PPIMpred: A webserver for high throughput screening of small molecules targeting Protein- Protein Interaction

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Supporting Information

Supporting Table legends

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Table S2 (b). List of 18 features of Bcl2/Bak dataset were taken, out of which 14 features were showed significantly different (p-value < 0.05) in PPIMs vs. random chemical structures. The symbol (*) implies that significant descriptors/features after t-test. Then HCA test was performed and finally 10 descriptors were chosen for prediction.

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Figure S5 (a). ROC plot of Mdm2/P53. The area under curve (AUC) of 0.99 similarity (blue), 0.9 similarity (red), 0.8 similarity (green) and randomization trial (black) are given respectively 0.88, 0.69, 0.63 and 0.55.

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Figure S15 (b). Position of ABT-263 & GX15-070 in frequency density plot of Bcl2/Bak.

Table S1 (a).

Target	Positive set	Negative set
Mdm2/P53 0.99 similarity	250	1790 (Random(1040) +Myc/Max +Bcl2/Bak)
Mdm2 0.9 similarity	75	390 (Random(200)+Myc(5)+Bcl2(185))
Mdm2 0.8 similarity	40	305 (Random(200)+Myc(5)+Bcl2(100))
Bcl2/Bak 0.99 similarity	735	1305 (Random(1040)+Myc/Max+Mdm2/P53)
Bcl2 0.9 similarity	185	280 (Random(200)+Myc(5)+Mdm2(75))
Bcl2 0.8 similarity	100	245 (Random(200)+Myc(5)+Mdm2(40))
Myc/Max 0.99 similarity	15	150 (Random)

Table S1 (b).

Target	Positive set	Negative set I (1:1)	Negative set II (1:10)
Mdm2/P53	30	30	330
Bcl2/Bak	100	100	1000
Myc/Max	5	5	50

Table S2 (a)

Molecular Descriptor	**Significant t-test**
Molecular Weight *	0.00
XLogP3 *	0.00
Hydrogen Bond Donor Count *	0.00
Hydrogen Bond Acceptor Count *	0.00
Rotatable Bond Count *	0.00
Exact Mass *	0.00
Monoisotopic Mass *	0.00
Topological Polar Surface Area *	0.00
Heavy Atom Count *	0.00
Formal Charge	0.13
Complexity *	0.00
Isotope Atom Count	0.12
Defined Atom Stereocenter Count *	0.00
Undefined Atom Stereocenter Count	0.49
Defined Bond Stereocenter Count*	0.00
Undefined Bond Stereocenter Count	0.47
Covalently-Bonded Unit Count *	0.00

Table S2 (b)

Molecular Descriptor	**Significant t-test**

Molecular Weight *	0.00
XLogP3 *	0.00
Hydrogen Bond Donor Count *	0.00
Hydrogen Bond Acceptor Count *	0.00
Rotatable Bond Count *	0.00
Exact Mass *	0.00
Monoisotopic Mass *	0.00
Topological Polar Surface Area *	0.00
Heavy Atom Count *	0.00
Formal Charge	0.16
Complexity *	0.00
Isotope Atom Count	0.23
Defined Atom Stereocenter Count *	0.00
Undefined Atom Stereocenter Count*	0.00
Defined Bond Stereocenter Count*	0.00
Undefined Bond Stereocenter Count	0.31
Covalently-Bonded Unit Count *	0.00

Table S2 (c)

Molecular Descriptor	**Significant t-test**
Molecular Weight	0.56
XLogP3	0.17
Hydrogen Bond Donor Count	0.05
Hydrogen Bond Acceptor Count *	0.00
Rotatable Bond Count	0.29
Exact Mass	0.05
Monoisotopic Mass	0.05
Topological Polar Surface Area *	0.00
Heavy Atom Count *	0.00
Formal Charge	-
Complexity *	0.00
Isotope Atom Count	-
Defined Atom Stereocenter Count	0.08
Undefined Atom Stereocenter Count	0.02
Defined Bond Stereocenter Count	0.05
Undefined Bond Stereocenter Count	-
Covalently-Bonded Unit Count	0.08

Table S3 (a)

Threshold	**Sensitivity**	**Specificity**	**Accuracy**	**F1 score**	**PPV**
1.00	0.48	0.95	0.89	0.6	0.52
0.90	0.56	0.93	0.89	0.59	0.56
0.80	0.62	0.92	0.88	0.56	0.58
0.70	0.66	0.91	0.88	0.55	0.59
0.60	0.72	0.89	0.87	0.54	0.60
0.50	0.74	0.88	0.86	0.52	0.60

0.40	0.76	0.87	0.86	0.51	0.59
0.30	0.77	0.85	0.84	0.48	0.58
0.20	0.77	0.85	0.84	0.48	0.57
0.10	0.79	0.84	0.83	0.46	0.57
0.00	**0.83**	**0.82**	**0.83**	**0.45**	**0.57**
-0.10	0.83	0.82	0.82	0.44	0.56
-0.20	0.84	0.80	0.80	0.41	0.54
-0.30	0.86	0.78	0.79	0.38	0.52
-0.40	0.87	0.76	0.76	0.37	0.51
-0.50	0.88	0.75	0.76	0.35	0.50
-0.60	0.89	0.73	0.75	0.34	0.48
-0.70	0.90	0.71	0.73	0.32	0.47
-0.80	0.91	0.68	0.71	0.31	0.45
-0.90	0.91	0.66	0.69	0.28	0.43
-1.00	**0.92**	**0.63**	**0.67**	**0.27**	**0.42**

Table S3 (b)

Threshold	Sensitivity	Specificity	Accuracy	F1 score	PPV
1.00	0.39	0.90	0.72	0.79	0.48
0.80	0.52	0.87	0.75	0.80	0.59
0.70	0.59	0.86	0.76	0.80	0.64
0.60	0.63	0.84	0.77	0.78	0.67
0.50	0.67	0.83	0.77	0.78	0.69
0.40	0.69	0.82	0.78	0.77	0.70
0.30	0.73	0.81	0.78	0.76	0.72
0.20	0.75	0.80	0.78	0.76	0.73
0.10	0.77	0.79	0.78	0.76	0.74
0.00	0.79	0.78	0.79	0.75	0.75
-0.10	0.80	0.77	0.78	0.74	0.75
-0.20	0.82	0.76	0.78	0.74	0.75
-0.30	0.84	0.76	0.79	0.73	0.76
-0.40	**0.86**	**0.75**	**0.79**	**0.72**	**0.77**
-0.50	0.87	0.74	0.79	0.72	0.77
-0.60	0.87	0.73	0.78	0.71	0.76
-0.70	0.88	0.73	0.78	0.71	0.76
-0.80	0.88	0.72	0.78	0.70	0.76
-0.90	0.89	0.70	0.77	0.68	0.75
-1.00	0.93	0.54	0.69	0.56	0.69

Table S3 (c)

Threshold	Sensitivity	Specificity	Accuracy	F1 score	PPV
1.00	0.27	0.59	0.56	0.50	0.34
0.90	0.40	0.59	0.58	0.53	0.45
0.80	0.47	0.59	0.58	0.47	0.47
0.70	0.53	0.57	0.56	0.37	0.44
0.60	0.53	0.57	0.56	0.37	0.44

0.50	0.53	0.57	0.56	0.37	0.44
0.40	0.60	0.75	0.73	0.42	0.49
0.30	0.67	0.75	0.74	0.45	0.53
0.20	0.67	0.74	0.73	0.44	0.52
0.10	0.73	0.91	0.89	0.47	0.56
0.00	0.73	0.90	0.88	0.44	0.54
-0.10	0.73	0.88	0.87	0.39	0.50
-0.20	0.80	0.87	0.86	0.40	0.52
-0.30	0.80	0.87	0.86	0.40	0.52
-0.40	0.80	0.87	0.86	0.40	0.52
-0.50	**0.87**	**0.85**	**0.86**	**0.40**	**0.54**
-0.60	0.87	0.82	0.82	0.34	0.48
-0.70	0.87	0.79	0.80	0.32	0.46
-0.80	0.93	0.72	0.74	0.27	0.41
-0.90	0.93	0.69	0.72	0.25	0.39
-1.00	0.93	0.61	0.64	0.20	0.33

Table S4 (a)

Dataset	Methods	Sensitivity	Specificity	Accuracy	F1 score	PPV	AUC
Mdm2 0.9_similarity	SVM RBF g=0.0001 c=2 j=2	0.67	0.65	0.66	0.31	0.4	0.69
Mdm2 0.8_similarity	SVM RBF g=0.0001 c=10 j=5	0.62	0.6	0.6	0.27	0.17	0.63

Table S4 (b)

Dataset	Methods	Sensitivity	Specificity	Accuracy	F1 score	PPV	AUC
Bcl2 0.9_similarity	SVM RBF g=0.0001 c=1 j=2	0.72	0.74	0.73	0.68	0.70	0.761
Bcl2 0.8_similarity	SVM RBF g=0.0001 c=1 j=2	0.74	0.73	0.73	0.61	0.56	0.763

Table S5 (a)

Threshold	Sensitivity	Specificity	Accuracy	PPV	F1	MCC
1.1	0.03	0.4	0.34	0.3	0.05	0.03
1	0.12	0.78	0.67	0.5	0.18	0.13
0.9	0.12	0.77	0.66	0.38	0.17	0.15
0.8	0.12	0.76	0.66	0.36	0.17	0.14
0.7	0.16	0.76	0.66	0.39	0.21	0.18
0.6	0.2	0.95	0.83	0.55	0.27	0.24
0.5	0.23	0.95	0.83	0.56	0.3	0.26
0.4	0.24	0.94	0.83	0.57	0.31	0.27
0.3	0.31	0.94	0.84	0.58	0.37	0.33
0.2	0.35	0.93	0.84	0.58	0.41	0.35
0.1	0.35	0.92	0.83	0.55	0.4	0.33
0	0.39	0.92	0.83	0.54	0.43	0.35

-0.1	0.4	0.9	0.82	0.5	0.42	0.33
-0.2	0.44	0.88	0.81	0.48	0.42	0.34
-0.3	0.45	0.86	0.79	0.44	0.41	0.31
-0.4	0.45	0.83	0.77	0.41	0.4	0.29
-0.5	0.48	0.81	0.76	0.4	0.4	0.29
-0.6	0.52	0.77	0.73	0.37	0.4	0.27
-0.7	0.57	0.73	0.71	0.36	0.41	0.29
-0.8	0.61	0.68	0.67	0.31	0.39	0.26
-0.9	**0.67**	**0.65**	**0.66**	**0.31**	**0.4**	**0.27**
-1	0.71	0.55	0.57	0.24	0.35	0.16
-1.1	0.79	0.36	0.43	0.19	0.31	0.09
-1.2	0.88	0.24	0.34	0.18	0.3	0.04
-1.3	0.92	0.16	0.28	0.17	0.29	0.00
-1.5	0.93	0.07	0.21	0.16	0.28	-0.02
-2	1	0.01	0.17	0.16	0.28	0
-2.5	1	0	0.16	0.16	0.28	0
-2.7	1	0	0.16	0.16	0.28	0
-3	1	0	0.16	0.16	0.28	0

Table S5 (b)

Threshold	Sensitivity	Specificity	Accuracy	PPV	F1	MCC
1	0.05	0.19	0.17	0.08	0.06	0.05
0.9	0.05	0.18	0.17	0.05	0.05	0.03
0.8	0.05	0.18	0.17	0.05	0.05	0.03
0.7	0.07	0.36	0.33	0.08	0.08	0.04
0.6	0.07	0.36	0.33	0.08	0.08	0.04
0.5	0.07	0.36	0.33	0.08	0.08	0.04
0.4	0.1	0.36	0.33	0.09	0.09	0.05
0.3	0.15	0.7	0.63	0.12	0.13	0.04
0.2	0.17	0.69	0.63	0.14	0.15	0.06
0.1	0.23	0.67	0.62	0.15	0.18	0.08
0	0.25	0.85	0.78	0.18	0.2	0.08
-0.1	0.25	0.83	0.76	0.16	0.19	0.06
-0.2	0.28	0.81	0.75	0.16	0.2	0.07
-0.3	0.33	0.8	0.75	0.18	0.22	0.1
-0.4	0.33	0.78	0.73	0.16	0.21	0.08
-0.5	0.33	0.76	0.71	0.15	0.2	0.06
-0.6	0.35	0.74	0.69	0.15	0.2	0.06
-0.7	0.35	0.71	0.67	0.14	0.19	0.05
-0.8	0.5	0.69	0.67	0.18	0.27	0.14
-0.9	0.57	0.65	0.64	0.18	0.27	0.15
-1	**0.62**	**0.6**	**0.6**	**0.17**	**0.27**	**0.15**
-1.5	0.8	0.42	0.46	0.16	0.26	0.09
-2	0.9	0.28	0.35	0.14	0.24	0.03

Table S6 (a)

