

Integrated adsorption, kinetic–thermodynamic, and computational assessment of cestrum nocturnum as a green corrosion inhibitor for Carbon Steel in 1 M HCl

Silas.O. Okuma^{*}, Martins Obaseki

Nigeria Maritime University, Faculty of Engineering, Mechanical Engineering Department, P.O. Box 1005, Okerenkoko, Nigeria

ARTICLE INFO

Keywords:

Cestrum nocturnum
Carbon steel corrosion
Green corrosion inhibitor
Chemi-physisorption mechanism
Computation studies

ABSTRACT

This study investigates Cestrum nocturnum leaf extract (CNLE) as an eco-friendly corrosion inhibitor for carbon steel in 1 M HCl. The extract was characterized using Fourier-transform infrared spectroscopy (FTIR) and thermogravimetric/differential thermal analysis (TGA/DTA). Corrosion inhibition was assessed via gravimetric analysis and atomic absorption spectrometry, while the interaction mechanism was evaluated using quantum-chemical (DFT) and molecular dynamics (MD) simulations. FTIR analysis identified O–H/N–H, carbonyl, and aromatic functional groups capable of strong adsorption onto iron surface sites. TGA/DTA confirmed the extract's thermal stability below 100 °C, a relevant range for industrial processes like acidizing and flowline operations. Thermometric and gravimetric tests demonstrated clear concentration-dependent inhibition, with efficiencies reaching 94.41 % (thermometric) and 92.44 % (gravimetric) at 0.8 g L⁻¹. Adsorption data were well-described by both Langmuir and Freundlich isotherms (R² up to 0.998). The negative ΔG_{ads} values indicated a spontaneous adsorption process, and the magnitudes suggested a mixed physisorption–chemisorption mechanism. Thermodynamic activation and adsorption parameters further corroborated an endothermic process with combined physical and chemical interactions. DFT and MD simulations of the dominant constituents, oleic acid and piperidine, revealed strong electron-donating character, favorable adsorption geometries, and robust binding on the Fe(110) surface, aligning with the experimental observations. In conclusion, CNLE presents a novel, plant-based corrosion inhibitor for carbon steel. It emerges as a promising and sustainable alternative to conventional synthetic inhibitors for mitigating corrosion in acidic environments such as pickling and oil-well acidization.

1. Introduction

Corrosion is the tendency of refined metals to revert to more thermodynamically stable oxide or hydroxide forms through interaction with their environment. It remains a major factor limiting the safe, reliable service life of carbon steel in process and energy infrastructures. Physical manifestations such as rust formation, discoloration, wall thinning, and cracking not only shorten equipment lifetime and disrupt production, but also degrade structural integrity and increase the likelihood of leaks, rupture, and catastrophic failure over an asset's life cycle [1–5]. Recent assessments continue to place the global cost of corrosion in the range of 1–5 % of gross domestic product, which have been accounted for directly as a result of mitigation and indirect losses [6–9]. At the same time, studies on pipelines and structural steels have shown

that localized corrosion and erosion–corrosion can sharply reduce load-bearing capacity, accelerate crack initiation, and compromise mechanical performance under pressure and cyclic loading [10]. To mitigate these impacts, industry typically adopts a multi-barrier strategy that combines materials selection, corrosion-resistant design, protective coatings, and chemical treatments that limit the interaction between steel and aggressive environments while maintaining stringent safety and sustainability requirements [11], corrosion inhibitors are now central to corrosion management, particularly in acidic conditions relevant to pickling, acid cleaning, and oil- and gas-well stimulation [12]. These compounds act primarily by suppressing the anodic metal dissolution and cathodic hydrogen-evolution reactions at the steel/electrolyte interface [13–17].

However, the toxicity, and costs of many conventional synthetic

^{*} Corresponding author.

E-mail address: silas.okuma@nmu.edu.ng (Silas.O. Okuma).

<https://doi.org/10.1016/j.ctta.2025.100261>

Received 20 November 2025; Received in revised form 22 December 2025; Accepted 25 December 2025

Available online 26 December 2025

2667-3126/© 2025 The Authors. Published by Elsevier B.V. This is an open access article under the CC BY-NC license (<http://creativecommons.org/licenses/by-nc/4.0/>).

organic inhibitors have prompted a significant shift toward a sustainable and eco-friendly alternatives [18–22]. Plant-based inhibitors, have gained significant attention because they are renewable, biodegradable, and easily available from agricultural or agro-industrial waste. Recent research have shown that plant extracts can achieve high inhibition efficiencies for carbon steels in acidic environment, but also emphasize ongoing challenges in identifying active constituents, clarifying adsorption mechanisms, and linking molecular structure to durability and performance under realistic flow and temperature conditions [23, 24]. Their secondary metabolites which includes phenolics, flavonoids, alkaloids, tannins, amino acids, and related species have shown to provide multiple adsorption-active sites and potential chelation centers, typically involving oxygen and nitrogen heteroatoms and π -electron systems, which can interact strongly with steel surfaces [25,26]. However the performance of inhibitor is governed by the formation and stability of adsorbed films, therefore, understanding the adsorption mechanism is critical for corrosion mitigation process. *Cestrum nocturnum* (night-blooming jasmine) is a widely distributed ornamental and medicinal plant whose leaf extracts are rich in nitrogen- and oxygen-containing compounds, including steroidal glycosides and other heteroatom-bearing species capable of donating lone pairs and engaging in π -interactions with metal surfaces [27,28]. Several plant-derived extracts have been investigated as green corrosion inhibitors, *Cestrum nocturnum* leaf extract remained unexplored, to the best our knowledge, in an acidic environment. This study focus on addressing this gap using 1 M HCl a standard benchmark for acidic corrosion and a representative medium for industrial processes such as pickling and oil-well acidizing. This research combined both gravimetric and thermometric measurements with adsorption and thermodynamic analysis, further supported by density functional theory and molecular dynamics simulations.

2. Materials and methods

2.1. Materials

Carbon steel (CS) coupons, *Cestrum nocturnum* leaves, methanol (99.8 %), hydrochloric acid (37 % w/w), and acetone (99.8 %) were used in this study. All chemicals were of analytical grade, supplied by Labscape Scientific Ltd., and were employed without further purification. Standard laboratory consumables and equipment, included borosilicate glassware, filter paper, funnels, a grinder, plastic containers, cotton thread, emery papers (grit sizes 400–1200), and masking tape .

2.1.1. Carbon steel specimen preparation

Carbon steel with the following composition (wt. %) was used in this study: C (0.42), Mn (0.90), Si (0.32), P (0.035), S (0.040), Cr (0.90), Mo (0.20), and Fe (balance). The steel was machined into rectangular coupons measuring 2.5 cm $\times$ 2.0 cm $\times$ 0.15 cm. The coupon surfaces were cleaned sequentially with silicon carbide abrasive papers (grit sizes 200 to 800), degreased with acetone, rinsed with distilled water, and air-dried. The cleaned specimens were stored in a desiccator until use [11,24].

2.1.2. Preparation of the plant for extract

Leaves samples of *Cestrum nocturnum* were collected in Ughoton, Okpe, Nigeria. After taxonomic identification, the leaves were rinsed with water to remove surface contaminants and shade-dried under ambient conditions for approximately two weeks. The dried leaves was then milled into a fine powder, sealed in a plastic bag, and stored at room temperature until extraction [29].

2.2. Methods

2.2.1. Extraction and characterization of *Cestrum nocturnum*

The extraction of *Cestrum nocturnum* leaves was performed via maceration. Briefly, 500 g of powdered *Cestrum nocturnum* leaves were

mixed with 1000 cm³ of methanol (99.8 %) and allowed to macerate for four days with intermittent stirring. The mixture was then filtered through Whatman filter paper, and the filtrate was concentrated using a rotary evaporator at 65 °C. The resulting crude extract was transferred to a sealed container for subsequent corrosion studies. For film analysis, carbon steel coupons were immersed in 1 M HCl containing 0.8 g/L of the crude extract for 24 h. Following exposure, the thin protective film formed on the steel surface was carefully removed. Both the crude extract of the *Cestrum nocturnum* leaves and the desorbed film were analyzed using a Nicolet iS5 FT-IR spectrometer (Thermo Fisher Scientific, USA) via the KBr pellet technique, over a wavenumber range of 400–4000 cm⁻¹ [30]. Thermogravimetric and differential thermal analyses (TGA/DTA) were conducted using a DTG-60H instrument (Shimadzu, Japan). Approximately 10 mg of the dried extract was placed in an alumina pan and heated from room temperature to 900 °C at a rate of 10 °C/min under a high-purity nitrogen gas flow of 60 mL/min [31,32].

2.2.2. Atomic absorption spectroscopic measurement(AAS)

The concentration of dissolved Fe in 1 M HCl solutions was determined using atomic absorption spectrometry (AAS) (Agilent 240FS AA, Australia). Measurements were performed under identical exposure conditions for solutions both with and without *Cestrum nocturnum* leaf extract [33].

2.2.3. Thermometric study

Thermometric measurements were performed using a three-neck round-bottom flask assembled according to established corrosion testing procedures as prescribe by [34]. To minimize heat loss, the flask was thermally insulated. In each experiment, 100 cm³ of 1 M HCl was used as the corrodent, with all tests initiated at an initial temperature of 50 °C. The corrosion reaction was monitored by recording temperature as a function of time using a calibrated thermometer (accuracy ± 0.05 °C, range 0–100 °C). The reaction number (RN) was calculated from the initial slope of the temperature–time curve, which corresponds to the rate of temperature increase, as defined in Eq. (1).

$$RN (^{\circ}C / min) = \frac{T_m - T_i}{t} \quad (1)$$

Here, T_i denotes the initial temperature at the start of each run, T_m is the maximum temperature attained by the reacting system, and t is the elapsed time. In parallel, the inhibition efficiency (%IE) of the acetone bio-waste extract derived from CNLE was evaluated using Eq. (2), following the same data-reduction procedure specified for the thermometric measurements.

$$\% I = \frac{RN_{uninhibited} - RN_{inhibited}}{RN_{uninhibited}} \times 100 \quad (2)$$

Where $RN_{uninhibited}$ and $RN_{inhibited}$ are the corresponding reaction numbers for the systems that for the uninhibited solution and the inhibited systems respectively.

