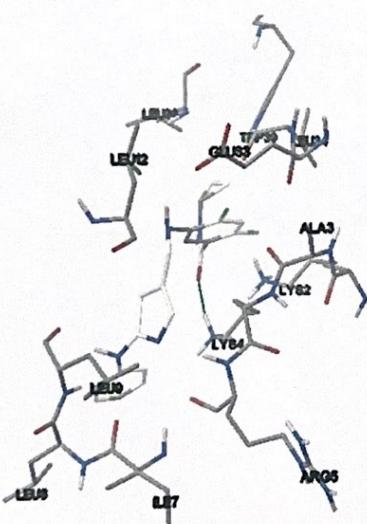
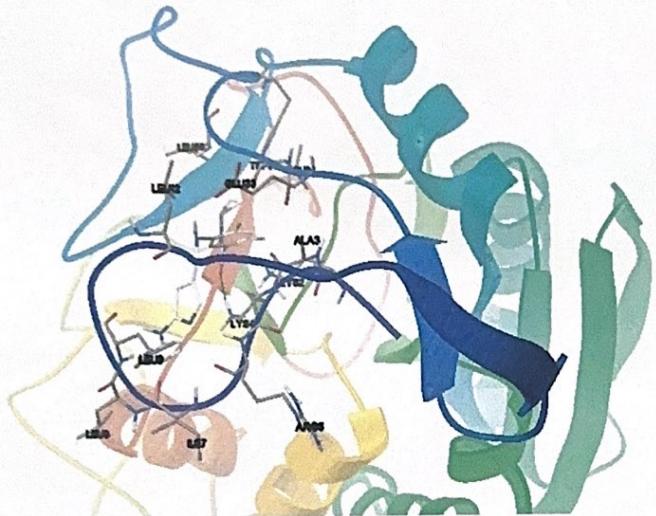
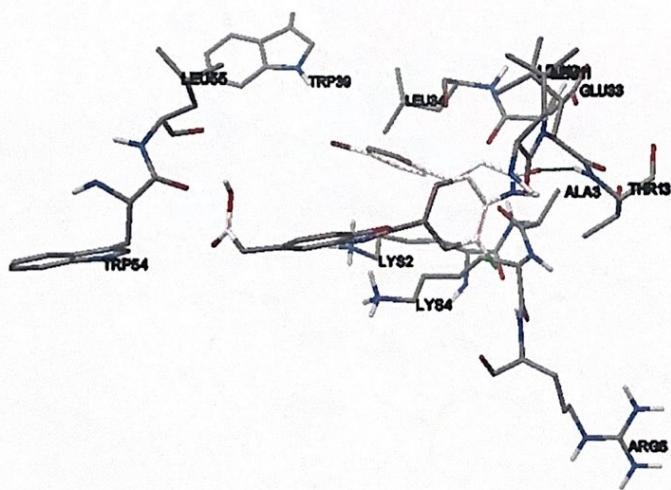
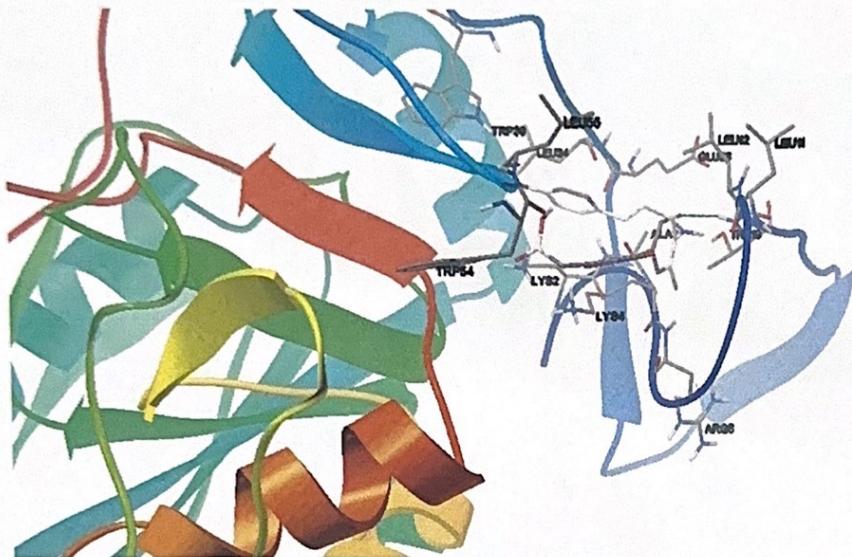


