Table S1. Druggability scores of the positive instances [a]

Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	Druggability score			
			Structural attributes	Drug/chemical attributes	Functional attributes	All attributes
ARF1	CYTH2	1s9d_A [b]	0.8602	0.9961	0.7766	0.8805
ARF1	CYTH2	1s9d_E [b]	0.6310	0.9961	0.7766	0.7037
ARF1	CYTH2	1r8q_A [b]	0.9793	0.9961	0.7766	0.8688
ARF1	CYTH2	1r8q_E [b]	0.5617	0.9961	0.7766	0.8922
ARF1	CYTH2	1r8q_B [b]	0.9816	0.9961	0.7766	0.8637
ARF1	CYTH2	1r8q_F [b]	0.5684	0.9961	0.7766	0.8899
ARF1	CYTH2	1r8q_BF [c]	0.9217	0.9961	0.7766	0.9691
ARF1	CYTH2	1s9d_AE [c]	0.6139	0.9961	0.7766	0.9281
ARF1	CYTH2	1r8s_AE [c]	0.8594	0.9961	0.7766	0.9779
ARF1	CYTH1	1s9d_A [b]	0.8602	0.7025	0.7189	0.8671
ARF1	CYTH1	1s9d_E [b]	0.6310	0.7025	0.7189	0.6614
ARF1	CYTH1	1r8q_A [b]	0.9793	0.7025	0.7189	0.8435
ARF1	CYTH1	1r8q_E [b]	0.5617	0.7025	0.7189	0.8834
ARF1	CYTH1	1r8q_B [b]	0.9816	0.7025	0.7189	0.8384
ARF1	CYTH1	1r8q_F [b]	0.5684	0.7025	0.7189	0.8796
ARF1	CYTH1	1r8q_BF [c]	0.9217	0.7025	0.7189	0.9635
ARF1	CYTH1	1s9d_AE [c]	0.6139	0.7025	0.7189	0.9129
ARF1	CYTH1	1r8s_AE [c]	0.8594	0.7025	0.7189	0.9748
BAK1	BCL2	2o2f_A	0.9943	0.6671	0.9432	0.9489
BAK1	BCL2	2o22_A	0.9884	0.6671	0.9432	0.9610
BAK1	BCL2	2o21_A	0.9905	0.6671	0.9432	0.9434
BAK1	BCL2	1ysw_A	0.9902	0.6671	0.9432	0.9461
BAK1	BCL2L1	2o2n_A	0.9867	0.4991	0.8962	0.9427
BAK1	BCL2L1	2o2m_A	0.9950	0.4991	0.8962	0.8553
BAK1	BCL2L1	2yxj_A	0.9938	0.4991	0.8962	0.9459
BAK1	BCL2L1	2yxj_B	0.9957	0.4991	0.8962	0.9332
BAK1	BCL2L1	1ysi_A	0.9802	0.4991	0.8962	0.9258
BAK1	BCL2L1	2w3l_A	0.9639	0.4991	0.8962	0.8404
BAK1	BCL2L1	2w3l_B	0.9739	0.4991	0.8962	0.8390
BAK1	BCL2L1	3inq_A	0.9391	0.4991	0.8962	0.9304
BAK1	BCL2L1	3inq_B	0.9967	0.4991	0.8962	0.8909
CALM1	CAMK1	1mux_A pocket1	0.9952	0.9998	0.9991	0.9866
CALM1	CAMK1	1mux_A pocket2	0.9855	0.9998	0.9991	0.9879
CALM1	MYLK	1mux_A pocket1	0.9952	0.9998	0.9971	0.9932
CALM1	MYLK	1mux_A pocket2	0.9855	0.9998	0.9971	0.9951
CALM1	PDE1A	1qiv_A	1.0000	1.0000	0.9838	0.9993
CD4	HLA-DQB1	1jl4_D	0.7982	0.9913	0.9991	0.9400
CREBBP	TP53	2d82_A	0.9815	0.7397	1.0000	0.9835
ESR1	NCOA2	3erd_A	0.7780	0.9998	0.9914	0.9589
ESR1	NCOA2	3erd_B	0.9159	0.9998	0.9914	0.9521
FKBP1A	TGFBR1	1fkj_A	0.9938	0.9999	0.9942	0.9532
FKBP1A	TGFBR1	1fkf_A	0.9825	0.9999	0.9942	0.9516
EGFR	GRB2	1cj1_B	0.9923	0.9998	0.9995	0.9992
EGFR	GRB2	1cj1_C	0.9928	0.9998	0.9995	0.9992
EGFR	GRB2	1cj1_D	0.9920	0.9998	0.9995	0.9992
EGFR	GRB2	1cj1_E	0.9943	0.9998	0.9995	0.9991
EGFR	GRB2	1cj1_F	0.9901	0.9998	0.9995	0.9992
EGFR	GRB2	1cj1_G	0.9903	0.9998	0.9995	0.9991
EGFR	GRB2	1cj1_H	0.9887	0.9998	0.9995	0.9991
EGFR	GRB2	1cj1_I	0.9952	0.9998	0.9995	0.9992
EGFR	GRB2	1cj1_J	0.9925	0.9998	0.9995	0.9992
GRB2	MET	1cj1_B	0.9923	0.9964	1.0000	0.9999
GRB2	MET	1cj1_C	0.9928	0.9964	1.0000	0.9999
GRB2	MET	1cj1_D	0.9920	0.9964	1.0000	0.9999
GRB2	MET	1cj1_E	0.9943	0.9964	1.0000	1.0000
GRB2	MET	1cj1_F	0.9901	0.9964	1.0000	0.9999
GRB2	MET	1cj1_G	0.9903	0.9964	1.0000	0.9999
GRB2	MET	1cj1_H	0.9887	0.9964	1.0000	0.9998
GRB2	MET	1cj1_I	0.9952	0.9964	1.0000	0.9999
GRB2	MET	1cj1_J	0.9925	0.9964	1.0000	0.9999
HOXB1	PBX1	1b72_B	0.8647	0.0000	0.7546	0.6464
IL1B	IL1R1	1itb_B	0.8352	0.9991	0.9967	0.8652
IL2	IL2RA	1py2_A	0.9474	0.9940	0.9980	0.8907
IL2	IL2RA	1py2_B	0.9560	0.9940	0.9980	0.8969
IL2	IL2RA	1py2_C	0.9920	0.9940	0.9980	0.8915

Table S1. (continued)

Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	Druggability score			
			Structural attributes	Drug/chemical attributes	Functional attributes	All attributes
IL2	IL2RA	1py2_D	0.9889	0.9940	0.9980	0.8844
IL2	IL2RA	1m48_A	0.8257	0.9940	0.9980	0.9074
IL2	IL2RA	1m48_B	0.9447	0.9940	0.9980	0.8985
IL2	IL2RA	1m4a_A	0.7358	0.9940	0.9980	0.7688
PTEN	MAGI3	1be9_A	0.9911	0.0000	0.2251	0.7637
MDM2	TP53	1t4e_A	0.9964	0.8004	1.0000	0.9883
MDM2	TP53	1t4e_B	0.9958	0.8004	1.0000	0.9871
MDM2	TP53	1ttv_A	0.9939	0.8004	1.0000	0.9848
MDM2	TP53	3jzk_A	0.9663	0.8004	1.0000	0.9575
MDM2	TP53	3lbk_A	0.9974	0.8004	1.0000	0.9816
MDM2	TP53	3lbl_A	0.9704	0.8004	1.0000	0.9448
MDM2	TP53	3lbl_C	0.9916	0.8004	1.0000	0.9744
MDM2	TP53	3lbl_E	0.9610	0.8004	1.0000	0.9605
MDM4	TP53	3lbj_E	0.9956	0.4991	0.9981	0.9943
PDGFRB	PIK3R1	1h9o_A	0.9636	0.9951	0.9997	1.0000
RAC1	TIAM1	1foe_B	0.8975	0.4991	1.0000	0.9978
RAC1	TIAM1	1foe_D	0.8895	0.4991	1.0000	0.9978
RAC1	TIAM1	1foe_F	0.9061	0.4991	1.0000	0.9966
RAC1	TIAM1	1foe_H	0.9508	0.4991	1.0000	0.9954
RAC1	TRIO	2nz8_A	0.9146	0.4991	0.9980	0.9995
RAF1	YWHAZ	3rdh_A	0.9201	0.4521	0.9996	0.9850
RAF1	YWHAZ	3rdh_B	0.8791	0.4521	0.9996	0.9873
RAF1	YWHAZ	3rdh_C	0.8529	0.4521	0.9996	0.9861
RAF1	YWHAZ	3rdh_D	0.8211	0.4521	0.9996	0.9723
S100B	TP53	3hcm_A	0.8769	0.8679	0.9730	0.9304
S100B	TP53	3hcm_B	0.7313	0.8679	0.9730	0.9142
STAT3	STAT3	1bg1_A	0.5700	0.0000	1.0000	0.9517
BIRC5	BIRC5	1e31_A	0.9929	0.0000	0.9998	0.6917
BIRC5	BIRC5	1e31_B	0.9950	0.0000	0.9998	0.6768
BIRC5	BIRC5	1f3h_A	0.9954	0.0000	0.9998	0.6724
BIRC5	BIRC5	1f3h_B	0.9970	0.0000	0.9998	0.6732
BIRC5	BIRC5	1xox_A	0.9941	0.0000	0.9998	0.6986
BIRC5	BIRC5	1xox_B	0.9923	0.0000	0.9998	0.6974
CTNNB1	TCF7L1	1g3j_A	0.9865	0.4991	0.9996	0.9906
CTNNB1	TCF7L1	1g3j_C	0.9784	0.4991	0.9996	0.9925
CTNNB1	TCF7L2	1g3j_A	0.9865	0.4991	1.0000	0.9896
CTNNB1	TCF7L2	1g3j_C	0.9784	0.4991	1.0000	0.9928
THRB	NCOA2	1bsx_B	0.9720	1.0000	0.7517	0.7834
TNF	TNF	2az5_AB	0.7129	0.9998	1.0000	0.8896
TNF	TNF	2az5_CD	0.7210	0.9998	1.0000	0.8856
XIAP	CASP3	1i3o_E pocket1	0.4319	0.9769	0.9990	0.7893
XIAP	CASP3	1i3o_E pocket2	0.5627	0.9769	0.9990	0.8624
XIAP	CASP3	1i3o_F pocket3	0.4088	0.9769	0.9990	0.7930
XIAP	CASP3	1i3o_F pocket4	0.4983	0.9769	0.9990	0.8897
XIAP	CASP9	1tft_A	0.8136	0.5387	0.9926	0.9300
XIAP	CASP9	1nw9_A	0.9305	0.5387	0.9926	0.8778
XIAP	DIABLO	1g73_C	0.8154	0.5387	0.7883	0.8305
XIAP	DIABLO	1g73_D	0.7672	0.5387	0.7883	0.8391
XIAP	DIABLO	2opy_A	0.9421	0.5387	0.7883	0.8336
CD247	ZAP70	2oq1_A pocket1	0.8303	0.7912	0.8296	0.2915
CD247	ZAP70	2oq1_A pocket2	0.2697	0.7912	0.8296	0.4264

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S2. Predicted highly druggable PPIs in Dr. PIAS.

Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	Druggability score			
			Structural attributes	Drug/chemical attributes	Functional attributes	All attributes
ABL1	CRK	1ju5_C	0.3825	0.4185	0.6486	0.9122
ARHGAP1	CDC42	1am4_F	0.4813	0.5387	0.9547	0.9327
BCL2L1	BCL2L1	3ilb_N	0.9646	0.7397	0.9642	0.9110
BRAF	RAF1	3q96_A	0.9704	0.6736	0.9975	0.9209
CALM1	CAMK2G	1cm4_A	0.9954	0.9968	0.9942	0.9754
CALM1	CAMKK1	1ckk_A	0.9944	0.9998	0.8502	0.9865
CALM1	CAMKK2	1ckk_A	0.9944	0.9998	0.4493	0.9737
CALM1	GRIN1	3bya_A	0.9969	0.8663	0.4556	0.9663
CALM1	KCNN2	1g4y_R	0.9478	0.9477	0.2900	0.9423
CALM1	RYR1	2bcx_A	0.9911	0.9544	0.4977	0.9434
CALM2	MARCKS	1iwq_A	0.9965	0.9998	0.2820	0.9487
CALM2	MYO6	2vas_B	0.9952	0.9998	0.1739	0.9186
CALM3	CAMK2A	1cm4_A	0.9954	0.9865	0.9514	0.9844
CALM3	MARCKS	1iwq_A	0.9965	0.9998	0.2798	0.9524
CALM3	MYO6	2vas_B	0.9952	0.9998	0.1861	0.9213
CDH1	CTNNB1	1i7w_C	0.9799	0.4991	0.9974	0.9925
CDH1	JUP	3ifq_A	0.8486	0.0000	0.7726	0.9256
CDH3	CTNNB1	1i7w_C	0.9799	0.4991	0.4372	0.9727
CTNNB1	CTNNBIP1	1luj_A	0.5249	0.4991	0.4217	0.9469
CTNNB1	LEF1	3oux_A	0.8720	0.4991	0.9528	0.9661
DOCK2	RAC1	2yin_A	0.9868	0.4991	0.9802	0.9800
EP300	TP53	2k8f_A	0.9227	0.4991	0.9936	0.9259
FKBP1A	PPP3CA	1tco_C	0.9110	0.7074	0.9427	0.9222
FKBP1A	PPP3R1	1tco_C	0.9110	0.7074	0.8777	0.9104
GRB2	GRB2	3n7y_A	0.9464	0.9961	0.9724	0.9424
GRB2	VAV1	1gcq_C	0.6600	0.7912	0.9860	0.9323
HRAS	RASA1	1wq1_G	0.5284	0.5691	0.9955	0.9314
MAPK14	MAPKAPK2	2oza_A	0.9730	0.6779	0.9948	0.9373
PAK1	RAC1	2qme_A	0.2748	0.4991	0.9992	0.9205
PAK2	RAC1	2qme_A	0.2748	0.4991	0.9989	0.9144
PRKACA	PRKAR1A	2qcs_A	0.6991	0.6077	0.9940	0.9227
PRKCE	YWHAZ	2wh0_B	0.9241	0.0000	0.9387	0.9601
RAC1	ARFIP2	1i4t_D	0.4861	0.4991	0.8991	0.9208
RAC1	KALRN	2nz8_B	0.5612	0.4991	0.9856	0.9092
RAC1	VAV1	3bji_C	0.9337	0.4991	0.9857	0.9829
RHOA	ARHGDIA	1cc0_A	0.8604	0.4991	0.9886	0.9480
RHOA	ARHGEF11	3kz1_A	0.8327	0.4991	0.9632	0.9480
RHOA	ARHGEF12	1x86_G	0.8101	0.4991	0.9921	0.9605
RHOA	GEFT	2rgn_F	0.8057	0.4991	0.7973	0.9562
RHOA	MCF2L	1lb1_F	0.8029	0.4991	0.9758	0.9614
RXRA	NCOA1	1fm6_U	0.6024	0.7966	0.3540	0.9183

Table S3. Matrix of the similarities of the positive instances assessed by our SVM model using all attributes [a]

