

Electronic Supplementary Information

Rapid Screening Anti-tumor Metastasis Drugs Targeting Integrin Macrophage Antigen-1 by Immobilized Cell Capillary Electrophoresis

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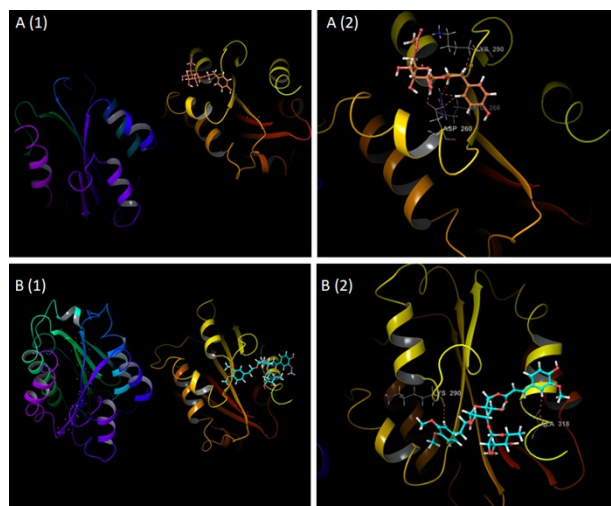


Fig. S2. Docked structures (1) and detailed interaction sites (2) of the representative inactive compounds (A) PhGs-6 and (B) PhGs-1 binding to α -subunit (CD11b) of MAC-1.

Table S1. The results of ICCE and molecular docking study of the twenty-nine compounds.

Compound	Results of ICCE	Ligand docking	GScore (E_{model} value)
PhGs-1	NS	G	-4.010
PhGs-2	NS	NG	-
PhGs-3	NS	G	-3.047
PhGs-4	NS	G	-4.117
PhGs-5	NS	G	-3.726
PhGs-6	N	G	-2.271
PhGs-7	NS	G	-4.321
PhGs-8	NS	NG	-
PhGs-9	N	NG	-
PhGs-10	NS	G	-3.769
PhGs-11	NS	G	-5.104
PhGs-12	Y	G	-10.055
PhGs-13	Y	G	-9.460
PhGs-14	NS	G	-4.709
PhGs-15	NS	G	-4.892
PhGs-16	NS	G	-6.405
PhGs-17	NS	G	-4.105
PhGs-18	NS	NG	-
PhGs-19	Y+NS	G	-10.582
PhGs-20	NS	G	-6.721
PhGs-21	NS	G	-2.782
PhGs-22	N	G	-4.121
PhGs-23	N	NG	-
PhGs-24	N	G	-3.390
PhGs-25	N	G	-4.055
PhGs-26	N	G	-3.227
PhGs-27	NS	G	-5.757
PhGs-28	N	G	-4.456
PhGs-29	N	NG	-

N: have no interaction with any cells;

NS: possess non-specific interaction with cells;

Y: possess specific interaction with MAC-1;

G: Glide docking showed that compounds could enter into the activity pocket of the receptor or had interactions with the receptor;

NG: Glide docking showed that compounds could not have interaction with the receptor;

GScore: the smaller the value of GScore is, the stronger the binding effect is. And it usually makes sense when less than -9.0.