INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

Research Article

Synthesis Insilico Screening and Evaluation of Novel Indole Derivatives for Possible Biological Activity

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ARTICLE INFO

Published: 15 Sept 2026
Keywords:
Osimertinib; EGFR-TKI; Antibacterial activity, Staphylococcus aureas, Molecualr docking, Indole derivatives, Dihdrofolate reductase protein.
DOI:
10.5281/zenodo.22769763

ABSTRACT

Indole is a heterocyclic aromatic compound that has gained considerable attention in medicinal chemistry because of its diverse pharmacological properties, particularly its promising antibacterial activity.Pharmacological agents that kills bacteria are essential drugs in some tropical countries. In this review ,a series of 2-(4-Bromophenyl)-1H-indole derivatives (5a-e) have been synthesized by the conventional method. The obtained derivatives were purufied by recrystallization using methanol as a solvent or columa chromatography. They are characterized by melting point, TLC, FT-IR, 13C NMR, 1H NMR, MASS spectral data. These compounds wewrw evaluated in silico by using softwaew's (Pubchem for novality, Lipinski's rule of 5, Molsoft molecular property explorer, OSIRIS for toxicity studies, PASS prediction and Molecular docking studies). These compounds were evaluted for their possible antibacterial activity against gram +ve bacteria (Staphylococcus aureas, Bacillus subtilis). These derivatives are compared with standard antibacterial drug (Norfloxacin).All the novel derivatives shows antibacterial activity but the derivative 5d shows high potent activity towards bacteria. Molecular docking studies guided and proved the biological activity against Dihydrofolate reductase protein (3SRQ). In conclusion these novel indole derivatives have promising potential as antibacterial activity for treatment of many bacterial infections.

INTRODUCTION

The widespread use of antibiotics has significantly improved public health by reducing the incidence and severity of bacterial infections. However, the inappropriate and excessive use of these agents has accelerated the emergence of antibiotic-resistant bacterial strains, thereby diminishing the effectiveness of conventional antimicrobial therapies. The rapid development of antimicrobial resistance has become a major global health concern and highlights the urgent need for the discovery of novel antibacterial agents. Among the promising heterocyclic scaffolds, benzimidazole

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Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

and indole derivatives have attracted considerable attention because of their broad spectrum of biological activities. These aromatic heterocyclic compounds serve as valuable structural frameworks in medicinal chemistry and are extensively utilized for the design, synthesis, and structural modification of new pharmaceutical agents with enhanced therapeutic potential.

The indole nucleus is a pharmacologically important bicyclic heterocyclic ring with nitrogen atom which exhibits a broad spectrum of biological activities. Owing to its versatile chemical structure, indole has been extensively employed in medicinal chemistry to enhance the antibacterial potential of therapeutic compounds. Furthermore, indole derivatives have demonstrated significant pharmacological activities, including antitumor, antimicrobial, antibacterial, antiviral, antifungal, and anti-HIV effects.

MATEERIALS AND METHODS

Phenylhydrazine, 4-bromo acetophenone, Ethanol, Glacial acetic acid, Dilute HCL, Rectified spirit, Polyphosphoric acid, Activated charcoal, Potassium carbonate, Dimethyl formamide, Alkyl halides (Chloro fluro benzene, 2-chloro ethanol, Chloroacetonitrile, 2-chloro acetamide, Trifluoromethyl).

All the reactions werw performed in dried borosilicate glass beakers, round bottemed flask, Heating mantle with reflux condenser. Precoated silica gel plates (MERCK) were useed for TLC to monitor progress of the reaction. Compounds melting points were determined by capillary method and are uncorrected. JASCO UV chamber was used for detection of spots in TLC. IR spectra were recorded on BRUKER FTIR spectrometer. 1H NMR spectra were recorded on 400MHZ spectrometer using DMSO as solvent. The chemical shift data were expressed as values relative to TMS in ppm. Mass spectra were recoded on a 3-5kvESI-MS instrument. 13C NMR spectra were recoded on 100MHZ spectrometer using DMSO as solvent. Elemental analyses (C,H, and N) of the compounds were obbtained from perki-Elmer 240B analyzer and were within ± 0.4% of the theoretical values.

