Supplementary File

Supplementary Table S1: GC–MS identified compounds of *Ipomoea aquatica* Forsk

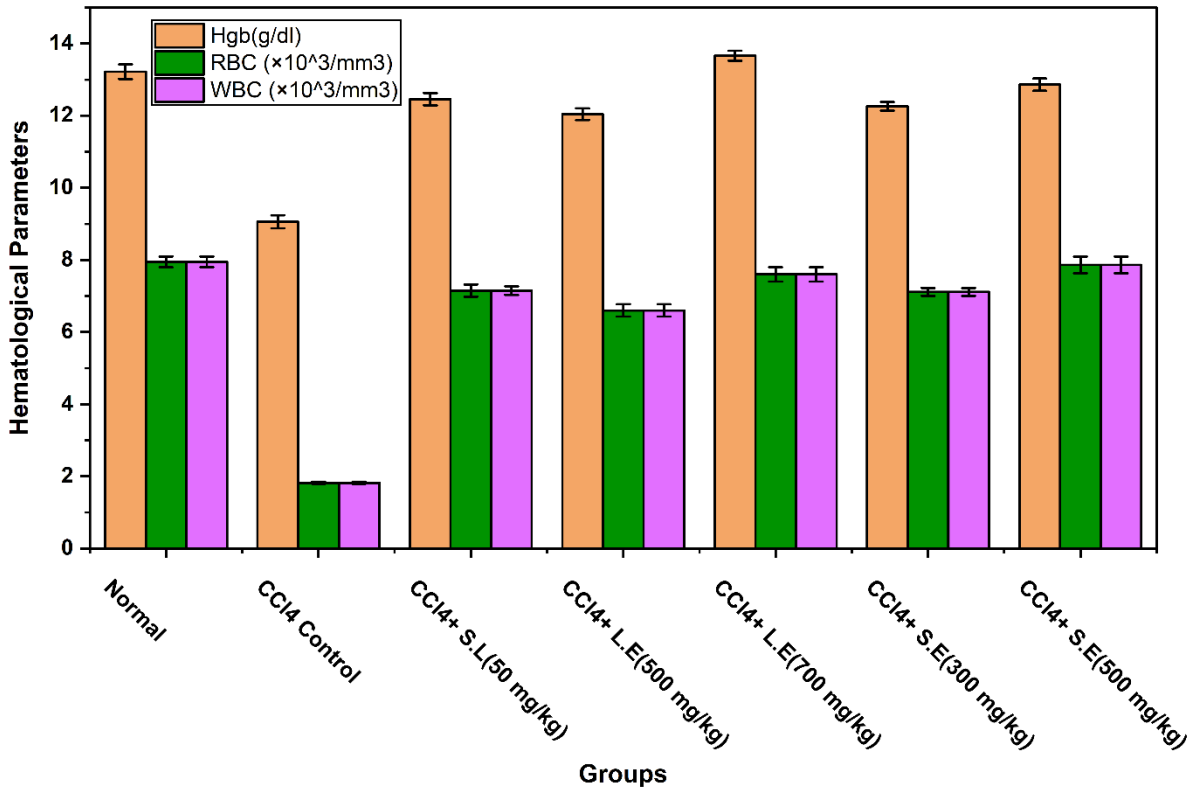
SL/ No.	Compound	R.Time (min)	m/z	Area	Conc. (µg/mL)
1	Erythritol	6.759	44	11004	0.613
2	Urea, butyl-	6.759	44	11004	0.613
3	1,2,3,4-Butanetetrol, [S-(R*,R*)]-	6.759	44	11004	0.613
4	Propanamide	6.759	44	11004	0.613
5	Diglycolamine	6.759	44	11004	0.613
6	Acetic acid, (2-propenylthio)-	6.759	44	11004	0.613
7	2-Heptanamine, 5-methyl-	7.333	44	3833	0.214
8	Cystine	7.333	44	3833	0.214
9	Tetrahydro-4H-pyran-4-ol	7.333	44	3833	0.214
10	Glutaraldehyde	7.333	44	3833	0.214
11	Erythritol	7.333	44	3833	0.214
12	Butanal, 3-hydroxy-	7.333	44	3833	0.214
13	Cyclopropyl carbinol	7.333	44	3833	0.214
14	Octodrine	7.333	44	3833	0.214
15	D-Alanine	7.755	44	3931	0.219
16	Benzenemethanol,Î±-[(methylamino)methyl]-	7.755	44	3931	0.219
17	2-Heptanamine, 5-methyl-	7.755	44	3931	0.219
18	3,6-Dimethylpiperazine-2,5-dione	7.962	44	4682	0.261
19	Piperazine, 2-methyl-	7.962	44	4682	0.261
20	3-Nitropropanoic acid	8.287	73	57939	3.23
21	[1,4]Dioxino[2,3-b]-1,4-dioxin, hexahydro-	8.287	73	57939	3.23
22	3-Pentanol, 2,4-dimethyl-	8.287	73	57939	3.23
23	Trimethylsilylmethanol	8.287	73	57939	3.23
24	Butanoic acid, 2-(methoxyimino)-3-methyl-, trimethylsilyl ester	8.287	73	57939	3.23
25	Erythritol	8.799	44	10675	0.595
26	Hexanal	8.799	44	10675	0.595
27	Butanamide	8.799	44	10675	0.595
28	L-Asparagine	8.799	44	10675	0.595
29	1,3-Dioxolane, 4-methyl-	8.799	44	10675	0.595
30	3-Nitropropanoic acid	9.26	73	27379	1.526
31	Î±-Ketoisovaleric acid, TMS derivative	9.26	73	27379	1.526
32	Sorbitol	9.26	73	27379	1.526

