Corrosion inhibition performance of 4-(4-methoxybenzylideneamino)-5-(4-pyridinyl)-2,4-dihydro-1,2,4-triazole-3-thione (MPDTT) for mild steel in acidic media: Experimental and theoretical insights

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Abstract

This study investigates the corrosion inhibition efficiency of a novel triazole-based compound, 4-(4-methoxybenzylideneamino)-5-(4-pyridinyl)-2,4-dihydro-1,2,4-triazole-3-thione (MPDTT), for mild steel in 1 M HCl, integrating both experimental and theoretical analyses. Unlike conventional triazole inhibitors, MPDTT features a unique molecular structure incorporating methoxy and pyridinyl groups, which enhance its adsorption capacity and corrosion inhibition performance. Weight loss experiments were performed across varying MPDTT concentrations (0.1–1.0 mM) and immersion times (1–48 hours) to evaluate its protective capabilities. The results revealed that inhibition efficiency increased with MPDTT concentration, achieving a maximum of 96.1% at 0.5 mM after 48 hours, with efficiency stabilizing after 10 hours of immersion. Temperature studies (303–333 K) over a 5-hour immersion indicated a slight enhancement in inhibition efficiency with rising temperature, suggesting a robust inhibitor-metal interaction. Adsorption behavior followed the Langmuir isotherm, confirming monolayer formation and indicating a mixed chemisorption and physisorption mechanism. Quantum chemical parameters derived from Density Functional Theory (DFT) calculations, such as HOMO and LUMO energy levels, provided insights into the electronic properties of MPDTT and its potential interaction with the mild steel surface, supporting the experimentally observed inhibition efficiency. This combined experimental-theoretical approach demonstrates MPDTT's enhanced efficiency, thermal stability, and potential as a highly effective and reliable

corrosion inhibitor for mild steel in acidic environments, offering a significant advancement over existing triazole-based compounds.

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Introduction

Mild steel is a primary structural material of construction work as well as the essential material for automotive and chemical processing equipment, but it is seriously susceptible to corrosion. Mild steel, when placed in an aggressive medium, such as a solution of HCl, makes the metal degrade massively and fail, culminating in increased maintenance costs. One of the oldest methods of preventing such problems is to inhibit corrosion by providing a protective barrier that reduces the metal dissolution [1, 2]. Among some of the categories, heteroatoms such as nitrogen, sulfur, and oxygen in organic compounds are significant inhibitors of corrosion. These show effective adsorption of these decomposable organic molecules on the metal surface that form a protective layer to mitigate corrosion. The above triazole derivatives are interesting as they can affect the potential adsorption of multipoint adsorbate-molecule interactions onto a metal surface [3, 4]. This study is relative to the efficiency of the new compound, the triazole derivative, MPDTT. Various studies have been done on the effectiveness of organic compounds as corrosion inhibitors that would highlight the adsorption behavior, inhibition efficiencies, and mechanics of interaction. Caldona *et al.* (2021) tested the ability of a series of triazole-based molecules in protecting mild steel samples from corrosion in acidic media and quite interestingly demonstrated that they were excellent corrosion inhibitors since they could lay down very stable adsorption layers [5]. Benzbiria *et al.* (2023) highlighted the role of heterocyclic compounds containing nitrogen and sulfur, demonstrating improved corrosion resistance due to chemisorption [6]. Rasheeda *et al.* (2022) confirmed that the adsorption of organic inhibitors often follows the Langmuir isotherm, indicating monolayer adsorption on the metal surface [7]. Shenoy *et al.* (2022) studied temperature influences and noted that inhibition efficiencies for certain compounds increase with rising temperature due to stronger adsorptive interactions [8]. Berrissoul *et al.* (2022) utilized Density Functional Theory (DFT) to analyze molecular properties of inhibitors, such as HOMO and LUMO energies, which correlate with adsorption efficiency [9]. Ouakki *et al.* (2022) observed stabilization in inhibition efficiency after prolonged immersion, attributed to equilibrium adsorption [10]. Sun *et al.* (2022) explained the dual adsorption behavior-chemisorption and physisorption-in heterocyclic inhibitors, enhancing overall corrosion protection [11]. Ghaderi *et al.* (2022) demonstrated that electron-donating groups, such as methoxy, improve inhibitor performance by enhancing electron density at the adsorption sites [12]. Kaban *et al.* (2021) emphasized the industrial relevance of developing environmentally friendly and efficient inhibitors for mild steel corrosion in acidic environments [13]. Damej *et al.* (2021) investigated the synergistic role of functional groups

in inhibitors, highlighting their importance in enhancing adsorption stability [14]. These studies collectively underscore the critical role of molecular structure, adsorption isotherms, and environmental parameters in designing effective corrosion inhibitors. However, the exploration of MPDTT, a triazole derivative with unique functional groups, remains underexplored, presenting a gap in the literature.

Corrosion of mild steel in acidic environments, such as those encountered during pickling and industrial cleaning processes, leads to significant material loss and operational inefficiencies [15, 16]. Current inhibitors often exhibit limitations in terms of stability, cost, and efficiency, particularly under varying immersion times and temperatures [17]. Additionally, the lack of systematic integration of theoretical and experimental analyses limits the comprehensive understanding of inhibitor performance.

The environmental impact of corrosion inhibitors is a crucial factor when considering their potential for industrial applications. In this study, 4-(4-methoxybenzylideneamino)-5-(4-pyridinyl)-2,4-dihydro-1,2,4-triazole-3-thione (MPDTT) was designed with a focus on both efficiency and environmental safety. The molecular structure of MPDTT incorporates eco-friendly functional groups, such as methoxy and triazole rings, which are known for their relatively low toxicity and biodegradability compared to traditional corrosion inhibitors containing heavy metals or toxic halogens. MPDTT's synthesis avoids the use of hazardous reagents and solvents, aligning with green chemistry principles. The functional groups present in MPDTT enhance its adsorption onto the mild steel surface, allowing effective inhibition at lower concentrations (maximum efficiency achieved at 0.5 mM). This reduces the overall chemical load required for corrosion protection, thereby minimizing its environmental footprint. Moreover, triazole-based compounds, including MPDTT, are reported to exhibit low aquatic toxicity and a reduced tendency for bioaccumulation, making them safer alternatives for large-scale industrial applications. The absence of heavy metals and persistent organic pollutants in MPDTT's structure further supports its classification as an environmentally friendly inhibitor. Considering its high inhibition efficiency, low effective concentration, and eco-friendly profile, MPDTT presents a sustainable solution for corrosion prevention in industries such as oil and gas, chemical processing, and water treatment. Future work will focus on conducting detailed ecotoxicological assessments and life cycle analyses to fully validate MPDTT's environmental compatibility for widespread industrial use.

The novelty of this study lies in the design, synthesis, and comprehensive evaluation of MPDTT (Figure 1) as a novel and highly efficient corrosion inhibitor for mild steel in acidic environments. Unlike conventional triazole-based inhibitors, MPDTT incorporates unique functional groups-specifically the methoxy and pyridinyl moieties-that enhance its electron-donating and accepting capabilities, leading to superior adsorption and inhibition performance. This work distinguishes itself by integrating experimental and theoretical approaches to thoroughly assess the corrosion inhibition behavior of MPDTT. The experimental investigation includes weight loss measurements, temperature-dependent studies, and adsorption isotherm analysis, providing a detailed understanding of MPDTT's

interaction with the mild steel surface. The study further employs Density Functional Theory (DFT) calculations to explore the electronic properties of MPDTT, offering molecular-level insights into its inhibition mechanism. A key novelty of this research is the demonstration of MPDTT's exceptional inhibition efficiency (up to 96.1% at 0.5 mM) achieved at lower concentrations compared to similar triazole-based inhibitors, alongside its stability across a range of temperatures. The combination of high efficiency, strong adsorption, and thermal stability positions MPDTT as a promising next-generation corrosion inhibitor, addressing existing gaps in the development of cost-effective, efficient, and environmentally friendly inhibitors for industrial applications.

The specific objectives are:

1. To evaluate the inhibition effectiveness of MPDTT with different concentrations and contact periods via weight screen tests.
2. Testing the effect of temperature on inhibiting efficiency to determine thermal stability as well as performance.
3. Study adsorption characteristics of MPDTT in various adsorption isotherm models.
4. Perform quantum chemical calculations to understand the molecular properties and adsorption mechanisms of MPDTT.
5. Reliance of experimental investigation in theoretical analysis for the acknowledgement of potential alone on the practical corrosion protective natures of MPDTT.

