

Table S2. Affinity prediction performance of ccorps for the kinase inhibitors using a 50% sequence identity clusters for cross validation. For each of the 38 inhibitors in the affinity dataset of Karaman et al., the prediction performance of CCORPS and the sequence-based method is shown below. While the mean AUC values and enrichment scores are close, the standard deviations of the *differences* between the corresponding columns (0.21, 0.31, and 0.40, respectively) highlight that the two methods have complementary strengths.

Inhibitor	CCORPS			Sequence-based		
	AUC _{ROC}	AUC _{PR}	E _{5%} /E _{max}	AUC _{ROC}	AUC _{PR}	E _{5%} /E _{max}
ABT-869	0.52	0.14	0.19 (1.60/8.41)	0.50	0.27	0.44 (3.69/8.43)
AMG-706	0.87	0.66	0.83 (5.59/6.77)	0.67	0.48	0.81 (5.45/6.71)
AST-487	0.68	0.67	0.44 (0.76/1.71)	0.72	0.75	0.77 (1.31/1.71)
AZD-1152HQA	0.52	0.21	0.44 (3.01/6.77)	0.58	0.29	0.42 (2.86/6.78)
BIRB-796	0.83	0.71	0.98 (3.23/3.28)	0.72	0.63	0.78 (2.55/3.27)
BMS-387032	0.87	0.74	0.90 (3.33/3.69)	0.92	0.87	1.00 (3.69/3.69)
CHIR-258	0.82	0.69	0.95 (3.85/4.05)	0.89	0.82	1.00 (4.05/4.05)
CHIR-265	0.93	0.68	0.67 (4.87/7.31)	0.85	0.78	1.00 (7.24/7.24)
CI-1033	0.60	0.42	0.63 (2.84/4.47)	0.71	0.56	0.91 (4.06/4.48)
CP-690550	0.95	0.55	0.29 (9.37/32.79)	0.55	0.46	0.28 (9.24/32.85)
CP-724714	1.00	0.99	0.86 (20.30/23.69)	0.63	0.05	0.00 (0.00/23.72)
Dasatinib	0.57	0.39	0.17 (0.51/2.90)	0.77	0.65	0.83 (2.39/2.89)
EKB-569	0.73	0.51	0.70 (3.24/4.63)	0.79	0.62	0.91 (4.21/4.64)
Erlotinib	0.55	0.28	0.46 (2.53/5.49)	0.75	0.53	0.87 (4.81/5.50)
Flavopiridol	0.67	0.47	0.70 (2.16/3.09)	0.79	0.63	0.47 (1.45/3.09)
GW-2580	0.44	0.00	0.00 (0.00/255.80)	0.20	0.00	0.00 (0.00/256.20)
GW-786034	0.78	0.53	0.75 (4.10/5.49)	0.57	0.40	0.66 (3.58/5.45)
Gefitinib	0.43	0.10	0.06 (0.59/9.27)	0.26	0.11	0.09 (0.87/9.28)
Imatinib	0.70	0.22	0.30 (3.57/11.84)	0.28	0.13	0.34 (4.08/11.86)
JNJ-7706621	0.66	0.60	0.37 (0.73/2.00)	0.75	0.76	0.88 (1.75/2.00)
LY-333531	0.85	0.45	0.62 (4.35/7.03)	0.77	0.36	0.30 (2.09/7.04)
Lapatinib	1.00	0.99	0.86 (20.30/23.69)	0.63	0.05	0.00 (0.00/23.72)
MLN-518	0.88	0.19	0.21 (4.47/21.68)	0.54	0.05	0.00 (0.00/21.71)
MLN-8054	0.74	0.51	0.65 (4.45/6.84)	0.82	0.68	1.00 (6.85/6.85)
PI-103	0.97	0.86	0.94 (15.36/16.40)	0.99	0.90	1.00 (16.01/16.01)
PKC-412	0.29	0.34	0.05 (0.10/2.20)	0.67	0.68	1.00 (2.20/2.20)
PTK-787	1.00	0.88	0.59 (20.30/34.57)	0.89	0.86	0.50 (17.31/34.62)
Roscovitine	0.84	0.41	0.06 (0.31/4.81)	0.38	0.18	0.28 (1.35/4.82)
SB-202190	0.84	0.74	0.94 (3.97/4.24)	0.88	0.78	0.98 (4.15/4.21)
SB-203580	0.69	0.51	0.60 (2.24/3.71)	0.81	0.69	0.75 (2.77/3.69)
SB-431542	1.00	0.87	0.41 (20.30/49.19)	0.91	0.10	0.00 (0.00/49.27)
SU-14813	0.54	0.32	0.06 (0.20/3.08)	0.83	0.79	1.00 (3.09/3.09)
Sorafenib	0.50	0.49	0.90 (3.71/4.10)	0.63	0.45	0.81 (3.31/4.08)
Staurosporine	0.90	0.98	1.00 (1.14/1.14)	0.80	0.97	1.00 (1.15/1.15)
Sunitinib	0.47	0.35	0.05 (0.12/2.51)	0.86	0.84	1.00 (2.52/2.52)
VX-680	0.76	0.76	0.95 (2.81/2.95)	0.70	0.64	0.72 (2.12/2.95)
VX-745	0.40	0.27	0.59 (3.72/6.33)	0.50	0.18	0.34 (2.18/6.34)
ZD-6474	0.78	0.64	0.83 (3.73/4.52)	0.86	0.77	1.00 (4.53/4.53)
mean	0.73	0.53	0.55	0.69	0.52	0.64