Supplementary file 1

Table S1: Validation of the MOE scoring functions pre-docking for all four targets

4Y14		
Scoring Function	**Docking Score**	**RMSD**
ASE	-8.3522	1.2180
Affinity dG	-8.3014	1.2927
Alpha/HB	-8.7310	2.8833
GBVI/WSA dG	-9.0354	1.4660
London dG	-8.2786	0.9873
2QV4		
Scoring function	**Docking Score**	**RMSD**
ASE	9.9611	2.9904
Affinity dG	-9.5040	2.3756
Alpha/HB	-9.3210	2.1340
GBVI/WSA dG	-9.1338	2.0913
London dG	-9.8893	0.9873
4PNZ		
Scoring function	**Docking Score**	**RMSD**
ASE	-7.8486	1.4465
Affinity dG	-8.5048	0.8675
Alpha/HB	-7.6911	2.8194
GBVI/WSA dG	-6.8456	2.1267
London dG	-8.675	0.9893
2QJM		
Scoring function	**Docking Score**	**RMSD**
ASE	-8.2616	3.6032
Affinity dG	-8.2378	2.2347
Alpha/HB	-8.5402	1.6400
GBVI/WSA dG	-6.0017	1.5285
London dG	-6.9774	2.4996

Table S2: Docking Binding Energies, Number of heavy atoms and computed Size-Independent Ligand Efficiencies of the top-ranked compounds selected post-docking in Human Pancreatic amylase (PDB ID:2QV4.)

S/N	**Compound PubChem ID**	**Compound Description**	**Docking Energy (D)**	**N**	**SILE**

1	101679366	Hypoxoside	-8.657	42	2.821
2	132989152	Licarin-type phenylpropanoid	-7.725	29	2.813
3	132989074	Barbigerone-type pyranoisoflavone	-7.719	29	2.811
4	393472	Acetogenin	-7.886	33	2.763
5	162944977	Cucurbitacin-type steroidal diterpene	-8.077	36	2.756
6	10219	Isoquinolone alkaloid	-7.917	35	2.725
7	10884656	Microfolian	-7.637	32	2.700
8	132989156	Calceolarioside- type hydroxy cinnamic acid glycosides	-7.443	32	2.630
9	5280805	Rutin	-8.101	43	2.621
10	163058659	Kulonate- type diterpene	-7.681	36	2.621
11	442664	Vicenin	-7.764	42	2.530
12	5280343	Quercetin	-5.689	22	2.251
13	Control (24755467)		-9.670	55	2.906

SILEs: size independent ligand efficiencies; **HA:** No of heavy atoms of the compound; **D:** Docking Score or Docking Binding energy, **N**=No of Heavy atoms

Table S3: Docking Binding Energies, Number of heavy atoms and computed Size-Independent Ligand Efficiencies of the top-ranked compounds selected post-docking in Human Maltase-Glucoamylase (PDB ID:2QMJ.)

S/N	Compound PubChem ID	Compound Description	Docking Score (D)	N	SILE
1	64982	Baicalin	-7.971	32	2.818
2	442435	Swertiamarin (a secoiridoid glycoside)	-7.471	26	2.811
3	161036	Sweroside (an iridoid glycoside)	-7.176	25	2.732
4	132988919	Prenylated flavonoid	-7.392	34	2.566
5	21721869	Hydroxy Mundulinol	-7.170	31	2.559
6	10363971	Mundulinol	-7.082	30	2.553
7	87691	Loganin (an iridoid monoterpenoid)	-6.854	27	2.550
8	10250777	Lupinifolin	-7.051	30	2.541
9	163085068	Flavonoid	-6.804	27	2.531
10	15895372	Mundulin	-6.926	29	2.522
11	163058856	Acetylated flavonoid	-7.186	34	2.495
12	10884656	Microfolian	-6.997	31	2.474
13	Control (445421)		-8.281	44	2.661

SILEs: size independent ligand efficiencies; **HA:** No of heavy atoms of the compound; **D:** Docking Score or Docking Binding energy, **N**:No of Heavy atoms

Table S4: Docking Binding Energies, Number of heavy atoms and computed Size-Independent Ligand Efficiencies of the top-ranked compounds selected post-docking in Human dipeptidyl peptidase IV (DPP4) (PDB ID:4PNZ)

