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ORIGINAL RESEARCH ARTICLE

Synthesis, in silico, and biological evaluation of new schiff base derivatives as antibacterial and anti-breast cancer agents

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ABSTRACT

Three new Schiff base compounds (S1-S3) from 1-([1,1'-biphenyl]-4-yl)ethan-1-amine and substituted-benzaldehydes are synthesized and biologically evaluated in this work. After microwave-assisted synthesis, the compounds were purified and structurally characterized by FTIR, 1H-NMR, and 13C-NMR. Agar diffusion was used to test their antibacterial activities against pathogens such Staphylococcus aureus, Escherichia coli, Bacillus anthracis, and Acinetobacter. The derivative S2 was the most antibacterial at all doses, with inhibitory zones greater than those of azithromycin in certain instances. The cytotoxicity studies on the MCF-7 breast cancer cell line using MTT assay showed that derivatives S2 and S3 significantly inhibited cancer cell growth in a dose-dependent manner, with derivative S2 having a lower IC50 than derivative S3, indicating greater potency, which depending on in silico molecular docking investigations, derivative S3 have substantial binding affinities to the EGFR receptor and glucosamine-6-phosphate synthase, respectively, with binding energies of -8.5 and -5.4 kcal/mol, and this study suggests Schiff base derivatives multipurpose antibacterial and anticancer applications, particularly against drug-resistant microorganisms and hormone-responsive breast cancer.

Keywords: antimicrobial; anticancer; schiff base; MCF-7; molecular docking; EGFR receptor; G6P synthase

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1. Introduction

Schiff bases are ligands with Imines of the RC group (-RC=N-) are formed by reacting primary amines (R-NH2) with carbonyl compounds (RCOR′). R and R′ might be alkyls or aryls. Schiff bases provide several functions that can replace bridged N, N′, or unbridged. Schiff bases usually include donor atoms. Schiff bases' coordinative solid ability allows them to be employed for liquid–liquid extraction, metal cation transport by means of liquid membranes, asymmetric reactions with organometallic reagents to aldehydes, and asymmetric Diels-Alder reactions[1,2]. Schiff bases have many industrial uses, study shows. They also have several physiological qualities, including antianxiety, antipyretic, antiinflammatory, antibacterial, and others[3]. Schiff bases are chemical compounds of the Schiff base family. As versatile ligands, they may combine with metallic ions and geometries in different oxidation states. When bases appear, d-block metals and lanthanides form complexes. Scientific and pharmacological activities favor metallic Sulphonamide Ligand complexes[4].

Ortho-hydroxy groups generate ketogenic tautomer isomerism at the azomethine group, and Schiff bases from chitosan are used in biochemistry, catalysis, sensing, and water treatment. Ocean crustaceans, molluscs, insects, and fungi produce polysaccharides, such as chitosan and others. The different diseases, such as antitumor, antiulcer, antidiabetic, antioxidant, and antibacterial effects of these derivatives are widely known[5], and these compounds assist breast cancer patients avoid drug resistance by targeting biological processes. Schiff base compounds mixed with traditional chemotherapeutic medicines boost treatment outcomes, according to additional research[6]. The molecular versatility of schiff base derivatives allows extensive structural modifications, which improves their biological activity and drug kinetics. Electron-donating or electron-withdrawing derivatives significantly impact antibacterial and anticancer action[7]. The computational investigations and molecular docking analysis have rationalized Schiff base compound design to optimize biological target interaction[8], and these compounds effects on clinical and preclinical studies continue to reveal their therapeutic potential, enabling their use in infectious illness and cancer therapy. Schiff base compounds are interesting therapeutic candidates for antibacterial and breast cancer treatment, especially against the MCF-7 cell line, because of their multifunctional capabilities. Because of the resistance of microbes to many drugs and synthetic compounds, a number of compounds have been synthesized[9].

Schiff base derivatives have been extensively studied for their biological potential, however few biphenyl-containing imine derivatives have been tested for antibacterial, cytotoxic, and docking purposes. The biological implications of hydroxyl- and methoxy-substitution patterns on this small structural class remain unknown. In this work, three imine derivatives based on 1-([1,1'-biphenyl]-4-yl)ethan-1-amine were synthesized, characterized spectroscopically, and investigated for antibacterial activity, cytotoxicity against MCF-7 breast cancer cells, and in silico binding to selected biological For scaffold optimization, this comprehensive technique may provide a draft structure-activity interpretation.

