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# A Series of Novel 4-(Benzo[D]Oxazol) Piperazine Derivatives as Potent Anti-Fungal Agents: Design, Synthesis, Biological Evaluation and Molecular Docking Studies

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**ABSTRACT:**

A series of 4-(benzo[d]oxazol) piperazine derivatives was designed and synthesized in excellent yield. All newly synthesized compound(s) were characterized by their infrared, proton nuclear magnetic resonance and mass spectral analysis. In order to evaluate their biological activity, all the compounds were screened for their antifungal activity against *Candida tropicalis* and *Aspergillus niger* employing a Agar well diffusion method. Furthermore, the experimental results were supported by molecular docking study. The results revealed that all newly synthesized compounds were exhibited moderate to potent antifungal activity. In case of potent antifungal activity, compound 1 gives prominent activity with comparison of all synthesized compounds. Significantly, we have designed, synthesized and characterized an interesting and biologically important series of 4-(benzo[d]oxazol) piperazine bridged analogues of Benzisoxazole derivatives. Most of the synthesized compounds were found more active as comparison with each other as manifested by theoretical as well as experimental results.

**Key-words:** Benzisoxazole, Antifungal**,** Piperazine, molecular docking.

## INTRODUCTION: [1-18]

Fungal infections are caused by microscopic organisms that can invade the epithelial tissue. The fungal kingdom includes yeasts, molds, rusts and mushrooms.[1-3] Most fungi are beneficial and are involved in biodegradation; however, a few can cause opportunistic infections if they are introduced into the skin through wounds, or into the lungs and nasal passages if inhaled. [4-5]

Benzisoxazole is an aromatic organic compound with a molecular formula $C_7H_5NO$ containing a benzene-fused isoxazole ring structure. It is a novel antiepileptic drug and is effective for the treatment of partial seizures. 1, 2-Benzisoxazole is a potential substrates of rabbit liver aldehyde oxidase. The supposed mechanism of action of benzisoxazole derived atypical antipsychotics is classified intoserotonergic, dopaminergic and combined regulatory effects. Since the above antipsychotics mainly exhibit antagonism to D2/5HT2A/H1/α adrenergic systems. It has a wide range of biological activities such an antimicrobial, anticonvulsant, antitumor, anti-psychotic, antithrombotic, analgesic activities. [6-17]

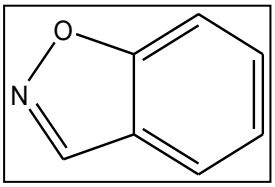


**Figure 1: Structure of Benzisoxazole**

In the field of Molecular modeling, docking is a computational method which estimates the preferred orientation of the ligand relative to the receptor as well as the confirmation of the ligand and receptor when bound to each other. [18-21]

The present research work deals with the synthesis of the title parent compounds starting from substituted 4-(benzo[d]oxazol) piperazine, followed by their molecular docking study and *in-vitro* antifungal evaluation.

## METHODS AND MATERIAL:

### Chemicals and Reagents

All of the chemicals were commercially available and procured from Aldrich, Merck and Vijay chemicals. All reactants and solvents were analytically pure and were used without further purification. The starting compounds, 2-bromobenzoxazole (I) and N-Boc piperazine (II) purchased from Vijay chemicals, Mehsana.

### Instrumentation

Thin layer chromatography (TLC) was performed on silica gel plates (silica gel GF254) visualized at 254 nm. Infrared (IR) spectra were measured on Bruker, Alpha- II. Nuclear Magnetic resonance (NMR) spectra were measured on a Bruker biospin AV400 instrument at 400 MHz for $^{1}$H NMR spectra. The high resolution mass spectra were acquired with a Q-TOF mass spectrometer (Impact II, Bruker).

## EXPERIMENTAL:

### Molecular Docking study:

**Software Used:** AutoDock Vina 4.2.6

**Procedure:** Protein-Ligand Docking

### Steps for AutoDock Vina software

Firstly, choose the protein target and ligand molecule.