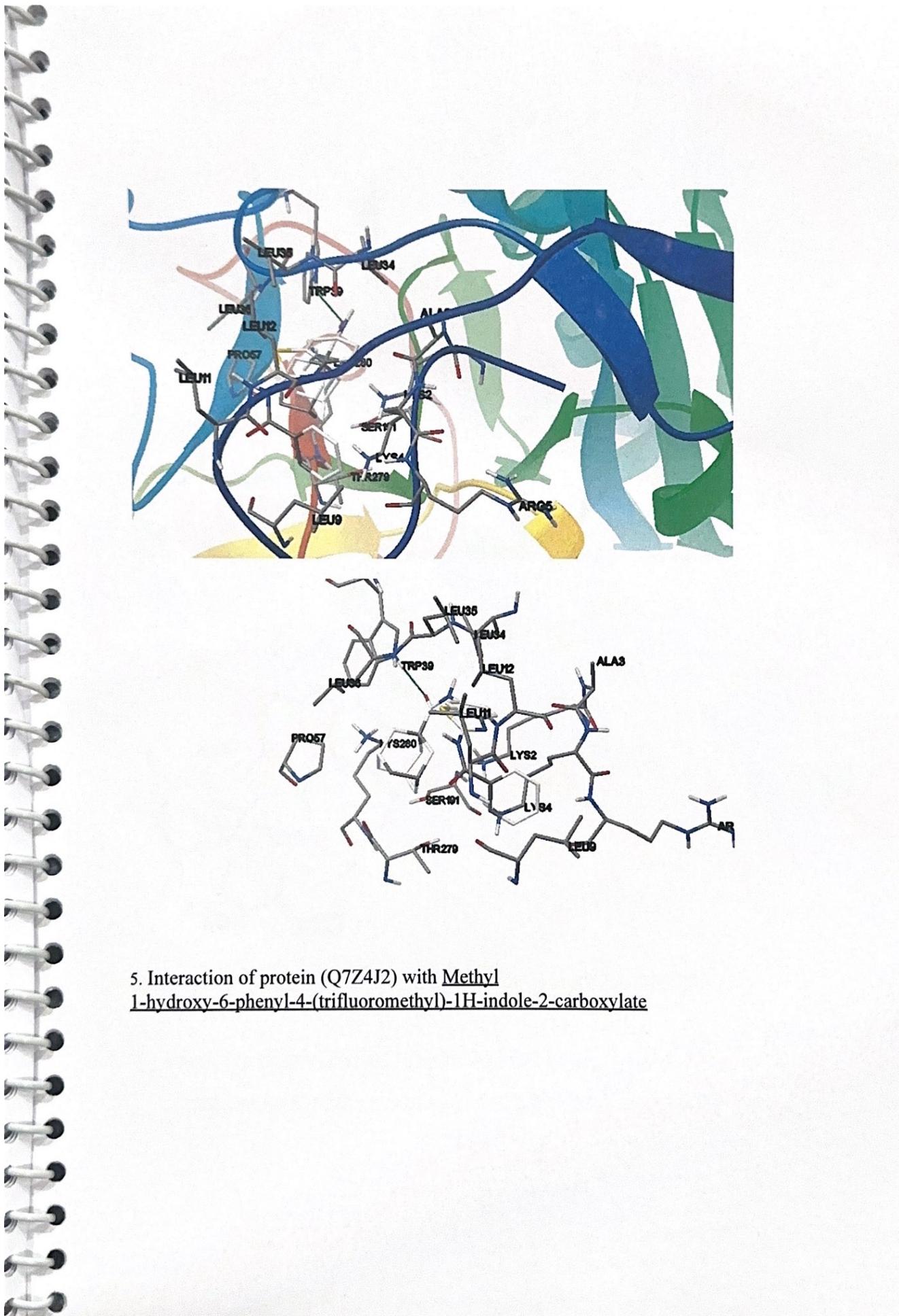
2. Interaction of protein (Q7Z4J2) with
N-cyclopropyl-2,4-difluoro-5-((2-(pyridin-2-ylamino)thiazol-5-yl)methylamino)benzamide (11632737)



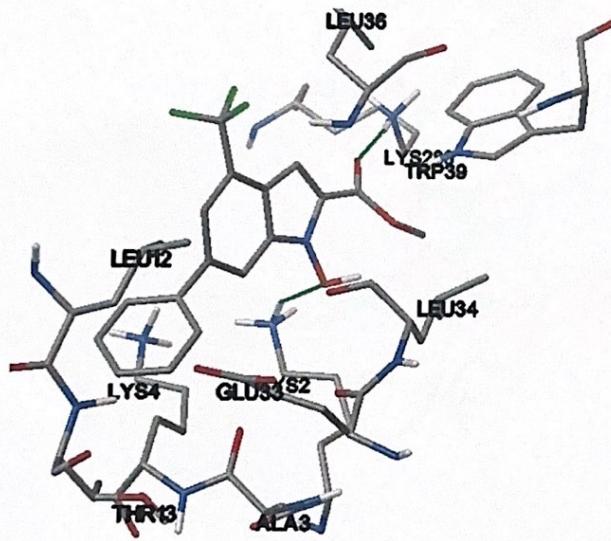
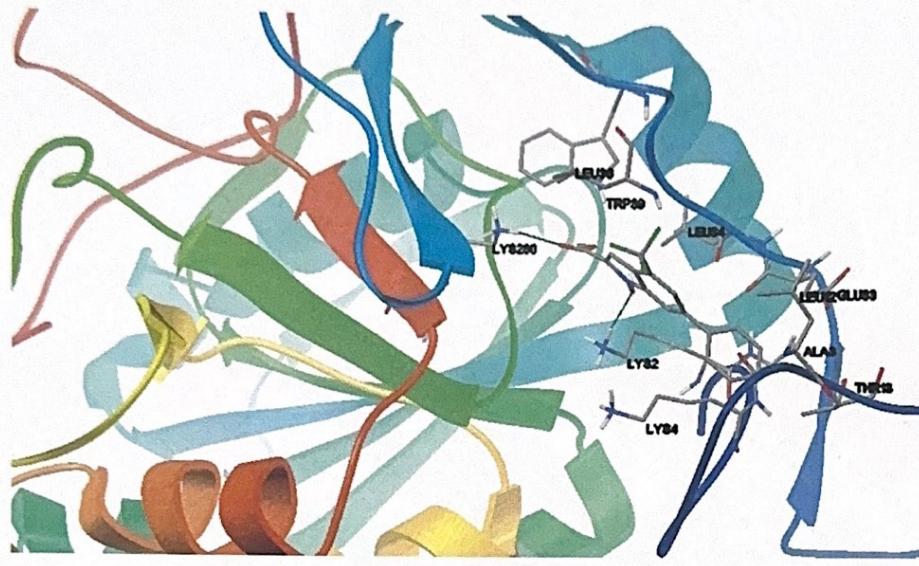
3. Interaction of protein (Q7Z4J2) with
(E)-2-(2-(4-(3-(4-bromophenyl)acrylamido)-3-fluorophenyl)benzo[d]oxazol-5-yl)acetic acid



