Supporting Information

The Biostructural Features of Additional Jasplakinolide Analogues

Katharine R. Watts,† Brandon Morinaka,† Taro Amagata,† Sarah J. Robinson,† Karen Tenney,† Walter M. Bray,†,‡ Nadine C. Gassner,†,‡ R. Scott Lokey,†,‡ Joseph Media,§ Frederick A. Valeriote,§ Phillip Crews†*

†Department of Chemistry and Biochemistry and ‡UCSC Chemical Screening Center, University of California, Santa Cruz, Santa Cruz, CA 95064

§Department of Internal Medicine, Division of Hematology and Oncology, Henry Ford Hospital, Detroit MI 48202

Index:

Figure S1. NOE spectra in CDCl₃ and DMSO- d_6 of **8**.

Figure S2. ¹³C chemical shift differences of the hydroxy-aryl substructures.

Figure S3. Likely pathways for the origin of 9-11 from 1, and 15 and 12 from 14.

Figure S4. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of **7**.

Figure S5. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of 8.

Figure S6. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of 9.

Figure S7. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of **10**.

Figure S8. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of 11.

Figure S9. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of **12**.

Figure S10. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of 13.

Figure S11. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of 14.

Figure S12. ¹H NMR, ¹³C NMR, gHMQC, and gHMBC spectra of 15.

Table S1. NCI 60 cell line evaluation of 1.

Table S2. NCI 60 cell line evaluation of 4.

Table S3. NCI 60 cell line evaluation of **5.**

Table \$4. NCI 60 cell line evaluation of 6.

Table S5. NCI 60 cell line evaluation of **7**.

Table S6. NCI 60 cell line evaluation of 8.

Table S7. NCI 60 cell line evaluation of 9.

Table S8. NCI 60 cell line evaluation of 11.

Table S9. NCI 60 cell line evaluation of 12.

Table S10. NCI 60 cell line evaluation of **13**.

Table S11. NCI 60 cell line evaluation of **14.**

Table S12. One dose mean graph for **15**.

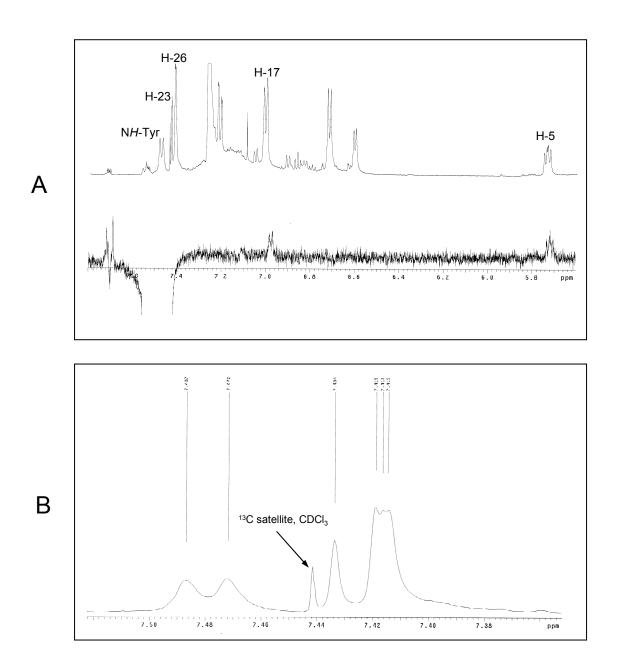
Figure S11. Microfilament effects of 10 in HCT-116 and HeLa cells.

Figure \$12. Above water photo of 00101.

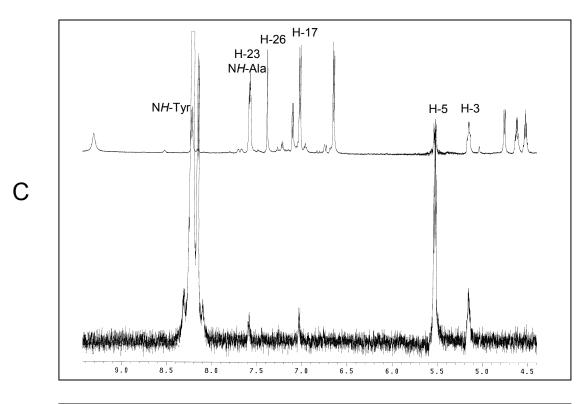
University of California, Santa Cruz.

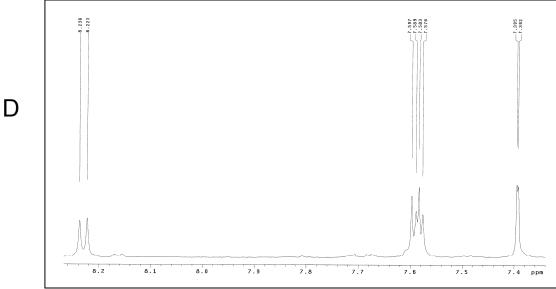
^{*}To whom correspondence should be addressed: Phone: 831-459-2603 Fax 831-459-2935 Email: phil@chemistry.ucsc.edu.

Figure S1. NOE correlations of $\bf 8$ in CDCl $_3$ and DMSO- $\bf d_6$



A. NOE in CDCl $_3$ **B.** Blowup of 1 H spectra region in CDCl $_3$ containing N*H*-Tyr, H-23, and H-26.





C. NOE in DMSO- d_6 **D.** Blowup of 1 H spectra region in DMSO- d_6 containing N*H*-Tyr, H-23, N*H*-Ala and H-26.

Figure S2. ¹³C chemical shift differences of the hydroxy-aryl substructures.

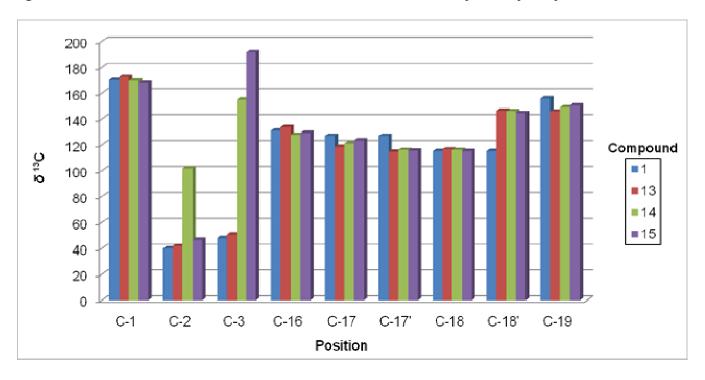
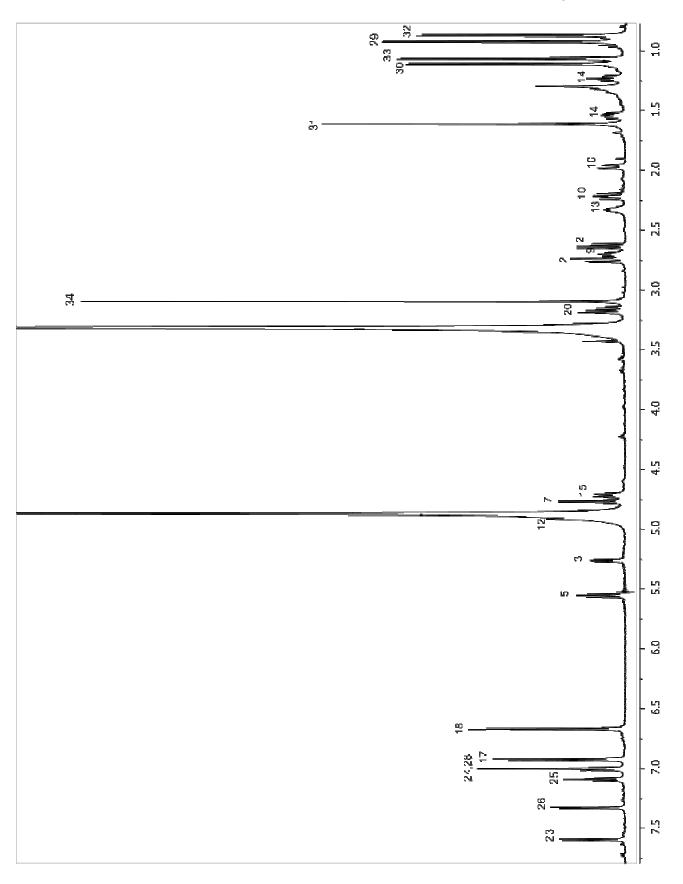
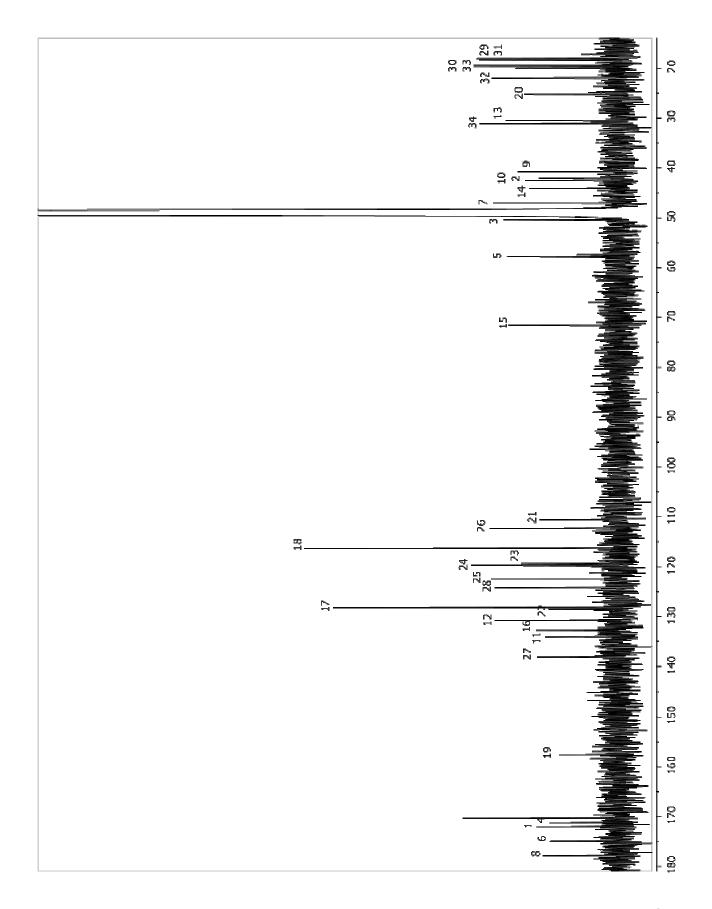
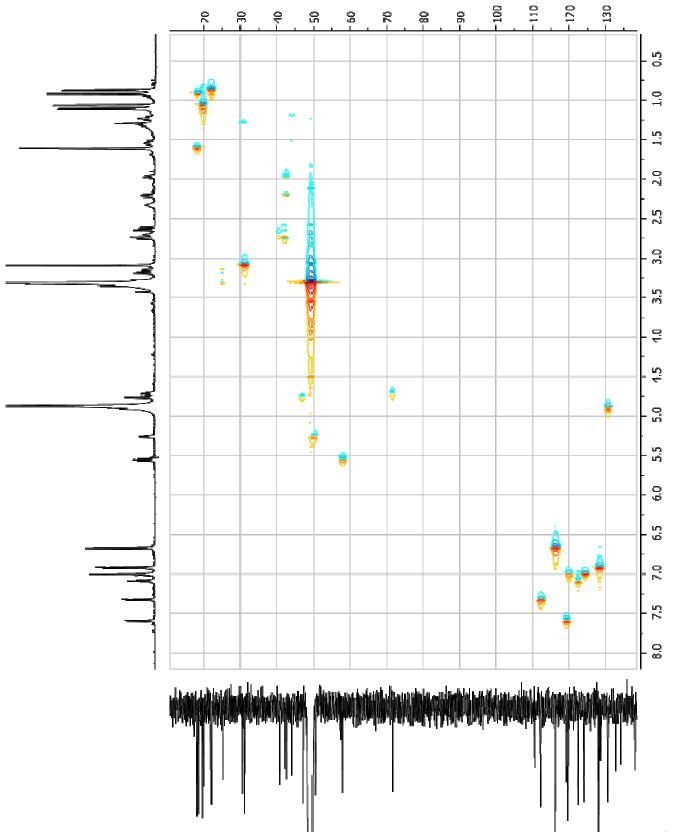


Figure S3. Likely pathways for the origin of **9-11** from **1**, and **15** and **12** from **14**.

Figure S4. 1 H, 13 C, gHMQC, and gHMBC spectra for **7** in CD $_{3}$ OD.







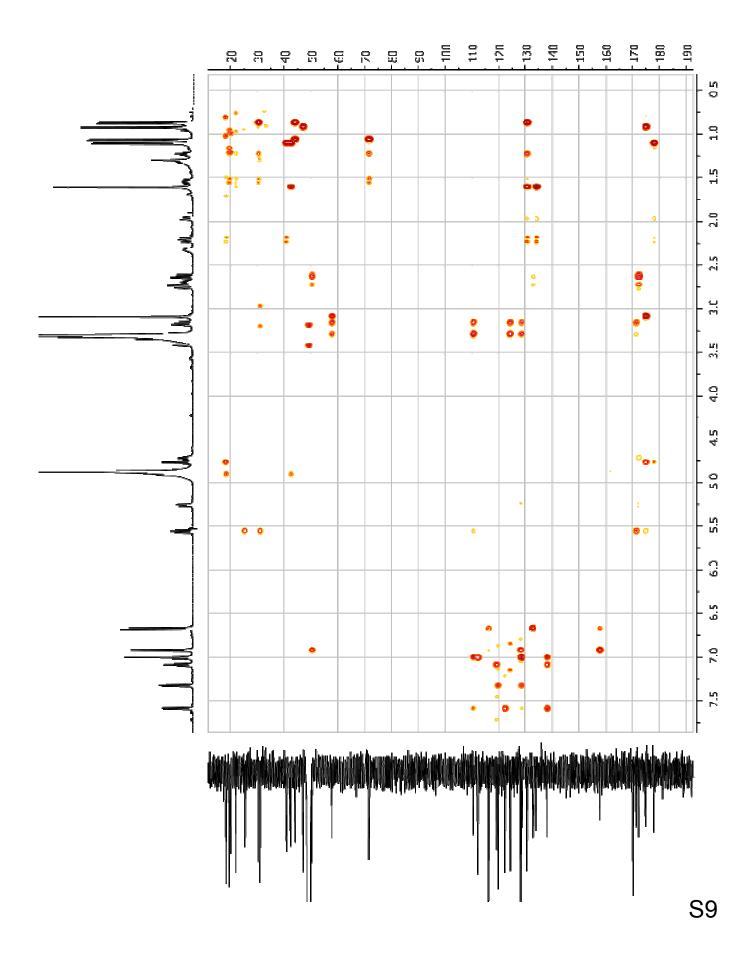
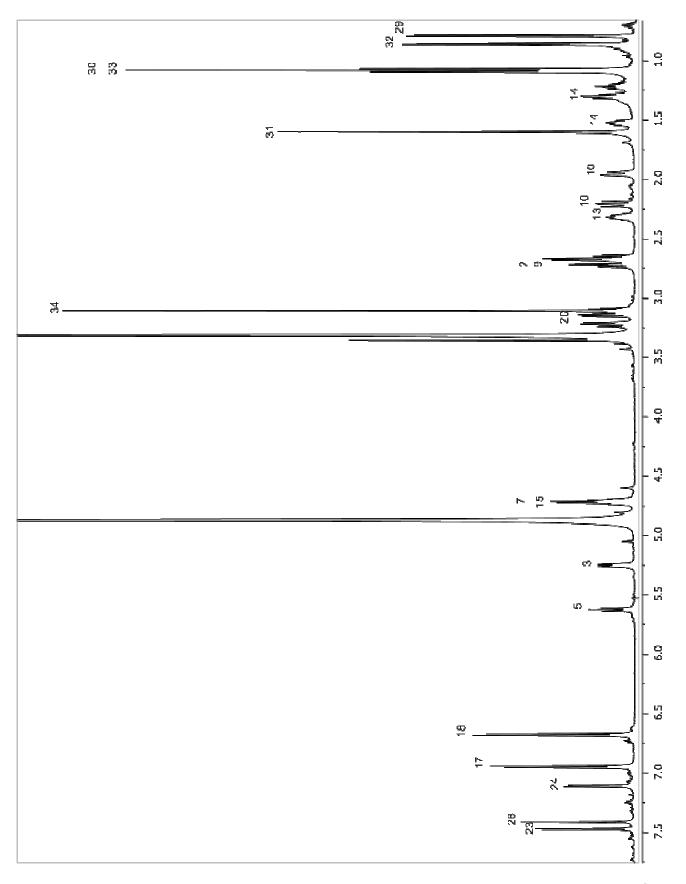
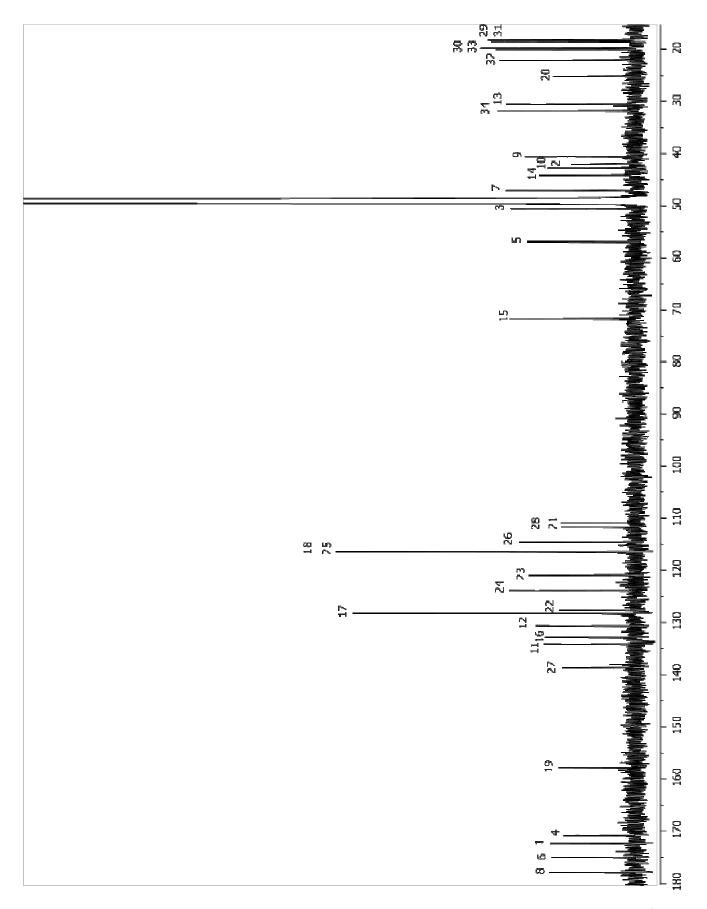
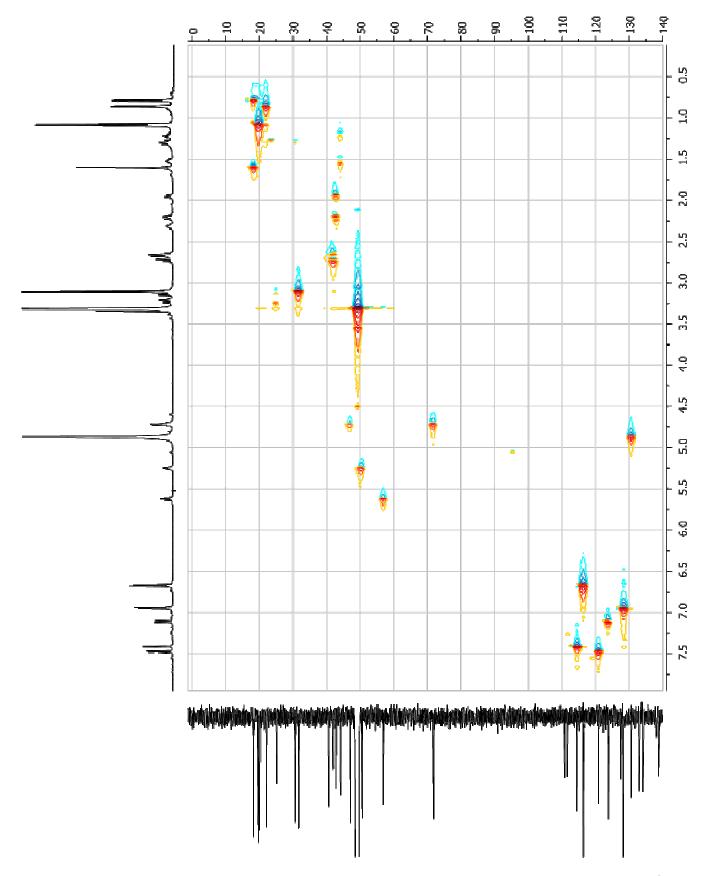


Figure S5. 1 H, 13 C, gHMQC, and gHMBC spectra for **8** in CD $_{3}$ OD.







