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Eco-Friendly Green Synthesis of Novel 1,2,3-Triazole Derivatives via Piperazine Scaffold and Their Antimicrobial Potential: *In Silico* Evaluation Targeting Serine Proteases 6RKS and 1BDD

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Abstract:

Background: *Microbes play several essential roles in human beings, impacting in both good and bad , few microbes are essential to our body and some few microbes cause harm to our body, this harmful microbes leads to various health issues. So the utilization of antimicrobial agents are important for the destructive organisms.*

Challenge: *The individual heterocyclic compounds of 1,2,3 triazole and piperazine have various biological activities, we took a challenge to find it out weather the combined form have the anti-microbial activity.*

Aim: *Aim of this work is to synthesize new potent 1,2,3 triazole appended piperazine derivatives and to evaluate antimicrobial activity*

Objectives: *All the synthesized compounds were isolated , recrystallized by using suitable solvents and characterized by FTIR, ^{1}H and ^{13}C NMR, Mass, Elemental analysis, melting point etc., Finally the compounds were purified by TLC and further assessed for in- vitro antibacterial activity by using the Disc diffusion method..*

Procedure: *A catalyst free one-pot synthesis of substituted 1,2,3-triazole has been described (Table-01). This reaction proceeds via the simple click chemistry as well as the formation of new combined heterocyclic compounds. In-silico design of novel analogues were carried out for fifty compounds using Auto Dock Vina by using (pdb id: 6RKS and 1PDD) (Fig-1,2,3,4,5,6,7,8) and compared with standard drug ciprofloxacin. Among all the tested compounds, some showed good to moderate antibacterial activities against both Gram-positive* Staphylococcus aureus *and Gram-negative* Escherichia coli *strains.*

Result: *Out of 50 compounds, 30 compounds which have good docking score were synthesized (Tables-03,04,05,06) by one-pot synthesis using CH_3CN as solvent in reflux condition which shows the good yield (Table-01). The synthesis were carried out by two step process with various primary aromatic amines (Tables 02, 08, 09) to determine their anti-microbial activity. Overall the observed results concluded that given synthetic compounds were effective against anti-bacterial activity. Out of these in A series 11A and 14A (Fig-10, 11) shows significant activity in both* E. coli and Staphylococcus aureus *(Table-10), and in B Series Compounds 38B, 39B (Fig-12) in* E. coli and 39B, 42B in Staphylococcus aureus (*Fig-13) (Table-11) shows significant anti-microbial activity.*

KEYWORDS: *Docking studies, Disc diffusion,* Staphylococcus aureus, Escherichia coli.

1. INTRODUCTION:

Nitrogen heterocyclic compounds have been extensively studied for their overall medicinal properties. Among that 1,2,3-Triazole and piperazine are individual heterocyclic compounds having five-membered ring that have significant attention in medicinal chemistry due to their diverse biological activities like Anti-microbial[1,2,3,4,5] Anti HIV[6], Antibacterial [7,8], Anticancer [9,10,11,12,13], Anti-proliferative agents[14,15], Anti tubercular activity [16,17] Anti-oxidant [18,19] Anthelmintic [20], Antipsychotic [21] , and Antimalarial [22] activities. The literature survey had demonstrated that now a days microorganisms like bacteria, viruses, fungi, and protozoa, are very infectious and moreover being its very tiny it founds in almost every environment on earth, soil and water. A few microorganisms are helpful to people like influencing wellbeing, processing, resistance, and synthesizing nutrients, some can be unsafe and cause

sicknesses in people like flu, HIV, Candida (which can cause yeast infections) Aspergillus (which can lead to respiratory infections). Giardia and Plasmodium (which causes malaria) and the normal cold infection can also attack cells and cause a scope of illnesses, from gentle to extreme. These infectious diseases pose a major challenge to human health, and there is an urgent need to develop new antimicrobial agents with excellent antibacterial activity. So we took a challenge to know wheather this combinational heterocyclic compounds of 1,2,3 triazole and piperazine have anti-microbial activity. We synthesised 1,2,3 triazole appended piperazine derivatives associated with various primary hetero aromatic amines moiety and to evaluate their antimicrobial activity. Insilico design were carried out for fifty derivatives using software Auto Dock Vina, by using pdb id: 6RKS and 1BDD and compared with standard drug ciprofloxacin. Thirty derivatives which have highest docking score (Tables 03,04,05,06) were synthesized (Tables 08,09) (Fig-9)by one-pot synthesis using CH_3CN as solvent in reflux condition which shows the good yield (Table-01) and their structures were elucidated with FTIR ,^{1}H NMR,^{13}C NMR, MASS and elemental analysis. The antimicrobial activity of synthesised compound have done by using disc diffusion method by using both Gram-positive *Staphylococcus aureus* and Gram-negative *Escherichia coli* strains, among this compounds 11A
,14A (Fig-1,2,3,4) shows significant activity in both *E. coli* and *Staphylococcus aureus* (Table-10), similarly compounds 38B, 39B (Fig-5,6) in *E. coli* and 39B, 42B(Fig-7,8) in *Staphylococcus aureus* (Table-11) shows significant antimicrobial activity when compared with standard drug ciprofloxacin.

2. .EXPERIMENT SECTION:

MATERIALS AND METHODS:

We purchased the synthetic chemicals from Vasa manufactured chemicals in Malleshwaram, Bangalore. Utilizing KBr pellets, ABB Bomem FTLA 2000-102 FTIR spectra were kept in the 400-4000 cm-1 territory. ^{1}H and ^{13}C NMR spectra were recorded using "500 MHz, $CDCl_3$ and 125 MHz, DMSO-d_6, δ ppm. TMS is utilized as the interior standard, and the compound movements are given in parts per million (ppm) at 500 and 125 MHz exclusively. Following material are used for anti-microbial activity.

Test Organisms:

Bacteria:

Escherichia coli (MTCC, Chandigarh, India)
Staphylococcus aureus (MTCC, Chandigarh, India)
Muller Hinton Agar (Cat No: M173, Himedia)
Nutrient Agar (Cat No:M001, Himedia)
SDA agar (Cat No: M063, Himedia)
Ciprofloxacin-5ug discs (Cat No: SD060, Himedia)
DMSO (Fisher Scientific)
Double distilled water

Environmenally Friendly Synthesis:

Green chemistry is one of the best sustainability of chemistry and the main object of this is to minimize the waste, decrease substance subsidiaries, less hazodous chemical synthesis and eliminates the use of solvents in chemical synthesis and also it is required to reduce the production of harmful side-product through sustainable, reliable, and eco-friendly synthesis procedure. These method of synthesis have incredible feature such as lower energy consumption, increase selectivity, proper utilization of raw ,material in green synthesis are available like microwave synthesis, multi-steps synthesis, one-pot synthesis etc. In this experiment we used one pot synthesis for the development of 1,2,3 triazole derivatives.

To commence our synthetic approach benzotriazole, and piperazine were taken as suitable reacting partners, so initially benzotriazole (0.01mmol) 4-Nitrobenzaldehyde (R) in A series and Benzaldehyde (R) in B series (0.01mmol) and piperazine (0.01mmol) were treated in CH_3CN at room temperature for 8hrs, under these condition only trace amount of desired product obtained however by increasing the reaction temperature to 50^{o}C

in the same reaction media the yield of the product was improved 60% In order to obtain an optimum reaction condition with improved efficiency, various reaction media were and also analysed under the same reaction temperature. Solvents such as EtOH, MeOH and toluene leads to our desired product with no significant improvement of yield, whereas solvents such as DMSO and DMF did not lead to our desired product. Our desired product compounds A& B obtained 80% yield when the reaction temperature met the reflux conditions withCH_3CN as reaction media. Interestingly, to achieve this higher efficiency of the product, only 45min-1 hr of reaction time was required. Further, using other solvents such as EtOH, MeOH and toluene under reflux conditions, no substantial improvement in yield was observed. In addition, increasing the reaction time to 8 h for CH_3CN under reflux conditions lowers the yield of the product. After achieving our optimal values, we subsequently explored the substrate scope for our synthetic protocol with various substituted amines (R1) and formaldehyde.

Table-01: Solvents used in Green chemistry:

Sl. NO	Solvent	Temperature(°*C*)	Time(h)	Yield[b](%)
1	CH_3CN	Room temperature	8	35
2	CH_3CN	50	6	60
3	EtOH	50	6	40
4	MeOH	50	6	45
5	Toluene	50	6	35
6	CH_3CN	Reflux	45min-1(h)	95
7	EtOH	Reflux	4	50
8	MeOH	Reflux	4	55
9	Toluene	Reflux	4	65
10	CH_3CN	Reflux	8	60
11	DMSO	50	6	ND
12	DMF	50	6	ND

3. BIOLOGICAL ACTIVITY:

Steps Followed For The Study:

The microorganisms used for antimicrobial analysis were purchased from Microbial Type Culture Collection and Gene Bank (***MTCC***), Chandigarh, India. The bacterial strains were maintained on nutrient agar (NA) medium.

Aerobic bacteria growth conditions:

Pure cultures from the plate were inoculated into Nutrient Agar plate and sub cultured at 37ºC for 24 h. Inoculum was prepared by aseptically adding the fresh culture into 2 ml of sterile 0.145 mol/L saline tube and the cell density was adjusted to 0.5 McFarland turbidity standard to yield a bacterial suspension of 1.5×10^8cfu/ml. Standardized inoculum used for Antimicrobial test.

Antibacterial Test by disc diffusion method:

The medium was prepared by dissolving 38 g of Muller Hinton Agar Medium (Hi Media) in 1000 ml of distilled water. The dissolved medium was autoclaved at 15 Lbs pressure at 121^0C for 15 min (pH 7.3). The autoclaved medium was cooled, mixed well and poured on petriplates (25 ml/plate). The plates were swabbed with Pathogenic Bacteria and incubated for 24hours. Ciprofloxacin loaded with 5microgram disc was placed in the center of plate on inoculated media with the help of sterile forceps in each plate and the Sample loaded discs with 1000ug/ml concentration were placed on the corners of plate and the plates were kept for incubation at 37°C for 24 hours. Empty disc loaded with distilled water was considered as negative control. At the end of incubation, inhibition zones were examined around the disc and measured with transparent ruler in millimeters. The absence of zone inhibition was interpreted as the absence of activity (Kohner et al., 1994; Mathabe et al., 2006). The activities are expressed as resistant, if the zone of inhibition (ZOI) was less than 7 mm, intermediate (8-10 mm) and sensitive if more than 11 mm.

4. MOLECULAR DOCKING: [23,24,25,26,27,28,29]

Now a days computer aided drug design is playing a major role in the development of significant drug over the past few decades. The docking study make us to predict some important binding interaction of the 1,2,3 triazole

derivatives with targeted protein receptors like a phage receptor binding protein for *e.coli* and pattern recognition receptors (PRRs) for *Staphylococcus aureus* . These receptors are actively involved for microbial growth. Molecular docking studies were carried out for all synthesized compounds (with Pdb id: 6rks and 1bdd). Finally Ciprofloxacine was employed as a standard drug method validation at the active site of receptor. Before the docking analysis, ligandswere prepared from the optimized compounds and saved in pdb file format. The 3D Compound was downloaded from the protein bank, and the enzyme was prepared with help of discovery studio visualizer for the docking analysis. The docking of the ligands to the active site was achieved with the help of pyrex software using Autodock vina. After successful docking protocol, reformation of the complexes (ligand-receptor) for further investigation was also achieved utilizing chimera software. Discovery studio visualizer and pyMOL were used to investigate the interactions of the complexes.

