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Novel 1,2,3-Triazole–Piperazine Compounds: Synthesis, HOMO–LUMO Gap Insights, And Antioxidant Potential Via Pharmacophore Modeling

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Abstarct

Background:*Free radicals are generated in the human body due to various factors such as environmental pollution, radiation, immune responses, and cellular respiration. These reactive species can lead to oxidative stress, causing significant damage to proteins, DNA, and cellular structures. Such oxidative damage is strongly associated with aging and the development of numerous diseases, including cancer and cardiovascular disorders. Antioxidants play a vital role in neutralizing free radicals by donating electrons, thereby stabilizing these reactive molecules and protecting the body from oxidative damage and related diseases.*

Aim: *The aim of the present study is to synthesize novel 1,2,3-triazole–appended piperazine derivatives and evaluate their antioxidant potential through in vitro assays.*

Objectives: *To synthesize a series of 1,2,3-triazole–piperazine derivatives using appropriate synthetic protocols.To isolate and purify the synthesized compounds using recrystallization, thin-layer chromatography (TLC), and column chromatography.To characterize the purified compounds using FTIR, ^{1}H NMR, ^{13}C NMR, Mass spectrometry, and Elemental analysis.To evaluate the antioxidant activity of the synthesized compounds using in vitro methods (DPPH assay)*

Procedure: *In-silico design(Fig 1) of novel analogues were carried out for fifteen compounds using Auto Dock Vina by using pdb id: (PDB id: 1XLY) (Fig 2) and compared with standard drug ascorbic acid. Pharmagist software will be used to analyse ‘parmacophore properties (Fig 3), which is responsible for a particular biological interaction. Guassian, Smarten, and Mastroes softwares will be used to find out the HOMO-LUMO gaps (Fig 4) which is used for examining the kinetic stability. Anti-oxidant activity are determined by DPPH technique (Fig 5).*

Result: *Out of 15 compounds, Five compounds which have highest docking score (Table2) better pharmacophore properties, and larger HOMO-LUMO gaps (Table 3& Table 4) were synthesized (Table-5). The synthesis were carried out by two step process with various primary aromatic amines (Table 1) to determine their anti-oxidant activity. Among this mixtures B1, B5, B11 shows good and B7 & B15 shows better anti-oxidant activity(Table-6).*

Keywords: *Benzotriazole, Homo-Lumo Studies, Pharmacophore, Docking studies.*

1.INTRODUCTION:

1,2,3-Triazole derivatives are of significant interest due to their potential to serve as versatile scaffolds for the synthesis of various heterocyclic compounds exhibiting diverse biological activities. These include antimicrobial [1–5], antioxidant [6–10], anti-tuberculosis [11–17], antifungal [18], and anticancer properties [19–24]. Given the broad spectrum of bioactivity demonstrated by 1,2,3-triazole-based compounds and the utility of hybrid pharmacophore systems, we were motivated to explore the synthesis of novel derivatives with enhanced antioxidant potential. In this context, we designed and synthesized a series of 1,2,3-triazole–piperazine derivatives and evaluated their antioxidant activity. These derivatives were constructed by linking the triazole and piperazine moieties with various biologically relevant aromatic amines, as outlined.Notably, several pyrazole-based drugs, such as Pyrazofurin, Encorafenib, Celecoxib, Crizotinib, and Lonazolac, are already available on the market [20–23], further underscoring the pharmacological importance of such heterocycles. Literature evidence suggests that compounds containing triazole and piperazine moieties possess considerable therapeutic relevance, especially in medicinal chemistry. However, examples of molecules that integrate both triazole and piperazine nuclei within a single framework are relatively limited. Inspired by their superior biological activity and existing research, we pursued the synthesis of hybrid molecules incorporating both these pharmacophores with the aim of achieving enhanced antioxidant efficacy. Accordingly, we report herein the synthesis and characterization of a new series of 1,2,3-triazole-appended piperazine derivatives, designed as potential antioxidant agents with improved therapeutic profiles.

2.EXPERIMENT SECTION:

MATERIALS AND METHODS:

We purchased the synthetic chemicals from Vasa Manufactured Substances in Malleshwaram, Bangalore. Utilizing KBr pellets, ABB Bomem FTLA 2000-102 FTIR spectra were kept in the 400-4000 cm-1 territory. The NMR spectra of the ^{1}H and ^{13}C were recorded (500 MHz- DMSO - d_6) and (125 MHz- DMSO - d_6). TMS is utilized as the standared and the and chemical shifts are reported in parts per million (ppm).

Preparation Of 1,2,3 Triazole Appended Piperazine(Compound A)

0.01 gram of benzotriazole, 0.008 gram of Piperzine, and 0.6 ml of chloro benzaldehyde were added in round bottomed flask (RBF) and dissolved in ethanol . Keep the above mixture for refluxing up to 8 hours. After 8 hours remove the mixture and filter it.. The product was kept for drying in hot air oven at temperature 120-160 degree Celsius for 5 minutes.

Synthesis of substituted triazole and piperazine derivatives Compounds (B1-B15):

The above product was weighed up to 0.29 grams and dissolved with ethanol in RBF. 0.1 gram of 5 different primary amines and 0.2 ml of formaldehyde were added and kept for refluxing for 8 hours. After refluxing, the product was taken out carefully and filtered.