4. Interaction of protein (Q7Z4J2) with
N-(2-benzamido-1,3-benzothiazol-6-yl)adamantane-1-carboxamide

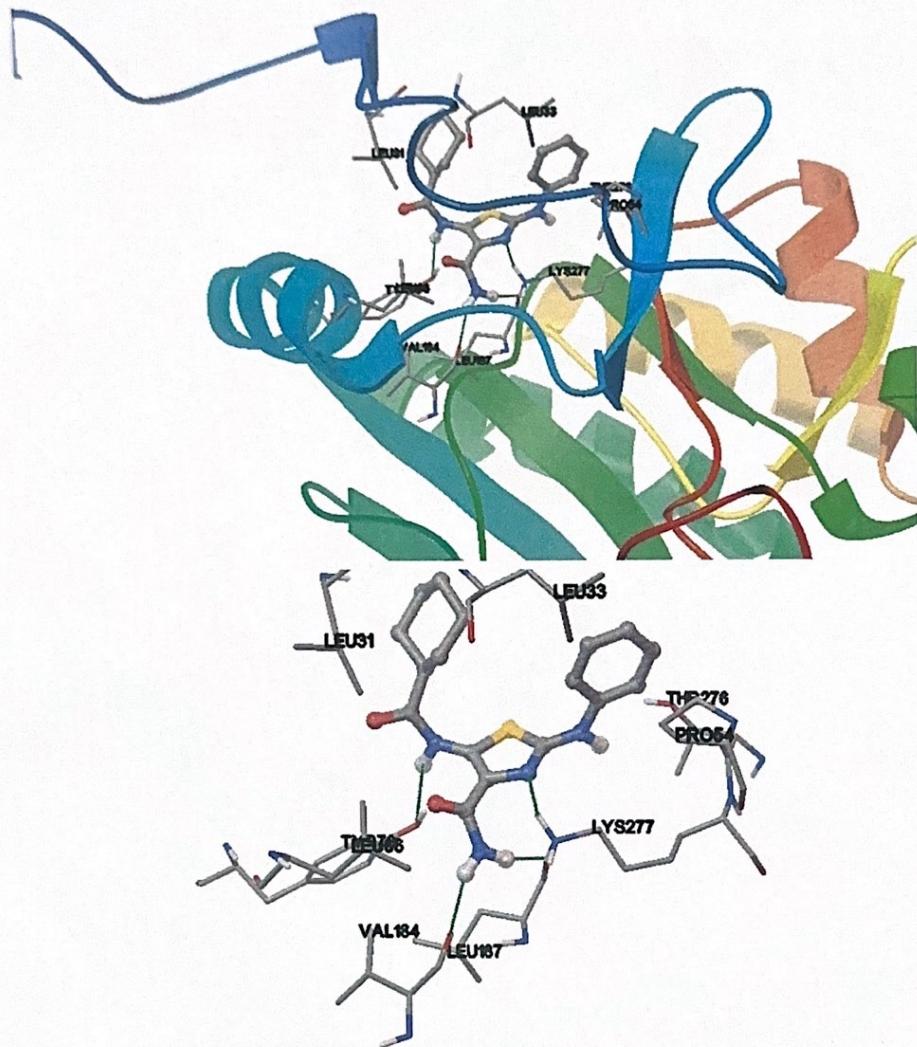


5. Interaction of protein (Q7Z4J2) with Methyl 1-hydroxy-6-phenyl-4-(trifluoromethyl)-1H-indole-2-carboxylate

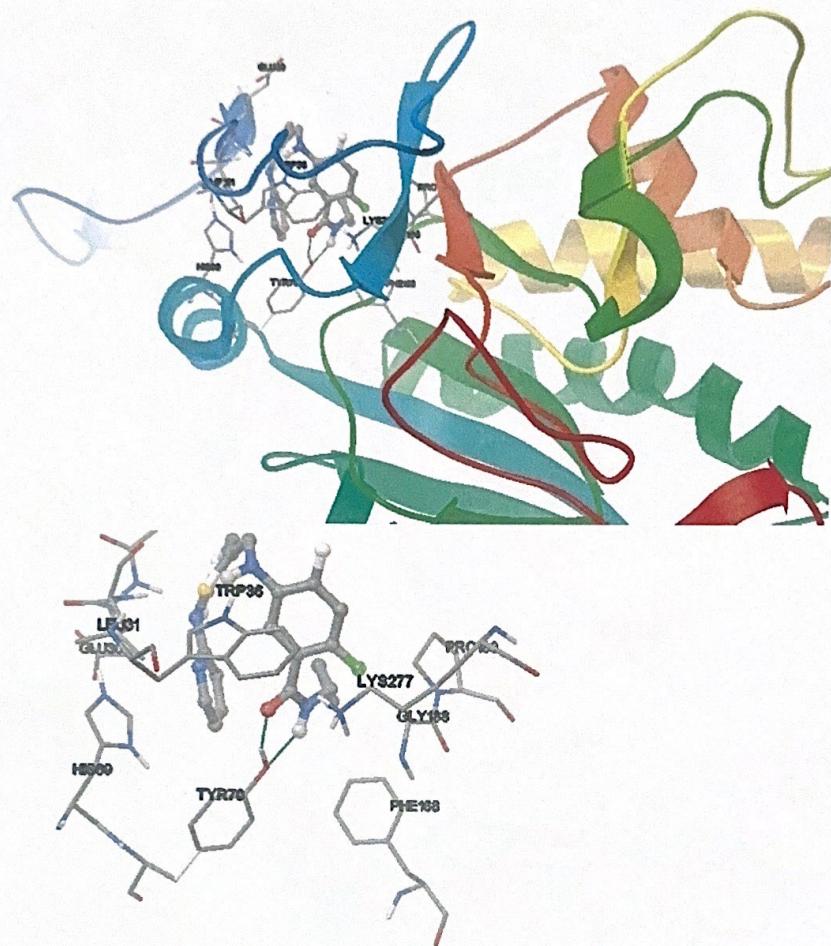


Interaction of glycotransferase(Q4R5T7) with LIGANDS

