Supporting information

Imidazolium derived ionic salts induce inhibition of cancerous cell growth through apoptosis

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NCI-60 Human Tumor Cell Line Screen: Details of the methodology are described at http://dtp.nci.nih.gov/branches/btb/ivclsp.html. Briefly, the panel is organized into nine subpanels representing diverse histologies: leukemia, melanoma, and cancers of lung, colon, kidney, ovary, breast, prostate, and central nervous system. The cells are grown in supplemented RPM1 1640 medium for 24 h. The test compounds were dissolved in DMSO and incubated with cells at five concentrations with 10-fold dilutions, the highest being 10^{-4} M and the others being 10^{-5} , 10^{-6} , 10^{-7} , and 10^{-8} M. The assay is terminated by addition of cold trichloroacetic acid, and the cells are fixed and stained with sulforhodamine B. Bound stain is solubilized, and the absorbance is read on an automated plate reader. Percentage growth inhibition (GI₅₀) is calculated from time zero, control growth, and the five concentration level absorbance. The inhibitory concentrations (LC₅₀) represent the average of two independent experiments.

Interpretation of One-Dose Data: The One-dose data of all the compounds is reported as a mean graph of the percent growth of treated cells and will be similar in appearance to

mean graphs from the 5-dose assay. The number reported for the One-dose assay is growth relative to the no-drug control, and relative to the time zero number of cells. This allows detection of both growth inhibition (values between 0 and 100) and lethality (values less than 0). For example, a value of 100 means no growth inhibition. A value of 40 would mean 60% growth inhibition. A value of 0 means no net growth over the course of the experiment. A value of -40 would mean 40% lethality. A value of -100 means all cells are dead. The one-dose data of all the four compounds is given in Figure 1-4, respectively.

The drug response curves from the five-dose data of these four compounds are given in Figure 5-8 respectively for all NCI-60 tumor cell lines.

Panel/Cell Line	Growth Percent	Mean	Growth Pe	rcent - Gro	wth Percent	t	
Non-Small Cell Lung Cancer							
A549/ATCC	32.62			_			
HOP-62	38.17						
HOP-92 NCI-H226	51.88						
NCI-H226 NCI-H23	30.42 28.79			L			
NCI-H23 NCI-H322M	57.06						
NCI-H460	23.64						
NCI-H522	-19.92						
Colon Cancer	-10.02						
COLO 205	8.80				•		
HCC-2998	31.07						
HCT-116	17.62						
HCT-15	82.04						
HT29	12.35						
KM12	14.03						
SW-620	44.11						
Breast Cancer							
HS 578T	30.28			•			
MCF7	3.94						
MDA-MB-231/ATCC	41.54				_		
MDA-MB-435	7.98				• <u> </u>		
MDA-MB-468	-42.10					•	
NCI/ADR-RES	82.17						
T-47D	24.65						
Ovarian Cancer	45.00						
OVCAR-3	45.92						
OVCAR-4 OVCAR-5	22.69						
OVCAR-5 OVCAR-8	45.62 11.53						
SK-OV-3	44.54						
Leukemia	44.04						
CCRF-CEM	110.51						
HL-60(TB)	51.90						
K-562	64.21						
MOLT-4	78.62						
RPMI-8226	116.34						
SR	103.60						
Renal Cancer	100.00						
786-0	47.82						
A498	12.45						
ACHN	45.02						
CAKI-1	28.77						
RXF 393	-20.81						
SN12C	19.36						
TK-10	-1.53						
UO-31	65.71						
Melanoma							
LOX IMVI	23.94						
M14	24.55						
MALME-3M	8.94				•		
SK-MEL-2	13.06						
SK-MEL-28	34.86			-			
SK-MEL-5	-33.13						
UACC-257	-12.38						
UACC-62 Prostate Cancer	31.07			ľ			
DU-145	75.39						
PC-3	6.60						
CNS Cancer	0.00				-		
SF-268	58.74		•				
SF-200	9.99		·				
SF-539	30.45						
SNB-19	45.54						
SNB-75	-10.60						
U251	21.74						
Mean	31.97						
Delta	74.07					•	
Range	158.44					•	
	150	100	50	0	-50	-100	-150

