

Neighbors of the tested compounds

NVP-AUY922			NSM-Tanespimycin			NMS-E973		
	well-known HSP90 inhibitors			well-known HSP90 inhibitors			well-known HSP90 inhibitors	
Distance	Compound	Community	Distance	Compound	Community	Distance	Compound	Community
0.6084	alvespimycin	28	0.4360	alvespimycin	28	0.4436	alvespimycin	28
0.6391	monorden	28	0.4913	geldanamycin	28	0.4891	geldanamycin	28
0.7123	geldanamycin	28	0.5176	monorden	28	0.5294	monorden	28
0.7506	puromycin	40	0.6315	tanespimycin	28	0.6568	tanespimycin	28
0.7608	tanespimycin	28	0.6533	puromycin	40	0.6723	puromycin	40
0.7756	gefitinib	60	0.7178	trifluoperazine	100	0.7308	trifluoperazine	100
0.8005	disulfiram	40	0.7542	parthenolide	104	0.7638	disulfiram	40
0.8023	trifluoperazine	100	0.7561	thiostrepton	104	0.7842	methylbenzethonium_chloride	100
			0.7608	withaferin_A	104	0.7850	parthenolide	104
			0.7724	disulfiram	40	0.7903	lanatoside_C	63
			0.7750	MG-262	40	0.7955	withaferin_A	104
			0.7896	1,4-chrysenequinone	40	0.7955	proscillaridin	63
			0.7915	digoxin	63	0.7957	etacrynic_acid	104
			0.7943	oxyphenbutazone	104	0.7964	0297417-0002B	100
			0.7943	proscillaridin	63	0.8036	MG-262	40
			0.7961	ouabain	63	0.8045	ouabain	63
			0.7970	0297417-0002B	100	0.8047	digoxin	63
			0.7991	perphenazine	100			
			0.7992	mefloquine	34			
			0.7995	etacrynic_acid	104			
			0.7997	digoxigenin	63			
			0.8019	tomelukast	98			
			0.8022	lanatoside_C	63			
			0.8027	helveticoside	63			
			0.8056	securinine	104			
Distance	Community		Distance	Community		Distance	Community	
0.128599	28		0.128599	28		0.131027	28	
0.129687	40		0.129687	104		0.199684	63	
			0.132954	63		0.24817	40	
			0.186359	40		0.256643	100	
			0.256786	100		0.264003	104	

