

Identifying new topoisomerase II poison scaffolds by combining publicly available toxicity data and 2D/3D-based virtual screening – Additional Information

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1 Additional Text

Commands used for ROCS (OpenEye Scientific Software, Santa Fe, NM) similarity calculations:

1) generate 3D conformers using OMEGA: `omega2 -mpi_np <n> -in <input> -out <output> -prefix <P> -strictstereo false`

n: number of processors n in MPI mode

input: the input sd file

output: the file containing the 3D conformers, used as input when running ROCS

strictstereo false: when stereocenters are not defined, random stereocenters are defined during the conformer generation

2) run ROCS to compare the structures: `rocs -mpi_np <n> -query <qfile> -dbase <dfile> mcquery true -rankby TanimotoCombo -stats best -subrocs -scoreonly`

n: number of processors n in MPI mode

mcquery: combine contiguous conformers in the query file into a multi-conformer query molecule

qfile: file containing the query molecule dfile: file containing the molecules to overlay against query

rankby ShapeTanimoto: rank molecular overlay by shape and color

stats best: the report includes stats for the best overlay(s) for every dbase molecule

subrocs: start the search at all heavy atoms of the larger molecule as well as the default inertial starts

scoreonly: perform scoring calculation only

Commands used for CFP (ChemAxon Ltd., Budapest, Hungary) similarity calculations:

`screenmd <target.sdf> <query.sdf> -k CF -c <cfp.xml> -M Tanimoto -e 2 -o <output.txt>`

target.sdf: sd file containing the target molecule(s)

query.sdf: sd file containing the query molecule(s)

-k CF: use the CFP descriptor

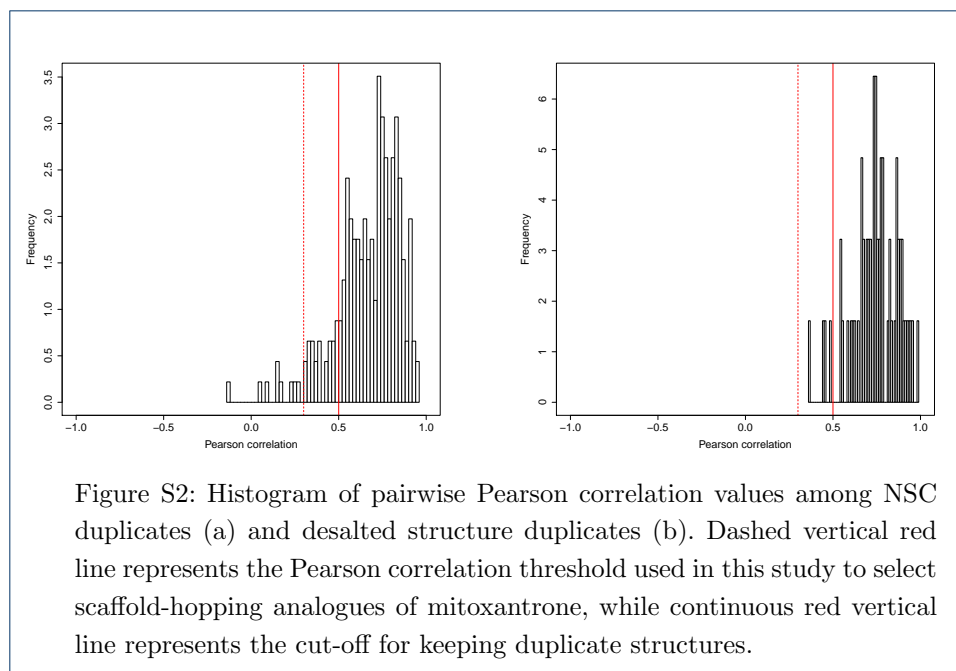
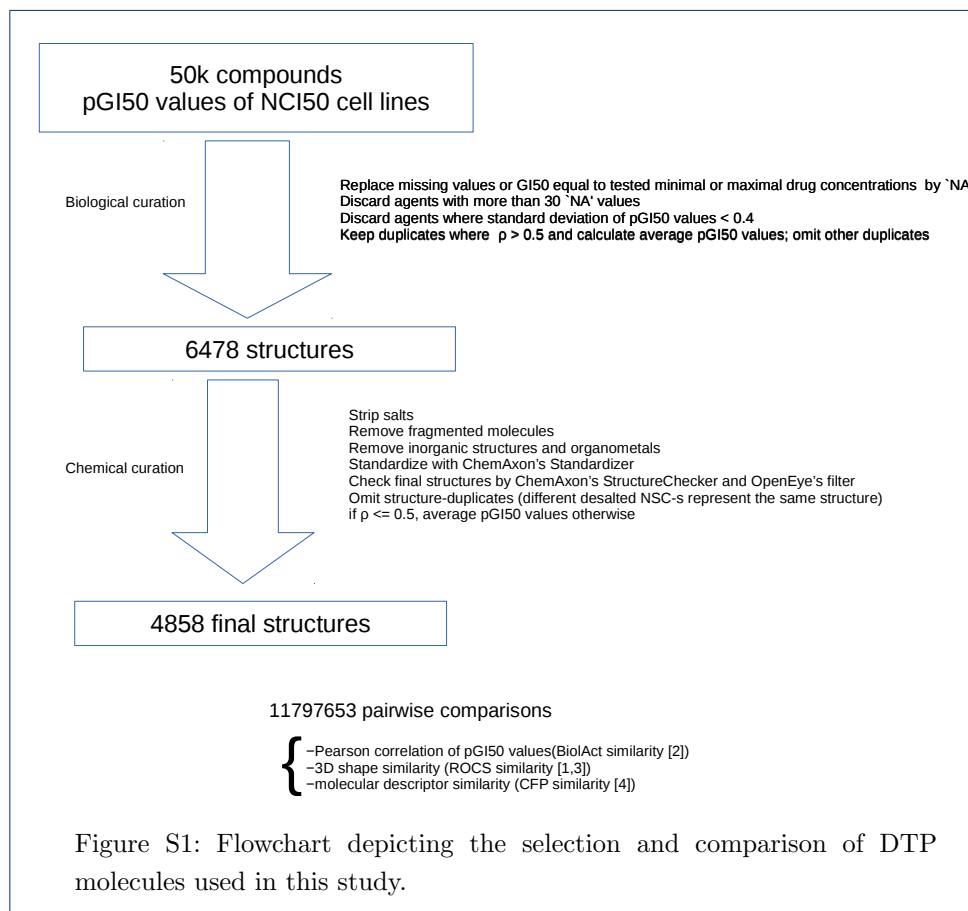
cfp.xml: the config file used, the cfp.xml available from `jchem16.7/examples/config`, where the Tanimoto threshold was set to 1.0, in order to report all similarity values