2.2.4. Corrosion inhibition investigation (Gravimetric)

Corrosion inhibition was assessed gravimetrically using carbon steel (CS) coupons over a temperature range of 313–333 K and *Cestrum nocturnum* leaf extract (CNLE) concentrations of 0.0 to 0.8 g L⁻¹. For blank tests, coupons were suspended in 200 cm³ of uninhibited 1 M HCl contained in 250 mL beakers. For inhibition experiments, identical setups were prepared with the appropriate CNLE concentrations added. Each coupon was immersed for 10 hrs, after which it was removed, cleaned to eliminate corrosion products, dried thoroughly, and reweighed. The weight loss (Δw) was calculated from the difference between the initial and final masses. From Δw , the corrosion rate (CR), inhibition efficiency (IE), and surface coverage (θ) were determined using Eqns (3)–(6), respectively [29].

$$\Delta w = m_i - m_f \quad (3)$$

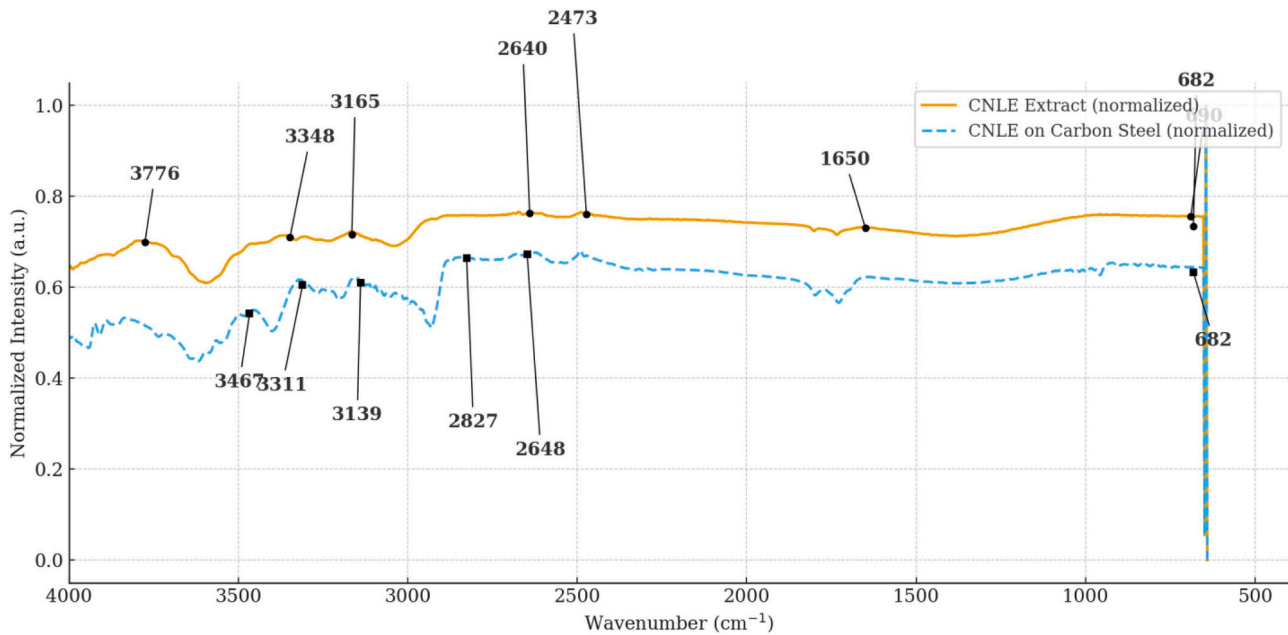


Fig. 1. FTIR plots of CNLE extract and carbon steel immersed in CNLE inhibitor.

$$CR = \frac{87.6 \Delta w}{DA T} \quad (4)$$

where Δw is the weight loss (g), m_i and m_f are the initial and final masses of the coupon (g), D is the density of carbon steel (g cm^{-3}), A is the exposed surface area (cm^2), and T is the exposure time (h).

$$IE = \frac{W_b - w}{W_b} \times 100 \quad (5)$$

Where W_b and W_i are the weight loss in the absence and presence of CNLE, respectively, expressed in g. In line with the procedure reported by [20], the degree of surface coverage, θ was then evaluated using Eqn. (6) as shown below.

$$\theta = 1 - \frac{W_b}{W_i} \quad (6)$$

2.2.5. Thermodynamics studies and adsorption parameters

The apparent activation energy (E_a) for the corrosion process was determined using the linearized form of the Arrhenius equation (Eqn. (7)), which describes the dependence of the corrosion rate on temperature [35], and is commonly expressed as:

$$\ln\left(\frac{R_1}{R_2}\right) = \left(\frac{E_a}{R}\right)\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \quad (7)$$

R is the universal molar gas constant; R_1 and R_2 are the corrosion rates measured at temperatures T_1 and T_2 , respectively. The temperature dependence of surface coverage, ($\% I = 100 \times \theta$), was then analysed to quantify heat absorption. Accordingly, the heat of adsorption for the inhibitors on carbon steel was determined from the using Eq. (8) as specified in [35].

$$Q_{ads} = 2.303R \left(\log \frac{\theta_1}{1 - \theta_2} \right) - \log \left(\log \frac{\theta_1}{1 - \theta_1} \right) \times \left[\frac{T_1 \times T_2}{T_2 - T_1} \right] \quad (8)$$

Where R is the universal gas constant; θ_1 and θ_2 are the surface coverages determined at $T_1=303$ K and $T_2=333$ K respectively. The adsorption behavior of the inhibitor was evaluated by fitting the experimental data to the Langmuir, Freundlich, and Temkin isotherm models, as expressed in Eqs. (8)–(11).

$$\frac{C}{\theta} = \frac{1}{K} + C \quad (9)$$

$$\log \theta + = \log k_m + n \log C \quad (10)$$

$$\ln C = 2a\theta - \ln K_{ads} \quad (11)$$

Where, K_{ads} are the adsorption equilibrium constants obtained from the Langmuir and Freundlich models, respectively; θ denotes the surface coverage; and C is the inhibitor concentration. The standard Gibbs free energy of adsorption was calculated using eqn. (12)

$$\Delta G_{ads} = -2.303RT \log (55.5K_{ads}) \quad (12)$$

where ΔH_{ads} is the standard enthalpy of adsorption, ΔG_{ads} is the standard Gibbs free energy of adsorption, and T is the absolute temperature. The entropy of adsorption ($T\Delta S_{ads}$) was calculated using eqn. (13).

$$\Delta G_{ads} = \Delta H_{ads} - T\Delta S_{ads} \quad (13)$$

2.2.6. Computational methods

Oleic acid and piperidine were identified as the dominant organic constituents of CNLE. Both compounds are well-studied corrosion inhibitors via computational approaches. In this work, their electronic structures were examined using density functional theory (DFT) as implemented in TeraChem [36,37]. Electron density distributions and molecular orbitals were calculated in both the gas phase and in aqueous solution; the latter was modeled using the COSMO continuum solvation model [24]. All DFT calculations employed the B3LYP functional with the aug-cc-pCVTZ basis set [38], augmented with D3 dispersion corrections to account for noncovalent interactions [39]. Geometry optimizations were performed using the geomeTRIC algorithm [40].

The adsorption of inhibitor molecules onto the steel surface and their lateral motion were further investigated using classical molecular dynamics (MD) with the ReaxFF reactive force field [41,42], implemented in the LAMMPS package [43]. Simulations were performed at 300 K with a time step of 0.3 fs. The iron substrate model, adopted directly from [44], comprised six atomic layers with an energetically favorable (110) crystallographic orientation, which is widely used in corrosion simulations. The model's lateral dimensions (on the order of a few nanometers) were sufficient to observe inhibitor diffusion and film

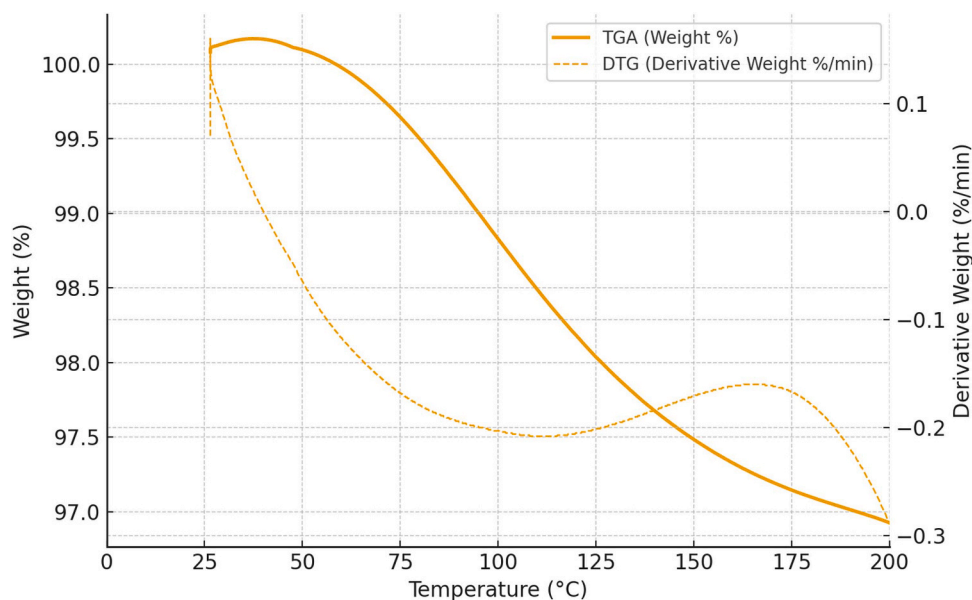


Fig. 2. Thermal stability plots of CNLE.

formation at the interface. Post-processing and visualization of electronic and structural data were conducted using Multiwfn [45,46] and Chemcraft [47], respectively.

3. Results and discussion

3.1. FTIR analysis

The FTIR analysis was used to identify and study the chemical composition and functional groups present in the CNLE [48]. Fig. 1 is an overlay of normalized spectra of the crude CNLE and the film adsorbed on the steel surface with the key bands highlighted. The widespread O—H/N—H stretching envelope of the neat extract, with peaks at 3776, 3348 and 3165 cm^{-1} shifts to lower wavenumber and reduced strength in the adsorbed film, where they are found at 3467, 3311 and 3139 cm^{-1} . Likewise, the aliphatic C—H stretching range which is indicated by the 2640 and 2473 cm^{-1} bands in the extract is shifted to 2827 and 2648 cm^{-1} in the film. Carbonyl/aromatic band of 1650 cm^{-1} becomes more broad and weak following the adsorption [49]. These orderly

down-shifts and attenuations are regular with the participation of O—H/N—H and C=O/C=C groups in coordination and reorganization of hydrogen bonds at the Fe surface sites. Most significantly, there is a band at approximately 682 cm^{-1} that is merely apparent in the neat extract, but is strong in the film spectrum, which is attributed to the Fe-O/Fe-N stretching modes, which offers a direct indication of metal-ligand bonding in the interface. The emergence of the 682 cm^{-1} band along with the measured changes in the O—H/N—H and carbonyl/aromatic bands is thus indicative of a hybrid physisorption-chemisorption reaction of CNLE on carbon steel [50].

