of -200 – 200 mV at a scan rate of 1 mV/s . EIS measurements used an AC signal with an amplitude of 10 mV and a frequency of 100 kHz – 10 mHz . Specifically, corrosion rate (PDP) was calculated based on the equation below [34]:

$$\text{Cr}(\text{mm.y}^{-1}) = 3.27 \times 10^{-3} \frac{i_{\text{corr}} \times \text{EW}}{\rho} \quad (1)$$

In this equation, EW is the equivalent weight (g/mol), and ρ is the metal density (g/cm^3). Meanwhile, the inhibition efficiency (IE) of MCLE inhibitors and PDP measurement was calculated based on the following equation [35]:

$$(\text{IE}) \% = \frac{i_{\text{corr}}^0 - i_{\text{corr}}(\text{inh})}{i_{\text{corr}}^0} \quad (2)$$

i_{corr}^0 and $i_{\text{corr}}(\text{inh})$ are the corrosion current density without and with the presence of MCLE inhibitor protection ($\mu\text{A/cm}^2$). Meanwhile, the effectiveness of the MCLE inhibitor in EIS measurements can be determined through the following Eq. 3:

$$\text{IE}(\%) = \frac{R_{p(\text{inh})} - R_p^0}{R_{p(\text{inh})}} \times 100\% \quad (3)$$

Where, R_p^0 and $R_{p(\text{inh})}$ are the corrosion charge transfer resistances under conditions without and with the inhibitor mixture.

PDP test was conducted with temperature variations ranging from 25 , 35 , 45 , and 55°C at the concentration with the best inhibition. To determine the inhibition mechanism and the relationship between inhibitor protection on the metal surface, the Langmuir, Temkin, Freundlich, and Frumkin adsorption isotherm theories were applied, as follows [36]:

Langmuir adsorption isotherm equation:

$$\frac{C}{\theta} = \frac{1}{K_{ads}} + C \quad (3)$$

Freundlich adsorption isotherm equation:

$$\log \theta = \log K_{ads} + n \log C \quad (4)$$

Frumkin adsorption isotherm equation:

$$\log \left[C \frac{\theta}{1-\theta} \right] = \log K_{ads} + g\theta \quad (5)$$

Temkin adsorption isotherm equation:

$$\log \frac{\theta}{C} = \log K_{ads} - g\theta \quad (6)$$

Where θ is the degree of surface coverage, C is the inhibitor concentration, and K_{ads} is the adsorption-desorption equilibrium constant, n is a constant, and g is a molecular interaction parameter.

2.4. Surface characterization of carbon steel

Protection capacity of carbon steel by MCLE inhibitors was investigated through surface characterization using scanning electron microscopy-energy dispersive x-ray (SEM-EDS) with a JEOL JSM 6510 LA, atomic force microscopy (AFM) with a Bruker, and X-ray diffraction (XRD) with a Rigaku Miniflex 600. This analysis was performed on carbon steel under pre-treatment conditions, in a 3.5% NaCl solution, and at a concentration of 1000 ppm.

2.5. Computational details

To elucidate the molecular mechanism underlying the corrosion inhibition performance of MCLE, a combined Density Functional Theory (DFT) and Density Functional Tight-Binding (DFTB) approach was employed. The major phytochemical constituents identified by GC-MS analysis, namely 5-hydroxymethylfurfural (5-HMF), methyl- β -D-glucopyranoside, methyl hexadecanoate, and 9,12,15-octadecatrienoate, were selected as representative inhibitor molecules for theoretical investigations.

Quantum chemical calculations were performed using Gaussian 09. Molecular structures were optimized using the B3LYP functional with the 6-311++G(d,p) basis set, selected for its reliability in describing molecular interactions and charge-transfer processes relevant to corrosion inhibition [37,38]. Solvent effects were considered using the CPCM model with water as the solvent. Frequency analysis was performed to confirm that the optimized structures corresponded to true minima on the potential energy surface.

The optimized molecular structures were used to determine the frontier molecular orbital energies, including the highest occupied molecular orbital (E_{HOMO}) and lowest unoccupied molecular orbital (E_{LUMO}). Furthermore, several quantum chemical descriptors were calculated, including the energy gap (ΔE), ionization potential (I), electron affinity (A), electronegativity (χ), global hardness (η), global softness (σ), electrophilicity index (ω), dipole moment (μ), and fraction of electron transfer (ΔN). ESP (Electrostatic Potential) analyses were also performed to identify the most probable adsorption sites and electron-rich regions involved in the interaction with the metallic surface [39].

The adsorption behavior of the selected phytochemicals on iron was investigated using the self-consistent charge density-functional tight-binding (SCC-DFTB) method implemented in the DFTB+ package. The Fe(110) surface was chosen as the adsorption substrate because it is the most stable crystallographic plane of α -Fe and is widely used as a representative model for carbon steel in corrosion studies, providing a realistic platform for evaluating adsorption and charge-transfer interactions between inhibitor molecules and the metal [40,41]. A

five-layer periodic Fe(110) slab was constructed with a 50 Å vacuum region along the surface normal to prevent interactions between periodic images. During geometry optimization, the bottom layers were fixed to represent the bulk phase, whereas the upper layers and adsorbed molecules were fully relaxed.

The SCC-DFTB calculations were performed using the trans3d Slater-Koster parameter set. Multiple initial adsorption geometries were considered by varying the orientation and position of each inhibitor molecule on the Fe(110) surface. Structural relaxation was carried out until the maximum atomic force converged below 1×10^{-3} a.u. SCC-DFTB was employed because it enables efficient and reliable modeling of large inhibitor-metal interfaces while accurately describing adsorption energies and charge-transfer interactions relevant to corrosion inhibition [37,42].

The adsorption energy was calculated according to:

$$E_{ads} = E_{Fe(110)+inh} - (E_{Fe(110)}|E_{inh}) \quad (7)$$

where $E_{Fe(110)+inh}$ is the total energy of the adsorbate-surface system, $E_{Fe(110)}$ is the energy of the clean Fe(110) slab, and E_{inh} is the energy of the isolated inhibitor molecule.

3. Results and discussion

3.1. MCLE characterization

The MCLE extract was analyzed to identify the constituents included in the corrosion protection system. Based on the results presented in Fig. 1, FTIR testing showed a spectrum of functional groups, with the peak at 3284 cm^{-1} indicating the hydroxyl (O-H) stretching. The peak at 2926 cm^{-1} corresponded to C-H stretching, typical of alkanes. Meanwhile, the peak between 1800 and 1600 cm^{-1} signified C=O stretching, representing a carbonyl group. Other functional groups were detected, including amines at 1360 – 1080 cm^{-1} and halogens at 418 cm^{-1} . These FTIR results confirm that the MCLE extract contains various bonds and heteroatoms crucial for protecting carbon steel from corrosion, indicating the presence of compounds contributing to protective film formation [43]. Therefore, the MCLE extract can be considered an effective natural anti-corrosion agent, which is consistent with the results from previous studies [23,24].

GC-MS analysis of the MCLE extract identified several main compounds, including 5-Hydroxymethylfurfural at 40.73%, Methyl- β -D-glucopyranoside at 13.00%, Methyl hexadecanoate at 6.36%, and 9, 12, 15-Octadecatrienoic acid at 6.10%, as shown in the chromatogram in Fig. 2 and Table 2 [32]. These compounds are known to actively inhibit corrosion reactions and limit the interaction of carbon steel with the

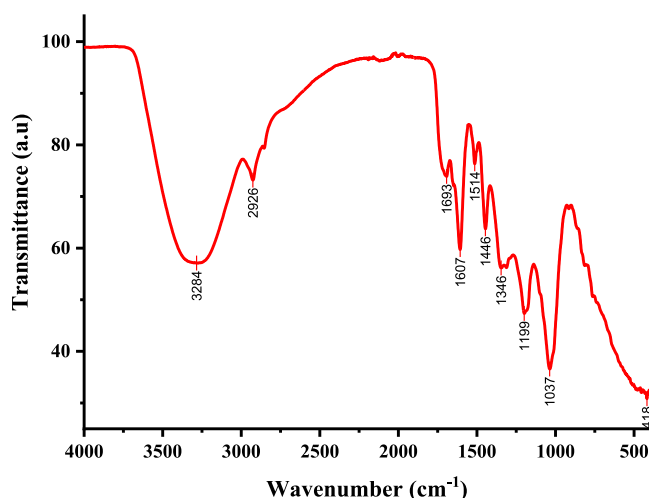


Fig. 1. FTIR of *Melastoma candidum* leaves.

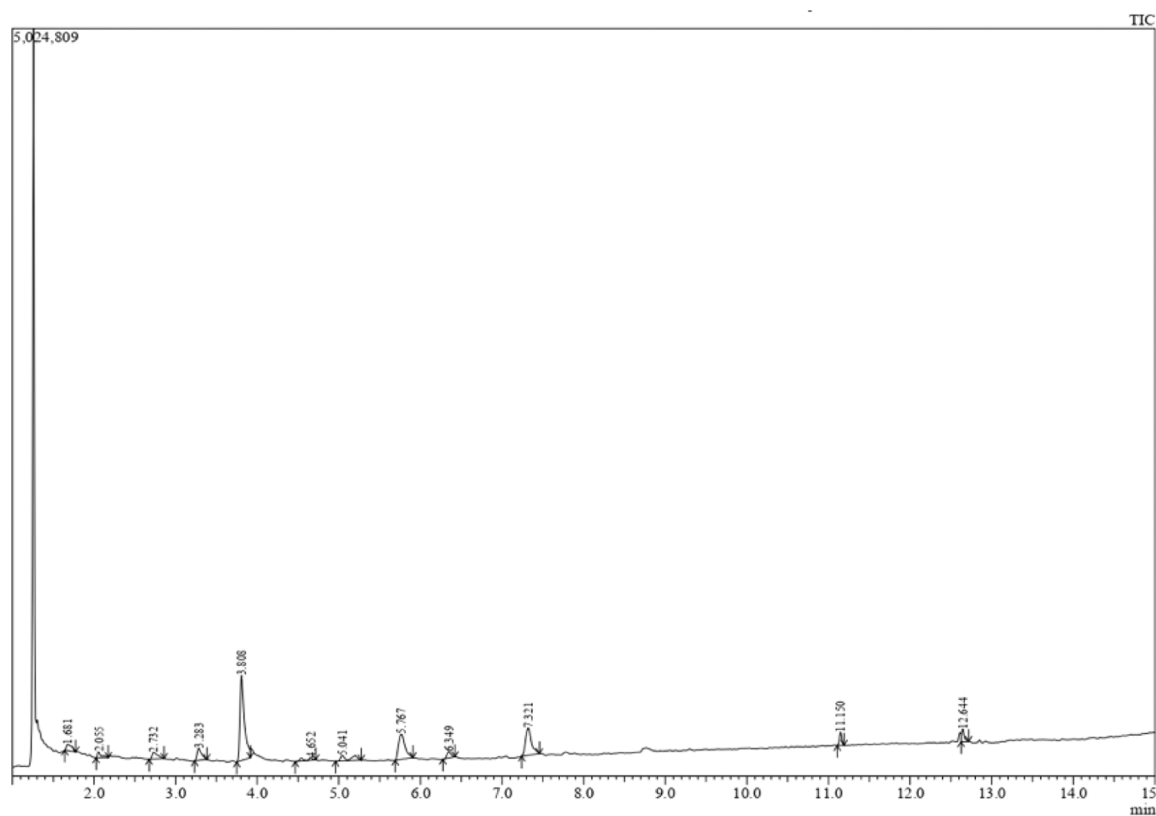


Fig. 2. Chromatogram of the MCLE extract.

Table 2

Content and ionic structure of the MCLE extract.

Compound	Ionic bonding
5-Hydroxymethylfurfural	
Methyl-β-D-glucopyranoside	
Methyl hexadecanoate	
9, 12, 15-Octadecatrienoic acid	

environment [40,41].

