

Synthesis and characterization of 5-benzyl-5-(4-benzyl-4-methyl piperazin-4-ium-1-yl)-1,3,5-dithiazinan-5-ium as corrosion inhibitor, antibacterial and antifungal.

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Abstract.

According to the domino reaction method, 5-benzyl-5-(4-benzyl-4-methylpiperazin-4-ium-1-yl)-1,3,5-dithiazinan-5-ium has prepared. The structure of the synthesized compound has been characterized by several techniques such as, Fourier Transform Spectroscopy (FT-IR), ¹H-NMR Spectroscopy, Elemental analysis (CHNS), and Mass spectroscopy. Finally, the synthesized compound has been tested as anti corrosion for carbon steel, antibacterial activity against Gram positive bacteria *Staphylococcus aureus*, Gram negative bacteria *Escherichia coli* and antifungal activity against *Candida albicans* (Human Pathogens) at concentrations 10, 20, 30, 40, and 50 µg/ml. The tests have been checked as antibacterial and antifungal according to the disk diffusion method, and it has been checked as anticorrosion by weight loss method in 15% HCl as corrosive medium at 3 hours. The mechanism of corrosion inhibition has been studied, and the adsorption of heterocyclic compound on the carbon steel surface has been studied which follows the Langmuir adsorption isotherm. On the other hand, the temperature affect on the corrosion rate has been studied. The results have shown that heterocyclic compound is a very effective to anticorrosion and moderate for antibiotic(antifungal and antibacterial).

Index: Corrosion inhibitors, Antibacterial, Antifungal, Heterocyclic compounds, Domino reaction, Weight loss method.

I. INTRODUCTION.

The corrosion of metal and its alloys is a common problem with economic implications costing billions of dollars in every year [1]. Metals and alloys are frequently used in industrial applications due to their convenience and low cost. Among these, carbon steel is one of the most important alloys which are widely used [2]. Corrosion degradation of steel reinforcement in concrete is due to aggressive agents present in the surrounding environment, which affects the durability of the structure and leads to the premature failure [3]. The inhibitors used are expected to be chemically stable to provide high protection [4].

Fungi and bacteria are everywhere: in the soil, on trees, in grass and in woodlands, the fur on our pets, our hair, they are on our skin and in our intestinal tract. Fungi, also known as mycophyta, include yeasts, moulds and rusts. Can be

made up of single cells (such as the yeasts) or composed of multi-cellular filaments which are called hyphae (e.g. with the dermatophytes) [5]. Medicinal chemistry is the application of chemical research techniques for the synthesis of pharmaceuticals. Heterocyclic compounds their application obvious in pharmacy medicine, photography, agriculture, antioxidant such as corrosion inhibitors and also the other fields [6].

Heterocyclic compounds, that containing particularly on nitrogen, and sulfur atoms successfully tested against several diseases and therefore received special attention in medicinal field, pharmaceutical and industry field. Heterocyclic compounds for example 1,2,4-triazole derivatives are associated with biological activity such as pesticidal potentialities, herbicides fungicides and anti bacterial [7]. Bacterial and fungal infections have been for many centuries a major cause of death in humans. M. Pitucha, et al. studied the effect of pyrazole derivatives were tested in vitro against two Gram-positive bacteria, that is a drug susceptible strain, *Staphylococcus aureus* FDA 209P and a multidrug resistant strain, *S. aureus* KMP9 (MRSA), and against two Gram-negative bacteria that is a susceptible strain, *Escherichia coli* NIHJ JC-2 and a multidrug efflux pump mutant, *Escherichia coli* W3110 DacrA. The obtained results show that (3-chlorophenyl)-5-(4-phenoxyphenyl)-3-(3-piperidyl) pyrazole hydrochloride and 1-(3-chlorophenyl)-3-[3-(N- methyl) aminopropyl]-5-(4-phenoxyphenyl) pyrazole hydrochloride exhibits comparatively strong antibacterial activity against tested *Staphylococcus aureus* and *Escherichia coli* W3110 DacrA [8,9]. The main objective of this research is evaluation of new heterocyclic compound as anticorrosion through weight loss method, also its evaluation as an antibacterial and fungi through disk diffusion method, and study of mechanism of corrosion inhibition.

II. EXPERIMENTAL.

2.1. Materials.

1-Amino-4-methylpiperazine 99%, 10% formaldehyde, chloroform 99%, sodium sulfate 98% and hydrochloric acid 37% were procured from Sigma-Aldrich. Di methyl sulfoxide DMSO, Benzyl chloride 99% were procured from Merck company, and absolute ethanol 99% were procured from BDH company. Double distilled water was used for all the experiments. Muller Hinton Agar was procured from Himedia, Carbon steel (pipeline) which used in the south oil company, Basra, IRAQ.

