Electronic supplementary materials *Mendeleev Commun*., 2013, **23**, 147−149

Synthesis of polyalkoxy-3-(4-methoxyphenyl)coumarins with antimitotic activity from plant allylpolyalkoxybenzenes

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^{1}H and ^{13}C NMR spectra were collected on a Bruker DRX-500 instrument [working frequencies of 500.13 MHz (^{1}H) and 125.76 MHz (^{13}C)]. Mass spectra were obtained on a Finnigan MAT/INCOS 50 instrument (70 eV) using direct probe injection.

7-Methoxy-1,3-benzodioxol-5-ol **4b.** 4.57 g, 57% yield; mp 88–89 °C (hexane) [lit.,[1] 88–89 °C (petroleum ether)]. ^{1}H NMR **(**DMSO-d_6): δ 3.75 (s, 3H, OCH_3); 5.84 (s, 2H, OCH_2O); 6.01 (d, 1H, J = 2.15 Hz, H_{Ar}); 6.03 (d, 1H, J = 2.15 Hz, H_{Ar}); 9.17 (br.s, 1H, OH). Anal. calc. for $C_8H_8O_4$ (%): C, 57.14; H, 4.80. Found (%): C, 57.22; H, 4.88.

4,7-Dimethoxy-1,3-benzodioxol-5-ol **4c.** 4.66 g, 50% yield; mp 84–85 °C (MeOH) [lit.,[2] 86 °C (cyclohexane)]. ^{1}H NMR **(**DMSO-d_6): δ 3.72 (s, 3H, OCH_3); 3.725 (s, 3H, $OCH_{3)}$; 5.88 (s, 2H, OCH_2O); 6.18 (s, 1H, H_{Ar}); 8.94 (s, 1H, OH). Anal. calc. for $C_9H_{10}O_5$ (%): C, 54.55; H, 5.09. Found (%): C, 54.63; H, 5.04.

6,7-Dimethoxy-1,3-benzodioxol-5-ol **4d.** 4.38 g, 47% yield; mp 84–85 °C [lit.,[3] 82–83 °C (cyclohexane)]. ^{1}H NMR **(** DMSO-d_6): δ 3.62 (s, 3H, OCH_3); 3.89 (s, 3H, OCH_3); 5.84 (s, 2H, OCH_2O); 6.19 (s, 1H, H_{Ar}); 8.83 (br.s, 1H, OH). EIMS *m/z* 198 $[M]^+$ (77), 183 (100), 137 (28). Anal. calc. for $C_9H_{10}O_5$ (%): C, 54.55; H, 5.09. Found (%): C, 54.67; H, 5.02.

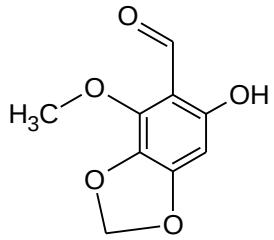
2,6-Dimethoxybenzo-1,4-quinone **5a.** 0.34 g, 20% yield; mp 251 °C (lit.,[4] 250–252 °C). ^{1}H NMR **(**DMSO-d_6): δ 3.75 (s, 6H, OCH_3); 5.97 (s, 2H, H_{Ar}). EIMS *m/z* 168 $[M]^+$ (100), 138 (73), 125 (36). 97 (38), 80 (71). Anal. calc. for $C_8H_8O_4$ (%): C, 57.14; H, 4.80. Found (%): C, 57.23; H, 4.87.

3-Hydroxy-2,5-dimethoxybenzo-1,4-quinone **5c.** 0.352 g, 19% yield; mp 210 °C (AcOH) [lit.,[2] 211 °C (AcOH)]. ^{1}H NMR **(**DMSO-d_6): δ 3.74 (s, 3H, OCH_3); 3.80 (s, 3H, OCH_3); 5.8 (s, 1H, OCH_2O); 5.8 (s, 1H, H_{Ar}); 10.3 (br.s, 1H, OH). EIMS *m/z* 184$[M]^+$ (100), 169 (82), 139 (76). Anal. calc. for $C_8H_8O_5$ (%): C, 52.18; H, 4.38. Found (%): C, 52.25; H, 4.43.

4,4',7,7'-Tetramethoxy-5,5'-bi-1,3-benzodioxole-6,6'-diol **6.** 0.44 g, 22% yield; mp 191–193 °C. ^{1}H NMR **(** DMSO-d_6): δ 3.62 (s, 6H, OCH_3); 3.79 (s, 6H, OCH_3); 5.93 (s, 4H, OCH_2O); 8.05 (s, 2H, OH). EIMS *m/z* 394 $[M]^+$ (100), 349 (29), 334 (20), 197 (235). Anal. calc. for $C_{18}H_{18}O_{10}$ (%): C, 54.83; H, 4.60. Found (%): C, 54.77; H, 4.56.