3.2. PDP

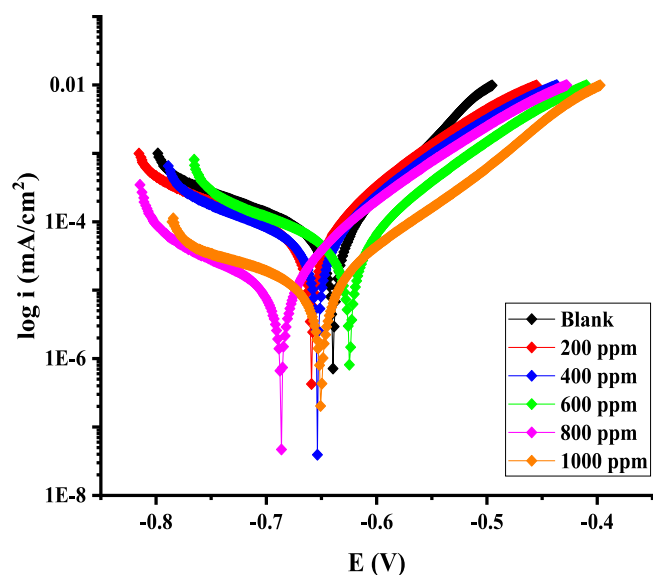
Corrosion rate of carbon steel was investigated using the PDP method. Each sample condition was tested three times to obtain more

accurate data, and the test parameters through Tafel extrapolation are presented in Table 3. The polarization curve of corrosion rate based on inhibitors concentration (ppm) at room temperature conditions (25 °C) was presented in Fig. 3. This test was conducted to investigate the effect of MCLE inhibitors in the role in protecting carbon steel from corrosive environment of 3.5% NaCl. The results showed distinct corrosion

Table 3

PDP test parameters on low-carbon steel.

Concentration (ppm)	E_{corr} (V)	i_{corr} (A/cm ²)	β_a (mV/dec)	$-\beta_c$ (mV/dec)	Resistant polarization (Ω)	Cr (mm/y)	IE (%)
Variation of MCLE concentration (ppm) at room temperature (25 °C)							
Blank	−0.640	9.23×10^{-5}	93.50	157.65	288.33	1.074	0
200	−0.659	7.68×10^{-5}	83.38	152.07	339.27	0.894	16.76
400	−0.654	6.66×10^{-5}	88.15	147.19	391.11	0.775	27.84
600	−0.625	5.78×10^{-5}	84.33	148.08	451.16	0.672	37.43
800	−0.687	1.79×10^{-5}	83.35	124.46	1457.26	0.208	80.63
1000	−0.651	1.49×10^{-5}	84.94	176.80	1751.96	0.173	83.89
Temperature variation at 1000 ppm MCPE concentration (°C)							
25 (blank)	−0.640	9.23×10^{-5}	93.50	157.65	288.33	1.074	0
25	−0.651	1.49×10^{-5}	84.94	176.80	1751.96	0.173	83.89
35 (blank)	−0.621	1.11×10^{-4}	92.19	148.24	234.38	1.293	0
35	−0.630	2.92×10^{-5}	64.26	276.36	892.02	0.339	73.78
45 (blank)	−0.678	1.25×10^{-4}	83.73	150.57	208.15	1.457	0
45	−0.692	4.04×10^{-5}	67.17	207.86	644.39	0.470	67.74
55 (blank)	−0.628	1.54×10^{-4}	104.09	179.78	169.75	1.786	0
55	−0.649	1.1×10^{-4}	77.38	144.57	235.72	1.286	27.99

**Fig. 3.** Polarization curve of carbon steel with varying inhibitor concentration at room temperature (25 °C).

behaviors in the absence and presence of inhibitors, with varying concentrations enabling the determination of the optimum concentration for effective corrosion protection.

From the tests conducted, corrosion current density (i_{corr}) of carbon steel in 3.5% NaCl solution decreased significantly along with increasing MCLE concentration, starting from 9.23×10^{-5} (blank) to 1.49×10^{-5} A/cm². The decrease in the i_{corr} value shows that MCLE inhibitor molecules are adsorbed on the surface of carbon steel, thereby successfully blocking the growth of corrosion compounds [25–27]. The adsorption that occurs affects electrochemical reaction (oxidation-reduction) to slow corrosion rate and estimate the durability of carbon steel during use. The corrosion rate decreases with increasing inhibitors concentration [28–30], ranging from 0, 200, 400, 600, 800, and 1000 ppm. Based on the results, the highest corrosion rate of 1.074 mm/year occurred when there was no protection and decreased from 0.894, 0.775, 0.672, 0.208, to 0.173 mm/year gradually as inhibitors concentration increased.

Tafel slope analysis was performed to evaluate the impact of inhibitor addition on the stability of the inhibition mechanism. Based on the experimental data, the cathodic Tafel slope constant (β_c) was found to be more influential than the anodic Tafel slope constant (β_a). This pattern occurred at all concentrations of MCLE inhibitor, with slope data

remaining consistent as the concentration increased. This suggests that the MCLE inhibitor primarily reduces corrosion by suppressing the reduction reaction (cathodic region). Therefore, the effectiveness of the inhibitor is more pronounced at the cathode, although some inhibition also occurs in the anodic region [29].

According to PDP analysis, inhibitors are categorized as anodic or cathodic when the difference in E_{corr} value with no protection exceeds a value of 85 mV [44]. Based on the results obtained, E_{corr} value is less than 85 mV. This shows that MCLE is in the mixed inhibitor category capable of blocking the anodic reaction area (dissolved metal ions) and the cathodic area (hydrogen reduction) through the reaction of molecules adsorbed on the surface [45,46]. The behavior inhibits the electrochemical corrosion process and slows down the corrosion rate. IE is very important in determining the performance of inhibitors. In this study, a concentration of 1000 ppm showed the best performance with the highest efficiency of 83.89%, indicating successful protection of carbon steel [31,32]. This high performance is attributed to the filling of empty orbitals by protonated active molecules on the surface of carbon steel [47]. The best inhibition value obtained at a maximum concentration of 1000 ppm shows that MCLE inhibitors perform effectively based on the continuity of protection mechanism.

Several factors affect corrosion rate and inhibitory activity of inhibitors, such as temperature [48]. In principle, higher temperature cause corrosion susceptibility in carbon steel to occur more quickly due to faster electrochemical reaction [49]. Based on the analysis conducted, the effect of changes in room temperature on carbon steel environment in a 3.5% NaCl environment and inhibitor protection was investigated through PDP testing, with the results obtained shown in Fig. 4 and Table 3. The polarization curve showed the comparison between samples without and with selected protection at maximum concentration conditions (1000 ppm) over temperature range of 25, 35, 45, and 55 °C.

Based on Table 3, corrosion rate increased with rising room temperature, both in conditions without and with the presence of inhibitors [36]. This phenomenon was due to faster diffusion of ions and oxygen, which accelerated corrosion of carbon steel. As presented in Fig. 5, corrosion rate at room temperature (25 °C) appeared lower than other conditions and increased with rising temperature. This process affects the acquisition of IE percentage value. However, the efficiency of MCLE decreased with increasing room temperature because of the damage to the protective film layer of inhibitors on carbon steel and the loss of molecules in its environment, causing direct interaction with corrosive compounds [38,39]. This was also supported by the data and parameters produced, where i_{corr} value was relatively higher with increasing temperature environment [50].

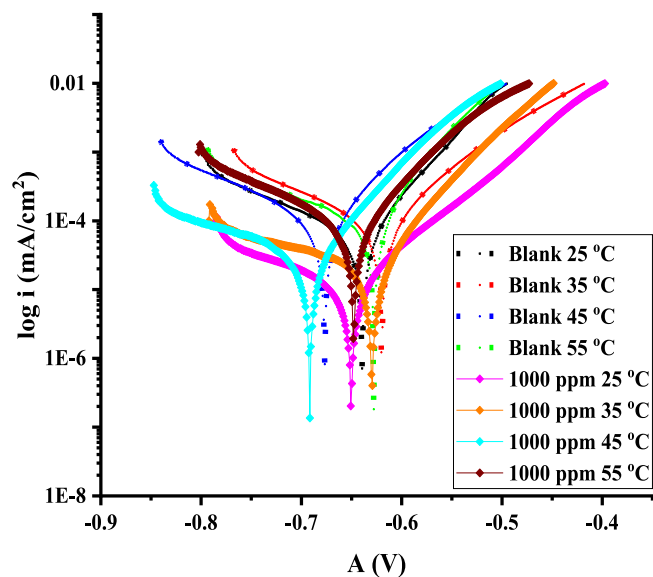


Fig. 4. Polarization curve of carbon steel with temperature variation.

3.3. EIS

EIS testing is an experimental method used to determine the corrosion inhibition of low-carbon steel by inhibitors. To ensure data reproducibility, each sample under different conditions was tested three times. In this study, EIS was applied to evaluate the electrochemical behavior of the low-carbon steel-electrolyte (NaCl) interface mixed with MCLE inhibitor. The analysis focused on inhibitor adsorption properties, charge-transfer mechanisms, and diffusion. The impedance of protected and unprotected low-carbon steel was shown through a semicircle (Nyquist) graph consisting of Z_{real} and Z_{img} in Fig. 6. The results showed distinct behavior under varying environmental conditions, where the loop diameter significantly affected corrosion rate in low-carbon steel.

Smaller capacitive loop diameters indicate very high corrosion rates, which are caused by low-carbon steel exposed to pure NaCl solutions without any protective coating [51]. However, larger capacitive loop diameters suggest lower corrosion rates [26,42]. This pattern occurs when inhibitors are mixed, and loop diameters increase with higher MCLE inhibitor concentrations ranging from 200, 400, 600, 800, to 1000 ppm. The corresponding increase is attributed to the natural molecular interactions of the inhibitor with the steel surface, which can displace the dispersion of corrosive ions.

The Nyquist diagram is supported by an electrical circuit consisting of R_s (solution resistance), CPE (constant phase element), and R_p (polarization resistance), as shown in Table 4. The presence of these elements indicates a double-layer capacitance treatment on the surface of low-carbon steel. Based on the results, the R_p value increased with higher concentration, from 154.15, 373.95, 491.17, 676.24, to 1032.8 Ω/cm^2 , and correlated with the size of the semicircle curve formed [8,43]. This behavior suggests enhanced corrosion resistance, as the inhibitor effectively limits chemical reactions by forming a protective film [52]. In line with the analysis, the highest inhibitor efficiency of 85.07% was achieved at the maximum concentration (1000 ppm), indicating that corrosion was significantly reduced through the adsorption of MCLE molecules on the surface of carbon steel.

The Bode curve in Fig. 7 further explains the performance of the MCLE molecules, showing that higher inhibitor concentration provides better protection [53]. The lowest impedance is observed without any inhibitor, while the addition of MCLE progressively increases the Bode curve magnitude. Characterization results in Fig. 1 and Table 2 confirm that the inhibitor molecules are adsorbed on the steel surface and can inhibit the growth of corrosion compounds. These results support the

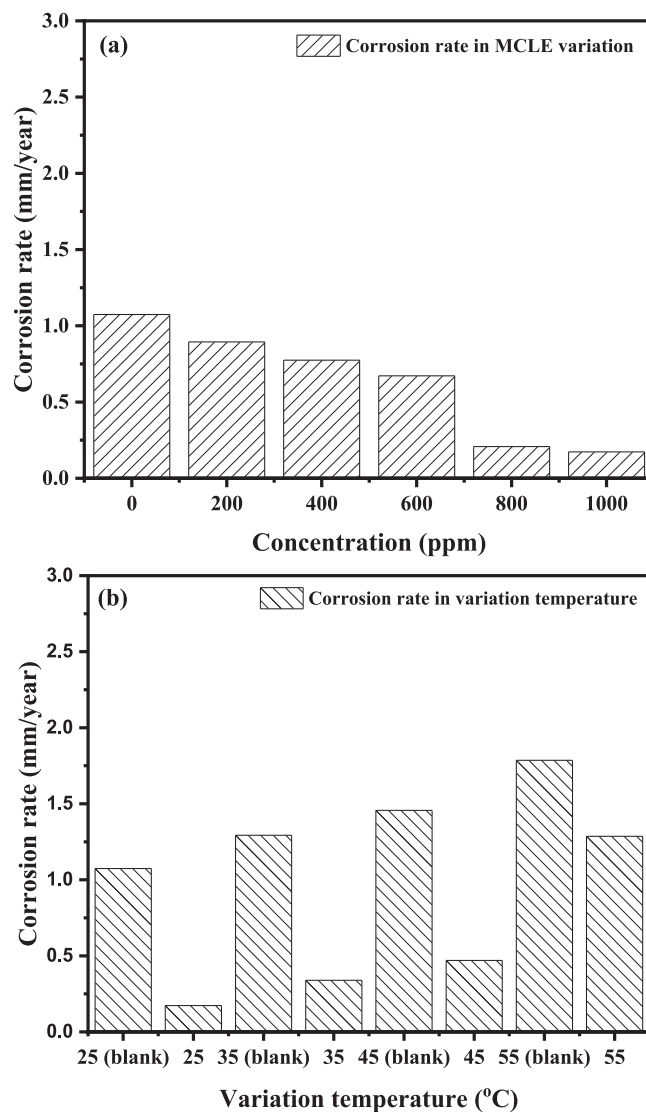


Fig. 5. Comparison of corrosion rates of concentration variations (a) and temperature variations (b).

