

(Supplementary Information)

Novel C₅-curcuminoid-4-aminoquinoline molecular hybrids: Design, synthesis and mechanistic investigation of anticancer activity

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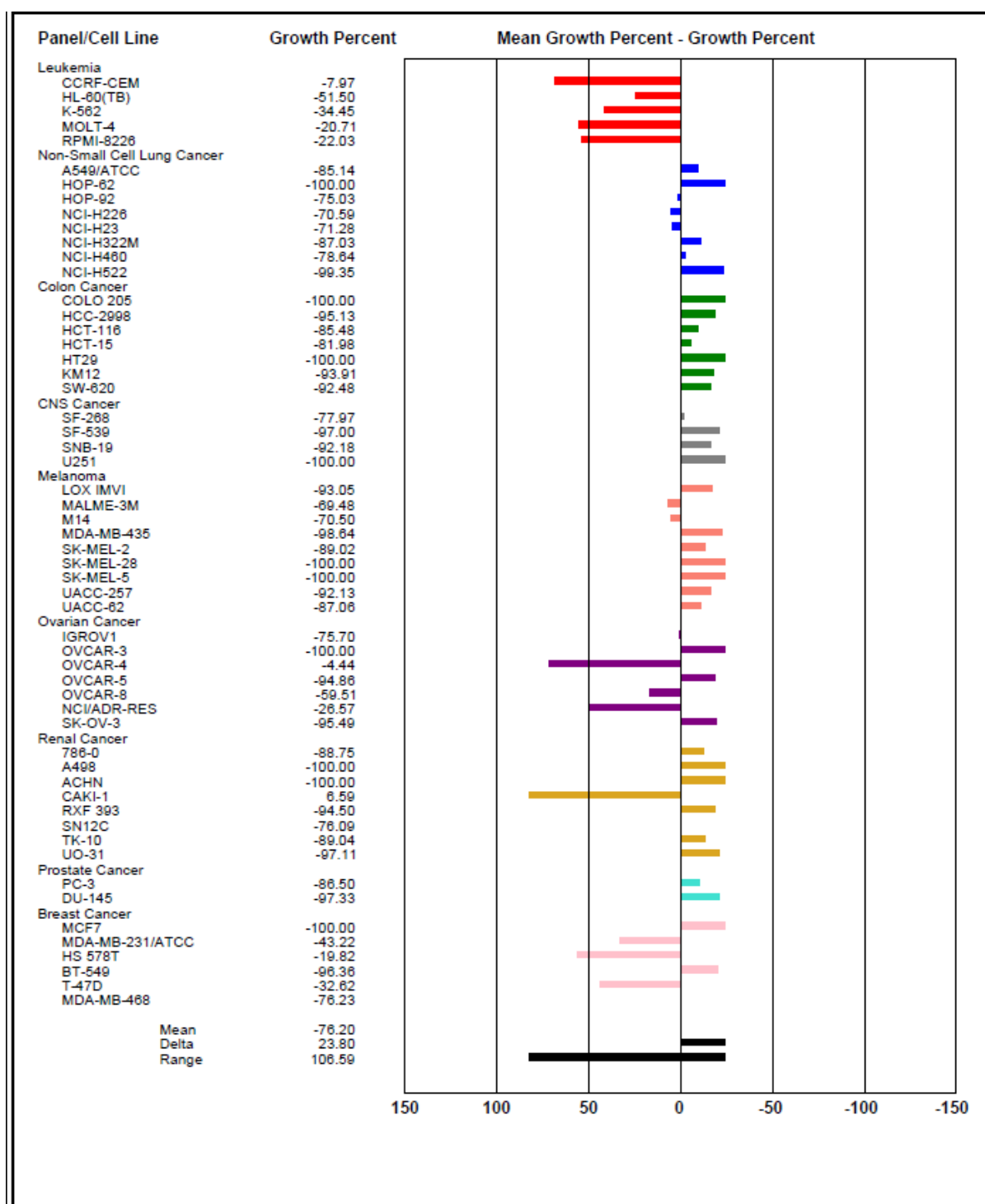
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Single Dose Data

Panel/Cell Lines	Growth Percent(7d)	Growth percent (7f)
Leukemia		
CCRF-CEM	-07.97	0.69
HL-60(TB)	-51.50	-11.33
K-562	-34.45	2.21
MOLT-4	-20.71	-3.65
RPMI-8226	-22.03	-1.73
Non-small cell Lung Cancer		
A549/ATCC	-85.14	22.74
HOP-62	-100.00	-7.73
HOP-92	-75.03	-16.12
NCI-H226	-70.59	17.02
NCI-H23	-71.28	47.96
NCI-H322M	-87.03	44.66
NCI-H460	-78.64	-28.51
NCI-H522	-99.35	-67.82
Colon Cancer		
COLO 205	-100.00	10.07
HCC-2998	-95.13	
HCT-116	-85.48	-85.29
HCT-15	-81.98	76.05
HT 29	-100.00	-42.42
KM 12	-93.91	-35.68
SW-620	-92.48	0.35
CNS Cancer		
SF-268	-77.97	9.60
SF-539	-97.00	-12.52
SNB-19	-92.18	58.09
U 251	-100.00	6.39
Melanoma		
LOX IMVI	-93.05	-28.31
MALME-3M	-69.48	-27.75
M 14	-70.50	3.70
MDA-MB-435	-98.64	-5.87
SK-MEL-2	-89.02	-19.66
SK-MEL-28	-100.00	21.60
SK-MEL-5	-100.00	10.80
UACC-257	-92.13	5.32
UACC-62	-87.06	7.74
Ovarian Cancer		
IGROV1	-75.70	7.35
OVCAR-3	-100.00	-13.94
OVCAR-4	-4.44	29.84
OVCAR-5	-94.86	18.09
OVCAR-8	-59.51	-3.77
NCI/ADR-RES	-26.57	103.20
SK-OV-3	-95.49	4.28

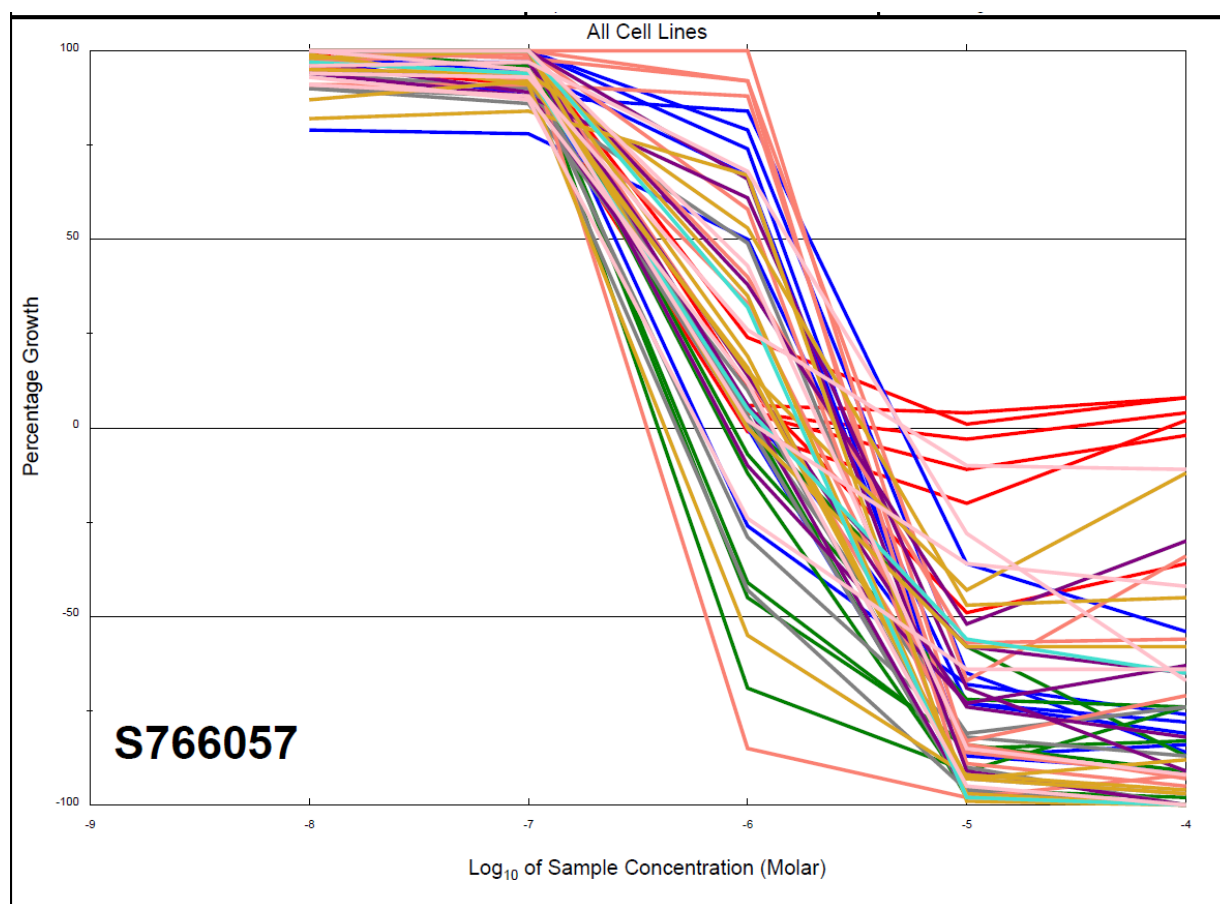
Renal Cancer		
786-0	-88.75	15.92
A498	-100.00	32.52
ACHN	-100.00	51.36
CAKI-1	6.59	97.44
RXF 393	-94.50	-52.09
SN 12C	-76.09	-0.66
TX-10	-89.04	8.71
UO-31	-97.11	80.49
Prostate Cancer		
PC-3	-86.50	12.09
DU-145	-97.33	0.08
Breast Cancer		
MCF7	-100.00	27.95
MDA-MB-231/ATCC	-43.22	-0.28
HS 578T	-19.82	23.38
BT-549	-96.36	-31.56
T-47D	-32.62	32.88
MDA-MB-468	-76.23	-37.67