6,6'-Methylenebis(4,7-dimethoxy-1,3-benzodioxol-5-ol) **7.** 0.33 g, 17% yield; mp 149–150 °C. ^{1}H NMR **(**DMSO-d_6): δ 3.63(s, 6H, OCH_3); 3.73 (s, 2H, CH_2) 3.75 (s, 6H, OCH_3); 5.86 (s, 4H, OCH_2O); 8.35 (br.s, 2H, OH). ^{13}C NMR **(**125,76 MHz, DMSO-d_6): 18.83 (CH_2); 59.56 (OCH_3); 60.44 (OCH_3); 101.06 (OCH_2O); 113,44; 128.31; 131.20; 137.19; 137.58; 142.47. EIMS *m/z* 408 $[M]^+$ (33), 210 (84), 198 (95), 183 (100). Anal. calc. for $C_{19}H_{20}O_{10}$ (%): C, 55.88; H, 4.94. Found (%): C, 55.81; H, 4.82.

6-Hydroxy-4-methoxy-1,3-benzodioxole-5-carboxaldehyde **8b.**



0.6 g (column chromatography), 25% yield; a mixture of aldehydes **8b** and **8'b** (3:1), mp **8b** 122–123 °C (white powder, HPLC) [lit.,[5] cream-coloured flakes, mp 124–125 °C (light petroleum), lit.,[6] white powder, 121 °C]. ^{1}H NMR **(**DMSO-d_6): δ 4.08 (s, 3H, OCH_3); 6.06 (s, 2H,OCH_2O); 6.29 (s, 1H, H_{Ar}); 9.95 (s, 1H, CHO); 12.42 (br. s, 1H, OH).

5-Hydroxy-7-methoxy-1,3-benzodioxole-4-carboxaldehyde **8'b.**

8'b (Separated by HPLC to record NMR spectra). ^{1}H NMR **(**DMSO-d_6): δ 3.85 (s, 3H, OCH_3); 6.04 (s, 2H, OCH_2O); 6.15 (s, 1H, H_{Ar}); 10.01 (s, 1H, CHO) 12.43 (br. s, 1H, OH).

6-Hydroxy-4,7-dimethoxy-1,3-benzodioxole-5-carboxaldehyde **8c.** 2.4 g, 73% yield; mp 125–127 °C (EtOH) (lit.,[6] 121.4 °C). ^{1}H NMR **(**DMSO-d_6): δ 3.79 (s, 3H, OCH_3); 4.01 (s, 3H, OCH_3);

6.10 (s, 2H, OCH_2O); 9.97 (s, 1H, CHO) 12.43 (s, 1H, OH). EIMS m/z 226 $[M]^+$ (100), 211 (62), 196 (13), 193 (7), 183 (11), 180 (5), 153 (11), 125 (14), 123 (7), 121 (8), 113 (5), 95 (13), 93 (16), 85 (20), 83 (22), 81 (5), 77 (5), 69 (58), 53 (54).

5-Hydroxy-6,7-dimethoxy-1,3-benzodioxole-4-carboxaldehyde **8d.** 1.0 g, 30% yield; mp 125–126 °C (AcOEt-petroleum ether). ^{1}H NMR **(**DMSO-d_6): δ 3.65(s, 3H, OCH_3); 4.05(s, 3H, OCH_3); 6.04 (s, 2H, OCH_2O); 10.02 (s, 1H, CHO); 12.40 (s, 1H, OH). EIMS m/z 226 $[M]^+$(68), 211 (41), 183 (25), 153 (8), 127 (7), 125 (7), 110 (6), 99 (16), 97 (25), 95 (12), 93 (14), 87 (46), 85 (17), 83 (64), 82 (56), 77 (8), 69 (61), 53 (100). Anal. calc. for $C_{10}H_{10}O_6$ (%): C, 53.10; H, 4.46. Found (%): C, 53.17; H, 4.52.

*9-Methoxy-7-(4-methoxyphenyl)-6*H-*[1,3]dioxolo[4,5*-g*]chromen-6-one* **9b.** 0.008 g, resin (column chromatography, AcOEt-petroleum ether = 1:4, R_f=0.4); 3% yield. ^{1}H NMR **(**$CDCl_3$): δ 3.85 (s, 3H, OCH_3); 4.15 (s, 3H, OCH_3); 6.01 (s, 2H, OCH_2O); 6.57 (s, 1H, H_{Ar}); 6.95 (d, *J* = 9.0 Hz, 1H, H_{Ar}); 7.68 (d, *J* = 9.0 Hz, 1H, H_{Ar}); 8.02 (s, 1H, C=CH). EIMS m/z 326 $[M]^+$ (100), 311 (28), 298 (31), 283 (78), 268 (16), 255 (11), 253 (13), 227 (13), 199 (10), 197 (11), 169 (22), 163 (11), 157 (10), 154 (9), 149 (16), 139 (11), 135 (27), 126 (19), 121 (19), 113 (13), 111 (16), 97 (30), 95 (27), 85 (28), 83 (38), 81 (29), 71 (62), 69 (70). Anal. calc. for $C_{18}H_{14}O_6$ (%): C, 66.26; H, 4.32. Found (%): C, 66.34; H, 4.37.