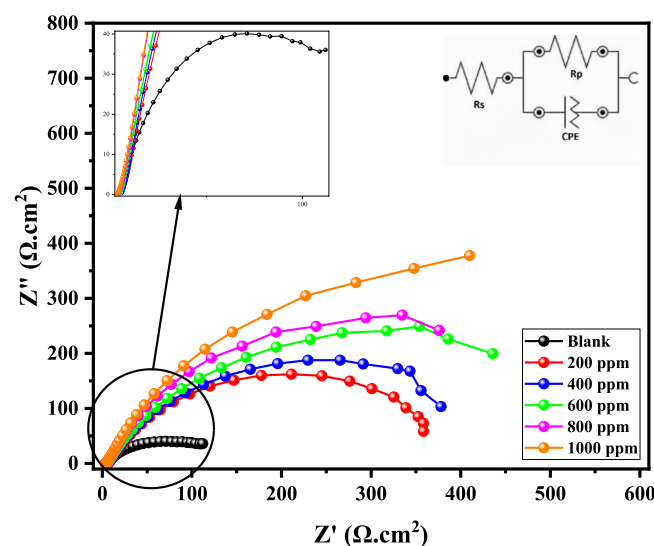


Fig. 6. Nyquist curve of low-carbon steel without and with varying MCLE inhibitor mixtures.

Table 4
Electrochemical impedance spectroscopy test parameters.

Concentration (ppm)	Rs (Ω/cm ²)	Rp (Ω/cm ²)	CPE		E _{EIS} (%)
			Y ₀ (Ω ⁻¹ S ⁿ cm ⁻²)	n	
Blank	4.11	154.15	2.37×10^{-3}	0.63	0
200 ppm	12.01	373.95	6.16×10^{-4}	0.91	21.98
400 ppm	6.22	491.17	9.33×10^{-4}	0.82	68.62
600 ppm	4.69	676.24	1.31×10^{-3}	0.79	77.20
800 ppm	4.53	687.87	1.97×10^{-3}	0.85	77.59
1000 ppm	3.63	1032.8	1.54×10^{-3}	0.82	85.07

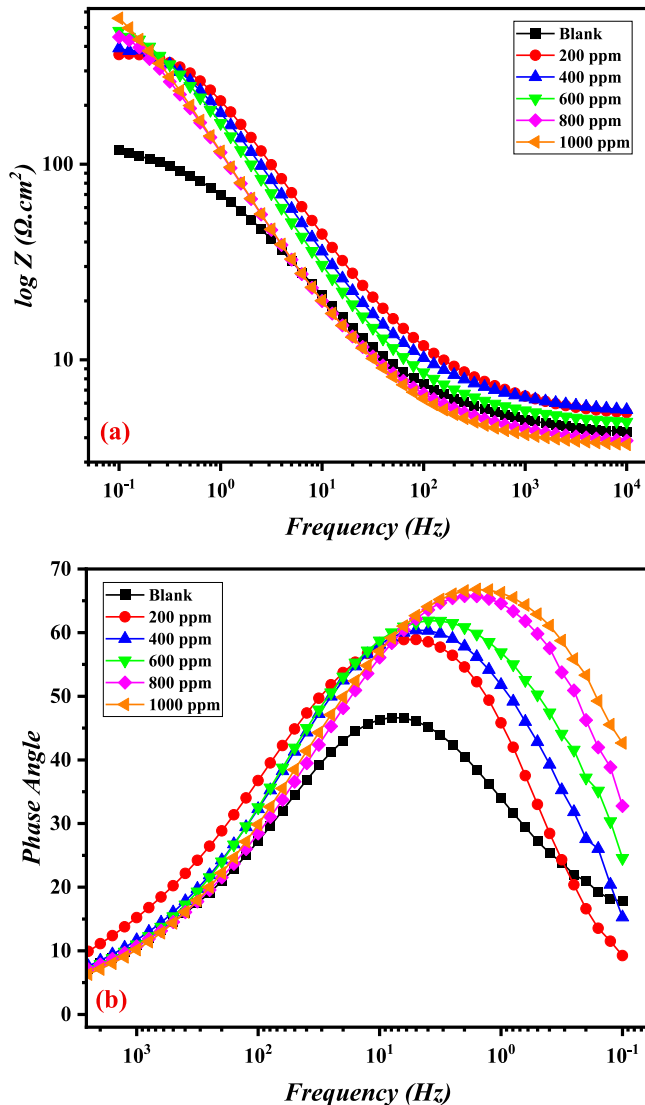


Fig. 7. Mode modulus (a) and phase angle (b) in carbon steel with and without inhibitor mixtures.

evidence that the MCLE inhibitor is highly effective in an environmentally friendly corrosion protection system.

3.4. Adsorption isotherm of MCLE inhibitor on low-carbon steel

The protection and adsorption mechanisms of organic molecules from MCLE inhibitors were investigated based on experimental data against the adsorption isotherm theory. Specifically, the adsorption isotherm equations were calculated using four isotherm Eqs. 3, 4, 5, and

6, namely, Langmuir, Freundlich, Frumkin, and Temkin. To identify the most suitable theory, the four equations were compared using the data of the linear fitting curve plot performed under varying MCLE inhibitor concentrations, with results shown in Table 5. The regression results were shown in Fig. 8 to confirm the best value and type of theory selected to determine inhibition mechanism. From the results obtained, a strong linear relationship between $\log (\theta/(1-\theta) \times C)$ against θ showed the best value with an R-squared of 0.97. This result was obtained in the Frumkin isotherm theory, which was selected for producing the strongest and most suitable value compared to others. Isotherm calculation showed adsorption equilibrium constant (K_{ads}) and the standard free energy ($\Delta G_{\text{ads}}^{\circ}$) according to Eq. 7 and 8.

$$K_{\text{ads}} = \frac{1}{55.5} \exp \left(\frac{-\Delta G_{\text{ads}}^{\circ}}{RT} \right) \quad (7)$$

$$\Delta G_{\text{ads}}^{\circ} = -n R T \ln (55.5 \times K_{\text{ads}}) \quad (8)$$

A negative value of $\Delta G_{\text{ads}}^{\circ}$ shows stable adsorption of inhibitors on carbon steel surface. Based on adsorption isotherm theory, the value of $\Delta G_{\text{ads}}^{\circ}$ obtained between -20 kJ/mol or higher, suggests that inhibition occurs predominantly through physisorption. Meanwhile, the value of $\Delta G_{\text{ads}}^{\circ}$ between -40 kJ/mol or lower, shows chemisorption mechanism [54]. From experimental data calculations, the value of $\Delta G_{\text{ads}}^{\circ}$ of -19.57 kJ/mol showed that the MCLE inhibitors protected carbon steel by physisorption. This occurred through an adsorption process driven by electrostatic interactions between the inhibitor molecules and the surface of carbon steel [55,56]. The mechanism also showed that protection by MCLE inhibitors occurred through weak van der Waals forces without the formation of chemical bonds.

The inhibition mechanism by MCLE inhibitors is shown in Fig. 9. Without any protection, carbon steel is directly attacked by corrosive compounds, namely chloride ions (Cl^-) from the dissolution of NaCl compounds in water. These ions penetrate and disrupt the passive layer on the steel surface, leading to the formation of corrosion products and progressive surface damage. After protecting carbon steel by MCLE inhibitors in a corrosive environment, the active compounds interact with the metal surface to inhibit corrosion. For example, 5-hydroxymethyl-furfural (5-HMF) donate their electrons to the empty orbital region of carbon steel. methyl- β -D-glucopyranoside compounds enable even hydrogen bonding on the metal surface. Methyl hexadecanoate forms a hydrophobic layer, and 9,12,15-octadecatrienoate plays an active role in electron donation, which facilitates the adsorption on the metal surface. The ongoing process shows that compounds from MCLE inhibitors are physically adsorbed on the metal surface, thereby limiting their spread and direct interaction with corrosive compounds (Cl^-).

3.5. SEM-EDX

SEM analysis was carried out to investigate the morphology of carbon steel before treatment, after exposure to a 3.5% NaCl solution, and with inhibitor protection (1000 ppm) at a temperature of 25°C . This analysis compared the surface conditions of carbon steel to determine the effectiveness of protection by MCLE inhibitors based on the level of damage. As presented in Fig. 10a, the untreated carbon steel shows a flat, and uniform surface, indicating the absence of corrosion or structural damage.

After exposure to a corrosive 3.5% NaCl solution, carbon steel was

Table 5
Adsorption isotherm parameters.

Adsorption equation	Linear equation	K_{ads}	ΔG_{ads} (kJ. mol ⁻¹)
Langmuir	$y = -0.2235x + 1.4175$	26.15	-18.04
Freundlich	$y = 1.0543x - 0.087$	1.222	-10.45
Frumkin	$y = 2.8471x - 1.6865$	48.585	-19.57
Temkin	$y = 0.1505x - 0.1766$	1.502	-10.96

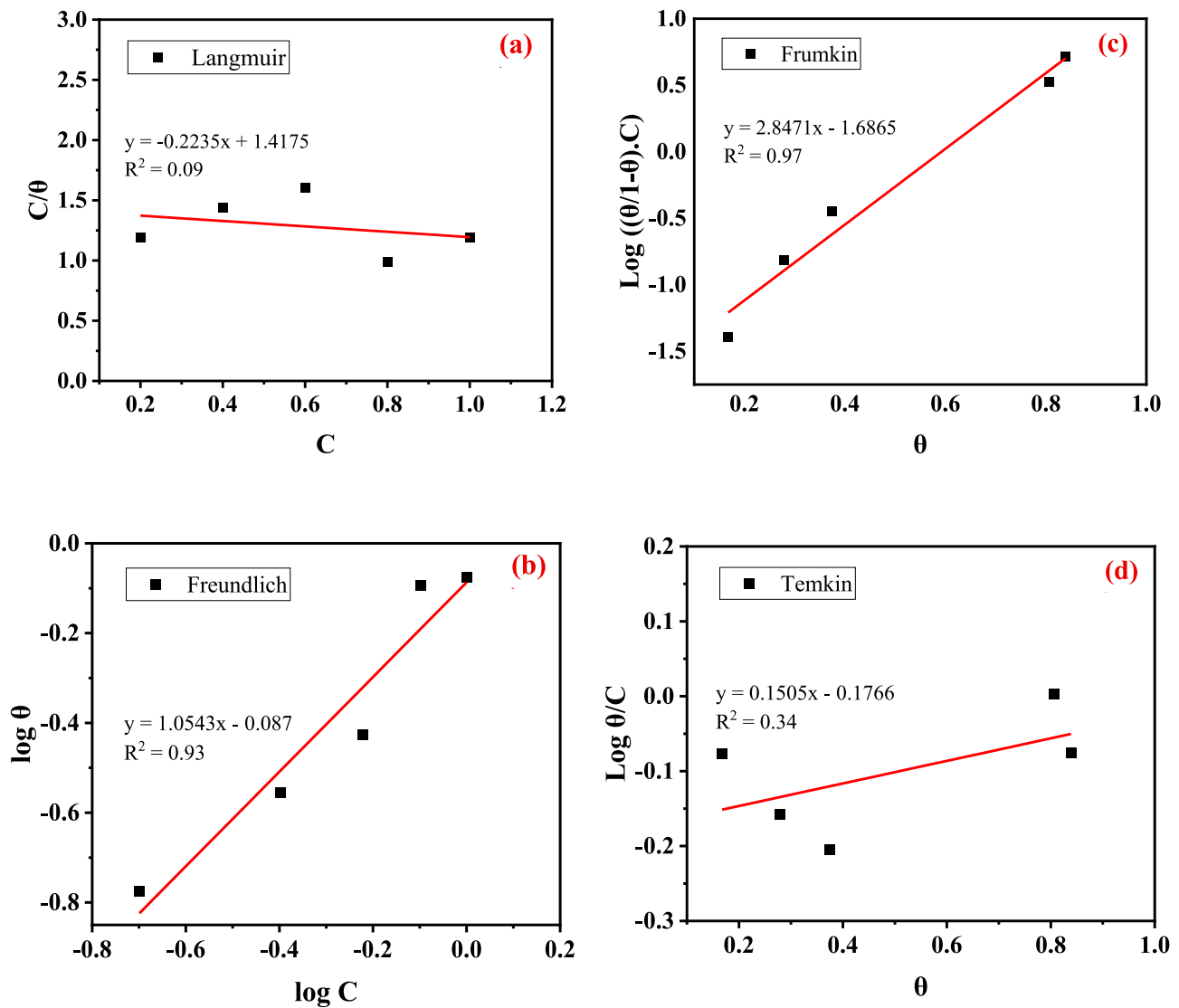


Fig. 8. Adsorption isotherms of Langmuir (a), Freundlich (b), Frumkin (c), and Temkin (d) on carbon steel.

