Supplementary Data for article

CompScore: boosting structure-based virtual screening performance by incorporating docking scoring functions components into consensus scoring

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Table TS1. Composition of the datasets employed in our studies

Target(a)	Num. Ligands(b)	Num. Decoys(c)	Total molecules(d)
aa2ar	480	31281	31761
abl1	181	10609	10790
ace	281	16795	17076
aces	442	22384	22826
ada	93	5427	5520
ada17	532	35723	36255
adrb1	247	15125	15372
adrb2	229	13230	13459
akt1	289	16048	16337
akt2	116	6770	6886
aldr	159	8925	9084
ampc	48	2829	2877
andr	222	13062	13284
aofb	119	6730	6849
bace1	279	18025	18304
braf	152	9903	10055
cah2	491	30981	31472
casp3	199	10674	10873
cdk2	474	27757	28231
comt	41	3824	3865
cp2c9	119	7246	7365
cp3a4	170	11760	11930
csf1r	166	12087	12253
cxcr4	40	3401	3441
def	99	5689	5788
dhi1	330	19107	19437
dpp4	532	40776	41308
drd3	480	33359	33839
dyr	229	17098	17327
egfr	540	34869	35409
esr1	379	20413	20792
esr2	366	20087	20453
fa10	536	28143	28679
fa7	114	6213	6327
fabp4	47	2683	2730
fak1	99	5316	5415
fgfr1	135	7785	7920
fkb1a	111	5793	5904
fnta	592	51258	51850

fpps	79	8536	8615
gcr	206	14146	14352
glcm	54	3739	3793
gria2	157	11688	11845
grik1	100	6478	6578
hdac2	179	10155	10334
hdac8	168	10426	10594
hivint	99	6631	6730
hivpr	533	35564	36097
hivrt	334	18293	18627
hmdh	170	8726	8896
hs90a	78	4822	4900
hxk4	92	4385	4477
igf1r	148	9267	9415
inha	44	2293	2337
ital	138	8459	8597
jak2	107	6450	6557
kif11	116	6832	6948
kit	166	10404	10570
kith	57	2845	2902
kpcb	133	8644	8777
lck	419	27279	27698
lkha4	167	7448	7615
mapk2	100	6112	6212
mcr	51	4157	4208
met	166	11207	11373
mk01	78	4423	4501
mk10	104	6574	6678
mk14	578	35715	36293
mmp13	572	37027	37599
mp2k1	120	8057	8177
nos1	99	8001	8100
nram	98	6181	6279
pa2ga	99	5139	5238
parp1	507	29928	30435
pde5a	398	27437	27835
pgh1	184	10312	10496
pgh2	415	21362	21777
plk1	106	6767	6873
pnph	103	6901	7004
ppara	372	17807	18179
ppard	240	11801	12041
pparg	482	25094	25576

prgr	247	14248	14495
ptn1	130	7198	7328
pur2	50	2683	2733
pygm	77	3927	4004
pyrd	111	6091	6202
reni	104	6943	7047
rock1	100	6274	6374
rxra	120	6270	6390
sahh	60	2821	2881
src	522	34184	34706
tgfr1	133	8409	8542
thb	97	6375	6472
thrb	456	26863	27319
try1	448	25787	26235
tryb1	148	7609	7757
tysy	109	6715	6824
urok	162	9810	9972
vgfr2	402	22623	23025
wee1	102	6136	6238
xiap	100	5130	5230

(a) Target identification on the DUD-E database (http://dude.docking.org/)

(b) Number of ligands

(c) Number of decoy molecules

(d) Total number of molecules per target

Table TS2. VS performance of different scoring methods for the DUD-E database when BEDROC with α is set to 160.9 is used as model selection criterion

Target(a)	CompScore					Exhaustive Search					Best Individual Scoring Component			All Scoring Components
	Model Size(b)	BEDROC(c)	Boot. BEDROC(d)	Std. Boot. BEDROC(e)	Time (seconds)(f)	Model Size(b)	BEDROC(c)	Boot. BEDROC(d)	Std. Boot. BEDROC(e)	Time (seconds)(f)	BEDROC(c)	Boot. BEDROC(d)	Std. Boot. BEDROC(e)	BEDROC(c)
aa2ar	15	0.73	0.73	0.02	1088.92	2	0.53	0.52	0.03	336.69	0.55	0.55	0.02	0.43
abl1	10	0.6	0.6	0.04	203.64	2	0.41	0.41	0.05	110.63	0.49	0.48	0.04	0.17
ace	15	0.52	0.51	0.03	388.91	2	0.32	0.32	0.03	172.19	0.3	0.3	0.03	0.04
aces	7	0.66	0.66	0.03	481.02	3	0.55	0.55	0.03	265.62	0.46	0.46	0.03	0.13
ada	14	0.75	0.74	0.04	93.63	2	0.59	0.59	0.06	60.19	0.33	0.33	0.06	0.12
ada17	5	0.78	0.78	0.02	1258.96	1	0.64	0.64	0.02	430.22	0.72	0.72	0.02	0.33
adrb1	9	0.48	0.48	0.04	349.04	5	0.26	0.26	0.03	175.22	0.16	0.16	0.03	0.16
adrb2	12	0.42	0.42	0.04	326.43	3	0.2	0.2	0.03	131.30	0.23	0.23	0.04	0.16
akt1	17	0.68	0.68	0.03	495.25	2	0.53	0.53	0.03	170.74	0.45	0.44	0.04	0.24
akt2	12	0.64	0.63	0.05	110.44	2	0.45	0.45	0.06	75.66	0.43	0.42	0.06	0.15
aldr	18	0.6	0.59	0.04	148.11	1	0.54	0.53	0.04	94.55	0.54	0.53	0.05	0.07
ampc	14	0.66	0.65	0.07	35.88	4	0.18	0.17	0.07	35.55	0.16	0.16	0.07	0
andr	13	0.54	0.54	0.04	208.22	6	0.28	0.28	0.04	129.88	0.28	0.28	0.04	0.19
aofb	18	0.4	0.4	0.05	107.99	8	0.28	0.28	0.05	71.74	0.21	0.21	0.05	0.06
bace1	11	0.32	0.32	0.03	523.42	4	0.23	0.23	0.03	187.28	0.23	0.23	0.03	0.16
braf	8	0.61	0.61	0.04	161.23	1	0.32	0.32	0.05	102.44	0.35	0.35	0.05	0.23
cah2	22	0.52	0.52	0.03	1252.91	3	0.23	0.23	0.02	374.27	0.17	0.17	0.02	0.08
casp3	12	0.37	0.37	0.05	306.41	2	0.21	0.21	0.04	107.80	0.19	0.19	0.04	0.04
cdk2	17	0.47	0.47	0.03	760.82	6	0.37	0.37	0.03	317.24	0.34	0.34	0.03	0.23
comt	21	0.99	0.99	0.01	56.58	1	0.92	0.92	0.03	43.52	0.94	0.94	0.02	0.45
cp2c9	17	0.25	0.25	0.05	121.45	6	0.12	0.12	0.04	76.81	0.11	0.11	0.04	0.06
cp3a4	16	0.26	0.26	0.04	275.18	3	0.18	0.17	0.04	115.98	0.16	0.17	0.04	0.07
csf1r	9	0.53	0.53	0.04	238.6	1	0.35	0.35	0.04	121.08	0.35	0.34	0.04	0.12

