

# **MEGADOCK: An all-to-all protein-protein interaction prediction system using tertiary structure data**

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**Additional tables (Table S1, S2, S3, S4, S5 and S6) and figures (Figure S1, S2 and S3) referred to in the main article.**

**Table S1. Docking prediction performance of MEGADOCK and ZDOCK for the bound docking test cases in Benchmark 4.0.** #NND denotes the number of near-native decoy in the top 3,600 predictions, Best Rank is the rank of first near-native decoy, and L-RMSD is the Ligand RMSD of first near-native decoy.

	MEGADOCK 1.0			MEGADOCK 2.0			MEGADOCK 2.1			ZDOCK 3.0		
	#NND	Best Rank	L-RMSD	#NND	Best Rank	L-RMSD	#NND	Best Rank	L-RMSD	#NND	Best Rank	L-RMSD
Rigid-body (121)												
1AHW	0	-	-	1	5	1.92	1	2	1.92	1	3	1.99
1BVK	0	-	-	4	250	4.85	4	183	1.75	3	91	2.07
1DQJ	0	-	-	5	3	1.99	6	4	1.99	4	1	1.51
1E6J	0	-	-	1	1258	1.92	0	-	-	2	170	2.33
1JPS	1	3517	4.72	3	4	1.99	3	4	1.99	2	38	2.41
1MLC	0	-	-	1	607	1.91	1	482	1.91	6	12	2.39
1VFB	0	-	-	2	107	1.51	2	130	1.59	1	77	1.65
1WEJ	0	-	-	2	883	1.55	3	872	1.55	5	17	1.57
2FD6	0	-	-	0	-	-	0	-	-	1	21	1.74
2I25	0	-	-	6	1	1.24	5	2	1.24	6	1	3.16
2VIS	0	-	-	0	-	-	0	-	-	2	252	3.27
1BJ1	0	-	-	3	39	3.15	3	69	2.10	3	2	2.70
1FSK	0	-	-	3	13	1.33	2	6	1.33	3	1	1.71
1I9R	0	-	-	0	-	-	0	-	-	1	514	3.07
1HQD	0	-	-	1	28	1.46	1	16	1.46	3	1	1.93
1K4C	0	-	-	1	34	2.16	2	10	2.16	3	2	2.25
1KXQ	6	10	3.01	5	8	1.33	5	10	1.33	5	1	1.36
1NCA	0	-	-	1	7	2.04	1	5	2.04	1	5	1.85
1NSN	3	719	4.87	3	727	4.33	3	291	1.36	4	39	2.16
2QFW	0	-	-	2	82	2.37	2	80	2.37	1	52	1.81
1QFW	0	-	-	1	214	3.88	1	116	3.88	1	375	3.65
2JEL	0	-	-	4	120	2.22	5	97	1.09	7	6	1.26
1AVX	0	-	-	3	8	2.56	3	7	2.56	4	1	2.47
1AY7	2	453	3.26	4	14	3.42	4	5	1.81	7	15	2.05
1BVN	7	3	3.70	10	1	4.28	8	1	2.93	15	1	1.91
1CGI	3	155	3.25	11	1	1.02	10	1	1.02	11	1	1.33
1CLV	24	1	2.95	23	1	1.99	25	1	1.51	35	1	1.78
1D6R	0	-	-	5	4	1.40	7	3	1.85	2	1597	1.51
1DFJ	2	10	3.46	2	62	2.21	2	19	2.21	2	1	4.10
1E6E	4	138	2.37	2	34	1.33	5	2	1.33	5	1	1.15
1EAW	1	1739	4.72	6	1	1.46	6	1	1.46	4	3	1.55
1EWY	6	798	4.94	2	833	1.03	1	607	1.18	6	5	1.71
1EZU	1	180	2.41	2	1	2.10	2	1	2.10	1	1	2.06
1F34	2	4	2.38	2	1	1.74	2	1	1.74	3	1	1.79
1FLE	5	1022	3.62	6	2	0.84	7	1	0.84	8	1	1.43
1GL1	12	31	2.14	14	1	0.99	14	1	0.99	15	1	1.38
1GXD	0	-	-	1	79	1.72	1	13	1.72	1	3	2.47
1HIA	3	612	2.69	10	1	1.05	12	1	1.23	10	3	1.39
1JTG	5	21	2.99	5	1	0.91	5	1	1.35	5	1	1.23
1MAH	6	187	1.99	9	1	1.52	9	1	1.37	8	1	1.52
1N8O	2	2397	1.90	3	1	2.44	3	1	2.44	2	1	2.99
1OC0	7	428	2.13	7	39	0.93	9	5	0.93	10	3	1.11
1OPH	0	-	-	3	329	1.53	4	212	1.53	5	67	1.42
BOYV	0	-	-	1	78	2.37	1	1178	2.37	0	-	-
1OYV	1	2124	4.06	5	1	1.69	5	1	1.69	4	1	1.86
1PPE	7	61	3.03	22	1	1.43	22	1	1.43	22	1	2.39
1R0R	6	155	3.13	13	3	1.01	13	3	1.01	11	3	1.29
1TMQ	3	124	1.20	2	1	1.81	2	1	1.81	5	1	2.07
1UDI	8	1	1.57	10	1	1.31	11	1	1.31	10	1	1.18
1YVB	1	761	3.02	1	4	2.63	1	10	1.57	2	1	2.76
2ABZ	5	348	4.09	11	3	2.57	9	7	2.57	8	21	3.16
2B42	2	215	2.67	6	1	1.42	5	1	1.42	5	1	1.68
2J0T	0	-	-	2	3	1.58	1	7	1.49	2	59	1.43
2MTA	0	-	-	5	126	1.25	5	79	1.25	11	1	2.57
2O8V	1	1451	3.90	7	1	1.08	7	1	1.08	9	1	1.47
2OUL	1	736	3.20	3	1	1.24	3	1	1.24	2	2	2.05
2PCC	3	1501	3.45	0	-	-	0	-	-	2	31	1.79
2SIC	1	1720	3.46	4	1	1.85	4	2	1.85	5	1	1.98
2SNI	0	-	-	9	1	1.61	9	1	1.61	8	1	2.01
2UUY	0	-	-	8	1	1.64	8	1	1.64	9	5	2.89
3SGQ	8	83	3.85	10	9	0.78	7	7	3.92	5	70	3.51
7CEI	3	1132	4.00	7	1	1.36	6	1	1.36	5	2	4.77
1A2K	0	-	-	2	143	1.75	2	79	1.75	3	1	2.30

