The corrosion inhibition effect of a pyridine derivative for low carbon steel in 1 M HCl medium: Complemented with antibacterial studies

M.A. Dawood,[1] Z.M.K. Alasady,[2] M.S. Abdulazeez,[3] D.S. Ahmed,[3] G.M. Sulaiman,[4] A.A.H. Kadhum,[5] L.M. Shaker[6] and A.A. Alamiery[6,7] ⓘ*

[1]*College of Dentistry, The University of Mashreq, Baghdad, 10001 Iraq*
[2]*General Directorate of Education in Baghdad, The third Al-Karkh Government, Baghdad, 10001 Iraq*
[3]*Department of Medical Instrumentation Engineering, Al-Mansour University College, Baghdad, 10001 Iraq*
[4]*Applied Science Department, University of Technology, Baghdad, 10001 Iraq*
[5]*University of Al-Ameed, Karbala, 56001 Iraq*
[6]*Department of Chemical and Process Engineering, University Kebangsaan Malaysia (UKM), P.O. Box: 43000, Bangi, Selangor, Malaysia*
[7]*Energy and Renewable Energies Technology Center, University of Technology, Baghdad, 10001 Iraq*
*E-mail: dr.ahmed1975@ukm.edu.my

Abstract

A pyridine derivative 4-chloro-2-((pyridin-2-ylimino)methyl)phenol (CPP) was synthesized and its anti-corrosion effect toward low carbon steel in 1 M hydrochloric acid medium was studied by mass loss measurements. The protective efficiency of CPP increased along with the inhibitor concentration. The effect of temperature on the corrosion performance of low carbon steel was studied in the temperature range of 303–333 K. The inhibition efficiency of CPP decreased with an increase in temperature. Experimental findings from weight loss measurements confirmed that the anti-corrosion efficiency of CPP was significant. The adsorption of inhibitor molecules on low carbon steel surface obeyed the Langmuir adsorption isotherm model. Moreover, quantum chemical calculations were conducted based on density functional theory (DFT) in order to study the relationship of inhibition efficiency and the structure of the inhibitor molecule. The quantum chemical parameters such as E_{HOMO}, E_{LUMO}, the energy gap (E), electron affinity (A), ionization potential (I), softness (S), hardness (η), absolute electronegativity (χ), and the fraction of electron transferred (N), were determined. The antibacterial efficiency against selected types of bacteria, namely *Escherichia coli* and *Staphylococcus aureus*, was also studied. The results show that CPP has a significant potential to inhibit the growth of gram negative and gram positive bacteria.

1. Introduction

Low carbon steel is one of the most flexible, widely utilized, and cheapest materials in almost all sectors [1–3]. The unavoidable damage caused by low carbon corrosion leading to an increase in production costs is one of the primary problems in an industrial process [4]. In corrosive conditions, several strategies are available for controlling and preventing corrosion [5–7]. An economical strategy used today to reduce corrosion attacks employs organic inhibitors. Corrosion inhibitors are usually employed in tiny amounts. Numerous studies demonstrated that the organic molecules that are most efficient for this function contain nitrogen, phosphorus, oxygen, and sulfur [8–11]. Their effectiveness for corrosion prevention is attributed to their interaction with a metal surface [12, 13]. Generally, the adsorption of organic molecules on the metal surface blocks corrosion sites [14–18]. Schiff bases are extremely efficient due to the existence of a nitrogen atom among the many heteroatom-containing molecules and numerous such chemicals have been reported in publications as possible corrosion inhibitors for metals and alloys in acid media. The increased use of Schiff bases as a corrosion inhibitor is mainly based on their minimal toxicity and simplicity of synthesis from extremely cheap precursor materials. Schiff bases are recognized for strong inhibition capacity and extensive study on natural compounds has revealed that the efficiency of Schiff bases is substantially higher than that of comparable aldehydes and amines. Schiff bases increase inhibitory efficiency significantly [19–22]. The aforesaid concerns have prompted us to use the weight loss technique in order to assess the inhibitory capacity, adsorption isotherm, and to perform quantum chemical calculations to estimate the adsorption properties of the Schiff base synthesized, namely 4-chloro-2-((pyridin-2-ylimino)methyl)phenol (CPP), on low carbon steel surface in 1 M HCl. Moreover, an antimicrobial study was conducted on selected types of *Escherichia coli* as Gram-negative bacteria and *Staphylococcus aureus* as Gram-positive bacteria.

2. Materials and Methods

2.1 Materials

The inhibitory effects of CPP were examined on mild steel with the chemical composition presented in Table 1.

Table 1. Chemical composition of mild steel coupons (wt.%).

Carbon	Manganese	Silicon	Aluminum	Sulfur	Phosphorus	Iron
0.210	0.050	0.380	0.010	0.050	0.090	balance

A mechanical press was used to cut low carbon steel into coupons with dimensions of 4.5×2×0.5 cm. All examined coupons were washed with double-distilled water and degreased with acetone. The coupons were utilized for weight loss procedures. The corrosive medium was prepared from hydrochloric acid reagent of analytical grade and double-

distilled water. Figure 1 shows the molecular structure of the examined inhibitor. In this article, CPP was synthesized similarly to the procedure in an earlier study *via* the reaction of 2-aminopyridine and 5-chloro-2-hydroxybenzaldehyde.
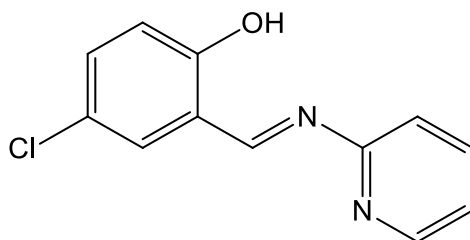
Figure 1. Molecule structure of 4-chloro-2-((pyridin-2-ylimino)methyl)phenol (CPP).

2.2 Weight Loss Analysis

The low carbon steel coupons were exposed to 1 M HCl medium with various concentrations (0.1, 0.2, 0.3, 0.4, 0.5, and 1.00 mM) of the tested inhibitor for 10 h. A thermostat aqueous bath at 303 K regulated the temperature. Moreover, the low carbon steel coupons were exposed to 1 M HCl environment with addition of the tested inhibitor, and the tests were carried over the temperature range from 303 to 333 K. After the exposure, the tested coupons were taken from the suspension, rinsed completely with distilled water, acetone, then dried and weighed accurately. The experiments were repeated in triplicate and the average values were determined [23]. The corrosion rate (C_R, $g \cdot m^{-2} \cdot h^{-1}$), protection efficacy (*IE%*) and the fractional surface coverage (θ) were calculated according to equations (1), (2) and (3) [24, 25]:

$$C_R = \frac{W_0 - W_i}{at} \tag{1}$$

$$IE(\%) = \frac{C_R^0 - C_R^i}{C_R^0} \cdot 100 \tag{2}$$

$$\theta = \frac{IE}{100} \tag{3}$$

where W_0 represents the value of the mass loss in the absence of CPP; and W_i is refers to the value of mass loss in the presence of CPP; a is the coupon area and t is the immersion time (h); C_R^0 is the corrosion rate ($g \cdot m^{-2} \cdot h^{-1}$) in the absence of CPP, and C_R^i is the corrosion rate ($g \cdot m^{-2} \cdot h^{-1}$) in the presence of CPP.