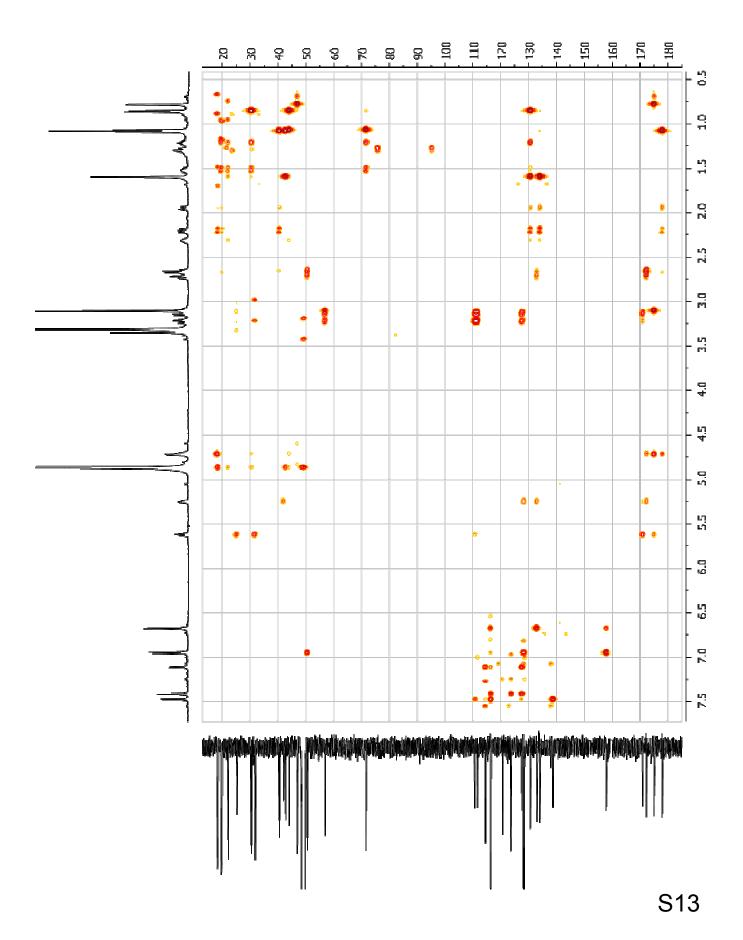
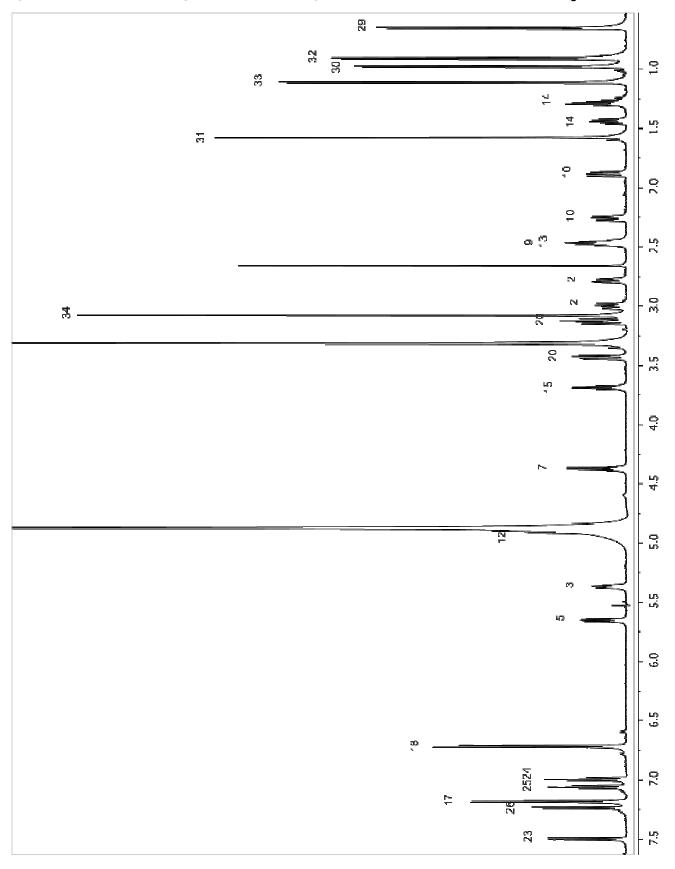
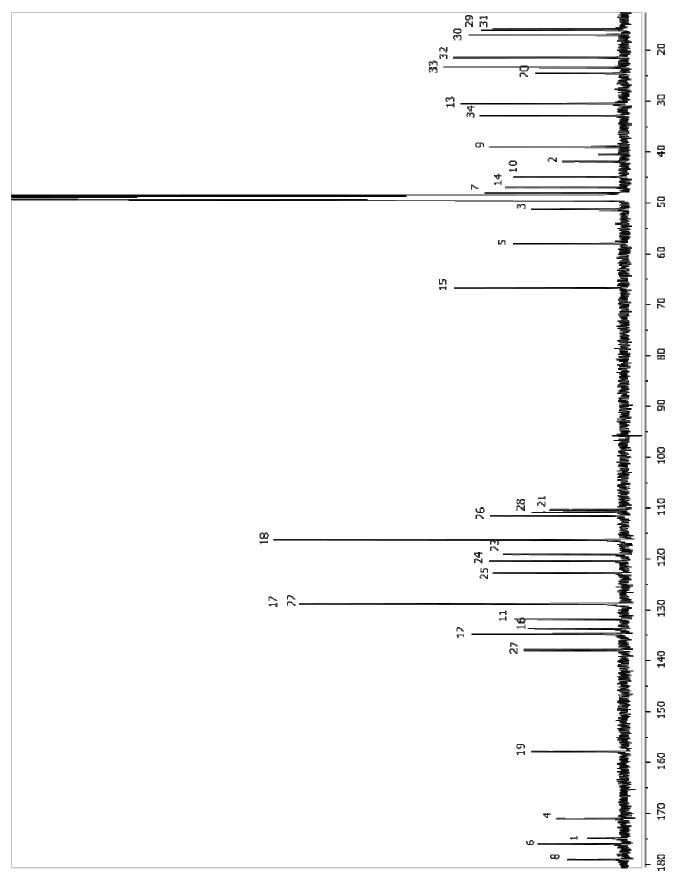
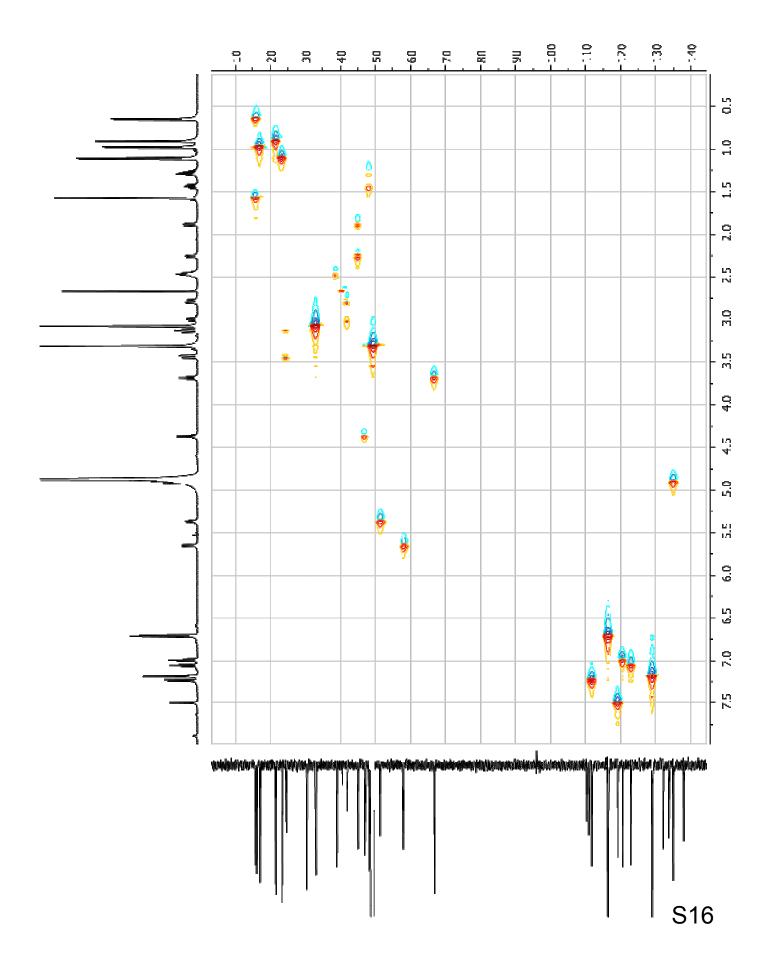


Figure S6. 1 H, 13 C, gHMQC, and gHMBC spectra for **9** in CD $_{3}$ OD.







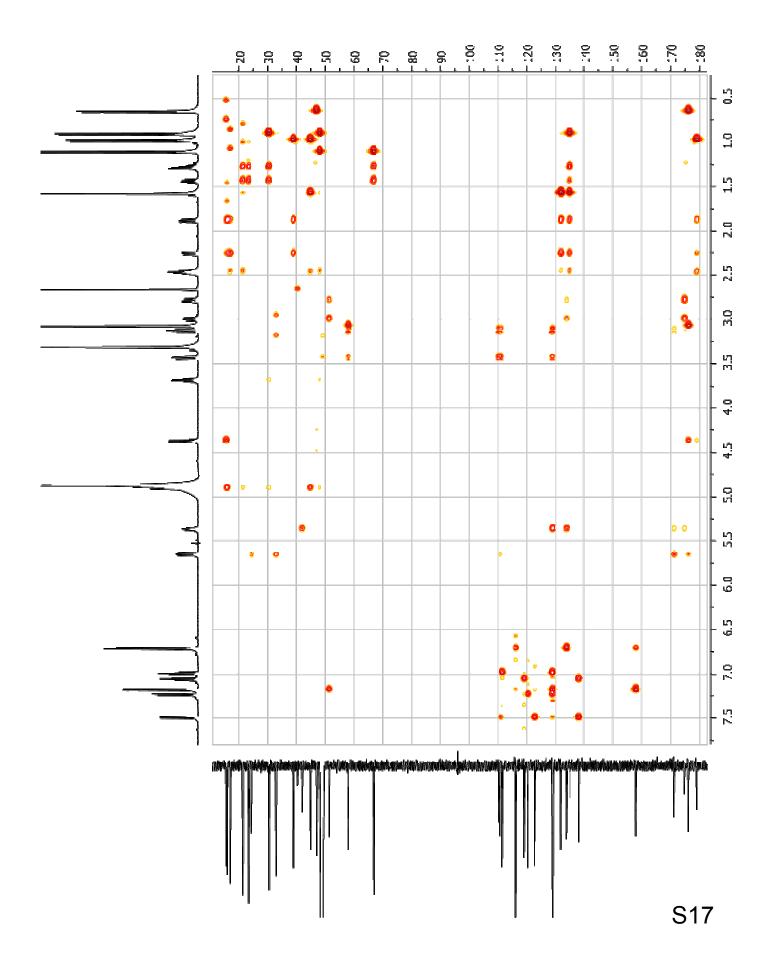
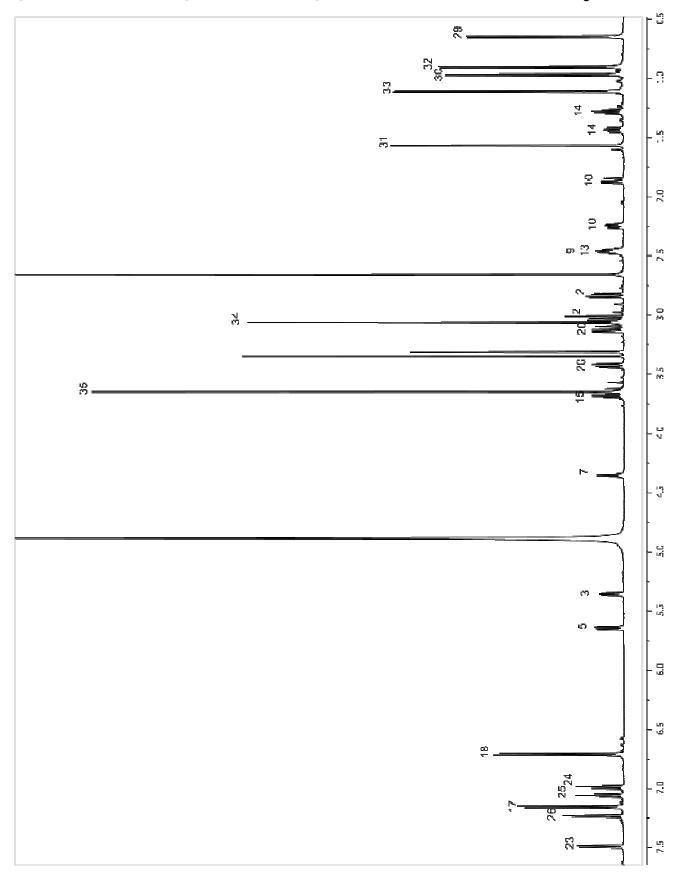
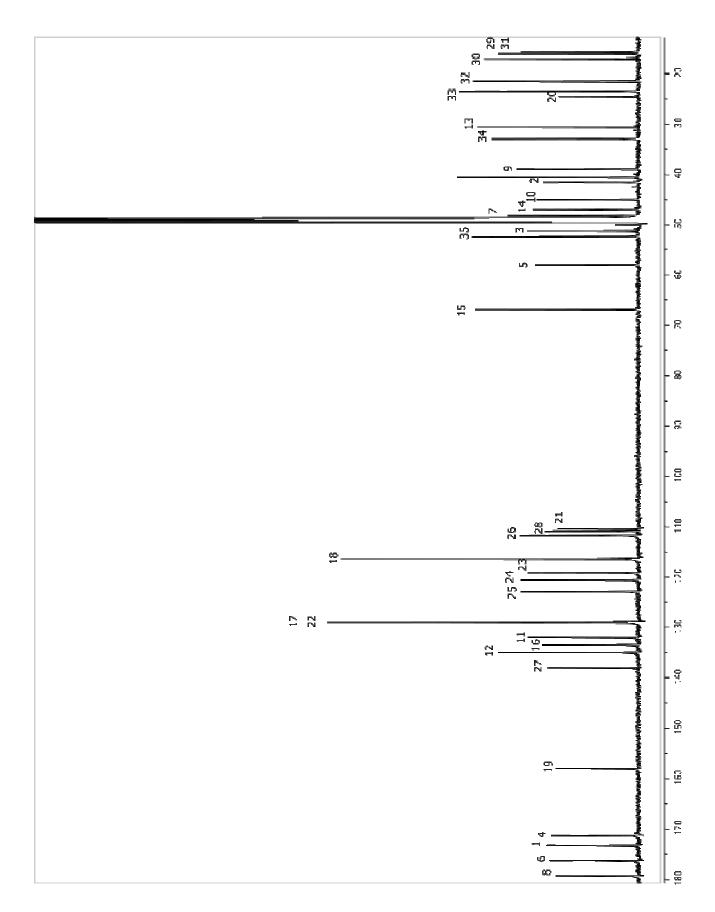
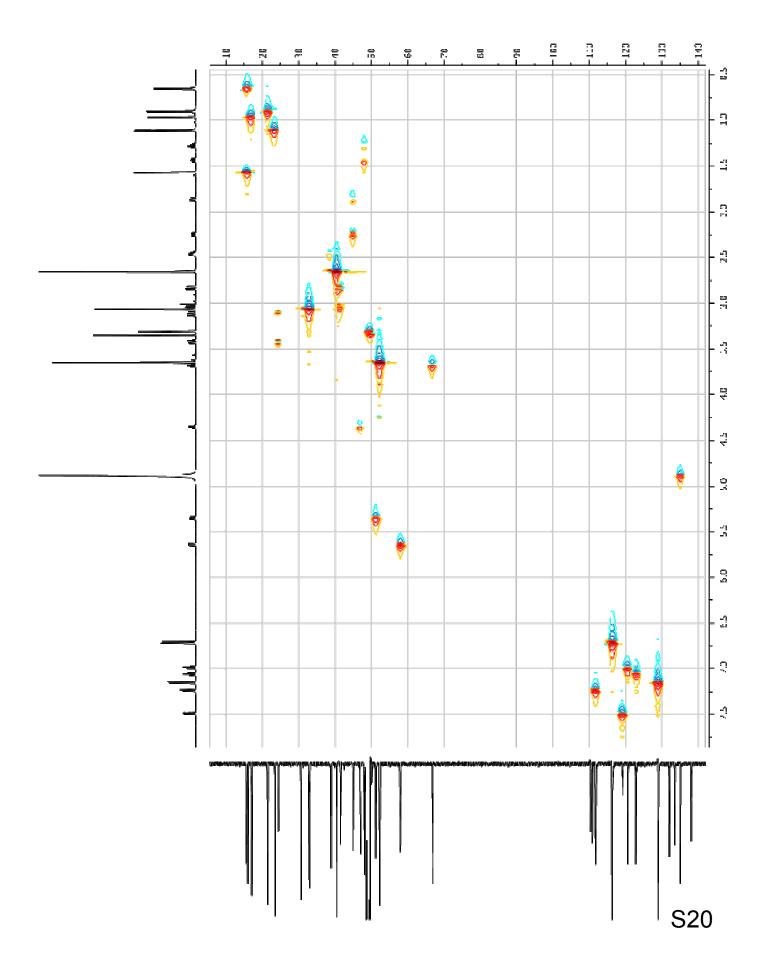


Figure S7. 1 H, 13 C, gHMQC, and gHMBC spectra for **10** in CD $_{3}$ OD.







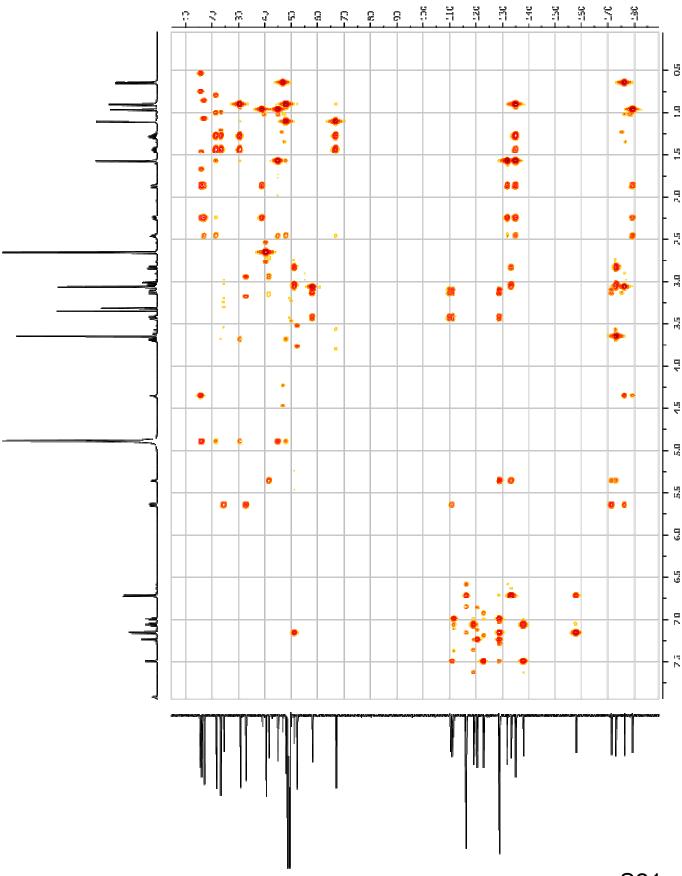
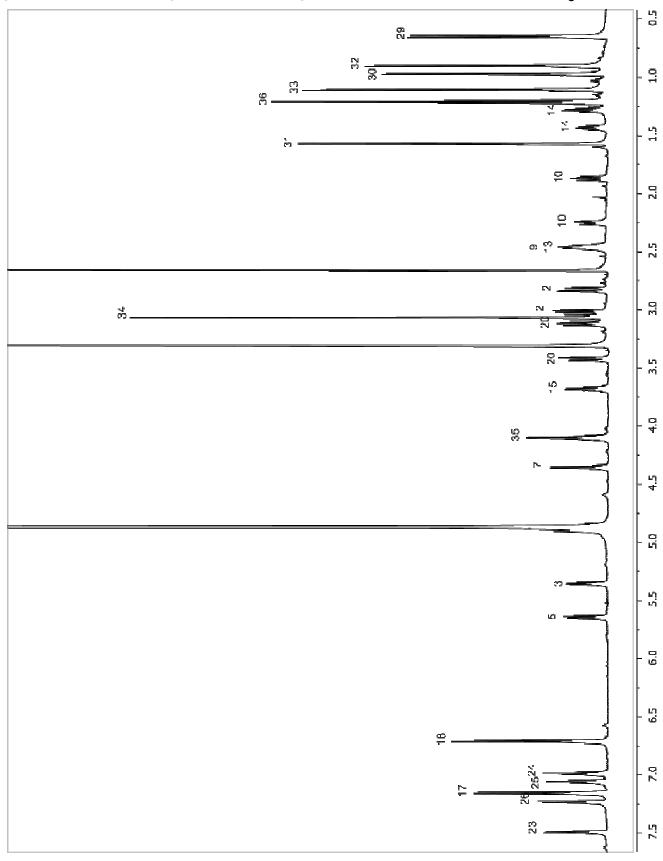
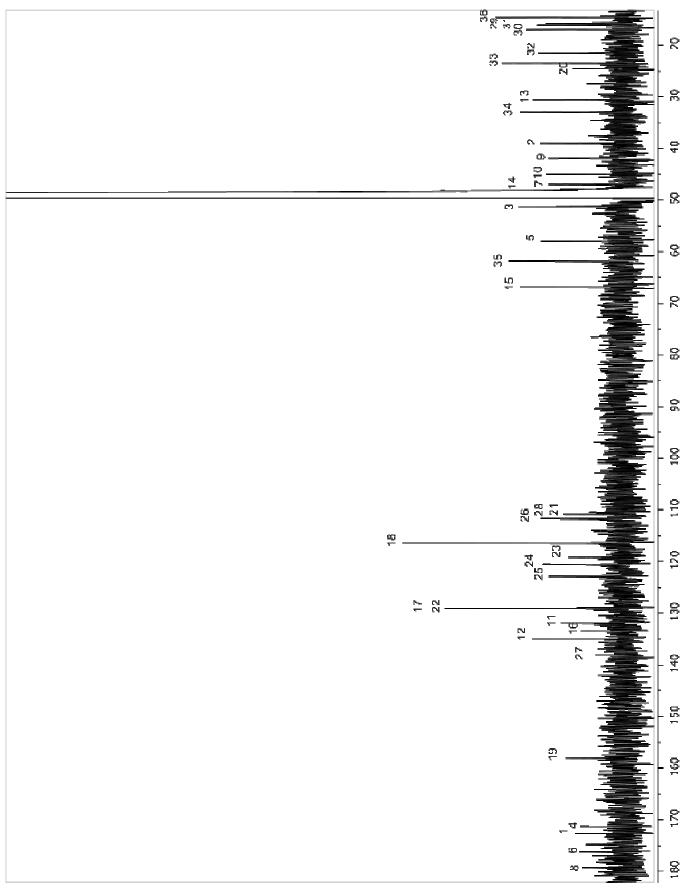
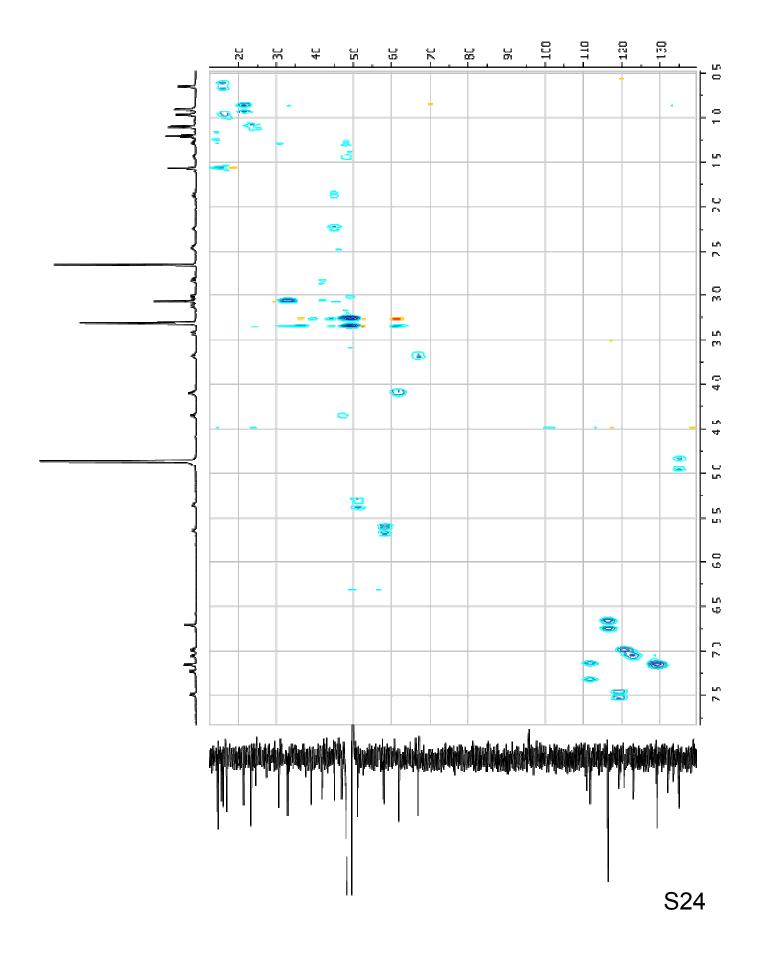


Figure S8. 1 H, 13 C, gHMQC, and gHMBC spectra for **11** in CD $_{3}$ OD.