1AK4	0	-	-	0	-	-	0	-	-	2	44	2.20
1AKJ	3	26	4.08	1	325	1.40	2	56	1.93	2	4	1.48
1AZS	0	-	-	2	158	1.78	2	37	1.84	2	1	2.34
1B6C	1	1188	2.81	2	2	1.92	2	3	1.92	1	1	1.76
1BUH	0	-	-	5	27	1.47	3	70	1.47	7	5	2.02
1E96	0	-	-	0	-	-	0	-	-	1	1825	4.73
1EFN	4	89	3.20	4	5	2.86	7	3	2.86	16	1	3.03
1F51	6	32	4.68	4	7	1.30	5	6	1.30	6	8	1.23
1FC2	0	-	-	2	36	1.71	2	41	1.71	2	7	4.15
1FCC	0	-	-	3	235	1.32	2	324	1.32	1	496	1.29
1FFW	4	623	4.98	2	526	0.89	3	123	0.89	14	2	3.29
1FQJ	0	-	-	1	376	1.81	1	205	1.81	2	193	1.68
1GCQ	8	37	3.01	9	1	1.35	8	1	1.35	9	3	1.37
1GHQ	0	-	-	0	-	-	0	-	-	0	-	-
1GLA	1	3311	1.27	1	3181	4.10	3	1538	1.95	8	14	2.18
1GPW	1	29	2.20	4	1	1.63	4	1	1.63	3	2	1.99
1H9D	2	60	1.95	4	1	3.32	5	1	1.64	5	1	2.36
1HCF	3	7	2.20	2	8	1.31	3	2	1.31	4	5	1.89
1HE1	1	26	2.54	5	1	1.44	4	1	1.44	4	1	1.77
1I4D	0	-	-	2	356	1.46	0	-	-	4	1	1.56
1J2J	1	992	1.83	5	115	1.15	6	71	1.15	10	1	1.91
1JWH	0	-	-	0	-	-	0	-	-	1	83	1.84
1K74	1	69	2.67	1	6	2.46	2	1	2.46	2	1	2.39
1KAC	0	-	-	1	492	1.76	1	41	1.76	5	5	3.42
1KLU	0	-	-	0	-	-	0	-	-	1	4	2.26
1KTZ	0	-	-	0	-	-	2	221	1.59	7	76	1.62
1KXP	1	1	1.69	1	1	2.51	1	1	2.51	1	1	2.14
1ML0	5	29	4.34	7	1	1.65	8	1	1.65	12	1	1.78
1OFU	0	-	-	0	-	-	0	-	-	2	1	1.74
1PVH	0	-	-	1	642	2.03	1	1051	2.03	2	75	1.81
1QA9	0	-	-	0	-	-	2	40	1.03	5	24	1.46
1RLB	0	-	-	0	-	-	0	-	-	2	14	1.79
1RV6	5	141	2.24	2	201	1.72	3	140	1.55	8	1	1.72
1S1Q	3	1298	3.43	3	538	0.99	3	175	1.08	3	54	1.60
1SBB	0	-	-	1	2278	4.71	1	2245	2.74	0	-	-
1T6B	0	-	-	1	118	1.66	1	49	1.66	3	1	2.66
1US7	0	-	-	0	-	-	0	-	-	1	310	2.81
1WDW	1	3	2.00	2	1	1.49	2	1	1.49	2	1	2.53
1XD3	0	-	-	3	1	1.05	3	1	1.05	8	1	1.77
1XU1	2	797	2.47	10	1	0.98	12	1	0.98	16	3	3.14
1Z0K	6	13	4.14	8	1	0.80	7	1	2.38	7	1	0.92
1Z5Y	0	-	-	3	43	2.00	3	67	2.00	3	1	2.11
1ZHH	0	-	-	2	7	1.52	1	6	1.52	3	1	2.28
1ZHI	0	-	-	2	465	1.13	2	196	1.13	2	4	2.14
2A5T	1	507	2.99	2	37	2.21	2	28	1.69	2	2	2.03
2A9K	1	770	2.45	2	1	2.20	2	1	1.70	1	1	2.03
2AJF	0	-	-	0	-	-	0	-	-	1	158	1.88
2B4J	0	-	-	3	79	1.77	3	24	1.77	5	81	3.65
2BTF	2	147	1.72	5	4	1.33	5	1	2.89	5	6	1.24
2FJU	0	-	-	0	-	-	0	-	-	2	3	1.39
2G77	4	42	2.81	5	1	1.85	5	1	1.43	4	1	2.18
2HLE	0	-	-	4	3	1.81	4	2	1.81	4	2	1.86
2HQS	4	11	1.86	3	4	1.09	5	2	1.09	3	3	1.71
2OOB	0	-	-	0	-	-	0	-	-	0	-	-
2OOR	2	718	2.01	3	1	1.73	3	1	2.20	4	1	1.68
2VDB	0	-	-	7	3	1.02	7	2	1.02	10	1	3.37
3BP8	0	-	-	2	952	0.99	1	1562	4.00	3	429	3.10
3D5S	1	202	3.07	3	6	0.88	4	6	0.88	4	5	1.28

