Supporting Information

Cytotoxic potential of A-azepano- and 3-amino-3,4-seco-triterpenoids

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Figure S1. Anticancer screening data of compound 1 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-797815 / 1	Conc: 1.00E-5 Molar	Test Date: May 01, 2017
Experiment ID: 1705OS96		Report Date: May 18, 2017

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	12.43
HL-60(TB)	-51.88
K-562	-26.59
MOLT-4	4.40
RPMI-8226	-36.88
SR	-40.44
Non-Small Cell Lung Cancer	
A549/ATCC	44.88
EKVX	63.26
HOP-62	78.96
HOP-92	81.99
NCI-H226	84.36
NCI-H23	62.57
NCI-H322M	69.84
NCI-H460	-54.44
NCI-H522	64.19
Colon Cancer	
COLO 205	-63.45
HCC-2998	-5.02
HCT-116	-78.86
HCT-15	3.28
HT29	2.58
KM12	23.20
SW-620	-66.45
CNS Cancer	
SF-268	61.21
SF-295	40.41
SF-539	34.26
SNB-19	49.62
SNB-75	77.06
U251	7.49
Melanoma	
LOX IMVI	-57.73
MALME-3M	-65.40
M14	-49.76
MDA-MB-435	13.55
SK-MEL-2	78.76
SK-MEL-28	-65.40
SK-MEL-5	-82.49
UACC-257	-8.72
UACC-62	43.16
Ovarian Cancer	
IGROV1	36.30
OVCAR-3	44.42
OVCAR-4	31.81
OVCAR-5	74.96
OVCAR-8	23.54
NCI/ADR-RES	44.82
SK-OV-3	92.20
Renal Cancer	
786-0	30.17
ACHN	50.20
CAKI-1	38.39
RXF 393	48.36
SN12C	45.93
TK-10	80.77
UO-31	53.76
Prostate Cancer	
PC-3	25.61
DU-145	49.53
Breast Cancer	
MCF7	-12.60
MDA-MB-231/ATCC	46.85
HS 578T	46.76
BT-549	77.10
T-47D	36.46
MDA-MB-468	11.74
Mean	20.76
Delta	103.25
Range	174.69

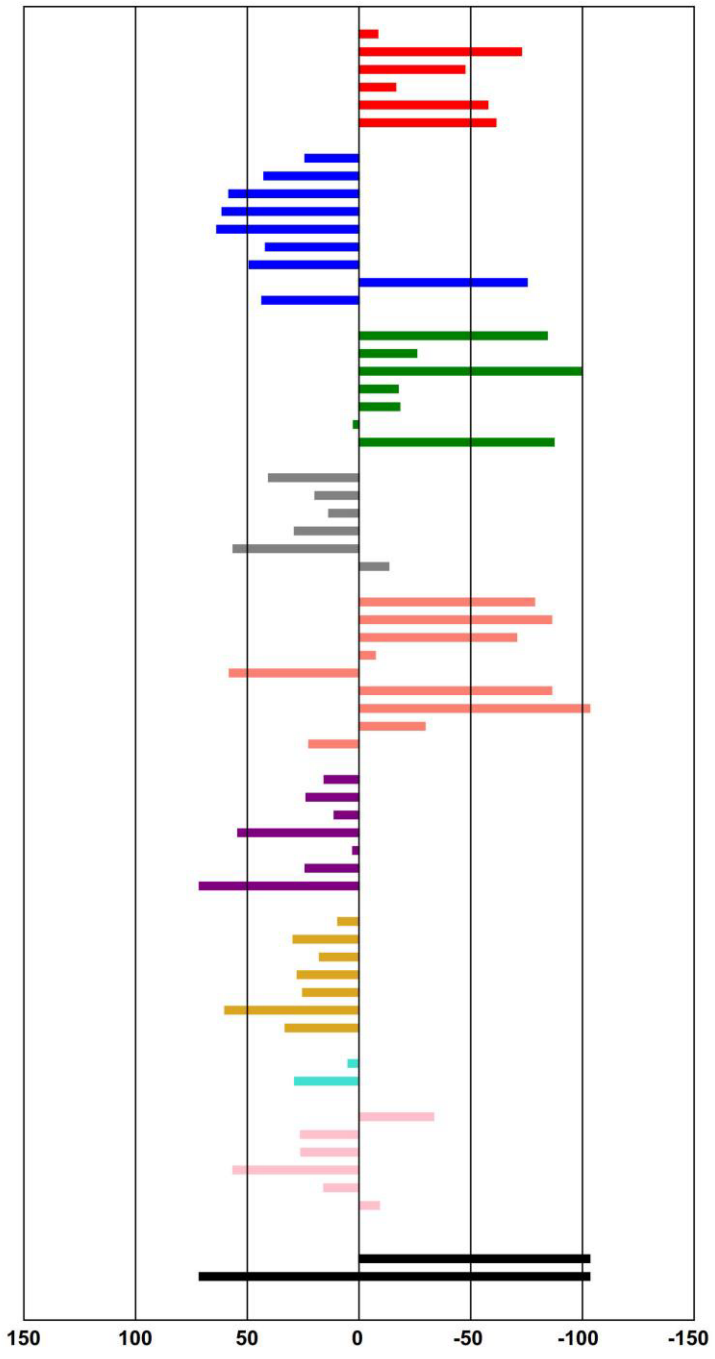

Figure S2. Anticancer screening data of compound 2 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-799588 / 1	Conc: 1.00E-5 Molar	Test Date: Jul 24, 2017
Experiment ID: 1707OS42		Report Date: Aug 17, 2017

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	103.44
HL-60(TB)	136.13
MOLT-4	95.32
RPMI-8226	98.64
SR	86.78
Non-Small Cell Lung Cancer	
A549/ATCC	111.67
EKVX	95.43
HOP-62	111.45
HOP-92	88.73
NCI-H226	106.68
NCI-H23	94.64
NCI-H322M	88.79
NCI-H460	100.32
NCI-H522	91.58
Colon Cancer	
COLO 205	105.64
HCC-2998	100.86
HCT-116	94.31
HCT-15	81.53
HT29	68.07
KM12	100.50
SW-620	102.99
CNS Cancer	
SF-268	91.20
SF-295	104.64
SF-539	105.10
SNB-19	99.05
SNB-75	86.05
U251	108.12
Melanoma	
LOX IMVI	95.60
MALME-3M	92.94
M14	93.63
MDA-MB-435	96.83
SK-MEL-2	105.21
SK-MEL-28	112.66
SK-MEL-5	92.71
UACC-257	123.03
UACC-62	94.66
Ovarian Cancer	
IGROV1	99.10
OVCAR-3	97.23
OVCAR-4	101.04
OVCAR-5	101.51
OVCAR-8	105.20
NCI/ADR-RES	96.36
SK-OV-3	121.52
Renal Cancer	
786-0	93.63
A498	95.26
ACHN	106.83
CAKI-1	97.14
RXF 393	103.51
SN12C	91.18
TK-10	110.20
UO-31	84.39
Prostate Cancer	
PC-3	86.01
DU-145	100.72
Breast Cancer	
MCF7	87.13
MDA-MB-231/ATCC	107.27
HS 578T	96.07
BT-549	100.88
T-47D	102.55
MDA-MB-468	106.17
Mean	99.25
Delta	31.18
Range	68.06