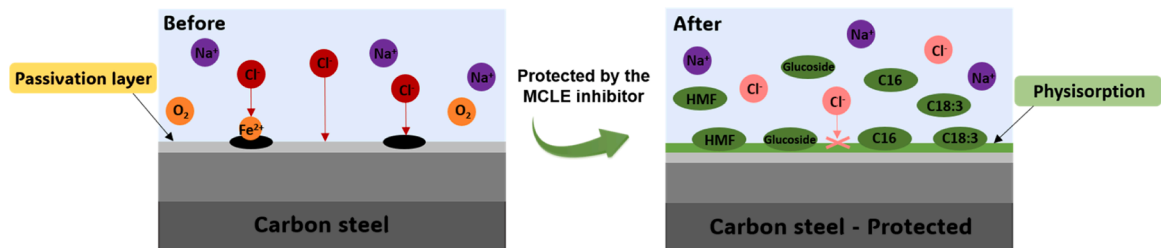


Fig. 9. Adsorption mechanism of MCLE inhibitor on carbon steel in 3.5% NaCl solution.

severely damaged (Fig. 10b) due to the formation of corrosion. The steel surface appeared rougher, showing a high level of corrosion product [57], which reduced the function and caused degradation in the form of cracks and lines on the surface. A different situation occurred after the presence of a protective inhibitor, where damage to steel was minimal, with the surface appearing smoother and more uniform than without the protective coating [46,58] (Fig. 10c). This phenomenon shows that MCLE inhibitor works effectively through the adsorption of organic molecules on the surface. The moving molecules form a layer that protects carbon steel surface from direct interaction with corrosive NaCl environment [59].

The EDX spectrum correspondence supports the assessment of carbon steel before and after protection by the MCLE inhibitor. As shown in Table 1, the composition of pure carbon steel is dominated by Fe, which accounts for at 97.68%. Fig. 11a shows the EDX spectrum of carbon steel exposed to a corrosive NaCl solution, indicating that the percentage of Fe element content decreases by 82.56% and the Cl element experiences a very significant increase of 15.13%. This indicates that the formation of a corrosion layer is attributed to direct attack by the Cl element, causing a decrease in the Fe peak [60]. Fig. 11b shows a different EDX spectrum after protection, with a significant increase in the content of several elements, such as Fe (90.14%). This event shows the formation

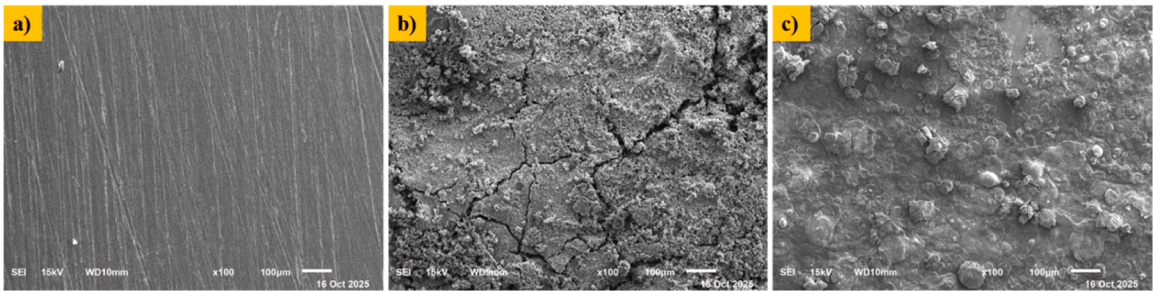


Fig. 10. SEM of carbon steel surface before treatment (a), in NaCl (b), and inhibitor protection (c).

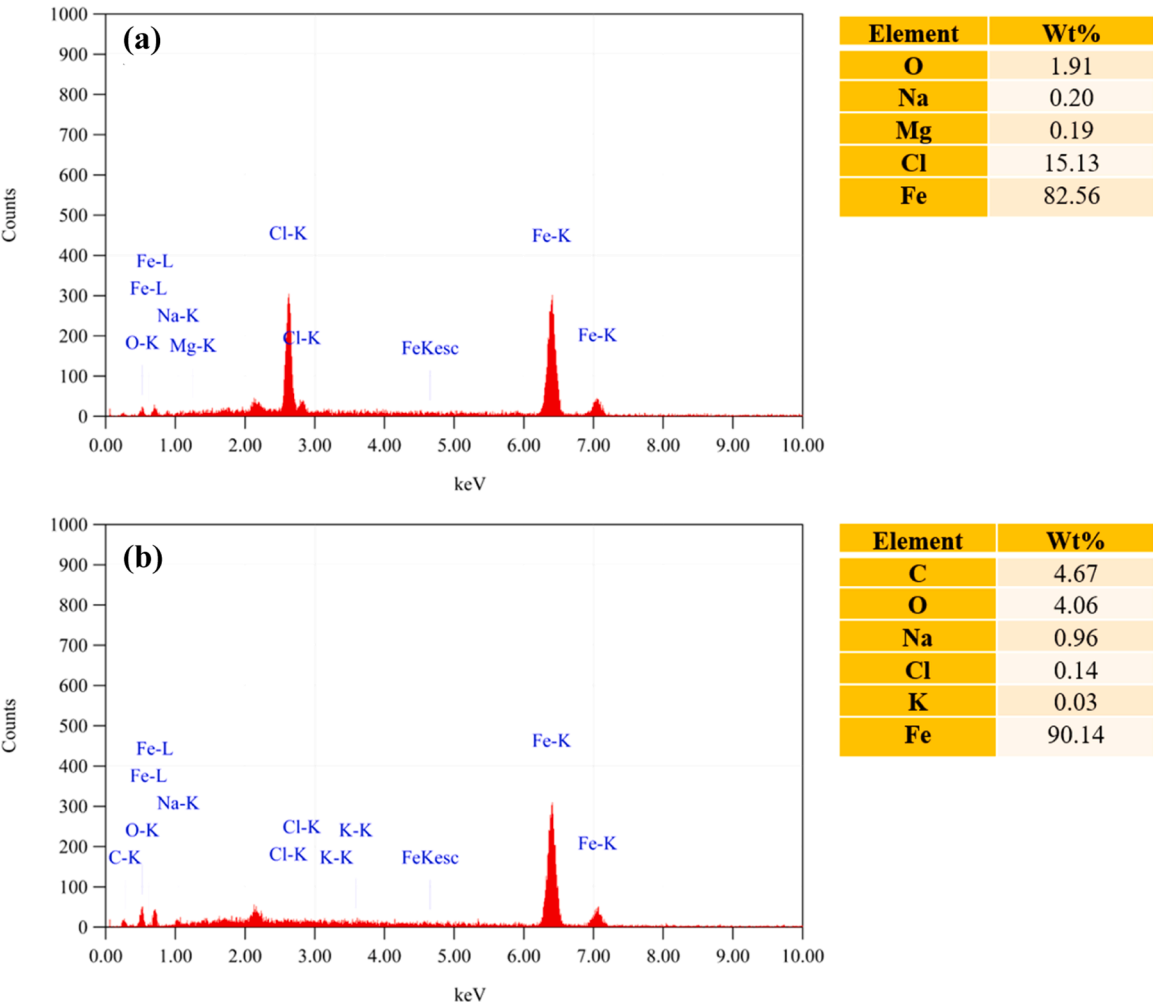


Fig. 11. EDX spectra of the surface of carbon steel after immersion (a) in a 3.5% NaCl solution and (b) in a 1000 ppm inhibitor solution.

of a protective layer that prevents the metal from corroding. The O content (4.06%) increases, showing the presence of inhibitor molecules, while the Cl content (0.14%) decreases due to a lack of direct contact with the steel surface [61].

3.6. AFM

AFM is a highly innovative method developed to investigate the morphology of carbon steel due to corrosion formation and inhibition by inhibitors in corrosive solutions. The results obtained using this method are shown in 2D and 3D images of carbon steel surfaces under various conditions, before, without, and with the presence of MCLE inhibitors

(Fig. 12). Based on AFM, surface roughness was determined by the parameters square roughness (Sq), average roughness (Sa), and maximum peak-to-valley height (St).

The surface of carbon steel before treatment was tested as a basis to show good condition, undamaged, smooth, and free from corrosion (Fig. 12a). Comparing Fig. 12b to Fig. 12c, carbon steel immersed in a 3.5% NaCl solution without inhibitors showed a surface with high roughness, a porous surface, and very wide scratches [62]. The presence of MCLE significantly affected steel surface, causing a smoother surface than without protection [41,44,63]. This shows that inhibitors play an essential role during steel contamination from corrosive solutions such as 3.5% NaCl. The AFM test parameters in Table 6 show the roughness

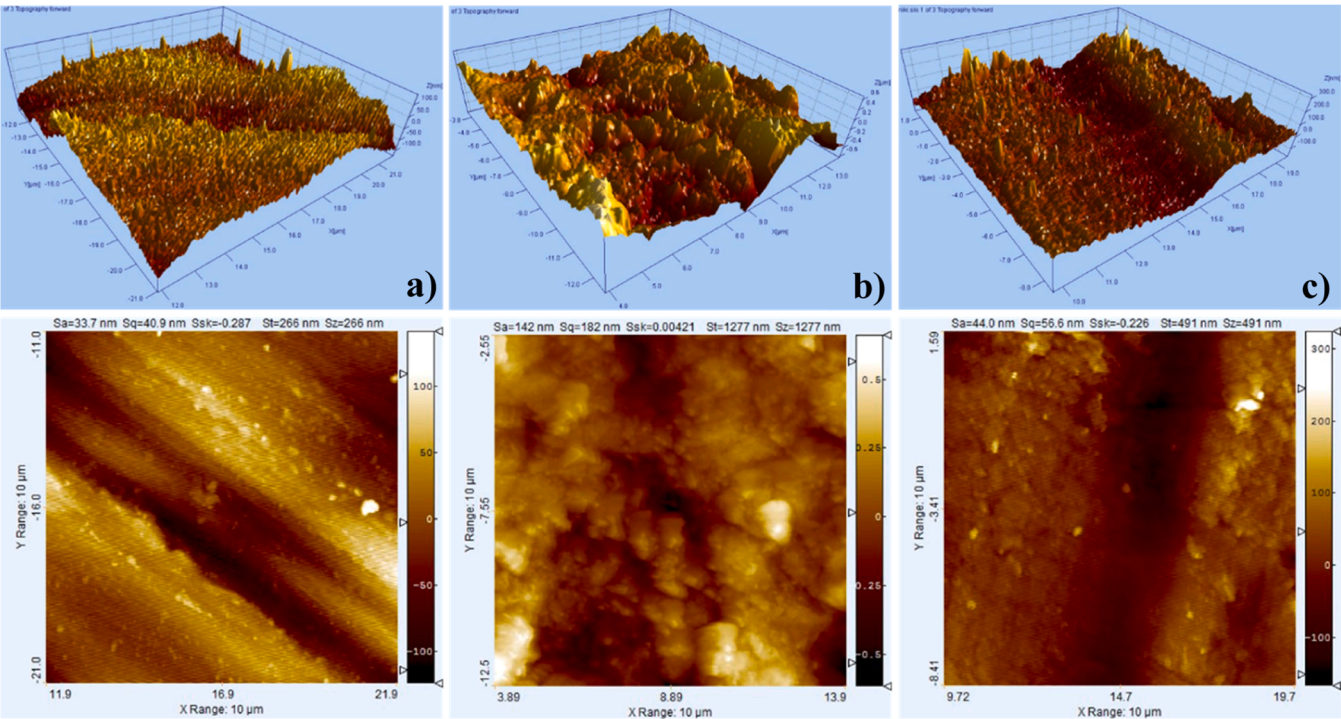


Fig. 12. AFM of carbon steel, before treatment (a), in NaCl (b), and in the presence of inhibitors (c).

Table 6

AFM parameters of carbon steel under different conditions.