Experimental

In Silico Screening

Lipinski's rule of 5 filtration

The molecular structures were prepared and uploaded in one of the supported formats, including *.pdb, *.mol, *.mol2, *.xyz, *.sdf, or *.smiles. The input file names were carefully checked to ensure they contained no blank spaces or unnecessary characters. After uploading the files, the pH was adjusted within the range of 0–14 according to the study requirements. The files were then submitted, and the molecular property results were generated following the method described by Lipinski (2004).

OSIRIS Property Explorer

In the present study, OSIRIS Property Explorer Version 2, a Java-based software application, was employed to predict the physicochemical and toxicity properties of the designed compounds. The chemical structures were either drawn directly within the software or imported in SMILES format for analysis. The software generated property predictions using a color-coded display, where green indicated a favorable or non-toxic property, while red signified a potential toxicity risk. This approach facilitated the preliminary assessment of the drug-likeness and safety profile of the synthesized compounds prior to further computational and experimental investigations.

Prediction of Activity Spectra for Substances (PASS)

Compounds that satisfied the Lipinski rule of five were further evaluated using the online PASS (Prediction of Activity Spectra for Substances) software to predict their potential biological activities. The prediction was based on the probability of activity (Pa) and probability of inactivity (Pi) values, which range from 0.000 to 1.000. These values were used as the selection criteria for assessing the likelihood of various biological activities of the designed molecules.

Molsoft Property Explorer

In the present study, Molsoft Property Explorer (Version 3.7-2) was employed to evaluate the physicochemical properties of the designed compounds. The molecular structures were either drawn directly within the software interface or imported in MOL, InChI, or SMILES formats. The software was used to calculate key molecular descriptors, including MlogP (octanol/water partition coefficient) and MlogS (aqueous solubility), which are important parameters for assessing the drug-likeness of the compounds.

Molecular Docking

Molecular docking studies were performed using AutoDock 4.2 to investigate the binding interactions of the synthesized indole derivatives (5a–5e) with the bacterial target enzyme Dihydrofolate Reductase (DHFR). The crystal structure of DHFR was retrieved from the Protein Data Bank (PDB) and prepared by removing water molecules and heteroatoms, followed by the addition of polar hydrogens and Kollman charges. The synthesized compounds and the standard drug, Norfloxacin, were drawn using ChemDraw, converted into 3D structures, energy minimized, and saved in PDBQT format. Docking simulations were carried out using the Lamarckian Genetic Algorithm (LGA) in AutoDock 4.2. The docked complexes were analyzed based on binding energy, hydrogen bonding, hydrophobic interactions, and interacting amino acid residues. The compound with the lowest binding energy was considered the most stable, and the results were compared with Norfloxacin to evaluate the antibacterial potential of the synthesized indole derivatives.

Chemistry

Synthesi of (E)-1-(4-bromophenyl)ethanone phenylhydrazone

A solution of 4-bromoacetophenone (1 mmol) in ethanol (10 mL) was treated with phenylhydrazine (1 mmol), followed by the addition of 2–3 drops of glacial acetic acid as a catalyst. The reaction mixture was refluxed at 70–80°C for 2–4 h, and the progress was monitored by TLC. After completion, the mixture was cooled to room temperature and then in an ice bath to induce precipitation of the hydrazone. The solid product was collected by filtration, washed successively with dilute hydrochloric acid and rectified spirit, and recrystallized from ethanol to afford pure (E)-1-(4-bromophenyl)ethanone phenylhydrazone.