2.2. Synthesis of 5-benzyl- 5-(4-benzyl-4-methyl piperazin-4-ium-1-yl)-1,3,5-dithiazinan-5-ium.

A mixture of aqueous solution 10 % formaldehyde (45ml) 150mmol and 50ml absolute ethanol were stirred with 50mmol (6ml) from 1- amino-4-methylpiperazin for 3 hour at a temperature of 0°C, after that the reaction allowed to reach room temperature, then added 100mmol of hydrogen sulfide gas for 1 hour and the product is extracted and dried with Na₂SO₄ for about 5 hrs, then filtered and evaporated even dryness under nitrogen to produce 5-(4-methylpiperazin-1-yl)-1,3,5-dithiazinan. After that, 100mmol of benzyl chloride and 100 ml absolute ethanol have been added to 50mmol of 5-(4-methyl piperazin-1-yl)-1,3,5-dithiazinan for 24 hrs (overnight) at 50°C to produce 5-benzyl- 5-(4- benzyl-4-methylpiperazin-4-ium-1-yl)-1,3,5-dithiazinan-5-ium (white solid). The yield was 62%, m.p. 122-124 °C. Figure (1) shown the structure of heterocyclic compound.

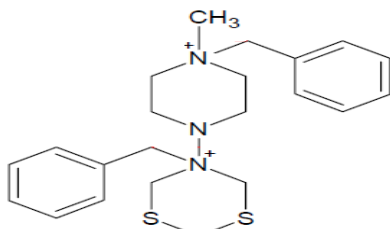


Fig. 1: General structure of heterocyclic compound 5-benzyl- 5-(4-benzyl-4-methylpiperazin-4-ium-1-yl)-1,3,5-dithiazinan-5-ium.

2.3 Instruments.

The mass spectrum was recorded on a Perkin-Elmer Hitachi RMU-6L QP2010 spectrometer at 70 e.V. and temperature 120 °C. Melting point was determined in open capillary tubes by a Gallenkamp apparatus, the IR spectrum obtained, was recorded in KBr disk on a Shimadzu FT-IR 8201 PC spectrometer in the region between 400 and 4000 cm⁻¹. The ¹H-NMR spectrum obtained, was recorded on a BRUKER spectrometer at 500 MHz in deuterium chloroform with TMS as internal reference. Elemental analysis for C, H, N and S, were carried out on elemental analyzer CHNS 628 from LECO company. Incubator, and autoclave apparatus.

2.4. Biological Activities.

The synthesized compound was studied and tested as (antibacterial and antifungal) activity by using agar disc diffusion method [10-12], against gram-positive bacteria *Staphylococcus aureus*, gram-negative bacteria *Escherichia coli* and antifungal, it was dissolved in DMSO-*d*₆ at a concentration 10, 20, 30,40 and 50 µg/ml, in test tube 20 ml. A filter paper, Sd400 type punched into 5 mm disc form and impregnated with different concentrations of the test compound for about 30 minutes (soaked in the test solution) with sterilized by autoclave apparatus, then dried. Muller-Hinton Agar medium was used for culturing bacteria and fungi, prepared from dissolved 38 gm per liter distilled water and neutralized to pH=8 under aseptic condition for about 15 minutes at 121°C and 15 lbs pressure, then it was

cooled to 45°C, after that added to petri plates in depth about 5mm. The bacterial cells were suspended according to the McFarland protocol in 2ml from normal saline, they were stricken by cotton swab on Muller Hinton, and left about 15 minutes to dry, then the synthesized compound disk was put on it, then incubated at 37°C for 22 hrs.. In case of fungi don't differ from the bacteria, in only the activation period and temperature, which lasted 72 hours at 25°C [13-16].

2.5. Anti Corrosion Activities.

The carbon steel cuts into (7×2.5×0.3)cm for length, width, and thickness respectively, and were polished by SiC (grade 140, 320), washed with distilled water, then acetone and finally dry it in a desiccator. Corrosion rate (C_R) in unit (mg cm⁻² h⁻¹), Inhibition efficiency (IE), and Surface coverage (θ) were calculated as follows [17]:

$$C_R = \frac{W_b - W_a}{At} \quad \text{----- (1)}$$

$$IE\% = \left(1 - \frac{W_i}{W_0}\right) \times 100 \quad \text{----- (2)}$$

$$\text{Surface coverage } (\theta) = \left(1 - \frac{W_i}{W_0}\right) \quad \text{----- (3)}$$

Where W_b and W_a are the specimen weight before and after immersion in the tested solution, W₀ and W_i are the values of corrosion right of carbon steel in uninhibited and inhibited solutions respectively. A is the total area of the carbon steel specimen in cm² (40.7cm²), and t is the exposure time (h).