3.BIOLOGICAL ACTIVITY:

In Vitro Antioxidant Activity:

The combined mixtures will be evaluated for *in vitro* Antioxidant Activity.

The anti-oxidant of all blended mixtures will be decided to use

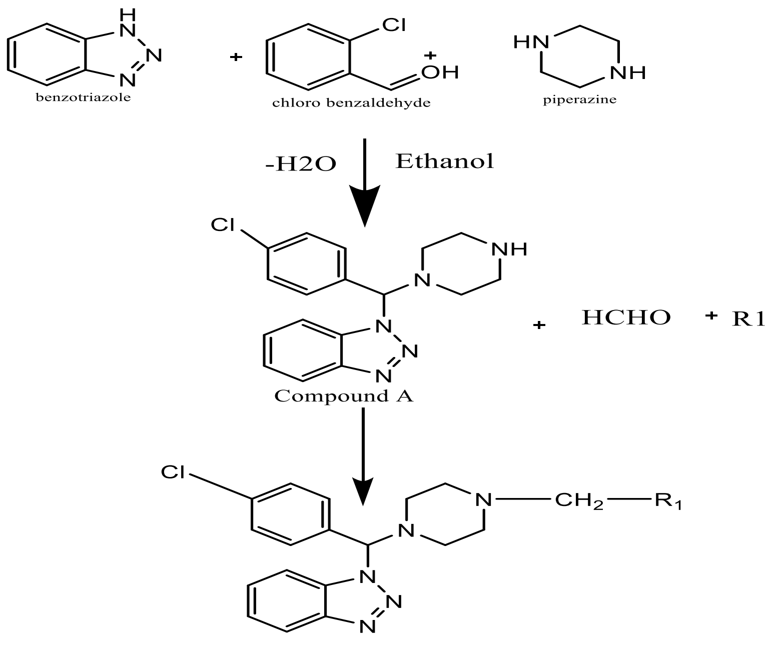
1. DPPH radical scavenging activity

DPPH Method:

Preparation of the reagent – 3.96 DPPH was accurately weighed and dissolved in 50 ml of methanol. Preparation of the test and standard solutions- Stock solutions of 2000 ug/ml of the synthesized compounds and ascorbic acid were prepared in methanol. These solutions were serially diluted with methanol to obtain the required concentrations. The antioxidant activity of the test compounds and standards were assessed using 96 well micro titre plate. Absorbance of solvent containing the same amount of methanol and DPPD radical solution was measured as well.

$$\text{Scavenging (\%)} = \frac{\text{Absorbance} - \text{Absorbance (Sample)}}{\text{Absorbance}} \text{ X } 100$$

4.SCHEME:



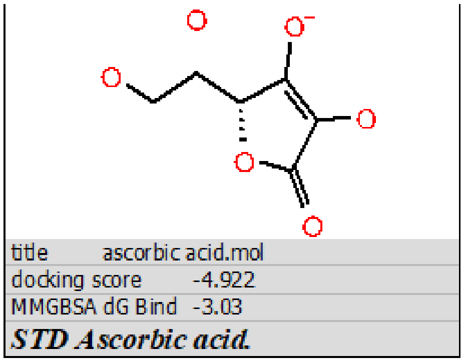
Compounds B1-B15

Fig 1: Schematic Represantation

Table 1: Amines used to design the compounds:

Sl No	Compounds	R1
1	B1	Aniline
2	B2	Ortho Anisidine
3	B3	Meta Anisidine
4	B4	Para Anisidine
5	B5	4-Chloro aniline
6	B6	2-Chloro aniline
7	B7	4-Bromo aniline
8	B8	2-Bromo aniline
9	B9	2-Nitro aniline
10	B10	3-Nitro aniline
11	B11	4-Nitro aniline
12	B12	2,4,Dimethyl aniline
13	B13	2,6 Dimethyl aniline
14	B14	Ortho toluidine
15	B15	Para toluidine

5.MOLECULAR DOCKING,PHARMACOPHORE & HOMO LUMO STUDIES:



title	ascorbic acid.mol
docking score	-4.922
MMGBSA dG Bind	-3.03

STD Ascorbic acid.

These compounds will be further evaluated computationally for their Molecular modelling , Pharmacophore and HOMO-LUMO gap analysis. Using Autodock Vina in the Pyrex programme, the ligands were docked to the active site (**PDB id: 1XLY**). If the docking procedure was successful, it was also feasible to reconstruct the complexes (ligand-receptor) using the Chimaera programme, enabling further research. The complexes' interactions were investigated using Discovery Studio Visualizer and pyMOL. By using Pharma gist software pharmacophore modelling can be performed and Gaussian, smarten, maestros soft wares can be utilized to find homo lumo gaps. Pharmacophore-based techniques are nowadays an important part of many computer-aided drug design workflows and have been successfully applied for tasks such as virtual screening, lead optimization and de novo design. Referance ligand that is cocrystal structure will be taken from online PDB protein and finding best fitting molecule, Cocrystal structure should have ligand height, fitting protein, binding pocket. The fifteen derivatives are subjected to these 6 pharmacaphore features (A2, A4, A1,R15, R16, H5).It should have minimum 3 matching sites so it resembles that it had 50% of matching cocrystal ligand.

