

Corrosion inhibition of low carbon steel in HCl medium using a thiadiazole derivative: weight loss, DFT studies and antibacterial studies

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Abstract

A thiadiazole derivative, namely 2-amino-5-(naphthalen-2-ylmethyl)-1,3,4-thiadiazole (ANYT), has been synthesized and its corrosion inhibition effect on low carbon steel in 1 M hydrochloric acid was examined by gravimetric technique. The protective efficiency of the examined inhibitor toward low carbon steel in 1 M HCl has been analyzed as a function of the inhibitor concentration, immersion time, and solution temperature. The experimental findings revealed that the inhibition efficiency (*IE*) reached 55% in 1 h and achieved above 95% in 1 h at 500 ppm of the tested inhibitor. The *IE* increased with concentration and immersion time, and decreased with an increase in temperature. The mass loss data showed that corrosion inhibition occurred due to efficient formation of an adsorbed film on the surface of low carbon steel. The adsorption of the tested inhibitor molecules obeyed the Langmuir adsorption model. The free energy value of adsorption of the tested inhibitor molecules indicated that both physisorption and chemisorption on low carbon steel surface occurred. Quantum chemical calculations were performed to compare the electronic structure parameters of the examined thiazole with its inhibition efficiency value. Frontier molecular orbitals, that is, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), the energy gap (ΔE), chemical hardness, softness, and electronegativity have been determined and explained. The DFT results were found to agree with gravimetric data showing that the examined compound was an efficient inhibitor for low carbon steel corrosion in HCl medium. The antibacterial

efficiency of ANYT against selected types of bacteria, namely *Escherichia coli*, and *Staphylococcus aureus*, was studied. The results showed that the examined inhibitor had a significant potential to inhibit the growth of gram negative and gram positive bacteria.

Keywords: *thiadiazole, corrosion inhibitor, Escherichia coli, Staphylococcus aureus, DFT.*

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1. Introduction

Low carbon steel is among the materials most widely used in both infrastructure and technology. Its importance has grown since its invention in the eighteenth century, and its mechanical properties, accessibility and low cost have supplanted the traditional concept of structural evolution [1–3]. As low carbon steels are widely used in human civilization and environmental sustainability, corrosion is a major problem [4–7]. The unfavourable decomposition of low carbon steels in an acidic environment has a significant impact on the global economy, as acid treatments are already used to remove rust and scale in acid pickling, boiler cleaning, oil well acidification and chemical processes. The main preventive method for protecting metal structures from corrosion is to limit their exposure to acidic conditions, although this is almost impossible [8–11]. However, corrosion can be controlled using anti-corrosion techniques including layer coating, alloying, chrome plating, and protective coatings. Barriers are one of the most cost-effective, easy-to-use and effective ways to protect a metal surface, and corrosion is the natural decomposition of a substance as a result of chemical reactions with its environment [12, 13]. It is a spontaneous, natural, relaxed and continuous action. It cannot be prevented, although it can be reduced by inhibitors, cathodic and anodic protection, and protective coatings. Inhibiting compounds coat the surface of low carbon steel, preventing acids from dissolving the metal further [14–18]. Adsorption of inhibitors goes through two paths: physical adsorption, which may result from charge transfer between two oppositely charged compounds on the surface of steel and inhibitor compounds, and chemical adsorption, which requires charge sharing or charge transfer from the inhibitor molecules to the surface of low carbon steel in order to form a coordination bond. In fact, new corrosion inhibitors with low cost and excellent corrosion protection performance are in great demand in a variety of sectors and industries. On the other hand, organic inhibitors distribute their molecules to cover the broad mineral surface area with a dense layer. Chemical adsorption is also a possibility. Electron pairs, or lone electrons, of the inhibitor molecules establish a coordinated covalent bond with the metal. In recent years, heterocyclic corrosion inhibitors have proven useful in preserving metal surfaces from oxidation by coating the surface with a continuous protective film that prevents or slows down metal cracking. Heterocyclic compounds containing electron donor atoms such as N, O, and S and aromatic ring and groups such as alkyl, amino and hydroxy groups are superior corrosion inhibitors because they can occupy the vacant orbitals of metals such as iron with the necessary electrons, and this allows the metal to return to stability and prevents oxidation

