Supplementary Materials

Table S1. The comparisons between the predictions with and without docking on 50 targets selected from the CAMEO-LB dataset between 2016-03-26 and 2016-04-16. [a] results without docking. [b] results after docking, where the ligand-binding pose was the one that matches the best with the consensus binding site prediction. [c] results after docking, where the ligand-binding pose was the one with lowest docking energy. The **Clash** column measures the total number of unique residues having steric clash with the ligand. One residue is defined to have steric clash with the ligand when their closest atomic distance is less than three quarters of the sum of their Van der Waals radii.

No.	PDB ID	Ligand ID	MCC[a]	MCC[b]	MCC[c]	Clash[a]	Clash[b]	Clash[c]
1	4za0B	PAH	0.67	0.41	0.23	3	1	2
2	5fsgA	MTT	0.92	0.92	0.92	1	0	0
3	5ed1D	IHP	0.97	0.8	0.8	0	0	0
4	4yuqB	KS1	0.77	0.77	0.77	2	0	0
5	4z6cA	0KX	0.14	0.14	0.14	0	0	0
6	5iqxA	HEM	0.97	0.85	0.85	2	2	2
7	4uhmA	PLP	1	0.9	0.61	1	0	0
8	5d3xB	4IP	1	0.92	0.76	1	0	0
9	4rfrB	RHN	1	0.9	0.86	0	0	0
10	5j94A	1XF	-0.04	-0.05	-0.04	1	0	0
11	5cfyE	ASP	0.81	0.79	0.79	1	0	0
12	4xf1A	CYS	0.95	0.91	0.79	0	0	0
13	5f8yB	X6X	0.81	0.83	0.83	3	0	0
14	5hv3A	ANP	1	0.89	0.73	0	0	0
15	5hi2A	BAX	0.54	0.62	0.62	2	0	0
16	5esxB	5GP	0.71	0.75	0.69	2	0	0
17	5d75A	FK5	0.78	0.83	0.91	0	0	0
18	5frzB	2MP	0.85	0.86	0.79	0	0	0
19	5et6D	AMP	0.88	0.85	0.78	1	0	0
20	4z7jA	RP5	0.69	0.57	0.57	1	0	0
21	5hidA	B1E	0.56	0.64	0.64	1	0	0
22	5fwjB	MMK	0.75	0.75	0.69	1	0	0
23	5d1nA	SAH	0.89	0.82	0.82	0	0	0
24	5ep4A	ATP	0.62	0.77	0.81	3	0	0
25	5anlA	RBQ	0.74	0.78	0.83	1	0	0
26	4uj1A	NVX	0.78	0.89	0.89	3	3	3
27	5hw0A	GLU	0.94	0.89	0.89	1	0	0
28	5ensC	RHQ	-0.02	-0.02	-0.02	6	1	1
29	5fsyA	AR6	0.82	0.87	0.81	2	0	0

30	5hr6A	SF4	0.18	0.34	0.5	1	0	0
31	5dlpA	MBT	0.2	0.56	0.56	1	0	0
32	4z51A	GNP	0.71	0.79	0.79	7	0	0
33	4y22B	SGA	0.66	0.63	0.63	3	0	0
34	5d0yB	FOL	0.94	0.69	0.69	0	0	0
35	4z6dA	1FZ	-0.04	-0.04	-0.04	1	1	1
36	4z07C	PCG	-0.05	-0.05	-0.05	0	0	0
37	5f8bA	GSH	0.69	0.72	0.65	6	0	0
38	5h8yF	FES	1	0.9	0.34	4	1	1
39	4yvnA	EBS	-0.02	-0.01	-0.01	0	0	0
40	5aniA	ES4	0.62	0.71	0.57	6	0	0
41	4ujaA	4L7	0.84	0.87	0.87	3	3	3
42	5hesB	032	0.65	0.73	0.75	1	0	0
43	5j3uA	CMP	-0.04	-0.05	-0.05	3	0	0
44	5eb4B	FAD	0.91	0.69	0.69	4	1	1
45	5j23B	A2R	0.65	0.64	0.65	0	0	0
46	5hraB	DAS	0.85	0.78	0.78	2	0	0
47	5bw4A	SAM	0.85	0.79	0.72	2	0	0
48	4yx6B	FMN	0.91	0.8	0.8	1	0	0
49	5ihxA	TYR	0.9	1	0.66	0	0	0
50	5fsxA	ADP	0.67	0.74	0.72	2	0	0
51	Average	--	0.67	0.66	0.62	1.72	0.26	0.28