2.3 DFT investigations

Quantum computations have been conducted utilizing density functional theory (DFT) with the basis set B3LYP/6-31G (d, p), using the Gaussian 03 program. The CPP molecular optimized geometry, the frontier molecular orbitals HOMO and LUMO were achieved by applying the DFT method. The important principal chemical parameters according to

Koopman's theorem [26] such as the ionization potential (I), electron affinity (A), softness (σ), absolute electronegativity (χ), and absolute hardness (η) in addition to the fraction of electron transferred (ΔN) were calculated.

2.4 Antimicrobial Efficiency

The antibacterial efficiency of the synthesized compound (CPP) was assessed for *Staphylococcus aureus* as gram-positive bacteria and *Escherichia coli* as gram-negative bacteria through the conventional approach, namely disc diffusion technique using nutrient agar. The incubation for the tested organisms in agar medium was conducted for 24 h at 37°C. The disks (5.0 mm diameter) were soaked in the studied solutions with the examined concentrations (0.1, 0.2, 0.3, 0.4, 0.5, and 1.00 mM) of CPP which was dissolved in dimethylsulphoxide as a sterilized solvent and were placed in Petri dishes on a proper medium earlier seeded with the examined bacteria and stored for 24 h in an incubator. The zone of inhibition around the tested discs was calculated in mm. To determine any inhibition activity of dimethylsulphoxide on the examined pathogens, further experiments were conducted using dimethylsulfoxide as control. Dimethylsulfoxide revealed no efficacy toward the examined bacteria.

3. Results and Discussion

3.1 Weight Loss Study

3.1.1 Effect of Concentration

The corrosion rate (C_R) of mild steel and the inhibition efficiency obtained from the mass loss measurements in 1 M HCl medium containing various concentrations of CPP (0.1, 0.2, 0.3, 0.4, 0.5, and 1.00 mM) at 303 K are exhibited in Figure 2. The weight loss findings obviously reveal that the inhibitory efficacy increases and the corrosion rate decreases with increasing concentration of the inhibitor studied. When the concentration of CPP changes from 0.1 mM to 1 mM, the inhibition efficacy of CPP improves from 47.3% to 92.8%. This implies that CPP acts as an inhibitor impeding mild steel corrosion in 1 M HCl environment. While the concentration of CPP corrosion inhibitor is low, additional molecules are required to effectively cover the mild steel surface. Furthermore, increasing the concentration above 0.5 mM did not bring any important differences in the inhibition efficiency, showing the realization of an optimum concentration value of the tested inhibitor. The result is due to the accumulation of CPP on the mild steel surface that is positively charged, therefore reducing direct interaction between the mild steel surface and the hydrochloric acid environment [27–31].
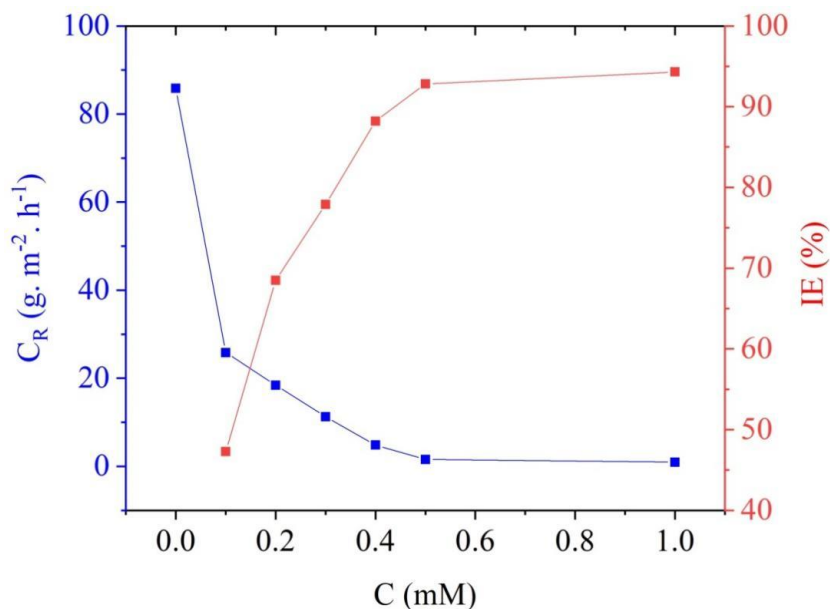
Figure 2. Mild steel corrosion characteristics in 1 M HCl medium with various concentration of CPP at 303 K.