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
1	ARF1	CYTH2	1s9d_A [b]	3657	0	0	0	0	0	6	165	0	1328	0	1196	0	996	0	2	86	0	22	47	37	45	2	0	0	21	93	0
2	ARF1	CYTH2	1s9d_E [b]	2848	0	0	0	0	470	0	94	0	0	1392	18	293	12	746	0	53	0	0	0	0	0	0	0	0	0	0	0
3	ARF1	CYTH2	1r8q_A [b]	3903	0	0	0	0	0	1	12	0	796	0	1326	0	1121	0	0	3	0	10	6	0	4	0	0	0	2	15	2
4	ARF1	CYTH2	1r8q_E [b]	3188	0	0	0	0	971	0	1	0	647	9	1273	14	1634	0	0	0	0	0	0	0	0	0	0	0	0	0	55
5	ARF1	CYTH2	1r8q_B [b]	3862	0	0	0	0	0	0	3	0	784	0	1083	0	1356	0	0	0	0	3	12	0	0	0	0	0	1	1	1
6	ARF1	CYTH2	1r8q_F [b]	2960	0	0	0	0	1232	0	3	0	660	4	930	21	1936	0	0	0	0	0	0	0	0	0	0	0	0	0	52
7	ARF1	CYTH2	1r8q_BF [c]	118	0	0	0	0	0	2463	1082	1082	10	1	60	0	40	0	2429	947	1292	0	0	0	0	0	0	0	0	0	0
8	ARF1	CYTH2	1s9d_AE [c]	61	0	0	0	0	0	1240	2753	705	1	0	20	0	15	0	1063	2506	642	0	0	0	0	0	0	0	0	0	0
9	ARF1	CYTH2	1r8s_AE [c]	45	0	0	0	0	0	1876	1124	1634	0	0	20	0	15	0	1851	973	1913	0	0	0	0	0	0	0	0	0	0
10	ARF1	CYTH1	1s9d_A [b]	3090	0	0	0	0	0	1	59	0	1396	0	1427	0	1216	0	3	104	0	34	68	47	52	1	0	0	22	87	0
11	ARF1	CYTH1	1s9d_E [b]	2275	0	0	0	0	354	0	51	0	0	1599	48	387	28	848	0	69	0	0	0	0	0	0	0	0	0	0	1
12	ARF1	CYTH1	1r8q_A [b]	3300	0	0	0	0	0	0	2	0	854	1	1559	0	1333	0	0	4	0	22	19	1	5	0	0	0	2	20	4
13	ARF1	CYTH1	1r8q_E [b]	2701	0	0	0	0	836	0	0	0	0	783	17	1442	20	1871	0	1	0	0	0	0	0	0	0	0	0	0	54
14	ARF1	CYTH1	1r8q_B [b]	3270	0	0	0	0	0	0	0	0	833	0	1314	0	1573	0	0	0	0	11	19	2	1	1	0	0	1	2	2
15	ARF1	CYTH1	1r8q_F [b]	2489	0	0	0	0	1066	0	0	0	0	809	6	1069	20	2219	0	0	0	0	0	0	0	0	0	0	0	0	49
16	ARF1	CYTH1	1r8q_BF [c]	89	0	0	0	0	0	1911	586	849	10	1	68	0	40	0	2964	1412	1526	0	0	0	0	0	0	0	0	0	0
17	ARF1	CYTH1	1s9d_AE [c]	16	0	0	0	0	0	647	2129	368	1	0	21	0	11	0	1577	3110	936	0	0	0	0	0	0	0	0	0	0
18	ARF1	CYTH1	1r8s_AE [c]	15	0	0	0	0	0	1389	621	1359	0	0	17	0	11	0	2323	1456	2194	0	0	0	0	0	0	0	0	0	0
19	BAK1	BCL2	2o2f_A	11	0	0	0	0	0	0	0	0	1	0	8	0	15	0	0	0	0	2290	2219	2322	1219	162	214	96	83	89	95
20	BAK1	BCL2	2o22_A	5	0	0	0	0	0	0	0	0	0	0	3	0	7	0	0	0	0	2297	2224	2324	1218	170	218	115	93	103	137
21	BAK1	BCL2	2o21_A	12	0	0	0	0	0	0	0	0	3	0	6	0	11	0	0	0	0	2152	2083	2336	1457	133	191	88	78	77	147
22	BAK1	BCL2	1ysw_A	11	0	0	0	0	0	0	0	0	3	0	10	0	10	0	0	0	0	2155	2086	2249	1560	126	192	88	79	84	144
23	BAK1	BCL2L1	2o2n_A	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1495	880	568	310	992	1062	390	419	697	64
24	BAK1	BCL2L1	2o2m_A	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	1627	931	793	409	917	1032	118	407	156	64
25	BAK1	BCL2L1	2yxj_A	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	543	547	560	307	736	776	926	732	772	90
26	BAK1	BCL2L1	2yxj_B	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	529	480	458	350	739	819	915	931	862	90
27	BAK1	BCL2L1	1ysi_A	2	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	1	517	474	457	349	737	806	900	888	972	37
28	BAK1	BCL2L1	2w3l_A	1	0	0	0	0	0	0	0	0	0	0	2	0	5	0	0	0	0	1331	1353	1643	1069	118	250	80	62	54	1018
29	BAK1	BCL2L1	2w3l_B	0	0	0	0	0	0	0	0	0	0	0	2	0	2	0	0	0	0	1279	1360	1638	1076	117	294	82	51	58	1011
30	BAK1	BCL2L1	3inq_A	3	0	0	0	0	0	0	0	0	0	0	1	0	6	0	0	0	0	1067	488	535	284	989	656	579	878	593	90
31	BAK1	BCL2L1	3inq_B	2	0	0	0	0	0	0	0	0	0	0	2	0	3	0	0	0	0	564	380	518	338	676	723	760	685	723	63
32	CALM1	CAMK1	1mux_A pocket1	86	0	0	0	0	0	0	0	0	9	28	48	0	36	0	0	1	0	0	0	8	5	0	0	0	0	0	66
33	CALM1	CAMK1	1mux_A pocket2	24	0	0	0	0	0	0	0	0	0	7	24	1	17	0	0	1	0	13	2	25	13	1	1	0	0	0	98
34	CALM1	MYLK	1mux_A pocket1	134	0	0	0	0	0	1	0	0	9	29	53	0	41	0	0	0	0	0	0	3	2	0	0	0	0	0	82
35	CALM1	MYLK	1mux_A pocket2	59	0	0	0	0	0	0	0	0	0	6	31	0	22	0	0	0	0	4	0	11	3	0	0	0	0	0	99
36	CALM1	PDE1A	1qiv_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	245	27	340	213	17	107	3	19	6	2
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	CREBBP	TP53	2d82_A	7	0	0	0	0	0	2	1	3	0	0	6	0	4	0	11	1	5	1	0	0	0	4	2	1	3	1	6
39	ESR1	NCOA2	3erd_A	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	ESR1	NCOA2	3erd_B	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	FKBP1A	TGFBR1	1fkj_A	712	0	0	0	0	0	0	0	0	0	2	228	0	151	0	0	0	0	306	16	13	4	0	68	0	0	0	14
42	FKBP1A	TGFBR1	1kf_A	649	0	0	0	0	0	0	0	0	0	4	161	0	168	0	0	0	0	668	89	57	39	0	125	0	5	0	69
43	EGFR	GRB2	1cj1_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
44	EGFR	GRB2	1cj1_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
45	EGFR	GRB2	1cj1_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
46	EGFR	GRB2	1cj1_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
47	EGFR	GRB2	1cj1_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
48	EGFR	GRB2	1cj1_G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
49	EGFR	GRB2	1cj1_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
50	EGFR	GRB2	1cj1_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	2	0	0	0	0
51	EGFR	GRB2	1cj1_J	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0
52	GRB2	MET	1cj1_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	5	3	0	0	0
53	GRB2	MET	1cj1_C	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	5	4	0	0	0
54	GRB2	MET	1cj1_D	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	4	2	0	0	0
55	GRB2	MET	1cj1_E	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	10	5	0	0	0
56	GRB2	MET	1cj1_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	4	3	0	0	0
57	GRB2	MET	1cj1_G	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	3	3	0	0	0
58	GRB2	MET	1cj1_H	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	3	2	0	0	0
59	GRB2	MET	1cj1_I	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	15	0	0	0	0	18	2	0	0	0
60	GRB2	MET	1cj1_J	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	6	3	0	0	0
61	HOXB1	PBX1	1b72_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	IL1B	IL1R1	1itb_B	18	0	0	0	0	0	0	0	0	13	1	0	0	0	0	0	0	0	2	1	0	0	3	1	0	0	0	2
63	IL2	IL2RA	1py2_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64	IL2	IL2RA	1py2_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	IL2	IL2RA	1py2_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66	IL2	IL2RA	1py2_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67	IL2	IL2RA	1m48_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	IL2	IL2RA	1m48_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69	IL2	IL2RA	1m4a_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	PTEN	MAGI3	1be9_A	1	0	0	0	0	0	0	2	0	0	0	0	1	0	0	3	0	1	1	0	0	0	0	0	0	0	1	0
71	MDM2	TP53	1t4e_A	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	2	0	2	1	9	8	2	5	7	0	0	1
72	MDM2	TP53	1t4e_B	6	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	9	0	2	1	7	6	2	6	0	0	0	0
73	MDM2	TP53	1ttv_A	4	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	1	0	1	0	1	0	0	8	1	1	0	0
74	MDM2	TP53	3jzk_A	16	0	0	0	0	0	0	0	0	4	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
75	MDM2	TP53	3lbk_A	5	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	2	0	15	7	0	7	0	1	0	6
76	MDM2	TP53	3lbl_A	19	0	0	0	0	0	0	7	0	6	1	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	2
77	MDM2	TP53	3lbl_C	14	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2
78	MDM2	TP53	3lbl_E	3	0	0	0	0	0	0	0	0	0	0	1	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
79	MDM4	TP53	3lbj_E	3	0	0	0	0	0	0	0	0	0	0	1	0	4	0	0	0	0	0	0	0	0	0	5	0	0	0	1
80	PDGFRB	PIK3R1	1h9o_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	5	0	0	0	0
81	RAC1	TIAM1	1foe_B	208	0	0	0	0	0	1	0	0	0	89	0	213	0	0	0	0	0	3	2	0	0	0	5	0	0	0	0
82	RAC1	TIAM1	1foe_D	206	0	0	0	0	0	1	0	0	0	80	0	215	0	0	0	0	0	3	2	0	0	0	5	0	0	0	0
83	RAC1	TIAM1	1foe_F	219	0	0	0	0	0	1	0	0	0	87	0	226	0	0	0	0	0	2	2	0	0	0	5	0	0	0	0
84	RAC1	TIAM1	1foe_H	208	0	0	0	0	0	1	0	0	0	86	0	197	0	0	0	0	0	3	2	0	0	0	5	0	0	0	0
85	RAC1	TRIO	2nz8_A	342	0	0	0	0	0	4	0	0	0	136	0	242	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0
86	RAF1	YWHAZ	3rdh_A	692	0	0	0	0	0	25	0	15	0	0	190	0	195	0	14	0	11	126	3	68	32	408	23	1	9	226	0
87	RAF1	YWHAZ	3rdh_B	315	0	0	0	0	0	5	7	15	1	0	50	0	105	0	4	2	10	20	2	4	2	378	0	2	70	233	0
88	RAF1	YWHAZ	3rdh_C	7	0	0	0	0	0	6	91	96	0	0	0	0	4	0	3	50	72	2	0	0	0	127	0	0	0	0	0
89	RAF1	YWHAZ	3rdh_D	1	0	0	0	0	0	237	0	35	0	0	0	0	0	0	234	0	39	1	0	0	0	3	0	0	11	0	0
90	S100B	TP53	3hcm_A	169	0	0	0	0	127	0	0	0	0	21	35	127	22	397	0	1	0	0	0	0	0	0	0	0	0	0	356
91	S100B	TP53	3hcm_B	0	0	0	0	0	0	0	0	0	0	0	3	0	4	0	0	0	0	191	45	423	331	27	192	12	32	74	354
92	STAT3	STAT3	1bg1_A	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
93	BIRC5	BIRC5	1e31_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94	BIRC5	BIRC5	1e31_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
95	BIRC5	BIRC5	1f3h_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	1	1	0	0	0	0	0	0	0
96	BIRC5	BIRC5	1f3h_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	1	2	1	0	0	0	1	0	0
97	BIRC5	BIRC5	1xox_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98	BIRC5	BIRC5	1xox_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
99	CTNNB1	TCF7L1	1g3j_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	2	0
100	CTNNB1	TCF7L1	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	2	0
101	CTNNB1	TCF7L2	1g3j_A	0	0	0	0	0	0	1	2	0	2	0	0	0	0	0	16	2	0	0	0	0	0	2	0	0	0	1	7
102	CTNNB1	TCF7L2	1g3j_C	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	4	3	0	0	0	0	0	11	0	0	1	7	0
103	THRB	NCOA2	1bsx_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
104	TNF	TNF	2az5_AB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
105	TNF	TNF	2az5_CD	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
106	XIAP	CASP3	1i3o_E pocket1	5	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	2	1	0	0	0	2	0	0	0	0
107	XIAP	CASP3	1i3o_E pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	4	1	2	0	6
108	XIAP	CASP3	1i3o_F pocket3	3	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	5	3	3	0	7
109	XIAP	CASP3	1i3o_F pocket4	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	5	0	3	3	7
110	XIAP	CASP9	1tft_A	33	0	0	0	0	0	0	0	0	0	0	9	0	28	0	0	3	0	3	0	0	0	0	2	0	0	0	0
111	XIAP	CASP9	1nw9_A	8	0	0	0	0	0	0	0	0	0	0	2	0	3	0	0	0	0	0	0	0	0	0	2	0	0	0	0
112	XIAP	DIABLO	1g73_C	7	0	0	0	0	0	0	0	0	0	0	3	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
113	XIAP	DIABLO	1g73_D	9	0	0	0	0	0	0	0	0	0	0	3	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
114	XIAP	DIABLO	2opy_A	8	0	0	0	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
115	CD247	ZAP70	2oq1_A pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
116	CD247	ZAP70	2oq1_A pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S3. (continued)

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56
1	ARF1	CYTH2	1s9d_A [b]	0	0	9	0	0	0	1	0	0	0	0	0	19	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	ARF1	CYTH2	1s9d_E [b]	0	0	0	1	0	3	1	0	0	0	0	0	672	218	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	ARF1	CYTH2	1r8q_A [b]	0	0	1	0	0	0	0	0	0	0	0	0	311	73	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	ARF1	CYTH2	1r8q_E [b]	28	0	0	1	11	5	19	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	ARF1	CYTH2	1r8q_B [b]	0	0	0	0	0	0	0	0	0	0	0	0	123	27	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	ARF1	CYTH2	1r8q_F [b]	22	0	0	0	3	0	6	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	ARF1	CYTH2	1r8q_BF [c]	0	0	0	0	0	0	0	0	0	81	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	ARF1	CYTH2	1s9d_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	ARF1	CYTH2	1r8s_AE [c]	0	0	0	0	0	0	0	0	0	54	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	ARF1	CYTH1	1s9d_A [b]	0	0	7	0	0	0	1	0	0	0	0	0	6	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	ARF1	CYTH1	1s9d_E [b]	0	0	0	1	0	6	1	0	0	0	0	0	423	123	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	ARF1	CYTH1	1r8q_A [b]	0	0	1	0	0	0	0	0	0	0	0	0	184	26	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	ARF1	CYTH1	1r8q_E [b]	29	0	0	1	11	5	20	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	ARF1	CYTH1	1r8q_B [b]	0	0	2	0	0	0	0	0	0	0	0	0	49	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	ARF1	CYTH1	1r8q_F [b]	24	0	0	0	4	0	6	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	ARF1	CYTH1	1r8q_BF [c]	0	0	0	0	0	0	0	0	0	67	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	ARF1	CYTH1	1s9d_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	ARF1	CYTH1	1r8s_AE [c]	0	0	0	0	0	0	0	0	0	40	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	BAK1	BCL2	2o2f_A	83	119	431	0	0	0	0	0	0	0	0	0	4	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	BAK1	BCL2	2o22_A	102	120	413	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	BAK1	BCL2	2o21_A	98	84	446	0	0	0	0	0	0	0	0	0	3	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	BAK1	BCL2	1ysw_A	93	85	457	0	0	0	0	0	0	0	0	0	3	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	BAK1	BCL2L1	2o2n_A	38	928	1437	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	BAK1	BCL2L1	2o2m_A	62	370	1583	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	BAK1	BCL2L1	2yxj_A	80	720	2573	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	BAK1	BCL2L1	2yxj_B	43	729	2284	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0
27	BAK1	BCL2L1	1ysi_A	7	712	2205	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	BAK1	BCL2L1	2w3l_A	983	81	272	0	1	1	9	0	0	0	0	0	4	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	BAK1	BCL2L1	2w3l_B	991	52	288	0	2	1	10	0	0	0	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	BAK1	BCL2L1	3inq_A	74	946	2039	0	0	0	0	0	0	0	0	0	4	6	0	0	0	0	0	0	0	0	0	0	0	0	1	0
31	BAK1	BCL2L1	3inq_B	62	660	2683	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
32	CALM1	CAMK1	1mux_A pocket1	50	0	0	3773	2178	2317	876	2	0	0	0	2	25	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	CALM1	CAMK1	1mux_A pocket2	82	0	1	2523	3422	1825	1390	9	0	0	3	2	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	CALM1	MYLK	1mux_A pocket1	55	0	0	1879	1449	4271	1605	0	0	0	0	0	53	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	CALM1	MYLK	1mux_A pocket2	87	0	0	641	2696	3779	2106	1	0	0	0	0	26	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	CALM1	PDE1A	1qiv_A	1	17	94	125	375	102	259	8014	0	0	0	0	11	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	CD4	HLA-DQB1	1j4_D	0	0	0	0	0	0	0	0	9318	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	CREBBP	TP53	2d82_A	2	2	3	0	0	0	0	0	0	9737	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	ESR1	NCOA2	3erd_A	0	0	0	5	57	1	12	0	0	0	3525	2673	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	ESR1	NCOA2	3erd_B	0	0	0	232	584	133	237	0	0	0	2807	3366	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	FKBP1A	TGFBR1	1fkj_A	1	2	1	0	0	0	0	0	0	0	0	0	4264	2271	0	0	0	0	0	0	0	0	0	2	1	1	1	1
42	FKBP1A	TGFBR1	1fkf_A	2	12	1	0	0	0	0	0	0	0	0	0	4117	2416	0	0	0	0	0	0	0	0	0	3	1	2	4	3
43	EGFR	GRB2	1cj1_B	0	0	2	0	0	0	0	0	0	0	0	0	8	6	417	359	391	361	308	362	389	375	389	507	472	530	462	505
44	EGFR	GRB2	1cj1_C	0	0	2	0	0	0	0	0	0	0	0	0	10	6	417	371	391	362	308	362	389	375	376	507	472	530	462	505
45	EGFR	GRB2	1cj1_D	0	0	1	0	0	0	0	0	0	0	0	0	10	7	405	359	408	361	322	362	389	375	370	507	472	530	462	505
46	EGFR	GRB2	1cj1_E	0	0	2	0	0	0	0	0	0	0	0	0	13	6	416	371	391	372	308	362	389	396	346	507	472	530	462	505
47	EGFR	GRB2	1cj1_F	0	0	1	0	0	0	0	0	0	0	0	0	8	7	405	359	408	361	322	375	406	375	340	507	472	530	462	505
48	EGFR	GRB2	1cj1_G	0	0	1	0	0	0	0	0	0	0	0	0	9	7	405	371	408	361	322	375	406	375	328	507	472	530	462	505
49	EGFR	GRB2	1cj1_H	0	0	1	0	0	0	0	0	0	0	0	0	8	7	417	360	408	361	322	375	406	375	327	507	472	530	462	505
50	EGFR	GRB2	1cj1_I	0	0	3	0	0	0	0	0	0	0	0	0	12	6	405	359	391	361	308	362	389	375	369	507	472	530	462	505
51	EGFR	GRB2	1cj1_J	0	0	2	0	0	0	0	0	0	0	0	0	9	6	405	359	391	361	308	362	389	375	401	507	472	530	462	505
52	GRB2	MET	1cj1_B	0	1	17	0	0	0	0	0	0	0	0	0	226	104	47	24	24	31	15	23	31	31	222	858	812	887	816	848
53	GRB2	MET	1cj1_C	0	0	16	0	0	0	0	0	0	0	0	0	247	106	47	36	24	32	15	23	31	31	209	858	812	887	816	848
54	GRB2	MET	1cj1_D	0	1	15	0	0	0	0	0	0	0	0	0	247	109	35	24	40	31	29	23	31	31	204	858	812	887	816	848
55	GRB2	MET	1cj1_E	0	0	29	0	0	0	0	0	0	0	0	0	256	117	46	36	25	42	15	23	31	52	179	858	812	887	816	848
56	GRB2	MET	1cj1_F	0	2	10	0	0	0	0	0	0	0	0	0	236	105	35	24	40	31	29	36	48	31	174	858	812	887	816	848
57	GRB2	MET	1cj1_G	0	2	9	0	0	0	0	0	0	0	0	0	255	105	35	36	40	31	29	36	48	31	162	858	812	887	816	848
58	GRB2	MET	1cj1_H	0	3	9	0	0	0	0	0	0	0	0	0	235	94	47	25	40	31	29	36	48	31	160	858	812	887	816	848
59	GRB2	MET	1cj1_I	0	0	73	0	0	0	0	0	0	0	0	0	258	126	35	24	25	42	15	23	31	52	202	858	811	887	816	848
60	GRB2	MET	1cj1_J	0	1	22	0	0	0	0	0	0	0	0	0	247	113	35	24	24	31	15	23	31	31	234	858	812	887	816	848
61	HOXB1	PBX1	1b72_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	IL1B	IL1R1	1itb_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	IL2	IL2RA	1py2_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64	IL2	IL2RA	1py2_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	IL2	IL2RA	1py2_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66	IL2	IL2RA	1py2_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67	IL2	IL2RA	1m48_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	IL2	IL2RA	1m48_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69	IL2	IL2RA	1m4a_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	PTEN	MAGI3	1be9_A	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	MDM2	TP53	1t4e_A	0	0	1	0	0	0	0	0	0	0	0	0	59	42	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72	MDM2	TP53	1t4e_B	0	0	1	0	0	1	0	0	0	0	0	0	87	44	0	0	0	0	0	0	0	0	0	0	0	0	0	0
73	MDM2	TP53	1ttv_A	0	0	0	0	0	0	0	0	0	1	0	0	58	44	0	0	0	0	0	0	0	0	0	2	0	2	0	0
74	MDM2	TP53	3jzk_A	0	0	0	0	0	3	0	0	0	0	0	0	89	44	0	0	0	0	0	0	0	0	0	0	0	0	0	0
75	MDM2	TP53	3lbk_A	0	0	1	0	0	1	0	0	0	1	0	0	58	44	0	0	0	0	0	0	0	0	0	0	0	0	0	0
76	MDM2	TP53	3lbl_A	28	0	0	2	5	97	17	0	0	0	0	0	585	189	0	0	0	0	0	0	0	0	0	0	0	0	0	0
77	MDM2	TP53	3lbl_C	3	0	0	1	1	12	0	0	0	0	0	0	689	281	0	0	0	0	0	0	0	0	0	0	0	0	0	0
78	MDM2	TP53	3lbl_E	0	0	0	0	0	2	1	0	5	0	0	0	65	44	0	0	0	0	0	0	0	0	0	0	0	0	0	0
79	MDM4	TP53	3lbj_E	1	0	0	0	0	0	1	0	0	0	0	0	93	66	0	0	0	0	0	0	0	0	0	0	0	0	0	0
80	PDGFRB	PIK3R1	1h9o_A	0	0	19	0	0	0	0	0	0	0	0	0	1	0	10	7	4	6	2	5	6	9	14	117	122	101	116	97
81	RAC1	TIAM1	1foe_B	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0
82	RAC1	TIAM1	1foe_D	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0
83	RAC1	TIAM1	1foe_F	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
84	RAC1	TIAM1	1foe_H	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
85	RAC1	TRIO	2nz8_A	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	2	0	1	0	0
86	RAF1	YWHAZ	3rdh_A	0	15	126	0	0	0	0	0	0	0	0	0	102	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0
87	RAF1	YWHAZ	3rdh_B	0	110	5	0	0	0	0	0	0	0	0	0	32	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
88	RAF1	YWHAZ	3rdh_C	0	1	0	0	0	0	0	0	0	0	0	0	4	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
89	RAF1	YWHAZ	3rdh_D	0	2	0	0	0	0	0	0	0	0	0	0	228	64	1	0	0	2	0	0	1	0	0	78	97	86	68	69
90	S100B	TP53	3hcm_A	167	0	0	16	55	11	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
91	S100B	TP53	3hcm_B	186	22	558	0	26	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
92	STAT3	STAT3	1bg1_A	0	0	0	0	0	0	0	0	0	0	0	0	1	5	0	0	0	0	0	0	0	0	0	2	2	5	1	2
93	BIRC5	BIRC5	1e31_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94	BIRC5	BIRC5	1e31_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
95	BIRC5	BIRC5	1f3h_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
96	BIRC5	BIRC5	1f3h_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
97	BIRC5	BIRC5	1xox_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98	BIRC5	BIRC5	1xox_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
99	CTNNB1	TCF7L1	1g3j_A	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
100	CTNNB1	TCF7L1	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
101	CTNNB1	TCF7L2	1g3j_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
102	CTNNB1	TCF7L2	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
103	THRB	NCOA2	1bsx_B	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
104	TNF	TNF	2az5_AB	0	0	0	0	0	0	0	0	0	5	0	0	0	0	5	3	1	1	2	4	1	5	1	0	0	0	0	0
105	TNF	TNF	2az5_CD	0	0	0	0	0	0	0	0	0	6	0	0	0	0	3	2	1	1	2	2	1	3	0	0	0	0	0	0
106	XIAP	CASP3	1i3o_E pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107	XIAP	CASP3	1i3o_E pocket2	1	0	9	0	0	0	0	0	0	3822	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108	XIAP	CASP3	1i3o_F pocket3	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
109	XIAP	CASP3	1i3o_F pocket4	1	5	6	0	0	0	0	0	0	4336	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1
110	XIAP	CASP9	1tft_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111	XIAP	CASP9	1nw9_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
112	XIAP	DIABLO	1g73_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
113	XIAP	DIABLO	1g73_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
114	XIAP	DIABLO	2opy_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
115	CD247	ZAP70	2oq1_A pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
116	CD247	ZAP70	2oq1_A pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S3. (continued)