-M Tanimoto: use the metric Tanimoto as specified in the config file

-e 2: two decimal places after the decimal point

output.txt: the name of the output file

2 Additional Figures



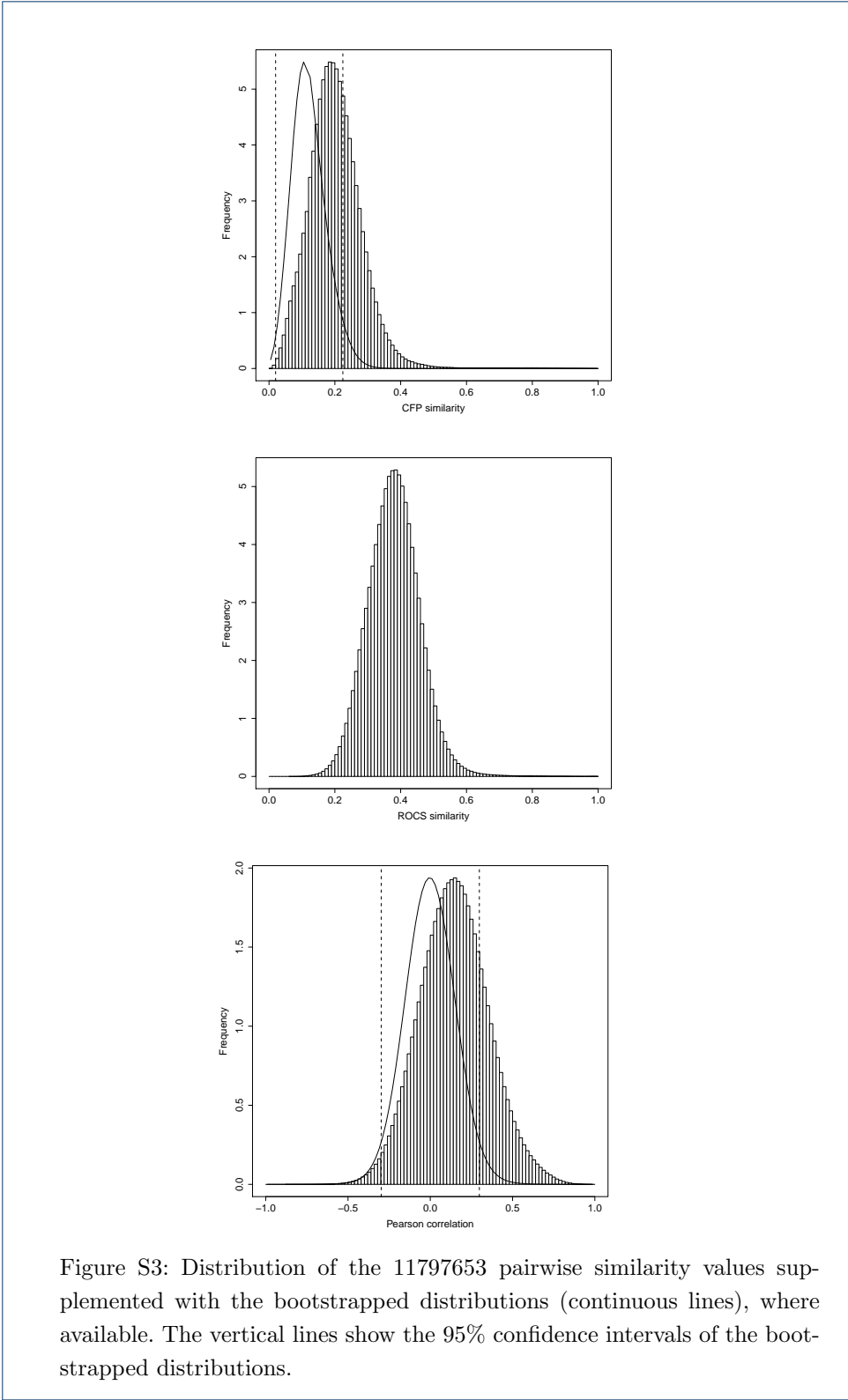
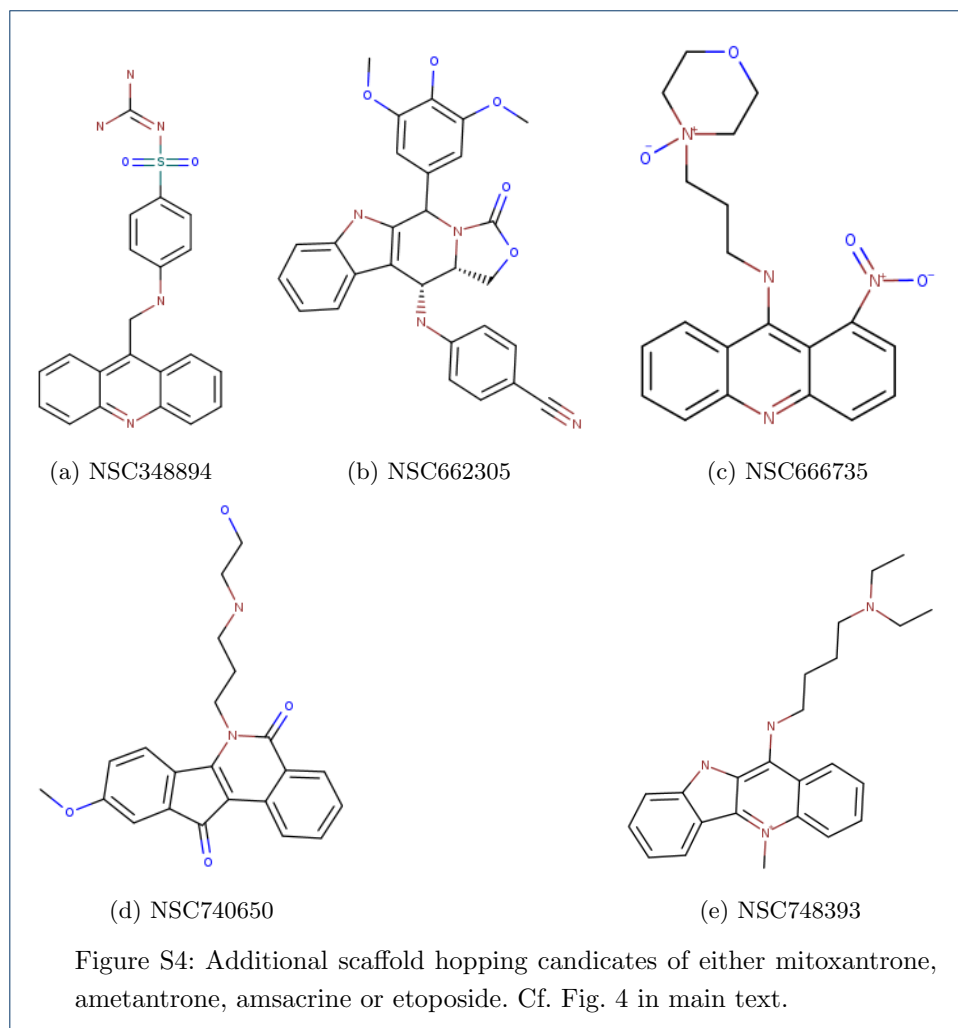
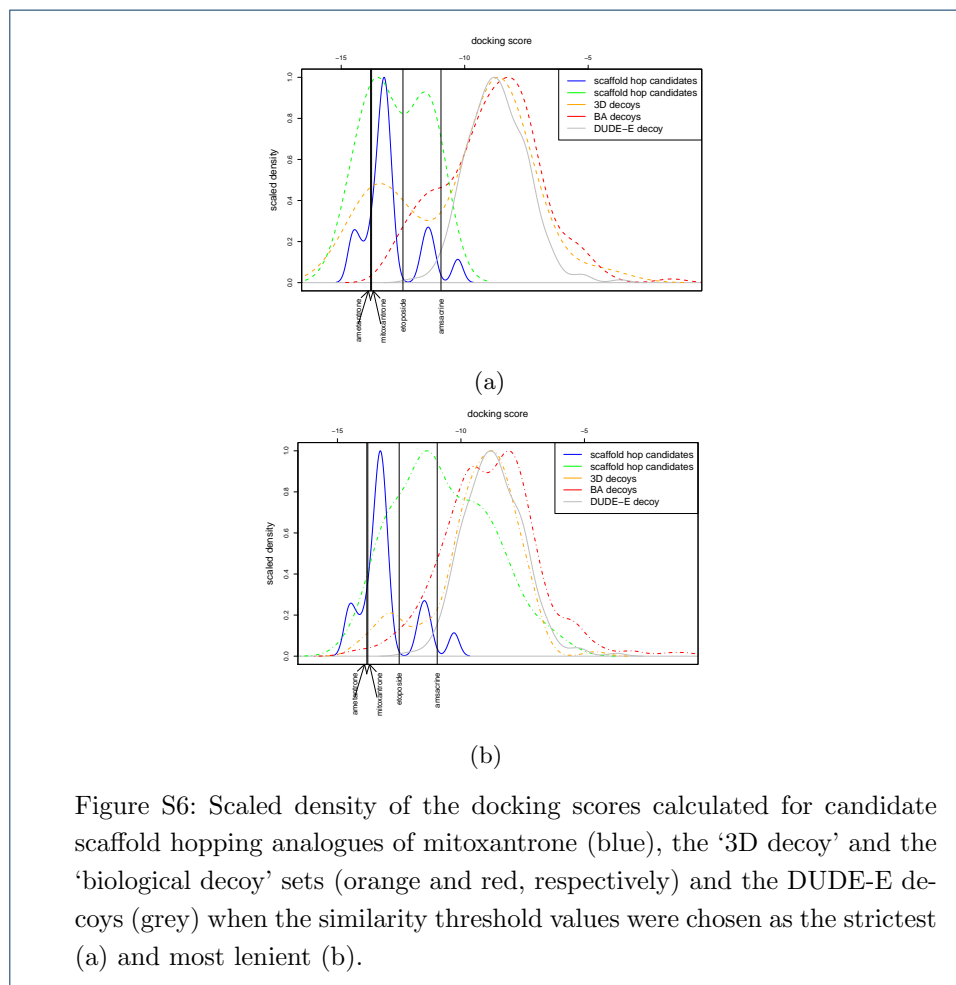
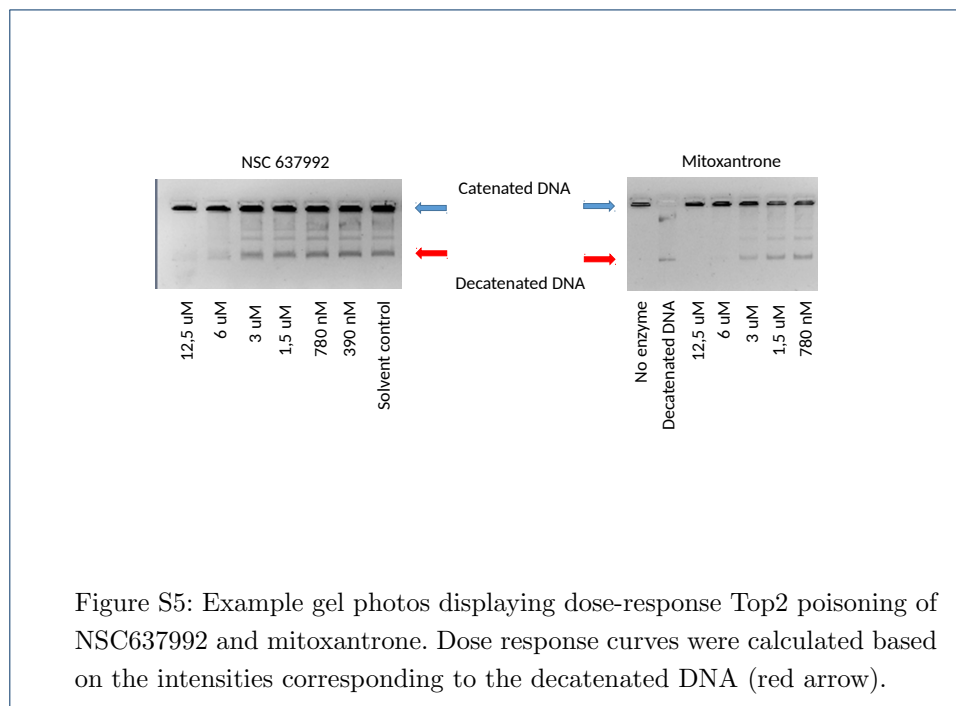


Figure S3: Distribution of the 11797653 pairwise similarity values supplemented with the bootstrapped distributions (continuous lines), where available. The vertical lines show the 95% confidence intervals of the bootstrapped distributions.





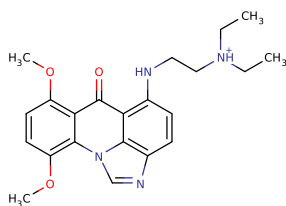


Figure S7: NSC660839, the '3D decoy' molecule tested in the *in vitro* decatenation assay.

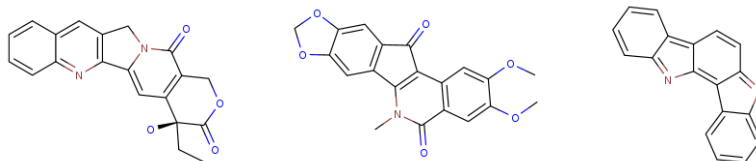


Figure S8: Known Top1 inhibitor scaffolds: camptothecins (NSC94600), indenoisoquinolines (NSC314622), indolocarbazoles.

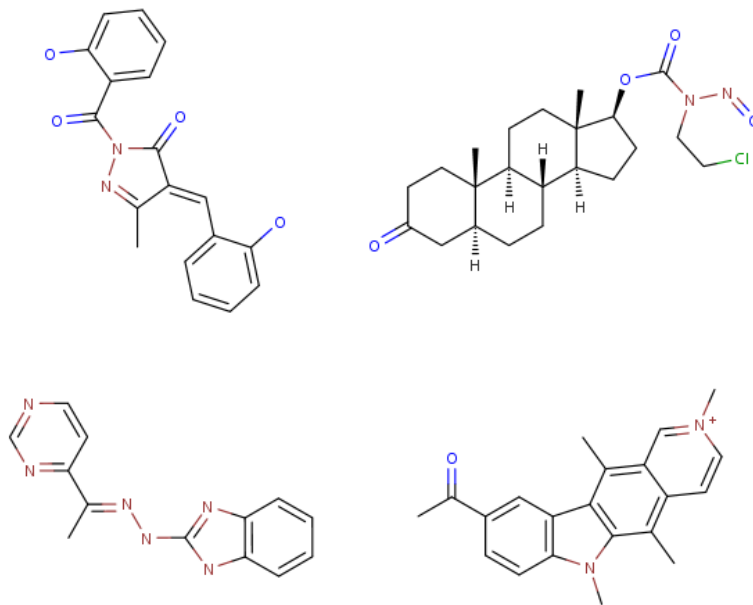


Figure S9: Scaffold hopping candidates of camptothecin obtained using threshold values $BA > 0.49$, $ROCS > 0.51$, $CFP \leq 0.34$.