Medium Difficulty (30)

1BGX	1	1	4.72	1	1	2.97	1	1	2.97	1	1	3.10
1ACB	2	1664	4.53	5	2	1.49	5	9	1.49	12	2	4.52
1IJK	1	400	1.94	1	1463	2.20	1	63	1.84	2	1	1.79
1JIW	0	-	-	3	10	1.22	3	6	0.88	4	1	1.28
1KKL	2	222	2.66	1	733	4.05	1	404	4.05	6	510	3.54
1M10	1	205	3.07	1	32	2.93	1	1	2.93	2	1	3.40
1NW9	6	7	1.82	6	1	1.43	6	1	1.22	7	1	2.07
4CPA	2	2301	3.67	16	6	2.95	14	5	2.95	21	2	4.10
1GP2	0	-	-	1	167	2.30	1	12	2.30	2	1	2.22
1GRN	0	-	-	4	1	1.42	4	1	1.42	3	1	1.74
1HE8	0	-	-	0	-	-	0	-	-	1	421	4.29
1I2M	2	1	2.46	2	1	1.69	1	1	1.69	1	1	1.73
1IB1	1	43	2.33	1	18	3.02	2	9	3.02	2	40	1.62
1K5D	1	455	2.34	1	5	1.69	1	1	1.69	2	1	1.73

1LFD	1	446	1.91	3	24	1.32	5	3	1.32	5	5	1.10
1MQ8	0	-	-	3	1144	4.94	2	1216	1.97	2	261	2.27
1N2C	1	24	2.26	2	1	2.17	2	2	2.17	2	1	2.08
1R6Q	4	679	1.97	4	16	1.40	4	7	1.40	3	66	1.39
1SYX	2	290	2.77	4	146	1.55	6	5	1.55	5	435	3.38
1WQ1	3	5	1.94	5	1	1.04	4	1	1.04	3	1	1.82
1XQS	0	-	-	1	1	1.81	2	1	1.81	1	1	1.79
2AYO	0	-	-	9	1	1.48	10	1	1.48	7	1	2.15
2CFH	4	32	2.71	5	1	1.28	5	1	1.28	6	1	1.57
2H7V	0	-	-	1	500	1.56	1	309	1.56	2	1	2.29
2HRK	4	318	1.94	4	15	1.17	3	8	1.17	5	5	2.54
2J7P	1	1	2.59	2	1	1.67	2	1	1.67	1	1	1.49
2NZ8	4	106	4.75	3	16	1.81	3	12	1.81	3	1	1.82
2OZA	1	2	3.49	1	1	1.66	1	1	1.66	1	1	1.98
2Z0E	2	110	3.11	2	1	1.16	2	1	2.12	3	1	1.55
3CPH	0	-	-	1	418	1.74	2	160	1.74	3	1	2.06
Difficult (25)												
1E4K	0	-	-	1	1000	1.91	1	552	1.91	1	688	2.55
2HMI	0	-	-	0	-	-	0	-	-	1	10	4.53
1F6M	2	456	2.55	5	18	1.02	7	15	4.07	8	1	2.16
1FQ1	1	612	2.54	1	253	1.58	1	48	1.58	1	11	1.98
1PXV	2	298	2.08	5	1	1.01	4	1	1.01	6	1	2.05
1ZLI	3	5	4.02	6	1	1.35	6	1	1.35	6	1	4.29
2O3B	2	38	2.49	2	142	1.27	2	22	1.29	2	1	1.41
1ATN	0	-	-	2	154	1.57	2	175	3.86	2	1	1.59
1BKD	3	1	2.08	5	1	1.99	5	1	1.99	4	1	1.94
1DE4	0	-	-	1	359	2.89	1	426	2.89	1	1	3.61
1EER	1	274	3.87	1	1	2.54	1	1	2.54	1	1	2.70
1FAK	2	42	2.76	4	1	1.95	4	1	1.95	3	1	1.95
1H1V	0	-	-	1	514	2.05	0	-	-	0	-	-
1IBR	1	8	3.32	1	3	2.50	1	1	2.09	1	1	2.13
1IRA	5	8	2.34	5	1	1.09	5	1	1.09	3	1	1.50
1JK9	2	1380	2.27	3	1	1.13	3	6	1.13	4	1	1.41
1JMO	2	892	2.41	3	1	1.34	3	1	1.34	3	1	1.71
1JZD	1	1368	1.97	1	32	1.24	2	19	1.42	4	1	1.98
1R8S	1	1	1.98	4	1	1.47	4	1	1.47	5	1	1.81
1Y64	1	911	1.61	1	64	1.83	1	9	1.83	1	114	2.28
1ZM4	0	-	-	1	1022	4.60	1	539	4.60	1	11	1.54
2C0L	1	1800	3.13	2	2	1.88	2	1	1.88	2	1	1.51
2I9B	1	973	1.80	2	2	1.60	3	1	1.60	3	1	1.83
2IDO	4	102	1.86	7	1	1.70	7	1	1.70	7	1	1.60
2OT3	1	498	2.60	4	1	2.03	4	1	1.84	5	1	1.31

**Table S2. Docking prediction performance of MEGADOCK and ZDOCK for the unbound docking test cases in Benchmark 4.0.** #NND denotes the number of near-native decoy in the top 3,600 predictions, Best Rank is the rank of first near-native decoy, and L-RMSD is the Ligand RMSD of first near-native decoy.