One Dose Mean Graph (Compound 7d)



FIVE dose results (Compound 7d)

Dose response curves

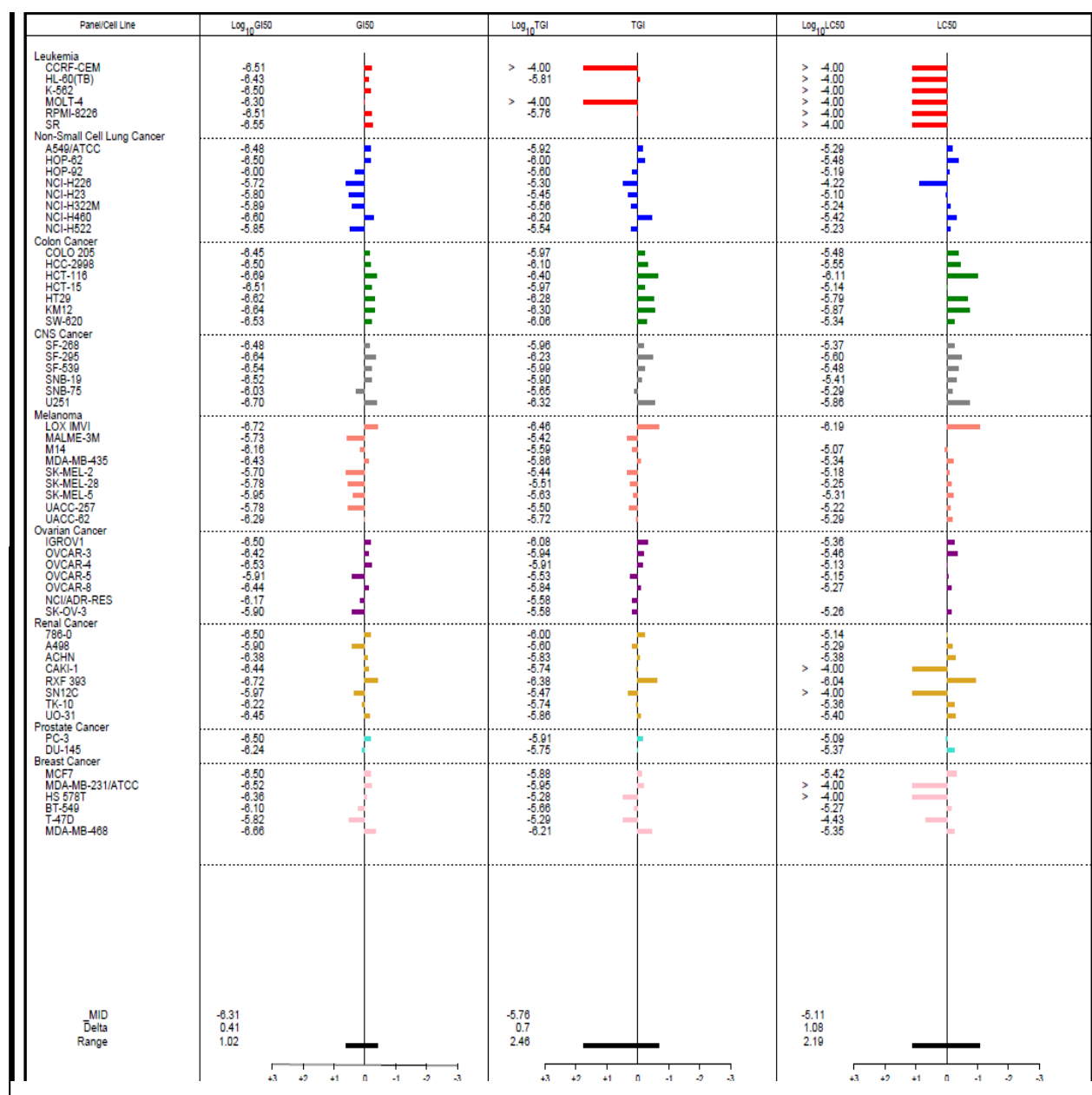


FIVE dose results (Compound 7d)