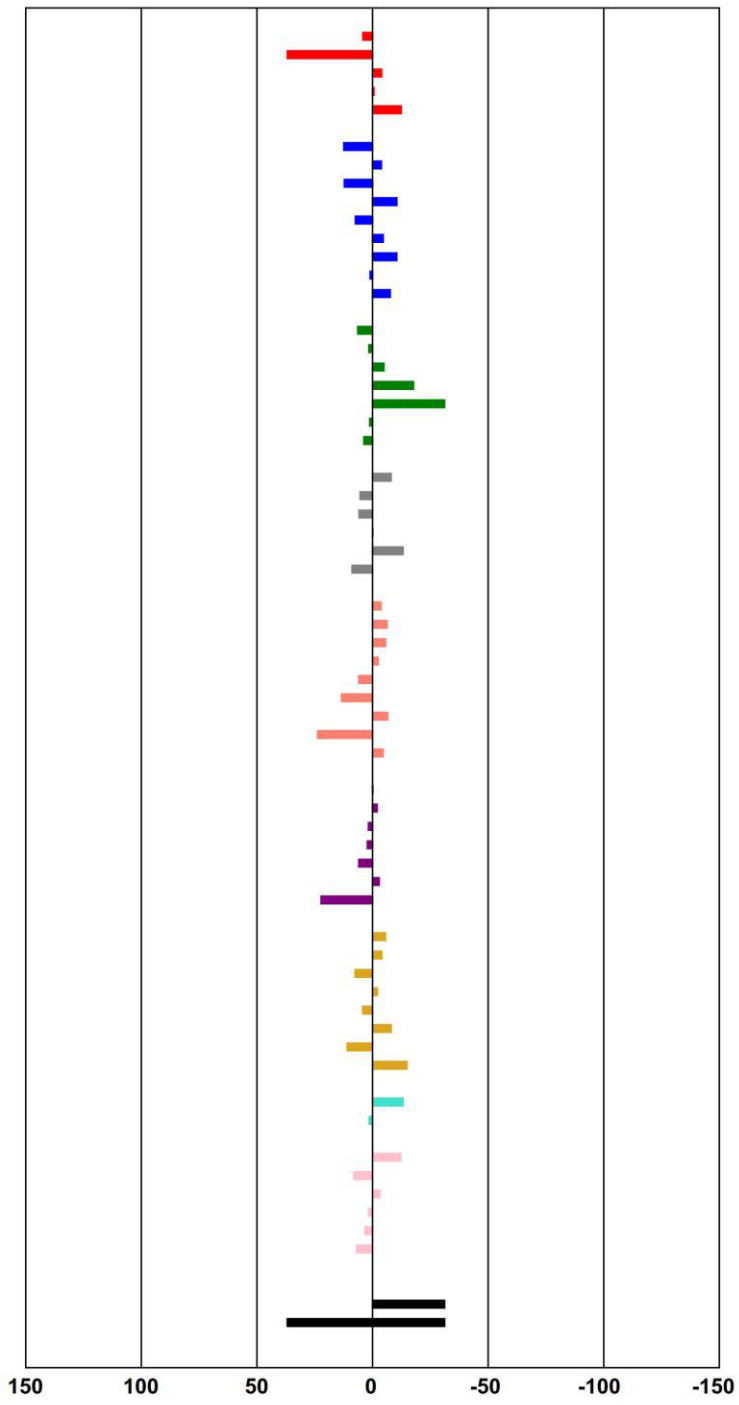

Figure S3. Anticancer screening data of compound 3 at single dose assay

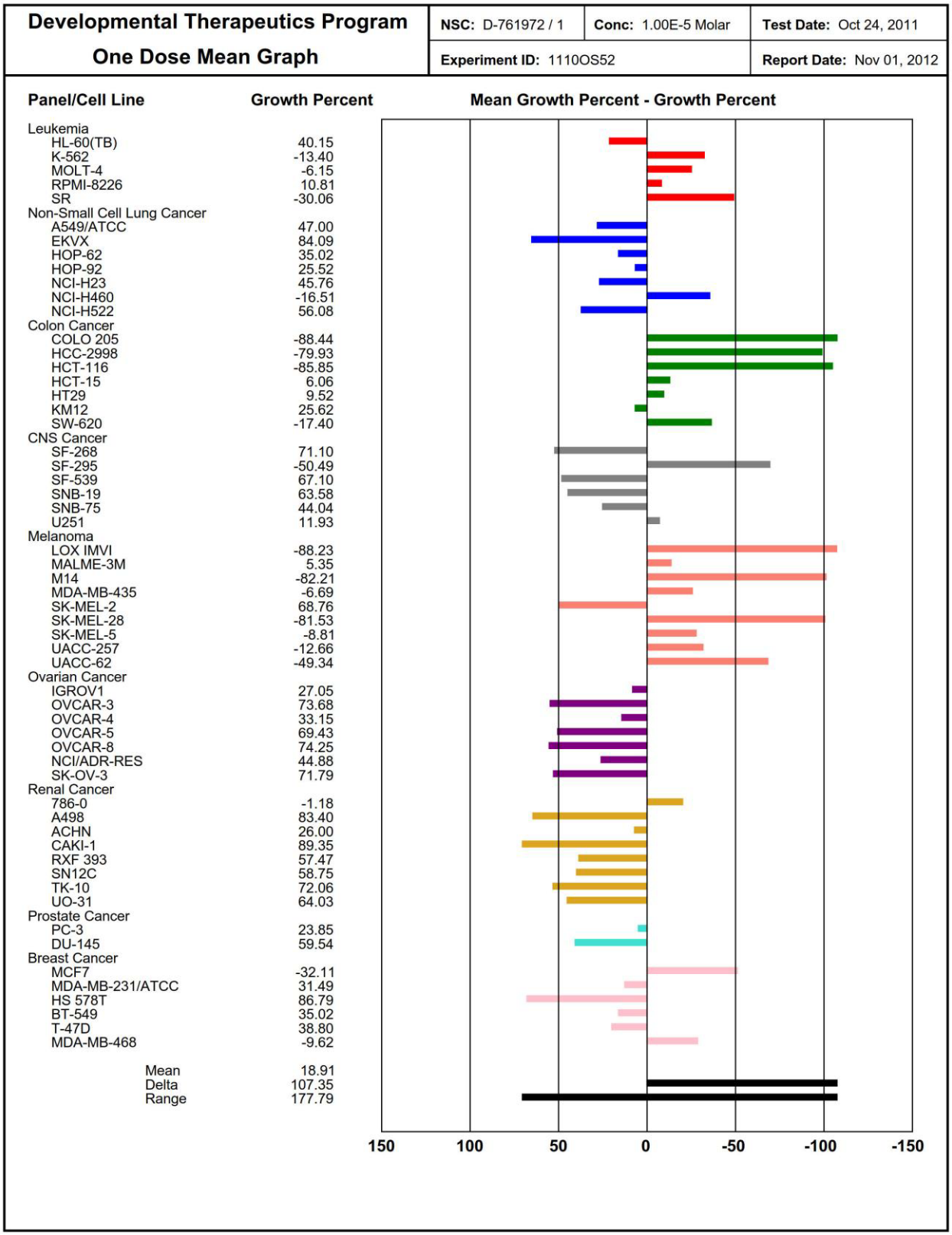

Figure S4. Anticancer screening data of compound 4 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-797816 / 1	Conc: 1.00E-5 Molar	Test Date: May 08, 2017
Experiment ID: 1705OS00		Report Date: May 26, 2017

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-34.70
HL-60(TB)	-54.98
K-562	-49.14
MOLT-4	-45.58
RPMI-8226	-39.72
SR	-49.90
Non-Small Cell Lung Cancer	
A549/ATCC	11.99
EKVX	19.40
HOP-62	-23.14
HOP-92	-5.92
NCI-H226	-99.04
NCI-H23	36.10
NCI-H322M	-17.88
NCI-H460	-83.30
NCI-H522	-77.84
Colon Cancer	
COLO 205	-78.29
HCC-2998	-38.73
HCT-116	-94.73
HCT-15	6.84
HT29	-75.38
KM12	0.12
SW-620	-69.61
CNS Cancer	
SF-268	5.71
SF-295	-64.59
SF-539	-36.47
SNB-19	-64.86
SNB-75	9.21
U251	-83.30
Melanoma	
LOX IMVI	-94.90
MALME-3M	-71.88
M14	-73.22
MDA-MB-435	-73.87
SK-MEL-2	13.06
SK-MEL-28	-84.86
SK-MEL-5	22.48
UACC-257	-36.88
UACC-62	-72.29
Ovarian Cancer	
IGROV1	-57.90
OVCAR-3	6.84
OVCAR-4	18.47
OVCAR-5	28.40
OVCAR-8	9.93
NCI/ADR-RES	17.62
SK-OV-3	69.60
Renal Cancer	
786-0	-80.95
ACHN	-66.33
CAKI-1	16.37
RXF 393	-27.89
SN12C	-1.54
TK-10	23.04
UO-31	12.51
Prostate Cancer	
PC-3	-43.18
DU-145	-17.44
Breast Cancer	
MCF7	-29.38
MDA-MB-231/ATCC	-54.76
HS 578T	10.53
BT-549	-65.99
T-47D	1.10
MDA-MB-468	-78.65
Mean	-31.86
Delta	67.18
Range	168.64