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S/N	Compound PubChem ID	Compound Description	Docking Score (D)	N	SILE
1	393472	Acetogenin	-9.759	33	3.419
2	163042290	Severifoline- type Acridone alkaloid	-9.019	33	3.159
3	132989036	Isodiscoloranone	-8.896	33	3.116
4	162887088	Obliquine alkaloid	-8.795	33	3.081
5	11995377	Discoloranone	-8.776	33	3.074
6	162912953	Prenylated flavonoid	-8.543	31	3.049
7	3037997	Corynantheine alkaloid	-8.143	27	3.029
8	5281633	Gartanin	-8.288	29	3.018
9	163065490	Flavonoid glycoside	-8.193	28	3.015
10	10366501	Parviflorone-type diterpene	-8.217	33	2.878
11	5280805	Rutin	-8.911	43	2.883
12	10884656	Microfolian	-8.161	33	2.860
13	Control (46209242)		-9.725	22	3.847

SILEs: size independent ligand efficiencies; **HA:** No of heavy atoms of the compound; **D:** Docking Score or Docking Binding energy, N: No of Heave atoms

Table S5: Docking Binding Energies, Number of heavy atoms and computed Size-Independent Ligand Efficiencies of the top-ranked compounds selected post-docking in Human protein tyrosine phosphatase 1B (PTP1B) (PDB ID:4Y14.)

S/N	Compound PubChem ID	Compound Description	Docking Score (D)	N	SILE
1	132988935	Limonianin-type flavone	-6.751	26	2.540
2	241097691	Lupinifolinol	-6.628	31	2.366
3	162856705	Pilostigmol-type phenylpropanoid	-6.245	28	2.298
4	509268	Tovophyllin B (Xanthone prenylated)	-6.538	34	2.270
5	5280805	Rutin	-6.987	43	2.261
6	393472	Acetogenin	-6.434	33	2.254
7	3085222	Diuvaretin (Hydrochalcones)	-6.600	36	2.252
8	132989074	Barbigerone-type pyranoisoflavone	-6.162	29	2.244
9	969516	Curcumin	-6.007	27	2.235
10	101967010	Parviflorone-type diterpene	-6.182	32	2.186
11	5280637	Luteolin-7-glucoside	-6.093	32	2.150
12	5281633	Gartanin	-5.889	29	2.140
13	Control (91826021)		-9.098	25	3.464

SILEs: size independent ligand efficiencies; **HA:** No of heavy atoms of the compound; **D:** Docking Score or Docking Binding energy, **N:** No of Heave atoms

