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# Original Research Article

# Synthesis, Characterization and Anti-corrosion Activity of New Triazole, Thiadiazole and Thiazole Derivatives Containing Imidazo[1,2-a]pyrimidine Moiety

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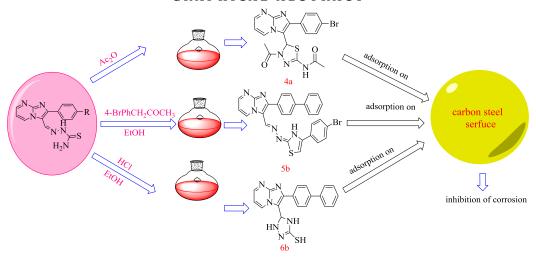
### KEYWORDS

Imidazo/pyrimidine Triazole Thiadiazole Thiazole Anti-corrosion

#### ABSTRACT

In this research, several heterocyclic rings (triazole, thiadiazol, thiazol) containing imidazo (1,2-a) pyrimidine moiety have been prepared via a series of reactions. To do this, synthesis of 2-substituted imidazo (1,2-a) pyrimidine was performed by condensation of 2-aminopyrimidine with (4-bromo phenacyl bromide) or (4-phenyl phenacyl bromide). Carbaldehyde group was prepared at position-3 of 2-substituted imidazo/pyrimidine rings by Vilsmeier-Haak reaction. Thiosemicarbazon derivatives (Schiff bases) were synthesized by condensation of 3-carbaldehyde derivatives thiosemicarbazide. Cyclization of thiosemicarbazone derivatives with Ac2O, 4bromophenacyl bromide and HCl afforded the thiadiazole(diacetyl) derivatives, 1,3-thiazole derivatives and 1,2,4-triazole derivatives respectively. Structures of the new derivatives were confirmed via FT-IR spectroscopy, some of which were confirmed via 1H-NMR spectroscopy. Three of these new derivatives were evaluated by their anti-corrosion activity.

# GRAPHICAL ABSTRACT



### Introduction

One of the most important core structure in organic compounds is Imidazo-fused heterocyclic scaffolding, which is found in many natural products and biologically active molecules that have antibacterial [1], anticancer [2], antimicrobial [3], antifungal [4], antiviral [5] and anti-inflammatory [6] activities. These are structural motifs of various marketed drugs [7] such as divaplon and fasiplon [8]. Because of their wide range of intriguing pharmacological imidazo-fused pyrimidines activity, are extremely important in the pharmaceutical industry [9]. Thiosemicarbazone was used as an intermediate in the production of a variety of heterocyclic compounds. Next, various reagents and conditions were used to cyclize the compounds to produce certain novel heterocyclic compounds (thiadiazole, thiazole and 1,2,4triazole) bearing imidazo/pyrimidine moiety. Thiadiazol is a five-membered heterocyclic structure of a sulfur atom and two nitrogen atoms that is well-known and commonly used. It contains several isomers, including 1,2,3thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, and 1,3,4- thiadiazole [10]. Thiadiazol system has great spectrum of biological activities such as

anti-cancer [11], anti-hypertensive [12], anti-

convulsants [13], anti-oxidant [11,14], anti-

inflammatory [15], anti-fungal [16], activity as

herbicides [17], anti-tubercular agents [18].

Moreover, many drugs contain 1,3,4-thiadiazole

core of clinical use such as acetazolamide,

methazolamide, sulfamethizole megazol, ancefazolin [19]. On the other hand, thiazoles (1,3-thiazoles) and isothiazoles (1,2-thiazoles) are aromatic heterocycles of five members containing one sulfur and one nitrogen atom [20]. A broad range of biologically active both natural and medicinal compounds, products, contain the thiazole ring [21]. This is present in natural products, such as peptides [22], epothilone [23], vitamins (thiamine), alkaloids [24] and chlorophyll [25]. Thiazole derivatives have shown numerous biological activities, which include antioxidant [26], antitubercular [27], antibacterial [28]. Many drugs known in the pharmaceutical field contain thiazole core, such nitazoxanide(antiparasitic), abafungin (antifungal), dasatinib (antineoplastic), meloxicam (anti-inflammatory) [29].