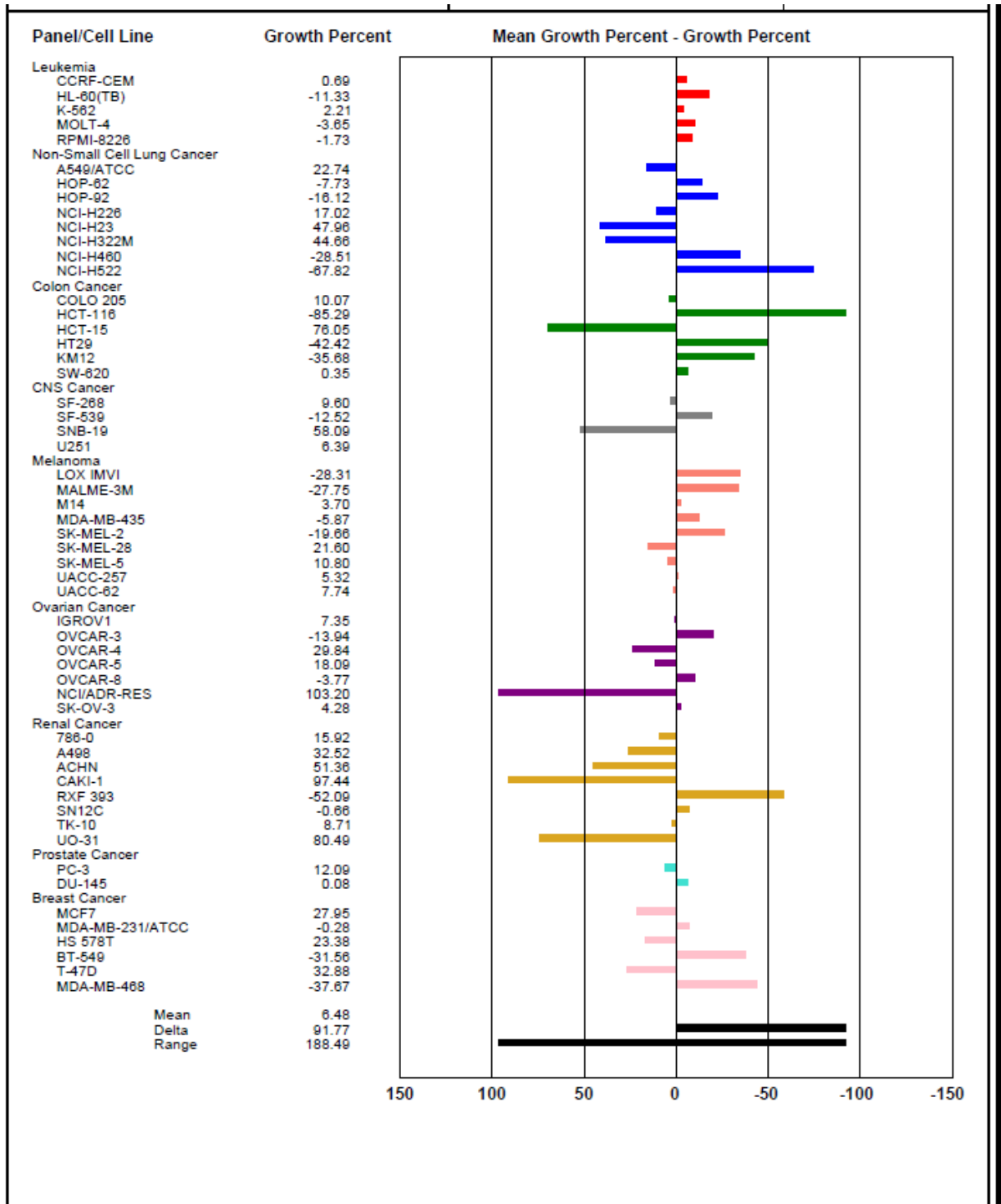
Panel/Cell Line	Time Zero	Ctrl	Log10 Concentration					Percent Growth					GI50	TGI	LC50	
			-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0				
Leukemia																
CCRF-CEM	0.413	2.341	2.248	2.188	0.531	0.493	0.571	95	92	6	4	8	3.09E-7	> 1.00E-4	> 1.00E-4	
HL-60(TB)	0.726	2.444	2.696	2.478	0.917	0.373	0.466	115	102	11	-49	-36	3.73E-7	1.53E-6	> 1.00E-4	
K-562	0.223	1.820	1.851	1.763	0.283	0.216	0.285	102	96	4	-3	4	3.17E-7	.	> 1.00E-4	
MOLT-4	0.825	2.811	2.935	3.029	1.295	0.844	0.978	106	111	24	1	8	4.99E-7	> 1.00E-4	> 1.00E-4	
RPMI-8226	0.766	2.758	2.745	2.638	0.837	0.681	0.750	99	94	4	-11	-2	3.06E-7	1.75E-6	> 1.00E-4	
SR	0.315	1.534	1.486	1.422	0.313	0.252	0.335	96	91	-1	-20	2	2.80E-7	.	> 1.00E-4	
Non-Small Cell Lung Cancer																
A549(ATCC)	0.517	2.255	2.194	2.199	0.628	0.141	0.098	97	97	6	-73	-81	3.29E-7	1.20E-6	5.15E-6	
HOP-62	0.438	1.179	1.161	1.176	0.440	0.016	-0.056	98	100	.	-96	-100	3.16E-7	1.01E-6	3.31E-6	
HOP-92	1.492	1.955	1.859	1.853	1.723	0.398	0.329	79	78	50	-73	-78	9.89E-7	2.54E-6	6.47E-6	
NCI-H226	0.689	1.319	1.308	1.244	1.218	0.443	0.316	98	88	84	-36	-54	1.92E-6	5.03E-6	5.96E-6	
NCI-H23	1.221	3.159	3.112	3.162	2.742	0.431	0.170	98	100	79	-65	-86	1.58E-6	3.53E-6	7.89E-6	
NCI-H322M	0.826	1.889	1.861	1.841	1.539	0.110	0.133	97	95	67	-87	-84	1.29E-6	2.73E-6	5.77E-6	
NCI-H460	0.303	2.684	2.736	2.686	0.225	0.098	0.073	102	100	-26	-68	-76	2.50E-7	6.24E-7	3.79E-6	
NCI-H522	1.093	2.476	2.473	2.530	2.117	0.138	0.097	100	104	74	-87	-91	1.41E-6	2.87E-6	5.86E-6	
Colon Cancer																
COLO 205	0.406	1.769	1.868	1.866	0.449	0.008	-0.050	107	107	3	-98	-100	3.54E-7	1.07E-6	3.35E-6	
HCC-2998	1.066	2.859	2.899	3.056	0.939	0.040	0.020	102	111	-12	-96	-98	3.13E-7	7.99E-7	2.83E-6	
HCT-116	0.234	2.145	2.267	2.217	0.073	0.022	0.062	106	104	-69	-91	-74	2.05E-7	3.99E-7	7.76E-7	
HCT-15	0.272	2.290	2.303	2.216	0.304	0.113	0.036	101	96	2	-58	-87	3.08E-7	1.06E-6	7.23E-6	
HT29	0.239	1.370	1.393	1.440	0.141	0.037	0.041	102	106	-41	-85	-83	2.41E-7	5.27E-7	1.61E-6	
KM12	0.471	2.414	2.466	2.491	0.261	0.074	0.042	103	104	-45	-84	-91	2.31E-7	5.00E-7	1.36E-6	
SW-620	0.321	2.199	2.195	2.208	0.299	0.089	0.085	100	100	-7	-72	-74	2.95E-7	8.63E-7	4.55E-6	
CNS Cancer																
SF-268	0.646	2.066	2.081	2.089	0.692	0.122	0.168	101	102	3	-81	-74	3.35E-7	1.09E-6	4.28E-6	
SF-295	0.932	2.638	2.728	2.721	0.666	0.164	0.125	94	94	-29	-82	-87	2.28E-7	5.84E-7	2.50E-6	
SF-539	0.922	2.558	2.519	2.428	0.933	0.026	-0.029	98	92	1	-97	-100	2.89E-7	1.02E-6	3.29E-6	
SNB-19	0.341	1.454	1.340	1.302	0.454	0.026	0.010	90	86	10	-93	-97	3.00E-7	1.26E-6	3.85E-6	
SNB-75	0.740	1.664	1.576	1.555	1.192	0.076	-0.030	90	88	49	-90	-100	9.36E-7	2.25E-6	5.17E-6	
U251	0.540	2.247	2.146	2.068	0.310	0.021	-0.021	94	90	-43	-96	-100	1.99E-7	4.75E-7	1.37E-6	
Melanoma																
LOX IMVI	0.507	2.689	2.616	2.715	0.078	0.011	0.041	97	101	-85	-98	-92	1.89E-7	3.50E-7	6.51E-7	
