Figure S1: Distributions of MCC and ACC for each window size (SVM parameters: gamma = 0.001, cost factor = 5, 5-fold cross validation) using the NR95 dataset.

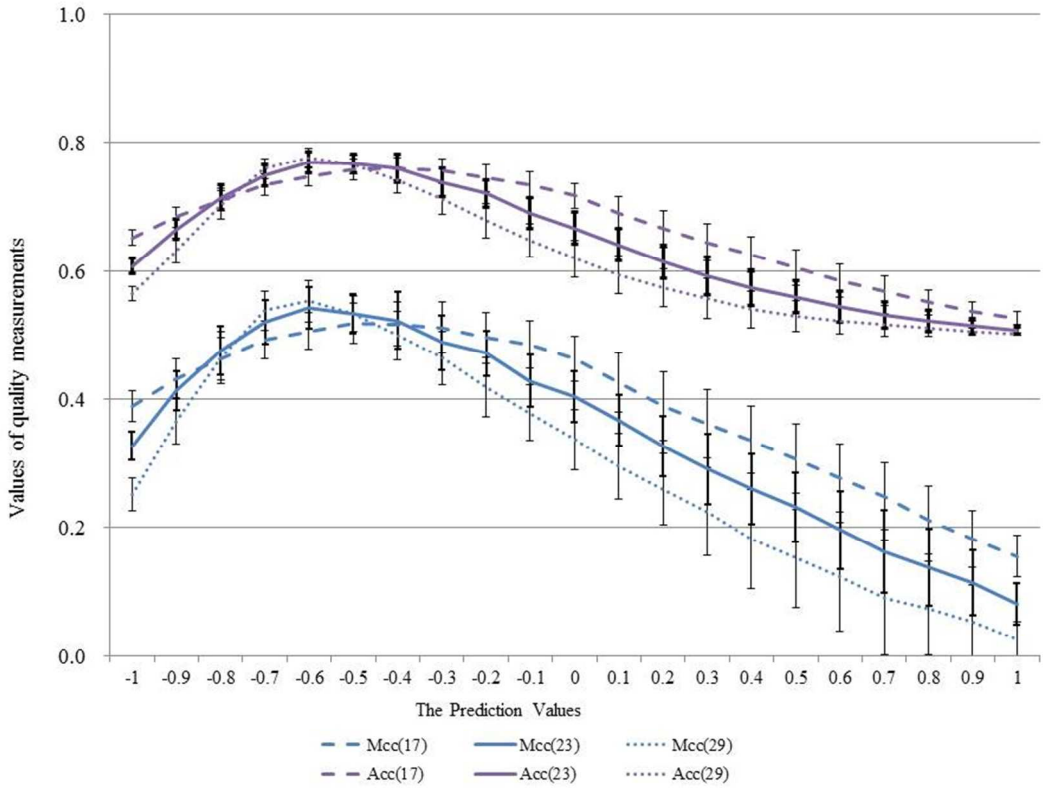
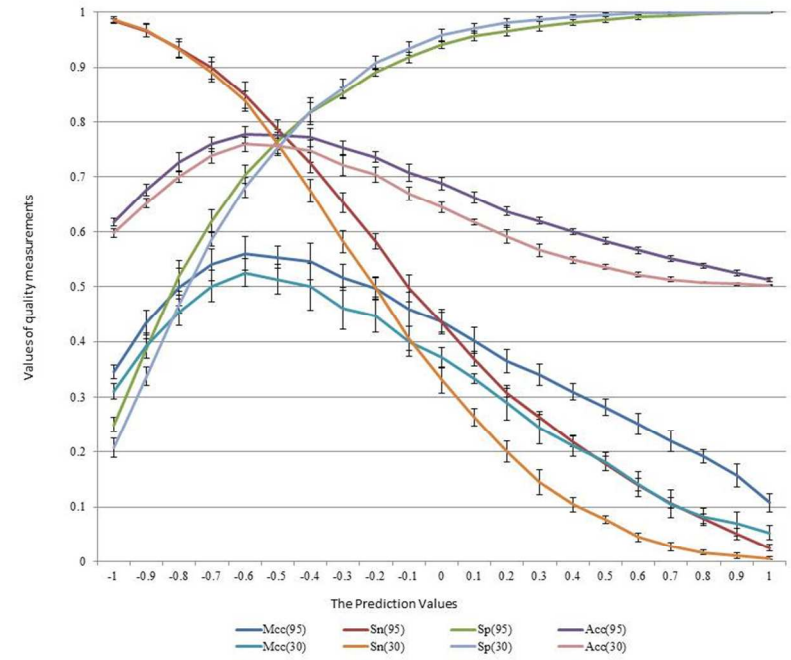


Figure S2: Distribution of all of the performance indicators (SVM parameters: gamma = 0.001, cost factor = 5, 5-fold cross validation) using the NR95 and NR30 datasets.



