Table S1 The test data.

GEO accession number	Treatment molecule	Primary target	Experiment type	Drug type	Target type
GSE10281	letrozole	CYP19A1	*in vivo*	small molecule	enzyme
GSE10311	BMP2	BMPR1A	*in vitro*	protein	/
GSE10311	dexamethasone	NR3C1	*in vitro*	small molecule	nuclear receptor
GSE10315	BMP2	BMPR1A	*in vitro*	protein	/
GSE10685	IL6	IL6R	*in vivo*	protein	/
GSE10943	IFNa	IFNAR1	*in vitro*	protein	/
GSE11115	TNF	TNFRSF1A	*in vitro*	protein	/
GSE11285	enzastaurin	PRKCB	*in vitro*	small molecule	enzyme
GSE11336	dexamethasone	NR3C1	*in vitro*	small molecule	nuclear receptor
GSE11352	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE11367	IL17	IL17RA	*in vitro*	protein	/
GSE11467	TNF	TNFRSF1A	*in vitro*	protein	/
GSE11467	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE11550	paclitaxel	TUBB1	*in vitro*	small molecule	other
GSE11791	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE11864	IFNg	IFNGR1	*in vitro*	protein	/
GSE11869	17a-ethynyl estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE11886	IFNg	IFNGR1	*in vitro*	protein	/
GSE11959	h10H5	IGF1R	xenograft	antibody	/
GSE11981	HhAntag	SHH	xenograft	small molecule	other
GSE12113	IPI-504	HSP90AA1	*in vitro*	small molecule	other
GSE12161	TNF	TNFRSF1A	*in vitro*	protein	/
GSE12198	IL2	IL2RA	*in vitro*	protein	/
GSE12261	2-methoxy estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE12446	tibolone	ESR1	*in vivo*	small molecule	nuclear receptor
GSE12446	estradiol	ESR1	*in vivo*	small molecule	nuclear receptor
GSE12517	tamoxifen	ESR1	*in vivo*	small molecule	nuclear receptor
GSE12791	paclitaxel	TUBB1	*in vitro*	small molecule	other
GSE12839	IL12	IL12RB1	*in vitro*	protein	/
GSE12949	cilingitide	ITGB5	xenograft	small molecule	other
GSE13168	IL1B	IL1R1	*in vitro*	protein	/
GSE13168	EGF	EGFR	*in vitro*	protein	/
GSE13168	fluticasone	NR3C1	*in vitro*	small molecule	nuclear receptor
GSE13604	BMP6	BMPR1A	*in vitro*	protein	/
GSE13762	calcitriol	VDR	*in vitro*	small molecule	nuclear receptor
GSE13987	rolipram	PDE4A	*in vitro*	small molecule	enzyme
GSE14386	IFNb1a	IFNAR1	*in vivo*	protein	/
GSE14491	TGFb	TGFBR1	*in vitro*	protein	/
GSE14581	LLNle	PSEN1	*in vitro*	small molecule	enzyme
GSE14581	DAPT	PSEN1	*in vitro*	small molecule	enzyme
GSE14630	mycophenolic acid	IMPDH2	*in vivo*	small molecule	enzyme
GSE14973	valproic acid	VDR	*in vitro*	small molecule	nuclear receptor
GSE14987	EGF	EGFR	*in vitro*	protein	/
GSE15389	R547	CDK2	*in vitro*	small molecule	enzyme
GSE15392	R547	CDK2	*in vitro*	small molecule	enzyme
GSE15395	R547	CDK2	*in vitro*	small molecule	enzyme
GSE15490	rituximab	MS4A1	*in vitro*	antibody	/
GSE15703	rapamycin	MTOR	*in vitro*	small molecule	enzyme
GSE15717	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE15918	torcetrapib	CETP	*in vitro*	small molecule	other
GSE15947	calcitriol	VDR	*in vitro*	small molecule	nuclear receptor
GSE1615	valproic acid	HDAC1	*in vitro*	small molecule	enzyme
GSE16179	lapatinib	EGFR	*in vitro*	small molecule	enzyme
GSE16179	foretinib	MET	*in vitro*	small molecule	enzyme
GSE16214	IFNb	IFNAR1	*in vivo*	protein	/
GSE16386	rosiglitazone	PPARG	*in vitro*	small molecule	nuclear receptor
GSE16416	TGFb	TGFBR1	*in vitro*	protein	/
GSE16450	IFNa	IFNAR1	*in vitro*	protein	/