III. RESULTS AND DISCUSSION.

3.1. Characterization of 5-benzyl- 5-(4-benzyl-4-methyl piperazin-4-ium-1-yl)-1,3,5-dithiazinan-5-ium.

Melting point of heterocyclic compound is 122-124 °C. ¹H-NMR, (CDCl₃) δ ppm: 1.993 (s, 3H, CH₃); 2.391-2.521 (t, 4H, CH₃-N-CH₂-CH₂); 2.766-2.916 (t, 4H, N-CH₂-CH₂-N⁺-CH₃); 3.719 (s, 2H, S-CH₂-S); 4.128 (s, 4H, N⁺-CH₂-S); 1.780 (s, 4H, N⁺-CH₂-ph); multiple signal (dd, 10H, Ar-H) in the region 7.66-7.982 ppm assigned to the aromatic protons of phenyl; 7.218 (s, 1H, CDCl₃). MS, m/z (I_{rel}, %): 401 [M]⁺ (13); 77 [C₆H₅]⁺ (67); 134 [C₄H₈NS₂]⁺ (26); 310 [C₁₅H₂₅N₃S₂]⁺ (100); 91 [C₇H₇]⁺ (17); 219 [C₈H₁₇N₃S₂]⁺ (45); 247 [C₁₀H₂₁N₃S₂]⁺ (37); 324 [C₁₆H₂₆N₃S₂]⁺ (66); 190 [C₁₂H₁₈N₂]⁺ (12); 211 [C₁₀H₁₃NS₂]⁺ (17); 295 [C₁₄H₂₁N₃S]⁺ (17); 233 [C₉H₁₉N₃S₂]⁺ (26); 386 [C₁₂H₂₉N₃S₂]⁺ (25); 15 [CH₃]⁺ (23). IR (KBr), ν_{max}/cm⁻¹: The stretching frequency at 690 corresponds to C-S; stretching frequency at 1301.95 corresponds to C-N; stretching frequency at 1051.2 corresponds to N-N; stretching frequency at 1585.49 corresponds to C=C; stretching frequency at 2989.66 corresponds to (C-H aliphatic); stretching frequency, almost at 3100.21 corresponds to (C-H aromatic); and frequencies at 1388.75 and 1415.75 corresponds to C-H bending [7], [18-22], and this pertinent details visible in spectra as shown in figures from (2) to (5) are as follows.

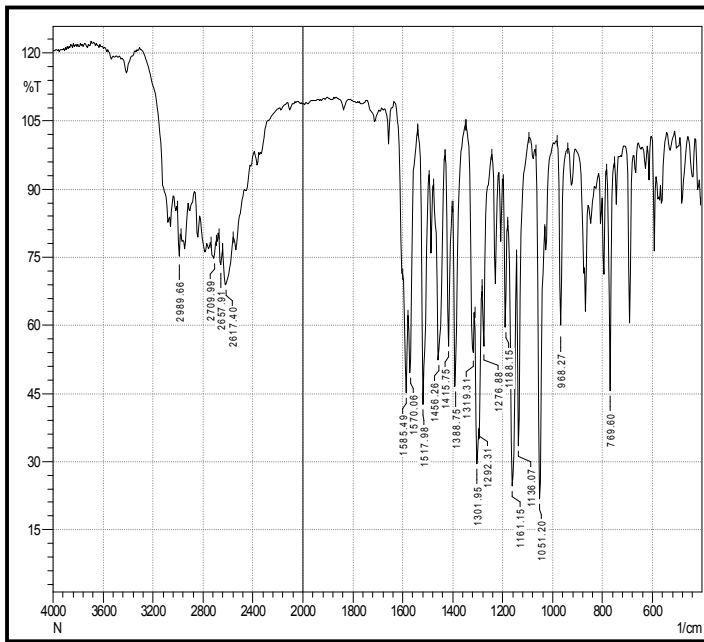


Fig. 2: IR spectrum of heterocyclic compound.