3.2. Thermal stability of *cestrum nocturnum* leaf extract (CNLE)

TGA and DTA are thermal analysis used to assess the thermal stability, composition and heat related behavior of the CNLE. Fig. 2 reveals that the material exhibits a very low mass loss of approximately 1.26 % over the temperature range 0–100 °C and shows no distinct decomposition. This suggests that the extract can be suitable for corrosion control in oil and gas acidizing or stimulation operations conducted in 1–15 % HCl, where

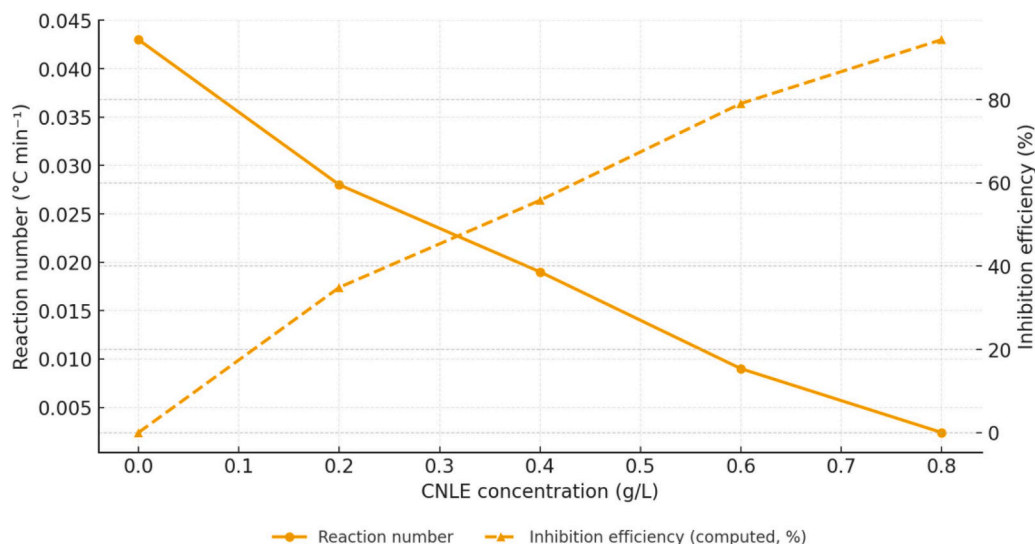


Fig. 3. Thermometric plots of CNLE.

Table 1

Values of reaction number and inhibition efficiency of Concentration-Dependent Inhibition of Carbon Steel Corrosion by CNLE in 1 M HCl at 50 °C.

Concentration/Systems (g/L)	Reaction Number($^{\circ}\text{C} / \text{min}$)	Inhibition Efficiency (%)
Blank	0.043	-
0.2	0.028	34.88
0.4	0.019	55.81
0.6	0.009	79.07
0.8	0.0024	94.41

typical operating temperatures range from ambient conditions up to about 80–90 °C. On this basis, the inhibitor can also serve as excellent candidate for corrosion mitigation in pipeline and flowline systems, tubulars subjected to acid cleaning and surface production facilities such as separators, heat exchangers, and produced-water handling units that operate under sub-boiling temperature conditions. For acidizing operations, the inhibitor may be blended directly with HCl-based treatment fluids without significant degradation before contact with steel surfaces. Once adsorbed, it can suppress both anodic metal dissolution and cathodic hydrogen evolution in pipelines [51].

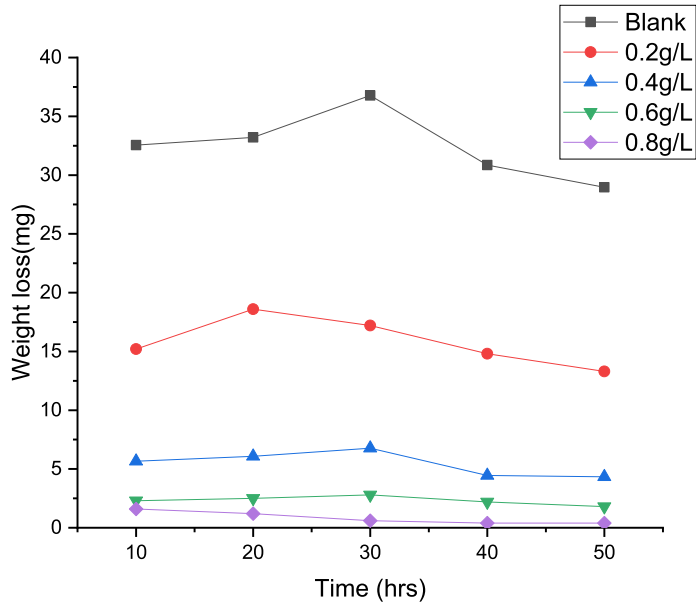


Fig. 4. Plots of weight loss in variation with time for carbon steel corrosion using CNLE as inhibitor at 313 K.

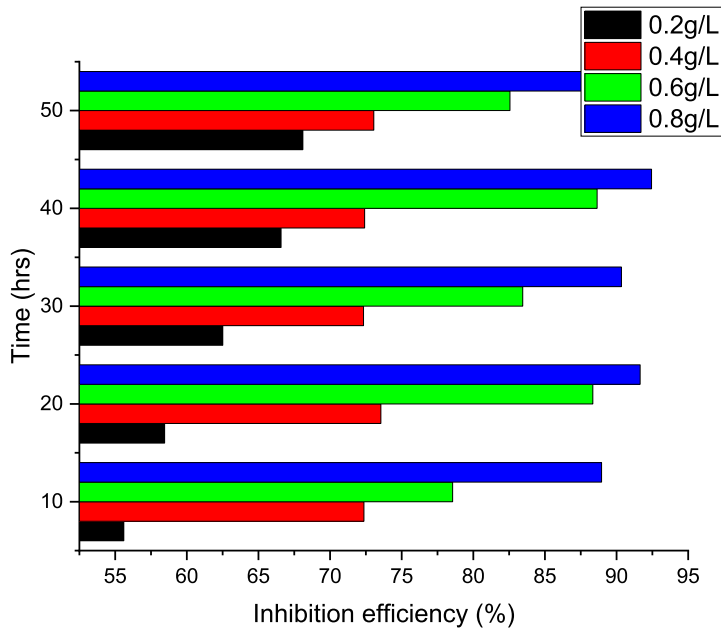


Fig. 5. Plots of inhibition efficiency in variation with time for carbon steel corrosion using CNLE as inhibitor at 313 K.

Table 2
Adsorption parameters for CNLE.

Isotherm	Temp (K)	R ²	Slope	Intercept	K _{ads}	n	ΔG _{ads}
Langmuir	313	0.9986	0.8365	0.1895	5.2977		−14.8
	323	0.9656	0.8966	0.227	5.497		−14.79
	333	0.967	0.9525	0.2496	3.405		−14.99
Freundlich	313	0.978	0.378	0.043	1.044	2.646	1.12
	323	0.963	0.363	−0.075	0.928	2.755	0.77
	333	0.975	0.359	−0.148	0.862	2.786	0.6

3.3. Thermometric analysis

Thermometric analysis was employed to evaluate the effect of temperature on the corrosion process by monitoring temperature variations during metal dissolution [52]. The thermometric reaction number (RN), which quantifies the corrosion rate, is presented for carbon steel in 1 M HCl in Fig. 3 and Table 1. A systematic trend is observed: all CNLE-containing solutions yield lower RN values than the uninhibited blank, confirming the extract's efficacy. Furthermore, the RN decreases progressively with increasing CNLE concentration (0.0 to 0.8 g L^{−1}), demonstrating a clear concentration-dependent inhibitory effect. Fig. 6 and Table 4 highlight the pronounced corrosion suppression. The highest RN, 0.043 °C min^{−1}, corresponds to the uninhibited blank. With the addition of CNLE at 0.2, 0.4, 0.6, and 0.8 g L^{−1}, the RN substantially decreases to 0.028, 0.019, 0.005, and 0.0024 °C min^{−1}, respectively [53]. Consequently, the calculated inhibition efficiency (IE) increases with concentration. The most significant gains occur up to approximately 0.6 g L^{−1}, beyond which improvements are more modest, suggesting a tendency toward surface saturation. For example, 0.6 g L^{−1} affords a high IE of 79.07 %, while 0.8 g L^{−1} approaches near-complete protection at ~94 % [54]. These results underscore both the strong inhibitory capability of CNLE and its distinct concentration dependence.

3.4. Weight loss analysis

The weight loss technique is a fundamental and reliable method for

evaluating corrosion rates by measuring the mass loss of a metal after exposure to a corrosive environment [55]. Figs. 4 and 5 present the weight loss and inhibition efficiency of carbon steel in 1 M HCl at 323 K as functions of CNLE concentration (0.2–0.8 g L^{−1}) and immersion time (10–50 h), compared with the uninhibited (blank) solution. The blank consistently exhibited the highest weight loss across all immersion times. In contrast, the mass loss of the steel progressively decreased with increasing CNLE concentration, confirming the extract's effectiveness in reducing the corrosion rate [56].

While cumulative metal loss is expected to increase with immersion time, the gravimetric data in Fig. 4 show a decrease in measured mass loss beyond 40–50 h. This suggests the measured values reflect not only the metal dissolved into solution but also the net balance between dissolved metal and corrosion products or adsorbed inhibitor species retained on the specimen surface. Over extended immersion, a tenacious layer composed of adsorbed CNLE constituents and corrosion products may form. If metal ions become incorporated or encapsulated within this layer, the measured mass loss can be reduced. Furthermore, organic residues from the inhibitor may remain on the surface, further contributing to an underestimation of true corrosion loss. Therefore, this trend indicates film thickening and surface stabilization over time. However, it also highlights a potential limitation of the gravimetric method when a stable, adherent film develops on the surface, as it can obscure accurate measurement of actual metal dissolution [57,58].