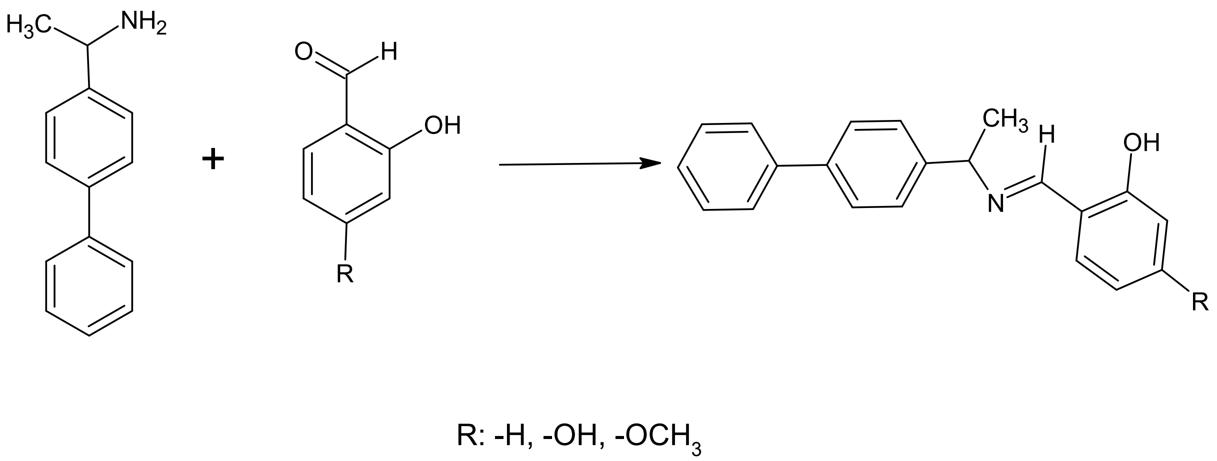
2. Methodology

2.1. Materials

All chemical materials used were high-purity, such as 1-([1,1'-biphenyl]-4-yl)ethan-1-amine, 2-hydroxybenzaldehyde, 2,4-dihydroxybenzaldehyde, and 4-methoxy-2-hydroxybenzaldehyde, which were obtained from Sigma Aldrich (Germany), anhydrous propanol from BDH Chemical Company (China), and absolute ethanol from CDH (India).

2.2. Synthesis of 2-[(E)-{[1-([1,1'-biphenyl]-4-yl)ethyl]imino}methyl]-5-subsutitedphenol (S1-S3)

To synthesize 2-[(E)-{[1-([1,1'-biphenyl]-4-yl)ethyl]imino}methyl]-5-subsutitedphenol , a mixture 0.01 mmole of 1-([1,1'-biphenyl]-4-yl)ethan-1-amine, reacted with 0.01 mmole of each 2-hydroxybenzaldehyde, 2,4-dihydroxybenzaldehyde, and 2-hydroxy-4-methoxybenzaldehyde were obtained three types of solutions. Subsequently, 15 mL of anhydrous propanol was included in the mixture and treated with microwave irradiation at power levels ranging from 400 W to 700 W for a duration of 10 to 15 minutes. The solvent was then evaporated using a rotary evaporator, and the resultant solid products were recrystallized using propanol and then dried at 35 °C. The products were further purified using a 1:10 ethanol-hexane mixture[10].



Scheme 1. Routs of schiff base derivatives (S1-S3).

2.3. Investigation of the antimicrobial activity of schiff base derivatives (S1-S3)

The newly synthesized derivatives (S1-S3) were tested for antibacterial activity utilizing cup-plate agar diffusion and millimeter-measured inhibitory zones. The synthesized compounds were tested for antibacterial activity against amoxicillin at 0.1 and 0.001 mg/mL, so, antibacterial activity against *Bacillus subtilis*, *Staphylococcus aureus*, *E. coli*, and *Acinetobacter* were assessed[11]. The sterilized agar material was placed on Petri plates to harden, and microbial suspensions were evenly applied to the press surface using a sterilized triangular loop, with micropipettes were used to deliver several synthetic chemicals into the cavities at doses of 0.1 and 0.001 mg/mL. DMSO was used as the solvent for all compounds, but sterile distilled water was only employed for pure Azithromycin. The plates were incubated at 37 °C for 48 hours. The diameter of the inhibitory zone around the cups was measured in millimeters after incubation[12].

3. Experimental Part of Molecular Docking

3.1. The derivative S3 with EGFR

The molecular docking research used Autodock (1.5.6). EGFR's cryptographic three-dimensional framework was downloaded from the RCSB protein data bank PDB ID:1M17, and the chemical structure of the synthesized compound was sketched using ChemDraw ultra (version 18.0). Pre-docking was done for receptor and ligand. The co-crystalized ligand and water molecules were removed, missing atoms rectified, and polar hydrogens added to EGFR. Swiss protein viewer (4.1) minimized energy. Both receptor and ligand were preserved as pdbqt. The receptor grid box was parametrized with dimensions of 24 x 26 x 22 (x, y, z) with center values of 20.663, 4.206, and 56.920 Å, with setting Autodock vina settings to default yielded 9 ligand-target protein poses. Discovery Studio (21.1.0.2) generated 2D and 3D images of docking findings[13].

3.2. The derivative S3 with Glucosamine-6-Phosphate

Protein data repository 1MOQ provided the crystallographic 3D structure of Glucosamine-6-Phosphate synthase. The synthesized derivative S3 was drawn in ChemDraw ultra (18.0). Docked using Autodock Tools (1.5.6) and saved as pdbqt. Molecular docking was done using Autodock vina and AutoGrid software with a 40 x 40 x 40 grid box with 21.067 x 20.007 x 12.729 grid center for x, y, and z dimensions[14].

4. Results and Discussion

Schiff base derivatives have been synthesized by condensing primary amines and carbonyl compounds, and amine nucleophilically attacks the carbonyl carbon to generate a carbinolamine intermediate, which dehydrates to form the imine compounds. The acid catalyst can eliminate water. Schiff bases are synthesized and stable and have biological functions[15].