cxcr4	19	0.71	0.7	0.07	45.11	2	0.43	0.42	0.08	40.11	0.3	0.3	0.08	0.15
def	15	0.91	0.91	0.02	93.7	1	0.67	0.67	0.05	60.94	0.78	0.78	0.04	0.19
dhi1	15	0.35	0.35	0.03	359.7	3	0.23	0.23	0.03	222.89	0.19	0.19	0.03	0.05
dpp4	10	0.64	0.64	0.02	1482.24	2	0.53	0.53	0.02	437.95	0.5	0.51	0.02	0.19
drd3	11	0.43	0.43	0.03	1093.71	5	0.24	0.24	0.02	410.68	0.17	0.17	0.02	0.04
dyr	17	0.75	0.75	0.03	517.59	3	0.64	0.64	0.03	190.07	0.61	0.61	0.03	0.45
egfr	10	0.75	0.75	0.02	1074.18	5	0.49	0.49	0.02	392.78	0.45	0.44	0.03	0.36
esr1	17	0.75	0.75	0.02	456.77	2	0.69	0.69	0.03	219.79	0.67	0.67	0.03	0.11
esr2	14	0.74	0.74	0.02	482.85	3	0.62	0.62	0.03	229.86	0.6	0.6	0.03	0.14
fa10	9	0.73	0.73	0.02	674.64	2	0.63	0.63	0.02	310.53	0.59	0.59	0.02	0.1
fa7	16	0.95	0.95	0.01	101.9	1	0.9	0.89	0.02	69.12	0.9	0.9	0.02	0.23
fabp4	18	0.78	0.78	0.06	35.86	1	0.7	0.69	0.07	34.33	0.7	0.69	0.07	0.1
fak1	12	0.69	0.69	0.05	100.95	4	0.54	0.54	0.06	60.17	0.5	0.49	0.07	0.27
fgfr1	12	0.55	0.54	0.05	152.11	4	0.39	0.39	0.05	83.57	0.26	0.26	0.04	0.23
fkb1a	22	0.71	0.71	0.05	106.23	7	0.38	0.38	0.06	64.28	0.34	0.34	0.06	0.14
fnta	17	0.23	0.23	0.02	1631.51	2	0.11	0.11	0.01	611.25	0.1	0.1	0.01	0.05
fpps	14	0.91	0.9	0.02	190.6	2	0.85	0.85	0.03	85.28	0.76	0.76	0.04	0.04
gcr	15	0.48	0.47	0.04	321.36	1	0.29	0.29	0.04	142.67	0.29	0.29	0.04	0.12
glcm	19	0.84	0.83	0.04	59.15	2	0.6	0.61	0.07	44.55	0.49	0.48	0.07	0.24
gria2	20	0.7	0.7	0.04	318.94	2	0.61	0.61	0.04	115.11	0.59	0.59	0.04	0.48
grik1	6	0.84	0.84	0.03	107.8	2	0.56	0.55	0.06	68.70	0.55	0.55	0.05	0.32
hdac2	14	0.74	0.74	0.03	240.08	3	0.52	0.52	0.04	104.52	0.45	0.45	0.04	0.37
hdac8	15	0.9	0.9	0.02	204.11	6	0.71	0.71	0.03	105.28	0.52	0.52	0.04	0.59
hivint	13	0.32	0.31	0.06	136.17	3	0.13	0.13	0.04	69.74	0.1	0.1	0.04	0.02
hivpr	12	0.3	0.3	0.02	1025.82	4	0.21	0.21	0.02	378.06	0.29	0.29	0.02	0.02
hivrt	18	0.43	0.43	0.03	554.53	3	0.2	0.2	0.03	207.14	0.18	0.18	0.03	0.21
hmdh	14	0.83	0.83	0.02	169.42	2	0.62	0.62	0.04	89.82	0.48	0.48	0.05	0.11
hs90a	19	0.77	0.77	0.04	87.98	6	0.49	0.48	0.07	53.58	0.27	0.27	0.05	0.42
hxk4	11	0.74	0.74	0.05	75.37	2	0.58	0.57	0.06	53.26	0.34	0.35	0.07	0.51
igf1r	20	0.54	0.54	0.05	209.16	3	0.38	0.38	0.05	103.68	0.34	0.34	0.05	0.23
inha	18	0.7	0.69	0.07	33.37	1	0.45	0.44	0.1	30.51	0.45	0.44	0.1	0.19
ital	7	0.46	0.46	0.05	161.09	3	0.39	0.39	0.05	90.02	0.28	0.28	0.05	0.06

jak2	14	0.8	0.8	0.04	117.05	3	0.56	0.56	0.05	68.63	0.51	0.51	0.06	0.37
kif11	15	0.84	0.83	0.03	130.06	4	0.79	0.79	0.03	77.14	0.77	0.77	0.04	0.05
kit	9	0.38	0.38	0.04	185.31	5	0.15	0.15	0.04	105.55	0.17	0.17	0.04	0.08
kith	14	0.96	0.96	0.01	40.43	2	0.89	0.89	0.03	35.29	0.88	0.88	0.03	0.62
kpcb	11	0.74	0.74	0.04	168.56	1	0.62	0.62	0.04	92.39	0.62	0.62	0.05	0.52
lck	10	0.61	0.61	0.02	993.33	2	0.34	0.34	0.03	314.28	0.31	0.31	0.03	0.31
lkha4	17	0.59	0.59	0.05	160.92	3	0.47	0.47	0.05	79.46	0.43	0.43	0.05	0.17
mapk2	21	0.92	0.91	0.02	134.9	5	0.79	0.79	0.03	65.26	0.7	0.7	0.04	0.64
mcr	18	0.52	0.52	0.08	50.35	3	0.27	0.27	0.08	48.13	0.25	0.25	0.08	0.12
met	10	0.67	0.67	0.04	215.84	4	0.5	0.5	0.05	118.48	0.61	0.61	0.04	0.13
mk01	19	0.63	0.62	0.06	126.09	3	0.5	0.49	0.07	50.39	0.34	0.34	0.06	0.26
mk10	19	0.56	0.55	0.05	90.35	5	0.41	0.41	0.06	71.09	0.31	0.31	0.06	0.23
mk14	14	0.41	0.41	0.02	1329.56	5	0.23	0.23	0.02	442.60	0.35	0.35	0.02	0.06
mmp13	8	0.68	0.68	0.02	1020.82	1	0.34	0.34	0.02	414.15	0.59	0.6	0.02	0.11
mp2k1	20	0.4	0.39	0.05	158.97	3	0.18	0.18	0.04	83.43	0.12	0.12	0.04	0.16
nos1	13	0.68	0.68	0.04	142.88	6	0.43	0.43	0.05	84.22	0.5	0.5	0.05	0.39
nram	16	0.95	0.95	0.01	119.16	3	0.73	0.73	0.04	66.72	0.47	0.47	0.05	0.24
pa2ga	15	0.73	0.72	0.05	83.15	2	0.56	0.55	0.06	57.22	0.45	0.45	0.06	0.04
parp1	17	0.9	0.9	0.01	812.95	2	0.76	0.76	0.02	356.11	0.71	0.71	0.02	0.7
pde5a	13	0.56	0.56	0.03	1007.22	2	0.48	0.48	0.03	297.26	0.47	0.47	0.03	0.29
pgh1	12	0.4	0.4	0.05	149.71	4	0.23	0.23	0.04	107.03	0.2	0.2	0.04	0.06
pgh2	15	0.63	0.63	0.03	687.72	7	0.4	0.4	0.03	233.66	0.33	0.33	0.03	0.32
plk1	20	0.7	0.7	0.04	126.04	3	0.56	0.56	0.05	70.85	0.49	0.49	0.05	0.31
pnph	23	0.9	0.9	0.02	135.09	2	0.78	0.77	0.04	76.44	0.76	0.75	0.04	0.74
ppara	10	0.41	0.42	0.03	369.56	4	0.23	0.23	0.03	191.24	0.14	0.14	0.02	0.07
ppard	8	0.46	0.46	0.04	231.32	1	0.28	0.28	0.04	117.60	0.28	0.28	0.03	0
pparg	14	0.46	0.46	0.03	922.63	1	0.22	0.22	0.03	274.90	0.22	0.22	0.03	0.07
prgr	21	0.75	0.75	0.03	416.19	8	0.39	0.39	0.04	154.05	0.38	0.38	0.04	0.54
ptn1	14	0.7	0.7	0.04	123.23	3	0.56	0.56	0.05	82.72	0.49	0.49	0.05	0.18
pur2	16	0.97	0.97	0.01	38.66	2	0.84	0.83	0.04	33.99	0.85	0.85	0.04	0.05
pygm	9	0.55	0.55	0.07	57.72	3	0.24	0.24	0.07	44.94	0.22	0.23	0.06	0.01
pyrd	20	0.81	0.81	0.03	107.26	6	0.56	0.56	0.05	70.84	0.61	0.61	0.05	0.22

reni	7	0.66	0.66	0.04	143.7	3	0.48	0.48	0.06	74.09	0.38	0.37	0.06	0.23
rock1	14	0.68	0.68	0.05	100.06	3	0.4	0.39	0.06	67.75	0.29	0.29	0.05	0.34
rxra	12	0.95	0.95	0.01	95.02	2	0.71	0.71	0.04	67.62	0.65	0.65	0.05	0.62
sahh	18	0.98	0.98	0.01	36.9	3	0.91	0.91	0.03	35.39	0.92	0.92	0.02	0.77
src	10	0.53	0.53	0.02	889.05	3	0.32	0.32	0.02	421.45	0.26	0.26	0.02	0.18
tgfr1	17	0.85	0.84	0.03	182.29	5	0.67	0.67	0.04	87.56	0.58	0.57	0.05	0.45
thb	15	0.81	0.81	0.03	104.52	2	0.69	0.69	0.05	68.33	0.6	0.6	0.06	0.4
thrb	9	0.76	0.76	0.02	946.82	3	0.59	0.59	0.02	310.40	0.49	0.49	0.03	0.12
try1	11	0.91	0.91	0.01	695	2	0.87	0.87	0.01	269.52	0.83	0.83	0.02	0.12
tryb1	13	0.79	0.79	0.03	140.13	1	0.54	0.54	0.05	81.62	0.54	0.54	0.05	0.13
tysy	19	0.62	0.62	0.05	116.44	2	0.43	0.42	0.06	72.73	0.38	0.38	0.06	0.28
urok	13	0.93	0.93	0.01	253.93	2	0.91	0.91	0.02	108.93	0.89	0.89	0.02	0.56
vgfr2	13	0.48	0.48	0.03	708.5	1	0.32	0.32	0.03	238.85	0.33	0.33	0.03	0.13
wee1	18	1	0.99	0	116.24	1	0.98	0.98	0.01	64.12	0.98	0.98	0.01	0.75
xiap	14	0.96	0.96	0.01	74.34	2	0.87	0.87	0.03	57.44	0.87	0.87	0.03	0.52
Mean	14.30	0.66	0.66	0.03	356.40	2.99	0.48	0.48	0.04	149.99	0.45	0.45	0.04	0.24