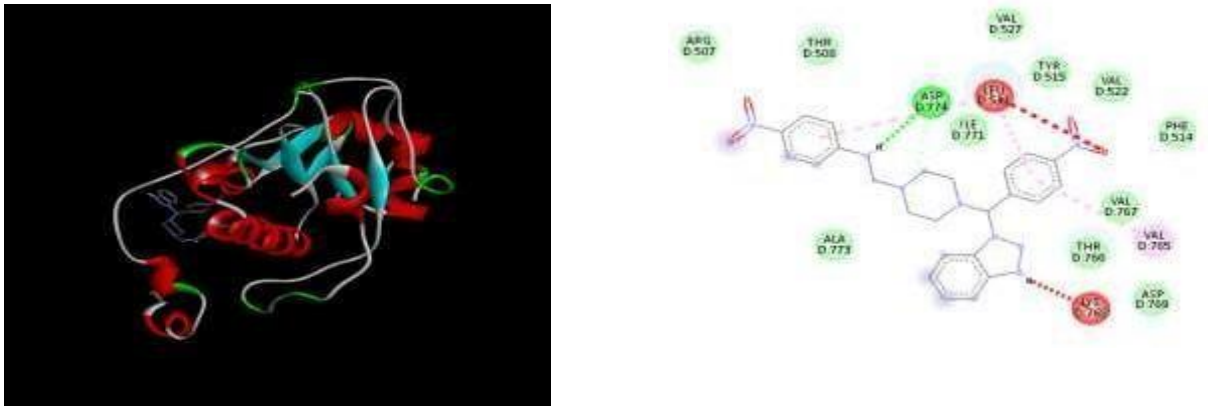
Table-02: Different primary Amines used for Designing the compounds:

Sl. No	Compounds 1-50		Amines
1	1A	26B	Aniline
2	2A	27B	*O*-Anisidine
3	3A	28B	*M*-Anisidine
4	4A	29B	*P*-Anisidine
5	5A	30B	4-Chloro Aniline
6	6A	31B	2-Chloro Aniline
7	7A	32B	4-Bromo Aniline
8	8A	33B	2-Bromo Aniline
9	9A	34B	2-Nitro Aniline
10	10A	35B	3-Nitro Aniline
11	11A	36B	4-Nitro-Aniline
12	12A	37B	2,4-Dimethyl Aniline
13	13A	38B	2,6 -Dimethyl Aniline
14	14A	39B	*O*-toludine
15	15A	40B	*P*- toludine
16	16A	41B	*M*-toludine
17	17A	42B	Sulphanilic acid
18	18A	43B	Anthranillic acid
19	19A	44B	Cyclohexylamine
20	20A	45B	Benzyl amine
21	21A	46B	3-Amino-9-ethylcarbazole
22	22A	47B	1- aminoanthraquinone
23	23A	48B	9-Aminophenanthrene
24	24A	49B	1-amino -9-fluorenone
25	25A	50B	4 Aminobezoic acid

Table -03: Docking Score Of 6RKS- *e.coli*

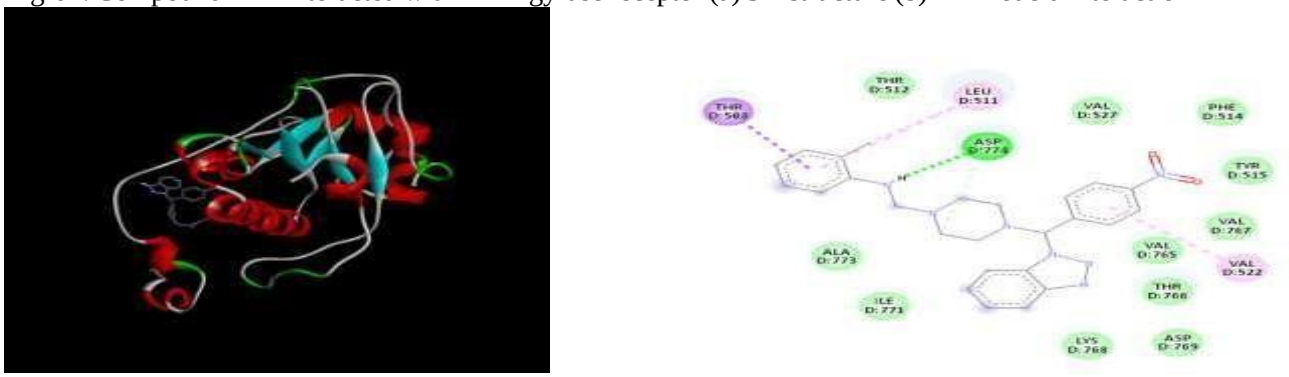
Sl. No	Compounds	6RKS	Interaction of amino acids
1.	Compound 1A	-7.5	Gln,Tyr,Val,Val
2.	Compound 2A	-6.0	Ser,Cys,Arg,Leu,Val
3.	Compound 3A	-5.6	Val,Ala,Leu
4.	Compound 4A	-7.7	Gln,Tyr,Val,Val,Ala
5.	Compound 5A	-7.2	Asp, Arg,Cys,Val,Lys,Leu,Ser
6.	Compound 6A	-7.6	Val,Lys,Ala,Arg,Cys,Asp
7.	Compound 7A	-7.6	Val,Leu,Cys,Leu,Arg,Cys,Asp
8.	Compound 8A	-5.5	Arg,Ser,Cys,Arg,Leu

9.	Compound 9A	-8.2	Tyr,Gln, Arg, Ala,Trp,Phe,Ile,Lys
10.	Compound 10A	-5.6	Val,Ala,Leu,Ser
11.	Compound 11A	-8.4	Arg,Ser,Cys,Arg,Leu,Val,Thr,Ala,Lys
12.	Compound 12A	-7.8	Lys,Val,Ala,Leu,Ser,Arg
13.	Compound 13A	-7.3	Leu,Val,Ala,Leu,Ser,Arg
14.	Compound 14A	-8.9	Val,Ala,Leu,Lys,Cys,Arg
15.	Compound 15A	-5.6	Val,Lys,Leu,Arg,Asp
16.	Compound 16A	-4.8	Val,Ala,Leu,Asp,Arg
17.	Compound 17A	-7.3	Cys,Val,Ala,Leu,Asp,Arg,Cys
18.	Compound 18A	-4.9	Cys,Arg,Leu,Val,Thr,Ala
19.	Compound 19A	-7.4	Leu,Val,Ala,Lys,Cys,Thr
20.	Compound 20A	-6.6	Ser,Arg,Val,Ala,Thr
21.	Compound 21A	-5.9	Lys,Leu,Arg,Asp
22.	Compound 22A	-5.8	Leu,Val,Ala,Lys
23.	Compound 23A	-6.0	Ala,Leu,Lys,Cys
24.	Compound 24A	-6.1	Val,Ala,Leu,Asp,Arg,Cys
25.	Compound 25A	-7.3	Ala,Val,Lys,Arg,Cys
Std	Ciprofloxacin	-8.0	Arg,Cys,Val,Lys,Leu,Ser



(a) (b)

Fig-01: Compound 11A interacted with DNA gyrase receptor (a) 3D structure (b) Aminoacid interaction

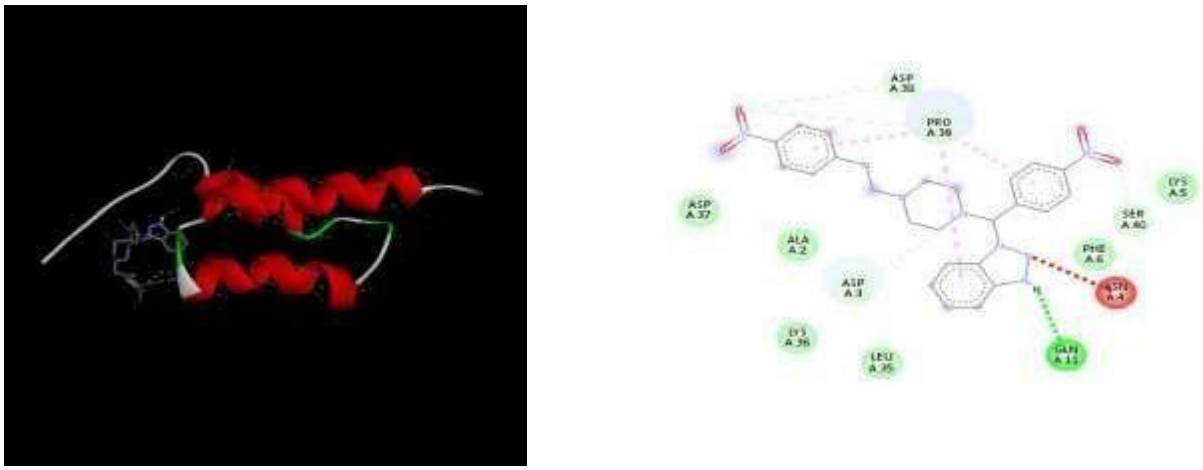


(a) (b)

Fig-2: compound 14 A interacted with DNA gyrase receptor (a) 3D structure (b) Aminoacidinteraction

Table -04: Docking Score Of 1BDD- *Staphylococcus aureus*

Sl. No	Compounds	1BDD	Interaction of amino acids
1.	Compound 1A	-6.8	Gln,Tyr,Val,Val
2.	Compound 2A	-5.9	Ser,Cys,Arg,Leu,Val,Thr,Ala
3.	Compound 3A	-5.9	Tyr,Gln, Arg, Ala,Trp
4.	Compound 4A	-6.7	Gln,Tyr,Val,Val,Ala
5.	Compound 5A	-6.8	ASP,ASP ARG,Cys,Val,Lys,Leu,Ser
6.	Compound 6A	-7.1	Val,Lys,Ala,Arg,Cys,Asp
7.	Compound 7A	-7.0	Ala,Leu,Asp,Arg,Cys
8.	Compound 8A	-5.7	Val,Ala,Leu,Ser,Arg
9.	Compound 9A	-7.6	Tyr,Gln, Arg, Ala,Trp,Phe,Ile,Lys
10.	Compound 10A	-5.9	Val,Ala,Leu,Asp,Arg,Cys
11.	Compound 11A	-7.7	Arg,Ser,Cys,Arg,Leu,Val,Thr,Ala,Lys
12.	Compound 12A	-7.5	Lys,Val,Ala,Leu,Ser,Arg
13.	Compound 13A	-7.0	Leu,Val,Ala,Leu,Ser,Arg
14.	Compound 14A	-7.8	Val,Ala,Leu,Lys,Cys,Arg
15.	Compound 15A	-6.6	Val,Lys,Leu,Arg,Asp
16.	Compound 16A	-5.9	Ala,Leu,Asp,Arg,Cys
17.	Compound 17A	-6.9	Cys,Val,Ala,Leu,Asp,Arg,Cys
18.	Compound 18A	-5.6	Ala,Leu,Ser,Arg
19.	Compound 19A	-6.8	Leu,Val,Ala,Lys,Cys,Thr
20.	Compound 20A	-6.6	Ser,Arg,Val,Ala,Thr
21.	Compound 21A	-5.7	Ala,Leu,Ser,Arg
22.	Compound 22A	-5.8	Arg, Ala,Trp
23.	Compound 23A	-5.8	Cys,Arg,Leu,Val
24.	Compound 24A	-4.8	Leu,Val,Ala
25.	Compound 25A	-6.9	Ala,Val,Lys,Arg,Cys
Std	Ciprofloxacin	-7.9	Phe,Glu,Gly,Lys,Ser