Threshold	Sensitivity	Specificity	Accuracy	PPV	F1	MCC
2.5	0	0	0	0	0	0

2	0	0	0	0	0	0
1.5	0	0	0	0	0	0
1.3	0	0	0	0	0	0
1.2	0.04	0.79	0.49	0.6	0.08	0.01
1.1	0.11	0.97	0.63	0.76	0.19	0.13
1	0.17	0.96	0.65	0.78	0.28	0.17
0.9	0.25	0.95	0.67	0.82	0.38	0.23
0.8	0.3	0.93	0.68	0.79	0.43	0.32
0.7	0.36	0.92	0.7	0.79	0.49	0.36
0.6	0.43	0.92	0.72	0.81	0.55	0.42
0.5	0.48	0.9	0.73	0.8	0.58	0.44
0.4	0.5	0.88	0.73	0.79	0.59	0.44
0.3	0.52	0.87	0.74	0.78	0.61	0.46
0.2	0.55	0.86	0.74	0.78	0.62	0.46
0.1	0.58	0.85	0.74	0.77	0.64	0.48
0	0.59	0.83	0.73	0.76	0.64	0.46
-0.1	0.62	0.82	0.74	0.76	0.65	0.48
-0.2	0.67	0.8	0.75	0.74	0.68	0.5
-0.3	0.69	0.79	0.75	0.75	0.69	0.52
-0.4	0.7	0.78	0.75	0.73	0.69	0.5
-0.5	0.71	0.75	0.74	0.71	0.68	0.49
-0.6	**0.72**	**0.74**	**0.73**	**0.7**	**0.68**	**0.48**
-0.7	0.74	0.71	0.72	0.67	0.67	0.46
-0.8	0.74	0.68	0.7	0.64	0.66	0.43
-0.9	0.77	0.62	0.68	0.61	0.66	0.4
-1	0.85	0.45	0.61	0.51	0.64	0.32
-1.1	0.96	0.06	0.42	0.4	0.57	0
-1.2	0.97	0.02	0.4	0.4	0.56	0.02
-1.3	0.99	0.01	0.4	0.4	0.57	0
-1.5	1	0	0.4	0.4	0.57	0
-2	1	0	0.4	0.4	0.57	0
-2.5	1	0	0.4	0.4	0.57	0
-2.7	1	0	0.4	0.4	0.57	0
-3	1	0	0.4	0.4	0.57	0

Table S6 (b)

Threshold	Sensitivity	Specificity	Accuracy	PPV	F1	MCC
2.5	0	0	0	0	0	0
2	0	0	0	0	0	0
1.5	0.01	0.2	0.14	0.2	0.02	0
1.3	0.03	0.4	0.29	0.4	0.06	0
1.2	0.06	0.59	0.44	0.48	0.1	0.09
1.1	0.13	0.98	0.74	0.81	0.22	0.14
1	0.19	0.98	0.75	0.85	0.3	0.19
0.9	0.25	0.97	0.76	0.82	0.37	0.2
0.8	0.31	0.93	0.75	0.72	0.41	0.26
0.7	0.33	0.91	0.74	0.7	0.42	0.25
0.6	0.37	0.89	0.74	0.63	0.45	0.33
0.5	0.4	0.89	0.75	0.65	0.48	0.35

0.4	0.48	0.88	0.76	0.67	0.54	0.41
0.3	0.54	0.87	0.78	0.69	0.58	0.46
0.2	0.56	0.87	0.78	0.69	0.59	0.47
0.1	0.6	0.86	0.78	0.7	0.61	0.49
0	0.61	0.82	0.76	0.65	0.59	0.46
-0.1	0.64	0.82	0.77	0.63	0.61	0.47
-0.2	0.65	0.79	0.75	0.6	0.6	0.45
-0.3	0.71	0.78	0.76	0.59	0.62	0.47
-0.4	0.72	0.76	0.75	0.58	0.62	0.47
-0.5	**0.74**	**0.73**	**0.73**	**0.56**	**0.61**	**0.3**
-0.6	0.75	0.7	0.71	0.54	0.6	0.29
-0.7	0.75	0.67	0.7	0.51	0.59	0.26
-0.8	0.8	0.63	0.68	0.49	0.59	0.2
-0.9	0.83	0.58	0.65	0.45	0.58	0.19
-1	0.87	0.39	0.53	0.37	0.52	0.12
-1.1	0.96	0.12	0.37	0.31	0.47	0.04
-1.2	0.96	0.05	0.31	0.29	0.45	-0.03
-1.3	0.97	0.01	0.29	0.29	0.44	-0.05
-1.5	1	0.01	0.3	0.29	0.45	0
-2	1	0	0.29	0.29	0.45	0
-2.5	1	0	0.29	0.29	0.45	0
-2.7	1	0	0.29	0.29	0.45	0
-3	1	0	0.29	0.29	0.45	0

Table S7 (a)

Threshold	Sensitivity	Specificity	Accuracy	F1 score	PPV
0.60	0.77	0.81	0.79	0.81	0.79
0.50	0.79	0.81	0.80	0.81	0.80
0.40	0.81	0.79	0.80	0.80	0.81
0.30	0.84	0.79	0.82	0.81	0.82
0.20	0.89	0.79	0.84	0.82	0.85
0.10	0.91	0.77	0.84	0.80	0.85
0.00	**0.93**	**0.77**	**0.85**	**0.80**	**0.86**
-0.10	0.93	0.76	0.85	0.80	0.86
-0.20	0.93	0.76	0.85	0.80	0.86
-0.30	0.94	0.76	0.85	0.80	0.86
-0.40	0.95	0.75	0.85	0.80	0.87
-0.50	0.95	0.75	0.85	0.80	0.87
-0.60	0.95	0.74	0.85	0.79	0.86

Table S7 (b)

Threshold	Sensitivity	Specificity	Accuracy	F1 score	PPV
0.60	0.77	0.68	0.69	0.19	0.31
0.50	0.79	0.66	0.67	0.19	0.30
0.40	**0.81**	**0.63**	**0.65**	**0.18**	**0.30**
0.30	0.84	0.61	0.63	0.18	0.29
0.20	0.89	0.59	0.62	0.18	0.30

0.10	0.91	0.56	0.59	0.17	0.29
0.00	0.93	0.53	0.57	0.17	0.28
-0.10	0.93	0.51	0.55	0.16	0.28
-0.20	0.93	0.49	0.53	0.15	0.27
-0.30	0.94	0.47	0.51	0.15	0.26
-0.40	0.95	0.45	0.49	0.15	0.25
-0.50	0.95	0.43	0.48	0.14	0.25
-0.60	0.95	0.41	0.46	0.14	0.24

Table S8 (a)

Threshold	Sensitivity	Specificity	Accuracy	F1 score	PPV
1.00	0.42	0.87	0.65	0.72	0.52
0.90	0.50	0.79	0.65	0.69	0.57
0.80	0.55	0.73	0.64	0.67	0.60
0.70	0.58	0.71	0.65	0.66	0.61
0.60	0.69	0.66	0.68	0.68	0.68
0.50	**0.71**	**0.62**	**0.67**	**0.66**	**0.68**
0.40	0.73	0.59	0.66	0.65	0.69
0.30	0.79	0.56	0.68	0.66	0.71
0.20	0.82	0.52	0.67	0.65	0.72
0.10	0.83	0.49	0.66	0.63	0.71
0.00	0.87	0.48	0.68	0.64	0.73
-0.10	0.90	0.47	0.69	0.65	0.75
-0.20	0.91	0.45	0.68	0.64	0.75
-0.30	0.93	0.43	0.68	0.64	0.75
-0.40	0.93	0.42	0.68	0.64	0.75
-0.50	0.94	0.39	0.67	0.63	0.75
-0.60	0.94	0.35	0.65	0.61	0.73
-0.70	0.96	0.34	0.65	0.61	0.74
-0.80	0.97	0.34	0.66	0.61	0.74
-0.90	0.98	0.32	0.65	0.60	0.74
-1.00	0.99	0.20	0.60	0.55	0.71

Table S8 (b)

Threshold	Sensitivity	Specificity	Accuracy	F1 score	PPV
1.00	0.42	0.83	0.80	0.21	0.27
0.90	0.50	0.78	0.76	0.19	0.27
0.80	0.55	0.75	0.73	0.18	0.27
0.70	0.58	0.71	0.70	0.17	0.26
0.60	0.69	0.68	0.68	0.18	0.29
0.50	0.71	0.66	0.66	0.18	0.28
0.40	**0.73**	**0.63**	**0.64**	**0.17**	**0.27**
0.30	0.79	0.60	0.62	0.17	0.28
0.20	0.82	0.58	0.60	0.17	0.27
0.00	0.87	0.54	0.57	0.16	0.27

-0.10	0.90	0.51	0.55	0.16	0.27
-0.20	0.91	0.49	0.53	0.15	0.26
-0.30	0.93	0.46	0.50	0.15	0.26
-0.40	0.93	0.44	0.49	0.15	0.25
-0.50	0.94	0.43	0.48	0.14	0.25
-0.60	0.94	0.41	0.46	0.14	0.24
-0.70	0.96	0.40	0.45	0.14	0.24
-0.80	0.97	0.39	0.45	0.14	0.24
-0.90	0.98	0.37	0.43	0.14	0.24
-1.00	0.99	0.27	0.33	0.12	0.21

Table S9 (a)

Threshold	Sensitivity	Specificity	Accuracy	F1 score	PPV
1.00	0.48	1.00	0.74	1.00	0.63
0.90	0.64	1.00	0.82	1.00	0.77
0.80	0.72	1.00	0.86	1.00	0.83
0.70	0.76	1.00	0.88	1.00	0.86
0.60	0.76	1.00	0.88	1.00	0.86
0.50	0.76	1.00	0.88	1.00	0.86
0.40	0.76	1.00	0.88	1.00	0.86
0.30	0.76	0.96	0.86	0.95	0.84
0.20	0.76	0.96	0.86	0.95	0.84
0.10	0.84	0.96	0.90	0.95	0.89
0.00	**0.84**	**0.96**	**0.90**	**0.95**	**0.89**
-0.10	0.88	0.96	0.92	0.95	0.91
-0.20	0.92	0.96	0.94	0.96	0.94
-0.30	0.96	0.96	0.96	0.97	0.96
-0.40	0.96	0.96	0.96	0.97	0.96
-0.50	1.00	0.88	0.94	0.9	0.95
-0.60	1.00	0.84	0.92	0.87	0.93
-0.70	1.00	0.84	0.92	0.87	0.93
-0.80	1.00	0.80	0.90	0.83	0.91
-0.90	1.00	0.80	0.90	0.83	0.91
-1.00	1.00	0.64	0.82	0.74	0.85

Table S9 (b)

Threshold	Sensitivity	Specificity	Accuracy	F1 score	PPV
1.00	0.48	0.92	0.88	0.40	0.42
0.90	0.64	0.91	0.88	0.44	0.50
0.80	0.72	0.89	0.88	0.44	0.53
0.70	0.76	0.86	0.85	0.36	0.48
0.60	0.76	0.82	0.82	0.31	0.43
0.50	0.76	0.78	0.79	0.26	0.39
0.40	0.76	0.73	0.73	0.23	0.35
0.30	0.76	0.69	0.70	0.20	0.32

0.20	0.76	0.66	0.67	0.19	0.30
0.10	**0.84**	**0.60**	**0.63**	**0.17**	**0.29**
0.00	0.84	0.58	0.60	0.17	0.28
-0.10	0.88	0.52	0.56	0.15	0.26
-0.20	0.92	0.48	0.52	0.15	0.26
-0.30	0.96	0.43	0.48	0.14	0.25
-0.40	0.96	0.39	0.44	0.14	0.24
-0.50	1.00	0.34	0.40	0.13	0.23
-0.60	1.00	0.34	0.40	0.13	0.23
-0.70	1.00	0.33	0.39	0.13	0.23
-0.80	1.00	0.29	0.36	0.12	0.22
-0.90	1.00	0.26	0.33	0.12	0.21
-1.00	1.00	0.22	0.29	0.11	0.20

Table S10.

Target	NCI cancer (< 250,000)	
	Threshold value from density plot	Number of PPIM
Mdm2/P53	Above 1.9	473
Bcl2/Bak	Above 1.4	467
Myc/Max	Above 1.7	233

Table S11.