*4,9-Dimethoxy-7-(4-methoxyphenyl)-6*H-*[1,3]dioxolo[4,5*-g*]chromen-6-one* **9c.** 0.1 g, 11% yield; mp 138–140 °C (AcOEt-petroleum ether = 1:4). ^{1}H NMR **(**DMSO-d_6): δ 3.79 (s, 3H, OCH_3); 3.92 (s, 3H, OCH_3); 4.02 (s, 3H, OCH_3); 6.15 (s, 2H, OCH_2O); 7.00 (d, J = 9.0 Hz, 1H, H_{Ar}); 7.64 (d, J = 9.0 Hz, 1H, H_{Ar}); 7.93 (s, 1H, C=CH). EIMS m/z 356 $[M]^+$ (100), 341 (20), 326 (2), 313 (24), 298 (9), 283 (7), 268 (6), 257 (14), 255 (14), 240 (11), 227 (13), 186 (9), 184 (19), 178 (17), 172 (17), 169 (22), 164 (14), 157 (17), 156 (20), 144 (12), 141 (13), 135 (82), 128 (11), 126 (16), 117 (12), 115 (17), 113 (30), 101 (24), 92 (14), 89 (19), 86 (10), 83 (15), 77 (18), 75 (25), 69 (12), 63 (21). Anal. calc. for $C_{19}H_{16}O_7$ (%): C, 64.04; H, 4.53. Found (%): C, 64.12; H, 4.59.

*4,5-Dimethoxy-8-(4-methoxyphenyl)-7*H-*[1,3]dioxolo[4,5*-f*]chromen-7-one* **9d.** 0.305 g, 28% yield; mp 171–174 °C (AcOEt-petroleum ether = 1:4). ^{1}H NMR **(**DMSO-d_6): δ 3.70 (s, 3H, OCH_3); 3.71 (s, 3H, OCH_3); 4.08 (s, 3H, OCH_3); 6.18 (s, 2H, OCH_2O); 7.00 (d, J = 9.0 Hz, 1H, H_{Ar}); 7.67 (d, J = 9.0 Hz, 1H, H_{Ar}); 7.82 (s, 1H, C=CH). EIMS m/z 356 $[M]^+$ (1), 313(1), 186 (6), 184 (18), 171 (8), 169 (17), 158 (10), 156 (26), 144 (14), 141 (22), 139 (10), 135 (100), 129 (11),

126 (17), 117 (19), 115 (29), 113 (63), 101 (29), 92 (18), 89 (29), 87 (18), 83 (33), 77 (29), 75 (26), 69 (14),63 (24). Anal. calc. for $C_{19}H_{16}O_7$ (%): C, 64.04; H, 4.53. Found (%): C, 64.16; H, 4.44.

Biology. Sea urchin embryo assay[7-9]

Adult sea urchins *Paracentrotus lividus* were collected from the Mediterranean Sea at the Cyprus coast and kept in an aerated seawater tank. Gametes were obtained by intracoelomic injection of 0.5 M KCl. Eggs were washed with filtered seawater and fertilized by adding drops of diluted sperm. Embryos were cultured at room temperature under gentle agitation with a motor-driven plastic paddle (60 rpm) in filtered seawater. The embryos were observed with a Biolam light microscope (LOMO, St. Petersburg, Russia). For treatment with the test compounds, 5 ml aliquots of embryo suspension were transferred to six-well plates and incubated as a monolayer at a concentration up to 2000 embryos/ml. Stock solutions of compounds were prepared in DMSO at 10 mM concentrations, followed by tenfold dilution with 95% EtOH. This procedure enhanced the solubility of the test compounds in the salt-containing medium (seawater), as evidenced by microscopic examination of the samples. The maximum tolerated concentrations of DMSO and EtOH in the *in vivo* assay were determined to be 0.05% and 1%, respectively.

The antiproliferative activity was assessed by exposing fertilized eggs (8–15 min after fertilization, 60–70 min before the first mitotic cycle completion) to 2-fold decreasing concentrations of a compound. Cleavage alteration and arrest were clearly detected at 2.5–5.5 h after fertilization**.** The effects were quantitatively estimated as a threshold concentration (EC) resulting in cleavage alteration and embryo death before hatching or full mitotic arrest. At these concentrations, all tested molecules caused 100% cleavage alteration and embryo death before hatching, whereas at 2-fold lower concentrations, the compounds failed to produce any effect. For microtubule destabilizing activity, the compounds were tested on free-swimming blastulae just after hatching (9–10 h post fertilization), originated from the same embryo culture. For spinning, embryos were observed after 2–20 h of treatment.