Supplementary file 1

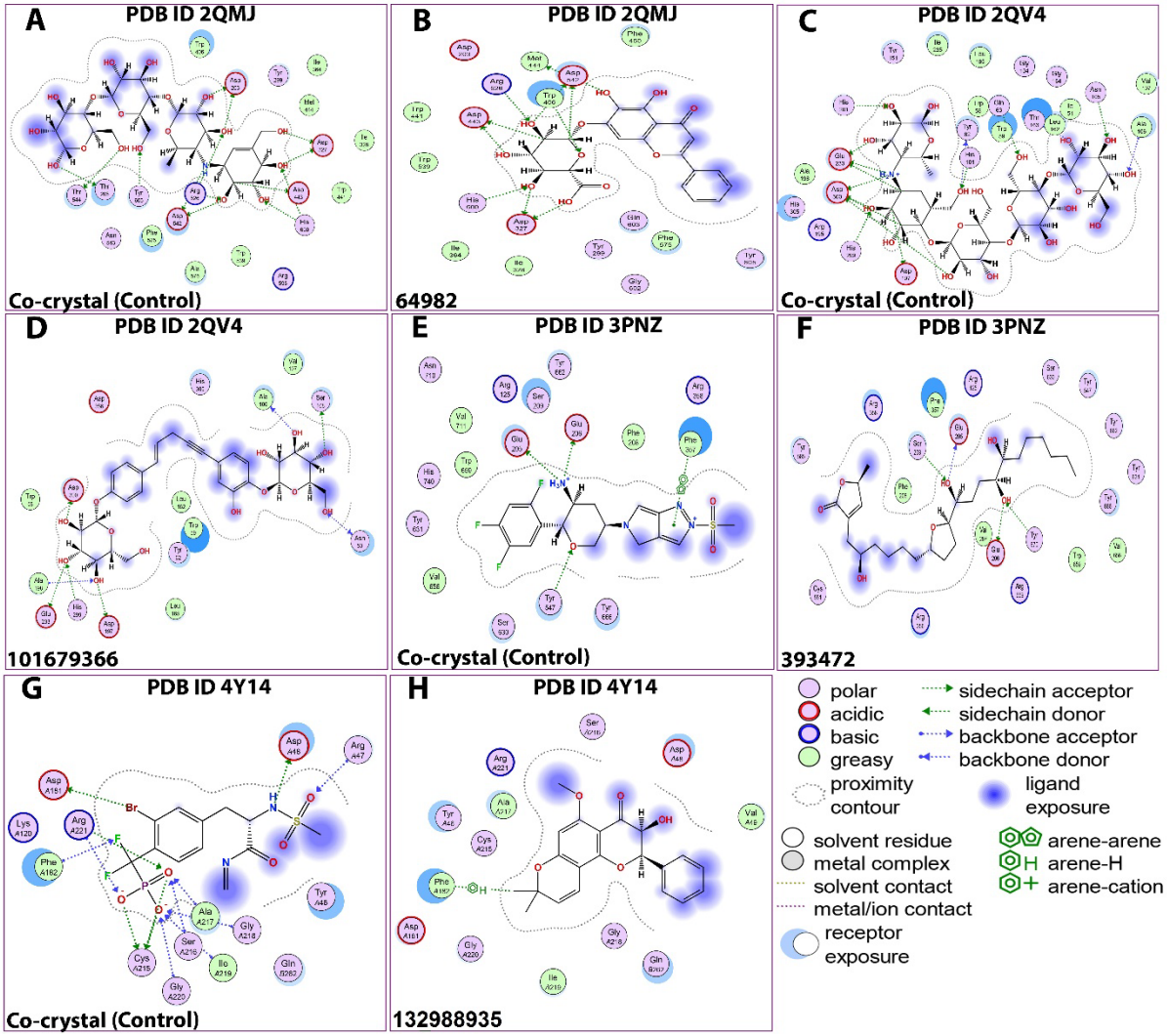

Figure S1: Post-docking compound-protein interactions displayed in 2-D (computed by MOE ligand interaction option)

Supplementary file 1

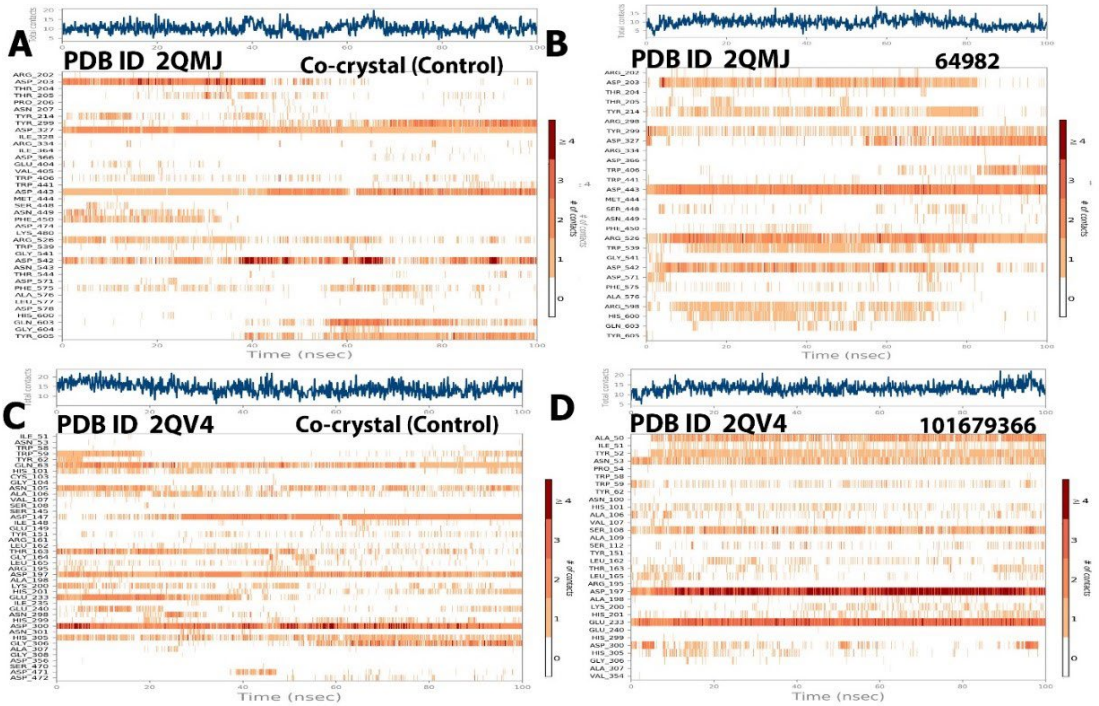

Figure S2: Heat map showing the number of hydrogen bond contacts/interactions contributed by the respective amino acids during the MD simulation for AMY1A (2QV4) and MGAM (2QMJ) compounds and their respective controls.