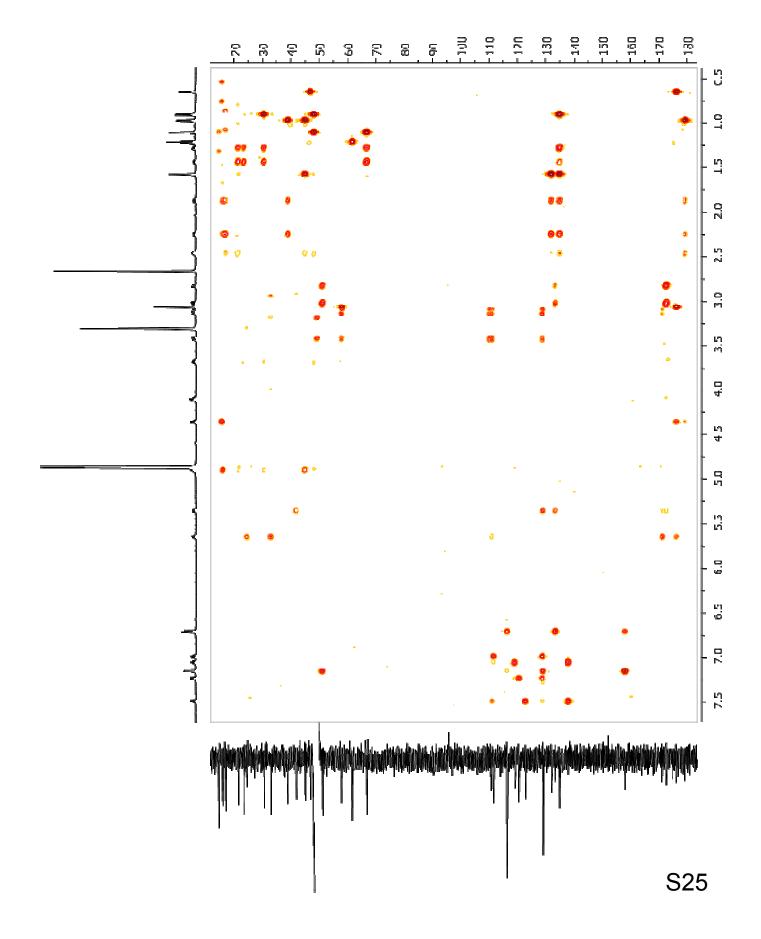
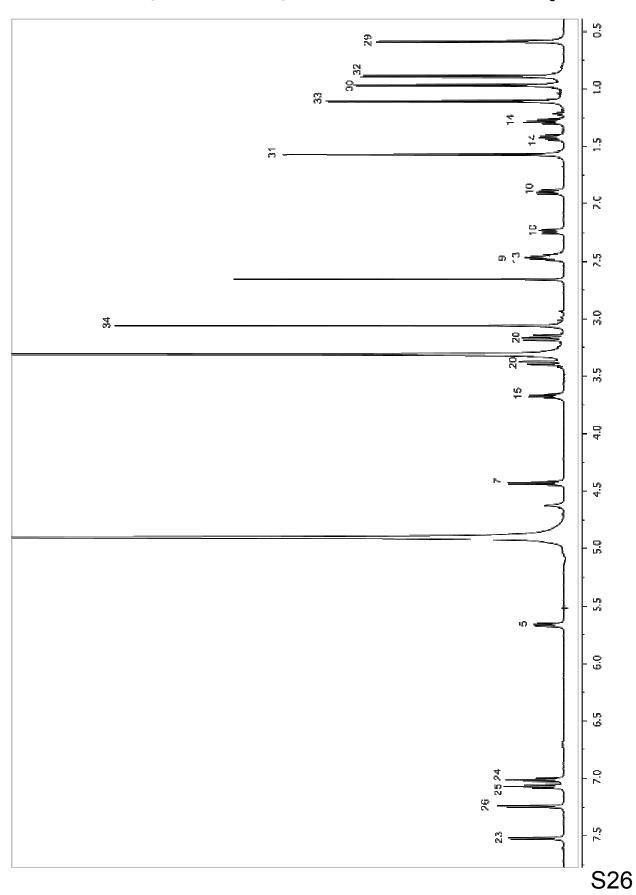
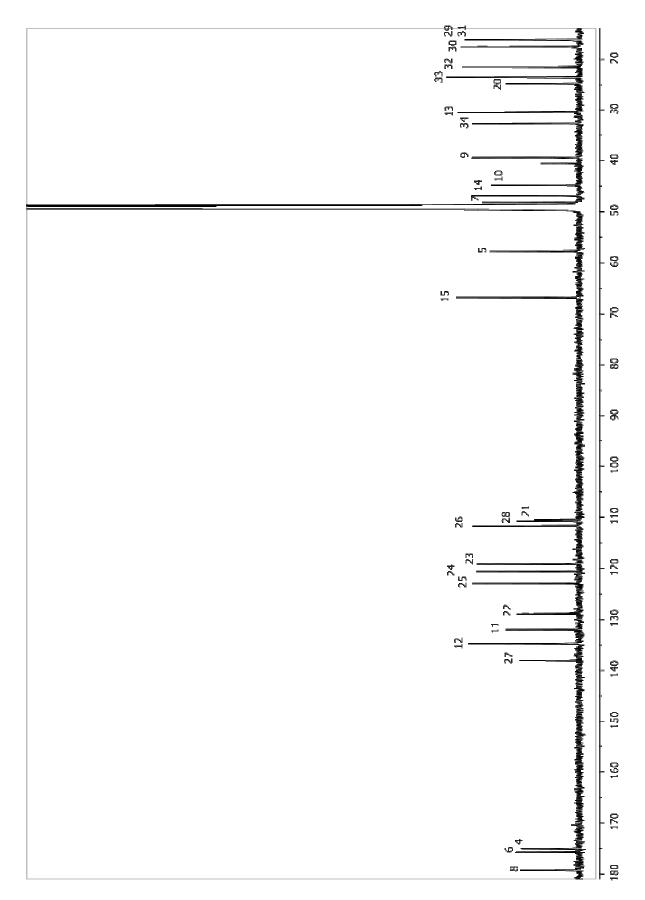
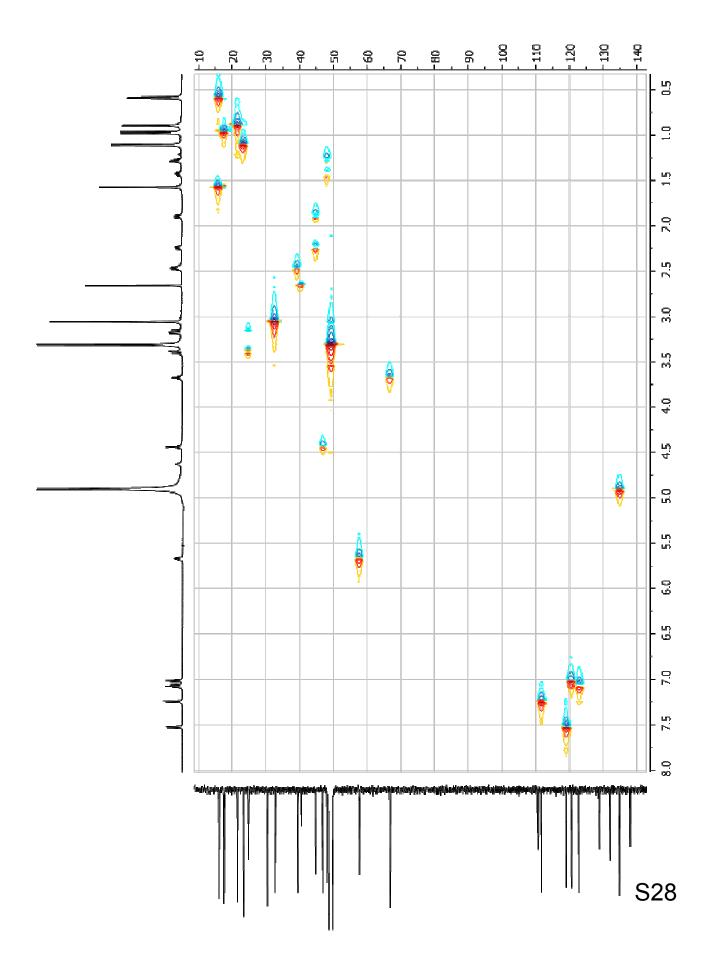


Figure S9. 1 H, 13 C, gHMQC, and gHMBC spectra for **12** in CD $_{3}$ OD.







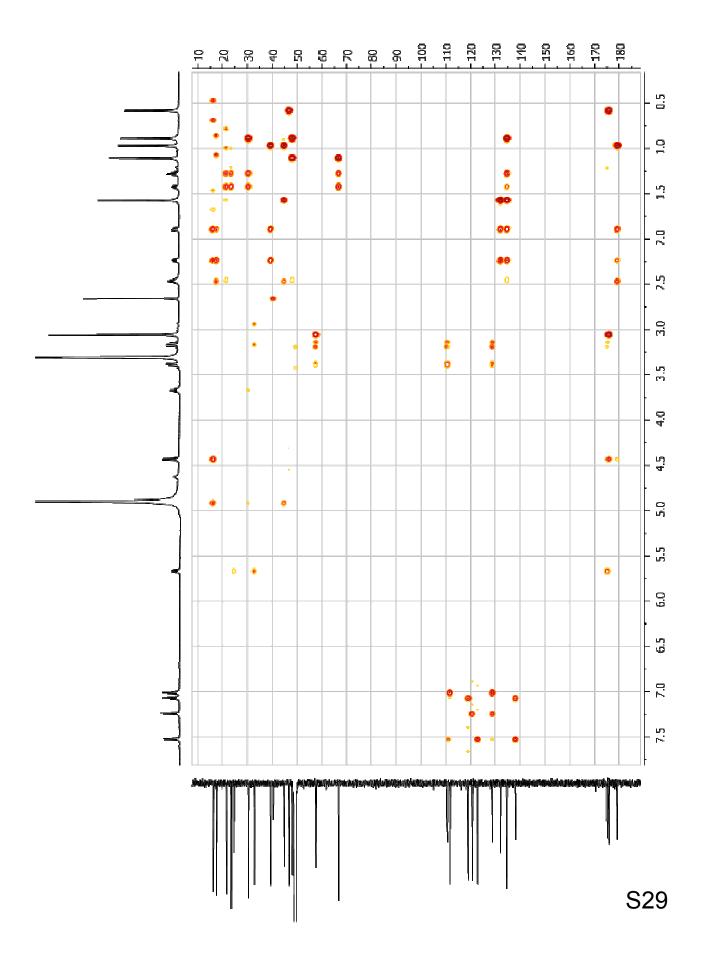
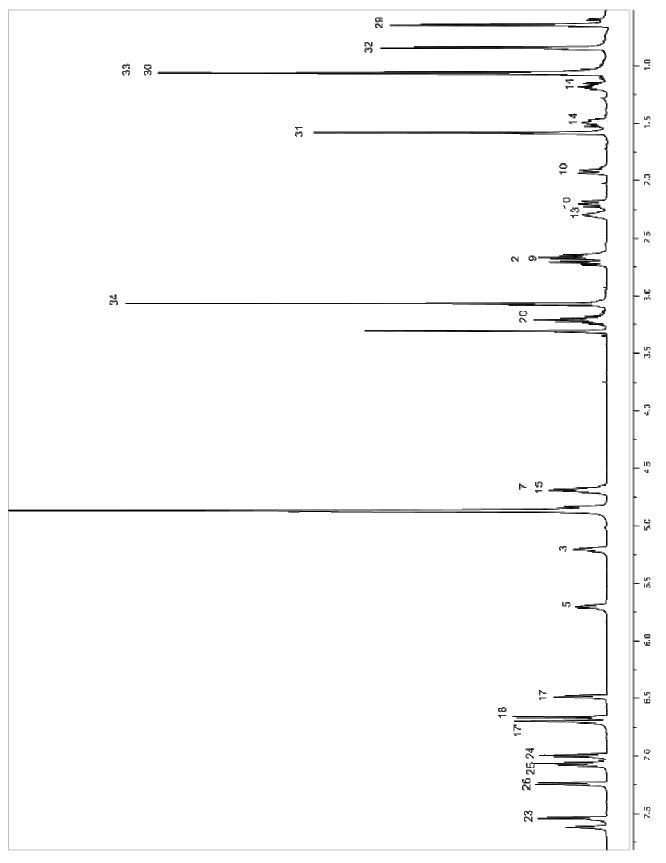
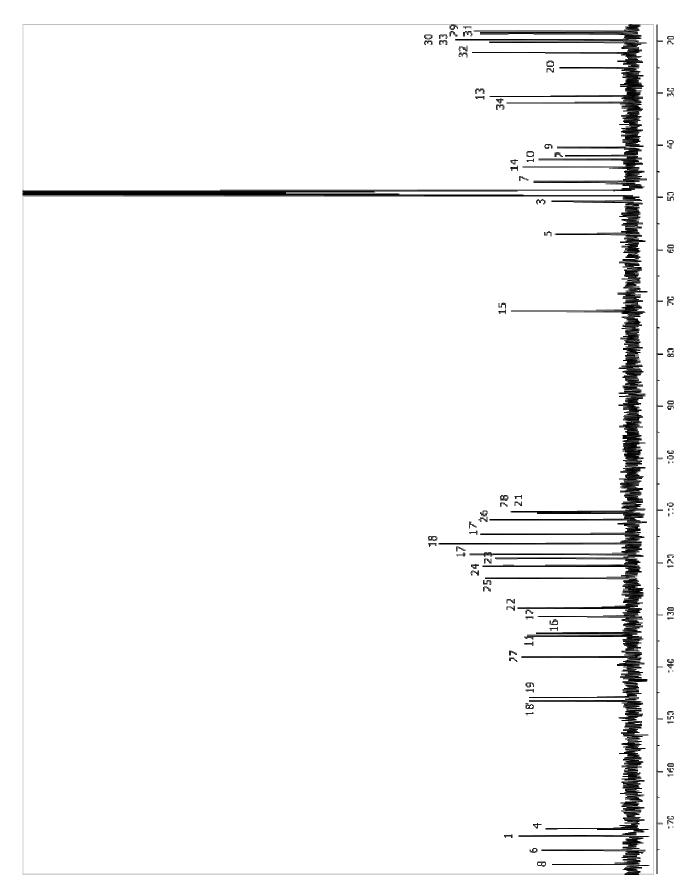
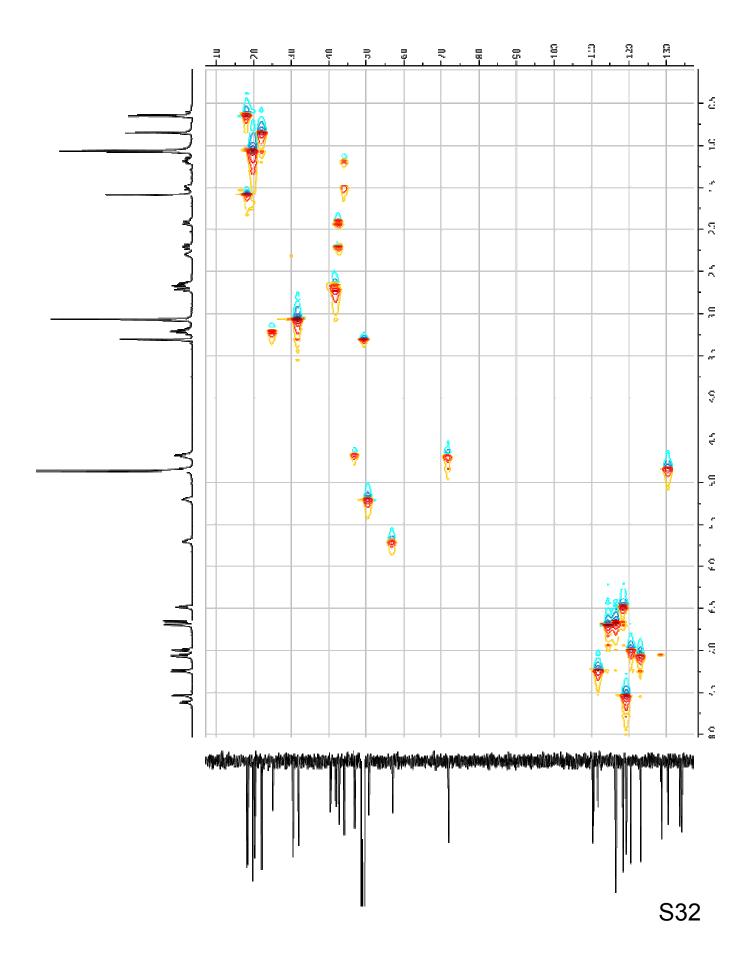


Figure S10. 1 H, 13 C, gHMQC, and gHMBC spectra for **13** in CD $_{3}$ OD.







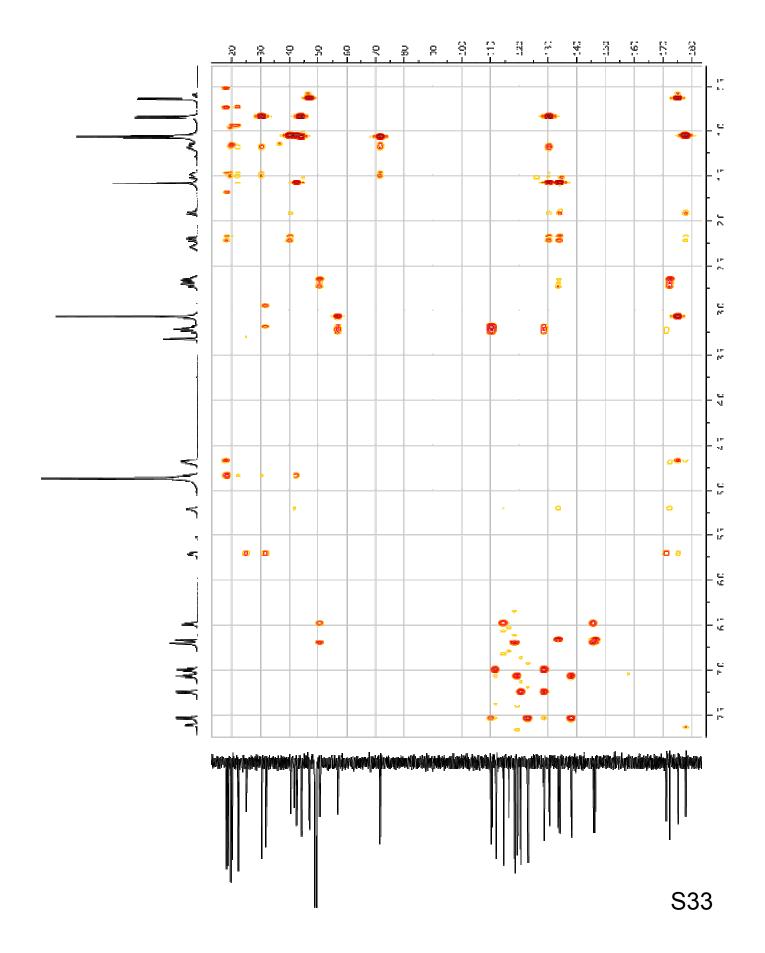
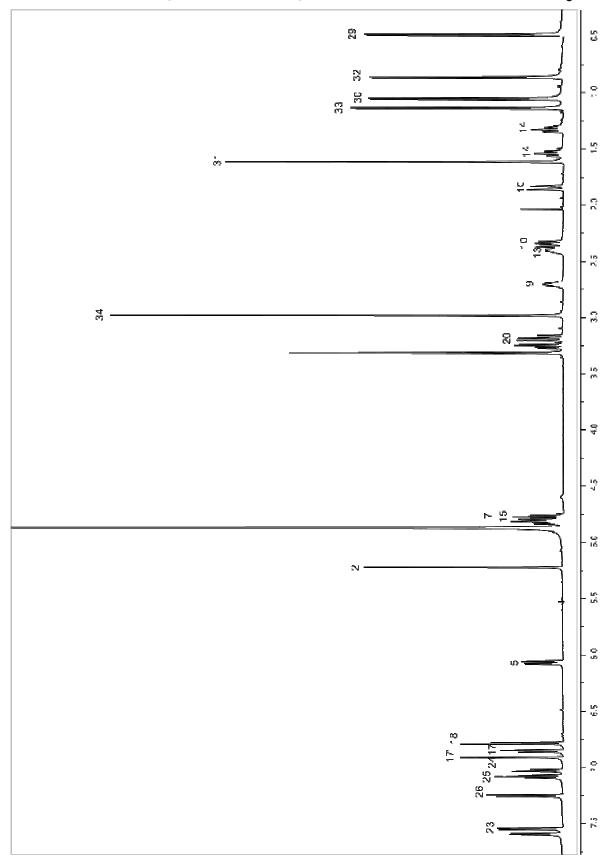
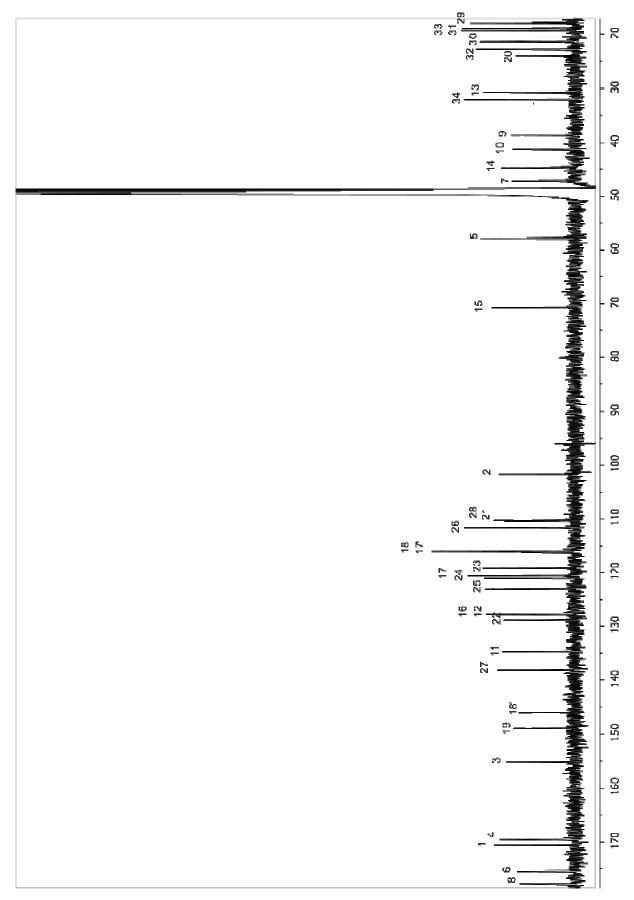
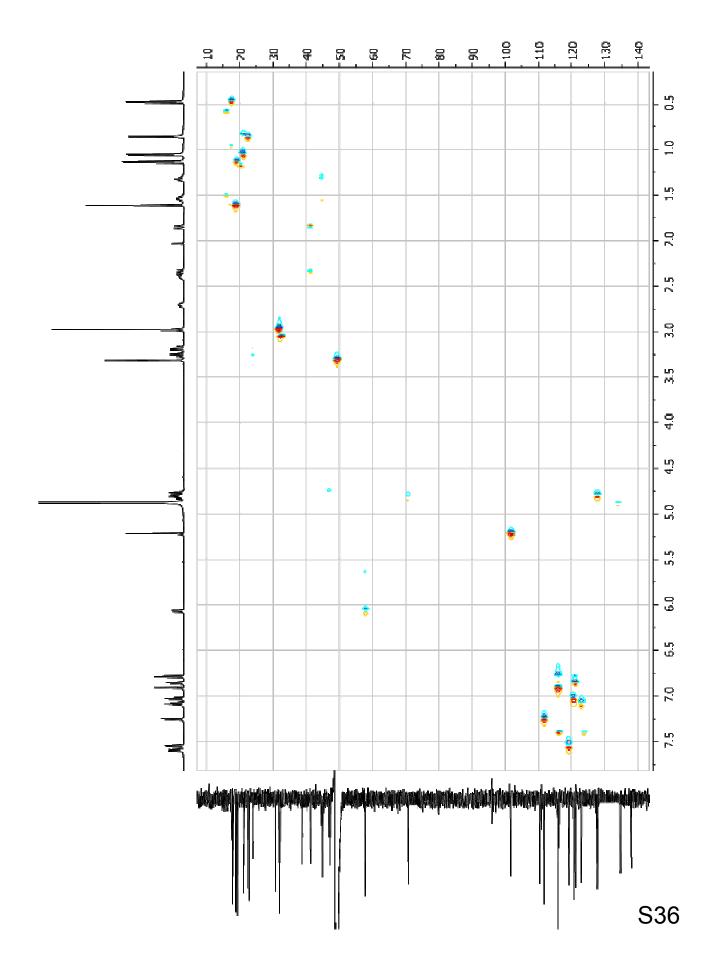


Figure S11. 1 H, 13 C, gHMQC, and gHMBC spectra for **14** in CD $_{3}$ OD.







