BIOINFORMATION

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Supplementary material:

Table 1: Possible Active Site

Active site searched by literature	Active Site predicted by CASTp	Active Site predicted by PASS	Active Site predicted by Q-Site Finder
ASP 67	ASP 67	ASP 67	ASP 67
VAL 106	VAL 106	VAL 106	VAL 106
ASP 110	ASP 110	ASP 110	TYR 181
TYR 181	MET 184	TYR 181	ASP 110
MET 184	ASP 185	MET 184	MET 184
ASP 185	ASP 186	ASP 185	ASP 185
ASP 186	TRP 229	ASP 186	ASP 186
LEU 228		LEU 228	LEU 228
TRP 229		TRP 229	TRP 229

Table 2: Characteristics of top seven ligand derivatives of 4-thiazolidinone identified form ChemBank database after virtual screening

ChemBank ID	Molecular weight (g/mol)	Log P value	Energy Score (kcal/mol) with active site	No. of Hydrogen Interaction of Ligand with Active site Residues	Rank of Molecule
3087795	254.32	1.38	-8.69 (VAL 106) -7.60 (ASP 186) -7.60 (ASP 185) -7.39 (MET 184) -7.13 (TYR 181) -6.34 (ASP 110)	6	1
1656714	266.36	3.003	-7.34 (ASP 185) -7.32 (ASP 186) -7.30 (VAL 106) -7.24 (MET 184) -6.88 (TYR 181) -6.34 (ASP 110)	6	5
1442532	288.34	2.3	-7.99 (MET 148)	1	2
1426866	266.0	1.32	-7.17 (ASP 185)	1	7
2061166	248.3	1.31	-7.43 (ASP 110)	1	4
1195053	264.34	1.55	-7.30 (ASP 185)	1	5
1187346	274.4	2.23	-7.60 (ASP 185)	1	3