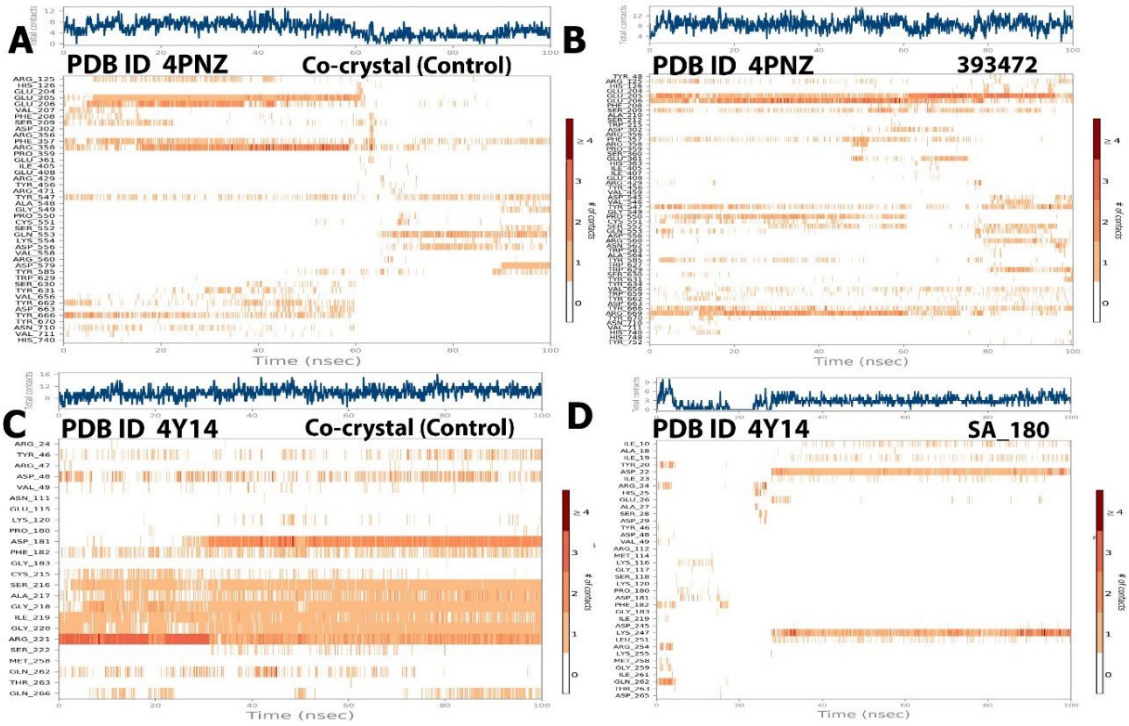

Figure S3: Heat map showing the number of hydrogen bond contacts/interactions contributed by the respective amino acids during the MD simulation for DPP 4 (4PNZ) and PTP1B (4Y14) compounds and their respective controls.