Bcl2_above1.40		Mdm2_above1.90		Myc_above1.70	
chemical_id	SVM scores	chemical_id	SVM scores	chemical_id	SVM scores
5203451	1.8721248	277440	3.790718	5986802	1.74747
315033	1.8717854	282617	3.424159	279854	1.747052
11969551	1.8404794	334894	3.41267	367880	1.745389
5384980	1.8270421	380480	3.272282	372001	1.743937
356231	1.8092628	233919	3.271427	9570040	1.743021
364723	1.7717167	406615	3.253142	9568301	1.74262
283075	1.7673921	24202650	3.238721	5911712	1.74105
299281	1.7502578	345161	3.229204	257491	1.739642
5383303	1.7456576	227727	3.19437	376217	1.739642
377172	1.7437165	3706625	3.168091	9560938	1.739192
334106	1.7215898	6332899	3.142773	5334	1.738893
406854	1.7170140	227722	3.113559	6508680	1.738129
261000	1.7155766	345162	3.112085	311764	1.73771
254013	1.7077260	345527	3.104941	362730	1.737376
5386495	1.6936428	403797	3.074339	9398	1.737261
5458646	1.6882574	6330467	3.043224	6101988	1.736532

300390	1.6703203	337231	3.024422	6161721	1.736493
339662	1.6670671	268891	3.02334	308460	1.73641
335659	1.6585095	330059	2.994196	328723	1.736397
300402	1.6557395	266556	2.979724	6512501	1.736247
5715120	1.6469042	275890	2.962487	371636	1.735706
6711234	1.6469042	418597	2.931016	283687	1.735631
330544	1.6380994	330313	2.915924	5473186	1.73547
290345	1.6364307	351813	2.878977	24203991	1.735379
334955	1.6360373	81345	2.857197	4125795	1.735338
258190	1.6208860	276372	2.844447	284731	1.735158
354868	1.6180335	418594	2.844104	285258	1.735158
5886902	1.6138779	18315	2.843106	9555601	1.734969
402646	1.6086908	435509	2.826279	434213	1.734155
278229	1.6079638	61049	2.806797	60147595	1.734074
45028638	1.6070719	377195	2.805623	352877	1.733473
325066	1.6059230	307198	2.795173	328149	1.733128
17757571	1.6040957	371792	2.790707	286223	1.732903
343206	1.6004212	54604916	2.782096	5384996	1.732365
343207	1.6004212	352818	2.777126	378495	1.732101
59563883	1.5994471	78115	2.769792	360258	1.731909
291384	1.5988708	418596	2.754102	230360	1.731827
387846	1.5971456	421504	2.750916	6109655	1.731685
5471461	1.5949172	389884	2.737871	389164	1.730951
72571	1.5943890	54613361	2.69582	54607064	1.730698
6917515	1.5925663	418598	2.691903	286740	1.730188
334701	1.5921442	231637	2.664569	9569314	1.729891
5899501	1.5912051	345998	2.662939	54607063	1.729208
237944	1.5899979	265647	2.662036	5494332	1.728607
45028632	1.5899190	228947	2.657825	335728	1.728576
54607418	1.5895034	418595	2.648003	9561605	1.727968
379535	1.5891029	231673	2.597939	3954182	1.727715
345994	1.5865426	293257	2.592211	252820	1.727606
54613090	1.5851639	3003741	2.589	367658	1.727303
395935	1.5840666	5359404	2.581667	406662	1.726596
54613127	1.5837552	322987	2.574418	363427	1.72633
5329370	1.5828984	69595	2.572477	325242	1.726053
5465290	1.5828984	306512	2.563193	101425	1.726043
344218	1.5824069	345526	2.561112	45028968	1.725968
54601834	1.5823299	383051	2.555135	45028969	1.725968
289382	1.5806791	383845	2.555135	54612325	1.725918
294929	1.5786527	348754	2.547198	24202956	1.725824
371681	1.5772442	349812	2.547198	5388164	1.7258
5468823	1.5766341	412252	2.542801	1549821	1.725435
338219	1.5752931	252928	2.540253	2511406	1.725309

330570	1.5746579	306996	2.540124	5354945	1.725303
60148352	1.5743231	280724	2.540086	286004	1.725054
363756	1.5728275	306995	2.539997	283686	1.725022
348076	1.5711799	266019	2.537583	392361	1.724988
335428	1.5696999	292104	2.537008	341847	1.724982
3004804	1.5691405	429365	2.535216	259796	1.724617
328374	1.5674673	225749	2.534293	6508559	1.724506
267433	1.5673626	373840	2.530214	3004351	1.724347
6377864	1.5660638	339491	2.528722	343738	1.723505
239595	1.5626672	364366	2.526136	54606727	1.723456
270224	1.5606890	68203	2.525271	269654	1.723443
9555905	1.5583882	226022	2.517609	262229	1.723393
398264	1.5568203	276420	2.51471	24205874	1.722687
335263	1.5558398	5468512	2.512714	284679	1.722427
249050	1.5549779	5286961	2.508375	364270	1.721744
5465865	1.5545052	66926	2.506352	5967551	1.721728
379196	1.5535424	286722	2.503552	46186589	1.72151
254626	1.5509898	434569	2.501911	308438	1.721487
273356	1.5505548	229453	2.498204	308915	1.721487
5386360	1.5504377	3677007	2.497497	24204200	1.721265
248585	1.5496332	260216	2.494929	3005882	1.721037
403006	1.5495001	275856	2.491927	254614	1.72102
429409	1.5486034	6098226	2.487364	270834	1.720973
373016	1.5484679	66219	2.485101	6044145	1.720966
390249	1.5480647	232399	2.484195	348069	1.720739
16092408	1.5470464	266021	2.483879	5465056	1.720733
302560	1.5466805	355098	2.478092	9561071	1.720576
294939	1.5466070	300560	2.471319	399277	1.720566
260469	1.5453141	369204	2.471173	6477364	1.720228
289323	1.5448804	406617	2.462453	225494	1.719819
332926	1.5438064	228958	2.453075	54717787	1.719609
282279	1.5436075	373843	2.449925	24205699	1.719529
54601406	1.5434529	285957	2.443211	308939	1.719348
5382633	1.5432384	310597	2.432857	304487	1.719246
259039	1.5429426	291859	2.431171	6400237	1.719024
5472796	1.5421737	304605	2.426551	374233	1.71852
5472821	1.5421737	341354	2.424909	5465749	1.718321
395585	1.5416046	306998	2.424384	326212	1.718077
188044	1.5412141	17357	2.419972	318920	1.71783
45028336	1.5407399	345160	2.419769	322179	1.717735
382254	1.5398415	257420	2.407836	289383	1.717724
2797269	1.5395433	410321	2.405989	355764	1.717644
6366966	1.5395133	17438	2.402862	267119	1.717479
389711	1.5390032	228456	2.395257	342713	1.717442

358208	1.5389167	5950593	2.392543	5943562	1.717395
6152359	1.5387471	286110	2.39194	101142	1.717109
277712	1.5383615	435508	2.388646	286915	1.717004
343445	1.5379802	423857	2.38574	275685	1.716743
278265	1.5372667	264098	2.385049	362696	1.716694
54612299	1.5371916	418550	2.381093	362697	1.716694
357293	1.5370409	375900	2.378276	6283355	1.716552
337370	1.5370014	363284	2.371323	275365	1.716486
403200	1.5368940	281774	2.370253	54609988	1.716407
60147931	1.5335443	5470694	2.366813	305190	1.716242
54612266	1.5331367	5355478	2.364606	330087	1.71613
60147788	1.5322647	397481	2.354045	6041104	1.716028
5387864	1.5295275	390675	2.35153	9699863	1.716028
396512	1.5279808	373332	2.345525	366855	1.716026
403194	1.5278765	54600268	2.344589	5380580	1.716002
297815	1.5275048	273178	2.341357	5464757	1.716002
257430	1.5273588	232405	2.339411	353302	1.715231
5466144	1.5263835	6712350	2.335676	5380581	1.715212
347913	1.5244969	72753	2.335253	281598	1.714843
337782	1.5244228	404275	2.334398	403847	1.71475
347914	1.5235224	326052	2.326524	336970	1.7142
401366	1.5228174	275864	2.323553	374170	1.714122
6712916	1.5225287	275891	2.320459	280976	1.713961
356859	1.5219798	275892	2.316982	54612216	1.713578
5472433	1.5204071	8265	2.316552	346529	1.71349
393247	1.5187820	264114	2.315467	381446	1.713431
406712	1.5186374	305821	2.314488	1121572	1.713376
254664	1.5176951	380064	2.313822	54604613	1.713365
370694	1.5170614	315725	2.312839	371522	1.713314
438262	1.5169667	220695	2.311874	353113	1.713277
431614	1.5152949	136630	2.310267	6185269	1.713126
54611485	1.5138265	43584	2.307588	54715262	1.712788
355605	1.5128269	435510	2.307015	6046001	1.712081
363760	1.5123775	94861	2.30442	300544	1.71201
5472772	1.5114249	327108	2.297066	315789	1.711991
5472785	1.5114249	369206	2.296701	381166	1.711847
9554587	1.5107190	297551	2.296428	362843	1.711842
339938	1.5083035	299895	2.294382	9556300	1.711673
286290	1.5082554	328362	2.294188	289386	1.711634
60198	1.5079568	356217	2.292567	337963	1.711562
309624	1.5075468	225654	2.292115	235562	1.710796
14952715	1.5067569	372284	2.291506	381635	1.710647
329157	1.5066911	367942	2.290847	362728	1.710312
386074	1.5066329	351391	2.283779	362729	1.710312

9572748	1.5065886	246183	2.283739	324810	1.710063
5472791	1.5058746	5710449	2.282722	5465002	1.709887
5472794	1.5058746	306515	2.28221	335211	1.709858
60147873	1.5056090	6330534	2.280529	6179266	1.709723
419137	1.5056072	382201	2.279844	375546	1.709662
286785	1.5053340	275961	2.279641	3721620	1.709655
6372930	1.5052989	24205043	2.277268	5465777	1.709444
355716	1.5048819	388208	2.276055	24195152	1.709372
290663	1.5046058	409127	2.275516	291933	1.709344
54599024	1.5044420	3002249	2.275387	6304386	1.709281
9572516	1.5039092	387756	2.269711	314751	1.708936
369436	1.5030612	232401	2.269037	285738	1.708854
386869	1.5029662	6081340	2.268906	353120	1.708854
5467895	1.5028747	306999	2.268261	336813	1.708773
314520	1.5016405	294835	2.267577	297857	1.708621
5382486	1.5015883	18363	2.266075	365126	1.708523
291333	1.5014492	266020	2.265694	237420	1.70844
54606497	1.5013004	249366	2.261423	401212	1.707968
454878	1.5011073	310814	2.258711	308459	1.707803
335660	1.5009280	293259	2.252537	379794	1.707777
54612675	1.5004064	256736	2.251659	97308	1.707594
367738	1.4991558	293547	2.249102	311768	1.707438
333310	1.4982715	285939	2.24858	242943	1.70689
333357	1.4982715	228959	2.244946	100658	1.706479
6327978	1.4982282	315788	2.244055	401240	1.706463
393279	1.4981919	264108	2.242032	399279	1.706144
337433	1.4969596	228492	2.239553	360892	1.705888
9568394	1.4966175	5384768	2.235214	5358633	1.705749
9568415	1.4966175	54611944	2.231513	5814880	1.705742
241778	1.4964410	6508767	2.229317	3094794	1.705642
317277	1.4962146	338483	2.228975	393674	1.705546
337314	1.4945402	417379	2.223487	5222453	1.70547
54601060	1.4940776	6508783	2.222365	3905395	1.705198
54607184	1.4940776	282917	2.222345	305468	1.705085
238205	1.4940400	420720	2.222214	388302	1.704931
370688	1.4939792	270791	2.220818	366582	1.704924
233377	1.4934741	54606293	2.220007	267143	1.704691
400739	1.4932156	384711	2.21984	333766	1.704688
5494449	1.4931617	381004	2.21517	4569488	1.704584
302409	1.4929711	373838	2.214983	9555411	1.704332
5470485	1.4927776	392957	2.210468	355762	1.704281
10067489	1.4919709	373841	2.209638	9555728	1.704046
405551	1.4917422	306513	2.208779	50990444	1.704029
328637	1.4915862	306997	2.208779	366580	1.703961

