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Synthesis, Characterization, and Evaluation of Schiff Base Derivatives from Sulfamethoxazole Drugs as Promising Antibacterial Agents Against Gram-positive and Gram-negative Bacteria

Zahraa M. Abdulmohsan [1*], Akram S. Karamallah [2], Andy N. S. Shamaya [3]

1. *College of Medicine, Al-Iraqia University, Baghdad, Iraq*
2. *Electromechanical Engineering Department, University of Technology, Baghdad, Iraq*
3. *Department of Chemistry, College of Science, University of Baghdad, Baghdad, Iraq*

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***Corresponding author:**
Zahraa M. Abdulmohsan,
College of Medicine, Al-Iraqia University, Baghdad, Iraq
Email:
zahraa.m.abdulmohsan@aliraqia.edu.iq

ABSTRACT

Background & Objective: Schiff bases are known to exhibit a wide range of biological activities, particularly antibacterial effects. Structural modification of existing antibacterial drugs, such as sulfamethoxazole, through Schiff base formation may enhance their therapeutic potential. This study aimed to synthesize novel Schiff base derivatives of sulfamethoxazole and evaluate their antibacterial activity using both in vitro and in silico approaches.

Materials & Methods: Four novel Schiff base derivatives of sulfamethoxazole were synthesized by condensation with differently substituted aromatic aldehydes (4-chloro-, 4-hydroxy-, 4-bromo-, and 4,4-dimethylbenzaldehyde). The synthesized compounds were characterized by melting point determination, Fourier-transform infrared (FT-IR) spectroscopy, and 1H-NMR spectroscopy. Their antibacterial activity was evaluated using in vitro antibacterial assays, while molecular docking studies against the bacterial enzyme dihydropteroate synthase (DHPS) were performed to investigate their binding affinity and potential mechanism of action.

Results: All synthesized Schiff base derivatives exhibited antibacterial activity against the tested bacterial strains. Among them, compounds 3 and 4 demonstrated the highest molecular docking scores and produced significantly larger antibacterial inhibition zones than the parent drug sulfamethoxazole. The findings indicate enhanced binding affinity toward dihydropteroate synthase, suggesting improved antibacterial efficacy. These results also suggest the potential of the synthesized derivatives to overcome bacterial resistance mechanisms.

Conclusion: The synthesized sulfamethoxazole-based Schiff base derivatives, particularly compounds 3 and 4, showed enhanced antibacterial activity in both in vitro and in silico evaluations. These findings highlight their potential as promising antibacterial agents and support further investigation into their development as candidates for combating antimicrobial resistance.

Keywords: Sulfamethoxazole; Schiff base; Antibacterial Agents; Molecular Docking; In Vitro Assay; Dihydropteroate Synthase; DHPS inhibitors.

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1. Introduction

Globally, the rise of antibiotic resistance poses a serious threat to public health. Consequently, the development of novel antibacterial agents has emerged as a critical area of research (1). One popular sulfonamide antibiotic that has been used consistently in combination chemotherapy for an assortment of bacterial diseases is sulfamethoxazole (2). Dihydropteroate synthase (DHPS), an essential enzyme responsible for the synthesis of folate in bacteria, is inhibited by this sulfonamide antibiotic. Folates are essential for bacterial growth and proliferation, as they are necessary for the synthesis of amino acids and nucleic acids (3). Nevertheless, the rising prevalence of the latter resistance emphasizes the need for novel compounds with more potent antibacterial efficacy. The chemical structure of sulfamethoxazole ($C_{10}H_{11}N_3O_3S$) is shown in Figure 1 (4).

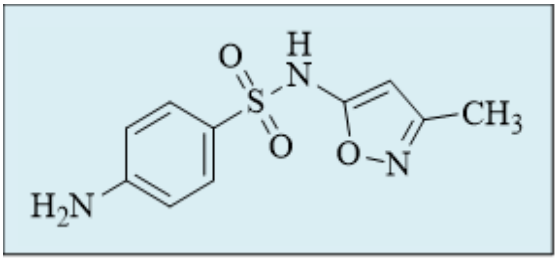


Figure 1. Structure of Sulfamethoxazole

Schiff base derivatives received an excessive amount of focus in the field of medicinal chemistry due to their variegated biological activities (5) and are compounds created by the condensation of an aldehyde or ketone with a primary amine.

