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Research Article

IN SILICO DOCKING STUDY OF -LAGERSTROEMIA SPECIOSA PLANT DERIVATIVES FOR ANTIDIABETIC ACTIVITY TARGETING ALPHA AMYLASE AND ALPHA GALACOSIDASE ENZYMES

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ABSTRACT

Diabetes mellitus is a chronic metabolic disorder characterized by persistent hyperglycemia, affecting millions worldwide and rapidly increasing in prevalence, particularly in developing countries. The inhibition of carbohydrate-hydrolyzing enzymes such as alpha-amylase and alpha-galactosidase is a key strategy in controlling postprandial hyperglycemia. Lagerstroemia speciosa (Jarul), a traditional medicinal plant, is well known for its antidiabetic properties due to the presence of bioactive phytochemicals including ellagic acid derivatives, gallic acid, corosolic acid, and other polyphenols. In the present study, an in silico molecular docking approach was employed to evaluate the interaction of selected phytochemicals from Lagerstroemia speciosa against alpha-amylase (PDB IDs: 7QQH, 3BAY, 1KGU) and alpha-galactosidase (PDB ID: 3HG5). ADME and toxicity analyses were performed to assess drug-likeness, pharmacokinetic behavior, and safety profiles. Docking results revealed that several phytochemicals exhibited strong binding affinities through multiple hydrogen bonds and favorable steric interactions, demonstrating significant inhibitory potential compared to standard ligands. Compounds A11–A14 were identified as the most promising, showing favorable docking scores, positive enzyme inhibition activity, and acceptable ADMET properties with non-mutagenic behavior. The findings suggest that phytochemicals from Lagerstroemia speciosa may serve as potential lead molecules for the development of novel antidiabetic drugs.

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INTRODUCTION

Diabetes is a metabolic disease that is rapidly increasing, and this problem is being seen in both urban and rural areas. Foot ulcers continue to be a growing challenge for healthcare as well as for vascular services. Diabetic neuropathy is a common complication of diabetes [2]. A neuroischaemic diabetic foot is far more common than is usually thought [1]. There is a need to prevent this disease and to develop effective medicines, especially for those who cannot afford expensive medications. The number of diabetes patients in India is increasing rapidly, and this problem is more pronounced in rural areas, where people have limited access to healthcare services. Therefore, it is essential to develop affordable and effective medicines [3]. The disease is becoming a significant health concern, and it is crucial to take steps to prevent and manage it. Research and development of new medicines, as well as awareness about the disease, are necessary to combat this growing health issue [3].

Plant profile-Lagerstroemia speciosa (L.) Pers., also known as Jarul or Queen's Crape Myrtle, is a medicinal plant belonging to the Lythraceae family Lagerstroemia speciosa (L.) Pers. (Family: Lythraceae) is used in traditional medicine in the treatment of diarrhea, diabetes[4] ,inflammation[5] hypertension,[6]antiviral[7] best cancer[8] urinary disorders, hyperlipidemia, diarrhea, and, decongestant, anti-diabetic , and anti-obesity properties[9]



Figure 1- ***Lagerstroemia speciosa plant***

Phytochemical Constituents — Lagerstroemia speciosa Leaves and Fruits

Lagerstroemia speciosa leaves and fruits contain various phytochemicals such as 4-O-methylgallic acid, 1-hydroxy-2-naphthoic acid, and ellagic acid derivatives:

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Ellagic acid derivatives:

- R1 = H, R2 = H, R3 = H (Ellagic acid)
- R1 = CH_3, R2 = H, R3 = H (3-O-methyl ellagic acid)
- R1 = CH_3, R2 = H, R3 = CH_3 (3,3′-di-O-methyl ellagic acid)
- R1 = CH_3, R2 = CH_3, R3 = CH_3 (3,3′,4-tri-O-methyl ellagic acid)

Other phytochemicals present include caffeic acid, protocatechuic acid, gallic acid, and triterpenes such as:

- R1 = H, R2 = H (Ursolic acid)
- R1 = OH, R2 = H (Corosolic acid)
- R1 = OH, R2 = OH (Asiatic acid)

Additional constituents include lagerstroemin, corosolic acid, and 4-O-methylgallic acid.

These phytochemical structures were drawn in 2D and 3D using ChemDraw and ChemSketch. The structures were cleaned, energy-minimized, and saved in. mol format. These structures are now ready for docking studies.

PROTEIN STRUCTURE FOR DOCKING

The 3D structures of alpha-amylase (PDB IDs: 7QQH, 3BAY, 1KGU) and alpha-galactosidase (PDB ID: 3HG5) were obtained from the Protein Data Bank (PDB).

PDB ID: 7QQH
This is the crystal structure of MYORG (D520N) in complex with Gal-α1,4-Glc.
Organism: Homo sapiens
Method: X-ray diffraction
Resolution: 2.25 Å
Selected ligand: NAG (2-acetamido-2-deoxy-β-D-glucopyranose) [11]

PDB ID: 3BAY
This structure represents the N298S variant of human pancreatic alpha-amylase in complex with nitrate and acarbose.
Organism: Homo sapiens
Method: X-ray diffraction
Resolution: 1.99 Å
Selected ligand: ARE (acarbose derivative pentasaccharide)[12]

PDB ID: 1KGU
This is the three-dimensional structure of the R337A variant of human pancreatic alpha-amylase [13].

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PDB ID: 3HG5
This structure represents the human alpha-galactosidase catalytic mechanism (product-bound form).
Method: X-ray diffraction
Resolution: 2.30 Å
Selected ligand: GAL (β-D-galactopyranose) [14]

ADME STUDIES-ADME STUDIES PHYTOCHEMICALSIN THE PRESENT OF JARUL PLANT BY USING ADMET TOOL

Table-1 Drug likeness

S.N.	Compound name	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
1	A1	-0.77	-0.26	-0.88	-0.52	-0.94	-0.17
2	A2	-0.77	-0.26	-0.88	-0.52	-0.94	-0.17
3	A3	-0.79	-0.45	-0.94	-0.43	-1.06	-0.38
4	A4	-0.00	-0.10	-0.09	0.24	-0.16	0.28
5	A5	-0.035	-0.16	-0.09	0.14	-0.20	0.22
6	A6	-0.01	-0.15	-0.10	0.16	-0.17	0.18
7	A7	-0.02	-0.16	-0.14	0.13	-0.18	0.15
8	A8	-0.48	-0.23	-0.81	-0.10	-0.79	-0.09
9	A9	-0.88	-0.35	-1.10	-0.58	-1.09	-0.34
10	A10						
11	A11	0.24	0.11	-0.40	0.74	0.21	0.55
12	A12	0.25	-0.01	-0.35	0.78	0.31	0.60
13	A13	0.23	0.12	-0.38	0.83	0.27	0.68
14	A14	0.20	-0.02	-0.41	0.76	0.22	0.52
15	A13	-0.77	-0.26	-0.88	-0.52	-0.94	-0.17

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Inactive / weak candidates:
A1–A3, A8–A9, A15 → Broad negative scores, unlikely to be useful leads.

Moderate candidates:
A4–A7 → Weak activity overall, but show **some nuclear receptor & enzyme inhibition potential**.

Promising candidates:
A11–A14 → Clear **positive signals** in nuclear receptor ligand activity (0.74–0.83) and enzyme inhibition (0.52–0.68). These stand out as the **most favorable compounds** for further exploration.

Table-2 Toxicity study (ADMET)

S.NO.	Compound	Ames test	Carcino_Mouse	Carcino_Rat	hERG_inhibition
1	A1	mutagen	negative	positive	low risk
2	A2	mutagen	negative	positive	low_risk
3	A3	mutagen	negative	positive	low_risk
4	A4	mutagen	negative	positive	low_risk
5	A5	mutagen	negative	positive	low_risk
6	A6	mutagen	negative	positive	low_risk
7	A7	mutagen	negative	positive	low_risk
8	A8	mutagen	negative	positive	medium risk
9	A9	mutagen	negative	positive	low_risk
11	A11	non-mutagen	negative	positive	low_risk
12	A12	non-mutagen	negative	positive	low_risk
13	A13	non-mutagen	negative	positive	low_risk
14	A14	non-mutagen	negative	positive	low_risk

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15	A15	Mutagen	negative	positive	low_risk

Compounds A6–A10:

- All are **mutagenic** (genotoxic risk).
- Show **rat carcinogenicity** but not mouse carcinogenicity.
- hERG inhibition is mostly **low risk**, except **A8** which is **medium risk** (potential cardiotoxicity).
- These are **less favorable candidates** due to mutagenicity concerns.

Compounds A13 & A14:

- Both are non-mutagenic (no genotoxicity).
- Still show rat carcinogenicity, but with low hERG risk.
- These are comparatively safer and more promising than A6–A10.

