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Synthesis, Characterization, and Effectiveness of Pyranopyrimidine Derivatives as Multi-function Additive for Lubricating Oils

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ABSTRACT

In the lubricating oil industry, multifunction additives have garnered considerable interest because of their ability to significantly enhance and add different functions. This study details the two-step synthesis of pyranopyrimidine derivatives. The initial step entails a three-component, one-pot reaction of pyrrole-2-carboxaldehyde, malononitrile, and 3-methyl-1-phenyl-2-pyrazoline-5-one, or dimedone, or barbituric acid, to produce compounds (1-3) using nanoparticles magnesium oxide (MgO-Nps) as the catalyst. In the second step, these products are cyclized with isothiocyanatobenzene to form the desired pyranopyrimidine derivatives (4, 5, and 6). The structures of synthesized compounds were confirmed using FTIR and ^{1}H-NMR spectroscopies. The pyranopyrimidine derivatives were blended with the base lubricating oil, and then evaluated as effective antioxidants, corrosion inhibitors, and anti-rust agents using the IP-280 test (Institute of Petroleum's testing method), ASTM-D-130 and ASTM-D-665 tests (American Society of Testing and Materials methods), respectively. Furthermore, pyranopyrimidine derivatives were investigated for antimicrobially induced corrosion (MIC) by molecular docking on the rubredoxin (2DSX) protein from *Desulfovibrio gigas* bacteria and the cytochrome-c_3 (2CTH) protein from *Desulfovibrio vulgaris* bacteria.

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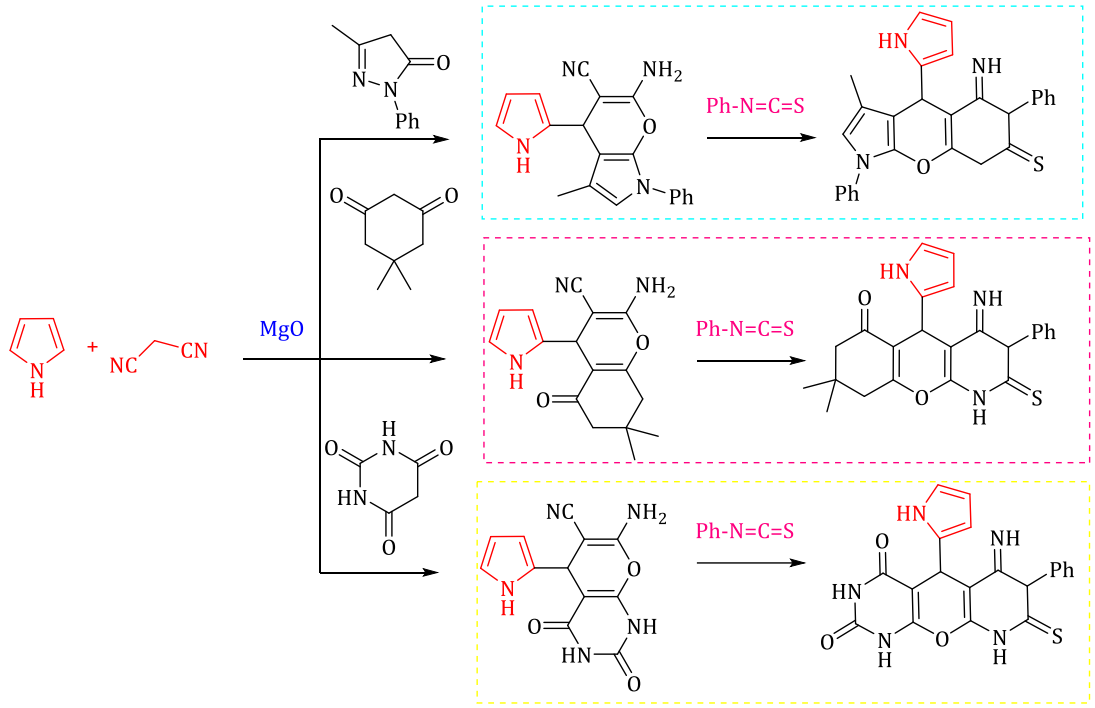
GRAPHICAL ABSTRACT



Introduction

Lubricants are oils used to reduce wear and friction between mechanical parts in contact. Lubricants with additives can help make equipment last longer and use less energy [1]. The base oils are mixed with different kinds of additives to make lubricants with better oxidation stability, viscosity index, pour point, corrosion resistance, wear resistance, and rust resistance [2]. Multifunctional additives are components used to improve multiple lubricant properties simultaneously. Zinc-dialkyl dithiophosphate (Zn-DTPs) are widely used as anti-wear and antioxidants to prevent the corrosion of copper and lead additives [3-5]. Polyacrylates are applied as pour point depressants, anti-wear, and viscosity index improvers [6, 7].

Pyrano[2,3-d]pyrimidine derivatives are unsaturated, six-membered heterocycles created by the fusion of pyrimidine and pyran rings. Pyranopyrimidines are among the most important chemicals with various pharmacological effects, including anti-inflammatory [8], antibacterial [9-12], anti-cancer [13, 14], and antioxidant [15, 16] properties. Some pyrano[2,3-d]pyrimidine compounds were synthesized and applied as lubricant anti-oxidant additives [17]. Recently, novel pyranopyrimidine compounds were found to be effective multifunctional lubricant additives [18, 19]. Some derivatives were shown anti-corrosion activity with carbon steel [20, 21].

This work aims to synthesize new pyranopyrimidine derivatives using MgO-Nps and evaluate their usage as multifunctional additives for lubricants, such as anti-corrosion, anti-rust, and antioxidants.

Experimental

Chemicals and base oil

All the chemicals were supplied by BDH, Fluka AG, and Merck, and the nano-powder magnesium oxide was by Nanoshel. For the preparation of oil blend, base lubricating oils (Sixty stock) were blended with 1% weight/weight of each of the prepared derivatives. Table 1 lists the specifications of sixty stock base lubricating oils provided by the Midland Refineries Company in Baghdad, Iraq, and the test methods employed.

