Table S1. Atom Types Used in Developing Pair Potentials.

Atom Types		Description	Atom Types		Description
Protein	Ligand		Protein	Ligand	
C.3	c.3	Carbon sp3	O.3	o.3	Oxygen sp3
C.2	c.2	Carbon sp2	O.2	o.2	Oxygen sp2
C.AR	c.ar	Carbon aromatic, sp1	O.CO2	o.co2	Oxygen in carboxylate and phosphate groups
C.CAT	c.cat	Carbocation	P.3	p.3	Phosphorous sp3, sulfoxide and sulfone sulfur
N.4	n.4	Nitrogen sp3, and sp3 positively charged	S.3	s.3	Sulfur sp3
N.AM	n.am	Nitrogen amide	MET	-	All metals
N.PL3	n.pl3	Nitrogen trigonal	-	f	Fluorine
N.2	-	Nitrogen sp1, sp2 and aromatic	-	cl	Chlorine, Bromine
-	n.2	Nitrogen sp1and sp2			
-	n.ar	Nitrogen aromatic			

Table S2. Enrichment Performance of Different Cluster Size on Test Set Using ROC-AUC Score for Other Scoring Functions.

	ChemScore					GoldScore					GBSA				
	AChE	AR	Mdm2	p38	trypsin	AChE	AR	Mdm2	p38	trypsin	AChE	AR	Mdm2	p38	trypsin
Crystal	0.55	0.21	0.38	0.33	0.20	0.54	0.36	0.34	0.38	0.34	0.43	0.70	0.54	0.57	0.30
5	0.58	0.17	0.45	0.29	0.08	0.49	0.41	0.35	0.30	0.23	0.52	0.43	0.59	0.54	0.32
10	0.53	0.18	0.45	0.25	0.08	0.51	0.42	0.34	0.24	0.29	0.51	0.44	0.59	0.49	0.33
20	0.53	0.14	0.40	0.30	0.06	0.51	0.38	0.33	0.28	0.32	0.55	0.46	0.57	0.47	0.28
30	0.52	0.13	0.39	0.32	0.08	0.55	0.37	0.30	0.29	0.32	0.58	0.42	0.56	0.48	0.29
50	0.53	0.12	0.42	0.31	0.11	0.53	0.38	0.33	0.31	0.27	0.50	0.47	0.48	0.46	0.30
100	0.50	0.15	0.48	0.36	0.12	0.55	0.36	0.36	0.38	0.31	0.56	0.57	0.52	0.44	0.32
250	0.49	0.12	0.48	0.35	0.11	0.51	0.39	0.34	0.33	0.27	0.55	0.46	0.50	0.41	0.37

Figure S1

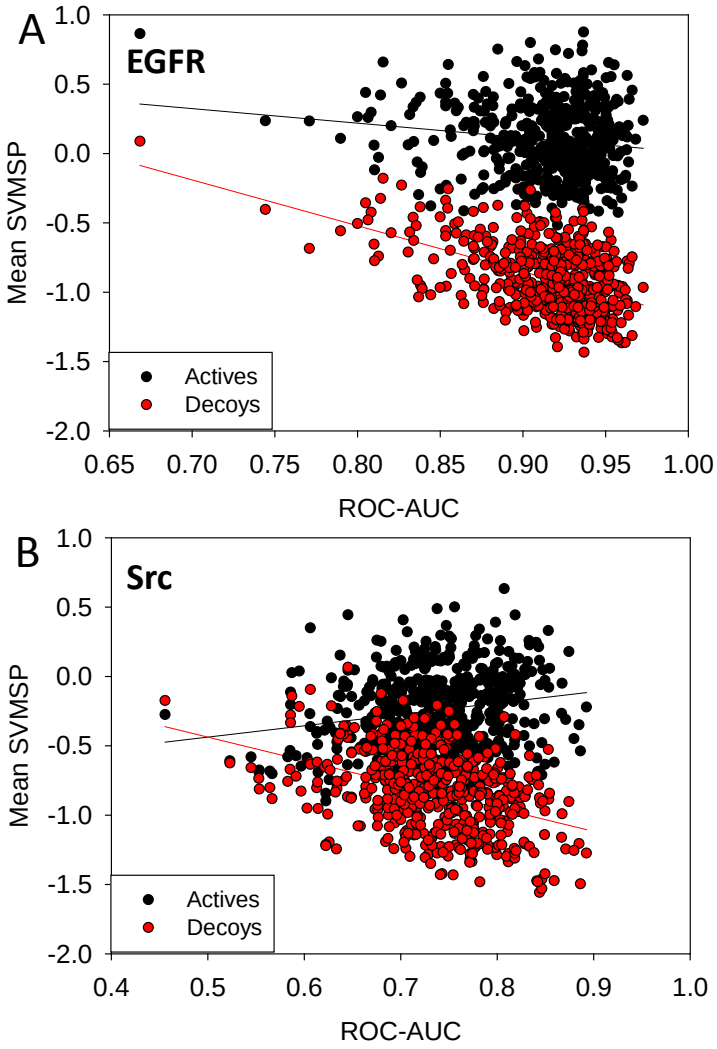

Figure S1. Regression plots between mean SVMSP score of DUD compounds and ROC-AUC of correspond snapshots. (A) EGFR; and (B) Src. Black dots illustrate ligands, red dots illustrate decoys.