These derivatives possess a wide range of pharmacological properties (6), including antimicrobial (7), hypoglycemic (8), anti-inflammatory (9), anti-proliferative (10), anti-tubercular (11), antitumor (12), and anticancer (13) activities.

The incorporation of Schiff bases into the structure of sulfamethoxazole provides a promising avenue for the development of novel antibacterial agents. The presence of a Schiff base component may alter the compound's pharmacokinetics and physicochemical characteristics, increase its antibacterial effectiveness and decrease susceptibility.

The principal amine group of sulfamethoxazole can react to distinct aldehydes or ketones in order to produce Schiff base derivatives. The structural variety of the resulting compounds allows for the discovery of active antibacterial medicines and the investigation of structure-activity relationships.

By emphasizing on Schiff base derivatives of sulfamethoxazole, this study aims to address the shortcomings of existing sulfonamide antibiotics and increase the variety of antibacterial medications. Integration in vitro and in silico methods will enable a comprehensive knowledge of the structure-activity relationship and potential therapeutic applications of these compounds.

2. Materials and Methods

All chemicals and reagents used in this study were obtained from Fluka or Aldrich starting chemical compounds. The melting points were marked using a Gallenkamp melting point apparatus, and the uncorrected FT-IR spectra were recorded on a SHIMADZU FTIR-8400 Fourier transform infrared spectrophotometer as KBr discs. ^{1}H-NMR spectra: Proton NMR was recorded on a Bruker model ultra shield 300 MHz instrument in Iran, using DMSO-d6 as a solvent and TMS (Tetramethylsilane) as an internal reference. UV-VIS spectra were recorded by a Shimadzu spectrophotometer and an Apel PD303 spectrophotometer (Japan).

2.1 Synthesis of Sulfamethoxazole derivatives

Schiff base compounds were synthesized through the reflux reaction of sulfamethoxazole with substituted aromatic aldehydes (1). (0.5 g, 0.002 moles) with various substituted aromatic aldehydes (0.002 moles) in 5 mL of absolute ethanol and 2-3 drops of glacial acetic acid. The refluxing process continued for 8 hours, maintaining a temperature range of (50-60) °C. After the reaction, the resulting precipitate was allowed to cool to room temperature, followed by filtration and recrystallization using ethanol/water (14).

2.2 *In silico* study of antibacterial activity

2.2.1 Ligand Preparation

Two-dimensional structures of synthesized compounds (**1-5**) were drawn using Chem Draw Ultra 12 software, subsequently converted to three-dimensional structures, and saved as MOL files. The energy minimization of synthesized compounds (**1-5**) was calculated using Avogadro 3.0 with the MMFF94s force field (15).

2.2.2 Protein Preparation

The three-dimensional arrangement of dihydropteroate synthase (PDB ID: 5jq9) (16) was collected from the Protein Data Bank (https://www.rcsb.org/) and made using the Protein Preparation wizard of the Maestro 12.5 software suite utilizing default settings.

These variables include bond order assignment, hydrogen addition, the generation of zero-order bonds for metals, the formation of disulfide bonds, and elimination of water molecules more than 5 A° from het groups, energy optimization, and limited minimization using the OPLS3e force field (17).

2.2.3 Molecular Docking

The protein grid for the docking of molecules analyses was generated with the Maestro 12.5 software suite's Glide-Grid wizard. The binding site was established by selecting one atom from the co-crystallized ligand. Other options have been included by default. Molecular docking investigations was carried out utilizing the Glide Docking wizard of the Maestro 12.5 software suite in standard precision (SP) mode. The additional parameters were set to their default values. The results were seen and assessed with BIOVIA Discovery Studio 2021 (17).

2.3 In vitro study of antibacterial activity

The agar well-diffusion method was used to establish the in vitro antibacterial activity of samples (1-5) against

two bacterial strains: *E. coli* and *Staphylococcus aureus*. Gentamicin at a concentration of 40 mg/1ml served as the standard reference. A 1 mg/ml solution of dimethyl sulfoxide (DMSO) was utilized to create test samples (1-5), along with standard references. The sterilized and liquefied agar was infected with a 1 ml/100 ml suspension of the microbe and placed in a Petri dish to a depth of approximately 3 mm. The test samples and references were put in wells created in the solidified substance.