	MEGADOCK 1.0			MEGADOCK 2.0			MEGADOCK 2.1			ZDOCK 3.0		
	#NND	Best Rank	L-RMSD	#NND	Best Rank	L-RMSD	#NND	Best Rank	L-RMSD	#NND	Best Rank	L-RMSD
Rigid-body (121)												
1AHW	0	-	-	1	526	3.29	1	1490	2.99	1	1621	2.52
1BVK	0	-	-	1	3510	4.69	0	-	-	3	321	4.32
1DQJ	0	-	-	0	-	-	0	-	-	0	-	-
1E6J	0	-	-	2	2146	4.15	1	2574	4.15	2	124	4.24
1JPS	1	3152	4.15	1	681	2.78	2	571	2.78	1	1171	3.53
1MLC	0	-	-	0	-	-	0	-	-	4	56	3.54
1VFB	0	-	-	1	3162	4.57	0	-	-	1	1905	4.93
1WEJ	0	-	-	1	2887	4.44	2	2980	4.12	6	155	1.88
2FD6	0	-	-	0	-	-	0	-	-	0	-	-
2I25	0	-	-	0	-	-	0	-	-	6	9	1.82
2VIS	0	-	-	0	-	-	0	-	-	0	-	-
1BJ1	0	-	-	1	222	4.67	1	785	4.11	3	1	4.29
1FSK	0	-	-	4	27	1.83	4	12	1.83	4	1	2.12
1I9R	0	-	-	0	-	-	0	-	-	0	-	-
1IQD	0	-	-	1	2348	4.38	1	1998	4.72	2	50	4.48
1K4C	0	-	-	0	-	-	0	-	-	2	2087	1.91
1KXQ	3	200	3.91	3	101	4.79	2	115	4.79	1	1	1.37
1NCA	0	-	-	1	68	2.73	1	106	2.73	1	188	1.97
1NSN	2	1409	4.53	0	-	-	0	-	-	0	-	-
2QFW	0	-	-	1	636	3.49	1	543	3.49	1	49	4.34
1QFW	0	-	-	0	-	-	0	-	-	1	291	3.26
2JEL	0	-	-	2	2156	3.33	1	1957	3.74	10	118	4.38
1AVX	0	-	-	1	471	4.25	1	686	4.25	1	235	3.16
1AY7	4	1233	3.69	4	1252	3.86	3	1225	4.43	3	1525	4.96
1BVN	4	5	4.25	8	42	4.68	8	11	4.08	8	2	4.28
1CGI	1	1019	4.77	1	107	4.29	1	96	4.29	6	154	4.86
1CLV	1	157	4.35	3	188	4.74	4	99	4.74	16	1	3.22
1D6R	0	-	-	2	1492	4.26	2	1409	4.26	0	-	-
1DFJ	2	32	4.07	1	17	2.69	1	3	2.69	1	2	2.83
1E6E	2	1600	2.98	1	2822	4.98	3	1202	2.99	7	16	3.16
1EAW	1	2586	4.85	7	24	3.36	6	42	4.13	7	45	4.64
1EWY	7	631	4.69	1	1896	3.69	3	259	4.96	6	10	4.78
1EZU	0	-	-	1	1405	3.53	1	2759	3.53	1	2498	3.02
1F34	2	488	2.80	1	515	2.00	1	128	2.55	1	702	3.12
1FLE	0	-	-	0	-	-	0	-	-	0	-	-
1GL1	0	-	-	6	562	4.72	2	1109	4.72	3	256	3.69
1GXD	0	-	-	0	-	-	0	-	-	0	-	-
1HIA	0	-	-	0	-	-	0	-	-	0	-	-
1JTG	4	2	3.87	4	3	2.65	4	2	3.32	4	1	3.39
1MAH	0	-	-	6	69	2.22	5	35	4.04	7	1	3.97
1N8O	0	-	-	1	132	2.67	1	215	2.67	2	4	2.86
1OC0	0	-	-	0	-	-	0	-	-	0	-	-
1OPH	0	-	-	0	-	-	0	-	-	0	-	-
BOYV	0	-	-	0	-	-	0	-	-	0	-	-
1OYV	2	936	4.67	3	79	3.92	3	128	4.15	2	157	4.39
1PPE	5	178	3.88	15	1	3.08	16	1	3.08	16	1	2.66
1R0R	4	935	3.78	7	148	2.74	7	199	2.74	6	605	2.42
1TMQ	1	89	2.32	3	104	2.30	1	1028	2.44	4	12	4.89
1UDI	2	1485	4.32	3	64	4.37	3	8	4.37	3	67	3.93
1YVB	0	-	-	1	163	3.94	1	180	4.47	0	-	-
2ABZ	1	801	4.49	0	-	-	1	1482	4.78	0	-	-
2B42	0	-	-	1	133	2.40	1	120	2.40	3	1	1.83
2J0T	0	-	-	0	-	-	1	929	4.91	0	-	-
2MTA	0	-	-	1	3384	1.84	1	3561	1.84	7	214	4.65
2O8V	0	-	-	0	-	-	0	-	-	0	-	-
2OUL	1	1246	2.48	2	1	1.92	3	1	1.92	3	1	2.26
2PCC	0	-	-	0	-	-	0	-	-	0	-	-
2SIC	0	-	-	1	844	3.08	1	1328	3.08	2	2	2.38
2SNI	0	-	-	0	-	-	0	-	-	3	1464	3.63
2UUY	0	-	-	1	1597	4.40	1	1484	4.40	1	3127	4.61
3SGQ	0	-	-	3	28	4.08	3	38	4.08	3	792	2.11
7CEI	0	-	-	2	374	3.77	2	38	2.84	2	23	3.94
1A2K	0	-	-	0	-	-	0	-	-	1	2973	4.56