SL/ No.	Compound	R.Time (min)	m/z	Area	Conc. (µg/mL)
33	N,N-Dimethylformamide dipropyl acetal	9.26	73	27379	1.526
34	Butyric acid, 2-hydroxy-3-methyl-, methyl ester	9.26	73	27379	1.526
35	1,2,3,4-Butanetetrol, [S-(R*,R*)]-	9.672	44	7371	0.411
36	Propanamide	9.672	44	7371	0.411
37	Norpseudoephedrine	9.672	44	7371	0.411
38	Cycloserine	9.672	44	7371	0.411
39	Tetrahydro-4H-pyran-4-ol	9.672	44	7371	0.411
40	Butanal, 3-hydroxy-	9.672	44	7371	0.411
41	1,3-Dioxolane, 4-methyl-	9.672	44	7371	0.411
42	Urea, butyl-	9.672	44	7371	0.411
43	Hexanal	9.672	44	7371	0.411
44	(-)-Norephedrine	9.672	44	7371	0.411
45	(-)-Norephedrine	9.672	44	7371	0.411
46	Amphetamine	9.672	44	7371	0.411
47	1,2,3,4-Butanetetrol, [S-(R*,R*)]-	9.672	44	7371	0.411
48	1,3-Dioxan-5-ol	10.456	73	45927	2.56
49	2-Methoxy-1,3-dioxolane	10.456	73	45927	2.56
50	Benzeneacetic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester	11.209	73	22289	1.243
51	Bis(dimethyl-t-butylsilyl) maleate	11.209	73	22289	1.243
52	2-Methoxy-1,3-dioxolane	11.209	73	22289	1.243
53	Heptanal	11.229	44	14361	0.801
54	Butanal, 3-hydroxy-	11.229	44	14361	0.801
55	1,2,3,4-Butanetetrol, [S-(R*,R*)]-	11.42	44	6322	0.352
56	Urea, butyl-	11.42	44	6322	0.352
57	1,3-Dioxolane, 4-methyl-	11.669	44	6135	0.342
58	Benzeneacetic acid, 3-[(trimethylsilyl)oxy]-, trimethylsilyl ester	12.318	73	34366	1.916
59	L-Asparagine, N,N2-bis(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester	12.318	73	34366	1.916
60	N-Ethylformamide	12.318	73	34366	1.916
61	Bis(dimethyl-t-butylsilyl) maleate	12.318	73	34366	1.916
62	3-Hydroxyphenylacetic acid, 2TMS derivative	12.318	73	34366	1.916
63	Glycolic acid, 2TMS derivative	12.993	73	26347	1.469
64	11-Tetradecen-1-ol, acetate, (Z)-	13.006	44	6887	0.384