[a] Target identification on the DUD-E database (http://dude.docking.org/)

[b] Number of aggregated scoring functions

[c] BEDROC of the best performing VS strategy

[d] Mean BEDROC on 1000 bootstrap simulations of the best performing VS strategy

[e] Standard deviation of the bootstrap cross-validation procedure

[f] Run time for each consensus scoring approach

Table TS3. VS performance of different scoring methods for the DUD-E database when EF at the first 1% of screened data is used as model selection criterion

Target(a)	Opt. EF(b)	CompScore						Exhaustive Search						Best Individual Scoring Component				All Scoring Components	
		Size(c)	EF(d)	Boot. EF(e)	Std. Boot. EF(f)	Fract. Opt. EF(g)	Time (seconds) (h)	Size(c)	EF(d)	Boot. EF(e)	Std. Boot. EF(f)	Fract. Opt. EF(g)	Time (seconds) (h)	EF(d)	Boot. EF(e)	Std. Boot. EF(f)	Fract. Opt. EF(g)	EF(d)	Fract. Opt. EF(g)
aa2ar	66.17	20	46.19	45.8	1.63	0.69	951.53	1	33.08	33.14	1.71	0.50	354.85	33.71	33.89	1.67	0.51	24.14	0.36
abl1	59.61	14	35.33	34.37	3.05	0.58	214.87	1	22.08	21.74	2.72	0.37	110.86	25.39	24.98	2.51	0.43	10.49	0.18
ace	60.77	14	29.5	28.97	2.26	0.48	418.39	2	17.06	17.19	2.02	0.28	177.24	15.99	16.17	2.05	0.26	2.13	0.04
aces	51.64	13	32.25	31.96	1.83	0.62	570.06	3	25.71	25.8	1.65	0.50	243.67	20.52	20.31	1.59	0.40	6.09	0.12
ada	59.35	21	45.58	43.08	3.75	0.73	114.91	2	32.86	32.44	4.36	0.55	60.43	19.08	18.68	3.45	0.32	5.3	0.09
ada17	68.15	8	51.06	50.82	1.63	0.75	937.72	1	37.92	37.75	1.74	0.56	415.39	46	45.67	1.5	0.67	19.15	0.28
adrb1	62.23	14	26.27	25.91	2.33	0.42	392.3	3	14.95	14.63	2.07	0.24	164.80	9.29	9.18	1.67	0.15	8.08	0.13
adrb2	58.77	18	23.94	23.28	2.42	0.40	329.11	4	10.88	10.48	1.83	0.19	141.97	11.75	11.49	1.93	0.20	7.84	0.13
akt1	56.53	14	37.57	37.51	2.23	0.66	413.34	2	26.89	26.81	2.11	0.48	167.90	23.44	23.28	2.07	0.41	12.41	0.22
akt2	59.36	17	36.13	34.9	3.55	0.59	136.22	4	24.95	24.66	3.3	0.42	71.50	23.23	23.06	3.73	0.39	10.32	0.17
aldr	57.13	18	32.02	30.75	2.97	0.54	201.36	1	27	27.72	2.93	0.47	90.45	27	27.56	2.92	0.47	2.51	0.04
ampc	59.94	14	39.27	37.13	5.5	0.62	45.26	2	10.33	10.74	4.25	0.17	35.09	8.27	7.59	3.7	0.14	0	0.00
andr	59.84	12	30.14	29.57	2.52	0.49	288.34	5	17.1	16.38	2.36	0.29	136.56	13.05	13.33	2.22	0.22	9.9	0.17
aofb	57.55	20	21.69	20.61	3.09	0.36	147.9	6	16.68	16.11	3.05	0.29	72.20	11.68	10.85	2.73	0.20	4.17	0.07
bace1	65.61	15	17.47	16.95	2.05	0.26	508.84	1	11.41	11.5	1.93	0.17	183.25	11.77	11.7	1.88	0.18	8.56	0.13
braf	66.15	11	36.68	36.27	3.16	0.55	231.19	3	17.68	17.37	2.81	0.27	101.97	19.65	19.64	2.8	0.30	11.79	0.18
cah2	64.1	23	31.74	31.51	1.71	0.49	1024.17	6	13.23	12.79	1.39	0.21	362.64	12.41	12.12	1.4	0.19	4.68	0.07
casp3	54.64	16	17.54	17.06	2.32	0.31	272.26	2	12.03	11.93	1.99	0.22	116.46	10.03	9.87	1.91	0.18	1.5	0.03
cdk2	59.56	21	27.36	26.92	1.69	0.45	807.19	5	20.2	19.86	1.55	0.34	297.64	17.05	16.87	1.43	0.29	13.47	0.23
comt	94.27	21	91.85	90.34	3.13	0.96	79.93	1	79.77	78.43	4.86	0.85	45.32	79.77	78.64	4.88	0.85	36.26	0.38
cp2c9	61.89	25	15.05	14.09	2.91	0.23	165.67	4	8.36	8.07	2.35	0.14	75.81	5.85	5.3	2.01	0.09	3.35	0.05
cp3a4	70.18	17	14.04	13.94	2.5	0.20	294.07	4	11.11	10.47	2.27	0.16	118.99	10.53	10.24	2.24	0.15	4.68	0.07
csf1r	73.81	17	33.01	32.17	3.09	0.44	303.65	1	24	23.63	2.93	0.33	120.77	24	23.68	2.9	0.33	7.2	0.10