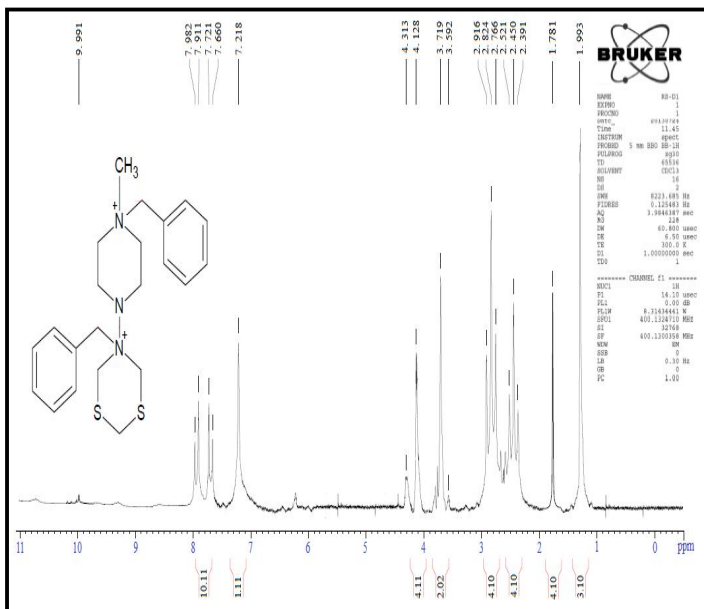


Fig. 3: ¹H-NMR spectrum of heterocyclic compound.

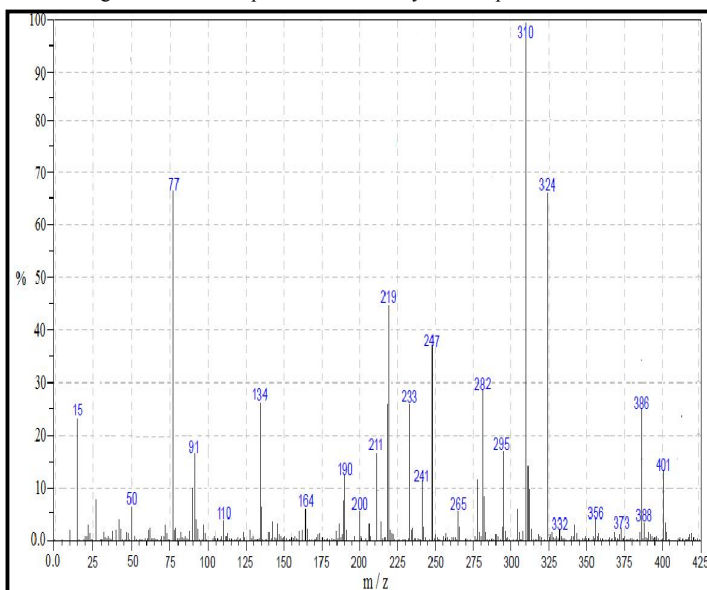


Fig. 4: Mass spectrum of heterocyclic compound.

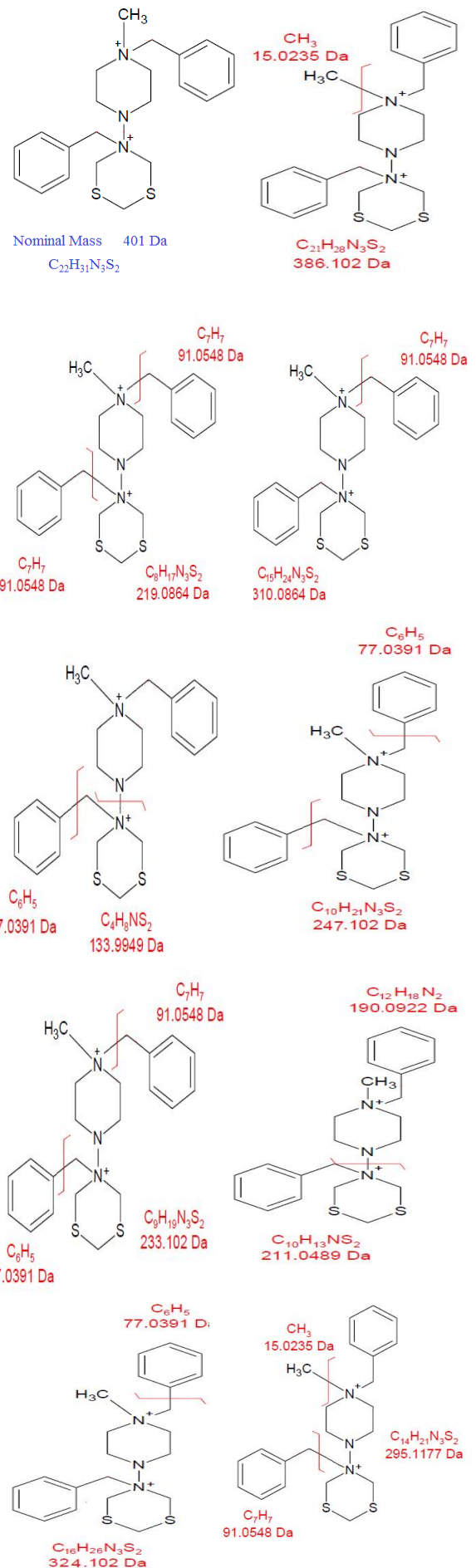


Fig. 5: The most important fragment structures in the mass spectrum of heterocyclic compound.