also organic Triazoles are heterocyclic five-membered compounds with a ring containing two carbon atoms and three nitrogen atoms. There are two isomeric groups of triazoles: 1,2,3-triazole, and1,2,4-Triazol [30]. Derivatives of triazole have various pharmacological properties, such as anti-malarial [31], anti-cancer [32], anti-tubercular [33], antibacterial [34]. Furthermore, a number of drugs that contain triazole ring such as (fluconazole, Ribavirin, Brassinazole) Finally, there are several synthesized derivatives of thiadiazole, thiazole and triazole possess anticorrosion activity (Figure 1) [36-41].

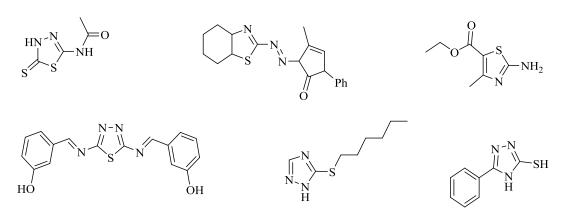


Figure 1: synthesized derivatives bearing thiadiazole, thiazole and triazole moiety

### Material and methods

1- In the College of Sciences, University of Baghdad, a SHIMADZU FT-IR 8300 Fourier transform infrared spectrophotometer was used to calculate infrared spectra for prepared derivatives as a KBr disc in the wave range (4000-400) cm<sup>-1</sup>.

NMR (¹H-NMR & ¹³C-NMR) spectral data were recorded on spectrophotometer of Bruker model Ultra shield 500 Mega Hertz using DMSO as solvent (Isfahan University of Technology (IUT), Iran) and (Sharif University of Technology (SUT). 2- The melting point was determined using an open capillary system with a hot stage Gallen Kamp melting point apparatus (m.p.).

General procedure for synthesis of 2-(4-bromo phenyl) / 2-(4-phenyl phenyl) imidazo(1,2-a)pyrimidine (1a, 1b)

In 20 ml of ethanol, a mixture of 2-amino pyrimidine (0.01 mol) and 4-bromo phenacyl bromide (0.01 mol) was dissolved. The mixture was refluxed for 6 hours. The solution was then cooled and basified with NaoH (5%) until pH10 was achieved. The resulting solid was purified

**Table 1:** Physical properties of compounds (1a-b)

and recrystallized with ethanol after being washed with water.

2-(4-bromo phenyl) imidazo[1,2-])pyrimidine (1a)

FT-IR (KBr/cm<sup>-1</sup>): 3087 (Ar-H), 1631(C=N) imidazo, 1596 (C=N) pyrimidine, 1596 and 1521(C=C).  $^{1}$ H-NMR (DMSO, 500 MHz)  $\delta$ : 8.83-8.78 ppm (m, 3H Ar-H), 7.78-7.55 ppm (m, 4H, Ar-H), 7.28 ppm (d, H, Ar-H).  $^{13}$ C-NMR (DMSO, 500 MHz)  $\delta$ : 155.5, 148.8 ppm (C=N), 140.1, 135.2, 132.1, 128.3, 123.1, 109.6, 107.4 ppm (C=C).

2-(4-phenyl) imidazo (1,2-a)pyrimidine (1b)

IR (KBr/cm<sup>-1</sup>): 3029(Ar-H), 1635 (C=N) imidazo, 1602 (C=N) pyrimidine, 1556 and 1533 (C=C).  $^{1}$ H-NMR (DMSO, 500 MHz)  $\delta$ : 8.79-8.63 ppm (m, 3H, Ar-H), 8.3 ppm (d, 2H, Ar-H), 7.85-7.75 ppm (m, 4H, Ar-H), 7.49 ppm (m, 3H, Ar-H), 7.23 ppm(d, Ar-H).  $^{13}$ C-NMR (DMSO, 500 MHz)  $\delta$ : 153.1, 146.3 ppm (C=N), 141.4, 135.1, 132.3, 128.2, 126.4, 125.7, 109.6, 106.3 ppm (C=C).