Table 1: Properties of base lubricating oils and the employed test methods

Specification	Properties	Test method
Kinematic viscosity at 40 °C	62.90 mm^2/s	ASTM-D445
Kinematic viscosity at 100 °C	8.35 mm^2/s	ASTM-D445
Viscosity Index (VI)	100	ASTM-D2270
Specific gravity	0.879	ASTM-D4052
Pour Point (P.P)	-6 °C	ASTM-D97
Flash Point	250 °C	ASTM-D92
Rust Preventing	Fail	ASTM-D665
Copper Corrosion	2a	ASTM-D130
TBN	0.75 mg KOH/g	ASTM-D4739
Color	2.0 Yellow	ASTM-D1500

Instrumentation

The melting points were measured with the Stuart Electro-Thermal melting point apparatus (SMP1). Infrared spectra were recorded on a Shimadzu FTIR-8400S spectrophotometer in the form of a potassium bromide disk at the University of Baghdad-College of Science, Iraq. Proton nuclear magnetic resonance (1H-NMR) spectra were recorded on a Varian model UltraShield Plus at a frequency of 500 MHz, using the DMSO-d6 solvent at the University of Isfahan in Iran, and the chemical shifts were expressed in parts per million (ppm) relatives to an internal reference of tetramethylsilane (TMS).

The general method to synthesize pyranopyrazole, pyranopyrimidine, and chromene derivatives (1, 2, and 3)

A mixture of pyrrole-2-carboxaldehyde (1.0 eq., 1.90 g, 0.02 mol), malononitrile (1.0 eq., 1.32 g, 0.02 mol), and 3-methyl-1-phenyl-2-pyrazoline-5-one (1.0 eq., 3.48 g, 0.02 mol), 5,5-dimethyl-1,3-cyclohexandion (Dimedone) (1.0 eq., 2.80 g, 0.02 mol), or pyrimidine-2,4,6-trione (Barbituric acid) (1.0 eq., 2.56 g, 0.02 mol) in the presence of a catalyst of nano-powder magnesium oxide (0.25 eq., 0.20 g, 0.005 mol) in (20 mL) ethanol, was refluxed for 2-4 hours. The mixture was cooled at the end of reaction, and the formed precipitate was filtered and crystallized from ethanol to afford the title derivatives (**1**, **2**, and **3**) [22].

*The general method to synthesize pyranopyrimidine derivatives (**4**, **5**, and **6**)*

A mixture of an appropriate compound (**1**, **2**, or **3**) (1.0 eq., 0.01 mol) and isothiocyanatobenzene (1.2 mL, 0.01 mol, 1.0 eq.) in dimethylformamide (DMF) (10 mL) was heated for 6-8 hours. The produced solution was poured into ice to give the solid product which was filtered, and then crystallized from ethanol to obtain the title derivatives (**4**, **5**, and **6**) [23].

*Some selected spectral data and physical properties for compounds (**1-6**)*

Compound (1): *6-Amino-3-methyl-1-phenyl-4-(1H-pyrrol-2-yl)-1,4-dihydro-pyrano[2,3-c]pyrazolo-5-carbonitril*

1 exhibits properties like yellow crystals, m.p. = 120-122 °C, F.W= $C_{18}H_{15}N_5O$, M.W= 317.35 g/mole, reaction yield = 95%.

The FT-IR (KBr) (ν_{max}/ cm^{-1}) spectral data are: 3472, 3328 (NH_2), 3271 (N-H), 3105 (C-H aromatic), 2981, 2839 (C-H aliphatic), 2195(CN), 1657 (C=N), and 1580 (C=C).

The ^{1}H-NMR chemical shifts (δ_H, in ppm): 13.7 (1H, singlet, N-H), 7.7-7.9 (5H, multiplet, Ar-H), 7.6 (1H, doublet, J=7.5 Hz, pyrrol), 7.4 (1H, doublet, J=7.5 Hz, pyrrol), 7.2 (1H, triplet, J=7.5 Hz, pyrrol), 6.5 (2H, singlet, NH_2), 3.4 (1H, singlet, C-H pyran), and 2.4 (3H, singlet, CH_3).

Compound (2): *7-Amino-2,4-dioxo-5-(1H-pyrrol-2-yl)-1,3,4,5-tetrahydro-2H-pyrano[2,3-d]pyrimidin-6-carbonitril*

Brown crystals of m.p.= 150-152 °C, F.W= $C_{12}H_9N_5O_3$, M.W = 271.24 g/mole, and yield= 86%.
The FT-IR (cm^{-1}) responses are: 3405, 3312 (NH_2), 3236 (N-H), 2199 (CN), 1700, 1691 (C=O), and 1597 (C=C).
The ^{1}H-NMR (δ_H, ppm) characteristics are: 12.8 (singlet, 1H, NH), 10.8, 10.9 (2H, singlet, 2NH), 7.3 (1H, doublet, J=7.5 Hz, pyrrol), 6.9 (1H, doublet, J=7.5 Hz, pyrrol), 7.1 (1H, triplet, J=7.5 Hz, pyrrol), 6.4 (2H, singlet, NH_2), and 3.5 (singlet, 1H, CH pyran).

Compound (3): *2-Amino-7-dimethyl-5-oxo-4-(1H-pyrrol-2-yl)-5,6,7,8-tetrahydro-chromen-3-carbonitril*

3 is a solid compound of brown color, m.p.= 248-250 °C, F.W= $C_{16}H_{17}N_3O_2$, M.W= 283.33 g/mole, and yield = 92%.
FT-IR (cm^{-1}) spectral data of **3** are: 3430, 3335 (NH_2), 3247 (N-H), 2958, 2872 (C-H aliphatic), 2191 (CN), 1674 (C=O), and 1600 (C=C).
^{1}H-NMR (δ_H, ppm): 13.4 (1H, singlet, N-H), 7.6 (1H, doublet, J=7.5 Hz, pyrrol), 7.2 (1H, doublet, J=7.5 Hz, pyrrol), 6.9 (1H, triplet, J=7.5 Hz, pyrrol), 5.6 (2H, singlet, NH_2), 3.3 (1H, singlet, C-H pyran), 2.3 (2H, singlet, CH_2), 2.1 (2H, singlet, CH_2), and 1.4 (6H, singlet, $2CH_3$).