GSE16683	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE16755	IFNa	IFNAR1	*in vitro*	protein	/
GSE16879	infliximab	TNF	*in vivo*	antibody	/
GSE17007	NC1153	JAK3	*in vitro*	small molecule	enzyme
GSE17044	metribolone	AR	*in vitro*	small molecule	nuclear receptor
GSE17251	Wy-14643	PPARA	*in vitro*	small molecule	nuclear receptor
GSE17307	dexamethasone	NR3C1	*in vitro*	small molecule	nuclear receptor
GSE17708	TGFb1	TGFBR1	*in vitro*	protein	/
GSE18195	bevacizumab	VEGFA	xenograft	antibody	/
GSE18486	PHA-848125	CDK2	*in vitro*	small molecule	enzyme
GSE18498	PHA-793887	CDK2	*in vitro*	small molecule	enzyme
GSE18501	PHA-848125	CDK2	*in vitro*	small molecule	enzyme
GSE18504	flavopiridol	CDK9	*in vitro*	small molecule	enzyme
GSE19136	paclitaxel	TUBB1	*in vivo*	small molecule	other
GSE19182	IL4	IL4R	*in vitro*	protein	/
GSE19182	IL13	IL13RA1	*in vitro*	protein	/
GSE19182	IFNg	IFNGR1	*in vitro*	protein	/
GSE19182	IFNb	IFNAR1	*in vitro*	protein	/
GSE19182	IFNa	IFNAR1	*in vitro*	protein	/
GSE1922	imatinib	KIT	*in vitro*	small molecule	enzyme
GSE19638	tanespimycin	HSP90AA1	*in vitro*	small molecule	other

GEO accession number	Treatment molecule	Primary target	Experiment type	Drug type	Target type
GSE19736	SB-216763	GSK3A	*in vitro*	small molecule	enzyme
GSE20181	letrozole	CYP19A1	*in vivo*	small molecule	enzyme
GSE20198	IL12	IL12RB1	*in vitro*	protein	/
GSE20198	IFNa	IFNAR1	*in vitro*	protein	/
GSE20719	GDC-0941	PIK3CA	*in vitro*	small molecule	enzyme
GSE20854	EGF	EGFR	*in vitro*	protein	/
GSE20854	gefitinib	EGFR	*in vitro*	small molecule	enzyme
GSE20876	panobinostat	HDAC1	*in vitro*	small molecule	enzyme
GSE20876	imatinib mesylate	KIT	*in vitro*	small molecule	enzyme
GSE20963	dexamethasone	NR3C1	*in vitro*	small molecule	nuclear receptor
GSE21327	GH	GHR	*in vitro*	protein	/
GSE22061	vorinostat	HDAC1	*in vitro*	small molecule	enzyme
GSE22061	romidepsin	HDAC1	*in vitro*	small molecule	enzyme
GSE22061	largazole	HDAC1	*in vitro*	small molecule	enzyme
GSE22172	calcitriol	VDR	*in vitro*	small molecule	nuclear receptor
GSE2225	letrozole	CYP19A1	*in vitro*	small molecule	enzyme
GSE2225	anastrozole	CYP19A1	*in vitro*	small molecule	enzyme
GSE2225	tamoxifen	ESR1	*in vitro*	small molecule	nuclear receptor
GSE22363	ORG-2058	PGR	*in vitro*	small molecule	nuclear receptor
GSE22445	piroxicam	PTGS1	*in vitro*	small molecule	enzyme
GSE22483	metribolone	AR	*in vitro*	small molecule	nuclear receptor
GSE22523	calcitriol	VDR	*in vitro*	small molecule	nuclear receptor
GSE22807	TNF	TNFRSF1A	*in vitro*	protein	/
GSE23399	paclitaxel	TUBB1	*in vitro*	small molecule	other
GSE23597	infliximab	TNF	*in vivo*	antibody	/
GSE23687	methotrexate	DHFR	*in vivo*	small molecule	enzyme
GSE23741	rottlerin	PRKCD	*in vitro*	small molecule	enzyme
GSE23764	blebbistatin	MYH2	*in vitro*	small molecule	other
GSE23909	valproic acid	HDAC1	*in vitro*	small molecule	enzyme
GSE23935	LY2109761	TGFBR1	*in vitro*	small molecule	enzyme
GSE23952	TGFb	TGFBR1	*in vitro*	protein	/
GSE23984	TX527	VDR	*in vitro*	small molecule	nuclear receptor
GSE24183	enzastaurin	PRKCB	*in vitro*	small molecule	enzyme
GSE24187	rosuvastatin	HMGCR	*in vitro*	small molecule	enzyme
GSE24187	rifampicin	HMGCR	*in vitro*	small molecule	enzyme
GSE24187	atorvastatin	HMGCR	*in vitro*	small molecule	enzyme
