

Supplementary Information (SI)

Pentafuhalol-B, a Phlorotannin from Brown Algae strongly Inhibit the PLK-1 overexpression in Cancer Cells as Revealed by Computational Analysis

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Table S1. Triplicate molecular docking of phlorotannins compounds against 2YAC receptor

Compounds	Binding energy (Kcal/mole)		
1	-7.665	-7.665	-7.665
2	-7.635	-7.635	-7.635
3	-6.846	-6.846	-6.846
4	-6.729	-6.729	-6.729
5	-6.511	-6.511	-6.511
6	-5.897	-5.897	-5.897
7	-5.767	-5.767	-5.767
8	-5.708	-5.708	-5.708
9	-5.656	-5.656	-5.656
10	-5.489	-5.489	-5.489
11	-5.348	-5.348	-5.348
12	-5.142	-5.142	-5.142
13	-4.976	-4.976	-4.976
14	-4.953	-4.953	-4.953
15	-3.087	-3.087	-3.087
16	-5.172	-5.172	-5.172

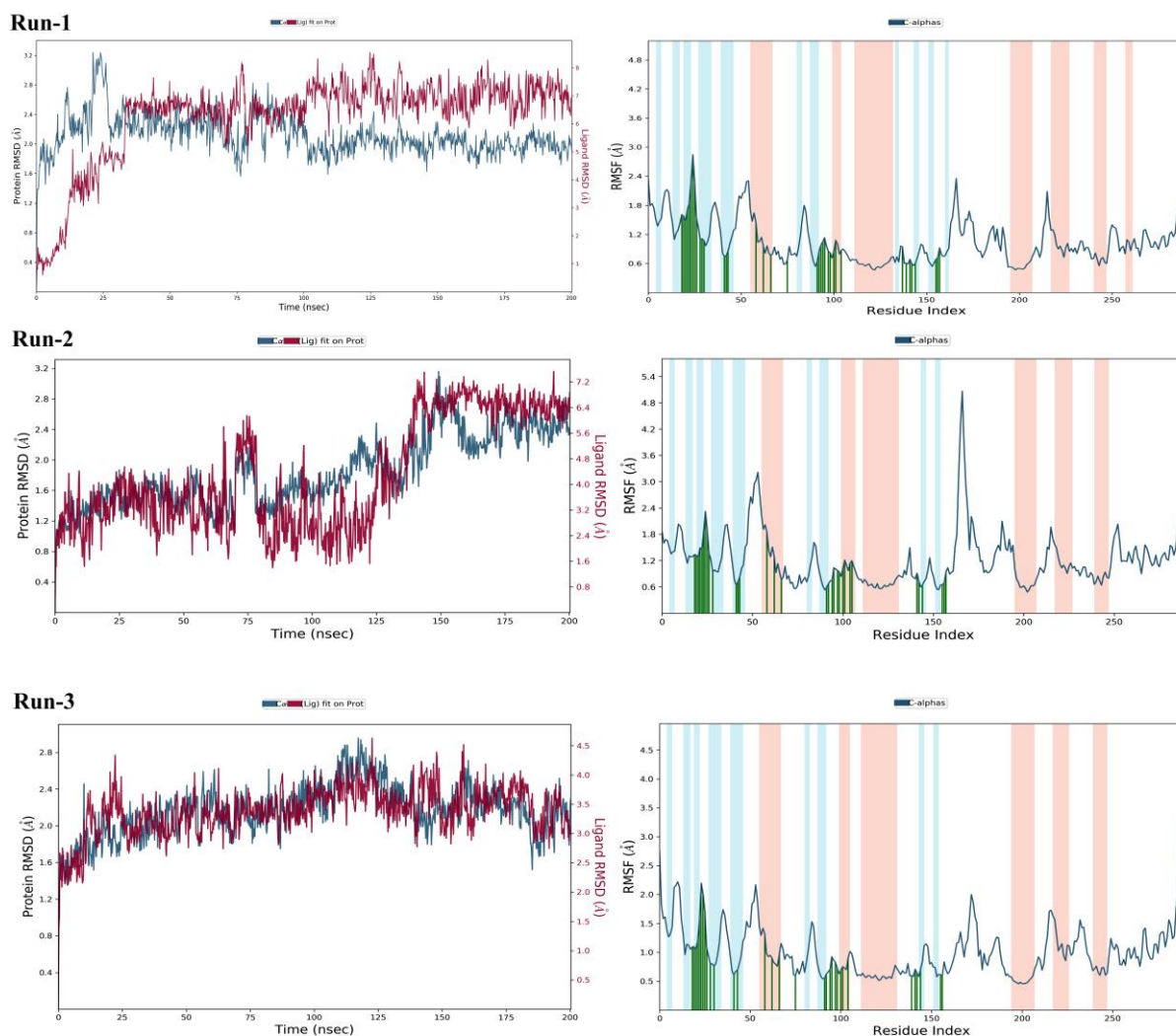


Figure S1. The triplicate RMSD and RMSF plots of PtB-2YAC complex throughout 200ns simulation

Table S2. The triplicate calculated parameters of PtB-2YAC complex throughout 200ns simulation

Parameters	PtB-2YAC complex		
RMSD of Protein (Å)	1.118 - 3.238	0.794 - 3.159	1.167 - 2.956
RMSD of PtB (Å)	0.606 - 8.550	1.394 - 7.526	1.394 - 4.630
RMSF of Protein (Å)	0.466 - 4.418	0.481 - 7.216	0.454 - 6.985
rGyr (Å)	4.481 - 6.060	4.401 - 5.765	4.588 - 5.316
MolSA (Å ²)	461.249 - 511.531	450.397 - 511.461	457.037 - 503.076
SASA (Å ²)	117.430 - 408.527	149.567 - 404.065	105.693 - 293.441
PSA (Å ²)	528.426 - 604.276	508.704 - 616.063	508.501 - 597.879

Table S3. The triplicate MMGBSA binding free energy study of PtB-2YAC complex

Complex	ΔG_{bind}	ΔG_{coul}	$\Delta G_{\text{H-bond}}$	ΔG_{lipo}	ΔG_{GB}	ΔG_{vdW}
PtB-2YAC	-61.766	-177.145	-6.458	-9.666	-23.537	-57.198
	-59.828	-174.863	-6.347	-9.590	-19.696	-52.335
	-67.915	-191.533	-5.742	-11.187	-7.178	-62.129