(a) (b)

Fig-03: Compound 11A interacted with *Staphylococcus aureus* protein (a) 3D structure (b) Aminoacid interaction

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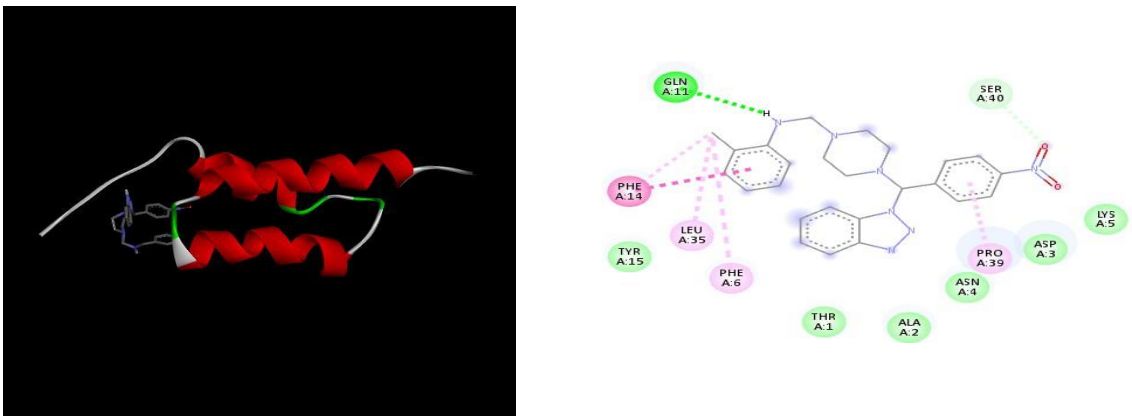
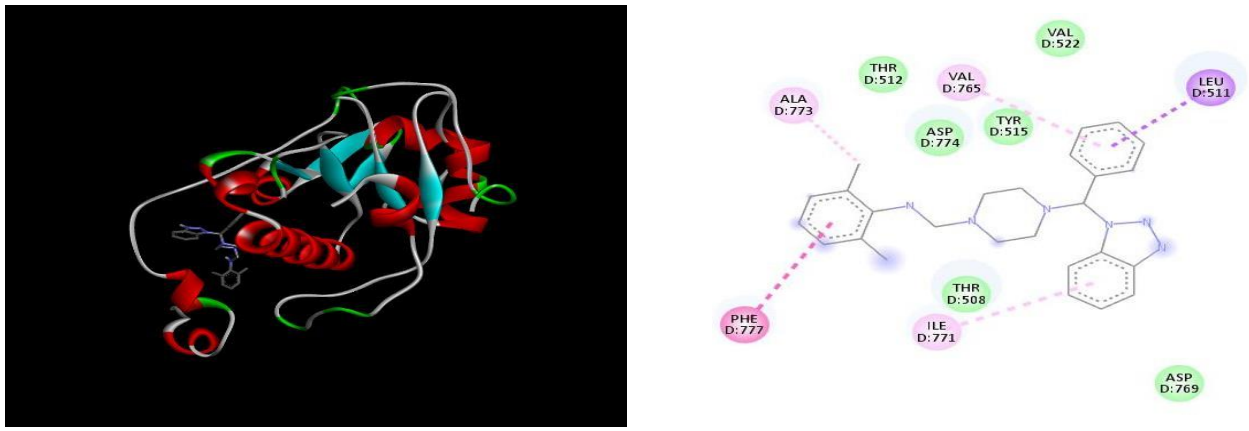


(b)

Fig-04: Compound 14A interacted with *Staphylococcus aureus* protein (a) 3D structure (b) Aminoacid interaction

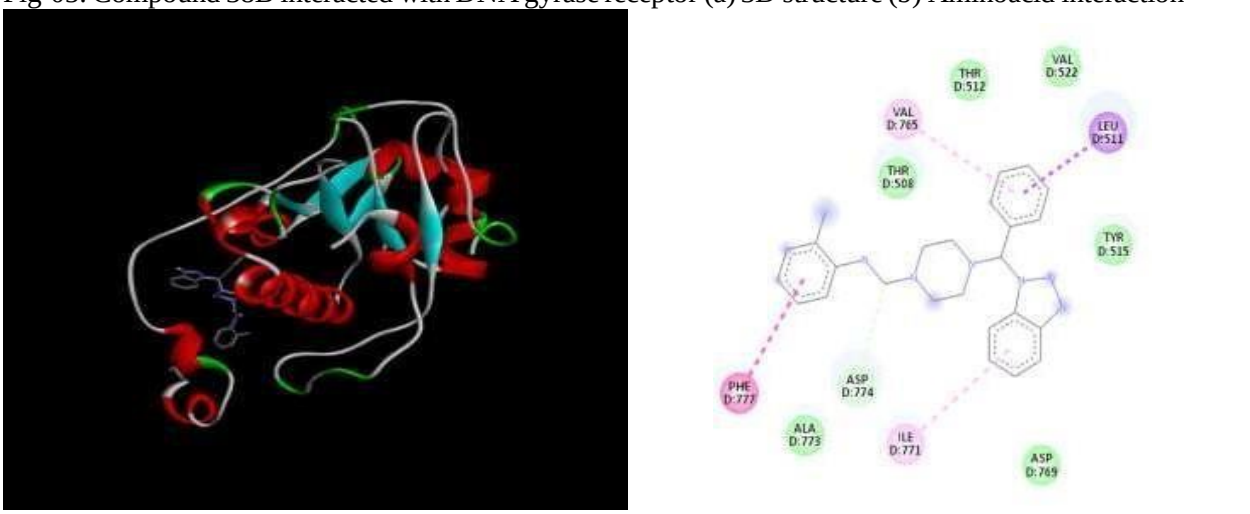
Table -05: Docking Score Of 6RKS- *E.coli*

Sl. No	Compounds	6RK	Interaction of amino acids
1.	Compound 26B	-7.6	Glu,Ser,Lys,Arg,Gly,Val,Ile,Ala
2.	Compound 27B	-5.6	Glu,Ser,Lys, , Leu, Phe
3.	Compound 28B	-4.8	Val,Ala, Leu, Asp, Cys
4.	Compound 29B	-7.8	Arg,Lys,Phe,Val,Trp
5.	Compound 30B	-7.8	Arg, Ala, Leu, Phe
6.	Compound 31B	-7.8	Val,Ala, Leu, Asp, Cys
7.	Compound 32B	-7.9	Arg, Ser,Lys, Phe, Ala, Thr
8.	Compound 33B	-4.6	Thr,Asp,Phe, Gly, Val
9.	Compound 34B	-4.8	Thr,Asp,Phe,Val
10.	Compound 35B	-7.3	Ala, Tyr, Val
11.	Compound 36B	-7.8	Gly, Val, Tyr, Ala,pro
12.	Compound 37B	-7.8	Val,Ala,Ser,Leu,Thr,Gly,
13.	Compound 38B	-8.1	Thr,Asp,Phe,Val,Lys,Leu,The,Arg
14.	Compound 39B	-8.2	Arg,Glu,Phe,Glu,Gly,Lys,Ser
15.	Compound 40B	-7.8	Gly,Leu,Met,Phe,Cys,Val,Thr
16.	Compound 41B	-5.3	Lys,Leu,The,Arg
17.	Compound 42B	-7.8	Asp,Tyr.Ala,Val,Arg,Ser
18.	Compound 43B	-5.6	Tyr.Ala,Val,Arg,Ser
19.	Compound 44B	-7.8	Phe,Arg,Gly,Ala,Leu,Cys
20.	Compound 45B	-6.7	Leu,Arg,Val,Asp,Cys,Ala
21.	Compound 46B	-5.7	Thr,Asp,Phe,Val
22.	Compound 47B	-5.4	Leu,Arg,Val,Asp
23.	Compound 48B	-5.1	Arg,Gly,Ala,Leu,Cys
24.	Compound 49B	-5.6	Val,Asp,Cys,Ala
25.	Compound 50B	-7.9	Tyr,Val, Thr,Asp,Phe
Std	Ciprofloxacin	-8.2	Arg,Leu,Val, Ala,Leu,Ser,Arg



(a) (b)

Fig-05: Compound 38B interacted with DNA gyrase receptor (a) 3D structure (b) Aminoacid interaction



(a) (b)

Fig-06: Compound 39B interacted with DNA gyrase receptor (a) 3D structure (b) Aminoacid interaction

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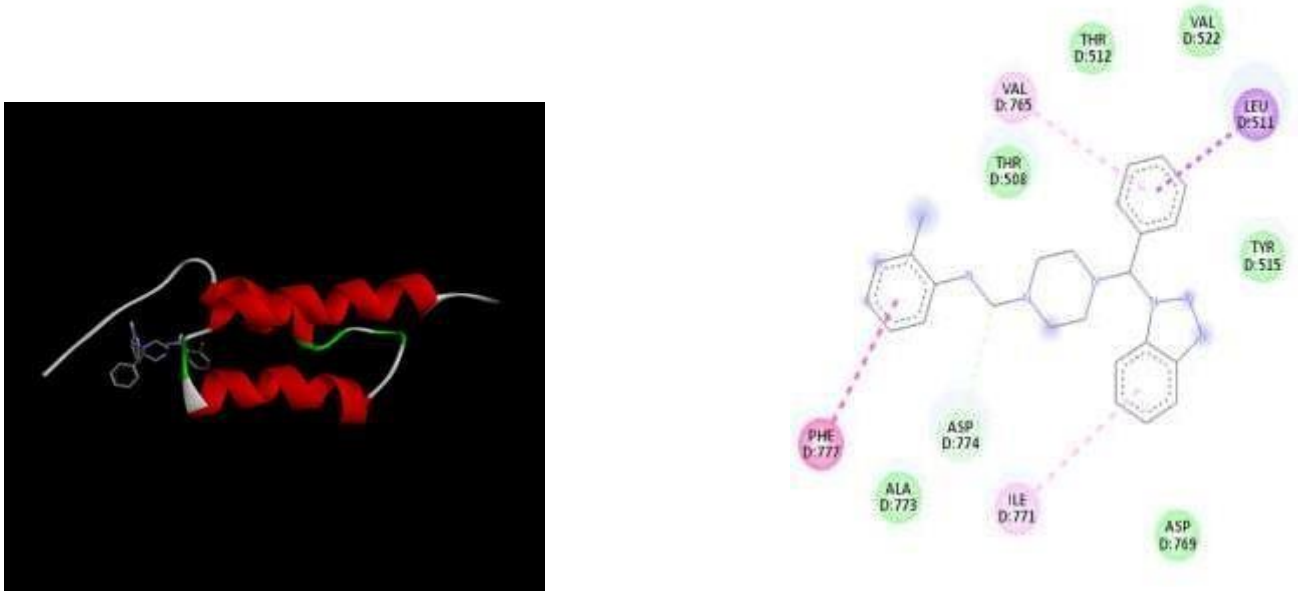
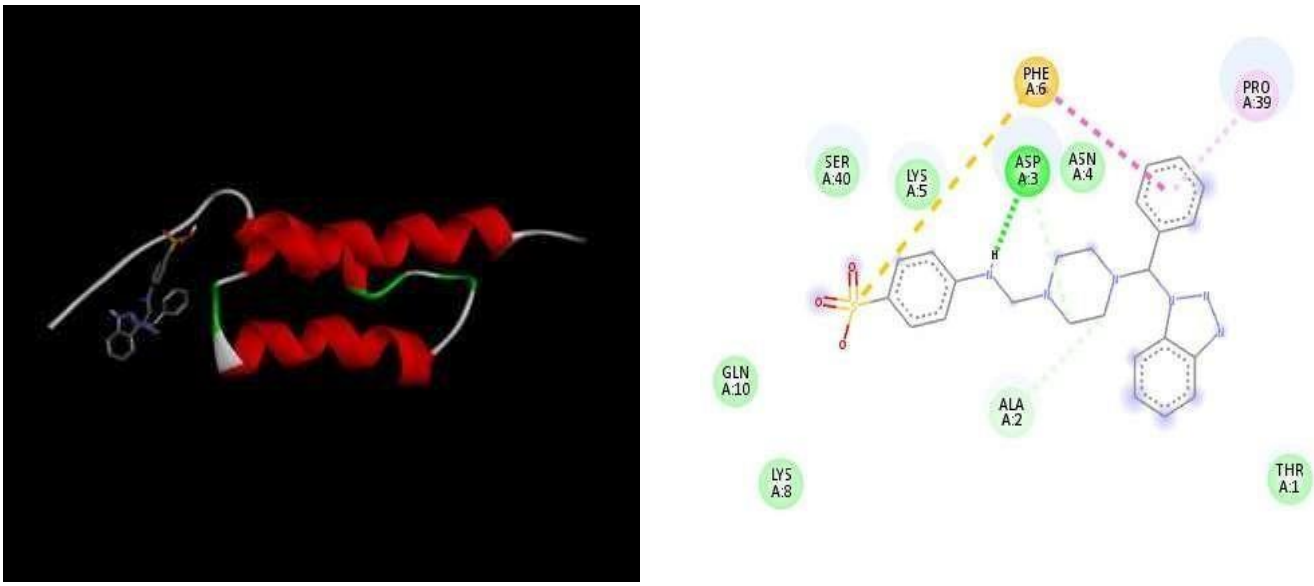
Table -06: Docking Score Of 1BDD- *Staphylococcus aureus*