1AK4	0	-	-	0	-	-	0	-	-	0	-	-
1AKJ	2	305	4.83	0	-	-	0	-	-	1	1455	3.33
1AZS	0	-	-	0	-	-	0	-	-	1	98	2.55
1B6C	0	-	-	1	740	3.33	1	885	3.33	1	24	3.18
1BUH	0	-	-	0	-	-	0	-	-	8	47	4.65
1E96	0	-	-	0	-	-	0	-	-	0	-	-
1EFN	0	-	-	0	-	-	0	-	-	0	-	-
1F51	2	2253	4.56	1	345	4.38	1	318	4.38	1	1516	3.06
1FC2	0	-	-	0	-	-	0	-	-	0	-	-
1FCC	0	-	-	0	-	-	0	-	-	0	-	-
1FFW	0	-	-	0	-	-	0	-	-	2	77	4.85
1FQJ	0	-	-	0	-	-	0	-	-	0	-	-
1GCQ	0	-	-	0	-	-	0	-	-	0	-	-
1GHQ	0	-	-	0	-	-	0	-	-	0	-	-
1GLA	0	-	-	0	-	-	0	-	-	0	-	-
1GPW	4	12	2.49	2	16	2.25	3	16	4.23	1	87	2.40
1H9D	1	1424	4.94	3	132	4.07	2	474	4.07	2	364	4.58
1HCF	0	-	-	0	-	-	0	-	-	3	90	4.28
1HE1	1	48	3.76	1	385	4.09	1	595	4.09	0	-	-
1I4D	0	-	-	0	-	-	0	-	-	1	1020	4.85
1J2J	0	-	-	0	-	-	0	-	-	0	-	-
1JWH	0	-	-	0	-	-	0	-	-	2	171	2.48
1K74	1	8	4.35	1	403	3.80	1	9	4.49	1	5	3.49
1KAC	1	805	4.63	1	2487	4.14	2	1351	4.27	1	1801	4.26
1KLU	0	-	-	0	-	-	0	-	-	0	-	-
1KTZ	0	-	-	0	-	-	0	-	-	0	-	-
1KXP	1	7	3.04	0	-	-	1	18	3.12	2	1	3.63
1ML0	3	529	4.17	3	70	3.85	4	45	3.85	6	35	3.59
1OFU	0	-	-	0	-	-	0	-	-	1	39	2.41
1PVH	0	-	-	0	-	-	0	-	-	3	1528	4.70
1QA9	0	-	-	0	-	-	0	-	-	0	-	-
1RLB	0	-	-	0	-	-	0	-	-	0	-	-
1RV6	2	3038	2.34	1	1642	2.24	1	2378	2.19	3	1	2.45
1S1Q	3	693	4.25	3	580	4.85	3	1167	2.62	4	494	4.48
1SBB	0	-	-	0	-	-	0	-	-	0	-	-
1T6B	0	-	-	0	-	-	0	-	-	1	234	3.16
1US7	0	-	-	0	-	-	0	-	-	2	849	4.24
1WDW	1	299	3.17	1	8	2.15	1	9	2.15	2	4	2.87
1XD3	0	-	-	0	-	-	0	-	-	8	5	4.85
1XU1	0	-	-	0	-	-	0	-	-	0	-	-
1Z0K	0	-	-	0	-	-	1	837	4.87	0	-	-
1Z5Y	0	-	-	0	-	-	0	-	-	3	104	4.99
1ZHH	0	-	-	0	-	-	0	-	-	0	-	-
1ZHI	0	-	-	0	-	-	0	-	-	2	87	4.47
2A5T	0	-	-	0	-	-	0	-	-	0	-	-
2A9K	0	-	-	0	-	-	0	-	-	0	-	-
2AJF	0	-	-	0	-	-	0	-	-	0	-	-
2B4J	0	-	-	0	-	-	0	-	-	0	-	-
2BTF	1	2945	4.55	0	-	-	0	-	-	4	179	3.93
2FJU	0	-	-	0	-	-	0	-	-	1	1381	4.84
2G77	0	-	-	0	-	-	1	131	4.86	5	23	3.83
2HLE	1	347	4.22	2	501	4.53	2	367	4.62	2	225	4.17
2HQS	2	1702	3.37	0	-	-	1	2740	4.95	0	-	-
2OOB	0	-	-	0	-	-	0	-	-	0	-	-
2OOR	0	-	-	0	-	-	0	-	-	1	898	4.55
2VDB	0	-	-	5	197	4.54	5	51	4.17	4	15	1.74
3BP8	0	-	-	0	-	-	0	-	-	0	-	-
3D5S	0	-	-	1	254	3.65	3	82	3.65	4	60	2.12