cxcr4	86.02	19	51.61	50.37	6.83	0.59	62.36	4	29.49	26.35	6.35	0.34	40.66	19.66	19.68	6.03	0.23	12.29	0.14
def	58.46	17	58.46	56.89	2.27	0.97	122.1	1	35.28	35.79	4	0.60	62.90	42.34	42.17	3.47	0.72	8.06	0.14
dhi1	58.9	14	19.94	19.51	1.88	0.33	452.78	3	11.78	11.7	1.74	0.20	212.26	8.76	8.84	1.5	0.15	2.42	0.04
dpp4	77.65	13	42.95	42.56	1.76	0.55	1172.21	2	34.13	34.17	1.81	0.44	478.41	33.38	33.44	1.74	0.43	13.5	0.17
drd3	70.5	19	26.41	26.09	1.8	0.37	964.27	5	14.97	14.66	1.52	0.21	358.36	9.77	10.11	1.3	0.14	3.33	0.05
dyr	75.66	20	52.18	51.67	2.86	0.68	462.34	2	40.01	39.61	2.82	0.53	171.22	39.14	39.26	2.68	0.52	26.96	0.36
egfr	65.57	10	49.32	48.83	1.54	0.74	971.57	5	28.45	28.59	1.61	0.43	415.57	22.72	22.82	2.3	0.35	20.32	0.31
esr1	54.86	17	43.26	42.5	1.61	0.77	502.85	1	36.4	36.4	2.11	0.66	215.12	34.29	33.97	2.14	0.63	6.07	0.11
esr2	55.88	11	41.71	41.64	1.84	0.75	472.16	3	32.17	32.27	2.12	0.58	214.72	29.99	30.2	1.98	0.54	8.45	0.15
fa10	53.51	14	39.34	38.95	1.68	0.73	786.81	3	31.32	31.3	1.53	0.59	294.69	28.71	28.61	1.46	0.54	5.03	0.09
fa7	55.5	17	55.5	55.47	0.25	1.00	130	1	55.5	54.97	1.12	1.00	68.47	55.5	55.02	1.04	1.00	11.27	0.20
fabp4	58.09	15	41.49	39.04	5.16	0.67	43.86	1	39.41	37.43	5.56	0.68	35.16	39.41	37.53	5.57	0.68	6.22	0.11
fak1	54.7	7	36.8	35.92	4.02	0.66	86.09	6	26.85	25.54	3.64	0.49	60.03	23.87	22.67	3.65	0.44	12.93	0.24
fgfr1	58.67	18	30.07	29.41	3.37	0.50	167.57	6	19.07	18.15	2.94	0.33	82.78	16.13	16.1	2.81	0.27	11	0.19
fkb1a	53.19	23	38.12	37.3	3.4	0.70	131.49	8	21.28	20.04	3.24	0.40	63.65	17.73	17.12	3.11	0.33	7.09	0.13
fnta	87.58	18	15.86	15.53	1.38	0.18	1528.55	3	7.93	7.8	1.05	0.09	583.78	7.09	7.21	1.05	0.08	4.05	0.05
fpps	97.77	14	81.47	80.23	3.73	0.82	184.69	2	72.7	72.4	4.73	0.74	86.18	66.43	66.5	4.56	0.68	1.25	0.01
gcr	69.67	20	27.09	26.77	2.68	0.38	324.83	1	17.42	17.65	2.39	0.25	138.15	17.42	17.6	2.52	0.25	7.74	0.11
glcm	70.24	19	61	58.32	4.15	0.83	67.52	3	36.97	36.23	5.27	0.53	44.52	35.12	33.2	5.63	0.50	16.64	0.24
gria2	75.45	25	46.92	46.45	3.64	0.62	298.11	3	38.67	37.8	3.42	0.51	122.71	36.14	36.11	3.64	0.48	29.16	0.39
grik1	65.78	13	56.81	56.38	2.7	0.86	146.64	1	30.9	31.25	4.18	0.47	71.32	30.9	31.64	4.25	0.47	16.94	0.26
hdac2	57.73	21	42.19	41.52	2.81	0.72	240	5	29.42	29.04	2.6	0.51	103.94	28.87	28.68	2.82	0.50	21.09	0.37
hdac8	63.06	12	63.06	62.26	1.28	0.99	208.54	6	45.21	43.92	3.01	0.72	111.70	32.72	32	2.88	0.52	36.88	0.58
hivint	67.98	18	16.99	16.36	3.46	0.24	151.65	3	9	8.64	2.82	0.13	70.73	6	6.03	2.36	0.09	1	0.01
hivpr	67.72	11	18.2	17.92	1.51	0.26	1043.03	4	12.76	12.67	1.37	0.19	396.82	17.26	17.09	1.46	0.25	0.75	0.01
hivrt	55.77	19	21.77	21.25	1.87	0.38	469.98	3	10.44	10.36	1.55	0.19	185.00	9.25	9.34	1.51	0.17	10.44	0.19
hmdh	52.33	16	46.45	45.27	2.32	0.87	208.51	2	31.16	30.52	2.64	0.60	93.81	25.87	25.18	2.66	0.49	4.12	0.08
hs90a	62.82	16	47.44	46.23	4.61	0.74	96.63	7	30.77	29.27	4.35	0.49	55.57	16.67	18.08	3.93	0.27	26.92	0.43
hxk4	48.66	21	36.77	35.84	3.96	0.74	81.76	2	25.95	26.89	3.99	0.53	50.75	16.22	15.11	3.23	0.33	21.63	0.44
igf1r	63.61	25	32.14	30.98	3.11	0.49	236.86	3	19.42	19.24	2.94	0.31	94.26	18.75	17.89	2.75	0.29	10.71	0.17
inha	53.11	19	42.05	39.51	5.07	0.74	43.59	1	19.92	20.05	5.94	0.38	32.27	19.92	19.64	5.83	0.38	8.85	0.17
ital	62.3	13	24.63	24.33	3.42	0.39	166.16	2	21.01	20.41	3.23	0.34	93.50	15.21	15.33	2.84	0.24	3.62	0.06

jak2	61.28	20	47.35	46.61	3.25	0.76	136.95	3	31.57	31.12	3.63	0.52	70.15	26	25.99	3.78	0.42	18.57	0.30
kif11	59.9	19	51.34	50.32	3.23	0.84	145.57	4	48.77	47.95	2.84	0.81	71.95	44.49	44.84	3.29	0.74	3.42	0.06
kit	63.67	12	23.43	22.79	2.96	0.36	218.1	4	8.41	7.92	2.04	0.13	107.33	9.61	9.55	2.17	0.15	4.2	0.07
kith	50.91	34	50.91	50.35	1.53	0.99	64.06	1	50.91	49.49	2.59	1.00	36.73	50.91	49.39	2.75	1.00	28.85	0.57
kpcb	65.99	20	47.24	46.15	3.37	0.70	193.44	1	34.5	34.36	3.83	0.52	89.69	34.5	34.56	3.61	0.52	30.75	0.47
lck	66.11	16	36.99	36.64	1.86	0.55	789.45	2	19.81	19.69	1.81	0.30	298.70	17.66	17.81	1.66	0.27	16.94	0.26
lkha4	45.6	16	28.43	27.43	2.42	0.60	164.68	3	21.32	20.97	2.48	0.47	82.32	17.77	18.45	2.57	0.39	10.07	0.22
mapk2	62.12	24	61.13	59.57	2.23	0.96	141.52	4	49.3	49.04	3.32	0.79	66.43	41.41	40.83	3.96	0.67	35.5	0.57
mcr	82.51	19	34.54	34.13	6.01	0.41	71.77	2	15.35	15.19	4.87	0.19	48.13	15.35	15.57	5.09	0.19	9.59	0.12
met	68.51	9	43.27	42.91	3.25	0.63	249.09	4	30.65	29.97	3.13	0.45	115.02	34.86	35.23	3.56	0.51	7.81	0.11
mk01	57.71	22	32.62	31.68	4.54	0.55	98.94	3	25.09	25.31	4.43	0.43	51.26	21.33	20.12	3.92	0.37	11.29	0.20
mk10	64.21	19	36.42	35.25	4.05	0.55	145	4	23.96	23.28	3.62	0.37	69.18	17.25	17.22	3.37	0.27	14.38	0.22
mk14	62.79	9	23.87	23.72	1.57	0.38	950.81	3	11.94	11.83	1.28	0.19	387.82	17.99	18.01	1.45	0.29	4.15	0.07
mmp13	65.73	17	38.29	37.79	1.72	0.57	1176.44	1	18.01	18.07	1.47	0.27	438.33	39.86	39.68	1.81	0.61	6.99	0.11
mp2k1	68.14	20	23.27	22.68	3.58	0.33	155.07	3	11.63	11.21	2.7	0.17	84.62	6.65	6.6	2.31	0.10	9.14	0.13
nos1	81.82	20	44.44	43.39	4.51	0.53	159.34	4	30.3	29.54	4.28	0.37	85.36	34.34	34.09	4.47	0.42	24.24	0.30
nram	64.07	16	64.07	63.01	1.75	0.98	136.21	2	45.77	45.04	3.52	0.71	65.71	27.46	27.84	3.88	0.43	14.24	0.22
pa2ga	52.91	17	40.93	39.37	3.68	0.74	103.74	2	25.96	26.07	3.68	0.49	56.60	22.96	22.75	3.47	0.43	2	0.04
parp1	60.03	26	58.26	57.94	0.8	0.97	971.19	2	45.86	45.64	1.36	0.76	339.21	40.54	40.51	1.56	0.68	39.95	0.67
pde5a	69.94	20	34.09	33.74	2.06	0.48	824.73	2	27.32	27.62	1.98	0.39	292.93	27.32	27.38	1.97	0.39	15.79	0.23
pgh1	57.04	12	20.1	19.21	2.58	0.34	182.59	4	13.04	12.69	2.19	0.23	111.23	10.32	10.34	2.13	0.18	2.17	0.04
pgh2	52.47	11	32.26	32.37	1.93	0.62	519.3	5	19.26	18.94	1.64	0.37	211.94	15.89	15.85	1.62	0.30	15.16	0.29
plk1	64.84	23	42.29	40.71	3.62	0.63	152.91	3	35.71	35.38	3.85	0.55	74.55	27.25	26.8	3.97	0.42	17.85	0.28
pnph	68	27	65.13	63.32	2.74	0.93	142.01	2	51.72	51.23	4.12	0.76	72.89	48.85	47.96	4.13	0.72	45.01	0.66
ppara	48.87	9	19.6	19.6	1.76	0.40	428.92	3	11.55	11.63	1.51	0.24	190.85	6.44	6.38	1.2	0.13	3.76	0.08
ppard	50.17	6	23.22	23	2.25	0.46	241.61	1	12.44	12.78	1.98	0.25	121.94	12.44	12.79	1.97	0.25	0	0.00
pparg	53.06	20	22.39	22.13	1.61	0.42	777.48	1	10.78	10.74	1.21	0.20	249.12	10.78	10.71	1.29	0.20	3.32	0.06
prgr	58.68	25	45.33	44.64	2.39	0.76	318.85	5	21.45	20.93	2.33	0.37	144.63	18.21	18.25	2.19	0.31	29.95	0.51
ptn1	56.37	14	38.85	38.06	3.54	0.68	146.85	2	29.71	29.87	3.13	0.53	78.34	26.66	26.94	3.4	0.47	7.62	0.14
pur2	54.66	22	54.66	53.97	1.89	0.99	53.85	1	48.8	47.4	3.48	0.89	34.15	50.76	48.59	3.62	0.93	1.95	0.04
pygm	52	21	16.49	15.14	3.65	0.29	82.01	2	12.68	11.63	3.36	0.24	46.72	13.95	13.68	3.52	0.27	1.27	0.02
pyrd	55.87	14	50.55	49	3.21	0.88	109.65	5	31.93	30.59	3.53	0.57	69.18	31.04	31.07	4.34	0.56	10.64	0.19