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84
1	ARF1	CYTH2	1s9d_A [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	ARF1	CYTH2	1s9d_E [b]	0	0	0	0	0	208	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	ARF1	CYTH2	1r8q_A [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	ARF1	CYTH2	1r8q_E [b]	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2	2
5	ARF1	CYTH2	1r8q_B [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	ARF1	CYTH2	1r8q_F [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	2	2	8	2
7	ARF1	CYTH2	1r8q_BF [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	ARF1	CYTH2	1s9d_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	268	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	ARF1	CYTH2	1r8s_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	118	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	ARF1	CYTH1	1s9d_A [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	ARF1	CYTH1	1s9d_E [b]	0	0	0	0	0	393	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	ARF1	CYTH1	1r8q_A [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	ARF1	CYTH1	1r8q_E [b]	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2	1
14	ARF1	CYTH1	1r8q_B [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	ARF1	CYTH1	1r8q_F [b]	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	3	2	8	2
16	ARF1	CYTH1	1r8q_BF [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	42	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	ARF1	CYTH1	1s9d_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	306	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	ARF1	CYTH1	1r8s_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	172	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	BAK1	BCL2	2o2f_A	0	0	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	BAK1	BCL2	2o22_A	0	0	0	0	0	0	0	0	0	0	0	0	0	50	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	BAK1	BCL2	2o21_A	0	0	0	0	0	0	0	0	0	0	0	0	0	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	BAK1	BCL2	1ysw_A	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	BAK1	BCL2L1	2o2n_A	0	0	0	0	0	0	0	0	0	0	0	0	0	130	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	BAK1	BCL2L1	2o2m_A	0	0	0	0	0	1	0	0	0	0	0	0	0	67	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	BAK1	BCL2L1	2yxj_A	0	0	0	0	0	0	0	0	0	0	0	0	0	87	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	BAK1	BCL2L1	2yxj_B	0	0	0	0	0	0	0	0	0	0	0	0	0	92	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	BAK1	BCL2L1	1ysi_A	0	0	0	0	0	0	0	0	0	0	0	0	0	181	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	BAK1	BCL2L1	2w3l_A	0	0	0	0	0	0	0	0	0	0	0	0	0	15	0	0	0	0	0	0	0	0	0	0	0	1	0	0
29	BAK1	BCL2L1	2w3l_B	0	0	0	0	0	0	0	0	0	0	0	0	0	49	0	0	0	0	0	0	0	0	0	0	0	1	0	0
30	BAK1	BCL2L1	3inq_A	0	0	0	0	0	0	0	0	0	0	0	0	0	50	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	BAK1	BCL2L1	3inq_B	0	0	0	0	0	0	0	0	0	0	0	0	0	54	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	CALM1	CAMK1	1mux_A pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	8	7	1	59	0	0	0	0	0
33	CALM1	CAMK1	1mux_A pocket2	0	0	0	0	0	2	0	0	0	0	0	0	0	45	0	0	0	0	0	0	0	0	101	0	0	0	0	0
34	CALM1	MYLK	1mux_A pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	1	17	7	1	78	0	0	0	0	0
35	CALM1	MYLK	1mux_A pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	32	0	0	0	0	0	2	0	0	176	0	0	0	0	0
36	CALM1	PDE1A	1qiv_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	0	0	0	0	0	0	0	0	0	15	1	0	2	0	0	0	0	0	61	0	0	0	0	0
38	CREBBP	TP53	2d82_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
39	ESR1	NCOA2	3erd_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
40	ESR1	NCOA2	3erd_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	FKBP1A	TGFBR1	1fkj_A	1	0	0	2	0	0	0	0	0	0	0	0	0	9	14	106	3	4	1	3	2	0	1321	0	0	0	0	0
42	FKBP1A	TGFBR1	1kff_A	1	0	1	3	0	0	0	0	0	0	0	0	0	0	7	8	67	3	2	0	3	0	818	0	0	0	0	0
43	EGFR	GRB2	1cj1_B	448	468	507	262	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	1	0	1	1153	0	0	0	0
44	EGFR	GRB2	1cj1_C	448	468	507	262	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	1	0	1	1153	0	0	0	0
45	EGFR	GRB2	1cj1_D	448	468	507	262	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	1	1146	0	0	1	0
46	EGFR	GRB2	1cj1_E	448	468	507	261	0	2	0	0	0	0	0	0	0	1	0	1	1	0	0	0	1	0	1	1155	0	0	0	0
47	EGFR	GRB2	1cj1_F	448	468	507	262	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	1	0	1	1125	0	0	1	0
48	EGFR	GRB2	1cj1_G	448	468	506	262	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	1	1118	0	0	0	0
49	EGFR	GRB2	1cj1_H	448	468	506	262	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	1	1087	0	0	1	0
50	EGFR	GRB2	1cj1_I	448	468	507	262	0	2	0	0	0	0	0	0	0	1	0	1	2	1	0	1	1	0	1	1160	0	0	0	0
51	EGFR	GRB2	1cj1_J	448	468	507	262	0	1	0	0	0	0	0	0	0	1	0	1	1	0	0	0	1	0	1	1154	0	0	0	0
52	GRB2	MET	1cj1_B	782	798	857	414	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	4	1156	1	0	0	0
53	GRB2	MET	1cj1_C	782	798	857	414	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	4	1153	1	0	0	0
54	GRB2	MET	1cj1_D	782	798	857	414	0	0	0	0	0	0	0	0	0	2	0	1	0	0	0	0	0	0	3	1146	1	0	0	0
55	GRB2	MET	1cj1_E	782	798	857	414	0	0	0	0	0	0	0	0	0	11	1	0	1	0	0	0	0	0	12	1159	1	0	0	0
56	GRB2	MET	1cj1_F	782	798	857	414	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	4	1137	1	0	0	0
57	GRB2	MET	1cj1_G	782	798	857	414	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	4	1122	1	0	0	0
58	GRB2	MET	1cj1_H	782	798	857	414	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	3	1103	1	0	0	0
59	GRB2	MET	1cj1_I	782	798	857	414	0	0	0	0	0	0	0	0	0	20	1	0	0	0	0	0	0	0	11	1159	1	0	0	0
60	GRB2	MET	1cj1_J	782	798	857	414	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	3	1156	1	0	0	0
61	HOXB1	PBX1	1b72_B	0	0	0	0	6413	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	IL1B	IL1R1	1itb_B	0	0	0	0	11	8600	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	IL2	IL2RA	1py2_A	0	0	0	0	343	4	1171	1137	1138	1165	1161	1188	467	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64	IL2	IL2RA	1py2_B	0	0	0	0	270	2	1172	1144	1139	1172	1169	1198	465	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	IL2	IL2RA	1py2_C	0	0	0	0	135	52	1151	1108	1169	1166	1136	1178	498	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66	IL2	IL2RA	1py2_D	0	0	0	0	242	6	1148	1086	1127	1154	1141	1169	528	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67	IL2	IL2RA	1m48_A	0	0	0	0	339	2	1162	1122	1129	1166	1189	1212	554	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
68	IL2	IL2RA	1m48_B	0	0	0	0	508	3	1138	1105	1127	1151	1173	1212	539	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69	IL2	IL2RA	1m4a_A	0	0	0	0	56	2	882	740	903	1032	1047	1044	575	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	PTEN	MAGI3	1be9_A	0	0	0	0	0	0	0	0	0	0	0	0	0	7625	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	MDM2	TP53	1t4e_A	0	1	0	0	0	0	0	0	0	0	0	0	0	48	891	967	1093	1030	1031	1058	1036	520	2034	0	0	0	0	0
72	MDM2	TP53	1t4e_B	0	0	0	1	0	0	0	0	0	0	0	0	0	29	891	967	1093	1036	1029	1064	1044	521	1979	0	0	0	0	0
73	MDM2	TP53	1ttv_A	2	2	2	1	0	0	0	0	0	0	0	0	0	6	871	959	1098	1043	1030	1054	1034	516	2027	10	0	0	0	0
74	MDM2	TP53	3jzk_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	846	927	1074	1053	1014	957	1009	491	1954	0	0	0	0	0
75	MDM2	TP53	3lbk_A	0	0	0	1	0	0	0	0	0	0	0	0	0	6	865	957	1096	1033	1032	1058	1033	511	2016	7	0	0	0	0
76	MDM2	TP53	3lbl_A	0	0	0	0	0	0	0	0	0	0	0	0	0	18	813	925	1043	965	1065	1034	0	517	1199	0	0	0	0	0
77	MDM2	TP53	3lbl_C	0	0	0	0	0	0	0	0	0	0	0	0	0	50	861	961	1084	1020	1023	1068	1044	518	1078	0	0	0	0	0
78	MDM2	TP53	3lbj_E	0	0	0	0	0	0	0	0	0	0	0	0	0	83	860	941	1064	933	1014	1062	1022	522	1959	0	0	0	0	0
79	MDM4	TP53	3lbj_E	0	0	0	0	0	0	0	0	0	0	0	0	0	45	15	30	67	31	47	11	10	19	9435	3	0	0	0	0
80	PDGFRB	PIK3R1	1h9o_A	107	104	126	64	0	0	0	0	0	0	0	0	0	42	0	4	0	0	0	0	0	0	639	7665	0	0	0	0
81	RAC1	TIAM1	1foe_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1409	1458	1508	764
82	RAC1	TIAM1	1foe_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1409	1458	1508	751
83	RAC1	TIAM1	1foe_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1404	1451	1508	764
84	RAC1	TIAM1	1foe_H	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1393	1350	1507	771
85	RAC1	TRIO	2nz8_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	132	174	187	101	0
86	RAF1	YWHAZ	3rdh_A	0	0	0	0	0	0	0	0	0	0	0	0	0	741	63	7	0	0	0	0	0	0	10	599	0	0	0	0
87	RAF1	YWHAZ	3rdh_B	0	0	0	0	0	0	0	0	0	0	0	0	0	761	118	27	0	0	0	0	0	0	6	4	0	0	0	0
88	RAF1	YWHAZ	3rdh_C	0	0	0	0	0	0	0	0	0	0	0	0	0	1703	0	1	0	0	0	0	0	0	370	0	0	0	0	0
89	RAF1	YWHAZ	3rdh_D	76	84	45	47	0	0	0	0	0	0	0	0	0	0	25	7	0	0	0	0	0	0	1	0	0	0	0	0
90	S100B	TP53	3hcm_A	0	0	0	0	1	5	0	0	0	0	0	0	0	58	0	0	0	0	0	0	0	0	1448	0	0	0	0	0
91	S100B	TP53	3hcm_B	0	0	0	0	0	31	0	0	0	0	0	0	0	83	0	0	0	0	0	0	0	0	139	0	1	0	2	0
92	STAT3	STAT3	1bg1_A	3	4	1	3	0	0	0	0	0	0	0	0	0	0	0	0	1	1	2	1	0	1	2	0	0	0	0	0
93	BIRC5	BIRC5	1e31_A	0	0	0	0	4	0	2	3	2	4	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
94	BIRC5	BIRC5	1e31_B	0	0	0	0	1	0	2	4	1	3	2	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
95	BIRC5	BIRC5	1f3h_A	0	0	0	0	11	0	1	1	1	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
96	BIRC5	BIRC5	1f3h_B	0	0	0	0	0	0	4	2	2	3	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
97	BIRC5	BIRC5	1xox_A	0	0	0	0	24	0	3	3	3	3	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
98	BIRC5	BIRC5	1xox_B	0	0	0	0	27	0	2	1	3	3	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
99	CTNNB1	TCF7L1	1g3j_A	0	0	0	0	0	0	0	0	0	0	0	0	0	240	0	0	0	0	0	0	0	0	11	0	0	0	0	0
100	CTNNB1	TCF7L1	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	235	0	0	0	0	0	0	0	0	14	0	0	0	0	0
101	CTNNB1	TCF7L2	1g3j_A	0	0	0	0	0	0	0	0	0	0	0	0	0	139	0	3	11	17	5	1	3	0	1	29	0	0	0	0
102	CTNNB1	TCF7L2	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	121	4	10	24	4	1	1	2	0	39	0	0	0	0	0
103	THRB	NCOA2	1bsx_B	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
104	TNF	TNF	2az5_AB	0	0	0	0	1446	0	0	0	0	0	0	0	0	3	51	55	51	13	27	24	33	22	1	0	0	0	0	0
105	TNF	TNF	2az5_CD	0	0	0	0	1454	0	0	0	0	0	0	0	0	3	50	48	45	10	23	23	31	22	1	0	0	0	0	0
106	XIAP	CASP3	1i3o_E pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107	XIAP	CASP3	1i3o_E pocket2	0	0	0	0	0	1	0	0	0	0	0	0	1	16	0	0	0	0	0	0	0	0	0	345	0	0	0	0
108	XIAP	CASP3	1i3o_F pocket3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109	XIAP	CASP3	1i3o_F pocket4	1	1	0	1	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	89	0	0	0	0
110	XIAP	CASP9	1tft_A	0	0	0	0	0	0	0	0	0	0	0	0	0	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111	XIAP	CASP9	1nw9_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
112	XIAP	DIABLO	1g73_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
113	XIAP	DIABLO	1g73_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
114	XIAP	DIABLO	2opy_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
115	CD247	ZAP70	2oq1_A pocket1	0	0	0	0	0	17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
116	CD247	ZAP70	2oq1_A pocket2	0	0	0	0	103	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S3. (continued)