Compound (4): *5-Amino-3-methyl-1,6-di-phenyl-4-(1H-pyrrol-2-yl)tetrahydro-pyrazolo [4',3':5,6]pyrano [2,3-d] pyrimidine-7(1H)-thione*

Orange crystals of **4** has m.p of 166-168 °C, F.W = $C_{25}H_{20}N_6OS$, M.W = 452.54 g/mole, and reaction yield = 71%.
FT-IR (cm^{-1}): 3207 (NH), 3100 (C-H aromatic), 2980 (C-H aliphatic), 1652 (C=N), 1591 (C=C), and 1433 (C=S).
^{1}H-NMR (δ_H, ppm): 13.7 (1H, singlet, N-H), 9.8 (1H, singlet, N-H), 7.1-7.9 (13H, multiplet, Ar-H), 3.3 (1H, singlet, C-H pyran), and 2.3 (3H, singlet, CH_3).

Compound (5): *6-Imino-7-phenyl-5-(1H-pyrrol-2-yl)-8-thioxo-1,5,6,7,8,9-hexahydro-2H-pyrano[2,3-d:6,5-d'] di-pyrimidin-2,4(3H)-dione*

5 has deep violet oily character, F.W= $C_{19}H_{14}N_6O_3S$; M.W= 406.42 g/mole; yield= 65%.
FT-IR (cm^{-1}): 3254 (N-H), 3107 (C-H aromatic), 1722, 1688 (C=O), 1610 (C=C), and 1415 (C=S).
^{1}H-NMR (δ_H, ppm): 12.7 (singlet, 1H, NH), 11.5 (singlet, 1H, NH), 10.8, 11.0 (2H, singlet, 2NH), 6.8-7.4 (8H, multiplet, Ar-H), and 3.8 (singlet, 1H, CH pyran).

Compound (6): *4-Imino-8,8-dimethyl-3-phenyl-5-(1H-pyrrol-2-yl)-2-thioxo-octa-hydro-6H-chromene [2,3-d] pyrimidines-6-one*

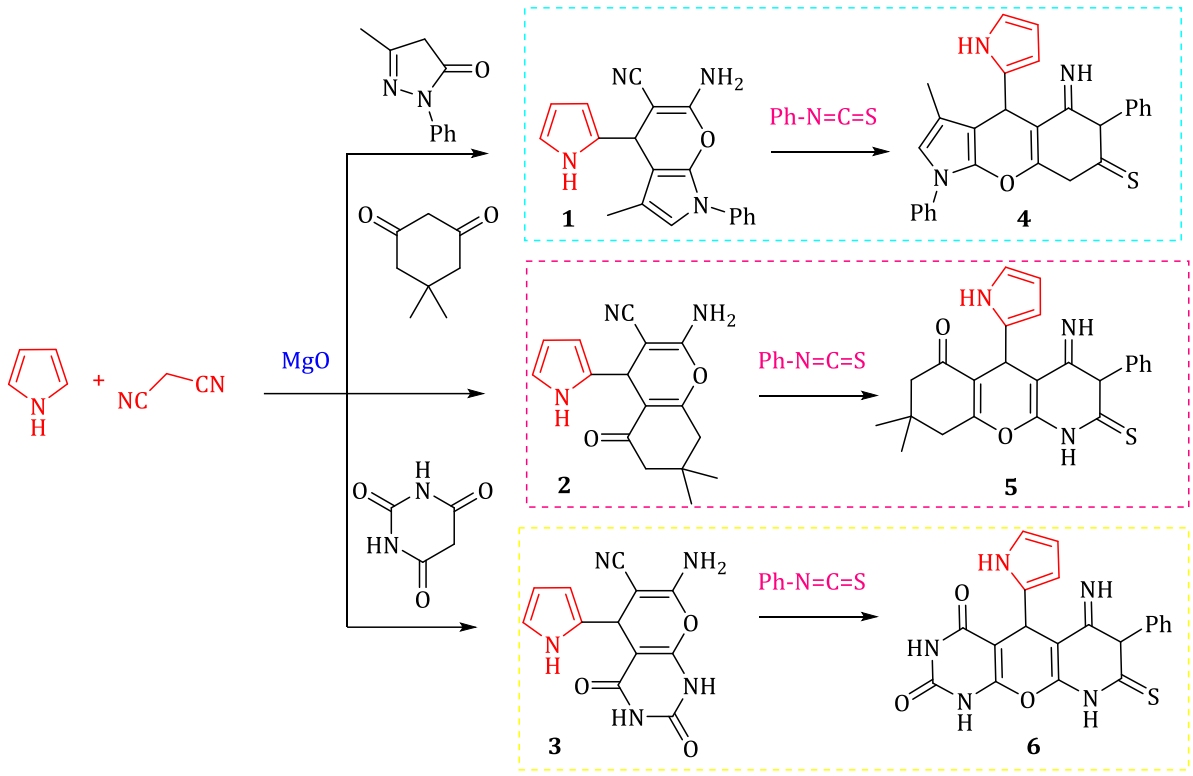
The brown solid product of **6** has m.p. = 156-160 °C, F.W= $C_{23}H_{22}N_4O_2S$, M.W = 418.52 g/mole, and yield = 73%.
FT-IR (cm^{-1}): 3210 (N-H), 3038 (C-H aromatic), 2978 (C-H aliphatic), 1680 (C=O), 1648 (C=N), 1595 (C=C), and 1445 (C=S).
^{1}H-NMR (δ_H, ppm): 13.6 (1H, singlet, N-H), 9.8 (1H, singlet, N-H), 7.1-7.5 (8H, multiplet, Ar-H), 3.4 (1H, singlet, C-H pyran), 2.3 & 2.2 (4H, singlet, $2CH_2$), and 1.0 (6H, singlet, $2CH_3$).

Oil Blend Formulation

The blends of the prepared derivatives (**1–6**) with a concentration of 1% weight/weight were prepared by dissolving and mixing one gram of each derivative in 100 grams of base oil (60 stock) for one hour at 80˚C, followed by stirring for two hours at room temperature [24].

Results and Discussion

The pyranopyrimidine derivatives (**4**, **5**, and **6**) were prepared in two stages. The first stage included the preparation of compounds (**1**, **2**, and **3**) from a three-component, one-pot reaction. The reaction involved two steps. In the initial step, Knoevenagel condensation of pyrrole-2-carboxaldehyde with malononitril in the presence of nanoparticles of magnesium oxide as a catalyst produced an intermediate derivative of (2-((1*H*-pyrrol-2-yl)methylene)malononitrile), and then the second step included a reaction of intermediate with 3-methyl-1-phenyl-2-pyrazoline-5-on, or dimedon, or barbituric acid (Scheme 1) [22].
The second stage involved the cyclization reaction of compounds (**1**, **2**, or **3**) with isothiocyanatobenzene to produce the desired derivatives (**4**, **5**, and **6**). Schemes 1 and 2 represent each of these reactions and mechanisms (Scheme 2).