353636	1.4909930	282912	2.206763	54607758	1.70395
60147605	1.4903728	435507	2.206138	381834	1.703922
225724	1.4899307	45028352	2.205529	375629	1.703905
5472779	1.4897580	5469930	2.205005	357198	1.703831
353633	1.4892042	255299	2.204597	9556472	1.703825
5472118	1.4881581	303440	2.204026	377200	1.703665
36238	1.4878578	361191	2.202077	374169	1.703578
404448	1.4876153	5472056	2.201991	334296	1.703487
278872	1.4872951	306994	2.197476	332470	1.703187
350191	1.4870246	340322	2.196427	5228004	1.70318
387845	1.4849430	382434	2.194964	362701	1.703149
278080	1.4838276	306511	2.19473	5465711	1.702929
270223	1.4827027	237514	2.189073	3004745	1.702895
314417	1.4826653	361146	2.187031	254766	1.702886
6711455	1.4825303	288588	2.187018	372013	1.702789
45027958	1.4822799	5387176	2.181702	24203333	1.702681
400546	1.4819717	345158	2.179567	350914	1.702373
50987505	1.4811284	45028255	2.178267	391093	1.702283
362710	1.4810929	98406	2.175814	336814	1.702268
362720	1.4809468	272879	2.175654	288191	1.702248
24205768	1.4805677	373836	2.174058	278799	1.702229
5468882	1.4803655	233941	2.173299	9555073	1.70212
5469855	1.4803655	411936	2.171452	2263390	1.701931
419169	1.4801360	263527	2.167061	100109	1.701704
267511	1.4795487	402243	2.1665	262382	1.70168
5356293	1.4790356	300231	2.166319	243231	1.70161
182193	1.4786922	54606684	2.164698	101409	1.701442
393762	1.4786564	403682	2.162882	3004315	1.701295
5472775	1.4778480	21961	2.162395	339443	1.701279
330976	1.4777460	338371	2.15814	362691	1.701243
419062	1.4775538	84720	2.15595	257337	1.701119
393237	1.4774905	232762	2.155894	339442	1.700987
395587	1.4774340	428600	2.153806	399816	1.700808
5472781	1.4772115	338368	2.153196	247217	1.700803
6057425	1.4771890	266849	2.15237	9572324	1.700717
5470926	1.4770280	227135	2.148439	54610171	1.700575
406860	1.4768724	5380673	2.146401	9572749	1.700398
100113	1.4762512	327306	2.14351	344248	1.700391
334924	1.4762512	339495	2.143365	313612	1.700262
5476765	1.4759683	12030674	2.138994	5792639	1.700143
353635	1.4757993	253596	2.138328	263477	1.700102
337371	1.4754997	230037	2.136333		
51353353	1.4746851	17755023	2.135791		
269831	1.4743623	6281424	2.135409		

54613531	1.4736324	356701	2.130734		
5358837	1.4732237	387780	2.128627		
384656	1.4719340	373771	2.12695		
16667705	1.4718009	5472313	2.126589		
54607778	1.4711040	273334	2.126321		
257421	1.4704064	273345	2.126321		
54610041	1.4693841	228956	2.123125		
285066	1.4691039	257927	2.120172		
387002	1.4690449	380876	2.118031		
391009	1.4690449	422412	2.115633		
368604	1.4680957	56946086	2.115444		
240036	1.4680832	314399	2.113607		
24203954	1.4677277	4999	2.111175		
401362	1.4676596	288854	2.109401		
5472792	1.4674825	369423	2.108782		
5472799	1.4674825	329828	2.108286		
5386774	1.4673179	67548	2.108035		
421848	1.4660086	5387174	2.106425		
53483672	1.4658941	54721825	2.102322		
60147797	1.4651440	342063	2.100872		
3001721	1.4651149	54613310	2.100419		
9572204	1.4650058	255298	2.098783		
405547	1.4647290	320731	2.098749		
405553	1.4647290	3465612	2.098527		
273187	1.4646081	381612	2.097367		
5465636	1.4644519	394333	2.097117		
291162	1.4640028	400634	2.096812		
219975	1.4640013	271612	2.093854		
56833684	1.4636813	384881	2.093481		
60147895	1.4636813	395441	2.09314		
405978	1.4634980	5472466	2.091704		
352616	1.4633745	5387017	2.090891		
352075	1.4616608	5472122	2.090453		
380022	1.4606643	54606105	2.087186		
343562	1.4597040	323505	2.085428		
331523	1.4596635	373133	2.085411		
258179	1.4595804	5845	2.085098		
330977	1.4592119	401622	2.085064		
5351422	1.4591040	3562869	2.078536		
397613	1.4590494	388286	2.078159		
328189	1.4577042	405011	2.077789		
5320815	1.4573584	395444	2.075988		
24936159	1.4567173	349834	2.073293		
401439	1.4566803	5469512	2.071909		

339663	1.4561011	241805	2.070165		
45028428	1.4554473	5472302	2.067947		
24204787	1.4552072	324956	2.067839		
272908	1.4546796	5800494	2.067091		
16092412	1.4545919	5473357	2.066748		
293627	1.4544880	280865	2.066544		
402725	1.4542305	276369	2.066173		
375341	1.4541940	6508605	2.065222		
292370	1.4536972	328584	2.063983		
60148006	1.4534213	5470441	2.063005		
6140848	1.4533491	5470442	2.063005		
60147576	1.4533228	5470831	2.063005		
5702275	1.4528633	5470833	2.063005		
60147634	1.4525619	363237	2.062796		
382342	1.4509524	23403	2.062475		
5835541	1.4497167	2690313	2.062121		
393669	1.4489319	291905	2.060879		
60147986	1.4487968	434171	2.060277		
3976461	1.4483146	404780	2.057061		
331739	1.4479150	252266	2.053479		
343166	1.4477058	256282	2.053479		
303943	1.4475592	392195	2.052733		
5035	1.4473644	60147989	2.052611		
99614	1.4470047	333824	2.051858		
4306816	1.4469450	245225	2.049801		
336168	1.4468486	1098360	2.049022		
60147630	1.4461823	304571	2.046059		
317279	1.4461261	312291	2.041749		
24204790	1.4453541	314010	2.041048		
390932	1.4447926	395677	2.040669		
51371333	1.4443470	401614	2.040103		
84923	1.4442858	5472758	2.039232		
5472776	1.4439745	236488	2.03875		
5468067	1.4430747	45029465	2.037244		
376183	1.4427294	314735	2.036869		
253422	1.4413485	247305	2.036215		
45028114	1.4410694	24203212	2.036139		
245972	1.4398950	6344347	2.034018		
251863	1.4394697	381503	2.033986		
54603054	1.4391493	5351862	2.030319		
24204596	1.4385348	219445	2.03024		
316872	1.4383521	1574964	2.028923		
5837709	1.4378499	403651	2.024617		
340847	1.4376413	240028	2.024571		

5464877	1.4375663	385403	2.023266		
5471435	1.4372409	349006	2.022134		
297833	1.4366183	333905	2.021372		
267454	1.4365901	335900	2.019468		
44118991	1.4362430	1179892	2.01906		
54610615	1.4362430	289863	2.016784		
9555397	1.4360425	99547	2.016641		
344766	1.4353267	342081	2.015873		
60807	1.4346520	306625	2.013071		
244720	1.4342066	297801	2.010152		
376621	1.4340711	364634	2.010056		
284515	1.4337227	54613583	2.010052		
60147787	1.4335685	363236	2.009221		
279194	1.4333874	6712782	2.009148		
5386713	1.4330808	335630	2.008974		
392427	1.4329812	381611	2.006964		
241533	1.4329784	329836	2.006143		
6519134	1.4329281	54719014	2.003359		
60147934	1.4329177	373412	2.003103		
273244	1.4328481	363797	2.00278		
433421	1.4326189	406613	2.002712		
359553	1.4325801	400485	2.002374		
429260	1.4325801	400486	2.002374		
45029303	1.4318017	357606	1.999705		
354164	1.4317476	399908	1.998617		
5359173	1.4313635	5470440	1.994684		
392426	1.4313157	5470832	1.994684		
402724	1.4309294	5470835	1.994684		
9572690	1.4306315	5470836	1.994684		
251861	1.4305633	403451	1.991612		
45028594	1.4303964	294871	1.989406		
320590	1.4303946	292152	1.989242		
394017	1.4303203	313998	1.987898		
299927	1.4302678	373051	1.985937		
6381032	1.4299810	343048	1.985929		
60147936	1.4299720	288059	1.985592		
363974	1.4299036	396571	1.984657		
9572669	1.4296271	262917	1.984163		
60147790	1.4293785	5467140	1.983807		
333234	1.4291971	5466455	1.982339		
296891	1.4285962	379824	1.982224		
391935	1.4280246	1576365	1.982057		
395201	1.4278641	354850	1.98154		
251643	1.4276767	263759	1.98076		

235314	1.4244235	435291	1.979856		
268591	1.4243307	280722	1.978994		
402426	1.4240675	393054	1.978515		
406709	1.4240507	5469517	1.978283		
304875	1.4235515	374305	1.976858		
392021	1.4235402	54599590	1.976359		
387339	1.4230822	308378	1.973308		
24205620	1.4229478	341989	1.972883		
341155	1.4229192	5472304	1.972103		
374920	1.4228770	138726	1.971558		
16092414	1.4228683	338370	1.971203		
16092428	1.4228683	434170	1.970827		
354229	1.4228355	354462	1.967886		
400001	1.4224297	45029455	1.965918		
394894	1.4222165	271900	1.965807		
297105	1.4221877	5382353	1.964315		
332927	1.4221854	401791	1.961904		
24189184	1.4206872	314734	1.961769		
364312	1.4206864	280718	1.959663		
5281545	1.4206584	54608971	1.959594		
6330209	1.4206584	300591	1.957416		
24204185	1.4204971	5386357	1.956835		
5387800	1.4202774	5469509	1.956099		
226469	1.4202257	5469510	1.956099		
324826	1.4193103	9572355	1.955047		
394209	1.4190783	340966	1.954756		
5912031	1.4188351	24205853	1.954613		
371062	1.4187239	395328	1.953267		
54601166	1.4182825	432769	1.951349		
5468254	1.4181776	383339	1.951213		
295833	1.4179786	5964761	1.949917		
385079	1.4177123	5988864	1.949466		
401356	1.4176415	4568312	1.949165		
240986	1.4172194	373602	1.949031		
9604729	1.4170966	375824	1.948855		
5291	1.4168860	54613736	1.948801		
400545	1.4168568	399521	1.948062		
9571961	1.4166759	319662	1.948037		
72499	1.4159276	1379641	1.94416		
406434	1.4157631	24205563	1.944038		
241544	1.4156204	287408	1.943469		
54605308	1.4155459	213803	1.942887		
243942	1.4153240	6309276	1.942593		
223997	1.4152164	306992	1.942274		

260116	1.4150839	393056	1.942167		
6111057	1.4150189	12319944	1.941718		
400183	1.4148394	60147988	1.941699		
111337	1.4145795	228502	1.941506		
5945673	1.4140776	5469508	1.940824		
6399642	1.4132099	261926	1.93987		
334736	1.4115161	318875	1.938701		
5867049	1.4114617	347885	1.938476		
5702095	1.4112325	236199	1.937348		
377037	1.4108773	54608442	1.936677		
24204377	1.4104508	434038	1.936172		
298316	1.4103847	24779697	1.935587		
10184653	1.4102434	297480	1.935308		
223249	1.4100661	403241	1.934897		
6710729	1.4099882	321168	1.934601		
24204844	1.4097041	367773	1.934046		
323905	1.4096772	9554599	1.934013		
299850	1.4094306	353833	1.933477		
5469821	1.4092886	351612	1.933475		
353595	1.4092791	45029473	1.932098		
6103807	1.4091371	399739	1.931172		
272214	1.4090259	399517	1.930191		
314402	1.4087612	296886	1.928712		
387429	1.4076943	24203025	1.927239		
54603490	1.4073639	401228	1.927119		
45028113	1.4071804	337978	1.924795		
309944	1.4071482	404860	1.923827		
241400	1.4070310	356718	1.923702		
9554930	1.4065719	334123	1.923198		
372977	1.4063725	373739	1.922675		
382321	1.4056729	373572	1.921907		
54602601	1.4050540	222104	1.920831		
381063	1.4048247	395325	1.919979		
261920	1.4048200	404580	1.919633		
382340	1.4044417	250324	1.918753		
9555370	1.4042532	5472467	1.917617		
241149	1.4040013	98407	1.916704		
337520	1.4039138	405217	1.91636		
233524	1.4037326	406175	1.915991		
5896574	1.4037233	293199	1.915854		
353546	1.4035030	5468713	1.915114		
313877	1.4034553	54604837	1.914781		
383300	1.4018206	224165	1.914421		
5470175	1.4014318	323345	1.913354		

270131	1.4013861	429734	1.911829		
6712058	1.4012439	17756600	1.911518		
6712059	1.4012439	281835	1.911088		
375302	1.4011573	382107	1.908085		
291145	1.4007053	436767	1.90722		
349861	1.4006148	357095	1.906582		
245352	1.4004213	54606088	1.905842		
24204303	1.4003853	374205	1.905635		
382258	1.4002471	381797	1.905337		
367609	1.4002402	313819	1.904131		
5388311	1.4000490	345159	1.903664		
		434035	1.902374		
		400755	1.901975		
		19656597	1.900937		
		17755849	1.900764		
		392196	1.900683		
		100815	1.900483		

Table S12.

	The median values:	The 25th percentile values:	The 75th percentile values:	T-test
Mdm2 top	-5.55	-4.30	-7.15	0.56
Mdm2 low	-6.00	-5.50	-6.55	
Mdm2 random	-5.74	-4.95	-6.66	
Bcl2 top	-7.60	-7.10	-8.20	0.11
Bcl2 low	-7.40	-6.70	-7.90	
Bcl2 random	-7.35	-6.80	-7.96	
Myc top	-5.70	-5.40	-6.10	0.14
Myc low	-5.50	-4.85	-6.05	
Myc random	-5.53	-4.95	-6.03	

Table S13 (a).