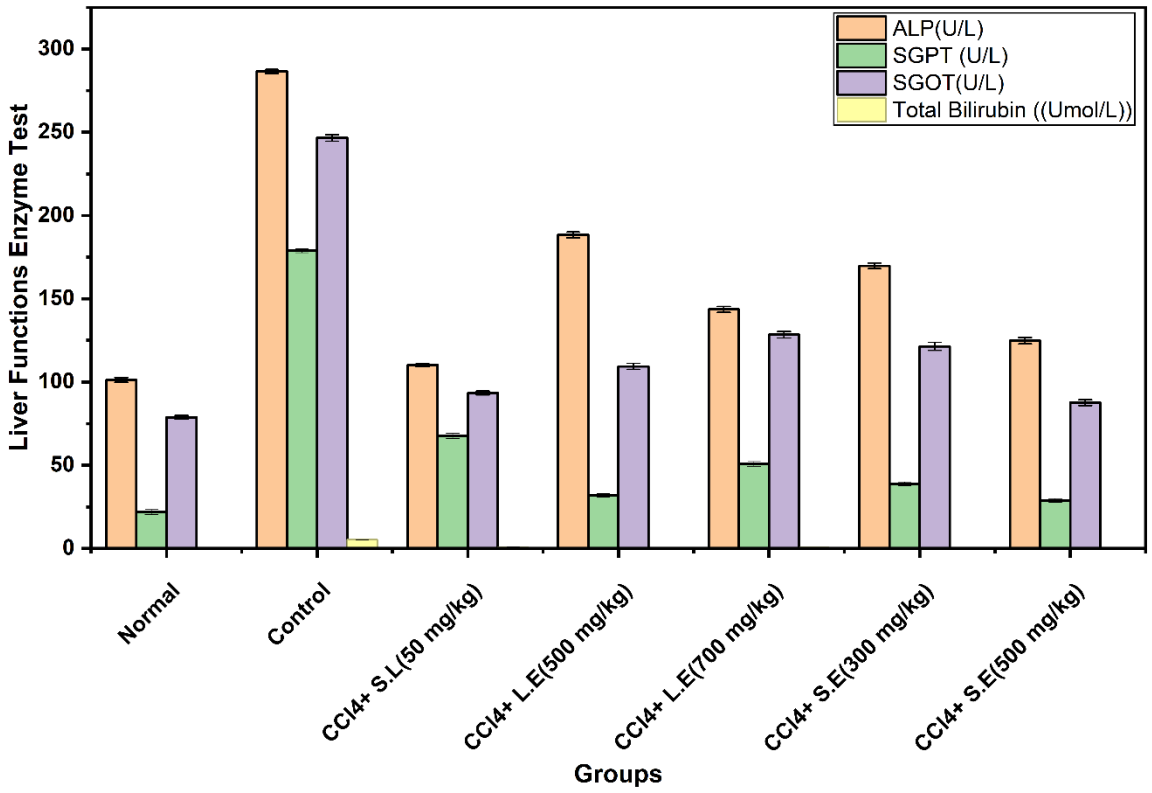
SL/ No.	Compound	R.Time (min)	m/z	Area	Conc. (µg/mL)
65	11-(2-Cyclopenten-1-yl)undecanoic acid, (+)-	13.006	44	6887	0.384
66	1-Nonyne	13.006	44	6887	0.384
67	4-Nonenoic acid, methyl ester	13.006	44	6887	0.384
68	trans-2-Undecen-1-ol	13.006	44	6887	0.384
69	Heptanal	13.006	44	6887	0.384
71	Tridecanoic acid, methyl ester	14.026	74	214465	11.956
72	Methyl stearate	14.026	74	214465	11.956
73	Pentadecanoic acid, methyl ester	14.026	74	214465	11.956

