

Table S1. All docking conformations of the pentapeptide WPMGF for ACE.

Conformational ranking	Binding energy (KJ mol ⁻¹)	Ligand efficiency	Inhibition constant (μM)
1	-29.97	-0.16	5.57
2	-28.67	-0.16	9.34
3	-27.55	-0.15	14.78
4	-27.42	-0.15	15.47
5	-27.38	-0.15	15.89
6	-25.50	-0.14	33.88
7	-25.00	-0.14	41.66
8	-23.95	-0.13	62.63
9	-23.49	-0.13	76.36
10	-23.45	-0.13	77.63
11	-22.74	-0.12	102.21
12	-22.53	-0.12	112.27
13	-22.45	-0.12	115.24
14	-22.36	-0.12	119.94
15	-22.24	-0.12	126.08
16	-22.11	-0.12	132.18
17	-21.44	-0.12	173.57
18	-21.02	-0.11	204.35
19	-20.98	-0.11	207.72
20	-20.94	-0.11	212.18
21	-20.94	-0.11	213.30
22	-20.90	-0.11	217.71
23	-20.44	-0.11	261.03
24	-20.27	-0.11	278.45
25	-19.65	-0.11	360.41
26	-19.44	-0.11	390.42
27	-18.64	-0.10	541.06
28	-18.52	-0.10	566.35
29	-18.48	-0.10	572.59
30	-18.48	-0.10	574.95
31	-18.10	-0.10	675.09
32	-17.81	-0.10	749.26
33	-17.43	-0.09	874.01
34	-16.84	-0.09	1120
35	-16.47	-0.09	1280
36	-16.30	-0.09	1370
37	-15.84	-0.09	1670
38	-15.76	-0.09	1730
39	-15.26	-0.08	2110
40	-15.09	-0.08	2270
41	-13.75	-0.07	3900
42	-13.67	-0.07	4000
43	-13.33	-0.07	4610
44	-13.17	-0.07	4910
45	-11.24	-0.06	10610
46	-10.32	-0.06	15350
47	-10.07	-0.05	17100
48	-9.78	-0.05	19160
49	-9.66	-0.05	20350
50	-3.38	-0.02	253970

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binding energy range in this cluster of 1 is 0.00
binding_energy=-7.17
ligand_efficiency=-0.16
inhib_constant=5.57
inhib_constant_units=uM
intermol_energy=-11.94
vdw_hb_desolv_energy=-10.7
electrostatic_energy=-1.24
total_internal=-1.74
torsional_energy=4.77
unbound_energy=-1.74
filename=WPMGF.dlg
cIRMS=0.0
refRMS=68.68
rseed1=None
rseed2=None
```

Figure S1. The calculation of binding energy between pentapeptide WPMGF and ACE

$$\begin{aligned}\Delta G_{\text{binding}} &= \Delta G_{\text{vdW+hb+desolv}} + \Delta G_{\text{elec}} + \Delta G_{\text{intern}} + \Delta G_{\text{tor}} - \Delta G_{\text{unb}} \\ &= -10.7 - 1.24 - 1.74 + 4.77 - (-1.74) = -7.17 \text{ kcal/mol} = -29.97 \text{ kJ/mol}\end{aligned}$$