CID_Mdm2	**Binding Free Energy (Kcal/mol)**	**SVM score**
231637	-9.40	2.66
68203	-9.20	2.53
282617	-9.10	3.42
435509	-9.10	2.83
348754	-9.10	2.55
349812	-8.80	2.55
6330467	-8.40	3.04
5.5E+07	-8.20	2.70
293257	-8.00	2.59
330059	-7.70	2.99

389884	-7.70	2.74
225749	-7.40	2.53
231673	-7.30	2.60
306512	-7.20	2.56
226022	-7.20	2.52
307198	-7.10	2.80
383051	-7.00	2.56
306996	-6.90	2.54
383845	-6.80	2.56
339491	-6.50	2.53
277440	-6.40	3.79
371792	-6.40	2.79
364366	-6.30	2.53
306995	-6.20	2.54
6332899	-6.10	3.14
268891	-6.10	3.02
228947	-6.00	2.66
412252	-5.90	2.54
292104	-5.70	2.54
330313	-5.60	2.92
380480	-5.50	3.27
418597	-5.50	2.93
265647	-5.50	2.66
266019	-5.50	2.54
233919	-5.40	3.27
421504	-5.40	2.75
418594	-5.30	2.84
61049	-5.30	2.81
418595	-5.30	2.65
418596	-5.10	2.75
406615	-4.90	3.25
418598	-4.80	2.69
322987	-4.60	2.57
345161	-4.40	3.23
345162	-4.30	3.11
3003741	-4.30	2.59
345526	-4.30	2.56
280724	-4.30	2.54
345527	-4.20	3.10
18315	-4.20	2.84
266556	-4.10	2.98
81345	-4.10	2.86
351813	-4.00	2.88
78115	-4.00	2.77
373840	-4.00	2.53
334894	-3.90	3.41
227727	-3.80	3.19
227722	-3.60	3.11

3706625	-3.50	3.17
69595	-2.80	2.57

Table S13 (b).

CID_Bcl2	Binding Free Energy (Kcal/mol)	SVM score
338219	-10.30	1.58
402646	-10.00	1.61
45028632	-9.80	1.59
45028638	-9.30	1.61
54607418	-8.80	1.59
5886902	-8.70	1.62
258190	-8.50	1.62
5899501	-8.50	1.6
54613090	-8.40	1.59
54601834	-8.40	1.59
300390	-8.30	1.67
354868	-8.30	1.62
72571	-8.30	1.6
345994	-8.30	1.59
59563883	-8.20	1.6
289382	-8.20	1.58
330570	-8.20	1.58
348076	-8.10	1.58
5329370	-8.00	1.59
254013	-7.90	1.71
5465290	-7.90	1.59
283075	-7.80	1.77
335659	-7.80	1.66
5715120	-7.80	1.65
395935	-7.80	1.59
3004804	-7.80	1.57
356231	-7.70	1.81
5386495	-7.70	1.7
17757571	-7.70	1.61
334955	-7.60	1.64
54613127	-7.60	1.59
339662	-7.50	1.67
5383303	-7.40	1.75
334106	-7.40	1.73
261000	-7.40	1.72
330544	-7.40	1.64
335428	-7.40	1.57
5203451	-7.30	1.88
300402	-7.30	1.66
6917515	-7.30	1.6

237944	-7.30	1.59
299281	-7.20	1.75
377172	-7.20	1.75
290345	-7.20	1.64
387846	-7.20	1.6
364723	-7.10	1.78
6711234	-7.10	1.65
328374	-7.00	1.57
267433	-7.00	1.57
315033	-6.90	1.88
294929	-6.90	1.58
60148352	-6.80	1.58
406854	-6.60	1.72
5384980	-6.50	1.83
325066	-6.50	1.61
11969551	-6.40	1.84
5471461	-6.40	1.6
363756	-6.40	1.58
5468823	-6.30	1.58
5458646	-6.10	1.69

Table S13 (c).

CID_Myc	**Binding Free Energy (Kcal/mol)**	**SVM score**
279854	-6.60	1.75
367658	-6.50	1.73
352877	-6.40	1.73
252820	-6.40	1.73
2511406	-6.40	1.73
328723	-6.30	1.74
286223	-6.30	1.73
367880	-6.20	1.75
9555601	-6.20	1.73
54607064	-6.20	1.73
5986802	-6.10	1.75
60147595	-6.10	1.73
328149	-6.10	1.73
360258	-6.10	1.73
101425	-6.10	1.73
5388164	-6.10	1.73
283687	-6.00	1.74
9569314	-6.00	1.73
3954182	-6.00	1.73
24202956	-6.00	1.73
5911712	-5.90	1.74
6109655	-5.90	1.74
54607063	-5.90	1.73

372001	-5.80	1.74
371636	-5.80	1.74
4125795	-5.80	1.74
230360	-5.80	1.73
308460	-5.70	1.74
286740	-5.70	1.73
335728	-5.70	1.73
45028968	-5.70	1.73
45028969	-5.70	1.73
1549821	-5.70	1.73
9568301	-5.60	1.74
376217	-5.60	1.74
363427	-5.60	1.73
257491	-5.50	1.74
9398	-5.50	1.74
6512501	-5.50	1.74
9561605	-5.50	1.73
9560938	-5.40	1.74
5334	-5.40	1.74
311764	-5.40	1.74
6101988	-5.40	1.74
6161721	-5.40	1.74
389164	-5.40	1.73
54612325	-5.40	1.73
284731	-5.30	1.74
5473186	-5.20	1.74
285258	-5.20	1.74
5494332	-5.20	1.73
325242	-5.20	1.73
6508680	-5.10	1.74
362730	-5.10	1.74
434213	-5.10	1.73
406662	-5.10	1.73
9570040	-5.00	1.74
378495	-4.60	1.73
24203991	-4.50	1.74
5384996	-4.50	1.73

Table S14.

2P2I full	Mdm2_reported(32)	Bcl2_reported (26)	common 2P2I and Mdm2	SVM score	common 2P2I and Bcl2	SVM score
03B	0R2	LIU	07G	0.96	398	1.15
07G	0R3	1E9	0R3	1	03B	1.12
0Q5	0Y7	1XJ	DIZ	1.01	0Q5	1.23
0R3	1MN	1XV	IMZ	1.13	43B	0.8
0RO	1MO	1Y1	K23	1.1	B50	0.87
307	1MQ	43B	MI6	1.33	DRO	1
398	1MT	398	YIN	1.54	HI0	1.3
434	1MY	DRO			LI0	1.12
43B	2SW	LI0			N3B	1.1
703	2TW	X0R			N3C	1.27
723	2TZ	X0J				
976	2U0	X0D				
997	2U1	X0B				
998	2U5	TN1				
9JZ	2U6	N3C				
B50	2U7	N3B				
BI6	2V8	LIW				
CL3	07G	LC6				
CMM	13Q	HI0				
CO9	28W	H1I				
CZ3	35S	H0Y				
DIZ	BLF	B50				
DRO	DIZ	38H				
FRB	IMZ	03B				
FRG	K23	0Q5				
FRI	LTZ	X8U				
HI0	MI6					
IMZ	NUT					
K23	TJ2					
LI0	VZV					
MI6	Y30					
N3B	YIN					
N3C						
TQ2						
TQX						
WAC						
WAI						
WW8						
Y30						
YIN						

Table S15.

Target	2P2I Hunter (40)		
	Threshold value from SVM prediction	Number of PPIM from SVM prediction	Number of PPIM reported in 2P2I target wise
Mdm2/P53	0.90	16	7
Bcl2/Bak	0.80	20	10
Myc/Max	Not reported	Not reported	Not reported

Table S16.

Mdm2/P53 (PubChem Id)	**Bcl2/Bak (PubChem Id)**
53470410	60169704
56973540	53470410
56965957	56973540
921795	56965957
5388929	54765302
4369343	5327044
25021179	56973535
5287936	5287508
656933	5388929
5288631	4369343
44825260	42609700
49867311	57339126
44199170	25113117
44198672	447945
11987780	656989
5594130	15991563
	49867311
	4369509
	11228183
	25011737

Table S17.

CID	Target	Svm Score	Positiveness	Negativeness
11433190(Nutlin)	MDM2/P53	1.1668327	52.14	23.27
24978538(ABT-263)	BCL2/BAK	1.0059592	42.86	3.46
46930996(GX15-070)	BCL2/BAK	0.56320301	17.02	13.27

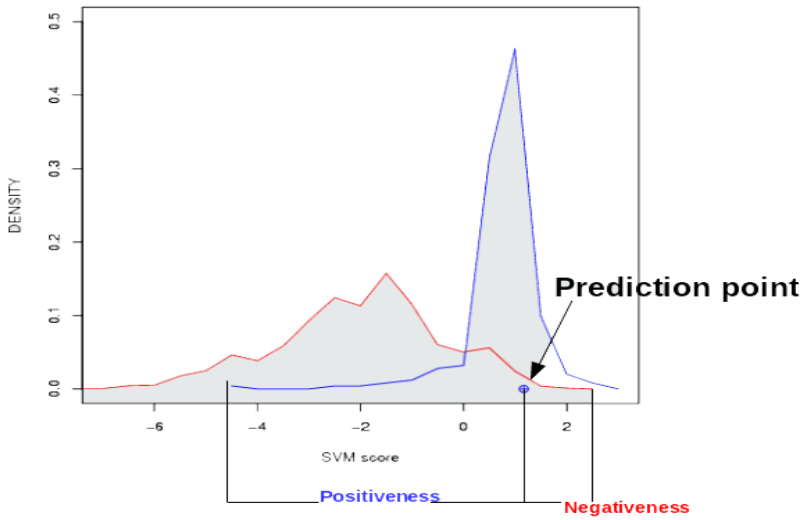
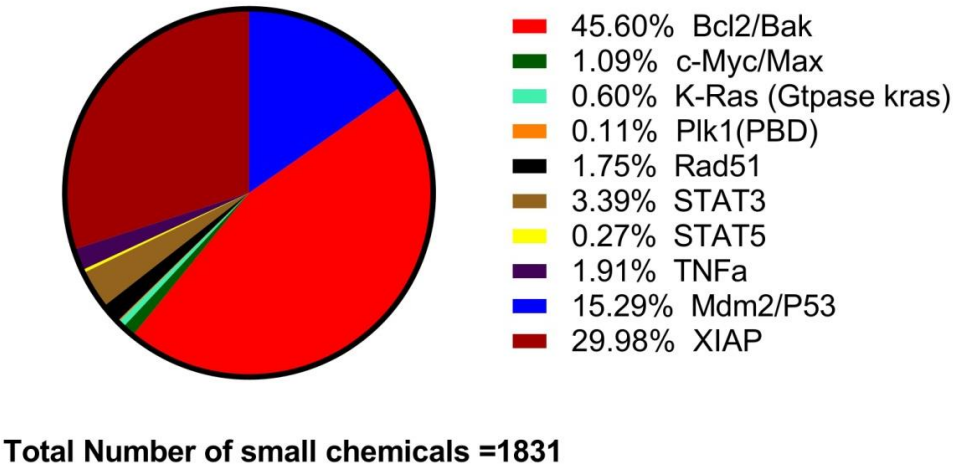


Figure S1.



Total Number of small chemicals =1831

Figure S2.

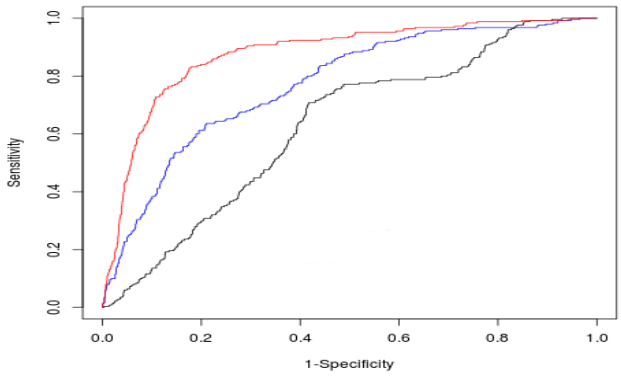


Figure S3 (a).

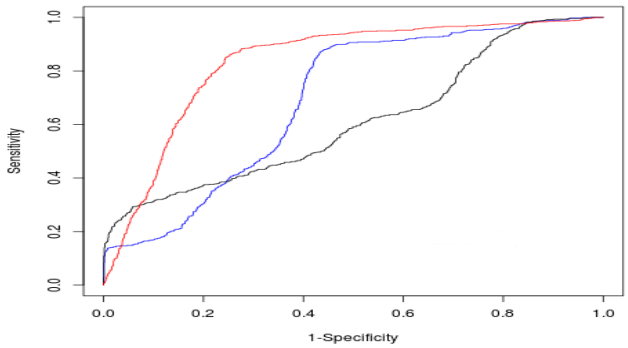


Figure S3 (b).