Sl .No	Compounds	**1BDD**	Interaction of amino acids
1.	Compound 26B	-6.5	Glu,Ser,Lys,Arg,Gly,Val,Ile,Ala
2.	Compound 27B	-5.6	Glu,Ser,Lys, , Leu, Phe
3.	Compound 28B	-5.7	Val,Ala, Leu, Asp, Cys
4.	Compound 29B	-6.5	Arg,Lys,Phe,Val,Trp
5.	Compound 30B	-6.7	Arg, Ala, Leu, Phe
6.	Compound 31B	-6.6	Val,Ala, Leu, Asp, Cys
7.	Compound 32B	-6.8	Arg, Ser,Lys, Phe, Ala, Thr
8.	Compound 33B	-5.8	Thr,Asp,Phe, Gly, Val
9.	Compound 34B	-5.8	Thr,Asp,Phe,Val
10.	Compound 35B	-7	Ala, Tyr, Val
11.	Compound 36B	-6.6	Gly, Val, Tyr, Ala,pro
12.	Compound 37B	-7.5	Val,Ala,Ser,Leu,Thr,Gly,
13.	Compound 38B	-7	Thr,Asp,Phe,Val,Lys,Leu,The,Arg
14.	Compound 39B	-7.1	Arg,Glu,Phe,Glu,Gly,Lys,Ser
15.	Compound 40B	-7	Gly,Leu,Met,Phe,Cys,Val,Thr
16.	Compound 41B	-5.8	Lys,Leu,The,Arg
17.	Compound 42B	-7.2	Asp,Tyr.Ala,Val,Arg,Ser
18.	Compound 43B	-5.9	Tyr.Ala,Val,Arg,Ser
19.	Compound 44B	-6.8	Phe,Arg,Gly,Ala,Leu,Cys
20.	Compound 45B	-6.4	Leu,Arg,Val,Asp,Cys,Ala
21.	Compound 46B	-5.7	Thr,Asp,Phe,Val
22.	Compound 47B	-5.6	Leu,Arg,Val,Asp
23.	Compound 48B	-4.8	Arg,Gly,Ala,Leu,Cys
24.	Compound 49B	-5.1	Val,Asp,Cys,Ala
25.	Compound 50B	-6.7	Tyr,Val, Thr,Asp,Phe
Std	Ciprofloxacin	-7.9	Phe,Glu,Gly,Lys,Ser



(a) (b)

Fig-07: Compound 39B interacted with *Staphylococcus aureus* receptor (a) 3D structure (b) Aminoacid interaction



(a) (b)

Fig-08: Compound 42B interacted with *Staphylococcus aureus* receptor (a) 3D structure (b) Aminoacid interaction

5. SCHEME:

Table -07: Different aldehydes used in Synthetic process:

Sl.No	R	Series	Compounds
1	4-Nitrobenaldehyde	A	Compounds 1-25A
2	Benzaldehyde	B	Compounds 26-50B

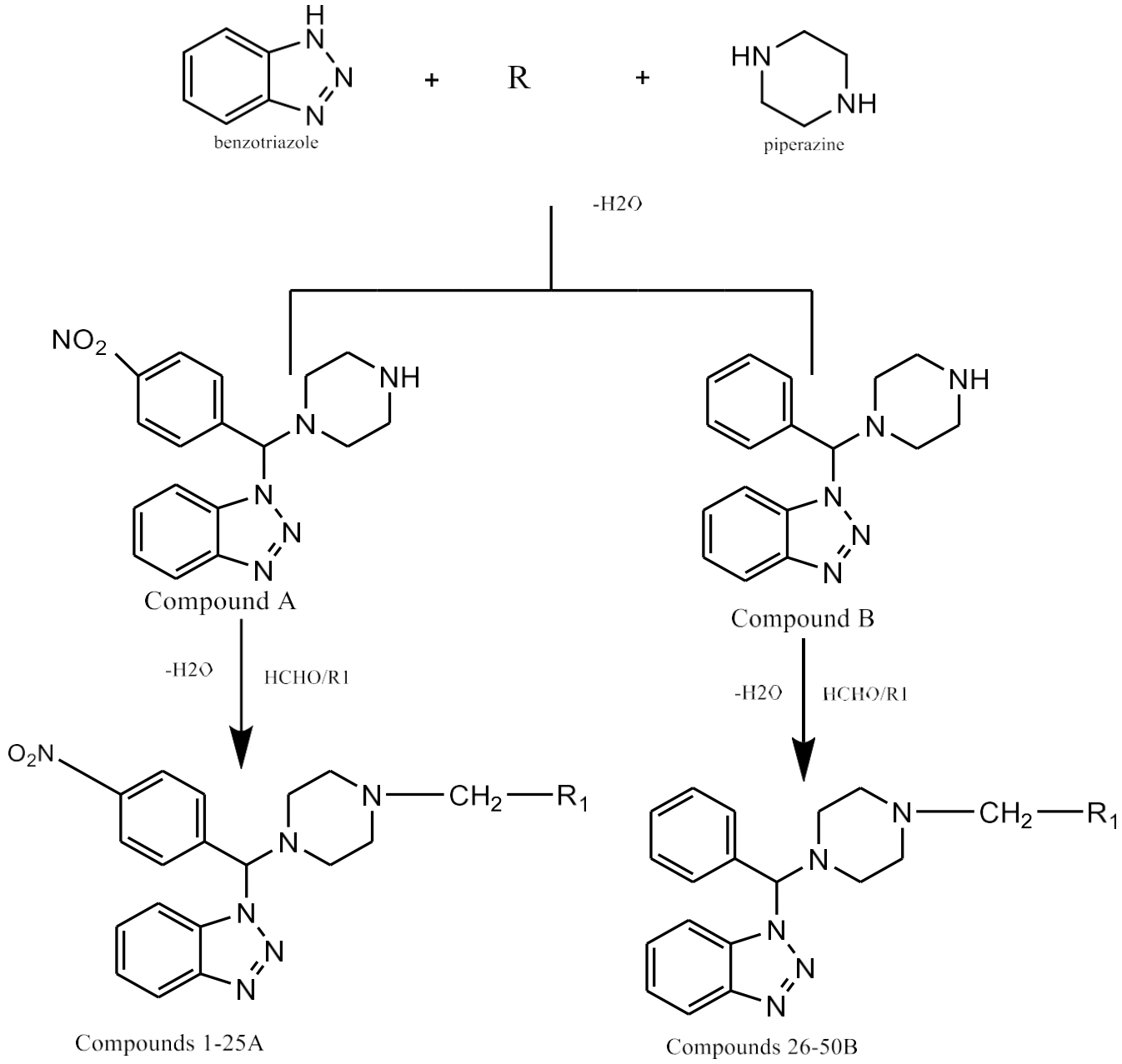


Fig-09: Schematic representation

A SERIES OF COMPOUNDS:

1-(phenyl(piperazin-1-yl)methyl)-1*H*-benzo[*d*] [1,2,3]triazole (Series –A):

Yellow to light orange, M.P.160-162 °C, Yield 93%, TLC (ethyl acetate/hexane) 3:7, Elemental Analysis calc.(%) for $C_{17}H_{20}N_6O_2$: C,72.84; H,7.19; N, 19.9 **,** Found (%): C, 72.65; H, 7.10; N, 19.85, Mol Wt. 338.37 g/mol, FTIR (KBR, ν_{max}/cm^{-1}): = 3300 (N–H), 3050 (Ar–C–H), 2950, 2850 (C–H aliphatic), 1600–1450 (C=C aromatic), 1300–1250 (C–N), 1220–1050 (triazole ring vibrations), 760 (C–H bending, aromatic) cm^{-1} .The ^{1}H NMR (500 MHz, DMSO - d_6): δ (ppm)= 8.01 (s, 1H, triazole-H), 7.93–7.89 (m, 1H, Ar-H), 7.69–7.65 (m, 1H, Ar-H), 7.53–7.46 (m, 3H, phenyl-H), 7.41–7.37 (m, 2H, phenyl-H), 7.28 (d, J = 8.0 Hz, 1H, Ar-H), 4.85 (s, 2H, benzylic –CH_2–) ppm, ^{1}*C NMR (125 MHz, DMSO - d_6): δ (ppm) = δ 147.8, 143.2, 134.5, 129.8, 129.4, 128.5, 127.6, 126.9, 124.3, 123.9,

122.7 (aromatic and triazole carbons), 61.2 (benzylic $–CH_2–$), 52.4, 50.8 (piperazine $–CH_2–$) ppm, *m/z* %: 341.2 $[M+H]^+$ (base peak)..

***N*-((4-((1*H* - benzo(*d*) (1,2,3)-triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) - *N* –benzyl methanamine (Compound 1A):**

Yellow to orange solid, M.P.180-182ºC,Yield 86%, TLC(ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{25}H_{27}N_7O_2$: C,65.63;H,5.95;N,21.43;O,6.99. FTIR (KBR,V_{max}/cm^{-1}): = (CH) bending 736, (NO) 1597 (N=N) 1661, (NH) 1582, (Aromatic) 1660 cm^{-1}. ^{1}HNMR (500 MHz, DMSO-d_6): δ (ppm)= (NH) 4.61(CH2)2.71,(CH)8.0, ^{13}C NMR (125MHz, DMSO-d_6): δ (ppm) = (CH2)52.8,(CH)119.6(C)140.2, *m/z*%: 457.22(base peak) 458.23$(M+1)^+$.