reni	67.76	7	41.99	41.02	3.65	0.61	139.59	2	24.81	24.88	4.36	0.37	72.66	19.09	19.05	3.78	0.28	12.41	0.18
rock1	63.74	26	40.83	39.75	4.13	0.62	122.19	5	25.89	24.96	3.53	0.41	68.16	15.94	15.95	3.18	0.25	19.92	0.31
rxra	53.25	21	53.25	52.87	0.89	0.99	127.75	4	39.11	38.61	3.06	0.73	69.61	32.45	32.95	3.09	0.61	34.11	0.64
sahh	48.02	28	48.02	47.98	0.33	1.00	56.47	2	48.02	46.06	2.83	1.00	36.47	46.36	45.74	2.78	0.97	38.08	0.79
src	66.49	12	32.67	32.22	1.68	0.48	955.4	2	17.96	18.02	1.48	0.27	399.24	14.52	14.85	1.44	0.22	9.17	0.14
tgfr1	64.23	18	56.76	55.32	2.92	0.86	176.39	2	39.58	39.06	3.06	0.62	89.37	34.35	33.74	3.21	0.53	24.64	0.38
thb	66.72	24	53.38	51.4	3.76	0.77	135.8	2	42.09	41.42	4.41	0.63	68.22	32.85	33.81	4.05	0.49	22.58	0.34
thrb	59.91	7	45.92	45.66	1.61	0.76	678.75	3	32.36	32.47	1.75	0.54	270.53	25.36	25.56	1.7	0.42	7.22	0.12
try1	58.56	9	58.34	58.05	0.59	0.99	693.85	2	53.44	53.41	1.12	0.91	262.63	50.54	50.56	1.62	0.86	6.01	0.10
tryb1	52.41	15	43.68	42.65	2.38	0.81	155.78	1	25.53	25.06	2.9	0.49	81.97	25.53	25.08	2.93	0.49	7.39	0.14
tysy	62.61	20	35.39	34.42	3.93	0.55	156.22	4	25.41	24.3	3.41	0.41	74.01	19.96	20.03	3.58	0.32	14.52	0.23
urok	61.56	20	60.94	59.56	2.04	0.97	256.66	2	60.94	60.85	0.9	0.99	104.03	57.86	57.35	2.02	0.94	32.01	0.52
vgfr2	57.28	10	26.78	26.6	1.85	0.46	509.54	2	15.87	15.93	1.71	0.28	244.17	15.62	15.52	1.68	0.27	5.95	0.10
wee1	61.16	24	61.16	61.16	0	1.00	137.18	1	61.16	61.15	0.12	1.00	65.02	61.16	61.1	0.32	1.00	46.6	0.76
xiap	52.3	24	52.3	52.1	0.72	1.00	112.78	1	49.34	48.53	1.92	0.94	58.19	49.34	48.59	1.92	0.94	24.67	0.47
Mean	62.24	17.26	39.64	38.85	2.68	0.63	346.47	2.83	28.12	27.73	2.78	0.46	147.08	25.71	25.53	2.76	0.42	13.16	0.21

(a) Target identification on the DUD-E database (http://dude.docking.org/)

(b) EF at 1% of screened data for a perfect ranking of the active compounds on the ranked list

(c) Number of aggregated scoring functions

(d) EF of the best performing VS strategy

(e) Mean EF on 1000 bootstrap simulations of the best performing VS strategy

(f) Standard deviation of the bootstrap cross-validation procedure

(g) Fraction of the maximum possible EF that the VS method achieves

(h) Run time for each consensus scoring approach

Table TS4. VS performance of different scoring methods for the DUD-E database when BEDROC with α is set to 160.9 is used as model selection criterion and weighted scoring components are employed

Target	CompScore					BISC			ASC
	Size	BEDROC	Boot. BEDROC	Std. Boot. BEDROC	Time	BEDROC	Boot. BEDROC	Std. Boot. BEDROC	BEDROC
aa2ar	22	0.74	0.74	0.02	1388.29	0.55	0.55	0.02	0.35
abl1	19	0.62	0.62	0.04	370.36	0.49	0.48	0.04	0.19
ace	21	0.54	0.54	0.03	799.7	0.3	0.3	0.03	0.04
aces	14	0.71	0.71	0.02	916.06	0.46	0.46	0.03	0.15
ada	17	0.77	0.77	0.04	135.22	0.33	0.33	0.06	0.07
ada17	14	0.79	0.79	0.01	1832.18	0.7	0.7	0.02	0.37
adrb1	14	0.53	0.53	0.04	589.61	0.16	0.16	0.03	0.13
adrb2	19	0.44	0.43	0.04	594.32	0.23	0.23	0.04	0.15
akt1	24	0.71	0.7	0.03	812.16	0.45	0.45	0.03	0.24
akt2	21	0.7	0.7	0.04	184.32	0.43	0.42	0.06	0.11
aldr	23	0.68	0.68	0.04	371.02	0.54	0.54	0.04	0.04
ampc	15	0.72	0.72	0.07	69.25	0.16	0.16	0.07	0.01
andr	15	0.6	0.6	0.03	420.84	0.28	0.28	0.04	0.17
aofb	18	0.42	0.42	0.06	164.75	0.21	0.21	0.05	0.06
bace1	28	0.33	0.32	0.04	870.06	0.18	0.18	0.03	0.13
braf	9	0.61	0.61	0.04	302.52	0.35	0.35	0.04	0.21
cah2	25	0.54	0.54	0.02	1500.49	0.17	0.17	0.02	0.05
casp3	17	0.41	0.4	0.05	392.34	0.19	0.19	0.04	0.04
cdk2	21	0.51	0.51	0.02	1070.25	0.34	0.33	0.03	0.21
comt	26	0.99	0.99	0.01	98.61	0.92	0.92	0.03	0.15
cp2c9	31	0.26	0.26	0.05	250.77	0.11	0.11	0.04	0.06
cp3a4	22	0.25	0.25	0.04	466.11	0.16	0.16	0.04	0.06
csf1r	13	0.59	0.59	0.04	353.53	0.35	0.35	0.04	0.11

cxcr4	27	0.73	0.72	0.06	87.07	0.3	0.29	0.09	0.12
def	18	0.91	0.91	0.02	168.79	0.74	0.74	0.04	0.1
dhi1	17	0.42	0.41	0.03	656.72	0.19	0.19	0.03	0.07
dpp4	27	0.66	0.66	0.02	2385.56	0.5	0.5	0.02	0.17
drd3	21	0.45	0.45	0.03	1728.59	0.17	0.17	0.02	0.02
dyr	22	0.76	0.76	0.03	752.26	0.61	0.61	0.03	0.36
egfr	13	0.75	0.75	0.02	1696.56	0.43	0.43	0.02	0.34
esr1	19	0.79	0.78	0.02	931.6	0.67	0.66	0.03	0.09
esr2	20	0.8	0.79	0.02	892.88	0.6	0.6	0.03	0.12
fa10	15	0.75	0.75	0.02	1404.37	0.59	0.59	0.02	0.2
fa7	17	0.95	0.95	0.01	167.68	0.9	0.9	0.02	0.23
fabp4	24	0.87	0.87	0.04	46.35	0.7	0.69	0.07	0.15
fak1	14	0.71	0.71	0.05	133.74	0.48	0.48	0.06	0.3
fgfr1	24	0.57	0.57	0.05	260.84	0.26	0.26	0.05	0.25
fkb1a	26	0.73	0.73	0.04	182.83	0.34	0.34	0.06	0.15
fnta	21	0.27	0.27	0.02	3158.1	0.1	0.1	0.01	0.04
fpps	16	0.94	0.93	0.02	284.27	0.87	0.87	0.03	0.02
gcr	17	0.54	0.54	0.04	445.71	0.29	0.29	0.04	0.12
glcm	24	0.86	0.85	0.04	94.21	0.39	0.39	0.07	0.09
gria2	31	0.73	0.72	0.03	499.57	0.57	0.57	0.04	0.43
grik1	20	0.82	0.82	0.03	313.45	0.55	0.55	0.06	0.32
hdac2	22	0.75	0.75	0.03	441.63	0.44	0.44	0.04	0.33
hdac8	16	0.9	0.9	0.02	343.87	0.52	0.52	0.04	0.48
hivint	19	0.4	0.4	0.05	178.8	0.14	0.14	0.04	0.03
hivpr	6	0.45	0.45	0.02	1395.58	0.29	0.29	0.02	0.02
hivrt	15	0.46	0.46	0.03	807.05	0.18	0.18	0.03	0.19
hmdh	19	0.86	0.86	0.02	276.17	0.4	0.4	0.05	0.11
hs90a	21	0.76	0.75	0.05	108.64	0.2	0.2	0.05	0.27
hxk4	18	0.78	0.78	0.04	94.63	0.48	0.47	0.07	0.45
igf1r	24	0.59	0.59	0.04	253.57	0.34	0.34	0.05	0.24
inha	21	0.72	0.71	0.07	47.37	0.45	0.44	0.1	0.19

