

PDB_ID	Functional class	Experiment	Experimental Kd (M)	delta_G	prediction	MAE
1AHW_AB:C	Antigen-Antibody	11.55	3.40E-09	-11.55	-10.47	1.082467
1BJ1_HL:VW	Antigen-Antibody	11.55	3.40E-09	-11.55	-11.54	0.005637
1BVK_DE:F	Antigen-Antibody	10.53	1.40E-08	-10.71	-9.7	1.005092
1DQJ_AB:C	Antigen-Antibody	11.67	2.80E-09	-11.67	-11.55	0.123082
1E6J_HL:P	Antigen-Antibody	10.28	2.90E-08	-10.28	-8.02	2.260912
1FSK_BC:A	Antigen-Antibody	13.12	2.40E-10	-13.12	-10.96	2.16494
1JPS_HL:T	Antigen-Antibody	13.64	1.00E-10	-13.64	-10.59	3.046062
1KXQ_H:A	Antigen-Antibody	11.54	3.50E-09	-11.54	-10.12	1.423957
1NCA_HL:N	Antigen-Antibody	11.02	8.30E-09	-11.02	-11.1	0.078871
1P2C_AB:C	Antigen-Antibody	13.63	1.02E-10	-13.63	-12.37	1.259263
1VFB_AB:C	Antigen-Antibody	11.46	3.70E-09	-11.5	-10.79	0.706213
1WEJ_HL:F	Antigen-Antibody	12.48	7.14E-10	-12.48	-11.57	0.911187
2I25_N:L	Antigen-Antibody	12.28	1.00E-09	-12.28	-11.37	0.908411
2JEL_HL:P	Antigen-Antibody	11.59	2.80E-09	-11.67	-11.05	0.623857
2VIR_AB:C	Antigen-Antibody	12.28	1.00E-09	-12.28	-11.59	0.69017
1ACB_E:I	Enzyme-Inhibitor	13.05	2.00E-10	-13.23	-13.06	0.174153
1AVX_A:B	Enzyme-Inhibitor	12.5	4.80E-10	-12.71	-12.41	0.29679
1BRS_A:D	Enzyme-Inhibitor	17.32	2.00E-13	-17.32	-13.91	3.40672
1BUH_A:B	Enzyme-Inhibitor	9.7	7.70E-08	-9.7	-8.73	0.973416
1BVN_P:T	Enzyme-Inhibitor	15.06	9.20E-12	-15.06	-13.35	1.709111
1DFJ_E:I	Enzyme-Inhibitor	18.05	5.90E-14	-18.05	-19.56	1.508156
1EAW_A:B	Enzyme-Inhibitor	14.06	4.97E-11	-14.06	-12.3	1.764493
1EMV_A:B	Enzyme-Inhibitor	18.58	2.40E-14	-18.58	-19.95	1.366268
1EZU_C:AB	Enzyme-Inhibitor	13.77	8.00E-11	-13.77	-11.97	1.798113
1F34_A:B	Enzyme-Inhibitor	14.19	1.00E-10	-13.64	-12.83	0.811887
1FLE_E:I	Enzyme-Inhibitor	12.28	1.00E-09	-12.28	-10.41	1.869282
1GXD_A:C	Enzyme-Inhibitor	11.3	5.20E-09	-11.3	-9.89	1.412392
1JIW_P:I	Enzyme-Inhibitor	15.55	4.00E-12	-15.55	-13.72	1.831613
1JTG_B:A	Enzyme-Inhibitor	12.82	4.00E-10	-12.82	-11.63	1.188641
1MAH_A:F	Enzyme-Inhibitor	14.51	2.50E-11	-14.46	-12.29	2.16909
1NB5_AP:I	Enzyme-Inhibitor	13.86	6.90E-11	-13.86	-11.37	2.490344
1OPH_A:B	Enzyme-Inhibitor	11.32	5.00E-09	-11.32	-10.15	1.172192
1PXV_A:C	Enzyme-Inhibitor	12.97	3.10E-10	-12.97	-11.3	1.672566
1ROR_E:I	Enzyme-Inhibitor	14.17	2.94E-11	-14.37	-12.55	1.823985
1YVB_A:I	Enzyme-Inhibitor	11.17	6.50E-09	-11.17	-10.43	0.735656
1ZLI_A:B	Enzyme-Inhibitor	12.04	1.30E-09	-12.12	-10.91	1.2053
2ABZ_B:E	Enzyme-Inhibitor	11.67	2.80E-09	-11.67	-13.75	2.07828
2B42_A:B	Enzyme-Inhibitor	12.11	1.07E-09	-12.24	-10.95	1.293821
