biomolecules

MDPI

Supplementary Materials

Compound Prunetin Induces Cell Death in Gastric Cancer Cell with Potent Anti-Proliferative Properties: In Vitro Assay, Molecular Docking, Dynamics, and ADMET Studies

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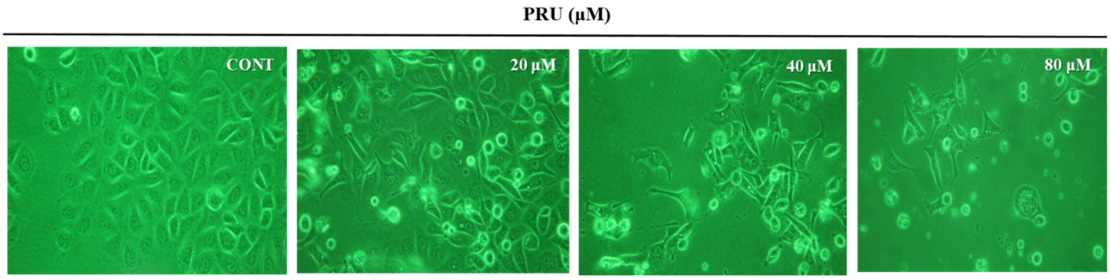


Figure S1. Cellular Morphological changes observed under light microscope upon three different concentrations of PRU (20, 40 and 80 μM) on AGS cells.

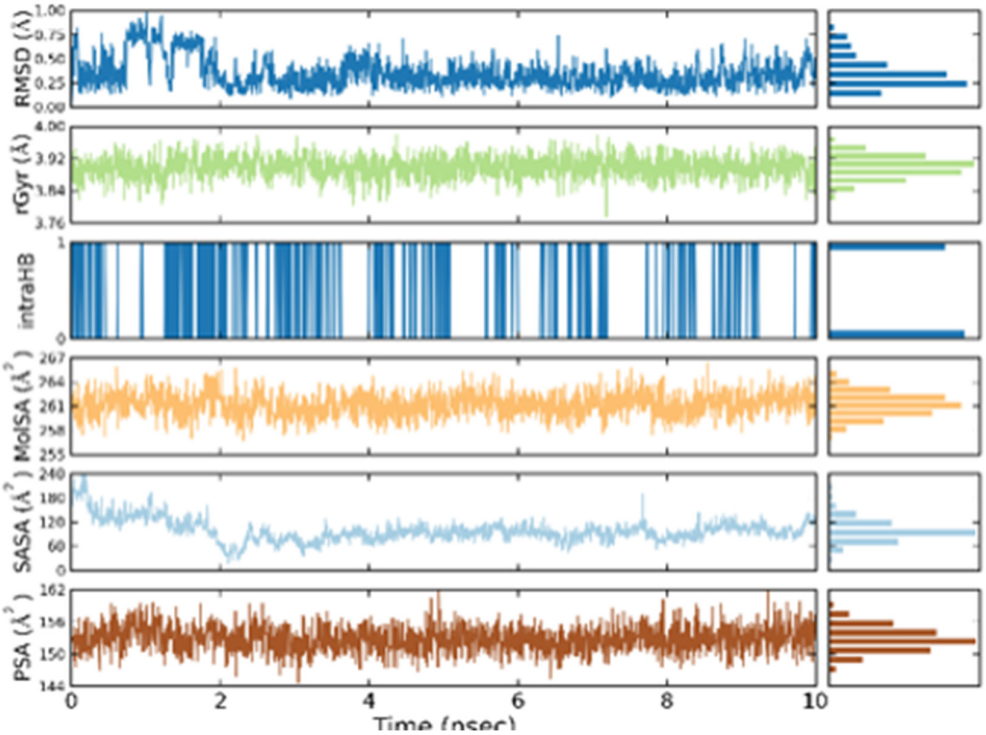


Figure S2. Fluctuations of the ligand properties during MD simulation for 10ns.