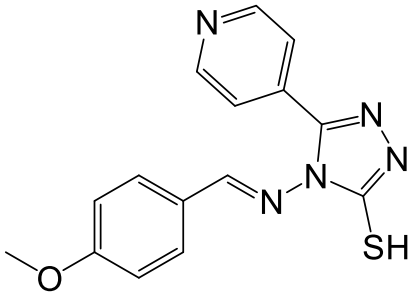

Figure 1. The chemical structure of tested inhibitor.

Experimental Section

Material and sample preparation

The mild steel specimens used in this study had the following weight composition: 0.21% carbon (C), 0.05% sulfur (S), 0.05% manganese (Mn), 0.38% silicon (Si), 0.09% phosphorus (P), 0.01% aluminum (Al), and the remainder being iron (Fe). To ensure consistency, the samples were prepared in uniform dimensions of $3 \times 2 \times 0.2$ cm. The surfaces of the specimens were polished sequentially using sandpapers with grit sizes ranging from 360 to 3000 to achieve a smooth and uniform finish. After polishing, the samples were thoroughly

cleaned following ASTM G1-03 [18] guidelines to remove any residual contaminants or surface oxides.

Solution preparation

A 1 M hydrochloric acid (HCl) solution was prepared by diluting concentrated HCl (37%) with bi-distilled water. MPDTT was dissolved in the acidic solution at concentrations of 0.1, 0.2, 0.3, 0.4, 0.5, and 1 mM for the corrosion inhibition studies.

Weight loss analysis

Weight loss experiments were performed to evaluate the corrosion inhibition efficiency of MPDTT, following ASTM G1 standards [18]. The tests were conducted at a controlled temperature of 303 K, with mild steel strips fully immersed in solutions containing the inhibitor. The initial and final weights of the specimens were measured using a precision digital balance at predetermined intervals of immersion (1, 5, 10, 24, and 48 hours). To study the effect of temperature, additional experiments were conducted at 313, 323, and 333 K, maintaining a fixed immersion time of 5 hours. The weight loss (in milligrams) was calculated as the difference between the initial and final weights of the specimens [19–22]. Each experiment was conducted in triplicate to ensure reproducibility and accuracy. The corrosion inhibition efficiency (*IE*%) and corrosion rate (C_R, in $g \cdot m^{-2} \cdot h^{-1}$) were calculated using the following Equations 1 and 2:

$$IE\% = \frac{W_0 - W_i}{W_0} \cdot 100\% \quad (1)$$

$$C_R = \frac{87.6 \cdot W}{A \cdot t \cdot D} \quad (2)$$

where W_0 and W_i represent the weight losses of mild steel in 1 M HCl without and with the inhibitor, respectively, W is the weight loss in milligrams, A is the exposed surface area of the steel specimen (in cm^2), t is the immersion time (in hours), and D is the density of mild steel.

Theoretical studies

Quantum chemical calculations were performed using Gaussian 09 software to investigate the electronic properties of the MPDTT molecule. The molecular structure was optimized using the B3LYP functional with the 6-31G++(d,p) [23–25] basis set. Based on Koopmans' theorem [26], the ionization potential (I) and electron affinity (A) were calculated, which are directly related to the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies, respectively (Equations 3–7):

$$E_{HOMO} = -I \quad (3)$$

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

$$\chi = \frac{I + A}{2} \tag{5}$$

$$\eta = \frac{I - A}{2} \tag{6}$$

$$\sigma = \frac{1}{\eta} \tag{7}$$

Additional molecular descriptors such as electronegativity (χ), hardness (η), and softness (σ) were derived using the equations.

To evaluate charge transfer interactions between the inhibitor and the metal surface, the fraction of electrons transferred (Δ*N*) was calculated as Equation 8:

$$\Delta N = \frac{\chi_{\text{Fe}} - \chi_{\text{inhibitor}}}{2\left(\eta_{\text{Fe}} + \eta_{\text{inhibitor}}\right)} \tag{8}$$

Hence, the absolute hardness of bulk iron (η) sets 0 as its elemental value while absolute required electronegativity lies at 4.5 eV. For these values, calculations provide good insight into the electronic interactions governing the adsorption of MPDTT on the steel mild surface and highly supported by experimental observations.

Results and Discussion

Effect of inhibitor concentration on corrosion rate and inhibition efficiency of MAPTT at 303 K

The effect of MPDTT concentration on corrosion rate (C_R) and inhibition efficiency (*IE*%) on mild steel in 1 M HCl at 303 K is shown in Figure 2. It can be observed that, with increasing inhibitor concentration, the corrosion rate decreased significantly by improving inhibition efficiency. At a inhibitor concentration of 0.1 mM, its C_R rate also fell down to 4.93 $g \cdot m^{-2} \cdot h^{-1}$ which is 0.82 $g \cdot m^{-2} \cdot h^{-1}$ with an inhibitory efficiency of 40.1%. By further increasing the concentration to 0.5 mM, performance results were realized at the corrosion rate of 0.34 $g \cdot m^{-2} \cdot h^{-1}$, producing the maximum inhibition rates of 92.7%. There was a small improvement in inhibition efficiency, which was found near 1.0 mM. In this instance, the corrosion rate recorded a value within 0.33 $g \cdot m^{-2} \cdot h^{-1}$ to yield a high efficiency of 94.3%. Generally, data tend to confirm that MPDTT significantly inhibits corrosion at relatively lesser degrees of concentration. An observation indicates that the excellence is reinforced due to the adsorption of MPDTT molecule onto the mild steel surface. This forms a protective layer with the acidic medium that will keep the metal from falling off [27]. This kind of behaviour has already been shown in previous studies on triazole derivatives according to which an inhibition efficiency typically increases with concentration until a saturation point is reached.

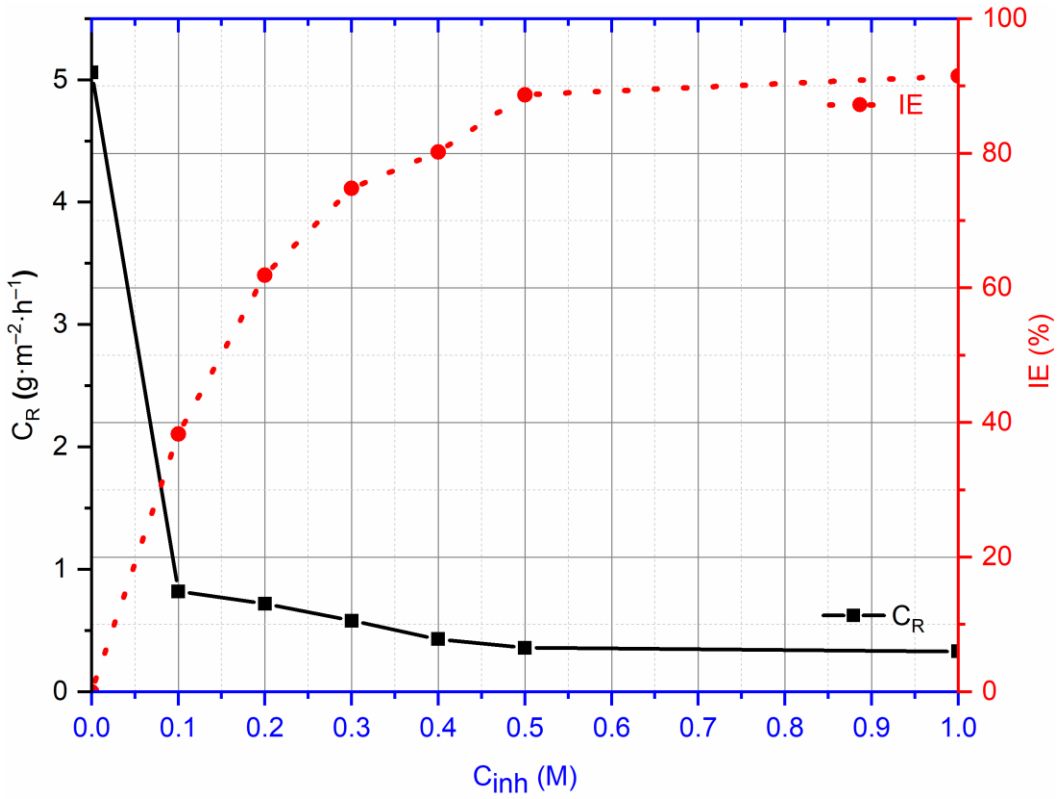

Figure 2. Effect of MPDTT concentration on corrosion rate and inhibition efficiency of mild steel in 1 M HCl at 303 K.