MALME-3M	0.498	0.807	0.828	0.800	0.784	0.165	0.327	107	98	92	-67	-34	1.85E-6	3.80E-6	.	
M14	0.381	1.691	1.696	1.726	0.903	0.165	0.170	100	103	40	-57	-56	6.89E-7	2.58E-6	8.50E-6	
MDA-MB-435	0.645	2.622	2.628	2.595	0.913	0.110	0.189	100	99	14	-83	-71	3.73E-7	1.38E-6	4.56E-6	
SK-MEL-2	1.130	2.256	2.408	2.372	2.358	0.160	0.086	113	110	109	-86	-92	2.01E-6	3.63E-6	6.55E-6	
SK-MEL-28	0.529	1.513	1.541	1.528	1.437	0.011	-0.044	103	102	92	-98	-100	1.67E-6	3.06E-6	5.59E-6	
SK-MEL-5	0.512	2.159	2.102	2.172	1.466	0.009	-0.009	97	101	58	-98	-100	1.12E-6	2.35E-6	4.91E-6	
UACC-257	0.859	1.817	1.735	1.732	1.704	0.094	0.047	91	91	88	-89	-95	1.64E-6	3.14E-6	6.02E-6	
UACC-62	0.738	2.929	2.880	2.753	1.457	0.121	0.053	98	92	33	-84	-93	5.12E-7	1.91E-6	5.14E-6	
Ovarian Cancer																
IGROV1	0.626	1.911	2.054	2.035	0.566	0.171	0.229	111	110	-10	-73	-63	3.16E-7	8.31E-7	4.36E-6	
OVCA-3	0.673	1.849	1.931	1.978	0.748	0.019	-0.027	107	111	6	-97	-100	3.83E-7	1.15E-6	3.50E-6	
OVCA-4	0.743	1.595	1.569	1.505	0.794	0.312	0.258	97	89	6	-58	-65	2.97E-7	1.24E-6	7.49E-6	
OVCA-5	0.703	1.670	1.615	1.558	1.295	0.217	0.066	94	88	61	-69	-91	1.22E-6	2.95E-6	7.12E-6	
OVCA-6	0.418	1.824	1.772	1.782	0.611	0.110	0.075	96	97	14	-74	-82	3.67E-7	1.43E-6	5.35E-6	
NCI/ADR-RES	0.709	2.358	2.420	2.491	1.334	0.344	0.499	104	108	38	-52	-30	6.73E-7	2.65E-6	.	
SK-OV-3	0.609	1.605	1.624	1.626	1.263	0.053	-0.051	102	102	66	-91	-100	1.26E-6	2.62E-6	5.45E-6	
Renal Cancer																
786-O	0.666	2.465	2.420	2.459	0.669	0.281	0.278	98	100	.	-58	-58	3.16E-7	1.01E-6	7.31E-6	
A498	1.472	2.372	2.210	2.225	2.074	0.019	-0.037	82	84	67	-99	-100	1.26E-6	2.53E-6	5.08E-6	
ACHN	0.359	1.759	1.808	1.769	0.618	0.027	0.042	104	101	19	-93	-88	4.14E-7	1.47E-6	4.13E-6	
CAKI-1	0.844	2.690	2.594	2.573	1.130	0.480	0.742	95	94	15	-43	-12	3.62E-7	1.84E-6	> 1.00E-4	
RXF 393	0.639	1.052	1.047	1.014	0.286	0.050	0.023	99	91	-55	-92	-96	1.90E-7	4.18E-7	9.20E-7	
SN12C	1.067	3.281	3.215	3.158	2.247	0.562	0.591	97	94	53	-47	-45	1.08E-6	3.38E-6	> 1.00E-4	
TK-10	0.758	1.500	1.530	1.534	1.016	0.025	-0.005	104	104	35	-97	-100	6.03E-7	1.84E-6	4.41E-6	
UO-31	0.836	2.276	2.096	2.155	1.061	0.058	0.027	87	92	16	-93	-97	3.52E-7	1.39E-6	4.01E-6	
Prostate Cancer																
PC-3	0.658	1.859	1.824	1.793	0.721	0.291	0.230	97	94	5	-56	-65	3.15E-7	1.22E-6	8.04E-6	
DU-145	0.565	1.957	1.993	2.056	1.015	0.013	0.002	103	107	32	-98	-100	5.80E-7	1.77E-6	4.30E-6	
Breast Cancer																
MCF7	0.433	2.421	2.250	2.181	0.681	0.020	-0.022	91	88	12	-95	-100	3.18E-7	1.31E-6	3.80E-6	
MDA-MB-231(ATCC)	0.640	1.567	1.570	1.518	0.657	0.410	0.374	100	95	2	-36	-42	3.03E-7	1.11E-6	> 1.00E-4	
HS 578T	0.925	1.895	1.835	1.830	1.174	0.834	0.828	94	93	26	-10	-11	4.36E-7	5.27E-6	> 1.00E-4	
BT-549	0.802	1.719	1.786	1.820	1.198	0.124	0.067	107	111	43	-85	-92	7.92E-7	2.18E-6	5.36E-6	
T-47D	0.716	2.004	1.957	1.963	1.587	0.517	0.239	96	97	68	-28	-67	1.53E-6	5.11E-6	3.73E-5	
MDA-MB-468	0.705	1.515	1.461	1.412	0.538	0.255	0.254	93	87	-24	-64	-64	2.17E-7	6.12E-7	4.51E-6	