Supplementary file 1

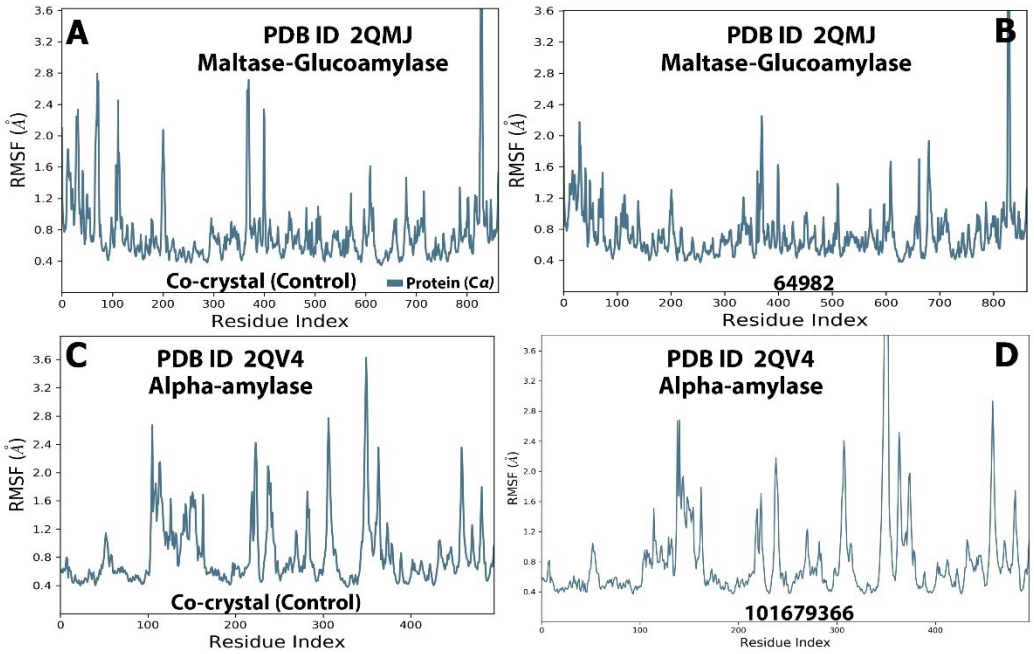

Figure S4: Molecular dynamics RMSF trajectory for AMY1A (2QV4) and MGAM (2QMJ) compounds and their respective controls.

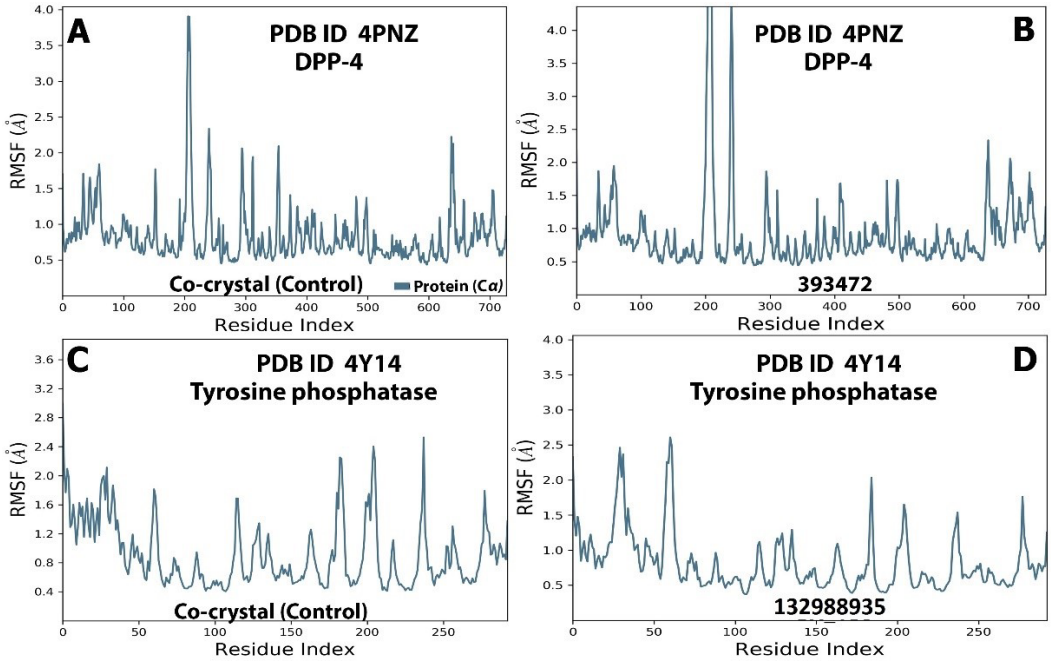

Figure S5: Molecular dynamics RMSF trajectory for DPP 4 (4PNZ) and PTP1B (4Y14) compounds and their respective controls.