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112
1	ARF1	CYTH2	1s9d_A [b]	13	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	212	440	3
2	ARF1	CYTH2	1s9d_E [b]	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	ARF1	CYTH2	1r8q_A [b]	67	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	559	119
4	ARF1	CYTH2	1r8q_E [b]	246	0	0	0	0	620	22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	142
5	ARF1	CYTH2	1r8q_B [b]	317	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	12	557	101
6	ARF1	CYTH2	1r8q_F [b]	362	0	0	0	0	611	24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	41
7	ARF1	CYTH2	1r8q_BF [c]	0	1	0	2	1	0	0	0	0	0	0	0	0	0	15	0	5	0	0	0	0	0	0	0	0	27	0	0
8	ARF1	CYTH2	1s9d_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	ARF1	CYTH2	1r8s_AE [c]	0	1	1	10	0	0	0	0	0	0	0	0	0	0	16	3	1	0	0	0	0	0	0	0	0	89	3	0
10	ARF1	CYTH1	1s9d_A [b]	11	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	221	438	3
11	ARF1	CYTH1	1s9d_E [b]	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	ARF1	CYTH1	1r8q_A [b]	60	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	515	145
13	ARF1	CYTH1	1r8q_E [b]	222	0	0	0	0	610	38	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	135
14	ARF1	CYTH1	1r8q_B [b]	289	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	10	505	105
15	ARF1	CYTH1	1r8q_F [b]	335	0	0	0	0	594	34	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	36
16	ARF1	CYTH1	1r8q_BF [c]	0	1	0	0	0	0	0	0	0	0	0	0	0	0	25	2	5	0	0	0	0	0	0	0	0	26	0	0
17	ARF1	CYTH1	1s9d_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	ARF1	CYTH1	1r8s_AE [c]	0	1	1	7	0	0	0	0	0	0	0	0	0	0	20	6	1	0	0	0	0	0	0	0	0	77	3	0
19	BAK1	BCL2	2o2f_A	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	4	0
20	BAK1	BCL2	2o22_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	BAK1	BCL2	2o21_A	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	BAK1	BCL2	1ysw_A	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0
23	BAK1	BCL2L1	2o2n_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	BAK1	BCL2L1	2o2m_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	BAK1	BCL2L1	2yxj_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	BAK1	BCL2L1	2yxj_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	BAK1	BCL2L1	1ysi_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	BAK1	BCL2L1	2w3l_A	0	0	0	0	0	25	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	BAK1	BCL2L1	2w3l_B	0	0	0	0	0	9	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	BAK1	BCL2L1	3inq_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	BAK1	BCL2L1	3inq_B	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	CALM1	CAMK1	1mux_A pocket1	0	0	0	0	0	198	64	0	0	0	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0
33	CALM1	CAMK1	1mux_A pocket2	0	0	0	0	0	163	77	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	CALM1	MYLK	1mux_A pocket1	0	0	0	0	0	126	12	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
35	CALM1	MYLK	1mux_A pocket2	0	0	0	0	0	126	30	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	CALM1	PDE1A	1qiv_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	2
38	CREBBP	TP53	2d82_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	17	0	15	0	0	0
39	ESR1	NCOA2	3erd_A	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	3298	0	0	0	0	0	0	0	0	0
40	ESR1	NCOA2	3erd_B	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	2151	0	0	0	0	0	0	0	0	0
41	FKBP1A	TGFBR1	1fkj_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	1	0
42	FKBP1A	TGFBR1	1fkf_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0
43	EGFR	GRB2	1cj1_B	0	1	0	0	1	0	0	1288	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0
44	EGFR	GRB2	1cj1_C	0	1	0	0	1	0	0	1286	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0
45	EGFR	GRB2	1cj1_D	0	1	0	0	1	0	0	1293	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0
46	EGFR	GRB2	1cj1_E	0	1	0	0	1	0	0	1280	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0
47	EGFR	GRB2	1cj1_F	0	1	0	0	1	0	0	1316	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0
48	EGFR	GRB2	1cj1_G	0	1	0	0	1	0	0	1322	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0
49	EGFR	GRB2	1cj1_H	0	0	1	0	2	0	0	1354	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0
50	EGFR	GRB2	1cj1_I	0	1	0	0	1	0	0	1274	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0
51	EGFR	GRB2	1cj1_J	0	1	0	0	1	0	0	1286	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1	0
52	GRB2	MET	1cj1_B	0	0	0	2	0	0	0	941	0	0	0	0	0	0	1	1	0	0	0	0	0	0	1	0	0	0	7	0
53	GRB2	MET	1cj1_C	0	0	0	1	0	0	0	922	0	0	0	0	0	0	2	3	0	0	0	0	0	0	1	0	0	0	7	0
54	GRB2	MET	1cj1_D	0	0	0	2	0	0	0	931	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0	8	0
55	GRB2	MET	1cj1_E	0	0	0	2	0	0	0	852	0	0	0	0	0	0	2	2	0	0	0	0	0	0	1	0	0	0	12	0
56	GRB2	MET	1cj1_F	0	0	0	1	0	0	0	960	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	0	0	7	0
57	GRB2	MET	1cj1_G	0	0	0	1	0	0	0	958	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	0	0	7	0
58	GRB2	MET	1cj1_H	0	0	0	1	0	0	0	1014	0	0	0	0	0	0	1	2	0	0	0	0	0	0	0	0	0	0	3	0
59	GRB2	MET	1cj1_I	0	0	0	3	0	0	0	773	0	0	0	0	0	0	3	0	0	0	0	0	0	1	1	0	0	1	13	0
60	GRB2	MET	1cj1_J	0	0	0	2	0	0	0	906	0	0	0	0	0	0	1	1	0	0	0	0	0	0	1	0	0	0	7	0
61	HOXB1	PBX1	1b72_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	IL1B	IL1R1	1itb_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	IL2	IL2RA	1py2_A	0	0	0	0	0	0	0	0	28	119	1	50	53	40	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64	IL2	IL2RA	1py2_B	0	0	0	0	0	0	0	0	110	143	0	72	42	33	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	IL2	IL2RA	1py2_C	0	0	0	0	0	0	0	0	115	140	8	81	81	56	0	0	0	0	0	4	0	0	0	0	0	0	0	0
66	IL2	IL2RA	1py2_D	0	0	0	0	0	0	0	0	111	134	4	71	63	22	0	0	0	0	0	0	0	0	0	0	0	0	0	0
67	IL2	IL2RA	1m48_A	0	0	0	0	0	0	0	0	82	139	0	8	0	0	0	0	0	0	0	105	0	0	0	0	0	0	0	0
68	IL2	IL2RA	1m48_B	0	0	0	0	0	0	0	0	30	119	0	3	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0
69	IL2	IL2RA	1m4a_A	0	0	0	0	0	0	2	0	4	3	2	0	0	0	0	0	0	0	0	328	0	0	0	0	0	0	0	0
70	PTEN	MAGI3	1be9_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	MDM2	TP53	1t4e_A	0	2	0	0	0	0	0	0	0	0	0	0	0	0	2	0	16	4	0	0	0	0	0	0	0	0	0	0
72	MDM2	TP53	1t4e_B	0	1	0	0	0	1	0	0	0	0	0	0	0	0	2	0	31	7	0	0	0	0	0	0	0	0	0	0
73	MDM2	TP53	1ttv_A	0	0	0	0	0	8	0	0	0	0	0	0	0	0	3	2	27	8	0	0	0	0	0	0	0	0	0	0
74	MDM2	TP53	3jzk_A	0	0	0	1	0	14	0	11	0	0	0	0	0	0	1	0	4	2	44	0	0	0	0	0	0	0	1	0
75	MDM2	TP53	3lbk_A	0	0	0	0	0	5	0	0	0	0	0	0	0	0	3	0	28	6	0	0	0	0	0	0	0	0	0	0
76	MDM2	TP53	3lbl_A	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	0	13	1	0	0	0	0	0	0	0	0	0	0
77	MDM2	TP53	3lbl_C	0	0	0	2	0	1	0	0	0	0	0	0	0	0	1	0	11	2	0	0	0	0	0	0	0	0	0	0
78	MDM2	TP53	3lbl_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	3	0	0	0	0	0	0	0	0	0	0
79	MDM4	TP53	3lbj_E	0	0	0	0	0	48	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0
80	PDGFRB	PIK3R1	1h9o_A	2	27	1	42	0	0	0	0	0	0	0	0	0	0	270	152	47	18	0	0	0	22	1	3	0	0	0	0
81	RAC1	TIAM1	1foe_B	3757	0	0	0	0	7	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	206	93
82	RAC1	TIAM1	1foe_D	3770	0	0	0	0	7	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	192	96
83	RAC1	TIAM1	1foe_F	3758	0	0	0	0	7	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	213	98
84	RAC1	TIAM1	1foe_H	3849	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	136	248
85	RAC1	TRIO	2nz8_A	8324	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	108	94
86	RAF1	YWHAZ	3rdh_A	1	1516	1343	1413	1128	0	0	0	0	0	0	0	0	0	285	31	407	8	0	0	0	0	0	0	0	0	0	0
87	RAF1	YWHAZ	3rdh_B	0	1516	1343	1409	1140	0	0	0	0	0	0	0	0	0	794	25	924	174	0	0	0	0	0	0	0	0	0	0
88	RAF1	YWHAZ	3rdh_C	0	1511	1339	1414	1124	0	0	0	0	0	0	0	0	0	843	46	1015	21	0	0	0	0	0	0	0	0	1	0
89	RAF1	YWHAZ	3rdh_D	2	1188	1036	1056	2024	0	0	24	0	0	0	0	0	0	573	957	822	489	0	0	0	0	0	0	0	0	0	0
90	S100B	TP53	3hcm_A	0	0	0	0	4148	2096	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0
91	S100B	TP53	3hcm_B	7	0	0	0	0	4055	2120	0	0	0	0	0	0	0	0	0	0	0	208	0	0	0	0	0	0	0	0	0
92	STAT3	STAT3	1bg1_A	3	1	0	0	1	0	0	9453	0	0	0	0	0	0	2	0	12	4	0	0	0	0	0	0	0	0	0	0
93	BIRC5	BIRC5	1e31_A	0	0	0	0	0	0	0	0	1316	1251	1129	1252	1079	831	0	0	0	0	28	0	0	0	0	0	0	0	0	0
94	BIRC5	BIRC5	1e31_B	0	0	0	0	0	0	0	0	1262	1266	762	1250	907	1262	0	0	0	0	31	0	0	0	0	0	0	0	0	0
95	BIRC5	BIRC5	1f3h_A	0	0	0	0	0	0	0	0	804	744	1200	800	895	2242	0	0	0	0	1	0	0	0	0	0	0	0	0	0
96	BIRC5	BIRC5	1f3h_B	0	0	0	0	0	0	0	0	1215	1229	1100	1308	1034	795	0	0	0	0	18	0	0	0	0	0	0	0	0	0
97	BIRC5	BIRC5	1xox_A	0	0	0	0	0	0	0	0	828	833	878	805	1210	2381	0	0	0	0	1	0	0	0	0	0	0	0	0	0
98	BIRC5	BIRC5	1xox_B	0	0	0	0	0	0	0	0	813	830	884	802	954	2640	0	0	0	0	1	0	0	0	0	0	0	0	0	0
99	CTNNB1	TCF7L1	1g3j_A	0	0	1	5	0	0	0	0	0	0	0	0	0	0	4359	2896	1669	725	0	0	0	0	0	0	0	0	0	0
100	CTNNB1	TCF7L1	1g3j_C	0	0	1	3	0	0	0	0	0	0	0	0	0	0	3552	3707	1667	741	0	0	0	0	0	0	0	0	0	0
101	CTNNB1	TCF7L2	1g3j_A	0	2	3	9	2	0	1	0	0	0	0	0	0	0	1692	1457	4408	2080	0	0	0	0	0	0	0	0	0	0
102	CTNNB1	TCF7L2	1g3j_C	0	2	3	8	5	0	0	5	0	0	0	0	0	0	904	2271	4409	2085	0	0	0	0	0	0	0	0	0	0
103	THRB	NCOA2	1bsx_B	0	0	0	0	0	0	1	0	1	0	1	0	0	0	0	0	0	0	7828	0	0	0	0	0	0	0	0	0
104	TNF	TNF	2az5_AB	0	0	0	0	0	0	0	9	0	0	0	0	0	0	10	0	9	0	0	4314	2789	0	0	0	0	0	0	0
105	TNF	TNF	2az5_CD	0	0	0	0	0	0	0	4	0	0	0	0	0	0	9	6	0	0	0	3975	3119	0	0	0	0	0	0	0
106	XIAP	CASP3	1i3o_E pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2279	0	2182	0	2	803	1185
107	XIAP	CASP3	1i3o_E pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	5	0	0	3	0	0	2068	0	2328	0	0	0	0
108	XIAP	CASP3	1i3o_F pocket3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2281	0	2193	0	4	897	1153
109	XIAP	CASP3	1i3o_F pocket4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	21	0	0	0	1786	0	2618	0	0	0
110	XIAP	CASP9	1tft_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2	0	3895	1957	585
111	XIAP	CASP9	1nw9_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	2	0	142	3423	1356
112	XIAP	DIABLO	1g73_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	2	0	2	1628	2929
113	XIAP	DIABLO	1g73_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	2	0	2	1701	2878
114	XIAP	DIABLO	2opy_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	2	0	1680	2059	598
115	CD247	ZAP70	2oq1_A pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
116	CD247	ZAP70	2oq1_A pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S3. (continued)

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	113	114	115	116	Druggability score (using all attributes)
1	ARF1	CYTH2	1s9d_A [b]	0	369	0	0	0.8793
2	ARF1	CYTH2	1s9d_E [b]	0	0	0	0	0.7030
3	ARF1	CYTH2	1r8q_A [b]	46	304	0	0	0.8687
4	ARF1	CYTH2	1r8q_E [b]	17	2	0	0	0.8917
5	ARF1	CYTH2	1r8q_B [b]	26	366	0	0	0.8636
6	ARF1	CYTH2	1r8q_F [b]	5	2	0	0	0.8893
7	ARF1	CYTH2	1r8q_BF [c]	0	9	0	0	0.9689
8	ARF1	CYTH2	1s9d_AE [c]	0	0	0	0	0.9274
9	ARF1	CYTH2	1r8s_AE [c]	0	30	0	0	0.9777
10	ARF1	CYTH1	1s9d_A [b]	0	356	0	0	0.8660
11	ARF1	CYTH1	1s9d_E [b]	0	0	0	0	0.6608
12	ARF1	CYTH1	1r8q_A [b]	40	330	0	0	0.8434
13	ARF1	CYTH1	1r8q_E [b]	21	1	0	0	0.8829
14	ARF1	CYTH1	1r8q_B [b]	30	360	0	0	0.8383
15	ARF1	CYTH1	1r8q_F [b]	6	2	0	0	0.8790
16	ARF1	CYTH1	1r8q_BF [c]	0	9	0	0	0.9633
17	ARF1	CYTH1	1s9d_AE [c]	0	0	0	0	0.9122
18	ARF1	CYTH1	1r8s_AE [c]	0	33	0	0	0.9746
19	BAK1	BCL2	2o2f_A	0	0	1	0	0.9489
20	BAK1	BCL2	2o22_A	0	1	0	0	0.9602
21	BAK1	BCL2	2o21_A	0	0	1	0	0.9432
22	BAK1	BCL2	1ysw_A	0	0	0	0	0.9459
23	BAK1	BCL2L1	2o2n_A	0	0	1	0	0.9412
24	BAK1	BCL2L1	2o2m_A	0	0	0	0	0.8538
25	BAK1	BCL2L1	2yxj_A	0	0	0	0	0.9451
26	BAK1	BCL2L1	2yxj_B	0	0	0	0	0.9325
27	BAK1	BCL2L1	1ysi_A	0	0	0	0	0.9248
28	BAK1	BCL2L1	2w3l_A	0	0	0	0	0.8393
29	BAK1	BCL2L1	2w3l_B	0	0	0	0	0.8379
30	BAK1	BCL2L1	3inq_A	0	0	0	0	0.9289
31	BAK1	BCL2L1	3inq_B	0	0	0	0	0.8898
32	CALM1	CAMK1	1mux_A pocket1	0	0	0	0	0.9860
33	CALM1	CAMK1	1mux_A pocket2	0	0	0	0	0.9877
34	CALM1	MYLK	1mux_A pocket1	0	0	0	0	0.9926
35	CALM1	MYLK	1mux_A pocket2	0	0	0	0	0.9946
36	CALM1	PDE1A	1qiv_A	0	0	0	0	0.9993
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	0.9400
38	CREBBP	TP53	2d82_A	0	0	0	0	0.9835
39	ESR1	NCOA2	3erd_A	0	0	0	0	0.9574
40	ESR1	NCOA2	3erd_B	0	0	0	0	0.9514
41	FKBP1A	TGFBR1	1fkj_A	0	0	0	0	0.9527
42	FKBP1A	TGFBR1	1fkf_A	0	0	0	0	0.9510
43	EGFR	GRB2	1cj1_B	0	0	9	0	0.9990
44	EGFR	GRB2	1cj1_C	0	0	8	0	0.9990
45	EGFR	GRB2	1cj1_D	0	0	9	0	0.9990
46	EGFR	GRB2	1cj1_E	0	0	8	0	0.9989
47	EGFR	GRB2	1cj1_F	0	0	9	0	0.9990
48	EGFR	GRB2	1cj1_G	0	0	8	0	0.9989
49	EGFR	GRB2	1cj1_H	0	0	9	0	0.9989
50	EGFR	GRB2	1cj1_I	0	0	8	0	0.9990
51	EGFR	GRB2	1cj1_J	0	0	9	0	0.9990
52	GRB2	MET	1cj1_B	0	0	1	0	0.9998
53	GRB2	MET	1cj1_C	0	0	0	0	0.9998
54	GRB2	MET	1cj1_D	0	0	0	0	0.9998
55	GRB2	MET	1cj1_E	0	0	0	0	0.9999
56	GRB2	MET	1cj1_F	0	0	1	0	0.9998
57	GRB2	MET	1cj1_G	0	0	0	0	0.9998
58	GRB2	MET	1cj1_H	0	0	0	0	0.9997
59	GRB2	MET	1cj1_I	0	0	0	0	0.9998
60	GRB2	MET	1cj1_J	0	0	1	0	0.9998
61	HOXB1	PBX1	1b72_B	0	0	38	11	0.6464
62	IL1B	IL1R1	1itb_B	0	0	0	0	0.8652
63	IL2	IL2RA	1py2_A	0	0	831	1	0.8897
64	IL2	IL2RA	1py2_B	0	0	825	3	0.8959
65	IL2	IL2RA	1py2_C	0	0	826	0	0.8904
66	IL2	IL2RA	1py2_D	0	0	827	2	0.8835
67	IL2	IL2RA	1m48_A	0	0	845	7	0.9061
68	IL2	IL2RA	1m48_B	0	0	847	12	0.8972
69	IL2	IL2RA	1m4a_A	0	0	847	202	0.7669
70	PTEN	MAGI3	1be9_A	0	0	0	0	0.7637
71	MDM2	TP53	1t4e_A	0	0	0	0	0.9869
72	MDM2	TP53	1t4e_B	0	0	0	0	0.9860
73	MDM2	TP53	1ttv_A	0	0	7	0	0.9838
74	MDM2	TP53	3jzk_A	0	0	0	0	0.9560
75	MDM2	TP53	3lbk_A	0	0	3	0	0.9806
76	MDM2	TP53	3lbl_A	0	0	0	0	0.9438
77	MDM2	TP53	3lbl_C	0	0	0	0	0.9732
78	MDM2	TP53	3lbl_E	0	0	0	0	0.9590
79	MDM4	TP53	3lbj_E	0	0	0	0	0.9943
80	PDGFRB	PIK3R1	1h9o_A	0	0	21	0	1.0000
81	RAC1	TIAM1	1foe_B	202	41	0	0	0.9973
82	RAC1	TIAM1	1foe_D	222	40	0	0	0.9973
83	RAC1	TIAM1	1foe_F	163	51	0	0	0.9962
84	RAC1	TIAM1	1foe_H	83	111	0	0	0.9945
85	RAC1	TRIO	2nz8_A	77	71	0	0	0.9995
86	RAF1	YWHAZ	3rdh_A	0	0	0	0	0.9848
87	RAF1	YWHAZ	3rdh_B	0	0	0	0	0.9867
88	RAF1	YWHAZ	3rdh_C	0	0	0	0	0.9853
89	RAF1	YWHAZ	3rdh_D	0	0	0	0	0.9713
90	S100B	TP53	3hcm_A	0	0	0	0	0.9297
91	S100B	TP53	3hcm_B	0	0	0	0	0.9134
92	STAT3	STAT3	1bg1_A	0	0	2	0	0.9517
93	BIRC5	BIRC5	1e31_A	0	0	0	0	0.6905
94	BIRC5	BIRC5	1e31_B	0	0	0	0	0.6757
95	BIRC5	BIRC5	1f3h_A	0	0	7	0	0.6714
96	BIRC5	BIRC5	1f3h_B	0	0	0	0	0.6721
97	BIRC5	BIRC5	1xox_A	0	0	2	0	0.6976
98	BIRC5	BIRC5	1xox_B	0	0	2	0	0.6964
99	CTNNB1	TCF7L1	1g3j_A	0	0	0	0	0.9906
100	CTNNB1	TCF7L1	1g3j_C	0	0	0	0	0.9925
101	CTNNB1	TCF7L2	1g3j_A	0	0	0	0	0.9894
102	CTNNB1	TCF7L2	1g3j_C	0	0	0	0	0.9926
103	THRB	NCOA2	1bsx_B	0	0	1	0	0.7834
104	TNF	TNF	2az5_AB	0	0	3	3	0.8891
105	TNF	TNF	2az5_CD	0	0	3	3	0.8850
106	XIAP	CASP3	1i3o_E pocket1	861	567	0	0	0.7888
107	XIAP	CASP3	1i3o_E pocket2	0	0	0	0	0.8621
108	XIAP	CASP3	1i3o_F pocket3	806	579	0	0	0.7926
109	XIAP	CASP3	1i3o_F pocket4	0	0	0	0	0.8894
110	XIAP	CASP9	1tft_A	453	2313	0	0	0.9292
111	XIAP	CASP9	1nw9_A	1453	2376	0	0	0.8767
112	XIAP	DIABLO	1g73_C	2709	1011	0	0	0.8300
113	XIAP	DIABLO	1g73_D	2831	952	0	0	0.8385
114	XIAP	DIABLO	2opy_A	400	3576	0	0	0.8329
115	CD247	ZAP70	2oq1_A pocket1	0	0	2464	426	0.2908
116	CD247	ZAP70	2oq1_A pocket2	0	0	2430	1720	0.4254

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S4. Matrix of the similarities of the positive instances assessed by our SVM model using structural attributes [a]