Concentration	Sq (nm)	Sa (nm)	St (nm)
Before treatment	40.9	33.7	266
NaCl 3.5%	182	142	1277
1000 ppm	56.6	44.0	491

values in each condition. Before treatment, surface roughness values were quite small, namely 40.9 (Sq), 33.7 (Sa), and 266 (St). Meanwhile, surface condition of steel contaminated with a corrosive 3.5% NaCl solution produced roughness values of 182 (Sq), 142 (Sa), 1277 (St), and the opposite after protection, namely 56.6 (Sq), 44.0 (Sa), and 491 (St). These parameters show the formation of a protective layer by MCLE inhibitors on carbon steel.

3.7. XRD

XRD is one of the most versatile methods for characterizing metals, particularly to identify compounds the material shows atomic-scale periodicity or crystallinity. The effectiveness of this method for in situ analysis of corrosion product species has led many studies to systematically apply XRD to carbon steel surface under various conditions. Fig. 13 shows XRD data corresponding to the phases present on carbon steel before treatment, when exposed to a 3.5% NaCl solution, and in the presence of MCLE inhibitors. Steel analysis before treatment showed no detectable compounds, indicating corrosion products. Meanwhile, in 3.5% NaCl environment, XRD detected corrosion products including FeOOH, FeOH₃, and Fe₂O₃ [64], showing strong diffraction peaks and a uniform distribution on carbon steel. Different results were observed when the surface of the carbon steel was protected by inhibitors at a concentration of 1000 ppm, which showed the formation of a very dominant Fe element along with higher diffraction peaks. On the protected surface, corrosion compounds such as Fe₂O₃ and FeOOH formed less frequently, while the intensity and number of corrosion product peaks were lower. The condition shows that corrosion products formed

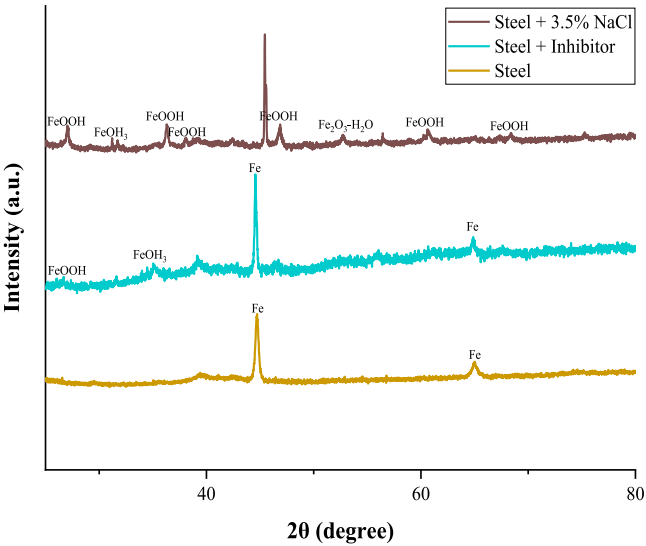


Fig. 13. XRD of carbon steel.

very little compared to when not protected [65]. This shows the effect of forming a protective film layer by the adsorbed inhibitor, thereby limiting the direct attack of corrosion-causing compounds [66].

3.8. Quantum chemical descriptors of MCLE phytochemical

To elucidate the adsorption behavior of the major phytochemicals identified in MCLE, DFT calculations were performed at the B3LYP/6–311++G(d,p) level. The optimized structures, frontier molecular orbital (FMO) distributions, and electrostatic potential (ESP) maps are presented in Fig. 14, while the calculated quantum chemical descriptors are summarized in Table 7.

The HOMO distributions are mainly localized around oxygen-containing functional groups, including hydroxyl, ether, ester, and

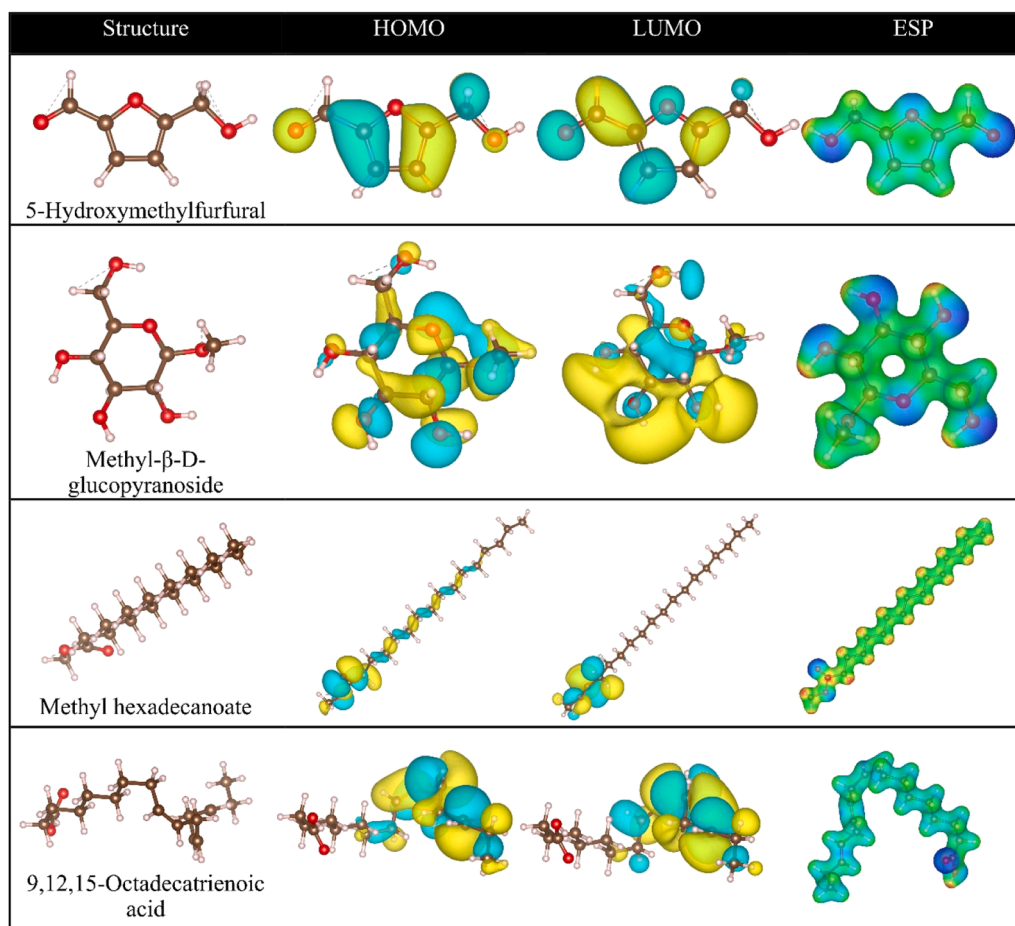


Fig. 14. Optimized molecular structures, frontier molecular orbital distributions (HOMO and LUMO), and electrostatic potential (ESP) maps of 5-hydroxymethylfurfural, methyl- β -D-glucopyranoside, methyl hexadecanoate, and 9,12,15-octadecatrienoate identified in MCLE.

Table 7

Quantum chemical descriptors of the major phytochemical constituents identified in MCLE obtained from DFT calculations. E_{HOMO} , E_{LUMO} , ΔE , η , μ , and ω are expressed in eV.

Compound	E_{HOMO}	E_{LUMO}	ΔE	Φ	η	μ	ω	ΔN
5-Hydroxymethylfurfural	−6.69	−1.96	4.73	4.32	2.36	−4.32	3.95	0.106
Methyl- β -D-glucopyranoside	−7.24	0.81	8.04	3.21	4.02	−3.21	1.28	0.200
Methyl hexadecanoate	−7.74	−0.12	7.62	3.93	3.81	−3.93	2.02	0.117
9,12,15-octadecatrienoate	−6.65	−0.12	6.53	3.39	3.27	−3.39	1.76	0.219

carbonyl moieties, indicating that these sites act as the primary electron-donating centers during adsorption. The corresponding ESP maps reveal highly negative electrostatic potential regions around oxygen atoms, confirming their role as the most favorable adsorption sites on the steel surface. Such localization of electron density facilitates donor–acceptor interactions between the inhibitor molecules and vacant Fe 3d orbitals, leading to the formation of a protective adsorbed layer. Similar adsorption behavior has been reported for oxygen-rich phytochemicals and green corrosion inhibitors, where heteroatoms and π -electron systems govern adsorption strength through charge-transfer interactions and surface complexation mechanisms [37,40].

Among the investigated compounds, 5-hydroxymethylfurfural exhibited the highest HOMO energy (−6.69 eV), the smallest HOMO–LUMO energy gap ($\Delta E = 4.73$ eV), and the lowest hardness value ($\eta = 2.36$ eV). These characteristics indicate a greater tendency for electron donation, higher molecular polarizability, and enhanced adsorption reactivity. In contrast, methyl- β -D-glucopyranoside showed the largest energy gap (8.04 eV) and highest hardness (4.02 eV), suggesting lower intrinsic reactivity. However, its multiple hydroxyl and ether groups

provide numerous adsorption centers capable of establishing multipoint interactions with surface iron atoms, thereby compensating for its less favorable frontier orbital characteristics. Similar correlations between high E_{HOMO} values, low ΔE values, low hardness, and improved corrosion inhibition efficiency have been widely reported for plant-derived and heteroatom-containing organic inhibitors [67,68].

The fraction of electrons transferred (ΔN) further supports the adsorption tendency of the investigated phytochemicals. Positive ΔN values were obtained for all compounds, indicating spontaneous electron donation from the inhibitor molecules to the metal surface. Among them, 9,12,15-octadecatrienoate exhibited the highest ΔN value (0.219), followed by methyl- β -D-glucopyranoside (0.200), methyl hexadecanoate (0.117), and 5-HMF (0.106). The enhanced electron-donating ability of 9,12,15-octadecatrienoate is attributed to its extended π -electron system associated with multiple C=C bonds, which promotes electron delocalization and facilitates charge transfer. Recent DFT and surface adsorption studies have demonstrated that unsaturated phytochemicals exhibit stronger adsorption on Fe surfaces through synergistic heteroatom coordination, π -electron donation, and

d- π orbital interactions [41].

The relatively high electrophilicity index (ω) of 5-HMF, together with its highest HOMO energy, lowest hardness, and smallest HOMO–LUMO energy gap, indicates superior adsorption reactivity among the investigated phytochemicals. Nevertheless, adsorption strength is determined by the combined effects of molecular reactivity, electron-transfer capability, and the availability of active adsorption centers rather than a single quantum descriptor [37,69]. Based on the calculated quantum chemical parameters, the adsorption reactivity follows the order: 5-hydroxymethylfurfural > 9,12,15-octadecatrienoate > methyl- β -D-glucopyranoside > methyl hexadecanoate. This suggests that 5-hydroxymethylfurfural is the principal contributor to corrosion inhibition, while the remaining phytochemicals enhance protection through complementary adsorption mechanisms. In particular, methyl- β -D-glucopyranoside provides multiple oxygen-containing adsorption sites, whereas the fatty acid derivatives improve surface coverage and barrier properties. The synergistic adsorption of these constituents is therefore expected to promote the formation of a compact and stable protective film on the steel surface, resulting in the overall inhibition performance of MCLE.

3.9. Molecular adsorption and interaction behavior of MCLE phytochemicals on the Fe(110) surface

Although DFT calculations provide valuable information regarding molecular reactivity, electronic structure, and charge-transfer capability, adsorption simulations are required to evaluate the interaction between inhibitor molecules and the metal surface. Therefore, SCC-DFTB calculations were performed on the Fe(110) surface, which is commonly employed as a representative model of α -Fe due to its high stability and relevance in corrosion inhibition studies of carbon steel [37,42].

The optimized adsorption geometries of MCLE phytochemicals on the Fe(110) surface are presented in Fig. 15. All investigated

Table 8

SCC-DFTB adsorption parameters of MCLE phytochemicals on the Fe(110) surface.

Compound	E_{ads} (kcal/mol)	Fe–Inhibitor Distance (Å)
5-Hydroxymethylfurfural	–122.3	O...Fe = 1.92; C...Fe = 2.18
Methyl- β -D-glucopyranoside	–39.54	Fe...H = 2.19; O...Fe = 2.74
Methyl hexadecanoate	–206.83	H...Fe = 3.33; H...Fe = 2.8
9,12,15-octadecatrienoate	–112.29	O...Fe = 1.92; C...Fe = 2.13

compounds exhibit negative adsorption energies (Table 8), indicating that the adsorption process is thermodynamically favorable and spontaneous. A more negative adsorption energy (E_{ads}) represents stronger interaction between the inhibitor molecule and the Fe surface, resulting in a more stable adsorbed protective layer [37,39,70].