Medium Difficulty (30)

1BGX	0	-	-	0	-	-	0	-	-	0	-	-
1ACB	1	2306	4.85	0	-	-	1	2567	4.61	4	212	4.78
1IJK	0	-	-	0	-	-	0	-	-	1	505	2.33
1JIW	0	-	-	0	-	-	0	-	-	0	-	-
1KKL	0	-	-	0	-	-	0	-	-	0	-	-
1M10	0	-	-	0	-	-	0	-	-	0	-	-
1NW9	0	-	-	0	-	-	2	2455	4.96	0	-	-
4CPA	0	-	-	9	2	4.66	8	4	4.03	16	1	3.55
1GP2	0	-	-	0	-	-	0	-	-	0	-	-
1GRN	0	-	-	1	663	3.05	0	-	-	1	2585	4.56
1HE8	0	-	-	0	-	-	0	-	-	0	-	-
1I2M	0	-	-	0	-	-	0	-	-	1	46	2.57
1IB1	0	-	-	0	-	-	0	-	-	0	-	-
1K5D	0	-	-	0	-	-	0	-	-	0	-	-

1LFD	0	-	-	0	-	-	1	1653	4.79	0	-	-
1MQ8	0	-	-	0	-	-	0	-	-	0	-	-
1N2C	0	-	-	0	-	-	0	-	-	0	-	-
1R6Q	0	-	-	0	-	-	1	1297	3.57	0	-	-
1SYX	1	14	4.93	0	-	-	1	67	4.87	1	20	4.91
1WQ1	0	-	-	0	-	-	0	-	-	1	1683	4.34
1XQS	0	-	-	0	-	-	1	576	3.75	1	80	4.46
2AYO	3	1234	4.66	1	877	3.40	3	237	3.40	6	62	4.72
2CFH	1	42	4.80	2	66	4.98	2	20	4.98	2	6	4.74
2H7V	0	-	-	0	-	-	0	-	-	0	-	-
2HRK	3	2678	3.95	0	-	-	0	-	-	1	825	4.92
2J7P	0	-	-	0	-	-	0	-	-	0	-	-
2NZ8	0	-	-	0	-	-	0	-	-	0	-	-
2OZA	1	1685	4.88	0	-	-	0	-	-	0	-	-
2ZOE	0	-	-	0	-	-	0	-	-	1	1688	4.81
3CPH	0	-	-	0	-	-	0	-	-	0	-	-
Difficult (25)												
1E4K	0	-	-	0	-	-	0	-	-	0	-	-
2HMI	0	-	-	0	-	-	0	-	-	0	-	-
1F6M	0	-	-	0	-	-	0	-	-	0	-	-
1FQ1	0	-	-	0	-	-	0	-	-	0	-	-
1PXV	0	-	-	0	-	-	0	-	-	0	-	-
1ZLI	0	-	-	0	-	-	0	-	-	0	-	-
2O3B	0	-	-	0	-	-	0	-	-	0	-	-
1ATN	0	-	-	0	-	-	0	-	-	0	-	-
1BKD	0	-	-	0	-	-	0	-	-	0	-	-
1DE4	0	-	-	0	-	-	0	-	-	0	-	-
1EER	0	-	-	0	-	-	0	-	-	0	-	-
1FAK	0	-	-	0	-	-	0	-	-	0	-	-
1H1V	0	-	-	0	-	-	0	-	-	0	-	-
1IBR	0	-	-	0	-	-	0	-	-	0	-	-
1IRA	0	-	-	0	-	-	0	-	-	0	-	-
1JK9	0	-	-	0	-	-	0	-	-	0	-	-
1JMO	0	-	-	0	-	-	0	-	-	0	-	-
1JZD	3	2187	4.90	0	-	-	0	-	-	1	88	4.95
1R8S	0	-	-	0	-	-	0	-	-	0	-	-
1Y64	0	-	-	0	-	-	0	-	-	0	-	-
1ZM4	0	-	-	0	-	-	0	-	-	1	26	3.29
2C0L	0	-	-	0	-	-	0	-	-	0	-	-
2I9B	0	-	-	0	-	-	0	-	-	0	-	-
2IDO	0	-	-	0	-	-	0	-	-	0	-	-
2OT3	0	-	-	0	-	-	0	-	-	0	-	-

**Table S3. Divided dataset located to the Nucleus subcellular location.**

PDBID	UniprotID	Subcellular location
1FQ1_r	P24941	Cytoplasm, Nucleus, Cytoplasm, Endosome
1GXD_r	P08253	Secreted, Membrane, Nucleus
1H9D_r	Q03347	Nucleus
1I2M_r	P62826	Nucleus, Cytoplasm, Melanosome
1IBR_r	P62825	Nucleus, Cytoplasm, Melanosome
1S1Q_r	Q99816	Cytoplasm, Membrane, Nucleus, Late endosome membrane
1SYX_r	P83876	Nucleus
1ZHI_r	P54784	Nucleus
2OZA_r	Q16539	Cytoplasm, Nucleus
1ATN_l	P00639	Secreted, Nucleus envelope
1FQ1_l	Q16667	Cytoplasm perinuclear region
1H9D_l	Q08024	Nucleus
1I2M_l	P18754	Nucleus, Cytoplasm
1IBR_l	Q14974	Cytoplasm, Nucleus envelope
1S1Q_l	P0CG48	Cytoplasm, Nucleus
1XD3_l	P0CG48	Cytoplasm, Nucleus
1ZHI_l	P21691	Nucleus, Chromosome
2AYO_l	P0CG48	Cytoplasm, Nucleus
2OOB_l	P0CH28	Cytoplasm, Nucleus
2OZA_l	P49137	Cytoplasm, Nucleus