Compound No.	Compound No. R		M.P. (°C)	Color	Yield (%) 89	
1a	-Br	C <sub>12</sub> H <sub>8</sub> BrN <sub>3</sub> 204		Dark orange		
1b		C <sub>18</sub> H <sub>13</sub> N <sub>3</sub>	180	Off orange	87	

General procedure for synthesis of 2-aryl imidazo[1,2-a[pyrimidine-3-carbaldehyde (2a, 2b)

Phosphorus oxychloride (POCl<sub>3</sub>) (5 ml) was added drop wise to a RB flask containing DMF (3 ml) and the temperature was held below 10 °C. 10 minutes was spent on stirring the reaction mixture and then a solution of compound (1a/1b) (2.5 g, 0,009 mol) in DMF (25 ml) was added. The reaction mixture was heated at 70 °C for 12 hours. The mixture was then allowed to cool before being poured onto crushed ice. After

that, the precipitate was washed with a lot of water and purified with a mixture of ethanol and acetone (1:1).

2-(4-bromophenyl)imidazo[1,2-a]pyrimidine-3-carbaldehyde (2a)

FT-IR (KBr/cm<sup>-1</sup>): 2852, 2923 (C-H aldehyde), 3085, 3060 (Ar-H), 1677(C=O), 1620 (C=N) imidazo, 1585 (C=N) pyrimidine, 1564 (C=C). <sup>1</sup>H-NMR (DMSO, 500 MH<sub>Z</sub>) δ: 10.01ppm (s, 1H, CHO), 7.91-7.88 ppm (d, 2H, Ar-H), 7.76-7.73 ppm (m, 4H, Ar-H), 7.32 ppm (d, 1H, Ar-H). <sup>13</sup>C-NMR (DMSO, 500 MH<sub>Z</sub>) δ: 179.2 ppm (C=O), 157.6,

153.1 ppm (C=N), 159.3, 136.7, 135.2, 133.6, 132.1, 128.3, 123.1, 109.6 ppm (C=C).

2-(4-phenyl phenyl) imidazo (1,2-a)pyrimidine-3-carbaldehyde (2b)

FT-IR (KBr/cm<sup>-1</sup>): 2962, 2827 (C-H aldehyde), 3083, 3058 (Ar-H), 1670 (C=O), 1639 (C=N) imidazo, 1583 (C=N) pyrimidine, 1533 (C=C). <sup>1</sup>H-

Table 2: Physical properties of compounds (2a-b)

NMR (DMSO, 500 MHz)  $\delta$ : 9.75 ppm (s, 1H, CHO), 8.01-7.87 ppm (m, 2H, Ar-H), 7.61-7.12 ppm (m, 6H, Ar-H), 6.97-6.54 ppm (m, 3H, Ar-H), 6.21 ppm (d, 1H, Ar-H),  $^{13}$ C-NMR (DMSO, 500 MHz)  $\delta$ : 183.2 ppm (C=O), 157.6, 155.3 ppm (C=N), 159.3, 140.8, 136.1, 134.3, 131.6, 129.2, 127.3, 126.4, 108.3 ppm (C=C).

Com. No.	R	M.F.	M.P. (°C)	Color	Yield (%)
2a	-Br	-Br C <sub>13</sub> H <sub>8</sub> BrN <sub>3</sub> O		white	89
2b		$C_{19}H_{13}N_3O$	184	Off white	93

General procedure for synthesis of thiosemicarbazone (3a, 3b)

In absolute ethanol (20 ml) with 2-3 drops of glacial acetic acid, an equimolar of aldehyde (2a/2b) (0.01 mol) and thiosimecarbazide (0.01 mol) were refluxed for 4hours. Following the end of the reflux, the mixture was cooled to room temperature, and the solid product was washed with cold water, purified with ethanol to yield compounds (3a/3b).

