Supporting Information for

Human and Server Docking Prediction for CAPRI Round 30-35 Using LZerD with Combined Scoring Functions

Lenna X. Peterson[†], Hyungrae Kim[†], Juan Esquivel-Rodriguez, Amitava Roy, Xusi Han, Woong-Hee Shin, Jian Zhang, Genki Terashi, Matt Lee, and Daisuke Kihara[*]

† Co-first authors
* To whom correspondence should be addressed
   E-mail: dkihara@purdue.edu

2

Table S1: Templates used for single models

CAPRI	CASP ID	Template(s) used	C_α RMSD (Å)	CASP Stage2 server model	C_α RMSD (Å)
T69	T0764	1qlw	7.9	-	-
T72	T0770	3mx3, 3gzs	5.8	-	-
T75	T0776	4jhl	2.8	Zhang-Server_TS1 (3w7vA 4jhlA 3rjtA 1yzfA)	2.8
T79	T0792	3rco	3.1	-	-
T80	T0801	3a7o	1.8	Baker-Server_TS5 (2fn6A)	1.4
T82	T0805	3bb8, 3dr4, 2oga	4.6	Baker-Server_TS2 (2isjA)	3.2
T84	T0811	4g1k, 1yya, 1btm, 3gvg, 1b9b	1.8	Baker-Server_TS2 (4iotA)	1.6
T85	T0813	3ggoA, 3ggpA, 3ggg_D	4.6	Baker-Server_TS4 (3ktdA)	2.3
T86	T0815	2bng, 4h3u, 2k54A, 3fh1A, 3ff2A	2.0	Baker-Server_TS1 (3ff2A)	2.4
T87	T0819	3get, 3ffh, 3hdoA, 3eucA, 1j32A	3.7	Baker-Server_TS5 (3cq4A)	7.9
T89	T0840	4fwwA, 2uzxB, 3okyA, 3al9A, 3ol2B	7.4	Baker-Server_TS3 (3oktA)	8.9
	T0841	2asuB	9.3	Baker-Server_TS4 (4duuA)	8.7
T90	T0843	3dr4A, 3bb8A, 3b8xA, 1mdoA, 3ogaA	2.6	Baker-Server_TS3 (2fnuA)	2.1
T91	T0847	1byr, 4gel, 1v0w, 3hsi, 2cil	5.4/5.5	Zhang-Server_TS1 (1byrA 1bysA 4gelA 4ggjA 3hsiA)	4.1/5.1
T92	T0849	1m0u, 2on7, 1zl9, 2on5, 2hnl, 1b48, 1yq1	9.6/9.7	Baker-Server_TS1 (3gtuB)	8.1/7.7
T93	T0851	3g79, 3gg2, 2gq4, 2y0c	6.4/7.2	Baker-Server_TS3 (3g79A)	3.1/3.7
T94	T0852	3gff, 2qm0, 1elwA, 4cgwA, 3sz7A, 3q49B	8.5/8.8	Baker-Server_TS1 (3gffB, 1a17A)	10.6/10.8

We did not dock CASP models for T69, T72, and T79.