**Table S4. Divided dataset located to the Mitochondrion subcellular location.**

PDBID	UniprotID	Subcellular location
1E6E_r	P08165	Mitochondrion matrix
1JK9_r	P40202	Cytoplasm, Mitochondrion intermembrane space
2PCC_r	P00431	Mitochondrion matrix
1E6E_l	P00257	Mitochondrion matrix
1JK9_l	P00445	Cytoplasm, Mitochondrion intermembrane space
2COL_l	O62742	Cytoplasm, Mitochondrion, Peroxisome
2PCC_l	P00044	Mitochondrion intermembrane space



**Table S5. Divided dataset located to the Golgi apparatus subcellular location.**

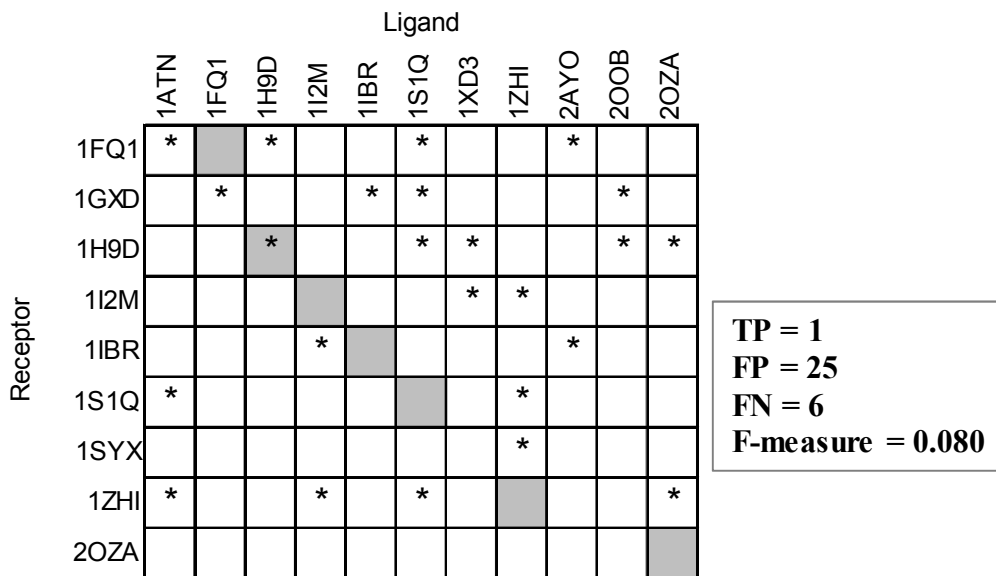
PDBID	UniprotID	Subcellular location
1HE8_r	P01112	Cell membrane, Golgi apparatus, Golgi apparatus membrane
1R8S_r	P84077	Golgi apparatus, Cytoplasm
1WQ1_r	P01112	Cell membrane, Golgi apparatus, Golgi apparatus membrane
2AJF_r	Q9BYF1	Processed angiotensin-converting enzyme, Secreted, Cell membrane
2CFH_r	O43617	Golgi apparatus, Endoplasmic reticulum
2G77_r	Q08484	Golgi apparatus
2OT3_r	Q9UL25	Endoplasmic reticulum membrane, Golgi apparatus membrane, Early endosome membrane, Cytoplasmic vesicle membrane, Cleavage furrow
1J2J_1	Q9UJY5	Golgi apparatus, Endosome membrane
2AJF_1	P59594	Virion membrane, Host endoplasmic reticulum-Golgi intermediate compartment membrane, Host cell membrane
2CFH_1	Q86SZ2	Golgi apparatus, Endoplasmic reticulum
2G77_1	O35963	Golgi apparatus membrane

*Note:* “\_r” represents receptor protein and “\_l” represents ligand protein in PDBID column.

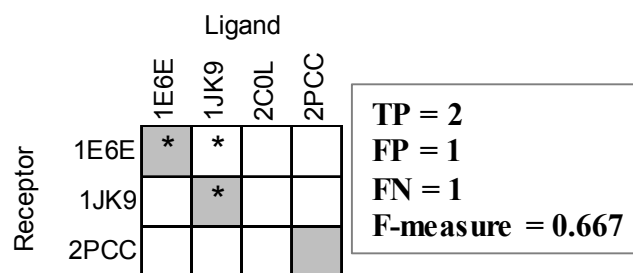
**Table S6: Chemotaxis dataset derived from PDB.**

