Table S1: predicted values by scoring functions and experimental pK_d for Set1 and Set2

Set1 Complex ID	Expt. pK_d	Pred. pK_d by QSBAR models	Medusa score	Pred. pK_d (consensus)	Set2 Complex ID	Expt. pK_d	Pred. pK_d by QSBAR models	Medusa score	Pred. pK_d (consensus)
1	3.34	4.06	-17.62	4.01	1	6.4	8.34	-29.74	8.27
2	4.41	4.36	-24.19	4.46	2	5.52	4.90	-25.38	5.32
3	3.28	3.90	-16.86	3.85	3	5.7	5.35	-7.16	5.18
5	8.47	6.59	-36.69	6.77	4	3.13	3.93	-18.14	4.32
6	9.7	4.42	-13.95	4.22	5	7.92	7.49	-57.19	8.34
7	4.4	4.72	-15.77	4.53	6	8.3	7.12	-48.82	7.80
8	4.82	5.30	-18.13	5.11	7	8.4	8.26	-60.52	9.06
9	5	6.46	-28.71	6.42	18	11.8	5.47	NA	NA
13	7.39	4.07	-22.65	4.17	19	4.36	6.68	-34.94	7.05
14	4.59	5.02	-45.51	5.64	20	4.94	5.78	-30.75	6.20
15	4.3	6.27	-36.75	6.49	23	7.12	8.80	-58.78	9.45
17	5.64	6.40	-37.23	6.61	26	6.89	4.97	-21.09	5.26
18	6.57	3.82	-12.90	3.67	27	6.43	4.91	-23.85	5.28
20	7.92	6.71	-29.48	6.66	28	6.82	5.03	-27.03	5.47
21	7.22	8.46	-40.82	8.51	29	7.96	7.95	-53.44	8.61
23	4.8	4.95	-25.58	5.01	34	6.96	5.79	-27.05	6.10
25	7.43	4.93	-21.00	4.86	35	5.22	5.29	-36.47	5.95
26	8.52	7.67	-61.84	8.43	36	5.37	6.79	-27.42	6.93
33	9.54	7.22	-40.87	7.43	39	3.64	4.87	-17.79	5.08
34	10.1	7.89	-66.88	8.76	40	3.51	4.28	-28.80	4.91
39	8	6.61	-21.56	6.35	41	3.49	4.06	-16.16	4.37
41	6.19	5.88	-26.68	5.86	42	9.1	7.71	-49.91	8.32
42	9.36	6.88	-42.64	7.18	43	8.35	7.98	-53.57	8.64
43	9.55	7.01	-46.08	7.40	44	3.57	7.04	-26.42	7.11
46	5.67	6.21	-25.24	6.10	45	5.54	7.23	-30.32	7.37
47	7.12	6.47	-18.63	6.14	47	6.24	5.41	-18.05	5.53
48	7.2	6.63	-17.43	6.24	48	6.4	6.28	-34.17	6.70
49	5.57	5.99	-17.43	5.68	49	6.19	5.02	-24.66	5.40
51	4.72	5.75	-25.84	5.72	53	8.7	7.69	-41.16	8.05
52	9.37	7.39	-44.10	7.67	56	10.39	8.68	-54.09	9.23
53	10.1	7.64	-48.77	8.03	62	8.7	7.66	-43.95	8.10
54	5.24	7.67	-48.93	8.05	63	6.82	6.91	-13.85	6.65
55	6.1	6.32	-36.39	6.52	67	6.12	6.17	-33.80	6.60
56	1	4.17	-16.52	4.07	68	5	5.41	-36.30	6.04
58	1.59	4.17	-18.48	4.13	71	3.59	4.58	-20.65	4.93
59	5.74	7.07	-31.94	7.05	74	5.21	6.13	NA	NA
60	9.52	8.06	-50.67	8.45	77	5.68	7.86	-31.15	7.91
61	5.35	4.38	-10.50	4.08	78	6.8	5.39	-17.33	5.50
63	4.68	5.04	-29.42	5.21	79	5.76	5.70	-17.52	5.76
64	4.79	5.06	-28.08	5.18	81	2.28	5.37	-21.02	5.58
65	5.68	5.11	-50.55	5.87	82	6.66	8.24	-41.53	8.51
66	6.82	5.21	-51.17	5.98	87	6.46	5.48	-21.74	5.69
68	8.7	7.46	-45.86	7.79	88	5.15	5.42	-19.73	5.59
71	7.24	8.91	-35.63	8.75	89	7.7	5.40	-15.64	5.46
73	7.92	8.98	-68.89	9.77	91	10.1	7.71	-59.89	8.60
74	8.3	8.99	-67.26	9.73	92	7.3	4.58	-12.78	4.71
75	9.01	9.52	-56.05	9.87	95	6.41	6.15	-28.10	6.42
77	6.35	4.69	-18.94	4.60	96	5.48	6.03	-29.40	6.36
78	6.03	4.16	-23.72	4.28	97	3.39	4.49	-21.58	4.88