Table-3 Pharmacokinetic studies

Pharmacokinetic	Compound-1	Compound-2	Compound-3	Compound-4	Compound-5	Compound-6	Compound-7
BBB	0.348084	0.348084	0.789889	0.321229	0.53886	0.340365	0.386059
Buffer_solubility_mg_L	1.56E+06	1.56E+06	2250.32	1.07E+07	495169	22924.8	1059.46
Caco2	13.8492	13.8492	20.0168	0.211332	0.21929	0.250772	0.758577
CYP_2C19_inhibition	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor
CYP_2C9_inhibition	Non	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor
CYP_2D6_inhibition	Non	Non	NON	Non	Non	Non	Non
CYP_2D6_substrate	Inhibitor	Inhibitor	NON	Non	Inhibitor	Non	Non
CYP_3A4_inhibition	53.696852	Inhibitor	Substrate	Inhibitor	Inhibitor	Inhibitor	Non
CYP_3A4_substrate	9.53976	Non	Inhibitor	Substrate	Weakly	Weakly	Substrate
HIA	Non	53.696852	67.006709	68.130701	81.029	89.6021	94.873526
MDCK	65.384676	9.53976	107.848	10.7463	22.5135	43.5336	73.622

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Pgp_inhibition	72333.4	Non	Inhibitor	Non	Non	Non	Non
Plasma_Protein_Binding	-3.62686	65.384676	76.812634	57.630394	63.1131	66.60218	67.905421
Pure_water_solubility_mg_L	0.13248	72333.4	76.812634	22809.6	4945.65	1070.25	231.192
Skin_Permeability	1.38048	-3.62686	-1.79015	-4.91033	1.21892	-4.3035	-4.28685
SKlogD_value	0.96271	0.13248	-0.46157	1.2743	1.21892	1.16354	1.10816
SKlogS_buffer	-0.37142	0.96271	0.78643	1.2743	1.21892	1.16354	1.10816

Table 4

Pharmacokinetis	Compound-8	Compound-9	Compound-11	Compound-12	Compound-13	Compound-14	Compound-15
BBB	0.4976	0.44288	7.95347	2.2666	0.456711	3.1976	0.348084
Buffer_solubility_mg_L	200243	184512	1590.06	3086.7	3141.74	3033.47	1.56E+06
Caco2	21.1076*	18.3046	21.702	21.1512	20.7789	21.2749	13.8492
CYP_2C19_inhibition	Non	Inhibitor	Non	Non	Non	Non	Inhibitor
CYP_2C9_inhibition	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor
CYP_2D6_inhibition	Non	Non	Non	Non	Non	Non	Non
CYP_2D6_substrate	Non	Non	Non	Non	Non	Non	Non
CYP_3A4_inhibition	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Inhibitor
CYP_3A4_substrate	Non	Non	subtract	Substrate	Substrate	Substrate	Non
HIA	82.301311	74.7496	95.91928	94.03245	90.348961	94.142639	53.696852
MDCK	109.433	23.6995	0.19339*	0.04769	0.0435362	0.0435145	9.53976
Pgp_inhibition	Non	Non	Inhibitor	Inhibitor	Inhibitor	Inhibitor	Non
Plasma_Protein_Binding	40.290625	27.1155	100	100	98.92759	100	65.384676

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Pure_water_solubility_mg_L	4878.52	15597.1	0.014619	0.049974	0.240847	0.020987	72333.4
Skin_Permeability	-2.66994	-3.3143	-2.28946	-2.74583	-3.241	-2.96545	-3.62686
SKlogD_value	0.56971	0.12502	5.00275	4.05906	3.28558	4.49242	0.13248
SKlogS_buffer	1.81771	1.37302	6.25075	5.30706	4.53358	5.74042	1.38048

Blood–Brain Barrier (BBB): Most compounds show moderate BBB penetration (0.3–0.5 range), but **Compound-11 (7.95)** and **Compound-12 (2.26)** demonstrate very high penetration, suggesting potential CNS activity.

Solubility: Several compounds (e.g., **Compound-4, Compound-2, Compound-15**) exhibit extremely high buffer or water solubility, which may aid absorption. In contrast, **Compound-11 and Compound-12** show very poor solubility, which could limit bioavailability.

Caco-2 Permeability: Most compounds demonstrate good intestinal permeability (>13), with **Compound-11 and Compound-12** showing particularly high values (>21), indicating strong absorption potential.

Cytochrome P450 (CYP) Interactions:

- CYP2C19: Majority act as inhibitors, which may cause drug–drug interactions.
- CYP2C9: Almost all compounds are inhibitors, suggesting metabolic interference risk.
- CYP2D6: Mostly non-inhibitors, reducing concerns for this pathway.
- CYP3A4: Many compounds act as inhibitors, with some substrates, indicating possible metabolism-related variability.

Human Intestinal Absorption (HIA): Most compounds show high absorption (>70%), with **Compound-11 (95.9%)** and **Compound-14 (94.1%)** being particularly strong candidates.

MDCK Permeability (Blood–Brain Barrier surrogate): Wide variation is observed. **Compound-11 and Compound-12** show extremely low values (<0.2), suggesting poor CNS penetration despite high BBB values, indicating possible efflux transporter involvement.

P-gp Inhibition: Some compounds (e.g., **Compound-3, Compound-11–14**) act as P-gp inhibitors, which may enhance CNS penetration but also risk transporter-related toxicity.

Plasma Protein Binding (PPB): Several compounds (e.g., **Compound-11, 12, 14**) show very high PPB (~100%), which may prolong half-life but reduce free drug concentration.

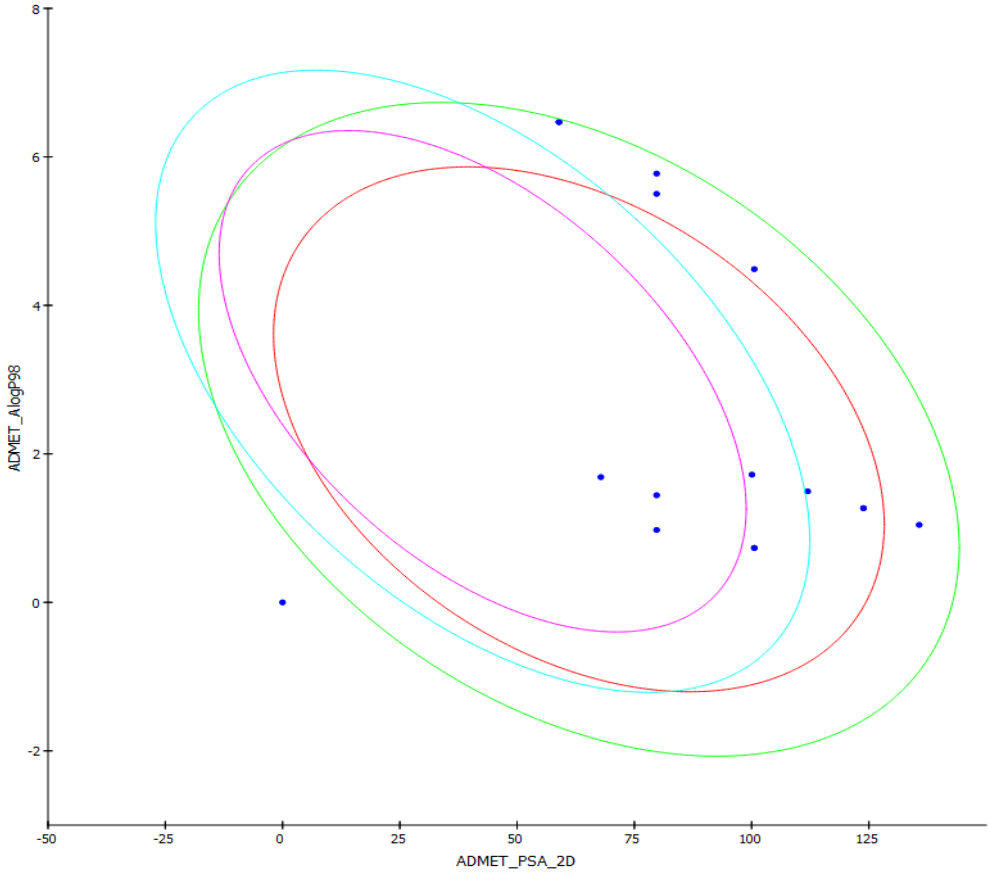
Skin Permeability & LogD/LogS: Most compounds show negative skin permeability values, indicating limited transdermal delivery. LogD values suggest moderate lipophilicity, while LogS values vary, reflecting solubility differences.