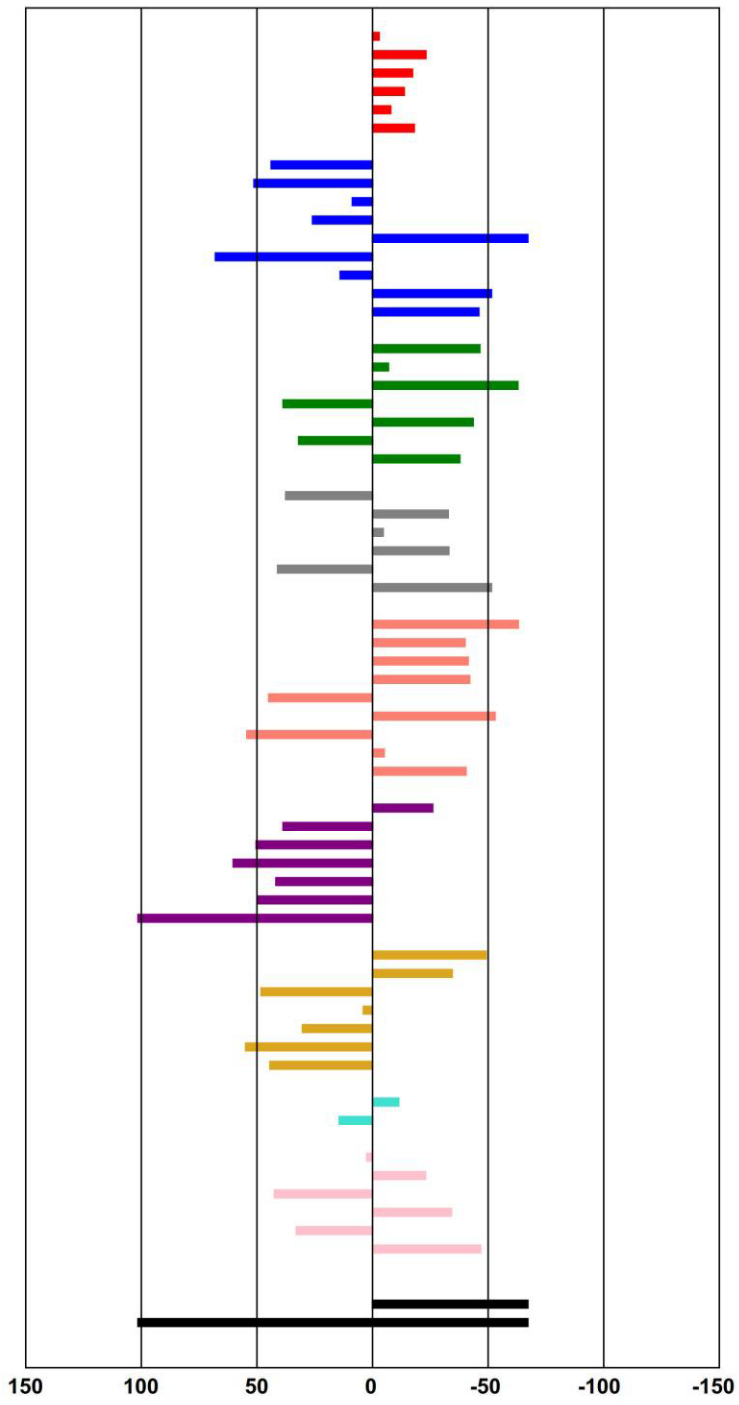

Figure S5. Anticancer screening data of compound 5 at single dose assay

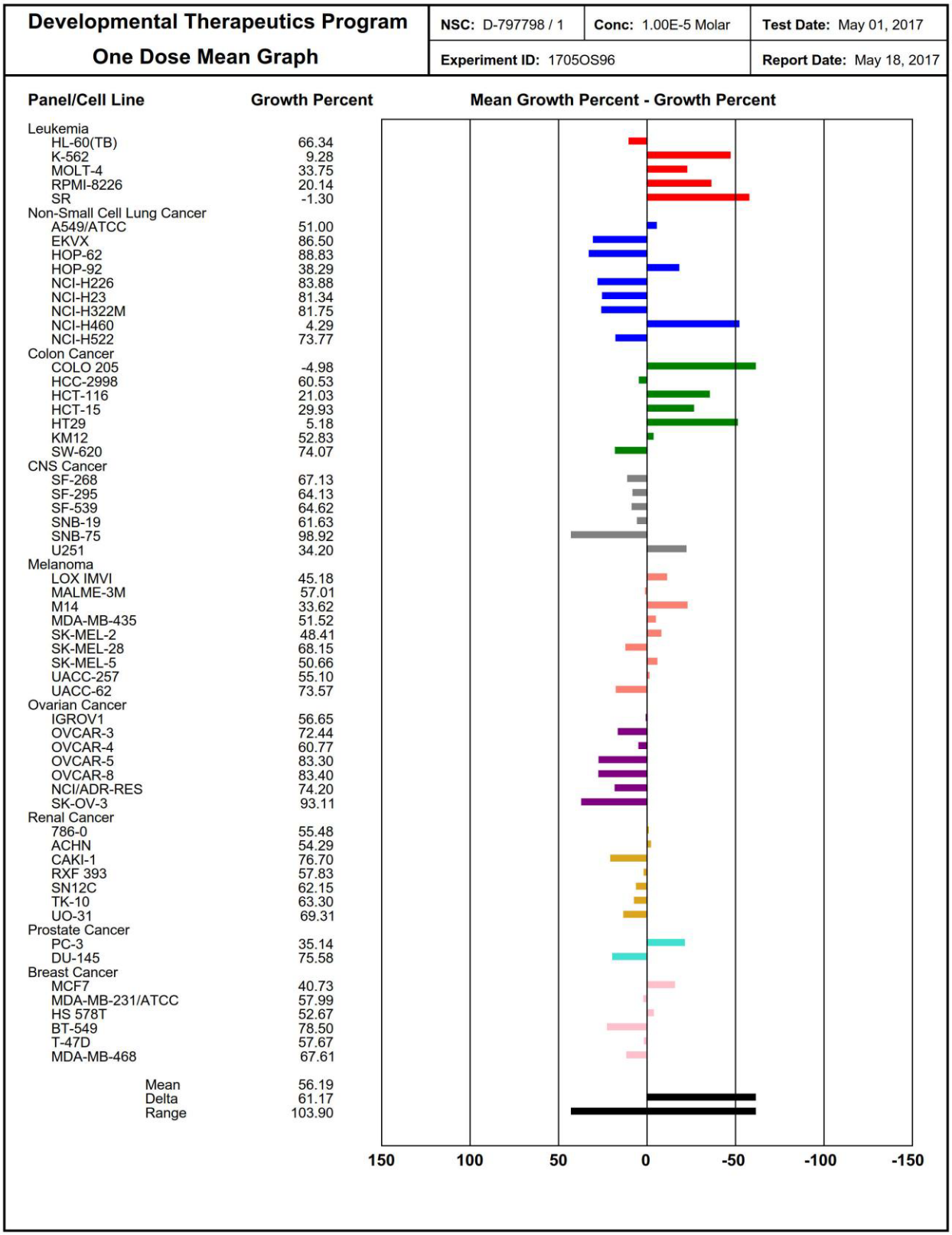

Figure S6. Anticancer screening data of compound 6 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-804743 / 1	Conc: 1.00E-5 Molar	Test Date: Apr 30, 2018
Experiment ID: 1804OS61		Report Date: May 16, 2018

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-44.06
HL-60(TB)	-52.80
K-562	-25.45
MOLT-4	-56.65
RPMI-8226	-43.82
SR	-5.08
Non-Small Cell Lung Cancer	
A549/ATCC	-66.53
EKVX	-87.12
HOP-62	-74.48
HOP-92	-76.37
NCI-H226	-59.08
NCI-H23	-84.89
NCI-H322M	-99.73
NCI-H460	-81.57
NCI-H522	-75.62
Colon Cancer	
COLO 205	-55.90
HCC-2998	-78.81
HCT-116	-77.38
HCT-15	-89.29
HT29	-62.15
KM12	-85.53
SW-620	-80.66
CNS Cancer	
SF-268	-69.91
SF-295	-90.09
SF-539	-93.29
SNB-19	-90.39
SNB-75	-97.70
U251	-59.66
Melanoma	
LOX IMVI	-91.45
MALME-3M	-82.63
M14	-82.08
MDA-MB-435	-95.56
SK-MEL-2	-84.91
SK-MEL-28	-97.33
SK-MEL-5	-91.52
UACC-257	-80.55
UACC-62	-94.26
Ovarian Cancer	
IGROV1	-84.51
OVCAR-3	-78.83
OVCAR-5	-98.74
OVCAR-8	-57.82
NCI/ADR-RES	-86.43
SK-OV-3	-80.14
Renal Cancer	
786-0	-71.98
A498	-88.73
ACHN	-95.35
CAKI-1	-96.49
RXF 393	-70.42
SN12C	-93.98
TK-10	-78.35
UO-31	-98.13
Prostate Cancer	
PC-3	-79.09
DU-145	-89.53
Breast Cancer	
MCF7	-70.69
MDA-MB-231/ATCC	-94.00
HS 578T	-46.83
BT-549	-87.92
T-47D	-63.85
MDA-MB-468	-79.54
Mean	-77.22
Delta	22.51
Range	94.65

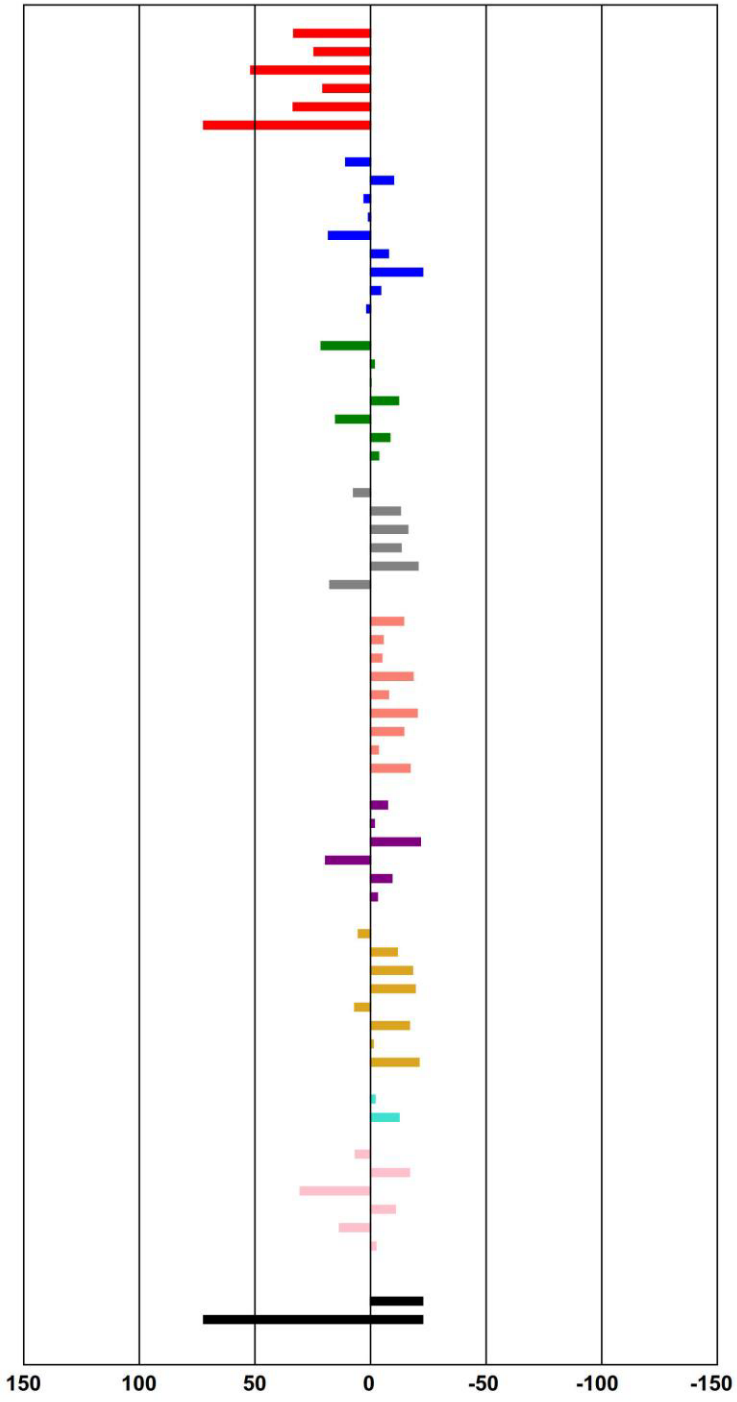

Figure S7. Anticancer screening data of compound 7 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-797792 / 1	Conc: 1.00E-5 Molar	Test Date: May 01, 2017
Experiment ID: 1705OS96		Report Date: May 18, 2017

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-6.07
HL-60(TB)	-65.48
K-562	-39.70
MOLT-4	-32.74
RPMI-8226	-29.65
SR	-30.19
Non-Small Cell Lung Cancer	
A549/ATCC	-45.63
EKVX	23.19
HOP-62	27.66
HOP-92	-37.20
NCI-H226	34.81
NCI-H23	41.22
NCI-H322M	-21.40
NCI-H460	-60.64
NCI-H522	9.35
Colon Cancer	
COLO 205	-68.17
HCC-2998	-55.47
HCT-116	-99.38
HCT-15	-63.69
HT29	-49.41
KM12	-69.00
SW-620	-71.93
CNS Cancer	
SF-268	38.23
SF-295	-65.01
SF-539	38.73
SNB-19	-20.21
SNB-75	3.81
U251	-75.61
Melanoma	
LOX IMVI	-94.90
MALME-3M	-63.41
M14	-77.21
MDA-MB-435	-80.01
SK-MEL-2	10.51
SK-MEL-28	27.70
SK-MEL-5	-7.69
UACC-257	45.08
UACC-62	-51.12
Ovarian Cancer	
IGROV1	-58.73
OVCAR-3	-31.21
OVCAR-4	-51.22
OVCAR-5	8.55
OVCAR-8	-45.63
NCI/ADR-RES	-19.60
SK-OV-3	75.76
Renal Cancer	
786-0	-96.23
ACHN	-88.31
CAKI-1	-92.03
RXF 393	-65.27
SN12C	17.72
TK-10	0.42
UO-31	2.86
Prostate Cancer	
PC-3	-10.65
DU-145	-8.90
Breast Cancer	
MCF7	-25.03
MDA-MB-231/ATCC	-62.85
HS 578T	-9.12
BT-549	76.37
T-47D	2.46
MDA-MB-468	-50.53
Mean	-27.32
Delta	72.06
Range	175.75

