

Table S1. 67 docking cases of the ZDock3-BM3 decoy set used in this study. For each case, i) ZDock 3.0 generated at least one near-native structure among a total of 54,000 decoys and ii) PS-HomPPI is able to generate interface predictions.

Case ID	Bound Complex PDB ID	Case ID	Bound Complex PDB ID	Case ID	Bound Complex PDB ID
1	2HLE	31	1DFJ	61	1KTZ
2	1MAH	32	1AK4	62	1KXQ
3	1B6C	33	2HRK	63	1NW9
4	1JPS	34	1GCQ	64	1EAW
5	1HE1	35	1IQD	65	1EZU
6	2QFW	36	1ML0	66	1OPH
7	1AVX	37	2AJF	67	1GRN
8	1XD3	38	1SBB		
9	1DQJ	39	2MTA		
10	1QA9	40	1ZHI		
11	1CGI	41	1Z5Y		
12	1KAC	42	1MLC		
13	1GPW	43	1KLU		
14	1AZS	44	2NZ8		
15	1GP2	45	1GLA		
16	2I25	46	2SNI		
17	1AHW	47	1AKJ		
18	1NCA	48	1T6B		
19	1K5D	49	1BVK		
20	2PCC	50	1S1Q		
21	2FD6	51	1BJ1		
22	1I4D	52	1Z0K		
23	2CFH	53	2B42		
24	1YVB	54	1PPE		
25	2UUY	55	1R0R		
26	1EWY	56	1VFB		
27	1AY7	57	7CEI		
28	1F51	58	1RLB		
29	1KKL	59	1EFN		
30	1UDI	60	1IJK		