(E)-2-((2-(4-bromophenyl)imidazo[1,2-a]pyrimidine-3-yl)methylene)hydrazine-1-carbothioamide (**3a**)

FT-IR (KBr/cm $^{-1}$ ): 3477, 3353 (-NH $_2$ ), 3234 (NH), 1623 (C=N) imine, 1583 (C=N) imidazo, 1519 (C=N) pyrimidine, 1477(C=C).  $^{1}$ H-NMR (DMSO, 500 MH $_2$ )  $\delta$ : 11.31 ppm (s, 1H, NH), 9.56-8.68 ppm (m, 2H, Ar-H), 8.26-7.52 ppm (m, 4H, Ar-H), 7.55 ppm (m, 2H, NH $_2$ ), 7.14 ppm (d, 1H, Ar-H), 7.11 ppm (s, 1H, N=CH).  $^{13}$ C-NMR (DMSO, 500

Table 3: Physical properties of compounds (3a-b)

MH<sub>z</sub>)  $\delta$ : 176.9 ppm (C=S), 148.9, 146.16 ppm (2C=N), 135.34 ppm (C=N Schiff), 132.4, 131.63, 129.84, 121.93, 122.23, 116.66, 115.13, 114.44 ppm (C=C).

(*E*)-2-((2-([1,1-biphenyl]-4-yl)imidazo[1,2-a]pyrimidine-3-yl)methylene)hydrazine-1-carbthioamide (**3b**)

FT-IR (KBr/cm<sup>-1</sup>): 3332, 3245 (NH<sub>2</sub>), 3168 (NH), 1649 (C=N) imine, 1579 (C=N) imidazo, 1558 (C=N) pyrimidine, 1479 (C=C). <sup>1</sup>H-NMR (DMSO, 500 MH<sub>Z</sub>)  $\delta$ : 11.29 ppm (s, 1H, NH), 8.83-8.73 ppm (m, 2H, Ar-H), 8.3-7.49 ppm (m, 8H, Ar-H), 7.85 ppm (m, 2H, NH<sub>2</sub>), 7.41,7.28 ppm (m, 2H, Ar-H), 7.13 ppm (s, 1H, N=CH Schiff). <sup>13</sup>C-NMR (DMSO, 500 MH<sub>Z</sub>)  $\delta$ : 178.7 ppm (C=S), 155.5, 148.8 ppm (2C=N), 139.2 ppm (C=N Sciff), 146.1, 140.8, 135.2, 129.3, 127.4, 116.4, 109.6 ppm (C=C).

$$N$$
 $N$ 
 $H$ 
 $N$ 
 $S$ 
 $H_2N$ 

				,	
Com. No.	R	M.F.	M.P. (°C)	Color	Yield (%)
3a	-Br	C <sub>14</sub> H <sub>11</sub> BrN <sub>6</sub> S	298	Yellow	78
3b		C <sub>20</sub> H <sub>16</sub> N <sub>6</sub> S	283	Dark yellow	73

General procedure for synthesis of (1,3,4-thiadiazol-2-yl) acetamide derivatives (4a/4b)

A mixture of thiosemicarbazone derivatives (3a/3b) and acetic anhydride (12 ml) was refluxed for 5hours with continuous stirring and then allowed to cool at room temperature. After that, the mixture was added to (400 ml) of ice-cold water and then stirred at room temperature for 1hours. The resulting precipitate was filtered, washed with water, dried, and purified with ethanol and DMF (2:1) to give the final product (4a/4b).

N-(4-acetyl-5-(2-(4-bromophenyl))imidazo[1,2-a]pyrimidin-3-yl)-4-5-dihydro-1,3,4-thiadiazol-2-yl)acetamide (4a)

FT-IR (KBr/cm<sup>-1</sup>): 1764, 1703 (C=O), 3114 (-NH), 3085 (Ar-H), 1633 (C=N) imidazo, 1595 (C=N) pyrimidine, 1450 (C=C).  $^1$ H-NMR (DMSO, 500 MH<sub>z</sub>)  $\delta$ : 13.86 ppm (s, 1H, NH), 8.81, 8.71 ppm (m, 2H, Ar-H), 7.78-7.28 ppm (m, 5H, Ar-H), 5.92 ppm (s, 1H, NCHS), 1.98, 1.83 ppm (s, 6H, 2CH<sub>3</sub>).