79	5.1	6.03	-26.72	5.99	98	2.47	4.27	-12.77	4.45
81	8.26	6.49	-40.04	6.78	99	5.85	5.56	-18.37	5.67
82	5.22	5.03	-23.82	5.04	101	4.22	5.38	-29.62	5.84
83	4.92	4.98	-28.12	5.11	102	5.91	4.64	-19.53	4.94
86	9.4	6.41	-66.06	7.45	104	7.06	4.33	-18.14	4.65
87	4.16	5.09	-53.05	5.93	105	5.82	4.64	-26.35	5.13
88	5.4	4.35	-22.83	4.41	107	3.01	4.31	-9.97	4.40
91	3.62	6.56	-23.75	6.37	109	5.98	4.93	-23.80	5.30
92	4.94	8.09	-56.48	8.64	110	6.89	5.00	-23.23	5.34
93	3.63	4.93	-20.06	4.83	111	3.4	4.38	-20.51	4.76
94	3.23	4.65	-17.48	4.52	113	6.32	4.90	-21.24	5.21
96	0.05	3.84	-10.21	3.61	114	4.82	4.04	-24.35	4.58
97	3.87	4.16	-12.52	3.95	115	4.57	5.15	-24.97	5.52
98	5.3	6.66	-32.27	6.70	119	3	4.47	-17.46	4.75
99	5.8	5.21	-21.75	5.13	121	2.21	3.74	-15.92	4.10
100	6.3	5.27	-20.07	5.14	122	3.96	5.63	-23.37	5.87
102	8.62	5.71	-25.46	5.68	124	4.68	5.22	-18.62	5.39
103	6.44	4.40	-26.38	4.56	126	9	6.88	-36.98	7.27
104	-0.15	4.18	-8.58	3.86	127	1.82	4.83	-17.05	5.03
105	8.48	8.92	-60.40	9.47	128	3.08	5.02	-15.76	5.15
106	7.01	5.60	-39.40	5.98	129	5.32	5.11	-13.65	5.17
107	4.61	4.64	-33.42	4.97	130	6.17	6.02	-32.96	6.45
108	7.55	4.86	-19.95	4.78	131	5.89	7.06	-24.10	7.06
109	7.96	6.59	-37.65	6.79	132	7.12	7.35	-44.23	7.86
110	6.26	6.97	-33.40	6.99	135	6.52	8.16	-50.26	8.69
111	5.71	4.78	-37.21	5.20	138	2.22	4.24	-22.05	4.68
113	5.61	5.16	-31.11	5.36	139	5.15	5.25	-19.79	5.45
114	5.42	5.18	-26.04	5.23	140	9.29	9.26	-60.77	9.90
116	12	6.09	-32.91	6.22	141	3.64	5.63	-19.37	5.76
117	3.29	3.69	-16.12	3.64	142	6.43	7.15	-25.81	7.18
119	4.05	5.25	-21.98	5.17	147	8.52	8.73	-43.35	8.97
120	2.54	3.90	-8.44	3.61	148	5.77	4.60	-7.01	4.56
121	3.22	5.12	-21.68	5.05	150	4.86	6.79	-32.24	7.07
122	2.27	5.08	-8.20	4.63	151	6	4.98	-28.31	5.47
123	3.19	5.12	-17.26	4.93	152	8.55	8.11	-50.07	8.64
124	6.85	6.36	-27.32	6.29	153	8.22	7.34	-44.54	7.86
126	3.1	5.56	-24.91	5.53	154	6.92	7.66	-29.52	7.70
127	6.6	6.35	-26.57	6.27	155	6.64	7.22	-30.81	7.38
128	3.7	5.15	-17.90	4.97	160	5.17	4.28	-34.23	5.05
129	2.46	4.19	-25.08	4.34	167	6.24	7.92	-36.63	8.11
130	13	6.05	-36.24	6.28	168	7.59	7.71	-58.47	8.56
131	4.74	5.25	-23.76	5.22	169	8.21	5.95	-26.51	6.22
132	7.22	5.00	-20.76	4.92	170	3.96	4.80	-17.87	5.03
133	4.7	5.71	-44.99	6.24	171	6.14	6.49	-13.35	6.29
134	4.85	4.68	-23.80	4.73	172	6.68	5.83	-29.61	6.20
136	6.72	4.15	-7.83	3.81	173	7.15	5.78	-33.12	6.26
137	4.37	4.42	-6.69	4.01	174	6.57	5.86	-26.31	6.13
139	4.23	4.55	-11.79	4.27	175	8.52	6.75	-33.78	7.07
141	11.3	7.17	-54.74	7.79	176	2.92	4.40	-17.03	4.68
143	9	8.02	-61.28	8.72	178	8.15	8.12	-55.50	8.80
144	6.53	6.46	-39.83	6.74	180	5.39	4.64	-31.60	5.28
145	5.74	4.22	-18.88	4.19	182	3.8	4.87	-19.64	5.14
147	6.31	5.63	-14.23	5.28	184	1.4	5.36	-10.60	5.29