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Graph-1: ADME

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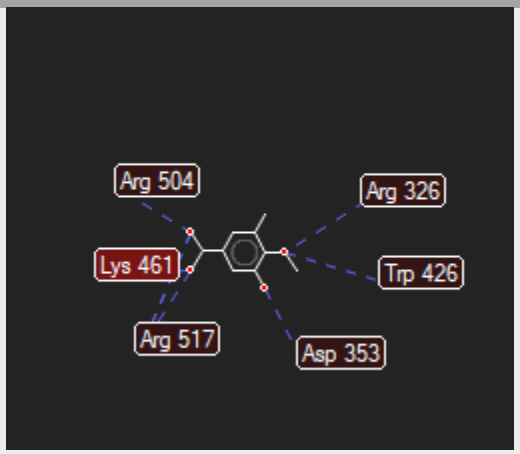
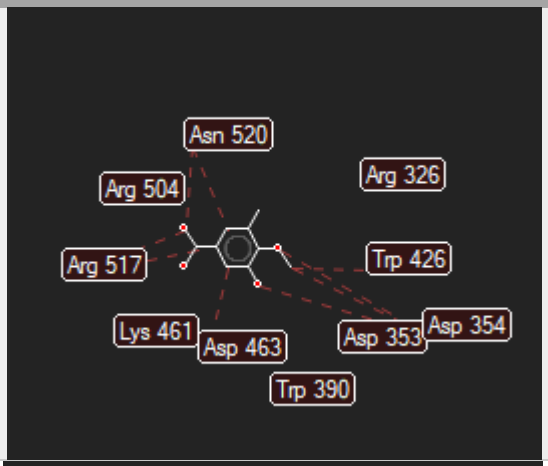
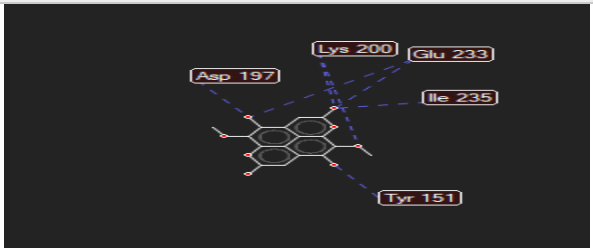
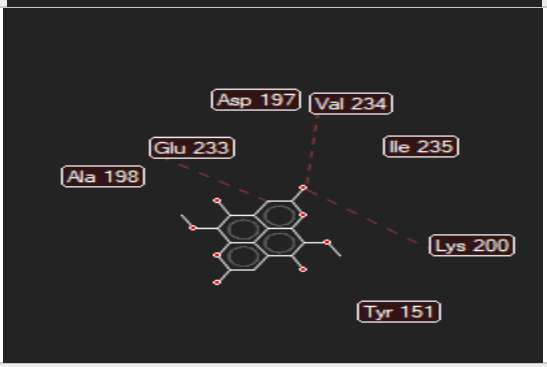
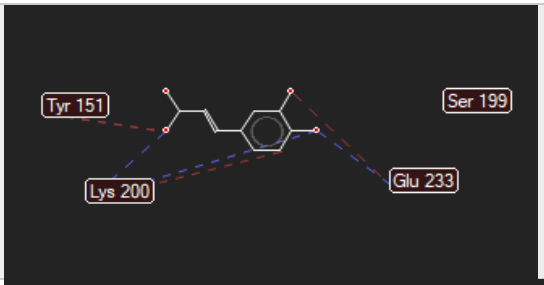
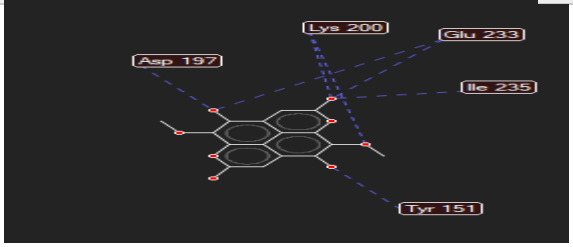
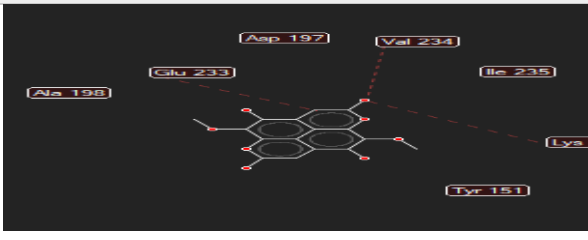
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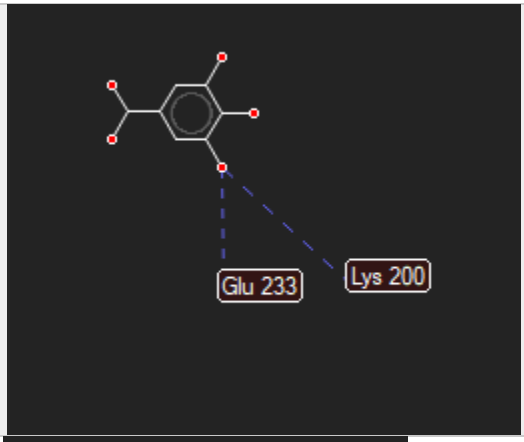
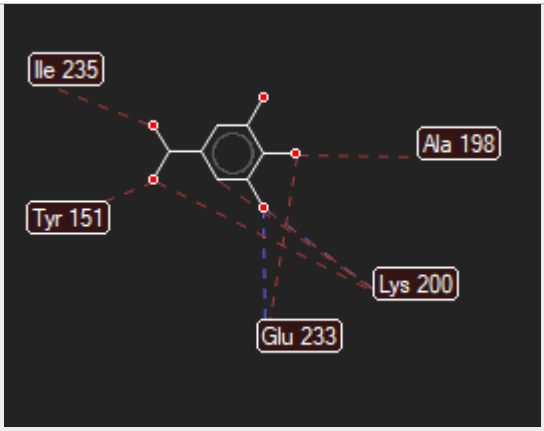
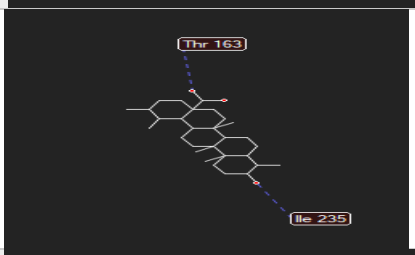
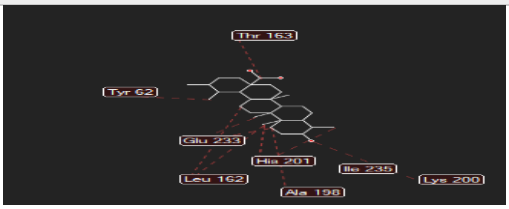
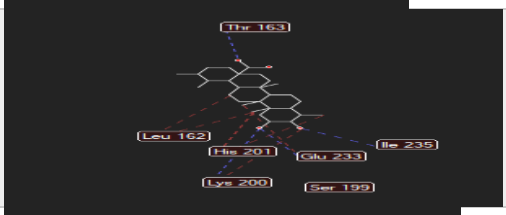
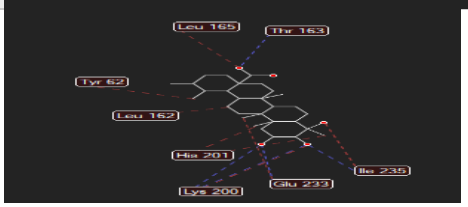
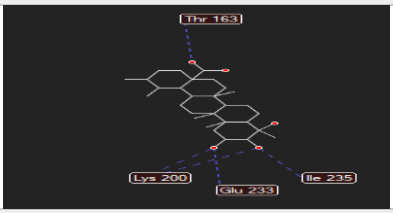
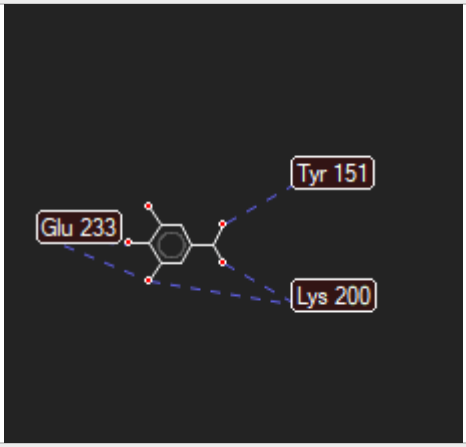
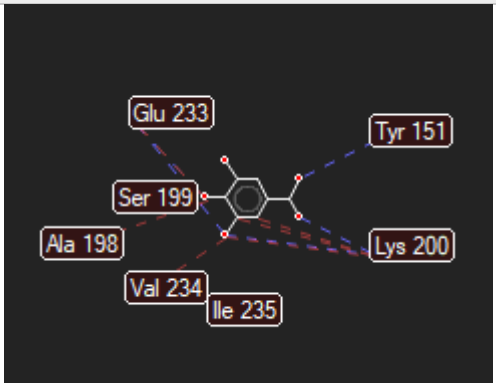
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RESULTS