Table 4: Physical properties of compounds (4a-b)

<sup>13</sup>C-NMR (DMSO, 500 MH<sub>z</sub>) δ: 169.2, 167.3 ppm (2C=0), 155.5, 148.7, 145.5 ppm (3C=N), 134.8, 132.1, 131.3, 123.1, 108.6 ppm(C=C), 47.9 ppm (N-C-S), 22.7 ppm (2CH<sub>3</sub>).

N-(5-(2-([1,1-biphenyl]-4-yl)imidazo[1,2-a]pyrimidin-3-yl)-4-acetyl-4-5-dihydro-1,3,4-thiadiazol-2-yl)acetamide (**4b**)

FT-IR (KBr/cm<sup>-1</sup>): 1691, 1666 (C=O), 3130 (-NH), 3056 (Ar-H), 1606 (C=N) imidazo, 1558 (C=N) pyrimidine, 1485, 1446 (C=C).  $^1$ H-NMR (DMSO, 500 MHz)  $\delta$ : 13.86 ppm (s, 1H, NH), 8.81, 8.69 ppm (m, 2H, Ar-H), 8.1-7.28 ppm (m, 10H, Ar-H), 5.92 ppm (s, 1H, NCHS), 1.72, 1.91 ppm (s, 6H, 2CH<sub>3</sub>).  $^{13}$ C-NMR (DMSO, 500 MHz)  $\delta$ : 171.1, 168.3 ppm (2C=O), 157.3, 149.1, 145.4 ppm (3C=N), 141.6, 135.3, 131.5, 131.1, 129.7, 128.3, 127.5, 111.3 ppm (C=C), 49.3 ppm (NCHS), 23.1 ppm (2CH<sub>3</sub>).

$$0 \longrightarrow N \longrightarrow N$$

$$N \longrightarrow N$$

Com. No.	R	M.F. M.P. (°C)		Color	Yield (%)
4a	4a -Br		175	Off yellow	80
4b		$C_{24}H_{20}N_6O_2S$	167	brown	83

General procedure for synthesis of 2,3-dihydrothiazole derivatives (5a,5b)

In the presence of anhydrous sodium acetate, a mixture of thiosemicarbazon derivatives (3a/3b) (0.01 mol) and 4-bromophenacylbromide (0.01 mol) in absolute ethanol (20 ml) was refluxed for 6 hours. After that, the mixture was cooled to room temperature. Then, the separated solid product was filtered off and recrystallized from ethanol to give (5a/5b) compounds.

(Z)-2-(((E)-(2-(4-bromophenyl)imidazo[1,2-a]pyrimidin-3-yl)methylene)hydrazono)-2,3-dihydrothiazole (5a)

FT-IR (KBr/cm<sup>-1</sup>): 3180 (NH), 3043 (Ar-H), 1631 (C=N) imine, 1595 (C=N) imidazo, 1556 (C=N) pyrimidine, 1402, 1373 (C=C), 740 (C-S-C).  $^{1}$ H-NMR (DMSO, 500 MHz)  $\delta$ : 10.13 ppm (s, 1H, NH), 8.83, 8.78 ppm (m, 2H, Ar-H), 7.69-7.12 ppm (m, 10H, Ar-H), 7.95 ppm (s, 1H, N=CH Schiff).  $^{13}$ C-NMR (DMSO, 500 MHz)  $\delta$ : 163.3, 158.7 ppm (2C=N imine), 155.3, 148.7 ppm (2C=N), 161.9,

146.6, 135.6, 133.5, 132.1, 131.5, 128.3, 123.1, 116.2, 108.3 ppm (C=C).