***N*-((4-((1*H* - benzo(*d*) (1,2,3)triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl)methyl)-4- methoxyaniline(Compound 4A):**

Orange to deep yellow solid, M.P. 172–174 °C ,Yield 90%, TLC(ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{25}H_{27}N_7O_3$: C,63.41;H,5.75:N,20.71;O,10.14, FTIR (KBR, V_{max} /cm^{-1}): = (CH) bending 736, (NO) 1597 (N=N) 1661, (NH) 1582, (Aromatic) 1660, (OCH3) 2800 cm^{-1}. ^{1}HNMR (500 MHz,DMSO-d_6): δ (ppm)= (NH) 6.34 (CH_2) 2.71, (CH) 8.0 (OH) 12.71 (CH_3) 3.81 ^{13}C NMR (125 MHz DMSO-d_6): δ (ppm) =(CH_2) 49.9 (C) 130.4,(C) In benzene 151.7 (CH) 110.0 Benzene, *m/z* %: 473.22(base peak) 474.22 $(M+1)^+$.

***N*-((4-((1*H* - benzo(*d*) (1,2,3)triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl)methyl)-4- chloroaniline(Compound 5A):**

Yellow to light brown solid, M.P. 182-185ºC, Yield 89%, TLC(ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{24}ClN_7O_2$: C,60.31;H,5.06:N,20.51; Cl 7.42, O,6.69, FTIR (KBR, V_{max} /cm^{-1}): = (CH) bending 736, (NO) 1597 (N=N) 1661, (NH) 1582, (Aromatic) 1660, (Cl) 800 cm^{-1}, ^{1}HNMR (500 MHz, DMSO-d_6):δ (ppm)=(NH) 6.34 (CH_2) 2.71, (CH_2) methylene(CH) 4.13 (OH) 12.71 (CH_3) 3.81 ^{13}C NMR (125 MHz,DMSO-d_6): δ (ppm) =(CH_2) 49.9 (CH_2) cyclohexane 52.6 (C) 130.4, (CH) 129.7 Benzene , *m/z*%:477.17(base peak) 479.17$(M+1)^+$.

***N*-((4-((1*H* - benzo(*d*) (1,2,3)triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl)methyl)-2- chloroaniline(Compound 6A):**

Pale yellow crystalline solid, M.P. 182-185 ºC, Yield 82%, TLC(ethylacetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{24}ClN_7O_2$: C,60.31;H,5.06: Cl 7.42, N,20.51;O,6.69, FTIR (KBR, V_{max} /cm^{-1}): = (CH) bending 736,(NO_2) 1650 (N=N) 1661, (NH) 1582,(Aromatic) 1660, (Cl) 800 cm^{-1} ^{1}HNMR, (500 MHz,DMSO-d_6): δ (ppm)= (NH) 5.80, (CH_2) 2.71,(CH_2) methylene 4.13 (CH) 6.11 ^{13}C NMR, (125 MHz,DMSO-d_6): δ (ppm) = (CH_2) 49.9 (CH_2) cyclohexane 52.8 (C) 130.7,(CH) 129.7 Benzene, *m/z* %: 477.17(base peak) 479.17$(M+1)^+$

***N*- (4-(1*H* - benzo[*d*] [1,2,3]-triazole-1-yl) (4-nitrophenyl)methyl)piperazine-1-yl)) methyl)- 4- bromoaniline (Compound 7A):**

Yellow to yellow-orange solid, M.P. 210-230 ºC ,Yield 73%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{25}BrN_7O_2$:C,55.18.38;H,4.63:N,18.77;Br,15.30;O,6.13, FTIR (KBR, V_{max} /cm^{-1}): = (CH) bending at 736 cm-1, (NO) 1597, (N=N) at 1661 cm-1, (NH) at 1582 cm-1, and (Br) at 702 cm-1. ^{1}HNMR, (500 MHz, DMSO-d_6) δ (ppm)= (NH) 6.34 (CH2) 4.13, (CH) 7.33 (CH2) 2.71 ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH2) 74.6 (C) 52.8 (CH) 128.4, (C) 110.0 *m/z* %: 523.12(base peak) 524.12 $(M+1)^+$.

***N*-((4-((1*H* - benzo[*d*) [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl)methyl)-2- nitroaniline(Compound 9A):**

Yellow to orange solid, M.P. 210-240ºC, Yield 83%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{24}N_8O_4$: C,59.01;H,4.95:N,22.94;O,13.10, FTIR (KBR, V_{max} /cm^{-1}) = (CH) bending at 736 cm-1, (NO) 1597, (N=N) at 1661 cm-1, (NH) at 1582 cm-1, and (Br) at 702 cm-1. ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34 (CH2) 4.13, (CH) 7.33 (CH2) 2.71 ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) =(CH2) 74.6 (C) 52.8 (CH) 128.4, (C) 110.0 *m/z* %:488.19(base peak) 489.19 $(M+1)^+$.

N-((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) methyl)-4- nitroaniline (Compound 11A):
Yellow orange solid, M.P. 210-230 ºC,Yield 83%, TLC (ethylacetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{24}N_8O_4$: C,59.01;H,4.95;N,22.94;0,13.10. FTIR (KBR, V_{max} /cm^{-1}) = (CH) bending 736, (CH_3) 1923, (NO) 1597 (N=N) 1661, (NH) 1582, cm^{-1} ^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm)= (NH) 6.34 (CH_2)4.13, (CH) 7.33 (CH_2) 2.71 ppm. ^{13}C NMR, (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 49.9 (CH_2)cyclohexane 52.8 (C) 130.7, (CH) 129.7 Benzene *m/z* %: 488.18 (base peak) 484.60(M^+) .

***N*- (4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) methyl) -2,4- Dimethylaniline (Compound 12A):**
Yellow solid, M.P 215–218 ºC ,Yield 85%, TLC (ethylacetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{26}H_{29}N_7O_2$,(C,66.22;H,6.20;N,20.79;0,6.79). FTIR (KBR, V_{max} /cm^{-1}) = bending CH-aromatic 811,(CH_3)1454, (NO) 1513, (N=N) 1598, (NH) 1627,cm^{-1}, ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm)= (NH)6.34 (CH_2) 4.13, (CH) 7.33 (CH_2) 2.71 ppm. ^{13}C NMR, (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 49.9 (CH_2)cyclohexane 49.9 (C) 130.4, (CH) 119.6,(CH_3) 17.9. Benzene. *m/z* %: 470.12 (base peak) , 471.32, (M^+) 315.24 $(M+1)^+$.

***N*- (4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) methyl) -2,6- Dimethylaniline (Compound 13A):**
Yellow solid, M.P. 224–227ºC,Yield 87%, TLC (ethylacetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{26}H_{29}N_7O_2$, (C,66. 22;H,6.20;N,20.79;0,6.79). FTIR (KBR, V_{max} /cm^{-1}): = (CH)-bending 737, 1443,(NO) 1520 (N=N) 1603, (NH) 1644 cm^{-1}. ^{1}H NMR (500 MHz, DMSO-d_6): δ (ppm)= (NH) 5.34 (CH_2) 4.13, (CH) 7.33 (CH_3) 2.12, (CH_2) 2.71 ppm. ^{13}C NMR, (125 MHz, DMSO-d_6): δ (ppm) = (CH_2)49.9 (CH_2) cyclohexane 52.8 (C) 130.4, (CH_3) 17.9, (CH) 119.6 Benzene. *m/z* %: 471.24, (base peak) 459.57$(M+1)^+$.

***N*- ((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) methyl) -2- Methylaniline (Compound 14A):**
Yellow solid, M.P. 219–222 ºC,Yield 85%, TLC (ethylacetate/hexane)3:7 Elemental Analysis calc.(%) for $C_{25}H_{27}N_7O_2$: C,60.31;H,5.06: Cl 7.42, N,20.51;O,6.69, FTIR (KBR, V_{max} /cm^{-1}): = (CH)-bending 737,1443,(NO) 1520 (N=N) 1603, (NH) 1644, (CH_3) 1400 cm^{-1}, ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 5.80, (CH_2) 2.71, (CH_2) methylene 4.13 (CH) 6.11 ^{13}C NMR, (125 MHz, DMSO-d_6): δ (ppm) = (CH_2)49.9 (CH_2) cyclohexane 52.8 (C) 130.7, (CH) 129.7 Benzene , *m/z* %: 478.12 (base peak) 479.17$(M+1)^+$.

***N*- ((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) methyl) -4- Methylaniline (Compound 15A):**
Yellow solid, M.P 226-229ºC,Yield 90%, TLC (ethylacetate/hexane)3:7 Elemental Analysis calc.(%) for $C_{25}H_{27}N_7O_2$, : C,65.63;H,5.95: Cl 7.42, N,21.43;O,6.99, FTIR (KBR, V_{max} /cm^{-1}): = (CH)- bending 737,1443,(NO) 1520 (N=N) 1603, (NH) 1644 (CH_3) 1350 cm^{-1}, ^{1}HNMR, (500 MHz, DMSO-d_6):δ (ppm)= (NH) 6.34, (CH_2) methylene 2.71 (CH)8.00 benztriazole(CH) 8.20 benzene ^{13}C NMR, (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 49.9 (CH_2) cyclohexane 52.8 (C) 130.7, (CH) 119.6 Benzene ,*m/z* %: 456.2 (base peak) 457.22$(M+1)^+$.

***N*- (((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) methyl) amino)benzenesulphonic acid(Compound 17A):**
Yellow to orange solid, M.P 248–251 ºC,Yield 86%, TLC (ethylacetate/hexane)3:7 Elemental Analysis calc.(%) for $C_{24}H_{25}N_7O_5S$:C,55.06;H,4.81;N,18.73;O,15.28;S,6.12; FTIR (KBR, V_{max} /cm^{-1}): = (CH) bending 736, (NO_2) 1660, (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34 (CH_2)4.13, (CH) 7.33 (CH_3) 2.01, (CH_2) 2.71 (OH) 8.5 ppm, ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2)75.2 (C) 52.8 (CH) 128.4, (C) 110.0 (CH_3) 17.6. *m/z*%: 523.16 (base peak) 524.12 $(M+1)^+$.

***N*- ((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) methyl) cyclohexanamine(Compound 19A):**

Yellow solid, M.P. 210–213 ºC ,Yield 78%, TLC (ethylacetate/hexane)3:7 , Elemental Analysis calc.(%) for $C_{24}H_{31}N_7O_2$: C,64.12; H,6.95;N,21.81; O,7.12; FTIR (KBR, V_{max} /cm^{-1}): = (CH) bending 736, (NO_2) 1660, (N=N) 1661, (NH) 1582, 1200 cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (CH_2) 3.62, (CH)7.33 (NH) 3.32 ppm, ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 70.3 (C) 52.8 (CH) 128.4 . *m/z* %:451.26 (base peak) .

***N*- (4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) –N- Benzylmethylamine(Compound 20A):**

Yellow solid, M.P. 226–229ºC, Yield 84.3%, Elemental Analysis calc.(%) for $C_{25}H_{27}N_7O_2$,: C,65.63;H,5.95;N,21.43;O,6.99; FTIR (KBR, V_{max} /cm^{-1}): = (CH) bending 736, (NO_2) 1660 , (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (CH_2) 3.62, (CH) 7.33 (NH) 4.16 ppm,^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 72.1 (C) 52.8 (CH) 128.4. m/z %: 457.24 (base peak).