Table-4 showing Hydrogen and Steric bonding

Compound name	Hydrogen Bonding	Steric bonding
1		
5		
7		
8		

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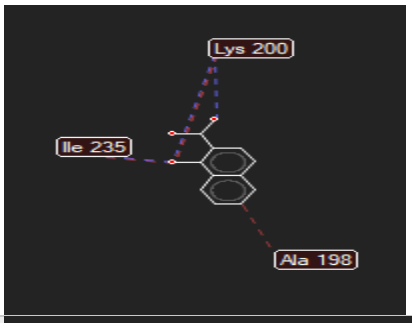
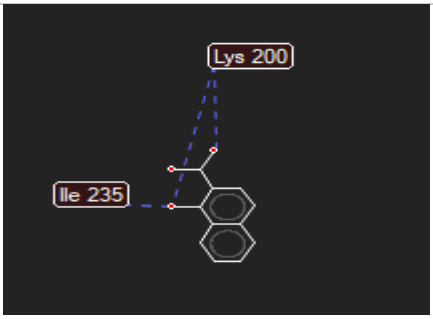
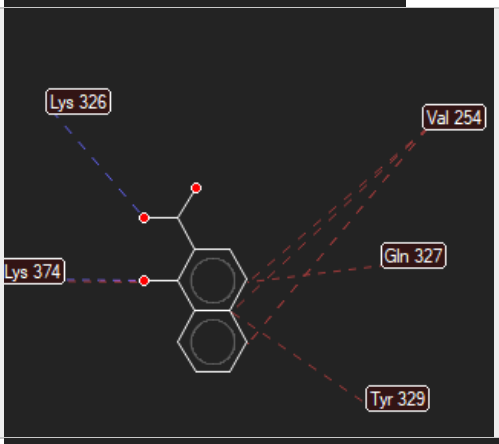
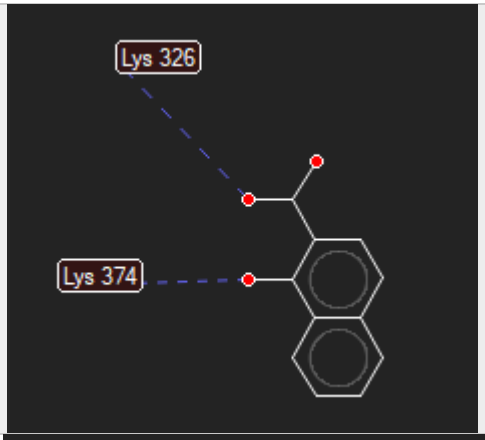
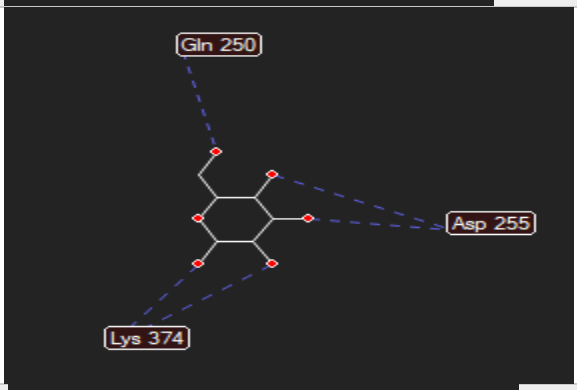
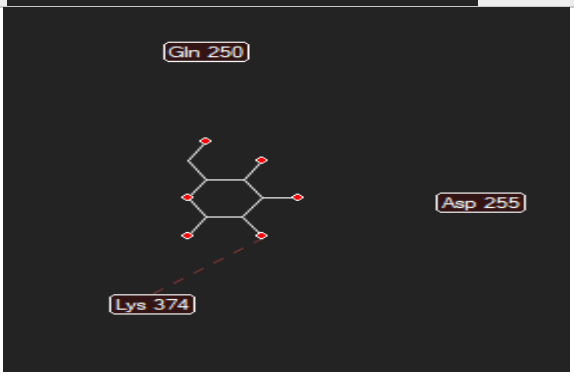
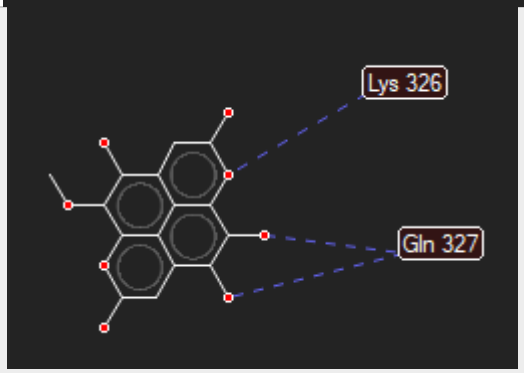
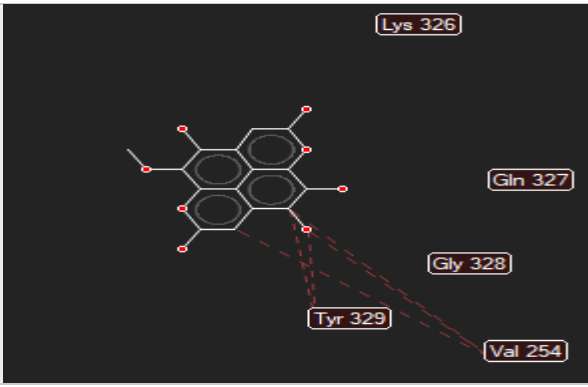
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Compound name	Hydrogen Bonding	Steric bonding