Figure 1: One dose mean graph for NSC747267 at $10\mu M$

Non-Small Cell Lung Cancer ASB/ATC2 HOP-R2	Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Percent
H0P-82 H0	Non-Small Cell Lung Cancer		
HOP-922 80.23 NCH-1322 40.54 NCH-1322 40.54 NCH-1422 87.38 Color Cancer 46.59 Color Cancer 87.54 Color Cancer 87.53 HC7-175 9.85 HC7-175 9.87 MAAM-84-88 -77.993 MOA-M8-231/ATCC -9.387 MAAM-84-88 -75.913 OVCAR-4 -24.763 OVCAR-5 -67.51 OVCAR-5 -77.913 H-60717 -83.57 H-707 -94.61 MOT-142 11.17 RK7 393 -60.19 SK-0V-3 -63.51 Lauren -64.71 SK-0V-3 -63.51 UACR-4 -77.31			
NCH-1226 -00.54 NCH-220 -51.99 NCH-1460 -87.94 NCH-1420 -87.94 NCH-1420 -87.93 NCH-1420 -87.93 HCT-15 -9.85 HCT-16 -7.9.92 MDA-MB-251ATCC -9.87 MDA-MB-25 -7.71 MOVAR-5 -7.71 MOVAR-5 -7.71 MOVAR-5 -7.71 Update Cancer -7.13 IGROVI -7.13 Update Cancer -7.14 Update Cancer -7.13 Update Cancer -7.14 Update Cancer -7.14 Update Cancer </td <td></td> <td></td> <td></td>			
NCI-H232			
NCI-H460 -47.94 NCI-H460 -47.93 Color Cancer -45.99 HCC-2958 -44.43 HCT-116 -97.23 Breast Cancer -66.7 Br-549 -65.21 HCC-2000 -77.33 MDA-MB-231/ATCC -98.67 MDA-MB-231/ATCC -98.67 MDA-MB-235 -77.33 MDA-MB-236 -77.37 OVCAR-3 -24.76 OVCAR-4 -44.68 OVCAR-5 -57.71 Sk-602 -57.71 Sk-602 -57.71 Sk-603 -77.73 Sk-604 -46.63 Ad98 -65.31 ACHN -06.02 Cold Cancer -96.64 Ad98 -63.31 ACHN -06.02 Sk-612 -46.47			
MOLH622 -47.38 Colon Cancer -49.43 HCT-116 -49.43 HCT-116 -9.85 HCT-116 -9.85 HT28 -100.00 KM22 -83.88 Prost Cancer -66.67 Brost Cancer -66.67 Brost Cancer -79.92 MDA-MB-2311/ATCC -63.97 MDA-MB-2311/ATCC -03.97 OvCAR-3 -77.99 MDA-MB-468 -78.99 NCLADA-RES -71.3 OvCAR-3 -92.78 OvCAR-4 -64.83 OVCAR-3 -33.77 WCOVAR-3 -33.77 VOCAR-4 -64.83 OVCAR-3 -65.37 MOL 4.2226 -73.57 MCLADA-RES -73.70 SR -94.61 TK-10 -80.37 MALME-3M -73.70 SN-12C -94.61 TK-10 -80.53 MALME-3M -73.70 SN-12C -94.63 OVCAR-3 -95.85 Mean -73.70 SN-12C -94.61 TK-10 -80.53 MALME-3M -73.70 SN-22S -94.63			
Colon Cancer CCUC 2058 4-459 HC 20			
COLO 205 - 45 99 HCC 2988 + 94 43 HCC 116 - 723 HT23 5 - 100.00 KM12 - 43.88 SW-620 - 66 67 Breat Cancer - 65 21 HS 5787 - 46 40 M67 - 79.92 M0A-MB-231/ATCC - 93.87 M0A-MB-231/ATCC - 94.83 OVCAR-4 - 45.83 OVCAR-5 - 67.51 OVCAR-5 - 67.51 OVCAR-6 - 50.44 ACMM - 0.60 CNC 20 CAR-6 - 50.44 ACMM - 0.60 CNS Cancer - 90.90 SN12C - 94.58 SN-75 UC-37 - 61.13 UC-37 M64.1 - 77.37 M64.1 - 77.37 M64.1 - 77.37 M64.1 - 77.37 M64.1 - 77.37 M64.2 - 94.59 SN12C - 94.58 SN-225 - 94.58 SN-225 - 94.58 SN-225 - 94.58 SN-225 - 94.58 SN-225 - 94.58 SN-225 - 94.58 SN-25 - 94.58 SN-2		-07.30	
HCC-2996 -94.43 HCT-116 -923 HCT-116 -923 HCT-116 -923 HCT-116 -923 HCT-116 -923 HCT-116 -9338 SW-620 -66.67 Brast Cancer BT-549 -65.21 HCT-117 -992 MDA-MB-231/ATCC -93.87 MDA-MB-468 -76.99 MDA-MB-468 -76.99 MDA-MB-465 -76.99 MDA-MB-465 -76.99 MDA-MB-465 -76.99 MCJADA-RES 37.13 OVCAR-3 -24.76 OVCAR-4 -64.83 OVCAR-4 -64.83 OVCAR-5 -63.97 HL-40/TB) -45.73 SK-CV-3 -33.78 Leukemia		-45.99	