148	4.61	4.62	-18.72	4.53	185	1.72	3.99	-10.93	4.17
149	6.29	6.90	-28.15	6.79	187	11.4	8.03	-44.87	8.43
150	5.68	5.06	-34.73	5.37	188	12.1	7.91	-44.82	8.34
151	7.44	5.80	-31.15	5.91	190	7.1	8.26	-59.29	9.03
152	6.33	5.87	-29.65	5.94	192	6.68	6.31	-29.34	6.59
153	6.68	5.67	-30.02	5.77	193	7.05	7.42	-36.74	7.71
154	5.19	3.77	8.41	3.01	194	7.82	7.13	-39.78	7.56
155	7.48	8.17	-44.35	8.36	195	9	7.24	-41.24	7.68
156	7.28	7.58	-45.89	7.89	196	6.42	4.86	-26.23	5.32
157	7.3	9.01	-40.45	8.98	201	3.7	4.22	-12.67	4.41
158	10.2	8.79	-39.14	8.75	202	3.84	4.43	-9.89	4.51
159	10.44	9.02	-46.82	9.17	204	8.85	8.38	-63.38	9.24
160	10.85	9.13	-48.61	9.31	205	8.36	8.01	-65.20	8.99
161	10.57	8.88	-43.21	8.95	207	9.7	8.37	-61.99	9.19
162	9.15	8.43	-61.02	9.07	208	9.4	8.12	-57.37	8.86
163	4.21	4.35	-28.67	4.58	209	8.49	8.22	-63.47	9.11
164	6.11	7.62	-49.29	8.02	210	8.92	8.77	-65.69	9.63
167	4	3.53	-12.39	3.40	211	10	8.33	-66.10	9.28
168	8.64	6.26	-38.95	6.54	213	5.08	5.39	-10.55	5.31
169	9.36	7.94	-56.05	8.49	214	3.05	4.74	-24.34	5.16
170	6.15	4.88	-41.41	5.41	215	5.96	5.75	-20.44	5.88
173	7.79	4.05	-9.81	3.77	217	4.28	5.19	-27.47	5.61
174	5.57	5.12	-22.58	5.08	218	4.28	5.87	-29.11	6.23
175	2.72	4.39	-6.68	3.99	220	6.42	5.76	-27.67	6.09
177	8.4	7.31	-31.30	7.23	222	8.12	7.13	-37.13	7.48
178	6.81	7.25	-32.73	7.23	223	6.46	5.13	-22.47	5.43
179	4.68	4.97	-16.77	4.78	224	9.04	8.05	-37.11	8.23
180	3.41	4.06	-10.20	3.80	225	7.96	7.63	-41.82	8.03
181	5.06	4.49	-22.27	4.52	226	2.06	3.89	-7.77	4.00
182	7.48	5.62	-40.85	6.04	227	1.84	3.79	-10.64	4.00
183	5.9	5.79	NA	NA	230	6.82	4.72	-23.28	5.12
184	6.66	5.60	-40.51	6.01	232	6.74	5.50	-21.96	5.72
187	5.09	5.76	-55.00	6.57	233	6.4	5.18	-16.07	5.29
189	8.74	8.65	-59.11	9.21	234	4.3	4.26	-24.43	4.77
191	3.02	3.67	-12.89	3.54	235	4.57	5.02	-9.41	4.97
193	6.72	5.40	-23.99	5.36	237	4.37	6.06	-36.53	6.58
194	3.82	6.74	-22.15	6.48	247	10.52	7.36	-53.33	8.12
195	8.52	6.71	-37.62	6.89	249	6.54	6.43	NA	NA
196	9.4	7.16	-40.85	7.38	251	7.8	6.32	-17.58	6.27
197	4.96	5.10	-29.52	5.26	257	4	4.94	-13.02	5.01
198	2.68	4.84	-4.54	4.31	260	7.35	7.92	-53.34	8.58
199	7.6	5.46	-28.40	5.54	261	2.1	4.48	-8.28	4.49
200	7.89	5.92	-29.39	5.97	262	5.59	4.49	-8.43	4.51
201	3.98	5.07	-13.36	4.76	266	8.16	8.11	-39.86	8.37
203	7.7	7.90	-33.42	7.81	269	9	5.47	-27.05	5.83
204	5.57	4.52	-24.25	4.60	270	5.85	5.20	-8.89	5.10
206	6.92	6.06	-13.75	5.65	271	5.85	5.09	-10.79	5.07
207	8.7	5.50	-23.45	5.44	272	6.6	5.36	-20.33	5.55
208	8.15	4.96	-13.17	4.66	273	7.19	5.27	-21.67	5.52
210	5.48	4.26	-17.76	4.19	274	7.24	5.49	-11.73	5.42
212	2	3.94	-10.77	3.71	276	5.35	4.40	-19.14	4.74
213	3.35	4.00	-9.24	3.71	277	5.18	4.73	-4.56	4.60
214	3.11	4.04	-7.72	3.71	278	7.26	8.26	-48.93	8.74