[19–22]. This study aims at testing the efficiency of a pre-synthesized thiadiazole derivative, namely 2-amino-5(naphthalene-2-ylmethyl)-1,3,4-thiadiazole (ANYT), as a corrosion inhibitor for low carbon steel by adding several electron-donating atoms, such as N and S atoms, and some electron-donating aggregates. Quantum chemical calculations were used to determine the corrosion inhibition of the investigated molecule. Figure 1 represents the chemical structure of the corrosion inhibitor.

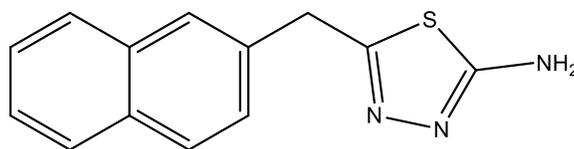


Figure 1. The structure of ANYT.

2. Materials and Methods

2.1 Low carbon steel coupons

The chemical composition of the tested low carbon steel coupons (wt.%) were 0.210% carbon, 0.050% manganese, 0.380% silicon, 0.010% aluminum, 0.050% sulfur, 0.090% phosphorus and balance iron. The low carbon steel was regularly split into coupons with an area of 4.0×2.5 cm. The coupons were smoothed utilizing sandpaper. The coupons were thereafter rinsed with distilled water and then acetone.

2.2 Hydrochloric acid solution

The hydrochloric acid solution used in this study has a concentration of 1 M. It was prepared from 37% HCl of analytical grade and double-distilled water.

2.3 Inhibitor concentration

The examined inhibitor was dissolved and diluted with 1 M HCl to provide a set of inhibitor stock suspensions with various concentrations (100, 200, 300, 400, 500 and 1000 ppm).

2.4 Weight loss measurements

Weight loss was determined, firstly, at various exposure periods (1, 5, 10, 24, 48, and 72 h) at 303 K, and secondly, at different temperatures (303, 313, 323 and 333 K) and 10 h exposure period to describe the interactions between the low carbon steel surface and the corrosive HCl solution and explain the inhibition process [23]. The low carbon steel specimens were prepared as above. The specimens were weighed before and after exposure to an HCl solution. From the weight loss data, the corrosion rates (C_R) and protection efficiency ($IE\%$) were calculated from the relations (1) and (2) [24, 25]:

$$C_R (\text{mmy}^{-1}) = \frac{87600\Delta W}{p \cdot a \cdot t} \quad (1)$$

where ΔW is the coupon weight difference before and after immersion (mg), ρ represents the coupon density (g cm^{-3}), a is the coupon surface area (cm^2), and t is the exposure time (h);

$$IE\% = \frac{C_{R(\text{blank})} - C_{R(\text{inhibitor})}}{C_{R(\text{blank})}} \cdot 100 \quad (2)$$

where $C_{R(\text{blank})}$ and $C_{R(\text{inhibitor})}$ are the corrosion rate values without and with the examined inhibitor, respectively.