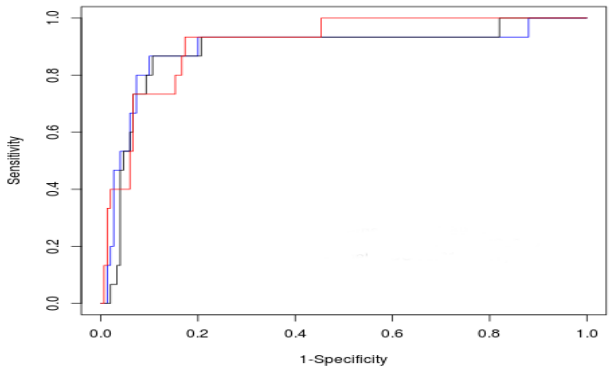


Figure S3 (c).

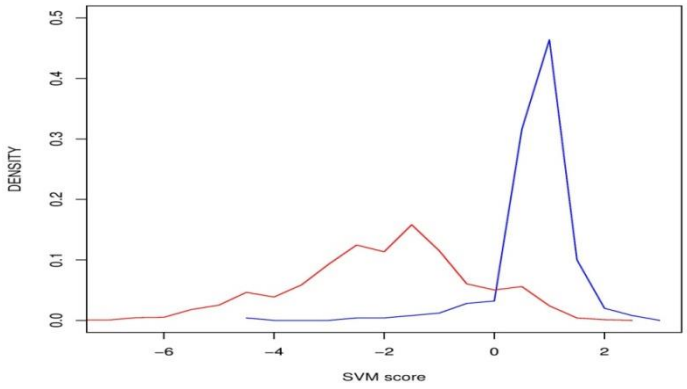


Figure S4 (a).

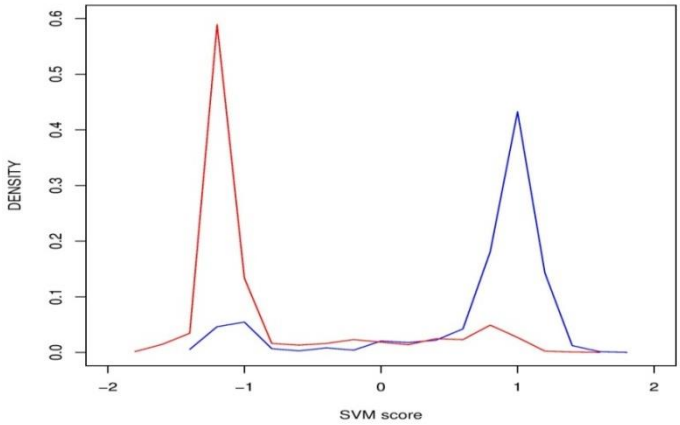


Figure S4 (b).

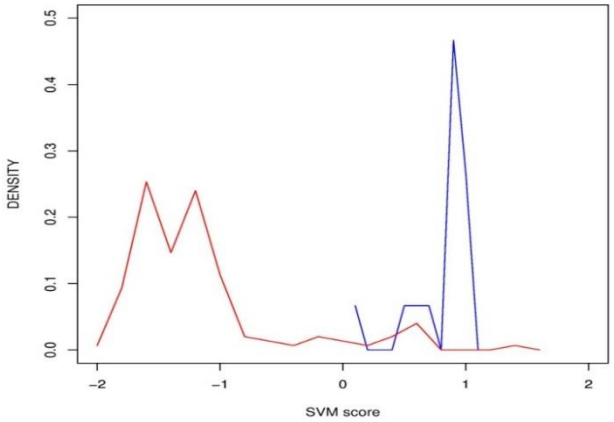


Figure S4 (c).

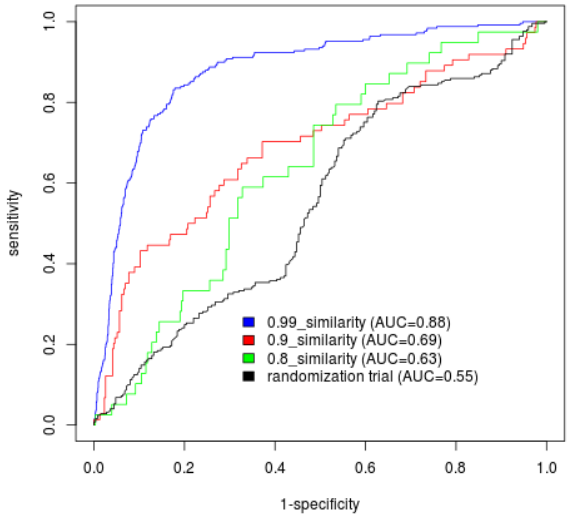


Figure S5 (a).

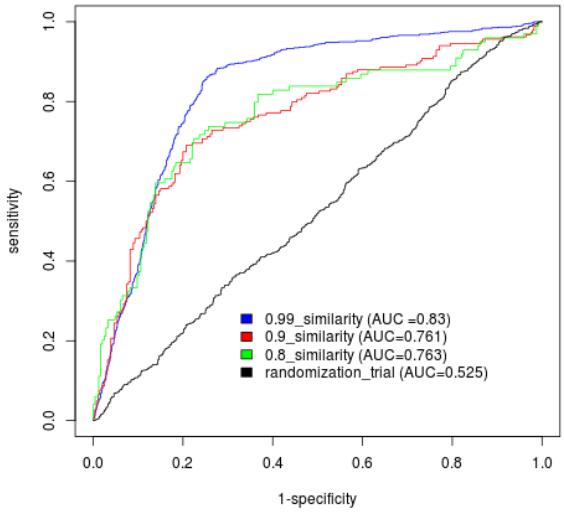


Figure S5 (b).

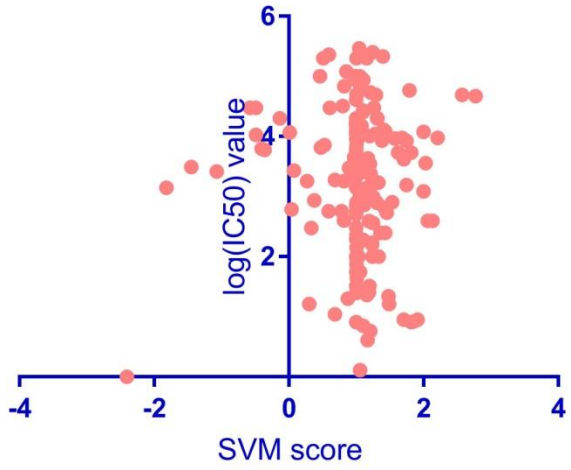


Figure S6 (a).

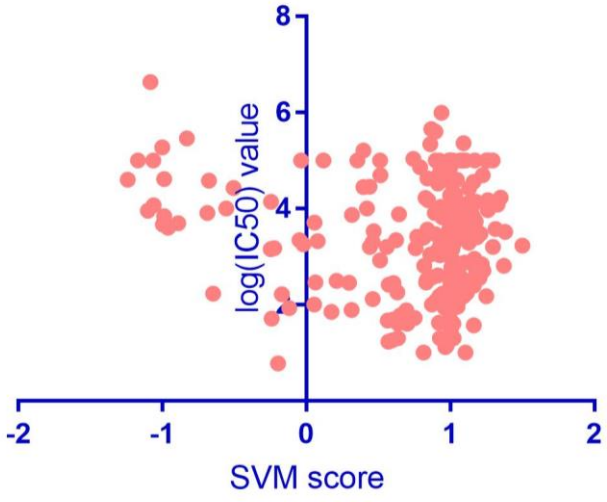


Figure S6 (b).

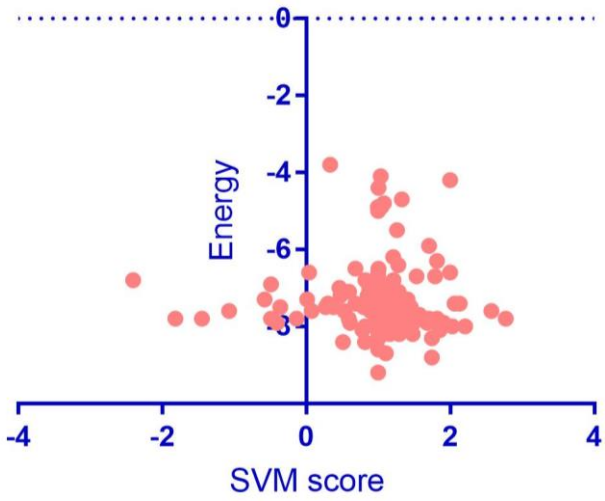


Figure S7 (a).

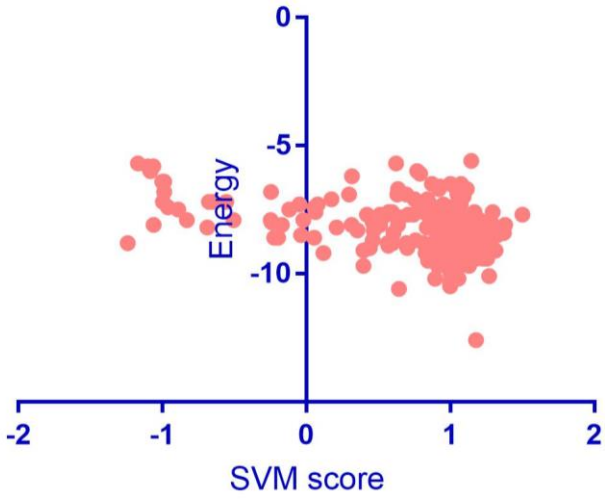


Figure S7 (b).

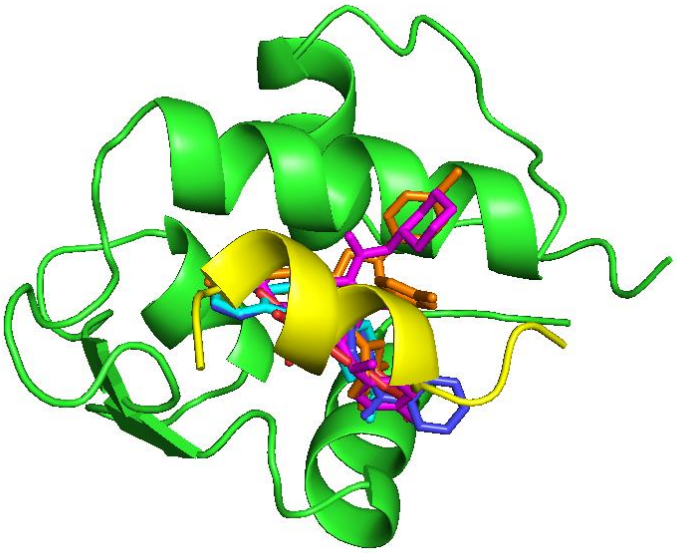


Figure S8 (a).

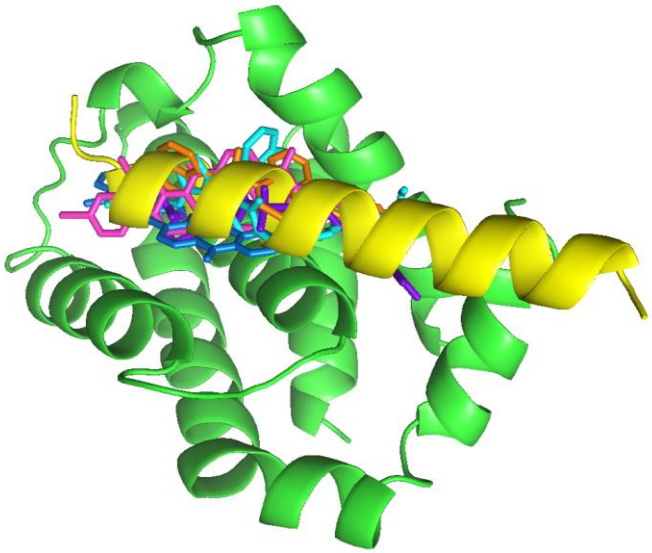


Figure S8 (b).

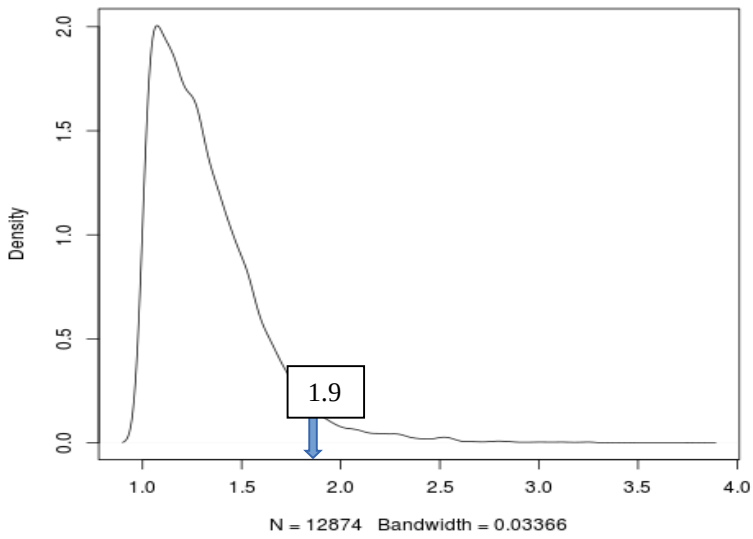


Figure S9 (a).