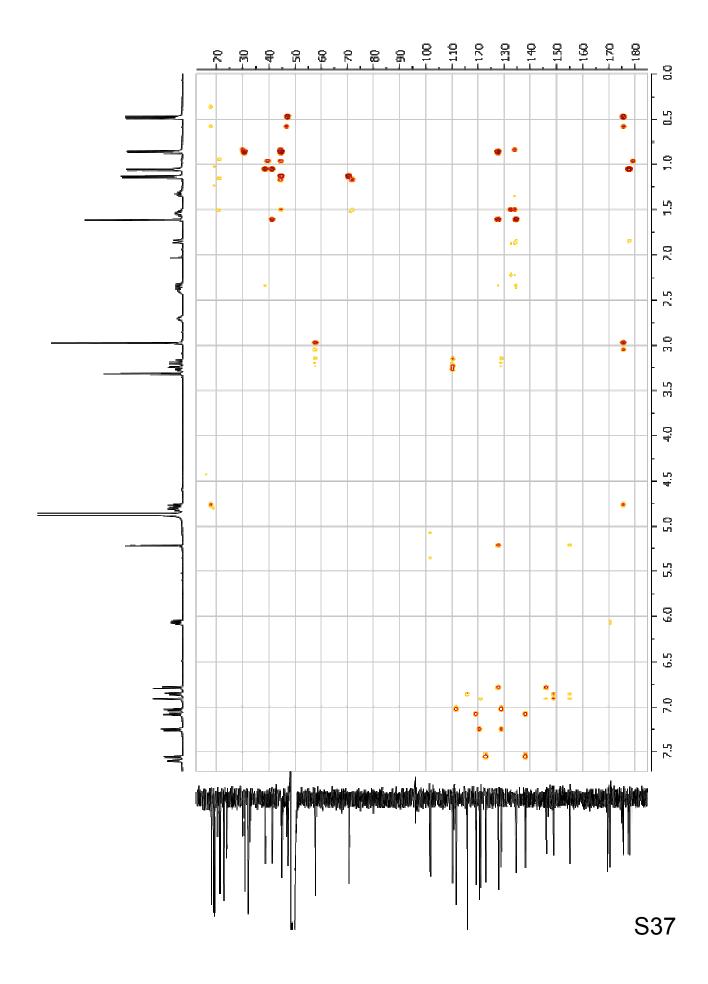
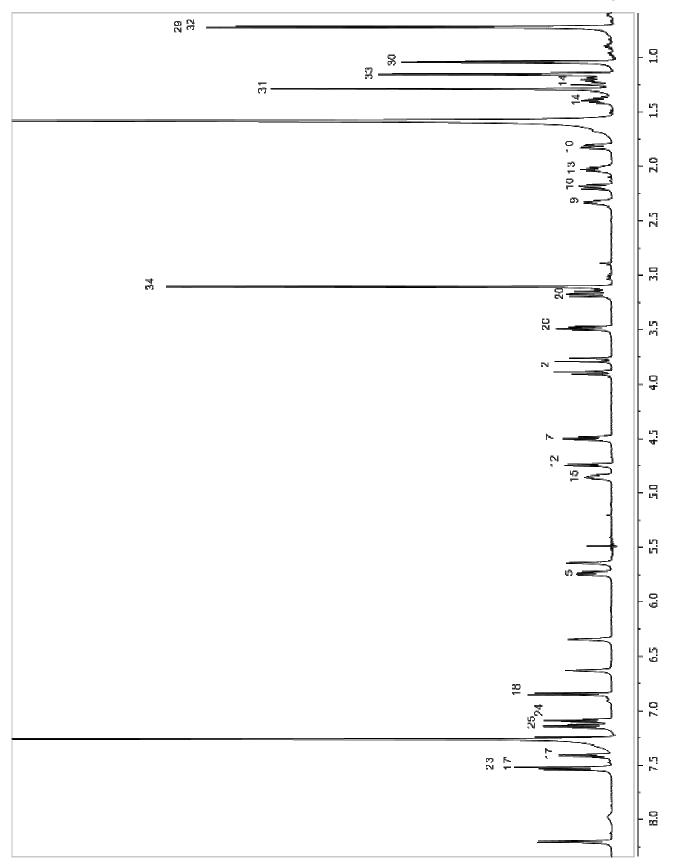
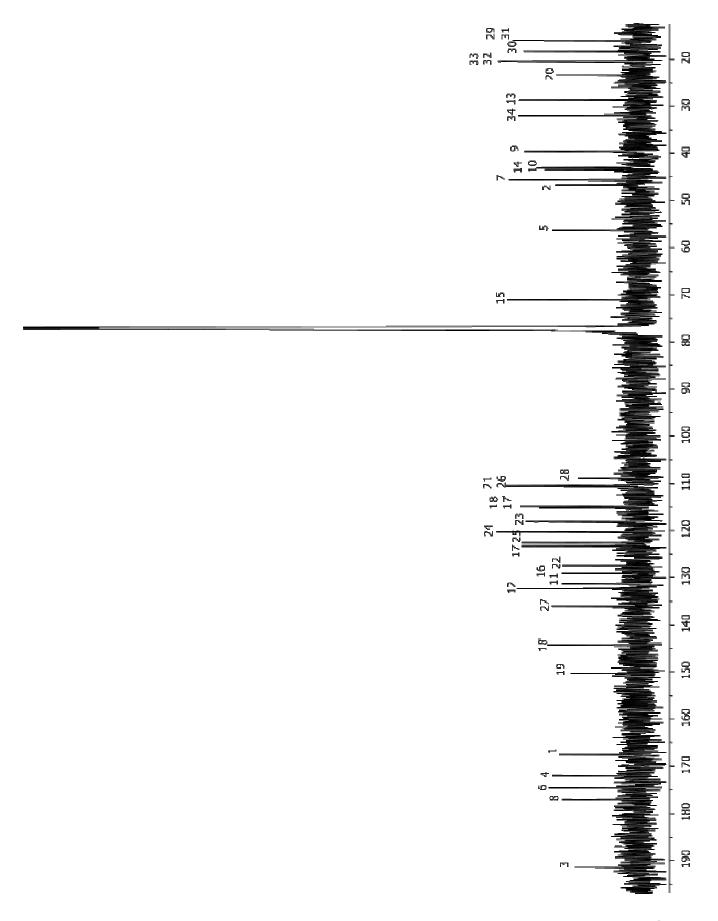
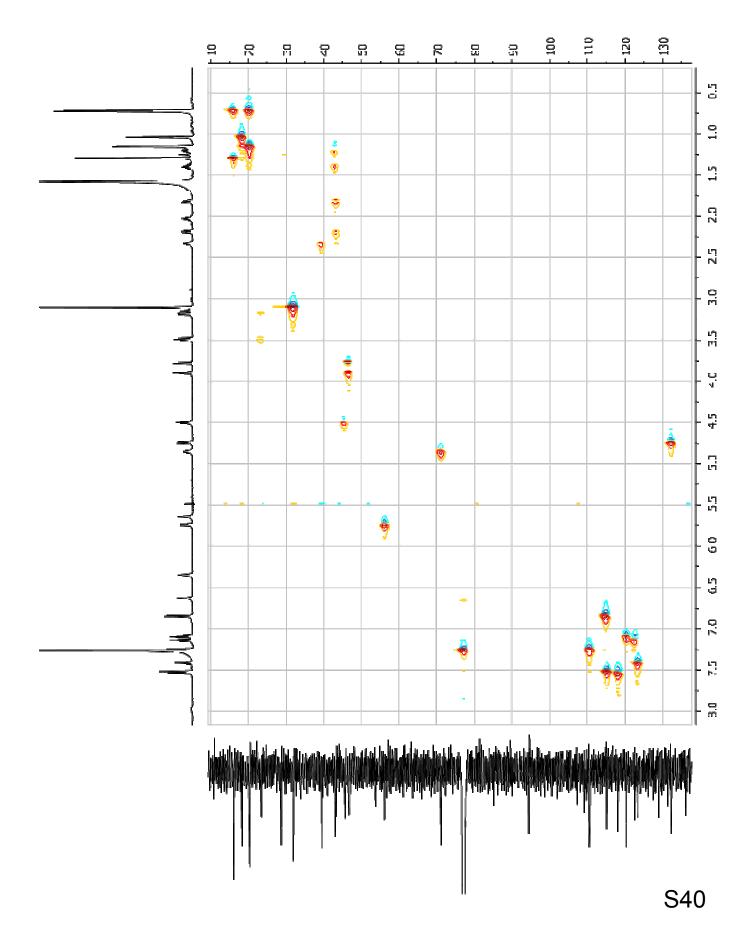


Figure S12. ¹H, ¹³C, gHMQC, and gHMBC spectra for **15** in CDCl₃.







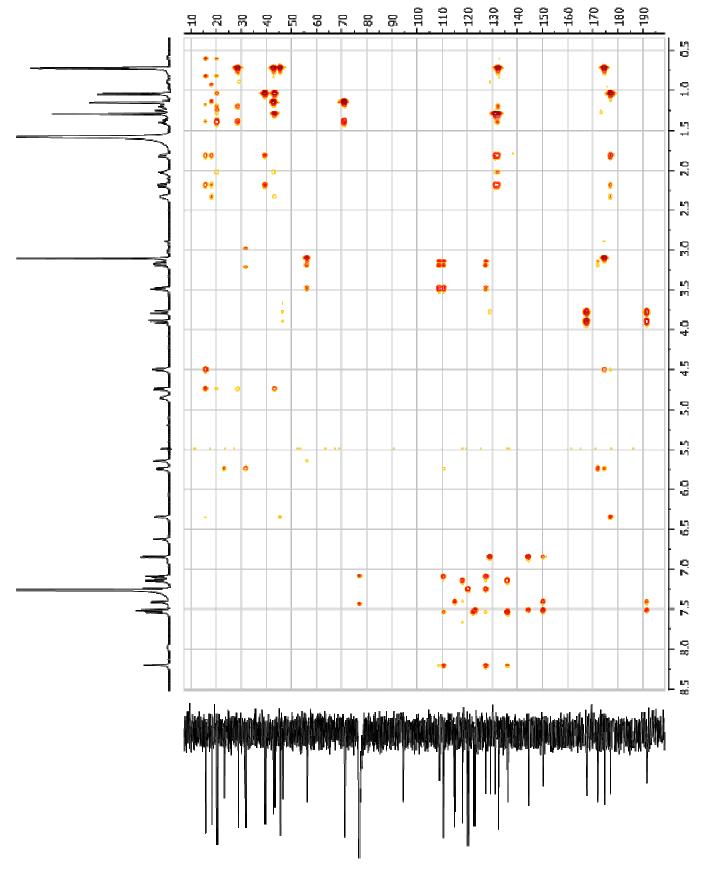


Table S1. NCI 60-cell line results for 1.

NSC: 613009 / 10	Experiment ID: 9704SR27	Test Type : 08	Units : Molar
Report Date : February 24, 2010	Test Date : April 14, 1997	QNS:	MC:
COMI : Jasplakinolide	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COM. Caopia		•					gont. o	TE Buu	. 400	tolutot	-		E . 1 CE 17 C		
						Lo	g10 Con	centration				•			
	Time			Mean	n Optica		-		Б	ercent 0	Srowth				
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
	2610	Out	-0.0	-7.0	-0.0	-0.0	-4.0	-0.0	-7.0	-0.0	-5.0	-4.0	3130	101	L030
Leukemia CCRF-CEM	0.419	1.454	1.025	0.604	0.568	0.585	0.528	59	18	14	16	11	1.62E-8	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.566	1.526	1.025	0.430	0.420	0.407	0.382	51	-24	-26	-28	-33	1.02E-8	4.78E-8	> 1.00E-4 > 1.00E-4
K-562	0.180	0.896	0.580	0.506	0.420	0.217	0.181	56	45	40	5	-55		> 1.00E-4	> 1.00E-4
RPMI-8226	0.610	0.762	0.510	0.524	0.462	0.353	0.317	-16	-14	-24	-42	-48		< 1.00E-8	> 1.00E-4
SR	0.568	0.927		0.762	0.598	0.537	0.470	93	54	8	-6	-17	1.23E-7	3.99E-6	> 1.00E-4
Non-Small Cell Lung	Cancor														
A549/ATCC	0.433	1.836	1.769	0.631	0.527	0.478	0.409	95	14	7	3	-6	3.61E-8	2.33E-5	> 1.00E-4
EKVX	0.325	0.820	0.792	0.510	0.326	0.312	0.312	94	37		-4	-4	6.01E-8	1.06E-6	> 1.00E-4
HOP-62	0.219	0.649	0.715	0.301	0.181	0.188	0.191	115	19	-17	-14	-13	4.77E-8	3.33E-7	> 1.00E-4
HOP-92	0.193	1.095	1.113	0.560	0.539	0.565	0.559	102	41	38	41	41	7.05E-8	> 1.00E-4	> 1.00E-4
NCI-H226	0.461	0.921	0.919	0.271	0.205	0.200	0.171	99	-41	-56	-57	-63	2.25E-8	5.09E-8	4.11E-7
NCI-H23	0.779	1.482	1.528	1.233	0.835	0.734	0.412	107	65	8	-6	-47	1.81E-7	3.80E-6	> 1.00E-4
NCI-H322M	0.239	0.790	0.728	0.449	0.308	0.233	0.239	89	38	12	-3	÷	5.82E-8	6.79E-6	> 1.00E-4
NCI-H460 NCI-H522	0.229 0.279	1.794 0.660	1.137 0.586	0.564	0.538	0.481 0.234	0.336 0.182	58 81	21 6	20 -11	16 -16	-35	1.65E-8 > 2.57E-8	> 1.00E-4 2.33E-7	> 1.00E-4 > 1.00E-4
NOI-HOZZ	0.279	0.000	0.300	0.303	0.250	0.234	0.102	01	0	-11	-10	-33	Z.37E-0	2.33E-7	> 1.00E-4
Colon Cancer															
COLO 205	0.117	0.591	0.398	0.214	0.200	0.218	0.193	59	20	18	21	16	1.73E-8 >	> 1.00E-4	> 1.00E-4
HCC-2998	0.001	0.642	0.473	0.287	0.251		0.200	74	45	39	37	31		> 1.00E-4	> 1.00E-4
HCT-116	0.143	1.477	1.237	0.484	0.217	0.218	0.101	82	26	6	6	-29	3.70E-8	1.44E-5	> 1.00E-4
HCT-15	0.773	1.630	1.565	1.036	0.756	0.781	0.787	92	31	-2	1	2	4.87E-8		> 1.00E-4
HT29	0.221	1.201	0.774	0.282	0.253	0.250	0.209	56	6	3	3	-5	1.34E-8	2.28E-5	> 1.00E-4
KM12 SW-620	0.280 0.281	1.459 1.291	1.257 0.919	0.926 0.723	0.666 0.652	0.473 0.580	0.204 0.431	83 63	55 44	33 37	16 30	-27 15	1.65E-7 4.76E-8	2.37E-5 > 1.00E-4	> 1.00E-4 > 1.00E-4
3VV-02U	0.201	1.231	0.919	0.723	0.032	0.560	0.431	03	44	31	30	13	4.700-0	1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.190	0.669	0.699	0.205	0.169	0.148	0.141	106	3	-11	-22	-26	3.52E-8	1.66E-7	> 1.00E-4
SF-295	0.430	1.390	1.335	0.691	0.345	0.235	0.318	94	27	-20	-45	-26	4.57E-8	3.81E-7	> 1.00E-4
SF-539	0.209	0.660	0.647	0.151	0.093	0.083	0.110	97	-28	-56	-60	-47	2.38E-8	5.97E-8	4 745 7
SNB-19 SNB-75	0.914 0.340	1.441 0.695	1.431 0.601	0.512	0.276 0.222	0.299	0.376 0.192	98 74	-44 -8	-70 -35	-67 -62	-59 -44	2.18E-8 1.94E-8	4.90E-8 7.93E-8	1.71E-7
U251	0.642	2.465	2.097	1.461	0.764	0.758	0.192	80	-o 45	-35 7	-62	-44	7.14E-8	6.73E-5	> 1.00E-4
	0.042	2.400	2.001	1.401	0.704	0.700	0.004	-	40	,		-	7.142-0	0.702-0	1.002-4
Melanoma															
LOX IMVI	0.124	0.922	0.265	0.104	0.091	0.073	0.069	18	-16	-27	-41	-44	< 1.00E-8	3.33E-8	> 1.00E-4
M14 MDA-MB-435	0.165 0.664	0.796 2.725	2.619	0.354 1.193	0.254	0.233	0.169 0.517	82 95	30 26	14 11	11 7	-22	4.11E-8 > 4.45E-8	> 1.00E-4 1.77E-5	> 1.00E-4 > 1.00E-4
SK-MEL-2	0.318	0.692	0.626	0.426	0.309	0.130	0.162	82	29	-3	-59	-49	4.03E-8	8.15E-7	7 1.00L-4
SK-MEL-28	0.592	1.848	1.787	0.771	0.734	0.847	0.572	95	14	11	20	-3	3.61E-8	7.15E-5	> 1.00E-4
UACC-257	0.710	1.932	1.938	1.633	1.059	1.016	0.630	100	75	29	25	-11	3.49E-7	4.88E-5	> 1.00E-4
UACC-62	0.680	1.705	1.691	1.003	0.866	0.738	0.447	99	31	18	6	-34	5.30E-8	1.39E-5	> 1.00E-4
Ovarian Cancer															
IGROV1	0.276	0.788	0.643	0.157	0.163	0.175	0.191	72	-43	-41	-37	-31	1.54E-8	4.21E-8	> 1.00E-4
OVCAR-3	0.498	1.488	1.421	0.730	0.469	0.252	0.389	93	23	-6	-49	-22	4.17E-8	6.37E-7	> 1.00E-4
OVCAR-4	0.238	1.162	1.108	0.875	0.510	0.237	0.224	94	69	29		-6	3.01E-7	9.68E-6	> 1.00E-4
OVCAR-5	0.292	0.831	0.860	0.577	0.472	0.449	0.460	105	53	33	29	31		> 1.00E-4	> 1.00E-4
OVCAR-8	0.233	0.962	0.968	0.273	0.096	0.017	0.091	101	5	-59	-93	-61	3.41E-8	1.22E-7	7.25E-7
NCI/ADR-RES	0.236	0.643	0.568	0.417	0.310	0.139	0.126	82	44	18	-41	-47	7.06E-8	2.02E-6	> 1.00E-4
Renal Cancer															
786-0	0.099	0.976	0.947	0.160	0.108	0.082	0.052	97	7	1	-17	-48	3.31E-8	1.13E-6	> 1.00E-4
A498	0.231	1.159	1.102	0.306	0.297	0.400	0.374	94	8	7	18	15		> 1.00E-4	> 1.00E-4
ACHN	0.266	0.620	0.405	0.178	0.140	0.179	0.171	39	-33	-48	-33	-36	< 1.00E-8	3.48E-8	> 1.00E-4
CAKI-1	0.164	0.431		0.078		0.070	0.126	93	-52	-66	-57	-23	1.98E-8	4.36E-8	
RXF 393	0.272	1.300			0.318			101	53	4	12	4		> 1.00E-4	> 1.00E-4
TK-10	0.336	1.033			0.262			88	7 51	-22 -59	-25	8	2.95E-8	2 01E 7	> 1.00E-4
UO-31	0.691	1.214	1.188	0.908	0.284	0.247	0.384	95	51	-09	-64	-44	1.02E-7	2.91E-7	
Prostate Cancer															
DU-145	0.147	0.542	0.499	0.202	0.137	0.175	0.175	89	14	-7	7	7	3.31E-8	-	> 1.00E-4
Breast Cancer															
MCF7	0.222	1.405			0.615			100	58	33	15	4		> 1.00E-4	> 1.00E-4
MDA-MB-231/ATC		0.411			0.085			78	-40	-54	-47	-36	1.71E-8	4.55E-8	
HS 578T	0.337	0.617		0.344		0.268		140	2	-17	-21	-9	4.51E-8	1.34E-7	> 1.00E-4
MDA-N T-47D	0.125 0.257	0.533 0.479	0.448		0.160 0.174			92	19 37	-32	-10 -25	-24 3	5.74E-8	2.83E-6	> 1.00E-4 > 1.00E-4
. 410	0.201	0.410	0.402	0.000	0.174	0.102	0.200	0L	31	J.E	20		0.1-7L-0	-	1.50L-4

Table S2. NCI 60-cell line results for 4.