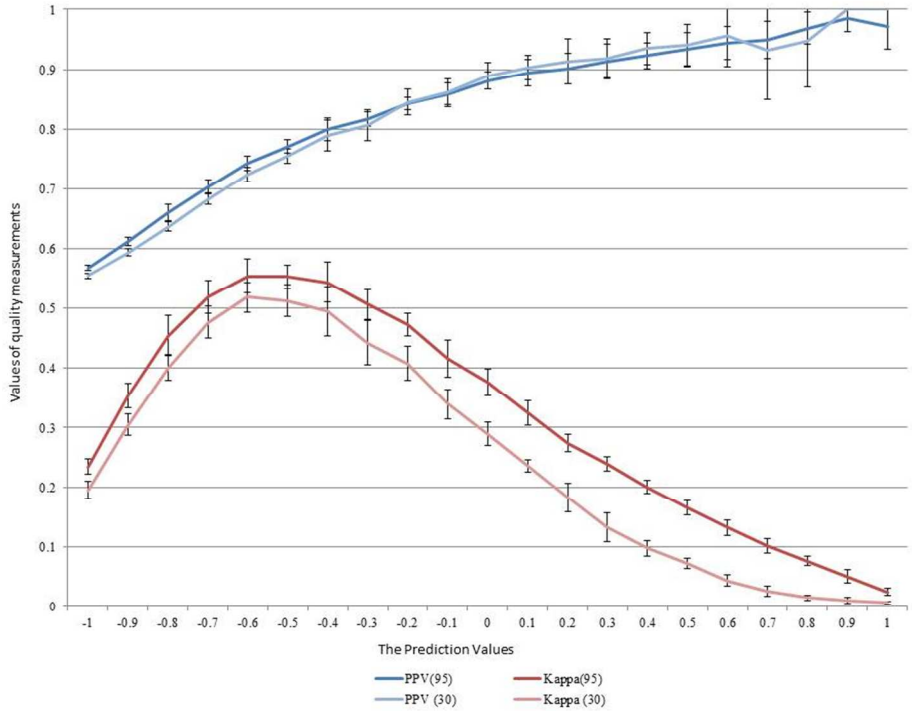


Table S1: All of the predicted induced-fit values for each residue in Turkey beta1 adrenergic receptor (PDB code 2VT4.A). If the value was more than the cutoff of -0.6, then the residue was predicted as an induced-fit residue.

Residue	PV
Met31	-0.661
Gly32	-0.661
Ala33	-0.646
Glu34	-0.627
Leu35	-0.62
Leu36	-0.587
Ser37	-0.529
Gln38	-0.471
Gln39	-0.363
Trp40	0.31
Glu41	0.299
Ala42	0.072
Gly43	-0.219
Met44	-0.374
Ser45	-0.431
Leu46	-0.439
Leu47	-0.499
Met48	-0.529
Ala49	-0.492
Leu50	-0.515
Val51	-0.519

Val52	-1.025
Leu53	-0.91
Leu54	-0.884
Ile55	-1.045
Val56	-0.878
Ala57	-1.006
Gly58	-1.097
Asn59	-1.238
Val60	-1.296
Leu61	-1.141
Val62	-1.196
Ile63	-1.204
Ala64	-1.175
Ala65	-1.143
Ile66	-0.98
Gly67	-1.09
Ser68	-0.978
Thr69	-0.871
Gln70	-0.647
Arg71	-0.716
Leu72	-0.884
Gln73	-1.139
Thr74	-1.009
Leu75	-1
Thr76	-0.961
Asn77	-1.038
Leu78	-1.098

Phe79	-1.182
Ile80	-1.363
Thr81	-1.526
Ser82	-1.37
Leu83	-1.17
Ala84	-1.313
Cys85	-0.988
Ala86	-1.109
Asp87	-1.13
Leu88	-1.021
Val89	-0.674
Val90	-0.69
Gly91	-0.797
Leu92	-0.918
Leu93	-1.104
Val94	-1.092
Val95	-0.917
Pro96	-0.928
Phe97	-0.929
Gly98	-1.059
Ala99	-1.098
Thr100	-0.94
Leu101	-0.666
Val102	-0.599
Val103	-0.592
Arg104	-0.46
Gly105	-0.448