Influence of immersion time and inhibitor concentration on corrosion inhibition efficiency of MAPTT at 303 K

Figure 3 below illustrates the end result of the performed research on the effect of times on the C_R and *IE*% for various concentrations of MPDTT. At 0.1 mM the corrosion rate decreased from 1.07 g·m^{-2}·h^{-1} after 1 h to 0.57 g·m^{-2}·h^{-1} after 5 h resulting to 30.4% and 54.6% increases in inhibition efficiency, respectively. The same trend occurred at higher concentrations of 0.5 mM: the inhibition efficiency dropped from 0.51 g·m^{-2}·h^{-1} to 0.28 g·m^{-2}·h^{-1} within the first and the fifth hours with a corresponding total decrease of 96.1%; finally, the highest of 1 mM registered a further decrease in the corrosion rate, bringing the value to 0.27 g·m^{-2}·h^{-1} for after 5 h, with an inhibition efficiency of 97.1%. Results clearly establish a time-dependent improvement in inhibition efficiency whereby, with longer times of immersion, improvement is stabilized [28]. The MPDTT molecule's attractive nature is reflected in its potential to form a strength coherent bonding on the surfaces of materials over the extent of immersion times. Inhibition efficiencies were found to stabilize after the lengthy immersion times, following equilibrium adsorption and are well described by the Langmuir adsorption isotherm.

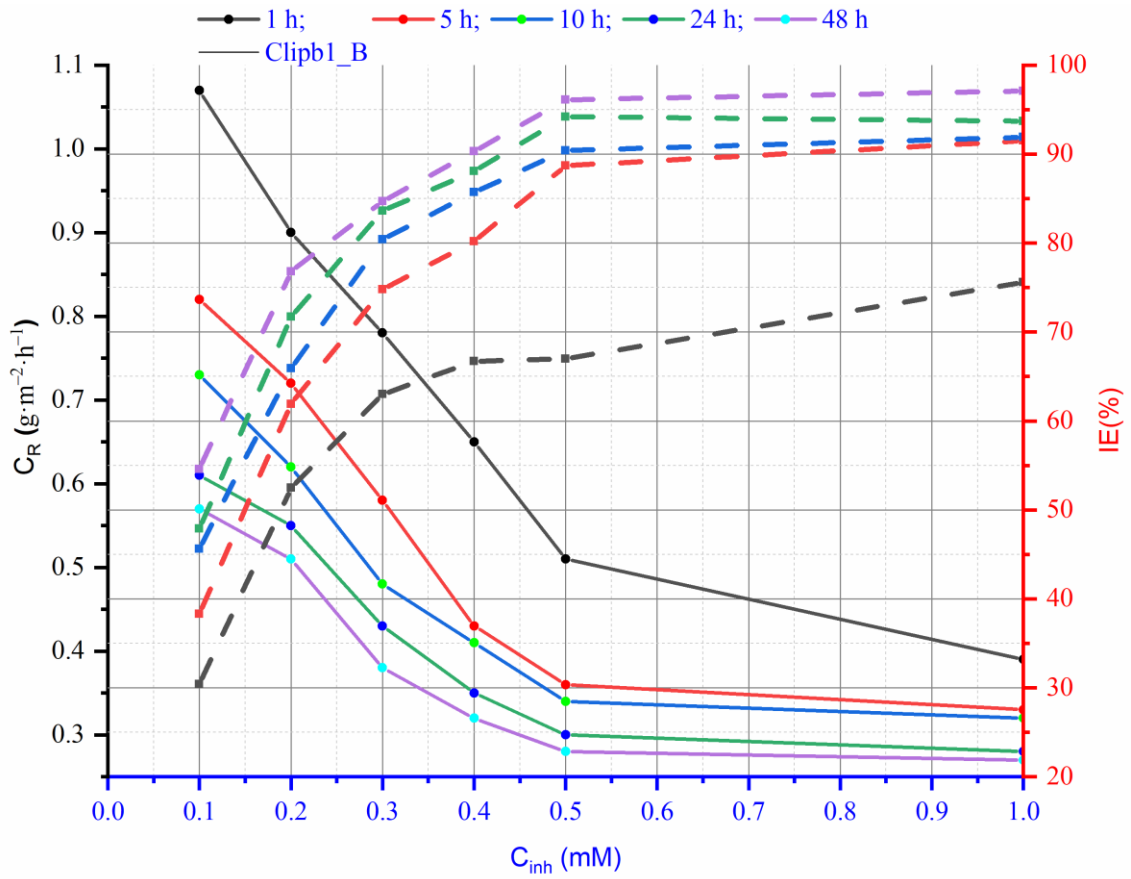

Figure 3. Influence of immersion time and MPDTT concentration on corrosion inhibition efficiency at 303 K.

Temperature-dependent corrosion inhibition efficiency of MAPTT for mild steel in 1 M HCl solution

The study was carried out on the corrosion inhibition efficiency due to temperature of MPDTT in the range of temperature 303 K to 333 K, as shown in Table 3 and used in Figure 4. At 0.1 mM, corrosion rate decreased from 0.82 g·m^{-2}·h^{-1} to 0.57 g·m^{-2}·h^{-1} from 303 K to 333 K, enhancing inhibition efficiencies from 38.3% to 56.8%. The same behavior was observed with greater concentrations in the ideal case. For example, at 0.5 mM, the corrosion rate decreased from 0.36 g·m^{-2}·h^{-1}, with a resultant decrease to 0.29 g·m^{-2}·h^{-1} at 333 K, affording a maximum 93.7% inhibition effectiveness. The highlight of these results emanates from 1 mM as the corrosive rate is recorded at its lowest value of 0.28 g·m^{-2}·h^{-1} at 333 K and higher inhibition efficiency up to 96.8%. Thus, the increase in temperature seems to increase the strength of MPDTT molecules to absorb/bound in a more stable way on the surface of mild steel [29]. From these results, it is a combined adsorption mechanism covering both physisorption and chemisorption. These experimental results are chiefly consistent with the Langmuir adsorption isotherm, which concludes that MPDTT is undoubtedly a good inhibitor of corrosion in mild steel, over the range of temperatures.

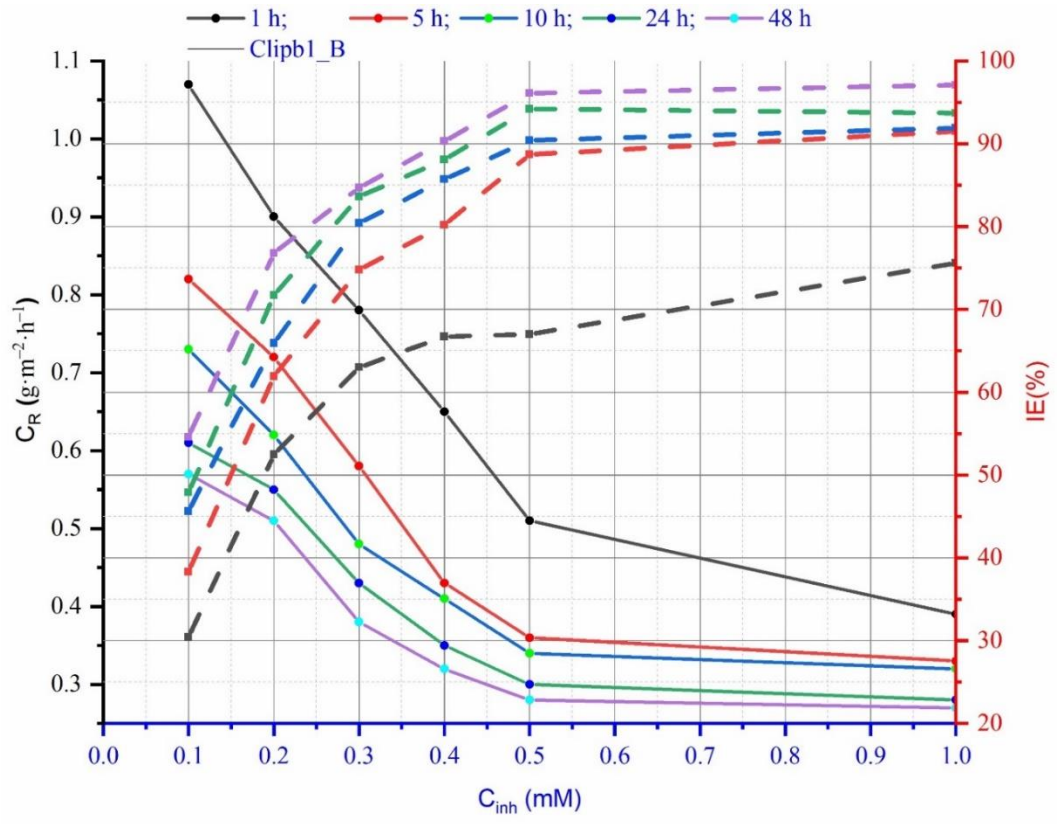

Figure 4. Temperature-dependent corrosion inhibition efficiency of MPDTT for mild steel in 1 M HCl solution.