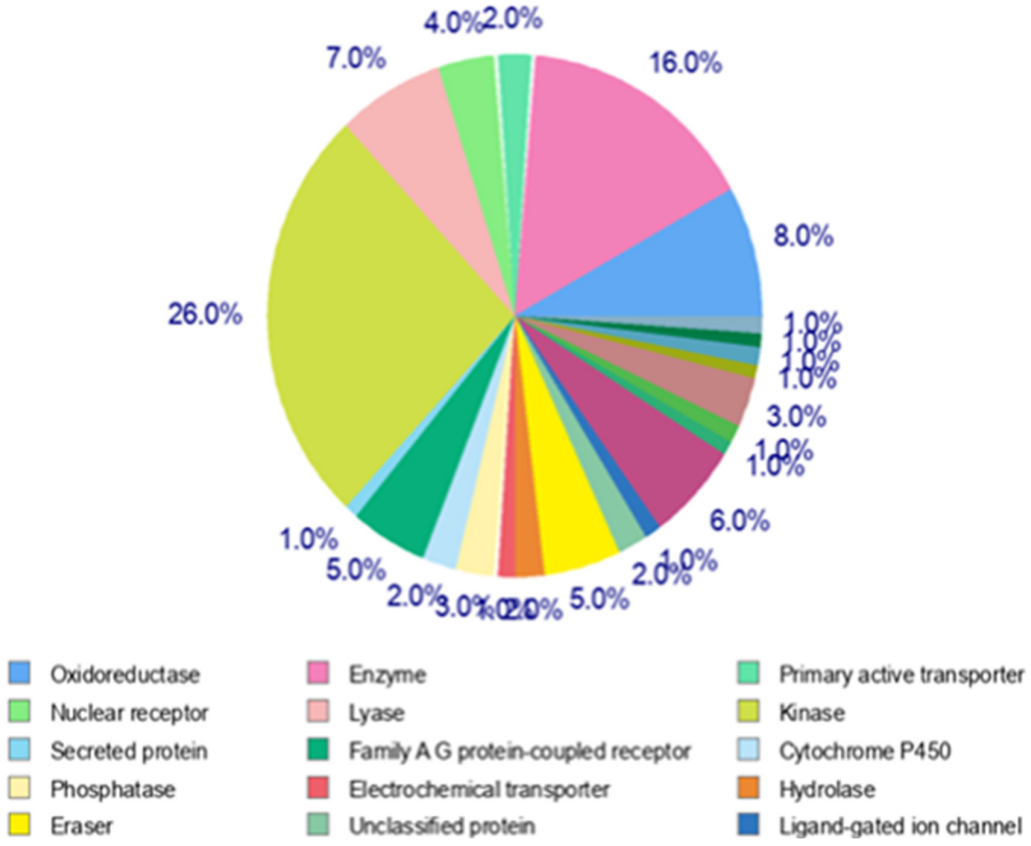
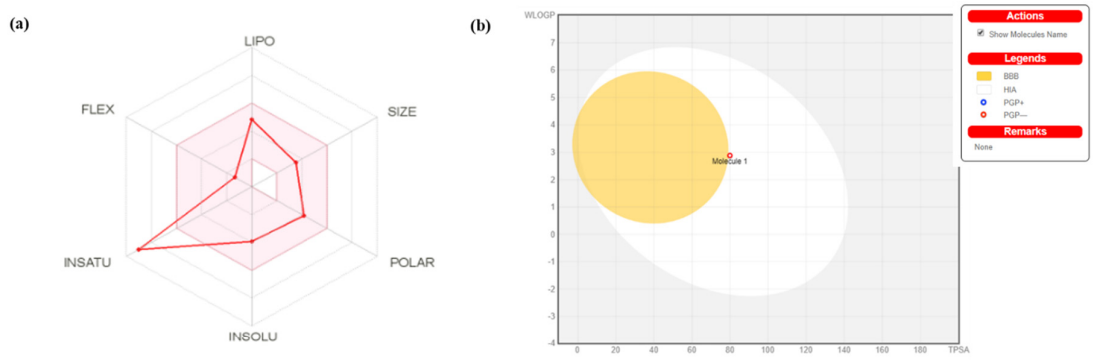


Figure S3. Swiss target prediction of compound Prunetin with its top class of predicted targets.



(c)

	Pharmokinetics								
	GI absorption	**BBB permeant**	**p-gp**	**CYP1A2 inhibitor**	**CYP2C19 inhibitor**	**CYP2C9 inhibitor**	**CYP2D6 inhibitor**	**CYP3A4 inhibitor**	**Log Kp (skin permeation)**
Prunetin	High	No	No	Yes	No	No	Yes	Yes	-5.91 cm/s

	Drug-likeness & Medicinal Chemistry									
	Lipinski	**Ghose**	**Veber**	**Egan**	**Muegge**	**Bioavailability score**	**PAINS**	**Brenk**	**Leadlikeness**	**Synthetic accessibility**
Prunetin	Yes	Yes	Yes	Yes	Yes	0.55	0 alert	0 alert	Yes	2.96

Figure S4. ADME prediction of the compound PRU.