3.1.2 Effect of Temperature

The temperature has a considerable effect on the corrosion rate of mild steel. The effect of environment temperature (303–333 K) on the corrosion rate and protection performance is illustrated in Figure 3. The corrosion rate decreased considerably upon addition of the inhibitor compared to the blank solution. In 1 M HCl, the corrosion is considerably inhibited by the addition of an inhibitor. It indicates that an increase in the concentration of the examined inhibitor considerably retards the corrosion of mild steel surface in 1 M HCl. The reduction in inhibitive efficacy and increase in corrosion rate was noted with a rise in temperature from 303 to 333 K, which is believed to be because the adsorption processes occur spontaneously and irreversible with rising temperature, and the temperature rise is not useful to the adsorption. The effect may further become stronger from weakening of electrostatic adsorption on the mild steel surface and the difficulty of inhibitor molecules desorption from the mild steel surface as the temperature rises. Moreover, mild steel corrosion in HCl solution is normally followed by hydrogen release, and the process of adsorption of the tested inhibitor molecules could be affected by the confusion generated by an acceleration hydrogen evolution at high temperatures that leads to a reduction in the protection efficacy [32–35].
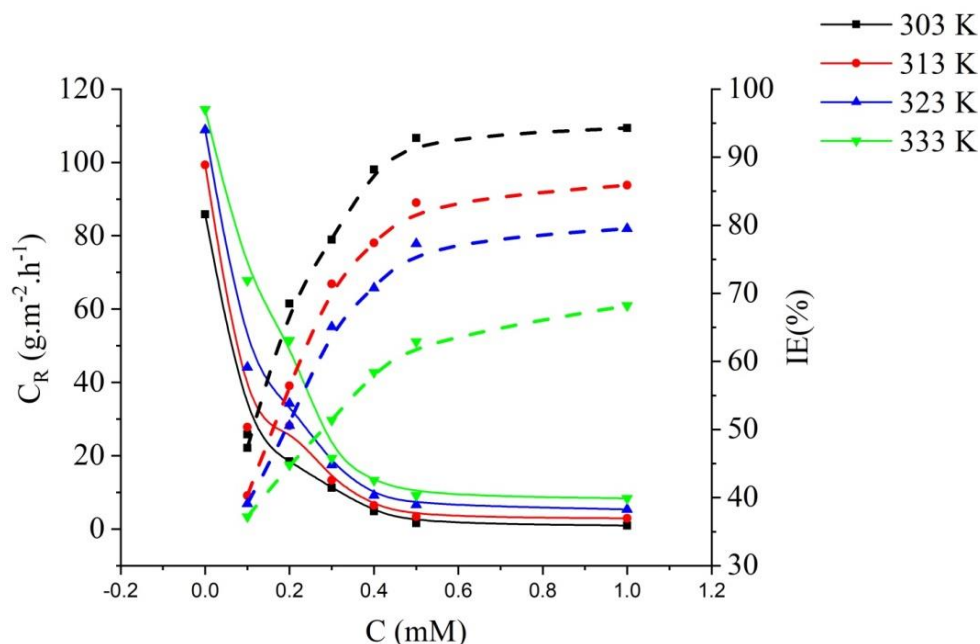
Figure 3. The variation of corrosion rate and inhibition efficiency of mild steel in 1 M HCl solution at various temperatures (303–333 K).

3.2 Adsorption Isotherm

The adsorption isotherm can be used to analyze the interactions between the inhibitor molecules and the mild steel surface. Different isotherm models, such as Frumkin, Langmuir, Freundlich, and Temkin, were studied in the adsorption mode, and Langmuir model was eventually judged to have been the most acceptable. Figure 4 shows the linear C/θ and C correlations for the CPP inhibitor [36–39].
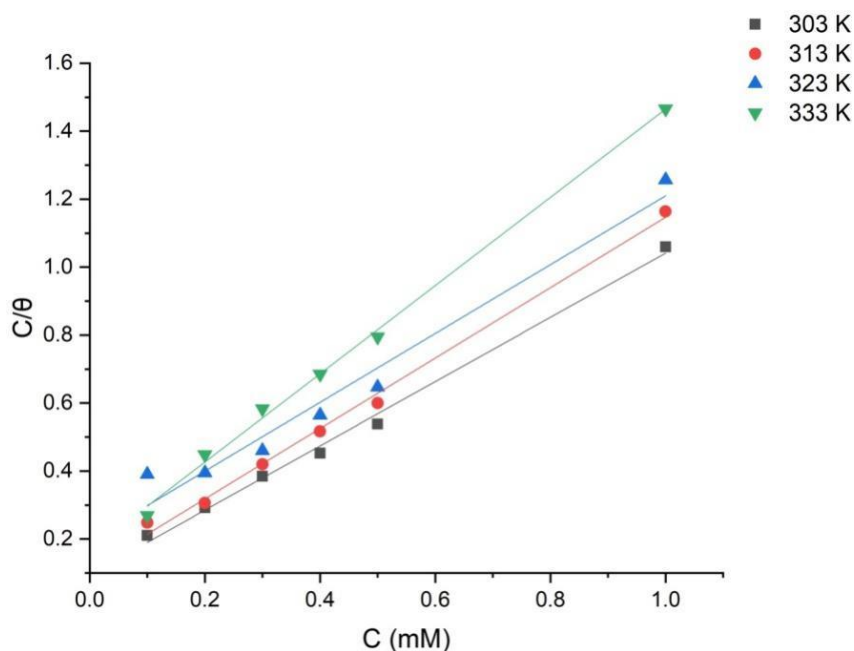

Figure 4. Langmuir adsorption model of CPP molecules in the corrosive environment.

As it is seen in Figure 4, R^2 (Table 2) which represents the linear regression parameter is relatively close to 1, revealing that the Langmuir adsorption model is valid at all the temperatures studied (303, 313, 323, and 333 K) in the adsorption of the examined CPP molecules on the mild steel surface. The adsorption isotherm could be determined according to Equation 4 [40–43]:

$$\frac{C}{\theta} = \frac{1}{K_{ads}} + C \tag{4}$$

where K_{ads} represents the adsorption equilibrium constant, C refers to the concentration of the tested inhibitor, and θ signifies the surface coverage.

Table 2. Physical parameters of CPP as a corrosion inhibitor of mild steel in HCl solution at various temperatures.

Temp. (K)	303	313	323	333
Slope	0.94552	1.03593	1.01246	1.29795
R^2	0.99756	0.99774	0.98398	0.9986

The free energy (ΔG^0_{ads}) can be calculated from K_{ads} as exhibited in Equation 5.

$$K_{ads} = \frac{1}{55.5} \exp\left(\frac{-\Delta G^0_{ads}}{RT}\right) \tag{5}$$

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

The values of K_{ads} and ΔG^0_{ads} are provided in Table 3. The negative values of ΔG^0_{ads} shows that the CPP molecule is spontaneously adsorbed on the mild steel surface to create a protective film. Moreover, a high K_{ads} value means that the CPP molecules are firmly adsorbed on mild steel surface. The presence of electron-negative active sites like nitrogen and oxygen in addition to π-bonds in the structure of the tested inhibitor molecules will provide strong inhibitor protection to mild steel surface [44–47].

Table 3. K_{ads} and ΔG^0_{ads} values of CPP molecules adsorbed on mild steel surface at 303–333 K.

Parameter	Temperature (K)			
	303	313	323	333
K_{ads} (mol·L^{-1})	117.49	104.34	93.85	77.94
ΔG^0_{ads} (kJ·mol^{-1})	–38.3	–34.9	–32.6	–31.7

Generally, if the value of ΔG_{ads}^0 is about -40 kJ·mol^{-1}, then the adsorption mechanism should be involve both physisorption and chemisorption. A value of ΔG_{ads}^0 more negative than -40 kJ·mol^{-1} may be suggestive of donation of electron pairs from the inhibitor molecules to the d-orbital of Fe atoms on the mild steel surface, whereas a value less negative than -20 kJ·mol^{-1} implies physical adsorption. As discussed earlier, it was suggested that both physisorption and chemisorption were reasonable for CPP at 303 to 333 K according to the values of ΔG_{ads}^0 values obtained in the current investigation as presented in Table 3.