Synthesis of 2-(4-bromophenyl)-1H-indole

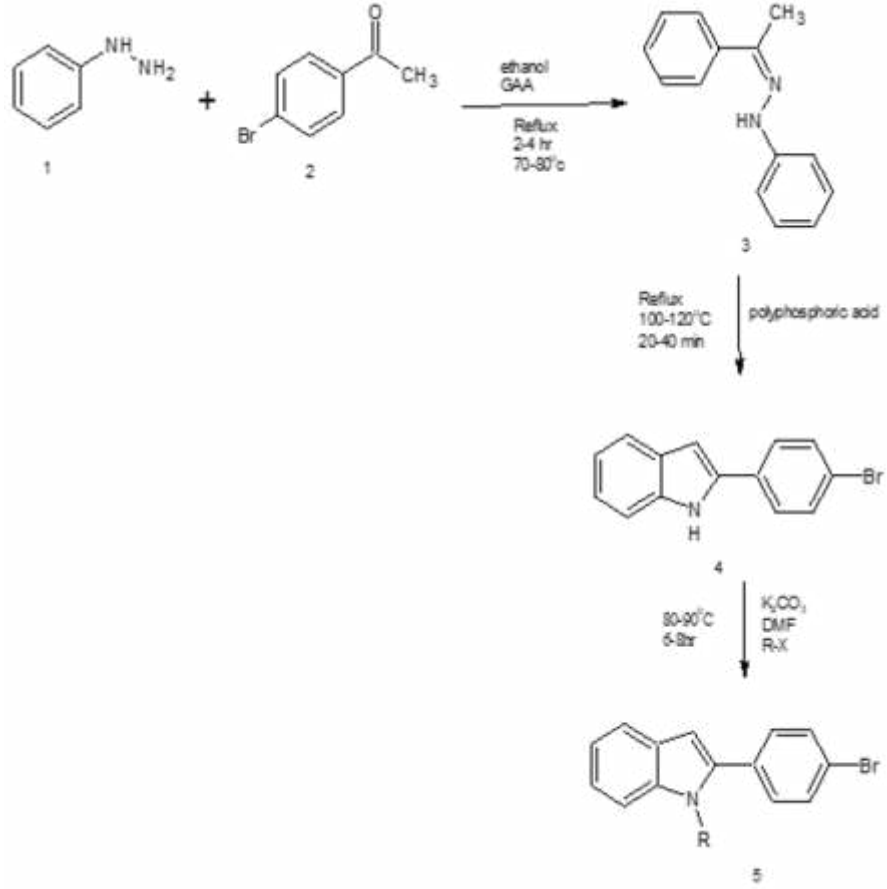
Polyphosphoric acid (PPA) was gently warmed until liquefied, and (E)-1-(4-bromophenyl)ethanone phenylhydrazone (1 mmol) was added portion-wise with continuous stirring. The reaction mixture was heated at 100–120°C for 20–30 min, and the progress was monitored by TLC. After completion, the mixture was cooled and poured onto crushed ice to precipitate the crude indole derivative. The solid was filtered, washed thoroughly with cold water, and dried. The crude product was purified by

recrystallization from hot ethanol using activated charcoal, filtered, and the filtrate was allowed to evaporate to obtain the purified indole derivative, which was stored in an airtight container.

Synthesis of N- substituted-2-(4-bromophenyl)-1H indole derivatives (1a-e)

2-(4-Bromophenyl)-1H-indole (1 mmol) was dissolved in dry DMF (10 mL), followed by the addition of K_2CO_3 (1.5 mmol). After stirring for 30 min at room temperature, the appropriate alkyl halide (1.2 mmol) was added dropwise. The reaction mixture was heated at 80–90°C for 6–8 h with continuous stirring, and the progress was monitored by TLC. Upon completion, the reaction mixture was cooled and poured into ice-cold water to precipitate the product. The crude solid was collected by filtration, washed with water, dried, and recrystallized from ethanol to afford the pure N-substituted indole derivatives.