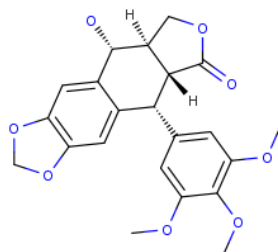
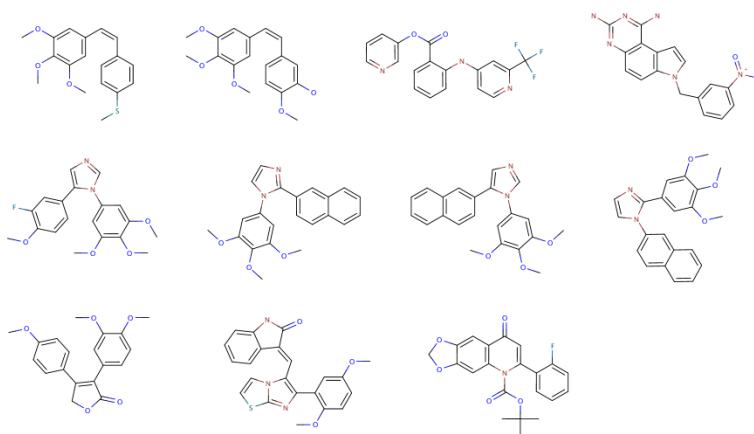


Figure S10: NSC24818 (podofilox).

Figure S11: Scaffold hopping candidates of NSC24818 obtained using threshold values $BA > 0.41$, $ROCS > 0.48$, $CFP \leq 0.30$.

3 Additional Tables

Table S1: Pearson correlation (BiolAct similarity) of the pIC50 values of annotated Top2 poisons to mitoxantrone.

name	NSC	BiolAct
ametantrone	196473	0.80
daunorubicin	83142	0.70
idarubicin	256439	0.72
N,N-dibenzyl Daunorubicin	268242	0.43
epirubicin	256942	0.65
doxorubicin	123127	0.80
rubidazon	164011	0.83
valrubicin	246131	0.79
menogaril	269148	0.85
piroxastrone	349174	0.89
bisantrene	337766	0.61
amsacrine	249992	0.87
2-methyllellipticinium	351710	0.44
2-N-Methyl-6-thiaellipticinium iodide	638066	0.59
etoposide	141540	0.66
teniposide	122819	0.86
dexrazoxane	169780	0.57

Table S2: Selected similarity thresholds to identify putative scaffold hopping analogues of mitoxantrone.

metric	threshold
BA	0.55
CFP	0.32
ROCS	0.51

Table S3: Docking scores and rankings (from 1173 compounds) of mitoxantrone and its scaffold hopping candidates.

chemotype	NSC	docking	rank
mitoxantrone	301739	-13.138	38
lucanthone derivatives	317003	-11.307	208
	317921	-11.474	187
	334352	-11.672	154
triazoloacridinones	645829	-13.412	24
	699148	-10.28	348
pyrimidoacridines	693117	-13.187	37
	693118	-14.476	2
	693119	-13.533	18
	693120	-14.573	1
	691849	-13.812	12
sedoxantrone	691852	-14.172	7
	635371	-13.322	32
imidazoacridinones	637991	-13.66	15
	637992	-13.254	35
	637994	-13.254	34
	645808	-13.326	31
	645809	-13.004	47
	645810	-13.269	33
5-substituted-9-aminoacridine 4 carboxamides	691240	-13.083	39
	693545	-12.952	52

Table S4: Maximum of biological, ROCS and 2D similarities compared to mitoxantrone, ametantrone, amsacrine or etoposide. Additionally, docking scores of these compounds.

NSC	BiolAct	ROCS	CFP	docking
348894	0.87	0.6	0.34	-11.23
662305	0.75	0.53	0.37	-12.72
666735	0.56	0.55	0.33	-9.47
740650	0.68	0.54	0.33	-13.00
748393	0.58	0.53	0.31	-12.12

Table S5: Similarities compared to published Top2 ligands and docking scores of 3D decoy agents.

NSC	lead	BiolAct	ROCS	CFP	docking
69600	amsacrine	0.07	0.54	0.32	-7.93
87034	amsacrine	0.10	0.57	0.28	-8.30
131734	amsacrine	0.43	0.59	0.32	-9.38
175636	amsacrine	0.43	0.54	0.18	-9.82
175639	amsacrine	0.34	0.54	0.24	-9.73
201873	amsacrine	-0.06	0.61	0.19	-8.82
208652	mitoxantrone	0.13	0.58	0.24	-6.67
225112	mitoxantrone	0.28	0.57	0.27	-7.93
280594	amsacrine	0.12	0.53	0.20	-8.56
348401	amsacrine	0.36	0.57	0.21	-7.12
348402	amsacrine	0.20	0.56	0.22	-7.38
601518	amsacrine	0.41	0.69	0.26	-9.34
612115	mitoxantrone	0.37	0.52	0.30	-7.10
625537	amsacrine	0.16	0.53	0.19	-9.59
627891	amsacrine	0.39	0.52	0.30	-8.09
637729	amsacrine	0.16	0.53	0.17	-8.53
637993	mitoxantrone	0.38	0.53	0.28	-12.47
645812	mitoxantrone	0.18	0.53	0.29	-12.72
645813	ametrantrone	0.31	0.54	0.22	-12.97
645827	mitoxantrone	0.36	0.56	0.26	-12.74
645828	mitoxantrone	0.41	0.56	0.26	-12.30
645830	mitoxantrone	0.48	0.55	0.24	-12.91
647751	ametrantrone	0.51	0.53	0.22	-12.02
648211	amsacrine	-0.03	0.52	0.25	-10.26
652183	amsacrine	0.31	0.54	0.18	-7.91
652884	amsacrine	0.26	0.53	0.33	-9.80
657348	ametrantrone	0.20	0.59	0.24	-8.90
659998	mitoxantrone	0.14	0.54	0.31	-8.21
659999	mitoxantrone	0.14	0.52	0.32	-8.37
660638	mitoxantrone	0.23	0.53	0.33	-9.70
660839	mitoxantrone	0.13	0.61	0.28	-12.76
660840	mitoxantrone	0.19	0.61	0.27	-12.86
660841	mitoxantrone	0.39	0.55	0.29	-12.51
664000	amsacrine	0.06	0.52	0.18	-8.46
664878	amsacrine	0.39	0.53	0.21	-8.13
665378	amsacrine	0.19	0.59	0.23	-8.66
665492	amsacrine	0.28	0.53	0.22	-9.61
665700	amsacrine	0.01	0.52	0.21	-8.88
666735	amsacrine	0.29	0.55	0.33	-9.46
667645	amsacrine	-0.05	0.53	0.33	-10.62
668495	mitoxantrone	-0.10	0.61	0.27	-8.08
669381	amsacrine	0.43	0.56	0.22	-8.71
669888	amsacrine	0.16	0.57	0.22	-9.29
669943	amsacrine	0.10	0.52	0.22	-9.20
673350	ametrantrone	0.37	0.56	0.32	-9.06
673805	amsacrine	0.11	0.53	0.33	-9.81
674220	mitoxantrone	0.25	0.55	0.25	-8.22
674256	amsacrine	0.31	0.56	0.20	-8.37
674257	amsacrine	0.35	0.57	0.20	-8.29
674258	amsacrine	0.44	0.60	0.25	-8.41
675370	amsacrine	0.10	0.55	0.22	-8.91
675985	mitoxantrone	0.39	0.53	0.24	-9.81
676514	amsacrine	0.12	0.56	0.30	-9.50
678866	amsacrine	0.29	0.53	0.19	-8.16
679813	mitoxantrone	0.33	0.56	0.12	-4.56
680781	amsacrine	0.25	0.53	0.15	-7.37
682011	amsacrine	0.08	0.54	0.28	-11.46
687308	mitoxantrone	0.29	0.56	0.21	-14.20
687311	amsacrine	0.24	0.77	0.26	-8.89
691850	mitoxantrone	0.51	0.57	0.24	-13.52
691851	mitoxantrone	0.27	0.56	0.25	-13.68
692309	amsacrine	0.03	0.52	0.22	-7.89
692646	amsacrine	0.28	0.65	0.27	-8.95
692738	ametrantrone	0.24	0.52	0.30	-12.96
693246	amsacrine	0.34	0.52	0.25	-7.39
693255	mitoxantrone	-0.10	0.54	0.23	-6.78
693620	amsacrine	0.30	0.53	0.22	-7.59

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NSC	lead	BiolAct	ROCS	CFP	docking
695177	amsacrine	0.41	0.55	0.27	-7.28
696991	mitoxantrone	-0.00	0.53	0.31	-7.15
698959	mitoxantrone	0.38	0.54	0.24	-13.35
698960	mitoxantrone	0.39	0.56	0.23	-13.35
699147	ametrantrone	0.23	0.53	0.22	-11.33
699149	ametrantrone	0.44	0.53	0.21	-10.93
699152	mitoxantrone	0.40	0.54	0.26	-10.91
700415	amsacrine	0.17	0.53	0.19	-11.60
701023	amsacrine	0.26	0.52	0.22	-10.18
710546	mitoxantrone	0.28	0.54	0.20	-12.91
710547	mitoxantrone	0.03	0.53	0.23	-14.07
710548	mitoxantrone	0.46	0.53	0.23	-14.02
710549	ametrantrone	0.15	0.53	0.21	-13.37
711725	amsacrine	0.27	0.56	0.30	-8.44
719923	amsacrine	0.33	0.58	0.22	-8.06
720558	amsacrine	-0.00	0.70	0.34	-10.69
720563	amsacrine	0.02	0.53	0.30	-8.55
720570	amsacrine	0.16	0.77	0.33	-10.19
720688	mitoxantrone	0.11	0.53	0.24	-12.74
723394	mitoxantrone	0.24	0.53	0.28	-6.96
723423	ametrantrone	0.25	0.70	0.17	-9.06
724686	amsacrine	0.30	0.70	0.33	-9.55
724693	amsacrine	0.04	0.64	0.28	-9.92
724699	amsacrine	0.30	0.58	0.33	-9.11
726438	ametrantrone	0.10	0.53	0.31	-11.17
727450	amsacrine	0.05	0.55	0.33	-10.20
727885	amsacrine	0.21	0.54	0.18	-9.01
731164	mitoxantrone	0.23	0.53	0.24	-8.42
734631	amsacrine	0.26	0.53	0.29	-9.11
736793	amsacrine	0.30	0.52	0.18	-9.89
740650	ametrantrone	0.51	0.54	0.28	-13.00
744231	ametrantrone	0.36	0.55	0.22	-11.51
745450	amsacrine	0.22	0.55	0.24	-8.58
745455	amsacrine	0.27	0.54	0.24	-8.66
745750	mitoxantrone	-0.18	0.53	0.26	-9.00
748392	amsacrine	0.20	0.54	0.31	-12.65
748393	amsacrine	0.25	0.53	0.31	-12.12
748533	amsacrine	0.18	0.58	0.22	-8.64
748870	amsacrine	0.24	0.52	0.23	-10.24
749804	amsacrine	0.16	0.55	0.22	-8.70
751830	amsacrine	-0.03	0.56	0.28	-8.62

Table S6: Similarities compared to published Top2 ligands and docking scores of biological activity decoy agents.