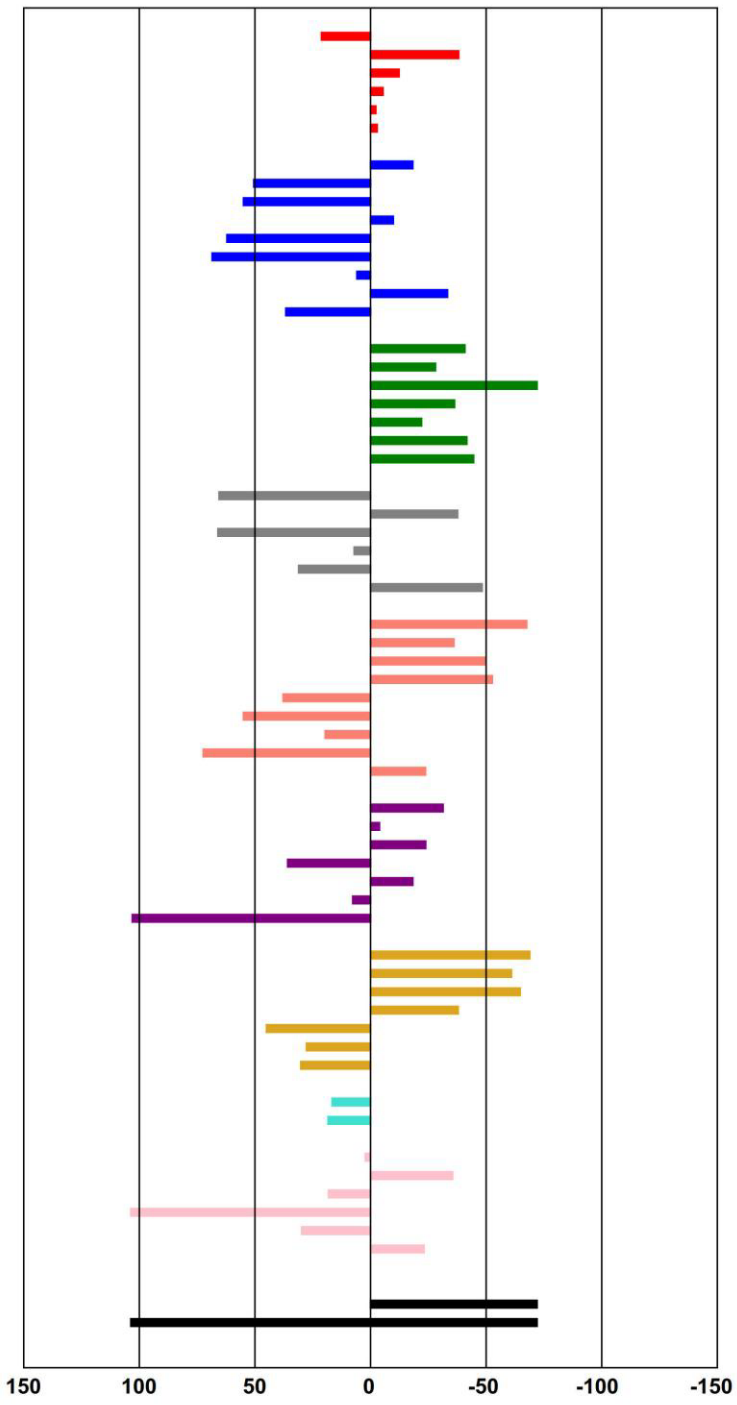

Figure S8. Anticancer screening data of compound 8 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-801866 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 13, 2017
Experiment ID: 1711OS00		Report Date: Dec 09, 2017

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-23.41
HL-60(TB)	-12.30
K-562	-44.63
MOLT-4	-46.37
RPMI-8226	-49.24
SR	-45.18
Non-Small Cell Lung Cancer	
A549/ATCC	-78.09
EKVX	-47.77
HOP-62	-63.53
HOP-92	-32.54
NCI-H226	23.24
NCI-H23	-58.81
NCI-H322M	-42.30
NCI-H460	-34.61
NCI-H522	-74.15
Colon Cancer	
COLO 205	-81.03
HCC-2998	-93.75
HCT-116	-96.24
HCT-15	-88.99
HT29	-83.75
KM12	-79.04
SW-620	-58.94
CNS Cancer	
SF-268	12.33
SF-295	-84.70
SF-539	9.45
SNB-19	-77.17
SNB-75	23.47
U251	-98.77
Melanoma	
LOX IMVI	-99.54
MALME-3M	-56.11
M14	-82.08
MDA-MB-435	-71.05
SK-MEL-2	-52.34
SK-MEL-28	-42.34
SK-MEL-5	64.23
UACC-257	-67.40
UACC-62	-79.00
Ovarian Cancer	
IGROV1	-94.22
OVCAR-3	-93.30
OVCAR-4	-67.50
OVCAR-5	16.76
OVCAR-8	-84.38
NCI/ADR-RES	-52.24
SK-OV-3	92.97
Renal Cancer	
786-0	-89.53
A498	69.82
ACHN	-82.43
CAKI-1	-92.49
RXF 393	-91.86
SN12C	-87.88
TK-10	-46.59
UO-31	18.40
Prostate Cancer	
PC-3	-21.40
DU-145	-36.79
Breast Cancer	
MCF7	-72.85
MDA-MB-231/ATCC	-76.55
HS 578T	-30.86
BT-549	75.89
T-47D	33.94
MDA-MB-468	-77.92
Mean	-46.72
Delta	52.82
Range	192.51

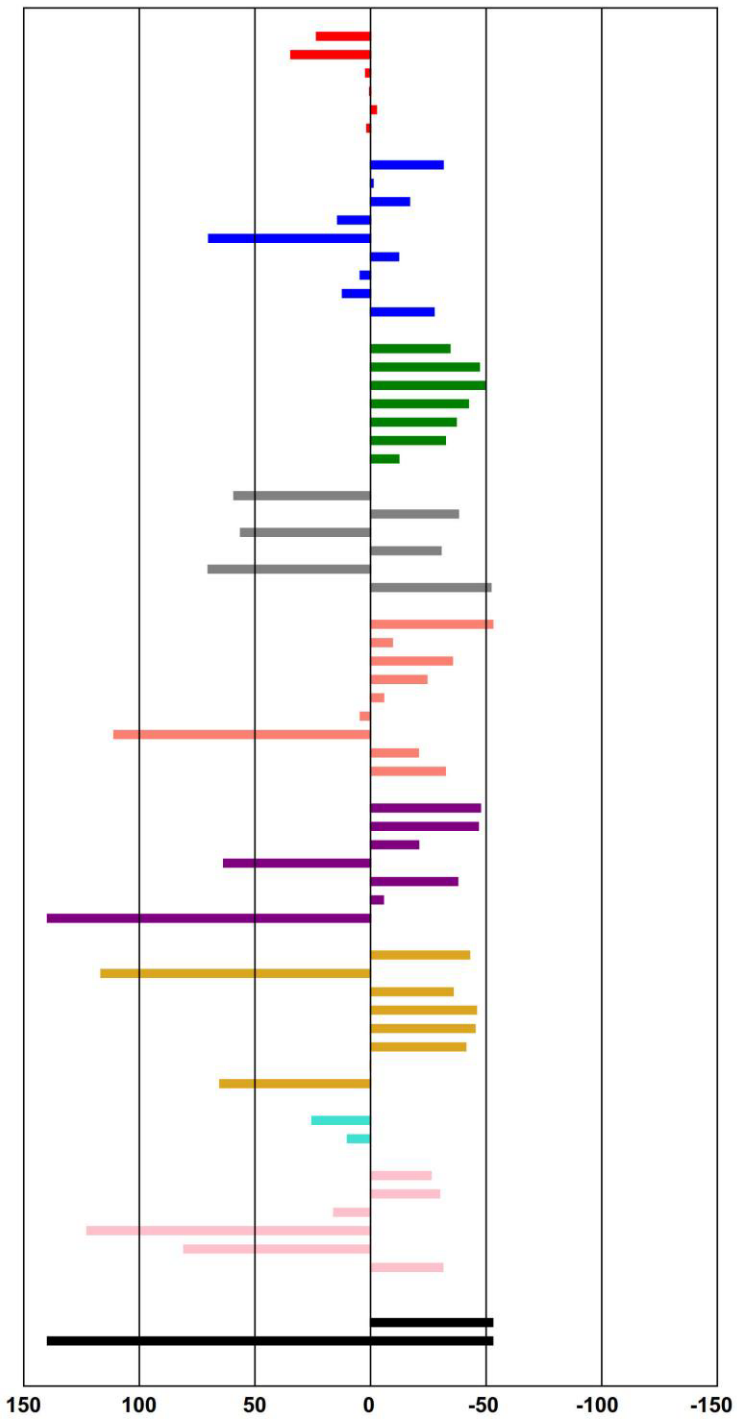

Figure S9. Anticancer screening data of compound 9 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-804757 / 1	Conc: 1.00E-5 Molar	Test Date: May 21, 2018
Experiment ID: 1805OS64		Report Date: Jun 08, 2018

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	5.21
HL-60(TB)	21.72
MOLT-4	-8.43
RPMI-8226	-32.81
SR	5.05
Non-Small Cell Lung Cancer	
A549/ATCC	-13.99
EKVX	84.53
HOP-62	104.59
HOP-92	23.79
NCI-H226	106.93
NCI-H23	63.08
NCI-H322M	20.66
NCI-H460	-70.37
NCI-H522	96.08
Colon Cancer	
COLO 205	-93.54
HCC-2998	-51.50
HCT-116	-32.08
HCT-15	-57.84
HT29	-55.24
KM12	-53.04
SW-620	-66.28
CNS Cancer	
SF-268	40.23
SF-295	-35.20
SF-539	77.48
SNB-19	18.12
SNB-75	76.51
U251	-90.81
Melanoma	
LOX IMVI	-100.00
MALME-3M	3.21
M14	15.48
MDA-MB-435	-17.26
SK-MEL-2	94.56
SK-MEL-28	63.75
SK-MEL-5	89.93
UACC-257	76.67
UACC-62	92.40
Ovarian Cancer	
IGROV1	40.52
OVCAR-3	-28.90
OVCAR-4	-40.99
OVCAR-5	41.09
OVCAR-8	-87.34
NCI/ADR-RES	-45.12
SK-OV-3	102.78
Renal Cancer	
786-0	-72.53
A498	60.16
ACHN	8.91
CAKI-1	30.45
SN12C	48.28
TK-10	80.51
UO-31	55.67
Prostate Cancer	
PC-3	27.74
DU-145	-7.26
Breast Cancer	
MCF7	-28.23
MDA-MB-231/ATCC	-7.94
HS 578T	92.86
BT-549	97.06
T-47D	65.05
MDA-MB-468	-47.15
Mean	13.57
Delta	113.57
Range	206.93

