Supplementary Information
The ClusPro web server for protein-protein docking

Dima Kozakov, David R. Hall, Bing Xia, Kathryn A. Porter, Dzmitry Padhorny, Christine Yueh, Dmitri Beglov, Sandor Vajda

TABLE S1 | Performance of ClusPro on Docking Benchmark 4.0[1]

Enzyme-Inhibitor pairs					
Easy (40/41)[a]		**Medium (3/6)[a]**		**Difficult (1/5)[a]**	
No. <10 Å[b]	**Min. IRMSD[c]**	**No. <10 Å**	**Min. IRMSD**	**No. <10 Å**	**Min. IRMSD**
172.3	2.94	42.5	8.21	19.0	15.9
Other type complexes					
Easy (28/59)[a]		**Medium (10/22)[a]**		**Difficult (6/18)[a]**	
No. <10 Å	**Min. IRMSD**	**No. <10 Å**	**Min. IRMSD**	**No. <10 Å**	**Min. IRMSD**
78.8	7.54	59.9	7.09	49.8	10.48
Antibody-antigen pairs (unbound structure of antigen)					
Unbound antibody (7/11)[a]		**Bound antibody (10/11)[a]**		**Unbound Ab + mask (8/11)[a]**	
No. <10 Å	**Min. IRMSD**	**No. <10 Å**	**Min. IRMSD**	**No. <10 Å**	**Min. IRMSD**
66.5	5.0	88.5	1.55	84.0	3.53

[a] Number of complexes that have clusters with < 10 Å IRMSD / Total number of complexes in the given category of the benchmark

[b] Average number of near-native docked structures with < 10 Å IRMSD among the 1000 lowest energy structures

[c] Average value of the lowest IRMSD

1 Hwang, H., Vreven, T., Janin, J. & Weng, Z. Protein-protein docking benchmark version 4.0. *Proteins* **78**, 3111-3114 (2010).