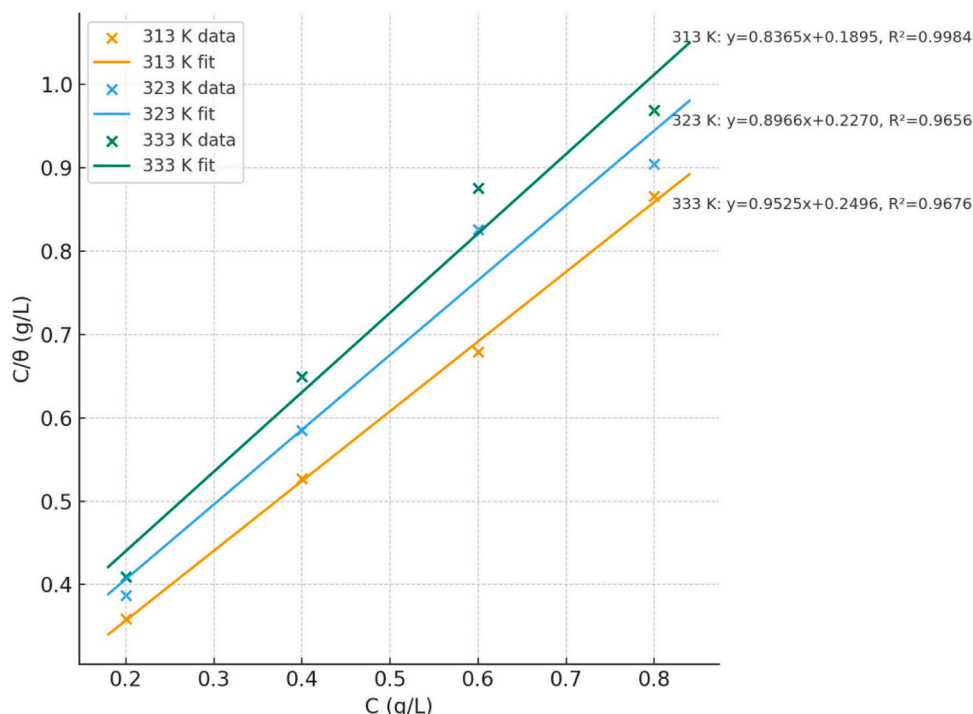


Fig. 6. Langmuir isotherm plots of CNLE adsorption at vary temperature.

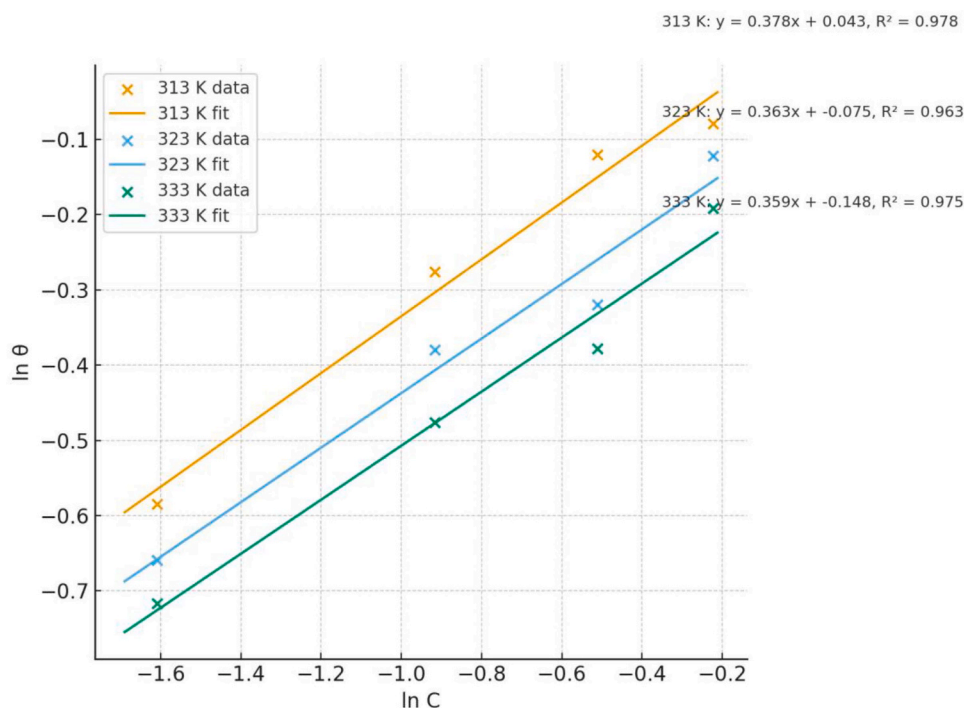


Fig. 7. Freundlich isotherm plots of CNLE adsorption at vary temperature.

3.5. Absorption studies

The adsorption behavior of CNLE on carbon steel was analyzed using both the Langmuir and Freundlich isotherm models (Tables 2 and Figs. 6 and 7). The experimental data correlate very well with both models, with correlation coefficients near unity for Langmuir and ranging from 0.996 to 0.999 for Freundlich across the temperatures studied. This excellent agreement aligns with findings reported in prior studies [41, 59]. Analysis of the gravimetric data at different temperatures using both models provides insight into the adsorption mechanism [60]. The good linear fits of both isotherm plots (Figs. 6 and 7) indicate that CNLE adsorption can be satisfactorily described by either model. The isotherm parameters exhibit distinct temperature dependence. For the Langmuir model, the adsorption equilibrium constant (K_{ads}) increases with temperature, which is characteristic of a process with a significant chemisorption component that becomes more favorable at elevated temperatures. This suggests that specific constituents in the extract form stronger bonds with the steel surface at higher temperatures. Conversely, the Freundlich constants decrease with increasing temperature. While this could indicate a reduction in average binding energy on a heterogeneous surface, it is more likely a reflection of the empirical nature of the Freundlich equation and its sensitivity to surface coverage and roughness effects [61].

In general, higher K_{ads} values correspond to stronger adsorbent-adsorbate interactions and greater inhibition efficiency [62]. The Langmuir slopes in this study (0.8365–0.9670) are close to the ideal value of 1.0 for monolayer adsorption. Slight deviations suggest that while the system largely follows Langmuir behavior, lateral interactions occur between adsorbed species and the active sites on the steel surface. Such deviations are typical for complex plant extracts containing a mixture of organic molecules that may interact attractively or repulsively, particularly high-molecular-weight compounds with multiple functional groups [63–65]. The negative values of the standard free energy of adsorption (ΔG_{ads}), calculated from the Langmuir K_{ads} , confirm that CNLE adsorption is spontaneous and that the resulting film is thermodynamically stable across all temperatures. In contrast, ΔG_{ads} values derived from the Freundlich constant are positive. This

Table 3

Thermodynamic parameters for CNLE.

S. No	CNLE Conc.(g/ L)	Ea (KJ/ mol)	$-\Delta G_{ads}$ (KJ/mol)			ΔH_{ads} (KJ/mol)	ΔS_{ads} (KJ/mol)
			313K	323K	333K		
1	0.0	33.05	-	-	-	-	-
2	0.2	21.15	71.93	72.93	74.62	18.39	-168.86
3	0.4	14.77	72.1	74	75.92	12.13	-191.55
4	0.6	24.4	75.18	76.83	75.68	21.72	-165.5
5	0.8	41.35	75.68	76.41	77.14	52.64	-173.57

discrepancy arises because the Freundlich constant is an empirical fitting parameter that does not satisfy the thermodynamic assumptions required for a meaningful ΔG_{ads} calculation. Therefore, the positive values should be interpreted as a limitation of the Freundlich model in this context, rather than as evidence of a non-spontaneous process [66].

3.6. Thermodynamic analysis

To further elucidate the inhibition mechanism, the activation energy (E_a), enthalpy of adsorption (ΔH_{ads}), and entropy of adsorption (ΔS_{ads}) were evaluated. The calculated values are summarized in Table 3. The enthalpy and entropy of activation (ΔH_{ads} and ΔS_{ads}) were derived from the slopes and intercepts of the linear Arrhenius and Eyring plots, shown in Figs. 8 and 9, respectively. Fig. 8 presents Arrhenius plots for corrosion at varying CNLE concentrations, while Fig. 9 displays the corresponding transition-state plots. The positive value of the activation enthalpy (ΔH_{ads}) indicates that the corrosion of carbon steel in HCl is an endothermic process [67], consistent with previous reports for similar steel-acid systems [64,68–71].

The Gibbs free energy of adsorption (ΔG_{ads}) provides further insight into the inhibition mechanism. According to the literature [72], ΔG_{ads} values more positive than approximately $-20 \text{ kJ}\cdot\text{mol}^{-1}$ are generally associated with physisorption, while values more negative than $-40 \text{ kJ}\cdot\text{mol}^{-1}$ suggest chemisorption. In this work, the ΔG_{ads} values fall within an intermediate range, indicating that CNLE adsorption proceeds

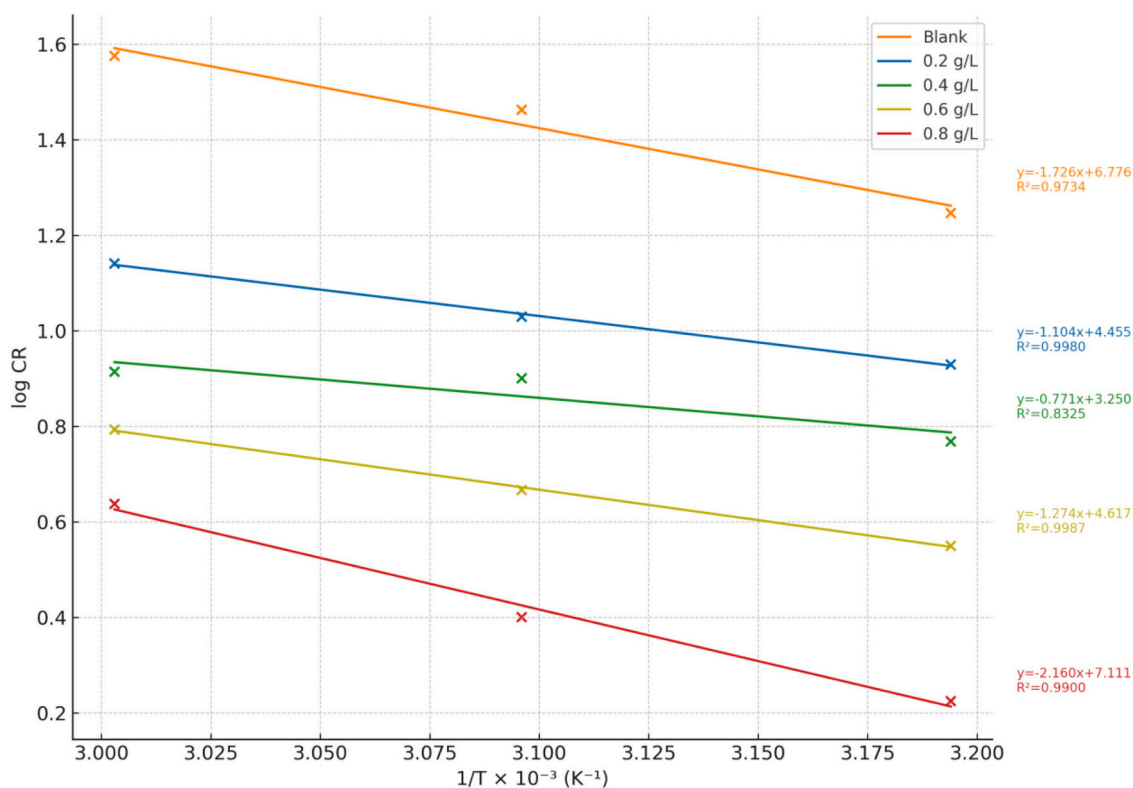


Fig. 8. Arrhenius plots (log CR Vs 1/T) for carbon steel corrosion in 1 M HCl in the presence and absence of CNLE.