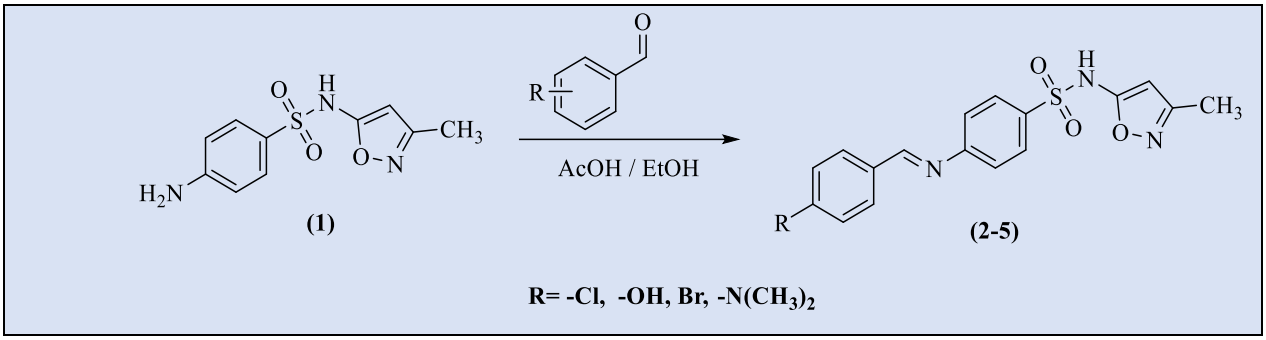
The plates were refrigerated for 1 hour at 5 °C before being incubated for 18 hours at 37 °C. The zones of bacterial growth inhibition formed by the test samples and standard references were measured in millimeters and recorded, Sulfamethoxazole tested as a control **(18)**.

2.4 Statistical Analysis:

The Statistical Packages of Social Sciences (SPSS) program (2019) was used to detect the effect of difference factors in study parameters. Least significant difference (LSD) was used to significantly compare between means (ANOVA/ One way) in this study **(19)**.

3. Result

The aimed Schiff base derivatives were prepared by reaction of Sulfamethoxazole compound 1 with different aromatic aldehydes (4-chloro Benzaldehyde, 4-hydroxy benzaldehyde, 4-bromo benzaldehyde, 4, 4 -di methyl benzaldehyde) to produce Schiff bases derivatives 2-5. The synthetic strategy of compounds 2-5 is represented in Scheme 1 and the physical properties and Fourier Transform Infrared (FT-IR) spectral data of compounds 1-5 can be found in Table 1, ^{1}H-NMR data in Table 2, Figure 2 and 3 ^{1}HNMR spectrum of compounds 1 and 2.



Scheme 1. The synthetic strategy of compounds 2-5. (**Prepared by Authors, 2026**).

Table 1. FT-IR spectral data of compounds 1-5.

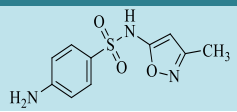
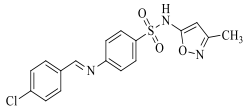
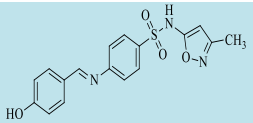
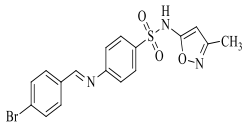
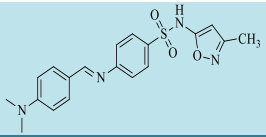
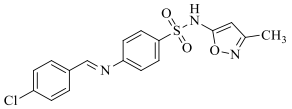
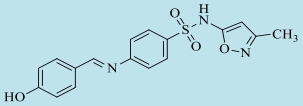
No.	Compound structure	Physical properties			Major FT-IR Absorptions cm^{-1}			
		Yield	Color	M.P° C	ν(N-H)	ν(C=O) amide	ν(C=N) ring	Other Bands
1		-	White	172-173	3400	1660	1620	νNH_2 Asym. 3485 Sym. 3261
2		90	White	150-152	3386	1667	1618	υC-Cl 1033 o-o-p-di-sub 831
3		92	Brown	122-124	3405	1665	1616	υO-H 3429 o-o-p-di-sub 835
4		91	White oily	182-183	3477	1701	1620	υC-Br 1035 o-o-p-di-sub 835
5		95	orange	184-186	3286	1656	1606	2995 o-o-p-di-sub815

Table 2. 1H-NMR data of some sulfamethoxazole derivatives.