SCHEME:



R = a = -C6H5F

b = -CH2CH2OH

c = -CH2CN

d = -CH2CONH2

e = -CF3

Spectral Characterisation

The synthesised indole derivatives were characterised using FTIR, ^1H NMR, and ESI-MS techniques to verify their chemical structures. FTIR spectroscopy was used to identify the characteristic functional groups, while ^1H NMR analyses confirmed the proton and carbon

environments within the molecules. ESI-MS was employed to determine the molecular mass and isotopic pattern. The combined spectral data confirmed the successful synthesis and structural identity of the target compounds. Among all (5a-e) derivatives 5d shows the maximum spectral acctiity as shown below.

FTIR (KBr, cm⁻¹): 3310 (N–H, str); 3075 (Ar–C–H, str); 2921 (Aliphatic C–H, str); 1620 (C=N, azomethine, str); 1585 (Ar C=C, str); 1585 (N–H, bend); 1456 (C–N, str); 1310 (C–N, str); 1175 (C–N, str); 1078 (C–C, str); 760 (Ar C–H, out-of-plane bend); 690 (C–Br, str).

ESI-MS (m/z): 367.0687 ($[M+H]^+$), 369.0666 ($[M+H+2]^+$, ^79Br/^81Br isotopic peak), 394.0481 ($[M+Na]^+$), 405.0300 ($[M+K]^+$), 733.1273 ($[2M+H]^+$); fragment ions at **m/z** 318.0764, 288.1016, 273.1135, 249.0922, 224.1079, 179.0828, 152.0706 and 121.0651.

^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 10.85 (s, 1H, NH), 7.75–7.68 (d, J = 8.4 Hz, 2H, Ar–H), 7.55–7.48 (d, J = 8.4 Hz, 2H, Ar–H), 7.42–7.18 (m, 5H, Ar–H), 2.28 (s, 3H, CH_3).

Evaluation of Antibacterial activity

Agar Well Diffusion Method

Mueller–Hinton agar was prepared according to the manufacturer's instructions, sterilized at 121°C for 15 min, and dispensed into sterile Petri plates. A standardized bacterial inoculum of *Staphylococcus aureus* or *Bacillus subtilis* (0.5 McFarland standard; approximately 1.5 × 10^8 CFU/mL) was uniformly spread over the agar surface using a sterile cotton swab. Wells of 6 mm diameter were prepared using a sterile cork borer. The synthesized indole derivatives were dissolved in DMSO to obtain concentrations of 25, 50, 75, and 100 µg/mL, while Norfloxacin at the same concentrations served as the positive control and DMSO as the negative control. Fifty microlitres (50 µL) of each test solution were dispensed into the respective wells, and the plates were incubated at 37°C for 24 h. Following incubation, the zone of inhibition (ZOI) surrounding each well was measured in millimetres (mm) to evaluate the antibacterial activity of the synthesized compounds.

Broth Dilution Method

The minimum inhibitory concentration (MIC) of the synthesized indole derivatives was determined using the broth dilution method. Serial dilutions of the test compounds (25, 50, 75, and 100 µg/mL) were prepared in sterile nutrient broth and inoculated with a standardized *Staphylococcus aureus* or *Bacillus subtilis* suspension. The inoculated tubes were incubated at 37°C for 24 h, and the lowest concentration exhibiting no visible bacterial growth was recorded as the minimum inhibitory concentration (MIC

RESULTS AND DISCUSSIONS

In Silico Screening

Lipinski Rule of 5 Filtration

All the synthesized indole derivatives obey the Lipinski rule of 5 (Table 1).

TABLE 1: Results of Lipinski's filtration

Compound	Molecular weight(daltons)	Hydrogen bond donors	Hydrogen bond acceptors	Log P	Molar refractivity m^3mol^{-1}
5a	366.23	0	1	5.77	96.37
5b	316.19	1	1	3.58	82.30
5c	311.18	0	1	3.89	80.89
5d	329.19	1	1	3.09	84.05

5e	340.14	0	3	5.23	76.37
Standard norfloxacin	319.33	2	5	0.69	92.55

Prediction of Activity Spectra for Substances (PASS)

The Pa values for all the synthesized compounds (5a-5e) were found greater than 0.1. Compound 5d exhibited the highest Pa value amongst the series. However, it wsas found to be less than the standard Norfloxacin (Table 2)

