**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 |

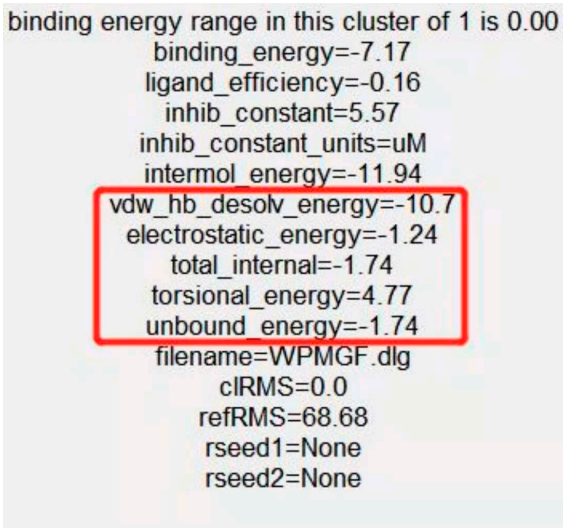


**Figure S1.** The calculation of binding energy between pentapeptide WPMGF and ACE

$$\Delta G_{\text{binding}} = \Delta G_{\text{vdW+hb+desolv}} + \Delta G_{\text{elec}} + \Delta G_{\text{intern}} + \Delta G_{\text{tor}} - \Delta G_{\text{unb}}$$

= -10.7-1.24-1.74+4.77-(-1.74) = -7.17 kcal/mol= -29.97 kJ/mol