Scheme 1: The synthesis routes for the prepared derivatives

The prepared compounds were identified by FT-IR and ^{1}H-NMR spectroscopies.

The FT-IR spectra of compounds 1, 2, and 3 showed stretching bands of the amine groups at 3472, 3405, and 3430 cm^{-1}, respectively. Also, bands at 3328, 3312, and 3335 cm^{-1} showed for asymmetric stretching and at 3328, 3312, and 3335 cm^{-1} for symmetric, while the nitrile (CN) showed a band in the region of 2191-2199 cm^{-1}.

The thione group (C=S) in compounds 4, 5, and 6 displayed stretching bands at 1433, 1415, and 1445 cm^{-1}. Another significant point is the disappearance of any band for amine (NH_2) and nitrile (CN) groups in the FT-IR spectra of these compounds [25].

The ^{1}H-NMR spectrum (in ppm) of compound 1 (pyrano[2,3-c]pyrazol derivative) showed a singlet signal at δ13.7 for pyrrole N-H, multiplet signals at the region δ=7.7-7.9 for phenyl protons, while the pyrrole ring protons appeared as doublet signals at δ=7.6 and δ=7.4, and as triplet signal at δ=7.2. The singlet signals at δ=6.5, δ3.4, and δ=2.4 were assigned for NH_2, C-H pyran, and methyl protons.

The ^{1}H-NMR spectrum after cyclization with phenyl isocyanate for compound 4 (pyrazolo-pyrano[2,3-d] pyrimidine-thione derivative) showed the appearance of a singlet signal at δ9.8 for N-H, and no signal disappearance of NH_2 protons.

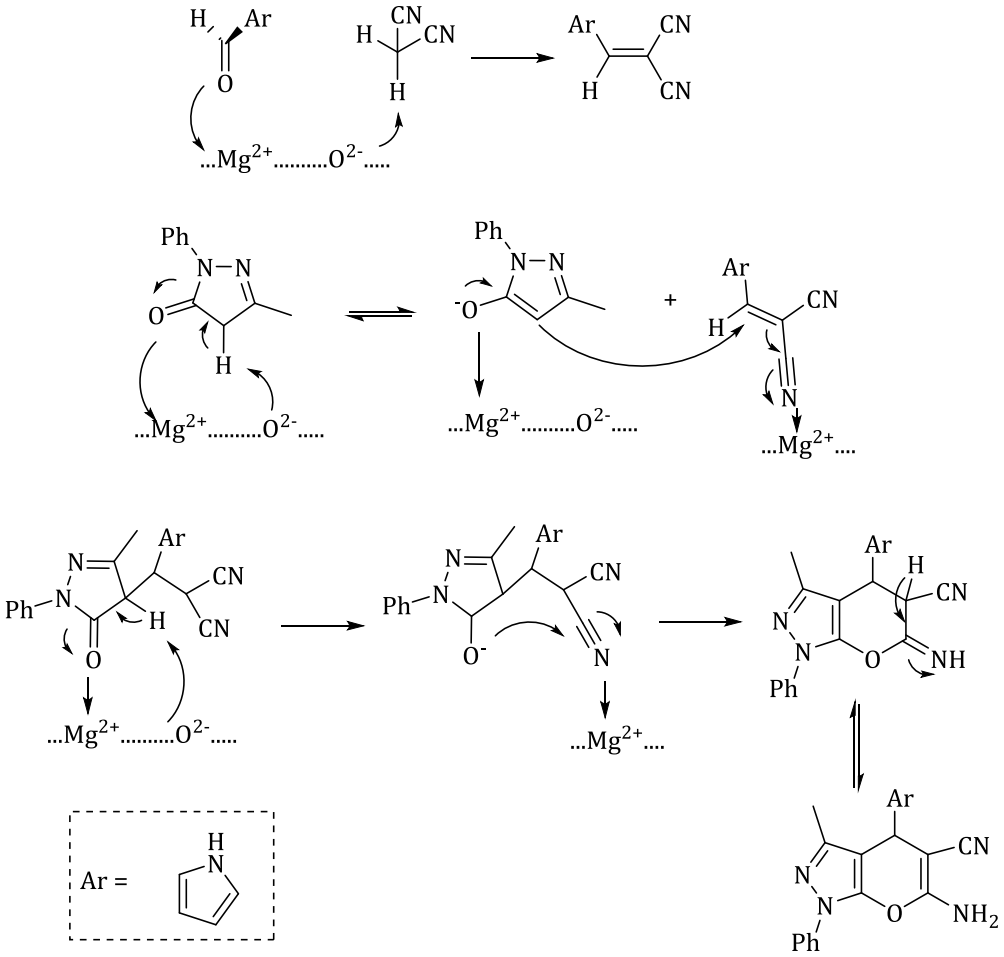
The structure of compound 2 (pyrano[2,3-d]pyrimidin derivative) was confirmed by ^{1}H-NMR, which showed singlet signals at δ12.8 for pyrrole N-H, δ10.8, and δ10.9 for pyrimidine ring 2N-H. The protons of pyrrole ring responded as doublet signals at δ 7.3 and δ 6.9, and a triplet signal at δ7.1. The singlet signals at δ6.4 and δ3.5 were assigned for NH_2 and C-H pyran, respectively.

After cyclization, the ^{1}H-NMR spectrum of compound 5 showed signal disappearance of NH_2 protons and appearance of a singlet signal at δ11.5 for C=N-H, and a multiplet signal at the region δ6.8-7.4 for aromatic protons [26].

The ^{1}H-NMR spectrum of compound 3 (tetrahydro-chromene derivative*)* exhibited a singlet signal at δ 13.4 for pyrrole N-H, while the pyrrole ring protons appeared as doublet signals at δ7.6 and δ7.2 and as triplet signal at δ6.9. The singlet signals at δ5.6, and δ3.3 were assigned for NH_2 and C-H pyran, respectively. While the protons for two methylene and two methyl groups

appeared as doublet signals at δ2.3, δ2.1, and δ1.4, respectively.

The ^{1}H-NMR spectrum after cyclization with phenyl isocyanate for compound 6 (chromene [2,3-d] pyrimidine derivative) displayed the appearance of a singlet signal at δ9.9 for N-H, multiplet signal at the region δ7.1-7.5 for protons of phenyl group, and the disappearance of NH_2 protons signal [27].