No.	Compounds	-CH_3	C-H Isoxazole ring	Aromatic benzene ring	Imine (N=CH)	N-H	-OH
1		2.2-2.3	6.2	7.7-8.1	8.0	8.9	-
2		2.2-2.3	6.1	6.5-7.0	7.8-7.9	8.0	10.1

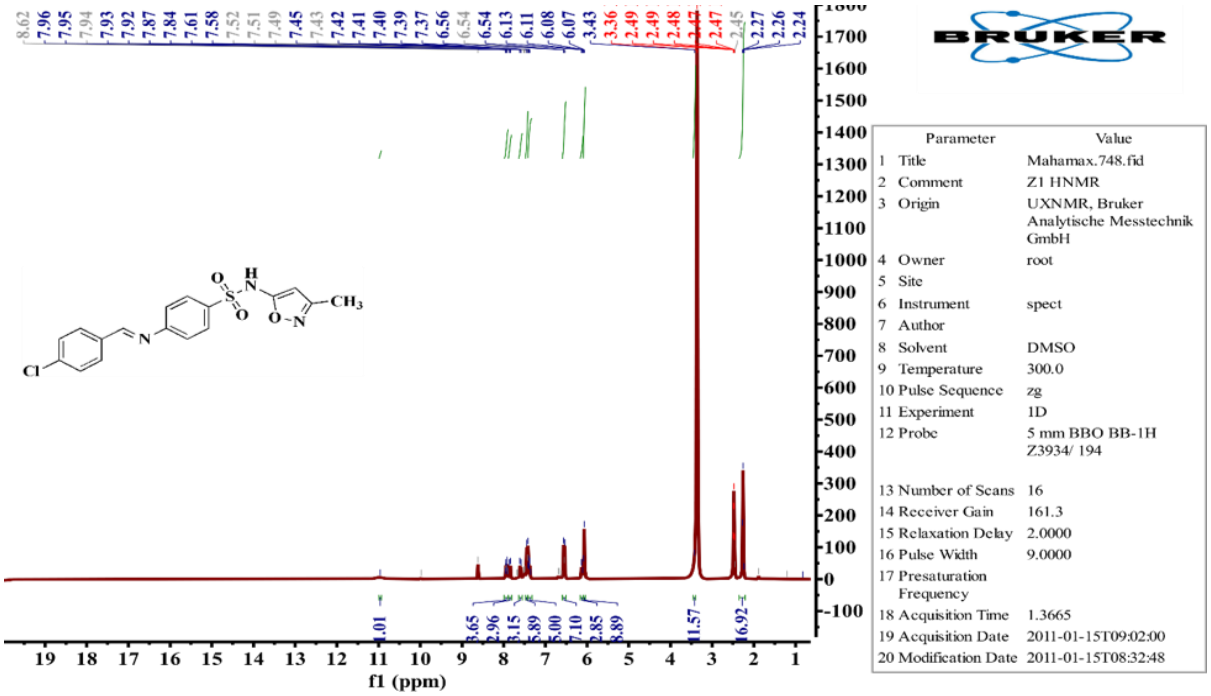


Figure 2. [1]HNMR spectrum of compound 1. (**Prepared by Authors, 2026**).