3.3 Computational studies

Quantum chemical calculations have become a really important technique for investigating the mechanism of inhibition. The optimized molecular structure of CPP molecules is demonstrated in Figure 5, and the theoretical parameters are presented in Table 4. It is noted that the frontier homo molecular orbital MO in the molecules studied is chiefly distributed over the entire inhibitor molecule including the heterocyclic ring and the imine bond [48–57]. It has been proved in recent studies that the HOMO energy is usually related to the ability of molecules to donate electrons. A HOMO with a high energy value is expected to show the ability of a molecule to donate an electron to a suitable acceptor molecule with an unoccupied orbital [58–63]. Moreover, the LUMO energy refers to the ability of a molecule to receive electron pairs. A lower energy gap of a molecule indicates the best inhibitory efficiency because the value of energy required to move an electron from the last occupied orbital is smaller. HOMO with high energy and low energy gap values were found in the CPP molecules, which shows that CPP has a superior protection performance as shown in Table 4.
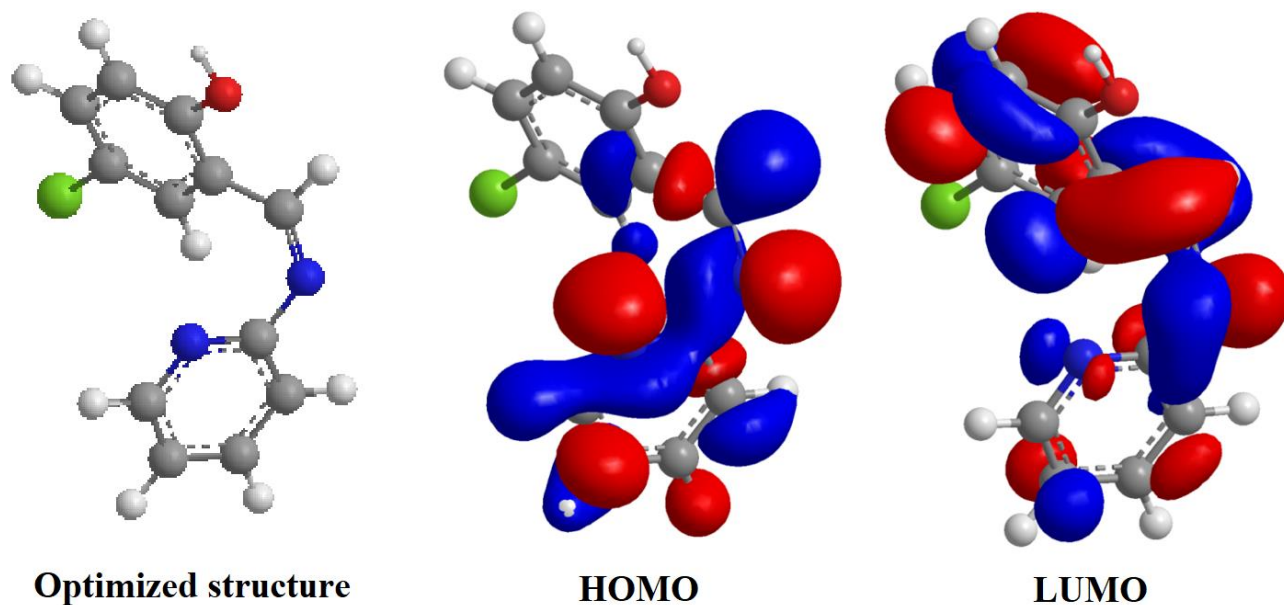

Optimized structure   **HOMO**   **LUMO**

Figure 5. Frontier MOs (HOMO and LUMO) and optimized structure of the CPP molecule.

Table 4. Quantum chemical parameters for CPP molecules.

Parameter	Value
E_{HOMO} (eV)	−10.030
E_{LUMO} (eV)	−3.162
ΔE (eV)	−6.868
$I = -E_{HOMO}$ (eV)	10.030
$A = -E_{LUMO}$ (eV)	3.162
$\chi = (I+A)/2$ (eV)	7.143
$\eta = (I-A)/2$ (eV)	3.034
$\sigma = 1/\eta$ (eV^{-1})	0.329
$\Delta N = [\chi_{Fe} - \chi_{inh}]/[2(\eta_{Fe} - \eta_{inh})]$	−0.0238
Dipole moment	2.195 (D)

Chemical hardness and softness are important factors that deal with the inhibitor molecule's reactivity and stability. A high value of hardness and low value of softness indicate excellent protection performance. Table 4 shows that the energy gap of CPP (6.868 eV) indicates that CPP is the best inhibitor for the corrosion of mild steel. The parameters ΔE, η, σ, and ΔN for CPP are in good agreement with weight loss findings. The energies of HOMO and LUMO were −10.030 eV and −3.162 eV respectively, which agrees with the experimental results. The number of electrons transferred was also determined. The values of ΔN revealed that the protection efficacy following electron donation is comparable with Lukovits's study. If $\Delta N < 3.6$, the inhibitive efficacy increases by increasing the ability to donate an electron to the Fe atoms on the mild steel surface. The value of ΔN is not specifically the number of leaving electrons from the donor and receiving the acceptor molecule. Dipole moment is the polarity strength of a polar covalent bond. Dipole moment is defined as the product of charges on the atoms and the distance between the two bonded atoms. The entire dipole moment, however, exhibits only the molecule polarity.
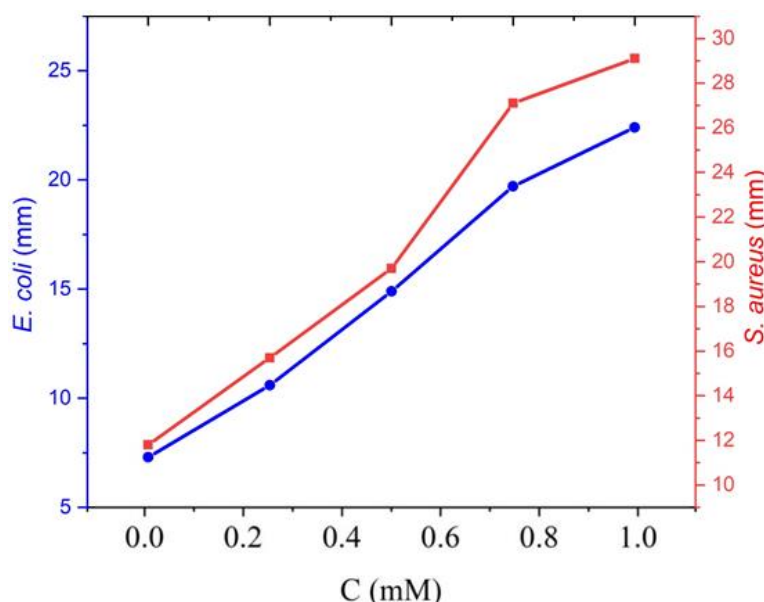
3.4 Atomic charges

The Mulliken charges are significant for figuring out the adsorption sites of corrosion inhibitor molecules. An atom with a high negative charge has the ability to be adsorbed on the mild steel surface. From Table 5, the CPP molecules have negative charges, which indicates that these atoms have the ability to coordinate with the empty d-orbital of Fe atoms on the mild steel surface.