(Z)-2-(((E)-(2-([1,1-biphenyl]-4-yl)imidazo[1,2-a]pyrimidin-3-yl)methylene)hydrazono)-2,3-dihydrothiazole (**5b**)

FT-IR (KBr/cm<sup>-1</sup>): 3321 (NH), 3031 (Ar-H), 1631 (C=N) imine, 1602 (C=N) imidazo,

Table 5: Physical properties of compounds (5a-b)

$$\begin{array}{c|c}
N & N \\
N & N
\end{array}$$

$$\begin{array}{c|c}
N & H \\
N & N
\end{array}$$

$$\begin{array}{c|c}
B1 & \\
\end{array}$$

Com. No.	R	M.F.	M.P. (°C)	Color	Yield (%)	
5a	-Br	$C_{22}H_{14}Br_2N_6S$	314	orange	71	
5b		C <sub>28</sub> H <sub>19</sub> BrN <sub>6</sub> S	308	brown	67	

General procedure for synthesis of 1,2,4-triazole-3-thiol derivatives (6a/6b)

A thiosemicarbazon derivative (3a/3b) (0.01 mol) was dissolved in absolute ethanol (15 ml) in the presence of few drops of HCl and then refluxed for 2 hours. The solid formed after cooling and dilution with water was filtered, washed with water, dried, and purified with ethanol to yield compounds (6a/6b) as powder.

5-(2-(4-bromophenyl)imidazo[1,2-a]pyrimidine-3-yl)-4,5-dihydro-1H-1,2,4-triazole-3-thiol (6a) FT-IR (KBr/cm<sup>-1</sup>): 3259, 3132(-NH-), 3089 (Ar-H), 1631 (C=N) imidazo, 1595(C=N) pyrimidine, 1544, 1492 (C=C), 2574 (SH). <sup>1</sup>H-NMR (DMSO, 500 MH<sub>Z</sub>) δ: 11.97, 9.95 ppm (s, 2H, 2NH), 8.83, 8.73 ppm (m, 2H, Ar-H), 7.69-7.28 ppm (m, Ar-H), 5.11 ppm(s, 1H, CH), 1.5 ppm(s, 1H, SH). <sup>13</sup>C-

**Table 6:** Physical properties of compounds **(6a-b)** 

NMR (DMSO, 500 MH<sub>z</sub>) δ: 155.5, 149.1, 148.7 ppm (3C=N), 145.5, 134.8, 132.3, 131.1, 128.3, 121.4, 110.3 ppm(C=C), 62.5 ppm(N-CH-N).

1562 (C=N) pyrimidine, 1494, 1473 (C=C), 732

(C-S-C).  ${}^{1}\text{H-NMR}$  (DMSO, 500 MHz)  $\delta$ : 10.13

ppm(s, 1H, NH), 8.83, 8.78 ppm (m, 2H, Ar-H),

8.3-7.12 ppm (m, Ar-H), 7.95 ppm (m, 1H, N=CH

Schiff).  $^{13}$ C-NMR (DMSO, 500 MH<sub>z</sub>)  $\delta$ : 163.7, 158.1 ppm (2C=N imine), 155.3, 148.1 ppm

(2C=N), 146.3, 135.5, 133.1, 132.3, 128.4, 123.3,

117.3, 109.5, 108.1 ppm (C=C).

5-(2-([1,1-biphenyl]-4-yl)imidazo[1,2-a]pyrimidin-3-yl)-4,5-1H-1,2,4-triazole-3-thiol (6b)
FT-IR (KBr/cm<sup>-1</sup>): 3296, 3161 (NH), 3029 (Ar-H), 1649 (C=N) iomidazo, 1596 (C=N) pyrimidine, 1523, 1488 (C=C), 2619(SH). <sup>1</sup>H-NMR (DMSO, 500 MH<sub>z</sub>) δ: 11.93, 9.89 ppm (s, 2H, 2NH), 8.81, 8.75 ppm (m, 2H, Ar-H), 8.78-8.28 ppm (m, Ar-H), 5.01 ppm (s, 1H, CH), 1.5 ppm (s, 1H, SH). <sup>13</sup>C-NMR (DMSO, 500 MH<sub>z</sub>) δ: 155.3, 151.2, 149.4 ppm (3C=N), 145.1, 135.3, 133.4, 131.01, 128.1, 122.3, 109.3 ppm (C=C), 61.04 ppm (CH)