215	5.64	5.73	-39.52	6.09	281	2.99	4.80	-21.33	5.12
216	7.87	7.50	-39.64	7.64	283	2.62	3.82	-24.94	4.42
217	7.29	7.19	-39.93	7.38	284	2.06	3.82	-25.92	4.44
218	7.84	7.56	-47.80	7.93	286	5.62	5.77	-19.93	5.88
222	7.8	5.70	-10.06	5.23	287	3.99	4.04	-18.17	4.41
225	5.48	4.87	-30.30	5.08	290	5.37	5.48	-18.96	5.62
226	4.15	4.52	-5.59	4.06	291	4.26	5.46	-25.11	5.77
227	8.36	8.00	-55.22	8.52	292	5.82	6.03	-14.70	5.95
228	6	5.31	-18.91	5.13	293	7.42	6.83	-27.71	6.97
229	7.37	5.84	-21.06	5.66	294	3.94	4.16	-14.12	4.39
230	8	7.32	-49.76	7.78	296	7.57	7.21	-41.72	7.68
232	6.7	5.31	-18.23	5.12	297	7.58	7.56	-45.42	8.06
233	5.55	6.53	-27.06	6.43					
234	6.24	6.08	-33.82	6.23					
235	8.7	7.28	-55.36	7.91					
237	6.63	5.49	-11.55	5.09					
238	5.48	5.03	-7.07	4.55					
239	3.49	4.94	-2.58	4.34					
240	7.68	7.65	-48.29	8.02					
241	7.64	5.67	-18.86	5.45					

Table S2: under-predicted complexes of scoring functions
(*: # of ill-predicted complexes in the family/ # of total complexes in the family)

QSBAR models			
Set ID	Complex ID	Family name	Ratio*
1	6	GLUTAMATE CARBOXYPEPTIDASE 2	1/1
1	13	Fumarylacetoacetase	1/1
1	18	TRAP-T family sorbitol/mannitol transporter, periplasmic binding protein, SmoM	1/1
1	25	Putative fructose-1,6-bisphosphate aldolase	1/1
1	33	Estrogen receptor	1/4
1	34	Vitamin D3 receptor	1/1
1	42	Estrogen receptor beta	2/2
1	43	ESTROGEN RECEPTOR BETA	2/2
1	53	Coagulation factor X (EC 3.4.21.6)(Stuart-Prower factor)	3/4
1	86	Enoyl-[acyl-carrier-protein] reductase [NADH]	1/1
1	102	D7R4 Protein	1/1
1	103	Fructose-1,6-bisphosphatase 1	1/1
1	108	Sialic acid-binding periplasmic protein siaP	1/1
1	116	CORE-STREPTAVIDIN	1/1
1	130	BIOTIN BINDING PROTEIN A	1/1
1	132	N-acetyl-beta-D-glucosaminidase	1/1
1	136	FUCOSE-BINDING LECTIN PA-IIL	1/4
1	141	Coagulation factor X	3/4
1	168	Thiamine-binding periplasmic protein	1/1
1	173	Glutamate [NMDA] receptor subunit 3B	1/1
1	196	ACTIVATED FACTOR XA HEAVY CHAIN	3/4
1	199	Tyrosine-protein phosphatase non-receptor type 1	1/9
1	207	Lipocalin	1/1
1	208	Lipocalin	1/1
1	222	Carbonic anhydrase 13	1/1
2	18	ORNITHINE TRANSCARBAMOYLASE	1/1
2	26	BETA-1,4-XYLANASE	3/3
2	27	BETA-1,4-XYLANASE	3/3

