



Fig. S1. The structures of the 34 diverse compounds.

Compounds	Docking Score
H1152	-11.9
1	-12.6
2	-12.3
3	-12.2
4	-12.2
5	-12.1
6	-11.9
7	-11.9
8	-11.7
9	-11.7
10	-11.7
11	-11.7
12	-11.6
13	-11.6
14	-11.1
15	-11.1
16	-11.0
17	-10.9
18	-10.8
19	-13.1
20	-12.7
21	-12.2
22	-12.1
23	-12.0
24	-11.7
25	-11.5
26	-11.3
27	-11.3
28	-11.2
29	-11.1
30	-11.1
31	-11.0
32	-10.9
33	-10.8
34	-10.8

Fig. S2. The docking score of compound candidates.