Table 5. The Mulliken charges of CPP molecule.

Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge
C(1)	0.297371	C(5)	−0.152666	N(9)	−0.533338	C(13)	−0.240084
C(2)	−0.051599	C(6)	−0.196630	C(10)	0.461847	C(14)	0.069906
C(3)	−0.143404	O(7)	−0.594288	C(11)	−0.201151	N(15)	−0.560322
C(4)	−0.272388	C(8)	0.138133	C(12)	−0.149386	Cl(16)	0.084310

3.5 The antimicrobial activity

The anti-microbial measurement data confirm that CPP has anti-microbial features in addition to better inhibition efficiency than the parent 2-aminopyridine or 4-chlorophenol. The most important inhibition efficacy of CPP molecules is attributed to the presence of an imine (C=N) group [64, 65]. It is understood that the imine group has the tendency to improve the efficacy of CPP molecules to be highly effective in approaching examined bacteria and CPP molecules become bactericidal agents, so killing pathogens better than the parent compounds which form the CPP. In CPP molecules, the partial (+*ve*) charge is given partly by the π-bond located in the CPP molecules, and there may be delocalization of π-electrons over the entire CPP molecules [64–67]. This could enhance the lipophilicity of the CPP molecules and favor their diffusion through the lipid membrane of the examined bacteria. The lipophilicity increasingly appears to be responsible for improving the efficiency of killing bacteria. It may be assumed that CPP molecules have the ability to inactivate different cellular enzymes that play a vital role in different pathways of metabolic of the examined pathogens. As observed from Figure 6, CPP showed less inhibition activity against *Escherichia coli* than against *Staphylococcus aureus*.

Figure 6. Effect of CPP against selected bacteria.

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].

Conclusions

The experimental findings may be summarized as follows:

1. 4-Chloro-2-((pyridin-2-ylimino)methyl)phenol (CPP) was found to work as an efficient corrosion inhibitor for mild steel surface in 1.0 M HCl.
2. The value of inhibition efficiency increases with CPP concentration, however, it diminishes with an increase in temperature suggesting physisorption, along with chemisorption based on the value of free energy (−38 kJ/mol).
3. Furthermore, the protection of mild steel surface by CPP molecules is usually demonstrated by the production of a coordination complex of 3d-orbital of iron atoms on the mild steel surface and the heteroatoms of CPP molecules.
4. The adsorption of CPP inhibitor on a mild steel surface in 1.0 M HCl was determined to obey the isothermal model of Langmuir adsorption.
5. The computational chemical quantum investigation showed that the protection efficacy improves with an increase in 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 a Fe-complex is formed as a layer that protects the surface of mild steel.
6. CPP was studied for antibacterial activities and its considerable antimicrobial inhibitive characteristics against selected types of bacteria were found.

References

1. K. Jacob and G. Parameswaran, Corrosion inhibition of mild steel in hydrochloric acid solution by Schiff base furoin thiosemicarbazone, *Corros. Sci.*, 2010, **52**, no. 1, 224–228. doi: 10.1016/j.corsci.2009.09.007
2. Z. Khiati, A. Othman, M. Sanchez-Moreno, M. Bernard, S. Joiret, E. Sutter and V. Vivier, Corrosion inhibition of copper in neutral chloride media by a novel derivative of 1,2,4-triazole, *Corros. Sci.*, 2011, **53**, no. 10, 3092–3099. doi: 10.1016/j.corsci.2011.05.042
3. B. Mert, M. Mert, G. Kardaş and B. Yazıcı, Experimental and theoretical investigation of 3-amino-1,2,4-triazole-5-thiol as a corrosion inhibitor for carbon steel in HCl medium, *Corros. Sci.*, 2011, **53**, no. 12, 4265–4272. doi: 10.1016/j.corsci.2011.08.038
4. W. Qafsaoui and H. Takenouti, Corrosion protection of 2024-T3 aluminium alloy by electro-polymerized 3-amino 1,2,4-triazole in sulphate solution containing chloride, *Corros. Sci.*, 2010, **52**, no. 11, 3667–3676. doi: 10.1016/j.corsci.2010.07.014

5. F. Bentiss, M. Traisnel, L. Gengembre and M. Lagrenée, Inhibition of acidic corrosion of mild steel by 3,5-diphenyl-4H-1,2,4-triazole, *Appl. Surf. Sci.*, 2000, **161**, no. 1–2, 194–202. doi: 10.1016/S0169-4332(00)00287-7

6. M. Finšgar and I. Milošev, Inhibition of copper corrosion by 1,2,3-benzotriazole: a review, *Corros. Sci.*, 2010, **52**, no. 9, 2737–2749. doi: 10.1016/j.corsci.2010.05.002

7. M. Zheludkevich, K. Yasakau, S. Poznyak and M. Ferreira, Triazole and thiazole derivatives as corrosion inhibitors for AA2024 aluminium alloy, *Corros. Sci.*, 2005, **47**, no. 12, 3368–3383. doi: 10.1016/j.corsci.2005.05.040

8. S. Zhang, Z. Tao, S. Liao and F. Wu, Substitutional adsorption isotherms and corrosion inhibitive properties of some oxadiazol-triazole derivative in acidic solution, *Corros. Sci.*, 2010, **52**, no. 9, 3126–3132. doi: 10.1016/j.corsci.2010.05.035

9. H. Wang, R. Liu and J. Xin, Inhibiting effects of some mercapto-triazole derivatives on the corrosion of mild steel in 1.0 M HCl medium, *Corros. Sci.*, 2004, **46**, no. 10, 2455–2466. doi: 10.1016/j.corsci.2004.01.023

10. F. Bentiss, M. Lagrenee, M. Traisnel and J. Hornez, The corrosion inhibition of mild steel in acidic media by a new triazole derivative, *Corros. Sci.*, 1999, **41**, no. 4, 789–803. doi: 10.1016/S0010-938X(98)00153-X