The FTIR spectroscopy is essential for establishing imine derivatives that synthesized by examining functional group vibrations, and successful synthesis is confirmed by the absence of the carbonyl, and C-H aldehyde bands with primary amine as two bands and the presence of an active imine (C=N) stretching band[15]. In addition, hydroxy groups (3390, 3352, and 3359 in FTIR), a methoxy group (55.62 in ^{1}HNMR), and the imine group of all synthesized derivatives in FTIR and ^{1}H-NMR appeared in the synthesized derivatives at FTIR, ^{1}HNMR, and ^{13}CHNMR. The experimental composition suggests the right synthesized derivatives S1-S3, as shown in **Table 1**.

Table 1. Experimental composition of synthesized derivatives S1-S3.

Compound No.	Experimental composition (Theory)			
	C	H	N	O
S1	83.55 (83.69%)	6.42(6.35%)	4.71 (4.65%)	5.32 (5.31%)
S2	79.51 (79.47%)	5.98 (6.03%)	4.46 (4.41%)	10.11 (10.08%)
S3	79.71 (79.73%)	6.45 (6.39%)	4.17 (4.23%)	9.67 (9.65%)

Azomethine derivative (S1): Color: Brown-Yellowish powder, melting point: 197-201 °C. FTIR (cm^{-1}): 3390 (OH), 3061 (C-H of aromatic ring), 2958 (C-H of the aliphatic group), 1638 (azomethine group), 1592 (C=C of aromatic ring)[16]. ^{1}H-NMR (ppm) used DMSO-d6 as a solvent, 9.83 (s, 1H, OH), 8.38 (s, 1H, CH=N), 6.88-7.70 (m, 13H, Ar), 1.36 (d, 3H, CH_3). ^{13}C-NMR: δ 161.01 for the carbon aromatic ring that linked OH, while 157.62 returned to the carbon of the azomethine group, 145.64 -116.33 returned to carbons of the aromatic ring, 64.33 returned to the carbon aliphatic group that linked to a methyl group, 24.39 for the carbon of methyl group[17].

Azomethine derivative (S2): Color: Yellow powder, melting point: 228-232 °C. FTIR (cm^{-1}): 3352 (OH), 3033 (C-H of aromatic ring), 2981 (C-H of aliphatic group), 1627 (azomethine group), 1599 (C=C of aromatic ring). ^{1}H-NMR (ppm) used DMSO-d6 as a solvent, 9.63 and 9.42 (s, 1H, OH in Ortho and Para), 8.42 (s, 1H, CH=N), 6.91-7.84 (m, 12H, Ar), 1.67 (d, 3H, CH_3)[18]. ^{13}C-NMR: δ 167.25 and 163.82 returned to the 2 carbons aromatic ring that linked OH, while 161.56 returned to the carbon of the azomethine group, 145.64 -105.54 returned to carbons of the aromatic ring, 67.64 returned to the carbon aliphatic group that linked to a methyl group, 22.42 for the carbon of methyl group[19].

Azomethine derivative (S3): Color: Yellow powder, melting point: 213-218 °C. FTIR (cm^{-1}): 3359 (OH), 3042 (C-H of aromatic ring), 2923 (C-H of aliphatic group), 1641 (azomethine group), 1597 (C=C of aromatic ring). ^{1}H-NMR (ppm) used DMSO-d6 as a solvent, 9.60 (s, 1H, OH), 8.45 (s, 1H, CH=N), 6.40-7.64 (m, 12H, Ar), 3.38 (s, 3H, OCH_3), 1.19 (d, 3H, CH_3)[20]. ^{13}C-NMR: δ 164.16 and 163.89 returned to the 2 carbons aromatic ring that linked methoxy and OH, while 158.72 returned to the carbon of the azomethine group, 146.20 -100.65 returned to carbons of the aromatic ring, 64.33 returned to the carbon aliphatic group that linked to a methoxy group, 55.62 for the carbon atom of methoxy group, 26.99 for the carbon of methyl group[21].

Cytotoxicity evaluation of synthesized derivatives S2 and S3

The results suggest that derivative S2 has cytotoxic effects on MCF-7 breast cancer cells at varying doses, with cell viability approximately 100% at 0 μppm and a mean of 100.16%. Cytotoxicity rises with concentration, and cell viability reduces to 71.543% at 20 ppm, to 43.72% at 80 μppm, and 31.56% at 160 μppm, with an IC50 for derivative S2 of 51.82 μppm, which inhibits cell viability by 50%. The dose-dependent decrease in cell viability shows that derivative S3 inhibits MCF-7 cell growth, as shown in **Table 2** and **Figures 1** and **2**.

Table 2. IC50 rates of synthesized derivative S2 on MCF-7 cell viability.

