

Table S1. Experimental and predictive activities of external set compounds (S1-S142).

Compound	Experimental pK_i	Predicted pK_i	Residual
S1	9.124	8.701	0.423
S2	9.387	9.537	-0.150
S3	9.795	8.974	0.821
S4	9.229	9.306	-0.077
S5	8.853	8.458	0.395
S6	9.251	8.312	0.939
S7	9.602	8.824	0.778
S8	9.585	9.146	0.439
S9	9.920	9.616	0.304
S10	8.795	9.276	-0.481
S11	9.259	8.796	0.463
S12	8.769	9.256	-0.487
S13	8.346	9.102	-0.756
S14	6.651	7.255	-0.604
S15	7.494	8.091	-0.597
S16	6.931	7.679	-0.748
S17	6.809	7.371	-0.562
S18	6.903	7.715	-0.812
S19	7.619	7.283	0.336
S20	6.850	7.010	-0.160
S21	7.221	7.748	-0.527
S22	6.679	7.257	-0.578
S23	6.818	7.469	-0.651
S24	7.124	6.601	0.523
S25	7.275	7.726	-0.451
S26	5.623	5.992	-0.369
S27	6.183	6.173	0.010
S28	6.293	6.819	-0.526
S29	6.958	7.738	-0.780
S30	7.229	6.461	0.768
S31	7.744	7.594	0.150
S32	6.191	5.783	0.408
S33	8.301	7.454	0.847
S34	7.602	7.271	0.331
S35	7.408	7.357	0.051
S36	6.692	6.854	-0.162
S37	7.481	6.641	0.840
S38	7.347	6.58	0.767
S39	6.337	6.581	-0.244
S40	6.625	7.125	-0.500
S41	6.501	7.125	-0.624
S42	6.522	6.447	0.075
S43	6.777	6.873	-0.096
S44	7.301	8.134	-0.833
S45	6.978	6.797	0.181
S46	6.623	6.818	-0.195
S47	8.327	7.856	0.471

S48	8.045	8.919	-0.874
S49	8.045	8.945	-0.900
S50	8.119	8.925	-0.806
S51	8.102	7.810	0.292
S52	8.421	8.933	-0.512
S53	8.283	8.628	-0.345
S54	7.522	7.003	0.519
S55	7.853	7.061	0.792
S56	7.522	7.651	-0.129
S57	8.000	7.714	0.286
S58	7.913	6.979	0.934
S59	7.309	7.549	-0.240
S60	7.921	7.283	0.638
S61	8.522	8.471	0.051
S62	7.886	7.664	0.222
S63	7.698	7.630	0.068
S64	7.886	7.749	0.137
S65	7.494	7.766	-0.272
S66	7.481	7.752	-0.271
S67	7.853	7.752	0.101
S68	7.619	7.765	-0.146
S69	7.221	7.167	0.054
S70	8.229	7.571	0.658
S71	8.657	8.912	-0.255
S72	8.744	7.684	1.060
S73	8.091	7.451	0.640
S74	8.508	7.691	0.817
S75	6.536	7.315	-0.779
S76	8.236	7.453	0.783
S77	8.229	7.854	0.375
S78	6.954	7.532	-0.578
S79	6.987	7.195	-0.208
S80	8.921	7.974	0.947
S81	8.638	8.057	0.581
S82	9.638	8.816	0.822
S83	8.522	8.023	0.499
S84	8.585	8.127	0.458
S85	8.921	8.216	0.705
S86	8.602	8.295	0.307
S87	6.986	7.041	-0.055
S88	7.009	7.079	-0.070
S89	5.680	6.569	-0.889
S90	5.659	6.714	-1.055
S91	5.421	6.461	-1.040
S92	5.658	6.318	-0.660
S93	5.851	6.481	-0.630
S94	5.750	6.298	-0.548
S95	6.059	6.766	-0.707
S96	6.000	6.656	-0.656
S97	6.229	6.563	-0.334

S98	7.105	6.412	0.693
S99	7.373	7.560	-0.187
S100	6.982	7.518	-0.536
S101	7.203	7.127	0.076
S102	8.136	7.387	0.749
S103	7.326	7.613	-0.287
S104	7.366	7.492	-0.126
S105	6.211	6.631	-0.420
S106	7.411	7.133	0.278
S107	7.869	7.613	0.256
S108	7.823	7.141	0.682
S109	6.101	6.399	-0.298
S110	7.809	7.477	0.332
S111	7.185	6.482	0.703
S112	6.782	6.898	-0.116
S113	7.065	7.715	-0.650
S114	6.735	6.887	-0.152
S115	6.728	6.333	0.395
S116	7.407	6.718	0.689
S117	7.108	6.528	0.580
S118	7.183	6.687	0.496
S119	7.651	6.757	0.894
S120	7.926	7.626	0.300
S121	6.872	6.674	0.198
S122	6.903	6.674	0.229
S123	7.756	7.658	0.098
S124	8.148	7.936	0.212
S125	8.207	8.407	-0.200
S126	7.958	7.974	-0.016
S127	7.593	7.701	-0.108
S128	6.657	7.534	-0.877
S129	6.570	7.534	-0.964
S130	7.619	7.497	0.122
S131	8.823	8.051	0.772
S132	7.853	8.033	-0.180
S133	7.600	8.056	-0.456
S134	8.440	7.923	0.517
S135	8.590	8.120	0.470
S136	8.470	8.059	0.411
S137	7.710	8.101	-0.391
S138	8.714	8.120	0.594
S139	8.396	8.122	0.274
S140	8.812	8.059	0.753
S141	8.573	8.124	0.449
S142	8.694	7.930	0.764