NSC : D - 751841 / 1	Experiment ID: 0912NS69	Test Type : 08	Units : Molar
Report Date : February 01, 2010	Test Date : December 14, 2009	QNS:	MC:
COMI : PC 1011 (92204)	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI : PC 10	11 (922	204)			Sta	in Rea	gent : S	RB Dual-	-Pass	Related	d	SSPI	L : K24A		
					•	L	og10 Con	centration				•			
	Time			Mean	n Optica	l Densiti	ies		P	ercent (
Panel/Cell Line	Zero	Ctrl	-9.3	-8.3	-7.3	-6.3	-5.3	-9.3	-8.3	-7.3	-6.3	-5.3	GI50	TGI	LC50
Leukemia CCRF-CEM	0.349	1.687	1.632	1.581	0.653	0.568	0.545	96	92	23	16	15	2.12E-8	> 5.25E-6	> 5.25E-6
HL-60(TB)	0.717	2.144	1.917	1.891	0.908	0.556	0.523	84	82	13	-22	-27	1.54E-8	1.24E-7	> 5.25E-6
K-562 MOLT-4	0.257 0.598	1.248 1.648	1.197 1.770	1.037 1.625	0.880 1.258	0.697 0.860	0.424 0.657	95 112	79 98	63 63	44 25	17 6	2.62E-7 1.14E-7	> 5.25E-6 > 5.25E-6	> 5.25E-6 > 5.25E-6
RPMI-8226	0.685	2.195	2.215	2.174	1.003	0.866	0.740	101	99	21	12	4	2.22E-8	> 5.25E-6	> 5.25E-6
Non-Small Cell Lung	Cancer														
A549/ATCC	0.353	1.013	0.996	0.880	0.276	0.216	0.231	97	80	-22	-39	-35	1.03E-8	3.20E-8	> 5.25E-6
EKVX HOP-62	0.633	1.534 0.851	1.609 0.872	1.556 0.868	0.671 0.290	0.619	0.459 0.150	108 104	102 103	4 5	-2 -22	-27 -42	1.79E-8 1.83E-8	2.38E-7 8.10E-8	> 5.25E-6 > 5.25E-6
HOP-92	1.146	1.965	1.911	1.910	1.852	0.516	0.683	93	93	86	-55	-40	9.47E-8	2.14E-7	
NCI-H226 NCI-H23	0.670 0.402	1.492 1.242	1.451 1.222	1.369	0.958	0.705 0.555	0.600	95 98	85 99	35 46	4 18	-11 13	2.63E-8 4.45E-8	1.01E-6 > 5.25E-6	> 5.25E-6 > 5.25E-6
NCI-H322M	0.461	0.773	0.785	0.762	0.750	0.465	0.388	104	96	26	1	-16	2.42E-8	6.24E-7	> 5.25E-6
NCI-H460	0.241	1.967	1.892	1.638	0.550	0.500	0.376	96	81	18	15	8	1.62E-8	> 5.25E-6	> 5.25E-6
NCI-H522	0.593	1.451	1.383	1.294	0.919	0.504	0.573	92	82	38	-15	-3	2.78E-8	2.73E-7	> 5.25E-6
Colon Cancer											_				
COLO 205 HCC-2998	0.195 0.747	1.194 1.776	1.211 1.669	1.082 1.594	0.432 0.525	0.251	0.172 0.155	102 90	89 82	24 -30	-35	-12 -79	2.07E-8 1.02E-8	1.09E-6 2.85E-8	> 5.25E-6 1.13E-6
HCT-116	0.239	1.641	1.589	1.467	0.570	0.417	0.296	96	88	24	13	4	2.03E-8	> 5.25E-6	> 5.25E-6
HCT-15	0.243	1.705	1.562	1.618	1.362	0.824	0.450	90	94	77	40	14	2.76E-7	> 5.25E-6	> 5.25E-6 > 5.25E-6
HT29 KM12	0.153 0.247	0.816 1.314	0.807 1.301	0.627 1.162	0.175 0.775	0.132	0.149 0.396	99 99	71 86	3 49	-14 31	-3 14	1.08E-8 5.08E-8	8.08E-8 > 5.25E-6	> 5.25E-6 > 5.25E-6
SW-620	0.205	1.161	1.106	0.972	0.448	0.340	0.310	94	80	25	14	11	1.87E-8	> 5.25E-6	> 5.25E-6
CNS Cancer															
SF-268	0.389	1.202	1.177	1.120 1.065	0.304 0.463	0.179	0.208	97	90 77	-22 -38	-54 -53	-47 -60	1.20E-8	3.35E-8	2 265 7
SF-295 SF-539	0.751 0.602	1.161 1.989	1.171 1.936	1.869	1.239	0.355	0.301 0.461	102 96	91	-36 46	-14	-60 -24	8.93E-9 4.27E-8	2.43E-8 3.09E-7	3.36E-7 > 5.25E-6
SNB-19	0.492	1.597	1.498	1.515	0.994	0.716	0.507	91	93	45	20	1	4.20E-8	> 5.25E-6	> 5.25E-6
SNB-75 U251	0.519 0.273	1.019 1.137	0.957 1.042	0.868 1.017	0.081	0.038	0.039 0.192	88 89	70 86	-84 -20	-93 -39	-93 -30	7.05E-9 1.15E-8	1.49E-8 3.41E-8	3.14E-8 > 5.25E-6
Melanoma	0.2.0	1.101	1.072	1.017	5.2.15	0.100	0.102	50	-	20	00	00	1.102 0	0.412.0	0.202 0
LOX IMVI	0.105	0.609	0.596	0.281	0.091	0.067	0.031	97	35	-13	-37	-71	3.01E-9	2.78E-8	1.29E-6
MALME-3M	0.844	1.401	1.328	1.157	0.757	0.654	0.611	87 97	56 90	-10	-23	-28	6.52E-9	3.68E-8	> 5.25E-6 > 5.25E-6
M14 MDA-MB-435	0.297	0.951 1.178	0.933 1.165	0.883	0.435	0.254	0.197 0.358	98	96	21 26	-15 10	-34 1	1.98E-8 2.36E-8	2.04E-7 > 5.25E-6	> 5.25E-6 > 5.25E-6
SK-MEL-2	0.714	1.526	1.552	1.469	0.585	0.408	0.265	103	93	-18	-43	-63	1.28E-8	3.61E-8	1.19E-6
SK-MEL-28 SK-MEL-5	0.451 0.409	1.277 2.186	1.270 2.156	1.217 2.059	0.432 1.167	0.178 0.318	0.266 0.228	99 98	93 93	-4 43	-61 -22	-41 -44	1.45E-8 3.74E-8	4.74E-8 2.38E-7	> 5.25E-6
UACC-257	0.559	0.895	0.824	0.847	0.415	0.320	0.320	79	86	-26	-43	-43	1.09E-8	3.08E-8	> 5.25E-6
UACC-62	0.662	2.016	1.942	1.771	1.217	0.988	0.719	95	82	41	24	4	3.16E-8	> 5.25E-6	> 5.25E-6
Ovarian Cancer															
IGROV1 OVCAR-3	0.479 0.536	0.809 1.382	0.858 1.357	0.745 1.331	0.149 0.425	0.216 0.244	0.150 0.179	115 97	81 94	-69 -21	-55 -54	-69 -67	8.41E-9 1.27E-8	1.82E-8 3.46E-8	3.92E-8 3.87E-7
OVCAR-5	0.488	1.177	1.150	1.127	0.425	0.646	0.590	96	93	53	23	15	6.71E-8	> 5.25E-6	> 5.25E-6
OVCAR-8	0.228	0.678	0.677	0.695	0.395	0.271	0.112	100	104	37	9	-51	3.37E-8	7.52E-7	5.04E-6
NCI/ADR-RES SK-OV-3	0.283	0.928 1.016	0.917 1.043	0.891	0.726	0.462	0.257 0.274	98 105	94 93	69 -3	28 -33	-9 -40	1.50E-7 1.48E-8	2.93E-6 4.88E-8	> 5.25E-6 > 5.25E-6
Renal Cancer										-					3.202
786-0	0.387	1.400	1.362	1.292	0.260	0.171		96	89	-33	-56	-62	1.10E-8	2.83E-8	2.93E-7
A498	0.736	1.773	1.365	1.179	0.253	0.121		61	43	-66 10	-84	-75	2.06E-9	1.30E-8	3.77E-8
ACHN CAKI-1	0.348 0.678	1.575 0.962	1.558 0.950	1.494 1.005	0.582 0.226	0.392	0.427 0.170	99 96	93 115	19 -67	-84	6 -75	2.01E-8 1.20E-8	> 5.25E-6 2.25E-8	> 5.25E-6 4.25E-8
RXF 393	0.649	1.194	1.166	1.151	0.384	0.298	0.140	95	92	-41	-54	-78	1.09E-8	2.59E-8	2.56E-7
SN12C	0.519 0.374	1.891 1.332	1.839 1.259	1.620 1.227		0.778 0.306		96	80	52	19	11	6.10E-8	> 5.25E-6 2.32E-7	> 5.25E-6 > 5.25E-6
TK-10 UO-31	0.569	1.136	1.259	1.033	0.092		0.322	92 91	89 82	33	-18 -70	-14 - 7 2	2.62E-8 1.38E-8	6.29E-8	2.87E-7
Prostate Cancer															
PC-3	0.397	1.634		1.577				97	95	72	21	.7	1.42E-7	> 5.25E-6	> 5.25E-6
DU-145	0.309	1.125	1.145	1.038	0.438	0.341	0.270	102	89	16	4	-13	1.80E-8	9.06E-7	> 5.25E-6
Breast Cancer MCF7	0.204	0.894	0.848	0.731	0.317	0.268	0.182	93	76	16	9	-11	1.44E-8	1.50E-6	> 5.25E-6
MDA-MB-231/ATCC	0.449	1.123	1.123	1.032	0.652	0.544	0.450	100	86	30	14		2.33E-8	> 5.25E-6	> 5.25E-6
HS 578T	0.514	1.222	1.103	1.114	0.505		0.403	83	85	-2	-10	-22	1.32E-8	5.01E-8	> 5.25E-6
BT-549 T-47D	0.792 0.443	1.348 1.111	1.350 1.068	1.245 1.092	0.183 0.784	0.079 0.568	0.061 0.485	100 94	82 97	-77 51	-90 19	-92 6	8.30E-9 5.65E-8	1.72E-8 > 5.25E-6	3.55E-8 > 5.25E-6
MDA-MB-468	0.536	1.400		1.244	0.300		0.206	98	82	-44	-57	-62	9.42E-9	2.35E-8	1.58E-7

Table S3. NCI 60-cell line results for 5.

NSC: D - 751842 / 1	Experiment ID: 0912NS69	Test Type : 08	Units : Molar
Report Date : February 01, 2010	Test Date : December 14, 2009	QNS:	MC:
COMI : PC 1010 (92205)	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMIT PC 10	10 (922	us)			Sta	in Rea	gent: S	KB Dual-	-Pass	Related	1	33P	L : KZ4A		
						L	and Con	centration				_			
	Time			Mear	n Optica		~	centiation	Р	ercent G	Srowth				
Panel/Cell Line	Zero	Ctrl	-8.7	-7.7	-6.7	-5.7	-4.7	-8.7	-7.7	-6.7	-5.7	-4.7	GI50	TGI	LC50
Leukemia	2010	001	0.11	7	0.1	0.1		4.7		0.,	0.1	***	0.00	101	2000
CCRF-CEM	0.349	1.687	1.546	1.580	0.674	0.612	0.544	89	92	24	20	15	7.51E-8 >	1.80E-5	> 1.80E-5
HL-60(TB)	0.717	2.144	2.104	2.198	1.378	0.542	0.611	97	104	46	-24	-15	1.55E-7	8.12E-7	> 1.80E-5
K-562	0.257	1.248	1.105	1.090	0.913	0.724	0.280	86	84	66	47	2		1.80E-5	> 1.80E-5
MOLT-4 RPMI-8226	0.598	1.648 2.195	1.652 2.182	1.659 2.067	1.262 1.284	0.863 0.927	0.542 0.700	100 99	101 92	63 40	25 16	-9 1	4.01E-7 1.14E-7 >	9.64E-6 1.80E-5	> 1.80E-5 > 1.80E-5
		2.193	2.102	2.007	1.204	0.927	0.700	90	92	40	10	'	1.146-7	1.00E-3	> 1.00E-0
Non-Small Cell Lung A549/ATCC		4.042	1.000	0.967	0.000	0.266	0.170	ne	02	40	o.e	40	4 26E 0	1 225 7	> 100E E
EKVX	0.353 0.633	1.013 1.534	1.429	1.428	0.286 1.191	0.200	0.179 0.582	98 88	93 88	-19 62	-25 -2	-49 -8	4.36E-8 2.76E-7	1.22E-7 1.65E-6	> 1.80E-5 > 1.80E-5
HOP-62	0.259	0.851	0.864	0.878	0.435	0.251	0.221	102	105	30	-3	-15	9.65E-8	1.43E-6	> 1.80E-5
HOP-92	1.146	1.965	1.911	1.803	1.928	0.636	0.919	93	80	95	-45	-20	3.80E-7	8.65E-7	> 1.80E-5
NCI-H226	0.670	1.492	1.380	1.487	1.230	0.754	0.601	86	99	68	10	-10	3.70E-7	5.62E-6	> 1.80E-5
NCI-H23 NCI-H322M	0.402 0.461	1.242 0.773	1.235 0.734	1.205 0.772	0.986 0.584	0.642 0.462	0.542 0.423	99 87	96 100	69 39	29	17 -8	5.38E-7 > 1.20E-7	1.80E-5 1.96E-6	> 1.80E-5 > 1.80E-5
NCI-H460	0.241	1.967	1.934	1.883	0.526	0.487	0.212	98	95	17	14	-12	6.75E-8	6.27E-6	> 1.80E-5
NCI-H522	0.593	1.451	1.405	1.439	1.342	0.735	0.371	95	99	87	16	-38	6.06E-7	3.64E-6	> 1.80E-5
0-1 0															
Colon Cancer COLO 205	0.195	1.194	1.251	1.086	0.465	0.241	0.294	106	89	27	5	10	7.69E-8 >	1.80E-5	> 1.80E-5
HCC-2998	0.747	1.776	1.674	1.639	0.660	0.729	0.114	90	87	-12	-2	-85	4.25E-8	1.37E-7	6.81E-6
HCT-116	0.239	1.641	1.550	1.605	0.776	0.477	0.114	93	97	38	17	-52	1.14E-7	3.16E-6	1.67E-5
HCT-15	0.243	1.705	1.637	1.710	1.533	1.152	0.490	95	100	88	62	17		1.80E-5	> 1.80E-5
HT29 KM12	0.153 0.247	0.816 1.314	0.787 1.243	0.764 1.280	0.211	0.198	0.123 0.291	96 93	92 97	9 49	7 42	-20 4	5.75E-8 1.71E-7 >	3.23E-6 1.80E-5	> 1.80E-5 > 1.80E-5
SW-620	0.205	1.161	1.116	1.140	0.769	0.096	0.261	95	98	36	19	6		1.80E-5	> 1.80E-5
	0.200				41001	0.001		••	-	••	10	•			11002
CNS Cancer SF-268	0.389	1.202	1.147	1.221	0.733	0.237	0.233	93	102	42	-39	-40	1.34E-7	5.95E-7	> 1.80E-5
SF-295	0.751	1.161	1.158	1.213	0.572	0.436	0.269	99	112	-24	-42	-64	5.17E-8	1.20E-7	4.13E-6
SF-539	0.602	1.989	1.950	1.841	1.626	0.701	0.416	97	89	74	7	-31	4.10E-7	2.77E-6	> 1.80E-5
SNB-19	0.492	1.597	1.463	1.504	1.239	0.785	0.524	88	92	68	26	3		1.80E-5	> 1.80E-5
SNB-75	0.519	1.019	0.920	0.977	0.844	0.066	0.095	80	92	65	-87	-82	2.26E-7 4.79E-8	4.81E-7	1.02E-6
U251	0.273	1.137	1.125	0.991	0.318	0.218	0.187	99	83	5	-20	-32	4./9E-0	2.88E-7	> 1.80E-5
Melanoma	0.405								70		40		0.405.0	4 055 7	4 44= 5
LOX IMVI MALME-3M	0.105 0.844	0.609 1.401	0.564 1.241	0.502 1.371	0.080	0.086 0.641	0.049 0.648	91 71	79 95	-24 63	-18 -24	-54 -23	3.43E-8 2.56E-7	1.05E-7 9.56E-7	1.41E-5 > 1.80E-5
M14	0.297	0.951	0.919	0.957	0.494	0.389	0.090	95	101	30	14	-70	9.40E-8	2.65E-6	1.04E-5
MDA-MB-435	0.349	1.178	1.113	1.110	0.655	0.540	0.204	92	92	37	23	-42	1.04E-7	4.09E-6	> 1.80E-5
SK-MEL-2	0.714	1.526	1.558	1.626	0.922	0.502	0.398	104	112	26	-30	-44	9.43E-8	5.22E-7	> 1.80E-5
SK-MEL-28 SK-MEL-5	0.451 0.409	1.277 2.186	1.196 2.121	1.301 2.128	0.889 1.643	0.347	0.285 0.293	90 96	103 97	53 69	-23 9	-37 -28	1.97E-7 3.75E-7	8.93E-7 3.07E-6	> 1.80E-5 > 1.80E-5
UACC-257	0.559	0.895	0.880	0.872	0.514	0.422	0.356	95	93	-8	-25	-36	4.79E-8	1.50E-7	> 1.80E-5
UACC-62	0.662	2.016	1.850	1.925	1.589	1.153	0.771	88	93	68	36	8		1.80E-5	> 1.80E-5
Overien Canaca															
Ovarian Cancer IGROV1	0.479	0.809	0.804	0.707	0.160	0.192	0.219	98	69	-67	-60	-54	2.49E-8	5.81E-8	1.36E-7
OVCAR-3	0.536	1.382	1.361	1.387	0.957	0.351	0.364	97	101	50	-35	-32	1.78E-7	7.00E-7	> 1.80E-5
OVCAR-5	0.488	1.177	1.111	1.159	1.054	0.742	0.649	90	97	82	37	23	9.22E-7 >	1.80E-5	> 1.80E-5
OVCAR-8	0.228	0.678	0.691	0.683	0.474	0.309	0.165	103	101	55	18	-28	2.41E-7	4.45E-6	> 1.80E-5
NCI/ADR-RES SK-OV-3	0.283 0.460	0.928 1.016	0.906 1.033	0.878 1.027	0.855 0.882	0.691 0.427	0.450 0.428	97 103	92 102	89 76	63 -7	26 -7	4.06E-6 > 3.68E-7	1.80E-5 1.47E-6	> 1.80E-5 > 1.80E-5
	0.400	1.010	1.003	1.027	0.002	0.727	0.720	103	102	70	-7	-1	0.00E-1	1.712-0	- 1.00E-0
Renal Cancer	A 207	1,400	1.299	1,417	1.026	0.213	0.336	90	102	62	-45	20	2 205 7	6 90E 7	> 1 00E F
786-0 A498	0.387 0.736	1.773	1.532	1.553	1.360	0.213	0.236 0.209	90 77	102 79	63 60	-45 -81	-39 -72	2.38E-7 2.12E-7	6.89E-7 4.79E-7	> 1.80E-5 1.08E-6
ACHN	0.348	1.575	1.554	1.477	1.200	0.550	0.419	98	92	69	16	6		1.80E-5	> 1.80E-5
CAKI-1	0.678	0.962	0.895	0.805	0.616	0.130	0.195	76	45	-9	-81	-71	1.22E-8	1.21E-7	6.68E-7
RXF 393	0.649	1.194	1.139	1.185	1.142	0.240	0.131	90	98	90	-63	-80	3.30E-7	6.99E-7	1.48E-6
SN12C TK-10	0.519 0.374	1.891 1.332		1.816 1.347				90 95	95 102	78 98	34 14	16 20		1.80E-5 1.80E-5	> 1.80E-5 > 1.80E-5
UO-31	0.569	1.136		1.094				89	93	86	-49	-32	3.31E-7	7.77E-7	> 1.80E-5 > 1.80E-5
Prostate Cancer PC-3	0.397	1.634	1.600	1.461	1 100	0.704	0.539	97	96	64	25	44	4.14E-7 >	1.80E-5	> 1.80E-5
DU-145	0.397	1.125		1.162				96	86 104	59	14	11 -3	4.14E-7 > 2.91E-7	1.80E-5 1.27E-5	> 1.80E-5 > 1.80E-5
Breast Cancer	4.000				0.754	V. Tal	0.50	-		50					
MCF7	0.204	0.894	0.786	0.865	0.357	0.335	0.127	84	96	22	19	-38	7.53E-8	3.88E-6	> 1.80E-5
MDA-MB-231/ATC	C 0.449	1.123	1.055	1.115	0.828	0.583	0.537	90	99	56	20	13	2.67E-7 >	1.80E-5	> 1.80E-5
HS 578T	0.514	1.222		1.372		0.709		105	121	129	27	23		1.80E-5	> 1.80E-5
BT-549 T-47D	0.792 0.443	1.348 1.111	1.297	1.371 1.042		0.125		91 95	104 90	115 66	-84 26	-87 -7	3.81E-7 4.45E-7	6.80E-7 1.09E-5	1.21E-6 > 1.80E-5
MDA-MB-468	0.536	1.400		1.338				90	93	-15	-50	-67	4.50E-8	1.09E-3	1.77E-6

Table S4. NCI 60-cell line results for 6.