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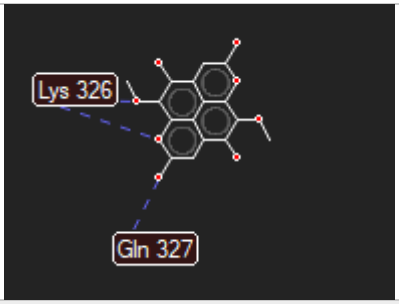
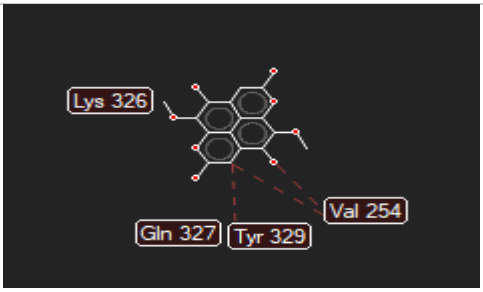
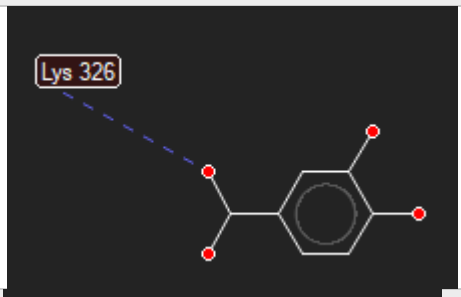
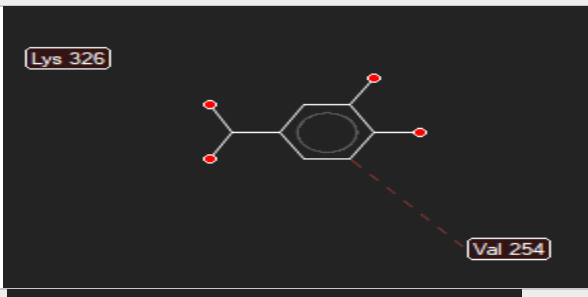
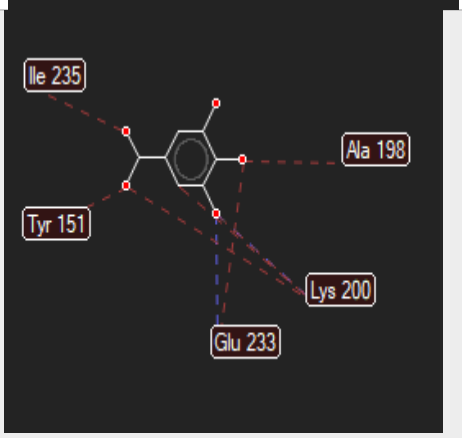
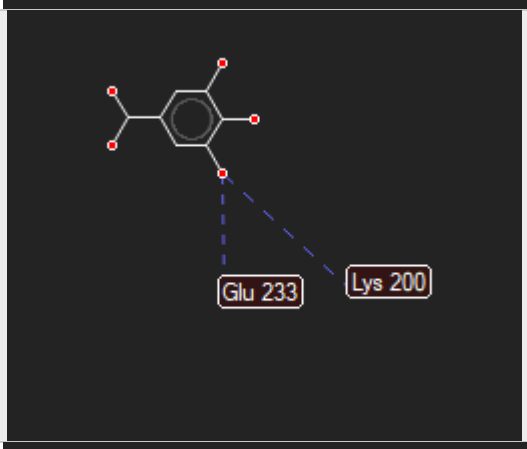
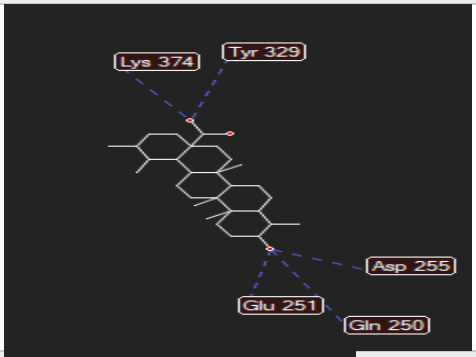
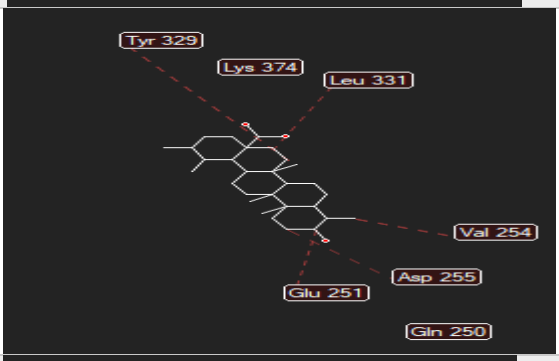
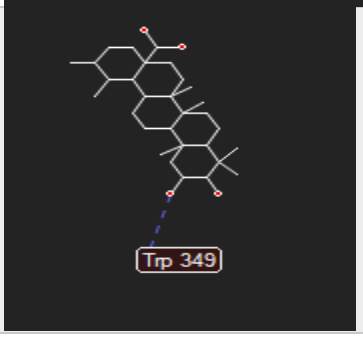
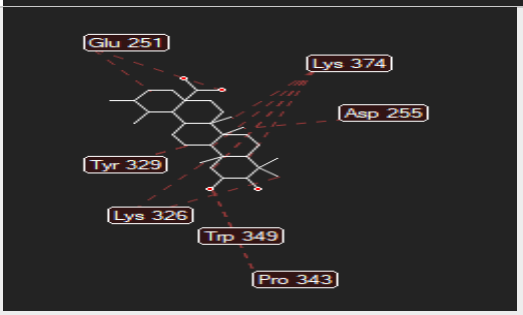
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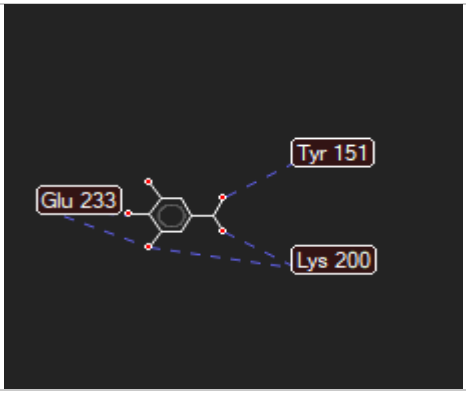
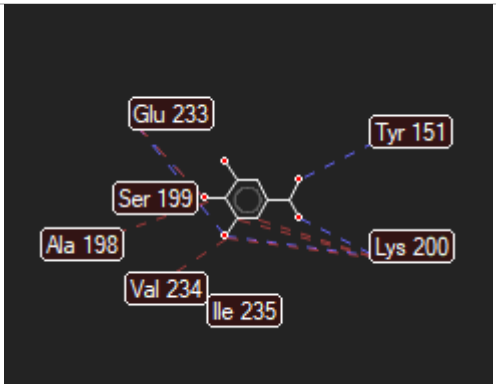
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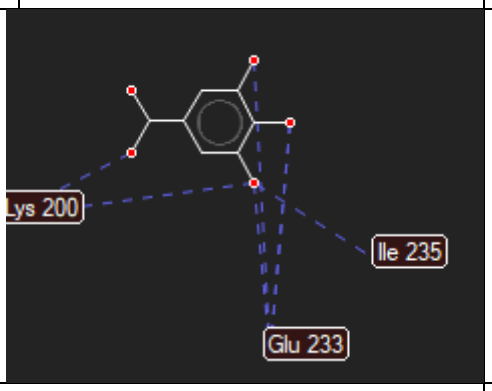
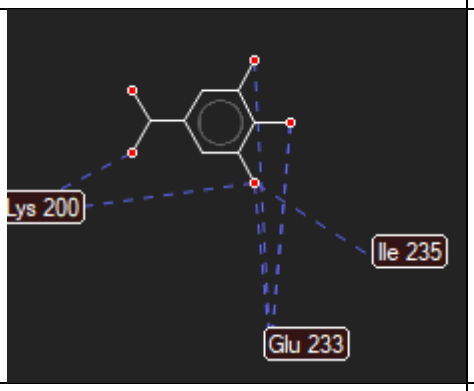
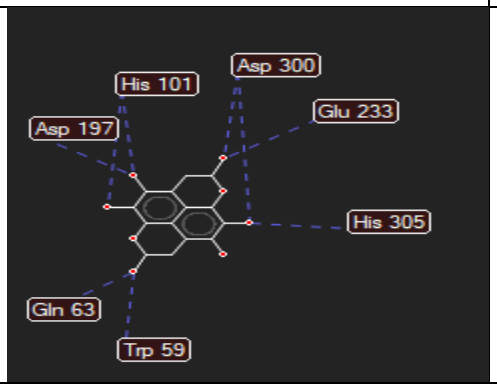
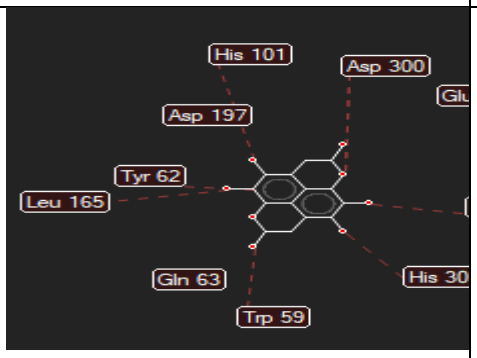
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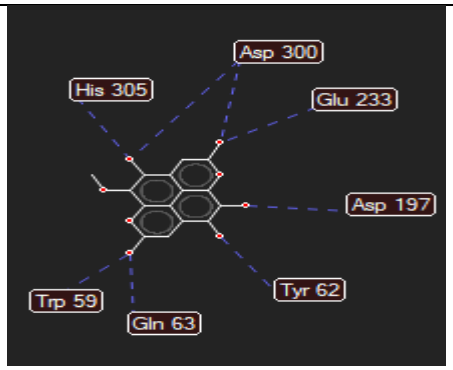
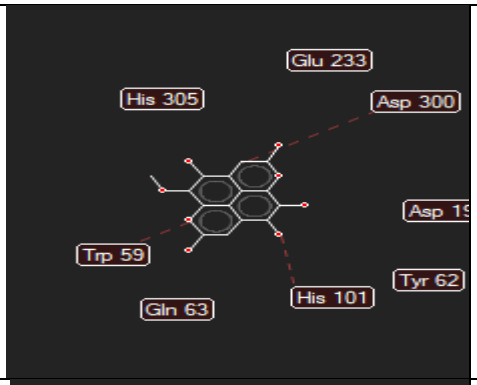
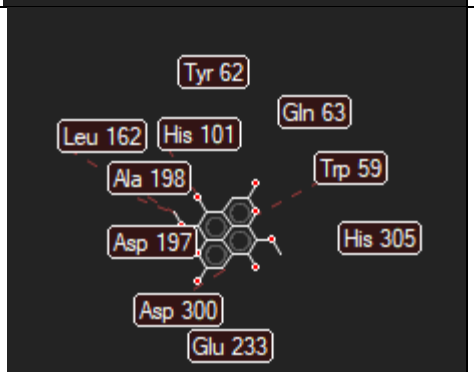
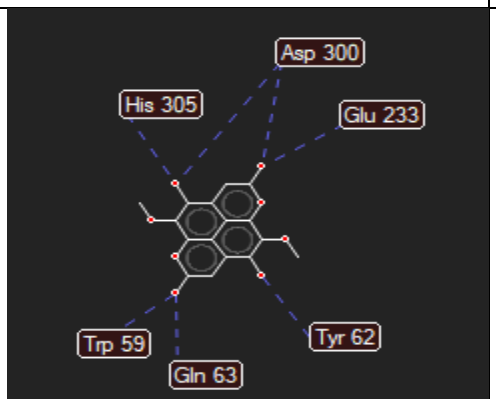
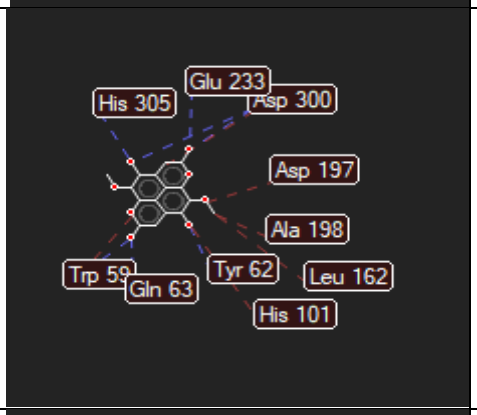
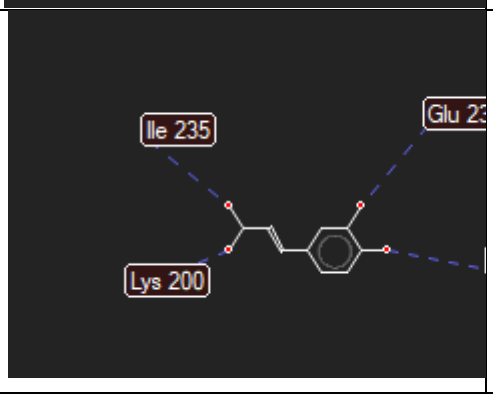
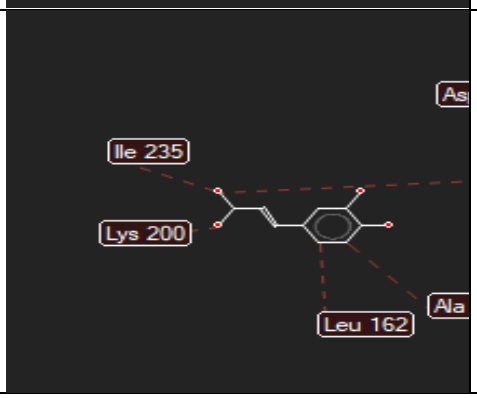
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Tablet-5