GSE24427	IFNb	IFNAR1	*in vivo*	protein	/
GSE24468	R5020	PGR	*in vitro*	small molecule	nuclear receptor
GSE2450	atorvastatin	HMGCR	*in vitro*	small molecule	enzyme
GSE24547	danusertib	AURKA	*in vitro*	small molecule	enzyme
GSE24742	rituximab	MS4A1	*in vivo*	antibody	/
GSE24869	LTB4	LTB4R	*in vitro*	small molecule	other
GSE25400	IL1A	IL1R1	*in vitro*	protein	/
GSE25547	GW7647	PPARA	*in vitro*	small molecule	nuclear receptor
GSE25725	lestaurtinib	JAK2	*in vitro*	small molecule	enzyme
GSE26104	IFNb1b	IFNAR1	*in vivo*	protein	/
GSE26104	IFNb1a	IFNAR1	*in vivo*	protein	/
GSE26114	vorinostat	HDAC1	*in vitro*	small molecule	enzyme
GSE26114	linifanib	PDGFRB	*in vitro*	small molecule	enzyme
GSE26351	BMP4	BMPR1A	*in vitro*	protein	/
GSE26351	BIO	GSK3A	*in vitro*	small molecule	enzyme
GSE2638	TNF	TNFRSF1A	*in vitro*	protein	/
GSE2639	TNF	TNFRSF1A	*in vitro*	protein	/
GSE26459	4-hydroxytamoxifen	ESR1	*in vitro*	small molecule	nuclear receptor
GSE26483	dihydrotestosterone	AR	*in vitro*	small molecule	nuclear receptor
GSE2677	prednisolone	NR3C1	*in vivo*	small molecule	nuclear receptor
GSE26790	panobinostat	HDAC1	*in vitro*	small molecule	enzyme
GSE26868	TNF	TNFRSF1A	*in vitro*	protein	/
GSE26903	calcitriol	VDR	*in vitro*	small molecule	nuclear receptor
GSE26949	IFNa	IFNAR1	*in vitro*	protein	/
GSE26950	IFNa	IFNAR1	*in vitro*	protein	/
GSE26951	IFNa	IFNAR1	*in vitro*	protein	/
GSE27220	calcitriol	VDR	*in vitro*	small molecule	nuclear receptor
GSE27526	TGFb	TGFBR1	*in vitro*	protein	/
GSE27615	givinostat	HDAC1	*in vitro*	small molecule	enzyme
GSE27858	SPC2996	BCL2	*in vivo*	nucleic acid	/
GSE28305	dihydrotestosterone	AR	*in vitro*	small molecule	nuclear receptor
GSE28645	tamoxifen	ESR1	*in vitro*	small molecule	nuclear receptor
GSE28646	belinostat	HDAC1	*in vitro*	small molecule	enzyme
GSE28995	TNF	TNFRSF1A	*in vitro*	protein	/
GSE28995	tretinoin	RARG	*in vitro*	small molecule	nuclear receptor
GSE29232	metribolone	AR	*in vitro*	small molecule	nuclear receptor
GSE29435	medroxyprogesterone acetate	PGR	*in vitro*	small molecule	nuclear receptor
GSE29868	atorvastatin	HMGCR	*in vitro*	small molecule	enzyme
GSE29881	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE30004	TGFb	TGFBR1	*in vitro*	protein	/
GSE30517	valproic acid	HDAC1	*in vitro*	small molecule	enzyme
GSE30531	MLN4924	NAE1	*in vitro*	small molecule	enzyme
GSE30644	salmeterol	ADRB2	*in vitro*	small molecule	other
GSE30644	dexamethasone	NR3C1	*in vitro*	small molecule	nuclear receptor
GSE31287	figitumumab	IGF1R	*in vivo*	antibody	/

GEO accession number	Treatment molecule	Primary target	Experiment type	Drug type	Target type
GSE32161	tretinoin	RARG	*in vitro*	small molecule	nuclear receptor
GSE32217	EGF	EGFR	*in vitro*	protein	/
GSE32280	venlafaxine	SLC6A4	*in vivo*	small molecule	other
GSE32473	betamethasone valerate	NR3C1	*in vivo*	small molecule	nuclear receptor
GSE33552	zoledronate	FDPS	*in vitro*	small molecule	enzyme
GSE33552	fluvastatin	HMGCR	*in vitro*	small molecule	enzyme
GSE3356	nebivolol	ADRB1	*in vitro*	small molecule	other
GSE3356	metoprolol	ADRB1	*in vitro*	small molecule	other
GSE33562	PF-03084014	PSEN1	*in vitro*	small molecule	enzyme
GSE33562	dexamethasone	NR3C1	*in vitro*	small molecule	nuclear receptor
GSE33585	infliximab	TNF	*in vitro*	antibody	/