Community Enriched for HSP90 inhibition

Neighbors of the tested compounds

PHA-848125						PHA-793887					
well Known CDK2 inhibitors			well Known CDK2 inhibitors			well-known CDK2 inhibitors			well-known CDK2 inhibitors		
Distance	Compound	Community	Distance	Compound	Community	Distance	Compound	Community	Distance	Compound	Community
0.6213	0175029-0000	32	0.7431	phenoxybenzamine	104	0.4715	0175029-0000	32	0.7509	digoxigenin	63
0.6352	apigenin	32	0.7440	digoxigenin	63	0.4846	GW-8510	14	0.7510	digitoxigenin	63
0.6504	harmine	32	0.7507	etoposide	3	0.5145	alsterpaullone	14	0.7547	mitoxantrone	14
0.6672	thioguanosine	32	0.7521	digoxin	63	0.5370	apigenin	32	0.7548	digoxin	63
0.6712	GW-8510	14	0.7539	harmol	32	0.5694	daunorubicin	14	0.7550	ciclopirox	3
0.6746	luteolin	32	0.7602	tyrphostin_AG-825	14	0.5976	doxorubicin	14	0.7590	etoposide	3
0.6795	daunorubicin	14	0.7610	doxorubicin	14	0.6014	ellipticine	14	0.7621	harmine	32
0.6828	irinotecan	32	0.7654	H-7	14	0.6353	tyrphostin_AG-825	14	0.7760	5109870	3
0.6877	camptothecin	14	0.7689	lanatoside_C	63	0.6582	luteolin	32	0.7781	lanatoside_C	63
0.6887	piperlongumine	40	0.7700	mebendazole	69	0.6607	camptothecin	14	0.7792	bisacodyl	63
0.6893	ellipticine	14	0.7818	bisacodyl	63	0.6825	staurosporine	14	0.7810	methotrexate	75
0.6905	alsterpaullone	14	0.7843	anisomycin	53	0.6940	H-7	14	0.7831	proscillaridin	63
0.7072	0297417-0002B	100	0.7853	sanguinarine	89	0.7018	irinotecan	32	0.7859	8-azaguanine	89
0.7121	proscillaridin	63	0.7889	resveratrol	3	0.7040	thioguanosine	32	0.7876	vorinostat	16
0.7201	digitoxigenin	63	0.7905	menadiione	89	0.7097	chrysin	32	0.7925	thiostrepton	104
0.7250	8-azaguanine	89	0.7938	STOCK1N-35215	104	0.7131	piperlongumine	40	0.7938	sanguinarine	89
0.7277	staurosporine	14	0.7957	thiostrepton	104	0.7165	fisetin	14	0.7942	resveratrol	3
0.7296	helveticoside	63	0.7969	azacitidine	14	0.7314	ouabain	63	0.8004	PNU-0293363	21
0.7297	ouabain	63	0.8012	fluspirilene	100	0.7369	helveticoside	63	0.8028	sulconazole	90
0.7353	nocodazole	69				0.7403	phenoxybenzamine	104			
0.7372	chrysin	32				0.7447	azacitidine	14			
	Distance			Community			Distance			Community	
	0.0722			14			0.0527			14	
	0.0846			32			0.0916			32	
	0.0927			63			0.0947			63	
	0.2554			89			0.1927			3	
	0.2590			104			0.383			104	
	0.3762			69							
	0.3764			100							
	0.3848			3							

Community Enriched for CDK/Topo inhibition

Neighbors of the tested compounds

NMS-Flavopyridol					
well-known CDK2 inhibitors			well-known CDK2 inhibitors		
Distance	Compound	Community	Distance	Compound	Community
0.4540	alsterpaullone	14	0.7810	scopoletin	90
0.4857	GW-8510	14	0.7811	digitoxigenin	63
0.5374	apigenin	32	0.7812	skimmianine	32
0.5534	0175029-0000	32	0.7851	ginkgolide_A	89
0.5789	daunorubicin	14	0.7875	hexestrol	90
0.5966	doxorubicin	14	0.7884	celastrol	40
0.5976	camptothecin	14	0.7890	meticrane	74
0.6196	ellipticine	14	0.7898	MS-275	14
0.6270	H-7	14	0.7898	tropicamide	90
0.6301	tyrphostin_AG-825	14	0.7905	etamsylate	89
0.6429	luteolin	32	0.7911	thiostrepton	104
0.6602	irinotecan	32	0.7915	antimycin_A	62
0.6722	chrysin	32	0.7924	verteporfin	89
0.6868	mitoxantrone	14	0.7939	omeprazole	90
0.6873	thioguanosine	32	0.7939	oxprenolol	85
0.7071	staurosporine	14	0.7953	tobramycin	95
0.7080	sanguinarine	89	0.7954	beta-escin	90
0.7089	azacitidine	14	0.7965	estriol	85
0.7098	8-azaguanine	89	0.7976	milrinone	85
0.7131	piperlongumine	40	0.7979	propylthiouracil	95
0.7159	fisetin	14	0.7987	dipyridamole	89
0.7228	phenoxybenzamine	104	0.7988	trioxysalen	32
0.7341	harmine	32	0.7991	napelline	55
0.7455	sulconazole	90	0.7991	fluorometholone	90
0.7493	doxazosin	52	0.7992	flunisolide	59
0.7578	carbachol	52	0.7998	cetirizine	90
0.7583	cantharidin	89	0.8002	denatonium_benzoate	90
0.7596	rimexolone	32	0.8009	ebesen	46
0.7616	proscillaridin	63	0.8011	reserpine	99
0.7654	bisacodyl	63	0.8027	ethaverine	52
0.7686	menadione	89	0.8033	PHA-00665752	19
0.7712	phthalylsulfathiazole	90	0.8042	repaglinide	85
0.7717	methotrexate	75	0.8043	bepiridil	100
0.7743	0297417-0002B	100	0.8046	sulfametoxydiazine	32
0.7747	triflusal	61	0.8050	metyrapone	
0.7747	gliclazide	61	0.8051	morantel	
0.7750	1,4-chrysenequinone	40	0.8051	cinchocaine	
0.7750	medrysone	90	0.8056	clomipramine	
0.7775	tyloxapol	90	0.8058	riboflavin	
0.7778	Prestwick-860	52	0.8059	chlorzoxazone	
0.7781	5109870	3	0.8059	N-acetyl-L-leucine	
0.7795	DL-thiorphan	13			
0.7809	norethisterone	90			
Distance			Community		
0.0480		14			
0.0603		90			
0.0625		32			
0.0954		89			
0.1929		52			
0.1995		85			
0.2527		40			
0.2564		63			
0.3781		104			
0.3874		61			
0.3946		100			
0.3983		95			