Supplementary Table S2: Comparative RMSD and RMSF Profiles of Apo and Ligand-protein complex During CABS-flex Simulation

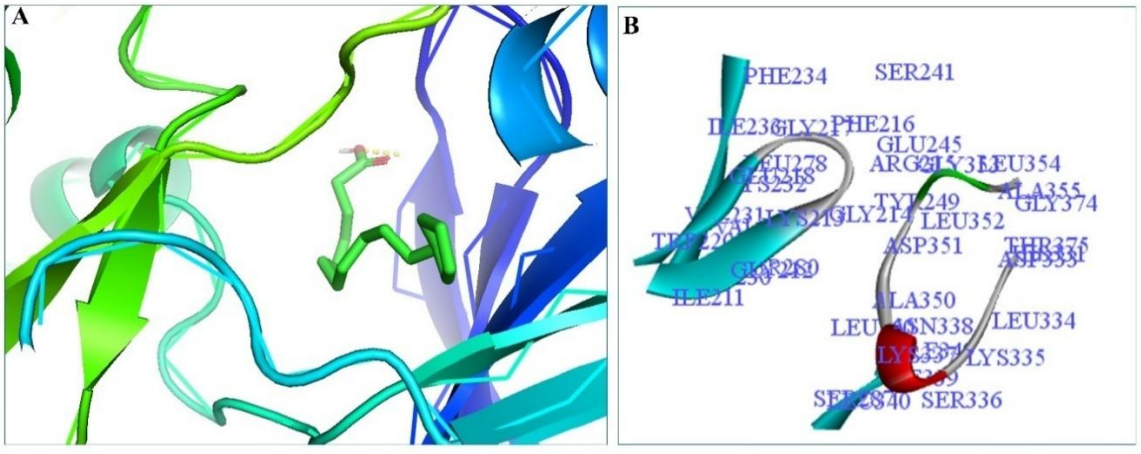
System	Mean RMSD ± SD (Å)	Maximum RMSD (Å)	Mean RMSF ± SD (Å)	Maximum RMSF (Å)
Apo	2.674 ± 0.052	3.029	0.850 ± 0.697	5.420
5213	2.583 ± 0.082	2.882	0.755 ± 0.595	3.291
110680	2.541 ± 0.065	2.906	0.811 ± 0.645	3.943
5367692	2.269 ± 0.072	2.428	0.763 ± 0.570	3.723
162265	2.426 ± 0.066	2.615	0.838 ± 0.731	5.386
10297	2.702 ± 0.084	2.886	0.915 ± 0.668	4.780



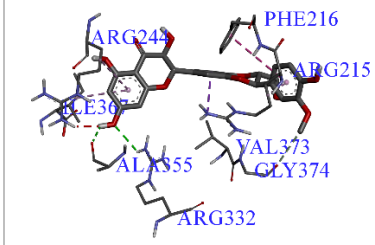
Supplementary Figure S1: Effect of methanolic extract of *Ipomoea aquatic* on CCl4-induced hepatotoxicity in rats for hematological parameters. RBC and WBC counts were brought back to ~97% normal with the 500 mg/kg stem extract, effects comparable to silymarin; the 700 mg/kg leaf extract effect to produce supranormal restoration of hemoglobin (>100%) is suggestive of a hematinic potential which might be attributed to the high phenolic and flavonoid content.