NSC	lead	BiolAct	ROCS	CFP	docking
762	mitoxantrone	0.60	0.17	0.05	-4.67
3424	mitoxantrone	0.59	0.42	0.27	-10.14
4623	etoposide	0.61	0.27	0.15	-6.89
6171	ametrantrone	0.55	0.24	0.06	-5.42
6396	mitoxantrone	0.72	0.19	0.05	-5.23
9706	mitoxantrone	0.73	0.36	0.08	-6.15
12150	ametrantrone	0.55	0.34	0.26	-10.37
12455	ametrantrone	0.53	0.30	0.22	-4.38
19781	etoposide	0.61	0.33	0.16	-6.71
22709	etoposide	0.55	0.17	0.10	-5.97
22984	etoposide	0.59	0.21	0.16	-5.97
26821	etoposide	0.60	0.28	0.11	-7.81
26980	mitoxantrone	0.74	0.40	0.20	-9.46
29228	etoposide	0.57	0.22	0.02	-2.96
30706	etoposide	0.61	0.21	0.11	-7.12
31717	amsacrine	0.58	0.31	0.08	-7.78
32065	mitoxantrone	0.54	0.14	0.04	-5.38
34462	mitoxantrone	0.72	0.30	0.14	-7.57
35915	mitoxantrone	0.69	0.25	0.11	-8.60
48006	amsacrine	0.52	0.40	0.16	-8.21

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NSC	lead	BiolAct	ROCS	CFP	docking
48034	mitoxantrone	0.70	0.32	0.24	-8.07
48956	mitoxantrone	0.60	0.29	0.25	-8.05
49520	etoposide	0.52	0.24	0.14	-8.13
50273	amsacrine	0.52	0.41	0.22	-7.92
56410	mitoxantrone	0.69	0.39	0.20	-10.48
57199	mitoxantrone	0.66	0.34	0.31	-8.52
58514	mitoxantrone	0.53	0.10	0.28	-8.59
62709	mitoxantrone	0.56	0.34	0.24	-6.72
63878	mitoxantrone	0.62	0.31	0.17	-8.48
64703	mitoxantrone	0.64	0.34	0.24	-8.01
72151	amsacrine	0.61	0.31	0.23	-7.98
73735	etoposide	0.62	0.32	0.25	-7.35
75520	mitoxantrone	0.54	0.39	0.19	-8.47
76919	mitoxantrone	0.60	0.34	0.27	-7.46
79037	etoposide	0.59	0.24	0.07	-5.56
80103	mitoxantrone	0.61	0.28	0.11	-8.60
81767	amsacrine	0.67	0.39	0.21	-8.38
82587	mitoxantrone	0.60	0.31	0.29	-9.52
83343	amsacrine	0.56	0.39	0.21	-7.88
85230	mitoxantrone	0.72	0.35	0.25	-8.92
86371	etoposide	0.59	0.31	0.22	-10.25
90810	etoposide	0.63	0.30	0.14	-7.67
92497	etoposide	0.62	0.22	0.13	-6.54
92498	etoposide	0.57	0.21	0.14	-6.97
92499	etoposide	0.57	0.20	0.14	-6.66
94600	mitoxantrone	0.63	0.37	0.27	-9.63
95382	mitoxantrone	0.73	0.35	0.26	-8.78
95466	mitoxantrone	0.60	0.31	0.12	-6.68
98572	amsacrine	0.53	0.43	0.18	-8.35
99445	mitoxantrone	0.53	0.36	0.18	-8.95
103704	amsacrine	0.54	0.40	0.15	-8.03
105132	mitoxantrone	0.69	0.37	0.27	-9.42
107124	mitoxantrone	0.68	0.42	0.27	-10.70
107392	etoposide	0.53	0.23	0.13	-7.96
111533	mitoxantrone	0.74	0.37	0.27	-9.34
112758	ametantrone	0.70	0.40	0.28	-10.33
112965	amsacrine	0.67	0.43	0.17	-7.36
114346	etoposide	0.56	0.33	0.30	-8.51
122870	amsacrine	0.57	0.35	0.24	-7.95
123115	mitoxantrone	0.66	0.39	0.20	-9.32
124147	ametantrone	0.58	0.36	0.21	-7.76
126849	amsacrine	0.54	0.36	0.13	-7.87
127763	etoposide	0.62	0.33	0.24	-9.14
128687	etoposide	0.65	0.33	0.26	-7.58
129943	amsacrine	0.58	0.38	0.06	-8.43
131547	ametantrone	0.56	0.36	0.23	-10.88
132313	mitoxantrone	0.70	0.31	0.05	-4.38
134459	etoposide	0.59	0.25	0.12	-6.90
134679	mitoxantrone	0.52	0.41	0.17	-8.70
134723	mitoxantrone	0.62	0.40	0.20	-9.10
134725	mitoxantrone	0.62	0.40	0.20	-9.19
134727	mitoxantrone	0.65	0.46	0.20	-9.51
135758	mitoxantrone	0.65	0.32	0.11	-9.45
135962	ametantrone	0.55	0.33	0.15	-7.55
138429	etoposide	0.55	0.39	0.31	-7.38
140701	mitoxantrone	0.71	0.34	0.18	-11.32
141537	etoposide	0.53	0.30	0.27	-6.98
143095	amsacrine	0.54	0.41	0.18	-6.97
143491	ametantrone	0.67	0.40	0.28	-11.57
145668	amsacrine	0.72	0.37	0.16	-9.29
146268	amsacrine	0.53	0.40	0.14	-8.66
146396	mitoxantrone	0.53	0.36	0.33	-8.88
146397	ametantrone	0.56	0.35	0.18	-10.19
149584	ametantrone	0.70	0.35	0.27	-11.08
150862	mitoxantrone	0.52	0.16	0.24	-11.87
152731	ametantrone	0.54	0.43	0.19	-10.11
154318	mitoxantrone	0.70	0.41	0.22	-10.71
155693	ametantrone	0.53	0.39	0.19	-11.06
155694	ametantrone	0.59	0.42	0.19	-11.62
156305	mitoxantrone	0.65	0.40	0.18	-10.58

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NSC	lead	BiolAct	ROCS	CFP	docking
157995	ametantrone	0.53	0.37	0.16	-10.20
162062	etoposide	0.53	0.26	0.12	-6.48
166199	mitoxantrone	0.66	0.31	0.10	-6.74
166224	amsacrine	0.56	0.34	0.21	-7.36
166237	etoposide	0.69	0.32	0.23	-8.08
166641	mitoxantrone	0.54	0.33	0.18	-9.54
167780	etoposide	0.69	0.29	0.28	-7.89
169534	ametantrone	0.68	0.40	0.28	-10.37
176323	amsacrine	0.70	0.40	0.26	-8.73
176878	ametantrone	0.54	0.27	0.20	-7.18
177365	ametantrone	0.53	0.34	0.20	-10.98
178248	mitoxantrone	0.57	0.32	0.14	-7.46
180510	ametantrone	0.60	0.40	0.29	-11.83
182986	mitoxantrone	0.68	0.38	0.13	-7.13
184692	amsacrine	0.54	0.35	0.23	-7.99
196473	etoposide	0.64	0.39	0.23	-13.45
201290	etoposide	0.58	0.30	0.25	-8.77
207895	mitoxantrone	0.55	0.40	0.26	-9.36
221265	ametantrone	0.68	0.34	0.28	-12.38
234714	amsacrine	0.69	0.44	0.07	-6.66
237538	mitoxantrone	0.53	0.30	0.17	-7.81
239336	etoposide	0.71	0.26	0.25	-6.98
243928	mitoxantrone	0.80	0.37	0.21	-11.01
243929	mitoxantrone	0.69	0.36	0.21	-10.82
243930	mitoxantrone	0.72	0.35	0.20	-9.46
249910	mitoxantrone	0.58	0.37	0.26	-8.71
249911	mitoxantrone	0.67	0.38	0.26	-9.72
249992	ametantrone	0.64	0.39	0.19	-10.94
250684	mitoxantrone	0.55	0.28	0.19	-9.35
250686	etoposide	0.60	0.29	0.25	-7.85
256438	amsacrine	0.69	0.37	0.18	-10.74
259968	ametantrone	0.53	0.26	0.25	-6.53
259969	ametantrone	0.59	0.26	0.24	-5.81
260610	ametantrone	0.56	0.29	0.23	-11.24
266068	mitoxantrone	0.52	0.31	0.26	-9.24
267707	etoposide	0.57	0.30	0.29	-6.83
268965	amsacrine	0.65	0.38	0.19	-7.78
269719	mitoxantrone	0.58	0.35	0.16	-8.46
269720	amsacrine	0.55	0.42	0.12	-6.79
269721	mitoxantrone	0.58	0.35	0.15	-7.75
275656	mitoxantrone	0.70	0.35	0.13	-6.93
280074	etoposide	0.56	0.27	0.28	-8.37
281272	mitoxantrone	0.55	0.33	0.16	-8.37
281612	amsacrine	0.62	0.41	0.19	-8.32
281613	mitoxantrone	0.57	0.27	0.27	-7.69
281617	mitoxantrone	0.54	0.27	0.28	-9.05
281817	mitoxantrone	0.53	0.27	0.27	-9.44
281818	mitoxantrone	0.53	0.26	0.29	-7.19
284682	amsacrine	0.56	0.35	0.19	-9.78
286628	ametantrone	0.54	0.37	0.27	-11.34
292463	etoposide	0.57	0.29	0.29	-5.93
294980	mitoxantrone	0.67	0.28	0.21	-6.99
295499	mitoxantrone	0.76	0.39	0.26	-9.41
295500	mitoxantrone	0.83	0.38	0.27	-9.27
295501	mitoxantrone	0.53	0.38	0.27	-10.03
296934	mitoxantrone	0.62	0.40	0.11	-5.44
300288	mitoxantrone	0.76	0.45	0.28	-11.14
301477	ametantrone	0.62	0.39	0.27	-11.09
301480	amsacrine	0.52	0.38	0.18	-8.67
301739	etoposide	0.75	0.38	0.31	-13.14
302325	amsacrine	0.53	0.40	0.17	-8.49
302991	amsacrine	0.66	0.39	0.25	-9.63
303812	mitoxantrone	0.61	0.41	0.11	-7.98
307990	ametantrone	0.56	0.37	0.26	-10.84
314622	mitoxantrone	0.55	0.39	0.33	-9.64
319726	amsacrine	0.53	0.41	0.16	-7.63
324646	ametantrone	0.64	0.29	0.12	-8.67
328410	mitoxantrone	0.78	0.37	0.26	-8.88
331269	mitoxantrone	0.61	0.40	0.14	-5.88
332488	amsacrine	0.67	0.38	0.13	-5.36