Community Enriched for CDK/Topo inhibition

Neighbors of the tested compounds

PHA-690509											
well-known CDK2 inhibitors			well-known CDK2 inhibitors			well-known CDK2 inhibitors			well-known CDK2 inhibitors		
Distance	Compound	Community	Distance	Compound	Community	Distance	Compound	Community	Distance	Compound	Community
0.3838	GW-8510	14	0.7572	ginkgolide_A	89	0.7822	methazolamide	42	0.7960	methotrexate	75
0.4613	doxorubicin	14	0.7593	bisacodyl	63	0.7823	verteporfin	89	0.7970	hexestrol	90
0.4794	alsterpaulone	14	0.7601	oxprenolol	85	0.7823	1,4-chrysenequinone	40	0.7975	levonorgestrel	58
0.5001	H-7	14	0.7632	carbachol	52	0.7840	trazodone	90	0.7975	ebseven	46
0.5593	daunorubicin	14	0.7658	lorglumide	90	0.7840	scopoletin	90	0.7978	ursodeoxycholic_acid	85
0.5873	camptothecin	14	0.7673	methacholine_chloride	13	0.7844	Prestwick-559	61	0.7979	piperidolate	90
0.5956	ellipticine	14	0.7673	apramycin	90	0.7850	norethisterone	90	0.7979	roxithromycin	74
0.6048	mitoxantrone	14	0.7682	Prestwick-1084	90	0.7851	thiostrepton	104	0.7983	moxonidine	95
0.6144	tyrphostin_AG-825	14	0.7684	meticrane	74	0.7868	etomidate	85	0.7987	acepromazine	90
0.6274	fisetin	14	0.7703	trioxysalen	32	0.7868	fusaric_acid	8	0.7992	cefalexin	90
0.6375	0175029-0000	32	0.7703	medrysone	90	0.7874	naftopidil	106	0.7993	molindone	106
0.6548	staurosporine	14	0.7704	phthalylsulfathiazole	90	0.7877	natamycin	52	0.7996	napelline	55
0.7091	azacitidine	14	0.7705	gliclazide	61	0.7879	etamsylate	89	0.7997	aminocaproic_acid	35
0.7120	sanguinarine	89	0.7716	chrysin	32	0.7879	cetirizine	90	0.7998	propafenone	61
0.7210	apigenin	32	0.7720	milrinone	85	0.7884	fluorometholone	90	0.8003	bezafibrate	90
0.7326	skimmianine	32	0.7726	propylthiouracil	95	0.7889	rimexolone	32	0.8004	3-nitropropionic_acid	18
0.7397	sulconazole	90	0.7739	aminohippuric_acid	58	0.7889	ethaverine	52	0.8005	difenidol	90
0.7399	triflusal	61	0.7767	flunixin	32	0.7892	thioguanosine	32	0.8009	urapidil	102
0.7401	cantharidin	89	0.7769	ethotoin	32	0.7905	atovaquone	99	0.8025	ipratropium_bromide	89
0.7435	DL-thiorphan	13	0.7772	denatonium_benzoate	90	0.7906	Prestwick-860	52	0.8029	5114445	4
0.7439	sitosterol	89	0.7777	pentoxifyverine	90	0.7908	sulfametoxydiazine	32	0.8031	roxarsone	41
0.7439	proxiphylline	74	0.7789	zomepirac	46	0.7913	talampicillin	89	0.8041	pancuronium_bromide	32
0.7450	dexverapamil	49	0.7795	hydrocotarnine	89	0.7924	halcinonide	59	0.8043	butoconazole	62
0.7476	repaglinide	85	0.7800	HC_toxin	16	0.7924	0297417-0002B	100	0.8046	oxetacaine	31
0.7518	doxazosin	52	0.7801	morantel	74	0.7940	procaine	82			
0.7528	piperlongumine	40	0.7803	omeprazole	90	0.7940	6-azathymine	8			
0.7536	riboflavin	90	0.7807	eucatropine	90	0.7941	dimethylxalylglycine	51			
0.7544	estriol	85	0.7809	menadione	89	0.7941	cycloserine	90			
0.7547	N-acetyl-L-leucine	89	0.7810	amiodarone	90	0.7941	metacycline	32			
0.7560	tyloxapol	90	0.7810	pargyline	89	0.7953	atropine	13			
0.7562	luteolin	32	0.7821	liothyronine	90	0.7955	piromidic_acid	52			
Distance	Community										
0.0300	90										
0.0464	14										
0.0585	32										
0.0639	89										
0.1283	85										
0.1299	52										
0.1931	74										
0.1933	61										
0.2561	13										
0.3837	40										
0.3927	95										
0.3928	58										
0.3941	46										
0.3952	8										
0.3967	106										

