Supporting Information

Identification and molecular mechanism study of novel small molecule inhibitor targeting Solute Carrier Family 7 Member 11 for the treatment of hepatocellular carcinoma

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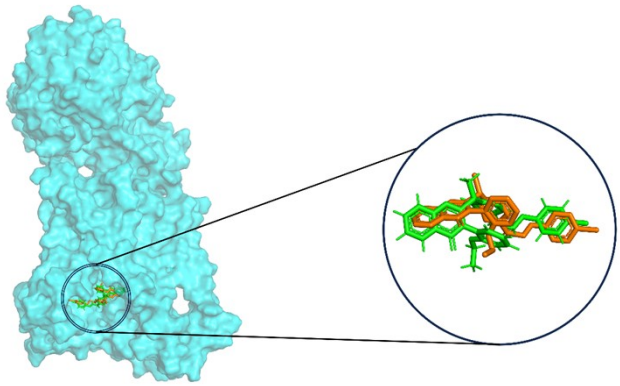

Figure S1. The result of re-docking. Original conformation(orange), The conformation of the re-docking(green)

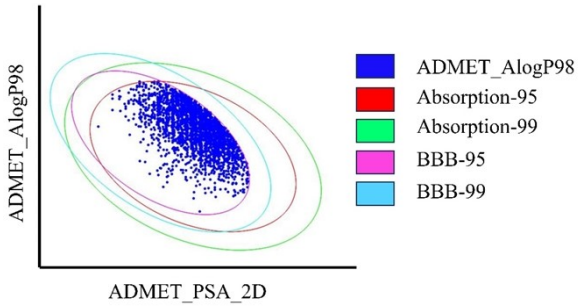

Figure S2. The ADME/T results.

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# *These authors contributed equally to this work.*

