

Hsp90 Inhibitors, Part 2: Combining Ligand-Based and Structure-Based Approaches for Virtual Screening Application

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SUPPORTING INFORMATION

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Table S1. Data set used for LB/SB alignment assessment

entry ^a	PDB Code	IC ₅₀ ATPase(μ M)	pIC ₅₀ ^b
1	1UY8	75	4.12
2	1UYC	41	4.39
3	1UYD	200	3.70
4	1UYE	200	3.70
5	1UYG	53.5	4.27
6	1UYH	14.3	4.84
7	1UYK	17.1	4.77
13	2BT0	5.7	5.24
14	2CCS	8.2	5.09
16	2CCU	1.3	5.89
17	3B25	9.6	5.02
18	3B26	6.9	5.16
20	3B28	3	5.52
21	3OWB	0.88	6.06
22	3OWD	0.55	6.26

^aEntry numbers are referred to the original paper (Table 1)¹

^bpIC₅₀ = -Log [IC₅₀ATPase(μ M) x 10⁻⁶]

¹Ballante, F.; Caroli, A.; Wickersham III, R. B.; Ragno, R., Hsp90 Inhibitors (I). Definition of 3-D QSAutogrid/R Models as a Tool for Virtual Screening *Journal of Chemical Information and Modeling* 2014, <http://dx.doi.org/10.1021/ci400759t>.

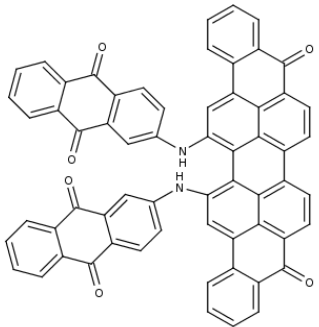
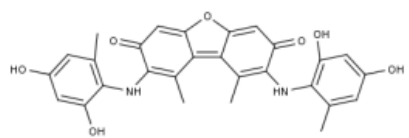
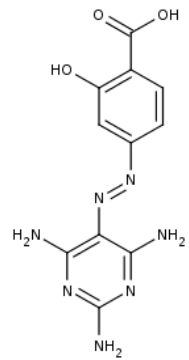
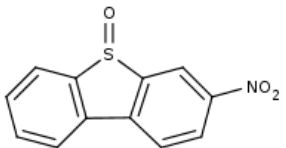
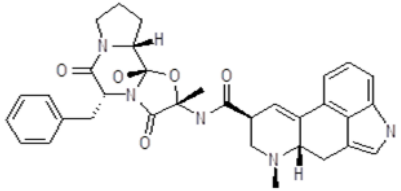
Table S2. Top 80 compounds selected by the VS procedure from the NCI Diversity Set

NCI ID	Autodock/3-D QSAR		Surflex/3-D QSAR		Autodock SF		Final Score	Rank
	BC	BC Score	MAXS	MAXS Score	Energy BC	Energy BC Score		
3364	7.183	1	6.577	22	-10.77	27	50	1
177383	6.534	42	6.534	34	-9.54	114	190	2
64111	6.394	82	6.28	127	-10.27	52	261	3
145612	6.647	16	6.245	172	-9.94	73	261	4
122140	6.504	48	6.486	45	-9.13	191	284	5
109197	6.382	88	6.194	217	-9.6	106	411	6
263220	6.173	259	6.416	64	-9.74	89	412	7
170578	6.226	211	6.226	188	-10.01	67	466	8
59620	6.498	49	6.168	239	-9.18	185	473	9
70127	6.579	35	6.288	120	-8.43	336	491	10
305831	6.012	429	6.571	24	-10.29	50	503	11
18877	6.096	335	6.332	98	-9.92	80	513	12
62914	6.103	328	6.829	3	-8.76	254	585	13
90318	6.046	384	6.435	57	-9.35	146	587	14
371688	6.334	112	6.053	376	-9.47	124	612	15
99543	6.237	196	6.236	176	-8.56	300	672	16
57725	6.089	341	6.315	110	-8.94	223	674	17
93352	6.739	9	5.803	673	-13.05	2	684	18
610930	6.498	50	6.288	121	-7.84	525	696	19
119889	6.146	285	6.232	183	-8.87	235	703	20
12363	5.911	572	6.335	97	-10.55	35	704	21
99550	6.28	158	6.003	442	-9.37	137	737	22
174267	6.506	47	6.506	42	-7.5	650	739	23
8797	6.603	29	5.99	460	-8.73	259	748	24
12181	6.029	404	6.128	290	-9.96	71	765	25
159631	6.612	24	6.323	106	-7.53	636	766	26