HT-15 9.85 HT28 -100.00 KH12 -83.88 SW122 -83.88 W122 -83.88 W122 -83.88 W122 -83.88 W122 -10000 HS 578T 448.40 MC7 -79.92 MOAMB-231/ATCC -93.87 MOAMB-231/ATCC -94.61 TK-10 -80.37 UC-31 -94.63 MALME-3M -77.38 MALME-3M -77.38 MALME-3M -77.38 MALME-3M -77.38 MALME-3M -77.38 MALME-3M -77.38 MALME-3M -77.38 MALME-3M -75.88 SMB-19 -75.88 SMB-1	HCC-2998	-94.43	
H129 H129 H129 H5 540 H5 557 H5 540 H5 5781 H5 579 H5 578 H5 579 H5 57			
KM12 83.88 SW-820 -66.67 Breast Cancor - BT 549 -64.40 M5 547 -79.92 MDA-MB-331/ATCC -79.92 MDA-MB-335 -55.77 MDA-MB-368 -78.99 NC/ADR-RES 37.13 OvcaR-4 -54.83 OVCAR-3 -4.76 OVCAR-4 -54.83 OVCAR-3 -57.51 OVCAR-3 -57.51 OVCAR-4 -54.83 OVCAR-5 -57.76 MDA-MB-468 -77.92 MDA-MB-468 -57.51 OVCAR-4 -54.83 OVCAR-5 -57.71 SK KOV3 -53.78 Leukemia -53.78 Leukemia -57.31 RAF 393 -66.19 SK K2C -72.68 MDH-1-26 15.177 RAF 393 -66.19 SK MEL-2 -64.47 SK MEL-2 -64.47 SK MEL-2 -64.47 SK MEL-28 -86.22 SK MEL-28 -96.20 MALME-344 -73.88 SK MEL-28 -96.99 SK MEL-28 -96.99 SK MEL-28 -96.99 </td <td></td> <td></td> <td></td>			
SW-620 -66.67 BTesat Cancer -65.21 H3 5781 -40.2 MD7 -231/ATCC MDA-MB-435 -76.99 NGLADR-RES 37.13 T-470 -0.13 Ovarian Cancer -77.13 OVCAR-3 -24.76 OVCAR-5 -67.51 OVCAR-8 -55.371 SK-602 72.56 MOLT-4 17.19 RPM-B2226 15.77 SR 75.11 SK-602 72.66 MOLT-4 17.19 RCH -90.44 ACHN -0.60 CAKI-1 -83.54 ACHN -0.60 CAKI-1 -83.54 MAMB-33 -66.19 SK-102 -94.61 TK-10 -80.37 MALME-34 -90.43 ACHN -0.60 CAKI-1 -83.54 MALME-34 -94.81 Prostate Cancer -90.43 TK-10 -80.37 MALME-34 -94.81 MALME-34 -94.81 MALME-34 -94.81 MALME-34 -94.81 MALME-34 -94.81 Moldrore			
BT-549 - 65.21 HS 5771 - 79.92 MDA-MB-231/ATCC - 79.92 MDA-MB-235 MDA-MB-2			
H 5 578T - 48.40 MCF7 - 79.92 MDA-MB-231/ATCC - 93.87 MDA-MB-435 - 76.93 MDA-MB-435 - 76.93 MDA-MB-435 - 76.93 MDA-MB-435 - 76.93 MDA-MB-435 - 76.93 OVAR-8 - 67.13 OVAR-8 - 67.51 OVCAR-3 - 24.76 OVCAR-3 - 24.76 OVCAR-3 - 24.76 OVCAR-3 - 24.76 OVCAR-3 - 24.76 OVCAR-3 - 24.76 OVCAR-4 - 54.83 OVCAR-3 - 33.78 Leukemia - 33.57 H-60(TB) - 45.73 K-562 - 72.56 MOLT-4 - 17.19 SK OV3 - 33.57 H-60(TB) - 45.73 K-562 - 72.56 MOLT-4 - 17.19 SK OV3 - 33.57 H-60(TB) - 45.73 K-562 - 72.56 MOLT-4 - 17.19 SK OV3 - 35.57 H-60(TB) - 45.73 K-562 - 72.56 MOLT-4 - 17.19 SK OV3 - 35.57 H-60(TB) - 45.51 ACHN - 0.60 CAKI-1 - 35.54 ACHN - 0.60 CAKI-1 - 45.54 ACHN - 0.60 CAKI-1 - 45.54 MOLT-4 - 77.38 MALME-28 - 46.22 SK MEL-5 - 96.20 UACC-257 - 61.13 UACC-62 - 94.58 Prostate Cancer DL-145 - 100.00 DL-145 - 100.00 DL-145 - 700.00 SF-295 - 39.458 SF-395 - 39.48 SF-395 - 39.48 SF-395 - 39.48 SF-539 - 39.48			
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RXF 393 -66.19 SN12C -94.61 TK-10 -80.37 UO-31 -85.85 Melanoma - LOX IMVI -50.37 M14 -77.30 MALME-3M -77.70 SK-MEL-2 -64.47 SK-MEL-28 -86.22 SK-MEL-5 -95.20 UACC-257 -61.13 UACC-62 -94.58 Prostate Cancer - DU-145 -100.00 PC-3 -69.69 CNS Cancer - SF-268 -22.98 SF-259 -39.48 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56			
TK-10 -80.37 UO-31 -85.85 Melanoma - LOX IMVI -50.37 M14 -77.38 MALME-3M -73.70 SK-MEL-2 -64.47 SK-MEL-28 -86.22 SK-MEL-5 -95.20 UACC-62 -94.58 Prostate Cancer - DU-145 -100.00 PC-3 -69.69 CNS Cancer - SF-295 -39.48 SF-295 -39.48 SF-295 -39.48 SF-295 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56			