ital	25	0.47	0.47	0.05	226.85	0.28	0.28	0.05	0.09
jak2	26	0.85	0.84	0.03	167.85	0.51	0.51	0.06	0.35
kif11	27	0.87	0.87	0.02	181.51	0.77	0.77	0.04	0.16
kit	18	0.41	0.41	0.05	365.22	0.16	0.16	0.03	0.07
kith	32	0.97	0.97	0.01	72.85	0.88	0.88	0.03	0.62
kpcb	18	0.77	0.77	0.03	271.21	0.62	0.62	0.05	0.53
lck	15	0.63	0.63	0.02	1074.97	0.31	0.31	0.03	0.29
lkha4	10	0.66	0.66	0.04	171.64	0.43	0.43	0.05	0.22
mapk2	35	0.93	0.93	0.02	169.57	0.7	0.7	0.05	0.66
mcr	11	0.65	0.65	0.06	70.06	0.25	0.24	0.08	0.1
met	20	0.71	0.71	0.03	315.02	0.61	0.61	0.04	0.15
mk01	21	0.64	0.64	0.06	120.41	0.34	0.34	0.06	0.23
mk10	19	0.57	0.57	0.05	148.8	0.29	0.29	0.06	0.23
mk14	20	0.45	0.45	0.03	1800.61	0.35	0.35	0.03	0.07
mmp13	18	0.74	0.74	0.02	1957.67	0.56	0.56	0.02	0.17
mp2k1	23	0.44	0.44	0.05	278.87	0.09	0.09	0.04	0.13
nos1	25	0.69	0.69	0.04	262.55	0.38	0.38	0.06	0.38
nram	24	0.95	0.95	0.01	178.38	0.47	0.47	0.05	0.34
pa2ga	22	0.76	0.75	0.04	119.99	0.45	0.45	0.06	0.06
parp1	26	0.91	0.9	0.01	1388.88	0.71	0.71	0.02	0.62
pde5a	22	0.59	0.59	0.03	1351.57	0.47	0.47	0.03	0.31
pgh1	13	0.41	0.4	0.05	356.61	0.2	0.2	0.04	0.05
pgh2	12	0.65	0.65	0.03	834.71	0.33	0.33	0.03	0.25
plk1	27	0.74	0.74	0.04	329.42	0.49	0.49	0.05	0.31
pnph	26	0.92	0.92	0.02	168.52	0.63	0.63	0.05	0.64
ppara	13	0.42	0.42	0.03	509	0.09	0.09	0.02	0.08
ppard	10	0.53	0.53	0.04	356.9	0.16	0.16	0.03	0
pparg	21	0.49	0.49	0.03	1016.67	0.22	0.22	0.03	0.05
prgr	25	0.77	0.77	0.02	571.18	0.34	0.34	0.04	0.4
ptn1	16	0.72	0.72	0.04	231.03	0.49	0.49	0.05	0.17
pur2	21	0.97	0.97	0.01	51.42	0.74	0.73	0.06	0.04

pygm	19	0.51	0.51	0.07	83.16	0.22	0.23	0.06	0
pyrd	19	0.84	0.84	0.03	143.15	0.61	0.61	0.05	0.23
reni	11	0.66	0.66	0.05	160.31	0.38	0.37	0.06	0.24
rock1	20	0.72	0.71	0.04	174.39	0.29	0.29	0.05	0.29
rxra	21	0.95	0.95	0.01	131.3	0.65	0.65	0.05	0.69
sahh	22	0.98	0.98	0.01	45.68	0.91	0.9	0.03	0.54
src	13	0.55	0.56	0.02	1596.35	0.26	0.26	0.02	0.15
tgfr1	18	0.87	0.87	0.02	272.91	0.58	0.57	0.04	0.43
thb	14	0.83	0.83	0.03	132.72	0.56	0.55	0.05	0.45
thrb	15	0.77	0.77	0.02	1122.75	0.44	0.44	0.03	0.11
try1	16	0.92	0.92	0.01	1158.06	0.77	0.77	0.02	0.12
tryb1	16	0.81	0.81	0.03	241.66	0.54	0.54	0.05	0.11
tysy	20	0.65	0.65	0.05	185.15	0.38	0.38	0.06	0.26
urok	20	0.94	0.94	0.01	439.94	0.89	0.89	0.02	0.44
vgfr2	14	0.53	0.53	0.03	958.08	0.33	0.33	0.03	0.14
wee1	22	1	1	0	156.2	0.97	0.97	0.01	0.7
xiap	24	0.97	0.97	0.01	124.81	0.87	0.87	0.03	0.56
Mean	19.68	0.69	0.68	0.03	553.31	0.44	0.44	0.04	0.22

Table TS5. VS performance of different scoring methods for the DUD-E database when EF at the first 1% of screened data is used as model selection criterion and weighted scoring components are employed

Target(a)	Opt. EF(b)	CompScore						BISC				ASC	
		Size(c)	EF(d)	Boot. EF(e)	Std. Boot. EF(f)	Fract. Opt. EF(g)	Time (seconds) (h)	EF(d)	Boot. EF(e)	Std. Boot. EF(f)	Fract. Opt. EF(g)	EF(d)	Fract. Opt. EF(g)
aa2ar	66.17	27	46.61	46.3	1.69	0.70	1360.07	33.71	33.97	1.71	0.51	19.35	0.29
abl1	59.61	24	29.81	28.81	2.84	0.50	343.29	25.39	24.98	2.63	0.43	11.59	0.19
ace	60.77	24	29.14	28.71	2.32	0.48	707.33	15.99	16.16	2.05	0.26	1.78	0.03
aces	51.64	15	35.86	35.65	1.92	0.69	835.67	20.52	20.23	1.65	0.40	6.99	0.14
ada	59.35	31	44.52	42.78	3.63	0.75	176.7	19.08	18.68	3.43	0.32	3.18	0.05
ada17	68.15	26	51.25	51.04	1.68	0.75	1621.2	42.8	42.83	1.97	0.63	21.59	0.32
adrb1	62.23	32	27.88	27.66	2.38	0.45	664.69	9.29	9.23	1.79	0.15	8.49	0.14
adrb2	58.77	23	24.82	24.03	2.43	0.42	511.15	11.75	11.64	2.05	0.20	6.97	0.12
akt1	56.53	22	38.61	38.11	2.23	0.68	640.26	23.44	23.34	2.05	0.41	11.72	0.21
akt2	59.36	24	39.57	39.04	4.14	0.67	236.88	23.23	22.8	3.69	0.39	6.88	0.12
aldr	57.13	20	38.93	38.09	2.93	0.68	345	27	27.69	2.95	0.47	2.51	0.04
ampc	59.94	25	37.2	34.5	5.37	0.62	78.06	8.27	7.57	3.54	0.14	0	0.00
andr	59.84	22	34.19	33.47	2.54	0.57	432.27	13.05	13.16	2.24	0.22	7.65	0.13
aofb	57.55	36	16.68	15.94	3.07	0.29	212.74	11.68	10.75	2.65	0.20	3.34	0.06
bace1	65.61	26	17.11	17.02	2.06	0.26	755.62	9.63	9.45	1.79	0.15	7.13	0.11
braf	66.15	28	32.09	31.09	3.07	0.49	388.47	19.65	19.56	2.85	0.30	11.79	0.18
cah2	64.1	28	32.35	32.36	1.73	0.50	1539.16	9.97	9.79	1.27	0.16	3.05	0.05
casp3	54.64	31	14.54	14.14	2.23	0.27	424.39	10.03	9.82	1.93	0.18	3.01	0.06
cdk2	59.56	26	29.25	28.93	1.73	0.49	1126.07	17.05	16.91	1.49	0.29	12.63	0.21
comt	94.27	30	91.85	90.53	3.1	0.97	120.68	79.77	78.29	4.9	0.85	7.25	0.08
cp2c9	61.89	40	15.05	13.84	3.07	0.24	300.88	5.85	5.41	1.95	0.09	4.18	0.07