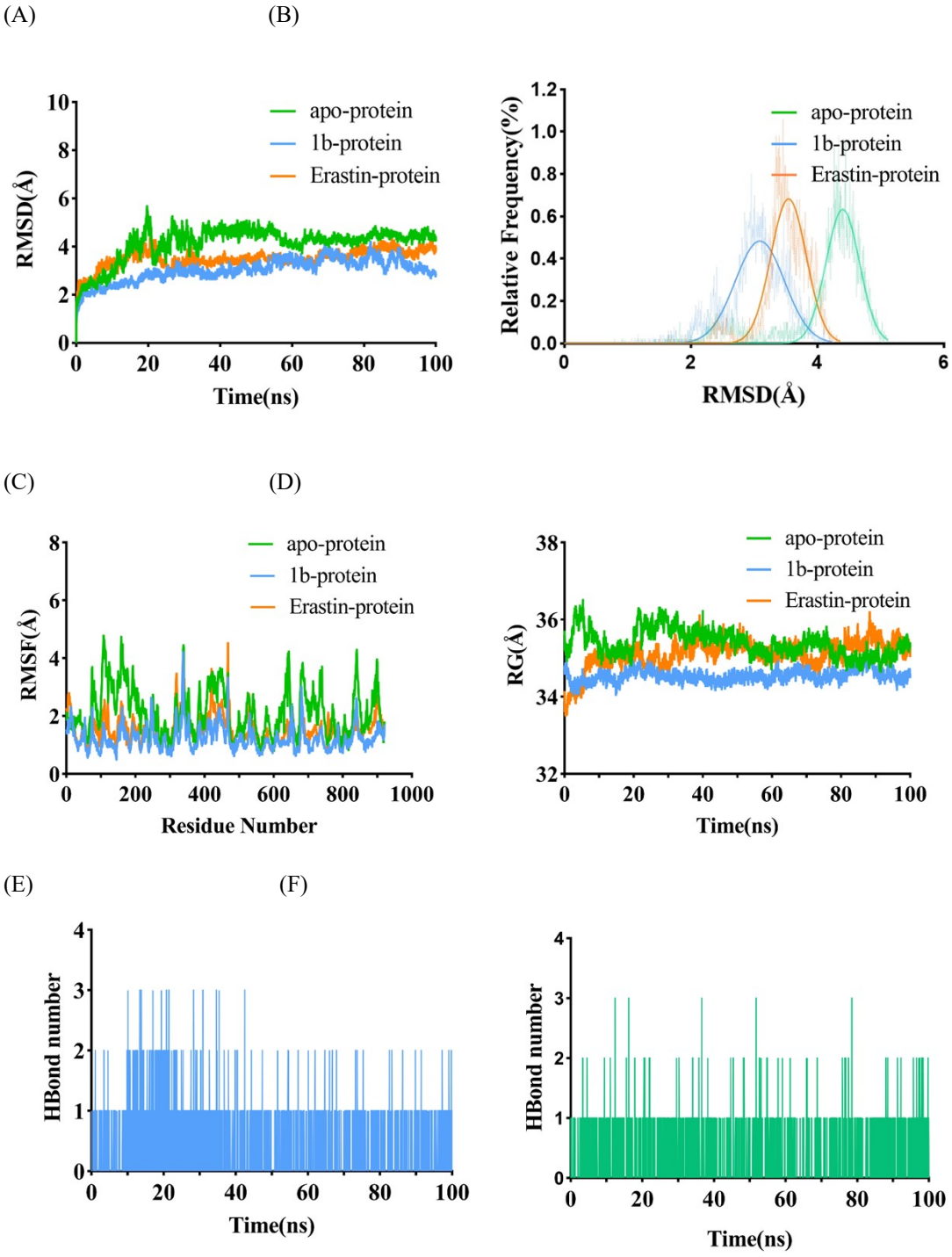

Figure S3. 1b could bind closely with SLC7A11. (A-B) RMSD of αC for apo/1b /Erastin-protein systems. (C) RMSF of each residue for apo/1b/Erastin-protein systems. (D)RG values of apo/1b/Erastin-protein systems. (E) The number of hydrogen bonds for 1b-SLC7A11. (F) The number of hydrogen bonds for Erastin-SLC7A11.

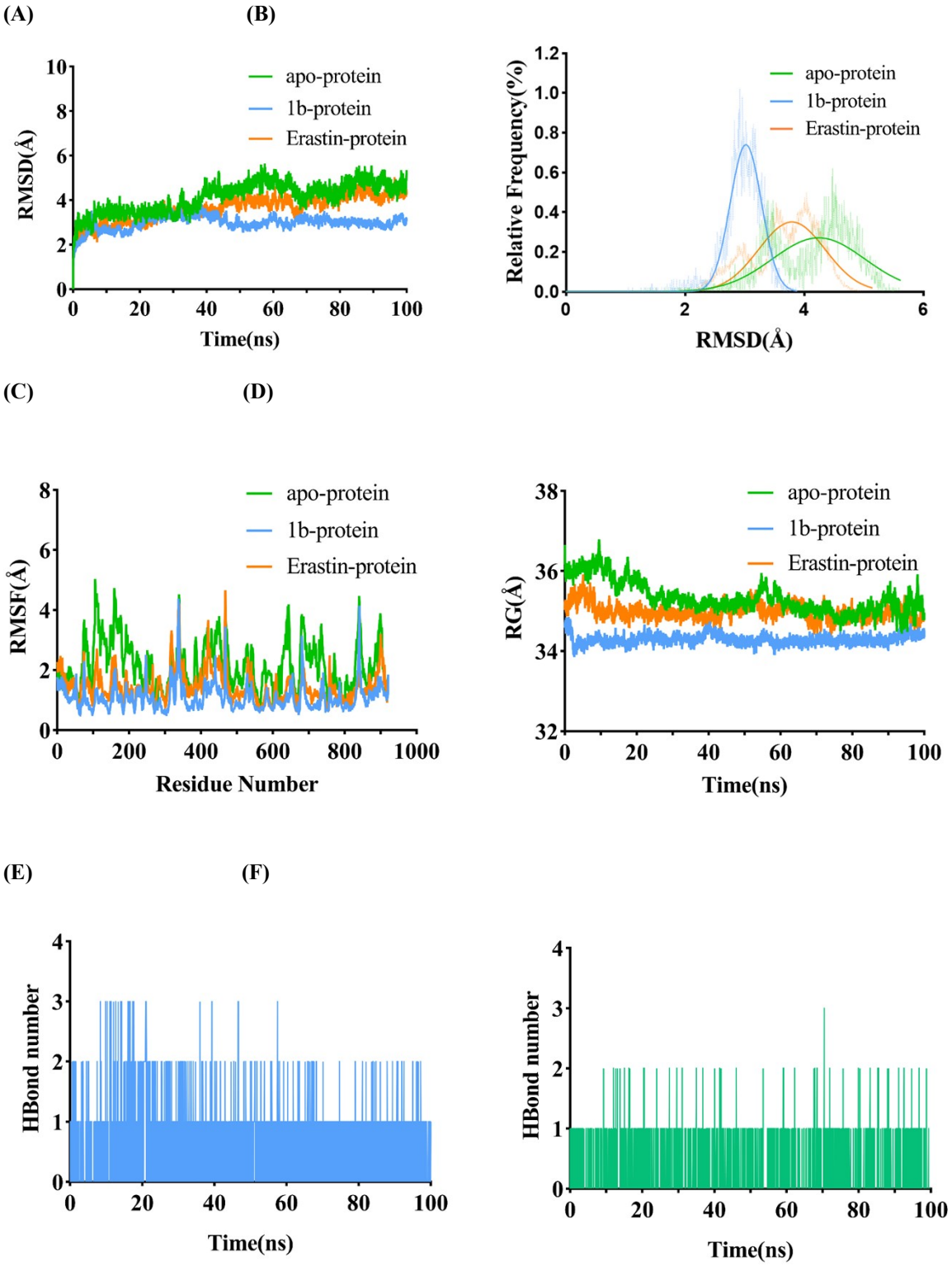

Figure S4. 1b could bind closely with SLC7A11. (A-B) RMSD of αC for apo/1b /Erastin-protein systems. (C) RMSF of each residue for apo/1b/Erastin-protein systems. (D)RG values of apo/1b/Erastin-protein systems. (E) The number of hydrogen bonds for 1b-SLC7A11. (F) The number of hydrogen bonds for Erastin-SLC7A11.