Compound name	Hydrogen Bonding	Steric bonding	Docking score
1			
2			
3			

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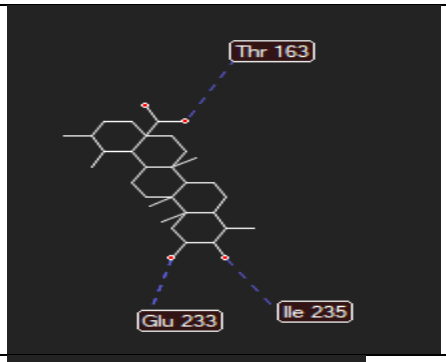
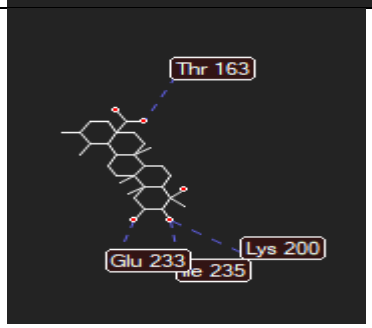
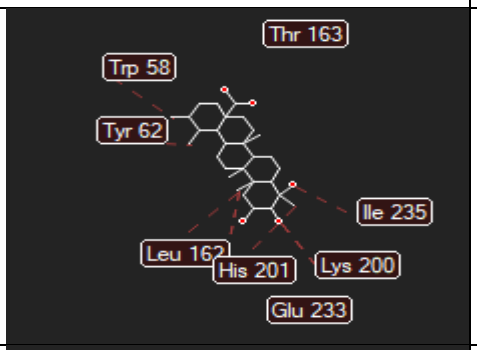
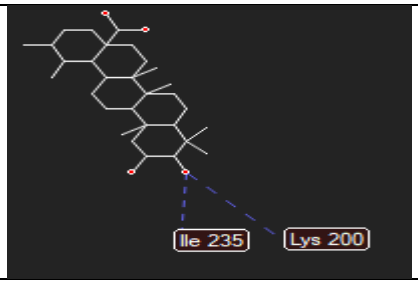
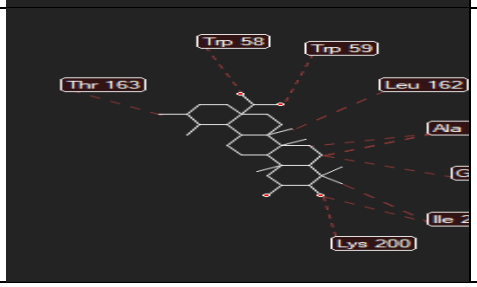
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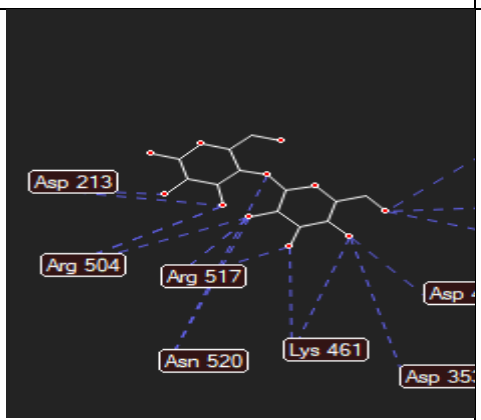
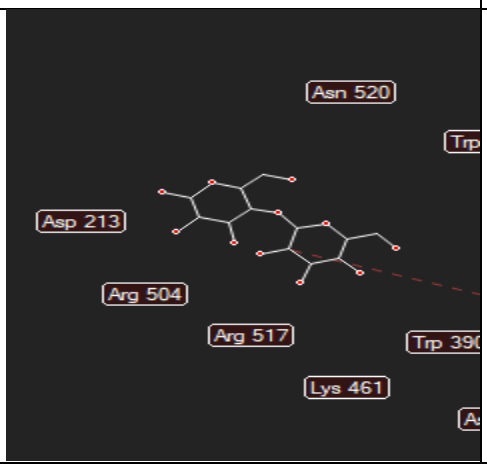
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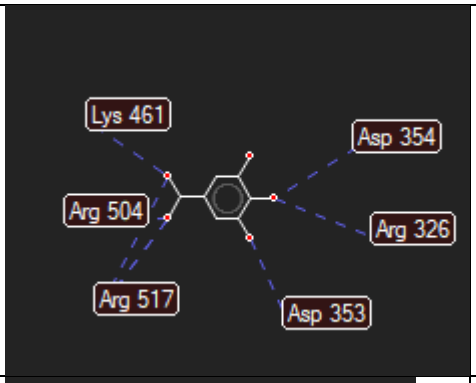
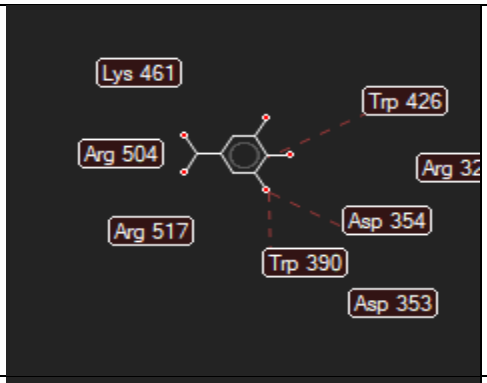
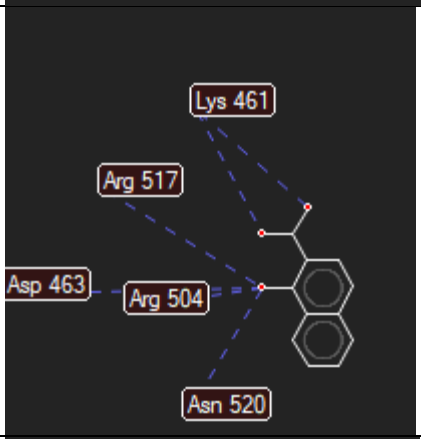
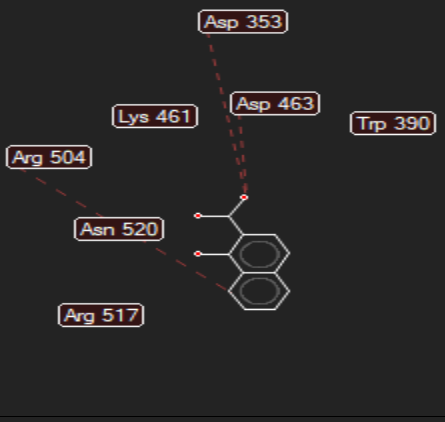
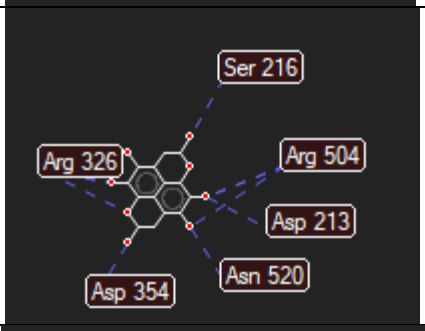
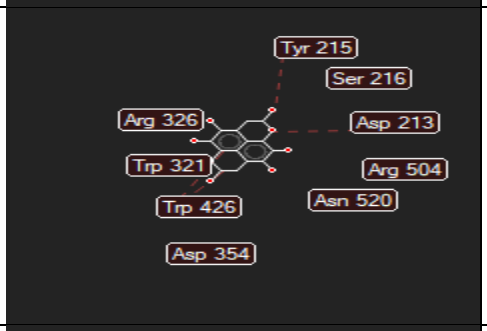
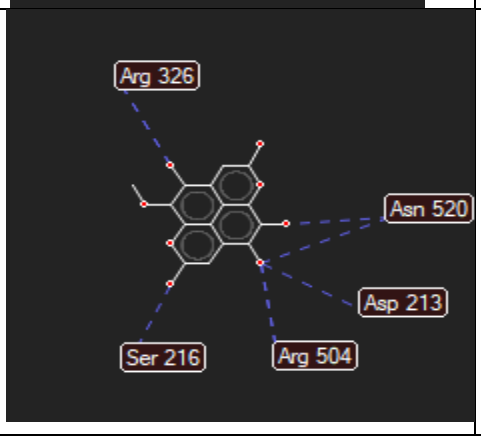
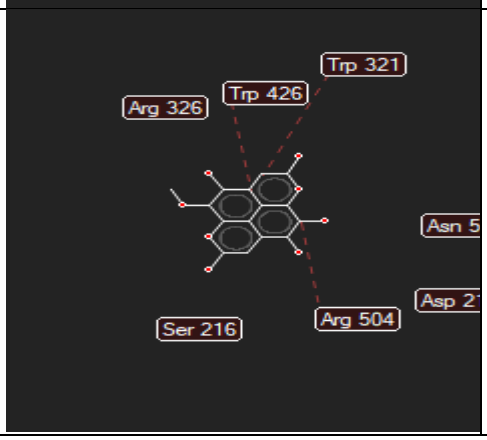
Compound name	Hydrogen Bonding	Steric bonding	Docking score
Bgc-qqa			