2.5 Quantum chemical calculation

The Gaussian 03 program, Revision C.01 was used to optimize the inhibitor molecules geometrically to a local optimum without symmetry constraints utilizing the polarisation basis set (6-31G++(d,p)). In the gas phase, a variation of the DFT approach combining the Becke three-parameter hybrid (B3) exchange functional and the Lee–Yang–Parr (LYP) correlations usable (B3LYP) was utilized to discover all optimum geometries. Various quantum variables were calculated using the following Equations (3)–(9) [26]:

$$\text{Energy gap } (\Delta E) = E_{\text{HOMO}} - E_{\text{LUMO}} \quad (3)$$

$$\text{Electron affinity } (EA) = -E_{\text{HOMO}} \quad (4)$$

$$\text{Ionisation potential } (IP) = -E_{\text{LUMO}} \quad (5)$$

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

$$\text{Global softness } (\sigma) = \frac{1}{\eta} \quad (7)$$

$$\text{Electronegativity } (\chi) = -\frac{E_{\text{HOMO}} + E_{\text{LUMO}}}{2} \quad (8)$$

$$\text{The fraction of electrons transferred } (\Delta N) = \frac{\chi_{\text{Fe}} - \chi_{\text{inh}}}{2(\eta_{\text{Fe}} + \eta_{\text{inh}})} \quad (9)$$

Where χ_{Fe} and η_{Fe} were 4.82 eV and 0 eV, respectively.

2.6 Antimicrobial efficiency

The antibacterial efficiency of the synthesized compound, namely 2-amino-5-(naphthalen-2-ylmethyl)-1,3,4-thiadiazole (ANYT), was assessed for *Staphylococcus aureus* chosen as gram-positive bacteria and *Escherichia coli* as gram-negative bacteria, through the conventional approach, namely disc diffusion technique utilizing nutrient agar. The examined organisms were incubated in an agar environment at 37°C for 24.0 h. A 5.0 mm diameter disc was soaked in the studied solutions in the presence of various concentrations (100, 200, 300, 400, 500 and 1000 ppm) of the examined inhibitor dissolved in DMSO

(dimethylsulphoxide), and then transferred to Petri dishes on a proper medium earlier seeded with the examined bacteria and stored for 24 hours. The inhibition zone around the tested disc was calculated (mm). In order to determine the inhibitive efficiency of DMSO on the examined pathogens, further experiments were conducted using the control namely DMSO. DMSO revealed no efficiency against the examined pathogens.

3. Results and Discussion

3.1 Gravimetric analysis

Gravimetric analysis is simple to execute because it does not require special facilities or materials and can be performed with many specimens at once. This strategy was intended to determine how the examined inhibitor concentration, immersion duration, and temperature affected the corrosion rate and inhibition efficiency.

3.2 Effect of concentration

The variation in the corrosion rate and protective efficiency with concentration at various measuring times is presented in Figure 2.

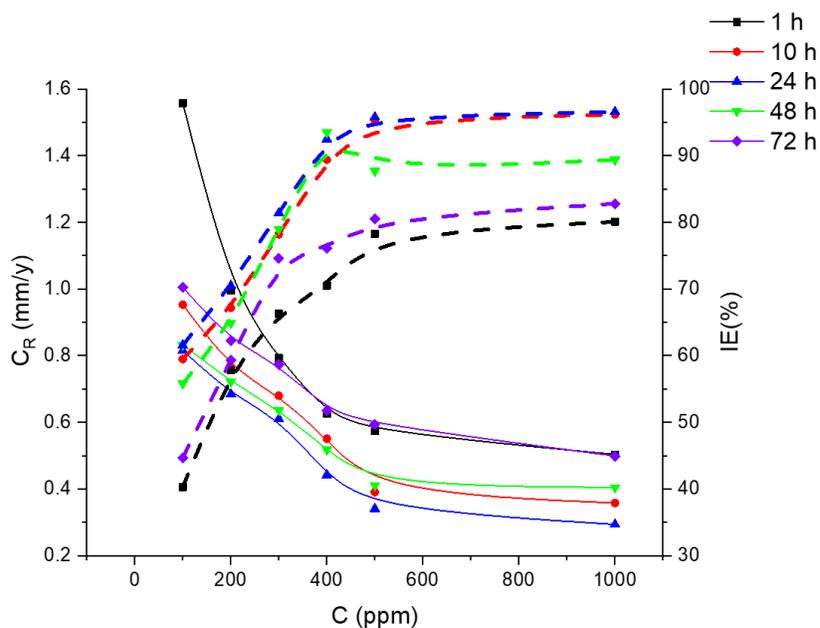


Figure 2. Low carbon steel corrosion characteristics in 1 M HCl medium with various concentrations of the investigated inhibitor at 303 K.