The synthesized molecule have these properties, so it is said to be more fitting. Here (R) represents Ring structure,(A) represents acceptor,(D) represents Donar and (H) represents Hydrophobic interaction. The larger a compounds HOMO-LUMO gap, the more stable the compound, gap tell us at what wavelength the compound can absorb. HOMO energy is firmly connected with reactivity to electrophilic assault, being the most elevated energy orbital containing electrons. LUMO energy is firmly connected with reactivity to nucleophilic assault. Since it is least energy orbital that can acknowledge electrons. The scaffolds which show better docking score, minimum 3 matching site of pharmacophore and larger HOMO-LUMO gaps will be taken up as the lead molecule for further synthesis.

Table- 2:Interaction of amino acids DHFR

Sl no	Compounds	Docking score	Interaction of amino acids
1.	Compound B1	-7.097	Tyr,met,ile,leu
2.	Compound B2	-6.121	Glu,Ser,asp, Leu, Phe
3.	Compound B3	-5.342	Val,Ala, Leu, Asp, Cys
4.	Compound B4	-4.564	Arg,Lys,Phe,Val,Trp
5.	Compound B5	-7.206	val, Asp, Tyr, Leu, Phe
6.	Compound B6	-4.523	Val,Ala, Leu, Asp, Cys
7.	Compound B7	-7.416	Phe, Leu, Tyr
8.	Compound B8	-5.689	Thr,Asp,Phe, Gly, Val
9.	Compound B9	-5.231	Thr,Asp,Phe,Val
10.	Compound B10	-6.234	Ala, Tyr, Val
11.	Compound B11	-6.696	Gly, Val, Tyr, Ala,pro
12.	Compound B12	-5.232	Val,Ala,Ser,Leu,Thr,Gly
13.	Compound B13	-4.432	Thr,Asp,Phe,Val,Lys,Leu,The,Arg
14.	Compound B14	-5.642	Arg,Glu,Phe,Glu,Gly,Lys,Ser
15.	Compound B15	-7.972	Phe,Asp, Val, Tyr
16.	Standard Ascorbic acid	-4.922	Gly, Val, Tyr, Ala.

Fig 2:Docking in an active site of human DHFR

Sl. No	Compounds	Structures

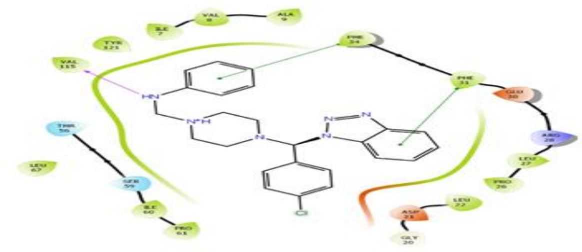
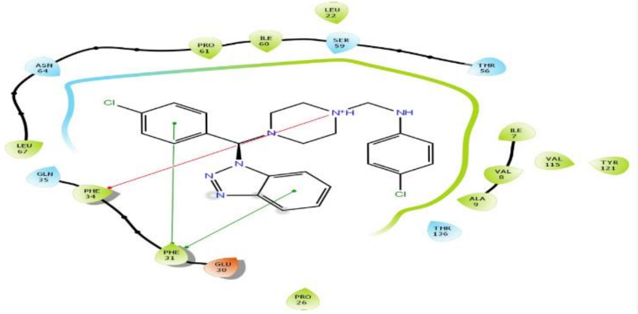
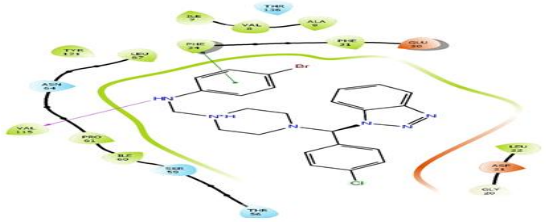
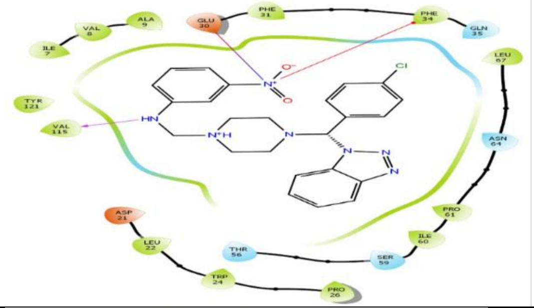
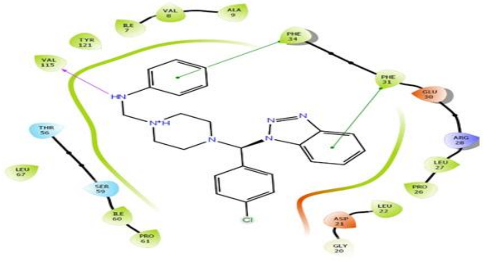
1	CompoundB1	
2	Compound B5	
3	Compound B7	
4	Compound B11	
5	Compound B15	

Table-3: Pharmacophore Modeling and Evaluation of Ligands Targeting DHFR (PDB ID: 1XLY)

Sl.No	Compounds	Matching ligand site	Fitness
1.	Compound B1	D(-) D(3) H(-) R(8) R(9) R(7)	1.172
2.	Compound B2	D(-) D(4) H(-) R(10) R(8) R(11)	1.218
3.	Compound B3	D(4) D(-) H(-) R(10) R(11) R(9)	1.05