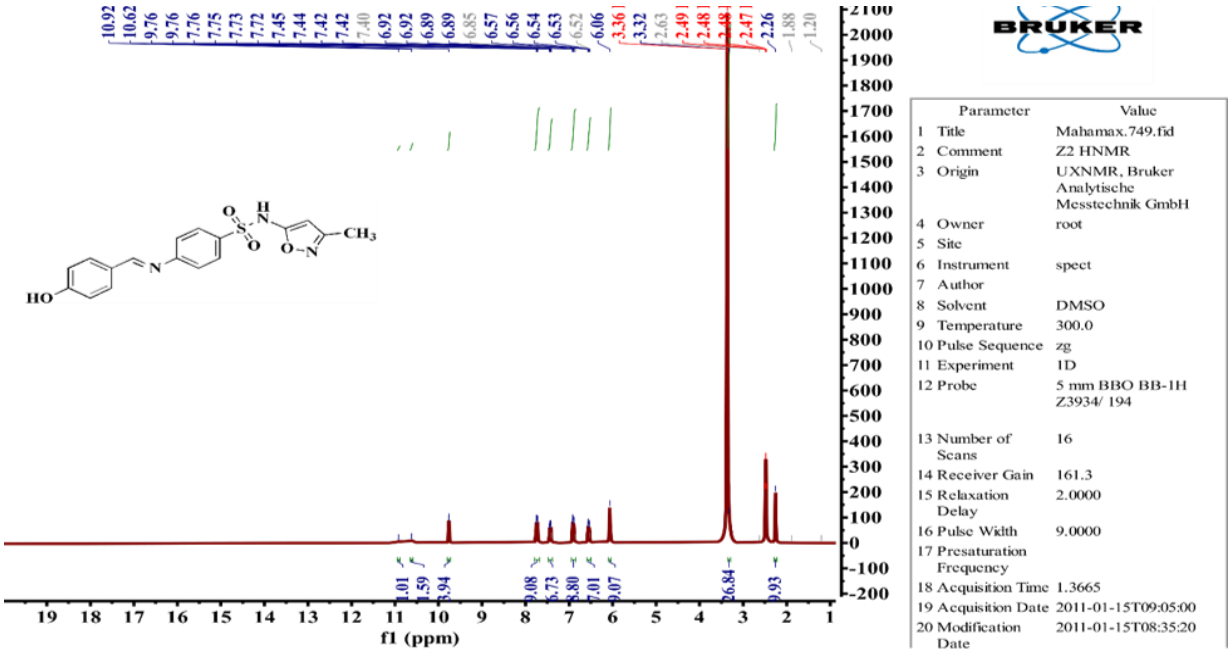


Figure 3. [1]HNMR spectrum of compound 2. (**Prepared by Authors, 2026**).

3.1 Anti-bacterial study- In silico study: Molecular Docking

Molecular docking was performed for the dihydropteroate synthase protein with the pterin–sulfonamide as a co-crystallized ligand, which acts as a protein inhibitor, in order to ensure the accuracy of the docking setting. Results indicated that the orientation of the co-crystallized ligand closely resembled its actual orientation in the binding site of dihydropteroate synthase, exhibiting high stability with a docking score of -5.706, as shown in Figure 4.

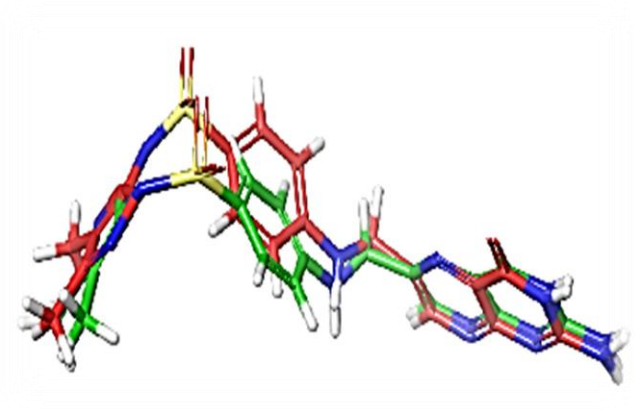


Figure 4. Orientation of co-crystallized ligand. (**Prepared by Authors, 2026**).

Furthermore, co-crystallized ligand demonstrated favorable interactions, including hydrogen bonds with residues (ARG235, ASN115, LYS221, SER222, ASP185, and GLY217) and hydrophobic interactions with residues (ARG255, ARG63, MET139, PHE190, and LYS221). Subsequently, molecular docking studies were conducted for all synthesized 1-5 compounds. The results revealed that these compounds bind to the dihydropteroate synthase at the same location as the co-crystallized ligand, with docking scores ranging between -4.161 and -3.927. Most of the synthesized compounds (**1-5**) exhibited weaker docking scores comparable to the co-crystallized ligand. Furthermore, all compounds demonstrated almost different orientations at the binding site, depending on their substituted groups. The results also indicated that all ligands generally formed hydrogen bonds with amino acid residues (ARG235, ARG255, ARG63, LYS221, and HID257) and exhibited hydrophobic interactions with amino acid residues (ARG235, ARG255, ARG63, LYS221, HID257, MET139, and PRO232). Additionally, a study was conducted to explore the molecular docking of the drug gentamicin with the synthase protein, aiming to evaluate its binding affinity. The results showed that gentamicin appeared a robust binding affinity of -4.169, primarily attributed to the formation of numerous hydrogen bonds. However, it's noteworthy that these interactions basically occurred outside the binding site, as shown in Table 3 Molecular docking scores of compounds 1-5.