2	28	BETA-1,4-XYLANASE	3/3
2	89	tRNA guanine transglycosylase	1/6
2	91	Progesterone receptor	1/1
2	92	osmoprotection protein (proX)	1/1
2	104	Uracil-DNA Glycosylase	1/1
2	110	BETA-GLUCOSIDASE A	2/2
2	126	Catalytic Antibody Fab 34E4 Light chain	1/1
2	169	IAG-nucleoside hydrolase	1/1
2	175	Cell division protein kinase 2	1/2
2	187	Protease	2/27
2	188	Protease	2/27
2	195	COAGULATION FACTOR X	1/7
2	196	BETA-GLUCOSIDASE A	2/2
2	230	FimH protein	1/1
2	247	ADAM 17	1/2
2	269	Fab 9B1, Light chain	1/1
2	273	Glutamate receptor, ionotropic kainate 2	1/4
2	274	Glutamate receptor, ionotropic kainate 1	1/2

MedusaScore

Set ID	Complex ID	Family name	Ratio*
1	6	GLUTAMATE CARBOXYPEPTIDASE 2	1/1
1	25	Putative fructose-1,6-bisphosphate aldolase	1/1
1	33	Estrogen receptor	2/4
1	39	ADAM 17	2/2
1	42	Estrogen receptor beta	2/2
1	43	ESTROGEN RECEPTOR BETA	2/2
1	48	Carbonic anhydrase 2	3/6
1	52	Factor Xa	4/4
1	53	Coagulation factor X (EC 3.4.21.6)(Stuart-Prower factor)	4/4
1	102	D7R4 Protein	1/1
1	108	Sialic acid-binding periplasmic protein siaP	1/1
1	116	CORE-STREPTAVIDIN	1/1
1	130	BIOTIN BINDING PROTEIN A	1/1
1	136	FUCOSE-BINDING LECTIN PA-IIL	1/4
1	141	Coagulation factor X	4/4
1	154	Metallo-beta-lactamase L1	1/1
1	158	Protease	7/27
1	159	Protease	7/27
1	160	Protease	7/27
1	161	Protease	7/27
1	173	Glutamate [NMDA] receptor subunit 3B	1/1
1	177	COAGULATION FACTOR X	2/7
1	196	ACTIVATED FACTOR XA HEAVY CHAIN	4/4
1	206	Carbonic anhydrase 2	3/6
1	207	Lipocalin	1/1
1	208	Lipocalin	1/1
1	222	Carbonic anhydrase 13	1/1
1	229	Glutamate receptor 3	1/1
1	237	Transporter	1/3
1	241	Glutamate receptor 4	2/2
1	242	Glutamate receptor 4	2/2
2	3	PUTRESCINE-BINDING PROTEIN	1/1
2	26	BETA-1,4-XYLANASE	1/3

2	56	Protease	7/27
2	63	auxin-binding protein 1	1/1
2	78	Glutamate receptor 2	4/4
2	89	tRNA guanine transglycosylase	1/6
2	92	osmoprotection protein (proX)	1/1
2	104	Uracil-DNA Glycosylase	1/1
2	126	Catalytic Antibody Fab 34E4 Light chain	1/1
2	148	PSEUDOMONAS AERUGINOSA LECTIN II	1/4
2	169	IAG-nucleoside hydrolase	1/1
2	171	S-ribosylhomocysteine lyase	1/1
2	175	Cell division protein kinase 2	1/2
2	187	Protease	7/27
2	188	Protease	7/27
2	195	COAGULATION FACTOR X	2/7
2	224	ESTRADIOL RECEPTOR	2/4
2	233	LEUCINE-SPECIFIC BINDING PROTEIN	1/1
2	247	ADAM 17	2/2
2	251	Carbonic anhydrase 2	3/6
2	262	PROTEIN (UREASE (CHAIN A))	1/1
2	269	Fab 9B1, Light chain	1/1
2	270	Glutamate Receptor 6	4/4
2	271	Glutamate receptor, ionotropic kainate 2 precursor	4/4
2	273	Glutamate receptor, ionotropic kainate 2	4/4
2	274	Glutamate receptor, ionotropic kainate 1	1/1
Consensus			
Set ID	Complex ID	Family name	Ratio*
1	6	GLUTAMATE CARBOXYPEPTIDASE 2	1/1
1	13	Fumarylacetoacetase	1/1
1	18	TRAP-T family sorbitol/mannitol transporter, periplasmic binding protein, SmoM	1/1
1	25	Putative fructose-1,6-bisphosphate aldolase	1/1
1	33	Estrogen receptor	1/4
1	42	Estrogen receptor beta	2/2
1	43	ESTROGEN RECEPTOR BETA	2/2
1	53	Coagulation factor X (EC 3.4.21.6)(Stuart-Prower factor)	3/4
1	86	Enoyl-[acyl-carrier-protein] reductase [NADH]	1/1
1	102	D7R4 Protein	1/1
1	108	Sialic acid-binding periplasmic protein siaP	1/1
1	116	CORE-STREPTAVIDIN	1/1
1	130	BIOTIN BINDING PROTEIN A	1/1
1	132	N-acetyl-beta-D-glucosaminidase	1/1
1	136	FUCOSE-BINDING LECTIN PA-IIL	1/4
1	141	Coagulation factor X	3/4
1	154	Metallo-beta-lactamase L1	1/1
1	168	Thiamine-binding periplasmic protein	1/1
1	173	Glutamate [NMDA] receptor subunit 3B	1/1
1	196	ACTIVATED FACTOR XA HEAVY CHAIN	3/4
1	199	Tyrosine-protein phosphatase non-receptor type 1	1/9
1	207	Lipocalin	1/1
1	208	Lipocalin	1/1
1	222	Carbonic anhydrase 13	1/1
1	241	Glutamate receptor 4	1/2
2	26	BETA-1,4-XYLANASE	3/3
2	27	BETA-1,4-XYLANASE	3/3