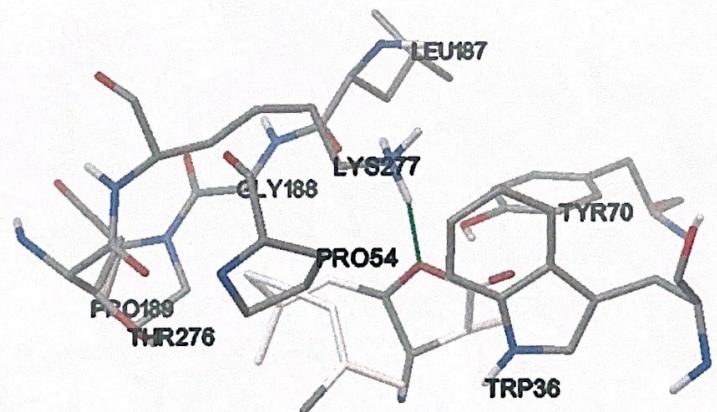
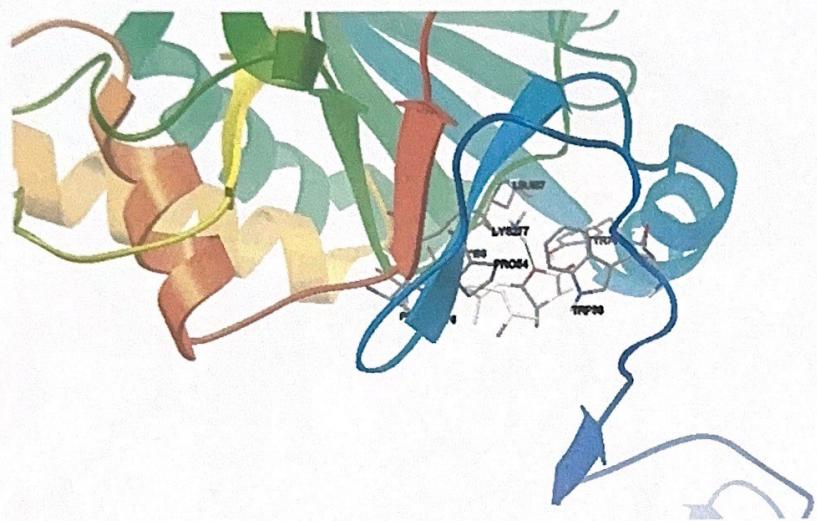
- 1) Interaction of protein (Q4R5T7) with 5-(Cyclohexanecarboxamido)-2-(phenylamino)thiazole-4-carboxamide (46355372)



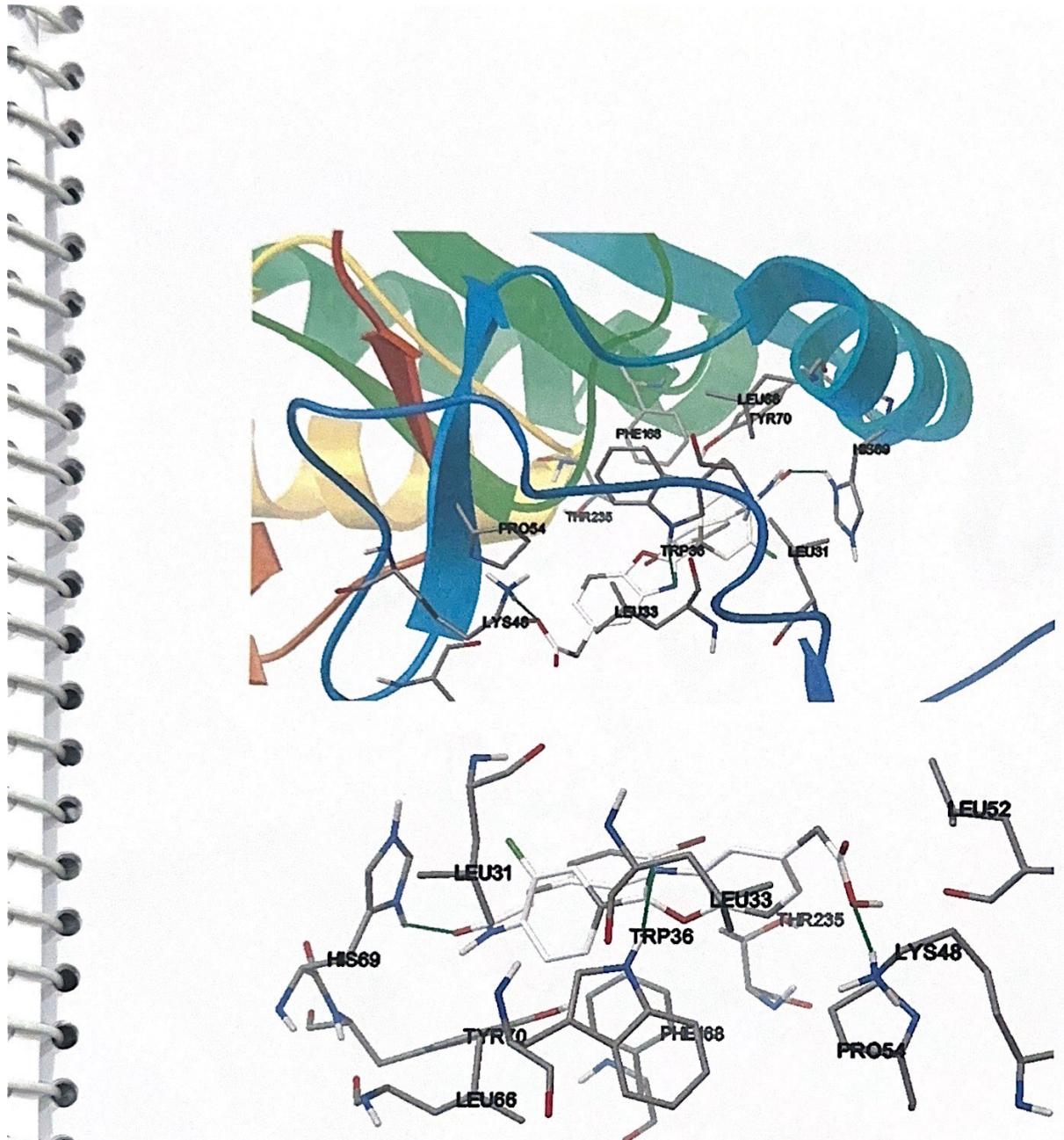
2)Interaction of protein (Q4R5T7) with
N-cyclopropyl-2,4-difluoro-5-((2-(pyridin-2-ylamino)thiazol-5-yl)methylamino)benza
mide (11632737)