Com. No.	R	M.F.	M.P. (°C)	Color	Yield (%)
6a	-Br	C <sub>14</sub> H <sub>11</sub> BrN <sub>6</sub> S	C <sub>14</sub> H <sub>11</sub> BrN <sub>6</sub> S 228 Off w		75
6b		C <sub>20</sub> H <sub>16</sub> N <sub>6</sub> S	276	white	68

The sequence of reactions that has led to the synthesis of the final products is shown in scheme 1. Synthesis of 2-substituted imidazo(1,2-a)pyrimidine is by condensation of 2-amino pyrimidine with  $\alpha$ -halo ketone (4-bromo phenacyl bromide ), (4-phenyl phenacyl bromide ) in refluxing ethanol to form 2-(4-bromophenyle)imidazo(1,2-a)pyrimidine (1a),2-(biphenyl)imidazo(1,2-a)pyrimidine(1b),

rrespectively. The FT-IR spectra of these compounds indicated that the peak of amino group disappeared and new absorption peak appeared at (1596 and 1602 cm-1) owing to (C=N) cyclic imidazo. In the second step, at position 3, there is subject electrophilic substitution via vilsmeier-haack reaction by using mixture of POCl3 and DMF to prepare aldehyde group (2-aryl imidazo[1,2a]pyrimidine-3-carbaldehydes) (2a, 2b). The FT-IR spectra of these carbaldehyde derivatives showed new absorption peak at (1677 and 1670 cm<sup>-1</sup>) due to C=O group stretching. The key intermediate thiosemicarbazone derivatives (3a**b**) were prepared by the reaction of 3carbaldehyd derivatives with thiosemicarbazide in refluxing ethanol containing acetic acid. Structures of compounds (3a-b) were confirmed by FT-IR spectra data that showed new peaks at (3477, 3353 cm<sup>-1</sup>) and (3332, 3245) owing to

amino group and also showed new peaks at (1623 and 1649 cm<sup>-1</sup>) owing to (C=N) imine.

Cyclization of thiosemicarbazone derivatives (3a-b) was realized by different cyclizing agents and reaction conditions. Thus, closure of thiosemicarbazone derivatives in the presence of acetic anhydride formed 1,3,4-thiadiazole derivatives (4a-b). A mechanism synthesis of (4a-b) derivatives is shown in scheme 2. The FT-IR spectra showed the disappearance of NH<sub>2</sub> bands of thiosemicarbazone derivatives and the presence of new peaks at 1764 and 1703 cm<sup>-1</sup> and at 1691 and 1666 cm<sup>-1</sup> due to C=0 group for diacetyl substituted thiadiazole.

Heterocyclization of thiosemicarbazone derivatives (3a-b) in the presence of 4-bromophwnacyl bromide and anhydrous sodium acetate yielded the corresponding 1,3-thiazole derivatives (5a-b). The FT-IR spectra showed peak at (1631 cm<sup>-1</sup>) owing to (C=N) imine.

At last, cyclization of thiosemicarbazone in acidic media (35% HCl) afforded 1,2,4-triazole-3-thiol derivatives (**6a-b**). The mechanism of the synthesis of these compounds (**6a-b**) is shown in scheme **3**. The FT-IR spectra showed absorption peaks at (2574 and 2619 cm<sup>-1</sup>) due to thiol group.