Community Enriched for CDK/Topo inhibitor

Neighbors of the tested compounds

NMS-SN38			NMS-Doxorubicin		
well-known TopoI inhibitors			well-known TopoII inhibitors		
Distance	Compound	Community	Distance	Compound	Community
0.3215	irinotecan	32	0.5587	daunorubicin	14
0.5641	camptothecin	14	0.6495	GW-8510	14
0.6158	apigenin	32	0.6536	hycanthone	3
0.6251	phenoxybenzamine	104	0.6555	ellipticine	14
0.6363	etoposide	3	0.6689	irinotecan	32
0.6596	luteolin	32	0.6900	camptothecin	14
0.6675	tyrphostin_AG-825	14	0.6921	etoposide	3
0.6877	daunorubicin	14	0.6926	mycophenolic_acid	75
0.6882	thioguanosine	32	0.6996	phenoxybenzamine	104
0.6903	hycanthone	3	0.7175	doxorubicin	14
0.7012	0175029-0000	32	0.7258	0175029-0000	32
0.7155	chrysin	32	0.7336	mepacrine	16
0.7251	resveratrol	3	0.7431	5151277	7
0.7360	GW-8510	14	0.7438	apigenin	32
0.7402	8-azaguanine	89	0.7521	5109870	3
0.7525	5109870	3	0.7579	vorinostat	16
0.7557	mycophenolic_acid	75	0.7598	scriptaid	16
0.7599	piperlongumine	40	0.7626	alsterpaullone	14
0.7635	methotrexate	75	0.7640	resveratrol	3
0.7805	5162773	7	0.7724	cytochalasin_B	100
0.7828	sanguinarine	89	0.7824	piperlongumine	40
0.7891	exemestane	49	0.7858	tyrphostin_AG-825	14
0.7901	ciclopirox	3	0.7896	HC_toxin	16
0.7902	digitoxigenin	63	0.7934	trifluridine	3
0.7937	harmine	32	0.7996	MG-262	40
0.8000	alsterpaullone	14			
0.8006	ellipticine	14			
0.8010	menadione	89			
0.8027	dopamine	44			
0.8041	sulindac_sulfide	91			
Distance	Community		Distance	Community	
0.0888	32		0.0978	14	
0.1174	14		0.1458	3	
0.1434	3		0.19	16	
0.2581	89		0.2374	32	
0.3798	75		0.3955	40	

Community Enriched for CDK/Topo inhibition