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
1	ARF1	CYTH2	1s9d_A [b]	4523	0	835	0	608	0	0	22	0	0	0	0	0	0	0	0	0	0	140	128	46	58	0	0	0	9	66	0
2	ARF1	CYTH2	1s9d_E [b]	1793	1192	0	6	0	11	0	37	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
3	ARF1	CYTH2	1r8q_A [b]	4411	0	986	0	759	0	0	0	0	0	0	0	0	0	0	0	0	0	94	37	0	4	0	0	0	0	20	0
4	ARF1	CYTH2	1r8q_E [b]	2496	42	0	1081	0	1707	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
5	ARF1	CYTH2	1r8q_B [b]	4413	0	784	0	960	0	0	0	0	0	0	0	0	0	0	0	0	0	41	14	0	0	0	0	0	0	0	0
6	ARF1	CYTH2	1r8q_F [b]	2020	40	0	612	0	2666	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
7	ARF1	CYTH2	1r8q_BF [c]	0	0	2	0	0	0	4796	1556	2693	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	ARF1	CYTH2	1s9d_AE [c]	3	0	1	0	0	0	579	4952	547	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	ARF1	CYTH2	1r8s_AE [c]	0	0	1	0	0	0	3016	1307	4124	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	ARF1	CYTH1	1s9d_A [b]	4523	0	835	0	608	0	0	22	0	0	0	0	0	0	0	0	0	0	140	128	46	58	0	0	0	9	66	0
11	ARF1	CYTH1	1s9d_E [b]	1793	1192	0	6	0	11	0	37	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
12	ARF1	CYTH1	1r8q_A [b]	4411	0	986	0	759	0	0	0	0	0	0	0	0	0	0	0	0	0	94	37	0	4	0	0	0	0	20	0
13	ARF1	CYTH1	1r8q_E [b]	2496	42	0	1081	0	1707	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
14	ARF1	CYTH1	1r8q_B [b]	4413	0	784	0	960	0	0	0	0	0	0	0	0	0	0	0	0	0	41	14	0	0	0	0	0	0	0	0
15	ARF1	CYTH1	1r8q_F [b]	2020	40	0	612	0	2666	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
16	ARF1	CYTH1	1r8q_BF [c]	0	0	2	0	0	0	4796	1556	2693	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	ARF1	CYTH1	1s9d_AE [c]	3	0	1	0	0	0	579	4952	547	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	ARF1	CYTH1	1r8s_AE [c]	0	0	1	0	0	0	3016	1307	4124	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	BAK1	BCL2	2o2f_A	46	0	13	0	13	0	0	0	0	0	0	0	0	0	0	0	0	0	2181	2156	2103	1138	233	165	77	112	121	178
20	BAK1	BCL2	2o22_A	46	0	10	0	13	0	0	0	0	0	0	0	0	0	0	0	0	0	2176	2155	2057	1088	279	178	86	108	131	209
21	BAK1	BCL2	2o21_A	31	0	6	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	2090	2057	2111	1297	210	151	90	107	128	212
22	BAK1	BCL2	1ysw_A	40	0	11	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	2087	2047	2012	1396	209	152	89	108	131	210
23	BAK1	BCL2L1	2o2n_A	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1684	1260	752	393	947	883	272	386	503	50
24	BAK1	BCL2L1	2o2m_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1761	1577	1103	572	948	888	114	418	189	189
25	BAK1	BCL2L1	2yxj_A	8	0	2	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	825	912	687	381	765	520	753	661	705	132
26	BAK1	BCL2L1	2yxj_B	10	0	3	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	819	726	583	417	763	635	733	821	760	81
27	BAK1	BCL2L1	1ysi_A	44	0	25	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	742	708	590	437	783	681	721	797	886	37
28	BAK1	BCL2L1	2w3l_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1343	1638	1640	1013	70	108	6	7	6	975
29	BAK1	BCL2L1	2w3l_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1391	1663	1663	1031	111	140	33	4	6	982
30	BAK1	BCL2L1	3inq_A	3	0	2	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	1445	821	625	328	919	432	388	764	507	120
31	BAK1	BCL2L1	3inq_B	7	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1156	811	849	488	644	419	624	637	649	189
32	CALM1	CAMK1	1mux_A pocket1	18	6	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	31
33	CALM1	CAMK1	1mux_A pocket2	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	73
34	CALM1	MYLK	1mux_A pocket1	18	6	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	31
35	CALM1	MYLK	1mux_A pocket2	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	73
36	CALM1	PDE1A	1qiv_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	383	31	356	196	101	135	9	69	27	3
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	CREBBP	TP53	2d82_A	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	3	0	0	0	2	0	0	0	1	4
39	ESR1	NCOA2	3erd_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	ESR1	NCOA2	3erd_B	22	0	4	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
41	FKBP1A	TGFBR1	1fkj_A	70	1	26	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	455	279	95	80	10	49	0	21	0	45
42	FKBP1A	TGFBR1	1fkf_A	44	1	11	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	636	353	247	133	23	53	0	24	0	48
43	EGFR	GRB2	1cj1_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	EGFR	GRB2	1cj1_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45	EGFR	GRB2	1cj1_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46	EGFR	GRB2	1cj1_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	EGFR	GRB2	1cj1_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	EGFR	GRB2	1cj1_G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49	EGFR	GRB2	1cj1_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	EGFR	GRB2	1cj1_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	EGFR	GRB2	1cj1_J	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52	GRB2	MET	1cj1_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53	GRB2	MET	1cj1_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54	GRB2	MET	1cj1_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55	GRB2	MET	1cj1_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56	GRB2	MET	1cj1_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57	GRB2	MET	1cj1_G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58	GRB2	MET	1cj1_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59	GRB2	MET	1cj1_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	GRB2	MET	1cj1_J	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	HOXB1	PBX1	1b72_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	IL1B	IL1R1	1itb_B	23	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	IL2	IL2RA	1py2_A	0	0	0	0	0	0	194	0	241	0	0	0	0	0	0	0	0	0	25	0	2	0	23	44	0	0	0	1
64	IL2	IL2RA	1py2_B	0	0	0	0	0	0	62	0	43	0	0	0	0	0	0	0	0	0	25	2	1	0	29	93	0	12	0	0
65	IL2	IL2RA	1py2_C	0	0	0	0	0	0	312	0	115	0	0	0	0	0	0	0	0	0	9	0	0	3	8	17	0	0	2	0
66	IL2	IL2RA	1py2_D	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	38	0	1	7	20	68	0	5	8	4
67	IL2	IL2RA	1m48_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	1	2	1	0	1	0	1	0	2
68	IL2	IL2RA	1m48_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	24	6	0	0	4	22	0	4	0	2
69	IL2	IL2RA	1m4a_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	1	1	1	0	1	0	0	0	12
70	PTEN	MAGI3	1be9_A	0	0	0	0	0	0	18	1	0	0	0	0	0	0	0	0	0	0	0	12	1	0	45	9	0	0	2	0
71	MDM2	TP53	1t4e_A	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	34	19	11	2	1	0	14	2	16
72	MDM2	TP53	1t4e_B	3	0	3	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	2	8	3	2	1	0	0	5	0	1
73	MDM2	TP53	1ttv_A	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
74	MDM2	TP53	3jzk_A	4	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
75	MDM2	TP53	3lbk_A	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	5	3	1	0	0	0	0	0
76	MDM2	TP53	3lbl_A	90	54	2	0	0	0	0	94	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
77	MDM2	TP53	3lbl_C	65	46	2	0	0	0	0	22	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	8
78	MDM2	TP53	3lbl_E	0	0	2	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
79	MDM4	TP53	3lbj_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
80	PDGFRB	PIK3R1	1h9o_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
81	RAC1	TIAM1	1foe_B	5	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82	RAC1	TIAM1	1foe_D	6	0	2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
83	RAC1	TIAM1	1foe_F	6	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
84	RAC1	TIAM1	1foe_H	6	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
85	RAC1	TRIO	2nz8_A	6	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
86	RAF1	YWHAZ	3rdh_A	9	0	4	0	5	0	9	0	23	0	0	0	0	0	0	0	0	0	33	5	18	11	137	0	0	0	0	26
87	RAF1	YWHAZ	3rdh_B	3	0	1	0	1	0	1	4	24	0	0	0	0	0	0	0	0	0	7	3	3	3	71	0	0	2	0	23
88	RAF1	YWHAZ	3rdh_C	1	0	0	0	0	0	2	41	132	0	0	0	0	0	0	0	0	0	1	1	0	0	14	0	0	0	0	0
89	RAF1	YWHAZ	3rdh_D	0	0	0	0	0	0	19	0	34	0	0	0	0	0	0	0	0	0	0	1	0	2	0	0	0	0	0	0
90	S100B	TP53	3hcm_A	346	7	6	89	1	467	0	9	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	109
91	S100B	TP53	3hcm_B	8	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	22	34	0	6	0	0	2	110
92	STAT3	STAT3	1bg1_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
93	BIRC5	BIRC5	1e31_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	25	14	4	1	0	14	0	23	1	7
94	BIRC5	BIRC5	1e31_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	1	3	0	0	5	0	4	0	2
95	BIRC5	BIRC5	1f3h_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	506	548	339	134	63	143	0	18	1	292
96	BIRC5	BIRC5	1f3h_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	293	387	88	42	139	194	81	255	99	44
97	BIRC5	BIRC5	1xox_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	58	36	113	59	11	119	0	0	0	187
98	BIRC5	BIRC5	1xox_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	49	31	128	38	16	107	0	0	0	218
99	CTNNB1	TCF7L1	1g3j_A	0	0	0	0	0	0	7	8	19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
100	CTNNB1	TCF7L1	1g3j_C	0	0	0	0	0	0	1	8	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
101	CTNNB1	TCF7L2	1g3j_A	0	0	0	0	0	0	7	8	19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
102	CTNNB1	TCF7L2	1g3j_C	0	0	0	0	0	0	1	8	15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
103	THRB	NCOA2	1bsx_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
104	TNF	TNF	2az5_AB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
105	TNF	TNF	2az5_CD	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
106	XIAP	CASP3	1i3o_E pocket1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107	XIAP	CASP3	1i3o_E pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
108	XIAP	CASP3	1i3o_F pocket3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
109	XIAP	CASP3	1i3o_F pocket4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
110	XIAP	CASP9	1tft_A	40	0	9	0	16	0	0	0	9	0	0	0	0	0	0	0	0	0	2	4	0	0	0	0	0	0	0	0
111	XIAP	CASP9	1nw9_A	8	0	4	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
112	XIAP	DIABLO	1g73_C	10	0	6	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
113	XIAP	DIABLO	1g73_D	12	0	5	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
114	XIAP	DIABLO	2opy_A	8	0	5	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
115	CD247	ZAP70	2oq1_A pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
116	CD247	ZAP70	2oq1_A pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method. see http://www.dropias.net/positives_attributes.txt and http://www.dropias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S4. (continued)

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56
1	ARF1	CYTH2	1s9d_A[b]	0	0	4	31	207	0	0	0	0	0	0	0	8	8	16	0	0	0	0	0	0	0	0	0	0	0	0	0
2	ARF1	CYTH2	1s9d_E[b]	0	0	0	22	12	0	0	0	0	0	0	0	7	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	ARF1	CYTH2	1r8q_A[b]	0	0	0	0	3	0	0	0	0	0	11	85	309	25	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	ARF1	CYTH2	1r8q_E[b]	0	0	0	0	10	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	ARF1	CYTH2	1r8q_B[b]	0	0	0	0	1	0	0	0	0	0	0	6	45	30	1	0	0	0	0	0	0	0	0	0	0	0	0	0
6	ARF1	CYTH2	1r8q_F[b]	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	ARF1	CYTH2	1r8q_BF[c]	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	ARF1	CYTH2	1s9d_AE[c]	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	ARF1	CYTH2	1r8s_AE[c]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	ARF1	CYTH1	1s9d_A[b]	0	0	4	31	207	0	0	0	0	0	0	0	8	8	16	0	0	0	0	0	0	0	0	0	0	0	0	0
11	ARF1	CYTH1	1s9d_E[b]	0	0	0	22	12	0	0	0	0	0	0	0	7	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	ARF1	CYTH1	1r8q_A[b]	0	0	0	0	3	0	0	0	0	0	11	85	309	25	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	ARF1	CYTH1	1r8q_E[b]	0	0	0	0	10	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	ARF1	CYTH1	1r8q_B[b]	0	0	0	0	1	0	0	0	0	0	0	6	45	30	1	0	0	0	0	0	0	0	0	0	0	0	0	0
15	ARF1	CYTH1	1r8q_F[b]	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	ARF1	CYTH1	1r8q_BF[c]	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	ARF1	CYTH1	1s9d_AE[c]	0	0	0	0	0	0	0	0	4	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	ARF1	CYTH1	1r8s_AE[c]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	BAK1	BCL2	2o2f_A	98	248	253	0	4	0	0	0	0	0	10	1	0	165	199	0	2	0	0	1	0	0	0	1	0	0	0	0
20	BAK1	BCL2	2o22_A	149	243	245	0	2	0	0	0	0	0	5	1	0	123	119	0	0	0	0	0	0	0	0	0	0	0	0	0
21	BAK1	BCL2	2o21_A	153	237	290	1	32	0	0	0	0	0	19	3	0	117	125	0	0	0	0	0	0	0	0	0	0	0	0	0
22	BAK1	BCL2	1ysw_A	151	236	302	2	32	0	0	0	0	0	15	3	0	123	124	0	0	0	0	0	0	0	0	0	0	0	0	0
23	BAK1	BCL2L1	2o2n_A	18	882	792	0	0	0	0	0	0	0	1	8	0	4	3	0	0	0	0	0	0	0	0	0	0	0	0	0
24	BAK1	BCL2L1	2o2m_A	115	374	860	0	0	0	0	0	0	0	0	23	0	70	34	0	0	0	0	0	0	0	0	0	0	0	0	0
25	BAK1	BCL2L1	2yxj_A	88	789	1772	0	0	0	0	0	0	0	21	24	0	11	7	0	0	0	0	0	0	0	0	0	0	0	0	0
26	BAK1	BCL2L1	2yxj_B	6	862	1577	0	0	0	0	0	0	0	11	10	0	186	175	1	5	1	4	2	2	2	0	1	0	0	0	0
27	BAK1	BCL2L1	1ysi_A	10	851	1452	0	0	0	0	0	0	0	4	27	0	7	1	0	0	0	0	0	0	0	0	0	0	0	0	0
28	BAK1	BCL2L1	2w3l_A	892	21	26	36	1081	0	0	0	0	0	6	9	0	61	23	0	0	0	0	0	0	0	0	0	0	0	0	0
29	BAK1	BCL2L1	2w3l_B	900	5	51	69	983	0	0	0	0	1	8	6	0	34	20	0	0	0	0	0	0	0	0	0	0	0	0	0
30	BAK1	BCL2L1	3inq_A	18	1019	1126	0	0	0	0	0	0	0	3	2	0	152	154	0	1	0	0	0	0	4	0	0	0	0	0	0
31	BAK1	BCL2L1	3inq_B	125	641	1902	0	0	0	0	0	0	0	4	18	0	56	59	0	0	0	0	0	0	0	0	0	0	0	0	0
32	CALM1	CAMK1	1mux_A pocket1	21	0	0	5916	3066	0	0	0	0	0	0	112	182	9	2	0	0	0	0	0	0	0	0	0	0	0	0	0
33	CALM1	CAMK1	1mux_A pocket2	50	0	0	3230	5667	0	0	0	0	0	0	178	223	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0
34	CALM1	MYLK	1mux_A pocket1	21	0	0	5916	3066	0	0	0	0	0	0	112	182	9	2	0	0	0	0	0	0	0	0	0	0	0	0	0
35	CALM1	MYLK	1mux_A pocket2	50	0	0	3230	5667	0	0	0	0	0	0	178	223	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0
36	CALM1	PDE1A	1qiv_A	5	101	33	0	99	0	0	7105	0	2	4	91	178	166	0	1	0	0	0	0	0	0	0	0	0	0	0	0
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	0	0	0	0	0	7952	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	CREBBP	TP53	2d82_A	0	0	0	0	0	0	0	0	0	0	9388	63	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	ESR1	NCOA2	3erd_A	0	0	0	0	0	0	0	0	8	3	4483	455	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	ESR1	NCOA2	3erd_B	0	0	0	52	1091	0	0	0	0	0	2746	3974	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	FKBP1A	TGFBR1	1fkj_A	0	27	1	0	0	0	0	0	0	0	0	1	3853	2397	14	19	6	12	15	23	15	6	15	0	0	0	0	0
42	FKBP1A	TGFBR1	1fkf_A	5	57	9	0	1	0	0	0	0	0	0	0	3753	2493	15	20	9	11	13	15	8	5	11	0	0	0	0	0
43	EGFR	GRB2	1cj1_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1498	1183	1201	586	1256	1098	1120	187	895	0	0	0	0	0
44	EGFR	GRB2	1cj1_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1338	1512	895	1026	961	1237	1117	187	756	0	0	0	0	0
45	EGFR	GRB2	1cj1_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1044	785	1532	422	1554	1336	1344	187	817	0	0	0	0	0
46	EGFR	GRB2	1cj1_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1062	1416	848	1342	820	996	938	1020	602	0	0	0	0	0
47	EGFR	GRB2	1cj1_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	894	722	1439	420	1635	1406	1641	187	659	0	0	0	0	0
48	EGFR	GRB2	1cj1_G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	745	986	1212	419	1489	1711	1712	187	544	0	0	0	0	0
49	EGFR	GRB2	1cj1_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	966	758	1211	419	1530	1459	1915	185	547	0	0	0	0	0
50	EGFR	GRB2	1cj1_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1143	999	852	1190	960	853	939	1327	790	0	0	0	0	0
51	EGFR	GRB2	1cj1_J	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1403	1095	1280	577	1265	1106	1120	189	991	0	0	0	0	0
52	GRB2	MET	1cj1_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1498	1183	1201	586	1256	1098	1120	187	895	0	0	0	0	0
53	GRB2	MET	1cj1_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1338	1512	895	1026	961	1237	1117	187	756	0	0	0	0	0
54	GRB2	MET	1cj1_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1044	785	1532	422	1554	1336	1344	187	817	0	0	0	0	0
55	GRB2	MET	1cj1_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1062	1416	848	1342	820	996	938	1020	602	0	0	0	0	0
56	GRB2	MET	1cj1_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	894	722	1439	420	1635	1406	1641	187	659	0	0	0	0	0
57	GRB2	MET	1cj1_G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	745	986	1212	419	1489	1711	1712	187	544	0	0	0	0	0
58	GRB2	MET	1cj1_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	966	758	1211	419	1530	1459	1915	185	547	0	0	0	0	0
59	GRB2	MET	1cj1_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1143	999	852	1190	960	853	939	1327	790	0	0	0	0	0
60	GRB2	MET	1cj1_J	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1403	1095	1280	577	1265	1106	1120	189	991	0	0	0	0	0
61	HOXB1	PBX1	1b72_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	IL1B	IL1R1	1itb_B	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	IL2	IL2RA	1py2_A	0	0	5	0	0	0	0	0	0	20	70	0	0	0	16	12	8	19	12	8	1	26	12	0	0	0	0	0
64	IL2	IL2RA	1py2_B	0	2	2	0	0	0	0	0	0	78	19	0	9	2	5	4	1	6	5	6	4	6	6	0	0	0	0	0
65	IL2	IL2RA	1py2_C	0	0	0	0	0	0	0	0	0	0	167	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
66	IL2	IL2RA	1py2_D	0	0	5	0	0	0	0	0	0	0	213	0	0	0	1	0	7	0	0	6	0	0	0	0	0	0	0	0
67	IL2	IL2RA	1m48_A	0	4	0	0	0	0	0	0	0	0	5	0	1	0	2	3	0	4	2	4	0	2	0	0	0	0	0	0
68	IL2	IL2RA	1m48_B	0	1	1	0	0	0	0	0	0	2	36	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69	IL2	IL2RA	1m4a_A	0	0	1	0	8	0	0	0	0	64	1107	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
70	PTEN	MAGI3	1be9_A	1	1	0	0	0	0	0	0	0	12	0	512	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
71	MDM2	TP53	1t4e_A	0	0	0	0	2	0	0	0	37	0	10	0	852	204	0	0	0	0	0	0	0	0	0	0	0	0	0	0
72	MDM2	TP53	1t4e_B	0	0	0	53	47	0	0	0	0	0	17	11	808	311	0	0	0	0	0	0	0	0	0	0	0	0	0	0
73	MDM2	TP53	1ttv_A	0	0	0	0	0	0	0	0	7	0	28	12	502	99	0	1	0	0	1	0	0	1	0	0	0	0	0	0
74	MDM2	TP53	3jzk_A	0	0	0	13	1	0	0	0	0	0	42	50	862	247	0	0	0	0	0	0	0	0	0	0	0	0	0	0
75	MDM2	TP53	3lbk_A	0	0	0	12	17	0	0	0	7	0	91	36	119	94	0	0	0	0	0	0	0	0	0	0	0	0	0	0
76	MDM2	TP53	3lbl_A	0	0	0	2033	1235	0	0	0	0	0	32	28	182	89	0	0	0	0	0	0	0	0	0	0	0	0	0	0
77	MDM2	TP53	3lbl_C	6	0	0	560	425	0	0	0	0	0	4	8	1045	557	0	0	0	0	0	0	0	0	0	0	0	0	0	0
78	MDM2	TP53	3lbl_E	0	0	0	71	257	0	0	0	38	0	134	14	789	223	0	0	0	0	0	0	0	0	0	0	0	0	0	0
79	MDM4	TP53	3lbj_E	0	0	0	0	11	0	0	0	282	0	117	165	46	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
80	PDGFRB	PIK3R1	1h9o_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6	6	4	8	5	13	14	5	1	0	0	0	0	0
81	RAC1	TIAM1	1foe_B	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
82	RAC1	TIAM1	1foe_D	0	0	0	0	0	0	0	0	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
83	RAC1	TIAM1	1foe_F	0	0	0	0	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
84	RAC1	TIAM1	1foe_H	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
85	RAC1	TRIO	2nz8_A	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
86	RAF1	YWHAZ	3rdh_A	0	1	4	0	0	0	0	0	0	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
87	RAF1	YWHAZ	3rdh_B	0	14	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
88	RAF1	YWHAZ	3rdh_C	0	0	0	0	0	0	0	0	0	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
89	RAF1	YWHAZ	3rdh_D	0	1	0	0	0	0	0	0	0	0	6	3	0	1	2	0	6	2	7	1	1	0	0	0	0	0	0	0
90	S100B	TP53	3hcm_A	9	0	0	168	586	0	0	0	0	0	52	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
91	S100B	TP53	3hcm_B	7	0	7	4	189	0	0	0	0	0	557	44	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
92	STAT3	STAT3	1bg1_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
93	BIRC5	BIRC5	1e31_A	0	21	0	0	0	0	0	0	0	0	13	0	41	2	2	5	1	1	8	8	9	0	3	0	0	0	0	0
94	BIRC5	BIRC5	1e31_B	0	3	0	0	0	0	0	0	0	0	41	0	3	1	1	2	0	1	3	2	6	0	0	0	0	0	0	0
95	BIRC5	BIRC5	1f3h_A	211	47	30	0	3	0	0	0	0	0	7	0	119	0	196	106	0	2	0	2	0	0	0	0	0	0	0	0
96	BIRC5	BIRC5	1f3h_B	2	184	213	0	0	0	0	0	0	0	0	0	4	0	14	7	14	20	5	18	6	8	2	13	9	0	0	0
97	BIRC5	BIRC5	1xox_A	143	0	2	0	0	0	0	0	0	3	0	71	0	260	107	0	3	0	14	0	2	0	10	0	0	0	0	0
98	BIRC5	BIRC5	1xox_B	166	0	2	0	1	0	0	0	0	3	0	65	0	187	85	5	6	0	10	0	2	0	5	0	0	0	0	0
99	CTNNB1	TCF7L1	1g3j_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
100	CTNNB1	TCF7L1	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
101	CTNNB1	TCF7L2	1g3j_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
102	CTNNB1	TCF7L2	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
103	THRB	NCOA2	1bsx_B	0	0	0	0	1	0	0	0	2	1	136	12	7	5	0	0	0	0	0	0	0	1	0	0	0	0	0	0
104	TNF	TNF	2az5_AB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
105	TNF	TNF	2az5_CD	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
106	XIAP	CASP3	1i3o_E pocket1	0	0	0	0	0	0	0	0	0	0	0	2	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
107	XIAP	CASP3	1i3o_E pocket2	0	0	0	0	0	0	0	0	0	0	635	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
108	XIAP	CASP3	1i3o_F pocket3	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0
109	XIAP	CASP3	1i3o_F pocket4	0	0	0	0	0	0	0	0	0	0	372	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
110	XIAP	CASP9	1tft_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111	XIAP	CASP9	1nw9_A	0	0	0	0	0	0	0	0	0	0	2	6	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
112	XIAP	DIABLO	1g73_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
113	XIAP	DIABLO	1g73_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
114	XIAP	DIABLO	2opy_A	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
115	CD247	ZAP70	2oq1_A pocket1	0	0	0	0	0	0	0	0	0	0	5	0	0	0	18	5	1	18	0	1	1	35	2	0	0	0	0	0
116	CD247	ZAP70	2oq1_A pocket2	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S4. (continued)