**For protein target:** use Protein Data Bank.

Process: go to PDB site------Search required PDB------click on download file click on PDF format -------- protein

was downloading in downloads.

**For ligand target:** Synthetically ligand molecule.

Process: go to PubChem------select download------select 3D conformers save it as SDF file format -------- Ligand

Was download in downloads. Both Protein and Ligand was saved in Docking Folder.

**Carry out protein and ligand preparation. For Protein Preparation:**

Go to AutoDock Vina tools -------- copy protein and paste in AutoDock Vina tools.

Step 1: Go to edit option -------- Delete water molecules.

Step 2: Go to Edit Option -------- Go to Hydrogen---------Add hydrogen------select on polar only ---------- click ok.

Step 3: Go to Edit-------- select charges-------- Add Kollaman charge ---------- click ok (Protein was prepared).

For PDBQT format: go to Grid ----- select Macromolecule----- click on choose----- select protein option-----

Select Molecules----- click ok ----- one tab is open--- save as PDBQT format---------- ok.

**For Ligand Preparation:**

Step 1: Convert SDF format to Ligand PDB format

go to PyMol tool----- copy and paste ligand to PyMol tool---- go to File---- Export Molecule-------- save as ligand in Docking Folder.

Step 2: Convert PDB format to PDBQT format.

Copy and paste Ligand to AutoDock Vina Tool---- go to Ligand---- select input----select Choose-------- select Ligand---- select molecule for AutoDock 4---------- click ok

Step 3: Save as PDBQT format.

Go to ligand---- select Output----save as PDBQT format -------Save in Docking Folder.

**Select the docking site in protein.**

Step 1: Preparation of Grid: copy and paste, protein and ligand in AutoDock Vina tool--- go to Grid-------Select Macromolecule----Click Choose-----Select Ligand and Protein-----Select Molecule-----Click No-----

Click ok.

Step 2: For Grid Formation: go to Grid----- select Grid Box---- select Grid Option Tab open----Click on file----

choose output Grid dimension file----Tab is open -----select Docking folder---------- save as grid.txt format in Docking folder.

**Docking process using AutoDock Vina Tool**

Installed AutoDock Vina tool----go to search--- type cmd (command prompt) ------- go to command prompt box----- "C:\Program Files (x86)\The Scripps Research Institute\Vina\vina.exe" --receptor 4dbn1.pdbqt -- ligand C36.pdbqt --config config.txt --log log.txt --out output.pdbqt -----click on enter log file and output .pdbqt file are generated in Docking folder.

**Different ligand poses are generated.**

Go to PyMol----copy protein----- copy output .pdbqt copy and paste.

**ANTIFUNGAL ACTIVITY:**

All the synthesized compounds were screened for the antifungal activity by Agar well diffusion method.

**Determination of antifungal activity by Agar well diffusion method:**

**Composition of Media:**

- Nutrient Agar: 15 %
- Peptic Digest of Animal Tissue: 5 %
- Sodium chloride: 5 %
- Bees extract: 1.5 %

- Yeast extract: 1.5 %
- Final pH (after sterilization): 7.5 ± 0.2
- Distilled water: up to 1000 ml

**Micro-organism used:**

- *Candida tropicalis* (Yeast)
- *Aspergillus niger* (Mould)

**Standard drug used:**

Fluconazole

**Preparation of synthetic compounds for microbiological assay:**

A stock solution of 10 mg of each synthetic compound dissolved in 1 mL of dimethyl sulfoxide (DMSO) as solvent was prepared. The antimicrobial activity of the synthesized compounds was evaluated by Agar well diffusion method.

**Preparation of Standard drug for microbiological assay:**

A stock solution of 1 mg of standard drug (Fluconazole) dissolved in 10 mL of dist. water as solvent was prepared.

**Procedure of Agar well diffusion method:**

1. Requisite quantity of the liquid agar media about 15-20 ml of molten agar was spread into each sterilized Petri dish by taking the usual precautions to avoid the contaminations.