Scheme 2: Formation mechanism using MgO-Nps catalyst

The effectiveness of synthesized compounds as anti-corrosion additives

The American Society of Testing and Materials (ASTM-D-130) method, which comprises dropping a copper strip in blended oil and heating it at 100 °C for about three hours, was used to test the activity of synthesized compounds' blends as anti-corrosion. After the heating period, the Cu-strip was taken out, and tarnish level was measured using the color-match scale of ASTM classification [28, 29]. All the compounds were discovered to be effective anti-corrosion lubricants additives, causing only a slight tarnish (1b), as opposed to a significant moderate tarnish (2a) on the blank.

The effectiveness of synthesized compounds as antirust additives

In the American Society of Testing and Materials (ASTM-D-665) procedure, a steel rod was dipped into a sample of blended oil mixed with water before being heated for four hours at 60 °C. This method was used to assess the anti-rust capabilities of blends of synthetic derivatives. Next, the test rod was checked for rust indicators. This test was conducted twice, and for it to be deemed successful, both test rods needed to be free of rust [30]. All synthetic derivative oil blends passed the rust-prevention test.

The effectiveness of synthesized compounds as antioxidant additives

Oil oxidation at high temperatures usually results in the formation of acidic components that cause sludge deposition, and metal corrosion. The Institute of Petroleum's (IP 280) testing method tested the oxidation stability of blended oils. This method has been utilized to determine the oxidation resistance under standard conditions of oxygen gas passing through an oil sample that has been mixed with an iron-copper metal catalyst for 72 hours at 120 °C [31]. Total sludge (T.S) and total acidity (T.A) levels in oil were determined after the period of the test was over, and the equation below was used to figure out the percentage of total oxidation products (TOP %):

$$TOP\% = T.S + (\frac{180 * T.A}{56.1 * 1000})100$$

Where, T.A denotes the total acidity in mg of KOH/g of oil, T.S is the total sludge in weight percentage, 56.1 represents the molecular weight of potassium hydroxide, and 180 is the mean molecular weight of oil oxidation acids. Figure 1 displays the results of the evaluation of oil blends. Accordingly, the findings show that all blends of synthetic derivatives **4**, **5**, and 6 have appropriate amounts of sludge and oxidation products and stronger oxidation stabilities than the base oil (blank). The oil blend with component 6 was about as stable against oxidation as the common antioxidant Hindered-Phenol derivative (HP) due to it structurally serves as a radical scavenger [32].

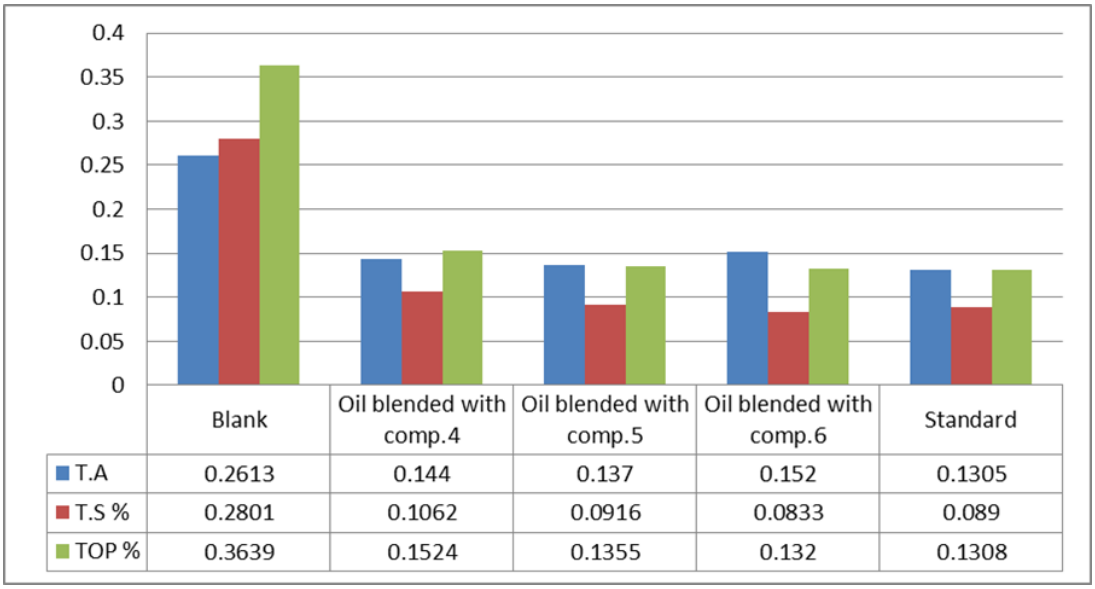


Figure 1: Graphical representation of total sludge, total oxidation products, and acidity of synthesized blended oils

Molecular docking study of synthesized compounds

Molecular docking is chosen to identify the interaction process and investigate potential binding simulations of the synthesized pyranopyrimidine derivatives **4, 5,** and **6** on the active sites of two different proteins: rubredoxin (2DSX) from *Desulfovibrio Gigas* and cytochrome-c_3 (2CTH) protein from *Desulfovibrio Vulgaris* bacteria. These two kinds of Sulfate Reducing Bacteria (SRB) are types of Microbial Influenced Corrosion (MIC) in pipelines oil [33]. The crystal structures of 2DSX and 2CTH proteins were found in the protein data bank (PDB) of the Research Collaborator for Structural Bioinformatics (RCSB) [34] and were molecularly docked using the Auto Dock Vina program version 15.6. The synthesized pyrimidine derivatives **4**, **5**, and **6** displayed binding energies determined to be -6.6, -6.8, and -7.0 Kcal/mole, respectively, which were favorable docking scores for bonding interaction with the 2DSX receptor. While these derivatives possessed binding energies of -8.0, -6.8, and -6.8 Kcal/mole, respectively, showed good docking scores for

bonding with the 2CTH receptor (a higher binding affinity was evident from more negative values of the binding energy). The docking outcomes are presented in Table 2.