Table S2: Interface prediction accuracy

Target	Merged			cons-PPISP			BindML -1.5			BindML -0.5		
	Precision	Recall	F1	Precision	Recall	F1	Precision	Recall	F1	Precision	Recall	F1
T69	0.59	0.29	0.39	0.85	0.25	0.39	0.45	0.13	0.20	0.40	0.43	0.41
T72	0.05	0.08	0.06	0.06	0.04	0.05	0.04	0.04	0.04	0.11	0.32	0.16
T75	0.00	0.00	-	0.00	0.00	-	0.00	0.00	-	0.00	0.00	-
T79	0.48	0.55	0.51	0.52	0.55	0.54	0.33	0.05	0.09	0.39	0.45	0.42
T80	0.83	0.56	0.67	1.00	0.38	0.56	0.68	0.25	0.37	0.58	0.77	0.66
T82	0.71	0.30	0.42	0.69	0.25	0.37	0.77	0.13	0.22	0.81	0.38	0.51
T84	0.92	0.55	0.69	0.95	0.45	0.61	0.92	0.29	0.44	0.57	0.60	0.58
T85	0.97	0.28	0.44	0.95	0.18	0.30	1.00	0.20	0.33	0.86	0.51	0.64
T86	0.21	0.67	0.32	0.23	0.56	0.32	0.14	0.11	0.13	0.15	0.44	0.22
T87	0.71	0.24	0.36	0.85	0.19	0.31	0.61	0.12	0.20	0.58	0.49	0.53
T89A	0.00	0.00	-	0.00	0.00	-	0.00	0.00	-	0.04	0.22	0.07
T89B	0.38	0.52	0.44	0.57	0.52	0.55	0.00	0.00	-	0.15	0.26	0.19
T90	0.74	0.38	0.50	0.80	0.26	0.40	0.71	0.20	0.31	0.61	0.70	0.65
T91	0.50	0.38	0.43	0.50	0.29	0.37	0.64	0.21	0.31	0.47	0.47	0.47
T92	0.52	0.29	0.37	0.59	0.25	0.35	0.35	0.12	0.17	0.41	0.35	0.38
T93	0.63	0.48	0.54	0.90	0.29	0.43	0.50	0.25	0.34	0.41	0.60	0.49
T94	0.23	0.30	0.26	0.10	0.07	0.08	0.33	0.27	0.30	0.23	0.60	0.33
Average	0.53	0.37	0.43	0.60	0.28	0.37	0.47	0.15	0.25	0.42	0.47	0.42

Merged: performance of the union of cons-PPISP and BindML -1.5 (residues predicted by either or both methods are predicted); BindML -1.5: using residues with a BindML score $\leq$ -1.5; BindML -0.5: using residues with a BindML score $\leq$ -0.5. Precision: (number of true positives)/(number of predicted positives); recall: (number of true positives)/(number of actual positives); F1: $2 \cdot$ precision $\cdot$ recall/(precision + recall). Dash (-) indicates that F1-score is not defined because both precision and recall are 0.

Table S3: Weights from logistic regression jackknife

Test Target	w0	w1	w2	w3	w4	w5
T75	-8.0912938449	-1.3688033399	-1.1778600548	0.7416239669	-0.3048333114	0.2545596097
T79	-8.3856541051	-0.9680873403	-0.9665509229	0.1769041945	-0.3535433522	0.2430590138
T80	-8.0451115545	-1.4163465989	-1.1499677208	0.7185715482	-0.3214804879	0.3597015568
T82	-8.0549823421	-1.4334898546	-1.2039798006	0.8042730071	-0.3320483466	0.3057084964
T84	-8.1089437095	-1.6282930902	-1.1467776187	1.0065735415	-0.3374461165	0.2614221816
T85	-8.2944007666	-1.6079657992	-1.3438787349	0.8290172284	-0.242946187	0.2611811393
T86	-8.0999457755	-1.4499203121	-1.1643743389	0.7705576998	-0.3393187931	0.3013481081
T87	-8.0494813094	-1.4498981529	-1.1939380594	0.8178968052	-0.3264398359	0.2869129142
T89	-8.3137167824	-1.4865869155	-1.2349909885	0.7694494879	-0.4017608443	0.3603071605
T90	-8.0749774294	-1.4170091338	-1.1734387315	0.6909266437	-0.3062337066	0.3124370648
T91	-8.2434229598	-1.3924785603	-0.9816516829	0.8970070256	-0.3508178207	-0.0322659103
T92	-8.1438700968	-1.435794271	-1.2643686133	0.8484427573	-0.3558522077	0.2885377551
T93	-8.0805300855	-1.3676542526	-1.1930640645	0.709531422	-0.3275865894	0.2726405379

Each row represents one subsample of the jackknife procedure. For example, in row T75, targets T79-T93 were used as the training set and target T75 was used as the test set. w0 is the intercept and w1-w5 are weights for the Z-scores of DFIRE, GOAP, ITScorePro, OPUS-PSP, and SOAP-PP, respectively.