TABLE 2: Results of PASS prediction

Compound	Antibacterial activity	
	Pa	Pi
5a	0.137	0.081
5b	0.288	0.069
5c	0.217	0.153
5d	0.325	0.066
5e	0.243	0.126
Standard norfloxacin	0.892	0.003

Pa =Probability to be active

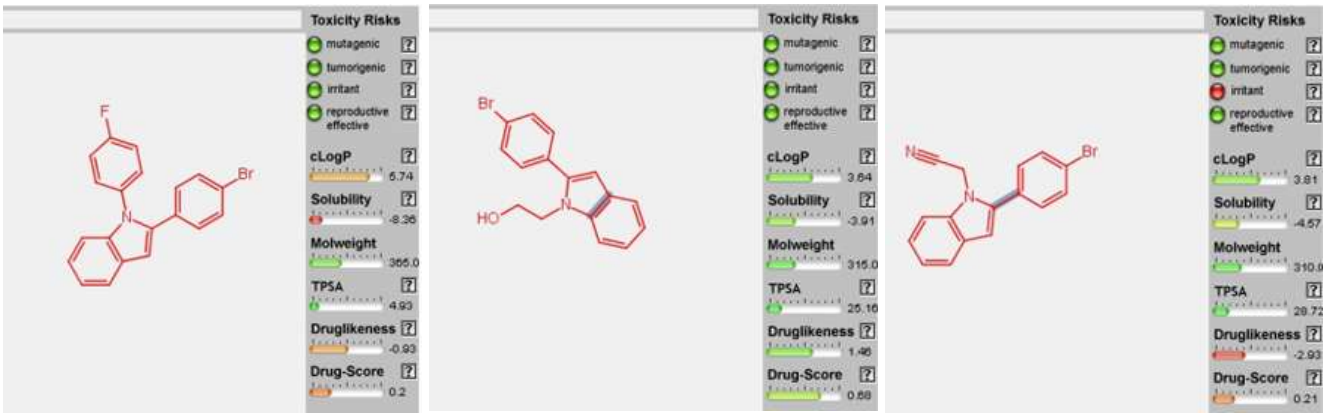
Pi =Probability to be inactive

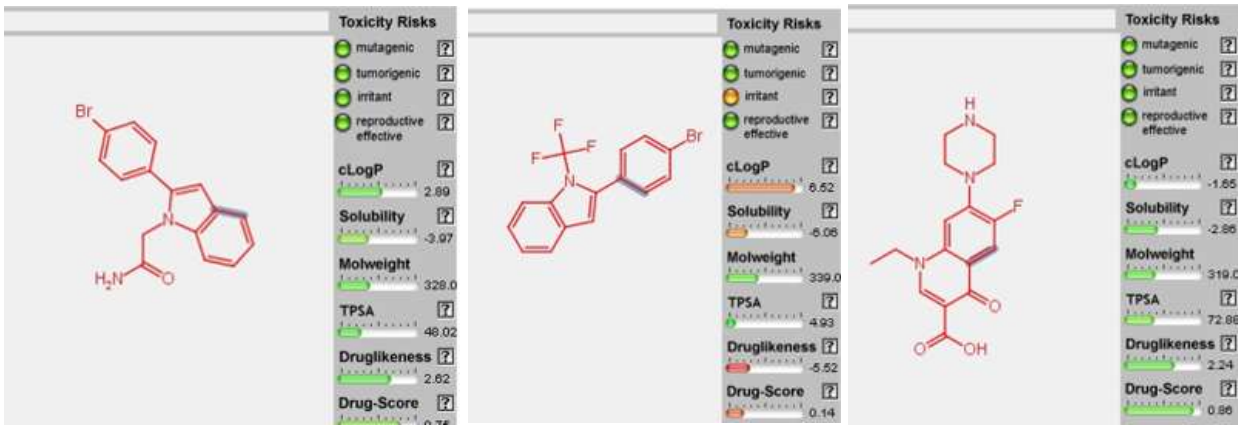
OSIRIS Molecular property Explorer

OSIRIS Molecular Property explorer revealed that the standard drug was non irritent, non-toxic to reproductive and non mutagenic. In the same way all synthesized compounds non- mutagenic, non-tumorigenic, non-reproductive effect. Where ony 5c and 5e shows the irritant effect. (Table 3).