Table 3. Molecular Docking scores of compounds 1-5

Title	docking score	Hydrogen bonding	Other interactions
1	-4.161	THR62, LYS221, HH12, LYS221, ARG255, ARG63	ARG63, LYS221
2	-3.822	ARG255, ARG255, LYS221, HID257	LYS221, HID257, ARG63
3	-4.104	ARG235, ASP96, LYS221	ARG255, ARG63, LYS221
4	-4.044	ARG63, ARG255, LYS221, GLY189, SER222	ARG255, ARG63, LYS221, HID257, ILE117,
5	-3.927	ARG63, LYS221, HID257, ARG235	HID257, ARG63, LYS221, PRO232
pterin–sulfonamide	-5.706	ARG235, ASN115, LYS221, SER222, ASP185, GLY217	ARG255, ARG63, MET139, PHE190, LYS221

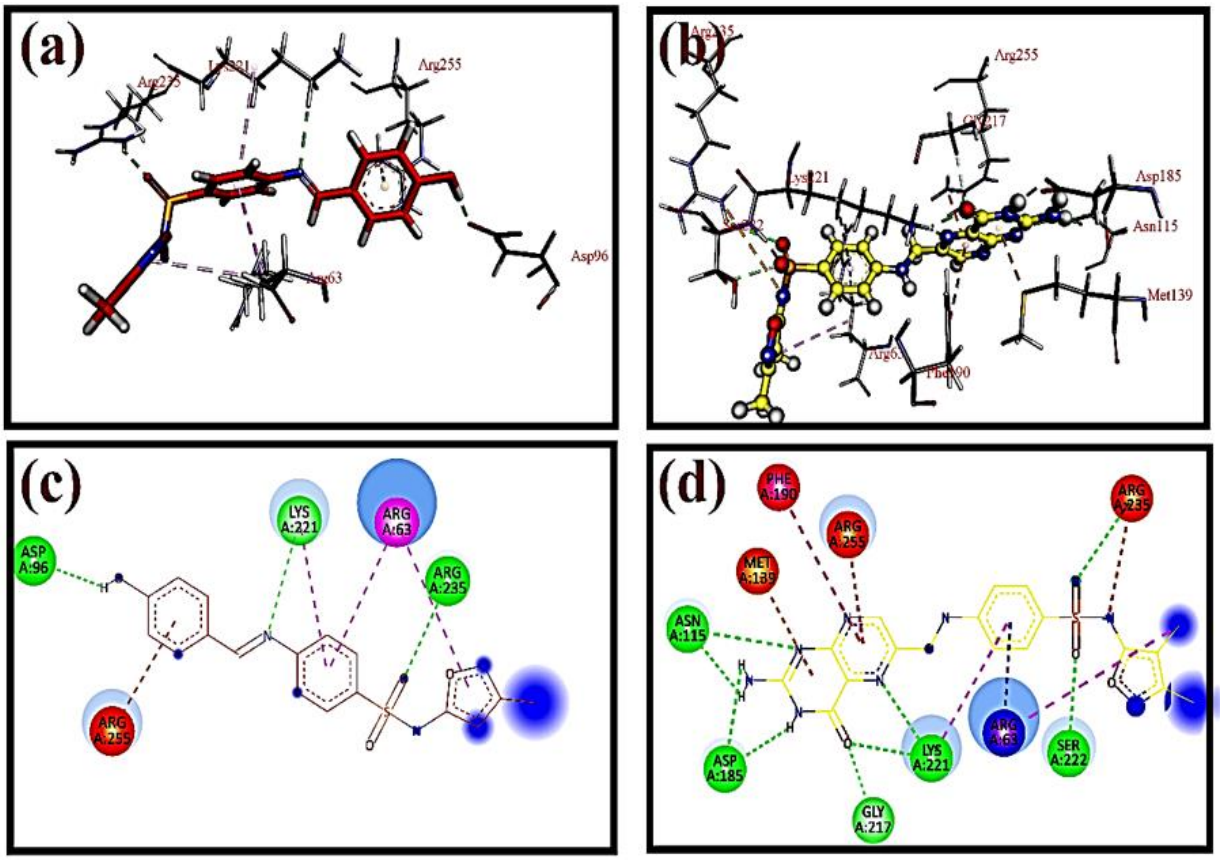


Figure 5. 2D and 3D interactions of compound 3 and co-crystalized ligand with dihydropteroate synthase. a. 3D interactions of compound 3. b. 3D interactions of co-crystalized. c. 2D interactions of compound 3. d. 2D interactions of co-crystalized. (**Prepared by Authors, 2026**).