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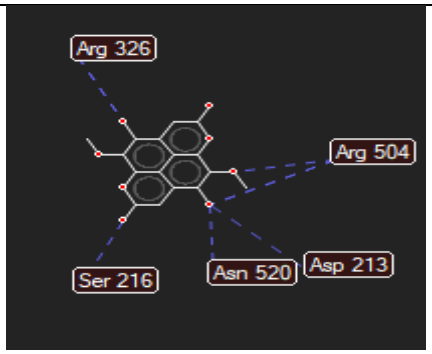
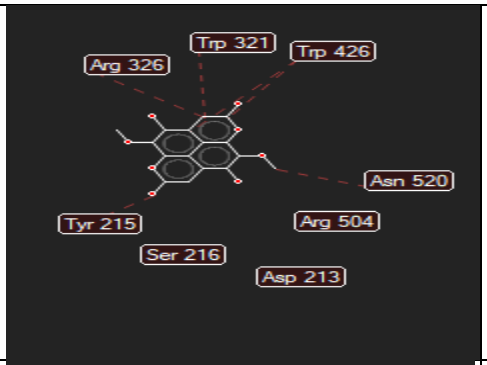
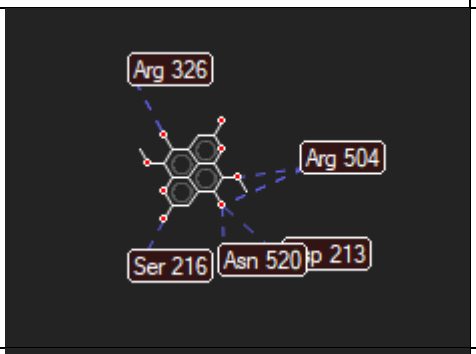
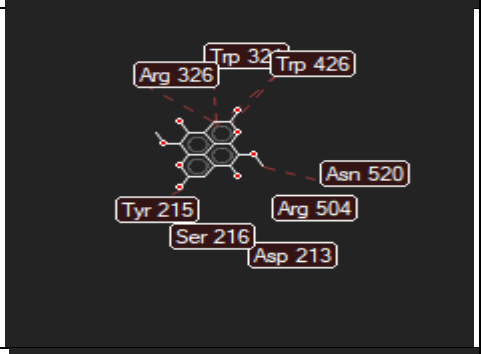
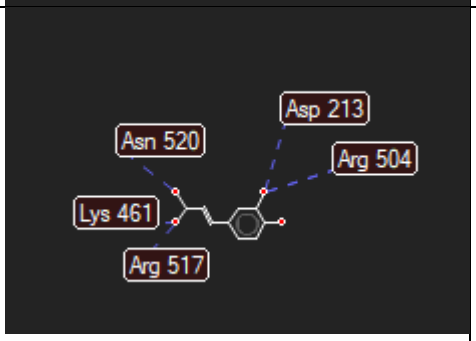
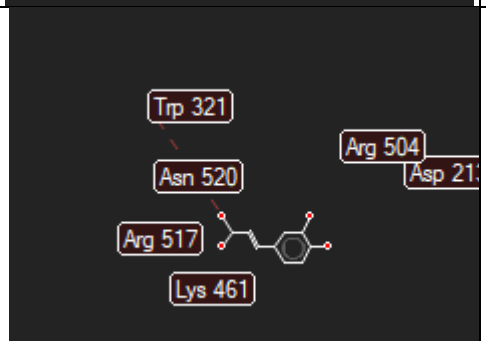
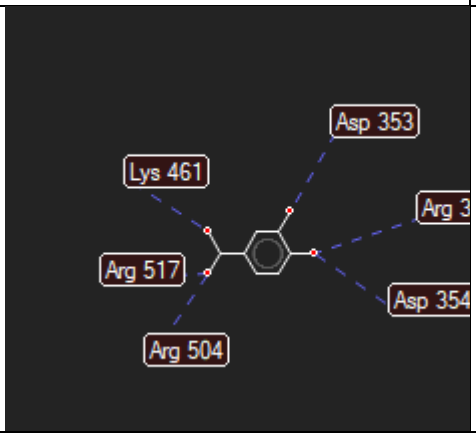
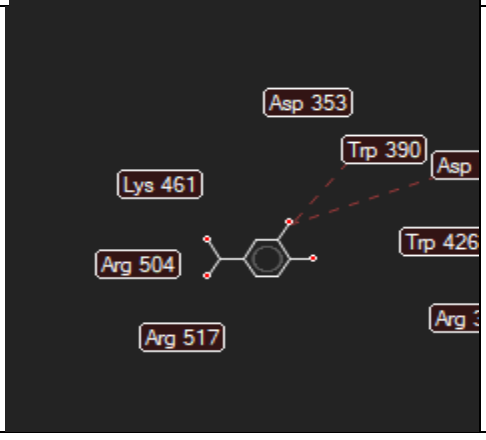
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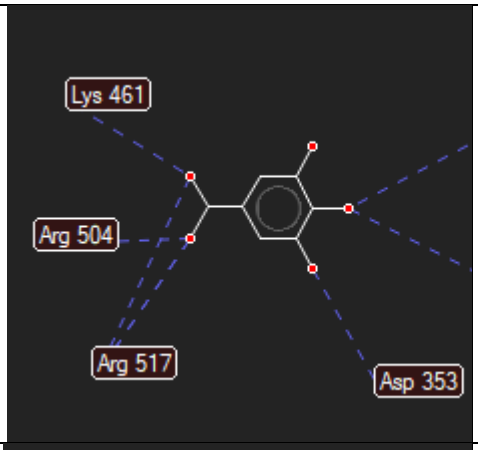
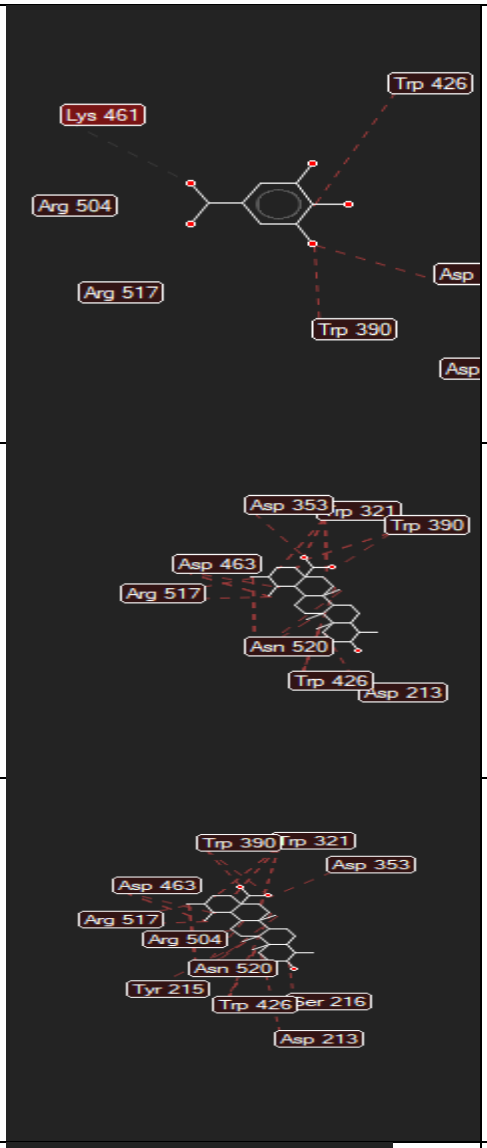
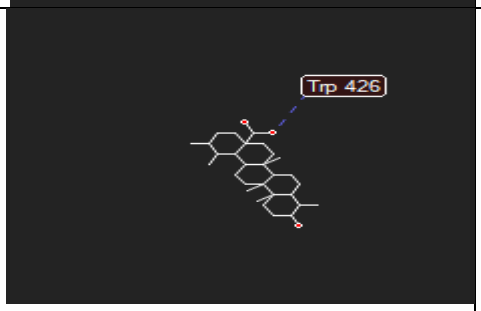
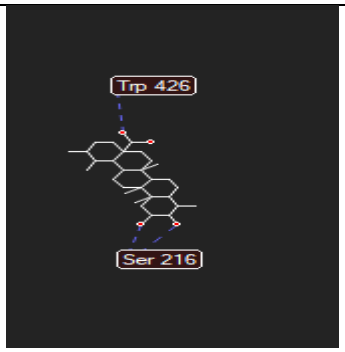
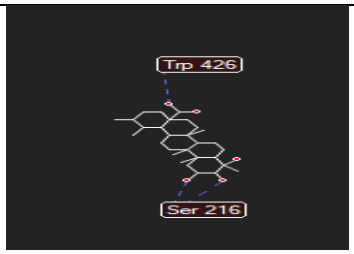
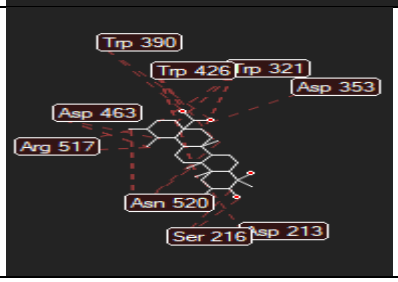
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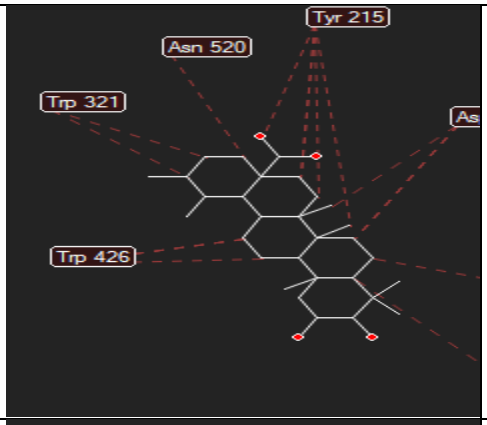
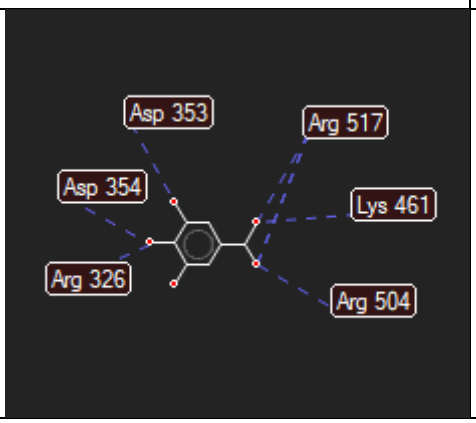
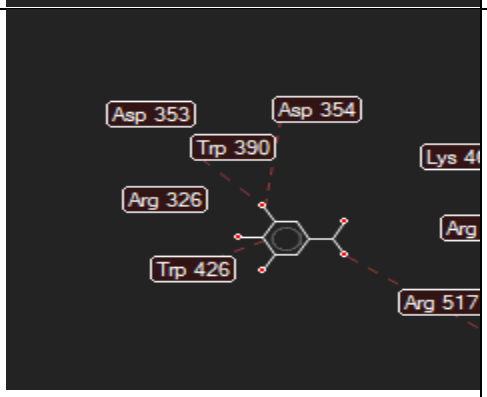
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Table-4 PDB 7QQH DOCKING SCORE