***N*- (4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1- yl)methyl)amino)benzoic acid(Compound 25A):**

Yellow crystalline solid, M.P. 236–239 °C,Yield 85%, TLC(ethylacetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{25}H_{25}N_7O_4$: C,61.59;H,5.17:N,20.11;O,13.13, FTIR(KBR,V_{max}/cm^{-1}): = (CH) bending 736, (NO_2) 1660 (N=N) 1661, (NH) 1582, (Aromatic) 1660, (COOH) 3100 .^{1}HNMR (500 MHz, DMSO-d_6): δ (ppm)= (NH)6.34 (CH_2) 2.71, (CH) 8.0 (OH) 12.71 ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 49.9 (C) 146.2(CH) 110.0 Benzene , *m/z* 487.20(base peak) 488.20$(M+1)^+$.

The synthesized compounds were structurally elucidated using FTIR,^{1}H NMR,^{13}C NMR and MASS. The spectral details of the synthesized compounds were given below

B SERIES OF COMPOUNDS:.

1-(phenyl(piperazin-1-yl)methyl)-1*H*-benzo[1,2,3]triazole (Series - B):

White solid, M.P. 145–165 °C, Yield 93%, TLC (ethyl acetate/hexane) 3:7, Elemental Analysis calc.(%) for $C_{17}H_{19}N_5$ C, 69.12; H, 7.17; N, 23.71**,** Found (%): C = 69.12, H = 6.73, N = 23.56 , Mol wt. 293.16 g/mol, FTIR (KBR, V_{max} /cm^{-1}): = aromatic C–H stretching 3030, aliphatic C–H stretching 2850–2950 , C=N and N=N 1575–1450 cm^{-1}.The ^{1}H NMR (500 MHz, DMSO -d_6): δ (ppm)= 7.90–7.20 (m, 9H, aromatic protons), 5.45 (s, 1H, benzylic CH), 3.50–2.45 (m, 8H, piperazine –CH_2–CH_2–) . ¹*C NMR (125 MHz, DMSO -d_6): δ (ppm) δ 147.8, 138.5, 130.2, 129.4, 128.6, 127.5, 126.8 (aromatic and triazole carbons), 62.1 (benzylic CH), 53.6, 51.2 (piperazine –CH_2–), *m/z* %: 296.2 $[M+H]^+$ (base peak).

N-((4-((1*H* - benzo[*d*][1,2,3]triazole-1-yl) (4-nitrophenyl)methyl) piperazin-1-yl) methyl)aniline(Compound 26B):

Yellow orange solid, M.P 180-200ºC, Yield 65%, TLC(ethylacetate/hexane)3:7 Elemental Analysis calc.(%) for $C_{24}H_{26}N_6$: C, 72. 33; H, 6.58;N,21.09. FTIR (KBR,V_{max}/cm^{-1}) = (CH) bending 736, (N=N) 1661, (NH) 3582, (CH_2) 1488, cm-1. ^{1}HNMR (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34(CH_2) 2.71, (CH) 7. 75 ppm.^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 49.9, (CH) 113.5, (C)52.8 , (C) 126.2ppm. *m/z* %:398.22 (base peak) 399.23 $(M+1)^+$.

N-((4-((1*H* – benzo [*d*] [1,2,3]triazole-1-yl) (phenyl)methyl) piperazin-1-yl)methyl)-4- methoxyaniline (Compound 29B):

Creamwhite, M.P 160-180ºCfor $C_{25}H_{25}N_7O_4$:C,70.07;H,6.59:N,19.61;O,3.73, FTIR (KBR,V_{max}/cm^{-1}) = (CH) bending 736, (N=N) 1661, (CH_2) 1488, (NH) 1582, (OCH3) 2840 , cm-1. ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34(CH2) 2.71, (CH) 8.0 ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 74.6, (C) 52.8, (CH) 128.4,(C) 126.2 , *m/z*% : 428.23(base peak) 429.44 $(M+1)^+$.

N-((4-((1*H*-benzo[*d*] [1,2,3]triazole-1-yl) (phenyl)methyl) piperazin-1-yl)methyl)-4-chloroaniline (Compound 30B): Pale yellow solid, M.P 170-190 ºC,Yield 71 %, TLC (ethylacetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{25}ClN_6$:C,66.58;H,5.82:N,19.41;Cl,8.19, FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736,(N=N) 1661, (NH) 1582, (Cl) 732 cm-1, ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34 (CH_2) 2.71, (CH) 7.33ppm. ^{13}C NMR, (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 74.6 (C) 52.8 (CH) 128.4, (C) 126.2. *m/z* %: 432.18(base peak) 433.12 $(M+1)^+$.

N-((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl)-2-chloroaniline (Compound 31B):

Pale yellow, M.P 175-195 ºC,Yield 75%, TLC (ethylacetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{25}ClN_6$: C,66.58;H,5.82:N,19.41;Cl,8.19, FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, (N=N) 1661, (NH) 1582, 1660, (Cl) 782 cm-1. ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 5.80 (CH_2) 4.13, (CH) 7.33 (CH_2) 2.71 ppm . ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 74.1 (C) 52.8 (CH) 128.4,(C) 126.2. *m/z* %: 432.18(base peak) 433.12 $(M+1)^+$.

N-((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl)-4-bromoaniline (Compound 32B):

Light Brown solid , M.P180-200ºC,Yield 63%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{25}BrN_6$:C,60.38;H,5.28:N,17.60;Br,16.74, FTIR (KBR,V_{max}/cm^{-1}) = (CH) bending 736, (N=N) 1661, (NH) 1582, (Br) 702 cm-1. ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34 (CH_2) 4.13, (CH)7.33 (CH_2) 2.71 ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 74.6 (C) 52.8 (CH) 128.4, (C)110.0 *m/z* %:476.13(base peak) 477.56 $(M+1)^+$.

N-((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl)-3-nitroaniline (Compound 35B):

Yellow orange solid , M.P 190-210ºC,Yield 73%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{25}N_7O_2$: C,65.00;H,5.68:N,22.11;O,7.21, FTIR (KBR,V_{max}/cm^{-1}) = (CH) bending 736, (NO_2) 1660 (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34 (CH_2) 4.13,(CH) 7.33 (CH_2) 2.71 ppm. ^{13}C NMR, (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 74.6 (C) 52.8 (CH) 128.4, (C) 110.0 *m/z*%: 443.21(base peak) 444.11$(M+1)^+$.

N-((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl)-4-nitroaniline (Compound 36B):

Orange Yellow solid, M.P 200-220ºC,Yield 74%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{25}N_7O_2$,C,65.00;H,5.68:N,22.11;O,7.2 : FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, (NO_2) 1660 (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34 (CH_2) 4.13, (CH) 7.33ppm. ^{13}C NMR(125 MHz, DMSO-d_6): δ (ppm) =(CH_2) 74.6 (C) 52.8 (CH) 128.4, (C) 110.0, *m/z* %:443.21(base peak).

N-((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl)-2,4-Dimethyl aniline (Compound 37B):

Pale yellow solid, M.P 160-180ºC,Yield 83% , TLC (ethyl acetate/hexane)3:7 , Elemental Analysis calc.(%) for $C_{26}H_{30}N_6$:C,73.21;H,7.09:N,19.70; FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, (NO_2) 1660 (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 5.80 (CH_2) 4.13, (CH) 7.33 (CH_3)2.12 (CH_2) 2.71 ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 74.9 (C) 52.8 .(CH) 128.4 , (C)110.0 (CH_3) 17.9 ,*m/z*%: 426.25(base peak).

N-((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl)-2,6-Dimethyl aniline (Compound 38B):

Pale yellow solid, M.P 155-175ºC,Yield 64%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{26}H_{30}N_6$C,73.21;H,7.09:N,19.70; FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, (NO_2) 1660 (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 5.34 (CH_2) 4.13, (CH) 7.33 (CH_3)2.12, (CH_2) 2.71 ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 75.2 (C) 52.8 (CH) 128.4 , (C)110.0 , (CH_3) 17.9.

m/z%: 426.25 (base peak) .

N-((4-((1*H* - benzo[*d*] 1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl)-2-Methyl aniline (Compound 39B):

Pale yellow solid, M.P 160-180ºC,Yield 78%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{25}H_{28}N_6$:C,72.79;H,6.84;N,20.37; FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, (NO_2) 1660 (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 5.80 (CH_2) 4.13, (CH) 7.33 (CH_3)2.01 , (CH_2) 2.71 ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 75.2 (C) 52.8 , (CH) 128.4, (C)110.0 (CH_3) 17.6. *m/z*%: 412.54 (base peak) .

N-((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl)-4-Methyl aniline (Compound 40B):

Off white , M.P 165-185ºC ,Yield 71%, TLC (ethyl acetate/hexane)3:7 , Elemental Analysis calc.(%) for $C_{25}H_{28}N_6$:C,72.79; H, 6.84; N,20.37; FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, (NO_2) 1660 (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= δ ppm (NH) 6.34 (CH_2) 4.13, (CH) 7.33 (CH_3) 2.32, (CH_2) 2.71 ppm. ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 75.2 (C) 52.8(CH) 128.4 , (C) 110.0 (CH_3) 17.6. *m/z*%: 412.54 (base peak) .

N-(((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl) amino) benzenesulphonic acid (Compound 42B):

Pale brown solid, M.P 210-250 ºC,Yield 76%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{24}H_{26}N_6O_3S$:C,60.23;H,5.48;N,17.56;O,10.03;S,6.70; FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, (NO_2) 1660 (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (NH) 6.34 (CH2)4.13, (CH) 7.33 (CH_3) 2.01, (CH_2) 2.71 (OH) 8.5 ppm, ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2)75.2 (C) 52.8 (CH) 128.4, (C) 110.0 (CH_3) 17.6. *m/z*% : 478.57 (base peak) .

N-((4-((1*H* - benzo [*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl) methyl) cyclohexanamine (Compound 44B):

Creamy white solid, M.P.160-180ºC,Yield 68%, TLC (ethyl acetate/hexane)3:7 Elemental Analysis calc.(%) for $C_{24}H_{32}N_6$:C,71.25; H,7.97;N,20.77; FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, 1660 (N=N) 1661, (NH) 1582, (C_6H_{12}) 1200 cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (CH_2) 3.62, (CH) 7.33 (NH) 3.32 ppm, ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 70.3 (C) 52.8 (CH) 128.4 . *m/z* %: 478.57 (base$_{peak}$) .