PDB ID	Chain	Organism	Molecule	Domain
1FFG	B,D	<i>E. coli</i>	CheA	P2
1FFS	B,D	<i>E. coli</i>	CheA	P2
1FFW	B,D	<i>E. coli</i>	CheA	P2
1A0O	A,C,E,G	<i>E. coli</i>	CheY	
1BDJ	A	<i>E. coli</i>	CheY	
1CHN	A	<i>E. coli</i>	CheY	
1F4V	A,B,C	<i>E. coli</i>	CheY	
1FFG	A,C	<i>E. coli</i>	CheY	
1FFS	A,C	<i>E. coli</i>	CheY	
1FFW	A,C	<i>E. coli</i>	CheY	
1FQW	A,B	<i>E. coli</i>	CheY	
1HEY	A	<i>E. coli</i>	CheY	
1JBE	A	<i>E. coli</i>	CheY	
1KMI	Y	<i>E. coli</i>	CheY	
1ZDM	A,B	<i>E. coli</i>	CheY	
2B1J	A,B	<i>E. coli</i>	CheY	
3CHY	A	<i>E. coli</i>	CheY	
1KMI <sup>†</sup>	Z	<i>E. coli</i>	CheZ	
1QU7	B	<i>E. coli</i>	MCP(Tsr)	Cytoplasmic domain
1H5N	A,B,C,D	<i>S. typhimurium</i>	CheA	P1
1A2O	A,B	<i>S. typhimurium</i>	CheB	
1CHD	A	<i>S. typhimurium</i>	CheB	C-terminal catalytic domain
1AF7	A	<i>S. typhimurium</i>	CheR	
1BC5	A	<i>S. typhimurium</i>	CheR	
2CHE	A	<i>S. typhimurium</i>	CheY	
2CHF	A	<i>S. typhimurium</i>	CheY	
2FKA	A	<i>S. typhimurium</i>	CheY	
2FLK	A	<i>S. typhimurium</i>	CheY	
2FLW	A	<i>S. typhimurium</i>	CheY	
2FMF	A	<i>S. typhimurium</i>	CheY	
2FMH	A	<i>S. typhimurium</i>	CheY	
2FMI	A	<i>S. typhimurium</i>	CheY	
2FMK	A	<i>S. typhimurium</i>	CheY	
2PL9	A,B,C	<i>S. typhimurium</i>	CheY	
2PMC	A,B,C,D	<i>S. typhimurium</i>	CheY	
1TQG	A	<i>T. maritima</i>	CheA	P1
1U0S	A	<i>T. maritima</i>	CheA	P2
2CH4	A,B	<i>T. maritima</i>	CheA	P4, P5 (Residues 355–671)
1XKR	A	<i>T. maritima</i>	CheC	
2F9Z	A,B	<i>T. maritima</i>	CheC	
2F9Z	C,D	<i>T. maritima</i>	CheD	
2CH4	W,Y	<i>T. maritima</i>	CheW	
1SQU	A,B	<i>T. maritima</i>	CheX	
1XKO	A,B	<i>T. maritima</i>	CheX	
1TMY	A	<i>T. maritima</i>	CheY	
1U0S	Y	<i>T. maritima</i>	CheY	
2TMY	A	<i>T. maritima</i>	CheY	
3TMY	A,B	<i>T. maritima</i>	CheY	
4TMY	A,B	<i>T. maritima</i>	CheY	
1LKV	X	<i>T. maritima</i>	FliG	C-terminal domain (Residues 104–335)
1QC7	A,B	<i>T. maritima</i>	FliG	C-terminal domain
2HP7	A	<i>T. maritima</i>	FliM	CheC-like domain
1O6A	A,B	<i>T. maritima</i>	FliN	C-terminal domain (Residues 59–154)
1YAB	A,B	<i>T. maritima</i>	FliN	Residues 68–154
2CH7	A,B	<i>T. maritima</i>	MCP	Cytoplasmic domain

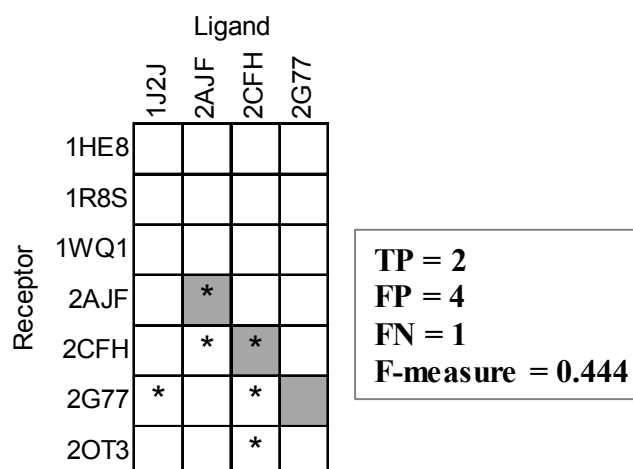
*Note:* CheA comprises five domains: P1 (Histidine phosphotransfer domain), P2 (Response regulator binding domain), P3 (Histidine kinase-like homodimeric domain), P4 (Histidine kinase-like ATPases) and P5 (Receptor coupling domain). <sup>†</sup>Includes a mutation in residue 134 (Glu→Lys).



**Figure S1. Result of the PPI predictions with nucleus sub-dataset.** The interactions estimated as positive are marked with asterisks. The gray colored cells correspond to the known interactions.



**Figure S2. Result of the PPI predictions with mitochondrion sub-dataset.** The interactions estimated as positive are marked with asterisks. The gray colored cells correspond to the known interactions.



**Figure S3. Result of the PPI predictions with Golgi apparatus sub-dataset.** The interactions estimated as positive are marked with asterisks. The gray colored cells correspond to the known interactions.