11. E. Sherif and S. Park, Effects of 1,4-naphthoquinone on aluminum corrosion in 0.50 M sodium chloride solutions, *Electrochim. Acta*, 2006, **51**, no. 7, 1313–1321. doi: 10.1016/j.electacta.2005.06.018

12. G. Mu, T. Zhao, M. Liu and T. Gu, Effect of metallic cations on corrosion inhibition of an anionic surfactant for mild steel, *Corrosion*, 1996, **52**, no. 11, 853–856. doi: 10.5006/1.3292077

13. D. Mahmood, A.K. Al-Okbi, M.M. Hanon, K.S. Rida, A.F. Alkaim, A.A. Al-Amiery, A. Kadhum and A.A.H. Kadhum, Carbethoxythiazole corrosion inhibitor: as an experimentally model and DFT theory, *J. Eng. Appl. Sci.*, 2018, **13**, no. 11, 3952–3959.

14. A. Kadhim, E.T. Salim, S.M. Fayadh, A.A. Al-Amiery, A.A.H. Kadhum and A. Mohamad, Effect of Multipath Laser Shock Processing on Microhardness, Surface Roughness And Wear Resistance of 2024-T3 Al Alloy, *Sci. World J.*, 2014, 1–6. doi: 10.1155/2014/490951

15. A. Alobaidy, A. Kadhum, S. Al-Baghdadi, A. Al-Amiery, A. Kadhum, E. Yousif and A.B. Mohamad, Eco-friendly corrosion inhibitor: experimental studies on the corrosion inhibition performance of creatinine for mild steel in HCl complemented with quantum chemical calculations, *Int. J. Electrochem. Sci.*, 2015, **10**, 3961–3972.

16. S. Junaedi, A.A.H. Kadhum, A. Al-Amiery, A.B. Mohamad and M.S. Takriff, Synthesis and characterization of novel corrosion inhibitor derived from oleic acid: 2-Amino-5-Oleyl 1,3,4-Thiadiazol (AOT), *Int. J. Electrochem. Sci.*, 2012, **7**, no. 4, 3543–3554.

17. A.Y.I. Rubaye, K.S. Rida, A.Q. Salam and A. Al-Amiery, Acetamidocoumarin as a based eco-friendly corrosion inhibitor, *Int. J. ChemTech Res.*, 2016, **9**, no. 11, 39–47.

18. H.J. Habeeb, H.M. Luaibi, T.A. Abdullah, R.M. Dakhil, A.A.H. Kadhum and A.A. Al-Amiery, Case study on thermal impact of novel corrosion inhibitor on mild steel, *Case Stud. Therm. Eng.*, 2018, **12**, 64–68. doi: 10.1016/j.csite.2018.03.005

19. S.S. Al-Taweel, K.W.S. Al-Janabi, H.M. Luaibi, A.A. Al-Amiery and T.S. Gaaz, Evaluation and characterization of the symbiotic effect of benzylidene derivative with titanium dioxide nanoparticles on the inhibition of the chemical corrosion of mild steel, *Int. J. Corros. Scale Inhib.*, 2019, **8**, no. 4, 1149–1169. doi: 10.17675/2305-6894-2019-8-4-21

20. H.R. Obayes, A.A. Al-Amiery, G.H. Alwan, T.A. Abdullah, A.A.H. Kadhum and A.B. Mohamad, Sulphonamides as corrosion inhibitor: experimental and DFT studies, *J. Mol. Struct.*, 2017, **1138**, 27–34. doi: 10.1016/j.molstruc.2017.02.100

21. D.M. Jamil, A.K. Al-Okbi, S.B. Al-Baghdadi, A.A. Al-Amiery, A. Kadhim, T.S. Gaaz, A.A.H. Kadhum and A.B. Mohamad, Experimental and theoretical studies of Schiff bases as corrosion inhibitors, *Chem. Cent. J.*, 2018, **12**, no. 7, 1–7. doi: 10.1186/s13065-018-0376-7

22. M.H.O. Ahmed, A.A. Al-Amiery, Y.K. Al-Majedy, A.A.H. Kadhum, A.B. Mohamad and T.S. Gaaz, Synthesis and characterization of a novel organic corrosion inhibitor for mild steel in 1M hydrochloric acid, *Results Phys.*, 2018, **8**, 728–733. doi: 10.1016/j.rinp.2017.12.039

23. ASTM G-31-72, Standard recommended practice for the laboratory immersion corrosion testing of metals, ASTM, Philaldelphia, PA, 1990, 401.

24. T.A. Salman, D.S. Zinad, S.H. Jaber, M. Shayaa, A. Mahal, M.S. Takriff and A.A. Al-Amiery, Effect of 1,3,4-thiadiazole scafold on the corrosion inhibition of mild steel in acid medium: an experimental and computational study, *J. Bio Tribo-Corros.*, 2019, **5**, no. 48, 1–11. doi: 10.1007/s40735-019-0243-7

25. H.J. Habeeb, H.M. Luaibi, R.M. Dakhil, A.A.H. Kadhum, A.A. Al-Amiery and T.S. Gaaz, Development of new corrosion inhibitor tested on mild steel supported by electrochemical study, *Results Phys.*, 2018, **8**, 1260–1267. doi: 10.1016/j.rinp.2018.02.015

26. T. Koopmans, Ordering of wave functions and eigenenergies to the individual electrons of an atom, Physica, 1933, **1**, 104–113. doi: 10.1016/S0031-8914(34)90011-2

27. A. Kadhim, A.K. Al-Okbi, D.M. Jamil, A. Qussay, A.A. Al-Amiery, T.S. Gaas, A.A.H. Kadhum, A.B. Mohamad and M.H. Nassir, Experimental and theoretical studies of benzoxazines corrosion inhibitors, *Results Phys.*, 2017, **7**, 4013–4019. doi: 10.1016/j.rinp.2017.10.027

28. A.A. Al-Amiery and L.M. Shaker, Corrosion inhibition of mild steel using novel pyridine derivative in 1 M hydrochloric acid, *Koroze Ochr. Mater.*, 2020, **64**, no. 2, 59–64. doi: 10.2478/kom-2020-0009

29. A.A. Al-Amiery, A.A.H. Kadhum, A.H.M. Alobaidy, A.B. Mohamad and P.S. Hoon, Novel corrosion inhibitor for mild steel in HCl, *Materials*, 2014, **7**, no. 2, 662–672. doi: 10.3390/ma7020662