Concentration	**24 h**	
(μppm)	Mean	SD
0	100.9808	4.563203
20	71.54341	4.087601
40	57.35048	2.674659
80	43.72347	4.221349
160	31.56592	4.08088
320	20.91865	2.522623

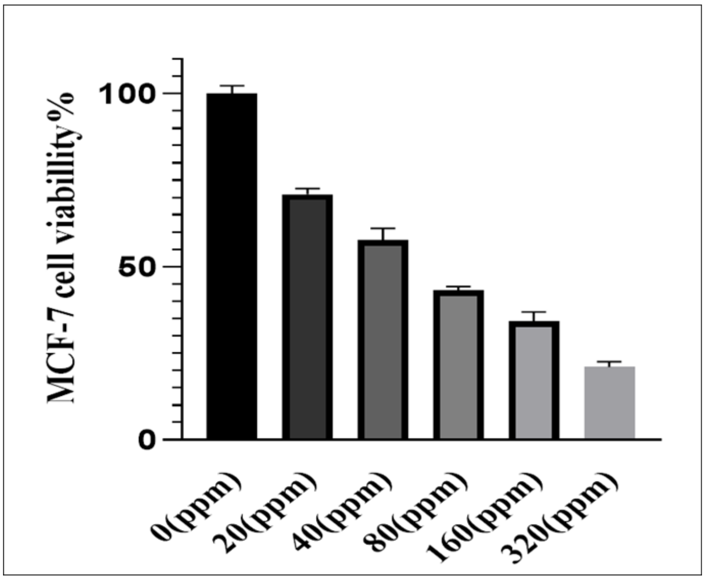


Figure 1. Effect of derivative S2 on MCF-7 cell viability.

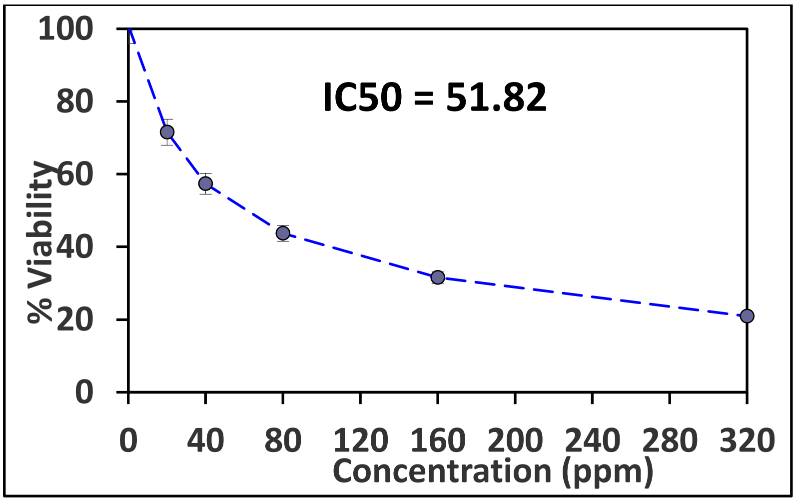


Figure 2. IC50 of derivative S2 on MCF-7 cell viability.

The derivative S3 cytotoxicity on MCF-7 breast cancer cell lines at different doses is shown. Cell viability averages 100.16% (SD = 3.38) at 0 µppm. Increased derivative S3 concentration drastically reduces cell viability. Cell viability reduces to 82.17% (SD = 1.02 at 20 µppm and 65.29% (SD = 2.08) at 40 µppm. The cytotoxicity increases with concentration, with cell viability at 56.43% (SD = 1.50) for 80 µppm, 34.75% (SD = 1.11) for 160 µppm, and 8.79% (SD = 1.28) for 320 µppm. The graph shows that derivative S3 inhibits

MCF-7 cell proliferation at 113.13 µppm, the IC50 value. Derivative S3 decreases cell viability dose-dependently and has strong cytotoxic effects at 40 µppm, making it a prospective cancer therapeutic option, as shown in **Table 3** and **Figures 3** and **4**.

Table 3. IC50 rates of derivative S3 on MCF-7 cell viability.

Concentration	**24 h**	
(µppm)	Mean	SD
0	100.0161	3.381016
20	82.17363	1.018785
40	65.28939	2.083698
80	56.43408	1.504772
160	34.75241	1.11068
320	8.7895	1.280397

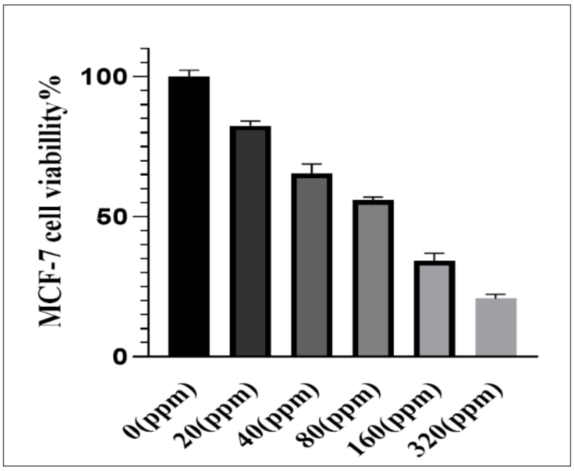


Figure 3. Effect of derivative S3 on MCF-7 cell viability.