This plot reveals that the corrosion rate diminishes with an increase in the inhibitor concentration and the inhibition efficiency increases with an increase in the inhibitor concentration. Furthermore, almost the highest inhibitor efficiency of 95.3% was obtained in the presence of 500 ppm, whereas, at a higher inhibitor concentration (1000 ppm), it became 96.2%. This means that no significant protection increase is achieved above 500 ppm and it is the optimum concentration. The increase in the inhibitor efficiency is due

to the adsorption of tested inhibitor molecules onto low carbon steel surface and formation of a protective layer that covers the coupon surface and thus reduces corrosion [27–31].

3.3 Effect of immersion time

The immersion periods were varied (1–72 h), and the weight loss results are exhibited in Figure 2. It is obvious that the inhibition efficiency decreased after long exposures of 48 or 72 h. The experimental results achieved for the corrosion rate and inhibition efficiency of low carbon steel in 1 M HCl without and with various concentrations of the tested inhibitor are exhibited in Figure 2. Analysis of results showed that the corrosion rate increased and the inhibiting efficiency decreased with increasing exposure time. The highest inhibition efficiency value obtained was 96.6% and diminished to 85.8% after exposure for 24 h or 72 h, respectively. This is due to the fact that the tested inhibitor molecules desorb from low carbon steel surface and enhance the contact between the immersed coupon and HCl solution thus causing low carbon steel to dissolve. The reduction in protection efficiency after a long immersion time may be due to a decrease in the number of inhibitor molecules ready in the corrosive environment to avert the low carbon steel dissolution. As the tested inhibitor molecules are desorbed from the metal surface, they become inefficient and have no value in the protection. Because of their biodegradability, these compounds will not be hazardous to the environment after disposal.

3.4 Effect of temperature

In this study, the effect of temperature on the protection efficiency of low carbon steel was investigated in the range of 303 to 333 K. The experimental findings shown in Figure 3 exhibit the inhibition efficiency values achieved by the gravimetric technique. It is obvious from Figure 3 that a rise in temperature decreases the inhibitive efficiency. However, as the inhibitor's concentration is increased, the inhibition efficiency improves as well. The time variation between the adsorption and desorption of inhibitor molecules on the low carbon steel surface gets smaller as the temperature rises. In a hydrochloric acid solution, corrosion is usually followed by emission of hydrogen. The process of adsorption is influenced by the excitement emanating from accelerated rates of hydrogen evolution at a high temperature, which leads to a decrease in the inhibition efficiency [32–35].

3.5 Adsorption isotherm

The interaction of the tested inhibitor with low carbon steel surface can be studied using adsorption isotherms. Different isotherms models, notably Langmuir and Temkin adsorption isotherms, were used to determine the adsorption isotherms model. The linear regression coefficients (R^2) values were equal to 1, as presented in Table 1. The Langmuir isotherm was found to be the best acceptable adsorption model. Figure 4 depicts the linear correlations of C/θ vs C for the tested inhibitor on low carbon steel surface at various temperatures [36–39].

$$\frac{C}{\theta} = \frac{1}{K_{\text{ads}}} + C \quad (10)$$

Where K_{ads} represents the adsorption constant, C refers to the concentration of the inhibitor, and θ signifies the surface coverage [40–43].