Thr106	-0.479
Trp107	-0.515
Leu108	-0.522
Trp109	-0.763
Gly110	-0.76
Ser111	-0.875
Phe112	-0.859
Leu113	-0.856
Cys114	-0.922
Glu115	-1.023
Leu116	-0.901
Trp117	-0.959
Thr118	-0.948
Ser119	-1.033
Leu120	-1.188
Asp121	-1.175
Val122	-1.166
Leu123	-1.067
Cys124	-0.784
Val125	-0.998
Thr126	-0.751
Ala127	-0.72
Ser128	-0.804
Ile129	-0.993
Glu130	-1.066
Thr131	-0.947
Leu132	-1.033

Cys133	-1.112
Val134	-1.201
Ile135	-1.222
Ala136	-1.235
Ile137	-1.172
Asp138	-0.955
Arg139	-0.959
Tyr140	-0.944
Leu141	-0.506
Ala142	-0.116
Ile143	0.135
Thr144	0.51
Ser145	0.526
Pro146	0.658
Phe147	0.857
Arg148	0.765
Tyr149	0.424
Gln150	-0.359
Ser151	-0.272
Leu152	-0.285
Met153	-0.655
Thr154	-0.704
Arg155	-0.737
Ala156	-0.651
Arg157	-0.882
Ala158	-0.809
Lys159	-0.903

Val160	-0.889
Ile161	-0.838
Ile162	-0.722
Cys163	-0.634
Thr164	-0.652
Val165	-0.72
Trp166	-0.755
Ala167	-0.714
Ile168	-0.781
Ser169	-0.965
Ala170	-1.216
Leu171	-0.818
Val172	-0.942
Ser173	-1.097
Phe174	-1.041
Leu175	-1.102
Pro176	-1.174
Ile177	-1.096
Met178	-1.104
Met179	-0.707
His180	-0.33
Trp181	-0.168
Trp182	0.078
Arg183	0.358
Asp184	0.582
Glu185	0.692
Asp186	0.817

Pro187	0.866
Gln188	0.753
Ala189	0.472
Leu190	0.457
Lys191	0.19
Cys192	0.136
Tyr193	-0.044
Gln194	0.059
Asp195	-0.315
Pro196	-0.161
Gly197	-0.528
Cys198	-0.598
Cys199	-0.731
Asp200	-0.897
Phe201	-0.73
Val202	-0.713
Thr203	-0.706
Asn204	-0.718
Arg205	-0.643
Ala206	-0.478
Tyr207	-0.7
Ala208	-0.77
Ile209	-0.709
Ala210	-0.721
Ser211	-0.827
Ser212	-0.722
Ile213	-0.891

Ile214	-0.941
Ser215	-1.139
Phe216	-1.07
Tyr217	-1.076
Ile218	-0.868
Pro219	-0.964
Leu220	-1.011
Leu221	-0.975
Ile222	-0.895
Met223	-1.152
Ile224	-1.199
Phe225	-1.118
Val226	-0.871
Ala227	-1.038
Leu228	-0.892
Arg229	-0.77
Val230	-0.835
Tyr231	-0.774
Arg232	-0.64
Glu233	-0.27
Ala234	-0.292
Lys235	-0.288
Glu236	-0.229
Gln237	-0.194
Ile238	0.033
Arg239	-0.462
Lys240	-0.607

Ile241	-0.671
Asp242	-0.695
Arg243	-0.669
Ala244	-0.659
Ser245	-0.654
Lys246	-0.645
Arg247	-0.639
Lys248	-0.641
Arg249	-0.641
Val250	-0.608
Met251	-0.557
Leu252	-0.527
Met253	-0.394
Arg284	0.265
Glu285	0.089
His286	-0.102
Lys287	-0.503
Ala288	-0.773
Leu289	-0.875
Lys290	-0.89
Thr291	-0.851
Leu292	-0.921
Gly293	-0.887
Ile294	-1.067
Ile295	-1.547
Met296	-1.488
Gly297	-1.52