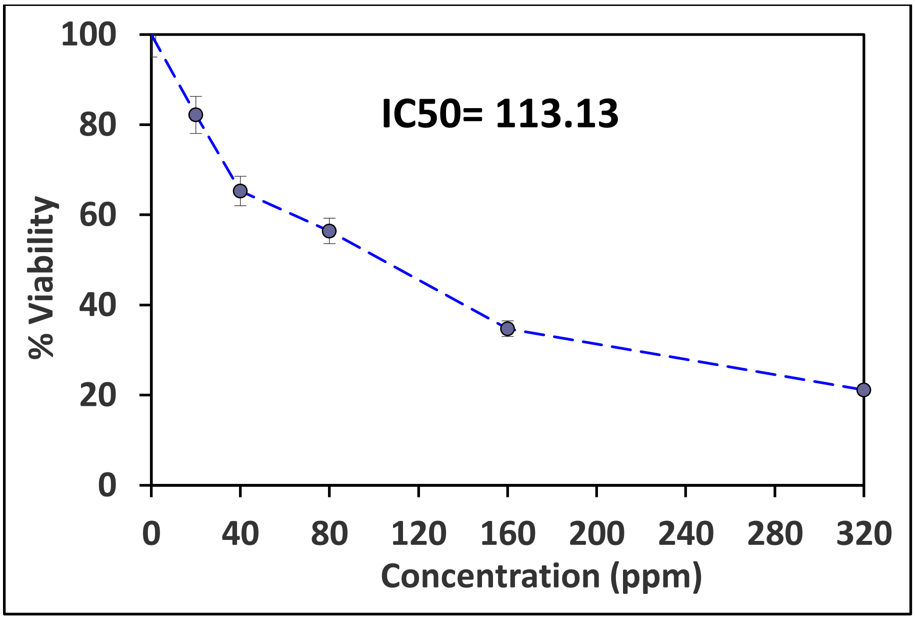


Figure 4. IC50 of derivative S3 on MCF-7 cell viability.

Compared to derivative S3, derivative S2 is more cytotoxic to MCF-7 breast cancer cells, and IC50 for derivative S2 is 51.82 µppm, showing a lower dosage needed to block 50% of cell viability, whereas S3 is 113.13 µppm, indicating lesser potency. These derivatives reduce cell viability at increasing doses, and derivative S2 kills cells at lower doses, indicating it may be better for cancer therapy.

5. Biological Activity

The different derivatives S1, S2, and S3 were tested for antibacterial activity against several microorganisms at 0.1 and 0.01 mg/ml. Derivative S2 was most bactericidal at 0.1 mg/ml. *Staphylococcus*, *E. coli*, and *Acinetobacter* had 26, 19, and 21mm inhibitory zones, while the derivative S2 had active inhibition zones of 20 mm against *E. coli* and 16 mm against *Acinetobacter* at 0.01 g/ml. The inhibitory zone of derivative S3 at 0.1 mg/ml was 23 mm for *Staphylococcus*, 25 mm for *E. coli*, and 16 mm for Acinetobacter. S3 remained effective against *E. coli* as 25 mm and Acinetobacter as 16 mm at 0.01 mg/ml. in addition, derivative S3 was efficient but has a smaller inhibition zone than synthesized derivative S2. At 0.1 mg/ml, derivative S1 inhibited *Staphylococcus* and *E. coli* with 24 and 18 mm zones, respectively, with did not inhibit *Bacillus anthracis* or *Acinetobacter*. Azithromycin, a known antibiotic, inhibited *Staphylococcus, E. coli*, and *Acinetobacter* at 0.1 mg/ml, suggesting that derivatives S1, S2, and S3 are comparable or better antimicrobials, but S2 is the most potent, as shown in **Table 4** and **Figures 5-8**.

Table 4. Biological activity of synthesized azomethine derivatives S1-S3.

Derivative No.	***staphylococcus***		***E.coli***		***Bacillus anthracis***		***Acinetobacter***	
	0.1 mg/ml	**0.01 mg/ml**	**0.1 mg/ml**	**0.01 mg/ml**	**0.1 mg/ml**	**0.01 mg/ml**	**0.1 mg/ml**	**0.01 mg/ml**
S1	24	13	18	8	5	-	9	-
S2	26	19	20	9	9	-	21	14
S3	32	15	25	11	8	-	16	9
Azithromycin	22	12	17	9	-	-	18	10
Control (D.w)	-	-	-	-	-	-	-	-

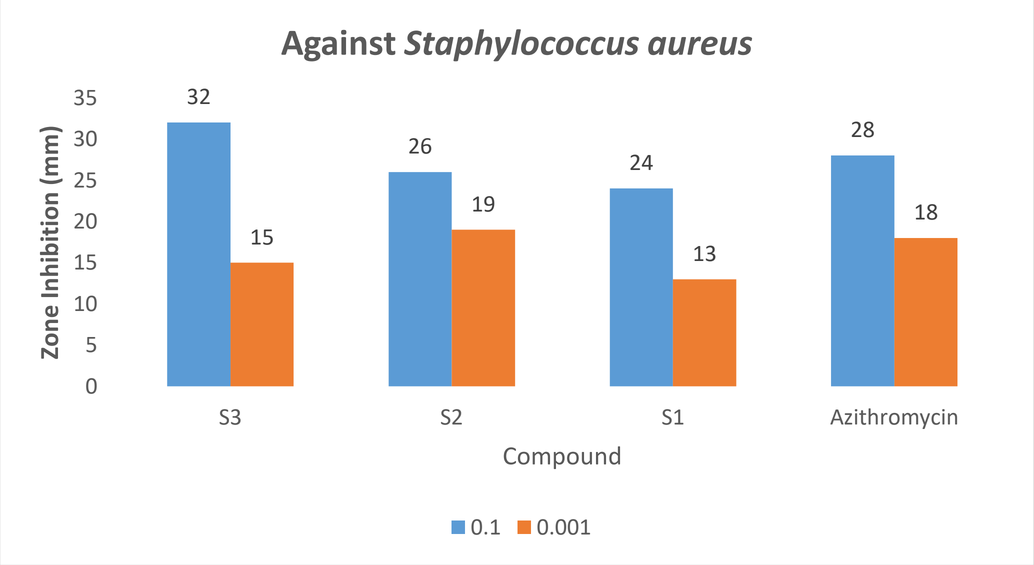


Figure 5. Biological activity of azomethine derivatives (S1-S3) against *Staphylococcus aureus*.

