

Supplementary Material

1 Supplementary Table and Figures

Compound Label	NSC Number	
3b	D-794940 / 1	
3d	D-794941 / 1	
4d	D-794939 / 1	
9b	D-795499 / 1	

Supplementary Table 1. Correlation of compound label and NSC number. The NSC numbers were assigned to each compound by the National Cancer Institute (NCI) before anticancer *in vitro* screening.

Developmental Ther	apeutics Program	NSC: D-794940 / 1	Conc: 1.00E-5 Molar	Test Date: Jan 03, 2017	
One Dose Mean Graph		Experiment ID: 1701OS37		Report Date: Feb 14, 201	
anel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	ent	
eukemia CCRF-CEM	77.63				
HL-60(TB)	75.93				
K-562	54.85				
MOLT-4	91.06				
RPMI-8226	81.05				
SR	51.24				
on-Small Cell Lung Cancer A549/ATCC	34.03				
EKVX	64.42				
HOP-62	28.04				
HOP-92	77.59				
NCI-H226	49.91				
NCI-H23 NCI-H322M	40.22 59.89				
NCI-H460	14.93				
NCI-H522	37.36				
olon Cancer					
COLO 205	72.17				
HCC-2998 HCT-116	93.71 45.29				
HCT-15	45.29 74.11				
HT29	43.76				
KM12	70.92				
SW-620	49.56		•		
NS Cancer SF-268	60.82				
SF-200 SF-295	53.13				
SF-539	56.65		-		
SNB-19	29.81				
SNB-75	30.40				
U251 elanoma	28.65				
LOX IMVI	50.89				
MALME-3M	48.24		•		
M14	67.96				
MDA-MB-435	51.21				
SK-MEL-2 SK-MEL-28	53.78 57.92				
SK-MEL-5	42.25				
UACC-257	66.45				
UACC-62	30.76				
Varian Cancer IGROV1	59.80				
OVCAR-3	56.08				
OVCAR-4	-5.56				
OVCAR-5	87.56				
OVCAR-8 NCI/ADR-RES	25.49				
SK-OV-3	84.49 31.00				
enal Cancer	51.00				
786-0	49.64		•		
A498	36.48				
ACHN RXF 393	66.17 48.12				
SN12C	40.50				
TK-10	84.02				
UO-31	79.77				
rostate Cancer	10.00				
PC-3 DU-145	19.36 33.58				
reast Cancer	00.00				
MCF7	22.55				
MDA-MB-231/ATCC	49.87				
HS 578T	49.76				
BT-549 T-47D	51.20 36.68				
MDA-MB-468	18.93				
Mean Delta	51.56 57.12				
Range	99.27				
		100 53		100	
	150	100 50	0 -50	-100 -15	

Supplementary Figure 2. NCI screening complete results for compound 3b.

Developmental Therapeutics Program One Dose Mean Graph		NSC: D-794941 / 1	Conc: 1.00E-5 Molar	Test Date: Jan 03, 2017
		Experiment ID: 1701OS37		Report Date: Feb 14, 201
Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Perc		cent
eukemia	01.01			
	61.81 57.35			
HL-60(TB) K-562	79.13			
MOLT-4	69.12			
RPMI-8226	91.77		•	
SR	78.15			
Non-Small Cell Lung Cancer				
A549/ATCC	91.54		• <u>•</u>	
EKVX HOP-62	75.80 90.61			
HOP-92	94.30			
NCI-H226	85.91			
NCI-H23	85.53		•	
NCI-H322M	90.76		• •	
NCI-H460	94.02			
NCI-H522	81.28		-	
Colon Cancer	100.00			
COLO 205 HCC-2998	100.92 97.44			
HCT-116	83.34			
HCT-15	87.50		•	
HT29	89.77		(L	
KM12	96.00			
SW-620	97.91			
CNS Cancer	100.17			
SF-268 SF-295	103.17 92.10			
SF-539	88.61		1	
SNB-19	97.79		_	
SNB-75	82.84		-	
U251	75.35			
<i>Aelanoma</i>	00.10			
	96.19			
MALME-3M M14	95.18 92.41			
MDA-MB-435	98.32			
SK-MEL-2	87.11			
SK-MEL-28	97.63			
SK-MEL-5	103.64			
UACC-257	94.84			
UACC-62	86.00		•	
Ovarian Cancer IGROV1	103.09			
OVCAR-3	100.46			
OVCAR-4	95.77		-	
OVCAR-5	105.81			
OVCAR-8	91.49			
NCI/ADR-RES	102.66			
SK-OV-3 Renal Cancer	87.08		r I	
786-0	95.59		–	
A498	91.13		•	
ACHN	96.15			
RXF 393	110.00			
TK-10	138.17			
UO-31	70.83			
rostate Cancer				
PC-3	102.36			
DU-145	113.04			
Breast Cancer	20.05			_
MCF7 MDA-MB-231/ATCC	29.05 89.91			-
HS 578T	106.68			
BT-549	83.39			
T-47D	39.50			
MDA-MB-468	48.30			
Mean	89.12			
Delta	60.07			■
Range	109.12			■
	150	100 50	0 -50	-100 -150

Supplementary Figure 2. NCI screening complete results for compound 3d.