UO-31 -85.85 Melanoma LOX IMVI -50.37 M14 -77.38 MALME-3M -73.70 SK-MEL-2 -64.47 SK-MEL-2 -64.47 SK-MEL-28 -86.22 SK-MEL-28 -86.22 SK-MEL-28 -86.22 UACC-257 -61.13 UACC-62 -94.58 Prostate Cancer DU-145 -100.00 PC-3 -69.69 CNS Cancer SF-268 -22.98 SF-295 -39.48 SF-539 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56			
Melanoma -50.37 M14 -77.38 MALME-3M -73.70 SK-MEL-2 -64.47 SK-MEL-28 -86.22 SK-MEL-5 -95.20 UACC-257 -61.13 UACC-62 -94.58 Prostate Cancer			
LOX IMVI -50.37 M14 -77.38 MALME-3M -77.70 SK-MEL-2 -64.47 SK-MEL-2 -64.47 SK-MEL-28 -86.22 UACC-257 -61.13 UACC-257 -61.13 UACC-62 -95.20 UACC-62 -94.58 Prostate Cancer DU-145 -100.00 PC-3 -69.69 CNS Cancer SF-268 -22.98 SF-295 -39.48 SF-539 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56		-05.05	
M14 -77.38 MALME-3M -77.370 SK-MEL-2 -64.47 SK-MEL-28 -86.22 SK-MEL-5 -95.20 UACC-62 -94.58 Prostate Cancer DU-145 -100.00 PC-3 -69.69 CNS Cancer SF-268 -22.98 SF-295 -39.48 SF-295 -39.48 SF-295 -98.62 U251 -69.96 Mean -54.13 Detta 45.87 Range 172.56		-50.37	
SK-MEL-2 -64.47 SK-MEL-28 -86.22 SK-MEL-5 -95.20 UACC-257 -61.13 UACC-62 -94.58 Prostate Cancer - DU-145 -100.00 PC-3 -69.69 CNS Cancer - SF-268 -22.98 SF-278 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56	M14	-77.38	
SK-MEL-28 -86.22 SK-MEL-5 -95.20 UACC-257 -61.13 UACC-62 -94.58 Prostate Cancer -100.00 PC-3 -69.69 CNS Cancer -22.98 SF-268 -22.98 SF-268 -39.48 SF-268 -25.93 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96			
SK-MEL-5 -95.20 UACC-257 -61.13 UACC-62 -94.58 Prostate Cancer - DU-145 -100.00 PC-3 -69.69 CNS Cancer - SF-268 -22.98 SF-275 -39.48 SF-295 -39.48 SF-539 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Detta 45.87 Range 172.56			
UACC-257 - 61.13 UACC-257 - 94.58 Prostate Cancer DU-145 - 100.00 PC-3 - 69.69 CNS Cancer SF-268 - 22.98 SF-295 - 394.8 SF-539 - 98.59 SNB-19 - 75.88 SNB-75 - 98.62 U251 - 69.96 Mean -54.13 Delta 45.87 Range 172.56			
Prostate Cancer DU-145 - 100.00 PC-3 -69.69 CNS Cancer SF-268 -22.98 SF-295 - 39.48 SF-539 - 98.59 SNB-19 -75.88 SNB-75 - 98.62 U251 - 69.96 Mean -54.13 Delta 45.87 Range 172.56	UACC-257	-61.13	
DU-145 -100.00 PC-3 -69.69 CNS Cancer SF-268 -22.98 SF-295 -39.48 SF-539 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56		-94.58	
PC-3 -69.69 CNS Cancer SF-268 -22.98 SF-295 -39.48 SF-539 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56		-100.00	
CNS Cancer SF-268 -22.98 SF-295 -39.48 SF-539 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56			
SF-268 -22.98 SF-295 -39.48 SF-539 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56	CNS Cancer		
SF-539 -98.59 SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56	SF-268		
SNB-19 -75.88 SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56	SF-295	-39.48	
SNB-75 -98.62 U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56		-98.59	
U251 -69.96 Mean -54.13 Delta 45.87 Range 172.56	SNB-75	-98.62	
Delta 45.87 Range 172.56	U251		
Delta 45.87 Range 172.56			
Range 172.56	Mean	-54.13	
		172.56	
150 100 50 0 -50 -100 -150			
150 100 50 0 -50 -100 -150		L	
		15	0 100 50 0 -50 -100 -150