Table 2: The molecular docking results of 4, 5, and 6 derivatives

Compound no.	Estimated binding energy (Kcal/mol)	Amino acid involved π -π interaction	Amino acid involved π -alkyl interaction	Amino acid involved π - sulfur interaction	Amino acid involved H-bonding interaction
Interactions of compounds with 2DSX protein					
4	-6.6	TYR A:11	LYS A:17 VAL A:41	CYS A:9	TYR A:11
5	-6.8	PRO A:20	PRO A:26 LYS A:17 PRO A:40	-	TYR A:11 GLY A:18
6	-7.0	GLY A:10	PRO A:20 LYS A:17 PRO A:40	-	TYR A:11 GLU A:12
Interactions of compounds with 2CTH protein					
4	-8.0	HIS B:35 PHE B:76	VAL A:86 LEU A:97 LYS B:75 ALA B:62	PHE B:76	
5	-6.8	-	PHE B:76 LYS B:77	-	THR B:74
6	-6.8	PHE A:76	PRO A:36 LYS A:75		HIS A:52

The best binding of derivative pyrano[2,3-d] pyrimidine-7-thione (**4**) with the active site of the 2CTH receptor from *Desulfovibrio Vulgaris* bacteria with a binding energy of -8.0 Kcal/mole was achieved through different interactions. In detail, the thione group interacts with phenylalanine (PHE B: 76) by π -S. The two phenyl groups interact with histidine (HIS B: 35) by π - π T-shaped, lysine (LYS B: 75), alanine (ALA B: 62), and valine (VAL A: 86), respectively, by π -alkyl. On the other hand, the pyrrole ring interacts with aspartic acid (ASP A: 96) by π-anion. While the best binding of derivative chromene [2,3-d] pyrimidines-6-one (**6**) is with the active site of 2DSX receptor from *Desulfovibrio Gigas* bacteria, binding energy of -7.0 Kcal/mole was achieved through different interactions. For example, hydrogen bonds with tyrosine (TYR A: 11) and glutamic acid (GLU A; 12), the phenyl group interacts with glycine (GLY A: 10) by π-Amide stacked, and the pyrrole ring interacts with tyrosine (TYR A: 11) by π - π stacked.

Figures 2, 3, 4, 5, 6, and 7 depict two- and three-dimensional (2D and 3D) interactions to visualize the interactions of the synthesized pyrimidine derivatives 4, 5, and 6 with rubredoxin (2DSX) and cytochrome-c_3 (2CTH) proteins (Figures 2-7).