2	28	BETA-1,4-XYLANASE	3/3
2	78	Glutamate receptor 2	1/4
2	89	tRNA guanine transglycosylase	1/6
2	91	Progesterone receptor	1/1
2	92	osmoprotection protein (proX)	1/1
2	104	Uracil-DNA Glycosylase	1/1
2	110	BETA-GLUCOSIDASE A	2/2
2	113	ENDO-1,4-BETA-XYLANASE A	1/1
2	126	Catalytic Antibody Fab 34E4 Light chain	1/1
2	148	PSEUDOMONAS AERUGINOSA LECTIN II	1/4
2	169	IAG-nucleoside hydrolase	1/1
2	175	Cell division protein kinase 2	1/2
2	187	Protease	2/27
2	188	Protease	2/27
2	195	COAGULATION FACTOR X	1/7
2	196	BETA-GLUCOSIDASE A	2/2
2	230	FimH protein	1/1
2	233	LEUCINE-SPECIFIC BINDING PROTEIN	1/2
2	247	ADAM 17	1/2
2	251	Carbonic anhydrase 2	1/6
2	262	PROTEIN (UREASE (CHAIN A))	1/1
2	269	Fab 9B1, Light chain	1/1
2	273	Glutamate receptor, ionotropic kainate 2	1/4
2	274	Glutamate receptor, ionotropic kainate 1	1/2

Table S3: over-predicted complexes of scoring functions
(*: # of ill-predicted complexes in the family/ # of total complexes in the family)

QSBAR models			
Set ID	Complex ID	Family name	Ratio*
1	9	Endoglycoceramidase II	1/1
1	15	TRYPTOPHAN SYNTHASE ALPHA CHAIN	1/1
1	21	Candidapepsin-3	1/1
1	54	GLUTAMATE RACEMASE	1/1
1	56	hypothetical protein slr0953	2/2
1	58	hypothetical protein slr0953	2/2
1	59	Soluble acetylcholine receptor	1/3
1	91	UDP-N-ACETYLMURAMOYLALANINE--D-GLUTAMATE LIGASE	1/1
1	92	Proto-oncogene tyrosine-protein kinase Src	1/1
1	94	Lysozyme	1/2
1	96	Ricin (EC 3.2.2.22)	2/2
1	98	Cysteine synthase A	1/1
1	104	Ricin A chain (EC 3.2.2.22)	2/2
1	121	Aspartate aminotransferase	2/4
1	122	TRYPSINOGEN	2/2
1	123	2-hydroxy-6-oxo-7-methylocta-2,4-dienoate hydrolase	1/2
1	126	EPOXIDE HYDROLASE	1/1
1	128	Trypsin	2/2
1	129	fructan 1-exohydrolase IIa	1/1
1	157	Protease	2/27
1	164	HIV-1 PROTEASE	2/27