TABLE 3

Compound	Toxicity	Clogp	Solubility	Molecular weight (grams)	TPSA	Drug Likeness	Drug Score
5a	NO	5.74	-8.36	365	4.93	-0.93	0.2
5b	NO	3.64	-3.91	315	25.16	1.46	0.68
5c	Irritant	3.81	-4.57	310	28.72	-2.93	0.21
5d	NO	2.89	-3.97	328	48.02	2.62	0.75
5e	Irritant	6.52	-6.06	339	4.93	-5.52	0.14
Standard Norfloxacin	NO	-1.65	-2.86	319	72.88	2.24	0.86





Molsoft Property Explorer

All the synthesized compounds and the Standard Norfloxacin shows the significant Molsoft values. (Table 4)

TABLE 4

Compound	Molecular formula	Mol.Weight (grams)	HBA	HBD	MlogP	MlogS	Mol PSA	Mol volume (m^3/mol)
5a	C20H13BrFN	365.02	0	0	6.67	-6.99	1.16 A^2	296.68 A^3
5b	C16H14BrNO	315.03	1	1	4.63	-4.78	17.33 A^2	257.71 A^3
5c	C16H11BrN2	310.01	1	0	4.85	-5.36	18.16 A^2	265.04 A^3
5d	C16H13BrN2O	328.02	1	2	3.91	-4.26	34.08 A^2	269.45 A^3
5e	C15H9BrF3N	338.99	0	0	5.87	-6.91	0.51 A^2	242.57 A^3
Standard Norfloxacin	C16H18FN3O3	319.13	4	2	-0.20	-2.14	59.08 A^2	323.78 A^3

Docking Analysis

Among the synthesized indole derivatives (5a–5e), compound 5d exhibited the highest binding affinity toward the DHFR active site, as indicated by its lowest (most negative) binding energy (-9.26) due to the presence of acetamide substitution suggesting that the strongest ligand–protein interaction with potential antibacterial activity.(Table 5).

TABLE 5

Compound	Key Residue	Distance (A°)	No.of Hydrogens	Docking Score (Kcal/Mol)
5a	-	-	0	-8.97
5b	SER	2.915 A°	1	-8.81
5c	-	-	0	-8.90
5d	-	-	0	-9.26
5e	-	-	0	-8.09
Standard Norfloxacin	TYR GLU TYR ARG	1.383A° 2.044A° 1.946A° 3.048 A°	4	-6.79

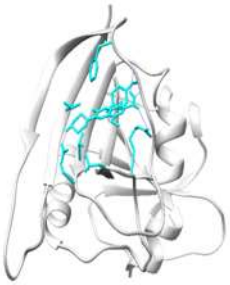
5a

5b

5c

5d

5e

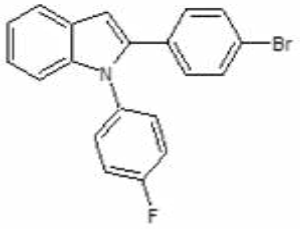
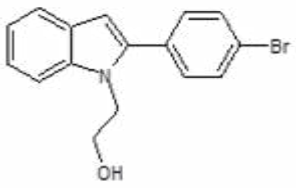


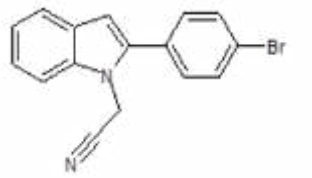
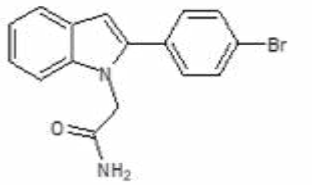
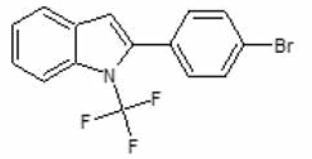
Standard(Norfloxacin)