Ligand	MolDock Score	Rerank Score	HBond
Compound 11	-98.0319	-70.2838	-5.19077
Compound13	-96.4877	-15.9954	-2.52149
Compound12	-95.2953	-47.4038	-3.58015
Compound10	-93.5096	-62.6618	-2.5
Compound14	-92.3333	-81.952	-15.4323
Compound15	-89.7553	-73.3615	-13.9519
Compound16	-88.9457	-73.3723	-13.7541
Compound3	-82.8068	-73.6006	-15.4654
Compound1	-67.6851	-50.6595	-9.90115
Compound 9	-67.0181	-51.91	-8.33502
Compound7	-70.45	-57.829	-8.274
Compound14	-66.9726	-50.0822	-8.13438
Compound2	-64.3243	-54.4976	-1.34544
Compound8	-64.0133	-53.2638	-4.16991
Compound 1 [Region: 0]	-63.301	-60.1059	-2.5

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PCA_1 [A]	-60.5864	-50.0995	-7.37051

Table-5 PDB 3HG5

Ligand	MolDock Score	Rerank Score	HBond
Compound4	-92.3333	-81.952	-15.4323
Compound10	-93.5096	-62.6618	-2.5
Compound12	-95.2953	-47.4038	-3.58015
Compound13	-96.4877	-15.9954	-2.52149
Compound11	-98.0319	-70.2838	-5.19077
Compound5	-89.7553	-73.3615	-13.9519
Compound6	-88.9457	-73.3723	-13.7541
Compound3	-82.8068	-73.6006	-15.4654
Compound7	-70.45	-57.829	-8.274
Compound8	-64.0133	-53.2638	-4.16991
Compound9	-67.0181	-51.91	-8.33502
Compound14	-66.9726	-50.0822	-8.13438
Compound2	-64.3243	-54.4976	-1.34544
Compound 1 [Region: 0]	-63.301	-60.1059	-2.5
PCA_1 [A]	-60.5864	-50.0995	-7.37051

Table 6- 3BAY Docking score

Ligand	MolDock Score	Rerank Score	HBond
Compound11	-103.71		-55.2547
Compound12	-100.692	-3.56204	-4.30326
Compound6	-98.4224	-87.7563	-10.8108
Compound10	-98.4105	-25.3296	-1.02151
Compound5	-98.0736	-87.5232	-10.7105
Compound13	-97.941	-19.4269	-6.45296
Compound4	-94.9817	-80.227	-10.2097
Compound3	-90.1243	-72.1133	-12.37
Compound7	-78.1701	-66.289	-4.13156
NAG_497 [A]	-76.7917	-66.7492	-7.2206
Compound 1 [Region: 0]	-74.5064	-68.6099	-2.20593
Compound2	-73.759	-61.9499	-3.65578
Compound 1	-69.8228	-58.3275	-6.27818
Compound8	-67.7622	-61.8863	-3.79703
Compound8	-67.7051	-59.8777	-7.98669
Compound14	-66.926	-54.1752	-9.69202

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CONCLUSION

The molecular docking analysis revealed that the ligands showing a higher number of hydrogen bonds and stronger steric interactions demonstrated better binding affinity toward the target protein. Compounds with the lowest docking scores exhibited more stable complexes, indicating strong inhibitory potential. Overall, the docking results suggest that hydrogen bonding and steric complementarity play a significant role in ligand–receptor stability. Therefore, the ligands with optimal hydrogen bonding patterns, favorable steric fit, and the most negative docking scores can be considered promising candidates for further in-vitro and in-vivo validation.

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Conflict of Interest

The authors declare that there is no conflict of interest.

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