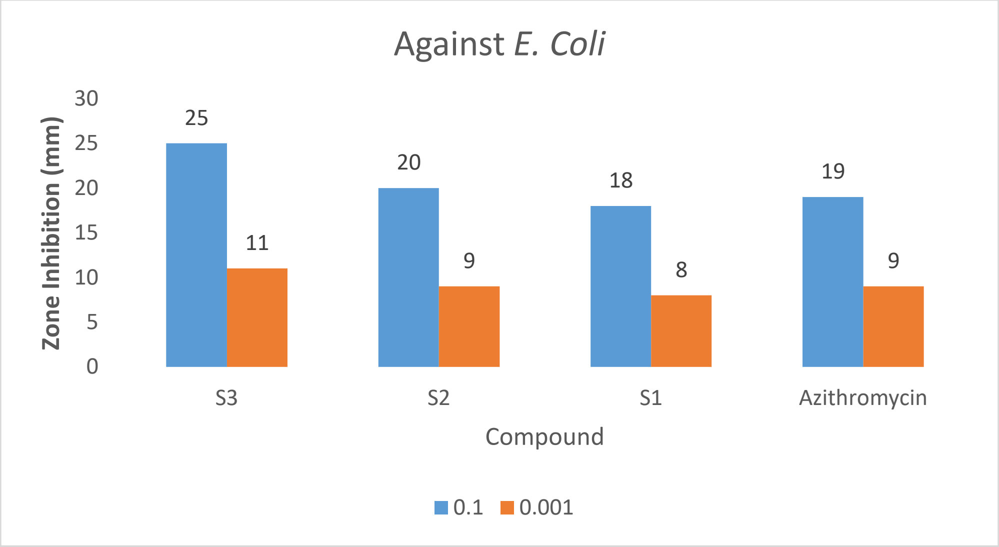


Figure 6a. Biological activity of azomethine derivatives (S1-S3) against *E. Coli.*

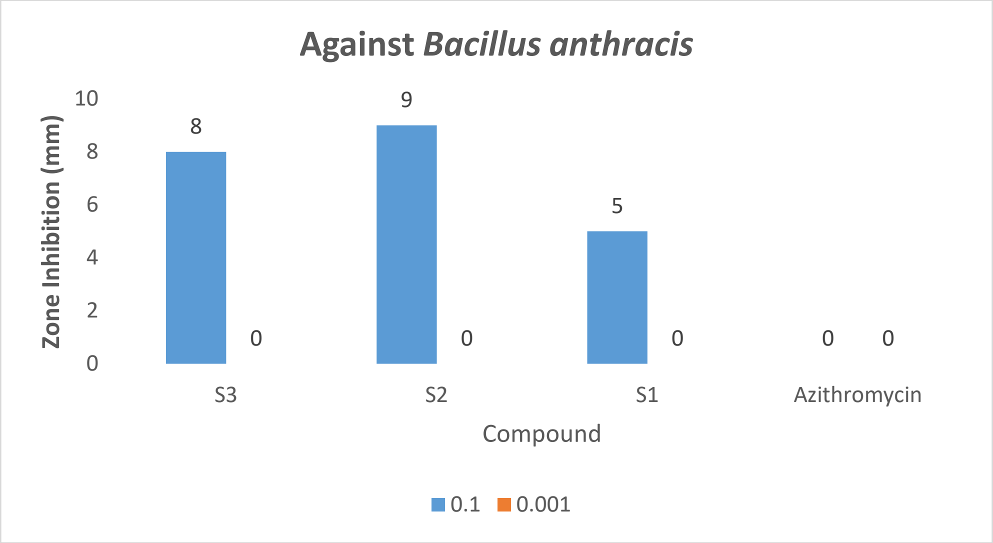


Figure 6b. Biological activity of azomethine derivatives (S1-S3) against *Bacillus anthracis*.