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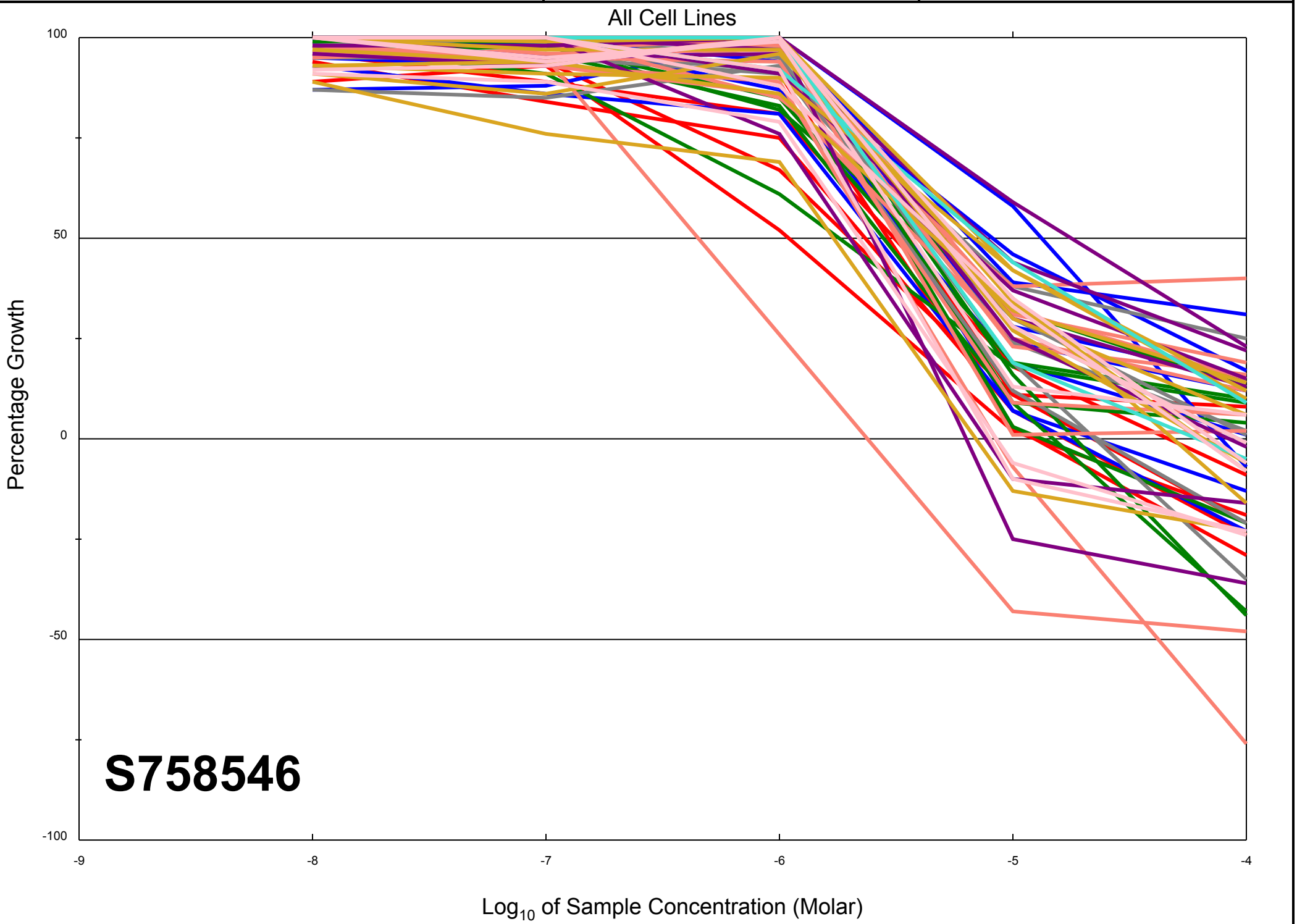
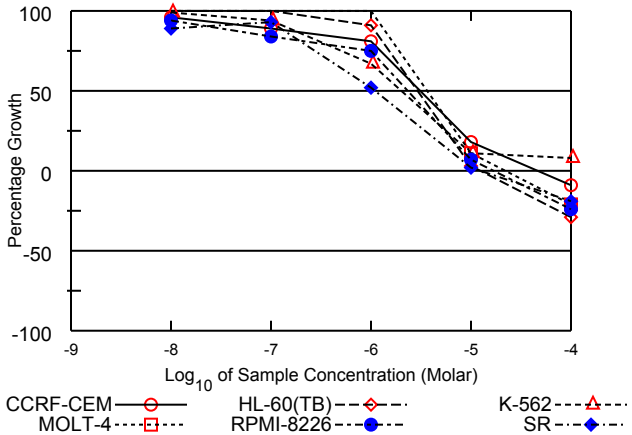
National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC:758546/1	SSPL:0YAR	EXP. ID:1106NS70
	Report Date:December 07, 2011	Test Date:June 27, 2011	



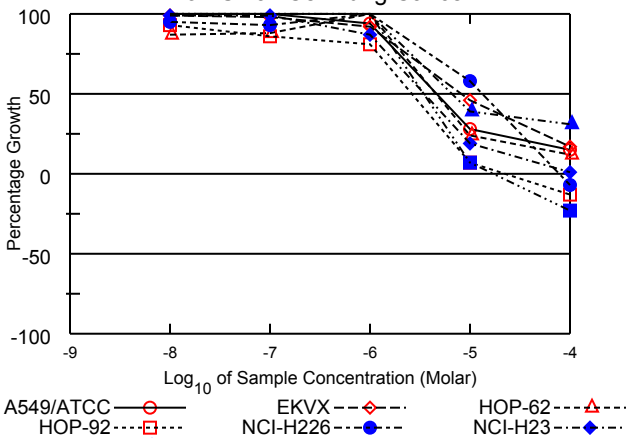
National Cancer Institute Developmental Therapeutics Program
Dose Response Curves

NSC: 758546 / 1	SSPL: 0YAR	EXP. ID: 1106NS70
Report Date: December 07, 2011	Test Date: June 27, 2011	

