

**Table S3. ClusPro2-BM3\_45 set.** This set contains 45 docking cases, for which i) ClusPro 2.0 returned at least one near-native conformation (a docked conformation with  $L\text{-}RMSD \leq 15$  Å), and ii) PS-HomPPI is able to generate interface predictions for the unbound component proteins.

Case ID	Bound Complex PDB ID	Case ID	Bound Complex PDB ID	Case ID	Bound Complex PDB ID
1	1ACB	16	1HIA	31	1XD3
2	1AVX	17	1IJK	32	1YVB
3	1AY7	18	1IQD	33	1Z0K
4	1B6C	19	1KKL	34	1Z5Y
5	1BVK	20	1KXQ	35	1ZHI
6	1CGI	21	1MAH	36	2B42
7	1D6R	22	1ML0	37	2CFH
8	1DFJ	23	1MLC	38	2HLE
9	1E6J	24	1NW9	39	2HRK
10	1EAW	25	1OPH	40	2MTA
11	1EWY	26	1PPE	41	2NZ8
12	1EZU	27	1R0R	42	2PCC
13	1F51	28	1R8S	43	2SNI
14	1GPW	29	1RLB	44	2UUY
15	1HE1	30	1UDI	45	7CEI