NSC : D - 751843 / 1	Experiment ID: 0912NS69	Test Type : 08	Units : Molar
Report Date : February 01, 2010	Test Date : December 14, 2009	QNS:	MC:
COMI : PC 1002 (92206)	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI : PC 100)2 (922	06)			Stai	n Rea	gent : S	RB Dual-	-Pass	Related	i	SSP	L : K24A		
Log10 Concentration															
Panel/Cell Line	Time Zero	Ctrl	-8.9	Mear -7.9	Optical	Densiti -5.9	es -4.9	-8.9	-7.9	ercent G -6.9	-5.9	-4.9	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.349 0.717 0.257 0.598 0.685	1.660 2.333 2.033 1.837 2.203	1.671 2.176 1.967 1.854 2.246	1.634 2.321 1.710 1.741 2.215	0.872 1.867 1.393 1.594 1.162	0.580 0.551 1.153 0.912 0.853	0.587 0.491 0.768 0.723 0.753	101 90 96 101 103	98 99 82 92 101	40 71 64 80 31	18 -23 50 25 11	18 -32 29 10 4	2.09E-7		> 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522	Cancer 0.353 0.633 0.259 1.146 0.670 0.402 0.461 0.241 0.593	1.345 1.451 0.942 1.963 1.472 1.272 0.745 1.964 1.500	1.292 1.542 0.930 1.889 1.425 1.248 0.787 1.911 1.371	1.295 1.548 0.908 1.911 1.369 1.254 0.748 1.772 1.324	0.529 1.396 0.809 1.987 1.169 1.131 0.673 0.558 1.204	0.281 0.602 0.223 0.616 0.717 0.574 0.451 0.448 0.494	0.245 0.472 0.136 0.734 0.580 0.540 0.387 0.353 0.390	95 111 98 91 94 97 115 97	95 112 95 94 87 98 101 89 81	18 93 81 103 62 84 75 18	-21 -5 -14 -46 6 20 -2 12	-31 -25 -48 -36 -14 16 -16 -6 -34	2.61E-7	3.63E-7 1.11E-6 8.91E-7 6.12E-7 2.51E-6 1.25E-5 1.17E-6 1.25E-5 7.91E-7	> 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.195 0.747 0.239 0.243 0.153 0.247 0.205	1.152 1.867 1.626 1.832 0.976 1.384 1.102	1.121 1.845 1.579 1.728 0.959 1.297 1.109	1.060 1.754 1.542 1.733 0.874 1.203 1.029	0.445 1.157 0.935 1.709 0.345 0.842 0.582	0.230 0.471 0.421 1.284 0.176 0.509 0.372	0.163 0.229 0.336 0.818 0.178 0.395 0.352	97 98 97 93 98 92 101	90 90 94 94 88 84 92	26 37 50 92 23 52 42	4 -37 13 65 3 23	-16 -69 7 36 3 13	5.32E-8 7.01E-8 1.26E-7 4.22E-6 4.80E-8 1.50E-7 8.63E-8	1.25E-5 1.25E-5	> 1.25E-5 3.15E-6 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.389 0.751 0.602 0.492 0.519 0.273	1.349 1.235 2.068 1.628 1.029 1.633	1.266 1.178 2.029 1.571 0.958 1.542	1.179 1.166 2.025 1.488 0.845 1.538	1.063 0.885 1.837 1.262 0.806 0.688	0.255 0.388 0.537 0.720 0.049 0.218	0.198 0.298 0.559 0.698 0.045 0.186	91 88 97 95 86 93	82 86 97 88 64 93	70 28 84 68 56 31	-34 -48 -11 20 -91 -20	-49 -60 -7 18 -91 -32	1.95E-7 5.16E-8 2.86E-7 2.94E-7 1.38E-7 6.09E-8	5.86E-7 2.89E-7 9.60E-7 1.25E-5 3.02E-7 5.00E-7	> 1.25E-5 1.72E-6 > 1.25E-5 > 1.25E-5 6.61E-7 > 1.25E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.105 0.844 0.297 0.349 0.714 0.451 0.409 0.559 0.662	0.570 1.389 0.989 1.173 1.610 1.231 2.175 0.993 2.014	0.530 1.349 1.013 1.183 1.590 1.243 2.160 0.976 1.950	0.443 1.211 0.970 1.175 1.529 1.170 2.036 1.007 1.792	0.102 0.872 0.569 0.597 0.717 0.490 1.338 0.606 1.309	0.060 0.585 0.322 0.422 0.460 0.173 0.340 0.336 1.007	0.071 0.518 0.231 0.422 0.328 0.201 0.220 0.296 0.924	91 93 103 101 98 101 99 96	73 67 97 100 91 92 92 103 84	-3 5 39 30 5 53 11 48	-43 -31 4 9 -36 -62 -17 -40 26	-32 -39 -22 9 -54 -55 -46 -47	3.53E-8 3.80E-8 1.36E-7 4.71E-8	1.15E-7 1.74E-7 1.71E-6 1.25E-5 1.27E-7 1.48E-7 7.12E-7 2.03E-7	> 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5 7.47E-6 8.36E-7 > 1.25E-5 > 1.25E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.479 0.536 0.488 0.228 0.283 0.460	0.771 1.427 1.231 1.041 0.910 1.125	0.828 1.472 1.175 1.044 0.916 1.210	0.733 1.317 1.168 1.078 0.903 1.327	0.373 1.056 1.192 0.924 0.882 0.602	0.206 0.246 0.651 0.323 0.635 0.314	0.150 0.116 0.655 0.220 0.445 0.246	120 105 93 100 101 113	87 88 92 105 99 130	-22 58 95 86 96 21	-57 -54 22 12 56 -32	-69 -78 22 -4 26 -47	2.73E-8 1.48E-7 5.14E-7 3.79E-7 2.00E-6 6.82E-8	7.84E-8 4.12E-7 1.25E-5 7.34E-6 1.25E-5 3.16E-7	7.88E-7 1.15E-6 > 1.25E-5 > 1.25E-5 > 1.25E-5 > 1.25E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.387 0.736 0.348 0.678 0.649 0.519 0.374 0.569	1.401 1.442 1.644 0.951 1.144 1.914 1.377 1.160	1.312	1.268 1.234 1.585 1.033 1.090 1.692 1.260 1.114	1.373	0,111 0.539 0.147 0.170 0.846 0.496	0.148 0.440 0.098 0.136 0.728 0.357	102 81 98 125 93 98 94	87 71 95 130 89 84 88 92	84 69 86 103 92 82 100 87	-56 -85 15 -78 -74 23 12 -45	-63 -80 7 -86 -79 15 -5	2.45E-7 2.23E-7	5.00E-7 3.50E-7 1.25E-5 4.62E-7 4.47E-7 1.25E-5 6.59E-6 5.70E-7	1.14E-6 7.41E-7 > 1.25E-5 8.72E-7 8.96E-7 > 1.25E-5 > 1.25E-5 1.69E-6
Prostate Cancer PC-3 DU-145	0.397 0.309	1.602 1.236		1.529 0.930				101 92	94 67	70 69	16 5	9 -18	2.93E-7 > 2.50E-7	1.25E-5 2.06E-6	> 1.25E-5 > 1.25E-5
Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	0.204 0.449 0.514 0.792 0.443 0.536	0.817 1.196 1.301 1.354 1.197 1.431	1.160 1.250 1.339 1.167	0.778 1.070 1.277 1.292 1.148 1.284	0.892 1.304 1.091 1.095	0.246 0.572 0.562 0.102 0.648 0.214	0.490 0.496 0.066 0.619	99 95 93 97 96 90	94 83 97 89 94 84	25 59 100 53 86 14	7 16 6 -87 27 -60	3 5 -4 -92 23 -65	2.06E-7 > 4.27E-7 1.32E-7	1.25E-5 1.25E-5 5.32E-6 2.99E-7 1.25E-5 1.93E-7	> 1.25E-5 > 1.25E-5 > 1.25E-5 6.79E-7 > 1.25E-5 9.12E-7

Table S5. NCI 60-cell line results for 7.

NSC : D - 751844 / 1	Experiment ID: 0912NS69	Test Type : 08	Units : Molar
Report Date : February 01, 2010	Test Date : December 14, 2009	QNS:	MC:
COMI : PC 1003 (92207)	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI : PC 1	003 (922	(70)			Sta	in Rea	gent : S	RB Dual	-Pass	Related	t	SSPI	_: K24A		
						L	og10 Con	centration							
	Time			Mean	n Optica		~		P	ercent G	Growth				
Panel/Cell Line	Zero	Ctrl	-9.1	-8.1	-7.1	-6.1	-5.1	-9.1	-8.1	-7.1	-6.1	-5.1	GI50	TGI	LC50
Leukemia											4.1		0.00		2000
CCRF-CEM	0.349	1.660	1.622	1.626	0.682	0.614	0.667	97	97	25	20	24	3.64E-8	> 8.00E-6	> 8.00E-6
HL-60(TB)	0.717	2.333	2.269	2.555	1.587	0.617	0.631	96	114	54	-14	-12	9.11E-8	4.98E-7	> 8.00E-6
K-562	0.257	2.033	1.978	2.035	1.808	1.153	1.078	97	100	87	50	46	1.02E-6	> 8.00E-6	> 8.00E-6
MOLT-4	0.598	1.837	1.804	1.786	1.518	0.982	0.830	97	96	74	31	19	2.90E-7	> 8.00E-6	> 8.00E-6
RPMI-8226	0.685	2.203	2.264	2.152	1.336	0.981	0.825	104	97	43	19	9	5.90E-8	> 8.00E-6	> 8.00E-6
Non-Small Cell Lun	ng Cancer														
A549/ATCC	0.353	1.345	1.285	1.288	0.368	0.383	0.355	94	94	_1	3	:	2.40E-8	> 8.00E-6	> 8.00E-6
EKVX	0.633	1.451	1.391	1.417	1.071	0.604	0.576	93	96	54 36	-5 -8	-9 -8	9.22E-8	6.67E-7	> 8.00E-6
HOP-62 HOP-92	0.259 1.146	0.942 1.963	0.943 1.925	1.008 1.848	0.508 1.824	0.238	0.238 0.717	100 95	110 86	83	-44	-8 -37	5.23E-8 1.46E-7	5.22E-7 3.60E-7	> 8.00E-6 > 8.00E-6
NCI-H226	0.670	1.472	1.397	1.419	1.241	0.770	0.686	91	93	71	12	2	1.84E-7	> 8.00E-6	> 8.00E-6
NCI-H23	0.402	1.272	1.257	1.228	0.970	0.666	0.594	98	95	65	30	22	2.18E-7	> 8.00E-6	> 8.00E-6
NCI-H322M	0.461	0.745	0.710	0.759	0.542	0.473	0.409	88	105	28	4	-11	4.18E-8	1.46E-6	> 8.00E-6
NCI-H460	0.241	1.964	2.031	1.952	0.576	0.579	0.459	104	99	19	20	13	3.31E-8	> 8.00E-6	> 8.00E-6
NCI-H522	0.593	1.500	1.435	1.427	1.204	0.690	0.497	93	92	67	11	-16	1.62E-7	1.99E-6	> 8.00E-6
Colon Cancer															
COLO 205	0.195	1.152	1.151	1.100	0.350	0.201	0.214	100	95	16	1	2	2.96E-8	> 8.00E-6	> 8.00E-6
HCC-2998	0.747	1.867	1.838	1.738	0.832	0.764	0.315	97	88	8	1	-58	2.39E-8	8.47E-7	5.90E-6
HCT-116	0.239	1.626	1.555	1.622	0.754	0.481		95	100	37	17	13	4.98E-8	> 8.00E-6	> 8.00E-6
HCT-15	0.243	1.832	1.743 0.946	1.721 0.913	1.609 0.246	1.116 0.224	0.649	94 96	93 92	86 11	55 9	26 5	1.18E-6	> 8.00E-6 > 8.00E-6	> 8.00E-6 > 8.00F-6
HT29 KM12	0.153 0.247	0.976 1.384	1.342	1.406	0.770	0.726	0.191 0.558	96	102	46	42	27	2.66E-8 6.78E-8	> 8.00E-6	> 8.00E-6 > 8.00E-6
SW-620	0.205	1.102	1.080	1.101	0.486	0.391	0.310	97	100	31	21	12	4.27E-8	> 8.00E-6	> 8.00E-6
	0.20				41.104		4.0.14	•						41442	*********
CNS Cancer	0.000	4 040	4 000	4 244	0.000	0.007	0.000	- 04	00	40	00	05	7.005.0	2 505 7	> 0.00E 0
SF-268 SF-295	0.389 0.751	1.349 1.235	1.268 1.139	1.344	0.860 0.648	0.287 0.467	0.293	91 80	99 65	49 -14	-26 -38	-25 -50	7.66E-8 1.24E-8	3.59E-7 5.36E-8	> 8.00E-6 7.52E-6
SF-539	0.602	2.068	1.916	1.895	1.637	0.701	0.637	90	88	71	7	2	1.68E-7	> 8.00E-6	> 8.00E-6
SNB-19	0.492	1.628	1.502	1.548	1,241	0.843	0.734	89	93	66	31	21	2.28E-7	> 8.00E-6	> 8.00E-6
SNB-75	0.519	1.029	0.954	1.014	0.783	0.078	0.057	85	97	52	-85	-89	8.24E-8	1.91E-7	4.43E-7
U251	0.273	1.633	1.540	1.443	0.630	0.350	0.299	93	86	26	6	2	3.20E-8	> 8.00E-6	> 8.00E-6
Melanoma															
LOX IMVI	0.105	0.570	0.547	0.480	0.072	0.090	0.066	95	81	-31	-14	-37	1.50E-8	4.20E-8	> 8.00E-6
MALME-3M	0.844	1.389	1.256	1.301	1.034	0.618	0.559	76	84	35	-27	-34	3.94E-8	2.94E-7	> 8.00E-6
M14	0.297	0.989	0.935	1.006	0.546	0.432	0.280	92	102	36	20	-6	4.91E-8	4.69E-6	> 8.00E-6
MDA-MB-435	0.349	1.173	1.129	1.129	0.682	0.558	0.446	95 97	95	40	25	12 -33	5.31E-8	> 8.00E-6	> 8.00E-6 > 8.00F-6
SK-MEL-2 SK-MEL-28	0.714 0.451	1.610 1.231	1.582 1.201	1.664 1.263	0.907 0.915	0.629	0.482 0.213	96	106 104	21 59	-12 -22	-33 -53	3.68E-8 1.04E-7	3.51E-7 4.27E-7	> 8.00E-6 6.44E-6
SK-MEL-5	0.409	2.175	2.045	2.108	1.550	0.691	0.383	93	96	65	16	-6	1.60E-7	4.12E-6	> 8.00E-6
UACC-257	0.559	0.993	0.972	0.968	0.580	0.500	0.386	95	94	5	-11	-31	2.50E-8	1.63E-7	> 8.00E-6
UACC-62	0.662	2.014	1.919	1.984	1.457	1.068	0.972	93	98	59	30	23	1.62E-7	> 8.00E-6	> 8.00E-6
0															
Ovarian Cancer IGROV1	0.479	0.771	0.777	0.672	0.154	0.136	0.172	102	66	-68	-72	-64	1.06E-8	2.49E-8	5.89E-8
OVCAR-3	0.536	1.427	1.353	1.409	1.064	0.365	0.302	92	98	59	-32	-44	1.01E-7	3.57E-7	> 8.00E-6
OVCAR-5	0.488	1.231	1.178	1.120	1.051	0.724	0.630	93	85	76	32	19	3.08E-7	> 8.00E-6	> 8.00E-6
OVCAR-8	0.228	1.041	1.037	0.989	0.770	0.458	0.328	99	94	67	28	12	2.17E-7	> 8.00E-6	> 8.00E-6
NCI/ADR-RES	0.283	0.910	0.901	0.881	0.833	0.684	0.434	99	95	88	64	24	1.79E-6	> 8.00E-6	> 8.00E-6
SK-OV-3	0.460	1.125	1.070	1.030	0.762	0.367	0.317	92	86	45	-20	-31	6.13E-8	3.93E-7	> 8.00E-6
Renal Cancer															
786-0	0.387	1.401	1.320	1.426	1.063	0.200	0.217	92	102	67	-48	-44	1.12E-7	3.04E-7	> 8.00E-6
A498	0.736	1.442	1.299	1.280	1.109	0.126	0.178	80	77	53	-83	-76	8.39E-8	1.96E-7	4.58E-7
ACHN	0.348	1.644	1.514	1.537	1.141		0.410	90	92	61	17	5	1.43E-7	> 8.00E-6	> 8.00E-6
CAKI-1	0.678	0.951	1.002	1.046	0.862	0.162		119	135	67	-76	-83	1.06E-7	2.36E-7	5.26E-7
RXF 393 SN12C	0.649	1.144 1.914		1.099				89 94	91 95	79 74	-79 39	-65 18	1.22E-7 3.84E-7	2.53E-7 > 8.00E-6	5.25E-7 > 8.00E-6
TK-10	0.374	1.377	1.276		1.313	0.535		90	94	94	16	8	2.92E-7	> 8.00E-6	> 8.00E-6
UO-31	0.569	1.160		1.074	0.984		0.147	77	86	70	-48	-74	1.19E-7	3.13E-7	9.28E-7
Prostate Cancer	0.207	4 000	4 004	4 540	4 400	0.507	0.500	400	00	04	40	40	4 00F 7	- 0.00F.0	- 0.00F.0
PC-3 DU-145	0.397 0.309	1.602 1.236		1.518 1.156	0.810			100 93	93 91	61 54	16 11	10 5	1.38E-7 9.94E-8	> 8.00E-6 > 8.00E-6	> 8.00E-6 > 8.00E-6
	0.309	1.230	1.174	1.130	0.010	0.413	0.337	93	91	34	11	9	9.34E-0	> 0.UUE-0	> 0.UUE-0
Breast Cancer	0.204	0.947	0.720	0.835	0.350	0.202	0.227	0.4	102	25	16	E	2 94⊑ 9	> 8.00E-6	> 8.00E-6
MCF7 MDA-MB-231/ATC	0.204	0.817 1.196		1.143	0.359	0.303		84 86	103 93	25 48	16 20	5 7	3.84E-8 7.35E-8	> 8.00E-6 > 8.00E-6	> 8.00E-6 > 8.00E-6
HS 578T	0.514	1.301		1.329	1.367	0.687		97	104	108	22	14	3.79E-7	> 8.00E-6	> 8.00E-6
BT-549	0.792	1.354		1.420	1.368	0.156		95	112	103	-80	-91	1.55E-7	2.91E-7	5.46E-7
T-47D	0.443	1.197	1.139	1.178	1.018	0.697	0.708	92	98	76	34	35	3.31E-7	> 8.00E-6	> 8.00E-6
MDA-MB-468	0.536	1.431		1.338			0.262	88	90	-9	-44	-51	2.02E-8	6.48E-8	5.37E-6

Table S6. NCI 60-cell line results for 8.

NSC : D - 751837 / 1	Experiment ID: 0912NS69	Test Type : 08	Units : Molar
Report Date : February 01, 2010	Test Date : December 14, 2009	QNS:	MC:
COMI : PC 811 (92196)	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI : PC 81	1 (9219	6)			Sta	n Rea	gent : S	RB Dual-	Pass I	Related	i	SSPI	L : K24A		
					•	Lo	og10 Con	centration				•			
	Time			Mear	n Optica	Densiti	es		Р	ercent G	Frowth				
Panel/Cell Line	Zero	Ctrl	-8.8	-7.8	-6.8	-5.8	-4.8	-8.8	-7.8	-6.8	-5.8	-4.8	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.349 0.717 0.257 0.598 0.685	1.710 1.972 1.311 1.681 2.244	1.766 2.059 1.312 1.699 2.343	1.734 2.071 1.103 1.604 2.203	0.793 0.942 0.873 1.305 1.400	0.647 0.566 0.716 0.894 1.074	0.536 0.489 0.218 0.449 0.768	104 107 100 102 106	102 108 80 93 97	33 18 58 65 46	22 -21 44 27 25	14 -32 -15 -25	8.01E-8 6.29E-8 5.24E-7 3.61E-7 1.19E-7	> 1.43E-5 4.12E-7 7.88E-6 4.76E-6 > 1.43E-5	> 1.43E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H322M NCI-H460	Cancer 0.353 0.633 0.259 1.146 0.670 0.402 0.461 0.241	1.063 1.554 0.792 2.045 1.448 1.274 0.894 1.866	1.096 1.614 0.763 2.004 1.405 1.222 0.895 1.967	0.946 1.458 0.823 1.997 1.347 1.257 0.884 1.232	0.304 1.037 0.448 1.959 1.079 0.800 0.735 0.581	0.285 0.590 0.292 0.582 0.842 0.644 0.624 0.573	0.183 0.523 0.104 1.115 0.509 0.339 0.394 0.132	105 107 95 95 94 94 100 106	83 90 106 95 87 98 98	-14 44 35 90 52 46 63 21	-19 -7 6 -49 22 28 38 20	-48 -17 -60 -3 -24 -16 -15 -45	3.15E-8 1.05E-7 8.88E-8 2.78E-7 1.73E-7 1.18E-7 4.69E-7 2.69E-8	1.03E-7 1.05E-6 1.77E-6 6.35E-7 4.29E-6 6.20E-6 7.49E-6 2.93E-6	> 1.43E-5 > 1.43E-5 1.01E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5
NCI-H522	0.593	0.802	0.729	0.637	0.365	0.336	0.150	65	21	-39	-43	-75	3.14E-9	3.21E-8	2.32E-6
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.195 0.747 0.239 0.243 0.153 0.247 0.205	1.210 1.727 1.640 1.573 0.553 1.278 1.218	1.250 1.719 1.594 1.613 0.548 1.253 1.217	1.240 1.483 1.330 1.596 0.452 1.155 1.017	0.534 0.677 0.725 1.481 0.148 0.715 0.702	0.221 0.705 0.453 0.947 0.131 0.680 0.446	0.208 0.114 0.119 0.357 0.098 0.156 0.187	104 99 97 103 99 98 100	103 75 78 102 75 88 80	33 -9 35 93 -4 45 49	3 -6 15 53 -14 42 24	1 -85 -50 9 -36 -37 -9	8.25E-8 2.83E-8 6.31E-8 1.67E-6 2.96E-8 1.11E-7 1.33E-7	> 1.43E-5 1.11E-7 2.44E-6 > 1.43E-5 1.29E-7 4.86E-6 7.58E-6	> 1.43E-5 5.20E-6 1.41E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.389 0.751 0.602 0.492 0.519 0.273	1.292 1.284 1.958 1.609 1.012 1.142	1.277 1.294 1.921 1.473 0.963 1.101	1.211 1.295 1.844 1.414 0.900 0.938	0.574 0.748 1.119 0.955 0.558 0.329	0.352 0.431 0.586 0.839 0.080 0.210	0.220 0.211 0.238 0.414 0.035 0.146	98 102 97 88 90 95	91 102 92 83 77 76	20 38 41 8 6	-10 -43 -3 31 -85 -23	-44 -72 -61 -16 -93 -47	5.45E-8 4.61E-8 8.57E-8 8.84E-8 3.54E-8 3.41E-8	6.83E-7 1.42E-7 1.23E-6 6.56E-6 1.74E-7 2.36E-7	> 1.43E-5 2.55E-6 9.39E-6 > 1.43E-5 6.04E-7 > 1.43E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.105 0.844 0.297 0.349 0.714 0.451 0.409 0.559 0.662	0.641 1.528 0.994 1.201 0.999 1.331 2.236 0.945 2.012	0.556 1.473 0.966 1.210 0.987 1.332 2.241 0.951 1.945	0.518 1.302 0.932 1.161 0.936 1.273 2.072 0.943 1.801	0.189 1.245 0.608 0.797 0.573 1.023 1.562 0.580 1.336	0.089 0.955 0.442 0.534 0.396 0.777 0.913 0.494 1.258	0.052 0.627 0.042 0.106 0.192 0.282 0.049 0.323 0.455	84 92 96 101 96 100 100 101 95	77 67 91 95 78 93 91 99	16 59 45 53 -20 65 63 5	-15 16 21 22 -45 37 28 -12	-50 -26 -86 -70 -73 -38 -88 -42 -31	3.93E-8 2.28E-7 1.10E-7 1.72E-7 2.75E-8 4.91E-7 3.34E-7 4.80E-8 1.42E-7	4.59E-7 3.49E-6 2.24E-6 2.47E-6 8.97E-8 4.49E-6 2.48E-6 2.97E-7 5.50E-6	1.39E-5 > 1.43E-5 6.58E-6 8.72E-6 2.21E-6 > 1.43E-5 6.70E-6 > 1.43E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.479 0.536 0.347 0.488 0.228 0.283 0.460	0.889 1.356 0.599 1.177 0.740 0.940 1.035	0.997 1.377 0.619 1.157 0.733 0.953 1.039	0.896 1.320 0.555 1.160 0.729 0.937 1.030	0.286 0.894 0.418 0.946 0.561 0.875 0.790	0.202 0.500 0.305 0.733 0.380 0.601 0.518	0.211 0.249 0.264 0.616 0.142 0.288 0.338	126 103 108 97 99 102 101	102 96 83 98 98 99	-40 44 28 66 65 90 57	-58 -7 -12 36 30 48 10	-56 -54 -24 19 -38 1	3.31E-8 1.08E-7 5.70E-8 4.88E-7 3.82E-7 1.31E-6 2.05E-7	7.44E-8 1.05E-6 7.12E-7 > 1.43E-5 3.94E-6 > 1.43E-5 2.69E-6	5.12E-7 1.20E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5 > 1.43E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.387 0.736 0.348 0.678 0.649 0.519 0.374 0.569	1.439 1.432 1.550 1.038 1.230 1.912 0.529 1.188	1.895 0.520	1.372 1.212 1.501 1.088 1.190 1.716 0.494 1.148	0.905 0.902 1.403	1.064 0.141	0.062	101 95 100 102 94 99 94 95	94 68 96 114 93 86 77 94	56 23 70 63 44 63 -34	-55 -83 12 -76 -71 39 -62 -54	-50 -70 1 -71 -90 9 -50	1.63E-7 3.63E-8 3.18E-7 1.78E-7 1.06E-7 5.10E-7 2.51E-8 2.55E-7	4.60E-7 2.36E-7 > 1.43E-5 4.06E-7 3.42E-7 > 1.43E-5 7.03E-8 5.84E-7	1.43E-5 7.03E-7 > 1.43E-5 9.30E-7 9.30E-7 > 1.43E-5
Prostate Cancer PC-3 DU-145	0.397 0.309	1.621 1.123		1.670 1.009	1.310 0.856	0.869 0.443	0.503 0.199	106 104	104 86	75 67	39 16	9 -36	6.87E-7 3.13E-7	> 1.43E-5 2.96E-6	> 1.43E-5 > 1.43E-5
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.204 0.449 0.514 0.792 0.443 0.536	1.049 1.138 1.108 1.372 0.940 1.361	1.125 1.107 1.349 0.922	0.916 1.022 1.124 1.322 0.948 1.124	0.733 0.926 1.020 0.818	0.476 0.613 0.571 0.213 0.703 0.352	0.412 0.388 0.065 0.338	98 98 100 96 96 94	84 83 103 91 102 71	46 41 69 39 76 6	32 24 10 -73 52 -34	-21 -8 -25 -92 -24 -76	1.10E-7 8.80E-8 3.01E-7 8.90E-8 1.54E-6 3.04E-8	5.71E-6 7.85E-6 2.72E-6 3.20E-7 6.98E-6 2.04E-7	> 1.43E-5 > 1.43E-5 > 1.43E-5 8.90E-7 > 1.43E-5 3.42E-6

Table S7. NCI 60-cell line results for 9.