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NSC	lead	BiolAct	ROCS	CFP	docking
333054	amsacrine	0.77	0.37	0.19	-10.52
335766	etoposide	0.57	0.30	0.27	-7.76
339705	mitoxantrone	0.62	0.41	0.30	-10.40
342443	ametrantrone	0.55	0.26	0.15	-11.05
344007	mitoxantrone	0.71	0.28	0.08	-6.84
344505	amsacrine	0.63	0.43	0.19	-9.25
348115	amsacrine	0.52	0.40	0.23	-10.09
348894	mitoxantrone	0.85	0.40	0.23	-11.23
350378	etoposide	0.54	0.36	0.25	-10.00
351520	etoposide	0.54	0.33	0.24	-9.22
353076	ametrantrone	0.56	0.43	0.20	-12.63
355457	mitoxantrone	0.53	0.37	0.34	-11.51
357885	etoposide	0.70	0.41	0.30	-14.19
360702	mitoxantrone	0.63	0.40	0.17	-7.97
364830	mitoxantrone	0.72	0.42	0.26	-9.39
365360	ametrantrone	0.69	0.30	0.25	-11.64
367428	amsacrine	0.66	0.34	0.09	-5.75
369395	amsacrine	0.60	0.38	0.24	-10.73
374028	mitoxantrone	0.69	0.40	0.27	-11.60
375575	amsacrine	0.59	0.40	0.16	-8.07
376254	mitoxantrone	0.58	0.36	0.30	-8.15
376739	ametrantrone	0.65	0.40	0.27	-9.25
378901	ametrantrone	0.61	0.39	0.27	-10.08
380212	amsacrine	0.53	0.40	0.18	-8.85
382001	etoposide	0.52	0.24	0.18	-7.73
382035	amsacrine	0.56	0.43	0.19	-8.43
400492	etoposide	0.58	0.26	0.16	-7.86
407335	mitoxantrone	0.56	0.33	0.17	-8.41
529180	amsacrine	0.60	0.40	0.17	-8.21
600167	mitoxantrone	0.59	0.28	0.18	-7.28
603071	amsacrine	0.60	0.38	0.25	-10.20
606172	mitoxantrone	0.66	0.40	0.27	-10.17
606173	mitoxantrone	0.77	0.43	0.26	-9.34
606174	amsacrine	0.55	0.37	0.25	-10.16
606497	mitoxantrone	0.69	0.42	0.26	-9.32
606498	mitoxantrone	0.62	0.41	0.26	-9.55
606499	mitoxantrone	0.82	0.42	0.26	-10.21
606985	mitoxantrone	0.58	0.39	0.26	-10.23
606986	amsacrine	0.67	0.37	0.25	-9.87
607347	mitoxantrone	0.57	0.33	0.08	-7.52
609699	mitoxantrone	0.67	0.38	0.28	-9.76
610456	mitoxantrone	0.56	0.38	0.26	-7.85
610457	mitoxantrone	0.57	0.40	0.26	-10.47
610458	mitoxantrone	0.79	0.34	0.26	-6.72
610459	mitoxantrone	0.67	0.40	0.26	-9.31
612828	amsacrine	0.58	0.43	0.14	-8.14
613327	mitoxantrone	0.54	0.34	0.19	-7.95
614049	etoposide	0.56	0.36	0.21	-11.78
616348	mitoxantrone	0.72	0.31	0.27	-10.52
617208	etoposide	0.57	0.22	0.20	-8.09
617806	etoposide	0.62	0.23	0.05	-7.21
617953	ametrantrone	0.52	0.43	0.25	-10.00
618939	mitoxantrone	0.67	0.42	0.26	-9.12
619003	amsacrine	0.84	0.35	0.18	-9.24
620480	mitoxantrone	0.61	0.29	0.25	-8.71
621199	etoposide	0.53	0.41	0.30	-10.14
623128	amsacrine	0.68	0.36	0.18	-9.84
623872	etoposide	0.65	0.26	0.20	-7.49
623905	etoposide	0.54	0.38	0.28	-8.11
624158	etoposide	0.58	0.33	0.12	-7.14
624414	etoposide	0.57	0.36	0.28	-9.66
624431	etoposide	0.57	0.41	0.32	-9.10
624432	etoposide	0.61	0.37	0.28	-8.25
624434	etoposide	0.52	0.27	0.28	-8.62
624851	etoposide	0.62	0.17	0.05	-5.45
625156	etoposide	0.53	0.28	0.22	-3.21
625174	etoposide	0.53	0.22	0.10	-6.86
626540	etoposide	0.53	0.37	0.21	-11.54
628497	mitoxantrone	0.63	0.43	0.28	-9.96
628498	mitoxantrone	0.53	0.44	0.26	-11.87

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NSC	lead	BiolAct	ROCS	CFP	docking
628662	amsacrine	0.87	0.37	0.22	-11.71
628663	ametrantrone	0.60	0.39	0.28	-12.42
628664	ametrantrone	0.57	0.37	0.29	-12.38
628665	mitoxantrone	0.70	0.38	0.34	-11.87
628666	mitoxantrone	0.70	0.37	0.33	-11.80
628667	amsacrine	0.83	0.36	0.22	-11.69
628668	ametrantrone	0.55	0.38	0.27	-12.48
628669	amsacrine	0.90	0.38	0.21	-12.20
628670	ametrantrone	0.53	0.38	0.29	-12.21
628671	amsacrine	0.83	0.39	0.21	-12.21
628672	ametrantrone	0.60	0.38	0.29	-12.15
628673	amsacrine	0.73	0.36	0.22	-10.04
628674	amsacrine	0.83	0.37	0.22	-11.66
628675	amsacrine	0.82	0.36	0.21	-12.49
628676	ametrantrone	0.61	0.38	0.28	-11.57
628677	amsacrine	0.79	0.37	0.22	-11.71
628678	amsacrine	0.87	0.36	0.22	-12.80
628679	mitoxantrone	0.76	0.37	0.34	-11.57
628680	amsacrine	0.86	0.38	0.21	-11.60
628681	amsacrine	0.53	0.38	0.20	-11.20
628908	etoposide	0.55	0.26	0.19	-8.25
628918	etoposide	0.59	0.32	0.23	-10.70
629266	mitoxantrone	0.53	0.39	0.26	-9.44
629874	etoposide	0.54	0.34	0.21	-7.60
629971	mitoxantrone	0.65	0.37	0.26	-10.20
630604	etoposide	0.55	0.33	0.21	-7.53
630699	mitoxantrone	0.52	0.46	0.27	-12.68
630700	mitoxantrone	0.66	0.42	0.26	-12.01
630701	ametrantrone	0.54	0.38	0.24	-12.55
630702	mitoxantrone	0.75	0.38	0.26	-11.79
631197	mitoxantrone	0.62	0.43	0.26	-11.72
631199	ametrantrone	0.56	0.44	0.25	-11.18
631939	amsacrine	0.61	0.32	0.07	-8.38
633403	etoposide	0.54	0.33	0.27	-11.24
634458	etoposide	0.62	0.25	0.06	-0.81
634724	amsacrine	0.77	0.37	0.25	-10.16
635405	etoposide	0.56	0.33	0.30	-7.60
637126	amsacrine	0.54	0.41	0.31	-10.37
637140	mitoxantrone	0.55	0.42	0.27	-9.12
637611	ametrantrone	0.56	0.29	0.30	-8.02
637651	ametrantrone	0.54	0.38	0.21	-9.60
638404	mitoxantrone	0.52	0.36	0.20	-7.65
638441	mitoxantrone	0.52	0.36	0.17	-9.08
638856	mitoxantrone	0.57	0.29	0.19	-8.93
639174	mitoxantrone	0.60	0.37	0.27	-9.81
639176	amsacrine	0.70	0.38	0.26	-9.46
639519	etoposide	0.53	0.29	0.18	-9.73
639659	ametrantrone	0.65	0.38	0.27	-9.69
639831	mitoxantrone	0.58	0.34	0.20	-10.25
639832	mitoxantrone	0.61	0.32	0.20	-10.22
640085	ametrantrone	0.61	0.30	0.21	-7.63
641454	amsacrine	0.54	0.39	0.23	-8.60
641533	etoposide	0.54	0.19	0.07	-6.05
642276	amsacrine	0.59	0.38	0.22	-11.43
642277	ametrantrone	0.59	0.44	0.28	-11.28
642278	mitoxantrone	0.84	0.39	0.34	-11.29
642279	mitoxantrone	0.83	0.40	0.32	-12.74
642280	mitoxantrone	0.74	0.41	0.34	-11.61
642281	mitoxantrone	0.76	0.41	0.31	-11.37
642282	mitoxantrone	0.75	0.40	0.31	-13.08
642283	mitoxantrone	0.56	0.40	0.31	-12.92
642284	mitoxantrone	0.76	0.42	0.31	-12.77
642285	mitoxantrone	0.76	0.38	0.34	-10.96
642286	mitoxantrone	0.73	0.39	0.33	-11.09
642287	mitoxantrone	0.74	0.42	0.31	-13.43
642288	mitoxantrone	0.53	0.40	0.33	-10.71
642289	mitoxantrone	0.77	0.40	0.31	-11.32
642290	mitoxantrone	0.73	0.38	0.34	-11.21
642291	mitoxantrone	0.73	0.40	0.32	-9.42
642292	mitoxantrone	0.67	0.38	0.32	-11.54