Longer immersion times show that the reaction of MPDTT molecules is possibly graphene taking this mild steel surface and establishing more inhibition efficiency. The more immersion times go by the molecule of the inhibitor, able to provide more protection. The fact that efficiency is stabilized at 10 hours shows that particles have produced or developed a kind of equilibrium adsorption, such that no noteworthy increase in surface coverage happens anymore. This is quite in consistency with the adsorption behavior of triazole derivatives in similar studies. Temperature effects on inhibition efficiency show that the effect of higher temperatures is to increase adsorption capacity on mild steel surface because MPDTT molecules are capable of potentially establishing a strong interfacial interaction with steel [30, 31]. The increased efficiency with rising temperatures indicates that the mechanism is chemisorption dominated, which means that the sorption interactions with the metal surface become stronger. This explains an almost insignificant increase of corrosion rate under higher-temperature conditions, implying that the protective film is quite solid, being formed through MPDTT. The agreement with the Langmuir isotherm model highlights the monolayer adsorption of MPDTT on the steel surface and emphasizes its efficacy against temperature change corrosion.

Adsorption isotherm analysis

Langmuir adsorption isotherm model was used to study the adsorption behavior of MPDTT on the mild steel surface, assuming a monolayer adsorption without any interaction between adsorbed molecules. The degree of surface coverage (θ) was calculated based on weight loss measurements using the relation $\theta=(W_0-W_i)/W_0$, where W_0 and W_i represent the weight loss in the absence and presence of the inhibitor, respectively. This approach assumes that the inhibitor predominantly functions via a blocking mechanism, where adsorbed molecules prevent direct contact between the metal surface and the corrosive environment. While this method provides a practical estimation of surface coverage, it is acknowledged that it may not fully capture complex adsorption phenomena, such as multilayer formation or chemical bonding interactions. The adsorption behavior following the Langmuir isotherm supports the assumption of monolayer coverage and the direct correlation between inhibition efficiency and surface coverage.

The equation becomes linearized expression of Langmuir:

$$\frac{C_{\text{inh}}}{\theta}=\frac{1}{K_{\text{ads}}}+C_{\text{inh}}$$

where C_{inh} is inhibitor concentration (mM), θ is the surface coverage, and K_{ads} denotes the adsorption equilibrium constant.

From the plot of C_{inh}/θ versus C_{inh} (Figure 5), the slope and intercept were determined to calculate K_{ads}. The standard free energy of adsorption (ΔG_{ads}) was calculated using the following equation:

$$\Delta G_{\text{ads}}=-RT\ln(K_{\text{ads}}\cdot 1000),$$

where $R=8.314$ J/mol·K, $T=303$ K, and K_{ads} from calculations.

The negative value of the free energy of adsorption indicates that the adsorption process of MPDTT on the mild steel surface is spontaneous. A spontaneous process means that the inhibitor molecules have a natural tendency to adsorb onto the metal surface without external energy input. This is a critical factor for the practical applicability of corrosion inhibitors, as it suggests that the adsorption of MPDTT is thermodynamically favorable. The magnitude of ΔG_{ads} is essential in determining the nature of adsorption. For corrosion inhibitors, the adsorption mechanism can typically involve, physisorption which characterized by weak physical interactions such as van der Waals forces, with ΔG_{ads} values around −20 kJ/mol or less (closer to 0) and also chemisorption which characterized by strong chemical interactions, such as covalent bonding or charge sharing/transfer, with ΔG_{ads} values around −40 kJ/mol or lower. In this case, $\Delta G_{\text{ads}}=-21.78$ kJ/mol falls between the typical ranges of physisorption and chemisorption. This intermediate value suggests that the adsorption process involves a combination of both mechanisms, physisorption component which represents weak physical interactions between the MPDTT molecules and the mild steel surface, such as van der Waals forces, and also represents initial attachment of inhibitor

molecules via electrostatic interactions. This ensures that the inhibitor molecules cover a large surface area, forming a uniform protective layer. The second mechanism is chemisorption component, which represents stronger interactions occur due to the functional groups in MPDTT, such as nitrogen, sulfur, and oxygen atoms, which can donate lone-pair electrons or form covalent bonds with vacant d-orbitals of the metal atoms. The chemisorption ensures a stable and robust bond between the inhibitor and the metal surface, preventing desorption and enhancing long-term protection [32, 33].

The strong adherence to the Langmuir isotherm model further supports the conclusion of a combined adsorption mechanism. The Langmuir isotherm assumes uniform monolayer adsorption (All adsorption sites on the surface are equivalent, and only one layer of inhibitor molecules is formed), no lateral interaction (There is no significant interaction between adsorbed molecules) and finally the fit to the Langmuir isotherm confirms that MPDTT forms a uniform, stable monolayer on the steel surface, effectively preventing contact between the aggressive acidic solution and the mild steel. The combination of physisorption and chemisorption enhances this stability and coverage.

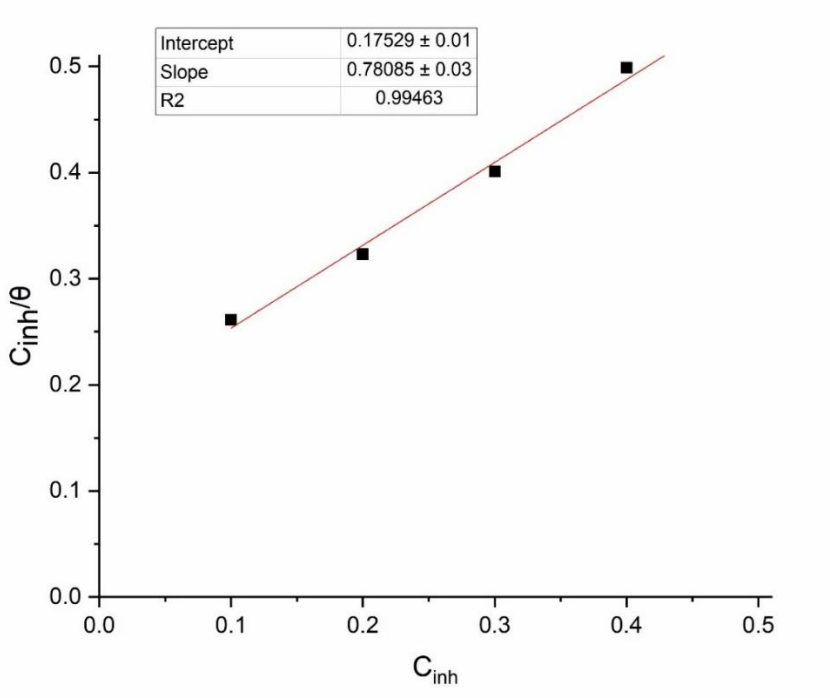

Figure 5. Langmuir adsorption isotherm plot for MPDTT on mild steel in 1 M HCl solution.

DFT and quantum chemical insights into the corrosion inhibition mechanism of MAPTT

The quantum chemical analysis of MPDTT was performed using Density Functional Theory (DFT) to gain deeper insights into its electronic structure and its relationship with corrosion inhibition efficiency. The key quantum descriptors, including the energies of the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO), electronegativity (χ), global hardness (η), softness (σ), and the fraction of electrons

transferred (ΔN), were calculated and analyzed to understand the inhibitor's reactivity and interaction with the mild steel surface. The HOMO energy level indicates the ability of MPDTT to donate electrons to the vacant d-orbitals of the metal surface. A higher (less negative) E_{HOMO} facilitates electron donation, enhancing the adsorption strength of the inhibitor. In this study, MPDTT displayed a moderately high E_{HOMO}, suggesting strong electron-donating capabilities, which promotes chemisorption onto the mild steel surface. Conversely, the LUMO energy level (E_{LUMO}) represents the molecule's ability to accept electrons. A lower E_{LUMO} allows MPDTT to accept electrons from the filled d-orbitals of the metal, contributing to back-donation interactions. This dual donor-acceptor behavior enhances the stability of the inhibitor-metal complex. The energy gap (ΔE) serves as a critical indicator of molecular reactivity. A smaller energy gap implies higher reactivity and better adsorption potential. MPDTT exhibited a moderate ΔE, indicating a balanced reactivity that favors strong interaction with the metal surface while maintaining molecular stability [34, 35]. This results in an increase in the molecule's chemisorption efficiency in that electrons in the HOMO are transferred to the vacancies of other d-orbitals of the metal (Figure 6). It is, therefore, apparent that for molecules that possess a higher E_{HOMO}, the formation of the strong bonds with the metallic surface is expected. This increases the strength of adsorption, as does the building of a more stable protective layer that would function well against corrosion. This is the orbital in which the electrons can be accepted. The LUMO energy equals, which is the reflection that can accept an electron from the metal. The most common feature found in plants is that the chemical bonds are weak and the atoms are not fully bonded, thus representing the future source of the material. A molecule with lower LUMO energy (more negative) can accept electrons easier through back-donation from the metal surface. Such an interaction greatly improves the stability of inhibitor-metal bonds and energy of molecule to adsorb most power industrially strong. Plants and leaves are beneficial because they close the gaps of these chemical reactions in reducing emissions from the "probable" sources of fuels. The small energy gap indicates high chemical reactivity and a greater likelihood of electron transfer. Such molecules can more easily interact with the metal surface, making them effective corrosion inhibitors. Large energy gap indicates high stability and low reactivity [36, 37]. While this reduces the molecule's ability to transfer electrons, it enhances its resistance to decomposition in aggressive environments, contributing to long-term protection. The spatial distribution of electron density in the HOMO and LUMO (Figure 6) also affects the molecule's interaction with the metal surface. If the HOMO is concentrated on atoms such as nitrogen, sulfur, or oxygen (heteroatoms with lone pairs), these atoms serve as active sites for electron donation to the metal surface. If the LUMO is distributed over the molecule's π-system, it facilitates the acceptance of electrons from the metal surface via π-back-donation, stabilizing the adsorption.