NSC : D - 666654 / 1	Experiment ID: 9312SR87	Test Type : 08	Units : Molar
Report Date : April 12, 2010	Test Date : December 14, 1993	QNS:	MC:
COMI : PC# 447	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI . FC# 4	41				Sta	iii Kea	gent. S	ND Dual	-rass	related	,	331	L. NZ4A		
						1,	anin Con	centration							_
	Time			Moor	Optica		-	centration		ercent G	Proudh				
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia	2010	Out	0.0	7.0	0.0	0.0	7.0	-0.0	-1.0	0.0	0.0	1.0	0100	101	2000
CCRF-CEM	0.347	0.902	0.944	0.925	0.551	0.552	0.507	107	104	37	37	29	6.34E-7	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.515	1.549	1.620	1.388	0.563	0.398	0.340	107	84	5	-23	-34	2.70E-7	1.48E-6	> 1.00E-4
K-562	0.161	0.871	0.845	0.726	0.492	0.499	0.294	96	80	47	48	19		1.00E-4	> 1.00E-4
MOLT-4 RPMI-8226	0.428	1.526 0.547	1.513 0.533	1.521 0.463	1.052 0.336	0.959	0.576 0.210	99 94	99 66	57 15	48 -3	13 -30	6.38E-6 2.03E-7	> 1.00E-4 6.40E-6	> 1.00E-4 > 1.00E-4
SR	0.396	1.452	1.549	1.394	1.015	0.859	0.365	109	95	59	44	-8	3.85E-6	7.06E-5	> 1.00E-4
Non-Small Call Luna	Concor														
Non-Small Cell Lung A549/ATCC	0.433	1.745	1.766	1.755	1.563	0.899	0.419	102	101	86	36	-3	5.18E-6	8.20E-5	> 1.00E-4
EKVX	0.823	1.964	1.943	1.939	1.842	1.281	0.823	98	98	89	40		6.29E-6	9.97E-5	> 1.00E-4
HOP-62	0.281	0.870	0.912	0.863	0.650	0.433	0.171	107	99	63	26	-39	2.20E-6	2.50E-5	> 1.00E-4
NCI-H226	1.117 0.825	1.590 2.225	1.538	1.519	1.546 1.502	1.028 1.323	0.386	89 96	85 97	91	-8	-65	2.59E-6	8.30E-6	5.39E-5 > 1.00E-4
NCI-H23 NCI-H322M	0.516	1.399	2.163 1.452	2.181 1.541	1.314	0.984	0.854 0.637	106	116	48 90	36 53	2 14		> 1.00E-4 > 1.00E-4	> 1.00E-4 > 1.00E-4
NCI-H460	0.209	1.818	1.773	1.587	0.757	0.501	0.235	97	86	34	18	2		1.00E-4	> 1.00E-4
NCI-H522	0.340	0.891	0.875	0.642	0.267	0.459	0.171	97	55	-22	22	-50	1.15E-7		> 1.00E-4
Colon Cancer															
COLO 205	0.191	1.745	1.688	1.760	0.774	0.409	0.410	96	101	38	14	14	6.36E-7	- 1.00E-4	> 1.00E-4
HCC-2998	0.243	0.472	0.433	0.424	0.274	0.301	0.142	83	79	13	25	-42	2.77E-7	2.38E-5	> 1.00E-4
HCT-116	0.170	1.451	1.375	1.222	0.339	0.525	0.271	94	82	13	28	8	2.92E-7		> 1.00E-4
HCT-15 HT29	0.308 0.184	1.306 1.421	1.385 1.373	1.387 1.382	1.358 0.721	1.257 0.335	0.529 0.273	108 96	108 97	105 43	95 12	22 7	4.15E-5 7.53E-7	> 1.00E-4 > 1.00E-4	> 1.00E-4 > 1.00E-4
KM12	0.395	1.660	1.676	1.593	1.048	1.060	0.620	101	95	52	53	18		1.00E-4	> 1.00E-4
SW-620	0.165	0.659	0.670	0.654	0.394	0.473	0.329	102	99	46	62	33			> 1.00E-4
CNS Cancer															
SF-268	0.514	1.095	1.114	1.135	1,116	0.569	0.398	103	107	104	9	-23	3.71E-6	1.97E-5	> 1.00E-4
SF-295	0.325	1.078	1.144	1.237	0.990	0.734	0.268	109	121	88	54	-18	1.15E-5	5.68E-5	> 1.00E-4
SF-539	0.635	1.496	1.508	1.630	1.419	0.668	0.368	101	116	91	4	-42	2.96E-6	1.21E-5	> 1.00E-4
SNB-19 SNB-75	0.746 0.417	1.915 1.394	1.969 1.349	1.874 1.278	1.581 1.079	1.091	0.575 0.174	105 95	97 88	71	30 -6	-23 -58	3.24E-6 6.53E-7	3.65E-5 7.62E-6	> 1.00E-4 6.97E-5
U251	0.677	2.236	2.245	2.072	1.280	0.901	0.565	101	89	39	14	-17	5.98E-7	2.92E-5	> 1.00E-4
Melanoma LOX IMVI	0.212	0.776	0.739	0.702	0.227	0.240	0.217	94	87	3	5	1	2.75E-7	1.00E-4	> 1.00E-4
MALME-3M	0.375	0.783	0.823	0.823	0.743	0.566	0.356	110	110	90	47	-5	8.43E-6	7.94E-5	> 1.00E-4
M14	0.176	0.662	0.725	0.602	0.556	0.328	0.146	113	88	78	31	-17	3.99E-6	4.48E-5	> 1.00E-4
SK-MEL-2 SK-MEL-28	0.452 0.622	1.139 1.919	1.074 1.870	1.109 1.862	0.679 1.431	0.546 1.199	0.226	91 96	96 96	33 62	14 44	-50 -25	5.36E-7 4.90E-6	1.64E-5 4.34E-5	9.96E-5 > 1.00E-4
SK-MEL-26	0.822	1.498	1.350	1.076	0.713	0.434	0.465 0.203	87	64	34	10	-36	2.93E-7	4.34E-5 1.66E-5	> 1.00E-4 > 1.00E-4
UACC-257	0.462	1.731	1.710	1.738	0.954	0.918	0.577	98	101	39	36	9		> 1.00E-4	> 1.00E-4
UACC-62	0.353	1.470	1.470	1.505	0.788	0.716	0.164	100	103	39	32	-54	6.71E-7	2.38E-5	9.06E-5
Ovarian Cancer															
IGROV1	0.323	1.474	1.418	1.413	1.116	0.297	0.164	95	95	69	-8	-49	1.76E-6	7.89E-6	> 1.00E-4
OVCAR-4	0.186	0.533	0.516	0.542	0.463	0.360	0.209	95	103	80	50	7	1.01E-5		> 1.00E-4
OVCAR-5	0.703	1.285	1.323	1.294	1.221	0.920	0.613	107	102	89	37 49	-13 4	5.67E-6	5.55E-5	> 1.00E-4 > 1.00E-4
OVCAR-8 NCI/ADR-RES	0.305 0.359	1.623 0.932	1.634 1.004	1.635 0.974	1.570 0.960	0.957 1.018	0.362 0.809	101 113	101 107	96 105	115	79		> 1.00E-4 > 1.00E-4	> 1.00E-4 > 1.00E-4
SK-OV-3	0.256	0.686	0.660	0.674	0.711	0.419	0.150	94	97	106	38	-42	6.61E-6	2.99E-5	> 1.00E-4
Renal Cancer															
786-0	0.207	1.159	1.192	1.189	1.131	0.581	0.140	104	103	97	39	-32	6.51E-6	3.53E-5	> 1.00E-4
ACHN	0.432	1.770	1.768	1.805	1.681	1.110	0.437	100	103	93	51	-	1.03E-5	> 1.00E-4	> 1.00E-4
CAKI-1	0.286	1.242	1.202	1.205	1.279	0.875	0.062	96	96	104	62	-78	1.21E-5	2.75E-5	6.26E-5
RXF 393 SN12C	1.144 0.320	1.485 1.134	1.456	1.532 1.123		0.867		91 101	114 99	119 82	-24 38	-82 14	3.03E-6 5.35E-6	6.77E-6 > 1.00E-4	2.82E-5 > 1.00E-4
TK-10	0.891	1.688		1.747				108	107	116	43	-53	7.95E-6	2.79E-5	9.26E-5
UO-31	1.124	2.188		2.055				86	87	101	92	-79	1.76E-5	3.45E-5	6.75E-5
Prostate Cancer															
PC-3	0.575	1.493	1.523	1.630	1.069	0.843	0.510	103	115	54	29	-11	1.43E-6	5.26E-5	> 1.00E-4
DU-145	0.495	1.589		1.690		1.239		108	109	102	68	3		> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.335	1.008		0.913			0.211	94	86	49	12	-37	9.27E-7	1.77E-5	> 1.00E-4
MDA-MB-231/ATCO HS 578T	0.360 0.577	0.970 1.568		0.982 1.493	0.825 1.438	0.423 0.846		105 88	102 93	76 87	10 27	-46 -5	2.50E-6 4.15E-6	1.52E-5 7.21E-5	> 1.00E-4 > 1.00E-4
MDA-N	0.377	2.058		2.041	1.859	1.209		101	99	88	49	-ə 9		1.21E-3 1.00E-4	> 1.00E-4 > 1.00E-4
BT-549	0.840	1.412	1.403	1.422	1.514	0.901	0.269	98	102	118	11	-68	4.29E-6	1.37E-5	5.90E-5
T-47D	0.534	1.185	1.122	1.255	1.359	1.193	0.622	90	111	127	101	13	3.83E-5	> 1.00E-4	> 1.00E-4

Table S8. NCI 60-cell line results for 11.

NSC : D - 751840 / 1	Experiment ID : 0912NS69	Test Type : 08	Units : Molar
Report Date : February 01, 2010	Test Date : December 14, 2009	QNS:	MC:
COMI : PC 889 (92203)	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI : PC 88	9 (9220	3)			Stai	n Rea	gent: S	KB Dual-	rass	Related	1	331	L : KZ4A		
					•	Lo	og10 Con	centration							
	Time			Mear	Optical	Densiti	es		Р	ercent G	Srowth				
Panel/Cell Line Leukemia	Zero	Ctrl	-8.8	-7.8	-6.8	-5.8	-4.8	-8.8	-7.8	-6.8	-5.8	-4.8	GI50	TGI	LC50
CCRF-CEM	0.349	1.583	1.524	1.547	1.156	0.845	0.647	95	97	65	40	24	6.73E-7	1.65E-5	> 1.65E-5
HL-60(TB)	0.717	2.326	2.129	2.097	1.136	0.623	0.562	88	86	26	-13	-22	6.55E-8	7.63E-7	> 1.65E-5
K-562 MOLT-4	0.257 0.598	1.337 1.723	1.249 1.706	1.223 1.545	0.960 1.404	0.782 1.116	0.327 0.535	92 98	89 84	65 72	49 46	-11	1.35E-6 > 1.15E-6	► 1.65E-5 1.07E-5	> 1.65E-5 > 1.65E-5
RPMI-8226	0.685	2.244	2.212	2.156	1.406	1.254	0.680	98	94	46	36	-1	1.38E-7	1.57E-5	> 1.65E-5
Non-Small Cell Lung		4.074	4.057	4.070	0.000	0.440	0.070		400	200	40	0.4	4.505.7	0.745.6	- 4 CEE E
A549/ATCC EKVX	0.353 0.633	1.074 1.567	1.057 1.506	1.072 1.516	0.928	0.446 0.895	0.270 0.618	98 93	100 95	80 82	13 28	-24 -2	4.59E-7 6.48E-7	3.71E-6 1.38E-5	> 1.65E-5 > 1.65E-5
HOP-62	0.259	0.766	0.840	0.767	0.654	0.442	0.255	115	100	78	36	-2	7.69E-7	1.50E-5	> 1.65E-5
HOP-92	1.146	1.967	1.928	1.797	1.834	1.481	1.010	95 90	79 104	84 99	41	-12	1.01E-6	9.81E-6	> 1.65E-5
NCI-H226 NCI-H23	0.670 0.402	1.461 1.268	1.384 1.256	1.496 1.202	1.452 0.879	1.129 0.788	0.819 0.592	99	92	55	58 45	19 22		> 1.65E-5 > 1.65E-5	> 1.65E-5 > 1.65E-5
NCI-H322M	0.461	0.875	0.846	0.873	0.844	0.689	0.493	93	100	93	55	8	2.12E-6		> 1.65E-5
NCI-H460	0.241	2.027	2.037	2.149	1.176	0.568	0.396	101	107	52	18	9		1.65E-5	> 1.65E-5
NCI-H522	0.593	1.325	1.236	1.103	0.712	0.609	0.579	88	70	16	2	-2	3.85E-8	4.89E-6	> 1.65E-5
Colon Cancer COLO 205	0.195	1.172	1.200	1.124	0.632	0.134	0.239	103	95	45	-32	5	1.29E-7		> 1.65E-5
HCC-2998	0.747	1.716	1.782	1.563	0.814	0.705	0.458	107	84	7	-6	-39	4.57E-8	5.84E-7	> 1.65E-5
HCT-116	0.239	1.618	1.567	1.612	0.623	0.572	0.358	96	100	28	24	9	8.10E-8	> 1.65E-5	> 1.65E-5
HCT-15	0.243	1.683	1.545 0.622	1.524	1.477 0.361	1.544	0.929	90	89	86	90	48 3		> 1.65E-5	> 1.65E-5
HT29 KM12	0.153 0.247	0.626 1.273	1.225	0.607 1.253	0.683	0.161 0.704	0.165 0.472	99 95	96 98	44 43	2 45	22		► 1.65E-5 ► 1.65E-5	> 1.65E-5 > 1.65E-5
SW-620	0.205	1.204	1.093	1.129	0.561	0.533	0.439	89	93	36	33	23		► 1.65E-5	> 1.65E-5
CNS Cancer															
SF-268	0.389	1.189	1.118	1.183	0.988	0.537	0.342	91	99	75	19	-12 -35	4.56E-7	6.64E-6	> 1.65E-5
SF-295 SF-539	0.751 0.602	1.251 1.924	1.166 1.931	1.174 1.871	0.913 1.703	0.884 0.961	0.489 0.731	83 101	85 96	32 83	27 27	10	7.60E-8 6.46E-7	4.45E-6 > 1.65E-5	> 1.65E-5 > 1.65E-5
SNB-19	0.492	1.645	1.510	1.543	1.459	0.954	0.809	88	91	84	40	28		1.65E-5	> 1.65E-5
SNB-75	0.519	1.003	0.915	0.979	1.022	0.557	0.160	82	95	104	8	-69	5.99E-7	2.08E-6	9.29E-6
U251	0.273	1.184	1.153	0.939	0.483	0.332	0.270	97	73	23	6	-1	4.78E-8	1.18E-5	> 1.65E-5
Melanoma LOX IMVI	0.105	0.588	0.599	0.518	0.346	0.157	0.088	102	86	50	11	-16	1.63E-7	4.14E-6	> 1.65E-5
MALME-3M	0.844	1.496	1.379	1.492	1.389	1.121	0.835	82	99	84	43	-1	1.09E-6	1.56E-5	> 1.65E-5
M14	0.297	1.004	0.937	0.968	0.977	0.681	0.340	90	95	96	54	6		1.65E-5	> 1.65E-5
MDA-MB-435 SK-MEL-2	0.349 0.714	1.179 1.285	1.118 1.292	1.104 1.294	1.084 0.948	0.723 0.637	0.394 0.347	93 101	91 102	89 41	45 -11	-51	1.27E-6 > 1.17E-7	1.65E-5 1.02E-6	> 1.65E-5 1.52E-5
SK-MEL-28	0.451	1.302	1.242	1.320	1.153	0.937	0.424	93	102	82	57	-6	2.14E-6	1.33E-5	> 1.65E-5
SK-MEL-5	0.409	2.204	2.118	2.148	1.086	0.524	0.360	95	97	38	6	-12	1.02E-7	3.65E-6	> 1.65E-5
UACC-257 UACC-62	0.559 0.662	0.953 1.886	0.912 1.768	0.929 1.853	0.888 1.659	0.579 1.267	0.376 0.809	90 90	94 97	83 81	5 49	-33 12	4.40E-7 1.58E-6	2.25E-6 > 1.65E-5	> 1.65E-5 > 1.65E-5
										•					
Ovarian Cancer IGROV1	0.479	0.901	0.801	0.824	0.693	0.267	0.255	76	82	51	-44	-47	1.68E-7	5.64E-7	> 1.65E-5
OVCAR-3	0.536	1.288	1.224	1.254	1.179	0.656	0.371	91	95	86	16	-31	5.34E-7	3.61E-6	> 1.65E-5
OVCAR-4 OVCAR-5	0.347 0.488	0.563 1.171	0.522 1.111	0.549 1.099	0.475 1.090	0.341	0.301 0.698	81 91	94 89	59 88	-2 49	-13 31	2.35E-7 1.52E-6	1.54E-6 1.65E-5	> 1.65E-5 > 1.65E-5
OVCAR-8	0.228	0.781	0.752	0.700	0.701	0.502	0.253	95	85	86	50	4		1.65E-5	> 1.65E-5
NCI/ADR-RES	0.283	0.933	0.968	0.916	0.912	0.940	0.740	105	97	97	101	70	> 1.65E-5	1.65E-5	> 1.65E-5
SK-OV-3	0.460	1.080	1.048	1.024	1.043	0.860	0.419	95	91	94	64	-9	2.60E-6	1.25E-5	> 1.65E-5
Renal Cancer 786-0	0.387	1.402	1.373	1.430	1.390	1.006	0.203	97	103	99	61	-48	2.08E-6	6.01E-6	> 1.65E-5
A498	0.736	1.636	1.426		1.383	0.922	0.203	77	81	72	21	-76	4.41E-7	2.70E-6	8.89E-6
ACHN	0.348	1.536	1.436	1.416	1.437		0.465	92	90	92	73	10	3.83E-6	> 1.65E-5	> 1.65E-5
CAKI-1 RXF 393	0.678 0.649	0.970 1.251	0.942 1.162	0.911 1.216	0.989 1.206	0.965 0.897	0.154 0.235	90 85	80 94	106 92	98 41	-77 -64	3.11E-6 1.11E-6	5.99E-6 4.07E-6	1.15E-5 1.22E-5
SN12C	0.549	1.800	1.706	1.727	1.637	1.283	0.800	93	94	92 87	60	22		+.07E-6 ► 1.65E-5	> 1.65E-5
TK-10	0.374	0.854		0.755		0.383	0.264	85	79	64	2	-29	2.74E-7	1.88E-6	> 1.65E-5
UO-31	0.569	1.186	1.080	1.150	1.143	1.182	0.200	83	94	93	99	-65	3.29E-6	6.64E-6	1.34E-5
Prostate Cancer	0.207	4 500	4 500	4.400	4 200	0.000	0.000	07	04	70	40	40	4.475.0	1055 5	> 1 CEE E
PC-3 DU-145	0.397	1.562 1.071	1.530	1.489 1.073	1.302 1.052	0.962	0.606	97 95	94 100	78 98	48 76	18 3	1.47E-6 3 3.72E-6	> 1.65E-5 > 1.65E-5	> 1.65E-5 > 1.65E-5
Breast Cancer															
MCF7	0.204	0.931	0.909		0.644		0.257	97	98	60	44	7		1.65E-5	> 1.65E-5
MDA-MB-231/ATCC HS 578T	0.449	1.112 1.153	1.041	1.066 1.159	0.968 1.146	0.680 0.756	0.494 0.530	89 95	93 101	78 99	35 38	7 3		► 1.65E-5 ► 1.65E-5	> 1.65E-5 > 1.65E-5
BT-549	0.792	1.362		1.445	1.609		0.405	95	115	143	37	-49	1.25E-6	4.47E-6	> 1.65E-5
T-47D	0.443	0.919		0.857	0.750		0.466	90	87	65	63	5		1.65E-5	> 1.65E-5
MDA-MB-468	0.536	1.371	1.282	1.178	0.362	0.530	0.272	89	77	-32	-1	-49	2.91E-8	8.33E-8	> 1.65E-5

Table S9. NCI 60-cell line results for 12.