cp3a4	70.18	32	12.87	12.58	2.46	0.18	476.93	10.53	10.21	2.19	0.15	2.92	0.04
csf1r	73.81	16	36.61	35.74	3.04	0.50	411.72	24	23.7	2.85	0.33	6.6	0.09
cxcr4	86.02	27	51.61	49.64	6.45	0.60	100.45	19.66	19.46	6.01	0.23	9.83	0.11
def	58.46	21	58.46	57.01	2.39	1.00	182.59	37.3	37.85	3.59	0.64	5.04	0.09
dhi1	58.9	26	19.63	19.46	2.04	0.33	749.89	8.76	8.82	1.5	0.15	3.62	0.06
dpp4	77.65	33	44.45	43.87	1.73	0.57	2007.78	33.38	33.42	1.84	0.43	10.5	0.14
drd3	70.5	27	27.24	26.89	1.78	0.39	1442.11	9.77	10.11	1.32	0.14	1.66	0.02
dyr	75.66	25	52.18	51.52	2.75	0.69	749.7	39.14	39.24	2.65	0.52	22.18	0.29
egfr	65.57	13	48.95	48.67	1.52	0.75	1431.16	25.86	25.4	1.57	0.39	19.39	0.30
esr1	54.86	23	46.16	45.57	1.81	0.84	786.89	34.29	34.05	2.07	0.63	4.48	0.08
esr2	55.88	20	46.34	45.76	1.64	0.83	773.7	29.99	29.95	1.96	0.54	6.54	0.12
fa10	53.51	22	41.2	40.76	1.5	0.77	1213.58	28.71	28.59	1.48	0.54	10.63	0.20
fa7	55.5	28	55.5	55.09	1.06	1.00	211.04	55.5	55	1.12	1.00	12.14	0.22
fabp4	58.09	29	47.71	46.56	5.71	0.82	71.02	39.41	37.53	5.73	0.68	12.45	0.21
fak1	54.7	23	32.82	32.59	4.25	0.60	162.36	23.87	22.58	3.45	0.44	14.92	0.27
fgfr1	58.67	33	30.8	29.52	3.3	0.52	275.61	16.13	16.18	2.87	0.27	11.73	0.20
fkb1a	53.19	26	41.66	40.14	3.36	0.78	193.73	17.73	17.45	3.14	0.33	7.09	0.13
fnta	87.58	29	15.69	15.44	1.37	0.18	2605.19	7.09	7.17	1.04	0.08	3.04	0.03
fpps	97.77	18	86.49	86.15	3.46	0.88	320.17	76.46	76.25	4.39	0.78	1.25	0.01
gcr	69.67	23	30.48	30.1	2.81	0.44	490.28	17.42	17.54	2.33	0.25	7.74	0.11
glcm	70.24	30	61	58.69	4.87	0.87	114.7	25.88	23.56	4.97	0.37	5.55	0.08
gria2	75.45	32	48.82	48.78	3.83	0.65	520.88	36.14	35.81	3.43	0.48	25.36	0.34
grik1	65.78	38	43.85	42.43	4.01	0.67	278.72	30.9	31.63	4.32	0.47	16.94	0.26
hdac2	57.73	31	41.08	40.44	3.11	0.71	428.48	28.31	28.29	2.88	0.49	18.87	0.33
hdac8	63.06	19	63.06	61.95	1.55	1.00	401.33	32.72	32.2	2.84	0.52	26.77	0.42
hivint	67.98	32	20.99	19.55	3.57	0.31	281.91	9	8.84	2.68	0.13	3	0.04
hivpr	67.72	14	24.95	24.6	1.61	0.37	1561.48	17.26	17.13	1.42	0.25	0.94	0.01
hivrt	55.77	26	22.37	22.09	1.96	0.40	696.29	8.65	8.69	1.43	0.16	9.25	0.17
hmdh	52.33	21	48.8	47.84	1.89	0.93	313.26	19.4	19.41	2.56	0.37	5.29	0.10
hs90a	62.82	22	46.15	45.72	4.97	0.73	142.66	14.1	14.91	3.68	0.22	19.23	0.31
hxk4	48.66	21	40.01	39.05	3.88	0.82	117.68	20.55	20.62	4.29	0.42	20.55	0.42

igf1r	63.61	30	34.82	33.83	3.13	0.55	353.42	18.75	17.88	2.73	0.29	11.38	0.18
inha	53.11	32	39.84	37.86	5.68	0.75	59.64	19.92	20.01	5.69	0.38	8.85	0.17
ital	62.3	33	23.9	22.84	3.03	0.38	314.91	15.21	15.39	2.88	0.24	5.07	0.08
jak2	61.28	25	52.92	52.02	3.3	0.86	226.61	26	25.68	3.74	0.42	19.5	0.32
kif11	59.9	27	55.62	53.86	2.95	0.93	254.08	44.49	44.89	3.25	0.74	10.27	0.17
kit	63.67	24	19.22	18.42	2.65	0.30	389.06	9.61	9.38	2.2	0.15	3.6	0.06
kith	50.91	39	50.91	50.54	1.12	1.00	95.72	50.91	49.42	2.73	1.00	28.85	0.57
kpcb	65.99	33	47.24	46.79	3.7	0.72	330.47	34.5	34.56	3.78	0.52	30.75	0.47
lck	66.11	21	36.75	36.5	1.96	0.56	1175.48	17.66	17.8	1.67	0.27	16.23	0.25
lkha4	45.6	27	26.06	25.46	2.73	0.57	250.72	17.77	18.41	2.51	0.39	11.25	0.25
mapk2	62.12	39	61.13	60.1	1.78	0.98	244.36	41.41	40.73	3.8	0.67	38.46	0.62
mcr	82.51	19	38.38	37.19	5.84	0.47	95.18	15.35	15.14	4.97	0.19	5.76	0.07
met	68.51	22	45.67	44.66	3.02	0.67	387.48	34.86	35.17	3.45	0.51	9.62	0.14
mk01	57.71	45	32.62	30.95	4.5	0.57	165.74	21.33	20.24	4.02	0.37	11.29	0.20
mk10	64.21	27	37.38	35.84	3.95	0.58	250.5	16.29	16.33	3.24	0.25	12.46	0.19
mk14	62.79	21	25.08	24.97	1.56	0.40	1519.57	17.99	18.07	1.43	0.29	3.63	0.06
mmp13	65.73	21	46.85	46.78	1.61	0.71	1684.44	34.79	34.64	1.61	0.53	10.84	0.16
mp2k1	68.14	21	24.93	24.06	3.66	0.37	276.09	6.65	6.57	2.27	0.10	9.14	0.13
nos1	81.82	32	47.47	45.67	4.1	0.58	319.46	24.24	24.26	3.76	0.30	22.22	0.27
nram	64.07	35	63.05	62.16	1.85	0.98	246.09	27.46	27.65	3.72	0.43	17.29	0.27
pa2ga	52.91	23	41.93	40.68	3.93	0.79	153	22.96	22.76	3.35	0.43	2.99	0.06
parp1	60.03	44	57.67	57.16	1.12	0.96	1542.55	40.54	40.46	1.61	0.68	32.87	0.55
pde5a	69.94	35	35.34	34.94	1.87	0.51	1241.17	27.32	27.28	1.95	0.39	17.8	0.25
pgh1	57.04	17	20.1	19.87	2.87	0.35	310.05	9.24	9.5	2.02	0.16	2.17	0.04
pgh2	52.47	22	32.5	32.13	1.8	0.62	808.63	15.89	15.84	1.59	0.30	13	0.25
plk1	64.84	30	46.99	45.36	3.3	0.72	229.59	27.25	26.82	4	0.42	16.91	0.26
pnph	68	30	66.08	64.68	2.61	0.97	235.27	40.23	40.17	4.26	0.59	36.39	0.54
ppara	48.87	22	19.06	18.7	1.75	0.39	602.02	3.76	3.68	0.98	0.08	3.49	0.07
ppard	50.17	10	24.88	24.55	2.23	0.50	371.88	8.29	8.25	1.7	0.17	0	0.00
pparg	53.06	28	24.67	24.31	1.64	0.46	1074.09	10.78	10.77	1.31	0.20	2.9	0.05
prgr	58.68	24	46.95	45.93	2.01	0.80	536.39	17.81	18.23	2.1	0.30	19.02	0.32