Figure 2: One dose mean graph for NSC747260 at 10µM

Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Percent
Non-Small Cell Lung Cancer	45.04	
A549/ATCC HOP-62	-15.21 -58.64	
HOP-92	-51.30	
NCI-H226	-54.04	
NCI-H23	-48.94	
NCI-H322M	5.30	
NCI-H460 NCI-H522	-62.94 -74.88	
Colon Cancer	-74.86	
COLO 205	1.82	
HCC-2998	-80.71	
HCT-116	-18.25	
HCT-15 HT29	3.30 -42.14	
KM12	-47.80	
SW-620	-45.24	
Breast Cancer		
BT-549	-55.64	
HS 578T	-26.09 -33.81	
MCF7 MDA-MB-231/ATCC	-66.25	
MDA-MB-231/A1000 MDA-MB-435	-56.40	
MDA-MB-468	-42.33	
NCI/ADR-RES	20.86	
T-47D	35.89	
Ovarian Cancer IGROV1	-43.92	
OVCAR-3	-48.71	
OVCAR-4	-19.32	
OVCAR-5	-61.54	
OVCAR-8	-20.19	
SK-OV-3 Leukemia	4.83	
CCRF-CEM	34.04	
HL-60(TB)	3.76	
K-562	28.31	
MOLT-4	16.78	
RPMI-8226	93.78	
SR Renal Cancer	4.33	
786-0	-74.92	
A498	-50.94	
ACHN	-12.35	
CAKI-1 RXF 393	-67.34 -28.27	
SN12C	-52.54	
TK-10	-70.24	
UO-31	-61.43	
Melanoma	0.10	
LOX IMVI	0.13 -62.43	
M14 MALME-3M	-33.70	
SK-MEL-2	-61.28	
SK-MEL-28	-49.38	
SK-MEL-5	-81.11	
UACC-257 UACC-62	-38.00 -70.86	
Prostate Cancer	-70.00	
DU-145	-54.01	
PC-3	-7.74	
CNS Cancer	45.40	
SF-268 SF-295	-45.40 -10.43	
SF-295 SF-539	-85.24	
SNB-19	-47.53	
SNB-75	-74.36	
U251	-0.67	
Mean	-33.24	
Delta	-33.24 52.00 179.02	
Range	179.02	
	150	100 50 0 -50 -100 -150