2JOT_A:D	Enzyme-Inhibitor	13.34	4.00E-10	-12.82	-12.5	0.316401
2O3B_A:B	Enzyme-Inhibitor	15.68	3.20E-12	-15.68	-13.97	1.706011
2OUL_A:B	Enzyme-Inhibitor	11.96	1.70E-09	-11.96	-11.43	0.530802
2PTC_E:I	Enzyme-Inhibitor	18.04	6.00E-14	-18.04	-19.32	1.280762
2SIC_E:I	Enzyme-Inhibitor	13.84	7.12E-11	-13.84	-12.78	1.058275
2SNI_E:I	Enzyme-Inhibitor	15.96	2.00E-12	-15.96	-13.12	2.835515
2UUY_A:B	Enzyme-Inhibitor	11.26	5.60E-09	-11.26	-12.12	0.863764
3SGB_E:I	Enzyme-Inhibitor	14.51	1.79E-11	-14.66	-12.92	1.73889
1A2K_C:AB	G-protein	9.31	1.50E-07	-9.31	-8.84	0.469277
1E96_A:B	G-protein	7.42	2.70E-06	-7.6	-9.96	2.358074
1FQJ_A:B	G-protein	9.79	6.70E-08	-9.79	-8.98	0.812681

1GRN_A:B	G-protein	9.03	2.39E-07	-9.03	-9.73	0.702596
1HE8_B:A	G-protein	7.37	3.20E-06	-7.5	-9.97	2.474724
1I2M_A:B	G-protein	15.83	2.50E-12	-15.83	-14.29	1.536096
1I4D_D:AB	G-protein	7.46	3.00E-06	-7.53	-7.75	0.219885
1IBR_A:B	G-protein	12.07	1.00E-09	-12.28	-9.83	2.452462
1K5D_AB:C	G-protein	12.77	3.00E-10	-12.99	-10.44	2.548942
1LFD_B:A	G-protein	7.79	1.94E-06	-7.79	-9.62	1.832218
1NVU_Q:S	G-protein	7.43	3.60E-06	-7.43	-9.98	2.553637
1WQ1_R:G	G-protein	6.62	1.70E-05	-6.51	-8.58	2.072509
1Z0K_A:B	G-protein	6.98	7.70E-06	-6.98	-8.25	1.27018
2FJU_B:A	G-protein	7.2	5.30E-06	-7.2	-7.31	0.112649
3CPH_G:A	G-protein	8.84	3.30E-07	-8.84	-9.76	0.920168
1NVU_R:S	G-protein	7.8	1.90E-06	-7.81	-9.98	2.173637
1E6E_A:B	Other enzymes	8.28	8.56E-07	-8.28	-9.05	0.765282
1EWY_A:C	Other enzymes	7.43	3.57E-06	-7.43	-8.66	1.231684
1F6M_A:C	Other enzymes	7.6	2.70E-06	-7.6	-9.59	1.98855
1GLA_G:F	Other enzymes	6.76	1.10E-05	-6.76	-6.13	0.628276
1IJK_A:BC	Other enzymes	10.42	2.30E-08	-10.42	-5.92	4.504447
1JMO_A:HL	Other enzymes	9.47	1.15E-07	-9.47	-10.04	0.570055
1JWH_CD:A	Other enzymes	11.14	1.26E-08	-10.78	-10.5	0.279707
1KKL_ABC:H	Other enzymes	10.02	4.50E-08	-10.02	-9.89	0.129859
1M10_A:B	Other enzymes	11.24	5.80E-09	-11.24	-10.51	0.729257
1NW9_B:A	Other enzymes	11.19	1.30E-08	-10.76	-10.02	0.741483
1OC0_A:B	Other enzymes	12.28	1.00E-09	-12.28	-10.89	1.393885
1R6Q_A:C	Other enzymes	8.84	3.30E-07	-8.84	-9.93	1.090388
1US7_A:B	Other enzymes	8.09	1.46E-06	-7.96	-9.07	1.113893
1WDW_BD:A	Other enzymes	12.72	2.50E-09	-11.74	-10.9	0.838462
1ZM4_A:B	Other enzymes	8.03	1.30E-06	-8.03	-8.41	0.382274
2A9K_A:B	Other enzymes	10.25	6.00E-08	-9.85	-9.4	0.445516
2MTA_HL:A	Other enzymes	7.42	4.50E-06	-7.29	-8.54	1.253234
2O0B_A:B	Other enzymes	5.66	6.00E-05	-5.76	-6.02	0.260944
2OOR_AB:C	Other enzymes	10.65	1.55E-08	-10.65	-6.09	4.556908
1E4K_AB:C	Receptor	7.87	1.70E-06	-7.87	-7.43	0.441456