GSE33585	certolizumab	TNF	*in vitro*	antibody	/
GSE33643	GDC-0941	PIK3CA	*in vitro*	small molecule	enzyme
GSE33643	BKM120	PIK3CA	*in vitro*	small molecule	enzyme
GSE33643	BEZ235	PIK3CA	*in vitro*	small molecule	enzyme
GSE34405	norepinephrine	ADRB2	*in vitro*	small molecule	other
GSE34652	KGF	FGFR2	*in vitro*	protein	/
GSE34880	vorinostat	HDAC1	*in vitro*	small molecule	enzyme
GSE35031	DPN	ESR2	*in vitro*	small molecule	nuclear receptor
GSE35031	4-hydroxytamoxifen	ESR1	*in vitro*	small molecule	nuclear receptor
GSE35907	sorafenib	RAF1	*in vivo*	small molecule	enzyme
GSE35925	calcitriol	VDR	*in vivo*	small molecule	nuclear receptor
GSE36149	obatoclax	BCL2	*in vitro*	small molecule	other
GSE36176	RO4929097	PSEN1	*in vitro*	small molecule	enzyme
GSE36287	TNF	TNFRSF1A	*in vitro*	protein	/
GSE36287	IL4	IL4R	*in vitro*	protein	/
GSE36287	IL17A	IL17RA	*in vitro*	protein	/
GSE36287	IL13	IL13RA1	*in vitro*	protein	/
GSE36287	IFNg	IFNGR1	*in vitro*	protein	/
GSE36287	IFNa	IFNAR1	*in vitro*	protein	/
GSE37373	vorinostat	HDAC1	*in vitro*	small molecule	enzyme
GSE37715	IFNa	IFNAR1	xenograft	protein	/
GSE38147	IFNg	IFNGR1	*in vitro*	protein	/
GSE38147	IFNa	IFNAR1	*in vitro*	protein	/
GSE39042	paclitaxel	TUBB1	*in vitro*	small molecule	other
GSE39091	MLN4924	NAE1	*in vitro*	small molecule	enzyme
GSE39091	nutlin	MDM2	*in vitro*	small molecule	other
GSE4636	RTI-6413-018	AR	*in vitro*	small molecule	nuclear receptor
GSE4636	dihydrotestosterone	AR	*in vitro*	small molecule	nuclear receptor
GSE4883	simvastatin	HMGCR	*in vivo*	small molecule	enzyme
GSE4917	dexamethasone	NR3C1	*in vitro*	small molecule	nuclear receptor
GSE5007	tretinoin	RARG	*in vitro*	small molecule	nuclear receptor
GSE5145	calcitriol	VDR	*in vitro*	small molecule	nuclear receptor
GSE6092	IFNg	IFNGR1	*in vitro*	protein	/
GSE6257	TNF	TNFRSF1A	*in vitro*	protein	/
GSE6653	TGFb	TGFBR1	*in vitro*	protein	/
GSE6800	tamoxifen	ESR1	*in vitro*	small molecule	nuclear receptor
GSE6800	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE6803	tamoxifen	ESR1	*in vitro*	small molecule	nuclear receptor
GSE6803	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE7035	rosiglitazone	PPARG	*in vitro*	small molecule	nuclear receptor
GSE7144	TGFb2	TGFBR1	*in vitro*	protein	/
GSE7144	TGFb1	TGFBR1	*in vitro*	protein	/
GSE7216	KGF	FGFR2	*in vitro*	protein	/
GSE7216	IL24	IL20RA	*in vitro*	protein	/
GSE7216	IL22	IL22RA1	*in vitro*	protein	/
GSE7216	IL20	IL20RA	*in vitro*	protein	/
GSE7216	IL1b	IL1R1	*in vitro*	protein	/
GSE7216	IL19	IL20RA	*in vitro*	protein	/
GSE7216	IFNg	IFNGR1	*in vitro*	protein	/
GSE7509	anti-FcgRIIB	FCGR2B	*in vitro*	antibody	/
GSE7524	etanercept	TNF	*in vivo*	protein	/
GSE8515	IL6	IL6R	*in vitro*	protein	/
GSE8515	IL1	IL1R1	*in vitro*	protein	/
GSE8597	estradiol	ESR1	*in vitro*	small molecule	nuclear receptor
GSE8615	exherin	CDH2	xenograft	small molecule	other
GSE8685	IL21	IL21R	*in vitro*	protein	/
GSE8685	IL2	IL2RA	*in vitro*	protein	/
GSE8685	IL15	IL15RA	*in vitro*	protein	/
GSE8772	KINK-1	NFKB1	*in vitro*	small molecule	other
GSE8853	IL13	IL13RA1	*in vitro*	protein	/
GSE9105	insulin	INSR	*in vivo*	protein	/
GSE9481	IFNa	IFNAR1	*in vitro*	protein	

Table S2 AUC values for kernel diffusion ranking using different diffusion rates α.