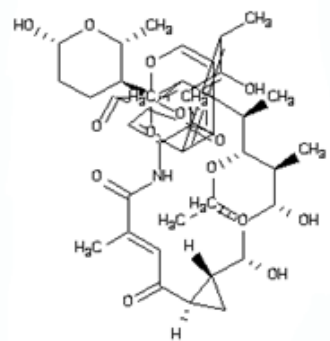
62349	5.935	541	6.437	55	-9.11	195	791	27
134755	5.929	551	6.233	179	-9.98	70	800	28
114449	6.169	262	6.144	268	-8.65	280	810	29
18312	6.169	261	6.271	135	-8.17	415	811	30
77037	6.636	19	5.742	749	-10.35	45	813	31
371880	6.069	359	6.157	253	-9.03	211	823	32
154389	6.436	67	6.252	160	-7.59	609	836	33
111326	6.208	224	5.899	567	-10.35	46	837	34
371682	5.858	659	6.272	134	-10.27	53	846	35
632536	6.466	57	6.363	82	-7.34	719	858	36
90615	6.593	34	6.634	15	-7.13	811	860	37
150817	5.88	629	6.581	21	-9.03	210	860	38
69573	5.858	658	6.582	20	-9.04	207	885	39
23833	6.353	101	6.165	241	-7.76	547	889	40
11668	6.207	226	6.208	197	-7.99	474	897	41
351123	6.022	415	6.325	105	-8.29	379	899	42
32673	6.154	275	6.326	104	-7.85	520	899	43
132498	5.997	449	6.022	414	-10.46	40	903	44
119886	6.295	136	5.82	662	-9.59	107	905	45
124029	5.957	502	6.083	348	-10.23	55	905	46
123993	6.672	14	6.252	158	-7.3	733	905	47
372060	5.696	899	6.736	8	-11.54	10	917	48
136472	6.17	260	6.053	375	-8.52	309	944	49
13726	5.882	625	6.125	292	-10.77	28	945	50
45236	5.879	632	6.892	2	-8.47	319	953	51
23128	5.697	892	6.411	66	-13.14	1	959	52
65828	5.853	664	6.405	69	-8.77	251	984	53
79563	6.574	38	5.747	742	-9.04	208	988	54
82802	5.883	623	6.394	72	-8.56	299	994	55
117285	6.212	217	5.932	526	-8.76	255	998	56
37245	5.938	534	6.108	308	-9.28	159	1001	57
118068	6.01	430	6.075	358	-9	216	1004	58

109593	5.911	573	6.519	39	-8.22	396	1008	59
109483	6.392	83	6.353	89	-7.06	839	1011	60
321578	6.271	166	5.834	648	-9.08	198	1012	61
7520	5.925	561	6.048	384	-9.92	79	1024	62
319440	5.809	733	6.416	65	-8.92	229	1027	63
42258	6.21	221	5.949	504	-8.54	305	1030	64
320870	6.343	106	6.344	93	-7.03	847	1046	65
112671	5.738	840	6.448	51	-9.3	155	1046	66
164460	6.388	85	6.535	33	-6.89	929	1047	67
360494	5.941	527	6.241	173	-8.36	358	1058	68
45208	5.933	543	6.284	123	-8.2	401	1067	69
45238	6.56	40	5.916	546	-7.98	481	1067	70
35949	6.284	154	5.83	652	-8.71	264	1070	71
95090	5.793	760	6.135	282	-10.76	29	1071	72
131612	5.99	457	5.879	603	-11.39	11	1071	73
126401	5.942	523	6.265	151	-8.21	400	1074	74
23173	6.764	8	5.886	589	-7.97	483	1080	75
95025	6.126	305	6.088	334	-8.07	448	1087	76
47949	6.049	377	5.89	580	-9.42	132	1089	77
13028	6.108	326	6.364	81	-7.41	682	1089	78
19976	5.792	763	6.142	271	-10.08	57	1091	79
52440	6.38	89	6	447	-7.72	559	1095	80

Table S3. Compounds with inhibitory activity

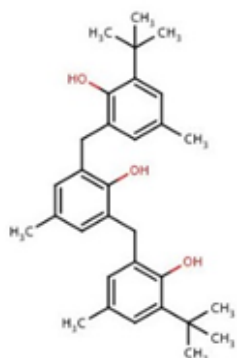
#	NCI ID	MW	Compound color	IC50 [μM]	
1		23128	899	dark brown	18
2		610930	500.51	dark brown	32
3		117285	289.25	dark brown	49
4		170578	245.25	clear	63
5		95090	581.67	brown	220

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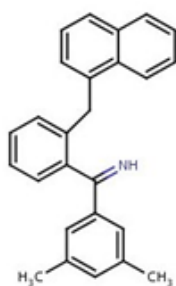
177383 822.9 dark brown 393

7



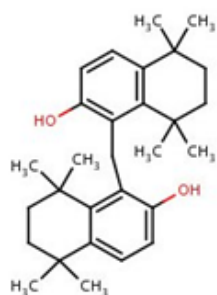
62914 460.66 clear >500

8



99543 349.47 yellowish >500

9



109197 420.63 clear >500