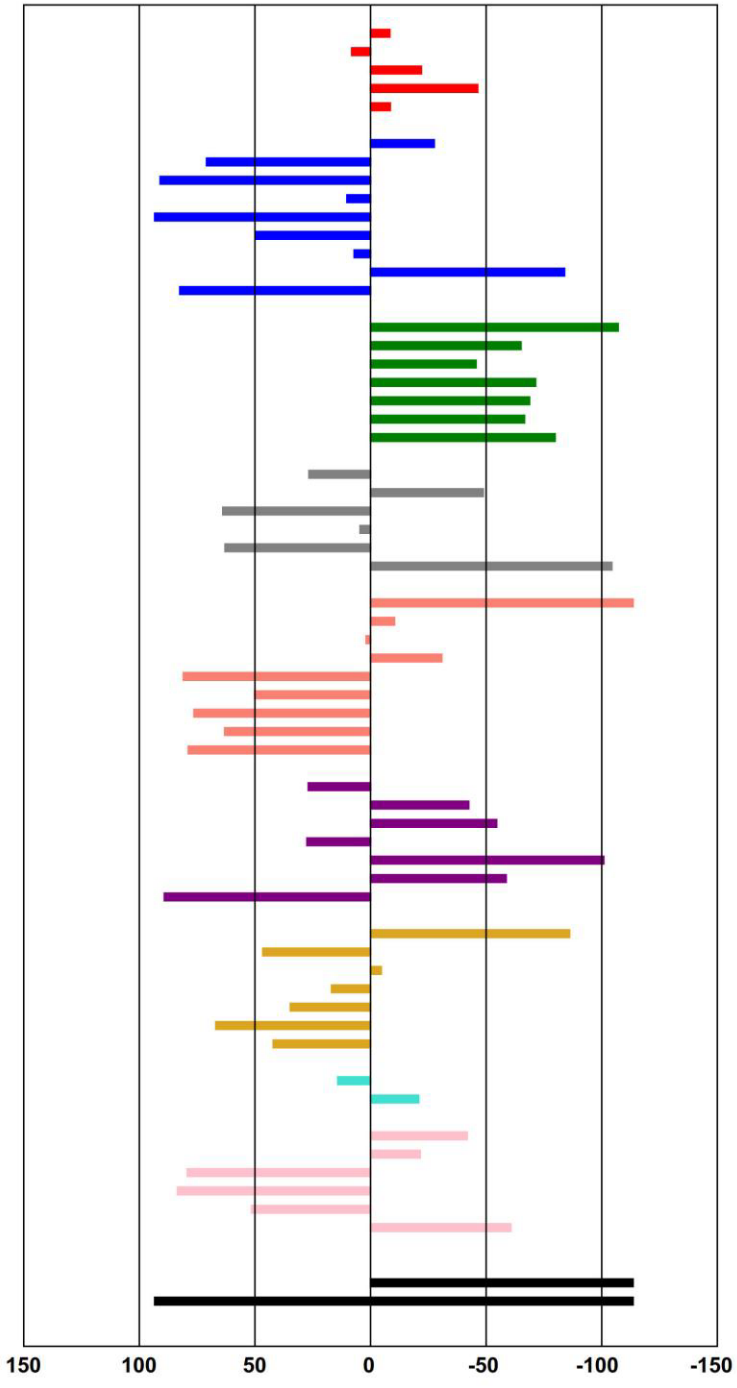

Figure S10. Anticancer screening data of compound 11 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-799581 / 1	Conc: 1.00E-5 Molar	Test Date: Jul 24, 2017
Experiment ID: 1707OS42		Report Date: Aug 17, 2017

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-46.66
HL-60(TB)	-73.26
MOLT-4	-62.57
RPMI-8226	-49.28
SR	-56.78
Non-Small Cell Lung Cancer	
A549/ATCC	-83.13
EKVX	-84.14
HOP-62	-86.15
HOP-92	-88.51
NCI-H226	-55.75
NCI-H23	-71.93
NCI-H322M	-86.00
NCI-H460	-86.20
NCI-H522	-79.22
Colon Cancer	
COLO 205	-83.45
HCC-2998	-84.68
HCT-116	-94.79
HCT-15	-82.28
HT29	-86.12
KM12	-80.70
SW-620	-82.33
CNS Cancer	
SF-268	-81.22
SF-295	-91.75
SF-539	-87.70
SNB-19	-88.04
SNB-75	-95.12
U251	-89.74
Melanoma	
LOX IMVI	-86.23
MALME-3M	-82.91
M14	-90.18
MDA-MB-435	-93.55
SK-MEL-2	-92.47
SK-MEL-28	-92.33
SK-MEL-5	-95.48
UACC-257	-88.77
UACC-62	-85.61
Ovarian Cancer	
IGROV1	-78.77
OVCAR-3	-95.88
OVCAR-4	-80.86
OVCAR-5	-93.52
OVCAR-8	-76.35
NCI/ADR-RES	-67.61
SK-OV-3	-96.25
Renal Cancer	
786-0	-90.70
A498	-97.92
ACHN	-95.87
CAKI-1	-93.50
RXF 393	-91.45
SN12C	-83.28
TK-10	-94.69
UO-31	-92.62
Prostate Cancer	
PC-3	-84.86
DU-145	-87.37
Breast Cancer	
MCF7	-69.74
MDA-MB-231/ATCC	-87.12
HS 578T	-60.53
BT-549	-88.14
T-47D	-58.03
MDA-MB-468	-90.49
Mean	-83.06
Delta	14.86
Range	51.26