Besides, the results analysis of C, H, N and S of heterocyclic compound given in Table 1, and as shown that the practical percentages to be identical to large extent with the theoretical percentages, furthermore, the physical data of heterocyclic compound listed in Table 2

TABLE I
SHOWS CHNS ANALYSIS.

Molecular formula	C%		H%		N%		S%	
	Cal.	Found	Cal.	Found	Cal.	Found	Cal.	Found
C ₂₂ H ₃₁ N ₃ S ₂ 401g/mol	65.83	65.87	7.73	7.66	10.47	10.44	15.96	15.99
		65.91		7.79		10.82		16.13
		65.81		7.57		10.32		15.54
		Average 65.86		Average 7.67		Average 10.52		Average 15.88

TABLE II
SHOWS THE PHYSICAL DADT OF HETEROCYCLIC COMPOUND

Molecular formula	Molecular weight	Melting point	Nature of substance	Yield %
C ₂₂ H ₃₁ N ₃ S ₂	401g/mol	122-123 °C	White solid	62

3.2. Anti Corrosion Measurements

Weight loss of carbon steel was calculated in the absence, and presence of different concentrations of inhibitor. Tables 3 and 4 have shown the results of weight loss method obtained in 15% hydrochloric acid solution as a corrosive medium. It was noted from these results that a decrease of both differences in weight loss, and corrosion rate when increasing concentration for both temperatures [23], as well as, they in 15% solution from hydrochloric acid (blank) more than inhibitor presence. Corrosion rate decreases with increasing inhibitor concentration as shows in Figure 6, thus the inhibition efficiency (% IE) increased. Subsequently, it can be concluded that the inhibitor has high efficiency for inhibition in acidic solution, reaching a maximum of (96.00). This may be due to the adsorption of heterocyclic compound onto the carbon steel surface through non-bonding electron pairs of sulfur, and nitrogen atoms as well as the JI- electrons in ring aromatic. Also, it is clear from results in Tables 3,4 and Figure 6, the corrosion rate, and differences in weight loss, increase with the raise of temperature in the absence, and presence of the inhibitor [11],[12],[24].

TABLE III
SHOWS RESULTS OF CORROSION, BY WEIGHT LOSS METHOD AT 298K AND PERIOD 3 HOURS.

Corrosion inhibitor Dosage	Specimen weight (before)	Specimen weight (after)	Difference in weight loss	Corrosion rate mg cm ² h ⁻¹	Inhibition efficiency IE%
15% HCl Blank	40.695	40.301	0.394	0.00322	----
10µg/ml	40.695	40.611	0.084	0.00068	78.90
20µg/ml	40.695	40.625	0.07	0.00057	82.30
30µg/ml	40.695	40.646	0.049	0.00040	87.60
40µg/ml	40.695	40.674	0.021	0.00017	94.80
50µg/ml	40.695	40.679	0.016	0.00013	96.00

TABLE IV
SHOWS RESULTS OF CORROSION, BY WEIGHT LOSS METHOD AT 308 K AND PERIOD 3 HOURS

Corrosion inhibitor Dosage	Specimen weight (before)	Specimen weight (after)	Difference in weight loss	Corrosion rate mg cm ² h ⁻¹	Inhibition efficiency IE%
15% HCl Blank	40.695	40.223	0.472	0.00386	----
10µg/ml	40.695	40.578	0.117	0.00095	75.20
20µg/ml	40.695	40.591	0.104	0.00085	78.00
30µg/ml	40.695	40.633	0.062	0.00050	87.10
40µg/ml	40.695	40.654	0.041	0.00033	91.50
50µg/ml	40.695	40.666	0.029	0.00023	94.10

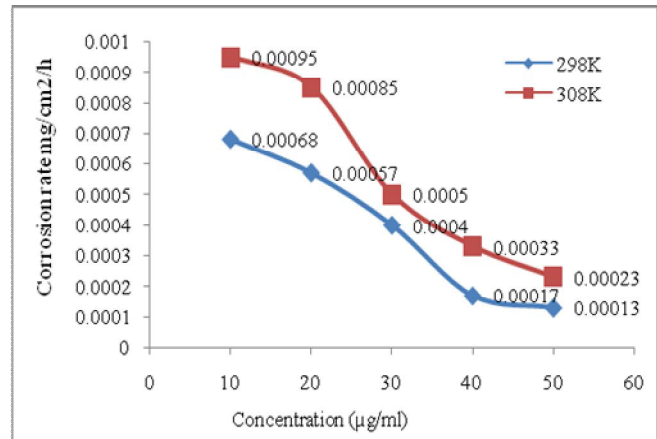


Fig. 6 : Shows decreases corrosion rate for carbon steel with increasing concentration at varying temperatures in 3 hours.