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NSC	lead	BiolAct	ROCS	CFP	docking
642293	mitoxantrone	0.69	0.40	0.32	-11.23
642318	amsacrine	0.53	0.40	0.21	-8.44
642321	etoposide	0.58	0.38	0.25	-7.98
642322	mitoxantrone	0.80	0.45	0.30	-11.64
642323	mitoxantrone	0.79	0.42	0.30	-11.96
642324	mitoxantrone	0.80	0.41	0.29	-11.24
642328	ametrantrone	0.57	0.38	0.28	-10.79
642329	ametrantrone	0.56	0.36	0.28	-10.54
642911	mitoxantrone	0.57	0.31	0.16	-7.33
642915	mitoxantrone	0.75	0.31	0.16	-8.69
643001	etoposide	0.56	0.31	0.22	-5.92
643006	mitoxantrone	0.65	0.33	0.16	-7.50
643833	mitoxantrone	0.55	0.39	0.26	-9.52
644945	mitoxantrone	0.79	0.46	0.33	-11.50
644946	mitoxantrone	0.81	0.44	0.33	-12.49
644947	ametrantrone	0.60	0.43	0.28	-11.67
644960	mitoxantrone	0.67	0.32	0.19	-9.10
644961	mitoxantrone	0.66	0.31	0.18	-8.95
644967	amsacrine	0.57	0.36	0.11	-7.93
645008	mitoxantrone	0.57	0.44	0.24	-11.91
645017	etoposide	0.73	0.31	0.30	-13.23
645018	etoposide	0.79	0.37	0.31	-13.57
645737	mitoxantrone	0.79	0.42	0.33	-12.30
646714	amsacrine	0.76	0.34	0.08	-7.68
648114	mitoxantrone	0.74	0.39	0.21	-10.29
648147	etoposide	0.54	0.30	0.21	-10.20
648316	mitoxantrone	0.58	0.40	0.19	-8.26
649677	mitoxantrone	0.80	0.39	0.22	-12.82
650259	ametrantrone	0.53	0.42	0.18	-10.57
650931	ametrantrone	0.60	0.39	0.27	-10.65
651777	amsacrine	0.54	0.49	0.19	-9.01
651850	mitoxantrone	0.73	0.43	0.32	-12.07
651855	mitoxantrone	0.67	0.40	0.32	-12.77
651857	mitoxantrone	0.71	0.42	0.33	-12.88
651861	mitoxantrone	0.75	0.42	0.32	-12.27
653438	mitoxantrone	0.58	0.47	0.25	-12.67
653842	amsacrine	0.54	0.44	0.17	-8.74
653860	mitoxantrone	0.78	0.47	0.32	-13.37
653862	amsacrine	0.55	0.12	0.22	-9.68
653863	mitoxantrone	0.67	0.43	0.32	-12.57
653864	ametrantrone	0.54	0.45	0.25	-12.57
654509	amsacrine	0.77	0.36	0.19	-10.13
654830	amsacrine	0.56	0.38	0.20	-9.24
656903	etoposide	0.52	0.39	0.33	-7.68
656904	etoposide	0.53	0.38	0.32	-7.38
657339	etoposide	0.58	0.31	0.22	-7.83
657446	etoposide	0.53	0.37	0.27	-9.88
658229	etoposide	0.55	0.27	0.18	-8.06
659687	mitoxantrone	0.79	0.44	0.30	-11.68
659948	amsacrine	0.83	0.36	0.18	-11.12
659949	amsacrine	0.73	0.36	0.18	-9.98
659950	ametrantrone	0.58	0.40	0.25	-9.48
660027	ametrantrone	0.60	0.43	0.29	-11.03
660028	ametrantrone	0.61	0.41	0.30	-11.07
660029	ametrantrone	0.57	0.40	0.28	-11.40
661226	etoposide	0.53	0.34	0.28	-9.66
662305	mitoxantrone	0.73	0.40	0.29	-12.72
663249	etoposide	0.63	0.25	0.11	-7.60
663291	etoposide	0.62	0.32	0.30	-8.91
663790	amsacrine	0.59	0.42	0.15	-8.02
663791	amsacrine	0.58	0.43	0.15	-7.64
665350	etoposide	0.62	0.35	0.30	-9.71
665534	mitoxantrone	0.61	0.13	0.29	-1.61
665934	mitoxantrone	0.80	0.44	0.32	-12.80
665935	mitoxantrone	0.77	0.47	0.33	-13.55
666871	amsacrine	0.53	0.39	0.16	-8.08
667047	amsacrine	0.59	0.40	0.20	-8.83
667070	etoposide	0.57	0.25	0.17	-6.53
667641	amsacrine	0.56	0.28	0.21	-8.96
667870	amsacrine	0.54	0.34	0.15	-7.16

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NSC	lead	BiolAct	ROCS	CFP	docking
668281	mitoxantrone	0.61	0.32	0.17	-7.93
668352	etoposide	0.52	0.27	0.16	-8.43
668370	etoposide	0.55	0.19	0.12	-6.51
668380	mitoxantrone	0.77	0.40	0.30	-12.81
668404	mitoxantrone	0.55	0.27	0.23	-7.92
668523	mitoxantrone	0.64	0.19	0.05	-5.47
668605	etoposide	0.57	0.30	0.21	-11.49
668834	etoposide	0.54	0.32	0.30	-7.01
668918	etoposide	0.59	0.30	0.27	-5.90
669727	mitoxantrone	0.58	0.42	0.18	-8.12
669728	mitoxantrone	0.54	0.17	0.18	-8.46
670013	mitoxantrone	0.67	0.30	0.31	-9.62
670430	etoposide	0.54	0.37	0.22	-8.09
670653	amsacrine	0.61	0.40	0.16	-8.39
670654	amsacrine	0.53	0.34	0.17	-9.60
670656	amsacrine	0.76	0.39	0.18	-7.90
670807	etoposide	0.53	0.24	0.08	-6.20
671002	mitoxantrone	0.57	0.34	0.14	-7.30
671014	etoposide	0.59	0.32	0.22	-9.26
671331	etoposide	0.57	0.26	0.25	-7.80
672974	etoposide	0.57	0.30	0.24	-8.13
672975	mitoxantrone	0.57	0.30	0.19	-8.12
673150	etoposide	0.60	0.27	0.19	-4.53
673347	etoposide	0.59	0.35	0.15	-5.93
673348	etoposide	0.54	0.34	0.24	-8.95
673804	ametrantrone	0.56	0.43	0.25	-11.35
673831	amsacrine	0.58	0.41	0.16	-6.86
673833	amsacrine	0.66	0.36	0.15	-7.17
673841	etoposide	0.55	0.26	0.19	-9.25
674182	amsacrine	0.65	0.39	0.17	-7.69
675249	mitoxantrone	0.64	0.32	0.28	-11.13
675250	mitoxantrone	0.65	0.30	0.28	-11.74
675251	mitoxantrone	0.53	0.32	0.30	-10.73
675255	mitoxantrone	0.65	0.36	0.31	-9.78
675256	mitoxantrone	0.53	0.28	0.25	-7.99
675574	mitoxantrone	0.69	0.49	0.19	-10.67
676316	etoposide	0.54	0.37	0.22	-8.25
678532	etoposide	0.58	0.31	0.24	-7.65
678880	etoposide	0.53	0.35	0.21	-7.92
678882	etoposide	0.53	0.40	0.22	-8.93
678914	mitoxantrone	0.59	0.49	0.25	-10.89
679108	etoposide	0.53	0.36	0.17	-8.51
679265	etoposide	0.55	0.36	0.23	-10.27
680417	mitoxantrone	0.57	0.17	0.20	-10.01
680420	mitoxantrone	0.55	0.30	0.20	-10.20
680715	etoposide	0.53	0.18	0.13	-7.72
680717	etoposide	0.54	0.31	0.23	-8.06
681152	etoposide	0.57	0.33	0.25	-8.71
681324	etoposide	0.54	0.27	0.20	-6.80
681326	etoposide	0.52	0.26	0.29	-9.34
681462	amsacrine	0.57	0.37	0.21	-9.68
681632	mitoxantrone	0.66	0.36	0.27	-10.73
681633	mitoxantrone	0.67	0.41	0.27	-11.05
681634	amsacrine	0.65	0.39	0.23	-8.30
681635	amsacrine	0.69	0.39	0.24	-10.66
681636	mitoxantrone	0.67	0.39	0.27	-10.49
681637	mitoxantrone	0.66	0.39	0.27	-10.68
681638	mitoxantrone	0.66	0.39	0.26	-10.73
681639	mitoxantrone	0.69	0.39	0.26	-10.76
681640	mitoxantrone	0.61	0.36	0.26	-10.76
681641	mitoxantrone	0.77	0.43	0.27	-9.95
681642	mitoxantrone	0.76	0.39	0.27	-10.60
681643	mitoxantrone	0.70	0.37	0.26	-10.20
681644	mitoxantrone	0.74	0.44	0.27	-10.10
681645	mitoxantrone	0.75	0.38	0.27	-9.59
681646	mitoxantrone	0.64	0.39	0.27	-10.13
682298	mitoxantrone	0.69	0.36	0.26	-10.12
682306	amsacrine	0.56	0.42	0.21	-8.78
683140	amsacrine	0.79	0.14	0.22	-13.39
683247	amsacrine	0.56	0.47	0.33	-13.36