FIVE dose results (Compound 7d)

Mean graph

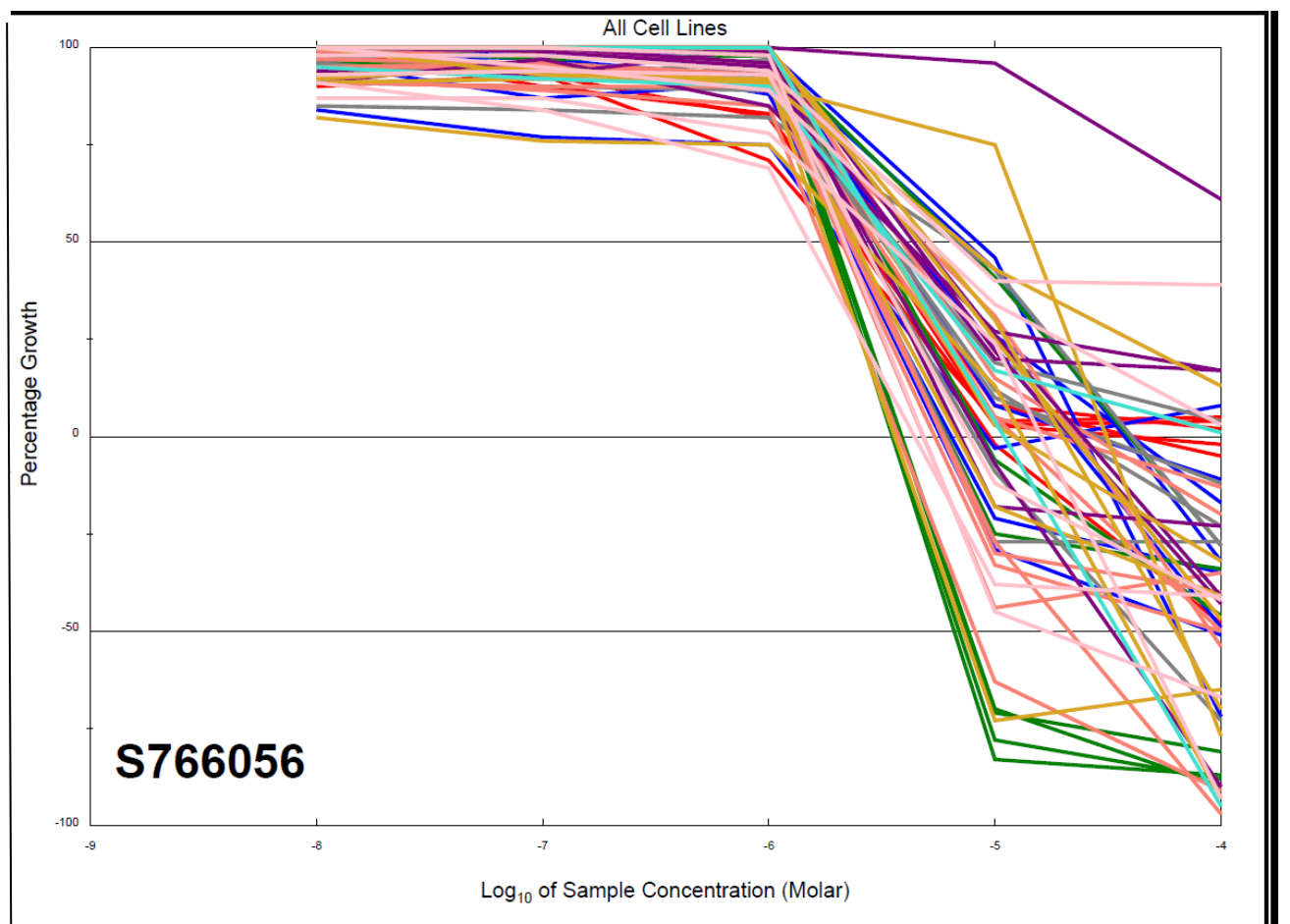


One dose Mean Graph (Compound 7f)



FIVE dose results (Compound 7f)