3.2.1. Adsorption Isotherm.

The adsorption depends on the structure of the inhibitor, type of the metal and the nature of its surface, the nature of the corrosion medium and its pH value, the temperature and the electrochemical potential of the metal-solution interface. Also, the adsorption provides information about the interaction between the adsorbed molecules with the metal surface [25]. It generally that the adsorption of the inhibitor on metal surface is an essential step to the explain of inhibition mechanism, and several adsorption isotherms were assessed such as, Langmuir, Temkin, Frumkin, and Freundlich isotherms. Langmuir adsorption isotherm was determined, by plotting C_{inh}/θ versus C_{inh} for various concentrations of inhibitor through using the equation (4) and was noted that it describes of the inhibitor adsorption behavior on the carbon steel surface. It can be concluded that concentration directly proportional with C_{inh}/θ , as shows in Figure 7. Besides, standard free energy of adsorption was calculated from equation 5 [22],[26-31].

$$\frac{C_{inh}}{\theta} = \frac{1}{K_{ads}} + C_{inh} \quad (4)$$

$$\Delta G_{ads}^{\circ} = - RT \ln(55.5 K_{ads}) \quad (5)$$

This equation can also be express in the form as follows

$$K_{ads} = \frac{1}{55.5} \exp\left(\frac{-\Delta G_{ads}^{\circ}}{RT}\right) \quad (6)$$

Where K_{ads} the equilibrium constant of the adsorption reaction, and its value calculated from the intercept line on the C_{inh}/θ axis, and by using the value of K_{ads} the value of ΔG_{ads} was calculate by equation 5. C_{inh} is the inhibitor concentration in the bulk of the solution, R is the gases constant $8.314 \text{ J.mol}^{-1} \text{ K}^{-1}$, T is the temperature in Kelvin 298K, and 55.5 is the concentration of water in solution in mol.L^{-1} . The intercept is represent $1/K_{ads}$, and all activation parameters are given in table 5.

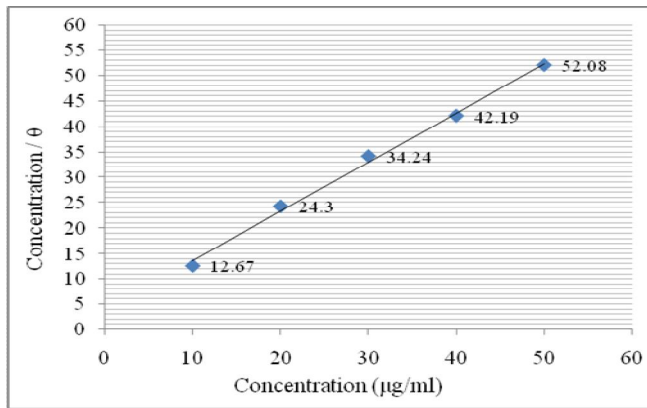


Fig.7 : Langmuir isotherm adsorption of heterocyclic compound on the surface of carbon steel in 15% HCl at 298K.

TABLE V
SHOWS THE LANGMUIR ISOTHERM PARAMETERS OF INHIBITOR IN 15% HCl SOLUTION.

Slope	Intercept	R ²	K _{ads}	- ΔG (KJ. mol ⁻¹)
0.9655	4.115	0.9979	0.243	-6.44

Generally, the value of ΔG_{ads} if the -20 kJ.mol^{-1} or less value that are consistent with the electrostatic interaction between the charged metal and the charged molecules (physical adsorption), while those more negative than $(-40 \text{ kJ.mol}^{-1})$ the adsorption is chemical adsorption, and ΔG_{ads} values between $(-20 \text{ and } -40 \text{ KJ.mol}^{-1})$ meaning they from type mixed- adsorption (physical adsorption and chemisorption occur tandem) [31-33].