1-(4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl)-*N*-Benzylmethylamine. (Compound 45B):

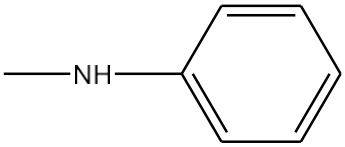
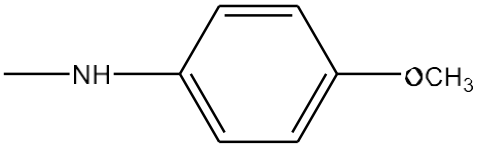
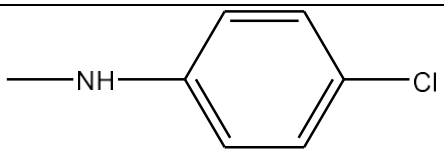
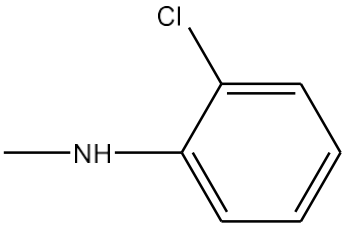
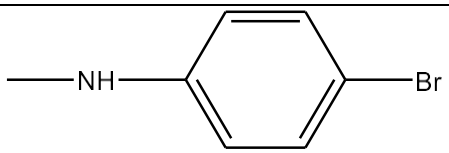
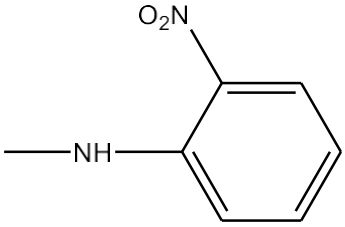
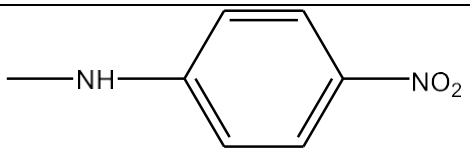
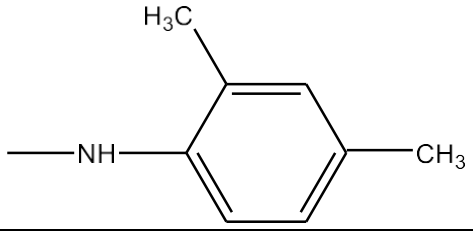
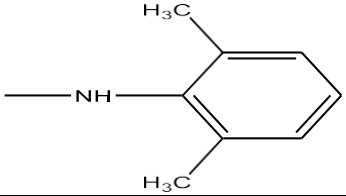
Off White, M.P .155-175ºC,Yield 74%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{25}H_{28}N_6$:C,72.79;H,6.84;N,20.37; FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, 1660 (N=N) 1661, (NH) 1582, cm-1 ^{1}HNMR, , (500 MHz, DMSO-d_6): δ (ppm)= (CH_2) 3.62, (CH) 7.33 (NH) 4.16 ppm, ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 72.1 (C) 52.8 (CH) 128.4 . *m/z* %: 412.24 (base peak) .

4-(((4-((1*H* - benzo[*d*] [1,2,3]triazole-1-yl) (Phenyl)methyl) piperazin-1-yl)methyl)amino)benzoic acid (Compound 50B):

Pale yellow solid, M.P. 210-230 ºC,Yield 72%, TLC (ethyl acetate/hexane)3:7, Elemental Analysis calc.(%) for $C_{25}H_{26}N_6O_2$: C,67.86;H,5.92;N,18.99,O17.23 ; FTIR(KBR,V_{max}/cm^{-1}) = (CH) bending 736, 1660 (N=N) 1661, (NH) 1582, (COOH) 2800 cm-1 ^{1}HNMR, (500 MHz, DMSO-d_6): δ (ppm)= (CH_2) 4.13, (OH)12.71 (CH) 7.33 (NH) 6.34 ppm, ^{13}C NMR (125 MHz, DMSO-d_6): δ (ppm) = (CH_2) 74.6 (C) 52.8 (CH)128.4 . *m/z*%: 442.21 (base peak) .

6. RESULT AND DISCUSSION: Out of 50 docking compounds 15 compounds in A series and 15 compounds in B series which shows highest docking score were synthesized.

Table -08: **Amines used in A series**

Sl.No	R_1	Colour	M.P	Yield %
1A		Yellow-white	182	86
4A		Slight Yellow crystals	195	90
5A		Yellow crystals	186	89
6A		Yellowish brown crystals	165	82
7A		Brown	250	73
9A		Yellow colour	181	83
11A		Yellow crystals	185	83
12 A		Brown colour	120	85
13A		Slighty Yellowish colour	158	87

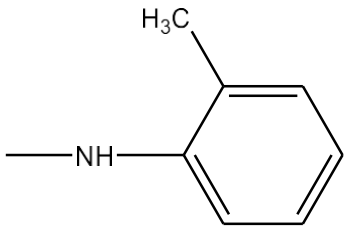
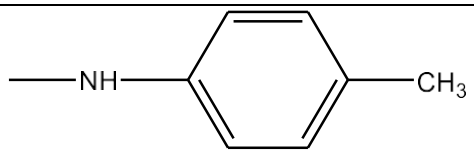
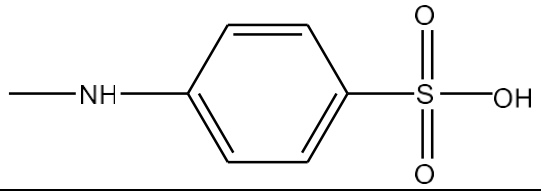
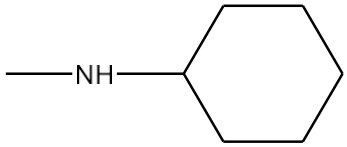
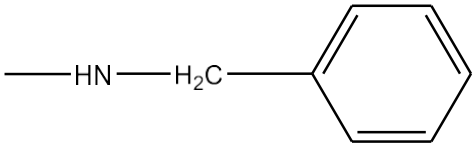
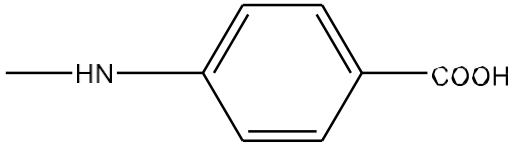
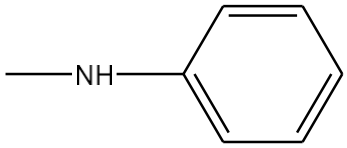
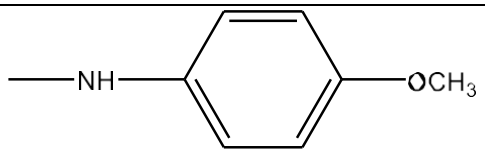
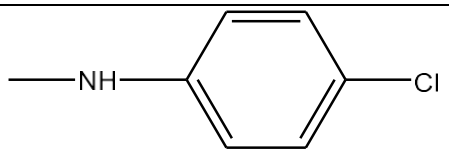
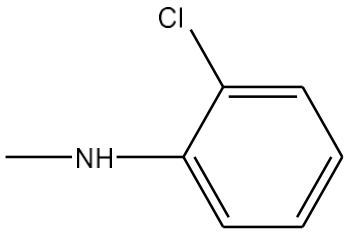
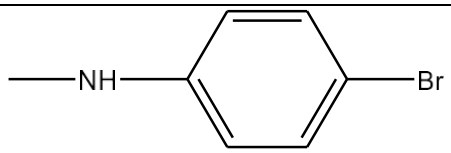
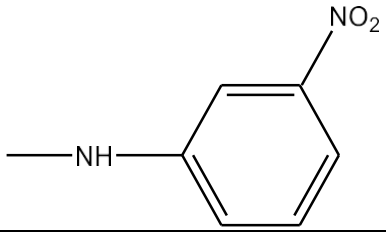
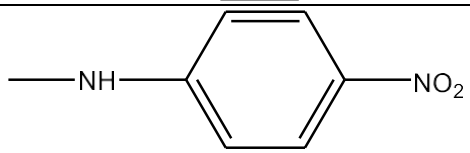
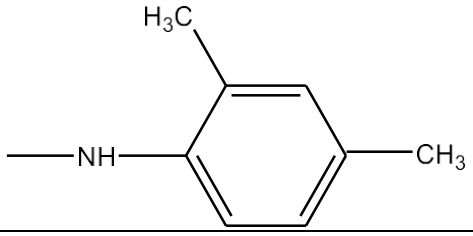
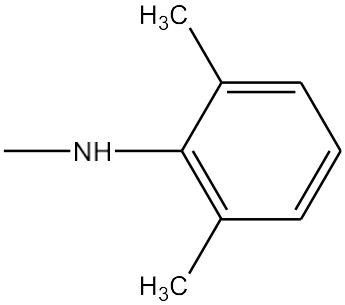
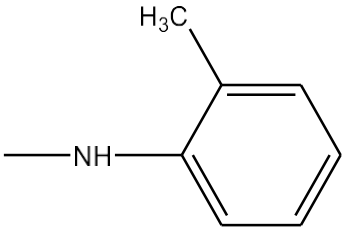
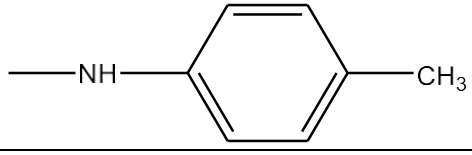
14A		Yellow colour	184	85
15A		Orange yellow colour	165	90
17A		Whitish yellow	183	86
19A		Creamy white	192	78
20A		White	220	84
25A		Yellow colour	160	85

Table -09: Amines used in B series

Sl.No	R_1	Colour	M.P	Yield%
26B		Yellowish white	260	65
29B		Cream white	240	76
30B		Cream white	270	71

31B		White	274	75
32B		Brown	250	63
35B		Yellow	181	73
36B		Yellow	180	74
37B		Creamy white	185	53
38B		white	189	64.64
39B		White	180	78
40B		Yellowish white	190	71

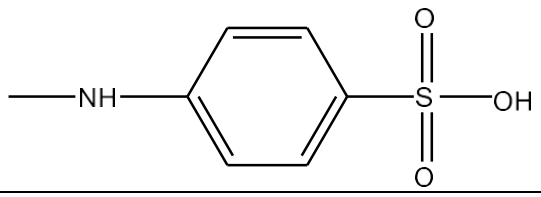
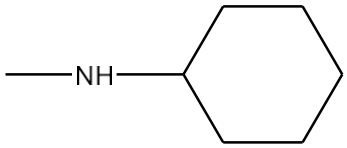
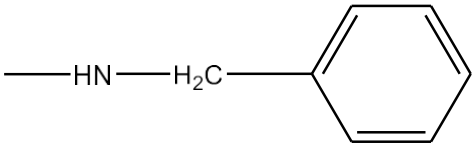
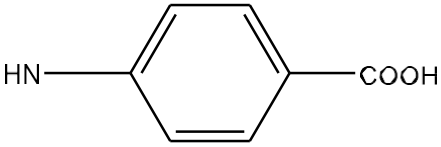
42B		Creamy white	183	76
44B		Creamy white	192	68
45B		White	220	74
50B		Brown	196	72

Table -10: Zone of Inhibition in A series

Sl. No	**Compounds**	**Antibacterial activity Zone of Inhibition(mm)**	
		Escherichia coli	*Streptococcus aureus*
1.	1A	20.33±1.53	18±2
2.	4A	12±1	12±2
3.	5A	14±1	13±0
4.	6A	19±1	20±1
5.	7A	14±1	22±1.73
6.	9A	18±1.73	22±2
7.	11A	22±1	25±2
8.	12A	15±2	12±1.73
9.	13A	22±0	22±1.73
10.	14A	22±1	24±1
11.	15A	14±1	13±2
12.	17A	15±2	20±2.65
13.	19A	20±3	22±1.73
14.	20A	17±1	20±1.73
15.	25A	15±1.73	15±2
16.	Ciprofloxacine(STD)	25.33±1.53	18.33±2.52
17.	Control	0	0

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Fig-10: 11A and 14A Compounds Zone of inhibition closer to STD Ciprofloxacine - *Escherichia coli*