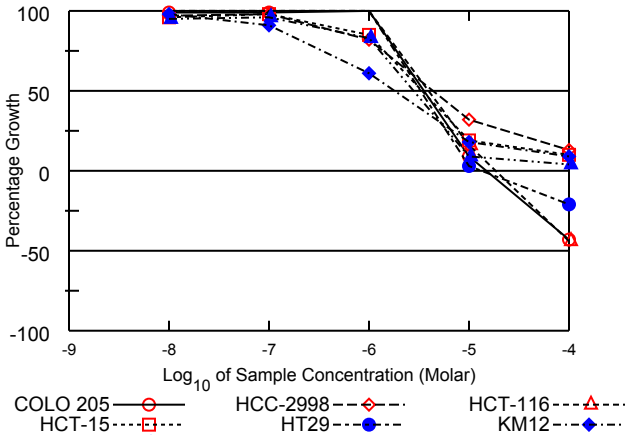
Leukemia



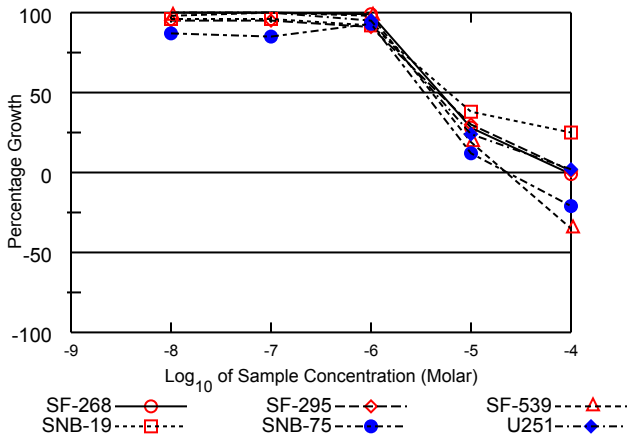
Non-Small Cell Lung Cancer



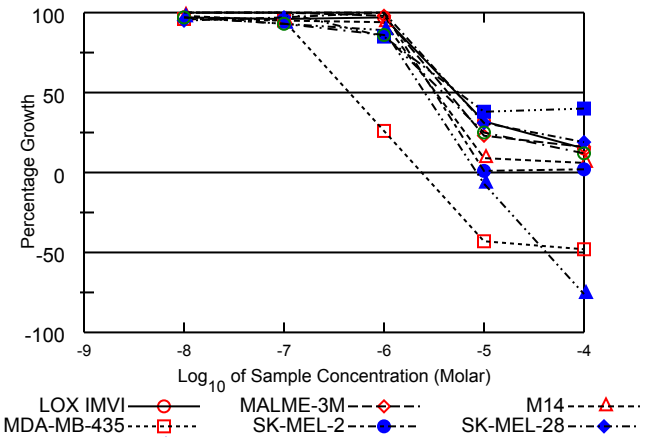
Colon Cancer



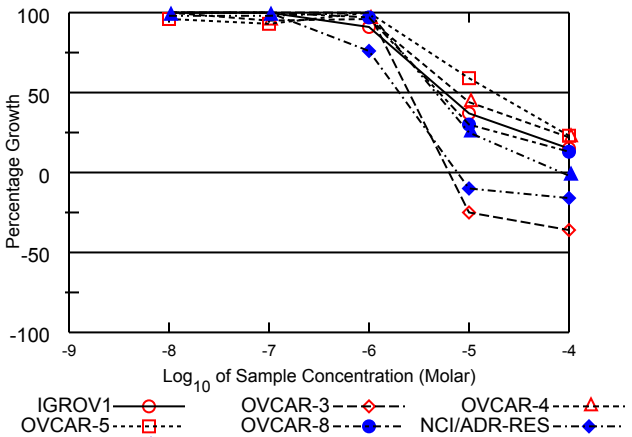
CNS Cancer



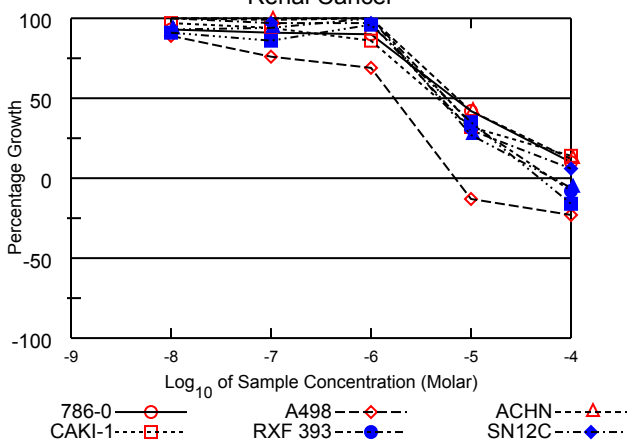
Melanoma



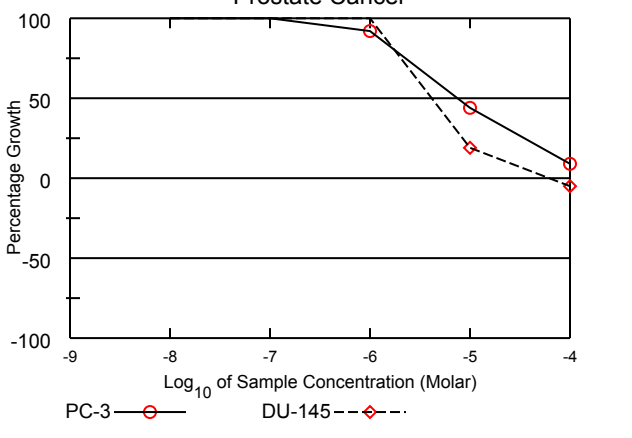
Ovarian Cancer



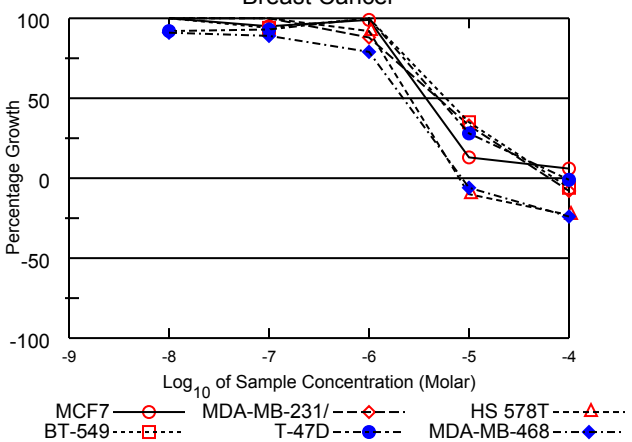
Renal Cancer



Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : 758546 / 1	Experiment ID : 1106NS70	Test Type : 08	Units : Molar
Report Date : December 07, 2011	Test Date : June 27, 2011	QNS :	MC :
COMI : A4535/0194125 (105298)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0YAR	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
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															
CCRF-CEM	0.557	1.585	1.539	1.474	1.390	0.742	0.506	96	89	81	18	-9	3.10E-6	4.59E-5	> 1.00E-4
HL-60(TB)	0.977	2.739	2.737	2.742	2.586	1.038	0.693	100	100	91	3	-29	2.95E-6	1.28E-5	> 1.00E-4
K-562	0.168	1.074	1.064	1.024	0.775	0.269	0.240	99	94	67	11	8	2.02E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.522	1.576	1.608	1.615	1.644	0.642	0.410	103	104	106	11	-21	3.92E-6	2.22E-5	> 1.00E-4
RPMI-8226	0.384	1.106	1.062	0.991	0.924	0.435	0.294	94	84	75	7	-24	2.32E-6	1.70E-5	> 1.00E-4
SR	0.374	1.375	1.265	1.302	0.897	0.396	0.304	89	93	52	2	-19	1.11E-6	1.27E-5	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.333	1.503	1.536	1.525	1.437	0.656	0.507	103	102	94	28	15	4.62E-6	> 1.00E-4	> 1.00E-4
EKVX	0.707	1.775	1.765	1.757	1.687	1.203	0.886	99	98	92	46	17	8.32E-6	> 1.00E-4	> 1.00E-4
HOP-62	0.364	1.117	1.023	1.027	1.136	0.546	0.458	87	88	103	24	12	4.68E-6	> 1.00E-4	> 1.00E-4
HOP-92	1.098	1.446	1.423	1.396	1.378	1.123	0.952	93	86	81	7	-13	2.61E-6	2.24E-5	> 1.00E-4
NCI-H226	0.752	1.514	1.480	1.464	1.542	1.195	0.702	95	93	104	58	-7	1.33E-5	7.88E-5	> 1.00E-4
NCI-H23	0.627	1.788	1.775	1.772	1.633	0.850	0.634	99	99	87	19	1	3.49E-6	> 1.00E-4	> 1.00E-4
NCI-H322M	0.347	0.758	0.764	0.761	0.794	0.506	0.474	101	101	109	39	31	6.87E-6	> 1.00E-4	> 1.00E-4
NCI-H460	0.224	1.964	2.011	1.967	1.979	0.344	0.173	103	100	101	7	-23	3.48E-6	1.70E-5	> 1.00E-4
Colon Cancer															