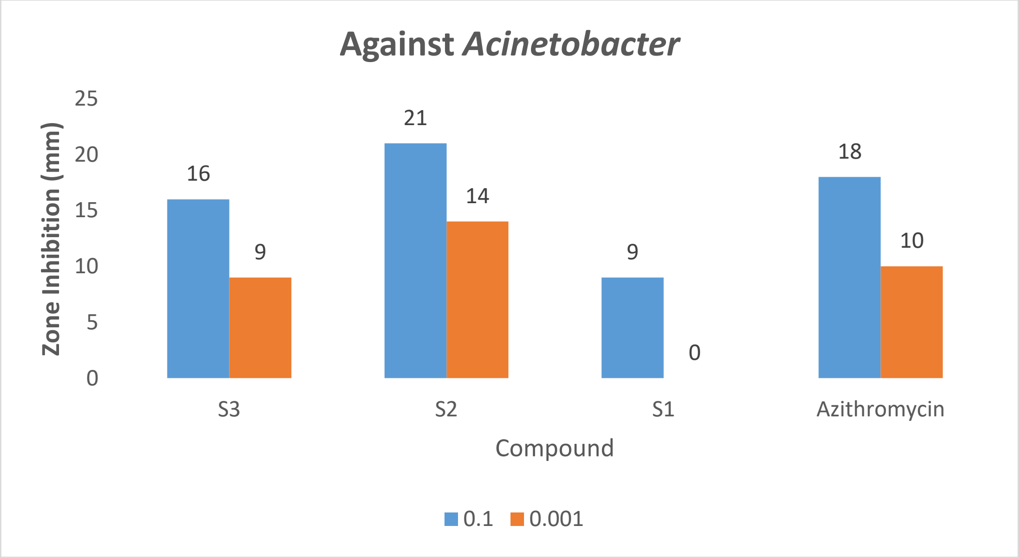


Figure 7. Biological activity of azomethine derivatives (S1-S3) against *Acinetobacter*.

Molecular Docking: The docking simulations have a major role in exploring the interacting modes of derivatives S1-S3 with a receptor molecule. Glucosamine-6-Phosphate synthase, known under the name (GlcnN-6-P synthase)[23] has attracted the interest of several researchers due to its importance in microbial cell wall synthesis[22]. The derivative S2 has a higher score as -5.85908 and rmsd as 1.270038, while derivative S1 has a score as -5.5406 and rmsd as 1.430602. Finally, the derivative S3 has a score of -5.43863 and an RMSD of 1.069565, as shown in **Table 5** and **Figures (8-11)**.

The Epidermal Growth Factor Receptor (EGFR) has been chosen as a target protein for molecular docking to enhance the cytotoxicity (MTT test) of produced derivative (S3) against the breast cancer cell line MCF-7. EGFR is a recognized pivotal signaling molecule that facilitates cellular proliferation, migration, and invasion in several cancer types[24]. The synthesized compound demonstrated a binding score of -8.5 kcal/mol and exhibited multiple interactions with the EGFR binding site, including a pi-sulfur interaction between MET742 and the pi-electrons of the aromatic ring, as well as pi-alkyl interactions with CYS773, LEU820, and VAL702 involving the ligand's backbone[13].

Table 5. Docking properties of synthesized derivatives S1-S3.

Compound No.	Smiles	rseq	mseq	S	rmsd_refine
S1	Oc1c(/C=N\C(C)c2ccc(-c3ccccc3)cc2)cccc1	1	1	-5.5406	1.430602
S2	Oc1c(/C=N\C(C)c2ccc(-c3ccccc3)cc2)ccc(O)c1	1	2	-5.85908	1.270038
S3	Oc1c(/C=N\C(C)c2ccc(-c3ccccc3)cc2)ccc(OC)c1	1	3	-5.43863	1.069565

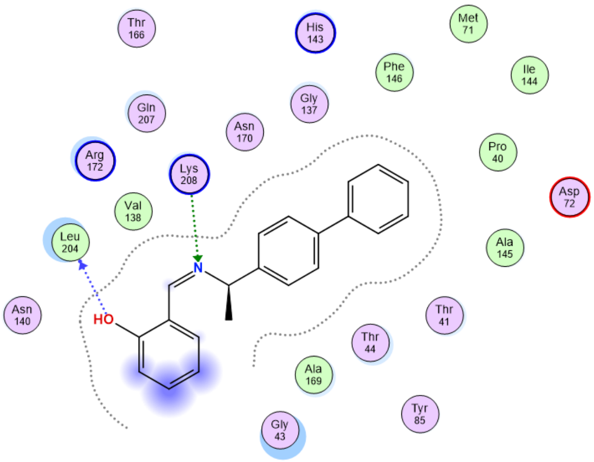


Figure 8. 2D of interaction between derivative S1 and GlcnN-6-P synthase Receptor.

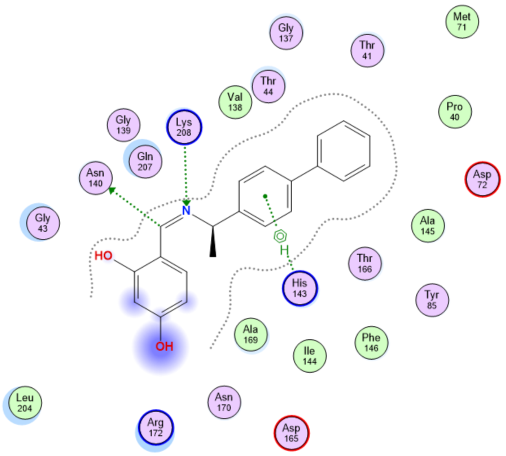


Figure 9. 3D of interaction between derivative S2 and GlcnN-6-P synthase Receptor.