3.2 In vitro antibacterial study:

All synthetic compound's function in biology (1-5) was evaluated against both negative and positive bacteria, specifically *Escherichia coli* and *Streptococcus auris*, to substantiate the potential compounds property to avoid the replication of bacteria. The findings, as presented in Table 4, Table 5 and Figure 6, indicate that the compounds exhibit a noteworthy inhibitory effect, with particular emphasis on compounds 3 and 4. The administered dose emphasize was 40 micrograms, and gentamicin was Participating as the standard inhibitor for comparison.

Table 4. Antibacterial activity of novel sulfamethoxazole

compound	Inhibition zone (mm)	
	E. coli	Staphylococcus aureus
1	13	10
2	16	12
3	25	24
4	24	23
5	17	16
Gentamicin standard	44	46

Table 5. Antibacterial activity of novel sulfamethoxazole, Schiff base derivatives

Compound	Inhibition zone (mm)	
	E. coli	Staphylococcus aureus
1	13 ±0.57 c	10 ±0.42 d
2	16 ±0.64 c	12 ±0.55 cd
3	25 ±1.09 b	24 ±1.17 b
4	24 ±1.17 b	23 ±0.96 b
5	17 ±0.62 c	16 ±0.64 c
Gentamicin	44 ±2.48 a	46 ±2.56 a
L.S.D. (P-value)	6.027 ** (0.0001)	5.962 ** (0.0001)

Note: Means having with the different letters in same column differed significantly. (P≤0.01).

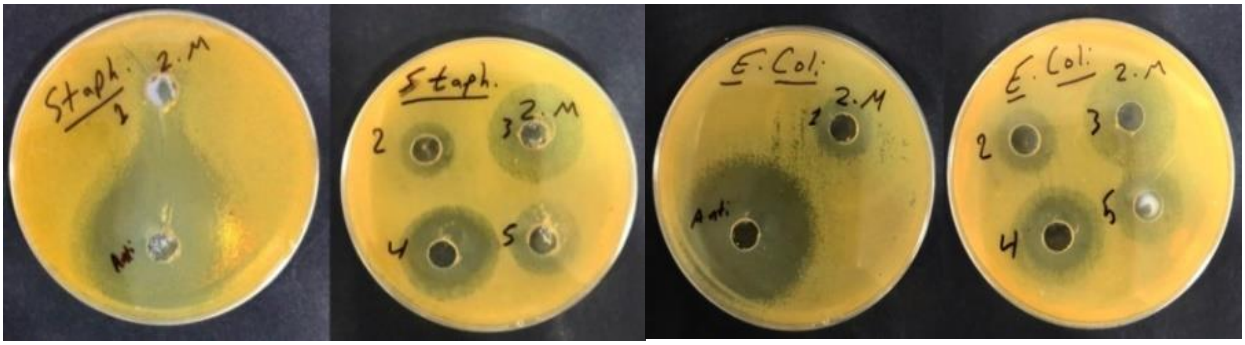


Figure 6. Antibacterial of Schiff base derivatives. (**Prepared by Authors, 2026**).