4.	Compound B4	D(-) D(4) H(-) R(10) R(11) R(9)	1.158
5.	Compound B5	D(-) D(-) H(5) R(9) R(10) R(7)	0.619
6.	Compound B6	D(-) D(3) H(-) R(9) R(7) R(10)	1.24
7.	Compound B7	D(-) D(-) H(-) R(10) R(7) R(9)	1.585
8.	Compound B8	D(-) D(3) H(-) R(10) R(9) R(7)	1.348
9.	Compound B9	D(-) D(3) H(-) R(9) R(6) R(8)	1.335
10.	Compound B10	D(3) D(-) H(-) R(9) R(8) R(7)	1.153
11.	Compound B11	D(3) D(-) H(-) R(9) R(8) R(7)	1.147
12.	Compound B12	D(-) D(-) H(4) R(11) R(10) R(8)	1.197
13.	Compound B13	D(-) D(3) H(4) R(-) R(8) R(10)	1.214
14.	Compound B14	D(-) D(-) H(4) R(10) R(9) R(7)	1.206
15.	Compound B15	D(3) D(-) H(-) R(10) R(9) R(8)	1.427
16.	Standard Ascorbic acid	D(-) D(3) H(-) R(-) R(9) R(-)	0.531

Fig 3: Cocrystal structure:

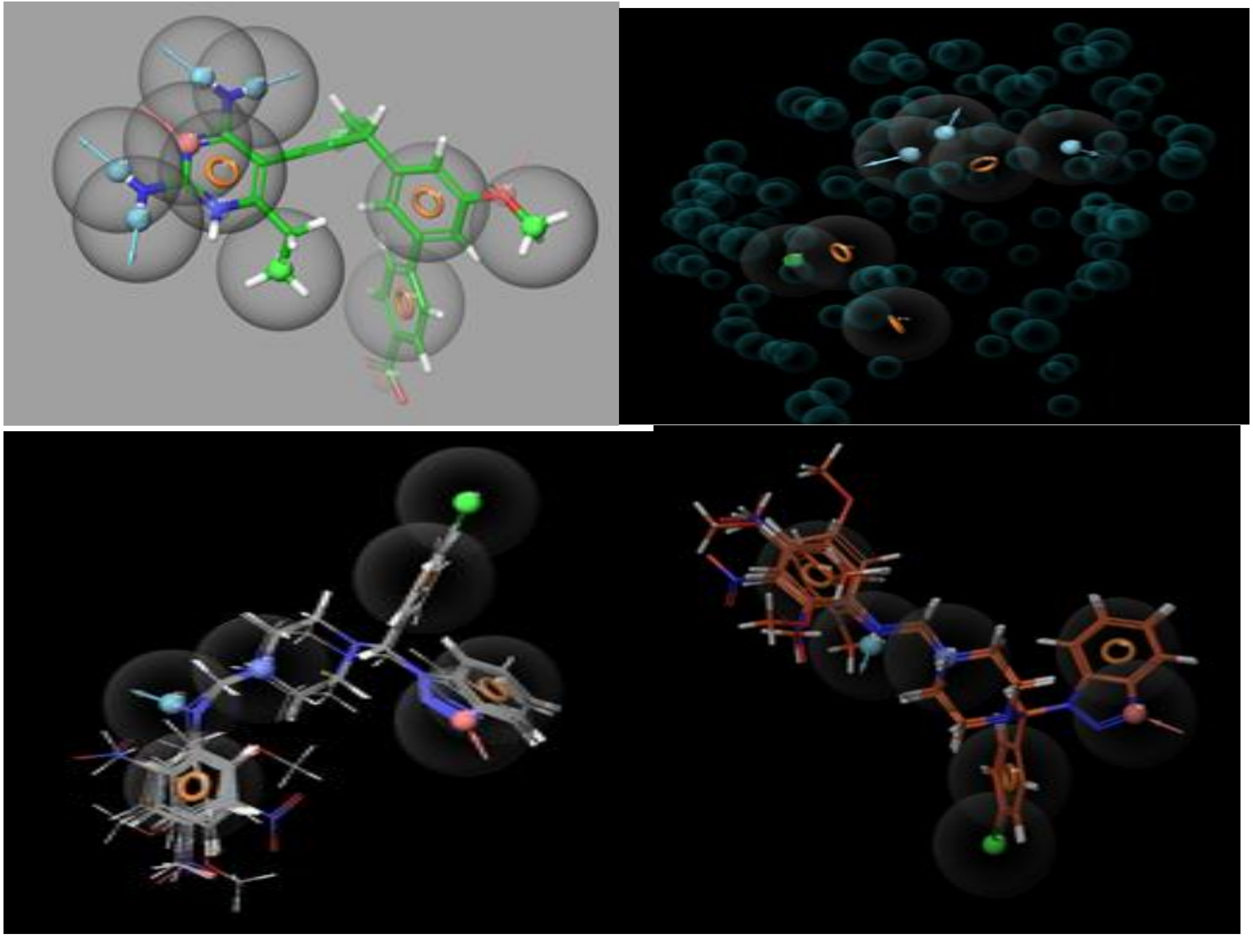
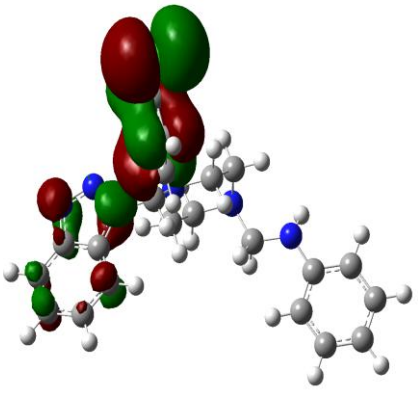
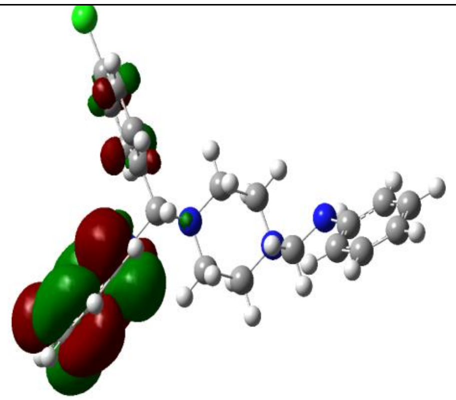
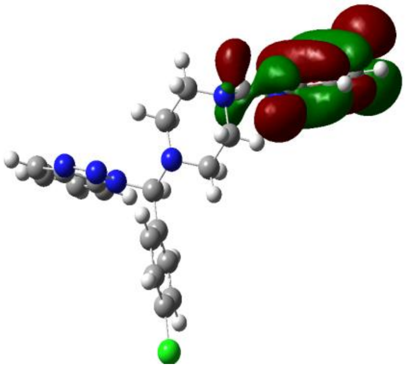
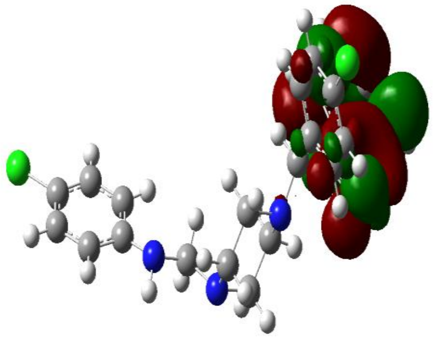
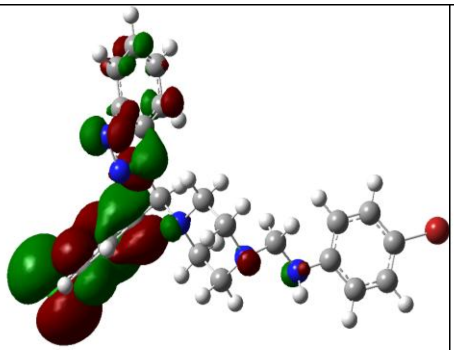
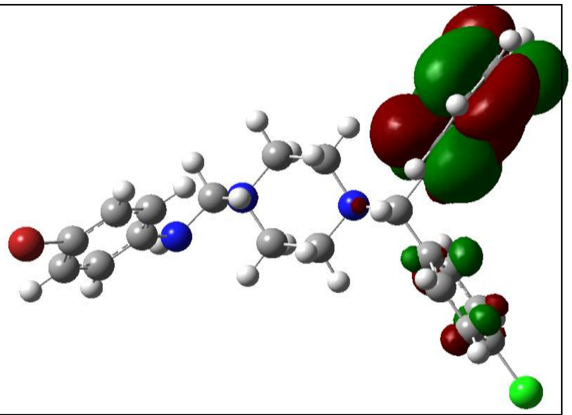
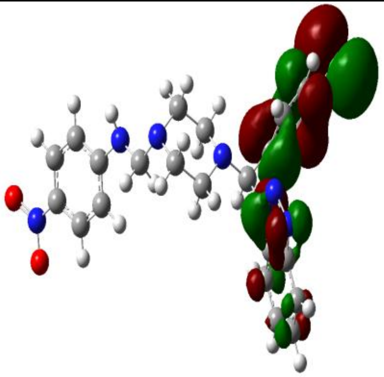
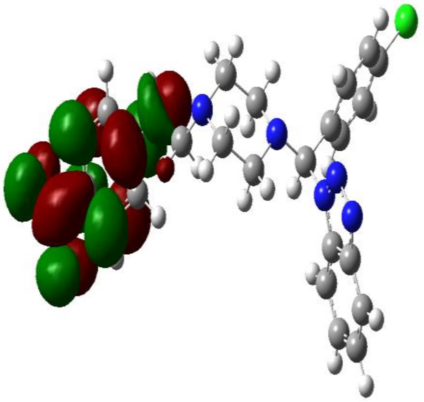
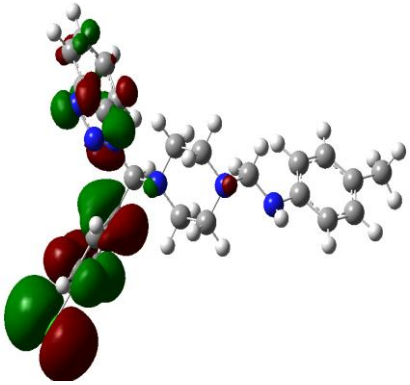
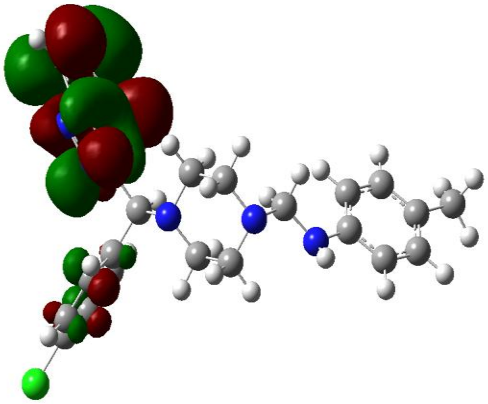
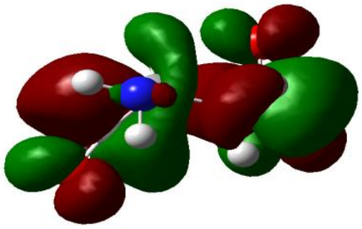
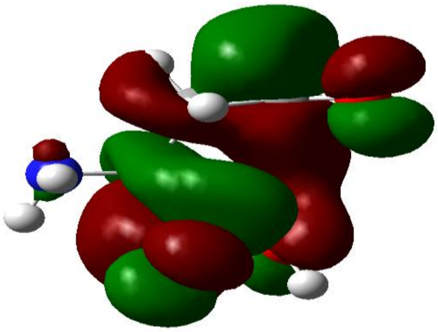