Figure 3: One dose mean graph for NSC747269 at $10\mu M$

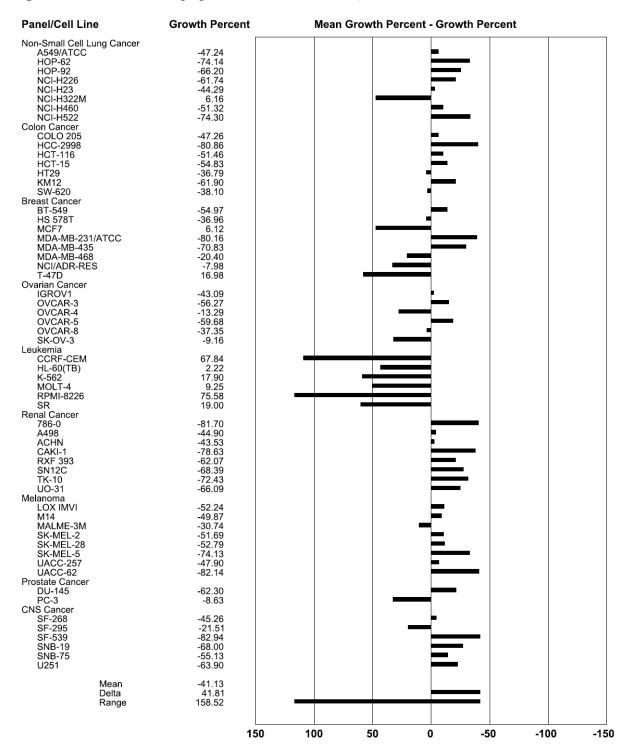


Figure 4: One dose mean graph for NSC747271 at 10µM

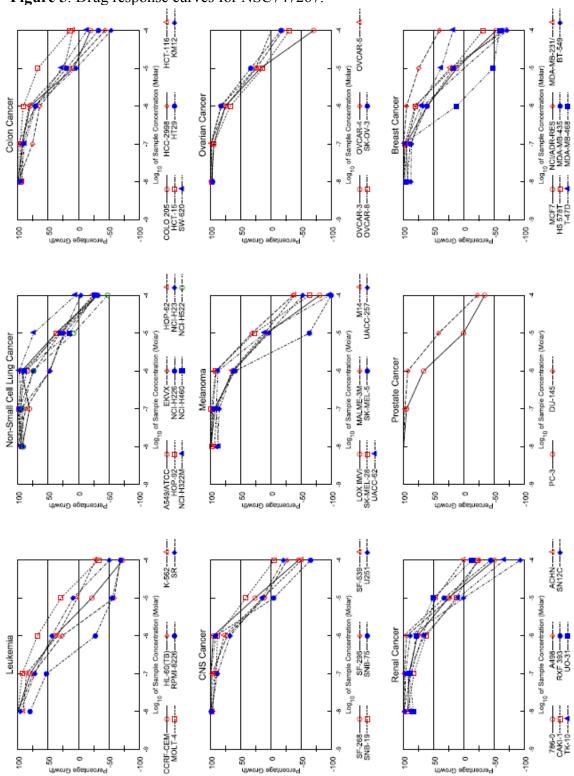


Figure 5: Drug response curves for NSC747267.