1EER_A:BC	Receptor	15.59	3.70E-12	-15.6	-15.94	0.340115
1HCF_AB:X	Receptor	13.08	2.60E-10	-13.08	-9.73	3.350063
1KAC_A:B	Receptor	10.68	1.48E-08	-10.68	-12.3	1.622022
1KTZ_A:B	Receptor	8.92	2.90E-07	-8.92	-9.33	0.413396
1PVH_A:B	Receptor	9.52	8.00E-08	-9.68	-10.63	0.94614
1RV6_VW:X	Receptor	13.86	1.70E-10	-13.33	-12.93	0.399999
1T6B_X:Y	Receptor	13.1	1.70E-10	-13.33	-10.64	2.686745
2AJF_A:E	Receptor	10.63	1.62E-08	-10.63	-11.68	1.050756
2HLE_A:B	Receptor	10.09	4.00E-08	-10.09	-10.9	0.810446
2I9B_E:A	Receptor	12.93	3.30E-10	-12.94	-9.92	3.023314
2NYZ_AB:D	Receptor	12.69	5.00E-10	-12.69	-10.23	2.460406
1ATN_A:D	Miscellaneous1	12.07	2.00E-09	-11.87	-10.28	1.589369
1DE4_AB:CF	Miscellaneous1	9.78	6.80E-08	-9.78	-8.74	1.04175
1FC2_C:D	Miscellaneous1	10.43	2.25E-08	-10.43	-9.63	0.795019
1H1V_A:G	Miscellaneous1	10.2	2.50E-08	-10.37	-10.72	0.346582
1IB1_AB:E	Miscellaneous1	9.76	2.00E-08	-10.5	-10.72	0.216582
1KLU_AB:D	Miscellaneous1	7.28	4.60E-06	-7.28	-9.86	2.575435

1KXP_A:D	Miscellaneous1	12.34	9.00E-10	-12.34	-8.74	3.60175
1XQS_A:C	Miscellaneous1	7.08	6.50E-06	-7.08	-7.66	0.576909
2B4J_AB:C	Miscellaneous1	10.86	1.09E-08	-10.86	-9.04	1.817672
2COL_A:B	Miscellaneous1	9.82	1.09E-07	-9.5	-10.32	0.823584
2VDB_A:B	Miscellaneous1	13.4	1.50E-10	-13.4	-10.72	2.683418
1AKJ_AB:DE	Miscellaneous2	5.32	0.000126	-5.32	-5.72	0.396582
1MQ8_A:B	Miscellaneous2	7.53	3.00E-06	-7.53	-10.34	2.812032
1RLB_ABCD:E	Miscellaneous2	8.18	8.00E-07	-8.32	-10.72	2.396582
1XD3_A:B	Miscellaneous2	8.9	3.00E-07	-8.9	-9.65	0.747713
1ZHI_A:B	Miscellaneous2	9.08	2.00E-07	-9.14	-10.34	1.202032
2BTF_A:P	Miscellaneous2	7.69	2.30E-06	-7.69	-10.23	2.544578
2HQS_A:H	Miscellaneous2	10.15	2.70E-08	-10.33	-10.28	0.054868
2HRK_A:B	Miscellaneous2	10.98	9.00E-09	-10.98	-9.44	1.536583
2OZA_B:A	Miscellaneous2	11.73	2.50E-09	-11.74	-9.22	2.518445
3BP8_AB:C	Miscellaneous2	11.44	4.14E-09	-11.44	-9.22	2.218445
1AK4_A:D	Miscellaneous3	6.43	1.60E-05	-6.54	-9.4	2.86297
1B6C_A:B	Miscellaneous3	8.94	2.80E-07	-8.94	-10.72	1.775541
1EFN_B:A	Miscellaneous3	10.12	3.80E-08	-10.12	-9.07	1.051129
1FFW_A:B	Miscellaneous3	8.09	1.35E-06	-8.01	-7.17	0.843381
1GCQ_B:C	Miscellaneous3	6.51	1.70E-05	-6.51	-6.63	0.116906
1GPW_A:B	Miscellaneous3	11.32	5.00E-09	-11.32	-10.36	0.963793
1H9D_A:B	Miscellaneous3	9.18	4.50E-08	-10.02	-9.48	0.536948
1QA9_A:B	Miscellaneous3	7.16	9.00E-06	-6.88	-7.32	0.438691
1S1Q_A:B	Miscellaneous3	4.29	0.000635	-4.36	-4.36	0.004024
2GOX_A:B	Miscellaneous3	12.08	1.40E-09	-12.08	-9.63	2.454475
3BZD_A:B	Miscellaneous3	9.57	9.60E-08	-9.57	-9.05	0.520191