Val298	-1.139
Phe299	-1.408
Thr300	-1.09
Leu301	-0.763
Cys302	-0.965
Trp303	-0.922
Leu304	-1.033
Pro305	-1.105
Phe306	-1.263
Phe307	-1.343
Leu308	-1.32
Val309	-1.209
Asn310	-1.093
Ile311	-1.046
Val312	-0.949
Asn313	-0.944
Val314	-0.635
Phe315	-0.613
Asn316	-0.616
Arg317	-0.781
Asp318	-0.86
Leu319	-0.764
Val320	-1.125
Pro321	-1.233
Asp322	-1.088
Trp323	-1.032
Leu324	-1.106

Phe325	-1.343
Val326	-1.461
Ala327	-1.227
Phe328	-1.467
Asn329	-1.546
Trp330	-1.631
Leu331	-1.582
Gly332	-1.433
Tyr333	-1.507
Ala334	-1.363
Asn335	-1.202
Ser336	-1.243
Ala337	-1.16
Met338	-0.937
Asn339	-0.911
Pro340	-1.119
Ile341	-0.855
Ile342	-0.359
Tyr343	-0.385
Cys344	-0.209
Arg345	-0.022
Ser346	-0.218
Pro347	0.059
Asp348	-0.622
Phe349	-0.837
Arg350	-0.881
Lys351	-0.731

Ala352	-0.668
Phe353	-0.216
Lys354	-0.208
Arg355	0.019
Leu356	-0.06
Leu357	-0.074
Ala358	0.151
Phe359	-0.359
Pro360	-0.616
Arg361	-0.686
Lys362	-0.71
Ala363	-0.702
Asp364	-0.704
Arg365	-0.686
Arg366	-0.667
Leu367	-0.659
His368	-0.653
His369	-0.649
His370	-0.622
His371	-0.622
His372	-0.622
His373	-0.622

Table S2: Predicted induced-fit values in the DFG-in motif residues from the kinase search by MOE kinase search 2010. A: Only the DFG-in motif is reported in MOE kinase db 2010. B: Both DFG-in and –out motifs are reported in MOE kinase db 2010. If the value was more than the cutoff of -0.6, then the residue was a predicted induced-fit residue.

A	PV Average	(N=14) SD	State	B	PV Average	N=7 SD	State
	-1.142	(0.124)			-1.108	(0.084)	
	-0.979	(0.212)			-0.989	(0.087)	
ASP	-0.972	(0.152)		ASP	-0.940	(0.069)	
PHE	-0.867	(0.147)		PHE	-0.723	(0.271)	
GLY	-0.772	(0.255)		GLY	-0.584	(0.294)	High
	-0.622	(0.156)			-0.300	(0.282)	High
	-0.358	(0.079)	High		-0.209	(0.267)	High

Table S3: All of the predicted induced-fit values for each residue in Eglin C (PDB code: 1ACB.I). If the value was more than the cutoff of -0.6, then the residue was a predicted induced-fit residue. The bold values mean the predicted induced-fit positive residues.

Residue	PV	Residue	PV	Residue	PV
Lys8	**0.059**	Tyr29	**-0.346**	Asn50	**-0.259**
Ser9	**-0.058**	Pro30	**-0.400**	Arg51	**-0.480**
Phe10	**-0.333**	Gln31	**-0.460**	Val52	-1.131
Pro11	**-0.492**	Tyr32	**-0.543**	Arg53	-1.185
Glu12	-0.616	Asp33	-0.646	Val54	-1.259
Val13	-0.699	Val34	-0.652	Phe55	-1.157
Val14	-0.882	Tyr35	-0.847	Tyr56	-1.018
Gly15	-0.942	Phe36	-0.878	Asn57	**-0.468**
Lys16	-0.941	Leu37	-0.649	Pro58	**0.240**
Thr17	-0.927	Pro38	**-0.190**	Gly59	**0.065**
Val18	-1.043	Glu39	**0.159**	Thr60	**0.209**
Asp19	-0.814	Gly40	**0.069**	Asn61	**0.069**
Gln20	**-0.322**	Ser41	**0.272**	Val62	**0.027**
Ala21	-0.664	Pro42	**0.094**	Val63	**-0.401**
Arg22	**-0.555**	Val43	**0.066**	Asn64	**-0.592**
Glu23	**-0.554**	Thr44	**0.135**	His65	-0.776
Tyr24	-0.621	Leu45	**0.174**	Val66	-0.765
Phe25	-0.627	Asp46	**0.079**	Pro67	-0.892
Thr26	**-0.566**	Leu47	**-0.032**	His68	-0.861
Leu27	-0.759	Arg48	**-0.099**	Val69	-0.974
His28	**-0.455**	Tyr49	**-0.164**	Gly70	**-0.199**