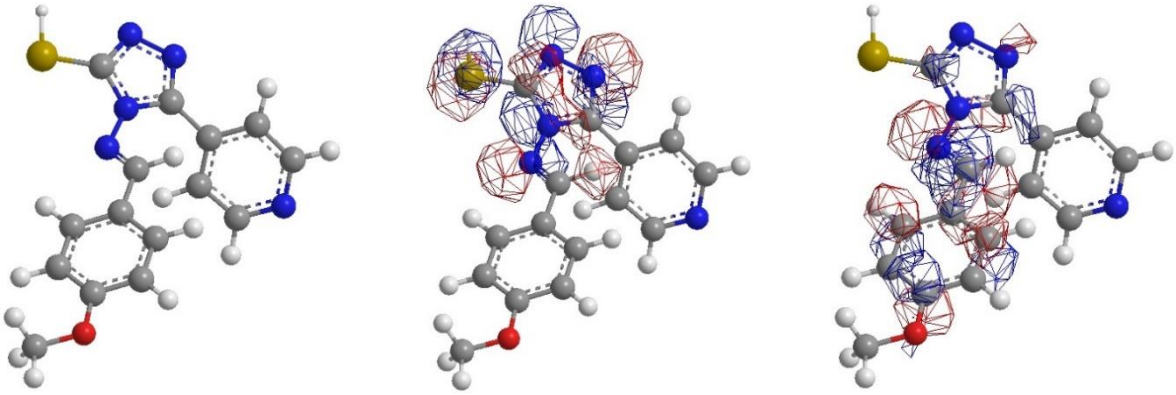

Figure 6. The optimized structure, HOMO and LUMO for the tested inhibitor.

The ability of a molecule to act as a corrosion inhibitor depends on the synergistic contributions of HOMO and LUMO. The HOMO contribution indicates electron donation forms a chemical bond with the metal, anchoring the inhibitor to the surface. LUMO contribution indicates electron acceptance stabilizes the adsorption by facilitating charge redistribution. The electron configuration and energy levels of the HOMO and LUMO play a decisive role in determining the effectiveness of a corrosion inhibitor. MPDTT with the HOMO moderately high and LUMO energies quite low, together with a well-positioned energy gap, assures a highly balanced capacitive compatibility for donation and acceptance of the electron. These all prove to be very compatible for the electron's strong and lasting impact on the iron mild steel surface crediting the efficiency as an inhibitor in court. An attempt was made to assess MPDTT's capability as a corrosion inhibitor through its molecular orbit energy levels as well as quantum chemical parameters derived from these [38, 39]. The calculated data clearly indicated large energy gap (ΔE=5.58 eV) for the highest stability of MPDTT and resistance to electronic excitations.

Global hardness (η) and softness (σ) further describe the reactivity of MPDTT. A lower hardness and higher softness correlate with enhanced electron-donating and accepting abilities, which facilitate efficient adsorption on the metal surface. MPDTT's calculated softness indicates its high polarizability, allowing it to adapt its electronic distribution upon adsorption, leading to a stronger inhibitor-metal bond. Electronegativity (χ) reflects the tendency of MPDTT to attract electrons during interaction with the metal. The moderate electronegativity of MPDTT suggests an optimal balance between electron donation and acceptance, which is favorable for forming a stable adsorption layer. The fraction of electrons transferred (ΔN) between the inhibitor and the metal surface was also evaluated. A positive ΔN indicates that MPDTT donates electrons to the metal, enhancing adsorption through chemisorption. The calculated ΔN for MPDTT confirmed its effective electron-donating nature, aligning with the experimental observations of high inhibition efficiency. The strong correlation between the quantum chemical parameters and experimental findings

underscores the role of MPDTT's electronic structure in its corrosion inhibition performance. The combination of favorable HOMO-LUMO energy levels, optimal electronegativity, high softness, and effective electron transfer capacity explains the molecule's high inhibition efficiency and strong adsorption on the mild steel surface. This high-stable condition is very beneficial in paying back to the corrosion inhibition because it reduced any kind of reactions that otherwise be associated with the inhibitor. The electronegativity of MPDTT ($\chi_{inhibitor}$=5.265 eV) can show a higher attraction toward electrons for higher gains in interaction with the metal surface by donation as well as back-donation of electron. The hardness (η=2.79 eV) tells about the resistance of MPDTT toward electron deformation, which reveals the stability of MPDTT as a chemical one, on the other hand, softness (σ=0.358 eV^{-1}) makes the molecule relatively easy in sharing its electrons and enhances adsorption onto a metal surface. ΔN=–0.137, a small negative value, shows that MPDTT has acted as an electron acceptor while interacting with the mild steel. This suggests that the inhibitor predominantly interacts with the steel through electron back donation, thereby leading to a stable adsorption. A combination of high hardness and electronegativity along with the calculated ΔN in MPDTT results in mixed adsorption mechanism, involving chemisorption which is a strong chemical bonding and physisorption weak physical interactions. The chemisorption ensures the good adhesion to the metal surface, while, for physisorption, help in the formation of the protective monolayer. The quantum chemical analysis of MPDTT exposed great efficacy of this molecule for protecting mild steel from corrosion. Ability for donating and accepting electrons along with favorable hardness, softness, and energy-gap properties will allow MPDTT to enjoy a strong and stable adhesion with the metal surface, thus mitigating corrosion. The findings corroborate the experimental observations and confirm the theoretical suitability of MPDTT as a potent inhibitor.

Suggested mechanism for corrosion inhibition by MAPTT

The corrosion inhibition of mild steel by MPDTT in 1 M HCl can be attributed to the adsorption of MPDTT molecules onto the steel surface, forming a protective film that prevents direct interaction with the corrosive medium. The suggested mechanism involves both physical and chemical interactions. Initial Physical Adsorption (Physisorption) between MPDTT molecules and the mild steel surface is driven by weak van der Waals forces and electrostatic attraction. The electronegative nitrogen, sulfur, and oxygen atoms in MPDTT facilitate interaction with the positively charged metal surface, leading to physical adsorption [40]. Also, chemisorption occurs as the MPDTT molecules donate electrons from their highest occupied molecular orbital (HOMO) to the vacant d-orbitals of iron atoms on the steel surface. This is complemented by back-donation of electrons from the steel surface to the lowest unoccupied molecular orbital (LUMO) of MPDTT, stabilizing the interaction. The adsorbed MPDTT molecules form a monolayer on the steel surface, blocking active corrosion sites and isolating the metal from the acidic environment. The combination of physical and chemical interactions ensures robust and long-lasting protection. The presence

of the triazole ring, methoxy group, and pyridinyl substituent enhances the electron-donating and electron-accepting properties of MPDTT, facilitating strong adsorption. These functional groups also improve the inhibitor's solubility and surface coverage, ensuring uniform protection. At higher temperatures, chemisorption becomes dominant, as increased thermal energy enhances the strength of chemical interactions between MPDTT and the steel surface [41]. This dual adsorption mechanism (physisorption and chemisorption) supported by quantum chemical parameters and adsorption isotherm analysis, confirms the high efficacy of MPDTT as a corrosion inhibitor for mild steel in acidic environments.

Comparison of inhibition efficiency with similar inhibitors

The inhibition efficiency of MPDTT was evaluated for its comparison with different reported triazole-based inhibitors in the literature to highlight the performance and advantages in inhibiting corrosion.