2. After solidify the liquid media test organism was spread over the solidified agar media. All the Petri dishes were marked in a specific way. Sterile cork borer was used to make well.

3. The agar plates were inoculated with the suspension of particular organism by spread plate technique.

4. Finally, the agar well plates were filled with the test solution. After the addition of the tested samples, the plates were kept in freeze for diffusion and incubated at 35ºC for 24 hours for fungi in B.O.D. incubator. The zone of inhibition if any was then measured in mm for the particular compound and specific organism.

5. Standard antifungal drug Fluconazole was used as positive control and sterile distilled water as negative control and incubated at 35°C for 4- 5 days.

6. All the microbial strains used were of non-invasive species of their genera and thus applicable for analytical work. *C. tropicalis* is the fungi and *A. niger* is the mould. Their zone of inhibition has been reported.

7. The MIC was determined by measuring the absorbance of microtitre plates at 530 nm for *C. tropicalis*. While for *A. niger*, MIC was determined visually. The optical density from each well was compared with optical density from the positive control wells, the lowest concentration with optical density <0.1 signifies inhibition and considered as MIC.

**RESULT AND DISCUSSION:**

**Chemistry**

Benzimidazole derivatives were synthesized according to **Scheme 1**. According to designed scheme, six derivatives were prepared. All the intermediate and target molecules were confirmed by TLC, IR, NMR and Mass Spectra.

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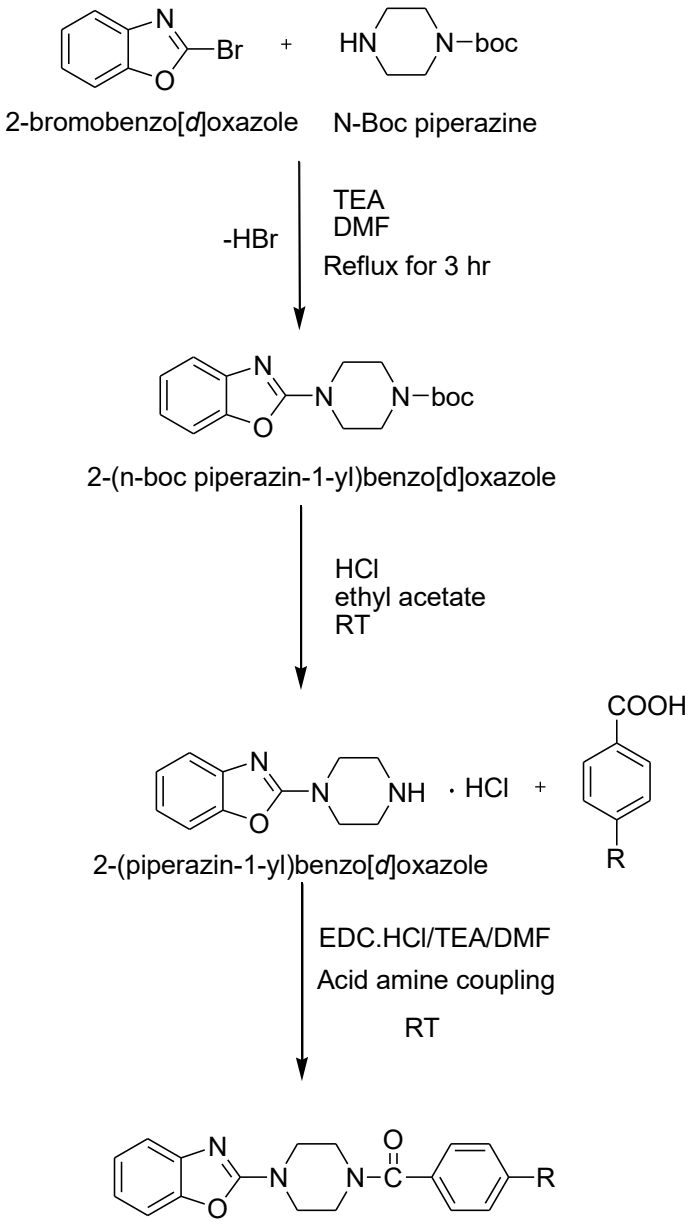