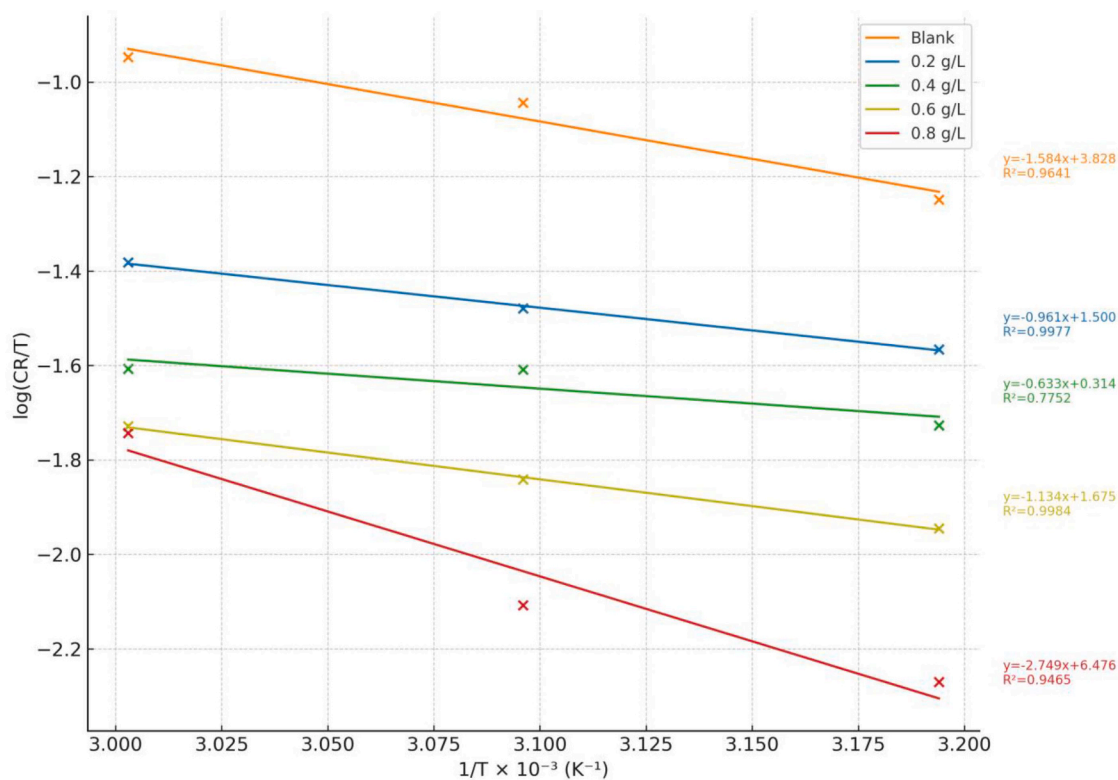


Fig. 9. Transition state plots ($\log \frac{CR}{T}$ Vs 1/T) for carbon steel corrosion in 1 M HCl in the presence and absence of CNLE.

via a mixed chemi-physisorption mechanism. The negative ΔG_{ads} values at all studied temperatures confirm the process is spontaneous and that the resulting inhibitor film is thermodynamically stable. Furthermore,

ΔH_{ads} and ΔS_{ads} were evaluated from the slope and intercept of the ΔG_{ads} versus temperature plot (Fig. 10). The positive ΔH_{ads} values and associated ΔS_{ads} trends support the proposed mixed adsorption

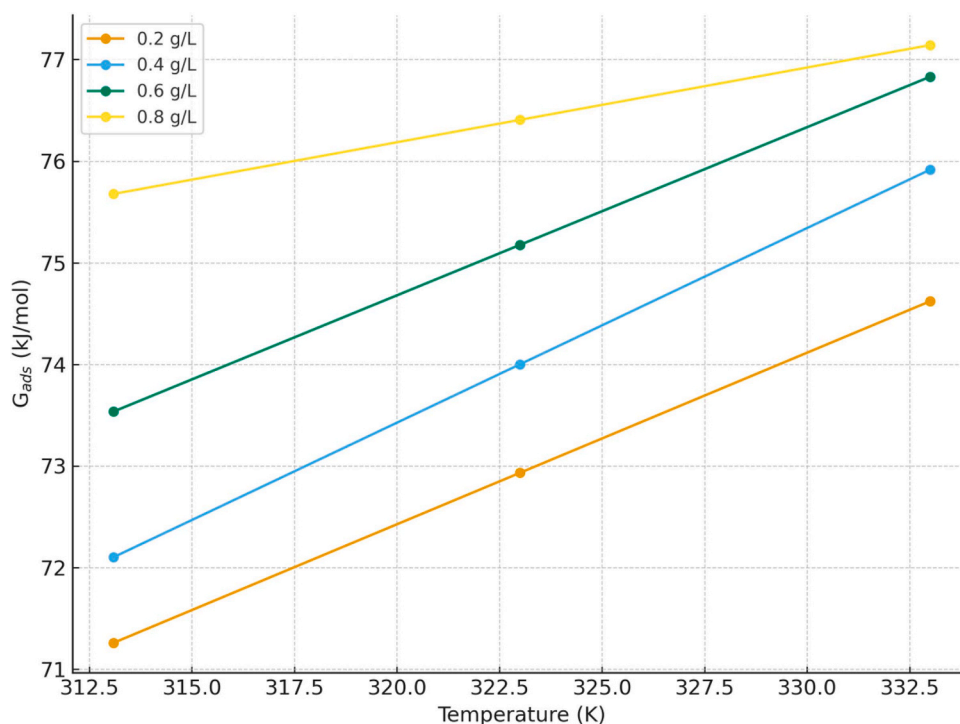


Fig. 10. ΔG_{ads} as a function of temperature in the presence of CNLE in 1 M HCl.

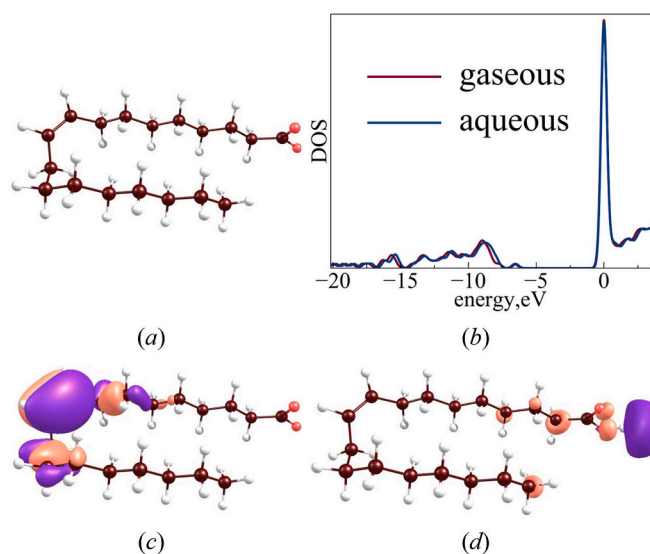


Fig. 11. Oleic acid (a), its density of electronic states (DOS) in both gaseous and aqueous phases (b), isosurfaces of frontier orbitals HOMO (c) and LUMO (d).

mechanism, aligning with findings for other plant-based inhibitors in acidic media [73]. The trend in activation energy (E_a) also informs the mechanism. An increase in E_a relative to the uninhibited solution typically indicates a physisorption-dominated process, whereas a decrease suggests chemisorption lowers the energy barrier [74]. The blank solution exhibits an E_a of 33.05 kJ·mol⁻¹. For inhibited systems, E_a values are 21.15, 14.77, 24.40, and 41.35 kJ·mol⁻¹ at CNLE concentrations of 0.2, 0.4, 0.6, and 0.8 g·L⁻¹, respectively (Table 3). The decrease in E_a at 0.2–0.6 g·L⁻¹ is consistent with a chemisorptive component, while the higher E_a at 0.8 g·L⁻¹ (exceeding the blank) points to an increased physisorption contribution at high surface coverage a trend observed for other plant extracts [75–78]. The adsorption enthalpy (ΔH_{ads}) offers

additional distinction. Physisorption is typically associated with $|\Delta H_{\text{ads}}| < 40$ kJ·mol⁻¹, while chemisorption involves higher values, often approaching 100 kJ·mol⁻¹ [79]. For CNLE, ΔH_{ads} ranges from 12.13 to 21.72 kJ·mol⁻¹ at 0.2–0.6 g·L⁻¹, consistent with physisorption or mixed adsorption. At 0.8 g·L⁻¹, ΔH_{ads} increases to 52.64 kJ·mol⁻¹, exceeding the 40 kJ·mol⁻¹ threshold and suggesting stronger chemisorptive interactions at higher inhibitor doses. When considered together with the strongly negative ΔG_{ads} values (–72 to –77 kJ·mol⁻¹), which signify a spontaneous, high-affinity binding process, the overall data support a concentration-dependent, mixed adsorption mechanism. At lower CNLE concentrations, physical interactions and film formation dominate. At higher concentrations, the rising ΔH_{ads} and E_a indicate a growing contribution from specific chemisorptive bonding [80].

3.7. Computational studies analysis

The optimized molecular structures, frontier molecular orbitals, and density of states (DOS) for oleic acid and piperidine are presented in Figs. 11 and 12. Key quantum chemical descriptors, calculated from the ionization potential (IP) and electron affinity (EA) via Koopmans' theorem, are compiled in Table 4. These include the highest occupied and lowest unoccupied molecular orbital energies (EHOMO, ELUMO), electronegativity (χ), global hardness (η), chemical softness (S), dipole moment (DM), electron transfer fraction (ΔN), and back-donation energy (Ebd) (for detailed definitions, see [81]). The computational results show that the aqueous medium, modeled with COSMO, increases the dipole moment but only weakly perturbs other electronic parameters compared to the gas phase. This minimal solvent effect is corroborated by the similarity of the DOS plots in both phases (Figs. 11 and 12).