The ΔG_{ads} negative value indication of adsorption of inhibitor on the carbon steel surface is spontaneous. Results this study shown in Table 5 and Figure 7, noted the ΔG_{ads} value obtained for heterocyclic compound on carbon steel surface in 15% HCl solution are $-6.44 \text{ KJ.mol}^{-1}$, this indicates that the adsorption of studied inhibitor is physical adsorption, and the negative value of ΔG_{ads} indicate also a spontaneous adsorption process, and stability of the adsorbed film on carbon steel surface [34-35]. The slope close to 0.9655, indicating that the adsorption of the inhibitor on the carbon steel surfaces is well depended to the Langmuir adsorption isotherm [36]. Also, in the present study found value of the adsorption equilibrium constant ($K_{ads} = 0.243$), this indicating the strong adsorption of heterocyclic compound (inhibitor) on the carbon steel surface [34]. A plot of C_{inh}/θ versus C_{inh} as shown in Figure 7 gives a straight line at correlation coefficient is close to 0.9979 was used to determine the best fit ($R^2=0.9979$ for the compound), suggests that the adsorption

of inhibitor molecules on the carbon steel surface obeys Langmuir adsorption isotherm, which can be expressed by the equation 4 previously mentioned [31-32],[37].

3.2.2. Mechanism of Corrosion Inhibition.

The results which obtained from characterization of heterocyclic compound which explained the structure is contain on nitrogen and sulfur hetero atoms, and π bond in ring aromatic. In addition, from adsorption isotherm results, can be concluded the corrosion process inhibition and adsorption of heterocyclic compound molecules on carbon steel surface in 15% HCl solution, discussed they as a following (i) Interaction between unshared electron pairs of hetero atoms (N,S) in the inhibitor molecule and vacant d- orbital of iron surface atoms by coordination bonds (Chemisorption adsorption) [28],[38-42],(ii) Interaction of π -electrons in aromatic rings with d-orbitals of iron surface atoms [40-41], (iii) Interaction between the positively charged molecules and the negatively charged metal surface by Vander Waals force [43-44], and (iv) A combination of mechanism the above- mentioned [45-46]. Besides possible explain the mechanism of inhibition according to the number of transferred electrons ΔN . If the value of $\Delta N < 3.6$ the inhibition efficiency increased with increasing electron donating ability of inhibitor at the metal surface (Chemical adsorption). It is observed from Table (6) that the value of ΔN is 0.546, and less than 3.6, thus the inhibition efficiency increased with increasing electron donating ability, another words increasing electron donating ability meaning increasing inhibitor molecular. The number of transferred electrons ΔN is depending on the quantum chemical method and calculated using the equation 7 [47-50].

$$\Delta N = (\chi_{Fe} - \chi_{inh}) / [2 (\eta_{Fe} + \eta_{inh})] \text{ ----- (7)}$$

Where χ_{Fe} and χ_{inh} are denote the absolute electro negativity of iron and inhibitor molecule respectively; η_{Fe} and η_{inh} are the global hardness of iron and the inhibitor molecules respectively. The theoretical values of χ_{Fe} and η_{Fe} are 7 and 0 eV/mol respectively. The χ_{inh} and η_{inh} calculated using the equations 8 and 9 respectively.

$$\chi_{inh} = -[(E_L + E_H)/2] \text{ -----(8)}$$

$$\eta_{inh} = (E_L - E_H)/2 \text{ -----(9)}$$

Where E_H is E_{HOMO} and E_L is E_{LUMO} . ΔE is energy of the gap and calculated using the equation 10

$$\Delta E = (E_{LUMO} - E_{HOMO}) \text{ -----(10)}$$

TABLE VI
QUANTUM CHEMICAL PARAMETERS OF THE INVESTIGATED INHIBITOR

E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)	χ_{inh} (eV mol ⁻¹)	$\eta_{inh} \Delta E/2$ (eV mol ⁻¹)	ΔN
-6.55	3.23	9.78	1.66	4.89	0.546

3.3. The Screening of Antibacterial and Antifungal.

The compound was tested as antibacterial and antifungal. The inhibition zones caused by the using various concentrations of heterocyclic compound were examined after 22 hrs for the bacteria and 72 hrs for fungus. It is clear from results as shown in Table 7 and Figures 8 and 9 that compound slightly active (moderate effectiveness) against gram negative bacteria *Escherichia coli* and against gram positive bacteria *Staphylococcus aureus*. But it more active in inhibition of fungi *Candida albicans*. The activity is may be due to that the compound contains on the hetero atoms like N and S which contenting electrons. It was found that molecules of inhibitor generally has passed through *Staphylococcus aureus* cell wall by passive diffusion but, the presence of outer membrane of peptidoglycon in *E. coli* may prevent the transport of molecules of inhibitor to the cell [57-58]. On the other hand, the passage across the outer membrane depended upon the chemical nature of inhibitor. The results shows that the varying concentrations of compound has given diameters of inhibitory zones different, and higher concentration 50 $\mu\text{g/ml}$ has been given the maximum for inhibiting of bacteria and fungi, against the *Staphylococcus aureus*, *Escherichia coli* and *Candida albicans*, thus, the maximum inhibition zone was obtained in *Staphylococcus aureus*, *Escherichia coli* and *Candida albicans* at 50 $\mu\text{g/ml}$ are, 13 mm, 12 mm and 18 mm respectively. The diameter of inhibition zone of *Staphylococcus aureus* is similar to a large extent to *Escherichia coli*, and inhibition zone (in mm) includes the diameter of disc (5 mm). Also, results noted to that bacterial more resistant from fungi when using heterocyclic compound. However, the discrepancies in the results obtained, relied on various intrinsic and extrinsic factors, such as molecular weight, and pH. [51-58].