1	175	Phosphoenolpyruvate carboxykinase, cytosolic [GTP]	1/1
1	194	CELLULAR TUMOR ANTIGEN P53	1/1
1	198	Glutamyl-Q tRNA(Asp) synthetase	1/1
1	212	Nicotinate-nucleotide pyrophosphorylase	1/3
1	239	Transporter	1/3
2	1	GLUTATHIONE S-TRANSFERASE P1-1	1/1
2	19	CELLOBIOHYDROLASE I	1/1
2	23	RETINOIC ACID RECEPTOR GAMMA-1	1/1
2	36	ACETYLCHOLINESTERASE	1/4
2	44	EXOGLUCANASE I	1/2
2	45	SERUM ALBUMIN	1/1
2	77	pheromone binding protein	1/1
2	81	Alpha-mannosidase II	1/3
2	82	Cell division protein kinase 2	1/2
2	98	Aspartate aminotransferase	2/4
2	122	Endoplasmic reticulum mannosyl-oligosaccharide 1,2-alpha-mannosidase	1/1
2	127	Glutamate [NMDA] receptor subunit zeta 1	2/3
2	128	Glutamate [NMDA] receptor subunit zeta 1	2/3
2	135	KES1 protein	1/2
2	138	ARAC	1/1
2	141	Tyrosine-protein phosphatase, non-receptor type 1	1/9
2	150	SERINE/THREONINE-PROTEIN KINASE CHK1	1/1
2	167	Estrogen receptor	1/1
2	184	Beta-lactamase	2/2
2	185	Beta-lactamase	2/2
2	214	N-ACETYL-NEURAMINATE LYASE	1/1
2	218	N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERASE	1/2
2	226	MANNOSE-BINDING PROTEIN-C	2/2
2	227	MANNOSE-BINDING PROTEIN-C	2/2
2	237	chitinase	1/1
2	261	Macrophage metalloelastase	1/1
2	281	Major Urinary Protein	1/1
2	284	beta-amylase	1/2
Medusascore			
Set ID	Complex ID	Family name	Ratio*
1	1	GALECTIN-1	1/1
1	14	Alpha-2,3/2,6-sialyltransferase/sialidase	2/2
1	15	TRYPTOPHAN SYNTHASE ALPHA CHAIN	1/1
1	54	GLUTAMATE RACEMASE	1/1
1	56	hypothetical protein slr0953	2/2
1	58	hypothetical protein slr0953	2/2
1	65	6,7-DIMETHYL-8-RIBITYLLUMAZINE SYNTHASE	1/2
1	87	Alpha-2,3/2,6-sialyltransferase/sialidase	2/2
1	91	UDP-N-ACETYLMURAMOYLALANINE--D-GLUTAMATE LIGASE	1/1
1	92	Proto-oncogene tyrosine-protein kinase Src	1/1
1	94	Lysozyme	1/1
1	96	Ricin (EC 3.2.2.22)	2/2
1	104	Ricin A chain (EC 3.2.2.22)	2/2
1	107	5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-1	1/1
1	120	meta-Cleavage product hydrolase	2/2
1	121	Aspartate aminotransferase	3/4
1	122	TRYPSINOGEN	1/2
1	123	2-hydroxy-6-oxo-7-methylocta-2,4-dienoate hydrolase	2/2

1	126	EPOXIDE HYDROLASE	1/1
1	129	fructan 1-exohydrolase IIa	1/1
1	133	Probable inorganic polyphosphate/ATP-NAD kinase 1	1/1
1	163	Maltase-glucoamylase, intestinal	1/1
1	187	ALANINE DEHYDROGENASE	1/1
1	212	Nicotinate-nucleotide pyrophosphorylase	1/3
2	4	LECTIN	1/5
2	19	CELLOBIOHYDROLASE I	1/1
2	23	RETINOIC ACID RECEPTOR GAMMA-1	1/1
2	40	ERYTHRINA CRISTA-GALLI LECTIN	1/5
2	44	EXOGLUCANASE I	1/2
2	68	MTA/SAH nucleosidase	1/2
2	71	Ribosome-inactivating protein alpha-trichosanthin	1/1
2	81	Alpha-mannosidase II	1/3
2	97	Aspartate aminotransferase	3/4
2	98	Aspartate aminotransferase	3/4
2	101	ADP-dependent glucokinase	1/1
2	111	MAN5A	1/1
2	119	Agglutinin beta-3 chain	1/2
2	121	Hypothetical protein yiiL	1/1
2	127	Glutamate [NMDA] receptor subunit zeta 1	2/3
2	128	Glutamate [NMDA] receptor subunit zeta 1	2/3
2	135	KES1 protein	1/2
2	138	ARAC	1/1
2	176	N5-carboxyaminoimidazole ribonucleotide mutase	1/1
2	184	Beta-lactamase	2/2
2	185	Beta-lactamase	2/2
2	190	Renin	1/1
2	214	N-ACETYL-NEURAMINATE LYASE	1/1
2	217	N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERASE	2/2
2	218	N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERASE	2/2
2	226	MANNOSE-BINDING PROTEIN-C	2/2
2	227	MANNOSE-BINDING PROTEIN-C	2/2
2	237	chitinase	1/1
2	261	Macrophage metalloelastase	1/1
2	281	Major Urinary Protein	1/1
2	283	beta-amylase	2/2
2	284	beta-amylase	2/2
Consensus			
Set ID	Complex ID	Family name	Ratio*
1	9	Endoglycoceramidase II	1/1
1	15	TRYPTOPHAN SYNTHASE ALPHA CHAIN	1/1
1	54	GLUTAMATE RACEMASE	1/1
1	56	hypothetical protein slr0953	2/2
1	58	hypothetical protein slr0953	2/2
1	73	POL PROTEIN	3/27
1	87	Alpha-2,3/2,6-sialyltransferase/sialidase	1/2
1	91	UDP-N-ACETYLMURAMOYLALANINE--D-GLUTAMATE LIGASE	1/1
1	92	Proto-oncogene tyrosine-protein kinase Src	1/1
1	96	Ricin (EC 3.2.2.22)	2/2
1	104	Ricin A chain (EC 3.2.2.22)	2/2
1	121	Aspartate aminotransferase	2/4
1	122	TRYPSINOGEN	1/2