30. A.A. Al-Amiery, A.A.H. Kadhum, A.B. Mohamad and S. Junaedi, A novel hydrazinecarbothioamide as a potential corrosion inhibitor for mild steel in HCl, *Materials*, 2013, **6**, no. 4, 1420–1431. doi: 10.3390/ma6041420

31. A. Nahlé, R. Salim, F. El Hajjaji, M. Aouad, M. Messali, E. Ech-Chihbi, B. Hammouti and M. Taleb, Novel triazole derivatives as ecological corrosion inhibitors for mild steel in 1.0 M HCl: experimental & theoretical approach, *RSC Adv.*, 2021, **11**, no. 7, 4147–4162. doi: 10.1039/D0RA09679B

32. A. Espinoza-Vázquez, F. Rodríguez-Gómez, I. Martínez-Cruz, D. Ángeles-Beltrán, G. Negrón-Silva, M. Palomar-Pardavé, L. Romero, D. Pérez-Martínez and A. Navarrete-López, Adsorption and corrosion inhibition behaviour of new theophylline–triazole-based derivatives for steel in acidic medium, *R. Soc. Open Sci.*, 2019, **6**, 181738. doi: 10.1098/rsos.181738

33. I. Merimi, R. Benkaddour, H. Lgaz, N. Rezki, M. Messali, F. Jeffali, H. Oudda and B. Hammouti, Insights into corrosion inhibition behavior of a triazole derivative for mild steel in hydrochloric acid solution, *Mater. Today: Proc.*, 2019, **13**, 1008–1022. doi: 10.1016/j.matpr.2019.04.066

34. L. Wang, M. Zhu, F. Yang and C. Gao, Study of a triazole derivative as corrosion inhibitor for mild steel in phosphoric acid solution, *Int. J. Corros.*, 2012, **2012**, no. 6. doi: 10.1155/2012/573964

35. F. Bentiss, M. Bouanis, B. Mernari, M. Traisnel, H. Vezin and M. Lagrenee. Understanding the adsorption of 4H-1,2,4-triazole derivatives on mild steel surface in molar hydrochloric acid, *Appl. Surf. Sci.*, 2007, **253**, no. 7, 3696–3704. doi: 10.1016/j.apsusc.2006.08.001

36. B. El Mehdi, B. Mernari, M. Traisnel, F. Bentiss and M. Lagrenee, Synthesis and comparative study of the inhibitive effect of some new triazole derivatives towards corrosion of mild steel in hydrochloric acid solution, *Mater. Chem. Phys.*, 2003, **77**, no. 2, 489–496. doi: 10.1016/S0254-0584(02)00085-8

37. H. Hassan, E. Abdelghani and M. Amin, Inhibition of mild steel corrosion in hydrochloric acid solution by triazole derivatives: Part I. Polarization and EIS studies, *Electrochim. Acta*, 2007, **52**, no. 22, 6359–6366. doi: 10.1016/j.electacta.2007.04.046

38. S. Ramesh and S. Rajeswari, Corrosion inhibition of mild steel in neutral aqueous solution by new triazole derivatives, *Electrochim. Acta*, 2004, **49**, 811–820. doi: 10.1016/j.electacta.2003.09.035

39. L. Qiu, A. Xie and Y. Shen, A novel triazole-based cationic gemini surfactant: synthesis and effect on corrosion inhibition of carbon steel in hydrochloric acid, *Mater. Chem. Phys.*, 2005, **91**, 269–273. doi: 10.1016/j.matchemphys.2004.11.022

40. B. Mert, M. Mert, G. Kardaş and B. Yazıcı, Experimental and theoretical investigation of 3-amino-1,2,4-triazole-5-thiol as a corrosion inhibitor for carbon steel in HCl medium, *Corros. Sci.*, 2011, **53**, no. 12, 4265–4272. doi: 10.1016/j.corsci.2011.08.038

41. A.A. Al-Amiery, A.A.H. Kadhum, A. Kadihum, A.B. Mohamad, C.K. How and S. Junaedi, Inhibition of mild steel corrosion in sulfuric acid solution by new Schiff base, *Materials*, 2014, **7**, no. 2, 787–804. doi: 10.3390/ma7020787

42. A.B. Mohamad, A.A.H. Kadhum, A.A. Al-Amiery, L.C. Ying and A.Y. Musa, Synergistic of a coumarin derivative with potassium iodide on the corrosion inhibition of aluminum alloy in 1.0 M H₂SO₄, *Met. Mater. Int.*, 2014, **20**, 459–467. doi: 10.1007/s12540-014-3008-3

43. H.R. Obayes, G.H. Alwan, A.H.MJ. Alobaidy, A.A. Al-Amiery, A.A.H. Kadhum and A.B. Mohamad, Quantum chemical assessment of benzimidazole derivatives as corrosion inhibitors, *Chem. Cent. J.*, 2014, **8**, no. 21, 1–8. doi: 10.1186/1752-153X-8-21

44. A.A. Al-Amiery, A.A.H. Kadhum, A.B. Mohamad, A.Y. Musa and C.J. Li, Electrochemical study on newly synthesized chlorocurcumin as an inhibitor for mild steel corrosion in hydrochloric acid, *Materials*, 2013, **6**, no. 12, 5466–5477. doi: 10.3390/ma6125466

45. AA. Abu-Hashem, Synthesis and antimicrobial activity of new 1,2,4-triazole, 1,3,4-oxadiazole, 1,3,4-thiadiazole, thiopyrane, thiazolidinone, and azepine derivatives, *J. Heterocycl. Chem.*, 2021, **58**, 74–92. doi: 10.1002/jhet.4149

46. A. Kadhim, A.A. Al-Amiery, R. Alazawi, M.K.S. Al-Ghezi and R.H. Abass, Corrosion inhibitors. A review, *Int. J. Corros. Scale Inhib.*, 2021, **10**, no. 1, 54–67. doi: 10.17675/2305-6894-2021-10-1-3

47. M. Quraishi and H. Sharma, 4-Amino-3-butyl-5-mercapto-1,2,4-triazole: a new corrosion inhibitor for mild steel in sulphuric acid, *Mater. Chem. Phys.*, 2003, **78**, no. 1, 18–21. doi: 10.1016/S0254-0584(02)00313-9

48. T. Poornima, J. Nayak and A. Shetty, Corrosion inhibition of the annealed 18 Ni 250 grade maraging steel in 0.67 m phosphoric acid by 3,4-dimethoxybenzaldehydethiosemicarbazone, *Chem. Sci. J.*, 2012, **69**, 1–13.