Dose response curves

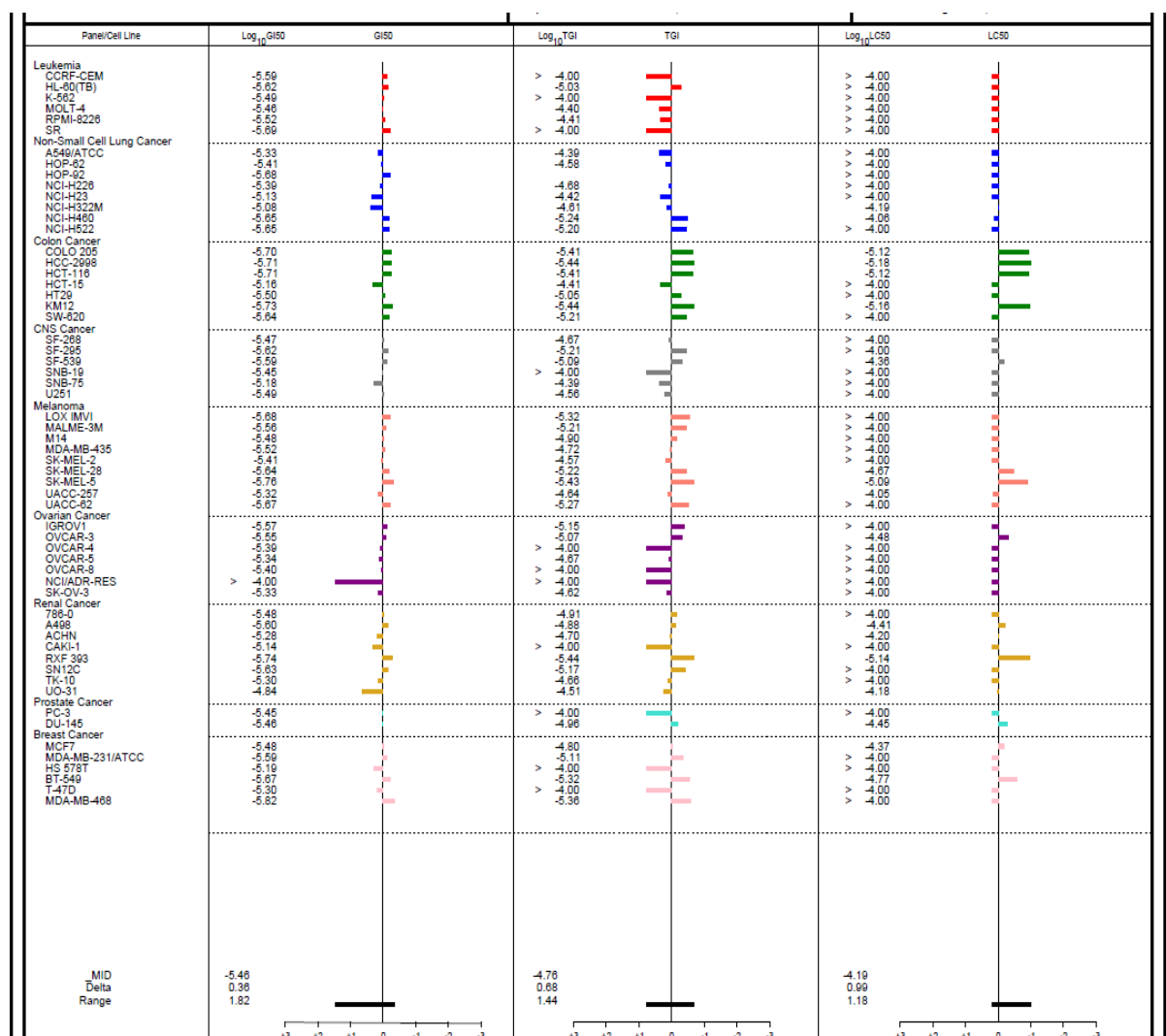


FIVE dose results (Compound 7f)

Panel/Cell Line	Time Zero	Ctrl	Log10 Concentration										GI50	TGI	LC50
			Mean Optical Densities					Percent Growth							
			-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0			
Leukemia															
CCRF-CEM	0.413	2.350	2.250	2.210	2.000	0.475	0.500	95	93	82	3	4	2.54E-6	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.726	2.327	2.415	2.170	2.050	0.709	0.378	106	90	83	-2	-48	2.42E-6	9.37E-6	> 1.00E-4
K-562	0.223	1.788	1.780	1.790	1.681	0.349	0.249	100	100	93	8	2	3.21E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.825	2.772	2.874	3.004	2.770	0.985	0.781	105	112	100	8	-5	3.50E-6	4.02E-5	> 1.00E-4
RPMI-8226	0.766	2.731	2.653	2.606	2.583	0.835	0.748	96	94	92	3	-2	3.00E-6	3.90E-5	> 1.00E-4
SR	0.315	1.567	1.438	1.478	1.200	0.365	0.373	90	93	71	4	5	2.04E-6	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549(ATCC)	0.517	2.270	2.245	2.228	2.258	0.977	0.429	99	98	99	26	-17	4.73E-6	4.04E-5	> 1.00E-4
HOP-62	0.438	1.146	1.147	1.157	1.221	0.495	0.390	100	102	111	8	-11	3.90E-6	2.62E-5	> 1.00E-4
HOP-92	1.492	1.806	1.757	1.735	1.727	1.451	1.516	84	77	75	-3	8	2.09E-6	.	> 1.00E-4
NCI-H226	0.689	1.234	1.212	1.163	1.188	0.815	0.353	96	87	91	23	-49	4.04E-6	2.10E-5	> 1.00E-4
NCI-H23	1.221	3.239	3.160	3.207	3.153	2.095	0.834	96	98	96	43	-32	7.45E-6	3.78E-5	> 1.00E-4
NCI-H322M	0.826	1.807	1.813	1.816	1.794	1.273	0.229	101	101	99	46	-72	8.25E-6	2.43E-5	6.46E-5
NCI-H460	0.303	2.720	2.707	2.642	2.528	0.215	0.148	99	97	92	-29	-51	2.22E-6	5.74E-6	8.72E-5
NCI-H522	1.093	2.500	2.439	2.474	2.337	0.859	0.707	96	98	88	-21	-35	2.24E-6	6.38E-6	> 1.00E-4
Colon Cancer															
COLO 205	0.406	1.833	1.952	1.913	1.851	0.122	0.039	108	106	101	-70	-90	1.99E-6	3.90E-6	7.65E-6
HCC-2998	1.066	2.994	2.997	3.034	3.085	0.183	0.135	100	102	105	-83	-87	1.96E-6	3.62E-6	6.68E-6
HCT-116	0.234	2.383	2.411	2.534	2.371	0.069	0.045	101	107	99	-71	-81	1.95E-6	3.85E-6	7.57E-6
HCT-15	0.272	2.225	2.249	2.171	2.192	1.065	0.195	101	97	98	41	-28	6.87E-6	3.87E-5	> 1.00E-4
HT29	0.239	1.384	1.413	1.457	1.441	0.225	0.128	102	106	105	-6	-46	3.13E-6	8.82E-6	> 1.00E-4
KM12	0.471	2.421	2.456	2.483	2.379	0.105	0.059	102	103	98	-78	-88	1.87E-6	3.61E-6	6.94E-6
SW-620	0.321	2.416	2.326	2.325	2.270	0.241	0.212	96	96	93	-25	-34	2.32E-6	6.15E-6	> 1.00E-4
CNS Cancer															
SF-268	0.646	1.951	1.917	1.999	1.854	0.798	0.495	97	104	93	12	-23	3.36E-6	2.15E-5	> 1.00E-4
SF-295	0.932	2.877	2.709	2.724	2.826	0.684	0.682	91	92	97	-27	-27	2.41E-6	6.10E-6	> 1.00E-4
SF-539	0.922	2.381	2.282	2.298	2.252	0.840	0.246	93	94	91	-9	-73	2.58E-6	8.14E-6	4.34E-5
SNB-19	0.341	1.455	1.355	1.345	1.328	0.554	0.380	91	90	89	19	4	3.59E-6	> 1.00E-4	> 1.00E-4
SNB-75	0.740	1.609	1.480	1.470	1.452	1.115	0.535	85	84	82	43	-28	6.67E-6	4.07E-5	> 1.00E-4
U251	0.540	2.254	2.188	2.116	2.100	0.709	0.473	96	92	91	10	-12	3.20E-6	2.77E-5	> 1.00E-4
Melanoma															
LOX IMVI	0.507	2.778	2.730	2.832	2.661	0.284	0.329	98	102	95	-44	-35	2.10E-6	4.82E-6	> 1.00E-4
MALME-3M	0.498	0.782	0.800	0.779	0.821	0.349	0.297	106	99	114	-30	-40	2.78E-6	6.19E-6	> 1.00E-4
M14	0.381	1.784	1.771	1.812	1.773	0.457	0.192	99	102	99	5	-50	3.35E-6	1.25E-5	> 1.00E-4
MDA-MB-435	0.645	2.675	2.621	2.603	2.502	0.745	0.564	97	96	91	5	-13	3.01E-6	1.91E-5	> 1.00E-4
SK-MEL-2	1.130	2.297	2.431	2.397	2.297	1.307	0.899	112	109	100	15	-20	3.88E-6	2.66E-5	> 1.00E-4
SK-MEL-28	0.529	1.501	1.453	1.465	1.435	0.387	0.014	95	96	93	-27	-97	2.29E-6	5.97E-6	2.12E-5
SK-MEL-5	0.512	2.102	1.980	1.922	1.865	0.189	0.045	92	89	85	-63	-91	1.72E-6	3.75E-6	8.15E-6
UACC-257	0.859	1.852	1.765	1.751	1.757	1.168	0.391	91	90	90	31	-54	4.80E-6	2.31E-5	8.86E-5
UACC-62	0.738	2.891	2.792	2.790	2.700	0.492	0.369	95	95	91	-33	-50	2.14E-6	5.39E-6	> 1.00E-4
Ovarian Cancer															
IGROV1	0.626	1.861	1.996	1.989	1.867	0.516	0.484	111	110	100	-18	-23	2.68E-6	7.09E-6	> 1.00E-4
OVCAR-3	0.673	1.803	1.885	1.860	1.757	0.627	0.067	107	105	96	-7	-90	2.80E-6	8.57E-6	3.30E-5
OVCAR-4	0.743	1.539	1.467	1.513	1.421	0.962	0.882	91	97	85	27	17	4.07E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.703	1.579	1.526	1.519	1.620	0.892	0.400	94	93	105	22	-43	4.55E-6	2.15E-5	> 1.00E-4
OVCAR-8	0.418	1.799	1.826	1.783	1.725	0.689	0.649	102	99	95	20	17	3.94E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.709	2.493	2.572	2.602	2.582	2.416	1.796	104	106	105	96	61	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-OV-3	0.609	1.556	1.605	1.589	1.549	0.851	0.358	105	103	99	26	-41	4.66E-6	2.41E-5	> 1.00E-4
Renal Cancer															
786-O	0.666	2.478	2.478	2.523	2.506	0.725	0.455	100	102	102	3	-32	3.35E-6	1.24E-5	> 1.00E-4
A498	1.472	2.436	2.267	2.201	2.197	1.594	0.103	82	76	75	13	-93	2.53E-6	1.32E-5	3.92E-5
ACHN	0.359	1.663	1.716	1.662	1.676	0.753	0.106	104	100	101	30	-70	5.25E-6	1.59E-5	6.26E-5
CAKI-1	0.844	2.773	2.607	2.614	2.608	1.677	1.101	91	92	91	43	13	7.22E-6	> 1.00E-4	> 1.00E-4
RFX 393	0.639	1.064	1.076	1.036	1.032	0.173	0.221	103	93	92	-73	-65	1.81E-6	3.62E-6	7.27E-6
SN12C	1.057	3.265	3.104	3.139	3.062	0.871	0.629	93	94	91	-18	-41	2.36E-6	6.79E-6	> 1.00E-4
TK-10	0.758	1.537	1.565	1.563	1.598	0.950	0.398	104	103	108	25	-47	4.96E-6	2.20E-5	> 1.00E-4
UO-31	0.836	2.303	2.186	2.237	2.151	1.932	0.191	92	95	90	75	-77	1.45E-6	3.10E-5	6.62E-5
Prostate Cancer															
PC-3	0.658	1.766	1.709	1.678	1.659	0.850	0.673	95	92	90	17	1	3.57E-6	> 1.00E-4	> 1.00E-4
DU-145	0.565	1.849	1.937	1.964	1.901	0.620	0.031	107	109	104	4	-95	3.48E-6	1.10E-5	3.54E-5
Breast Cancer															
MCF7	0.433	2.445	2.185	2.176	2.007	0.911	0.032	87	87	78	24	-93	3.30E-6	1.60E-5	4.30E-5
MDA-MB-231/ATCC	0.640	1.482	1.422	1.428	1.420	0.563	0.369	93	94	93	-12	-42	2.55E-6	7.67E-6	> 1.00E-4
HS 578T	0.925	1.930	1.914	1.912	1.870	1.326	1.322	98	98	94	40	39	6.49E-6	> 1.00E-4	> 1.00E-4
BT-549	0.802	1.718	1.761	1.823	1.697	0.442	0.262	105	112	98	-45	-67	2.16E-6	4.84E-6	1.68E-5
T-47D	0.716	1.960	1.964	1.902	1.818	1.136	0.757	100	95	89	34	3	5.05E-6	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.705	1.490	1.419	1.363	1.248	0.436	0.414	91	84	69	-38	-41	1.51E-6	4.41E-6	> 1.00E-4