**Scheme 1: Synthetic Scheme of Target compounds**

**General procedure for synthesis of newer compounds:**

***Synthesis of 2-(n-boc piperazin-1-yl)benzo[d]oxazole [Intermediate of STEP- 1(C-N COUPLING BY $SN_2$ REACTION)]:***

To a stir solution of 2-bromobenzoxazole (5 gm, 1 equ) in DMF, N-Boc piperazine (1.5 equ) is added followed by drop wise addition of TEA. The reaction mixture is refluxed on the water for 3 hr and the progress of the reaction is checked by TLC. After completion of the reaction, the reaction mixture was poured into ice-cold water to obtain a precipitate. Final crude products isolated by filtration and dry it. Recrystallization was done with hot methanol.

***Synthesis of 2-(piperazin-1-yl)benzo[d]oxazole hydrochloride [Intermediate of STEP- 2(Deprotection)]:***

Concentrated hydrochloric acid (5 mL) was added to N-Boc piprazinyl benzoxazole (step 1 product) (4.0 g). The resulting solution was stirred for 2 h and Ethyl acetate (20 mL) was then added over a period of 1 h at room temperature. The progress of the reaction was checked by TLC and after completion of the reaction, the resulting slurry was filtered. The filter cake was dried and then dissolved in ethyl acetate (20 mL) and $H_2O$ (10 mL). The crude product was isolated by extraction with 2 gm.

**Synthesis of substituted benzisoxazole (Acid-Amine coupling):**

Take solution of 2-piperazinyl benzoxazole (1.2 equ) in DMF in a round-bottomed flask. EDC HCl (1 equ) and TEA (1.5 equ) were added and the reaction mixture was stirred at RT for about 5-10 min. After that benzoic acid derivatives (1.2 equ) were added and the reaction mixture was stirred at room temperature for 3 hours. After the completion of the reaction monitored by TLC, the reaction mixture was diluted with water and extracted with DCM, dried in sodium sulphate and distilled in reduced pressure to obtain the final product.

**Physical and Spectral characterization of newer compounds:**

**Table 1: Physical characterization data of Intermediates**

| Intermediates | Molecular Formula | IUPAC name | Mol. Wt. (g/mol) | Melting Point ($^{o}$C) | Yield % | *Rf |
|---|---|---|---|---|---|---|
| Step- 1 Intermediate | $C_{16}H_{14}N_2O_2$ | 2-(n-boc piperazin-1-yl)benzo[d]oxazole | 420.49 | 88-90 | 90.21 | 0.2 |
| Step- 2 Intermediate | $C_{11}H_{14}ClN_3O$ | 2-(piperazin-1-yl)benzo[d]oxazole hydrochloride | 239.08 | 172-175 | 45.62 | 0.4 |

Mobile phase combination used for TLC:*Hexane: Ethyl acetate (9:1)

**Table 2: Physical characterization data of synthesized compounds**

| Compound | R | Molecular formula | IUPAC name | Mol. Wt. (g/mol) | Melting Point ($^{o}$C) | Yield % | *Rf |
|---|---|---|---|---|---|---|---|
| 1 | -H | $C_{18}H_{17}N_3O_2$ | (4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(phenyl)methanone | 307.35 | 165-168 | 80.0 | 0.8 |
| 2 | -$NO_2$ | $C_{18}H_{16}N_4O_4$ | (4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(4-nitrophenyl)methanone | 352.34 | 184-187 | 79.0 | 0.8 |
| 3 | -$CH_3$ | $C_{19}H_{19}N_3O_2$ | (4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(p-tolyl)methanone | 321.37 | 154-157 | 83.0 | 0.7 |
| 4 | -Cl | $C_{18}H_{16}ClN_3O_2$ | (4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(4-chlorophenyl)methanone | 341.79 | 178-182 | 67.0 | 0.75 |
| 5 | -$OCH_3$ | $C_{19}H_{19}N_3O_3$ | (4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(4-methoxyphenyl)methanone | 337.37 | 138-142 | 82.0 | 0.8 |
| 6 | -Br | $C_{18}H_{16}BrN_3O_2$ | (4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(4-bromophenyl)methanone | 386.24 | 170-173 | 45.0 | 0.7 |