ptn1	56.37	18	39.61	39.07	3.87	0.70	220.75	26.66	26.92	3.4	0.47	7.62	0.14
pur2	54.66	34	54.66	53.47	2.65	1.00	70.3	39.04	38.83	4.74	0.71	1.95	0.04
pygm	52	29	16.49	15.1	3.75	0.32	118.73	13.95	13.8	3.46	0.27	0	0.00
pyrd	55.87	27	50.55	49.15	3.38	0.90	179.65	31.04	31.1	4.26	0.56	10.64	0.19
reni	67.76	17	37.22	36.64	4.04	0.55	201.44	19.09	18.97	3.88	0.28	14.32	0.21
rock1	63.74	26	43.82	41.46	3.86	0.69	212.65	15.94	15.94	3.31	0.25	16.93	0.27
rxra	53.25	25	53.25	52.9	0.94	1.00	166.48	32.45	33	3.17	0.61	35.78	0.67
sahh	48.02	34	48.02	47.65	1.03	1.00	70	46.36	45.59	2.87	0.97	28.15	0.59
src	66.49	14	34.01	33.95	1.71	0.51	1373.12	14.52	14.66	1.43	0.22	8.22	0.12
tgfr1	64.23	29	59	57.11	2.68	0.92	288.13	34.35	33.81	3.1	0.53	23.15	0.36
thb	66.72	32	55.43	53.54	3.57	0.83	195.05	31.82	31.45	3.89	0.48	26.69	0.40
thrb	59.91	16	47.23	46.99	1.66	0.79	1174.91	25.36	25.4	1.65	0.42	5.9	0.10
try1	58.56	21	58.11	57.95	0.6	0.99	1123.07	44.76	44.62	1.45	0.76	5.57	0.10
tryb1	52.41	16	44.35	43.59	2.29	0.85	256.36	25.53	24.95	2.87	0.49	5.38	0.10
tysy	62.61	36	35.39	33.72	3.66	0.57	272.54	19.96	19.87	3.54	0.32	12.7	0.20
urok	61.56	28	60.94	59.83	1.77	0.99	419.33	57.86	57.2	1.92	0.94	25.24	0.41
vgfr2	57.28	17	28.51	28.16	1.8	0.50	831.42	15.62	15.67	1.78	0.27	8.43	0.15
wee1	61.16	38	61.16	61.15	0.09	1.00	222.52	61.16	61.12	0.24	1.00	40.77	0.67
xiap	52.3	44	52.3	52	0.82	1.00	194.12	49.34	48.61	1.98	0.94	27.63	0.53
Mean	62.24	26.46	40.40	39.59	2.72	0.65	545.77	25.09	24.92	2.74	0.41	12.02	0.20

[a] Target identification on the DUD-E database (http://dude.docking.org/)

[b] EF at 1% of screened data for a perfect ranking of the active compounds on the ranked list

[c] Number of aggregated scoring functions

[d] EF of the best performing VS strategy

[e] Mean EF on 1000 bootstrap simulations of the best performing VS strategy

[f] Standard deviation of the bootstrap cross-validation procedure

[g] Fraction of the maximum possible EF that the VS method achieves

[h] Run time for each consensus scoring approach

Table TS6. VS performance on external validation experiments. Enrichment is computed as BEDROC with α is set to 160.9. Results are presented as the average BEDROC over the 100 training/external partitions of each target

Target[a]	BEDROC			
	Train[b]	Std (Train)[c]	Ext.[d]	Std (Ext.)[e]
aa2ar	0.73	0.01	0.71	0.05
abl1	0.60	0.02	0.57	0.07
ace	0.52	0.02	0.48	0.06
aces	0.65	0.01	0.62	0.06
ada	0.76	0.02	0.64	0.10
ada17	0.78	0.01	0.77	0.04
adrb1	0.48	0.02	0.41	0.07
adrb2	0.44	0.02	0.35	0.07
akt1	0.69	0.01	0.63	0.06
akt2	0.64	0.02	0.59	0.11
aldr	0.60	0.03	0.53	0.10
ampc	0.67	0.04	0.52	0.19
andr	0.54	0.02	0.50	0.07
aofb	0.41	0.03	0.26	0.10
bace1	0.33	0.02	0.24	0.07
braf	0.61	0.02	0.55	0.09
cah2	0.52	0.01	0.49	0.05
casp3	0.38	0.03	0.30	0.09
cdk2	0.48	0.01	0.43	0.06
comt	0.99	0.01	0.96	0.04
cp2c9	0.27	0.02	0.09	0.07
cp3a4	0.26	0.02	0.14	0.07
csf1r	0.51	0.03	0.44	0.09
cxcr4	0.73	0.03	0.51	0.16
def	0.91	0.01	0.88	0.05

dhi1	0.35	0.02	0.30	0.08
dpp4	0.64	0.01	0.63	0.05
drd3	0.43	0.01	0.41	0.05
dyr	0.75	0.01	0.72	0.06
egfr	0.75	0.01	0.73	0.04
esr1	0.76	0.01	0.74	0.05
esr2	0.74	0.01	0.72	0.05
fa10	0.72	0.01	0.71	0.04
fa7	0.95	0.01	0.93	0.03
fabp4	0.77	0.04	0.60	0.16
fak1	0.70	0.03	0.58	0.12
fgfr1	0.56	0.03	0.47	0.11
fkb1a	0.71	0.03	0.64	0.11
fnta	0.22	0.01	0.19	0.04
fpps	0.91	0.01	0.89	0.05
gcr	0.48	0.02	0.41	0.08
glcm	0.85	0.02	0.72	0.13
gria2	0.70	0.02	0.65	0.07
grik1	0.84	0.02	0.77	0.08
hdac2	0.74	0.02	0.70	0.07
hdac8	0.90	0.01	0.88	0.04
hivint	0.33	0.02	0.15	0.07
hivpr	0.30	0.01	0.27	0.04
hivrt	0.44	0.02	0.37	0.06
hmdh	0.83	0.01	0.80	0.07
hs90a	0.77	0.02	0.69	0.11
hxk4	0.75	0.02	0.67	0.10
igf1r	0.55	0.02	0.43	0.10
inha	0.73	0.04	0.43	0.18
ital	0.45	0.03	0.39	0.12
jak2	0.80	0.02	0.72	0.09

kif11	0.83	0.02	0.78	0.07
kit	0.38	0.02	0.30	0.09
kith	0.96	0.01	0.92	0.05
kpcb	0.74	0.02	0.69	0.08
lck	0.61	0.01	0.60	0.05
lkha4	0.61	0.02	0.48	0.10
mapk2	0.92	0.01	0.87	0.06
mcr	0.53	0.04	0.43	0.14
met	0.67	0.02	0.64	0.08
mk01	0.63	0.03	0.43	0.15
mk10	0.57	0.02	0.41	0.11
mk14	0.41	0.01	0.39	0.05
mmp13	0.68	0.01	0.66	0.04
mp2k1	0.40	0.02	0.31	0.10
nos1	0.68	0.02	0.61	0.10
nram	0.95	0.01	0.93	0.04
pa2ga	0.74	0.02	0.66	0.12
parp1	0.90	0.01	0.90	0.02
pde5a	0.57	0.01	0.54	0.05
pgh1	0.41	0.02	0.33	0.09
pgh2	0.63	0.01	0.60	0.05
plk1	0.71	0.02	0.61	0.10
pnph	0.91	0.01	0.87	0.05
ppara	0.41	0.04	0.36	0.08
ppard	0.46	0.02	0.40	0.09
pparg	0.46	0.02	0.44	0.06
prgr	0.76	0.01	0.72	0.05
ptn1	0.71	0.02	0.62	0.10
pur2	0.97	0.01	0.92	0.05
pygm	0.43	0.06	0.23	0.13
pyrd	0.82	0.02	0.76	0.07

reni	0.67	0.02	0.61	0.09
rock1	0.69	0.02	0.57	0.11
rxra	0.95	0.01	0.94	0.03
sahh	0.98	0.01	0.93	0.06
src	0.53	0.01	0.52	0.05
tgfr1	0.85	0.01	0.83	0.06
thb	0.81	0.02	0.74	0.08
thrb	0.76	0.01	0.75	0.04
try1	0.92	0.01	0.91	0.02
tryb1	0.79	0.01	0.76	0.07
tysy	0.63	0.02	0.53	0.11
urok	0.93	0.01	0.91	0.03
vgfr2	0.48	0.02	0.45	0.06
wee1	1.00	0.00	0.98	0.01
xiap	0.96	0.01	0.94	0.03

(a) Target identification on the DUD-E database (http://dude.docking.org/)

(b) Mean BEDROC on the training set over 100 data splits

(c) Standard deviation of BEDROC on the training set over 100 data splits

(d) Mean BEDROC on the external set over 100 data splits

(e) Standard deviation of BEDROC on the external set over 100 data splits