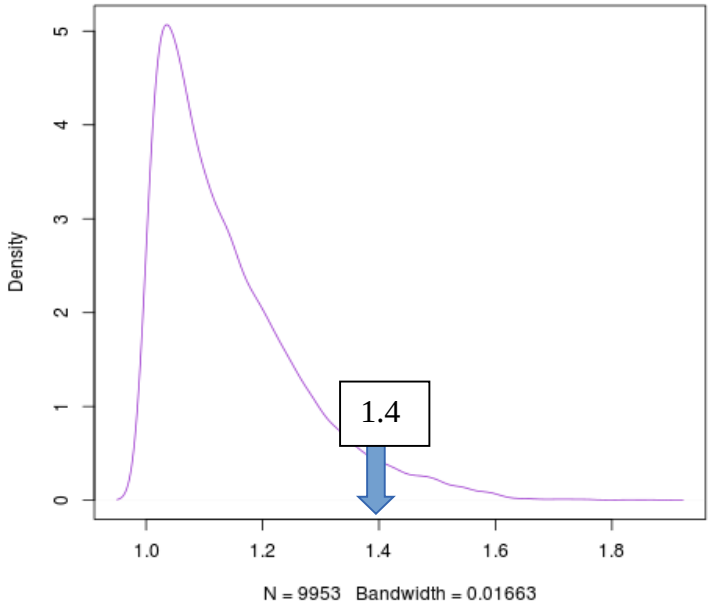


Figure S9 (b).

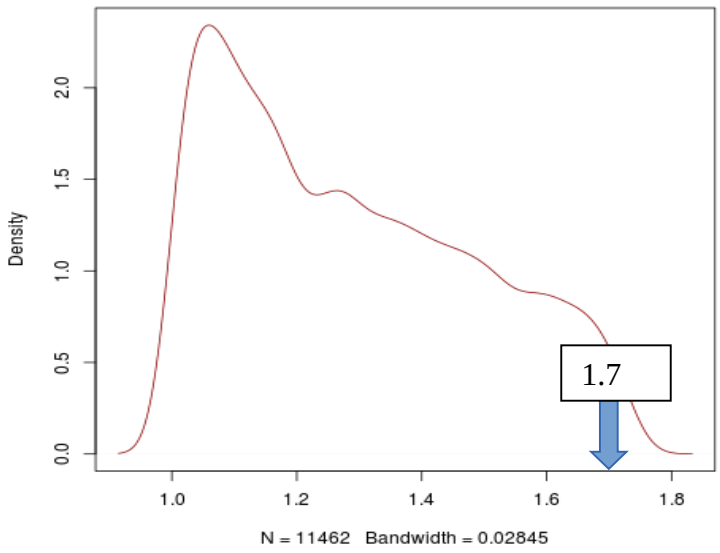


Figure S9 (c).

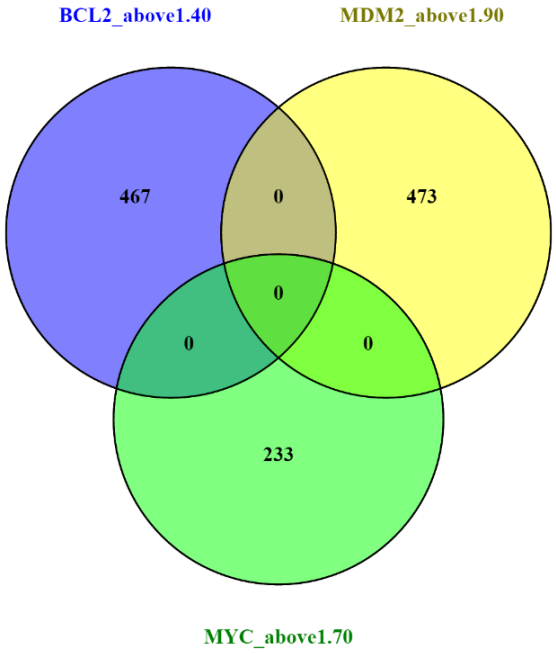


Figure S10.

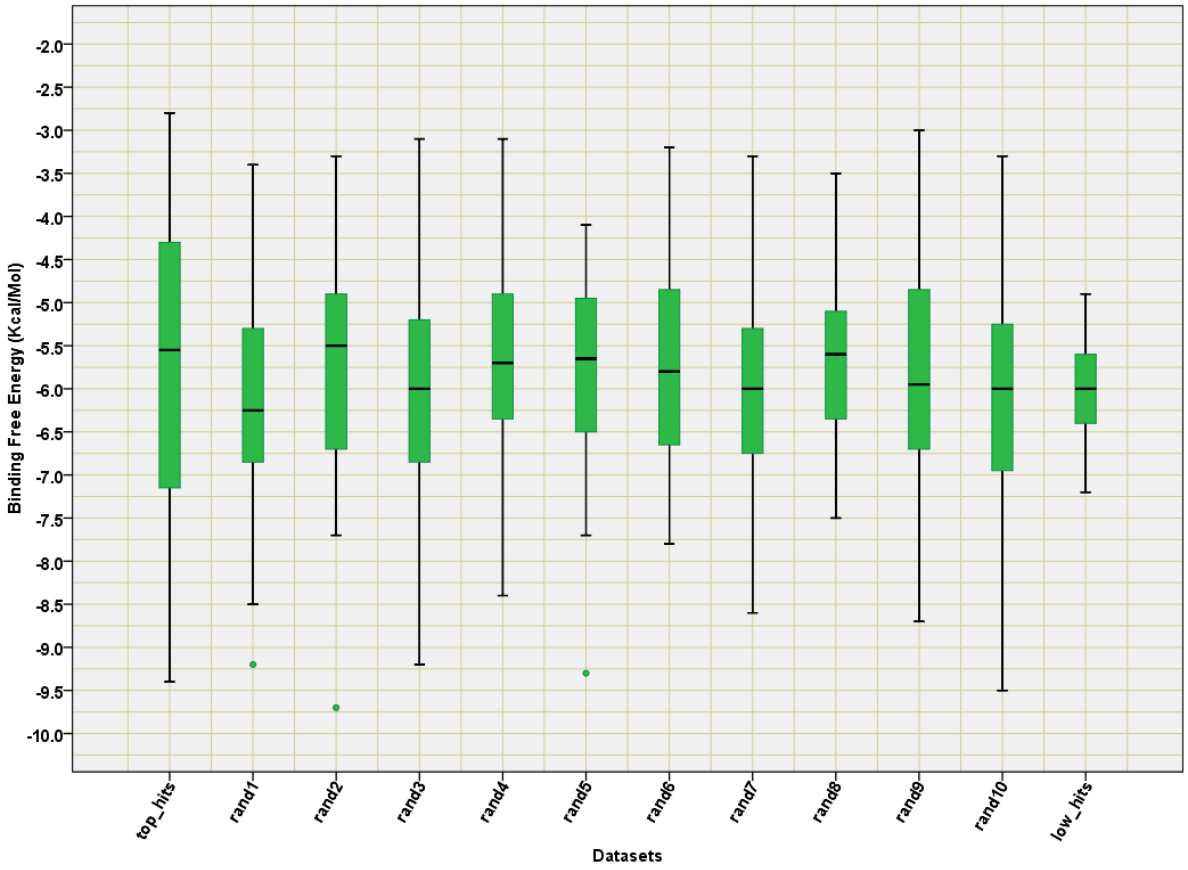


Figure S11 (a).

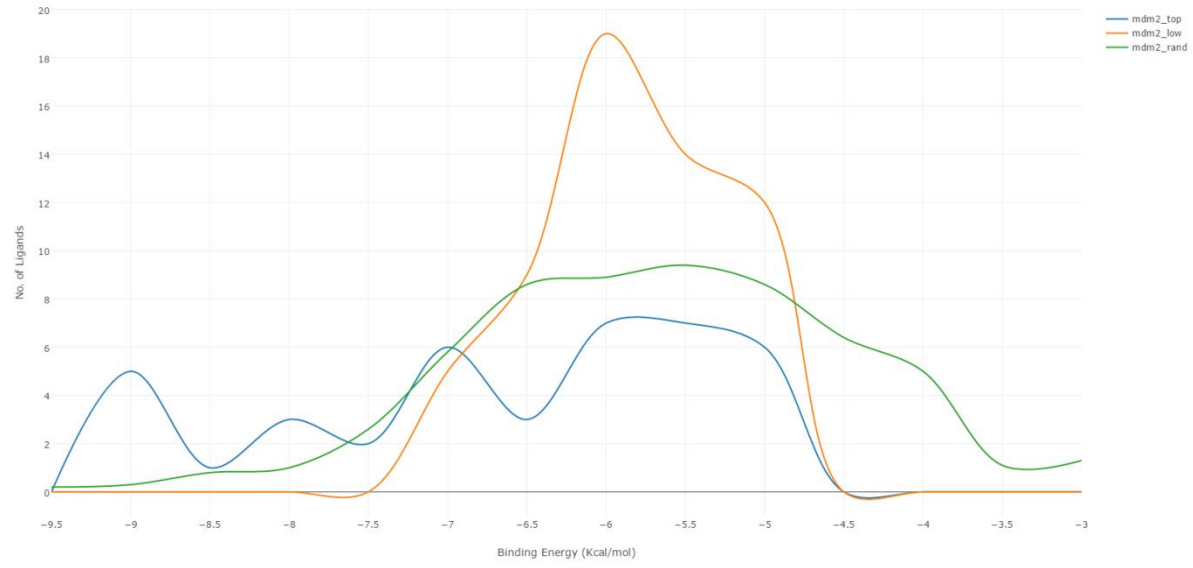


Figure S11 (b).

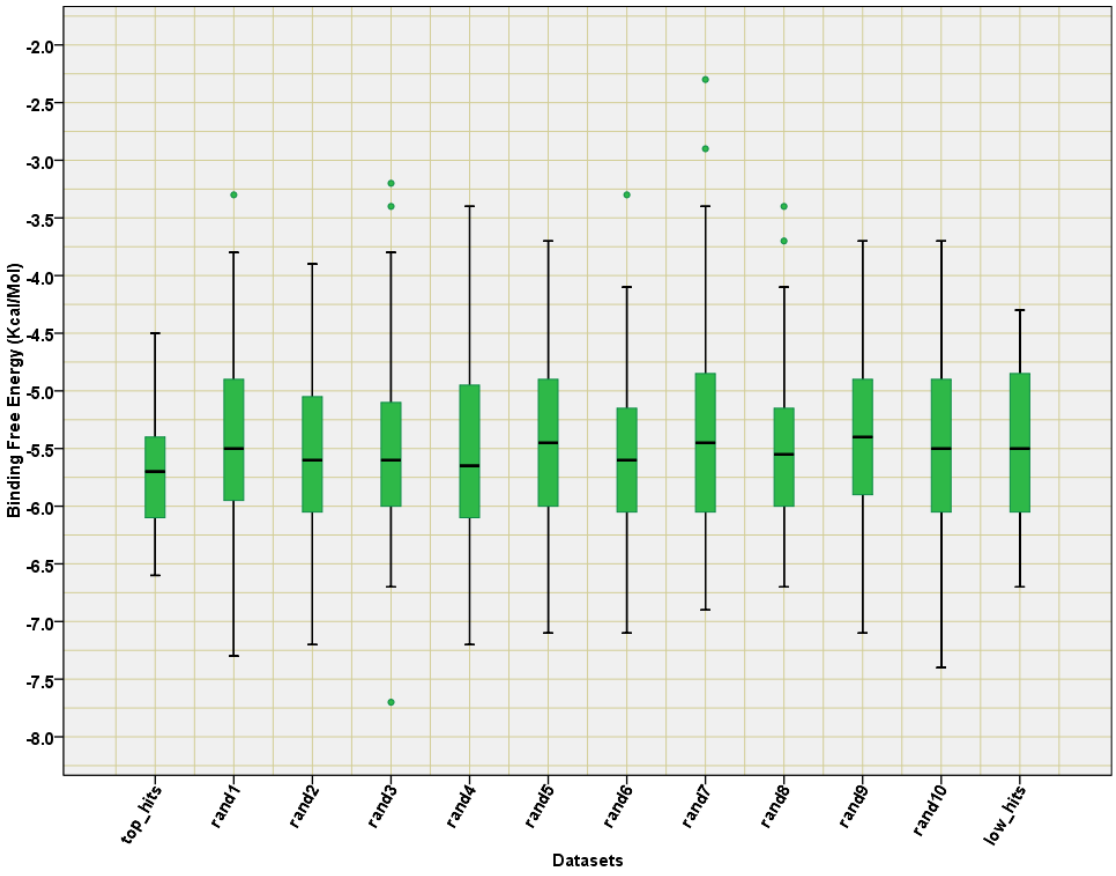


Figure S12 (a).