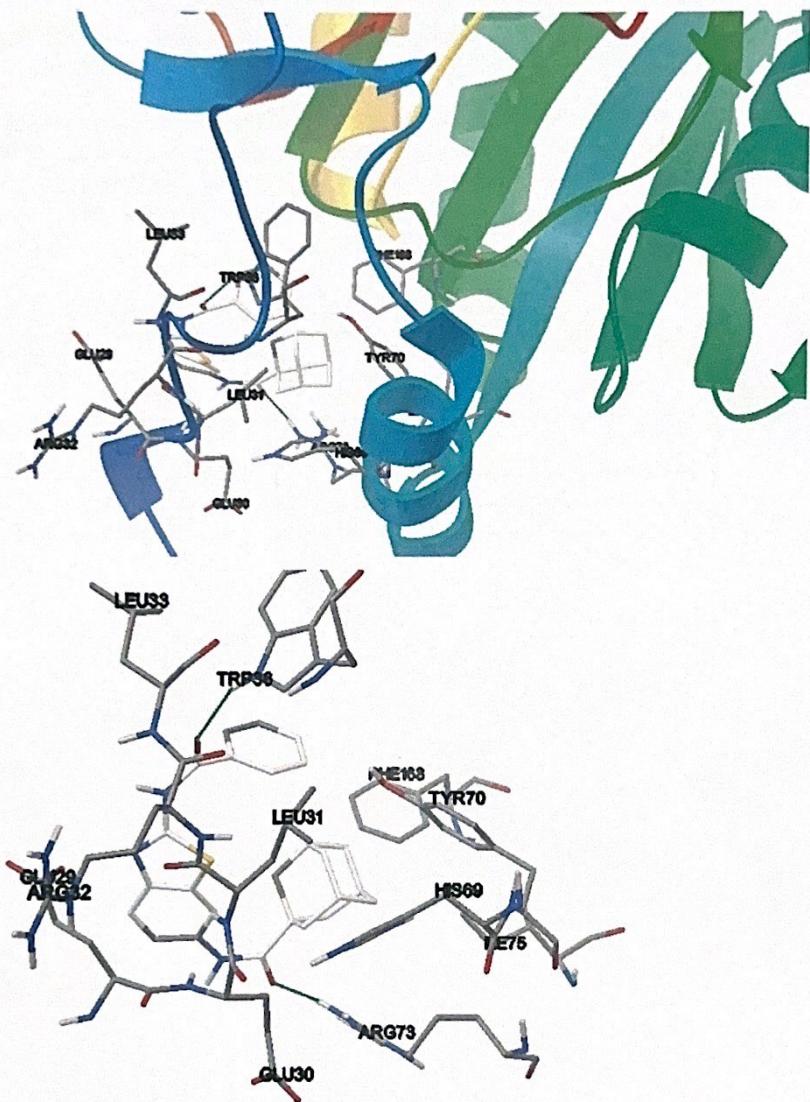
2. Interaction of protein (Q4R5T7) with Costunolide



3. Interaction of protein (Q4R5T7) with
(E)-2-(2-(4-(3-(4-bromophenyl)acrylamido)-3-fluorophenyl)benzo[d]oxazol-5-yl)acetic acid



4. 5)Interaction of protein (Q4R5T7) with
N-(2-benzamido-1,3-benzothiazol-6-yl)adamantane-1-carboxamide



RESULTS AND DISCUSSION:

Homology modelling with model evaluation:

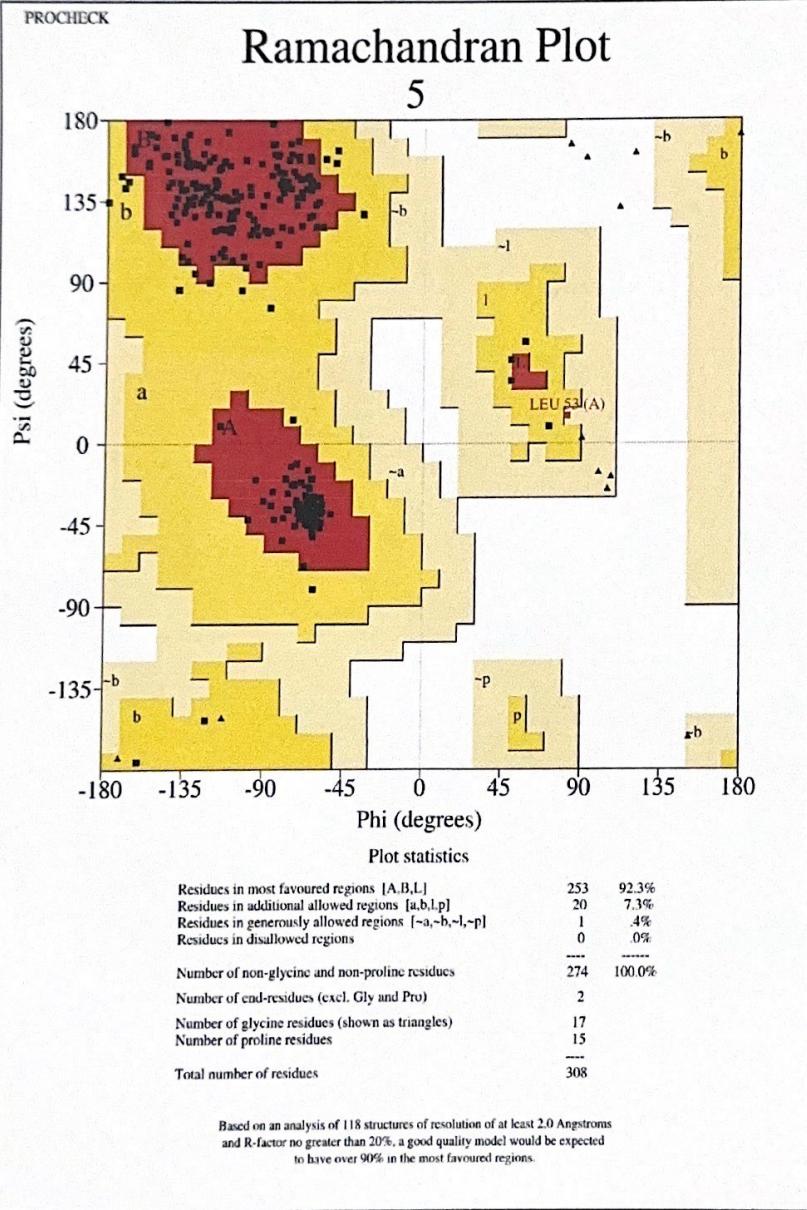
The current study reported the protein having high degree of homology with 1G8O which used as a template,with the excellent atomic resolution using BLAST, Upon using modeller 10.1 the structure was generated.It was validated with the help of its protein structure and PROCHECK where the generated model exhibited 92.3% of amino acid residues with .4% in the additionally

allowed region with 0.0% residues in disallowed region therefore,no amino acid in disallowed regions.

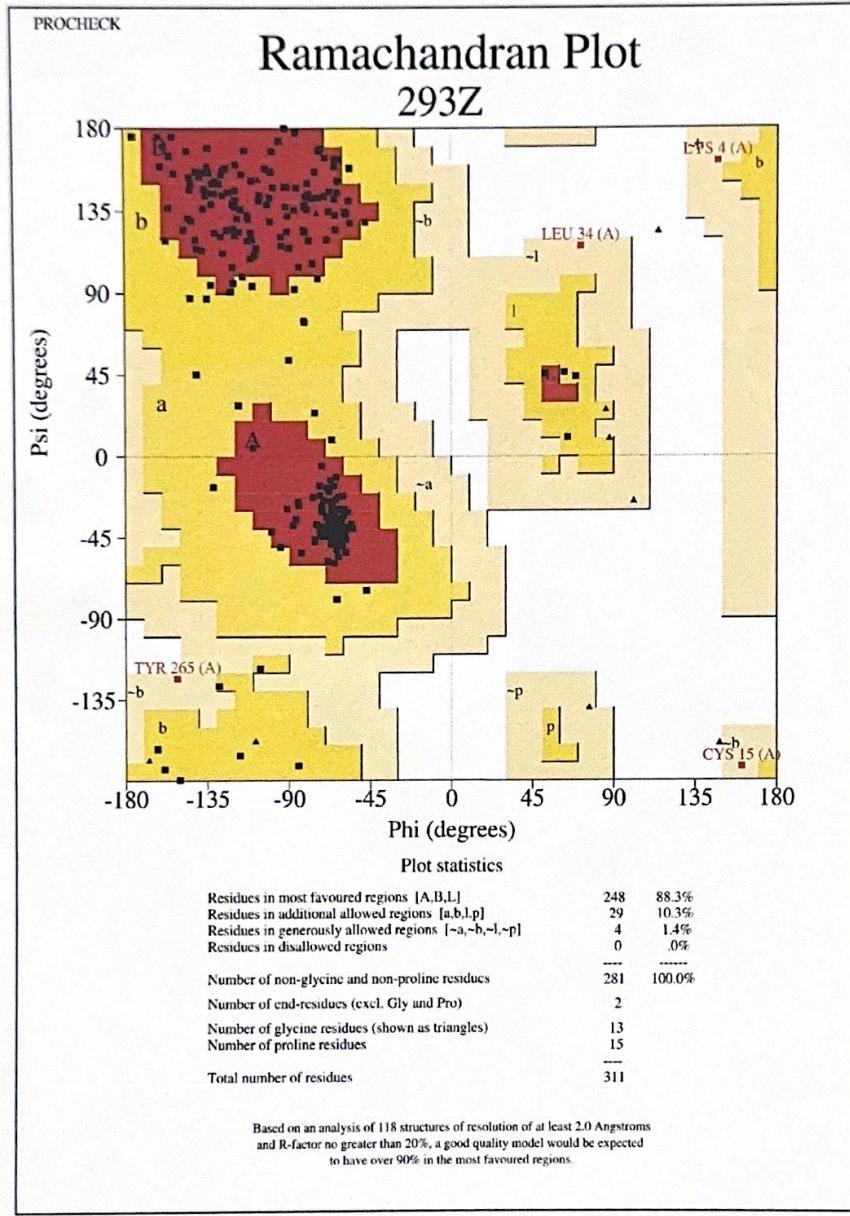
The Ramchandra plot of modelled protein is demonstrated.Calculation of root mean square deviation i.e., RMSD was done for the generated model and template.The two models were loaded and are superimposed together using carbon alpha and calculated RMSD which indicates the generated model exhibited a similar function as template.