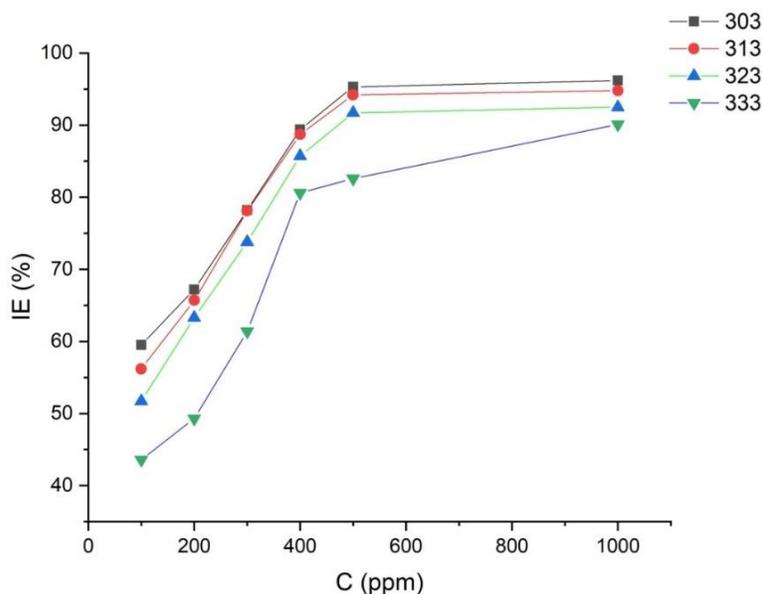


Figure 3. The variations in inhibitive efficiency of low carbon steel in corrosive solution for 10 h immersion time at different temperatures (303–333 K).

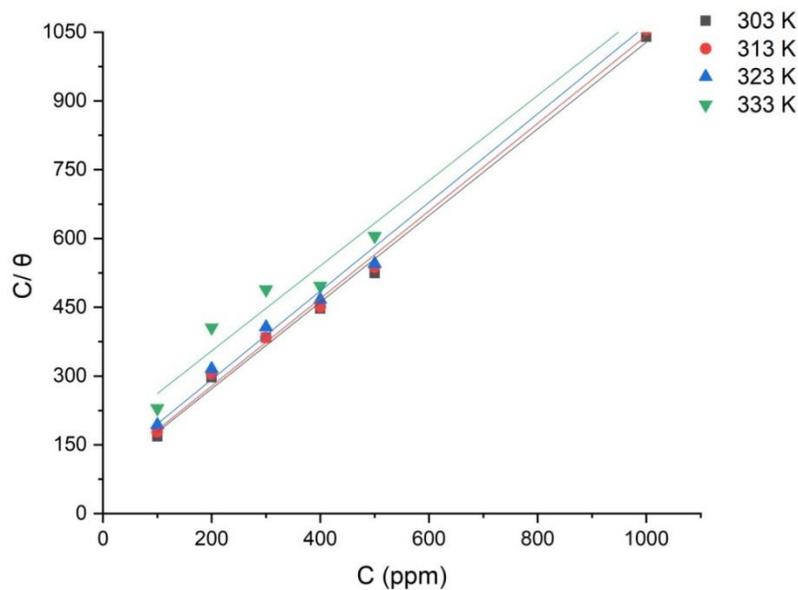


Figure 4. Langmuir adsorption model of investigated inhibitor molecules in the corrosive environment.

The surface coverage can be calculated according to Equation (11):

$$\theta = \frac{IE}{100} \quad (11)$$

The free energy ($\Delta G_{\text{ads}}^{\theta}$) can be determined from K_{ads} according to Equation (12):

$$K_{\text{ads}} = \frac{1}{55.5} \exp\left(\frac{-\Delta G_{\text{ads}}^{\theta}}{RT}\right) \quad (12)$$

where 55.5 is the water concentration ($\text{mol}\cdot\text{L}^{-1}$), T is the temperature (K), and R is the universal gas constant ($\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$).