Table S1. The binding free energy for 1b/Erastin-SLC7A11 (kcal/mol)

system	Polar contributions		Non-polar contributions		
	ΔG_{ele}	$\Delta G_{ele,sol}$	ΔG_{vdw}	$\Delta G_{nonpol,sol}$	ΔG_{bind}
1b-SLC7A11	-23.133	36.688	-46.067	-5.671	-38.183
Erastin-SLC7A11	-2.667	18.139	-38.525	-4.928	-27.981

(A) (B)

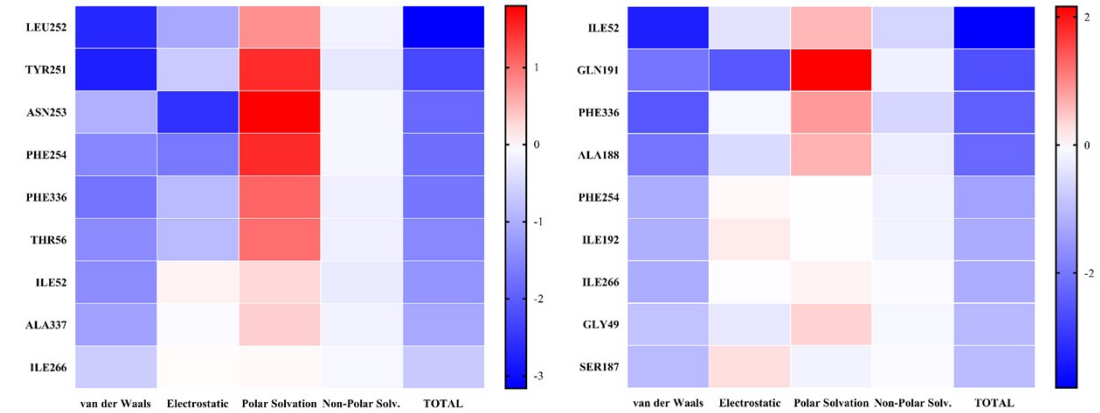

Figure S5. The free energy contribution of key residues. (A)1b-protein. (B) Erastin-protein.

Table S2. The binding free energy for 1b/Erastin-SLC7A11 (kcal/mol)

system	Polar contributions		Non-polar contributions		
	ΔG_{ele}	$\Delta G_{ele,sol}$	ΔG_{vdw}	$\Delta G_{nonpol,sol}$	ΔG_{bind}
1b-SLC7A11	-23.778	36.686	-46.129	-5.616	-38.837
Erastin-SLC7A11	-3.149	18.752	-39.117	-4.900	-28.414

(A) (B)

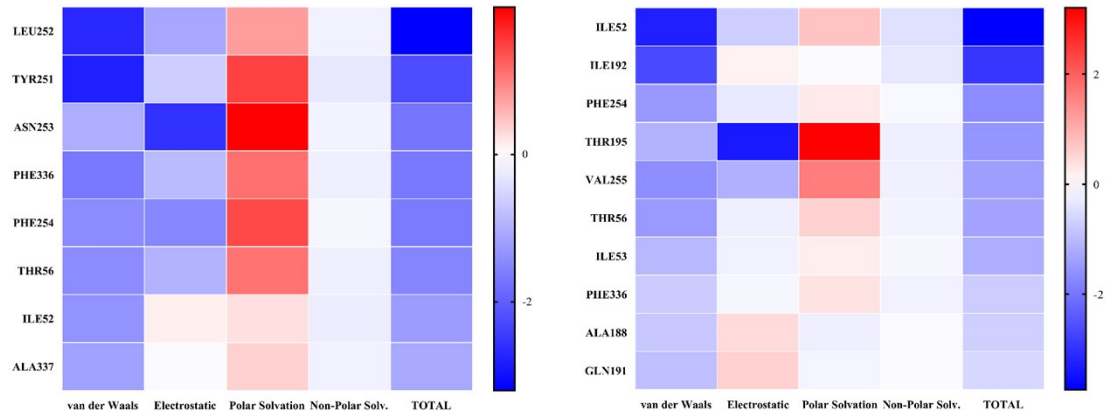

Figure S6. The free energy contribution of key residues. (A)1b-protein. (B) Erastin-protein.