Supplementary file 1

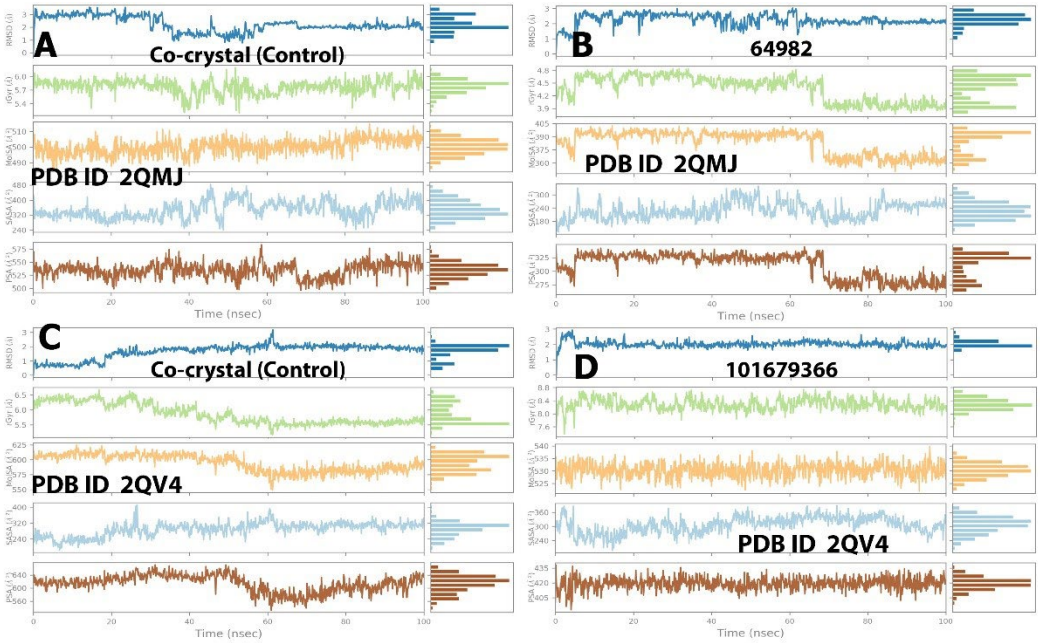

Figure S6: Molecular dynamics simulation analysis of, Radius of Gyration (rGyr), Molecular Surface Area (MolSA), Solvent Accessible Surface Area (SASA) and Polar Surface Area (PSA) for AMY1A (2QV4) and MGAM (2QMJ) compounds and their respective controls.

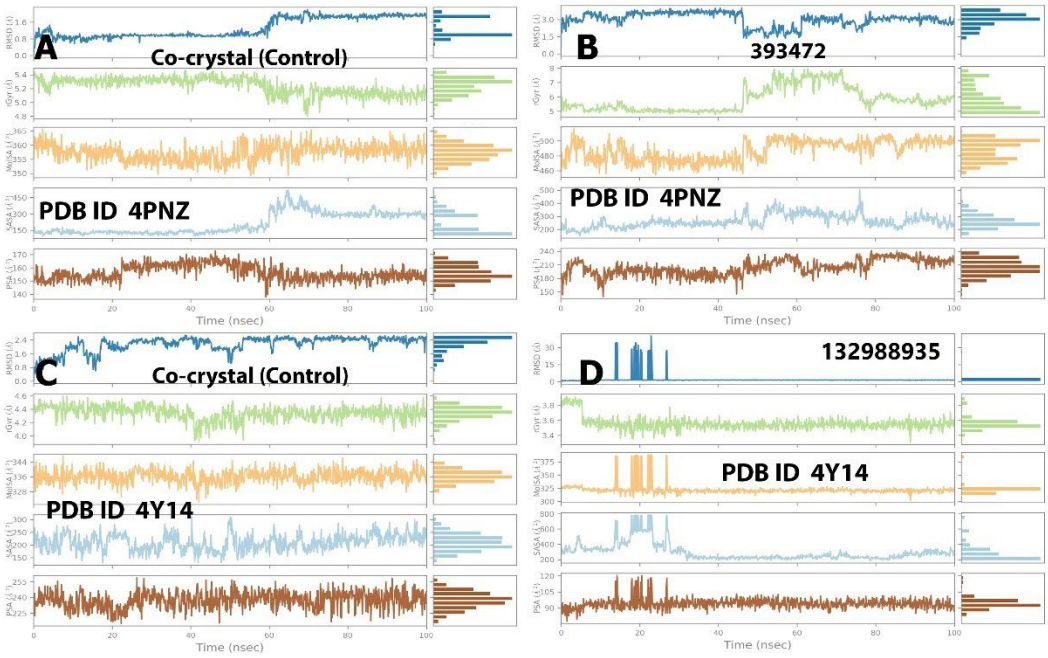

Figure S7: Post-molecular dynamics simulation analysis of protein and ligand properties, Radius of Gyration (rGyr), Molecular Surface Area (MolSA), Solvent Accessible Surface Area (SASA) and Polar Surface Area (PSA) for DPP 4 (4PNZ) and PTP1B (4Y14) compounds and their respective controls.