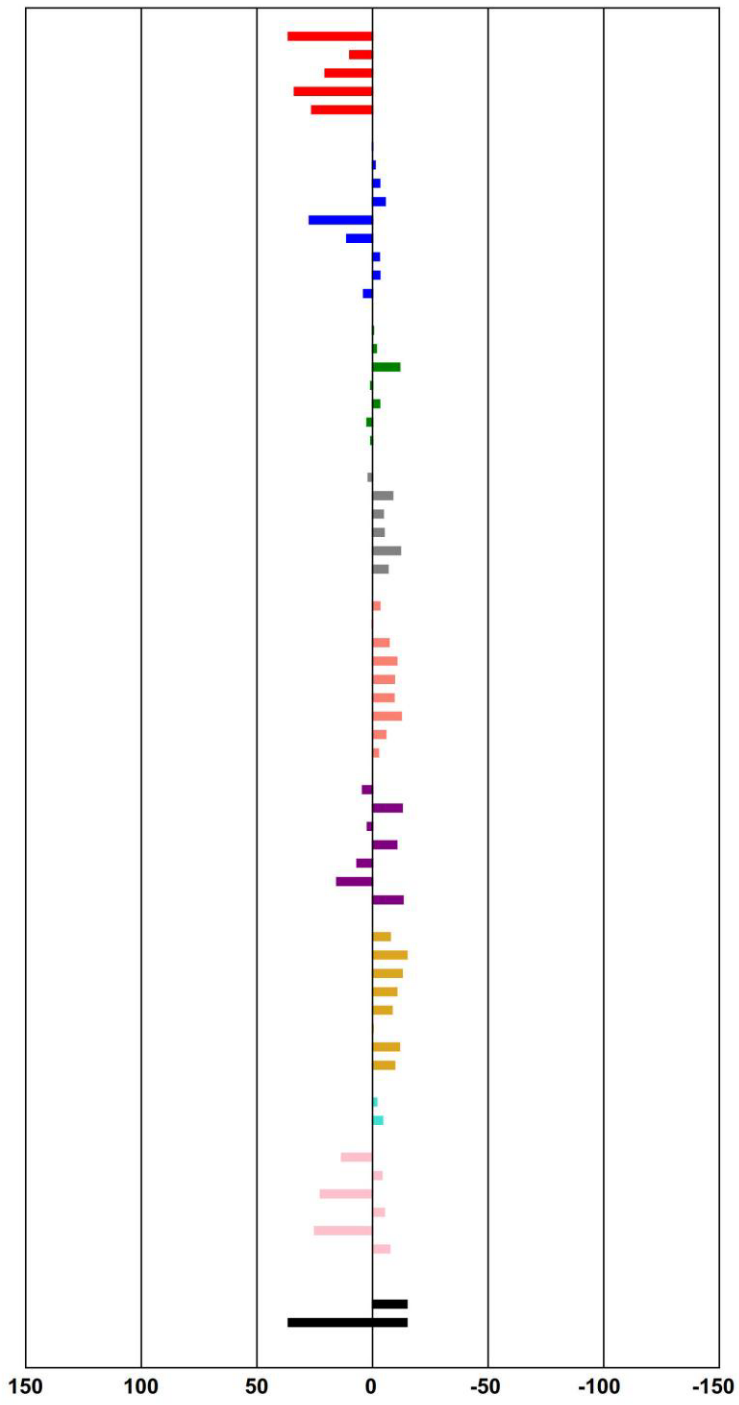

Figure S11. Anticancer screening data of compound 12 at single dose assay

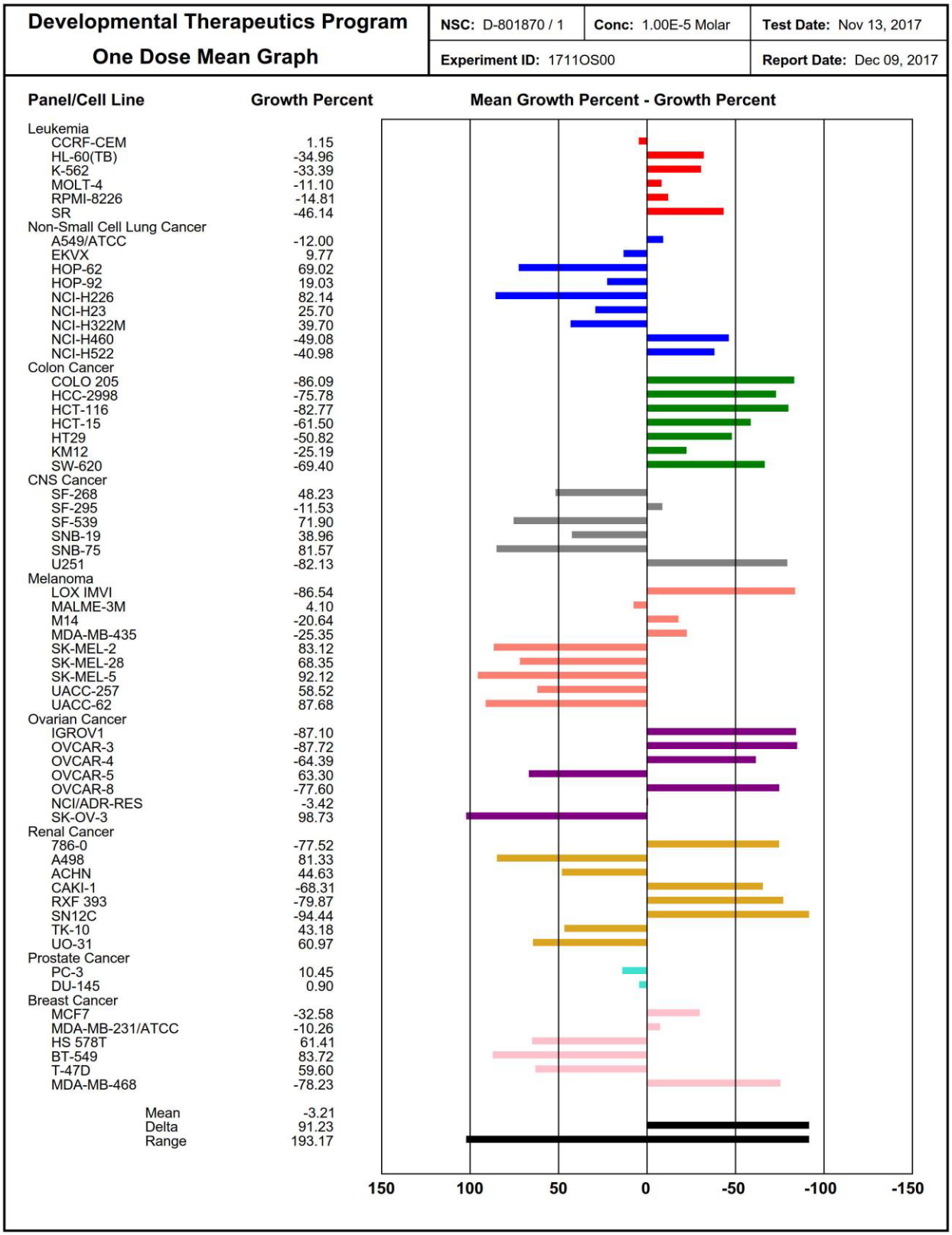

Figure S12. Anticancer screening data of compound 13 at single dose assay

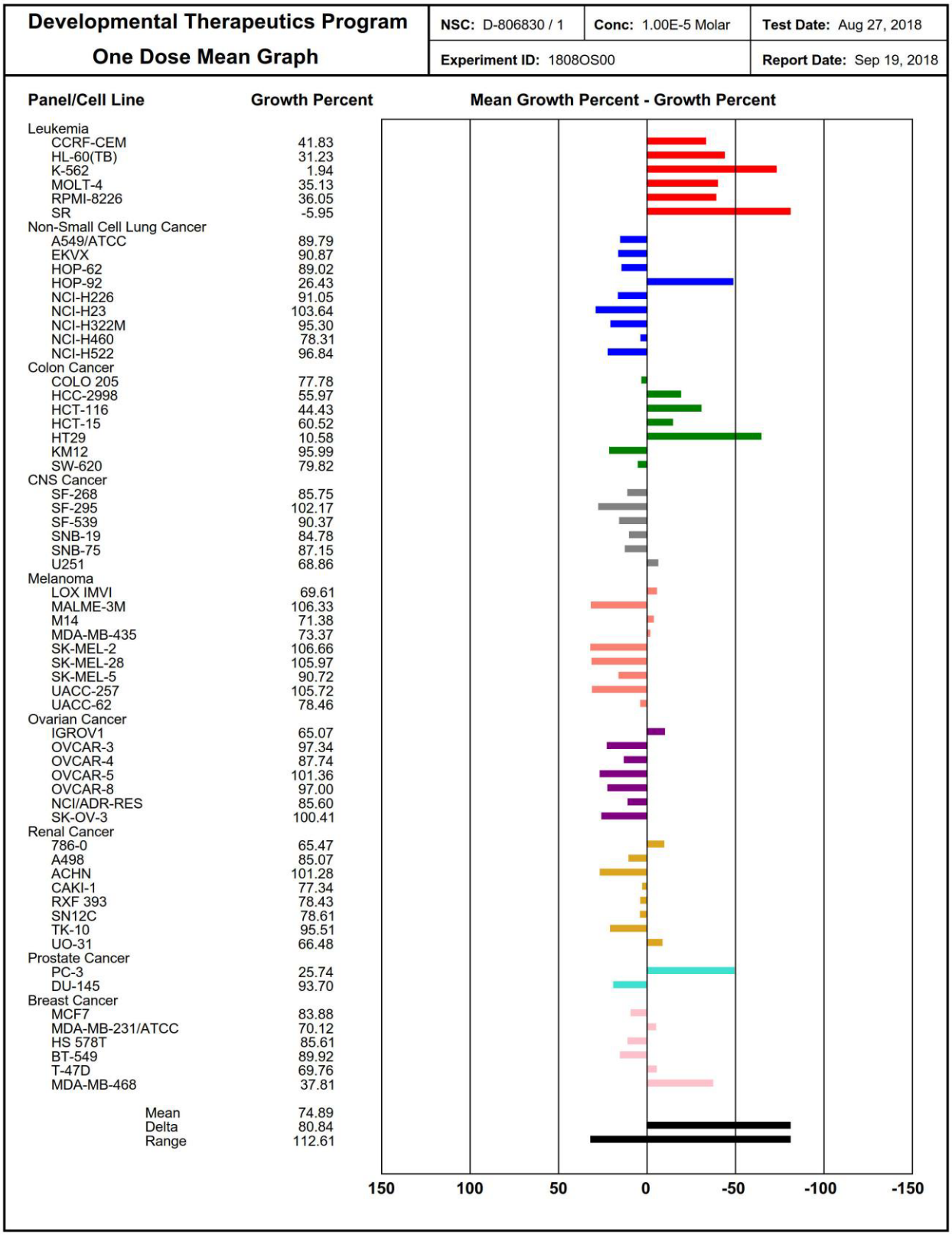

Figure S13. Anticancer screening data of compound 14 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-799580 / 1	Conc: 1.00E-5 Molar	Test Date: Jul 24, 2017
Experiment ID: 1707OS42		Report Date: Aug 17, 2017

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-25.46
HL-60(TB)	-45.18
MOLT-4	-47.91
RPMI-8226	-42.28
SR	-49.21
Non-Small Cell Lung Cancer	
A549/ATCC	-92.14
EKVX	76.61
HOP-62	95.22
HOP-92	60.23
NCI-H226	110.43
NCI-H23	50.99
NCI-H322M	63.12
NCI-H460	-79.81
NCI-H522	9.94
Colon Cancer	
COLO 205	-82.70
HCC-2998	-84.44
HCT-116	-100.00
HCT-15	-83.72
HT29	-88.52
KM12	-60.51
SW-620	-83.86
CNS Cancer	
SF-268	-40.43
SF-295	-50.76
SF-539	-72.93
SNB-19	-59.64
SNB-75	78.21
U251	-86.32
Melanoma	
LOX IMVI	-89.72
MALME-3M	-78.47
M14	-92.02
MDA-MB-435	-91.82
SK-MEL-2	90.55
SK-MEL-28	-67.28
SK-MEL-5	-18.81
UACC-257	-86.95
UACC-62	-74.49
Ovarian Cancer	
IGROV1	-73.28
OVCAR-3	-45.12
OVCAR-4	27.84
OVCAR-5	74.88
OVCAR-8	-80.46
NCI/ADR-RES	-48.63
SK-OV-3	103.04
Renal Cancer	
786-0	-96.25
A498	98.30
ACHN	-75.06
CAKI-1	26.66
RXF 393	-84.83
SN12C	-86.14
TK-10	101.82
UO-31	-76.54
Prostate Cancer	
PC-3	-4.73
DU-145	-74.13
Breast Cancer	
MCF7	-83.40
MDA-MB-231/ATCC	-71.91
HS 578T	-53.27
BT-549	92.03
T-47D	77.96
MDA-MB-468	-55.72
Mean	-27.92
Delta	72.08
Range	210.43