% of Residues falling in different regions of Ramachandran plot of 2 proteins

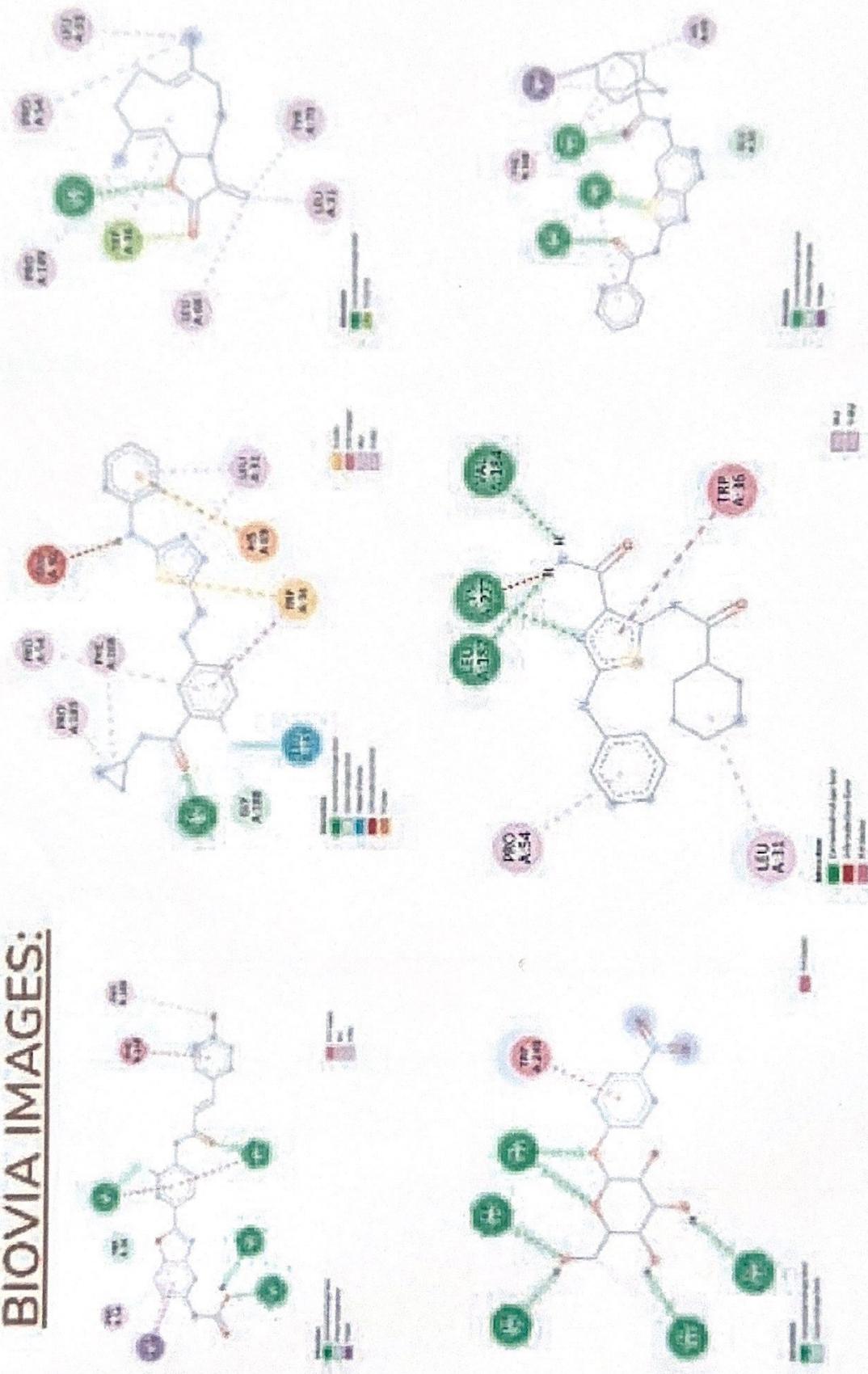
Name of the protein	Core region		Allowed region		Generously allowed region		Disallowed region	
	No of residues	%	No of residues	%	No of residues	%	No of residues	%
Q7Z4J2	248	88.3	29	10.3	4	1.4	0	0
Q4R5T7	253	92.3	20	7.3	1	.4	0	0