COLO 205	0.246	1.218	1.213	1.210	1.252	0.330	0.141	99	99	103	9	-43	3.66E-6	1.47E-5	> 1.00E-4
HCC-2998	0.650	2.080	2.040	2.054	1.828	1.110	0.842	97	98	82	32	13	4.41E-6	> 1.00E-4	> 1.00E-4
HCT-116	0.170	1.288	1.306	1.311	1.292	0.352	0.096	102	102	100	16	-44	3.97E-6	1.86E-5	> 1.00E-4
HCT-15	0.310	1.840	1.785	1.806	1.617	0.604	0.462	96	98	85	19	10	3.43E-6	> 1.00E-4	> 1.00E-4
HT29	0.223	1.028	1.072	1.092	1.062	0.245	0.177	105	108	104	3	-21	3.42E-6	1.31E-5	> 1.00E-4
KM12	0.398	1.734	1.706	1.620	1.212	0.635	0.516	98	91	61	18	9	1.79E-6	> 1.00E-4	> 1.00E-4
SW-620	0.189	1.077	1.030	1.044	0.929	0.266	0.223	95	96	83	9	4	2.79E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.327	0.974	0.972	0.987	0.967	0.511	0.323	100	102	99	28	-1	4.95E-6	9.09E-5	> 1.00E-4
SF-295	0.783	2.425	2.342	2.342	2.274	1.268	0.808	95	95	91	30	1	4.63E-6	> 1.00E-4	> 1.00E-4
SF-539	0.824	2.056	2.036	2.072	2.033	1.064	0.539	98	101	98	19	-35	4.09E-6	2.29E-5	> 1.00E-4
SNB-19	0.436	1.496	1.459	1.457	1.408	0.838	0.704	96	96	92	38	25	5.95E-6	> 1.00E-4	> 1.00E-4
SNB-75	0.617	1.242	1.162	1.146	1.196	0.693	0.485	87	85	93	12	-21	3.39E-6	2.30E-5	> 1.00E-4
U251	0.291	1.175	1.187	1.187	1.133	0.499	0.309	101	101	95	24	2	4.27E-6	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.314	1.969	1.912	1.902	1.916	0.849	0.555	97	96	97	32	15	5.32E-6	> 1.00E-4	> 1.00E-4
MALME-3M	0.544	0.857	0.856	0.857	0.850	0.617	0.594	100	100	98	23	16	4.37E-6	> 1.00E-4	> 1.00E-4
M14	0.369	1.364	1.345	1.314	1.309	0.459	0.429	98	95	94	9	6	3.31E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.384	1.751	1.699	1.681	0.734	0.220	0.201	96	95	26	-43	-48	4.44E-7	2.37E-6	> 1.00E-4
SK-MEL-2	0.846	1.753	1.830	1.749	1.824	0.855	0.862	108	100	108	1	2	3.48E-6	> 1.00E-4	> 1.00E-4
SK-MEL-28	0.321	0.955	0.924	0.936	0.955	0.517	0.441	95	97	100	31	19	5.28E-6	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.644	1.909	1.876	1.826	1.775	0.601	0.154	97	93	89	-7	-76	2.57E-6	8.51E-6	4.20E-5
UACC-257	0.691	1.343	1.473	1.346	1.245	0.936	0.953	120	100	85	38	40	5.47E-6	> 1.00E-4	> 1.00E-4
UACC-62	0.566	2.252	2.203	2.141	2.021	0.996	0.777	97	93	86	25	12	3.95E-6	> 1.00E-4	> 1.00E-4
Ovarian Cancer															