FIVE dose results (Compound 7f)

Mean graph



¹H and ¹³C NMR spectra of representative compounds

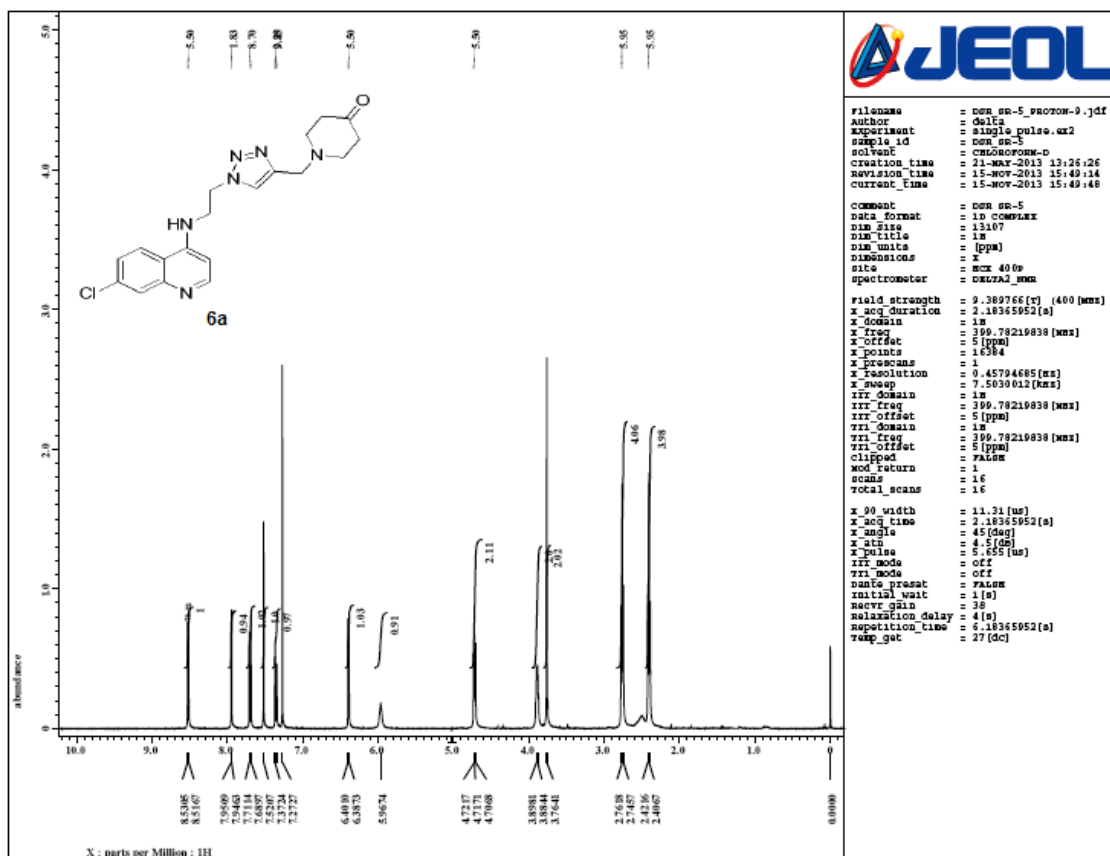


Fig. 1: ¹H NMR of compound 6a

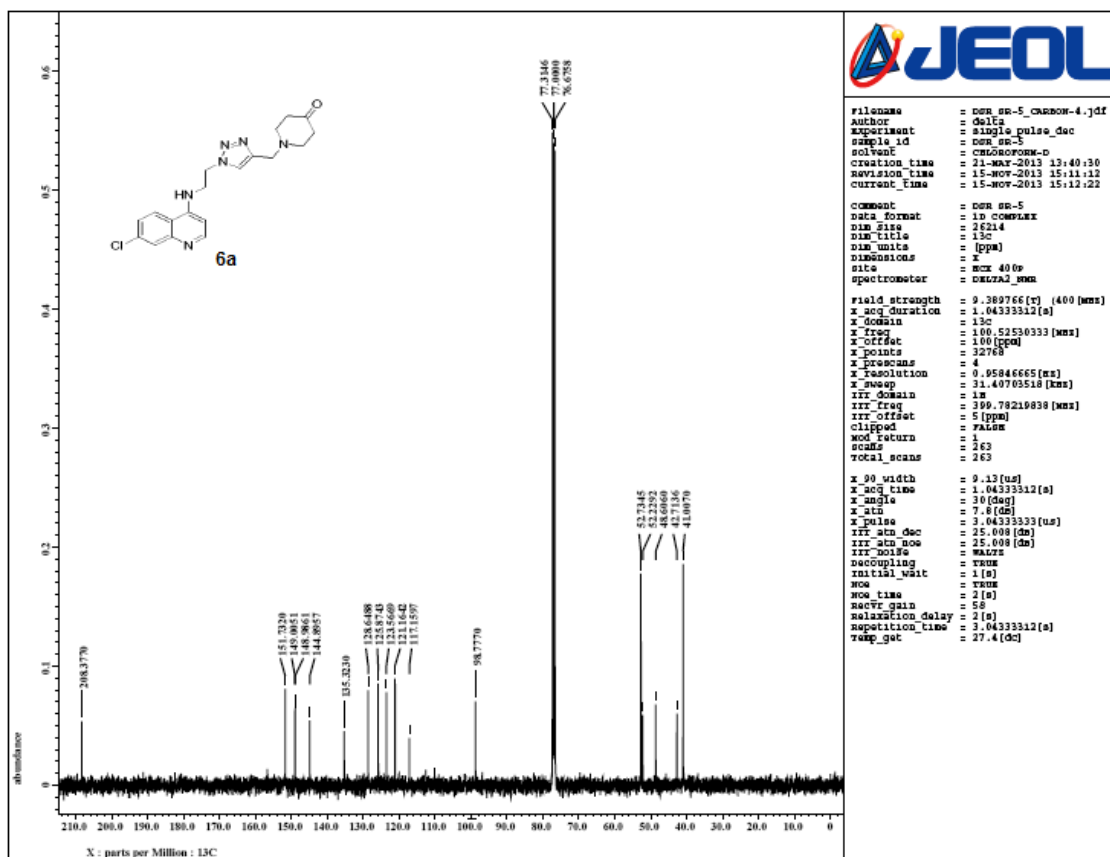


Fig. 2: ¹³C NMR of compound 6a

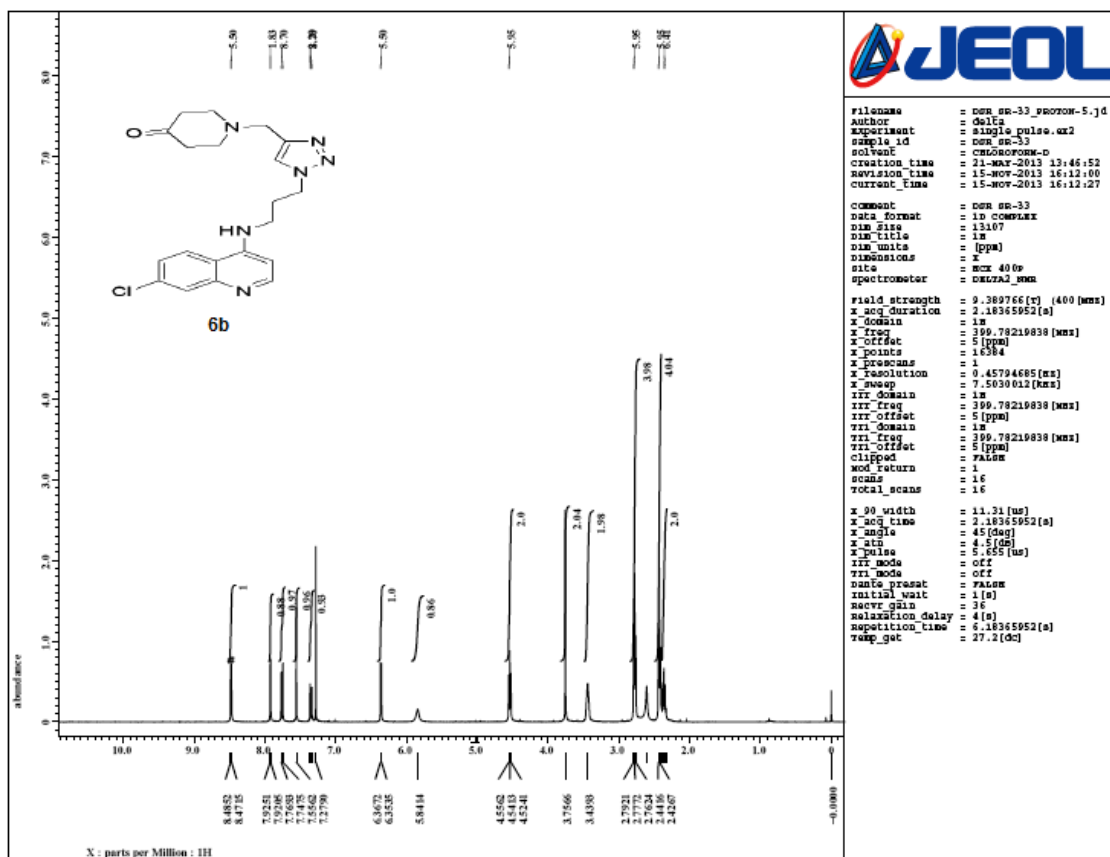


Fig. 3: ^1H NMR of compound 6b