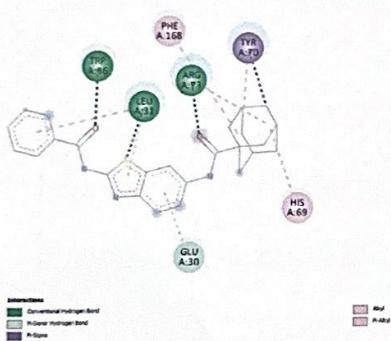
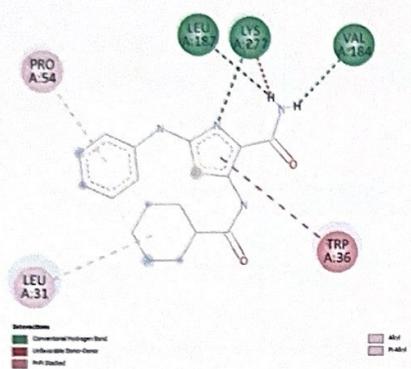


5_01.ps



BIOVIA IMAGES:





DOCKING TABLE:

Interactions of 46355372

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	TRP39, LYS2, GLU33, ALA3	-9.34	142.16 nM
Q4R5T7	LEU187, LYS277, VAL184	-8.30	822.73 μM

Interactions of 11632737

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	LYS4, LEU9, LYS2(2)	-8.46	627.97 nM
Q4R5T7	TYR70	-7.76	2.06 μM

Interactions of 54445

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	GLU33, THR13, LEU34(2), LYS4	-5.36	117.72 μM
Q4R5T7	THR259, TRP250, GLN247(2), GLU317	-5.33	124.75 μM

Interactions of 5281437

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	LYS2	-6.73	11.59 μM
Q4R5T7	LYS277	-6.88	8.98 μM

Interactions of 44402523

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	ARG5, THR13, TRP54	-9.10	213.98 nM
Q4R5T7	LEU31, LYS48, LEU52, HIS69	-9.26	161.93 nM

Interactions of 4096211

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	TRP39	-11.09	7.39 nM
Q4R5T7	TRP36, LEU31, ARG73	-9.32	147.66 nM

Interactions of 72376

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	LEU9, ILE7(2), ARG5(2), THR13, LEU34	-6.54	15.97 μM
Q4R5T7	LEU52, THR276(2), LYS277, LEU187, TYR70	-6.20	28.69 μM

Interactions of 874733

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	ILE(2)7, LEU9, ARG5	-7.00	7.45 μM
Q4R5T7	LEU52, THR276(2), LYS277, LEU187, TYR70	-6.20	28.42 μM

Interactions of 4652

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	ALA3(2), GLU33, LYS4, LYS2	-5.63	74.19 μM
Q4R5T7	GLU30(3), ARG24	-4.99	220.79 μM

Interactions of 51355147

Name of Protein	Interacting amino acids	Binding energy ΔG (Kcal/Mol)	Dissociation constant (kI)
Q7Z4J2	LEU36, LYS280, LYS2	-7.29	4.54 μM
Q4R5T7	—	-5.07	193.72 μM

Drug likeness

Results of the phytochemical molecules drug likeness properties.

Drug Likeness Properties	46355372	11632737	54445	5281437	44402523	4096211	72376
MW g/mol	344.43g/mol	401g/mol	189.21g/mol	232.32g/mol	495.30g/mol	431.55g/mol	307.26g/mol
Consensus Log Po/w	2.94	3.64	-1.55	2.97	4.80	4.57	-0.61
No. of H-bond Acceptors	3	5	5	2	6	3	7
No. of H-bond Donors	3	3	4	0	2	2	5
Molar Refractivity	95.99	103.66	47.80	69.85	122.57	124.81	75.21
Lipinski	Yes	yes	yes	yes	yes	yes	yes
Veber	yes	yes	yes	yes	yes	yes	yes
Bioavailability Score	0.55	0.55	0.55	0.55	0.56	0.55	0.55

Synthetic accessibility (SA)	3.42	3.23	3.37	4.29	3.38	5.41	4.09
TPSA (Å²)	125.35 Å²	107.18 Å²	84.16 Å²	26.30 Å²	92.43 Å²	99.33 Å²	128.48 Å²
No of rotatable bonds	6	8	0	0	7	6	0
solubility (mg/ml)	9.66e-03 mg/ml ; 2.81e-05 mol/l	1.15e-02 mg/ml ; 2.86e-05 mol/l	4.73e+02 mg/ml ; 2.50e+00 mol/l	5.88e-01 mg/ml ; 2.53e-03 mol/l	4.45e-04 mg/ml ; 8.98e-07 mol/l	6.58e-04 mg/ml ; 1.53e-06 mol/l	1.87e+01 mg/ml ; 6.08e-02 mol/l

Drug Likeness Properties	874733	4652	513551 47
MW g/mol	261.13 g/mol	199.63 g/mol	335.28 g/mol
Consensus Log Po/w	2.56	0.66	4.21
No. of H-bond Acceptors	2	3	6
No. of H-bond Donors	2	2	1
Molar Refractivity	62.74	50.51	81.20
Lipinski	yes	yes	yes
Veber	yes	yes	yes
Bioavailability Score	0.55	0.55	0.55
Synthetic accessibility (SA)	2.48	1.69	2.71
TPSA (Å²)		63.32 Å²	

	83.36 Å ²		51.46 Å ²
No of rotatable bonds	2	3	4
solubility (mg/ml)	5.22e-02 mg/ml ; 2.00e-04 mol/l	2.41e+01 mg/ml ; 1.21e-01 mol/l	1.12e-03 mg/ml ; 3.35e-06 mol/l

CONCLUSION:

Homology modelling and Molecular docking is a key tool in structural molecular biology and computer assisted drug design.the use of informatics and complementary experimental techniques increase the chances of success in many stages of the drug discovery process.The 3-dimensional model of Glycosyltransferase protein was developed using the molecular modelling method.The expected models showed 92.3% and 88.3% of maximum number of amino acid residues in the highly favoured region.The active site amino acid residues of the model identified.Molecular docking studies were also achieved to the modelled protein by taking all ten natural compounds.

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