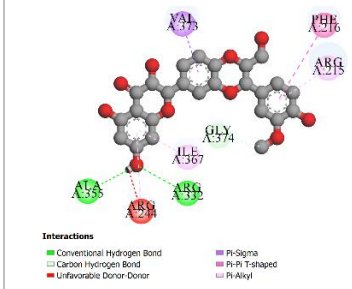


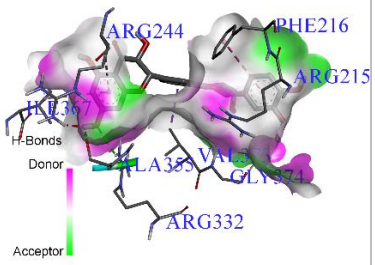
Supplementary Figure S2: Effect of methanolic extract of *Ipomoea aquatica* on CCl_4 CCl4-induced hepatotoxicity in rats for liver function parameters. Stem extract (SE) at 500 mg/kg concentration showed maximum protection, by 98.3% for SGPT, 95.6% for SGOT, and 98.9% for bilirubin, and was more effective than silymarin in some of the cases. Treatment with the leaf extract (LE) (700 mg/kg) also provided significant hepatoprotection. However, it was to a lesser extent in normalizing ALP and SGOT levels as compared to the stem extract.



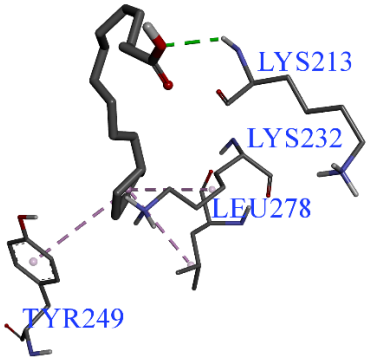
Supplementary Figure S3: Predicted binding pocket of Receptor 1VJY.A. Overall 3D view of the receptor with target ligands. **B.** View of the ligand-binding site, illustrating key amino acid residues involved in molecular interactions.