Table 1 demonstrates the $\Delta G_{\text{ads}}^{\theta}$ with negative values, suggesting the spontaneous adsorption of the tested inhibitor molecules on low carbon steel surface to form a protective layer. Generally, $\Delta G_{\text{ads}}^{\theta}$ values that are higher than ($-40 \text{ kJ}\cdot\text{mol}^{-1}$) refers to chemisorption. In contrast, a value of $\Delta G_{\text{ads}}^{\theta}$ lower than ($-20 \text{ kJ}\cdot\text{mol}^{-1}$) refers to physisorption. In the current investigation, the $\Delta G_{\text{ads}}^{\theta}$ values are located in the range of -35 to $-39 \text{ kJ}\cdot\text{mol}^{-1}$. Therefore, this suggests that the tested inhibitor molecules may inhibit the corrosion of low carbon steel through both physical and chemical adsorption. As shown in Figure 5, the process is near the chemical adsorption process in the temperature range of 313 to 333 K [44–47].

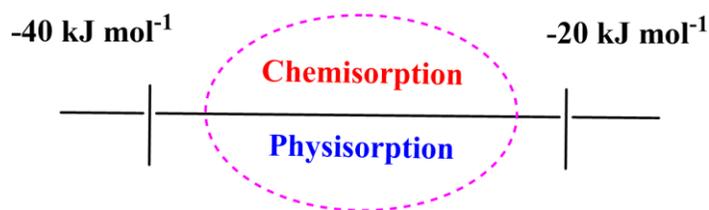


Figure 5. Adsorption process according to $\Delta G_{\text{ads}}^{\theta}$ values for adsorption of tested inhibitor molecules on low carbon steel surface in corrosive environment.

Table 1. Physical parameters of the tested inhibitor.

Parameter	Temperature (K)			
	303	313	323	333
Slope	0.994	0.954	0.966	0.928
R^2	1	1	1	1
K_{ads} ($\text{L}\cdot\text{mol}^{-1}$)	4.73	3.85	2.88	1.93
$\Delta G_{\text{ads}}^{\theta}$ ($\text{kJ}\cdot\text{mol}^{-1}$)	-35.14	-36.43	-36.94	-39.10

3.6 Computational studies

The computational parameters of the tested inhibitor molecules presented in Table 2 were determined to explain the inhibition mechanism suggested by inhibitor on Fe-atom. The achievement of an inhibitor can be divined by applying its values of HOMO, LUMO, and ΔE . The capability of the inhibitor molecule to add an electron to low carbon steel surface is explained by the HOMO energy, whereas the inhibitor capacity to take electron from the low carbon steel surface is explained by the LUMO energy [48–57]. Inhibitor molecules with a high HOMO energy are more likely to transfer electrons to the vacant d-metal orbitals on the surface [44]. Adsorption on the low carbon steel surface is facilitated by raising the HOMO energy, which improves the inhibitory efficiency.

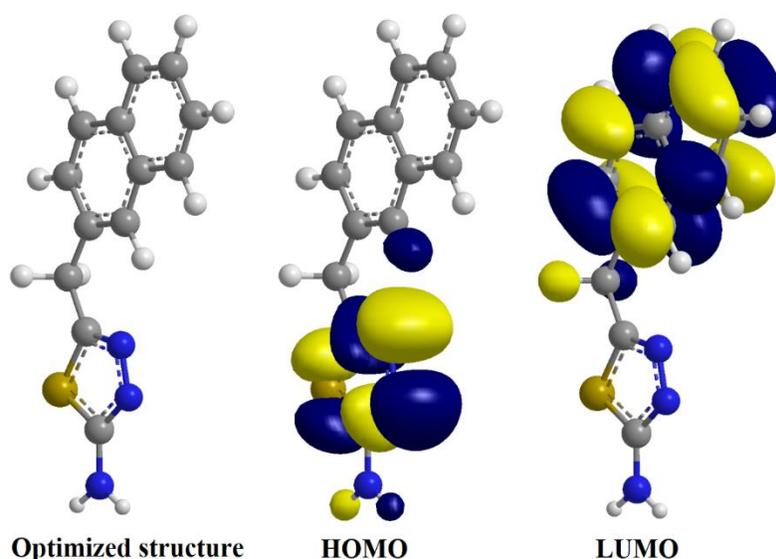


Figure 6. Frontier MOs (HOMO and LUMO) and optimized structure of the investigated inhibitor molecule.