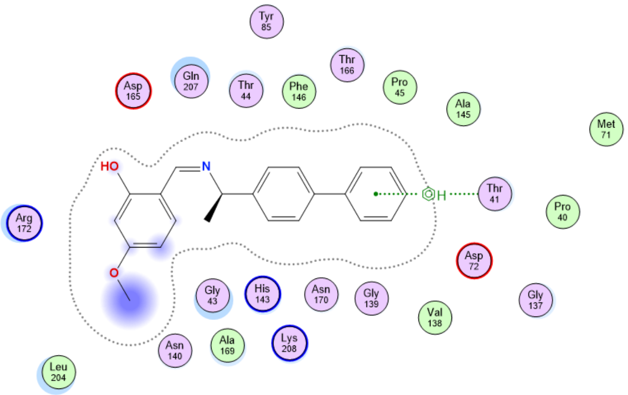


Figure 10. 3D of interaction between derivative S3 and GlcnN-6-P synthase Receptor.

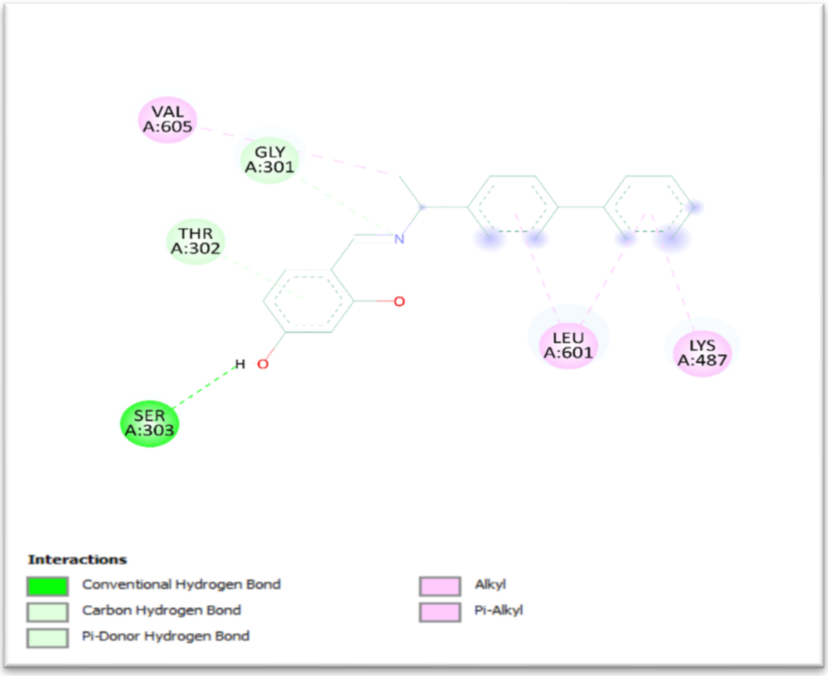


Figure 11. 2D of interaction between derivative S3 and Epidermal Growth Factor Receptor.

The calculated physicochemical properties differ significantly between synthesized derivatives S1-S3, in which derivative S2 had a molecular weight of 317.38 g/mol, a consensus LogP of 4.10, and the highest TPSA value (52.82 Å²), with 2 hydrogen-bond donors and 3 acceptors. A greater balance between lipophilicity and polarity may improve interactions with biological targets. While, derivative S1, with a lower molecular weight (301.38 g/mol), higher LogP (4.51), lower TPSA (32.59 Å²), and less hydrogen-bonding properties (HBD = 1, HBA = 2), derivative S1 showed poorer polarity and interaction synthesized derivative S3 is a larger and more flexible structure with a greater molecular weight (331.41 g/mol), intermediate TPSA (41.82 Å²), 3 hydrogen-bond acceptors, and high molar refractivity (103.14) with 5 rotatable bonds synthesized derivative S2 has the finest descriptor profile in this little series, as shown in **Table 6**.

Table 6. Selected physicochemical descriptors of synthesized derivatives S1-S3.

Compound	MW (g/mol)	Consensus LogP	TPSA (Å²)	HBD	HBA	Molar Refractivity	Rotatable Bonds
S1	301.38	4.51	32.59	1	2	96.65	4
S2	317.38	4.10	52.82	2	3	98.68	4
S3	331.41	4.46	41.82	1	3	103.14	5

A structure-activity relationship proposed for these synthesized derivatives, the derivative S2, bearing two hydroxyl groups, showed the most favorable overall profile, which attributed to increased polarity and stronger hydrogen-bonding capacity, because has these active groups that pull electrons to sharing. While derivative S1, containing only one hydroxyl group, exhibited lower activity, derivative S3, with one hydroxyl and one methoxy substituent as two active groups that share electrons and increase electron density, but the methoxy may result in bulk for this compound and suggest less activity.

6. Conclusion

The successful synthesis of Schiff base derivatives S1-S3 were characterised by spectrscopy, such as FTIR, ^{1}H-NMR, and ^{13}C-NMR, which confirmed the formation of the azomethine compounds, and biological evaluation indicated that tested derivatives exhibited measurable antibacterial and cytotoxic against MCF-7, with derivative S2 suggest most favourable overall profile among these derivatives S1-S3. The docking results suggested that these derivatives interact with target proteins via different bonds with amino acids in the protein according to docking results. However, these results suggest antibacterial activity was limited to agar diffusion, in addition to cytotoxicity evaluation was performed only against MCF-7 cell line. These derivatives are exploratory potential, not proven medicinal drugs. MIC/MBC, normal cell line, and mechanistic assessment investigations are needed to evaluate the cellular viability.

Conflict of interest

The authors declare no conflict of interest.

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