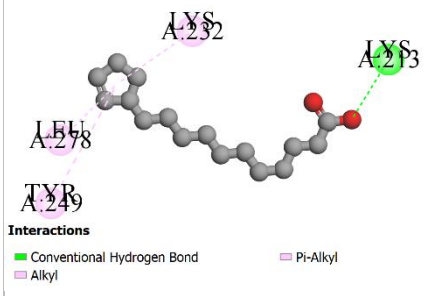


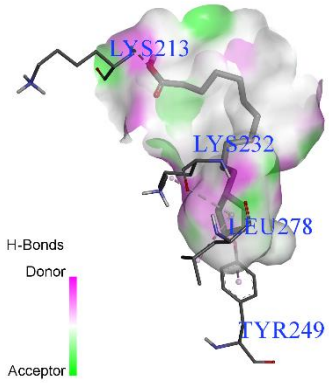




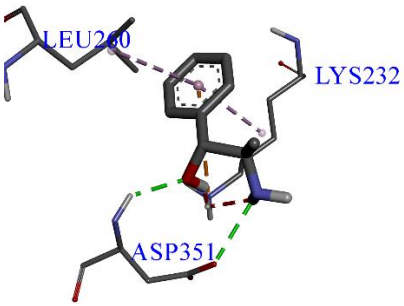
Standard VS 1VJY

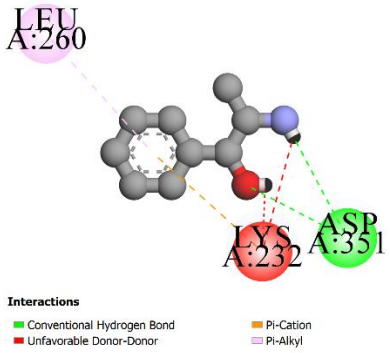


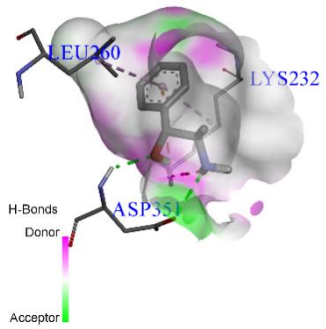




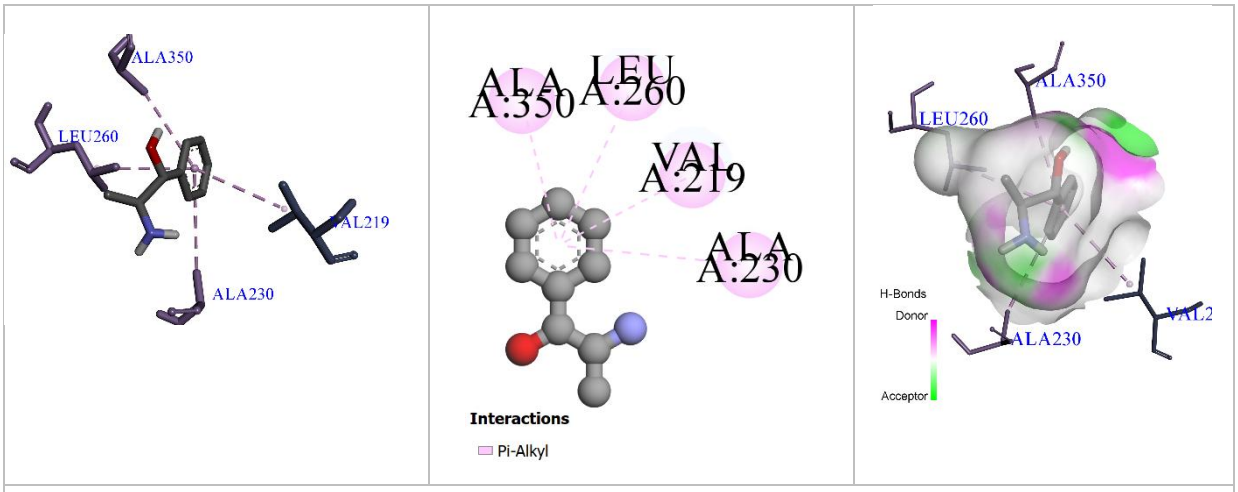
110680 VS 1VJY



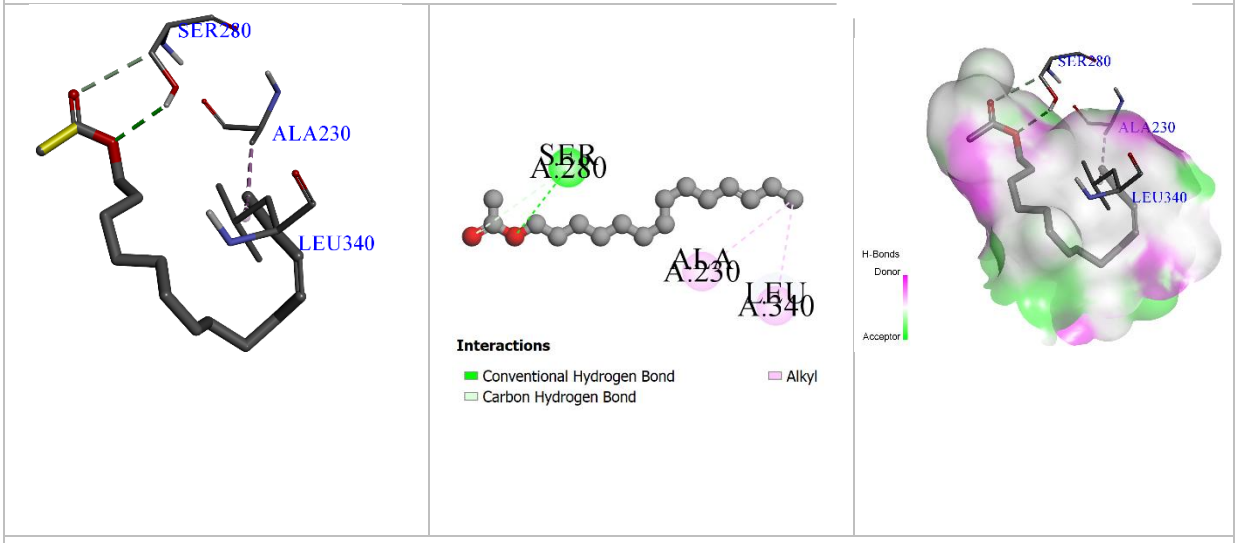




162265 VS 1VJY

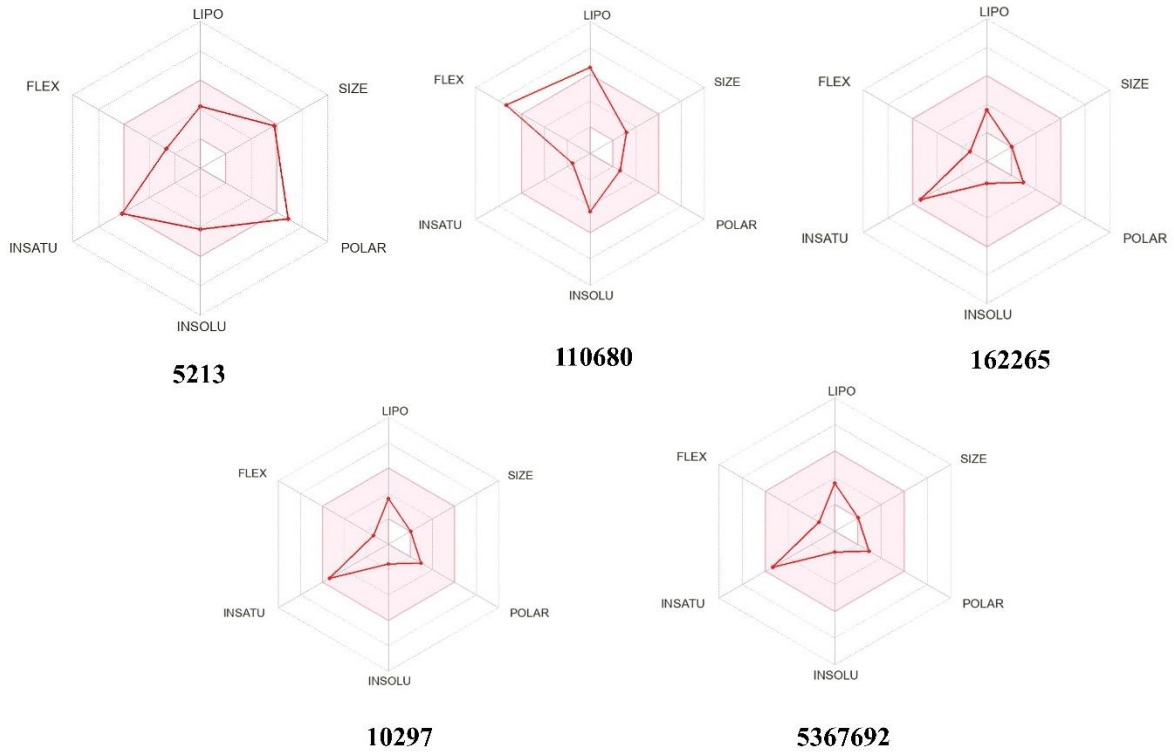


10297 VS 1VJY



5367692 VS 1VJY

Supplementary Figure S4:2D and 3D visualization of *I. aquatica* selected metabolites interactions with TGF-beta Type I Receptor [PDB: 1VJY]



Supplementary Figure S5: Summary of physicochemical, toxicological, and pharmacokinetic properties of selected compounds. [The colored zone is the suitable physicochemical space for oral bioavailability; SIZE: 150 g/mol<MV<500 g/mol; INSOLU (Insolubility):−6<log S (ESOL)<0; LIPO (Lipophilicity):−7<XLOGP3< +5.0; INSATU (In saturation): 0.25<Fraction Csp3<1; POLAR (Polarity): 20 Å2<TPSA<130 Å2; FLEX (Flexibility): 0<num of rotatable bonds<9