Continued on next page

NSC	lead	BiolAct	ROCS	CFP	docking
683252	mitoxantrone	0.62	0.41	0.26	-6.47
683414	amsacrine	0.86	0.37	0.21	-9.86
683415	mitoxantrone	0.69	0.37	0.32	-9.86
683416	amsacrine	0.63	0.11	0.21	-9.07
683556	mitoxantrone	0.56	0.08	0.27	-7.78
683558	mitoxantrone	0.67	0.21	0.27	-10.66
684667	mitoxantrone	0.68	0.48	0.24	-11.17
684902	mitoxantrone	0.56	0.09	0.26	-5.42
684906	mitoxantrone	0.56	0.10	0.24	-5.57
684907	mitoxantrone	0.59	0.09	0.25	-6.88
684908	mitoxantrone	0.57	0.09	0.26	-6.81
684913	amsacrine	0.53	0.38	0.18	-8.64
685803	amsacrine	0.55	0.47	0.23	-7.57
687305	amsacrine	0.59	0.41	0.27	-8.49
687353	mitoxantrone	0.57	0.47	0.21	-11.27
688021	mitoxantrone	0.56	0.31	0.15	-6.89
688022	mitoxantrone	0.56	0.32	0.20	-6.30
688274	etoposide	0.54	0.36	0.34	-5.15
690266	etoposide	0.58	0.35	0.30	-9.53
690269	etoposide	0.62	0.36	0.31	-10.15
690760	etoposide	0.57	0.35	0.30	-8.73
690983	etoposide	0.57	0.35	0.30	-7.00
691244	amsacrine	0.56	0.43	0.26	-8.77
691247	mitoxantrone	0.65	0.41	0.25	-11.74
691249	mitoxantrone	0.64	0.42	0.26	-12.00
691251	amsacrine	0.61	0.40	0.29	-12.20
691277	etoposide	0.52	0.34	0.23	-10.09
691656	mitoxantrone	0.56	0.40	0.25	-12.12
692228	etoposide	0.71	0.31	0.32	-14.27
692736	mitoxantrone	0.57	0.37	0.28	-9.68
693167	amsacrine	0.54	0.35	0.16	-8.11
693169	etoposide	0.57	0.26	0.26	-10.45
693325	amsacrine	0.60	0.36	0.06	-5.46
693335	amsacrine	0.57	0.40	0.17	-6.88
693539	etoposide	0.52	0.38	0.33	-7.72
693543	mitoxantrone	0.57	0.48	0.23	-12.99
693546	etoposide	0.53	0.44	0.30	-9.28
693563	amsacrine	0.58	0.31	0.26	-9.25
693858	amsacrine	0.59	0.40	0.20	-9.06
694456	mitoxantrone	0.54	0.34	0.26	-10.17
694501	mitoxantrone	0.61	0.30	0.30	-7.65
695590	mitoxantrone	0.56	0.05	0.30	-11.22
695804	etoposide	0.54	0.34	0.22	-9.17
695936	etoposide	0.56	0.33	0.25	-13.53
696125	amsacrine	0.62	0.39	0.27	-9.10
697535	amsacrine	0.58	0.35	0.25	-9.81
697653	amsacrine	0.55	0.41	0.22	-8.18
697685	mitoxantrone	0.54	0.31	0.12	-8.61
697686	etoposide	0.71	0.28	0.25	-7.63
697726	mitoxantrone	0.53	0.37	0.15	-7.89
698104	amsacrine	0.55	0.42	0.24	-10.94
699087	etoposide	0.54	0.40	0.31	-9.48
699150	mitoxantrone	0.57	0.43	0.27	-11.06
699724	mitoxantrone	0.55	0.48	0.23	-10.86
701022	etoposide	0.58	0.34	0.26	-8.89
701029	etoposide	0.57	0.39	0.18	-10.30
701599	mitoxantrone	0.54	0.29	0.19	-8.65
701616	ametrantrone	0.65	0.46	0.23	-11.20
701660	etoposide	0.60	0.35	0.27	-8.38
701743	mitoxantrone	0.58	0.05	0.27	-10.64
701745	ametrantrone	0.56	0.39	0.24	-11.63
701747	etoposide	0.64	0.36	0.26	-11.33
701973	mitoxantrone	0.68	0.33	0.20	-12.81
702045	etoposide	0.54	0.33	0.25	-8.71
702047	etoposide	0.55	0.37	0.17	-8.13
703104	amsacrine	0.61	0.41	0.21	-7.54
703327	etoposide	0.61	0.37	0.19	-11.59
703445	etoposide	0.53	0.37	0.23	-9.81
703874	etoposide	0.57	0.34	0.24	-7.79
704533	mitoxantrone	0.54	0.33	0.18	-8.02

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NSC	lead	BiolAct	ROCS	CFP	docking
706000	ametantrone	0.59	0.29	0.22	-12.61
706003	mitoxantrone	0.53	0.28	0.22	-12.51
706737	etoposide	0.54	0.30	0.34	-7.89
706743	mitoxantrone	0.54	0.48	0.33	-12.92
706744	amsacrine	0.74	0.40	0.24	-12.92
707059	etoposide	0.56	0.37	0.25	-7.91
707068	etoposide	0.54	0.36	0.21	-5.61
707696	etoposide	0.53	0.35	0.31	-8.61
708061	etoposide	0.57	0.20	0.12	-6.96
708411	etoposide	0.52	0.31	0.20	-6.63
708417	amsacrine	0.53	0.31	0.20	-7.52
708446	etoposide	0.57	0.35	0.26	-8.74
708447	mitoxantrone	0.57	0.18	0.20	-9.99
709317	etoposide	0.68	0.44	0.34	-7.33
709358	mitoxantrone	0.54	0.30	0.29	-9.52
710112	etoposide	0.54	0.33	0.29	-10.12
710403	etoposide	0.60	0.32	0.31	-8.77
710525	etoposide	0.60	0.34	0.26	-8.60
710551	ametantrone	0.59	0.34	0.24	-13.52
710578	etoposide	0.55	0.31	0.27	-8.22
710770	etoposide	0.62	0.35	0.28	-8.27
710861	etoposide	0.57	0.31	0.19	-8.68
711312	etoposide	0.54	0.26	0.21	-7.95
711693	ametantrone	0.53	0.26	0.28	-11.73
711694	ametantrone	0.56	0.26	0.28	-12.00
711695	mitoxantrone	0.54	0.29	0.32	-12.23
711696	ametantrone	0.65	0.24	0.28	-12.31
711946	mitoxantrone	0.58	0.27	0.32	-12.63
712583	mitoxantrone	0.62	0.18	0.03	-5.46
712741	amsacrine	0.53	0.45	0.25	-9.58
713309	etoposide	0.67	0.41	0.31	-9.02
713649	etoposide	0.66	0.34	0.27	-8.18
713663	etoposide	0.57	0.34	0.33	-7.56
713672	mitoxantrone	0.55	0.32	0.26	-10.00
715974	etoposide	0.61	0.31	0.16	-7.93
716095	etoposide	0.53	0.36	0.28	-7.50
718163	etoposide	0.54	0.39	0.21	-7.78
718303	etoposide	0.54	0.32	0.30	-8.52
718630	mitoxantrone	0.68	0.37	0.26	-7.62
718631	etoposide	0.69	0.33	0.24	-7.91
718810	etoposide	0.60	0.30	0.18	-6.82
720538	mitoxantrone	0.59	0.30	0.20	-9.00
720555	etoposide	0.53	0.37	0.22	-10.31
720597	etoposide	0.56	0.32	0.17	-8.93
720689	ametantrone	0.63	0.37	0.28	-14.43
720861	etoposide	0.60	0.35	0.23	-9.40
721385	mitoxantrone	0.56	0.34	0.20	-8.53
721386	amsacrine	0.58	0.35	0.18	-9.83
721387	mitoxantrone	0.64	0.37	0.23	-11.06
721514	mitoxantrone	0.59	0.39	0.25	-8.87
721685	etoposide	0.53	0.35	0.24	-8.90
722900	mitoxantrone	0.69	0.40	0.31	-9.62
723387	amsacrine	0.74	0.42	0.24	-11.13
723554	etoposide	0.53	0.32	0.31	-9.55
723733	etoposide	0.67	0.28	0.32	-9.58
724562	amsacrine	0.53	0.39	0.24	-11.29
724563	mitoxantrone	0.54	0.45	0.32	-12.68
724995	amsacrine	0.61	0.39	0.24	-10.84
724998	mitoxantrone	0.59	0.45	0.32	-10.59
725026	amsacrine	0.55	0.38	0.18	-7.06
725665	etoposide	0.59	0.38	0.33	-10.41
725666	amsacrine	0.63	0.39	0.24	-10.54
725669	etoposide	0.54	0.31	0.24	-11.58
725671	amsacrine	0.66	0.40	0.21	-11.94
725775	amsacrine	0.66	0.40	0.24	-10.96
725776	amsacrine	0.53	0.40	0.24	-11.58
725981	etoposide	0.66	0.33	0.34	-9.12
726112	etoposide	0.57	0.39	0.34	-11.32
726331	amsacrine	0.54	0.38	0.25	-11.00
726332	amsacrine	0.59	0.43	0.24	-10.22

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NSC	lead	BiolAct	ROCS	CFP	docking
726627	etoposide	0.52	0.33	0.24	-9.31
726764	ametantrone	0.55	0.38	0.24	-13.06
726769	mitoxantrone	0.64	0.48	0.29	-11.98
726770	amsacrine	0.67	0.40	0.20	-10.48
726796	etoposide	0.56	0.30	0.22	-8.47
726863	etoposide	0.59	0.28	0.15	-6.30
726971	amsacrine	0.66	0.40	0.24	-11.12
727212	etoposide	0.53	0.36	0.33	-13.05
727354	mitoxantrone	0.61	0.32	0.31	-10.63
727356	mitoxantrone	0.63	0.44	0.32	-11.56
727572	etoposide	0.63	0.36	0.32	-8.06
727620	mitoxantrone	0.62	0.06	0.32	-14.04
727621	etoposide	0.53	0.38	0.33	-11.37
727722	mitoxantrone	0.58	0.39	0.30	-10.97
727729	mitoxantrone	0.70	0.30	0.28	-9.76
728086	etoposide	0.55	0.29	0.24	-8.39
728089	mitoxantrone	0.69	0.44	0.33	-12.15
728091	mitoxantrone	0.63	0.42	0.32	-9.88
728134	etoposide	0.66	0.36	0.26	-8.31
728219	etoposide	0.60	0.32	0.17	-7.54
728316	mitoxantrone	0.76	0.43	0.32	-10.79
728318	mitoxantrone	0.55	0.46	0.33	-12.16
728457	etoposide	0.60	0.26	0.22	-8.62
728594	etoposide	0.58	0.27	0.13	-7.54
728856	mitoxantrone	0.54	0.45	0.28	-13.04
728979	amsacrine	0.57	0.40	0.23	-9.37
729352	mitoxantrone	0.55	0.34	0.31	-10.86
729812	amsacrine	0.66	0.40	0.23	-9.54
729813	amsacrine	0.66	0.38	0.23	-11.23
730001	etoposide	0.53	0.32	0.26	-10.15
730435	ametantrone	0.54	0.42	0.24	-12.87
731155	mitoxantrone	0.53	0.44	0.30	-11.26
731981	amsacrine	0.60	0.41	0.18	-8.51
732534	mitoxantrone	0.55	0.18	0.21	-4.48
732693	etoposide	0.56	0.37	0.23	-8.14
732787	etoposide	0.61	0.36	0.29	-9.12
732836	etoposide	0.65	0.35	0.23	-8.97
732851	etoposide	0.52	0.35	0.25	-8.58
733465	etoposide	0.62	0.38	0.25	-8.54
733654	amsacrine	0.70	0.40	0.23	-9.86
733883	mitoxantrone	0.56	0.39	0.32	-9.70
734294	amsacrine	0.64	0.41	0.20	-9.39
734296	etoposide	0.65	0.37	0.32	-9.12
734430	amsacrine	0.58	0.34	0.17	-10.29
734561	etoposide	0.53	0.34	0.29	-10.91
734562	etoposide	0.66	0.34	0.29	-11.06
734799	amsacrine	0.58	0.41	0.21	-9.74
735004	etoposide	0.55	0.27	0.10	-8.31
735036	amsacrine	0.72	0.40	0.24	-12.35
735037	mitoxantrone	0.71	0.42	0.32	-10.00
735356	etoposide	0.56	0.42	0.22	-8.28
735404	etoposide	0.56	0.29	0.22	-9.60
735493	amsacrine	0.61	0.43	0.25	-11.53
735798	ametantrone	0.58	0.26	0.24	-12.27
735799	etoposide	0.57	0.31	0.34	-10.47
736101	etoposide	0.55	0.37	0.24	-9.75
736116	mitoxantrone	0.55	0.43	0.31	-11.46
736198	mitoxantrone	0.67	0.41	0.29	-9.50
736200	mitoxantrone	0.68	0.41	0.29	-9.67
736201	mitoxantrone	0.60	0.43	0.29	-9.77
736202	mitoxantrone	0.64	0.42	0.29	-9.09
736268	etoposide	0.53	0.33	0.30	-7.46
736394	amsacrine	0.64	0.41	0.21	-11.68
736493	etoposide	0.58	0.34	0.27	-10.72
736611	mitoxantrone	0.63	0.49	0.19	-12.61
736624	mitoxantrone	0.61	0.43	0.29	-9.66
736681	etoposide	0.63	0.37	0.29	-9.89
736829	mitoxantrone	0.55	0.48	0.29	-11.77
736913	etoposide	0.61	0.36	0.29	-9.91
736916	etoposide	0.65	0.36	0.29	-9.62