Mobile phase combination used for TLC:*Chloroform: methanol (9.5:0.5)

**Spectral characteristics:**

**(4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(phenyl)methanone**

IR in $cm^{-1}$ (KBr**)** Aromatic CH: 3063, 3033, C=O (Amide): 1689, C=N: 1607, C-O:1195, C-N:1461;

$^{1}$H NMR in δ ppm (DMSO, 400 MHz) 3.36-3.43 (-$CH_2$, Methylene), 7.44-7.95 (Aromatic- H, 1-benzene), 7.26 (Aromatic- H,

Benzene);

Mass $M^+$peak (m/z) 307.35 $(M+H)^+$

**(4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(4-nitrophenyl)methanone**

IR in $cm^{-1}$ (KBr**)** Aromatic CH: 3077 C=O: 1688, C=N: 1608, C-O:1084, $NO_2$ : 1577, 1462, C-N:1310;

$^1H$ NMR in δ ppm (DMSO, 400 MHz) 3.36-3.43 ($-CH_2$, Methylene), 8.21-8.37 (Aromatic- H, 1-benzene), 7.26 (Aromatic- H, Benzene);

Mass $M^+$peak (m/z) 386.24 $(M+H)^+$

**(4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(p-tolyl)methanone**

IR in $cm^{-1}$ (KBr**)** Aromatic CH: 3059, 3031, 3007, Aliphatic CH: 2923, 2871, C=O (Amide): 1688, C=N: 1607, C-O:1025, C-N:1461;

$^1H$ NMR in δ ppm (DMSO, 400 MHz) 3.36-3.43 ($-CH_2$, Methylene), 7.24-7.83 (Aromatic- H, 1-benzene), 7.26 (Aromatic- H, Benzene), 2.35 ($-CH_3$, Methyl);

Mass $M^+$ peak (m/z) 341.79 $(M+H)^+$

**(4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(4-chlorophenyl)methanone**

IR in $cm^{-1}$ (KBr**)** Aromatic CH: 3069, C=O (Amide): 1679, C=N: 1609, C-O:1116, C-N:1460;

$^1H$ NMR in δ ppm (DMSO, 400 MHz) 3.36-3.43 ($-CH_2$, Methylene), 7.45-7.89 (Aromatic- H, 1-benzene), 7.26 (Aromatic- H, Benzene);

Mass $M^+$ peak (m/z) 352.34 $(M+H)^+$

**(4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(4-methoxyphenyl)methanone**

IR in $cm^{-1}$ (KBr**)** Aromatic CH: 3077, Aliphatic CH: 2974, C=O (Amide): 1690, C=N: 1608, C-O:1116, C-N:1409;

$^1H$ NMR in δ ppm (DMSO, 400 MHz) 3.36-3.43 ($-CH_2$, Methylene), 6.95-7.84 (Aromatic- H, 1-benzene), 7.26 (Aromatic- H, Benzene), 3.73 ($-CH_3$, Methyl);

Mass $M^+$peak (m/z) 321.37 $(M+H)^+$

**(4-(benzo[d]oxazol-2-yl)piperazin-1-yl)(4-bromophenyl)methanone**

IR in $cm^{-1}$ (KBr**)** Aromatic CH: 3077, C=O (Amide): 1690, C=N: 1609, C-O:1121, C-N:1462;