Physical Characterisation for Synthesized Derivatives

The synthesized indole derivatives (5a–5e) were evaluated for their physical characteristics, including appearance, color, percentage yield, melting point, molecular weight, and Rf values. The compounds exhibited satisfactory yields and distinct melting points, indicating a good degree of purity, while the Rf values confirmed the successful synthesis of the intended derivatives are shown in (Table 6)

TABLE 6

Compound	Structure	Molecular formula	Molecular weight	Melting point	Rf value	Percentage Yeild
5a		C20H13BrFN	365	188	0.62	78%
5b		C16H14BrNO	315	153	0.46	80%

5c		C16H11BrN2	310	172	0.58	82%
5d		C16H13BrN2O	328	198	0.40	78%
5e		C15H10BrF3N	339	118	0.68	84%

Evaluation of antibacterial activity

The novel indole derivatives (5a-5e) are screened for their antibacterial activity by using the gram positive bacteria Staphylococcus aureas and bacillus subtilis and compared with standard drug norfloxacin. All the synthesized compounds shows the potential activity towards the bacteria among all 5d shows the high antibacterial activity with more zone of inhibition and Low minimum inhibitory concentration. These significant activity displayed in (Table 7) and (Table 8)

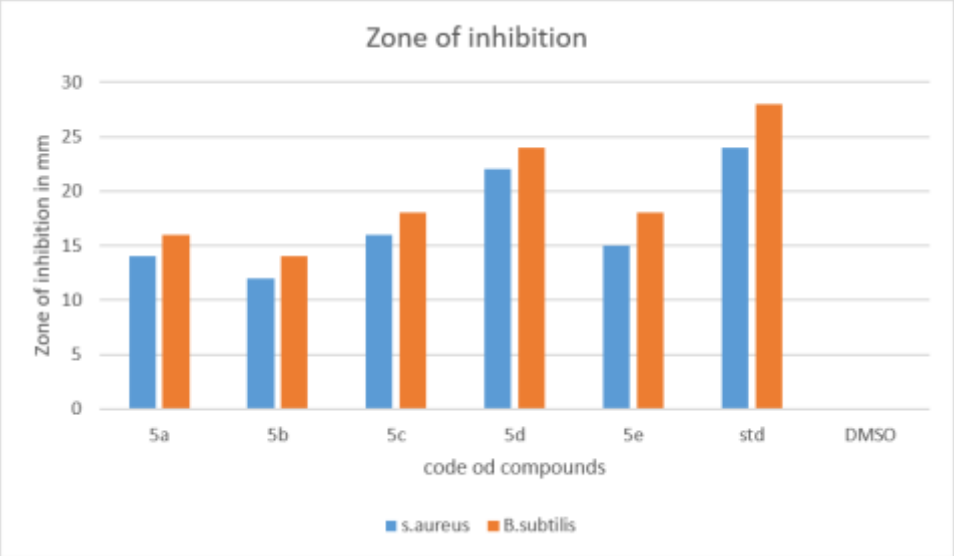
TABLE 7: Zone oF Inhibition (Concentration µ/ml)