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84
1	ARF1	CYTH2	1s9d_A [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	43	21	0	0	0	0	0	0	1	1	0	0	1	0
2	ARF1	CYTH2	1s9d_E [b]	0	0	0	0	0	3076	0	0	0	0	0	0	0	0	0	6	0	14	2	12	109	3	0	0	0	0	0	0
3	ARF1	CYTH2	1r8q_A [b]	0	0	0	0	0	0	3	0	0	0	0	0	0	0	11	1	1	0	0	0	0	0	0	2	5	1	4	1
4	ARF1	CYTH2	1r8q_E [b]	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0
5	ARF1	CYTH2	1r8q_B [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	11	6	10	1
6	ARF1	CYTH2	1r8q_F [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	1	0
7	ARF1	CYTH2	1r8q_BF [c]	0	0	0	0	0	0	23	4	8	7	7	0	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	1
8	ARF1	CYTH2	1s9d_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	31	0	1	0	0	0	2	0	3	0	0	0	0	0	0
9	ARF1	CYTH2	1r8s_AE [c]	0	0	0	0	0	0	18	0	2	2	9	2	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	ARF1	CYTH1	1s9d_A [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	43	21	0	0	0	0	0	0	1	1	0	0	1	0
11	ARF1	CYTH1	1s9d_E [b]	0	0	0	0	0	3076	0	0	0	0	0	0	0	0	0	6	0	14	2	12	109	3	0	0	0	0	0	0
12	ARF1	CYTH1	1r8q_A [b]	0	0	0	0	0	0	3	0	0	0	0	0	0	0	11	1	1	0	0	0	0	0	0	2	5	1	4	1
13	ARF1	CYTH1	1r8q_E [b]	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0
14	ARF1	CYTH1	1r8q_B [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	1	0	11	6	10	1
15	ARF1	CYTH1	1r8q_F [b]	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	1	0
16	ARF1	CYTH1	1r8q_BF [c]	0	0	0	0	0	0	23	4	8	7	7	0	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	1
17	ARF1	CYTH1	1s9d_AE [c]	0	0	0	0	0	0	0	0	0	0	0	0	0	31	0	1	0	0	0	2	0	3	0	0	0	0	0	0
18	ARF1	CYTH1	1r8s_AE [c]	0	0	0	0	0	0	18	0	2	2	9	2	0	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	BAK1	BCL2	2o2f_A	0	0	0	0	1	0	9	6	1	33	45	19	8	19	6	0	0	0	0	0	0	0	2	4	0	0	0	0
20	BAK1	BCL2	2o22_A	0	0	0	0	6	0	0	1	0	12	18	3	3	272	17	0	0	0	0	0	0	0	2	1	2	1	0	1
21	BAK1	BCL2	2o21_A	0	0	0	0	0	0	4	1	1	26	37	4	6	9	23	8	2	0	2	0	3	0	1	5	0	0	0	0
22	BAK1	BCL2	1ysw_A	0	0	0	0	0	0	4	1	2	30	43	8	6	3	22	9	2	0	1	0	2	0	1	3	0	0	0	0
23	BAK1	BCL2L1	2o2n_A	0	0	0	0	3	0	1	1	0	8	3	3	0	787	2	0	0	0	0	0	0	0	0	1	12	0	0	0
24	BAK1	BCL2L1	2o2m_A	0	0	0	0	8	4	17	30	0	66	5	17	1	348	6	0	0	0	0	0	0	0	2	4	0	0	0	0
25	BAK1	BCL2L1	2yxj_A	0	0	0	0	0	0	1	2	0	8	15	12	2	676	12	3	0	0	0	0	0	0	0	21	0	0	0	0
26	BAK1	BCL2L1	2yxj_B	0	0	0	0	0	0	3	21	2	45	102	30	2	210	58	26	1	0	0	0	0	0	0	1	2	0	0	0
27	BAK1	BCL2L1	1ysi_A	0	0	0	0	1	1	0	1	0	36	1	1	0	731	8	0	0	0	0	0	0	0	0	2	0	0	0	0
28	BAK1	BCL2L1	2w3l_A	0	0	0	0	10	0	0	0	0	4	33	0	13	14	25	1	0	0	0	0	4	0	6	2	0	0	0	0
29	BAK1	BCL2L1	2w3l_B	0	0	0	0	8	0	0	0	0	6	5	0	6	130	15	1	0	0	0	0	9	6	5	0	0	0	0	0
30	BAK1	BCL2L1	3inq_A	0	0	0	0	0	0	9	0	0	14	94	16	3	101	0	0	0	0	0	0	0	0	2	0	1	0	1	0
31	BAK1	BCL2L1	3inq_B	0	0	0	0	12	0	4	0	0	54	42	18	4	90	19	0	0	0	0	0	0	0	0	50	0	0	0	0
32	CALM1	CAMK1	1mux_A pocket1	0	0	0	0	1	0	0	0	0	0	0	0	0	4	0	36	5	22	0	61	29	38	39	0	0	0	0	0
33	CALM1	CAMK1	1mux_A pocket2	0	0	0	0	0	1	0	0	0	1	0	0	6	4	0	6	0	1	32	8	20	65	0	0	0	0	0	0
34	CALM1	MYLK	1mux_A pocket1	0	0	0	0	1	0	0	0	0	0	0	0	0	4	0	36	5	22	0	61	29	38	39	0	0	0	0	0
35	CALM1	MYLK	1mux_A pocket2	0	0	0	0	0	1	0	0	0	1	0	0	6	4	0	6	0	1	32	8	20	65	0	0	0	0	0	0
36	CALM1	PDE1A	1qiv_A	0	0	0	0	0	0	16	58	37	68	1	2	0	0	19	7	0	4	0	0	0	0	0	287	0	0	0	0
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	1	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	1	10	0	0	0	0
38	CREBBP	TP53	2d82_A	0	0	0	0	0	0	4	7	0	2	5	1	11	0	0	0	0	0	0	0	0	0	1	3	0	0	0	0
39	ESR1	NCOA2	3erd_A	0	0	0	0	1	0	0	0	0	2	0	0	13	1275	0	0	0	0	0	0	0	0	4	0	0	0	0	0
40	ESR1	NCOA2	3erd_B	0	0	0	0	0	3	0	0	0	1	0	0	1	6	0	2	0	4	0	0	0	0	1	1104	0	0	0	0
41	FKBP1A	TGFBR1	1fkj_A	0	0	0	0	3	17	0	0	0	1	1	5	0	0	261	285	333	189	193	119	299	171	134	0	0	0	0	0
42	FKBP1A	TGFBR1	1fkf_A	0	0	0	0	1	1	0	0	1	0	0	22	0	0	206	248	305	147	150	38	213	123	78	0	0	0	0	0
43	EGFR	GRB2	1cj1_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14	0	0	0	0
44	EGFR	GRB2	1cj1_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0
45	EGFR	GRB2	1cj1_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
46	EGFR	GRB2	1cj1_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	53	0	0	0	0
47	EGFR	GRB2	1cj1_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	EGFR	GRB2	1cj1_G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49	EGFR	GRB2	1cj1_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	EGFR	GRB2	1cj1_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	184	0	0	0	0
51	EGFR	GRB2	1cj1_J	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	16	0	0	0	0
52	GRB2	MET	1cj1_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14	0	0	0	0
53	GRB2	MET	1cj1_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0
54	GRB2	MET	1cj1_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0
55	GRB2	MET	1cj1_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	53	0	0	0	0
56	GRB2	MET	1cj1_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57	GRB2	MET	1cj1_G	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58	GRB2	MET	1cj1_H	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59	GRB2	MET	1cj1_I	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	184	0	0	0	0
60	GRB2	MET	1cj1_J	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	16	0	0	0	0
61	HOXB1	PBX1	1b72_B	0	0	0	0	8469	8	0	0	0	3	3	0	0	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0
62	IL1B	IL1R1	1itb_B	0	0	0	0	7	8220	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
63	IL2	IL2RA	1py2_A	0	0	0	0	48	0	1205	1212	921	1258	1365	1270	76	52	0	0	0	0	0	0	0	0	0	0	0	0	0	0
64	IL2	IL2RA	1py2_B	0	0	0	0	61	0	1202	1217	936	1258	1384	1273	8	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0
65	IL2	IL2RA	1py2_C	0	0	0	0	9	46	1198	1211	979	1287	1394	1285	54	8	44	0	1	0	0	0	0	0	1	0	0	0	0	0
66	IL2	IL2RA	1py2_D	0	0	0	0	121	0	1205	1211	972	1287	1388	1289	203	68	4	0	0	0	0	0	0	0	0	0	0	0	0	0
67	IL2	IL2RA	1m48_A	0	0	0	0	16	0	1056	1058	639	1064	1340	1191	292	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
68	IL2	IL2RA	1m48_B	0	0	0	0	243	2	1178	1187	909	1230	1378	1281	431	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
69	IL2	IL2RA	1m4a_A	0	0	0	0	1	0	4	2	4	168	524	252	662	8	0	0	0	0	0	0	0	0	0	527	0	0	0	0
70	PTEN	MAGI3	1be9_A	0	0	0	0	118	0	0	0	0	0	0	0	2	9013	3	0	0	0	0	0	0	0	1	4	0	0	0	0
71	MDM2	TP53	1t4e_A	0	0	0	0	0	0	0	0	0	0	0	0	0	61	859	969	1047	22	876	543	928	540	2667	0	0	0	0	0
72	MDM2	TP53	1t4e_B	0	0	0	0	0	1	0	0	0	0	0	0	0	19	854	969	1046	816	878	1052	996	540	1246	0	0	0	0	0
73	MDM2	TP53	1ttv_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	840	968	1048	477	875	44	925	385	3344	36	0	0	0	0
74	MDM2	TP53	3jzk_A	0	0	0	0	0	0	2	0	0	0	0	0	0	0	396	942	1031	1025	861	16	510	33	3127	0	0	0	0	0
75	MDM2	TP53	3lbk_A	0	0	0	0	0	0	0	0	0	0	0	0	0	1	856	969	1049	376	878	235	975	458	3531	36	0	0	0	0
76	MDM2	TP53	3lbl_A	0	0	0	0	0	0	0	0	0	0	0	0	0	14	435	951	775	73	850	1055	991	541	60	0	0	0	0	0
77	MDM2	TP53	3lbl_C	0	0	0	0	1	9	0	0	0	0	0	0	0	59	848	965	1040	361	872	1055	997	542	286	0	0	0	0	0
78	MDM2	TP53	3lbl_E	0	0	0	0	0	1	0	0	0	0	0	0	0	21	829	944	1012	12	847	1033	966	542	1813	0	0	0	0	0
79	MDM4	TP53	3lbj_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	22	33	52	39	11	1	4	49	9009	24	0	0	0	0
80	PDGFRB	PIK3R1	1h9o_A	0	0	0	0	0	0	0	0	0	0	0	0	6	2	0	0	1	0	0	0	0	0	11	9374	0	0	0	0
81	RAC1	TIAM1	1foe_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2184	2163	2081	155
82	RAC1	TIAM1	1foe_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2167	2149	2067	9
83	RAC1	TIAM1	1foe_F	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2197	2179	2095	316
84	RAC1	TIAM1	1foe_H	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	452	105	1712	954
85	RAC1	TRIO	2nz8_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	95	86	74	6
86	RAF1	YWHAZ	3rdh_A	0	0	0	0	62	0	0	0	0	1	0	18	0	179	4	0	0	0	0	0	0	0	0	8	0	0	0	0
87	RAF1	YWHAZ	3rdh_B	0	0	0	0	7	0	0	0	0	0	1	3	0	114	12	0	0	0	0	0	0	0	0	9	0	0	0	0
88	RAF1	YWHAZ	3rdh_C	0	0	0	0	0	0	0	0	0	0	0	0	0	402	0	0	0	0	0	0	0	0	0	9	0	0	0	0
89	RAF1	YWHAZ	3rdh_D	0	0	0	0	0	0	0	1	0	0	0	0	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0
90	S100B	TP53	3hcm_A	0	0	0	0	0	0	0	0	0	30	8	0	20	0	0	0	0	0	0	0	0	0	77	0	0	0	1	0
91	S100B	TP53	3hcm_B	0	0	0	0	0	1	3	0	0	48	60	1	87	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
92	STAT3	STAT3	1bg1_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
93	BIRC5	BIRC5	1e31_A	0	0	0	0	0	0	59	172	11	364	337	186	0	11	1	0	0	0	0	0	0	0	0	0	0	0	0	0
94	BIRC5	BIRC5	1e31_B	0	0	0	0	0	0	48	169	4	416	278	124	0	38	3	0	0	0	0	0	0	0	0	0	0	0	0	0
95	BIRC5	BIRC5	1f3h_A	0	0	0	0	0	0	4	2	0	75	1	1	0	378	58	0	0	0	0	0	0	0	2	21	0	0	0	0
96	BIRC5	BIRC5	1f3h_B	0	0	0	0	0	0	110	113	11	292	112	62	0	325	87	0	0	0	0	0	0	0	0	0	0	0	0	0
97	BIRC5	BIRC5	1xox_A	0	0	0	0	21	0	234	168	71	336	64	108	0	637	140	0	0	0	0	0	0	0	7	9	0	0	0	0
98	BIRC5	BIRC5	1xox_B	0	0	0	0	24	0	169	132	41	311	39	75	0	845	148	0	0	0	0	0	0	0	8	32	0	0	0	0
99	CTNNB1	TCF7L1	1g3j_A	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	146	0	0	0	0
100	CTNNB1	TCF7L1	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	134	0	0	0	0
101	CTNNB1	TCF7L2	1g3j_A	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	146	0	0	0	0
102	CTNNB1	TCF7L2	1g3j_C	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	134	0	0	0	0
103	THRB	NCOA2	1bsx_B	0	0	0	0	0	0	3	3	0	3	16	13	6	2	0	1	3	4	0	0	0	1	1	1	0	0	0	0
104	TNF	TNF	2az5_AB	0	0	0	0	31	557	0	0	0	0	0	0	0	4	3	0	0	4	0	0	0	0	0	7	0	0	0	0
105	TNF	TNF	2az5_CD	0	0	0	0	13	619	0	0	0	0	0	0	0	4	1	0	0	2	0	0	0	0	0	8	0	0	0	0
106	XIAP	CASP3	1i3o_E pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
107	XIAP	CASP3	1i3o_E pocket2	0	0	0	0	0	0	3	0	0	0	0	0	35	1	0	0	0	0	0	0	0	0	0	194	0	0	0	0
108	XIAP	CASP3	1i3o_F pocket3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
109	XIAP	CASP3	1i3o_F pocket4	0	0	0	0	8	0	0	0	0	0	0	3	0	21	0	0	0	0	0	0	0	0	0	79	0	0	0	0
110	XIAP	CASP9	1tft_A	0	0	0	0	0	0	0	0	0	1	0	0	0	23	0	0	0	0	0	0	0	0	0	0	0	0	0	0
111	XIAP	CASP9	1nw9_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
112	XIAP	DIABLO	1g73_C	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
113	XIAP	DIABLO	1g73_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	1	5	0
114	XIAP	DIABLO	2opy_A	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
115	CD247	ZAP70	2oq1_A pocket1	0	0	0	0	31	0	0	0	0	3	0	1	0	7	1	0	0	0	0	0	0	0	0	0	3212	0	0	0
116	CD247	ZAP70	2oq1_A pocket2	0	0	0	0	79	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	14	0	0