Among the studied phytochemicals, methyl hexadecanoate exhibited the strongest adsorption affinity toward the Fe(110) surface with an adsorption energy of –206.83 kcal/mol, followed by 5-hydroxymethylfurfural (–122.30 kcal/mol), 9,12,15-octadecatrienoate (–112.29 kcal/mol), and methyl- β -D-glucopyranoside (–39.54 kcal/mol). The strong adsorption of methyl hexadecanoate is mainly attributed to its long hydrocarbon chain, which provides a large contact area with the Fe surface and enhances van der Waals interactions. This interaction promotes the formation of a compact hydrophobic layer that can effectively block the penetration of aggressive corrosive species [71].

The adsorption behavior of 9,12,15-octadecatrienoate is associated with its extended unsaturated hydrocarbon structure. The presence of multiple C=C bonds increases molecular polarizability and facilitates stronger interaction with Fe atoms through dispersion forces and electron redistribution, resulting in a stable adsorbed configuration [70,72].

For 5-hydroxymethylfurfural, the adsorption energy of –122.30 kcal/mol confirms strong interaction with the Fe(110) surface. As shown in Fig. 15(a), adsorption occurs mainly through oxygen-containing functional groups, with the shortest interaction distance of

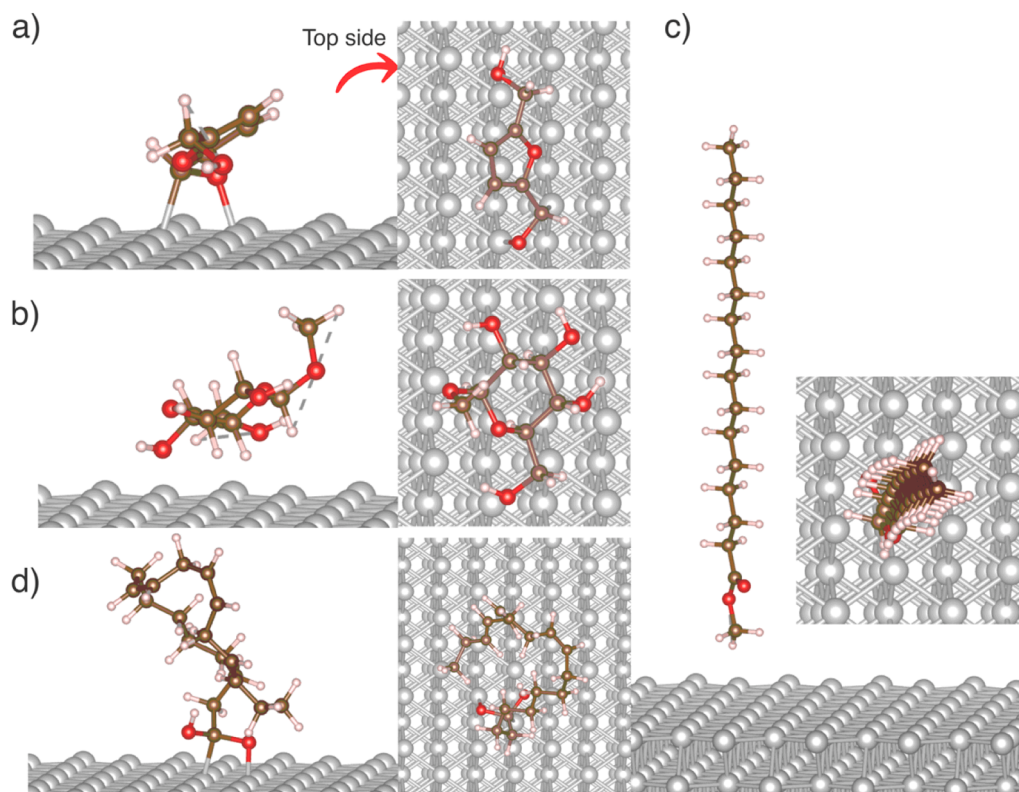


Fig. 15. Optimized adsorption geometries of MCLE phytochemicals on the Fe(110) surface obtained by SCC-DFTB calculations. All bond lengths are expressed in Å. (a) 5-hydroxymethylfurfural, (b) methyl- β -D-glucopyranoside, (c) methyl hexadecanoate, and (d) 9,12,15-octadecatrienoate.

O...Fe = 1.92 Å and C...Fe = 2.18 Å. The hydroxyl and carbonyl oxygen atoms act as electron-donating centers, facilitating coordination with surface Fe atoms. In addition, the furan ring may contribute to additional π -electron interactions, further stabilizing the adsorption structure [73].

Although methyl- β -D-glucopyranoside exhibits the lowest adsorption energy among the investigated compounds (−39.54 kcal/mol), it still shows favorable adsorption on the Fe(110) surface. The multiple hydroxyl groups provide several adsorption sites through electron donation and possible hydrogen-bond interactions. However, the absence of an extended hydrophobic chain or conjugated π -system results in weaker surface interaction compared with methyl hexadecanoate and other unsaturated compounds.

SCC-DFTB calculations confirm that MCLE phytochemicals possess strong affinity toward the Fe(110) surface. The adsorption mechanism involves a combination of surface coordination through oxygen-containing functional groups and enhanced surface coverage provided by hydrocarbon chains. These complementary interactions facilitate the formation of a stable protective adsorption film, which contributes to the corrosion inhibition performance of MCLE.

3.10. Comparative studies

Several recent studies have examined various applications of plant-derived green inhibitors that effectively inhibit corrosion on metals. These studies have been conducted at varying inhibitor concentrations, room temperature, as well as certain acidic and salty corrosive environments, with very promising results. The use of various plant materials has also gained significant attention in several investigations due to their environmentally friendly properties, rich organic compounds that can be adsorbed onto metal surfaces, and the formation of a film limiting direct interaction with the environment. A comparison of various plant-based green corrosion inhibitors is shown in Table 9. Based on the data, the MCLE inhibitors used in this study achieved a maximum inhibition rate of 85.07%, showing suitability in very competitive conditions in the scope of corrosion inhibitors, particularly salt (NaCl) environments. Therefore, these results show the advantages of MCLE inhibitors, promoting their use as an environmentally friendly metal protection system.

4. Conclusion

In conclusion, this study shows that MCLE has potential as natural inhibitors for carbon steel in 3.5% NaCl solution. The inhibitors function by forming a thin protective film based on the donation of organic molecules that fill the empty spaces in carbon steel. The results show that the best inhibition occurs at concentration of 1000 ppm, with the highest efficiency obtained at 83.89% (PDP) and 85.07% (EIS), showing optimal concentration. Based on the mechanism of operation, inhibitors are a type of mixed inhibitor that suppresses both anode and cathode reactions, as shown by the E_{corr} difference of less than 85 mV between carbon steel with and without treatment. Furthermore, the Frumkin isotherm theory completes the inhibition mechanism by producing a ΔG_{ads}^o value of −19.57 kJ/mol, showing that adsorption of molecules on the steel surface occurs by physisorption. DFT analysis revealed that MCLE phytochemicals exhibit favorable electronic characteristics, where oxygen-containing functional groups act as active adsorption centers. Furthermore, SCC-DFTB simulations confirmed strong interactions between MCLE constituents and the Fe(110) surface, with negative adsorption energies ranging from −39.54 to −206.83 kcal/mol, supporting the formation of a stable protective layer. Surface characterization using SEM-EDX, AFM, and XRD testing shows smoother surface conditions and minimal degradation after adding the inhibitor to corrosive media. Meanwhile, minimal damage and low formation of corrosion products show that MCLE inhibitors are very effective in

Table 9
Comparison of corrosion rates and inhibitor efficiency from previous studies.

Inhibitor	Corrosive materials and solutions	Concentration	Efficiency	References
<i>Musa paradisica</i> Extract	Carbon steel in 1 M HCl	200–1000 ppm	75–94%	[74]
<i>Azadirachta indica</i> Leaf Extract	Steel in 1 M HCl and 1 M NaCl	2.5–10 g	85.94% in NaCl	[75]
Cempedak (<i>Artocarpus integer</i>) Peel Extract	Carbon steel in 3.5% NaCl	200–1000 ppm	90.60%	[24]
<i>Justicia brandegeana</i>	Carbon steel in 1 M H ₂ SO ₄	250–1500 ppm	82.41%	[76]
<i>Euphorbia heterophylla</i> L. Extract	Mild steel in 1.5 M HCl	1000–2000 ppm	69%	[77]
Sweet potato native starch	Galvanized steel in 1 M HCl	100–700 ppm	64.26%	[78]
<i>Chromolaena odorata</i> Leaf Extract	Mild steel in 1 M HCl	100–900 ppm	83.33%	[79]
Ekstrak <i>Calotropis Gigantea</i>	Low carbon steel in 3.5% NaCl	100–500 ppm	66%	[80]
<i>Nephelium lappaceum</i> peel extract	Weldment in 3,5% NaCl	10–60 ppm	83%	[81]
Catechin	Iron in 1.5% NaCl + 1.5% Na ₂ SO ₄	3000 ppm	73.26%	[82]
<i>Melastoma candidum</i> Leaf Extract	Carbon steel in NaCl	200–1000 ppm	85.07%	This study

protecting carbon steel from attacks by corrosive media of 3.5% NaCl. Thus, MCLE inhibitors are excellent candidates for corrosion protection systems, and these results strongly support further research, particularly in acidic corrosive environments.

Author contributions: CRediT

Nurdin Ali and Syarizal Fonna played the role of conceptualization, Husni Usman played the role of resources, Yumaidi Saputra wrote the manuscript, Muhibul Jamal provided software, and Ali Imran played the role of project administration. Lala Adetia Marlina contributed to computational analysis and simulations.

CRediT authorship contribution statement

Nurdin Ali: Conceptualization. **Syarizal Fonna:** Conceptualization. **Muhibul Jamal:** Software. **Ali Imran:** Project administration. **Husni Usman:** Resources. **Yumaidi Saputra:** Writing – original draft. **Lala Adetia Marlina:** Formal analysis.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

The author would like to thank Universitas Syiah Kuala, Indonesia, for the financial support provided through the Professor Research Assignment Agreement (PP) Fiscal Year 2025 Number: 1251/UN11/KPT/2025 dated July 7, 2025. The authors acknowledge the Fugaku

high-performance computing facility at the RIKEN Center for Computational Science for providing the computational resources used in this study.