Analysis of the frontier orbitals reveals distinct characteristics. For oleic acid, the HOMO is localized on the hydrocarbon chain, while the LUMO resides on the carboxyl group. This spatial separation suggests the carboxyl group can act as an effective electron donor to the iron surface. In contrast, both the HOMO and LUMO of piperidine are delocalized across the entire molecule, a feature common in cyclic structures. Heteroatoms (N in piperidine, O in oleic acid) contribute significantly to these frontier orbitals, underscoring their key role in

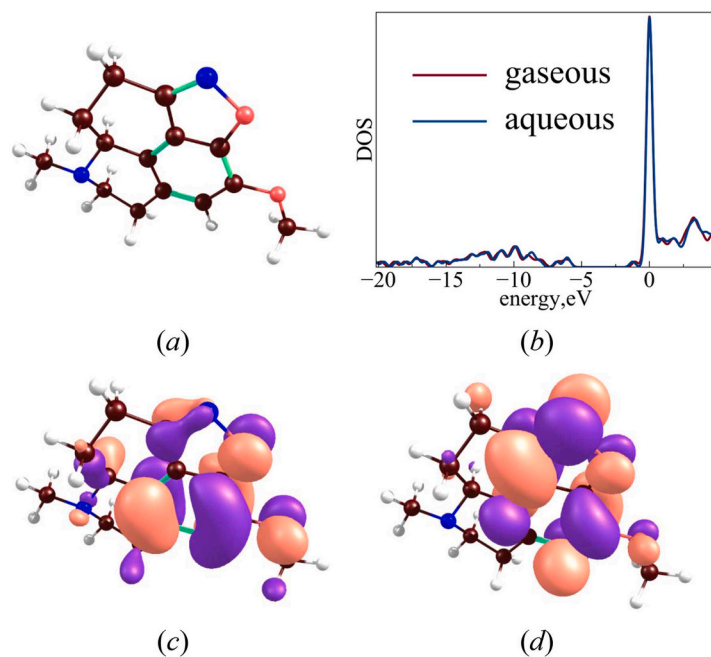


Fig. 12. Piperidine (a), its density of electronic states (DOS) in both gaseous and aqueous phases (b), isosurfaces of frontier orbitals HOMO (c) and LUMO (d).

Table 4

Electronic properties oleic acid and piperidine in both gaseous phase and in aqueous medium.

parameter	oleic acid		piperidine	
	gaseous	aqueous	gaseous	aqueous
E_{HOMO}	-6.59	-6.50	-5.92	-5.97
E_{LUMO}	-0.33	-0.19	-1.07	-1.24
gap	6.26	6.31	4.85	4.73
DM	1.50	2.46	4.88	7.40
IP	6.59	6.50	5.92	5.97
EA	0.33	0.19	1.07	1.24
χ	3.46	3.35	3.50	3.61
η	3.13	3.16	2.43	2.37
S	0.32	0.32	0.41	0.42
ΔN	0.22	0.23	0.27	0.26
E_{bd}	-0.78	-0.79	-0.61	-0.59

reactivity. As indicated in Table 4, both molecules exhibit comparable reactivity. Oleic acid possesses a marginally wider HOMO-LUMO gap, correlating with its slightly higher chemical hardness [82]. Molecular dynamics (MD) simulation results after 12 ps at 300 K are shown in Figs. 13 and 14. Both inhibitor molecules rapidly adsorb onto the iron (110) surface and remain firmly anchored without lateral sliding. The radial distribution functions (RDFs) in these figures quantify this interaction, with distinct peaks near 2 Å confirming strong, direct adhesion of the inhibitors to the metal surface [83].

4. Conclusion

This study demonstrates that CNLE is a highly efficient and thermally stable green inhibitor for carbon steel in 1 M HCl. CNLE maintained its integrity up to 100 °C and achieved inhibition efficiencies above 90 % at 0.8 g L⁻¹, indicating that it can withstand typical temperatures encountered in industrial acidic operations. Gravimetric and thermometric results consistently revealed a strong concentration-dependent reduction in corrosion rate. Adsorption analyses using the Langmuir model, together with thermodynamic parameters, indicate a mixed physical-chemical adsorption mechanism that is endothermic and driven in part by favorable entropy changes. Complementary DFT and

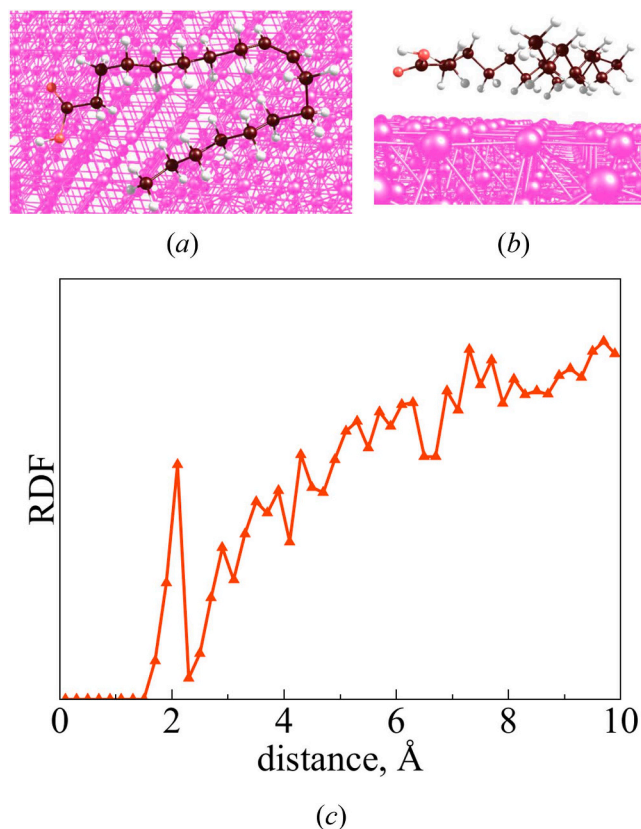


Fig. 13. Top (a) and side view (b) of the oleic acid on Fe(110) slab and slab-inhibitor radial distribution function (RDF) (c).

molecular dynamics simulations of the main CNLE components, oleic acid and piperidine, confirmed their high electronic reactivity, strong interactions with the Fe(110) surface, and ability to form stable adsorbed films, supporting the experimental observations. Overall, the combined experimental and computational evidence positions CNLE as a

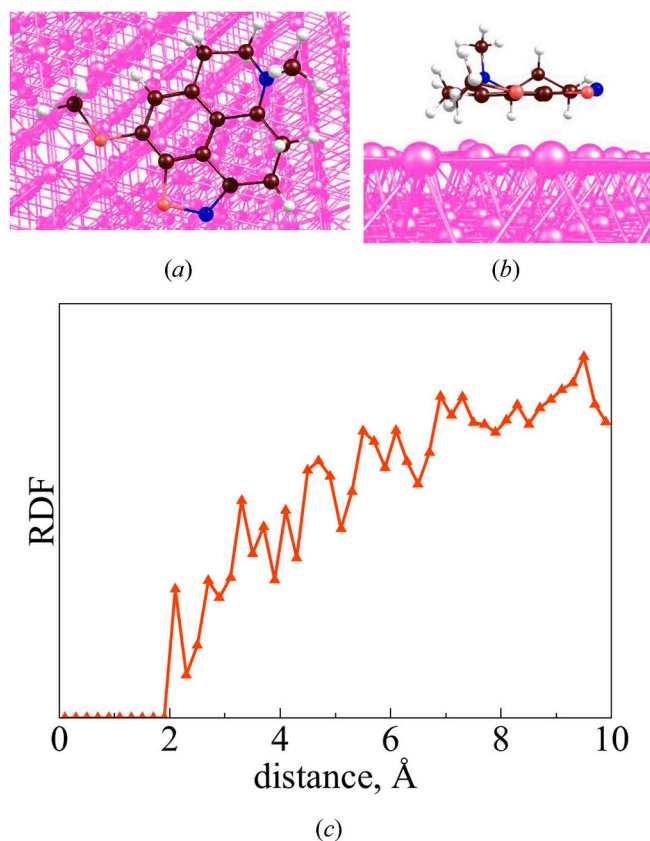


Fig. 14. Top (a) and side view (b) of the piperidine molecule on Fe(110) slab and slab-inhibitor radial distribution function ((c).

promising, sustainable alternative to conventional synthetic inhibitors for protecting carbon steel in acidic environments. However, the experimental efficiency decline at high temperatures and the restriction to 1 M HCl under laboratory conditions indicate that additional research is needed on harsh and realistic service conditions. Investigations into formulation strategies to improve the thermal and operational stability of CNLE-based inhibitor systems are also required. This work also provides a useful framework for integrating plant-derived chemistry, adsorption thermodynamics, and atomistic simulations in the design and evaluation of next-generation green corrosion inhibitors.

Availability of data and materials

The datasets used and/or analyzed during the current paper are available from the corresponding author on reasonable request.

Funding declaration

No funding

CRediT authorship contribution statement

Silas.O. Okuma: Writing – original draft, Validation, Supervision, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Martins Obaseki:** Supervision, Methodology, Investigation, Conceptualization.

Declaration of competing interest

The author confirms that there is no conflict of interest to declare.

Data availability

Data will be made available on request.