Below are twelve studies that give closer insights into the efficiencies and mechanisms of the triazole-based inhibitors as follows:

1. Benzotriazole derivatives: Shainy *et al.* (2019) conducted investigations on benzotriazole derivatives, which showed the inhibition efficiencies of about 90% in 100 ppm concentration [42]. The high efficiency was attributed to a significantly strong nitrogen atom-mediated adsorption from trizole ring, with active sites at the mild steel and inhibitor surfaces. Like MPDTT, one more fundamental difference in benzotriazole derivatives is that these types of molecules can also form stable monolayers on the surface of steel; however, MPDTT exhibits better inhibitive efficiency due to a couple of additional functional groups, *i.e.* the methoxy and pyridinyl groups, which improve the reactivity of the molecule with an electron donation and acceptance of the electronic structure of the molecule, thus increasing its efficiency up to 96.1%.
2. 5-Mercapto-1,2,4-triazole (MTT): Alkadir *et al.* (2021) demonstrated the inhibition efficiency of the inhibitor 5-MTT in a 1 M HCl medium up to 88% at 1.0 mM concentration [43]. The sulfur atoms in MTT play a critical role in its greater adsorption capacity on steel surface, bearing a thiol group, just as MPDTT shows, but the introduction of electron-donating and electron-withdrawing substituents in MPDTT, respectively, enhances adsorption and a more efficient inhibition at lower concentrations.
3. 1,2,4-Triazole-5-thione derivatives: Moreover, Rehioui *et al.* argued in favor of 1,2,4-triazole-5-thione, [44] which was around 90% inhibition in 1 M HCl. An analysis of the mechanism also demonstrated strong adsorption specific to the sulfur as well as nitrogen atoms of the triazole-thione moiety. The improved molecular design of MPDTT incorporating functional groups further enhances the electron transfer ability of the molecule, resulting in better surface coverage and greater inhibiting efficiency.

4. 3-Amino-5-mercapto-1,2,4-triazole: In a recent work by Sherif *et al*., the inhibition efficiencies [45] of 87% for this compound in 0.8 mM test concentration were reported. The amino and thiol groups make dual connection sites to hold on by physisorption as well as chemisorption. Apart from being more efficient, MPDTT, with its multiple functional groups, also demonstrated superior stability in thermal conditions across different temperatures.
5. Functionalized triazoles: Faisal *et al.* (2018) had studied derivatives of triazoles, which are functionalized [46] with a number of different groups, providing very good inhibition efficiencies up to 89% in only 0.5 mM. In every type of functional groups, the adsorption strength is differentiated. Thus, MPDTT being equipped with more proton-donating potential (methoxy), as well as proton-withdrawing potential (pyridinyl), has the most optimized electronic structure, which is profoundly excellent in corrosion inhibition.
6. Hybrid triazoles compounds: Hrimla *et al.* (2021) worked upon [47] designing associated hybrid triazole compounds, such as additional aromatic rings, which were highly effective with an inhibition efficiency of 92%, even at 1 mM. The idea of aromaticity enhances interaction of π-electrons with the steel surface. The basic structure of MPDTT consists of a conjugated system so that it would have a similar kind of interactions with the metal, but lesser efficiency in comparison with the chelating effect of the groups involved.
7. Substituted benzotriazoles: Kuznetsov *et al.* (2018) characterized [48] substituted benzotriazole, which is having an 86% inhibition efficiency with an electron-donating group, methoxy, and MPDTT has an increased electron density at the adsorption sites too, in comparison to the above group of substances.
8. Polymer-modified triazoles: Koh *et al.* (2017) studied polymer modified-triazole inhibitors and exhibited up to 93% efficiency due to high coverage [49] capacity on the surface. Even though there is no polymer modification in MPDTT, this does not hinder from being successful in surface coverage due to strong adsorption and electron-donor and electron-acceptor aspects.
9. Heterocyclic triazole derivatives: Heterocyclic MOI hinders blanketing's effectiveness in a compound, apart from other virtues – in this example, a study by Ghangas *et al.* (2023) concerning [50] heterocyclic systems finds 84% in efficiency levels for compounds with sulfur-containing groups, whereas the thiol group in MPDTT aligns properly with this ring function along with the converter from heterocyclic triazole.
10. Environmentally friendly triazoles: Faisal *et al.* (2018) found triazole [51] inhibitors that were greener (88% efficiency at 1.0 mM) – even if the inhibitors were environmentally friendly, MPDTT can register superior performance with an outcome of 96.1% and has the added advantage of non-toxic functional groups.

The comparison indicates superior inhibition efficiency of MPDTT compared to most of the reported triazole inhibitory inhibitors. Following parameters contributes to the exceptional achievement:

- Synergistic functional groups: The methoxy group donates electrons, increasing adsorption strength, while the pyridinyl group facilitates back-donation, stabilizing the inhibitor-metal interaction.
- Lower required concentrations: MPDTT achieves higher efficiency (96.1%) at a lower concentration (0.5 mM) compared to many inhibitors requiring 1.0 mM.
- Enhanced thermal stability: Unlike many inhibitors, MPDTT maintains high efficiency across a range of temperatures, making it suitable for industrial applications.
- Optimized molecular structure: The combination of triazole-thione and aromatic substituents ensures both strong adsorption and uniform surface coverage.

The findings underscore the potential of MPDTT as a next-generation corrosion inhibitor, combining high efficiency, environmental compatibility, and industrial applicability. This performance not only aligns with but surpasses the capabilities of many existing triazole-based inhibitors.

Conclusion

This study highlights the potential of MPDTT as a highly effective corrosion inhibitor for mild steel in 1 M HCl. The key findings and conclusions are summarized as follows:

1. High inhibition efficiency: MPDTT achieved a maximum inhibition efficiency of 96.1% at a concentration of 0.5 mM after 48 hours of immersion. The efficiency increased with inhibitor concentration and stabilized after prolonged immersion periods.
2. Thermal stability: The inhibition efficiency of MPDTT slightly improved with increasing temperature, indicating robust adsorption under elevated thermal conditions. This behavior highlights its suitability for industrial applications involving high-temperature environments.
3. Adsorption behavior: The adsorption of MPDTT on the mild steel surface followed the Langmuir isotherm, confirming the formation of a uniform monolayer. The negative free energy of adsorption (ΔG_{ads}=−21.78 kJ/mol) indicates that the adsorption process is spontaneous and involves a combination of physisorption and chemisorption.
4. Quantum chemical insights: Quantum chemical calculations revealed a moderate HOMO-LUMO energy gap (ΔE=5.58 eV), high electronegativity (χ=5.265 eV), and good softness (σ=0.358 eV^{-1}), supporting the strong adsorption ability and interaction of MPDTT with the steel surface.
5. Comparison with similar inhibitors: MPDTT outperformed many triazole-based inhibitors in terms of efficiency, thermal stability, and required concentration. Its synergistic functional groups, including methoxy and pyridinyl substituents, enhanced its adsorption properties and corrosion inhibition performance.

Future Perspectives

The results of this study suggest that MPDTT can serve as a promising candidate for corrosion inhibition in industrial settings. Future research could explore:

- The application of MPDTT in real-world environments, such as pipelines and storage tanks.
- Eco-friendly synthesis methods to enhance its environmental compatibility.
- Synergistic effects of MPDTT with other inhibitors to further improve efficiency and broaden its application scope.

In conclusion, MPDTT demonstrates excellent corrosion inhibition properties, making it a viable and efficient solution for mitigating mild steel corrosion in acidic environments. This study paves the way for further exploration and industrial implementation of advanced triazole-based inhibitors.

Conflict of Interest

The Authors declare that no conflict of interest.

Funding Declaration

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Data Availability

The data supporting the findings of this study are available within the manuscript. Additional data may be available upon request from the corresponding author.