References

- [1] N.M. Dube-johnstone, U. Tshishonga, S.S. Mnyakeni-moleele, L.C. Murulana, Investigation of synthesized as an effective corrosion inhibitor for mild steel in 1 M HCl: a gravimetric, electrochemical, and spectroscopic study, *Heliyon* 9 (4) (2023) e14753, <https://doi.org/10.1016/j.heliyon.2023.e14753>.
- [2] R. Jalab, M. Saad, A. Benali, I.A. Hussein, M. Khaled, Biodegradable polysaccharide grafted polyacrylamide inhibitor for corrosion in CO₂-saturated saline solution, *Heliyon* 9 (10) (2023) e20304, <https://doi.org/10.1016/j.heliyon.2023.e20304>.
- [3] D.I. Udunwa, O.D. Onukwuli, M.C. Menkiti, V.C. Anadebe, M.A. Chidiebere, 1-Butyl-3-methylimidazolium methane sulfonate ionic liquid corrosion inhibitor for mild steel alloy: Experimental, optimization and theoretical studies, *Heliyon* 9 (7) (2023) e18353, <https://doi.org/10.1016/j.heliyon.2023.e18353>.
- [4] O.I. El, et al., Anti-corrosive properties of two new green heterocyclic azole derivatives on C38 steel in 1 M (HCl) medium, experimental and theoretical study, *Results Chem.* 5 (July 2022) (2023) 100641, <https://doi.org/10.1016/j.rechem.2022.100641>.
- [5] U. Mamudu, M. Sahban, R. Chong, Adsorption isotherm and molecular modeling of phytoconstituents from *Dillenia suffruticosa* leaves for corrosion inhibition of mild steel in 1.0 M hydrochloric acid solution, *Results Surf. Interfaces* 13 (September) (2023) 100145, <https://doi.org/10.1016/j.rsufri.2023.100145>.
- [6] N. Islam, Corrosion And Its Effect: A Critical Appraisal ([Online]. Available), *J. Surv. Fish. Sci.* 9 (1) (2022) 396–408, <https://doi.org/10.53555/sfs.v9i1.1516>.
- [7] Z. Ahmad, *Princ. Corros. Eng. Corros. Control*, 11 (1) (2006).
- [8] A. Hafazeh, A. Balooch, Z.D. Shanbaraki, M. Azadi, Corrosion inhibition of steel in sulphuric acid using *Ferula Assa foetida* L. extract as an eco-friendly inhibitor: Experimental and computational study, *Results Eng.* 25 (December 2024) (2025) 103736, <https://doi.org/10.1016/j.rineng.2024.103736>.
- [9] H.A. Jaddoa, B.A. Abdulhussein, J.M. Ali, Novel efficiency of turmeric extract as a green inhibitor of low carbon steel corrosion in 3.5% NaCl solution, *Case Stud. Chem. Environ. Eng.* 11 (October 2024) (2025) 101086, <https://doi.org/10.1016/j.csee.2024.101086>.
- [10] N. Ali, M.A. Fulazzaky, The empirical prediction of weight change and corrosion rate of low-carbon steel, *Heliyon* 6 (9) (2020) e05050, <https://doi.org/10.1016/j.heliyon.2020.e05050>.
- [11] N. Ali, T.E. Putra, V.Z. Iskandar, M. Ramli, A simple empirical model for predicting weight loss of mild steel due to corrosion in NaCl solution, *Int. J. Automot. Mech. Eng.* 17 (1) (2020) 7784–7791, <https://doi.org/10.15282/ijame.17.1.2020.24.0579>.
- [12] X.T. Xu, H.W. Xu, Y. Wang, X.Y. Zhang, X.J. Tan, Cerium chloride and L-arginine as effective hybrid corrosion inhibitor for 5052 aluminum alloy in 3.5% NaCl solution, *Int. J. Electrochem. Sci.* 17 (2022), <https://doi.org/10.20964/2022.12.24>.
- [13] S.C. Joycee, A.S. Raja, A.S. Amalraj, S. Rajendran, Inhibition of corrosion of mild steel in simulated oil well water by an aqueous extract of *Daucus carota* (Carrot), *Int. J. Corros. Scale Inhib.* 14 (1) (2025) 269–287, <https://doi.org/10.17675/2305-6894-2025-14-1-17>.
- [14] S. Bilgiç, Plant extracts as corrosion inhibitors for carbon steel in HCl media, *A Compr. Rev.* (2) (2025) 503–559, <https://doi.org/10.17675/2305-6894-2025-14-2-6>.
- [15] S. A. T.P.W.Y. Stiadi, Emriadi Rahmayeni, Anticorrosive effectiveness of mild steel by dragon scale fern (*Drymoglossum piloselloides* L.) leaf extract in hydrochloric acid medium: A combined experimental and computational approach, *Int. J. Corros. Scale Inhib.* 14 (2) (2025) 566–588, <https://doi.org/10.17675/2305-6894-2025-14-2-8>.
- [16] M.M. El-Toony, A.M. Wahba, A.S. Fouda, *Withania somnifera* extract (WSE) as eco-friendly corrosion inhibitor for Al in acidic solutions: experimental and mathematical analyses ([Online]. Available), *Int. J. Corros. Scale Inhib.* 14 (2) (2025) 793–822, <https://doi.org/10.17675/2305-6894-2025-14-2-19>.
- [17] A. Nomozov, et al., Inhibition potential of *Salsola oppositifolia* extract as a green corrosion inhibitor of mild steel in an acidic solution, *Int. J. Corros. Scale Inhib.* 14 (3) (2025) 1103–1115, <https://doi.org/10.17675/2305-6894-2025-14-3-5>.
- [18] Q. A. Yousif, M.A. Bedair, A.M. Abuelela, High-performance corrosion inhibitors for carbon steel in hydrochloric acid: electrochemical and DFT, *RSC Adv.* 15 (2025) 28666–28688, <https://doi.org/10.1039/d5ra04952k>.
- [19] Q.A. Yousif, Z. Fadel, A.M. Abuelela, E.H. Alosaimi, Insight into the corrosion mitigation performance of three novel benzimidazole derivatives of amino, *RSC Adv.* 13 (2023) 13094–13119, <https://doi.org/10.1039/d3ra01837g>.
- [20] L. Feng, et al., *Cucumis sativus* L. Leaf Extract as a Green Corrosion Inhibitor for Carbon Steel in Acidic Solution ([Online]. Available), *Molecules* 27 (2022), <https://doi.org/10.3390/molecules27123826>.
- [21] O.O. Ogunleye, et al., Green corrosion inhibition and adsorption characteristics of *Luffa cylindrica* leaf extract on mild steel in hydrochloric acid environment, *Heliyon* 6 (1) (2020) e03205, <https://doi.org/10.1016/j.heliyon.2020.e03205>.
- [22] H. Septya, et al., Effect of spinach (*Spinacia oleracea*) leaf extract on the aluminum (Al) as a green corrosion inhibitor in HCl medium, *Hybrid. Adv.* 7 (August) (2024) 100283, <https://doi.org/10.1016/j.hybadv.2024.100283>.
- [23] R. Tambun, et al., Natural corrosion inhibitors derived from powder, concentrated extract and tannin of ketapang (*Terminalia catappa* L.) leaves for iron protection in sodium chloride solutions, *Curr. Res. Green. Sustain. Chem.* 11 (June) (2025) 100471, <https://doi.org/10.1016/j.crgsc.2025.100471>.
- [24] Y. Saputra, N. Ali, S. Fonna, P. Ramadhani, The effect of cempedak (*Artocarpus integer*) peel extract as a natural inhibitor in protecting carbon steel corrosion in salty environments, *Int. J. Corros. Scale Inhib.* 15 (1) (2026) 429–448, <https://doi.org/10.17675/2305-6894-2026-15-1-22>.
- [25] M. Zdravkovi, R. Vianello, V. Grekulovi, N. Strbac, Blackberry leaf extract as a green inhibitor for copper corrosion: Insights from coordination complexes, thermodynamics, RSM optimization, and DFT calculations, *Results Eng.* 29 (January) (2026), <https://doi.org/10.1016/j.rineng.2026.109812>.
- [26] F. Gapsari, et al., Efficacy of *Andrographis paniculata* leaf extract as a green corrosion inhibitor for mild steel in concentrated sulfuric acid: Experimental and computational insights, *Results Surf. Interfaces* 18 (September 2024) (2025) 100361, <https://doi.org/10.1016/j.rsufri.2024.100361>.
- [27] O.G. Echem, V.I. Chukwuikwe, T. Tubonemi, V.C. Anadebe, F.E. Abeng, L.G. Barine, Rubber leaf extract: A green inhibitor for mild steel corrosion in 1.0 M HCl medium, response surface analyzer and electrochemical approach, *Results Surf. Interfaces* 20 (July) (2025) 100607, <https://doi.org/10.1016/j.rsufri.2025.100607>.
- [28] E.S.J. Ahmed, G.M. Ganesh, Neem leaf extract as a sustainable green inhibitor for corrosion inhibition in RCC and strength improvement in concrete, in conjunction with spectroscopic characterization and statistical evaluation, *Results Surf. Interfaces* 23 (January) (2026) 100771, <https://doi.org/10.1016/j.rsufri.2026.100771>.
- [29] A.A. Adamu, O. Risikat, A. Iyuni, J.D. Habila, Evaluation of *Desmodium adscendens* (Sw.) DC. extract as an eco-friendly corrosion inhibitor for carbon steel in hydrochloric acid: Gravimetric with statistical modeling, electrochemical, and surface analysis, *Mater* 11 (December 2025) (2026) 101624, <https://doi.org/10.1016/j.nxmate.2026.101624>.
- [30] Q.A. Yousif, S. Malhotra, M.A. Bedair, A. Ansari, A.K. Hadi, Safflower plant extract as a sustainable corrosion inhibitor for carbon steel in acidic media: a combined electrochemical and computational study, *RSC Adv.* 15 (2025) 21006–21025, <https://doi.org/10.1039/d5ra03333k>.
- [31] W.L. Ng, Y. Cai, W. Wu, R. Zhou, The complete chloroplast genome sequence of *Melastoma candidum* (Melastomataceae, Mitochondrial DNA Part. B Resour. Vol. 2359 (2017), <https://doi.org/10.1080/23802359.2017.1318680>.
- [32] J. Supardi, et al., Comparative study of performance of temik (*Melastomacandidum*) and rubek (*Calotropis gigantea*) extract inhibitors for carbon steel in corrosive media, *J. Polimesin* 21 (6) (2023) 583–588.
- [33] M.A. Jafar Mazumder, Global Impact of Corrosion: Occurrence, Cost and Mitigation, *Glob. J. Eng. Sci.* 5 (4) (2020) 0–4, <https://doi.org/10.33552/gjes.2020.05.00618>.
- [34] G. Palumbo, et al., Effect of Grain Size on the Corrosion Behavior of Fe-3wt%Si-1wt%Al Electrical Steels in Pure Water Saturated with CO₂ ([Online]. Available), *Mater. (Basel)* 14 (2021) 1–19, <https://doi.org/10.3390/ma14175084>.
- [35] H. Yang, S. Deng, X. Li, *Eupatorium adenophorum* Spreng root extract as an efficient inhibitor for the corrosion of steel in sulfamic acid solution, *Int. J. Electrochem. Sci.* 19 (10) (2024) 100790, <https://doi.org/10.1016/j.ijeos.2024.100790>.
- [36] F. Gapsari, P.H. Setyarin, F. Kurniawan, A. Ahnaf, M.S. Anwar, U.K. Zuryati, Corrosion inhibition of weldment by *Nephelium lappaceum* peel extract in 3.5% NaCl solution, *South. Afr. J. Chem. Eng.* 41 (April) (2022) 223–232, <https://doi.org/10.1016/j.sajce.2022.06.006>.
- [37] J.M. Castillo-Robles, E. de, F. Martins, P. Ordejón, I. Cole, Molecular modeling applied to corrosion inhibition: a critical review, *npj Mater. Degrad.* 2 (2024), <https://doi.org/10.1038/s41529-024-00478-2>.
- [38] Z. Liu, D. Wang, D. Li, H. Wang, The inhibition efficiencies of some organic corrosion inhibitors of iron: An insight from density functional theory study, *Comput. Theor. Chem.* 1214 (May) (2022) 113759, <https://doi.org/10.1016/j.comptc.2022.113759>.
- [39] A.I. Ikeuba, et al., Review of computational methods used in the evaluation corrosion inhibition of metallic materials, *Discov. Chem. Eng.* (2024), <https://doi.org/10.1007/s43938-024-00065-6>.
- [40] H. Lgaz, A. Aldalbahi, H.-S. Lee, Atomic-Level Insights into the Adsorption of Methyl-Substituted Quinoxalinones on Fe(110): A Dispersion-Corrected DFT Analysis, *Molecules* (110) (2024).
- [41] H. Hamidi, F. Shojaei, M. Pourfath, M. Vaez-zadeh, Adsorption behavior of some green corrosion inhibitors on Fe (110) surface: the critical role of π - π interactions in binding strength, *Appl. Surf. Sci.* 655 (July 2023) (2024) 159425, <https://doi.org/10.1016/j.apsusc.2024.159425>.
- [42] L. Guo, C. Qi, X. Zheng, R. Zhang, X. Shen, S. Kaya, Toward understanding the adsorption mechanism of large size organic corrosion inhibitors on an Fe(110) surface using the DFTB method, *RSC Adv.* (2017) 29042–29050, <https://doi.org/10.1039/c7ra04120a>.
- [43] N.H. Kurshed, A.A. Khadom, R.K. Ismail, S. Khalil, N. Kadhim, A. Alamiery, Green biosynthesis of silver nanoparticles from *Citrus aurantium* leaves plant as corrosion inhibitor for carbon steel in sulfuric acid, *Nanotechnol* 9 (ember 2025) (2026) 100331, <https://doi.org/10.1016/j.nxnano.2025.100331>.
- [44] M.E. Eissa, S.H. Etaiw, E.S. El-hussieny, A.A. El, A.E.S. Fouda, Sweet Orange Peel Extract as green sustainable corrosion inhibitor for Al in 1 M HCl, *Int. J. Electrochem. Sci.* 20 (1) (2025) 100882, <https://doi.org/10.1016/j.ijeos.2024.100882>.
- [45] A. Zarebidaki, M. Mehrdar, S. Tavakoli, Cerium nitrate as a green corrosion inhibitor for 304 stainless steel: Efficacy and mechanism ([Online]. Available), *Mater. Today Commun.* 50 (December 2025) (2026) 1–10, <https://doi.org/10.1016/j.mtcomm.2025.114514>.