$^1H$ NMR in δ ppm (DMSO, 400 MHz) 3.36-3.43 ($-CH_2$, Methylene), 7.61-7.84 (Aromatic- H, 1-benzene), 7.26 (Aromatic- H, Benzene);

Mass $M^+$ peak (m/z) 337.37 $(M+H)^+$

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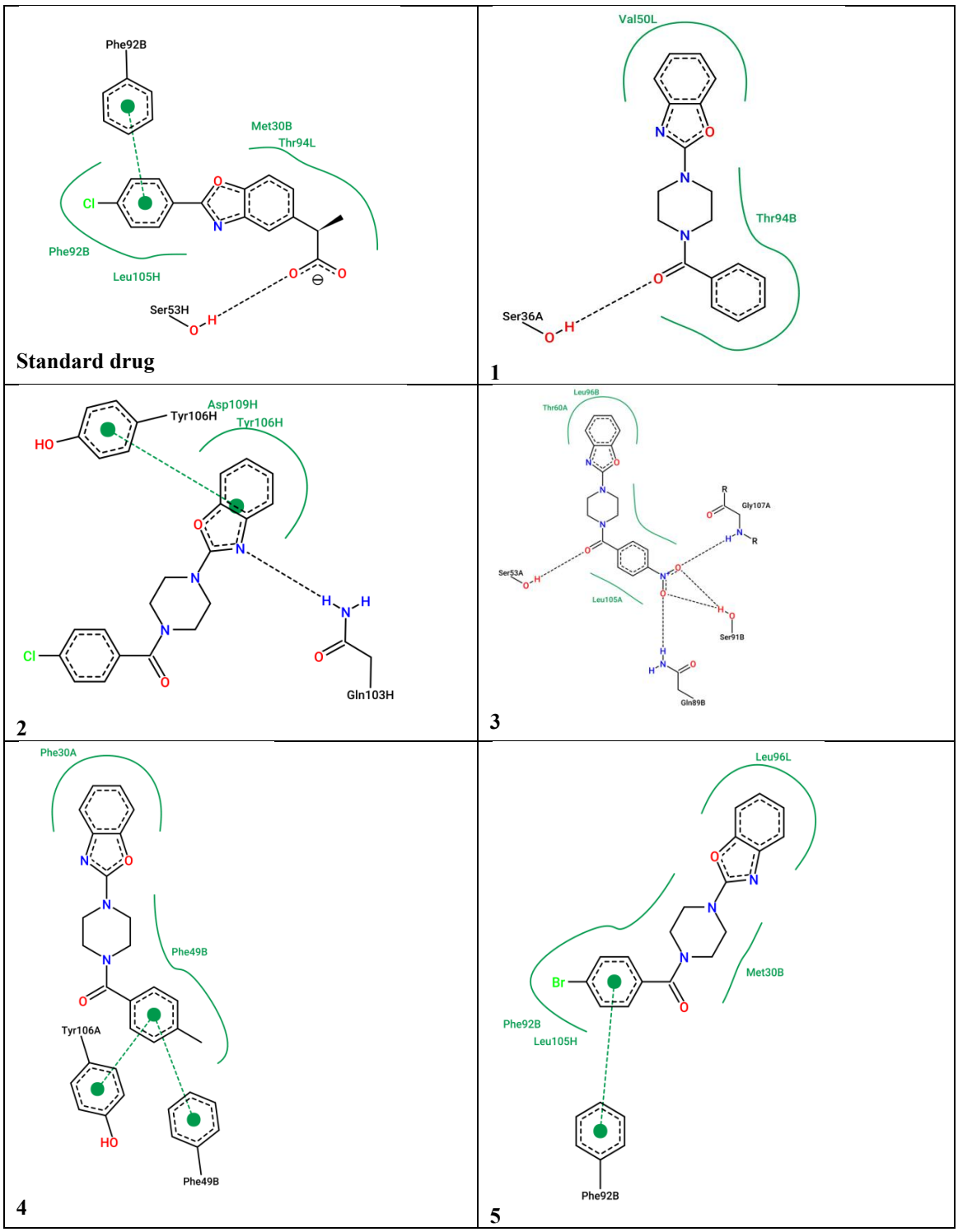
**Docking score**