Table-4: HOMO LUMO GAP ANALYSIS:

Sl no	Compounds	HOMO	LUMO
1.	Compound B1	-0.29433	-0.17836
2.	Compound B2	-0.29234	-0.17835
3.	Compound B3	-0.29432	-0.17835
4.	Compound B4	-0.28511	-0.17835
5.	Compound B5	-0.27739	-0.17836
6.	Compound B6	-0.28353	-0.17835
7.	Compound B7	-0.29431	-0.17835
8. .	Compound B8	-0.29430	-0.17835
9.	Compound B9	-0.29421	-0.20242
10.	Compound B10	-0.29431	-0.20885
11.	Compound B11	-0.029433	-0.19779
12.	Compound B12	-0.29432	-0.17836
13.	Compound B13	-0.29434	-0.17836
14.	Compound B14	-0.29433	-0.17835
15.	Compound B15	-0.29432	-0.17836
16.	Standard Ascorbic acid	-0.34408	-0.12473

Fig 4: HOMO-LUMO gap analysis:

1	B 1		
2	B5		

3	B7		
4	B611		
5	B15		
	STD Ascorbic Acid		

6.RESULT AND DISCUSSION:

The structural details of the produced chemicals were clarified by using FTIR, ^{1}H NMR, ^{13}C NMR, and MASS. The spectra of the substances that were synthesised are listed below.

1-((4-chlorophenyl)(piperazin-1-yl)methyl)-1*H*-benzo[*d*][1,2,3]triazole(Compound A): Off white solid, M.P 150-152 ^{o}C, Yield 83%, Mol Formula: $C_{20}H_{30}ClN_5$,,Mol Wt: 375, Elemental Analysis: C, 58.44; H, 5.21; N, 25.55, IR (KBr, cm^{-1}): 3320 (N–H, triazole), 3025 (Ar–C–H), 2940 & 2850 (C–H, aliphatic), 1615 (C=N, triazole ring), 1580 (C=C, aromatic), 1465 (C–N), 1260 (C–N piperazine), 755 (C–Cl) δ 8.01 (s, 1H, triazole–H), 7.85–7.20 (m, 7H, Ar–H), 5.12 (s, 1H, CH), 3.65–2.85 (m, 8H, piperazine). ^{13}C NMR (100 MHz, DMSO-d_6): δ 155.6, 145.3, 132.4, 128.7, 127.5, 125.3, 122.8, 118.9, 55.6, 53.3, 49.2. *m/z* %:375.95(base peak)376.22 (M+1)$^{+}$.

Synthesis of *N*-((4-((1*H*-Benzo[*d*][1,2,3]triazole-1-yl)(4-chlorophenyl)methyl)piperazine-1-yl)methyl)aniline(Compound B1): Pale yellow solid, M.P 158-160^{o}C ,Yield 83%,Mol Formula: $C_{24}H_{25}ClN_6$,Mol Wt: 432.18, Elemental Analysis C,66.58;H,5.82,Cl8.19;N,19.41 . IR cm^{-1} (KBr): 550,820, and 3200 cm-1. ^{1}HNMR (500 MHz, DMSO - d_6): δ ppm (NH) 6.34 (CH2) 4.13,(CH)6.11 ppm, ^{13}C NMR (125 MHz, DMSO - d_6) *δ* ppm: (CH2)74.6,(CH)126.2(C)146.2 ppm, *m/z* %: 432.18 (base peak) 433.23 (M+1)$^{+}$.