4. Discussion

The FT-IR and ^{1}H NMR spectral data confirm the effective synthesis of the Schiff base derivatives through imine bond formation. The disappearance of (-NH_2) stretching bands and the appearance of (-C=N) stretching peaks strongly support this transformation with water molecule exit. Additionally, the structures were confirmed by the existence of distinctive functional group peaks for halogenated and substituted derivatives. The mechanism involves a nucleophilic addition reaction to create Schiff base derivatives when an amine nucleophilically attacks a carbon atom in an aldehyde as an electrophile to give a carbinolamine that loses a water and acetate ion to give the required compounds **(20)**. Synthesis of compounds was characterized by using FT-IR and ^{1}H NMR spectra. FT-IR spectra confirm the synthesis of compounds 2-5 by the disappearance of symmetric and asymmetric stretching bands of (-NH_2) group (3485, 3261) and the appearance of stretching bands at (1606–1620) cm^{-1} due to formation of (-C=N) bonds of imine groups. In addition, FT-IR spectra showed the appearance of some characteristic bands for the formation of derivatives (2-4), such as the C-Cl group bands of compound (2) at (1033) cm^{-1}, the hydroxyl (- OH) stretching band of compound (3) at (3429) cm^{-1}, the C-Br band of compound (4) at (1035) cm^{-1} and the -$N(CH_3)_2$ band of compound (5) at (2995) cm^{-1} **(21)**, the other bands of compounds 2-5 mentioned in Table1.^{1}H NMR spectra confirm the synthesis of compounds 1 and 2 by the appearance signals at (7.8-8.0) ppm due to C–H proton of imine groups. In addition, singlet signals at (6.1-6.2) ppm due to C-H of Isoxazole ring protons and singlet signals at (2.2-2.3) ppm due to (-CH_3) protons as present in Table 2 and chart ^{1}HNMR spectrum of compounds 1,2 in Figures (2) and (3) **(21)**.

The synthesized sulfamethoxazole Schiff base derivatives showed differing degrees of inhibitory efficacy against both Gram-positive (Staphylococcus

aureus) and Gram-negative (E. coli) bacteria in the antibacterial assessment. All novel synthesized compounds showed significant inhibitory zones, according to the data (Table 4) and statistical analysis (Table 5) demonstrating that Schiff base synthesis usually enhanced antibacterial potency in a comparison with the parent medication.

According to docking studies, all of the synthesized compounds bind to the same active site as the co-crystallized ligand, their binding affinities were slightly weaker. Compounds 3 and 4 showed stronger binding interactions, which is consistent with their high antibacterial activity observed in vitro because of biological activity is frequently related to the chemical structure of the substance. The presence of function groups like -OH, -Br, or extra aromatic rings in drugs may increase their capacity to permeate bacterial cell walls or inhibit key enzymes. However, it should be identified that, while compounds 3 and 4 shown higher activity among the analyzed compounds, gentamicin had the strongest effect (44-46 mm) because of its outstanding effectiveness as a standard antibiotic. These chemicals can inhibit dihydropteroate synthase through methods comparable to those of commonly used sulfonamide medications, considering the consistency between docking results and biological activity. In contrast to its results of molecular docking, which indicate that bacteria are resistant to this substance. Overall, compounds 3 and 4 demonstrate promising antibacterial potential and may serve as candidates for future drug development **(22)**.

5. Conclusion

This study aimed to develop novel antibacterial agents to combat antibiotic resistance by synthesizing and evaluating Schiff base derivatives of sulfamethoxazole. The derivatives were synthesized through condensation reactions between the amino group of sulfamethoxazole and various substituted aromatic aldehydes and were characterized by melting point determination, FT-IR spectroscopy, and 1H NMR spectroscopy. Both in vitro antibacterial assays and in silico molecular docking studies demonstrated that compounds 3 and 4 exhibited the highest antibacterial activity against both Gram-positive and Gram-negative bacteria, whereas compound 1 (a control) showed comparatively lower activity, likely due to existing bacterial resistance mechanisms. These findings identify compounds 3 and 4 as the most promising derivatives and demonstrate that Schiff base modification of sulfamethoxazole is a promising strategy for developing new antibacterial agents with enhanced activity against resistant bacterial strains.

6. Declarations

6.1 Acknowledgments

The authors acknowledge the Department of Chemistry, College of Science, Baghdad University for their encouragement.

6.2 Ethical Considerations

This study was approved by Ethics Committee of [Al-Iraqia University/College of Medicine], Approval Code: [FM.SA242].

6.3 Authors' Contributions

Zahraa M. Abdulmohsan did the study design, drawing the scheme of reaction, supervising sample reaction; conducted sampling, sample testing, measuring melting point, record the results, finally characterization, determination and spectral techniques such as FT-IR, H^1NMR for all new compounds; Akram S. Karamallah and Andy N. S. Shamaya did study and design of molecular docking.

6.4 Conflict of Interest

The authors declare that there are no conflicts of interest.

6.5 Fund or Financial Support

This study did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

6.6 Using Artificial Intelligence Tools (AI Tools)

The authors declare that no artificial intelligence (AI) tools were used in the writing or analysis of this study.

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