References

- [1] R.W. Revie, H.H. Uhlig, *Corrosion and Corrosion Control*, John Wiley & Sons, 2025.
- [2] K. Rashid, A. Khadom, Evaluation of environmentally friendly inhibitor for corrosion of mild steel in phosphoric acid solution: unconventional approach, *Anti-corros. methods mater.* 65 (5) (2018) 506–514.
- [3] M. Obaseki, P.B. Alfred, P.T. Elijah, S.O. Okuma, Corrosion rate prediction in oil and gas pipelines based on multiphase flow modelling, *Int. J. Eng. Res. Afr.* 67 (2023) 27–48.
- [4] S.A. Hussein, A.A. Khadom, A.A.H. Kadhum, H.B. Mahood, K.H. Rashid, Mass transfer influence on the corrosion inhibition of N80 steel in 1 M H₂SO₄ by green corrosion inhibitor using MATLAB, *Int. J. Electrochem. Sci.* 19 (10) (2024) 100764.
- [5] K.H. Rashid, A.A. Khadom, H.B. Mahood, Aluminum ASA 6061 anodizing process by chromic acid using Box–Wilson central composite design: optimization and corrosion tendency, *Met. Mater. Int.* 27 (10) (2021) 4059–4073.
- [6] H.S. Hassan, K.H. Rashid, K.F. Al-Azawi, A.A. Khadom, H.B. Mahood, Synthesis and diagnosis of new heterocyclic compound as corrosion inhibitor for mild steel in acidic solution, *Diyala J. Eng. Sci.* (2024) 180–196.
- [7] M. Obaseki, P.B. Alfred, P.T. Elijah, S.O. Okuma, Corrosion rate prediction in oil and gas pipelines based on multiphase flow modelling, *Int. J. Eng. Res. Afr.* 67 (2023) 27–48.
- [8] H. Kania, Corrosion and anticorrosion of alloys/metals: the important global issue, *Coatings* 13 (2) (2023) 216.
- [9] S.M. Musa, F.B. Abudaia, E.O. Khalil, A.A. Elbasir, Corrosion cost in power plants of general electric company of Libya, *Alostath* (29) (2025).
- [10] W. Shao, X. Du, W. Zhang, D. Shi, J. Zhang, P. Tang, Corrosion mechanisms, responses, and mitigation strategies for steel piles in offshore wind turbines: a comprehensive review, *Mater. Corros.* (2025).
- [11] S.O. Okuma, E.O. Ogagavwodia, V.E. Ajokperiniowo, J.E. Emurotu, Performance of acetone extract of anthocleista grandiflora as a potential bioinhibitor on corrosion behavior of carbon steel in seawater environment, *Period. Polytech. Chem. Eng.* 68 (4) (2024) 597–608.
- [12] Z.I. Jasim, K.H. Rashid, A.A. Khadom, Corrosion and corrosion control of the steel in acidizing oil wells processes: an overview of organic inhibitors, *Russ. J. Appl. Chem.* 97 (1) (2024) 56–74.
- [13] N. Bhardwaj, P. Sharma, V. Kumar, Phytochemicals as steel corrosion inhibitor: an insight into mechanism, *Corros. Rev.* 39 (1) (2021) 27–41.
- [14] S. Mustapha, R. Elabor, A.T. Amigun, M.B. Etsuyankpa, T.C. Egbosiuba, D. T. Shuaib, A.K. Mohammed, Phytochemicals/plant extracts as corrosion inhibitors for zinc in various electrolytes, *Phytochemistry in Corrosion Science*, CRC Press, 2024, pp. 263–295.
- [15] A. Miralrio, A. Espinoza Vázquez, Plant extracts as green corrosion inhibitors for different metal surfaces and corrosive media: a review, *Processes* 8 (8) (2020) 942.
- [16] C. Verma, A. Kumar, A. Thakur (Eds.), *Phytochemistry in Corrosion Science: Plant Extracts and Phytochemicals as Corrosion Inhibitors*, CRC Press, 2024.
- [17] A. Saxena, J. Kumar, Phytochemical screening, metal-binding studies and applications of floral extract of *Sonchus oleraceus* as a corrosion inhibitor, *J. Bio-Tribo-Corros.* 6 (2) (2020) 55.
- [18] W.F. Hameed, K.H. Rashid, A.A. Khadom, Optimization of inhibition performance of hexa methylene tetra amine for corrosion of mild steel in CO₂-saturated brine produced water, in: *AIP Conference Proceedings* 2443, AIP Publishing LLC, 2022 030047.
- [19] K.H. Rashid, K.F. Al-Azawi, Z.I. Jasim, A.A. Khadom, Optimization for corrosion inhibition of steel in hydrochloric acid by DHOT as a novel corrosion inhibitor, *Pet. Chem.* 64 (8) (2024) 996–1001.
- [20] W.A. Mohammed, K.H. Rashid, K.F. AL-Azawi, A.A. Khadom, A.A.H. Kadhum, A. A. Al-Amiery, A review on corrosion inhibition performance of chalcones: a multi-technique study using weight loss, eis, polarization, and quantum chemical calculations, *Moroc. J. Chem.* 13 (3) (2025). *J-Chem.*
- [21] W.A. Mohammed, K.H. Rashid, K.F. AL-Azawi, A.A. Khadom, Novel chalcone-derived bases as efficient corrosion inhibitor for carbon steel in 1M HCl: synthesis, diagnosis, gravimetric, electrochemical, morphological, and computational insights, *ChemistrySelect.* 10 (34) (2025) e03378.
- [22] C.N. Njoku, T.U. Maduoma, W. Emori, R.E. Odey, B.M. Unimke, E. Yakubu, K. B. Oyoh, Natural and synthetic drugs as eco-friendly and sustainable corrosion inhibitors for metals: a review, *Pigment Resin Technol.* 53 (6) (2024) 1074–1087.
- [23] S.D. Tidke, S.S. Kulkarni, A.C. Marathe, Comprehensive review of green corrosion inhibitors for safe and sustainable protection of mild steel in acidic environments, *Discov. Electrochem.* 2 (1) (2025) 40.
- [24] C. Verma, D.S. Chauhan, R. Aslam, P. Banerjee, J. Aslam, T.W. Quadri, T. Rasheed, Principles and theories of green chemistry for corrosion science and engineering: design and application, *Green. Chem.* 26 (8) (2024) 4270–4357.
- [25] Chhetri Sapkota, S., Dahal, D., Yadav, A., Dhakal, D., Sharma, R.K., & Saini, G. (2024). A paradigm shift in corrosion inhibition using botanical extracts: from conventional methods to advanced methods for reinforcing steel.
- [26] P. Shathani, E.N. Ogunmuyiwa, B.A. Obadele, O.P. Oladijo, Plant leaf extracts as green corrosion inhibitors of steel in acidic and seawater environments: a review, *Environ. Sci. Pollut. Res.* (2025) 1–22.