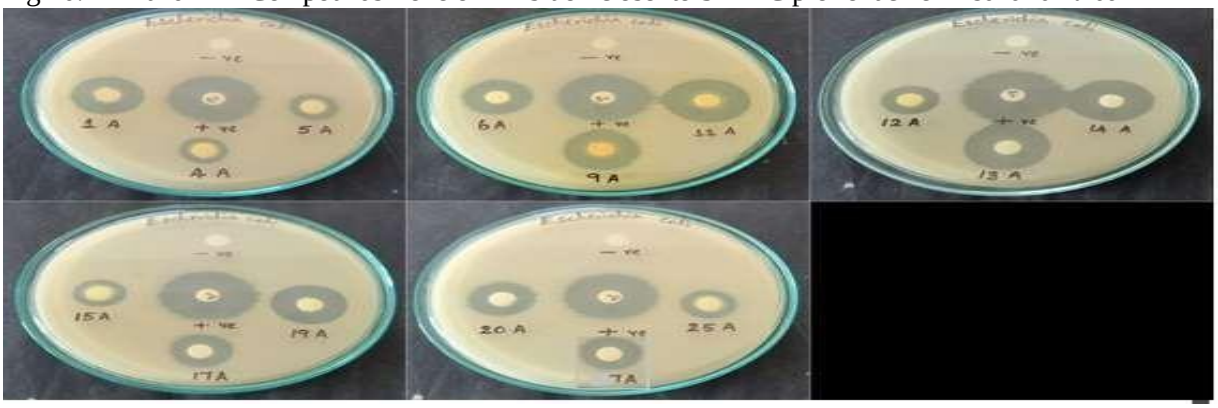


Fig-11:11A and 14A Compounds Zone of inhibition closer to STD Ciprofloxacine -*Staphylococcus aureus*

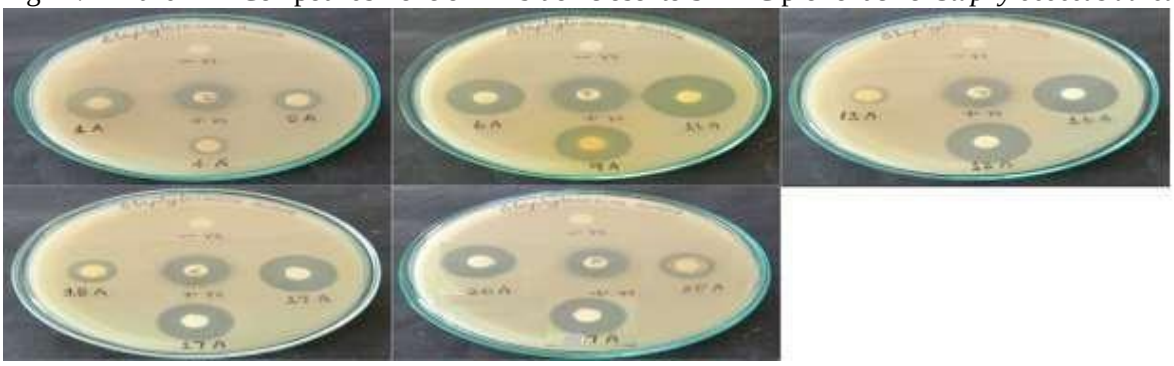


Table -11: Zone of Inhibition in B series

Sl.No	**Compounds**	**Antibacterial activity Zone of Inhibition(mm)**	
		Escherichia coli	*streptococcus*
1.	26B	6.8±1	0.5±0
2.	29B	2±1	6±2
3.	30B	5.18±1	3.8±1
4.	31B	0.5±1	1±0
5.	32B	3.14±0	0.8±1
6.	35B	7.18±0	3.8±0
7.	36B	2±2	2.6±1
8.	37B	1±1	2±2
9.	38B	10±2	8±0
10.	39B	12±0	9±2
11.	40B	2.6±0	4±0
12.	42B	7±2	10±2
13.	44B	6±1	7±2
14.	45B	5±0	4±1

15.	50B	7±1	3±0
16.	Ciprofloxacine (Std)	14±2	19±0
17.	Control	0	0

Fig -12:38B and 39B Compounds Zone of inhibition closer to STD Ciprofloxacine - *Escherichia coli*

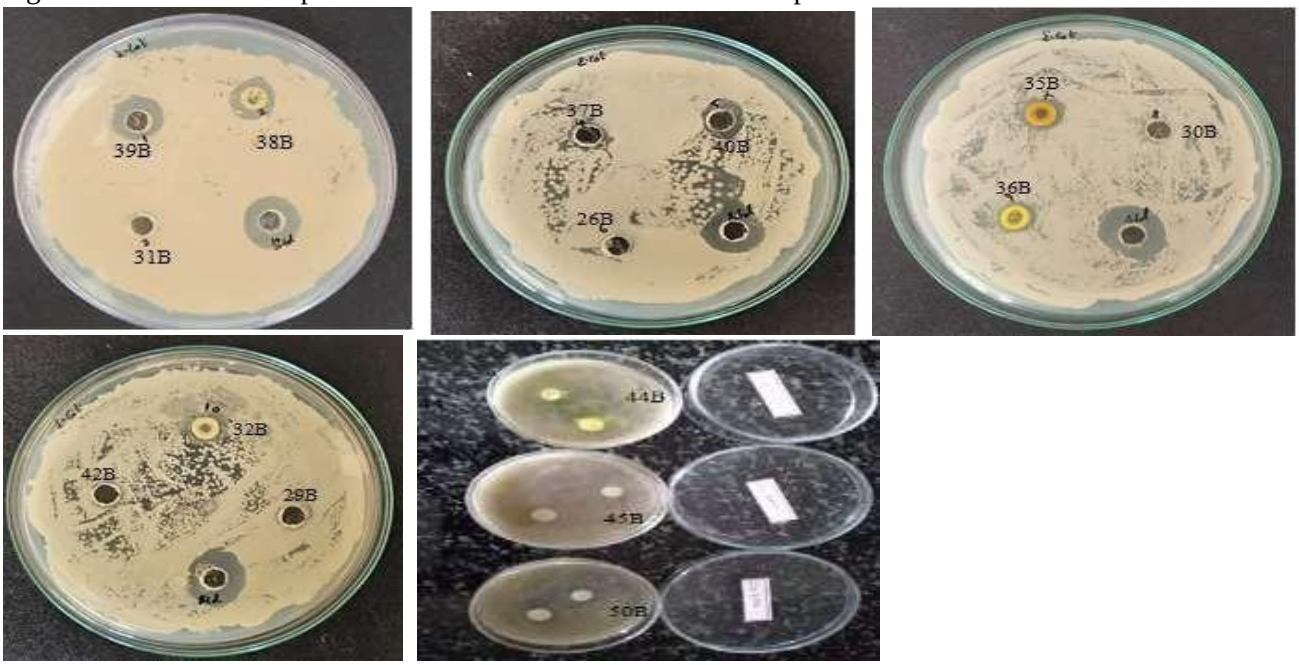
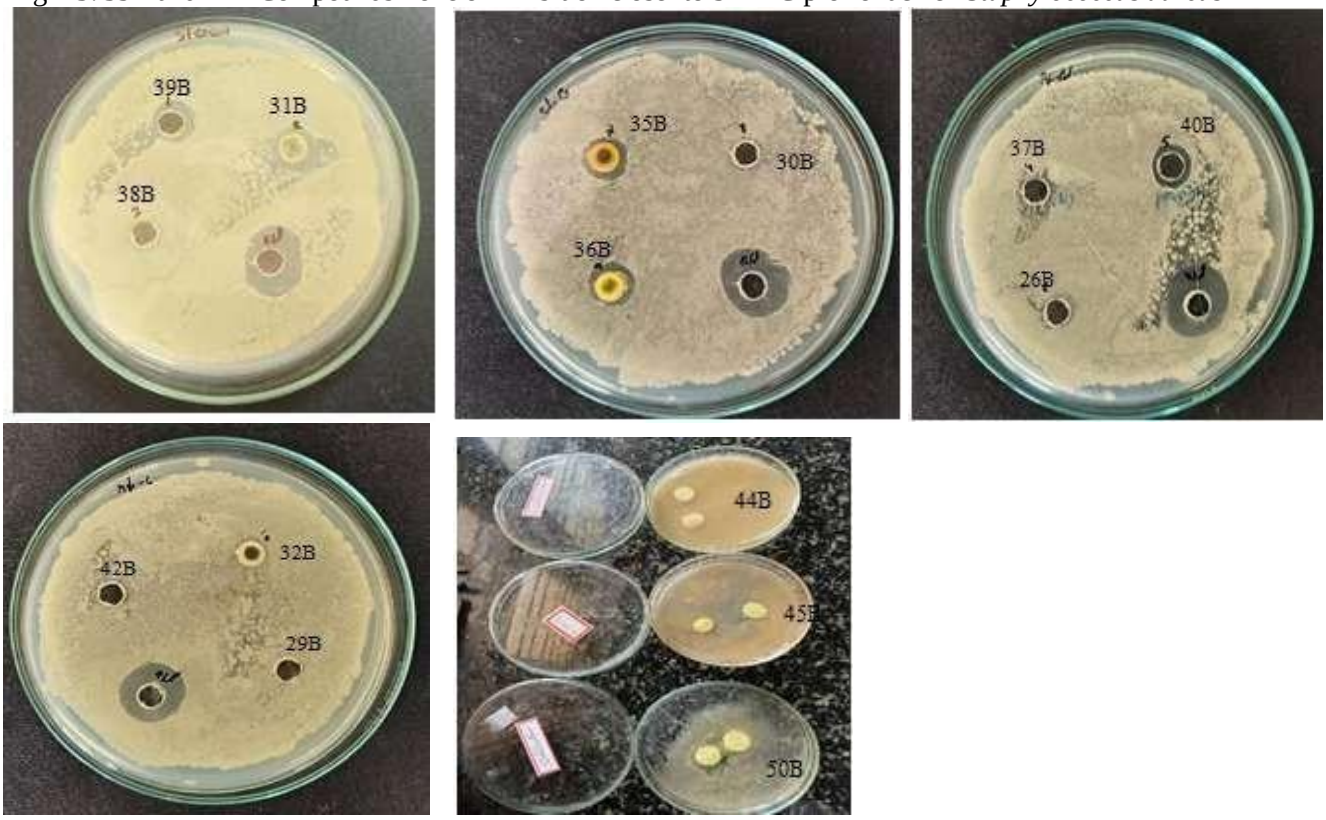


Fig -13: 39B and 42B Compounds Zone of inhibition closer to STD Ciprofloxacine - *Staphylococcus aureus*



7. ANTIMICROBIAL ACTIVITY

Anti-microbial activity refers to the capacity of a compound or material to inhibit the growth or destroy pathogenic microorganisms such as bacteria, fungi, viruses, and protozoa. This activity plays a vital role in fields like medicine, food preservation, agriculture, and water treatment. Anti-microbial agents function through various mechanisms, including disrupting microbial cell walls, inhibiting protein synthesis, or interfering with metabolic pathways. The investigation and development of new antimicrobial agents have become crucial area of scientific research**.** Even our challenge also the same to find out effective and potent anti-microbial agents.

8. CONCLUSION:

As a result of current study, the in-vitro anti bacterial activity shows that the synthesized thirty compounds were effective against on both gram positive and gram negative organism (*E.coli* & *Staphylococcus aureus)* The zone of inhibition observed against test and standard compounds were summarized in (Table 10 and 11). Ciprofloxacin with 5ug was used as a reference std control for the current study. Out of thirty compounds, nitro group in para position and methyl group in ortho position 11A and 14A shows more effective in both *E. coli and Staphylococcus aureus* (Fig-9,10) (Table-10). Similarly 2,6 dimethyl aniline and methyl group in ortho position 38B, 39B (Fig-11) in *E. coli* and methyl group in ortho position and acid group in para position 39B,42B (Fig-12) in *Staphylococcus aureus* (Table-11) shows significant anti-microbial activity. The overall result concluded that methyl group in ortho position imparted more on anti-bacterial activity. Thus further substitution with methyl group in ortho position needed to be studied in future.

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