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S4. (continued)

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112
1	ARF1	CYTH2	1s9d_A [b]	509	23	36	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	501	591	11
2	ARF1	CYTH2	1s9d_E [b]	0	0	0	0	0	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	ARF1	CYTH2	1r8q_A [b]	1178	1	0	0	0	36	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	81	1150	236
4	ARF1	CYTH2	1r8q_E [b]	11	0	0	0	0	250	16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	ARF1	CYTH2	1r8q_B [b]	2079	0	0	0	0	4	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	82	1015	94
6	ARF1	CYTH2	1r8q_F [b]	19	0	0	0	0	301	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	ARF1	CYTH2	1r8q_BF [c]	1	16	5	26	2	0	0	0	0	0	0	0	0	0	34	20	0	0	0	0	0	0	0	0	0	5	0	0
8	ARF1	CYTH2	1s9d_AE [c]	0	0	1	6	0	2	0	0	0	0	0	0	0	0	4	1	0	0	0	0	0	0	0	0	0	0	0	0
9	ARF1	CYTH2	1r8s_AE [c]	0	14	9	33	0	0	0	0	0	0	0	0	0	0	21	15	0	0	0	0	0	0	0	0	0	8	1	0
10	ARF1	CYTH1	1s9d_A [b]	509	23	36	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	501	591	11
11	ARF1	CYTH1	1s9d_E [b]	0	0	0	0	0	4	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	ARF1	CYTH1	1r8q_A [b]	1178	1	0	0	0	36	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	81	1150	236
13	ARF1	CYTH1	1r8q_E [b]	11	0	0	0	0	250	16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	ARF1	CYTH1	1r8q_B [b]	2079	0	0	0	0	4	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	82	1015	94
15	ARF1	CYTH1	1r8q_F [b]	19	0	0	0	0	301	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	ARF1	CYTH1	1r8q_BF [c]	1	16	5	26	2	0	0	0	0	0	0	0	0	0	34	20	0	0	0	0	0	0	0	0	0	5	0	0
17	ARF1	CYTH1	1s9d_AE [c]	0	0	1	6	0	2	0	0	0	0	0	0	0	0	4	1	0	0	0	0	0	0	0	0	0	0	0	0
18	ARF1	CYTH1	1r8s_AE [c]	0	14	9	33	0	0	0	0	0	0	0	0	0	0	21	15	0	0	0	0	0	0	0	0	0	8	1	0
19	BAK1	BCL2	2o2f_A	9	19	14	12	0	0	11	0	5	4	13	4	1	6	0	0	0	0	0	0	0	0	0	0	0	0	6	0
20	BAK1	BCL2	2o22_A	2	5	8	4	0	2	2	0	4	1	17	6	3	6	0	0	0	0	0	0	0	2	0	0	0	2	2	0
21	BAK1	BCL2	2o21_A	6	23	17	3	0	4	82	0	1	4	16	5	8	17	0	0	0	0	4	0	0	0	0	0	0	0	0	0
22	BAK1	BCL2	1ysw_A	1	24	14	3	0	4	100	0	2	3	11	3	6	11	0	0	0	0	4	0	0	0	0	0	0	0	0	0
23	BAK1	BCL2L1	2o2n_A	0	17	24	11	0	0	2	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
24	BAK1	BCL2L1	2o2m_A	0	0	0	0	0	0	5	0	1	6	12	22	3	2	0	0	0	0	2	0	0	0	0	0	0	0	0	0
25	BAK1	BCL2L1	2yxj_A	0	15	12	9	0	0	12	0	2	0	5	49	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0
26	BAK1	BCL2L1	2yxj_B	0	5	13	0	0	0	5	0	18	17	12	123	0	0	0	0	0	0	22	0	0	0	0	0	0	0	0	0
27	BAK1	BCL2L1	1ysi_A	0	43	54	8	0	0	16	0	2	0	2	40	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	BAK1	BCL2L1	2w3l_A	0	0	0	0	0	252	142	0	6	9	57	8	22	50	0	0	0	0	11	0	0	0	0	1	0	2	0	0
29	BAK1	BCL2L1	2w3l_B	0	0	0	0	0	123	59	0	1	1	96	8	46	102	0	0	0	0	0	0	0	5	0	1	0	0	0	0
30	BAK1	BCL2L1	3inq_A	0	7	37	7	0	0	15	0	18	13	14	17	0	0	0	0	0	0	1	0	0	0	1	0	0	1	0	0
31	BAK1	BCL2L1	3inq_B	0	8	0	2	0	0	77	0	0	3	19	26	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0
32	CALM1	CAMK1	1mux_A pocket1	0	0	0	0	0	247	48	0	0	0	0	0	0	0	0	0	0	0	25	0	0	0	0	0	0	0	0	0
33	CALM1	CAMK1	1mux_A pocket2	0	0	0	0	0	197	54	0	0	0	0	0	0	1	0	0	0	0	4	0	0	0	0	0	0	0	0	0
34	CALM1	MYLK	1mux_A pocket1	0	0	0	0	0	247	48	0	0	0	0	0	0	0	0	0	0	0	25	0	0	0	0	0	0	0	0	0
35	CALM1	MYLK	1mux_A pocket2	0	0	0	0	0	197	54	0	0	0	0	0	0	1	0	0	0	0	4	0	0	0	0	0	0	0	0	0
36	CALM1	PDE1A	1qiv_A	1	0	0	0	13	0	0	0	24	45	32	26	59	156	0	0	0	0	50	0	0	0	0	0	0	0	0	0
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	1	0	1	0	0
38	CREBBP	TP53	2d82_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	0	114	0	193	0	0	0	0
39	ESR1	NCOA2	3erd_A	0	0	0	0	0	1	4	0	4	0	0	0	0	0	0	0	0	0	1449	0	0	0	0	0	0	0	0	0
40	ESR1	NCOA2	3erd_B	0	0	0	0	0	19	12	0	0	0	0	0	0	0	0	0	0	0	28	0	1	0	0	0	0	0	48	4
41	FKBP1A	TGFBR1	1fkj_A	0	0	0	0	0	0	0	0	12	11	9	2	3	1	0	0	0	0	141	0	0	0	0	0	0	0	1	0
42	FKBP1A	TGFBR1	1fkf_A	0	0	0	0	0	0	0	0	1	5	5	7	4	4	11	0	0	0	115	0	0	0	0	0	0	0	2	0
43	EGFR	GRB2	1cj1_B	0	0	0	0	0	0	570	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	EGFR	GRB2	1cj1_C	0	0	0	0	0	0	614	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45	EGFR	GRB2	1cj1_D	0	0	0	0	0	0	706	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46	EGFR	GRB2	1cj1_E	0	0	0	0	0	0	437	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	EGFR	GRB2	1cj1_F	0	0	0	0	0	0	759	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	EGFR	GRB2	1cj1_G	0	0	0	0	0	0	775	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49	EGFR	GRB2	1cj1_H	0	0	0	0	0	0	825	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	EGFR	GRB2	1cj1_I	0	0	0	0	0	0	258	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	EGFR	GRB2	1cj1_J	0	0	0	0	0	0	584	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52	GRB2	MET	1cj1_B	0	0	0	0	0	0	570	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53	GRB2	MET	1cj1_C	0	0	0	0	0	0	614	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54	GRB2	MET	1cj1_D	0	0	0	0	0	0	706	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55	GRB2	MET	1cj1_E	0	0	0	0	0	0	437	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56	GRB2	MET	1cj1_F	0	0	0	0	0	0	759	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57	GRB2	MET	1cj1_G	0	0	0	0	0	0	775	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58	GRB2	MET	1cj1_H	0	0	0	0	0	0	825	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59	GRB2	MET	1cj1_I	0	0	0	0	0	0	258	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	GRB2	MET	1cj1_J	0	0	0	0	0	0	584	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
61	HOXB1	PBX1	1b72_B	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0
62	IL1B	IL1R1	1itb_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	50	32	0	0	0	0	0
63	IL2	IL2RA	1py2_A	0	0	0	0	0	6	5	10	41	104	1	54	32	36	0	0	0	0	23	0	0	0	0	0	0	0	2	6
64	IL2	IL2RA	1py2_B	0	0	0	0	1	0	1	56	134	157	0	85	44	57	0	0	0	0	416	0	0	0	0	0	0	0	3	10
65	IL2	IL2RA	1py2_C	0	2	0	0	0	0	2	0	109	166	0	77	94	70	0	0	0	0	254	0	0	0	0	0	0	0	2	4
66	IL2	IL2RA	1py2_D	0	0	0	0	0	30	29	2	168	185	5	115	96	54	0	0	0	0	105	0	0	0	0	0	0	0	0	10
67	IL2	IL2RA	1m48_A	0	0	0	0	0	4	19	5	24	120	0	2	0	0	0	0	0	0	1117	0	0	0	0	0	0	0	0	0
68	IL2	IL2RA	1m48_B	0	11	2	0	0	0	1	0	51	117	0	10	0	0	0	0	0	0	445	0	0	0	0	0	0	0	0	1
69	IL2	IL2RA	1m4a_A	0	1	0	0	0	44	313	0	0	0	0	0	0	0	0	0	0	0	1175	0	0	0	1	0	1	1	1	0
70	PTEN	MAGI3	1be9_A	0	1	1	12	0	0	0	0	0	1	1	0	2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
71	MDM2	TP53	1t4e_A	0	0	0	0	0	0	0	0	0	1	3	4	5	8	0	0	0	0	97	9	0	2	0	0	0	1	0	0
72	MDM2	TP53	1t4e_B	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	84	51	20	0	0	0	0	0	0	0
73	MDM2	TP53	1ttv_A	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	165	3	0	0	0	0	0	0	0	0
74	MDM2	TP53	3jzk_A	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	488	0	0	0	0	0	0	0	0	0
75	MDM2	TP53	3lbk_A	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	48	0	0	0	0	0	0	0	0	0
76	MDM2	TP53	3lbl_A	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	33	0	0	0	0	0	0	0	0	0
77	MDM2	TP53	3lbl_C	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	24	0	0	0	0	0	0	0	0	0
78	MDM2	TP53	3lbl_E	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	21	0	0	0	0	0	0	0	0	0
79	MDM4	TP53	3lbj_E	0	0	0	0	0	4	0	0	0	0	0	0	0	1	0	0	0	0	9	0	0	0	0	0	0	0	0	0
80	PDGFRB	PIK3R1	1h9o_A	0	0	0	3	0	0	0	0	0	0	0	0	0	0	6	7	0	0	0	0	0	0	0	0	0	0	0	0
81	RAC1	TIAM1	1foe_B	2334	0	0	0	0	2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	5
82	RAC1	TIAM1	1foe_D	2445	0	0	0	0	2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	5
83	RAC1	TIAM1	1foe_F	2215	0	0	0	0	2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7	5
84	RAC1	TIAM1	1foe_H	6227	0	0	0	0	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	6	11
85	RAC1	TRIO	2nz8_A	8827	0	0	0	0	3	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	8
86	RAF1	YWHAZ	3rdh_A	0	2209	2395	2322	547	0	0	0	0	0	0	0	0	0	307	53	0	0	0	0	0	0	0	0	0	0	0	0
87	RAF1	YWHAZ	3rdh_B	0	2162	2379	2237	964	0	0	0	0	0	0	0	0	0	339	235	0	0	0	0	0	11	1	0	0	0	0	0
88	RAF1	YWHAZ	3rdh_C	0	2069	2285	2327	47	0	0	0	0	0	0	0	0	0	798	150	0	0	0	0	0	0	0	0	0	0	1	0
89	RAF1	YWHAZ	3rdh_D	0	1341	1643	1159	2757	0	0	73	0	0	0	0	0	0	386	758	0	0	0	0	0	0	0	0	0	0	0	0
90	S100B	TP53	3hcm_A	8	0	0	0	0	4549	2218	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
91	S100B	TP53	3hcm_B	76	0	0	0	0	3652	2285	0	0	0	0	0	0	0	0	0	0	0	69	0	0	0	0	0	0	0	0	0
92	STAT3	STAT3	1bg1_A	0	0	0	0	0	0	0	5700	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
93	BIRC5	BIRC5	1e31_A	0	0	0	0	0	0	0	0	1090	1054	1093	996	1063	1063	0	0	0	0	2083	0	0	0	0	0	0	0	141	0
94	BIRC5	BIRC5	1e31_B	0	0	0	0	0	0	1	0	1090	1056	522	1000	917	1380	0	0	0	0	2816	0	0	0	0	0	0	0	0	0
95	BIRC5	BIRC5	1f3h_A	0	0	0	0	0	0	0	0	838	796	1112	762	858	2039	0	0	0	0	3	0	0	0	1	0	0	1	16	0
96	BIRC5	BIRC5	1f3h_B	0	0	0	0	0	0	0	0	1090	1053	1100	1001	1023	1032	0	0	0	0	412	0	0	0	0	0	0	0	2	0
97	BIRC5	BIRC5	1xox_A	0	0	0	0	0	0	0	0	837	796	875	757	1077	2059	0	0	0	0	80	0	0	0	0	0	0	0	2	0
98	BIRC5	BIRC5	1xox_B	0	0	0	0	0	0	0	0	832	795	875	757	861	2275	0	0	0	0	73	0	0	0	0	0	0	0	2	0
99	CTNNB1	TCF7L1	1g3j_A	0	43	69	82	5	0	0	1	0	0	0	0	0	40	6295	3162	0	0	0	0	0	0	0	0	0	0	141	0
100	CTNNB1	TCF7L1	1g3j_C	0	28	69	78	20	0	0	0	3	0	0	0	0	0	3509	5867	0	0	0	0	0	0	0	0	0	0	0	0
101	CTNNB1	TCF7L2	1g3j_A	0	43	69	82	5	0	0	1	0	0	0	0	0	40	6295	3162	0	0	0	0	0	0	0	0	0	0	141	0
102	CTNNB1	TCF7L2	1g3j_C	0	28	69	78	20	0	0	0	3	0	0	0	0	0	3509	5867	0	0	0	0	0	0	0	0	0	0	0	0
103	THRB	NCOA2	1bsx_B	0	0	0	0	0	0	11	0	4	4	0	0	0	0	0	0	0	0	9463	0	0	0	0	0	0	0	0	0
104	TNF	TNF	2az5_AB	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4204	2319	0	0	0	0	0	0	0
105	TNF	TNF	2az5_CD	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3682	2881	0	0	0	0	0	0	0
106	XIAP	CASP3	1i3o_E pocket1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2107	0	1895	0	23	60	112
107	XIAP	CASP3	1i3o_E pocket2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8	0	0	2201	0	2541	0	0	0	0
108	XIAP	CASP3	1i3o_F pocket3	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1981	0	1864	0	19	56	73
109	XIAP	CASP3	1i3o_F pocket4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	43	0	0	1452	0	3001	0	0	0	0
110	XIAP	CASP9	1tft_A	2	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	12	0	18	0	4698	1441	262
111	XIAP	CASP9	1nw9_A	25	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	14	0	0	16	0	16	0	350	3434	1648
112	XIAP	DIABLO	1g73_C	26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	42	0	0	42	0	0	0	118	1589	2790
113	XIAP	DIABLO	1g73_D	70	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	47	0	0	19	0	0	0	67	1515	2544
114	XIAP	DIABLO	2opy_A	25	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	16	0	0	21	0	0	0	2694	2510	562
115	CD247	ZAP70	2oq1_A pocket1	0	0	0	1	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
116	CD247	ZAP70	2oq1_A pocket2	0	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S4. (continued)