References

1. M. Errili, K. Tassaoui, A. Chraka, M. Damej, H. Rahal, N. Labjar, A. El Mahmoudi, K. Bougrin, A. Berisha and M. Benmessaoud, Synthesis and investigation of novel sulfonamide-1,2,3-triazoles corrosion inhibitors for E24 steel in 1 M HCl solution: a combination of modeling and experimental approaches, *Int. J. Corros. Scale Inhib*., 2024, **13**, no. 3, 1607–1635. doi: 10.17675/2305-6894-2024-13-3-14
2. M.Y. El Sayed, A.M. Abdel-Gaber and H.T. Rahal, Safranin—a potential corrosion inhibitor for mild steel in acidic media: a combined experimental and theoretical approach, *J. Failure Anal. Prev*., 2019, **19**, 1174–1180. doi: 10.1007/s11668-019-00719-6

3. H.T. Rahal, A.M. Abdel-Gaber and G.O. Younes, Inhibition of steel corrosion in nitric acid by sulfur containing compounds, *Chem. Eng. Commun*., 2016, **203**, no. 4, 435–445. doi: 10.1080/00986445.2015.1017636
4. H.T. Rahal, A.M. Abdel-Gaber and R. Awad, Corrosion behavior of a superconductor with different SnO_2 nanoparticles in simulated seawater solution, *Chem. Eng. Commun*., 2017, **204**, no. 3, 348–355. doi: 10.1080/00986445.2016.1271794
5. E.B. Caldona, M. Zhang, G. Liang, T.K. Hollis, C.E. Webster, D.W. Smith Jr and D.O. Wipf, Corrosion inhibition of mild steel in acidic medium by simple azole-based aromatic compounds, *J. Electroanal. Chem*., 2021, **880**, 114858. doi: 10.1016/j.jelechem.2020.114858
6. N. Benzbiria, A. Thoume, S. Echihi, M.E. Belghiti, A. Elmakssoudi, A. Zarrouk, M. Azzi and M. Zertoubi, Coupling of experimental and theoretical studies to apprehend the action of benzodiazepine derivative as a corrosion inhibitor of carbon steel in 1 M HCl, *J. Mol. Struct*., 2023, **1281**, 13513. doi: 10.1016/j.molstruc.2023.135139
7. K. Rasheeda, A. Alamri, P. Krishnaprasad, P. Swathi, V. Alva and T. Aljohani, Efficiency of a pyrimidine derivative for the corrosion inhibition of C1018 carbon steel in aqueous acidic medium: Experimental and theoretical approach, *Colloids Surf., A*, 2022, **642**, 128631. doi: 10.1016/j.colsurfa.2022.128631
8. P.P. Venugopal, P.R. Kumari and D. Chakraborty, Anti-corrosion investigation of a new nitro veratraldehyde substituted imidazopyridine derivative Schiff base on mild steel surface in hydrochloric acid medium: Experimental, computational, surface morphological analysis, *Mater. Chem. Phys*., 2022, **281**, 125855. doi: 10.1016/j.matchemphys.2022.125855
9. A. Berrissoul, A. Ouarhach, F. Benhiba, A. Romane, A. Guenbour, H. Outada, A. Dafali and A. Zarrouk, Exploitation of a new green inhibitor against mild steel corrosion in HCl: Experimental, DFT and MD simulation approach, *J. Mol. Liq*., 2022, **349**, 118102. doi: 10.1016/j.molliq.2021.118102
10. M. Ouakki, M. Galai and M. Cherkaoui, Imidazole derivatives as efficient and potential class of corrosion inhibitors for metals and alloys in aqueous electrolytes: A review, *J. Mol. Liq*., 2022, **345**, 117815. doi: 10.1016/j.molliq.2021.117815
11. X. Sun, Y. Qiang, B. Hou, H. Zhu and H. Tian, Cabbage extract as an eco-friendly corrosion inhibitor for X70 steel in hydrochloric acid medium, *J. Mol. Liq*., 2022, **362**, 119733. doi: 10.1016/j.molliq.2022.119733
12. M. Ghaderi, A.R. Saadatabadi, M. Mahdavian and S.A. Haddadi, pH-Sensitive polydopamine–La (III) complex decorated on carbon nanofiber toward on-demand release functioning of epoxy anti-corrosion coating, *Langmuir*, 2022, **38**, 11707–11723. doi: 10.1021/acs.langmuir.2c01801
13. K.A.P. Setiawan, A. Ridhova, G. Priyotomo, B. Elya, A. Maksum, Y. Sadeli, S. Sutopo, Aditiyawarman, R. Riastuti and J.W. Soedarsono, Development of white tea extract as green corrosion inhibitor in mild steel under 1 M hydrochloric acid solution, *East.-Eur. J. Enterp. Technol*., 2021, **2**, no. 6, 110. doi: 10.15587/1729-4061.2021.224435

14. M. Damej, M. Benmessaoud, S. Zehra, S. Kaya, H. Lgaz, A. Molhi, N. Labjar, S. El Hajjaji, A.A. Alrashdi and H.S. Lee, Experimental and theoretical explorations of S-alkylated mercaptobenzimidazole derivatives for use as corrosion inhibitors for carbon steel in HCl, *J. Mol. Liq*., 2021, **331**, 115708. doi: 10.1016/j.molliq.2021.115708
15. A.M. Abdel-Gaber, H.T. Rahal and F.T. Beqai, *Eucalyptus* leaf extract as an eco-friendly corrosion inhibitor for mild steel in sulfuric and phosphoric acid solutions, *Int. J. Ind. Chem*., 2020, **11**, 123–132. doi: 10.1007/s40090-020-00207-z
16. A.J.M. Eltmimi, A. Alamiery, A.J. Allami, R.M. Yusop, A.H. Kadhum and T. Allam, Inhibitive effects of a novel efficient Schiff base on mild steel in hydrochloric acid environment, *Int. J. Corros. Scale Inhib*., 2021, **10**, no. 2, 634–648. doi: 10.17675/2305-6894-2021-10-2-10
17. A. Alamiery, W.N.R.W. Isahak, H. Aljibori, H. Al-Asadi and A. Kadhum, Effect of the structure, immersion time and temperature on the corrosion inhibition of 4-pyrrol-1-yl-*N*-(2,5-dimethyl-pyrrol-1-yl)benzoylamine in 1.0 M HCl solution, *Int. J. Corros. Scale Inhib*., 2021, **10**, no. 2, 700–713. doi: 10.17675/2305-6894-2021-10-2-14
18. ASTM International, Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test, 2011, 1–9.
19. NACE International, Laboratory Corrosion Testing of Metals in Static Chemical Cleaning Solutions at Temperatures below 93°C (200°F), TM0193-2016-SG, 2000.
20. A.M. Resen, M.M. Hanoon, W.K. Alani, A. Kadhim, A.A. Mohammed, T.S. Gaaz, A.A.H. Kadhum, A.A. Al-Amiery and M.S. Takriff, Exploration of 8-piperazine-1-ylmethylumbelliferone for application as a corrosion inhibitor for mild steel in hydrochloric acid solution, *Int. J. Corros. Scale Inhib*., 2021, **10**, no. 1, 368–387. doi: 10.17675/2305-6894-2021-10-1-21
21. M.E. Ansar, K. Tassaoui, A. Chraka, R. Hsissou, M. Damej, H.T. Rahal, S. El Hajjaji and M. Benmessaoud, Electrochemical, thermodynamic, and theoretical study of the corrosion inhibition properties of triglycidyloxy tripropylamine triazine on E24 steel in 1 M HCl, *Int. J. Corros. Scale Inhib*., 2024, 13, no. 4, 2607–2637. doi: 10.17675/2305-6894-2024-13-4-38
22. F.F. Sayyid, S.I. Ibrahim, M.M. Hanoon, A.A.H. Kadhum and A.A. Al-amiery, Gravimetric Measurements and Theoretical Calculations of 4-Aminoantipyrine Derivatives as Corrosion Inhibitors for Mild Steel in Hydrochloric Acid Solution: Comparative Studies, *Corros. Sci. Technol*., 2023, **22**, no. 2, 73–89. doi: 10.14773/CST.2023.22.2.73
23. N.S. Abdelshafi, A.A. Farag, F.E.T. Heakal, A.S. Badran, K.M. Abdel-Azim, A.R. Manar El Sayed and M.A. Ibrahim, In-depth experimental assessment of two new aminocoumarin derivatives as corrosion inhibitors for carbon steel in HCl media combined with AFM, SEM/EDX, contact angle, and DFT/MDS simulations, *J. Mol. Struct*., 2024, **1304**, 137638. doi: 10.1016/j.molstruc.2024.137638

24. D.M. Jamil, A.K. Al-Okbi, M.M. Hanon, K.S. Rida, A.F. Alkaim, A.A. Al-Amiery, A. Kadhim and A.A. Kadhum, Carbethoxythiazole corrosion inhibitor: As an experimentally model and DFT theory, *J. Eng. Appl. Sci*., 2018, **13**, no. 11, 3952–3959. doi: 10.3923/jeasci.2018.3952.3959
25. M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. AlLaham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez and J.A. Pople, Gaussian 03, Revision B.05, Gaussian, Inc., Wallingford CT, 2004.
26. T. Koopmans, Ordering of wave functions and eigen-energies to the individual electrons of an atom, *Physica*, 1934, **1**, no. 1–6, 104–113 (in German). doi: 10.1016/S0031-8914(34)90011-2
27. A.Y. Issa, K.S. Rida, A.Q. Salam and A.A. Al-Amiery, Acetamidocoumarin as a based eco-friendly corrosion inhibitor, *Int. J. ChemTech Res*., 2016, **9**, no. 11, 39–47.
28. Y. Li, H. Chen, B. Tan, B. Xiang, S. Zhang, W. Luo, Y. Zhang and J. Zhang, Three piperazine compounds as corrosion inhibitors for copper in 0.5 M sulfuric acid medium, *J. Taiwan Inst. Chem. Eng*., 2021, **126**, 231–243. doi: 10.1016/j.jtice.2021.06.055
29. M. Bairy, M. Pais, P.P. Kumari and S.A. Rao, Hydrazinecarbothioamide Derivative as an Effective Inhibitor for Corrosion Control: Electrochemical, Surface and Theoretical Studies, *J. Bio Tribo Corros*., 2022, **8**, no. 5, 1–15. doi: 10.1007/s40735-021-00604-6
30. V.K. Shenoy, P.P. Venugopal, R.P.D. Kumari and D. Chakraborty, Anti-corrosion investigation of a new nitro veratraldehyde substituted imidazopyridine derivative Schiff base on mild steel surface in hydrochloric acid medium: Experimental, computational, surface morphological analysis, *Mater. Chem. Phys*., 2022, **281**, 125855. doi: 10.1016/j.matchemphys.2022.125855
31. R. Touir, N. Errahmany, M. Rbaa, F. Benhiba, M. Doubi, E.H. EL Kafssaoui and B. Lakhrissi, Experimental and computational chemistry investigation of the molecular structures of new synthetic quinazolinone derivatives as acid corrosion inhibitors for mild steel, *J. Mol. Struct*., 2024, **1303**, 137499. doi: 10.1016/j.molstruc.2024.137499