$$R = Br, C_{6}H_{5}$$

$$(3a-b)$$

$$R = Br, C_{6}H_{5}$$

**Scheme 1:** synthesis of (thiadiazole, thiazole and triazole) derivatives bearing imidazo(1,2-a)perimidine moiety. Reagents and condensations: (a) EtOH, reflux 6h; (b) POCl<sub>3</sub>, DMF, 70 °C 12h; (c) EtOH,NH<sub>2</sub>NHCSNH<sub>2</sub>, reflux 4h; (d) Ac<sub>2</sub>O, reflux 5h; (e) EtOH, anhydrous sodium acetate, 4-bromophenacyl bromide, reflux 6h; (f) EtOH, HCl, reflux 2h

#### Corrosion inhibition

The electrochemical corrosion data are illustrated in Table 7 as corrosion potential (Ecorr), cathodics and anodics. Tafel slopes (bc, ba) and corrosion current density (Icorr) were obtained by cathodic and anodic regions of the Tafel lines. Figures 2, 3 and 4 present potentiodynamic polarization curves for C-steel in sea water containing 3.5% NaCl. IE% was calculated in the equation below:

IE%= (Icorr (blank)- (icorr)/ Icorr (blank)) × 100

Compounds (4a, 5b and 6b) exhibited a good inhibition efficiency due to adsorption of the compounds with C-steel in 3.5% NaCl, which determines that these atoms bind the carbon surface atoms to protect them from corrosion. The atoms of compounds are ready in this case to bind to the carbon surface atoms, thus protecting surface from corrosion.

**Table 7:** Electrochemical data of the C-steel corrosion in sea water (3.5% NaCl) for the compounds (**4a,5b and 6b**)

Sub.	-Ecorr (mV)	icorr (A/cm²)*10 <sup>-6</sup>	-Bc (mV/Dec)	Ba (mV/Dec)	WL (g/m².d).d)	PL (mm/y)	IE%
blank	-331.6	630.58	-125.1	68.5	158	7.32	-
4a	-231.9	75.19	-128.9	56.4	18.8	0.873	88
5b	-300.7	117.56	-201.6	120.2	29.4	1.36	81
6b	-228.8	46.93	-127.4	90.6	11.7	0.545	92

Ecorr: corrosion potential, Icorr: corrosion current density, bc: cathodic Tafel slope, ba: anodic Tafel slope, WL: weight loss, PL: penetration loss, IE% inhibition efficiency

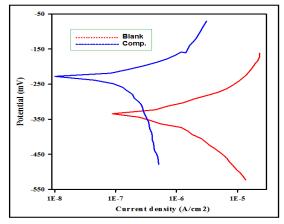


Figure 2: Polarization curve of C-steel in sea water (NaCl 3.5%) in presence 20 ppm of compound (4a)

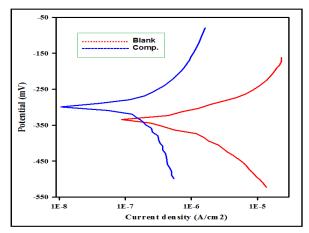


Figure 3: Polarization curve of C-steel in sea water (NaCl 3.5%) in presence 20 ppm of compound (5b)

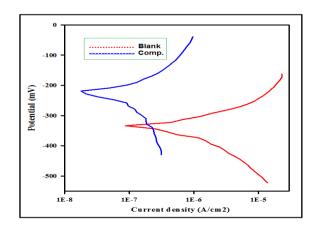


Figure 4: Polarization curve of C-steel in sea water (NaCl 3.5%) in presence 20 ppm of compound (6b)

### Conclusion

We have synthesized new imidazo[1,2-a]pyrimidine derivatives bearing thiadiazole, thiazol and triazole moiety at position 3. The structures of these compounds were confirmed with FT-IR, <sup>1</sup>H NMR, and <sup>13</sup>C NMR. Compounds (4a, 5b and 6b) were evaluated their anticorrosion activity on the surface of carbon steel in sea water 3.5% NaCl. These compounds exhibited a good anti-corrosion activity by forming adsorbed layer on the carbon steel surface. Thus, the metal surface was protected from corrosion.

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#### **Authors' contributions**

All authors contributed toward data analysis, drafting and revising the paper and agreed to be responsible for all the aspects of this work.

# **Conflict of Interest**

We have no conflicts of interest to disclose.

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