49. M. Abdallah, E.A. Helal and A.S. Fouda, Aminopyrimidine derivatives as inhibitors for corrosion of 1018 carbon steel in nitric acid solution, *Corros. Sci.*, 2006, **48**, no. 7, 1639–1654. doi: 10.1016/j.corsci.2005.06.020

50. M. Hanoon, D.S. Zinad, A.M. Resen and A.A. Al-Amiery, Gravimetrical and surface morphology studies of corrosion inhibition effects of a 4-aminoantipyrine derivative on mild steel in a corrosive solution, *Int. J. Corros. Scale Inhib.*, 2020, **9**, no. 3, 953–966. doi: 10.17675/2305-6894-2020-9-3-10

51. E. Yousif, Y.F. Win, A.H. Al-Hamadani, A. Al-Amiery, A.A.H. Kadhum and A.B. Mohamad, Furosemide as an environmental-friendly inhibitor of corrosion of zinc metal in acid medium: Experimental and theoretical studies, *Int. J. Electrochem. Sci.*, 2015, **10**, 1708–1718.

52. S.B. Al-Baghdadi, F.T.M. Noori, W.K. Ahmed and A.A. Al-Amiery, Thiadiazole as a potential corrosion inhibitor for mild steel in 1 M HCl, *J. Adv. Electrochem.*, 2016, **2**, 67–69.

53. K.F. Al-Azawi, I.M. Mohammed, S.B. Al-Baghdadi, T.A. Salman, H.A. Issa, A.A. Al-Amiery, T.S. Gaaz and A.A.H. Kadhum, Experimental and quantum chemical simulations on the corrosion inhibition of mild steel by 3-((5-(3,5-dinitrophenyl)-1,3,4-thiadiazol-2-yl)imino)indolin-2-one, *Results Phys.*, 2018, **9**, 278–283. doi: 10.1016/j.rinp.2018.02.055

54. S. Junaedi, A. Al-Amiery, A. Kadihum, A.H. Kadhum and A. Mohamad, Inhibition Effects of a Synthesized Novel 4-Aminoantipyrine Derivative on the Corrosion of Mild Steel in Hydrochloric Acid Solution together with Quantum Chemical Studies, *Int. J. Mol. Sci.*, 2013, **14**, 11915–11928. doi: 10.3390/ijms140611915

55. M.H.O. Ahmed, A.A. Al-Amiery, Y.K. Al-Majedy, A.A.H. Kadhum, A.B. Mohamad and T.S. Gaaz, Synthesis and characterization of a novel organic corrosion inhibitor for mild steel in 1 M hydrochloric acid, *Results Phys.*, 2018, **8**, 728–733. doi: 10.1016/j.rinp.2017.12.039

56. A.A. Al-Amiery, F.A.B. Kassim, A.A.H. Kadhum and A.B. Mohamad, Synthesis and characterization of a novel eco-friendly corrosion inhibition for mild steel in 1 M hydrochloric acid, *Sci. Rep.*, 2016, **6**, 19890. doi: 10.1038/srep19890

57. A.A.H. Kadhum, A.B. Mohamad, L.A. Hammed, A.A. Al-Amiery, N.H. San and A.Y. Musa, Inhibition of mild steel corrosion in hydrochloric acid solution by new coumarin, *Materials*, 2014, **7**, no. 6, 4335–4348. doi: 10.3390/ma7064335

58. K. Al-Azawi, S. Al-Baghdadi, A. Mohamed, A.A. Al-Amiery, T.K. Abed, S.A. Mohammed, A.H. Kadhum and A. Mohamad, Synthesis, inhibition effects and quantum chemical studies of a novel coumarin derivative on the corrosion of mild steel in a hydrochloric acid solution, *Chem. Cent. J.*, 2016, **10**, no. 23. doi: 10.1186/s13065-016-0170-3

59. T.A. Salman, Q.A. Jawad, M.A.M. Hussain, A.A. Al-Amiery, L.M. Shaker, A.A.H. Kadhum, M.S. Takriff and R.R. Hussain, New environmental friendly corrosion inhibitor of mild steel in hydrochloric acid solution: Adsorption and thermal studies, *Cogent Eng.*, 2020, **7**, no. 1, 1–17. doi: 10.1080/23311916.2020.1826077

60. A.A. Al-Amiery, Y.K. Al-Majedy, A.A.H. Kadhum and A.B. Mohamad, New coumarin derivative as an eco-friendly inhibitor of corrosion of mild steel in acid medium, *Molecules*, 2015, **20**, no. 1, 366–383. doi: 10.3390/molecules20010366

61. A. Al-Amiery, Coumarin-3-Amine as New Corrosion Inhibitor, *Preprints*, 2017, 2017070096. doi: 10.20944/preprints201707.0096.v1

62. F.G. Hashim, T.A. Salman, S.B. Al-Baghdadi, T. Gaaz and A.A. Al-Amiery, Inhibition Effect of Hydrazine-Derived Coumarin on a Mild Steel Surface in Hydrochloric acid, *Tribologia*, 2020, **37**, no. 3–4, 45–53. doi: 10.30678/fjt.95510

63. A. Al-Amiery, New Corrosion Inhibitor Derived from Coumarin, *Preprints*, 2017, 2017080021. doi: 10.20944/preprints201708.0021.v1

64. I. Abulyazid, E. Mahdy and R. Ahmed, Biochemical study for the effect of henna (*Lawsonia inermis*) on Escherichia coli, *Arabian J. Chem.*, 2013, **6**, no. 3, 265–273. doi: 10.1016/j.arabjc.2010.10.005

65. Y. Sáenz, L. Briñas, E. Domínguez, J. Ruiz, M. Zarazaga, J. Vila and C. Torres, Mechanisms of resistance in multiple-antibiotic-resistant Escherichia coli strains of human, animal, and food origins, *Antimicrob. Agents Chemother.*, 2004, **48**, no. 10, 3996–4001. doi: 10.1128/AAC.48.10.3996-4001.2004

66. J. Meng, S. Zhao, M. Doyle and S. Joseph, Antibiotic resistance of Escherichia coli O157: H7 and O157: NM isolated from animals, food, and humans, *J. Food Prot.*, 1998, **61**, no. 11, 1511–1514. doi: 10.4315/0362-028X-61.11.1511

67. L. Soufi, Y. Sáenz, L. Vinué, M. Abbassi, E. Ruiz, M. Zarazaga, A. Hassen, S. Hammami and C. Torres, *Escherichia coli* of poultry food origin as reservoir of sulphonamide resistance genes and integrons, *Int. J. Food Microbiol.*, 2011, **144**, no. 3, 497–502. doi: 10.1016/j.ijfoodmicro.2010.11.008

♦ ♦ ♦