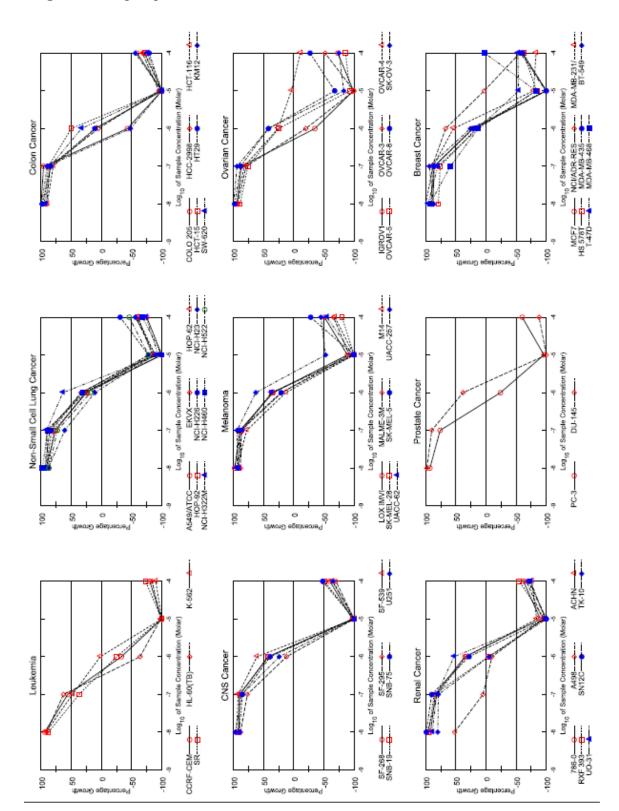


Figure 5: Drug response curves for NSC747260.

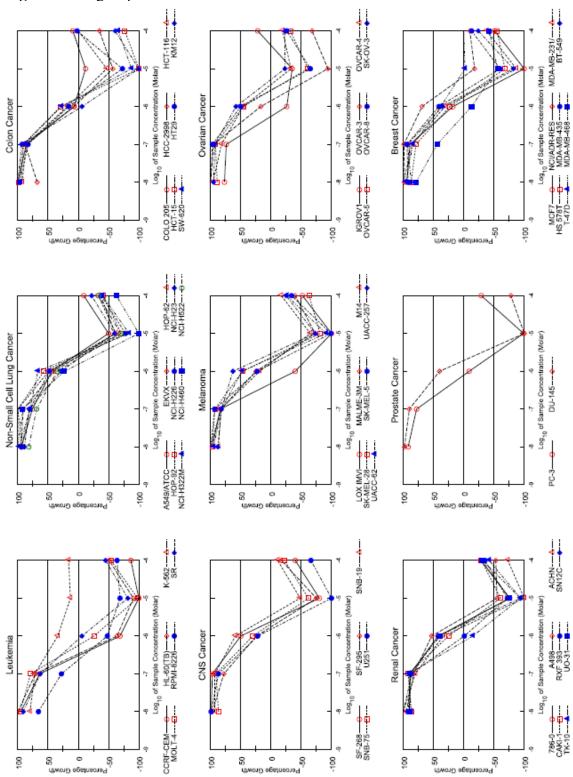


Figure 7: Drug response curves for NSC747269.

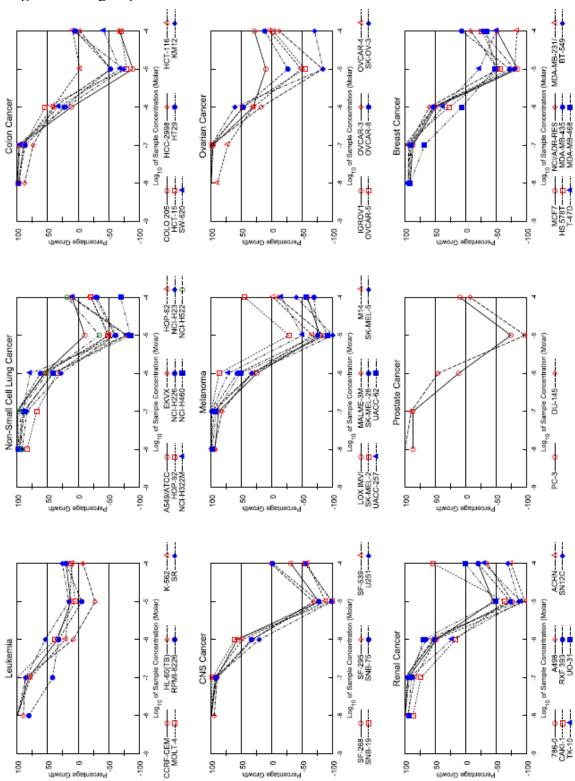


Figure 8: Drug response curves for NSC747271