

Supporting Materials

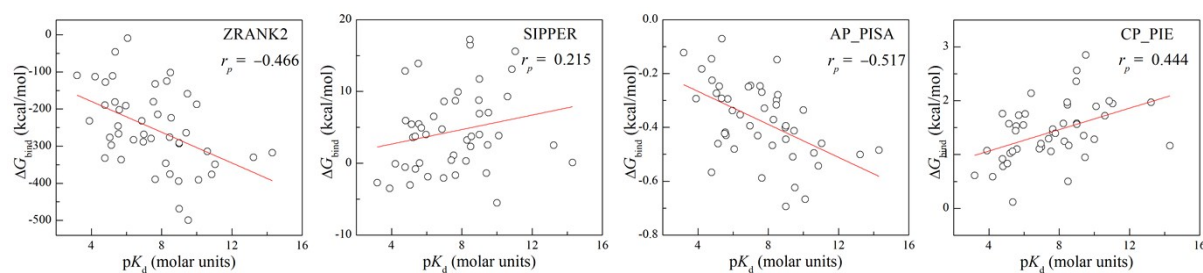


Figure S1. The scatter plots of the experimental binding affinities ($-\log(K_d)$) versus the scores predicted by four scoring functions

Table S1. The interaction features for the interfaces of 43 protein-protein complexes

PDB ID	Number of interacting residues Molecule1	Number of interacting residues Molecule2	Number of hydrophilic- hydrophobic interaction	Number of hydrophilic- hydrophobic interaction	Number of hydrophilic- hydrophobic interaction	Buried area upon the complex formation (Å ²)	Buried area upon the complex formation (%)	Interface area (Å ²)	Interface area MOL1 (%)	Interface area MOL2 (%)	<u>POLAR Buried area upon the complex formation (Å²)</u>	POLAR Buried area upon the complex formation (%)	POLAR Interface area (Å ²)	NO POLAR Buried area upon the complex formation (Å ²)	NO POLAR Buried area upon the complex formation (%)	NO POLAR Interface area (Å ²)	Residues at the interface_ TOT (n)	Residues at the interface_ Mol1 (n)	Residues at the interface_ Mol2 (n)	ϵ_{in} for re-rank
1WEJ_HL:F	43	34	69	112	5	1177.4	4.58	588.7	3.02	9.47	597.6	50.76	298.8	579.7	49.24	289.85	35	20	15	1
7CEI_A:B	38	33	73	101	10	1383.9	10.57	691.95	12.95	8.92	653.2	47.2	326.6	730.8	52.81	365.4	40	22	18	1
2I25_L:N	46	32	79	120	16	1424.6	10.92	712.3	10.83	11.01	698.3	49.02	349.15	726.3	50.98	363.15	39	21	18	1
4CPA_A:I	48	20	69	60	24	1188	8.21	594	5.05	21.91	720.8	60.67	360.4	467.2	39.33	233.6	38	23	15	2
1I9R_ABC:HL	56	52	103	157	13	1497.8	4.17	748.9	4.35	4	753.3	50.29	376.65	744.4	49.7	372.2	51	28	23	1
1BUH_A:B	31	33	73	70	32	1323.9	6.98	661.95	4.66	13.88	820.4	61.97	410.2	503.5	38.03	251.75	34	16	18	1
1J2J_A:B	29	35	62	37	47	1209.7	9.97	604.85	7.2	16.18	888.9	73.48	444.45	320.7	26.51	160.35	30	17	13	1
1FSK_BC:A	51	35	122	99	14	1622.8	5.81	811.4	4.15	9.65	912.6	56.24	456.3	710.1	43.76	355.05	44	23	21	1
1AZS_AB:C	37	38	74	87	25	1499.3	4.5	749.65	4.7	4.31	927.4	61.86	463.7	571.9	38.14	285.95	41	22	19	1
1BJ1_HL:VW	43	35	115	108	14	1730.8	5.69	865.4	4.42	7.97	980	56.62	490	750.7	43.37	375.35	45	26	19	1
1PPE_E:I	67	22	138	74	40	1687.8	14.52	843.9	9.25	33.72	1003.9	59.48	501.95	684	40.53	342	47	30	17	1
1NCA_N:LH	50	55	116	147	14	1953.4	5.68	976.7	6.52	5.04	1040.3	53.26	520.15	913.2	46.75	456.6	60	29	31	1
1XQS_A:C	71	48	125	168	13	2350.4	10.86	1175.2	9.47	12.73	1041.3	44.3	520.65	1309.1	55.7	654.55	60	32	28	1
1JWH_A:CD	42	37	95	47	45	1451.9	3.76	725.95	4.43	3.27	1065.9	73.41	532.95	386	26.59	193	43	23	20	1
2SIC_E:I	64	24	118	62	78	1616.8	10.21	808.4	8.16	13.64	1087.4	67.26	543.7	529.4	32.74	264.7	45	31	14	1
2QFW_HL:AB	44	38	147	60	32	1737.8	7.6	868.9	7.4	7.82	1113.6	64.08	556.8	624.2	35.92	312.1	48	26	22	1
1GL1_A:I	56	28	110	90	28	1595.7	11.98	797.85	7.54	29.14	1123	70.38	561.5	472.7	29.62	236.35	45	27	18	2
1RV6_VW:X	47	33	96	53	32	1636.6	9.73	818.3	7.43	14.09	1182.2	72.24	591.1	454.5	27.77	227.25	46	25	21	1
2OUL_A:B	59	38	135	101	58	1930.3	10.56	965.15	8.05	15.35	1220.5	63.23	610.25	709.9	36.78	354.95	61	32	29	1
1OYV_B:I	76	41	167	114	62	1961.2	11.57	980.6	9.99	13.74	1221.5	62.28	610.75	739.6	37.71	369.8	62	38	24	1
1IQD_AB:C	64	31	122	85	55	1976	7.52	988	5.37	12.55	1225.4	62.01	612.7	750.4	37.98	375.2	51	32	19	1
1GPW_A:B	67	47	156	102	47	2097.1	10.24	1048.55	9.16	11.6	1236.6	58.97	618.3	860.6	41.04	430.3	60	36	24	2