- [46] F.E. Abeng, et al., *Milletia aboensis* leaves extract as eco-friendly corrosion inhibitor for mild steel in acidizing solution: From experimental to molecular level prediction, *Results Eng.* 24 (July) (2024) 102950, <https://doi.org/10.1016/j.rineng.2024.102950>.
- [47] A. Singh, K.R. Ansari, X. Xu, Z. Sun, A. Kumar, Y. Lin, An impending inhibitor useful for the oil and gas production industry: Weight loss, electrochemical, surface and quantum chemical calculation, *Sci. Rep.* (October) (2017) 1–17, <https://doi.org/10.1038/s41598-017-13877-0>.
- [48] H.A. Almashhadani, Adsorption, thermodynamic and corrosion study of enalapril malate pharmaceutical drug as corrosion inhibitor for carbon steel in saline solution, *Results Mater.* 26 (February) (2025) 100706, <https://doi.org/10.1016/j.rinma.2025.100706>.
- [49] A. Khormali, S. Ahmadi, Experimental and modeling analysis on the performance of 2-mercaptobenzimidazole corrosion inhibitor in hydrochloric acid solution during acidizing in the petroleum industry, *J. Pet. Explor. Prod. Technol.* 13 (11) (2023) 2217–2235, <https://doi.org/10.1007/s13202-023-01675-6>.
- [50] G.S. Sajadi, F. Salமானian, R. Naghizade, S. Mohammad, A. Hosseini, The inhibitive action of lemon verbena plant extract as an economical and eco-friendly corrosion inhibitor for mild steel in acidic solutions, *Int. J. Electrochem. Sci.* 19 (8) (2024) 100699, <https://doi.org/10.1016/j.ijeoes.2024.100699>.
- [51] K. Krishnanjana, G.M. Ganesh, Evaluation of Punica granatum peel as an eco-friendly green corrosion inhibitor for different structural steels in comparison with commercial inhibitors, *J. Mol. Struct.* 1352 (P2) (2026) 144573, <https://doi.org/10.1016/j.molstruc.2025.144573>.
- [52] Y. Liu, S. Deng, B. Fan, J. Xu, D. Shao, X. Li, Investigation of benzyltrimethylstearyl ammonium chloride as an effective cationic surfactant inhibitor for steel corrosion in Cl[−] 2 CHCOOH solution, *Results Eng.* 27 (July) (2025) 106399, <https://doi.org/10.1016/j.rineng.2025.106399>.
- [53] J. Pan, X. Huang, H. Jiang, K. Cao, 3-Hydroxy-2-naphthoylamide as corrosion inhibitor for carbon steel in 1 M HCl, *Int. J. Electrochem. Sci.* 21 (2) (2026) 101279, <https://doi.org/10.1016/j.ijeoes.2025.101279>.
- [54] J. Pan, X. He, K. Cao, Electrochemical and theoretical studies of two amino acid ionic liquids as corrosion inhibitors for mild steel in 3.5 wt% NaCl solution, *Int. J. Electrochem. Sci.* 20 (2) (2025) 100916, <https://doi.org/10.1016/j.ijeoes.2024.100916>.
- [55] A. Khanra, M. Srivastava, M.P. Rai, R. Prakash, Application of Unsaturated Fatty Acid Molecules Derived from Microalgae toward Mild Steel Corrosion Inhibition in HCl Solution: A Novel Approach for Metal – Inhibitor Association, *ACS Omega* 3 (2018), <https://doi.org/10.1021/acsomega.8b01089>.
- [56] I.M. Iloaemaeke, S. Ezenwa, L. Olasunkanmi, K. Lobb, N. Nnaji, Biomass of *Anthothona macrophylla* leaf extract as a mild steel acid corrosion inhibitor: Experimental and theoretical study, *Mater* 7 (July 2024) (2025) 100344, <https://doi.org/10.1016/j.nxmate.2024.100344>.
- [57] O.E. Elazabawy, O.A.A. El-shamy, N.E.A. El-sattar, Corrosion inhibitory characteristics, thermodynamics, and theoretical studies of N-((2-aminoethyl) carbamothioyl) acrylamide for carbon steel in 1 M HCl, *Egypt. J. Pet.* 32 (3) (2023) 7–14, <https://doi.org/10.1016/j.ejpe.2023.07.001>.
- [58] A. Hafazeh, A. Balooch, Z.D. Shanbaraki, M. Azadi, Corrosion inhibition of steel in sulphuric acid using *Ferula Assa foetida* L. extract as an eco-friendly inhibitor: Experimental and computational study, *Results Eng.* 25 (September 2024) (2025) 103736, <https://doi.org/10.1016/j.rineng.2024.103736>.
- [59] R.K. Kosireddi, S. Mandal, K. Mondal, Cattle manure extract inhibiting corrosion in Al-Cu alloy and commercially pure Mg against NaCl solution, *Bioresour. Technol. Rep.* 32 (July) (2025) 102378, <https://doi.org/10.1016/j.biteb.2025.102378>.
- [60] O.E. Elazabawy, E.M. Attia, N.H. Shawky, A.M. Hyba, Eco - friendly orange peel extract as corrosion resistant for carbon steel 's deterioration in petroleum formation water, *Sci. Rep.* 13 (2023) 1–18, <https://doi.org/10.1038/s41598-023-47916-w>.
- [61] E.-S.M. Sherif, A.H. Ahmed, Alleviation of Iron Corrosion in Chloride Solution by N,N'-bis[2-Methoxynaphthylidene]amino]oxamide as a Corrosion Inhibitor El-Sayed, *crystals* 11 (2021).
- [62] X. Sun, Exploring *Metasequoia glyptostroboides* leaf extract as an eco-friendly corrosion inhibitor for Q235 steel, *Int. J. Electrochem. Sci.* 19 (2) (2024) 100494, <https://doi.org/10.1016/j.ijeoes.2024.100494>.
- [63] F. Gapsari, et al., A convolutional neural network -VGG16 method for corrosion inhibition of 304SS in sulfuric acid solution by timoho leaf extract, *J. Mater. Res. Technol.* 30 (January) (2024) 1116–1127, <https://doi.org/10.1016/j.jmrt.2024.03.156>.
- [64] M. Akbari Shahmirzadi, M. Azadi, A new study on the corrosion inhibition mechanism of green walnut husk extract as an agricultural waste for steel protection in HCl solution, *Heliyon* 10 (9) (2024) e29962, <https://doi.org/10.1016/j.heliyon.2024.e29962>.
- [65] F.D. Fernandes, L.M. Ferreira, M.L.C.P. Silva, Application of *Psidium guajava* L. leaf extract as a green corrosion inhibitor in biodiesel: Biofilm formation and encrustation, *Appl. Surf. Sci. Adv.* 6 (2021) 100185, <https://doi.org/10.1016/j.apsadv.2021.100185>.
- [66] M.B. Bahtiar, L. Sulistijono, T.N. Noerochim, B.A. Rohmannudin, R.K. Kurniawan, Pramadewardaru, Improved corrosion behaviour of A36 carbon steel in 3.5 % NaCl solution via bio-inhibitor of mangkok leaf extract (*Polyscias scutellaria*), *Results Eng.* 29 (September 2025) (2026) 109412, <https://doi.org/10.1016/j.rineng.2026.109412>.
- [67] N. Wazzan, I.B. Obot, H. Lgaz, Z. Safi, O. Al-qurashi, Multiscale computational modeling of phytochemicals for iron corrosion inhibition: Bridging DFT, SCC-DFTB, and molecular dynamics for eco-friendly solutions, *J. Mol. Liq.* 406 (January) (2024) 125070, <https://doi.org/10.1016/j.molliq.2024.125070>.
- [68] W. Mohamad, et al., Experimental, DFT and molecular dynamic simulation of *Andrographis paniculata* as corrosion inhibitor for mild steel in artificial seawater, *Mater. Chem. Phys.* 312 (2023) 128642, <https://doi.org/10.1016/j.matchemphys.2023.128642>.
- [69] O.I. El Mouden, et al., BMPD-Assisted Enhancement of Corrosion Resistance of Carbon Steel: Experimental and First-Principle DFTB Insights, *Met. (Basel)* (2024), <https://doi.org/10.3390/met14010069>.
- [70] F. Wang, et al., First-principles study of Ti adsorption on Al 4C 3 (0001) surface, *Appl. Surf. Sci.* 679 (July 2024) (2024) 161271, <https://doi.org/10.1016/j.apsusc.2024.161271>.
- [71] M. Sofi, et al., A recent review on theoretical studies of Gemini surfactant corrosion inhibitors, *J. Mol. Liq.* 368 (2022) 120649, <https://doi.org/10.1016/j.molliq.2022.120649>.
- [72] A.A. Bahraq, I.B. Obot, M.A. Al-osta, M. Ibrahim, Molecular simulations of anticorrosion behavior of inhibitors for steel in concrete: A review on recent advances and progress, *Constr. Build. Mater.* 412 (October 2023) (2024) 134808, <https://doi.org/10.1016/j.conbuildmat.2023.134808>.
- [73] E.E. Ebenso, D.A. Isabirye, and N.O. Eddy, "Adsorption and Quantum Chemical Studies on the Inhibition Potentials of Some Thiosemicarbazides for the Corrosion of Mild Steel in Acidic Medium," pp. 2473–2498, 2010, doi: 10.3390/ijms11062473.
- [74] J.R. Torres-Hernandez, E. Del Ángel-Meraz, F. Corvo-Pérez, M.G. Rivera-Ruedas, M.A. Hernández-Rivera, J. Barajas-Fernández, Musa paradisiaca extract as a corrosion inhibitor of steel. Role of KI as a synergistic additive, *Int. J. Corros. Scale Inhib.* 12 (4) (2023) 2391–2418, <https://doi.org/10.17675/2305-6894-2023-12-4-50>.
- [75] J.A. E. S, M.G. G, Evaluation of the corrosion inhibition potential of *Azadirachta indica* leaves on thermo mechanically treated steel rebars using an artificial neural network, electrochemical and spectroscopic approach, *Cogent Eng.* 11 (1) (2024), <https://doi.org/10.1080/23311916.2024.2392208>.
- [76] G.K.P. Barboza, M.C.C. De Oliveira, M.A. Neves, Justicia brandegeana as a green corrosion inhibitor for carbon steel in sulfuric acid, *Green. Chem. Lett. Rev.* 17 (1) (2024), <https://doi.org/10.1080/17518253.2024.2320254>.
- [77] O. Alaba, O. Johnson, E. Leke, Thermodynamics and adsorption study of the corrosion inhibition of mild steel by *Euphorbia heterophylla* L. extract in 1.5 M HCl, *Results Mater.* 5 (ember 2019) (2020) 100074, <https://doi.org/10.1016/j.rinma.2020.100074>.
- [78] C.K. Anyiam, O.O.E.E. Oguzie, I.C.M.S.C. Nwanonenyi, G.C.O.H.C. Obasi, Corrosion inhibition of galvanized steel in hydrochloric acid medium by a physically modified starch, *SN Appl. Sci.* 2 (4) (2020) 1–11, <https://doi.org/10.1007/s42452-020-2322-2>.
- [79] E.E. Mbamalu, A.P. Chinedu, Assessment of the Corrosion Inhibitory Potentials of *Chromolaena odorata* Leaf Extract on Mild Steel in Hydrogen Chloride Acid Environment, *Moroc. J. Chem.* 11 (1) (2023) 188–204, doi: //doi.org/10.48317/IMIST.P.RSM/morjchem-v10i3.30521.
- [80] J. Supardi, S. Rizal, N. Ali, S. Fonna, I. Ikramullah, Investigating an environmentally in aqueous solution of potassium chloride, *J. Mater. Res. Technol.* 29 (January) (2024) 303–310, <https://doi.org/10.1016/j.jmrt.2024.01.137>.
- [81] F. Gapsari, P.H. Setyarini, F. Kurniawan, A. Ahnaf, M. Syaiful, U. Khairi, Corrosion inhibition of weldment by *Nephelium lappaceum* peel extract in 3.5 % NaCl solution, *South African, J. Chem. Eng.* 41 (June) (2022) 223–232, <https://doi.org/10.1016/j.sajce.2022.06.006>.
- [82] M. Jia, et al., Corrosion Inhibition and Rust Conversion of Catechin on Archaeological Iron of Nanhai I, *Met. (Basel)* 12 (2022), <https://doi.org/10.3390/met12050714> (Academic).