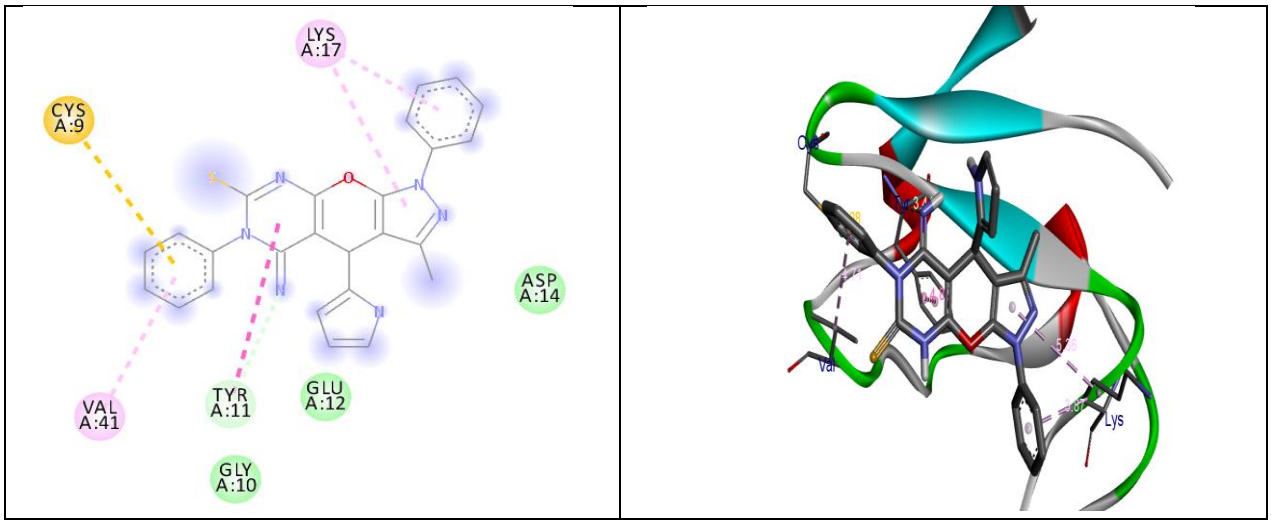


Figure 2: 2D and 3D interactions pose of derivative **4** with 2DSX protein

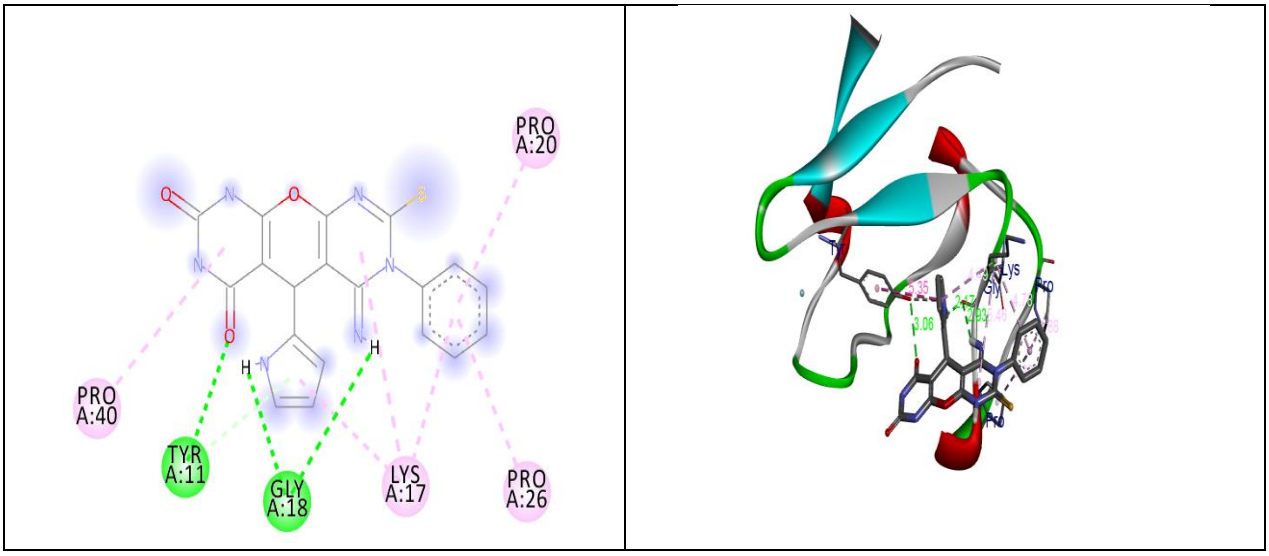


Figure 3: 2D and 3D interactions pose of derivative **5** with 2DSX protein

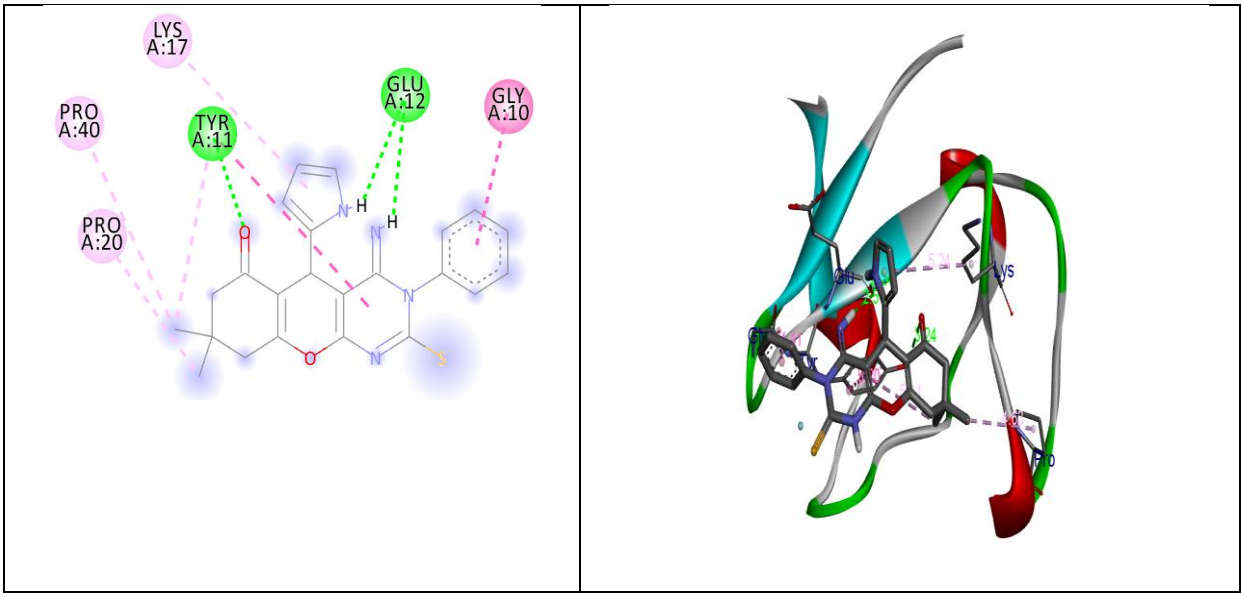


Figure 4: 2D and 3D interactions pose of derivative 6 with 2DSX protein

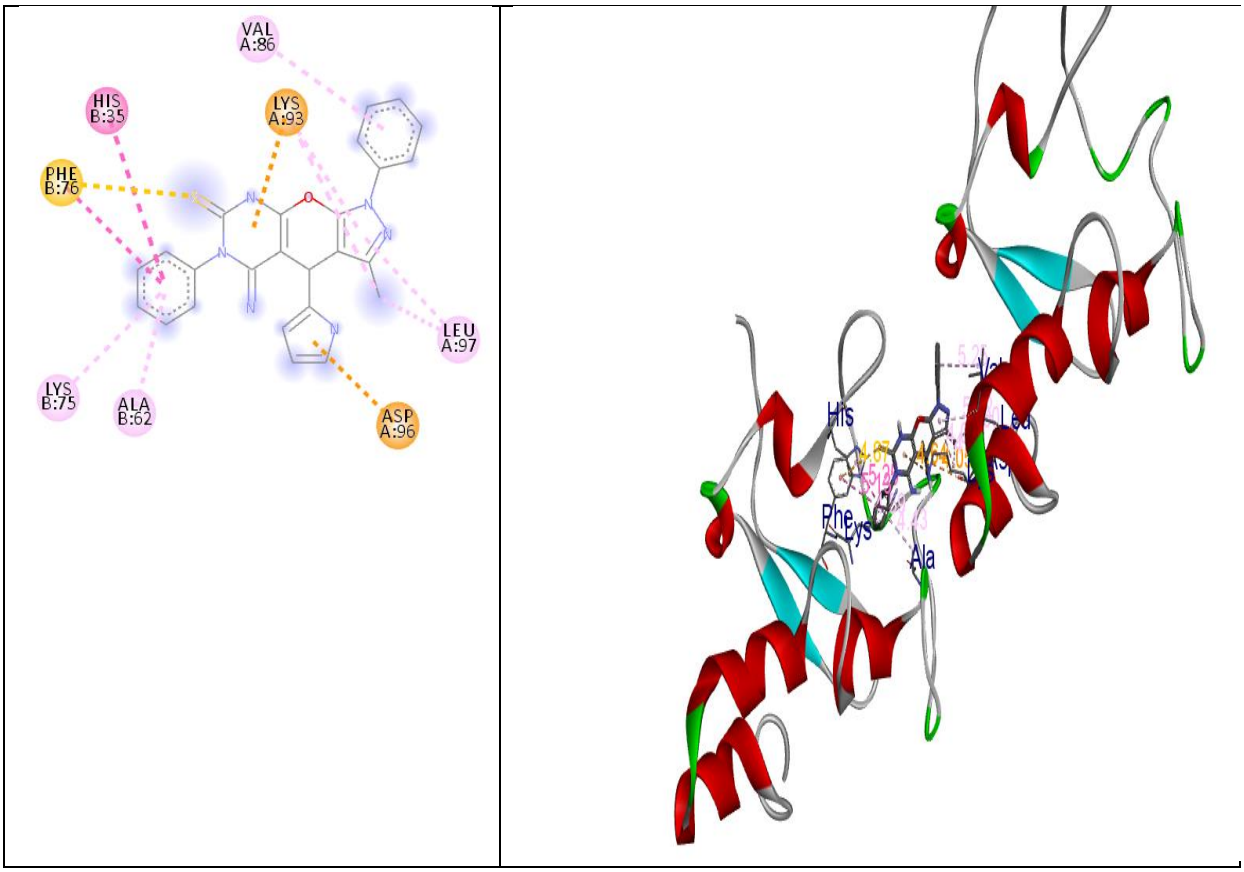


Figure 5: 2D and 3D interactions pose of derivative **4** with 2CTH protein

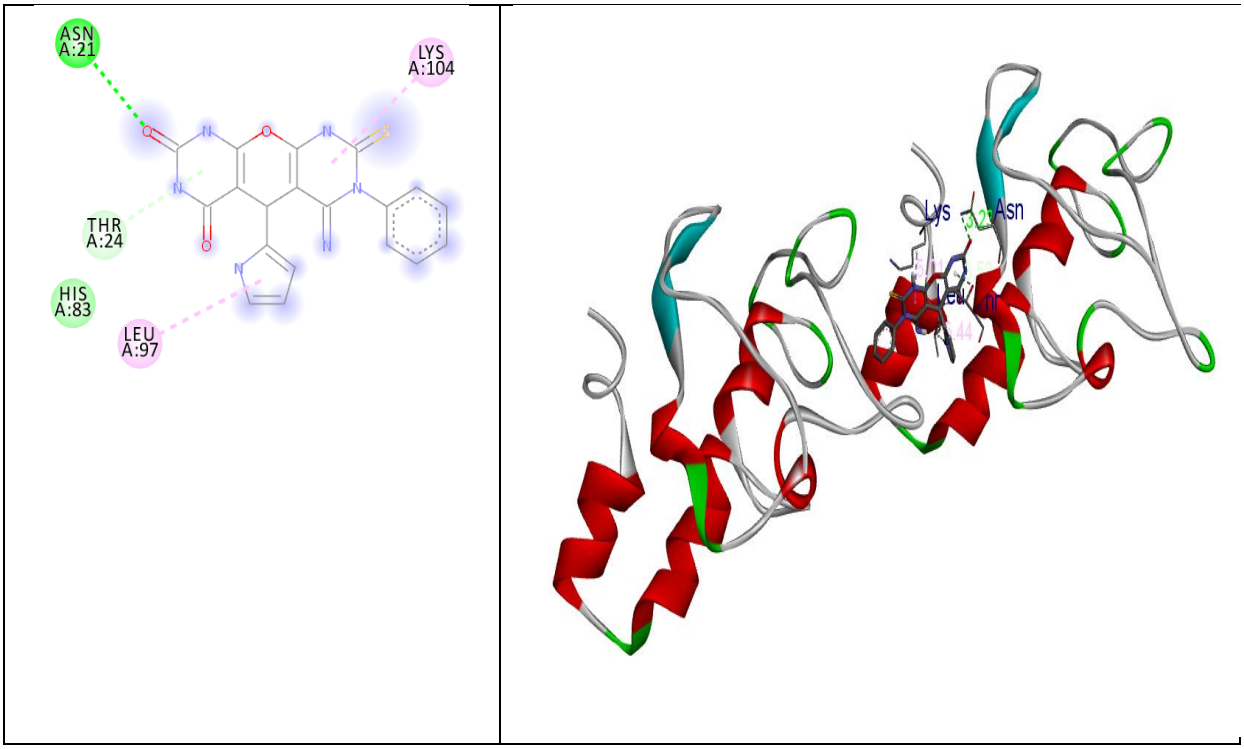


Figure 6: 2D and 3D interactions pose of derivative **5** with 2CTH protein

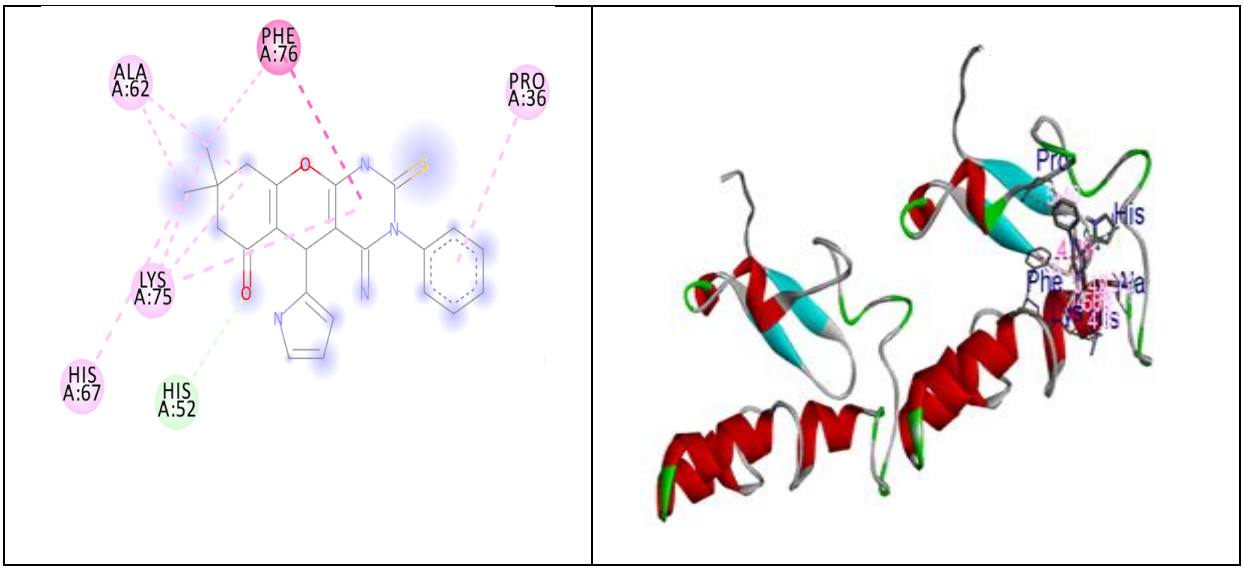


Figure 7: 2D and 3D interactions pose of derivative **6** with 2CTH protein

Conclusion

This work succeeded in synthesizing new efficient lubricant additives of pyranopyrimidine derivatives. Many tests have evidenced the multi-functionality of these additives as antioxidant, antirust, and anti-corrosion. Moreover, theoretical means have also proven the capability of these derivatives as microorganism-influenced corrosion inhibitors (MIC) against the *Desulfovibrio Gigas* bacteria and *Desulfovibrio Vulgaris* bacteria.

Disclosure Statement

No potential conflict of interest was reported by the authors.

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Authors' Contributions

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

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