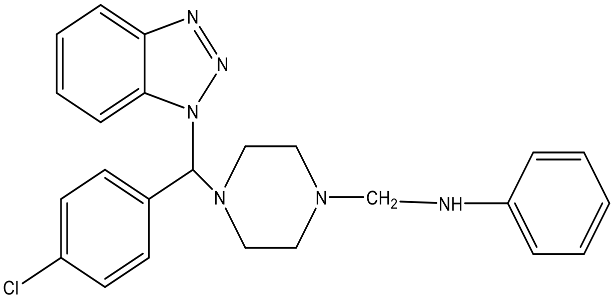
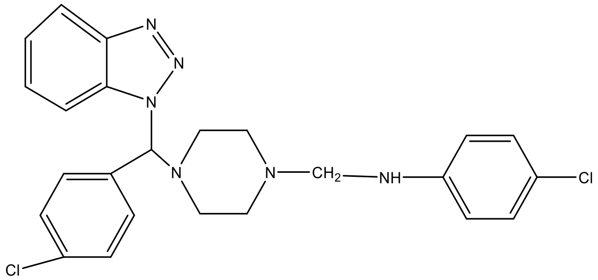
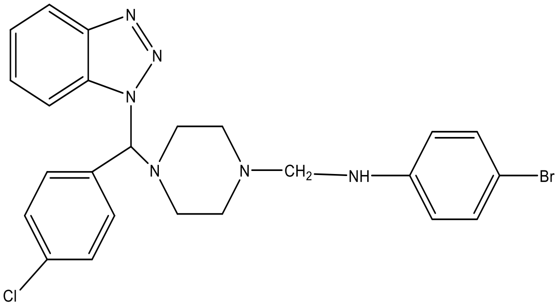
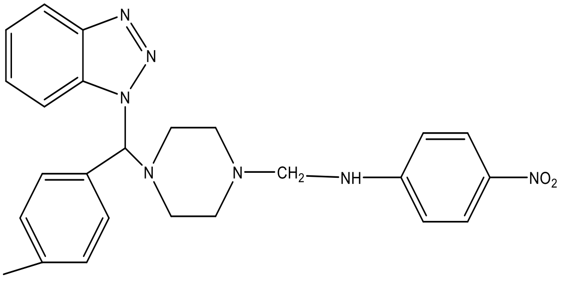
Synthesis of *N*-((4-((1*H*-Benzo[*d*][1,2,3]triazole-1-yl)(4-chlorophenyl)methyl)piperazine-1-yl)methyl)-4-chloroaniline (Compound B5): Light yellow solid, M.P 162-164^{o}C ,Yield 83%,Mol Formula: $C_{24}H_{24}Cl_2N_6$,Mol Wt: 466.14, Elemental Analysis C,61.67;H,5.18,Cl,15.17;N,17.98. IR cm^{-1} (KBr): 560,3320 and 3200 cm-1. ^{1}HNMR (500 MHz, DMSO - d_6): δ ppm (NH) 6.34 (CH2) 4.13,(CH)6.11 ppm, ^{13}CNMR (125 MHz, DMSO - d_6) *δ* ppm: (CH2)74.6,(CH)126.2(C)130.4 ppm, *m/z*%: 466.14 (base peak) 467.23 (M+1)$^{+}$.

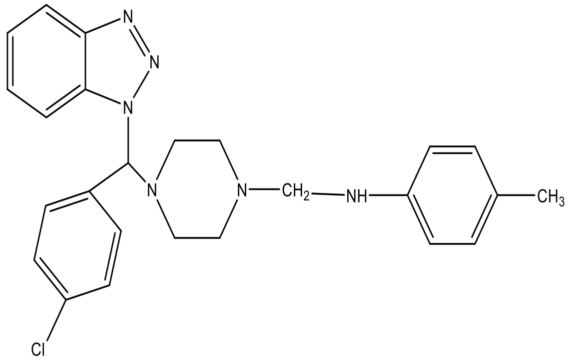
Synthesis of *N*-((4-((1*H*-Benzo[*d*][1,2,3]triazole-1-yl)(4-chlorophenyl)methyl)piperazine-1-yl)methyl)-4-bromoaniline (Compound B7): Yellow solid, M.P 168-170^{o}C ,Yield 83%,Mol Formula:$C_{24}H_{24}BrClN_6$,MolWt:510.09,ElementalAnalysisC,56.32;H,4.73,Br,15.61,Cl,6.93;N,16.42. IR cm^{-1} (KBr): 530,3340 and 3250 cm-1. ^{1}HNMR (500 MHz, DMSO - d_6): δ ppm (NH) 6.34 (CH2) 4.13,(CH)6.11 ppm, ^{13}CNMR (125 MHz, DMSO - d_6) *δ* ppm: (CH2)74.6,(CH)126.2(C)130.4 ppm, *m/z*%: 510.09 (base peak) 511.12 (M+1)$^{+}$.

Synthesis of *N*-((4-((1*H*-Benzo[*d*][1,2,3]triazole-1-yl)(4-chlorophenyl)methyl)piperazine-1-yl)methyl)-4-nitroaniline (Compound B11): Yellowish orange solid, M.P 172-174^{o}C ,Yield 83%,Mol,Formula:$C_{24}H_{24}ClN_7O_2$,MolWt:477.95,ElementalAnalysisC,60.31;H,5.06,Cl,7.42;N,20.51,O,6.69. IR cm^{-1} (KBr): 540, 1550,3200 and 1700 cm-1. ^{1}HNMR (500 MHz, DMSO - d_6): δ ppm (NH) 6.94 (CH2) 4.13,(CH)6.11 ppm, ^{13}CNMR (125 MHz, DMSO-d_6): *δ* ppm (CH2)74.6,(CH)126.2(C)130.4 ppm, *m/z*%: 477.95 (base peak) 478.17 (M+1)$^{+}$.