				STRING 8.3	STRING 9.0
α = 0.9	**L_1**	**N=1**	log2 ratio	0.835	0.785
			t-statistic	0.828	0.767
			sign. log2 ratio	0.821	0.780
		N=2	log2 ratio	0.829	0.801
			t-statistic	0.822	0.792
			sign. log2 ratio	0.830	0.805
		N=3	log2 ratio	0.820	0.797
			t-statistic	0.812	0.784
			sign. log2 ratio	0.825	0.801
	L_2	**N=1**	log2 ratio	0.909	0.903
			t-statistic	0.911	0.901
			sign. log2 ratio	0.887	0.876
		N=2	log2 ratio	0.828	0.822
			t-statistic	0.814	0.806
			sign. log2 ratio	0.846	0.840
		N=3	log2 ratio	0.812	0.805
			t-statistic	0.795	0.792
			sign. log2 ratio	0.840	0.834
α = 0.7	**L_1**	**N=1**	log2 ratio	0.825	0.788
			t-statistic	0.817	0.778
			sign. log2 ratio	0.813	0.782
		N=2	log2 ratio	0.805	0.782
			t-statistic	0.796	0.770
			sign. log2 ratio	0.816	0.792
		N=3	log2 ratio	0.800	0.778
			t-statistic	0.789	0.764
			sign. log2 ratio	0.814	0.794
	L_2	**N=1**	log2 ratio	0.835	0.826
			t-statistic	0.822	0.816
			sign. log2 ratio	0.841	0.834
		N=2	log2 ratio	0.790	0.783
			t-statistic	0.772	0.767
			sign. log2 ratio	0.826	0.823
		N=3	log2 ratio	0.780	0.772
			t-statistic	0.760	0.756
			sign. log2 ratio	0.824	0.819
α = 0.5	**L_1**	**N=1**	log2 ratio	0.792	0.768
			t-statistic	0.782	0.754
			sign. log2 ratio	0.794	0.772
		N=2	log2 ratio	0.775	0.760
			t-statistic	0.763	0.742
			sign. log2 ratio	0.800	0.781
		N=3	log2 ratio	0.771	0.755
			t-statistic	0.757	0.739
			sign. log2 ratio	0.799	0.781
	L_2	**N=1**	log2 ratio	0.769	0.764
			t-statistic	0.752	0.746
			sign. log2 ratio	0.811	0.806
		N=2	log2 ratio	0.751	0.745
			t-statistic	0.729	0.727
			sign. log2 ratio	0.814	0.806
		N=3	log2 ratio	0.744	0.739
			t-statistic	0.725	0.723
			sign. log2 ratio	0.812	0.808

Table S3 AUC values for correlation diffusion ranking using different correlation thresholds s.

		STRING 8.3	STRING 9.0
s = 0.1	log2 ratio	0.919	0.893
	t-statistic	0.919	0.891
	sign. log2 ratio	0.918	0.896
s = 0.3	log2 ratio	0.842	0.861
	t-statistic	0.868	0.860
	sign. log2 ratio	0.772	0.795
s = 0.5	log2 ratio	0.730	0.729
	t-statistic	0.729	0.732
	sign. log2 ratio	0.611	0.617