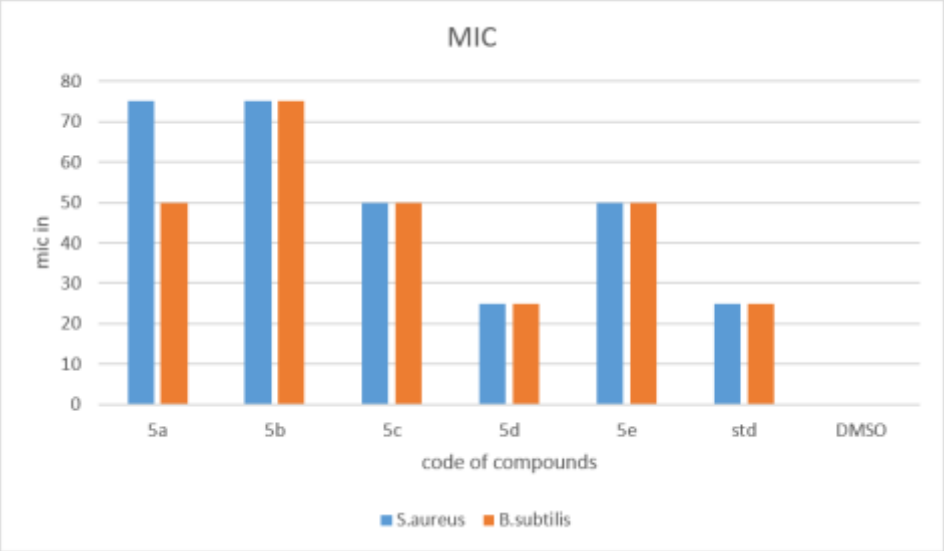
Sr. No	Compound	Staphylococcus aureas				Bacillus subtilis			
		25 µg/mL	50 µg/mL	75 µg/mL	100 µg/mL	25 µg/mL	50 µg/mL	75 µg/mL	100 µg/mL
1	5a	-	-	14 ±0.2	18 ± 0.3	-	12 ± 0.3	16 ± 0.3	20 ± 0.3
2	5b	-	-	12 ±0.3	16 ± 0.3	-	-	14 ± 0.3	18 ± 0.3
3	5c	-	12 ±0.3	16 ±0.2	20 ± 0.3	-	14 ± 0.3	18 ± 0.3	22 ± 0.3
4	5d	14±0.3	18 ±0.3	22 ±0.3	26 ± 0.3	16 ± 0.3	20 ± 0.3	24 ± 0.3	28 ± 0.3
5	5e	-	12 ±0.3	15 ±0.3	20 ± 0.3	-	14 ± 0.3	18 ± 0.3	22 ± 0.3
6	Standard norfloxacin	16±0.3	20 ±0.3	24 ±0.2	38 ± 0.3	18 ± 0.3	22 ± 0.3	28 ± 0.3	40 ± 0.3
7	DMSO	-	-	-	No mimimal inhibition	-	-	-	No mimimal inhibition

TABLE 8: Minimum inhibitory concentration

Sr. No	Compound	MIC (µ/ml)	
		Staphylococcus aureas	Bacillus subtilis
1	5a	75	50
2	5b	75	75
3	5c	50	50
4	5d	25	25
5	5e	50	50

6	Standard norfloxacin	25	25
7	DMSO	-	-





CONCLUSION

The present study successfully designed, synthesized, and characterized a series of novel indole derivatives (5a–5e). The synthesized compounds were confirmed by spectroscopic techniques such as FTIR, ^1H NMR, ^13C NMR, and mass spectrometry. Biological evaluation against *Staphylococcus aureus* and *Bacillus subtilis* demonstrated that several derivatives exhibited promising antibacterial activity, with compound **5d** showing the Potent inhibitory effect. Molecular docking studies with Novel indole derivative, Standard Norfloxacin and the DHFR (3SRQ) target protein further supported the experimental findings, as the most active compounds exhibited favorable binding affinities and stable interactions within the active site. Overall, the combined experimental and computational results indicate that the synthesized indole derivatives possess significant potential as antibacterial agents and may serve as promising lead molecules for the development of new antimicrobial drugs. Further optimization and in

vivo studies are recommended to establish their therapeutic efficacy and safety.

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HOW TO CITE: K. Shiva Ramulu, M. Ajitha, Guduru Sai Krishna, Synthesis Insilico Screening and Evaluation of Novel Indole Derivatives for Possible Biological Activity, Int. J. of Pharm. Sci., 2026, Vol 4, Issue 9, 1895-1906. https://doi.org/10.5281/zenodo.22769763