Synthesis of *N*-((4-((1*H*-Benzo[*d*][1,2,3]triazole-1-yl)(4-chlorophenyl)methyl)piperazine-1-yl)methyl)-4-methylaniline (Compound B15): Pale Yellow solid, M.P 154-156^{o}C ,Yield 83%,Mol Formula: $C_{25}H_{27}ClN_6$, Mol Wt:446.20, Elemental Analysis C,67.18;H,6.09,Cl,7.93;N,18.80. IR cm^{-1} (KBr): 520, 820, and 2830 cm-1. ^{1}HNMR (500 MHz, DMSO - d_6): δ ppm (NH) 6.94 (CH2) 4.13,(CH)6.11 ppm, ^{13}CNMR (125 MHz, DMSO - d_6) *δ* ppm: (CH2)74.6,(CH)126.2(C)130.4 ppm, *m/z*%: 446.20 (base peak) 447.20 (M+1)$^{+}$.

Table-5: Synthesized compounds

Com	**Structures**	**Yield(%)**
B 1	 *N*-((4-((1*H*-benzo[*d*][1,2,3]triazol-1-yl)(4-chlorophenyl)methyl)piperazin-1-yl)methyl)aniline	83
B5	 *N*-((4-((1*H*-benzo[*d*][1,2,3]triazol-1-yl)(4-chlorophenyl)methyl)piperazin-1-yl)methyl)-4-chloroaniline	81
B7	 *N*-((4-((1*H*-benzo[*d*][1,2,3]triazol-1-yl)(4-chlorophenyl)methyl)piperazin-1-yl)methyl)-4-bromoaniline	88
B11	 *N*-((4-((1*H*-benzo[*d*][1,2,3]triazol-1-yl)(4-chlorophenyl)methyl)piperazin-1-yl)methyl)-4-nitroaniline	84

B15	 *N*-((4-((1*H*-benzo[*d*][1,2,3]triazol-1-yl)(4-chlorophenyl)methyl)piperazin-1-yl)methyl)-4-methylaniline	85

7.ANTI-OXIDANT ACTIVITY

The DPPH technique has been used to study the antioxidant activity of compounds B1,B5,B7,B11,B15. When compared to ascorbic acid (IC 50 = 6.1 μg/ml), B15 (IC $_{50}$ = 25.94 μg/ml) among the 10 compounds in the anti-oxidant activity showed superior antioxidant capabilities.

Table-6: DPPH Radical Scavenging Activity and IC$_{50}$ Values of Selected Compounds Compared to Ascorbic Acid:

Sl.No	Compound	% Inhibition	IC$_{50}$ μg/mL
1	B1	64.19%	46.51
2	B5	60.81%	47.75
3	B7	80.44%	45.25
4	B11	55.44%	49.9
5	B15	83.63%	25.94
6	Ascorbic acid	55.12%	6.1

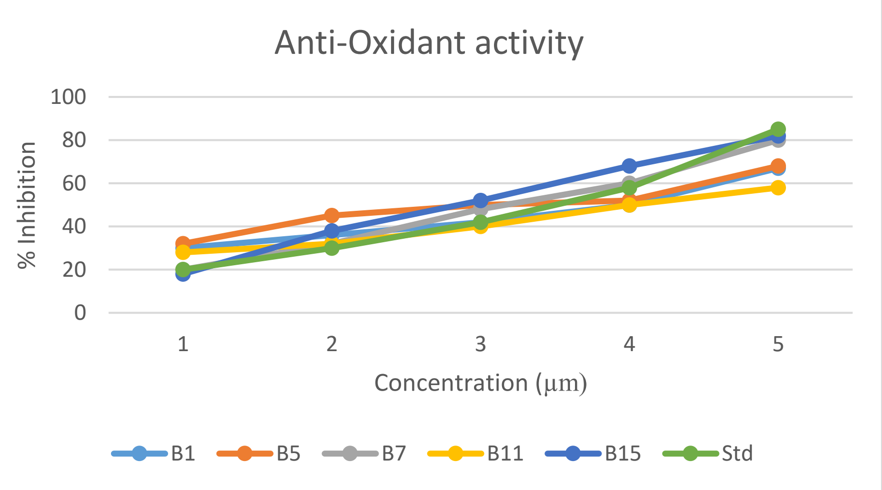


Fig 5: Plot Showing Antioxidant Activity of Synthesized Compounds

8.CONCLUSION:

In the present study, a novel series of 1,2,3-triazole-appended piperazine derivatives (B1–B15) was successfully synthesized and structurally confirmed by ^{1}H NMR, ^{13}C NMR, and mass spectrometry**.** The antioxidant potential of the synthesized compounds was evaluated using the DPPH radical scavenging assay. Among them, compounds B1, B5, and B11 exhibited notable activity, while B7 and B15 demonstrated enhanced antioxidant potential. As a result of current study the invitro anti-oxidant activity shows that the compound containing methyl group in the para position shows good activity, and the compounds containing chloro, bromo and nitro group in the para position shows better activity. The conclusion revealed that the methyl aniline imparted more on anti-oxidant activity. Thus the further substitutions with need to be studied potentially valuable new anti-cancer leads in future.

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Conflicts Of Interest:

The authors declare no conflict of interest.

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