Developmental Ther	apeutics Program	NSC: D-794939 / 1	Conc: 1.00E-5 Molar	Test Date: Jan 03, 2017	
One Dose Mean Graph		Experiment ID: 1701OS37		Report Date: Feb 14, 201	
Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Perc		cent	
eukemia CCRF-CEM	85.99		_		
HL-60(TB) K-562	74.63				
K-562	84.16		—		
MOLT-4 RPMI-8226	74.79 108.80				
SB	76.68				
Non-Small Cell Lung Cancer A549/ATCC	70.00				
A549/ATCC	93.68				
EKVX	80.85				
HOP-62 HOP-92	101.13 97.61				
NCI-H226	93.05		7 1		
NCI-H23	92.23				
NCI-H322M	90.48				
NCI-H460 NCI-H522	101.58				
Colon Cancer	80.85				
COLO 205	109.04				
HCC-2998	101.66		–		
HCT-116	91.76		I		
HCT-15 HT29	97.75 100.95				
KM12	89.35				
SW-620	107.19				
CNS Cancer					
SF-268	98.80				
SF-295 SF-539	94.78 92.83		1		
SNB-19	100.16		-		
SNB-75	62.55				
U251	92.76				
Aelanoma LOX IMVI	97.14		_ I		
MALME-3M	99.92				
M14	99.27		-		
MDA-MB-435	94.89				
SK-MEL-2 SK-MEL-28	106.53 101.26				
SK-MEL-5	101.34				
UACC-257	96.23		•		
UACC-62	85.24		—		
Ovarian Cancer	07.00				
IGROV1 OVCAR-3	97.32 93.23				
OVCAR-4	88.07		– 1		
OVCAR-5	105.13				
OVCAR-8	95.48 102.34				
NCI/ADR-RES SK-OV-3	88.24				
Renal Cancer					
786-0	99.34		_		
A498	102.79				
ACHN RXF 393	101.20 123.52				
SN12C	91.69				
TK-10	149.82	🔶			
UO-31	75.42				
Prostate Cancer PC-3	96.93				
DU-145	99.48				
Breast Cancer					
MCF7	30.30			-	
MDA-MB-231/ATCC HS 578T	92.09 104.30				
BT-549	77.03				
T-47D	55.16				
MDA-MB-468	62.83				
Mean	93.04				
Delta	62.74			■	
Range	119.52			■	
	150	100 50	0 -50	-100 -15	

Supplementary Figure 3. NCI screening complete results for compound 4d.

Developmental Therapeutics Program One Dose Mean Graph		NSC: D-795499 / 1	Conc: 1.00E-5 Molar	Test Date: Jan 30, 2017
		Experiment ID: 1701OS49		Report Date: Mar 23, 201
anel/Cell Line	Growth Percent	Mean Growth Percent - Growth Perc		cent
eukemia	68.00			
CCRF-CEM HL-60(TB)	68.09 89.72			
K-562	66.97			
MOLT-4	83.15			
RPMI-8226	64.35			
SR	79.17			
Ion-Small Cell Lung Cancer A549/ATCC	74.48			
EKVX	75.62			
HOP-92	64.68			
NCI-H226	72.65			
NCI-H23	62.17			
NCI-H322M	74.02			
NCI-H460 NCI-H522	84.07 62.43			
Colon Cancer	02.45			
HCC-2998	90.19			
HCT-116	75.10		P	
HCT-15	97.27			
HT29 KM12	86.46 79.92			
SW-620	79.92 85.81			
NS Cancer	03.01			
SF-268	78.05			
SF-295	71.91		—	
SF-539	88.17			
SNB-19	86.23			
SNB-75 U251	70.26 84.20			
Ielanoma	04.20			
LOX IMVI	78.78			
MALME-3M	97.03			
M14 MDA-MB-435	87.24			
SK-MEL-2	87.84 87.70			
SK-MEL-28	102.52			
SK-MEL-5	89.79		_	
UACC-257	81.06		•	
UACC-62	62.35			
Ovarian Cancer IGROV1	81.11			
OVCAR-3	87.74			
OVCAR-4	65.57			
OVCAR-5	95.80			
OVCAR-8	76.27			
NCI/ADR-RES SK-OV-3	83.14			
Renal Cancer	86.25			
786-0	85.33		-	
A498	78.28			
ACHN	83.82			
RXF 393 SN12C	93.69			
TK-10	89.87 106.80			
UO-31	50.42			
Prostate Cancer				
PC-3	60.18			
DU-145	93.31			
Breast Cancer MCF7	66.64			
MDA-MB-231/ATCC	76.37			
HS 578T	91.48			
BT-549	71.47			
T-47D MDA-MB-468	49.04 59.06			
	53.00			
Mean	79.32			
Delta	30.28			
Range	57.76			
	150	100 50	0 -50	-100 -150
	100		J -00	100 100

Supplementary Figure 4. NCI screening complete results for compound 9b.