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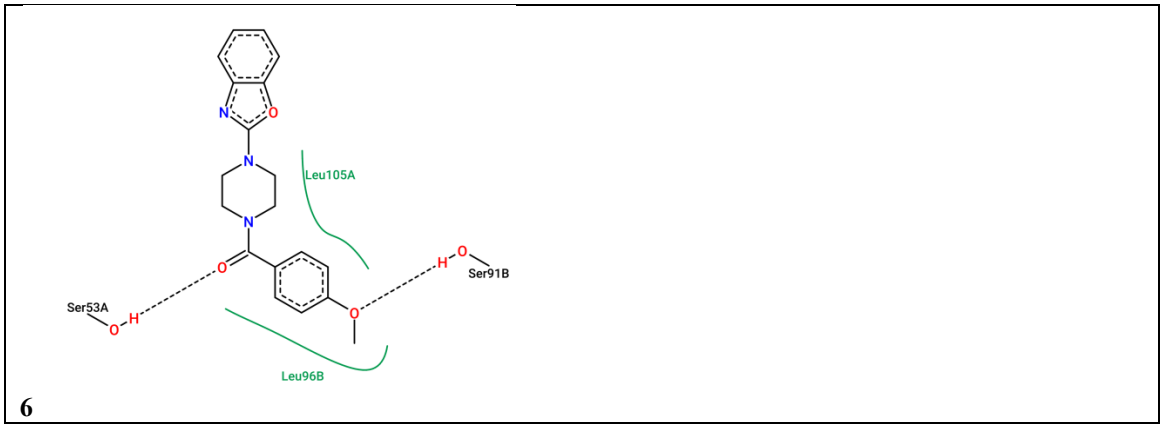



**Figure 2: 2D interaction image Molecular docking study of derivatives**

**Table 3: Docking score of benzisoxazole derivatives**

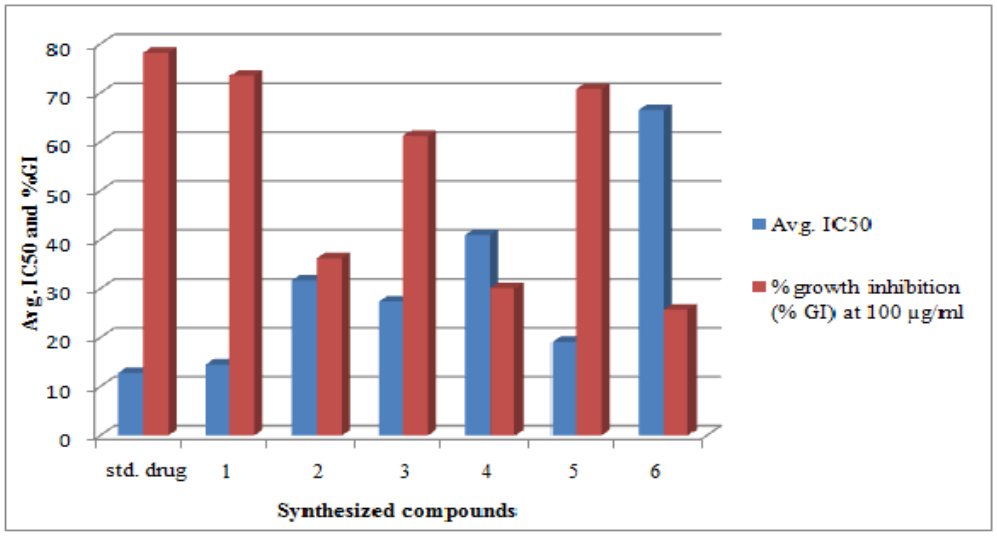
| Compounds | Docking Binding energy (kcal/mol) |
|---|---|
| Fluconazole | -9.7 |
| 1 (Phenyl) | -8.3 |
| 2 (p-nitro) | -9.3 |
| 3 (p-methyl) | -8.4 |
| 4 (p-chloro) | -8.6 |
| 5 (p-methoxy) | -8.7 |
| 6 (p-bromo) | -8.0 |