1	123	2-hydroxy-6-oxo-7-methylocta-2,4-dienoate hydrolase	1/2
1	126	EPOXIDE HYDROLASE	1/1
1	129	fructan 1-exohydrolase IIa	1/1
1	133	Probable inorganic polyphosphate/ATP-NAD kinase 1	1/1
1	157	Protease	3/27
1	164	HIV-1 PROTEASE	3/27
1	187	ALANINE DEHYDROGENASE	1/1
1	194	CELLULAR TUMOR ANTIGEN P53	1/1
1	198	Glutamyl-Q tRNA(Asp) synthetase	1/1
1	212	Nicotinate-nucleotide pyrophosphorylase	1/3
2	1	GLUTATHIONE S-TRANSFERASE P1-1	1/1
2	19	CELLOBIOHYDROLASE I	1/1
2	23	RETINOIC ACID RECEPTOR GAMMA-1	1/1
2	44	EXOGLUCANASE I	1/2
2	45	SERUM ALBUMIN	1/1
2	77	pheromone binding protein	1/1
2	81	Alpha-mannosidase II	1/3
2	82	Cell division protein kinase 2	1/2
2	98	Aspartate aminotransferase	2/4
2	121	Hypothetical protein yiiL	1/1
2	122	Endoplasmic reticulum mannosyl-oligosaccharide 1,2-alpha-mannosidase	1/1
2	127	Glutamate [NMDA] receptor subunit zeta 1	2/3
2	128	Glutamate [NMDA] receptor subunit zeta 1	2/3
2	135	KES1 protein	1/2
2	138	ARAC	1/1
2	141	Tyrosine-protein phosphatase, non-receptor type 1	1/9
2	150	SERINE/THREONINE-PROTEIN KINASE CHK1	1/1
2	167	Estrogen receptor	1/1
2	184	Beta-lactamase	2/2
2	185	Beta-lactamase	2/2
2	190	Renin	1/1
2	214	N-ACETYL-NEURAMINATE LYASE	1/1
2	218	N-ACETYLLACTOSAMINIDE ALPHA-1,3-GALACTOSYLTRANSFERASE	1/2
2	226	MANNOSE-BINDING PROTEIN-C	2/2
2	227	MANNOSE-BINDING PROTEIN-C	2/2
2	237	chitinase	1/1
2	261	Macrophage metalloelastase	1/1
2	281	Major Urinary Protein	1/1
2	283	beta-amylase	2/2
2	284	beta-amylase	2/2

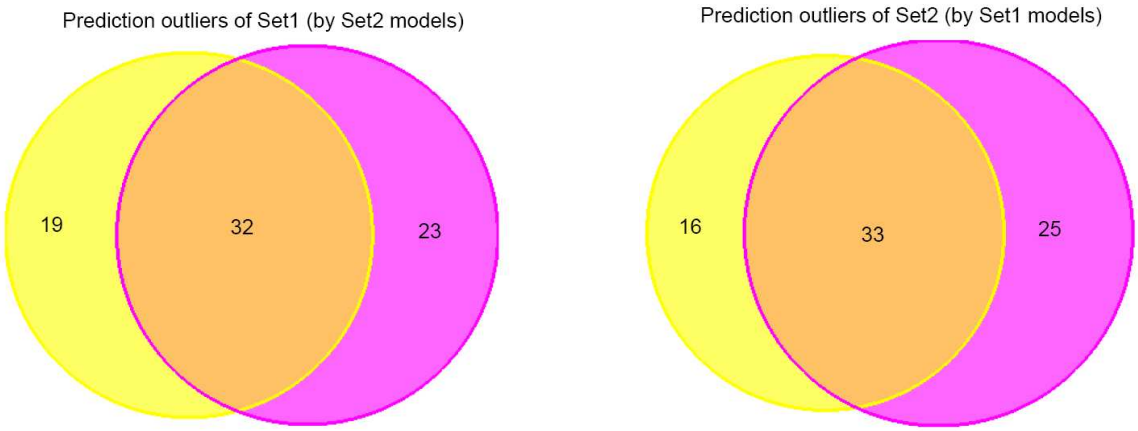

Figure S1: Venn diagrams of prediction outliers by either Set1 or Set2 QSBAR models. (yellow: prediction outliers by QSBAR models; Magenta: prediction outliers by MedusaScore)