Table 2. The quantum parameters of the examined inhibitor.

Parameter	Value
E_{HOMO} (eV)	-7.363
E_{LUMO} (eV)	-3.859
ΔE (eV)	-3.504
$I = -E_{\text{HOMO}}$ (eV)	7.363
$A = -E_{\text{LUMO}}$ (eV)	3.859
$\chi = (I+A)/2$	5.611
$\eta = (I-A)/2$	1.752
$\sigma = 1/\eta$	0.570

Parameter	Value
$\Delta N = [\chi_{\text{Fe}} - \chi_{\text{inh}}] / [2(\eta_{\text{Fe}} - \eta_{\text{inh}})]$	0.24
Dipole moment (D)	2.579

The frontier molecular orbital energies (E_{HOMO} and E_{LUMO}) are important characteristics for predicting the reactivity of organic compounds. The E_{HOMO} is frequently related with a molecule's capacity to donate electrons. Based on published findings, rising E_{HOMO} values suggests a greater likelihood of electron donation to a proper acceptor that has an empty orbital and a low energy value. Based on Eddy and Ebenso findings [58], increasing E_{HOMO} facilitates the inhibitor's adsorption. As a result, enhancing the transport mechanism *via* the adsorbed layer would improve the inhibitor's efficiency. The LUMO energy value denotes the molecule's capacity to take electrons. Based on research findings, E_{LUMO} with low energy refers to a high ability to accept electrons. Due to the relationship of ΔE with hardness or softness of a chemical compound, a larger value of ΔE suggests a lower reactivity of organic molecules, according to the literature. Due to the wide ΔE of a hard molecule it is more reactive than a soft molecule [59–63].

Table 2 shows the results of the I and A calculations. The findings show that the inhibitor's efficiency increases with rising I but reduces with a decrease in A . This is because the E_{HOMO} is directly related to the ionization potential (I), but E_{LUMO} is directly related to the ionization potential (A). This clarifies why the pattern in inhibition efficiency variation with I and A is comparable to that found in E_{HOMO} and E_{LUMO} data. It is clear that the inhibitor with the lowest global hardness value (and hence the greatest global softness value) is the optimum, and conversely. Hence soft molecules are much more reactive than hard molecules, which was the case. This discovery is in accordance with the finding of the percent inhibition efficiency experiment.

The calculated value of ΔN is shown in Table 2. The DFT findings suggest that the fraction of electron transferred value is associated highly with the inhibitive efficiency from the weight loss experiments. Hence, a high ΔN is correlated with an excellent inhibitor, whereas a lower ΔN correlates with a lower inhibitive performance.

The dipole moment (μ) is a parameter that may be utilized to determine the orientation of a corrosive protection mechanism. It is a polarity measurement in a bond that is related to the electron distribution in a molecule. However, the value of μ used as a prediction for the direction of a corrosion inhibition response is controversial, it is widely acknowledged that the adsorption of polar compounds with large μ on the metal surface should result in improved inhibition effectiveness. When the findings of quantum chemical calculations were compared to experimental inhibition effectiveness, it was observed that the inhibitor's inhibition efficiency increased as the μ increased.