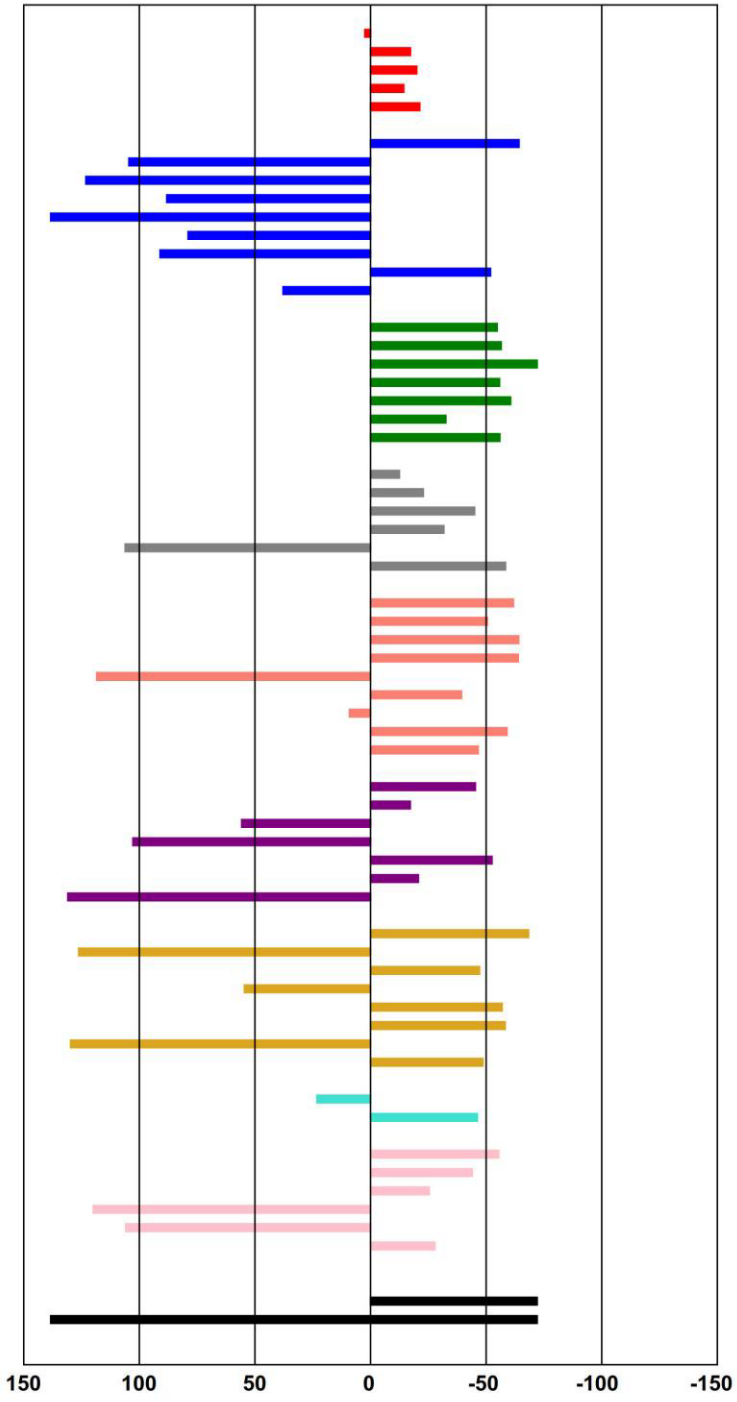

Figure S14. Anticancer screening data of compound 15 at single dose assay

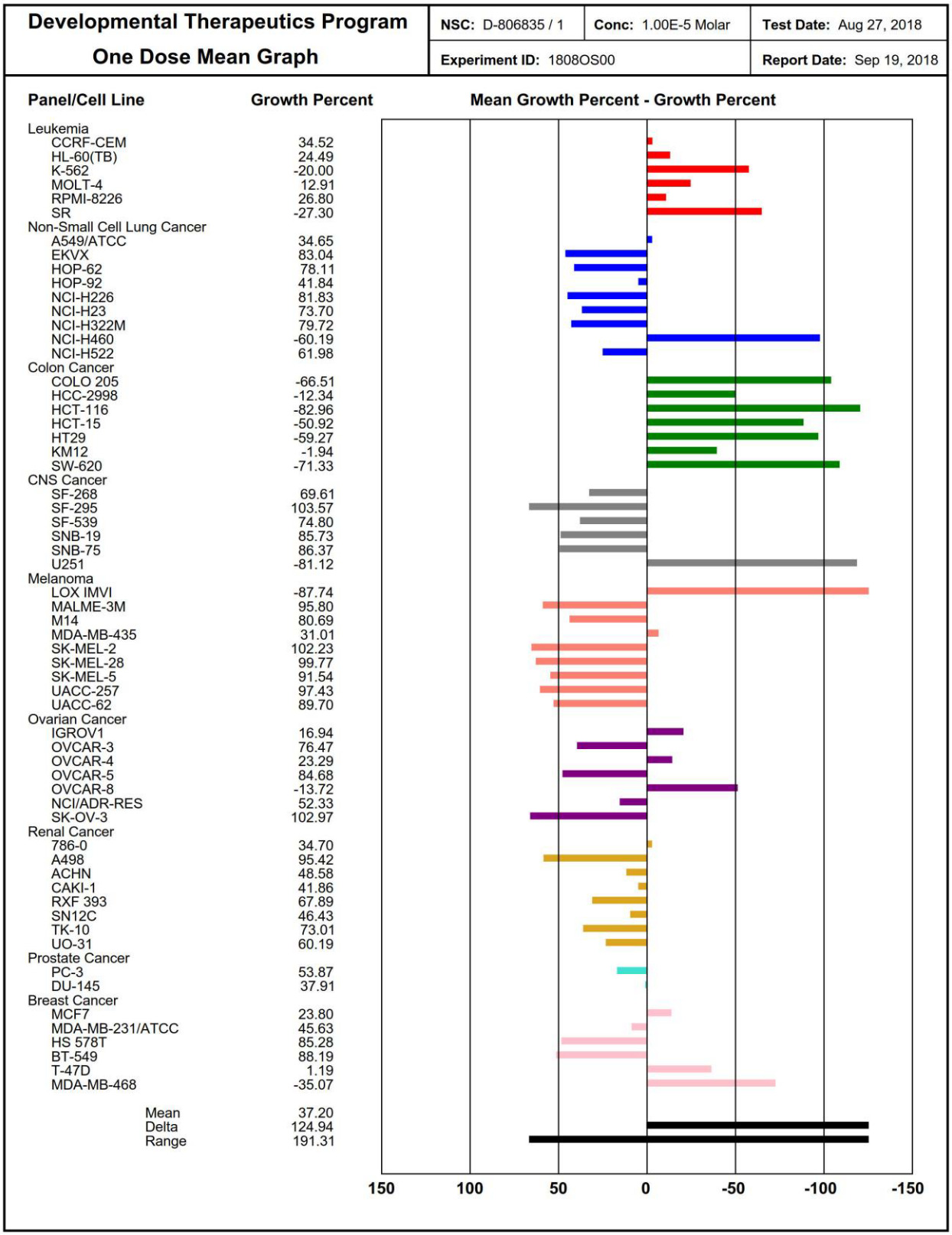

Figure S15. Anticancer screening data of compound 16 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-806829 / 1	Conc: 1.00E-5 Molar	Test Date: Aug 27, 2018
Experiment ID: 1808OS00		Report Date: Sep 19, 2018

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	0.85
HL-60(TB)	-58.40
K-562	-28.05
MOLT-4	-24.79
RPMI-8226	-66.03
SR	-30.93
Non-Small Cell Lung Cancer	
A549/ATCC	-38.22
EKVX	88.86
HOP-62	53.71
HOP-92	28.55
NCI-H226	66.78
NCI-H23	59.17
NCI-H322M	26.93
NCI-H460	-65.44
NCI-H522	-47.12
Colon Cancer	
COLO 205	-77.97
HCC-2998	-28.96
HCT-116	-91.45
HCT-15	-74.52
HT29	-69.23
KM12	-75.84
SW-620	-85.81
CNS Cancer	
SF-268	74.71
SF-295	102.41
SF-539	1.10
SNB-19	47.81
SNB-75	82.88
U251	-95.86
Melanoma	
LOX IMVI	-99.17
MALME-3M	15.09
M14	-64.90
MDA-MB-435	-38.22
SK-MEL-2	9.43
SK-MEL-28	96.70
SK-MEL-5	76.48
UACC-257	61.85
UACC-62	61.11
Ovarian Cancer	
IGROV1	-2.07
OVCAR-3	23.54
OVCAR-4	-40.54
OVCAR-5	34.76
OVCAR-8	-65.62
NCI/ADR-RES	-19.72
SK-OV-3	103.84
Renal Cancer	
786-0	-90.69
A498	103.72
ACHN	-46.63
CAKI-1	1.61
RXF 393	-7.17
SN12C	7.76
TK-10	68.56
UO-31	71.55
Prostate Cancer	
PC-3	43.55
DU-145	-1.23
Breast Cancer	
MCF7	-4.17
MDA-MB-231/ATCC	-43.73
HS 578T	83.36
BT-549	83.61
T-47D	-57.74
MDA-MB-468	-88.46
Mean	-.81
Delta	98.36
Range	203.01

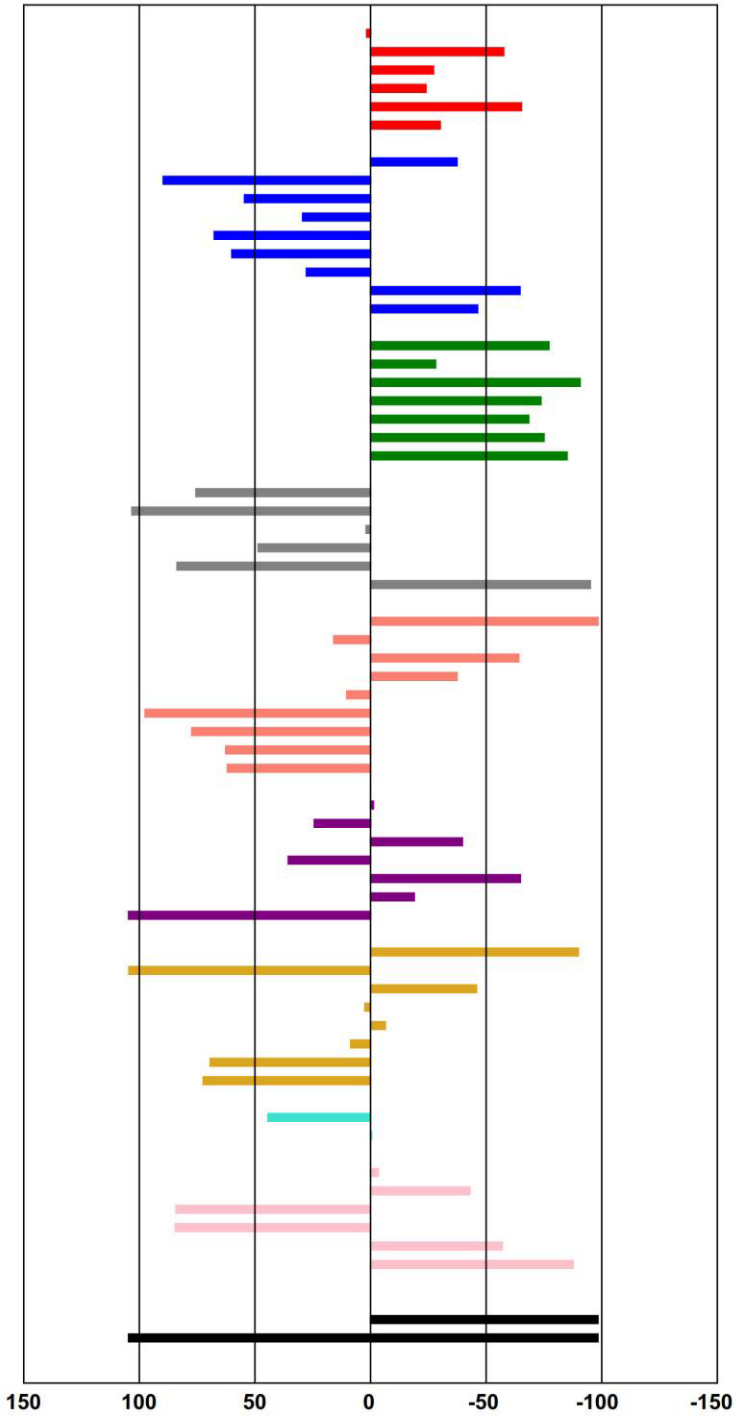

Figure S16. Anticancer screening data of compound 17 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-799582 / 1	Conc: 1.00E-5 Molar	Test Date: Jul 24, 2017
Experiment ID: 1707OS42		Report Date: Aug 17, 2017