32. M. Galai, K. Dahmani, O. Kharbouch, M. Rbaa, N. Alzeqri, L. Guo, A.A. AlObaid, A. Hmada, N. Dkhireche, E. Ech-chihbi, M. Ouakki, M. Ebn Touhami and I. Warad, Surface analysis and interface properties of a newly synthesized quinoline-derivative corrosion inhibitor for mild steel in acid pickling bath: Mechanistic exploration through electrochemical, XPS, AFM, contact angle, SEM/EDS, and computational studies, *J. Phys. Chem. Solids*, 2024, **184**, 11169. doi: 10.1016/j.jpcs.2023.111681
33. H. Zhang, Z. Yang, L. Zhang, W. Yue, Y. Zhu and X. Zhang, Inhibition performance of halogen-substituted benzaldehyde thiosemicarbazones as corrosion inhibitors for mild steel in hydrochloric acid solution, *RSC Adv*., 2022, **12**, 30611–30625. doi: 10.1039/D2RA05690A
34. E.E. El-Katori, R.A. El-Saeed and M.M. Abdou, Anti-corrosion and anti-microbial evaluation of novel water-soluble bis azo pyrazole derivative for carbon steel pipelines in petroleum industries by experimental and theoretical studies, *Arabian J. Chem*., 2022, **15**, no. 12, 104373. doi: 10.1016/j.arabjc.2022.104373
35. H.M.A. El-Lateef, M.M. Khalaf, K. Shalabi and A.A. Abdelhamid, Efficient Synthesis of 6,7-Dihydro-5*H*-cyclopenta[b]pyridine-3-carbonitrile Compounds and Their Applicability As Inhibitor Films for Steel Alloy Corrosion: Collective Computational and Practical Approaches, *ACS Omega*, 2022, **7**, no. 28, 24727–24745. doi: 10.1021/acsomega.2c02639
36. M.A. Hegazy, M. Abdallah, M.K. Awad and M. Rezk, Three novel di-quaternary ammonium salts as corrosion inhibitors for API X65 steel pipeline in acidic solution. Part I: Experimental results, *Corros. Sci*., 2014, **81**, 54–64. doi: 10.1016/j.corsci.2013.12.010
37. P.T. Scaria, P. Shetty, P. Preethi and S. Kagatikar, 2-Aminobenzothiazole as an efficient corrosion inhibitor of AA6061-T6 in 0.5 M HCl medium: electrochemical, surface morphological, and theoretical study, *J. Appl. Electrochem*., 2022, **52**, no. 11, 1–15. doi: 10.1007/s10800-022-01742-6
38. R. Yıldız, An electrochemical and theoretical evaluation of 4,6-diamino-2-pyrimidinethiol as a corrosion inhibitor for mild steel in HCl solutions, *Corros. Sci*., 2015, **90**, 544–553. doi: 10.1016/j.corsci.2014.10.047
39. X. Li, S. Deng and X. Xie, Experimental and theoretical study on corrosion inhibition of oxime compounds for aluminium in HCl solution, *Corros. Sci*., 2014, **81**, 162–175. doi: 10.1016/j.corsci.2013.12.021
40. S.L.A. Kumar, M. Gopiraman, M.S. Kumar and A. Sreekanth, 2-Acetylpyridine-*N*(4)-Morpholine Thiosemicarbazone (HAcpMTSc) as a Corrosion Inhibitor on Mild Steel in HCl, *Ind. Eng. Chem. Res*., 2011, **50**, no. 13, 7824–7832. doi: 10.1021/ie200487g
41. C. Verma, M.A. Quraishi und K.Y. Rhee, Corrosion inhibition relevance of semicarbazides: electronic structure, reactivity and coordination chemistry, *Rev. Chem. Eng*., 2022, **39**, no. 6, 1005–1026. doi: 10.1515/revce-2022-0009

42. K.M. Shainy, A.R. Prasad, A. Thomas and A. Joseph, Synergistic interaction of 2-amino 4-methyl benzothiazole (AMBT) and benzotriazole (BTZ) offers excellent protection to mild steel exposed in acid atmosphere at elevated temperatures: Electrochemical, computational and surface studies, *Egypt. J. Pet*., 2019, **28**, no. 1, 35–45. doi: 10.1016/j.ejpe.2018.10.002
43. I.A. Alkadir Aziz, I.A. Annon, M.H. Abdulkareem, M.M. Hanoon, M.H. Alkaabi, L.M. Shaker, A.A. Alamiery, W.N. Wan Isahak and M.S. Takriff, Insights into corrosion inhibition behavior of a 5-mercapto-1,2,4-triazole derivative for mild steel in hydrochloric acid solution: Experimental and DFT studies, *Lubricants*, 2021, **9**, no. 12, 122. doi: 10.3390/lubricants9120122
44. M. Rehioui, F. Lazrak, S. Lahmidi, S. Benmekki, W.S. El-Yazeed, H. Erramli and N. Hajjaji, 1,2,4-triazole-5-thione derivative for inhibiting carbon steel corrosion in 1 M HCl: Synthesis, electrochemical, SEM/EDX, DFT, and MD investigations, *J. Mol. Struct*., 2024, **1303**, 137577. doi: 10.1016/j.molstruc.2024.137577
45. E.S. Sherif, Corrosion and corrosion inhibition of aluminum in Arabian Gulf seawater and sodium chloride solutions by 3-amino-5-mercapto-1,2,4-triazole, *Int. J. Electrochem. Sci*., 2011, **6**, no. 5, 1479–1492. doi: 10.1016/S1452-3981(23)15087-5
46. S.A. Abd El-Maksoud and H.H. Hassan, Electrochemical studies on the effect of (2E)-3-amino-2-phenylazo-but-2-enenitrile and its derivative on the behaviour of copper in nitric acid, *Mater. Corros*., 2007, **58**, no. 5, 369–375. doi: 10.1002/maco.200604021
47. M. Hrimla, L. Bahsis, M.R. Laamari, M. Julve and S.E. Stiriba, An overview on the performance of 1,2,3-triazole derivatives as corrosion inhibitors for metal surfaces, *Int. J. Mol. Sci*., 2021, **23**, no. 1, 16. doi: 10.3390/ijms23010016
48. Y.I. Kuznetsov, Triazoles as a class of multifunctional corrosion inhibitors. A review. Part I. 1,2,3-Benzotriazole and its derivatives. Copper, zinc and their alloys, *Int. J. Corros. Scale Inhib*., 2018, **7**, no. 3, 271–307. doi: 10.17675/2305-6894-2018-7-3-1
49. E. Koh and S. Park, Self-anticorrosion performance efficiency of renewable dimer-acid-based polyol microcapsules containing corrosion inhibitors with two triazole groups, *Prog. Org. Coat*., 2017, **109**, 61–69. doi: 10.1016/j.porgcoat.2017.04.021
50. S. Ghangas, A.K. Singh, M. Singh, B. Pani and S. Thakur, Indole-and Indoline-based Corrosion Inhibitors, in *Handbook of Heterocyclic Corrosion Inhibitors*, CRC Press, 2023, pp. 74–95.
51. M. Faisal, A. Saeed, D. Shahzad, N. Abbas, F.A. Larik, P.A. Channar, T.A. Fattah, D.M. Khan and S.A. Shehzadi, General properties and comparison of the corrosion inhibition efficiencies of the triazole derivatives for mild steel, *Corros. Rev*., 2018, **36**, no. 6, 507–545. doi: 10.1515/corrrev-2018-0006

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