IGROV1	0.420	1.220	1.282	1.244	1.145	0.720	0.536	108	103	91	37	15	5.81E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.433	0.999	1.005	1.001	1.035	0.325	0.278	101	100	106	-25	-36	2.68E-6	6.45E-6	> 1.00E-4
OVCAR-4	0.396	1.329	1.361	1.284	1.289	0.805	0.605	103	95	96	44	22	7.60E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.467	1.162	1.137	1.116	1.173	0.876	0.630	96	93	102	59	23	1.78E-5	> 1.00E-4	> 1.00E-4
OVCAR-8	0.311	1.218	1.221	1.251	1.189	0.582	0.429	100	104	97	30	13	5.00E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.532	1.590	1.604	1.598	1.340	0.481	0.446	101	101	76	-10	-16	2.02E-6	7.72E-6	> 1.00E-4
SK-OV-3	0.566	1.451	1.430	1.437	1.461	0.785	0.553	98	98	101	25	-2	4.67E-6	8.22E-5	> 1.00E-4
Renal Cancer															
786-0	0.607	2.094	1.991	1.955	1.941	1.238	0.763	93	91	90	42	10	6.91E-6	> 1.00E-4	> 1.00E-4
A498	0.970	1.508	1.451	1.377	1.340	0.847	0.745	89	76	69	-13	-23	1.70E-6	6.98E-6	> 1.00E-4
ACHN	0.438	1.660	1.675	1.645	1.755	0.947	0.588	101	99	108	42	12	7.47E-6	> 1.00E-4	> 1.00E-4
CAKI-1	0.599	2.176	2.135	2.084	1.953	1.099	0.819	97	94	86	32	14	4.59E-6	> 1.00E-4	> 1.00E-4
RXF 393	0.605	0.959	0.961	0.957	0.969	0.727	0.554	101	100	103	34	-8	5.91E-6	6.35E-5	> 1.00E-4
SN12C	0.469	1.695	1.692	1.657	1.657	0.839	0.545	100	97	97	30	6	5.04E-6	> 1.00E-4	> 1.00E-4
TK-10	0.590	1.148	1.108	1.116	1.182	0.740	0.554	93	94	106	27	-6	5.11E-6	6.50E-5	> 1.00E-4
UO-31	0.674	1.467	1.392	1.359	1.432	0.948	0.569	91	86	96	35	-16	5.59E-6	4.88E-5	> 1.00E-4
Prostate Cancer															
PC-3	0.524	1.605	1.622	1.659	1.516	0.998	0.617	102	105	92	44	9	7.42E-6	> 1.00E-4	> 1.00E-4
DU-145	0.342	1.010	1.057	1.024	1.070	0.468	0.324	107	102	109	19	-5	4.51E-6	5.99E-5	> 1.00E-4
Breast Cancer															
MCF7	0.212	1.033	1.038	0.993	1.022	0.317	0.259	101	95	99	13	6	3.69E-6	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.437	1.047	1.060	1.064	0.975	0.638	0.400	102	103	88	33	-8	4.91E-6	6.25E-5	> 1.00E-4
HS 578T	0.898	1.380	1.383	1.383	1.344	0.807	0.693	100	100	92	-10	-23	2.59E-6	7.96E-6	> 1.00E-4
BT-549	0.905	1.798	1.819	1.749	1.800	1.216	0.852	102	94	100	35	-6	5.85E-6	7.16E-5	> 1.00E-4
T-47D	0.448	1.194	1.131	1.143	1.209	0.655	0.444	92	93	102	28	-1	5.02E-6	9.23E-5	> 1.00E-4
MDA-MB-468	0.682	1.464	1.390	1.381	1.303	0.640	0.520	91	89	79	-6	-24	2.21E-6	8.46E-6	> 1.00E-4