3.7 The antimicrobial activity

The antimicrobial assay result confirms the antimicrobial property of the examined inhibitor as well as additional inhibition efficiency over parent 2-amino-1,3,4-thiadiazole or naphthalene. The most important inhibition efficiency of examined inhibitor molecules is due to C=N functional group [64, 65]. Generally, Schiff bases have the ability to improve the efficiency against bacteria for any compound, so the examined inhibitor has significant abilities toward the examined microbes (bactericidal agents). The partial positive charges in the examined inhibitor molecule with π -bonds located in the ANYT molecules may delocalize with π -electrons over the entire examined inhibitor molecules [64–67]. The lipophilicity of ANYT molecules could enhance and favour diffusion through the tested bacteria membrane. The lipophilicity increasingly appears to be responsible for improving the efficiency of killing bacteria. It may be suggested that the examined inhibitor molecules have the ability to inactivate various cellular enzymes that possess a vital role in different pathways of the metabolism of the examined pathogens [64, 65]. As it is seen from Figure 7, ANYT showed a lower inhibition activity against *Escherichia coli* than against *Staphylococcus aureus*. Infectious problems acquired in hospitals affect around 1.4 billion individuals globally at any given time. *Escherichia coli* and *Staphylococcus aureus* are two microorganisms that are frequently implicated in these illnesses [64–67].

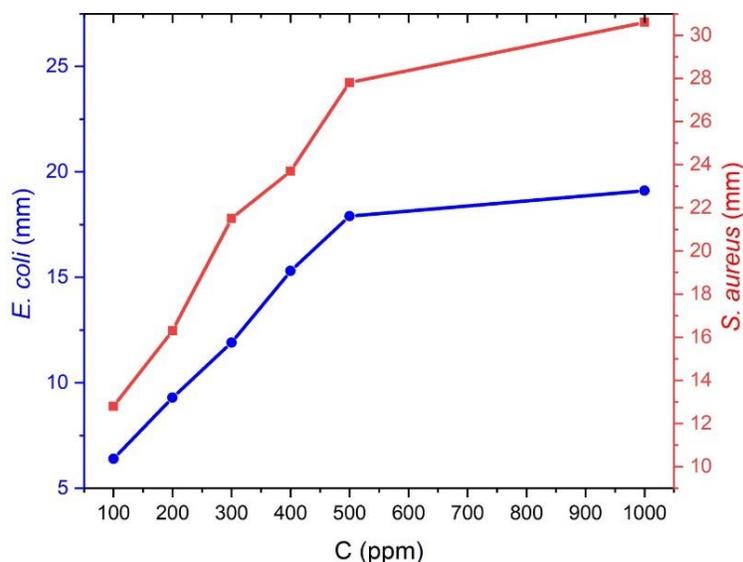


Figure 7. Effect of ANYT against selected bacteria.

Conclusions

The experimental findings may be summarized as follows:

1. 2-Amino-5-(naphthalen-2-ylmethyl)-1,3,4-thiadiazole (ANYT) was found to work as a corrosion inhibitor for low carbon steel surface in a corrosive environment.
2. The value of protection efficiency increases with increasing concentration of the examined inhibitor, however, diminishes with an increase in temperature proposing physisorption,

- and also chemisorption according to the calculated free energy values ($-35.14 \text{ kJ}\cdot\text{mol}^{-1}$ to $-39.10 \text{ kJ}\cdot\text{mol}^{-1}$).
3. Furthermore, the protection of low carbon steel surface by the examined inhibitor molecules is usually demonstrated by the production of a coordination complex of 3d-Fe-orbitals on the coupon surface with heteroatoms of ANYT molecules.
 4. The adsorption of the examined inhibitor on a low carbon steel surface in 1.0 M HCl was found to obey the isothermal model of Langmuir adsorption.
 5. Quantum chemical computations showed that the protective performance improves with an increase in the HOMO energy and a reduction in the LUMO energy and energy gap ΔE in addition to dipole moment (μ). The atomic charges describe the heteroatoms coupled with the 3d-orbital of Fe-atoms and formation of a Fe-complex as a layer that protects the surface of low carbon steel.
 6. The tested inhibitor shows high antibacterial activity against selected types of bacteria.

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