- [27] T. Satapathy, B. Banjare, H. Sahu, A comprehensive analysis of *Cestrum nocturnum*: its phytochemical composition, pharmacological applications and toxicity profile in the context of traditional medicinal practices, *J. Drug Deliv. Ther.* 14 (9) (2024).
- [28] S. Ahmad, M. Alrouji, S. Alhajlah, O. Alomeir, R.P. Pandey, M.S. Ashraf, S. Khan, Secondary metabolite profiling, antioxidant, antidiabetic and neuroprotective activity of *cestrum nocturnum* (night scented-jasmine): use of in vitro and in silico approach in determining the potential bioactive compound, *Plants* 12 (6) (2023) 1206.
- [29] S.O. Okuma, O.D. Ofuyekpone, C.C. Nwaeju, M. Obaseki, E.O. Ogagavwodia, Response optimisation and modelling of experimental data on the performance of *lasianthera africanum* leaves extract as a corrosion inhibitor on mild steel in hydrochloric-induced environment, *Eng. Chem.* 7 (2024) 25–40.
- [30] S.H. Abbas, A.M. Ridha, K.H. Rashid, A.A. Khadom, Biosorption of Congo red dye removal from aqueous solution using fennel seed spent and garlic peel, *Int. J. Environ. Sci. Technol.* 20 (12) (2023) 13845–13858.
- [31] S. Sutariya, A.A. Shah, A.B. Bajpai, R.J. Sharma, C.P. Pandhurnekar, A. Gupta, Fourier transform infrared spectroscopy (FTIR) analysis, antioxidant and anti-inflammatory activities of leaf and fruit extracts of *Gymnosporia montana*, *Mater. Today* 73 (2023) 134–141.
- [32] J. Adhikari, A. Bhattarai, N.K. Chaudhary, Data analysis for SEM-EDX, thermokinetics, surfactant, and corrosion inhibition activity of Co (II) and Zn (II) complexes of pyrrole-based surfactant ligand, *Data Br.* 48 (2023) 109124.
- [33] M.M. Mchihi, N.W. Odozi, A.O. Nurudeen, M.C. Emesiani, B.O. Seriki, Assessment of *Helianthus tuberosus* leaves extract as eco-friendly corrosion inhibitor for Aluminum in sodium hydroxide: insights from electrochemical, gravimetry and computational consideration, *Moroc. J. Chem.* 12 (4) (2024) 1462–1483.
- [34] O.D. Ofuyekpone, S.O. Okuma, S. Iweriolor, O.G. Utu, Chemical compounds from GC/MS analysis, functional investigations, and corrosion inhibition efficacy of a bio-based and sustainable extract against HCl solution-activated corrosion, *J. Bio-Tribo-Corros.* 11 (2) (2025) 37.
- [35] S.O. Okuma, E.O. Ogagavwodia, M. Obaseki, C.C. Nwaeju, Kinetic and thermodynamic assessment of the potency of *irvingia gabonensis* plant extract as an eco-friendly inhibitor for mild steel in an acidic environment, *Eur. J. Mater. Sci. Eng.* 8 (3) (2023) 142–155.
- [36] J. Kästner, J.M. Carr, T.W. Keal, W. Thiel, A. Wander, P. Sherwood, DL-FIND: an Open-Source Geometry Optimizer for Atomistic Simulations, *J. Phys. Chem. A* 113 (43) (2009) 11856–11865, <https://doi.org/10.1021/jp9028968>.
- [37] A.V. Titov, I.S. Ufimtsev, N. Luehr, T.J. Martinez, Generating efficient quantum chemistry codes for novel architectures, *J. Chem. Theory. Comput.* 9 (1) (2012) 213–221, <https://doi.org/10.1021/ct300321a>.
- [38] F. Liu, N. Luehr, H.J. Kulik, T.J. Martínez, Quantum chemistry for solvated molecules on graphical processing units using polarizable continuum models, *J. Chem. Theory. Comput.* 11 (7) (2015) 3131–3144, <https://doi.org/10.1021/acs.jctc.5b00370>.
- [39] K.L. Schuchardt, B.T. Didier, T. Elsethagen, L. Sun, V. Gurumoorhi, J. Chase, J. Li, T.L. Windus, Basis set exchange: a community database for computational sciences, *J. Chem. Inf. Model.* 47 (3) (2007) 1045–1052, <https://doi.org/10.1021/ci600510j>.
- [40] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, *J. Chem. Phys.* 132 (15) (2010), <https://doi.org/10.1063/1.3382344>.
- [41] L.-P. Wang, C. Song, Geometry optimization made simple with translation and rotation coordinates, *J. Chem. Phys.* 144 (21) (2016), <https://doi.org/10.1063/1.4952956>.
- [42] Y.K. Shin, H. Kwak, A.V. Vasenkov, D. Sengupta, A.C.T. van Duin, Development of a ReaxFF reactive force field for Fe/Cr/O/S and application to oxidation of butane over a pyrite-covered Cr₂O₃ catalyst, *ACS. Catal.* 5 (12) (2015) 7226–7236, <https://doi.org/10.1021/acscatal.5b01766>.
- [43] E. Moerman, D. Furman, D.J. Wales, Development of ReaxFF reactive force field for aqueous iron–sulfur clusters with applications to stability and reactivity in water, *J. Chem. Inf. Model.* 61 (3) (2021) 1204–1214, <https://doi.org/10.1021/acs.jcim.0c01292>.
- [44] A.P. Thompson, H.M. Aktulga, R. Berger, D.S. Bolintineanu, W.M. Brown, P. S. Crozier, P.J. in 't Veld, A. Kohlmeyer, S.G. Moore, T.D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott, S.J. Plimpton, LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales, *Comput. Phys. Commun.* 271 (2022) 108171, <https://doi.org/10.1016/j.cpc.2021.108171>.
- [45] S. Kaya, F. Siddique, D.O. Isin, K.P. Katin, V. Asati, A. Berisha, Inhibition performances of new pyrazole derivatives against the corrosion of C38 steel in acidic medium: computational study, *Results Surf. Interfaces* 14 (2024) 100184, <https://doi.org/10.1016/j.rsufi.2024.100184>.
- [46] T. Lu, F. Chen, Multiwfn: a multifunctional wavefunction analyzer, *J. Comput. Chem.* 33 (5) (2011) 580–592, <https://doi.org/10.1002/jcc.22885>. Portico.
- [47] Chemcraft (Version 1.8, Build 682) [Computer software]. (n.d.). <https://www.chemcraftprog.com>.
- [48] A.S. Jasim, A.A. Khadom, K.H. Rashid, K.F. AL-Azawi, (3, 5-dimethyl-1H-pyrazol-1-yl)(4-(3, 4-dimethoxybenzylidene) amino) phenyl) methanone as a novel corrosion inhibitor for low-carbon steel in hydrochloric acid: synthesis, diagnosis, and application, *Results. Chem.* 4 (2022) 100569.
- [49] P. Ragavendran, D. Sophia, C. Arul Raj, V.K. Gopalakrishnan, Functional group analysis of various extracts of *Aerva lanata* (L.) by FTIR spectrum, *Pharmacologyonline* 1 (2011) 358–364.
- [50] N. Al Otaibi, H.H. Hammud, Corrosion inhibition using harmal leaf extract as an eco-friendly corrosion inhibitor, *Molecules.* 26 (22) (2021) 7024.
- [51] A. Rahimi, A. Farhadian, A. Berisha, A. Shaabani, M.A. Varfolomeev, V. Mehmeti, R. Djimasbe, Novel sucrose derivative as a thermally stable inhibitor for mild steel corrosion in 15% HCl medium: an experimental and computational study, *Chem. Eng. J.* 446 (2022) 136938.
- [52] O. Onukwuli, M. Omotoma, I. Obiora-Okafo, Thermometric and gravimetric analyses of aluminum corrosion control in a HCl medium, using *ricinus communis* extract, *Port. Electrochim. Acta* 38 (1) (2020) 19–28.
- [53] J. Adhikari, A. Bhattarai, N.K. Chaudhary, Data analysis for SEM-EDX, thermokinetics, surfactant, and corrosion inhibition activity of Co (II) and Zn (II) complexes of pyrrole-based surfactant ligand, *Data Br.* 48 (2023) 109124.
- [54] Z.K. Sulay, A.U. Victor, B. Obed, A.O. Olufemi, Kinetics and thermodynamic study of inhibition potentials by ethoxyethane extracts of *cochlospermum tinctorium* for the oxoacid corrosion of mild steel, *Int. J. Mater. Chem.* 5 (3) (2015) 64–76.
- [55] F. Malaret, X.S. Yang, Exact calculation of corrosion rates by the weight-loss method, *Exp. Results.* 3 (2022) e13.
- [56] B. El Ibrahimia, E. Berdimurodovb, Weight loss technique. Electrochemical and Analytical Techniques For Sustainable Corrosion Monitoring: Advances, Challenges and Opportunities, 2023, p. 81.
- [57] S.O. Okuma, E.O. Ogagavwodia, V.E. Ajokperiniov, M. Obaseki, Predictive modeling and adsorption behavior, kinetics, and thermodynamic studies of *anthocleista grandiflora* leaf extract for corrosion inhibition of carbon steel in seawater, *Solid State Phenom.* 365 (2024) 33–52.
- [58] H.A. Al Salhi, R.R. Mahdi, A. Al-Amiry, W.K. Al-Azzawi, A.A.H. Kadhum, Exploring the efficacy of polysaccharides as green corrosion inhibitors: a comprehensive review, *Starch-Stärke* 76 (7–8) (2024) 2300234.
- [59] O. Oyewole, A.P. Oluyori, J.B. Adeoye, C.C. Chukwuma, A.O. Dada, Thermodynamics and adsorption studies of blended guava and mango leaves extract as inhibitors for 7075 aluminium, *Results. Chem.* 7 (2024) 101518.
- [60] S.A. Umoren, A.A. AlAhmary, Z.M. Gasem, M.M. Solomon, Evaluation of chitosan and carboxymethyl cellulose as ecofriendly corrosion inhibitors for steel, *Int. J. Biol. Macromol.* 117 (2018) 1017–1028.
- [61] O.A. Akinbulumo, O.J. Odejobi, E.L. Odekanle, Thermodynamics and adsorption study of the corrosion inhibition of mild steel by *Euphorbia heterophylla* L. extract in 1.5 M HCl, *Results Mater.* 5 (2020) 100074.
- [62] P.A. Andoor, K.B. Okeoma, U.S. Mbamara, Adsorption and thermodynamic studies of the corrosion inhibition effect of *Rosmarinus officinalis* L. leaves on aluminium alloy in 0.25 M HCl and effect of an external magnetic field, *Int. J. Phys. Sci.* 16 (2) (2021) 79–95.
- [63] Z. Tao, W. He, S. Wang, S. Zhang, G. Zhou, A study of differential polarization curves and thermodynamic properties for mild steel in acidic solution with nitrophenyltriazole derivative, *Corros. Sci.* 60 (2012) 205–213.
- [64] S.A. Umoren, M.M. Solomon, I.B. Obot, R.K. Suleiman, Comparative studies on the corrosion inhibition efficacy of ethanolic extracts of date palm leaves and seeds on carbon steel corrosion in 15% HCl solution, *J. Adhes. Sci. Technol.* 32 (17) (2018) 1934–1951.
- [65] N.O. Eddy, S.A. Odoemelam, E.C. Ogoko, R.A. Ukpe, R. Garg, B. Anand, Experimental and quantum chemical studies of synergistic enhancement of the corrosion inhibition efficiency of ethanol extract of *Carica papaya* peel for aluminum in solution of HCl, *Results. Chem.* (2022) 100290.
- [66] P. Shathani, E.N. Ogunmuyiwa, O.P. Oladijo, B.A. Obadele, Thermodynamics and adsorption behaviour of *Sclerocarya birrea* leaf extract as a potential green corrosion inhibitor for mild steel in a simulated seawater (3.5% NaCl) environment, *Chem. Thermodyn. Therm. Anal.* (2025) 100197.
- [67] G.A. Ijuo, H.F. Chahul, I.S. Enjeji, Kinetic and thermodynamic studies of corrosion inhibition of mild steel using *Bridelia ferruginea* extract in acidic environment, *J. Adv. Electrochem.* (2016) 107–112.
- [68] M.H. Hussin, M.J. Kassim, N.N. Razali, N.H. Dahon, D. Nasshorudin, The effect of *Tinospora crispa* extracts as a natural mild steel corrosion inhibitor in 1 M HCl solution, *Arab. J. Chem.* 9 (2016) S616–S624.
- [69] A. Ayodeji, D. Bamidele, F. Sunday, A. Oluranti, A. Edith, O. Oladokun, N. Daniel, Corrosion inhibitive performance of the waste orange peels (*Citrus Sinensis*) on A36 mild steel in 1M HCl, *Int. J. Electrochem. Sci.* 17 (1) (2022) 22011.
- [70] M. Alimohammadi, M. Ghaderi, S.A. Ramazani, A. M. Mahdavian, *Falcaria vulgaris* leaves extract as an eco-friendly corrosion inhibitor for mild steel in hydrochloric acid media, *Sci. Rep.* 13 (1) (2023) 3737.
- [71] S.O. Okuma, E.O. Ogagavwodia, M. Obaseki, C.C. Nwaeju, Kinetic and thermodynamic assessment of the potency of *irvingia gabonensis* plant extract as an eco-friendly inhibitor for mild steel in an acidic environment, *Eur. J. Mater. Sci. Eng.* 8 (3) (2023) 142–155.
- [72] S. Salmi, H. Boudellouia, Y. Hamlaoui, M. Fedel, Evaluating the corrosion inhibition performance of cerium oxide/cerium nitrate inhibitors on carbon steel in chloride solutions, *Mater. Corros.* (2025).
- [73] M.A. Ibrahim, I.H. Elshamy, M.I. Elshamy, A. Elaraby, An experimental and computational investigation on the performance of cefotaxime in mitigating Ti6Al4V alloy corrosion, *Corros. Eng. Sci. Technol.* (2025) 1478422X251348976.
- [74] X. Qin, Z. Xie, Y. Li, L. Chen, P. Tang, X. Liu, X. Wang, Synthesis and Properties of a New Environmentally Friendly Bicyclic Imidazoline Quaternary Ammonium Salt as a Corrosion Inhibitor of Carbon Steel, *Corrosion* 81 (3) (2025) 258–266.
- [75] M.H. Sliem, N.M. El Basyony, E.G. Zaki, M.A. Sharaf, A.M. Abdullah, Corrosion inhibition of mild steel in sulfuric acid by a newly synthesized Schiff base: an electrochemical, DFT, and Monte Carlo simulation study, *Electroanalysis.* 32 (12) (2020) 3145–3158.
- [76] M.S. Bejandi, M.H. Behrooz, M.R. Khalili, R. Sharifi, A.A. Javidparvar, E. Oguzie, Pharmaceuticals for materials protection: experimental and computational studies

- of expired closantel drug (C₂₂H₁₄Cl₂I₂N₂O₂) as a potent corrosion inhibitor, *J. Ind. Eng. Chem.* 131 (2024) 662–675.
- [77] J.A.A Al Aseel, Doctoral dissertation, Université de Lille, 2024.
- [78] A.I. Ikeuba, B.I. Ita, C.P. Okonkwo, P.E. Ekuri, H.O. Edet, J. Amajama, P.C. Iwuji, Review of computational methods used in the evaluation corrosion inhibition of metallic materials, *Discov. Chem. Eng.* 4 (1) (2024) 28.
- [79] M. Belhadi, M. Oubahou, I. Hammoudan, A. Chraka, M. Chafi, S. Tighadouini, A comprehensive assessment of carbon steel corrosion inhibition by 1, 10-phenanthroline in the acidic environment: insights from experimental and computational studies, *Environ. Sci. Pollut. Res.* 31 (53) (2024) 62038–62055.
- [80] I.A. Annon, K.K. Jlood, M.M. Hanoon, F.F. Sayyid, W.K. Al-Azzawi, A. Al-Amiery, Corrosion inhibition of mild steel in HCL solution using MPO: experimental and theoretical insights, *J. Mater. Eng.* 2 (2) (2024) 104–118.
- [81] Mostafa H. Sliem, Ahmed Bahgat Radwan, Farida S. Mohamed, Nasser A. Alnuaimi, Aboubakr M. Abdullah, An efficient green ionic liquid for the corrosion inhibition of reinforcement steel in neutral and alkaline highly saline simulated concrete pore solutions, *Sci. Rep.* 10 (1) (2020) 14565.
- [82] M.A. El-Haddad, A. Bahgat Radwan, M.H. Sliem, W.M. Hassan, A.M. Abdullah, Highly efficient eco-friendly corrosion inhibitor for mild steel in 5 M HCl at elevated temperatures: experimental & molecular dynamics study, *Sci. Rep.* 9 (1) (2019) 3695.
- [83] S. Kaya, F. Siddique, D.O. Isin, K.P. Katin, V. Asati, A. Berisha, Inhibition performances of new pyrazole derivatives against the corrosion of C38 steel in acidic medium: computational study, *Results Surf. Interfaces* 14 (2024) 100184.