National Cancer Institute Developmental Therapeutics Program

Mean Graphs

NSC :758546/1 | Units :Molar | SSPL :0YAR | EXP. ID :1106NS70

Report Date :December 07, 2011 | Test Date :June 27, 2011

Panel/Cell Line	Log_{10}GI50	GI50	Log_{10}TGI	TGI	Log_{10}LC50	LC50
Leukemia						
CCRF-CEM	-5.51		-4.34		> -4.00	
HL-60(TB)	-5.53		-4.89		> -4.00	
K-562	-5.70		> -4.00		> -4.00	
MOLT-4	-5.41		-4.65		> -4.00	
RPMI-8226	-5.63		-4.77		> -4.00	
SR	-5.96		-4.90		> -4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	-5.34		> -4.00		> -4.00	
EKVX	-5.08		> -4.00		> -4.00	
HOP-62	-5.33		> -4.00		> -4.00	
HOP-92	-5.58		-4.65		> -4.00	
NCI-H226	-4.88		-4.10		> -4.00	
NCI-H23	-5.46		> -4.00		> -4.00	
NCI-H322M	-5.16		> -4.00		> -4.00	
NCI-H460	-5.46		-4.77		> -4.00	
Colon Cancer						
COLO 205	-5.44		-4.83		> -4.00	
HCC-2998	-5.36		> -4.00		> -4.00	
HCT-116	-5.40		-4.73		> -4.00	
HCT-15	-5.47		> -4.00		> -4.00	
HT29	-5.47		-4.88		> -4.00	
KM12	-5.75		> -4.00		> -4.00	
SW-620	-5.55		> -4.00		> -4.00	
CNS Cancer						
SF-268	-5.31		-4.04		> -4.00	
SF-295	-5.33		> -4.00		> -4.00	
SF-539	-5.39		-4.64		> -4.00	
SNB-19	-5.23		> -4.00		> -4.00	
SNB-75	-5.47		-4.64		> -4.00	
U251	-5.37		> -4.00		> -4.00	
Melanoma						
LOX IMVI	-5.27		> -4.00		> -4.00	
MALME-3M	-5.36		> -4.00		> -4.00	
M14	-5.48		> -4.00		> -4.00	
MDA-MB-435	-6.35		-5.63		> -4.00	
SK-MEL-2	-5.46		> -4.00		> -4.00	
SK-MEL-28	-5.28		> -4.00		> -4.00	
SK-MEL-5	-5.59		-5.07		-4.38	
UACC-257	-5.26		> -4.00		> -4.00	
UACC-62	-5.40		> -4.00		> -4.00	
Ovarian Cancer						
IGROV1	-5.24		> -4.00		> -4.00	
OVCAR-3	-5.57		-5.19		> -4.00	
OVCAR-4	-5.12		> -4.00		> -4.00	
OVCAR-5	-4.75		> -4.00		> -4.00	
OVCAR-8	-5.30		> -4.00		> -4.00	
NCI/ADR-RES	-5.69		-5.11		> -4.00	
SK-OV-3	-5.33		-4.09		> -4.00	
Renal Cancer						
786-0	-5.16		> -4.00		> -4.00	
A498	-5.77		-5.16		> -4.00	
ACHN	-5.13		> -4.00		> -4.00	
CAKI-1	-5.34		> -4.00		> -4.00	
RXF 393	-5.23		-4.20		> -4.00	
SN12C	-5.30		> -4.00		> -4.00	
TK-10	-5.29		-4.19		> -4.00	
UO-31	-5.25		-4.31		> -4.00	
Prostate Cancer						
PC-3	-5.13		> -4.00		> -4.00	
DU-145	-5.35		-4.22		> -4.00	
Breast Cancer						
MCF7	-5.43		> -4.00		> -4.00	
MDA-MB-231/ATCC	-5.31		-4.20		> -4.00	
HS 578T	-5.59		-5.10		> -4.00	
BT-549	-5.23		-4.15		> -4.00	
T-47D	-5.30		-4.03		> -4.00	
MDA-MB-468	-5.66		-5.07		> -4.00	
_MID	-5.4		-4.31		-4.01	
Delta	0.95		1.32		0.37	
Range	1.6		1.63		0.38