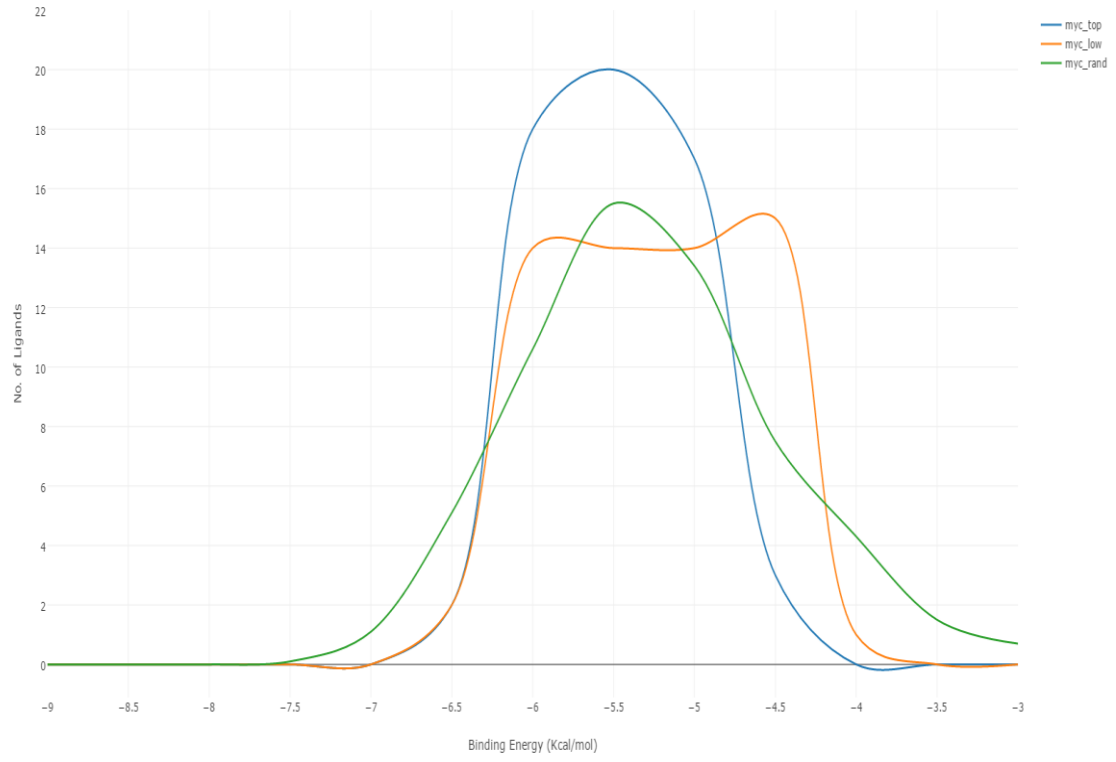


Figure S12 (b).

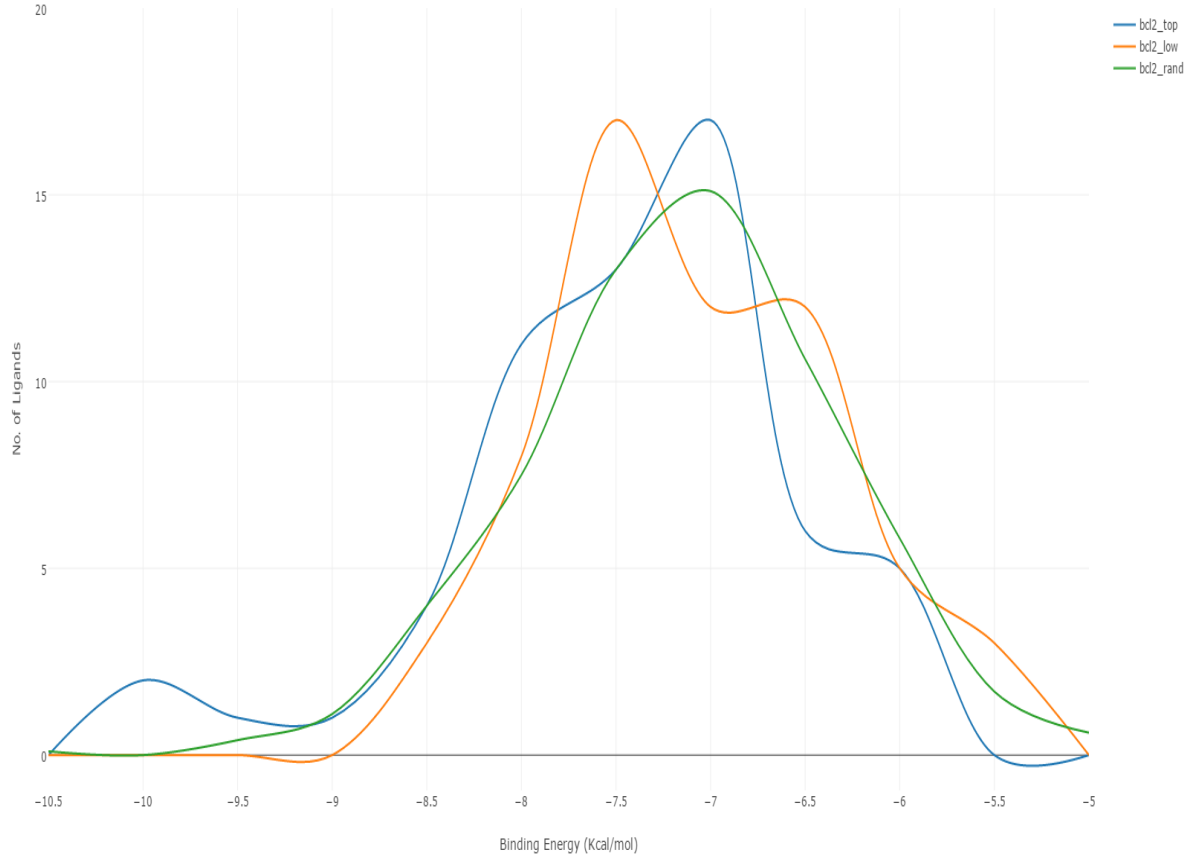


Figure S13.

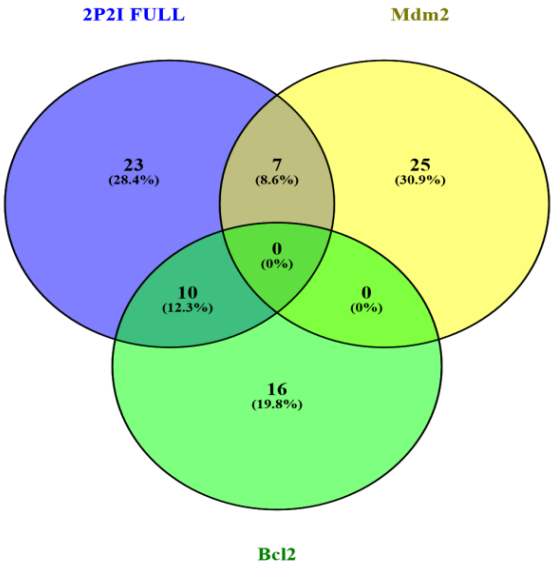


Figure S14 (a).

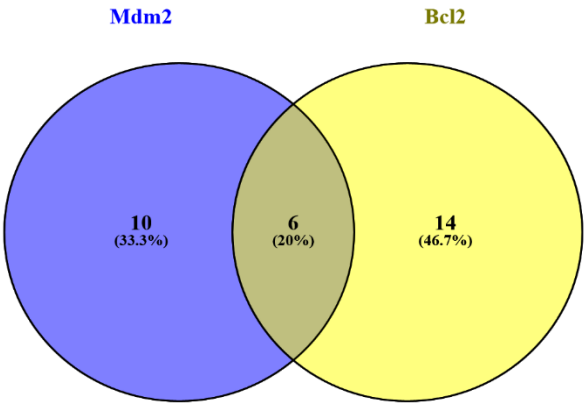


Figure S14 (b).

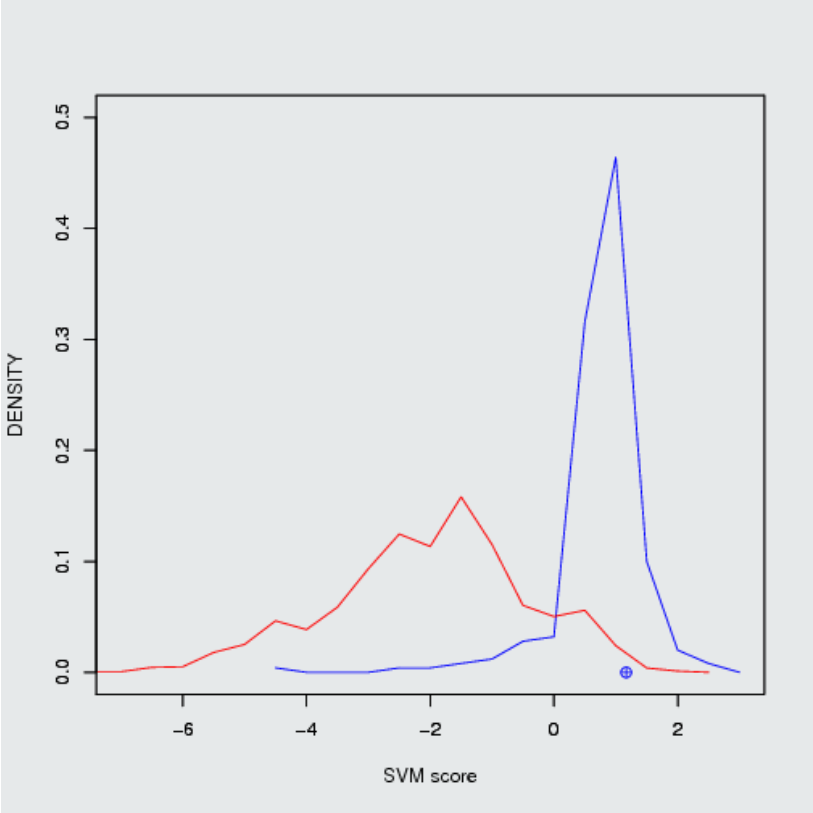


Figure S15 (a).

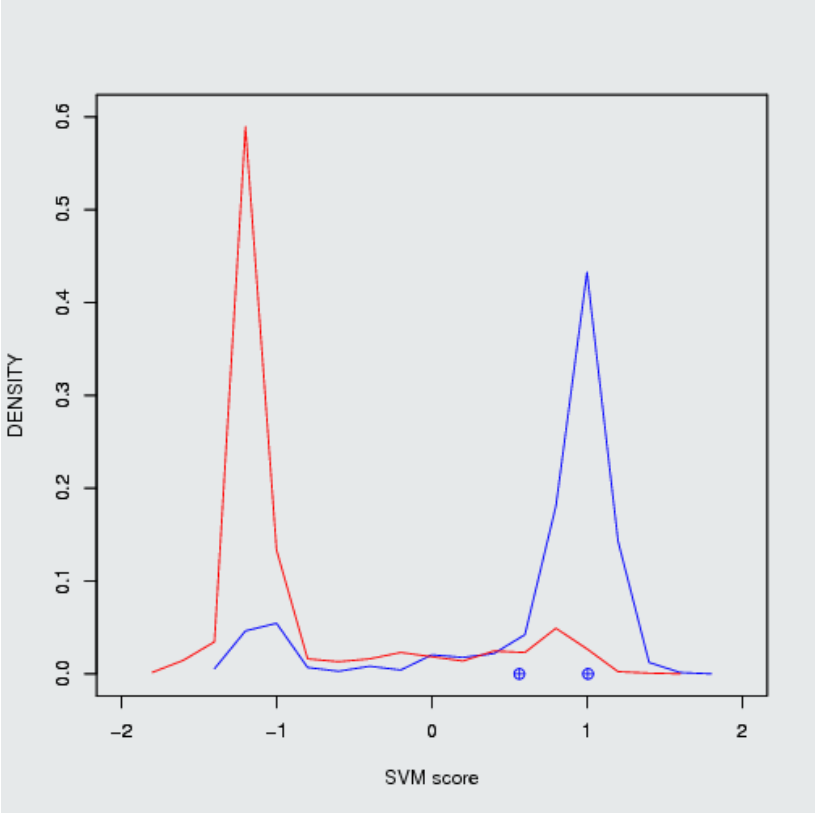


Figure S15 (b).