NSC : D - 751838 / 1	Experiment ID: 0912NS69	Test Type : 08	Units : Molar
Report Date : February 01, 2010	Test Date : December 14, 2009	QNS:	MC:
COMI : PC 812 (92197)	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI : PC 81	2 (9219	7)			Sta	in Rea	gent : SI	RB Dual-	-Pass	Related	d	SSP	L : K24A		
					•	L	og10 Con	centration				•			
Panel/Cell Line	Time Zero	Ctrl	-8.7	Mear -7.7	Optica -6.7	Densiti	es -4.7	-8.7	-7.7	ercent 6	Frowth -5.7	-4.7	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.349 0.717 0.257 0.598 0.685	1.710 1.972 1.311 1.681 2.244	1.620 2.008 1.279 1.612 2.262	1.571 2.016 1.349 1.689 2.215	1.591 1.959 1.305 1.695 2.210	1.743 2.086 1.187 1.723 2.259	1.121 1.020 0.952 1.120 1.562	93 103 97 94 101	90 103 104 101 98	91 99 99 101 98	102 109 88 104 101	57 24 66 48 56	> 2.23E-5 1.11E-5 > 2.23E-5 2.07E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522	Cancer 0.353 0.633 0.259 1.146 0.670 0.402 0.461 0.241 0.593	1.063 1.554 0.792 2.045 1.448 1.274 0.894 1.866 0.802	1.069 1.573 0.773 1.941 1.364 1.227 0.847 1.911 0.738	1.058 1.432 0.768 1.875 1.428 1.218 0.892 1.891 0.752	1.071 1.463 0.768 1.892 1.338 1.197 0.892 1.912 0.751	1.035 1.477 0.746 1.901 1.371 1.191 0.940 1.782 0.751	0.652 1.392 0.629 1.954 1.355 0.792 0.843 0.750 0.371	101 102 96 88 89 95 89 103 69	99 87 96 81 97 94 99 102 76	101 90 95 83 86 91 100 103 75	96 92 91 84 90 90 111 95 75	42 82 69 90 88 45 88 31 -38	1.59E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 1.71E-5 > 2.23E-5 1.13E-5 3.75E-6	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 1.04E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.195 0.747 0.239 0.243 0.153 0.247 0.205	1.210 1.727 1.640 1.573 0.553 1.278 1.218	1.211 1.758 1.542 1.635 0.532 1.203 1.103	1.229 1.688 1.598 1.422 0.561 1.242 1.155	1.150 1.678 1.585 1.494 0.550 1.194 1.055	1.062 1.706 1.658 1.476 0.513 1.255 1.107	0.522 0.880 0.627 1.549 0.300 0.834 0.627	100 103 93 105 95 93 89	102 96 97 89 102 97 94	94 95 96 94 99 92 84	85 98 101 93 90 98 89	32 14 28 98 37 57 42	1.03E-5 8.24E-6 1.11E-5 > 2.23E-5 1.26E-5 > 2.23E-5 1.49E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.389 0.751 0.602 0.492 0.519 0.273	1.292 1.284 1.958 1.609 1.012 1.142	1.222 1.236 1.829 1.544 0.912 1.125	1.235 1.230 1.829 1.594 0.942 1.103	1.193 1.272 1.787 1.487 0.910 1.124	1.180 1.199 1.894 1.583 0.937 1.088	0.987 0.726 1.869 1.397 1.033 0.525	92 91 90 94 80 98	94 90 90 99 86 95	89 98 87 89 79 98	88 84 95 98 85 94	66 -3 93 81 104 29	> 2.23E-5 5.46E-6 > 2.23E-5 > 2.23E-5 > 2.23E-5 1.06E-5	> 2.23E-5 2.04E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.105 0.844 0.297 0.349 0.714 0.451 0.409 0.559 0.662	0.641 1.528 0.994 1.201 0.999 1.331 2.236 0.945 2.012	0.542 1.315 0.927 1.136 0.992 1.300 2.047 0.946 1.887	0.568 1.431 0.954 1.161 1.010 1.335 2.200 0.908 1.936	0.567 1.378 0.937 1.144 0.962 1.301 2.127 0.894 1.798	0.607 1.393 0.949 1.219 1.014 1.371 2.058 0.948 1.849	0.081 1.377 0.915 0.957 0.692 1.168 0.875 0.791 1.547	81 69 90 92 97 97 90 100 91	86 94 95 104 100 98 90	86 78 92 93 87 97 94 87	94 80 94 102 105 105 90 101 88	-23 78 89 71 -3 81 25 60 66	5.26E-6 > 2.23E-5 > 2.23E-5 > 2.23E-5 7.20E-6 > 2.23E-5 9.33E-6 > 2.23E-5 > 2.23E-5	1.41E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 2.09E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.479 0.536 0.347 0.488 0.228 0.283 0.460	0.889 1.356 0.599 1.177 0.740 0.940 1.035	0.822 1.296 0.584 1.129 0.764 0.936 0.987	0.877 1.322 0.602 1.079 0.708 0.923 0.982	0.794 1.296 0.587 1.026 0.720 0.920 0.989	0.780 1.275 0.578 1.134 0.731 0.869 0.951	0.671 1.299 0.514 1.058 0.685 0.928 1.090	84 93 94 93 105 99	97 96 101 86 94 97 91	77 93 95 78 96 97 92	73 90 92 94 98 89 85	47 93 66 83 89 98 110	1.69E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.387 0.736 0.348 0.678 0.649 0.519 0.374 0.569	1.439 1.432 1.550 1.038 1.230 1.912 0.529 1.188	1.007 1.155 1.792	1.435 1.320 1.480 0.988 1.176 1.815 0.514 1.108		1.077 1.183 1.756	1.034 1.182	96 78 96 91 87 91 91 87	100 84 94 86 91 93 90 87	99 75 89 73 88 88 95 85	102 78 93 111 92 89 88 78	99 73 69 99 92 85 2	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 6.20E-6 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5
Prostate Cancer PC-3 DU-145	0.397 0.309	1.621 1.123		1.534 1.157				96 93	93 104	90 95	92 94	70 84	> 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5	> 2.23E-5 > 2.23E-5
Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	0.204 0.449 0.514 0.792 0.443 0.536	1.049 1.138 1.108 1.372 0.940 1.361	1.073 1.057 1.355 0.904	1.018 1.133 1.092 1.378 0.925 1.336		1.033 1.046 1.404 0.933	0.921 1.028 1.449 0.880	91 91 91 97 93 87	96 99 97 101 97 97	96 88 89 98 95 86	103 85 89 105 99 56	58 68 86 113 88 -9	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 2.71E-6	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 1.61E-5	> 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5 > 2.23E-5

Table S10. NCI 60-cell line results for 13.

NSC : D - 751839 / 1	Experiment ID: 0912NS69	Test Type : 08	Units : Molar
Report Date : February 01, 2010	Test Date : December 14, 2009	QNS:	MC:
COMI : PC 1009 (92198)	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI : PC 100	9 (921	98)			Sta	in Rea	gent : S	RB Dual-	Pass I	Related		SSP	L : K24A		
					•	Lo	og10 Con	centration				•		•	
Panel/Cell Line	Time Zero	Ctrl	-8.7	Mear	Optical	Densiti	es -4.7	-8.7	-7.7	ercent G	rowth -5.7	-4.7	GI50	TGI	LC50
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226	0.349 0.717 0.257 0.598 0.685	1.583 2.326 1.337 1.723 2.244	1.605 2.137 1.141 1.731 2.228	1.458 2.052 1.088 1.533 2.043	0.599 0.585 0.736 0.977 0.967		0.524 0.482 0.271 0.516 0.683	102 88 82 101 99	90 83 77 83 87	20 -18 44 34 18	16 -32 27 5	14 -33 1 -14		2.08E-5 1.37E-7	> 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H223 NCI-H322M NCI-H460 NCI-H522		1.074 1.567 0.766 1.967 1.461 1.268 0.875 2.027 1.325	1.118 1.656 0.827 1.941 1.414 1.236 0.910 1.862 1.314	0.820 1.573 0.790 1.966 1.351 1.245 0.856 1.200 1.263	0.279 0.728 0.231 0.487 0.793 0.663 0.604 0.453 0.591		0.247 0.470 0.164 0.872 0.576 0.472 0.446 0.191 0.201	106 110 112 97 94 96 108 91	65 101 105 100 86 97 96 54 92	-21 10 -11 -58 16 30 34 12	-29 -24 -42 -4 19 14 6	-30 -26 -37 -24 -14 8 -3 -21 -66	3.09E-8 7.55E-8 6.20E-8 4.31E-8 6.75E-8	1.18E-7 2.12E-6 1.68E-7 8.97E-8 1.31E-6 2.08E-5 1.33E-5 3.53E-6 2.06E-7	> 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5 1.61E-6
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.195 0.747 0.239 0.243 0.153 0.247 0.205	1.172 1.716 1.618 1.683 0.626 1.273 1.204	1.162 1.750 1.584 1.584 0.610 1.233 1.118	0.804 1.620 1.379 1.569 0.440 1.112 0.817	0.214 0.621 0.555 1.402 0.140 0.673 0.399	0.307 0.395 0.394 0.644 0.107 0.496 0.292	0.336 0.210 0.292 0.444 0.123 0.349 0.273	99 103 98 93 97 96 91	62 90 83 92 61 84 61	2 -17 23 80 -9 42 19	11 -47 11 28 -30 24 9	14 -72 4 14 -20 10 7	4,93E-8 7,33E-8 7,89E-7 2,96E-8 1,32E-7	2.08E-5 1.45E-7 2.08E-5 2.08E-5 1.55E-7 2.08E-5 2.08E-5	> 2.08E-5 2.70E-6 > 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5
CNS Cancer SF-268 SF-295 SF-39 SNB-19 SNB-75 U251	0.389 0.751 0.602 0.492 0.519 0.273	1.189 1.251 1.924 1.645 1.003 1.184	1.170 1.212 1.894 1.560 0.937 1.134	1.125 1.129 1.920 1.417 0.858 0.937	0.249 0.446 0.740 0.868 0.080 0.243	0.211 0.350 0.581 0.724 0.045 0.196	0.245 0.315 0.418 0.676 0.090 0.212	98 92 98 93 86 95	92 76 100 80 70 73	-36 -41 10 33 -85 -11	-46 -53 -3 20 -91 -28	-37 -58 -31 16 -83 -22	4.42E-8 3.45E-8 7.49E-8 8.97E-8 2.80E-8 3.90E-8	1.09E-7 9.29E-8 1.17E-6 2.08E-5 5.90E-8 1.54E-7	> 2.08E-5 1.11E-6 > 2.08E-5 > 2.08E-5 1.24E-7 > 2.08E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.105 0.844 0.297 0.349 0.714 0.451 0.409 0.559 0.662	0.588 1.496 1.004 1.179 1.285 1.302 2.204 0.953 1.886	0.534 1.446 0.981 1.160 1.355 1.321 2.157 0.938 1.844	0.181 1.455 0.942 1.032 1.171 1.247 2.021 0.868 1.731	0.099 0.742 0.356 0.471 0.411 0.387 0.501 0.386 1.100	0.101 0.671 0.266 0.379 0.236 0.323 0.285 0.335 0.845	0.066 0.617 0.161 0.300 0.192 0.340 0.048 0.311 0.385	89 92 97 98 112 102 97 96 97	16 94 91 82 80 94 90 78 87	-6 -12 8 15 -42 -14 5 -31	-4 -20 -10 4 -67 -28 -30 -40 15	-38 -27 -46 -14 -73 -25 -88 -44 -42	7.06E-9 5.39E-8 6.54E-8 6.25E-8 3.66E-8 5.28E-8 6.13E-8 3.78E-8 1.10E-7	1.12E-7 1.60E-7 5.79E-7 3.32E-6 9.37E-8 1.54E-7 2.89E-7 1.08E-7 3.81E-6	> 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5 4.22E-7 > 2.08E-5 4.53E-6 > 2.08E-5 > 2.08E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.479 0.536 0.347 0.488 0.228 0.283 0.460	0.901 1.288 0.563 1.171 0.781 0.933 1.080	0.899 1.326 0.552 1.139 0.736 0.950 1.076	0.777 1.266 0.494 1.195 0.741 0.917 1.093	0.210 0.319 0.284 0.767 0.372 0.800 0.407	0.237 0.247 0.254 0.641 0.263 0.514 0.356	0.197 0.216 0.281 0.671 0.143 0.368 0.268	100 105 95 95 92 103 99	71 97 68 104 93 98 102	-56 -40 -18 41 26 80 -12	-51 -54 -27 22 6 35 -23	-59 -60 -19 27 -37 13 -42	9.10E-8	7.50E-8 1.06E-7 1.28E-7 2.08E-5 2.89E-6 2.08E-5 1.65E-7	1.86E-7 1.05E-6 > 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5 > 2.08E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.387 0.736 0.348 0.678 0.649 0.519 0.374 0.569	1.402 1.636 1.536 0.970 1.251 1.800 0.854 1.186	0.871	1.259 1.111 1.489 1.041 1.156 1.728 0.817 1.124	0.287 1.028 0.282	0.189 0.129 0.415 0.122 0.246 0.756 0.162 0.152	0.175 0.185 0.481 0.211 0.076 0.634 0.133 0.228	100 62 100 101 92 108 103 93	86 42 96 124 84 94 92 90	-19 -81 24 -56 -56 40 -25 -10	-51 -83 6 -82 -62 18 -57 -73	-55 -75 11 -69 -88 9 -64 -60	5.36E-8 3.65E-8	1.36E-7 4.55E-8 2.08E-5 1.01E-7 8.30E-8 2.08E-5 1.28E-7 1.67E-7	1.89E-6 1.16E-7 > 2.08E-5 1.92E-7 1.89E-7 > 2.08E-5 1.29E-6 8.95E-7
Prostate Cancer PC-3 DU-145	0.397 0.309	1.562 1.071	1.569 1.100	1.464 1.044	0.836 0.409	0.587 0.343		101 104	92 96	38 13	16 4	8 -12	1.23E-7 7.50E-8	2.08E-5 3.84E-6	> 2.08E-5 > 2.08E-5
Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	0.204 0.449 0.514 0.792 0.443 0.536	0.931 1.112 1.153 1.362 0.919 1.371	1.138 1.275 1.373 0.912	0.663 1.063 1.213 1.362 0.902 1.033	0.336 0.621 0.477 0.147 0.563 0.219	0.293 0.508 0.397 0.082 0.508 0.202	0.235 0.388 0.287 0.063 0.408 0.193	97 104 119 102 99 94	63 93 109 100 96 59	18 26 -7 -81 25 -59	12 9 -23 -90 14 -62	4 -14 -44 -92 -8 -64	4.06E-8 9.04E-8 6.72E-8 3.92E-8 9.34E-8 2.50E-8	2.08E-5 5.15E-6 1.80E-7 7.40E-8 8.84E-6 6.60E-8	> 2.08E-5 > 2.08E-5 > 2.08E-5 1.40E-7 > 2.08E-5 1.74E-7

Table S11. NCI 60-cell line results for 14.

NSC : D - 662466 / 1	Experiment ID: 9306NS84	Test Type : 08	Units : Molar
Report Date : February 04, 2010	Test Date : June 28, 1993	QNS:	MC:
COMI : PC#278	Stain Reagent : SRB Dual-Pass Related	SSPL : K24A	

COMI : PC#27	8				Sta	ın Kea	gent : S	RB Dual-	Pass I	Related	1	SSF	'L : K24A		
					•	Lo	og10 Con	centration				•		•	
	Time			Mear	Optical	l Densiti	es		Р	ercent C	Growth				
Panel/Cell Line	Zero	Ctrl	-9.0	-8.0	-7.0	-6.0	-5.0	-9.0	-8.0	-7.0	-6.0	-5.0	GI50	TGI	LC50
Leukemia CCRF-CEM K-562 MOLT-4 RPMI-8226	0.347 0.213 0.393 0.413	1.173 1.367 1.349 1.447	1.224 1.412 1.365 1.459	1.219 1.429 1.396 1.414	1.271 1.273 1.427 1.546	1.155 1.226 1.386 1.412	0.357 0.466 0.568 0.410	106 104 102 101	106 105 105 97	112 92 108 110	98 88 104 97	1 22 18 -1		1.00E-5 1.00E-5 1.00E-5 9.80E-6	> 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522 Colon Cancer COLO 205 HCC-2998	Cancer 0.416 0.621 0.608 0.668 0.612 0.478 0.636 0.253 0.505	1.807 1.597 1.453 1.039 1.284 1.248 1.493 1.144 1.466	1.824 1.516 1.413 1.090 1.291 1.236 1.493 1.217 1.319	1.800 1.556 1.385 1.120 1.336 1.305 1.456 1.165 1.432	1.690 1.571 1.431 1.021 1.333 1.327 1.460 1.313 1.467	1.688 1.527 1.493 1.074 1.331 1.271 1.524 1.217 1.473	0.572 0.760 0.655 0.545 0.913 0.845 1.165 0.292 0.486	101 92 95 114 101 99 100 108 85	100 96 92 122 108 107 96 102 97	92 97 98 95 107 110 96 119 100	91 93 105 109 107 103 104 108 101	11 14 6 -19 45 48 62 4 -4	2.91E-6 8.26E-6 9.08E-6 > 1.00E-5 3.64E-6 3.06E-6	1.00E-5 1.00E-5 7.17E-6 1.00E-5	> 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5
HCT-116 HCT-15 HT29 KM12 SW-620	0.266 0.460 0.224 0.355 0.201	1.428 1.907 1.161 1.351 0.984	1.463 2.008 1.178 1.358 1.001	1.401 1.908 1.201 1.292 0.947	1.431 1.928 1.176 1.391 0.914	1.409 1.878 1.145 1.374 0.847	0.448 1.090 0.270 0.661 0.438	103 107 102 101 102	98 100 104 94 95	100 101 102 104 91	98 98 98 102 83	16 44 5 31 30	3.84E-6 > 7.61E-6 > 3.29E-6 > 5.38E-6 >	1.00E-5 1.00E-5	> 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.585 0.580 0.500 0.754 0.625 0.347	1.492 1.695 1.143 1.561 0.979 1.378	1.539 1.617 1.151 1.631 1.008 1.375	1.561 1.681 1.095 1.561 1.005 1.293	1.579 1.660 1.147 1.544 1.037 1.315	1.568 1.619 1.117 1.583 1.013 1.304	0.820 0.988 0.307 1.421 0.287 0.451	105 93 101 109 108 100	108 99 93 100 107 92	110 97 101 98 116 94	108 93 96 103 110 93	26 37 -39 83 -54 10	5.78E-6 > 2.19E-6 > 1.00E-5 > 2.31E-6	1.00E-5 1.00E-5 5.16E-6 1.00E-5 4.67E-6 1.00E-5	> 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 9.43E-6 > 1.00E-5
Melanoma MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257	0.656 0.225 0.409 0.632 0.481 0.396 0.527	1.323 0.827 1.463 1.046 1.152 1.953 1.403	1.294 0.802 1.480 1.055 1.157 1.850 1.374	1.312 0.676 1.484 1.084 1.153 1.856 1.497	1.295 0.819 1.512 1.069 1.161 1.843 1.498	1.325 0.872 1.525 1.093 1.274 1.839 1.484	0.947 0.405 0.697 0.397 0.615 0.565 0.798	96 96 102 102 101 93 97	98 75 102 109 100 94 111	96 99 105 106 101 93 111	100 108 106 111 118 93 109	44 30 27 -37 20 11 31	5.50E-6 > 5.14E-6 > 2.59E-6	1.00E-5 5.61E-6 1.00E-5 1.00E-5	> 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.483 0.563 0.399 0.554 0.278 0.392 0.600	1.623 1.497 1.003 1.277 1.101 1.087 1.211	1.642 1.497 1.015 1.273 1.075 1.062 1.138	1.628 1.413 0.974 1.285 1.066 1.054 1.179	1.477 1.434 1.018 1.272 1.049 1.082 1.161	1.494 1.465 0.952 1.291 1.003 1.046 1.154	0.317 0.610 0.374 0.824 0.373 0.710 0.594	102 100 102 99 97 96 88	101 91 95 101 96 95 95	87 93 102 99 94 99	89 97 92 102 88 94 91	-35 5 -6 37 12 46 -1	2.66E-6 6.36E-6 3.15E-6	5,25E-6 1,00E-5 8,63E-6 1,00E-5 1,00E-5 1,00E-5 9,73E-6	> 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.268 0.920 0.668 0.553 0.556 0.477 1.168 0.683	1.199 1.449 1.927 1.572 1.141 1.370 1.632 1.979	1.205 1.380 1.923 1.577 1.206 1.355 1.655 1.928	1.110 1.358 1.937 1.627 1.202 1.202 1.785 1.921	1.178 1.409 1.961 1.544 1.191 1.346 1.757 1.911	1.141 1.448 1.968 1.493 1.180 1.286 1.857 1.900	0.259 0.642 0.954 0.595 0.675 1.597	101 87 100 101 111 98 105 96	90 83 101 105 110 81 133 96	98 92 103 97 109 97 127 95	94 100 103 92 107 91 149 94	-36 -72 -4 39 7 22 92 -46	3.68E-6 > 3.92E-6 >	5.30E-6 3.81E-6 9.21E-6 1.00E-5 1.00E-5 1.00E-5 1.00E-5 4.72E-6	> 1.00E-5 7.46E-6 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5
Prostate Cancer PC-3 DU-145 Breast Cancer	0.622 1.129	1.893 2.399	1.773 2.414	1.850 2.428	1.795 2.364	1.695 2.460	0.675 2.069	91 101	97 102	92 97	84 105	4 74		1.00E-5 1.00E-5	> 1.00E-5 > 1.00E-5
MCF7 MDA-MB-231/ATCC HS 578T MDA-N BT-549 T-47D	0.469 0.363 0.524 0.233 0.597 0.553	1.939 0.804 1.269 1.024 1.354 1.089	0.818 1.263 1.122 1.319	1.879 0.679 1.255 0.962 1.273 1.140	0.802 1.303 1.071		0.314 0.692 0.518 0.348	95 103 99 112 95 98	96 72 98 92 89 110	101 99 105 106 82 123	96 87 100 80 90 115	27 -14 23 36 -42 57	2.32E-6 4.40E-6 4.80E-6 2.01E-6	1.00E-5 7.33E-6 1.00E-5 1.00E-5 4.81E-6 1.00E-5	> 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5 > 1.00E-5

Table S12. One dose mean graph for 15.

Developmental Therapeutics Program
One Dose Mean Graph

 NSC: D-752380 / 1
 Conc: 1.00E-5 Molar
 Test Date: Mar 08, 2010

 Experiment ID: 1003OS13
 Report Date: Apr 16, 2010

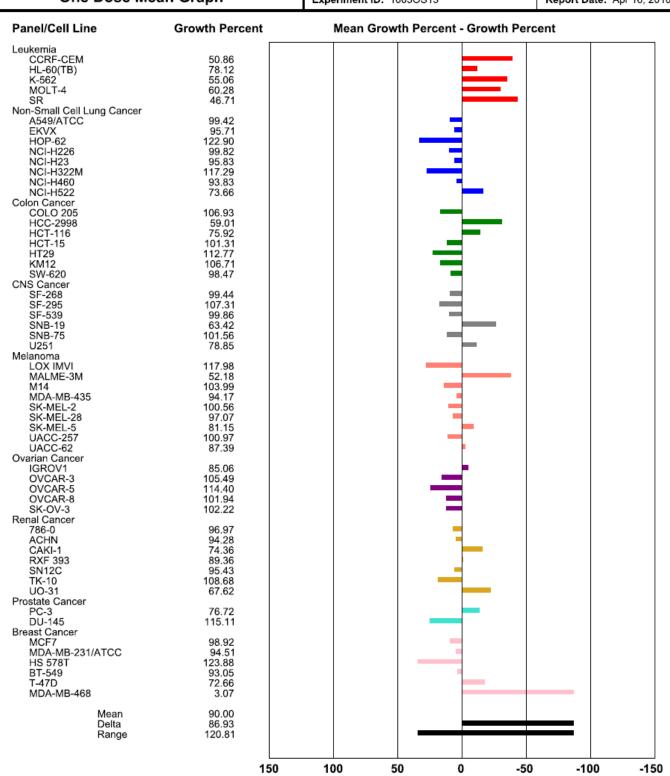


Figure S11. Microfilament effects of **10** in HCT-116 and HeLa cells.

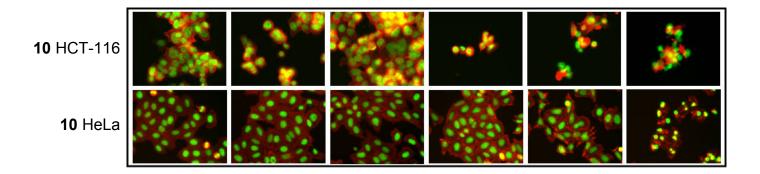


Figure S12. Above water photo of 00101.