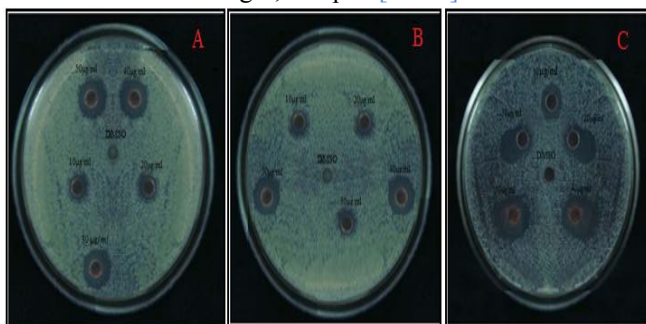


Fig.8: Inhibition zone of heterocyclic compound at different concentrations , against *Staphylococcus aureus* (A), *Escherichia coli* (B) and *Candida albicans* (C).

TABLE VII
DIAMETERS OF INHIBITORY ZONES OF HETEROCYCLIC COMPOUND.

Zone of Inhibition (in mm.)			
Concentrations	Gram- positive bacteria <i>S. aureus</i>	Gram- negative bacteria <i>E.coli</i>	Antifungal <i>C. albicans</i>
10 $\mu\text{g/ml}$	9	9	11
20 $\mu\text{g/ml}$	9	9	14
30 $\mu\text{g/ml}$	13	9	14
40 $\mu\text{g/ml}$	13	12	17
50 $\mu\text{g/ml}$	13	12	18
DMSO negative control	No zone	No zone	No zone

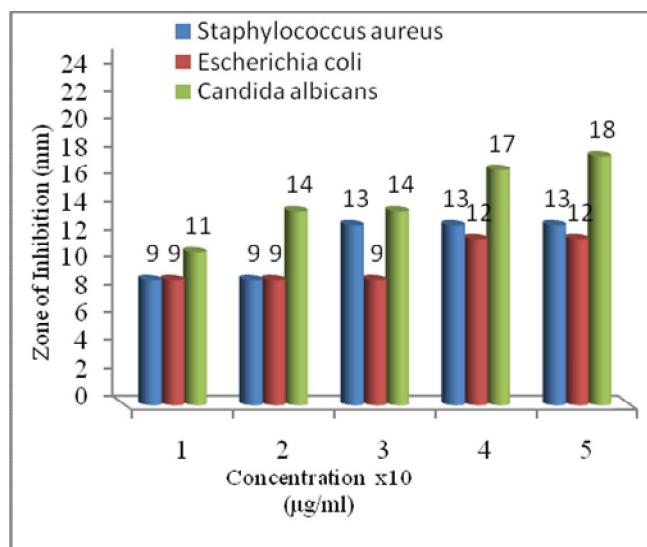


Fig. 9 : Shows the zone of inhibition of heterocyclic compound , against bacterial and fungal by disc diffusion method.

IV. CONCLUSIONS.

In the present study the heterocyclic compound has been evaluated for anticorrosion, antibacterial, and antifungal. The results of weight loss method explained that the heterocyclic compound has excellent inhibition properties for carbon steel. Furthermore, it has a moderate efficiency as a antibacterial and antifungal, in other words, its inhibition for corrosion more than antibiotics. The adsorption of heterocyclic compound on the carbon steel surface follows the Langmuir adsorption isotherm. ΔG_{ads} value obtained of heterocyclic compound on carbon steel $-6.44 \text{ KJ.mol}^{-1}$ this indicates that the adsorption of inhibitor is physical adsorption. Besides, quantum chemical explained the inhibition efficiency increases with increasing electron donating ability of inhibitor to the metal surface (Chemical adsorption) thus the occurs chemical adsorption and physical adsorption together (mixture of both processes). It is observed that the inhibition efficiency decreases with increase temperature in acidic medium.

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