1YVB_A:I	53	32	135	68	54	1743.2	9.23	871.6	7.46	12.08	1242.7	71.29	621.35	500.4	28.71	250.2	52	33	19	1
1KXQ_H:A	65	42	141	137	26	2171.6	9.2	1085.8	6.22	17.66	1251.9	57.65	625.95	919.7	42.35	459.85	64	36	28	1
1CLV_A:I	66	29	117	127	30	2085	11.03	1042.5	6.31	43.8	1290.2	61.88	645.1	794.8	38.12	397.4	57	36	21	4
1UDI_E:I	47	52	152	80	65	2021.9	12.95	1010.95	9.62	19.83	1297	64.15	648.5	725	35.86	362.5	59	29	30	4
1E6E_A:B	56	50	132	123	34	2312.3	8.55	1156.15	5.59	18.12	1297.9	56.13	648.95	1014.3	43.87	507.15	58	29	29	1
1ML0_AB:D	62	43	122	109	39	2069.4	5.63	1034.7	3.22	22.17	1305.7	63.1	652.85	763.7	36.9	381.85	63	33	30	1
1N8O_ABC:E	65	34	145	85	58	1850.5	10.37	925.25	9.25	11.8	1320.8	71.38	660.4	529.6	28.62	264.8	52	32	20	1
1MAH_A:F	59	32	124	100	43	2145.5	8.84	1072.75	5.34	25.68	1331.6	62.06	665.8	813.9	37.94	406.95	56	35	21	2
1DFJ_E:I	68	87	105	231	12	2582	10.01	1291	18.45	6.87	1350	52.29	675	1231.9	47.71	615.95	82	35	47	2
1BVN_P:T	79	41	143	134	47	2221.7	10.01	1110.85	6.23	25.48	1368.1	61.58	684.05	853.7	38.43	426.85	62	38	24	1
2B42_B:A	73	56	199	152	42	2520.1	10.6	1260.05	7.95	15.9	1373.5	54.5	686.75	1146.6	45.5	573.3	80	39	41	1
2G77_A:B	69	52	142	131	43	2524.3	10.09	1262.15	7.99	13.69	1373.8	54.42	686.9	1150.5	45.58	575.25	65	37	28	4
1CGI_E:I	67	31	126	139	29	2052.6	14.03	1026.3	9.7	25.31	1398.6	68.14	699.3	653.9	31.86	326.95	54	34	20	2
1F51_AB:F	64	53	146	93	53	2277.4	9.13	1138.7	6.16	17.63	1437.3	63.11	718.65	840.1	36.89	420.05	64	34	30	4
1TMQ_A:B	75	49	183	117	66	2401	10.73	1200.5	7.36	19.8	1554.1	64.73	777.05	846.9	35.27	423.45	70	39	31	1
1JTG_B:A	65	66	152	161	28	2617.1	13.67	1308.55	11.87	16.12	1574.5	60.16	787.25	1042.6	39.84	521.3	75	39	36	1
2NZ8_A:B	44	90	148	148	46	2598.8	10.17	1299.4	14.13	7.94	1637.4	63.01	818.7	961.4	36.99	480.7	67	27	40	6
2AYO_A:B	103	53	203	154	64	3035.2	12.09	1517.6	7.41	32.74	1722.7	56.76	861.35	1312.5	43.24	656.25	86	52	34	6
2CFH_A:C	51	50	122	60	115	2383.6	12.97	1191.8	12.43	13.55	1773.4	74.4	886.7	610.2	25.6	305.1	58	30	28	6
1WDW_A:BD	68	58	186	113	83	3156.4	8.09	1578.2	5.63	14.33	1906.5	60.4	953.25	1249.8	39.6	624.9	83	40	43	6
1KXP_A:D	81	95	194	186	69	3341.3	8.47	1670.65	10.62	7.04	2277.4	68.16	1138.7	1063.8	31.84	531.9	94	40	54	6