Continued on next page

NSC	lead	BiolAct	ROCS	CFP	docking
736988	amsacrine	0.65	0.43	0.25	-11.47
737318	mitoxantrone	0.56	0.41	0.32	-10.13
737344	amsacrine	0.65	0.37	0.24	-11.28
737518	amsacrine	0.70	0.40	0.24	-10.47
737672	mitoxantrone	0.58	0.43	0.34	-8.86
737707	amsacrine	0.54	0.41	0.20	-7.78
737737	mitoxantrone	0.65	0.36	0.24	-8.78
740051	etoposide	0.57	0.41	0.31	-9.06
740121	etoposide	0.58	0.30	0.21	-10.44
740268	mitoxantrone	0.64	0.41	0.33	-9.35
740504	etoposide	0.56	0.36	0.27	-13.06
740520	mitoxantrone	0.63	0.40	0.30	-9.98
740524	amsacrine	0.60	0.41	0.24	-10.16
740564	mitoxantrone	0.58	0.44	0.30	-11.47
740609	etoposide	0.52	0.34	0.28	-11.36
740643	amsacrine	0.63	0.42	0.24	-9.81
740644	amsacrine	0.65	0.40	0.24	-9.85
740645	amsacrine	0.66	0.40	0.24	-11.14
740648	amsacrine	0.67	0.46	0.25	-12.30
740974	mitoxantrone	0.60	0.43	0.30	-9.88
740975	mitoxantrone	0.59	0.41	0.29	-9.84
741106	amsacrine	0.60	0.43	0.20	-11.26
741107	amsacrine	0.57	0.40	0.22	-11.31
741459	mitoxantrone	0.76	0.30	0.28	-9.12
741695	etoposide	0.59	0.25	0.22	-8.64
742417	etoposide	0.57	0.30	0.27	-8.19
742801	etoposide	0.58	0.38	0.23	-7.78
743864	mitoxantrone	0.54	0.33	0.28	-8.88
744330	mitoxantrone	0.66	0.26	0.28	-8.80
744622	amsacrine	0.53	0.27	0.17	-9.49
746351	amsacrine	0.58	0.41	0.18	-7.28
747292	amsacrine	0.53	0.34	0.21	-8.17
751393	etoposide	0.61	0.37	0.27	-7.71

Table S7: Docking scores of DUDE-E decoys.

Title	docking_score
C65469915	-12.20
C00636200	-11.64
C02582595	-11.14
C14992360	-11.09
C57773689	-11.05
C20132031	-10.84
C15721960	-10.83
C76971785	-10.74
C09239600	-10.67
C97334294	-10.63
C71788398	-10.57
C98178696	-10.49
C39500252	-10.45
C05980708	-10.43
C38517546	-10.41
C19229474	-10.40
C02348787	-10.36
C63698417	-10.33
C63855242	-10.23
C15722286	-10.23
C33697219	-10.23
C08076202	-10.20
C64158213	-10.17
C02437529	-10.16
C38999931	-10.16
C13539040	-10.15
C64067023	-10.15
C34250406	-10.13
C65405674	-10.12
C40801473	-10.07

Continued on next page

Title	docking_score
C39560948	-10.05
C77357347	-10.02
C20116877	-9.99
C40570282	-9.99
C65407120	-9.97
C00636047	-9.95
C13539043	-9.93
C38486049	-9.91
C38517641	-9.90
C39015840	-9.89
C39015836	-9.88
C72434813	-9.86
C26896594	-9.80
C33450962	-9.79
C43773452	-9.79
C25585272	-9.79
C72477679	-9.77
C06510920	-9.76
C08740221	-9.74
C39953335	-9.74
C38546965	-9.73
C14472334	-9.71
C34001737	-9.70
C03840128	-9.68
C01698989	-9.65
C72380005	-9.65
C95869711	-9.63
C01062118	-9.57
C96336260	-9.55
C14086129	-9.52
C21146606	-9.52
C14744245	-9.52
C43773453	-9.50
C25605891	-9.45
C09490572	-9.42
C73374099	-9.42
C06614498	-9.40
C19741840	-9.38
C39932294	-9.38
C93791735	-9.37
C39946867	-9.37
C49061297	-9.37
C15066260	-9.36
C44358916	-9.34
C63818501	-9.29
C20805442	-9.29
C22576466	-9.28
C64683770	-9.27
C57761945	-9.27
C20463116	-9.22
C20436792	-9.22
C97945339	-9.20
C67616676	-9.18
C89943041	-9.18
C34914020	-9.18
C42182418	-9.14
C65374419	-9.14
C89943040	-9.14
C20915747	-9.12
C92455417	-9.12
C00623661	-9.12
C13555666	-9.12
C06501754	-9.11
C21866363	-9.10
C04066639	-9.09
C63503255	-9.09
C12504524	-9.08
C05192427	-9.08
C20836850	-9.05
C40756782	-9.05

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Title	docking_score
C40801537	-9.00
C04221602	-9.00
C14476043	-8.95
C01355376	-8.95
C97405180	-8.94
C40701948	-8.94
C58379195	-8.93
C49421241	-8.91
C40701949	-8.90
C86066393	-8.89
C88943634	-8.88
C08613448	-8.88
C67634894	-8.88
C02429161	-8.87
C72099787	-8.84
C18158775	-8.82
C09003806	-8.82
C39952927	-8.80
C88757913	-8.79
C03009215	-8.77
C15772708	-8.75
C01325000	-8.73
C12134269	-8.73
C06161920	-8.71
C08636781	-8.68
C20922520	-8.68
C04827638	-8.67
C09242812	-8.66
C20922598	-8.64
C20550368	-8.61
C08643875	-8.60
C22839320	-8.57
C39007764	-8.56
C14276867	-8.56
C97527879	-8.56
C37866073	-8.56
C11661801	-8.56
C20921837	-8.55
C22056694	-8.53
C02474720	-8.52
C08152480	-8.50
C35981790	-8.49
C02584814	-8.49
C15962384	-8.48
C97648044	-8.47
C63426950	-8.44
C50440563	-8.44
C05414593	-8.41
C63920236	-8.41
C03464393	-8.41
C12859983	-8.40
C54804688	-8.39
C89054088	-8.38
C09750214	-8.37
C89943835	-8.37
C16756749	-8.37
C04502846	-8.36
C39012857	-8.35
C97648048	-8.34
C14551099	-8.33
C08905668	-8.32
C06074140	-8.29
C03583996	-8.28
C85425716	-8.26
C04388372	-8.23
C19827453	-8.23
C09350731	-8.17
C41021336	-8.16
C27420460	-8.16
C16210468	-8.14

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Title	docking_score
C31157904	-8.14
C07742097	-8.11
C63752986	-8.08
C13608616	-8.05
C36127331	-8.03
C44443373	-8.00
C06550815	-7.98
C97337215	-7.95
C08763931	-7.94
C14674332	-7.88
C27570104	-7.87
C04221674	-7.86
C10248529	-7.84
C40679521	-7.83
C01754852	-7.83
C20566341	-7.83
C35555986	-7.83
C13608697	-7.80
C20566737	-7.80
C40734699	-7.77
C01037587	-7.76
C08740529	-7.75
C88464716	-7.74
C40686541	-7.71
C03807172	-7.68
C03043911	-7.66
C59612440	-7.65
C92477162	-7.61
C09325300	-7.60
C23379430	-7.59
C36006179	-7.59
C70671778	-7.59
C44137709	-7.56
C01511355	-7.55
C16283587	-7.55
C11883249	-7.51
C19940784	-7.50
C12930324	-7.46
C59147401	-7.46
C18098320	-7.43
C13513671	-7.40
C96147944	-7.38
C20922797	-7.38
C21819441	-7.38
C16430580	-7.36
C05362734	-7.34
C20407810	-7.33
C71789697	-7.32
C12516987	-7.31
C64684229	-7.30
C14609098	-7.30
C02751023	-7.29
C06560016	-7.25
C58441612	-7.25
C96395303	-7.21
C64948688	-7.09
C01452524	-7.08
C08116979	-6.98
C33257185	-6.89
C05819214	-6.85
C36694022	-6.76
C32996316	-6.75
C09366196	-6.68
C01820789	-6.66
C64684771	-6.66
C07260781	-6.61
C96333100	-6.52
C36693907	-6.51
C09824460	-6.51
C04742125	-6.22

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Title	docking_score
C98046891	-5.98
C29559740	-5.43
C03874159	-5.23
C16923900	-5.07
C67911450	-3.71