No.	Interactor1	Interactor2	PDB entries used for detecting the pockets located on PPI interface	113	114	115	116	Druggability score (using structural attributes)
1	ARF1	CYTH2	1s9d_A [b]	4	148	1	0	0.8602
2	ARF1	CYTH2	1s9d_E [b]	0	0	0	0	0.6310
3	ARF1	CYTH2	1r8q_A [b]	100	223	2	0	0.9793
4	ARF1	CYTH2	1r8q_E [b]	0	0	0	0	0.5617
5	ARF1	CYTH2	1r8q_B [b]	48	160	3	0	0.9816
6	ARF1	CYTH2	1r8q_F [b]	0	0	0	0	0.5684
7	ARF1	CYTH2	1r8q_BF [c]	0	0	0	0	0.9217
8	ARF1	CYTH2	1s9d_AE [c]	0	0	0	0	0.6139
9	ARF1	CYTH2	1r8s_AE [c]	0	0	1	0	0.8594
10	ARF1	CYTH1	1s9d_A [b]	4	148	1	0	0.8602
11	ARF1	CYTH1	1s9d_E [b]	0	0	0	0	0.6310
12	ARF1	CYTH1	1r8q_A [b]	100	223	2	0	0.9793
13	ARF1	CYTH1	1r8q_E [b]	0	0	0	0	0.5617
14	ARF1	CYTH1	1r8q_B [b]	48	160	3	0	0.9816
15	ARF1	CYTH1	1r8q_F [b]	0	0	0	0	0.5684
16	ARF1	CYTH1	1r8q_BF [c]	0	0	0	0	0.9217
17	ARF1	CYTH1	1s9d_AE [c]	0	0	0	0	0.6139
18	ARF1	CYTH1	1r8s_AE [c]	0	0	1	0	0.8594
19	BAK1	BCL2	2o2f_A	0	0	168	0	0.9943
20	BAK1	BCL2	2o22_A	0	0	51	0	0.9884
21	BAK1	BCL2	2o21_A	0	0	106	0	0.9905
22	BAK1	BCL2	1ysw_A	0	0	90	0	0.9902
23	BAK1	BCL2L1	2o2n_A	0	0	146	3	0.9867
24	BAK1	BCL2L1	2o2m_A	0	0	154	0	0.9950
25	BAK1	BCL2L1	2yxj_A	0	0	13	0	0.9938
26	BAK1	BCL2L1	2yxj_B	0	0	41	0	0.9957
27	BAK1	BCL2L1	1ysi_A	0	0	46	0	0.9802
28	BAK1	BCL2L1	2w3l_A	0	0	6	0	0.9639
29	BAK1	BCL2L1	2w3l_B	0	0	5	0	0.9739
30	BAK1	BCL2L1	3inq_A	0	0	158	26	0.9391
31	BAK1	BCL2L1	3inq_B	0	0	258	0	0.9967
32	CALM1	CAMK1	1mux_A pocket1	0	0	24	0	0.9952
33	CALM1	CAMK1	1mux_A pocket2	0	0	28	0	0.9855
34	CALM1	MYLK	1mux_A pocket1	0	0	24	0	0.9952
35	CALM1	MYLK	1mux_A pocket2	0	0	28	0	0.9855
36	CALM1	PDE1A	1qiv_A	0	0	0	0	1.0000
37	CD4	HLA-DQB1	1jl4_D	0	0	0	0	0.7982
38	CREBBP	TP53	2d82_A	0	0	3	0	0.9815
39	ESR1	NCOA2	3erd_A	0	0	82	0	0.7780
40	ESR1	NCOA2	3erd_B	0	2	20	0	0.9159
41	FKBP1A	TGFBR1	1fkj_A	0	0	204	0	0.9938
42	FKBP1A	TGFBR1	1fkf_A	0	0	135	0	0.9825
43	EGFR	GRB2	1cj1_B	0	0	315	0	0.9923
44	EGFR	GRB2	1cj1_C	0	0	281	0	0.9928
45	EGFR	GRB2	1cj1_D	0	0	191	0	0.9920
46	EGFR	GRB2	1cj1_E	0	0	409	0	0.9943
47	EGFR	GRB2	1cj1_F	0	0	139	0	0.9901
48	EGFR	GRB2	1cj1_G	0	0	123	0	0.9903
49	EGFR	GRB2	1cj1_H	0	0	72	0	0.9887
50	EGFR	GRB2	1cj1_I	0	0	457	0	0.9952
51	EGFR	GRB2	1cj1_J	0	0	299	0	0.9925
52	GRB2	MET	1cj1_B	0	0	315	0	0.9923
53	GRB2	MET	1cj1_C	0	0	281	0	0.9928
54	GRB2	MET	1cj1_D	0	0	191	0	0.9920
55	GRB2	MET	1cj1_E	0	0	409	0	0.9943
56	GRB2	MET	1cj1_F	0	0	139	0	0.9901
57	GRB2	MET	1cj1_G	0	0	123	0	0.9903
58	GRB2	MET	1cj1_H	0	0	72	0	0.9887
59	GRB2	MET	1cj1_I	0	0	457	0	0.9952
60	GRB2	MET	1cj1_J	0	0	299	0	0.9925
61	HOXB1	PBX1	1b72_B	0	0	65	76	0.8646
62	IL1B	IL1R1	1itb_B	0	0	4	3	0.8352
63	IL2	IL2RA	1py2_A	0	5	1003	0	0.9474
64	IL2	IL2RA	1py2_B	0	0	822	0	0.9560
65	IL2	IL2RA	1py2_C	0	6	980	0	0.9920
66	IL2	IL2RA	1py2_D	0	3	954	0	0.9889
67	IL2	IL2RA	1m48_A	0	0	266	0	0.8257
68	IL2	IL2RA	1m48_B	0	0	865	0	0.9447
69	IL2	IL2RA	1m4a_A	0	0	2472	0	0.7358
70	PTEN	MAGI3	1be9_A	0	0	130	0	0.9911
71	MDM2	TP53	1t4e_A	0	0	109	0	0.9964
72	MDM2	TP53	1t4e_B	0	0	107	0	0.9958
73	MDM2	TP53	1ttv_A	0	0	170	4	0.9939
74	MDM2	TP53	3jzk_A	0	0	9	0	0.9663
75	MDM2	TP53	3lbk_A	0	0	172	0	0.9974
76	MDM2	TP53	3lbl_A	0	0	84	0	0.9704
77	MDM2	TP53	3lbl_C	0	0	107	0	0.9916
78	MDM2	TP53	3lbl_E	0	0	30	0	0.9609
79	MDM4	TP53	3lbj_E	0	0	71	0	0.9956
80	PDGFRB	PIK3R1	1h9o_A	0	0	139	25	0.9636
81	RAC1	TIAM1	1foe_B	23	0	0	0	0.8975
82	RAC1	TIAM1	1foe_D	23	0	0	0	0.8895
83	RAC1	TIAM1	1foe_F	22	0	0	0	0.9060
84	RAC1	TIAM1	1foe_H	21	2	0	0	0.9508
85	RAC1	TRIO	2nz8_A	18	0	0	0	0.9146
86	RAF1	YWHAZ	3rdh_A	0	0	798	2	0.9201
87	RAF1	YWHAZ	3rdh_B	0	0	160	1	0.8790
88	RAF1	YWHAZ	3rdh_C	0	0	240	0	0.8529
89	RAF1	YWHAZ	3rdh_D	0	0	3	0	0.8211
90	S100B	TP53	3hcm_A	0	0	2	0	0.8769
91	S100B	TP53	3hcm_B	0	0	32	0	0.7313
92	STAT3	STAT3	1bg1_A	0	0	0	0	0.5700
93	BIRC5	BIRC5	1e31_A	0	2	0	0	0.9929
94	BIRC5	BIRC5	1e31_B	0	0	7	0	0.9950
95	BIRC5	BIRC5	1f3h_A	0	0	219	0	0.9954
96	BIRC5	BIRC5	1f3h_B	0	0	4	0	0.9970
97	BIRC5	BIRC5	1xox_A	0	0	459	0	0.9941
98	BIRC5	BIRC5	1xox_B	0	0	505	0	0.9923
99	CTNNB1	TCF7L1	1g3j_A	0	0	26	0	0.9865
100	CTNNB1	TCF7L1	1g3j_C	0	0	51	0	0.9784
101	CTNNB1	TCF7L2	1g3j_A	0	0	26	0	0.9865
102	CTNNB1	TCF7L2	1g3j_C	0	0	51	0	0.9784
103	THRB	NCOA2	1bsx_B	0	0	17	0	0.9720
104	TNF	TNF	2az5_AB	0	0	0	0	0.7129
105	TNF	TNF	2az5_CD	0	0	0	0	0.7210
106	XIAP	CASP3	1i3o_E pocket1	85	30	0	0	0.4319
107	XIAP	CASP3	1i3o_E pocket2	0	0	4	0	0.5627
108	XIAP	CASP3	1i3o_F pocket3	64	15	2	0	0.4088
109	XIAP	CASP3	1i3o_F pocket4	0	0	1	0	0.4982
110	XIAP	CASP9	1tft_A	255	1342	0	0	0.8136
111	XIAP	CASP9	1nw9_A	1828	1965	0	0	0.9305
112	XIAP	DIABLO	1g73_C	2794	734	0	0	0.8154
113	XIAP	DIABLO	1g73_D	2823	555	0	0	0.7672
114	XIAP	DIABLO	2opy_A	582	2986	0	0	0.9421
115	CD247	ZAP70	2oq1_A pocket1	0	0	4663	296	0.8303
116	CD247	ZAP70	2oq1_A pocket2	0	0	920	1680	0.2697

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes and pocket-constituting amino acids of the positive instances used for our SVM-based method. see http://www.drpias.net/positives_attributes.txt and http://www.drpias.net/positives_amino_acids.txt.

[b] Brefeldin-binding pocket.

[c] Target pocket in Viaud,J., Zeghouf,M., Barelli,H., Zee,J.C., Padilla,A., Guibert,B., Chardin,P., Royer,C.A., Cherfils,J. and Chavanieu,A. (2007) Structure-based discovery of an inhibitor of Arf activation by Sec7 domains through targeting of protein-protein complexes. *Proc. Natl. Acad. Sci. U. S. A.*, **104**, 10370-10375.

Table S5. Matrix of the similarities of the positive instances assessed by our SVM model using drug/chemical attributes. [a]

No.	Interactor1	Interactor2	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	Druggability score (using drug/chemical attributes)
1	XIAP	CASP3	2744	597	0	0	238	3670	206	162	0	0	0	0	0	905	0	0	0	0	2	191	0	0	3	484	0	0	0	0	0	170	397	0	0	0	0.9769
2	XIAP	CASP9	0	2420	0	0	0	0	0	2967	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5387
3	XIAP	DIABLO	0	2420	0	0	0	0	0	2967	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.5387
4	BIRC5	BIRC5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0000
5	ARF1	CYTH2	1450	88	0	0	2222	607	0	399	0	0	0	0	0	1770	0	0	0	0	13	72	0	0	0	1281	0	0	0	0	0	0	2058	0	1	0	0.9961
6	ARF1	CYTH1	179	1347	0	0	0	3691	0	1454	0	0	0	0	0	0	0	0	0	0	0	24	0	0	0	220	0	0	0	0	0	0	110	0	0	0	0.7025
7	BAK1	BCL2	0	0	0	5	0	0	4818	101	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1747	0	0	0	0	0.6671
8	BAK1	BCL2L1	0	55	0	2	0	0	0	4934	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.4991
9	CALM1	MYLK	307	11	0	0	1	216	1399	1	7329	470	0	2	0	0	0	0	0	0	3	17	0	0	39	1	0	2	0	0	0	182	15	0	3	0	0.9998
10	CALM1	PDE1A	309	7	0	0	11	94	1073	1	1827	5978	0	1	0	1	0	0	0	0	39	21	0	0	18	11	0	132	0	0	0	97	376	0	3	1	1.0000
11	CALM1	CAMK1	307	11	0	0	1	216	1399	1	7329	470	0	2	0	0	0	0	0	0	3	17	0	0	39	1	0	2	0	0	0	182	15	0	3	0	0.9998
12	CD247	ZAP70	0	25	0	0	0	0	0	1271	0	0	0	6542	0	0	0	0	0	0	0	74	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.7912
13	CD4	HLA-DQB1	0	0	0	484	0	0	0	0	0	0	0	671	6903	0	0	0	0	0	0	8	0	1847	0	0	0	0	0	0	0	0	0	0	0	0	0.9913
14	CREBBP	TP53	0	39	0	2	0	0	0	1724	0	0	0	0	0	5525	0	0	0	0	0	0	0	0	0	104	0	0	0	0	0	0	3	0	0	0	0.7397
15	CTNNB1	TCF7L2	0	55	0	2	0	0	0	4934	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.4991
16	CTNNB1	TCF7L1	0	55	0	2	0	0	0	4934	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.4991
17	EGFR	GRB2	4	0	0	0	0	0	56	0	0	0	0	161	1123	0	0	0	4432	0	5	31	0	1487	1907	0	0	748	0	0	0	36	8	0	0	0	0.9998
18	ESR1	NCOA2	166	0	0	0	117	111	130	0	1517	263	0	0	0	0	0	0	19	6566	66	59	0	222	56	5	0	456	0	0	0	14	182	0	49	0	0.9998
19	FKBP1A	TGFBR1	1725	2	0	0	516	1610	543	0	0	0	0	0	0	72	0	0	0	0	2840	236	0	2	58	68	0	570	0	0	0	86	521	0	1150	0	0.9999
20	GRB2	MET	306	156	0	0	5	3056	0	154	0	0	0	3528	0	211	0	0	0	0	0	2395	0	0	0	135	0	0	0	0	0	0	18	0	0	0	0.9964
21	HOXB1	PBX1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0000
22	IL1B	IL1R1	0	0	0	17	0	0	379	5	0	0	0	43	4314	0	0	0	17	0	0	4	0	4503	2	0	0	516	0	0	0	191	0	0	0	0	0.9991
23	IL2	IL2RA	15	0	0	0	0	27	80	0	0	0	0	1556	31	0	0	0	314	0	0	236	0	30	6088	0	0	1517	0	0	0	46	0	0	0	0	0.9940
24	MDM2	TP53	0	645	0	0	0	0	0	1117	0	0	0	0	0	3083	0	0	0	0	0	0	0	0	0	3153	0	0	0	0	0	0	6	0	0	0	0.8004
25	MDM4	TP53	0	55	0	2	0	0	0	4934	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.4991
26	PDGFRB	PIK3R1	31	0	0	0	0	0	2548	2	0	0	0	125	0	1	0	0	7	0	12	1	0	988	74	2	0	5247	0	0	0	901	12	0	0	0	0.9951
27	PTEN	MAGI3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0000
28	RAC1	TIAM1	0	55	0	2	0	0	0	4934	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.4991
29	RAC1	TRIO	0	55	0	2	0	0	0	4934	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.4991
30	RAF1	YWHAZ	0	0	0	106	0	0	549	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3866	0	0	0	0	0.4521
31	S100B	TP53	0	1536	0	0	0	338	0	512	0	0	0	0	0	1451	0	0	0	0	0	1	0	0	0	1827	0	0	0	0	0	0	3014	0	0	0	0.8679
32	STAT3	STAT3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0000
33	THRB	NCOA2	615	22	0	0	1080	1964	17	95	0	0	0	0	0	650	0	0	0	0	482	345	0	0	2	300	0	0	0	0	0	0	354	0	4074	0	1.0000
34	TNF	TNF	0	0	0	0	0	0	38	0	17	330	0	102	1058	0	0	0	104	0	0	19	0	1327	16	0	0	108	0	0	0	24	8	0	0	6847	0.9998

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt.

Table S6. Matrix of the similarities of the positive instances assessed by our SVM model using functional attributes. [a]

No.	Interactor1	Interactor2	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	Druggability score (using functional attributes)
1	XIAP	CASP3	4190	66	5358	0	31	21	0	31	290	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0.9990
2	XIAP	CASP9	0	6717	3089	0	0	0	2	118	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.9926
3	XIAP	DIABLO	0	3	7700	0	0	2	0	178	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.7883
4	BIRC5	BIRC5	0	0	0	6325	0	0	0	0	0	0	0	3	0	0	0	0	0	351	0	0	707	0	1895	0	0	0	0	0	0	0	0	0	717	0	0.9998
5	ARF1	CYTH2	1	0	6	0	5747	2009	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.7766
6	ARF1	CYTH1	1	0	6	0	65	7114	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.7189
7	BAK1	BCL2	0	6	16	0	0	0	8895	515	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.9432
8	BAK1	BCL2L1	0	0	34	0	0	0	589	8339	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.8962
9	CALM1	MYLK	375	0	2	0	20	1216	0	0	7870	416	72	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.9971
10	CALM1	PDE1A	0	0	0	0	0	0	0	0	538	7678	452	0	0	0	0	0	0	0	0	0	630	0	0	0	385	0	0	0	155	0	0	0	0	0	0.9838
11	CALM1	CAMK1	0	0	731	0	0	0	0	62	763	2778	5653	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0.9991
12	CD247	ZAP70	0	0	0	0	0	0	0	0	0	0	0	8045	0	0	0	0	0	10	0	0	0	0	2	0	0	0	0	0	0	0	0	0	239	0	0.8296
13	CD4	HLA-DQB1	0	824	27	0	0	0	15	750	45	0	26	0	8303	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.9991
14	CREBBP	TP53	294	50	2	0	2	0	8	88	21	0	0	0	0	3744	2153	99	449	0	197	137	0	0	0	1773	574	58	0	1	40	274	1	35	0	0	1.0000
15	CTNNB1	TCF7L2	42	0	0	0	0	42	0	184	63	0	0	0	1	237	6706	1353	0	263	25	0	0	0	0	666	274	0	0	0	132	0	0	12	0	0	1.0000
16	CTNNB1	TCF7L1	0	0	0	0	0	0	0	0	0	6	0	0	0	0	0	6414	0	0	0	0	0	0	0	0	0	0	2030	0	0	0	1546	0	0	0	0.9996
17	EGFR	GRB2	1191	181	0	0	0	0	2	106	33	0	0	0	0	362	0	610	4758	0	43	354	0	0	0	282	144	573	14	197	159	986	0	0	0	0	0.9995
18	ESR1	NCOA2	0	0	0	0	0	0	8	0	0	4	0	0	0	0	0	5	0	6923	0	0	2	1	0	0	0	3	0	0	0	0	117	0	2851	0	0.9914
19	FKBP1A	TGFBR1	27	0	1	0	1259	700	0	0	7	0	0	0	0	0	0	0	0	0	7030	0	0	0	0	916	0	0	0	0	2	0	0	0	0	0	0.9942
20	GRB2	MET	2797	224	217	0	0	0	0	13	178	0	1	0	0	0	0	424	163	0	70	2522	0	0	0	0	878	496	0	639	1358	20	0	0	0	0	1.0000
21	HOXB1	PBX1	0	0	0	0	0	0	0	0	0	33	0	0	0	0	0	0	0	0	0	0	7492	0	0	0	0	2	0	0	0	0	0	0	19	0	0.7546
22	IL1B	IL1R1	0	1518	1429	0	0	0	71	14	0	77	0	0	0	0	0	0	0	0	0	0	0	6842	0	0	0	0	0	0	0	0	16	0	0	0	0.9967
23	IL2	IL2RA	0	0	0	2	0	0	0	0	0	0	0	1943	0	0	0	0	0	23	0	0	52	0	7901	0	0	0	0	0	0	0	0	0	59	0	0.9980
24	MDM2	TP53	58	47	0	0	0	0	9	84	30	0	0	0	0	721	2156	118	435	0	366	60	0	0	0	4796	812	32	3	2	30	192	9	40	0	0	1.0000
25	MDM4	TP53	249	0	3	0	1	285	0	1	192	0	0	0	0	262	0	0	1767	172	0	0	0	0	0	0	6596	0	0	0	139	2	312	0	0	0	0.9981
26	PDGFRB	PIK3R1	388	138	0	0	0	0	0	0	316	0	1	0	0	0	0	231	349	0	76	326	0	0	0	0	440	3910	172	611	2313	726	0	0	0	0	0.9997
27	PTEN	MAGI3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2251	0	0	0	0	0	0	0	0.2251
28	RAC1	TIAM1	132	0	0	0	0	0	0	0	54	0	0	0	0	0	0	1257	1	0	0	596	0	0	0	0	0	1216	1393	3189	2162	0	0	0	0	0	1.0000
29	RAC1	TRIO	81	0	0	0	338	242	0	0	537	0	0	0	0	0	0	0	0	0	1114	332	0	0	0	0	547	395	0	87	6275	32	0	0	0	0	0.9980
30	RAF1	YWHAZ	478	9	0	0	225	116	0	0	127	0	0	0	0	0	0	0	354	0	605	284	0	0	0	19	208	640	0	2	1695	5234	0	0	0	0	0.9996
31	S100B	TP53	0	0	0	0	0	0	0	0	0	117	1	0	0	0	0	343	0	2	0	0	0	0	0	0	146	0	262	0	0	0	8859	0	0	0	0.9730
32	STAT3	STAT3	16	0	0	0	371	168	0	1	1	0	0	0	0	950	1758	0	245	0	791	60	0	0	0	1351	0	17	0	11	100	491	0	3669	0	0	1.0000
33	THRB	NCOA2	0	0	0	0	0	0	0	0	0	0	0	12	0	0	0	0	0	114	0	0	0	0	0	4	0	0	0	124	0	0	0	0	7263	0	0.7517
34	TNF	TNF	0	64	0	0	0	0	11	0	0	0	0	5144	1	8	29	19	15	0	0	0	0	27	0	35	0	1	0	0	0	0	0	0	8	4638	1.0000

When the druggability of a positive instance (in row) was assessed by our SVM-based method, the number of times each positive instance (in column) was located nearest to the assessed positive instance in a feature space was shown in a cell.

[a] For the details of the attributes of the positive instances used for our SVM-based method, see http://www.drpias.net/positives_attributes.txt.