From the docking study, we conclude that compound 2, compound 4 and compound 5 may give anti fungal activity. Among all these compounds, **compound 2 may give better antifungal activity.**

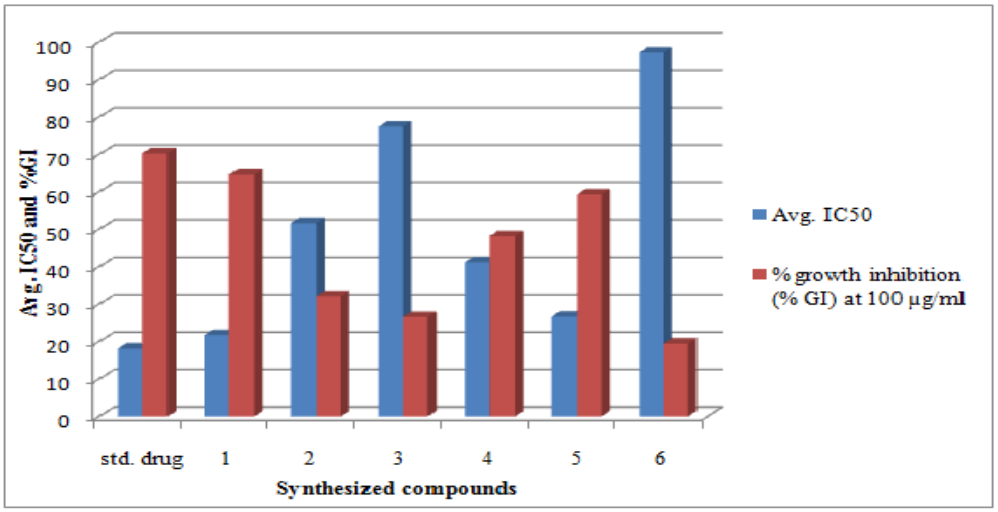
**Antifungal activity:**

**Table 4: Comparison of IC 50 of synthesized Compounds with standard drug**

| Compounds | *A. niger (715)* | | *C. tropicalis (2168)* | |
|---|---|---|---|---|
| | **Avg. IC50** | **% growth inhibition (% GI) at 100 µg/ml** | **Avg. IC50** | **% growth inhibition (% GI) at 100 µg/ml** |
| 1 | 14.48 | 73.5 | 21.71 | 64.7 |
| 2 | 31.67 | 36.2 | 51.64 | 32.1 |
| 3 | 27.36 | 61.2 | 77.51 | 26.6 |
| 4 | 40.95 | 30.1 | 41.19 | 48.2 |
| 5 | 19.11 | 70.8 | 26.71 | 59.4 |
| 6 | 66.48 | 25.7 | 97.30 | 19.5 |
| Std. Drug (Fluconazole) | 12.74 | 78.2 | 18.21 | 70.3 |




**Graph 1: Comparison of avg. IC50 and %GI against *A. niger* of all compounds with standard drug**




**Graph 2: Comparison of avg. IC50 and %GI against *C. tropicalis* of all compounds with standard drug**

## CONCLUSION

In this study, we designed, synthesized the series of 4-(benzo[d]oxazol) piperazine derivatives. All compounds are successfully characterized with TLC, IR, NMR, Mass Spectra and screened for their chemotherapeutics anti fungal activity. From the graph I and II, It concluded that compound 1 and compound 5 gives better activity against *A. niger* (715) and *C. tropicalis* (2168). Whereas **compound 1 gives better activity** then compound 5 because it contains phenyl group giving stable compound compare to compound 5 contains methoxy group at p- position.

## CONFLICT OF INTEREST:

The authors declare no conflict of interest.

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