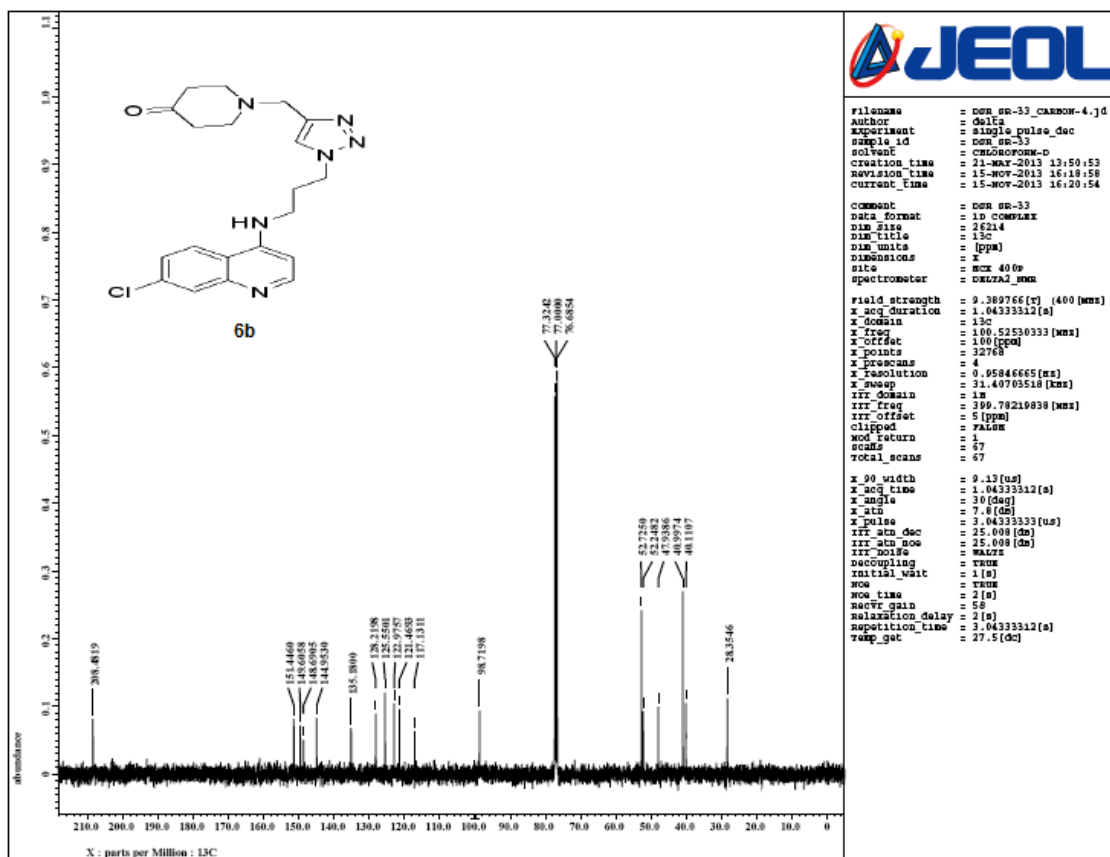


Fig. 4: ¹³C NMR of compound 6b

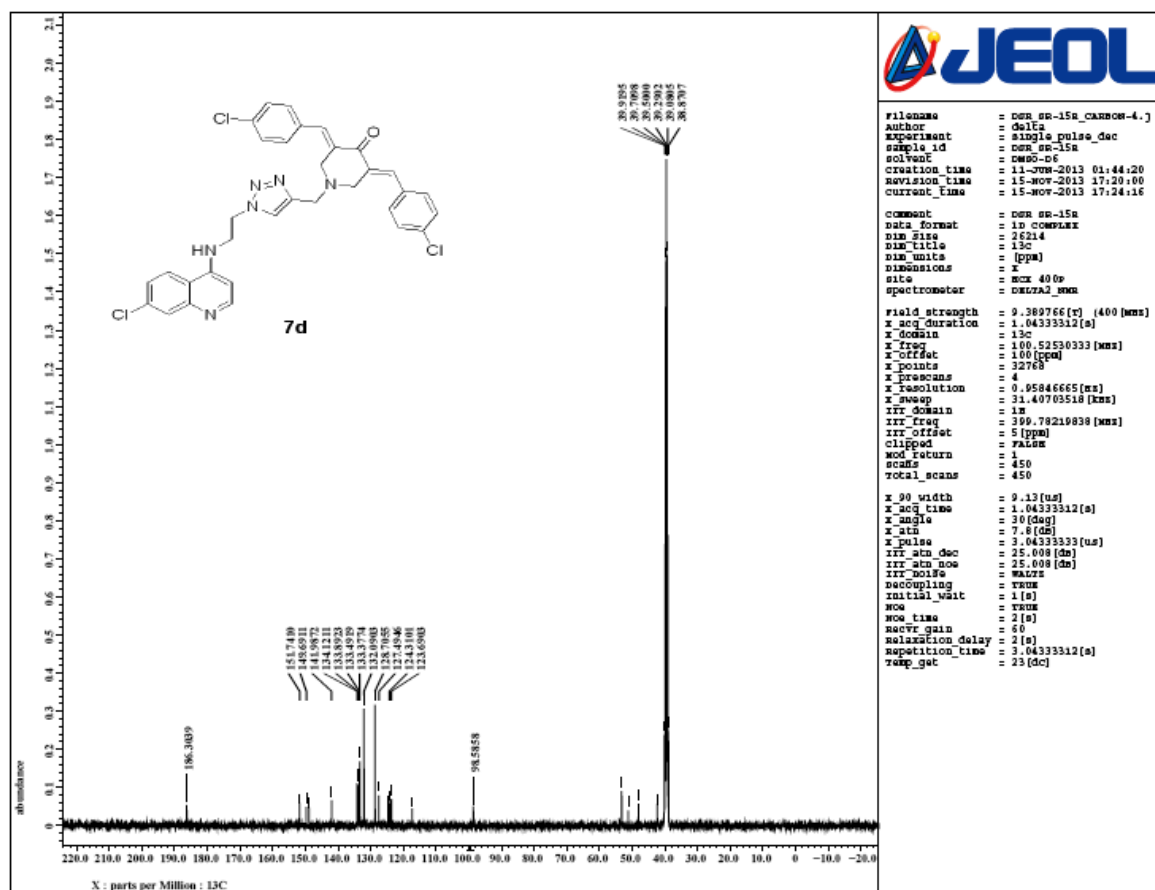


Fig. 6: ¹³C NMR of compound 7d

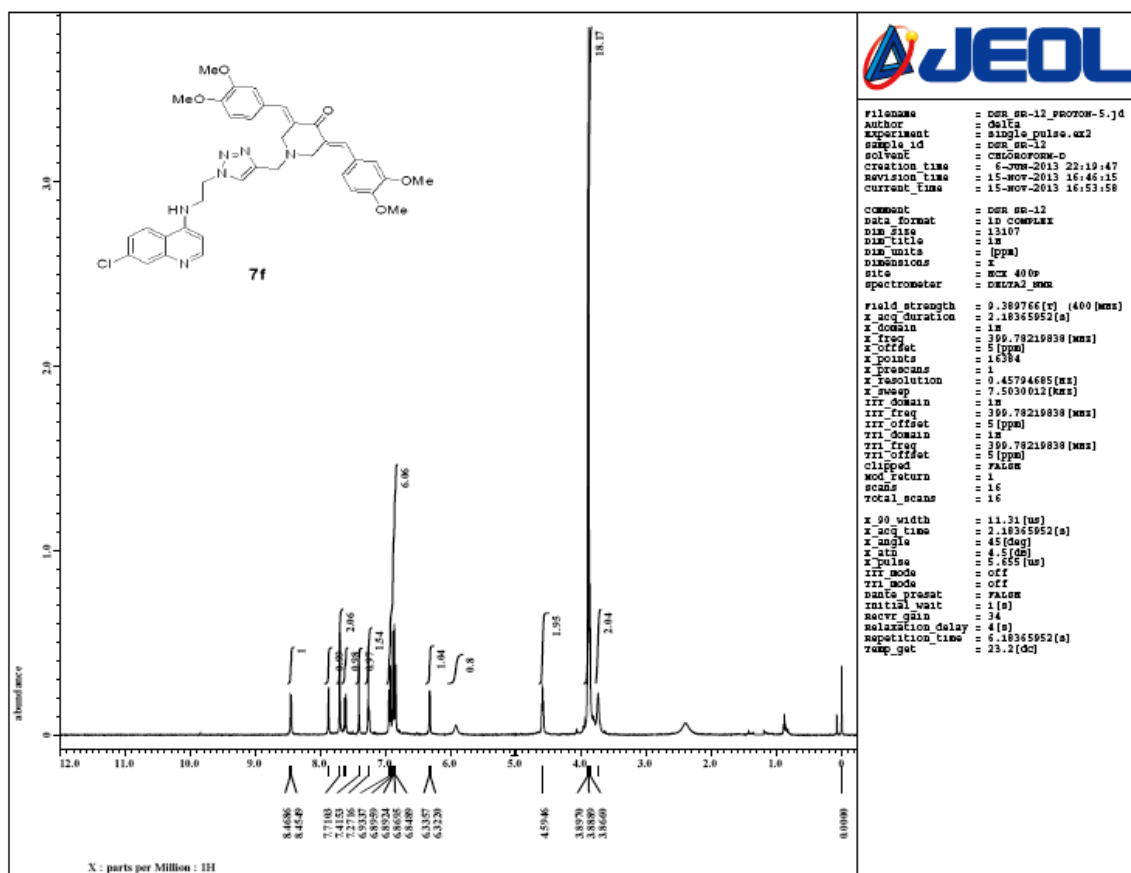


Fig. 7: ^1H NMR of compound 7f

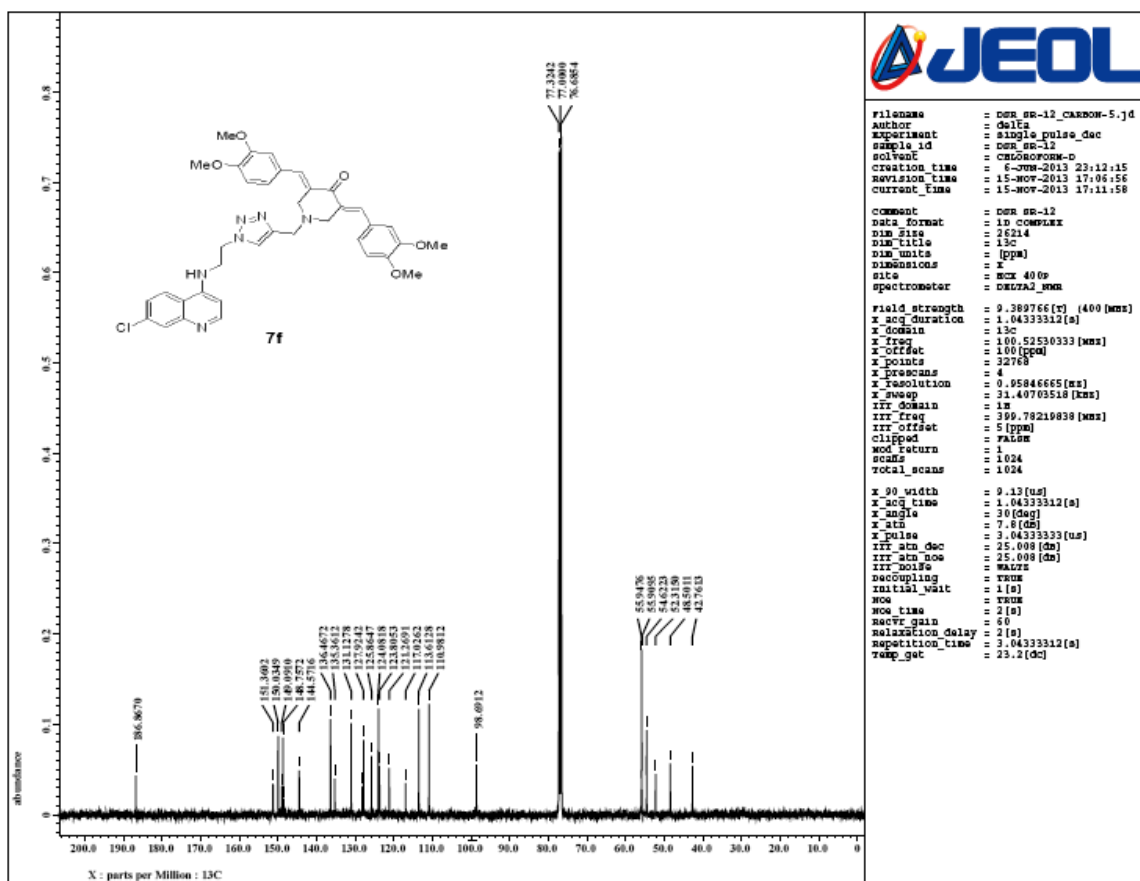


Fig. 8: ¹³C NMR of compound 7f