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	93.13
HL-60(TB)	101.91
MOLT-4	66.97
RPMI-8226	95.01
SR	81.99
Non-Small Cell Lung Cancer	
A549/ATCC	92.00
EKVX	96.88
HOP-62	92.38
HOP-92	83.99
NCI-H226	97.86
NCI-H23	104.36
NCI-H322M	98.16
NCI-H460	99.60
NCI-H522	100.64
Colon Cancer	
COLO 205	94.17
HCC-2998	100.27
HCT-116	84.05
HCT-15	98.94
HT29	69.79
KM12	95.42
SW-620	98.64
CNS Cancer	
SF-268	85.30
SF-295	105.62
SF-539	91.23
SNB-19	99.35
SNB-75	78.07
U251	91.42
Melanoma	
LOX IMVI	97.13
MALME-3M	101.93
M14	92.64
MDA-MB-435	92.16
SK-MEL-2	99.51
SK-MEL-28	104.73
SK-MEL-5	98.32
UACC-257	113.98
UACC-62	97.99
Ovarian Cancer	
IGROV1	98.11
OVCAR-3	89.77
OVCAR-4	91.97
OVCAR-5	98.33
OVCAR-8	113.99
NCI/ADR-RES	105.43
SK-OV-3	110.01
Renal Cancer	
786-0	94.03
A498	100.24
ACHN	102.50
CAKI-1	81.57
RXF 393	91.38
SN12C	101.25
TK-10	100.39
UO-31	95.49
Prostate Cancer	
PC-3	83.47
DU-145	96.45
Breast Cancer	
MCF7	87.35
MDA-MB-231/ATCC	118.35
HS 578T	99.38
BT-549	102.81
T-47D	87.51
MDA-MB-468	86.90
Mean	95.46
Delta	28.49
Range	51.38

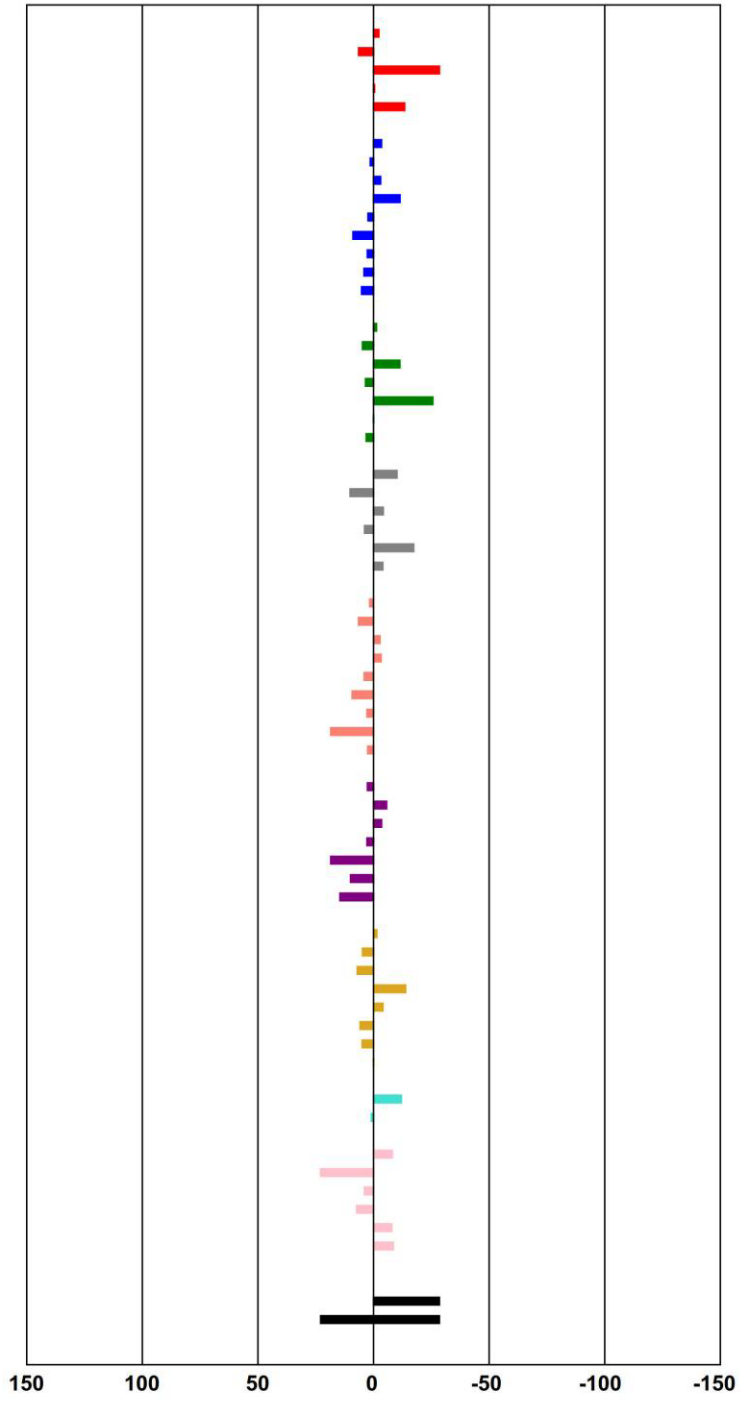

Figure S17. Anticancer screening data of compound 19 at single dose assay

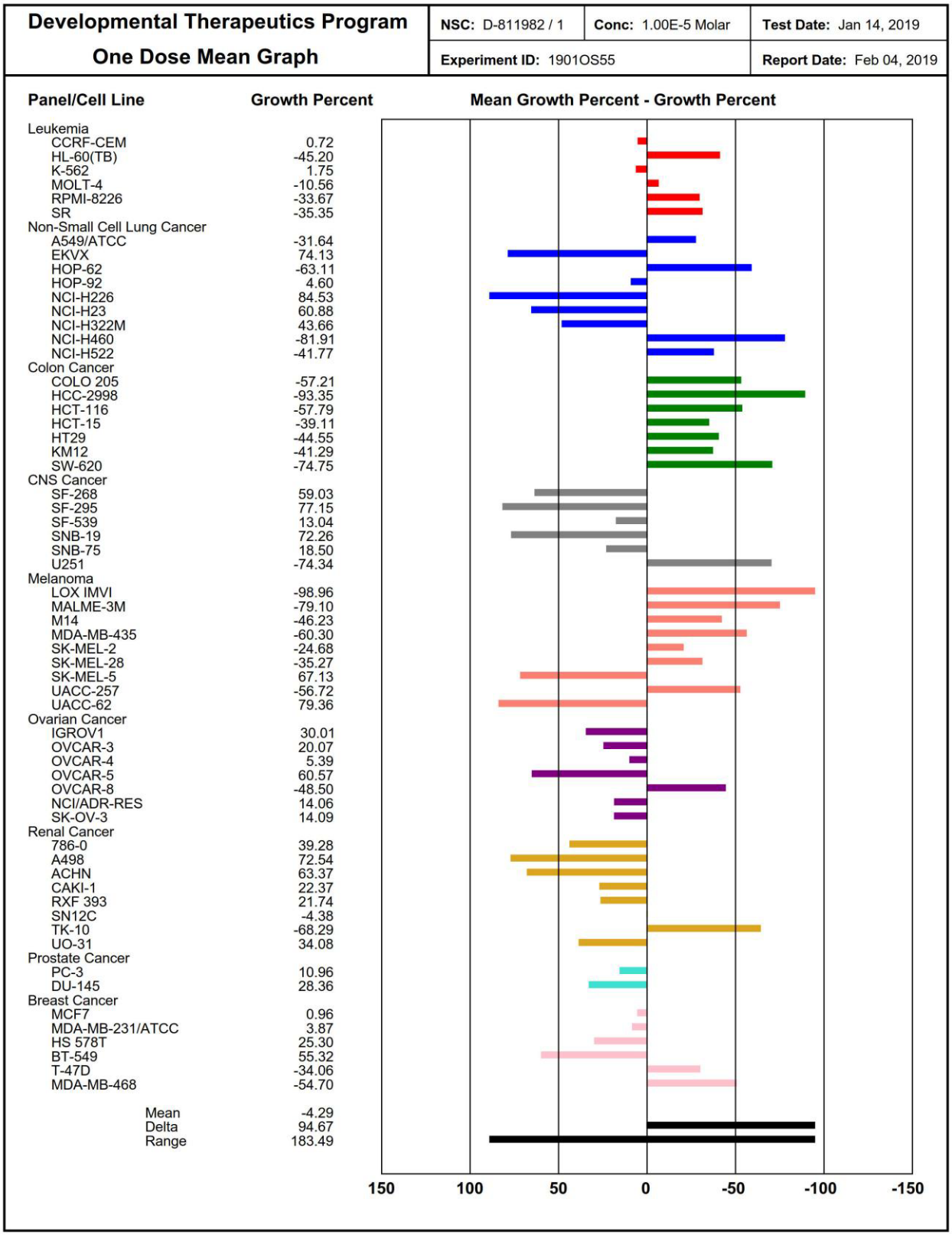

Figure S18. Anticancer screening data of compound 20 at single dose assay

Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-811985 / 1	Conc: 1.00E-5 Molar	Test Date: Jan 14, 2019
Experiment ID: 1901OS55		Report Date: Feb 04, 2019

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	0.79
HL-60(TB)	-57.96
K-562	0.27
MOLT-4	-10.47
RPMI-8226	-33.32
SR	-31.42
Non-Small Cell Lung Cancer	
A549/ATCC	-62.20
EKVX	42.52
HOP-62	-54.91
HOP-92	-52.89
NCI-H226	90.80
NCI-H23	-37.10
NCI-H322M	-14.29
NCI-H460	-86.19
NCI-H522	-43.10
Colon Cancer	
COLO 205	-64.41
HCC-2998	-92.03
HCT-116	-86.55
HCT-15	-82.03
HT29	-38.71
KM12	-71.73
SW-620	-80.83
CNS Cancer	
SF-268	-55.77
SF-295	73.26
SF-539	-89.96
SNB-19	34.30
SNB-75	-6.45
U251	-64.47
Melanoma	
LOX IMVI	-100.00
MALME-3M	-45.18
M14	-66.22
MDA-MB-435	-96.77
SK-MEL-2	-52.49
SK-MEL-28	-79.83
SK-MEL-5	17.55
UACC-257	-60.39
UACC-62	77.64
Ovarian Cancer	
IGROV1	6.46
OVCAR-3	-58.79
OVCAR-4	-55.44
OVCAR-5	19.15
OVCAR-8	-38.66
NCI/ADR-RES	-40.75
SK-OV-3	8.02
Renal Cancer	
786-0	-97.28
A498	68.30
ACHN	-94.94
CAKI-1	-81.62
RXF 393	-69.50
SN12C	-13.45
TK-10	-68.36
UO-31	47.22
Prostate Cancer	
PC-3	-33.98
DU-145	-72.65
Breast Cancer	
MCF7	-78.49
MDA-MB-231/ATCC	-75.70
HS 578T	-51.23
BT-549	80.04
T-47D	-43.69
MDA-MB-468	-62.10
Mean	-36.47
Delta	63.53
Range	190.80

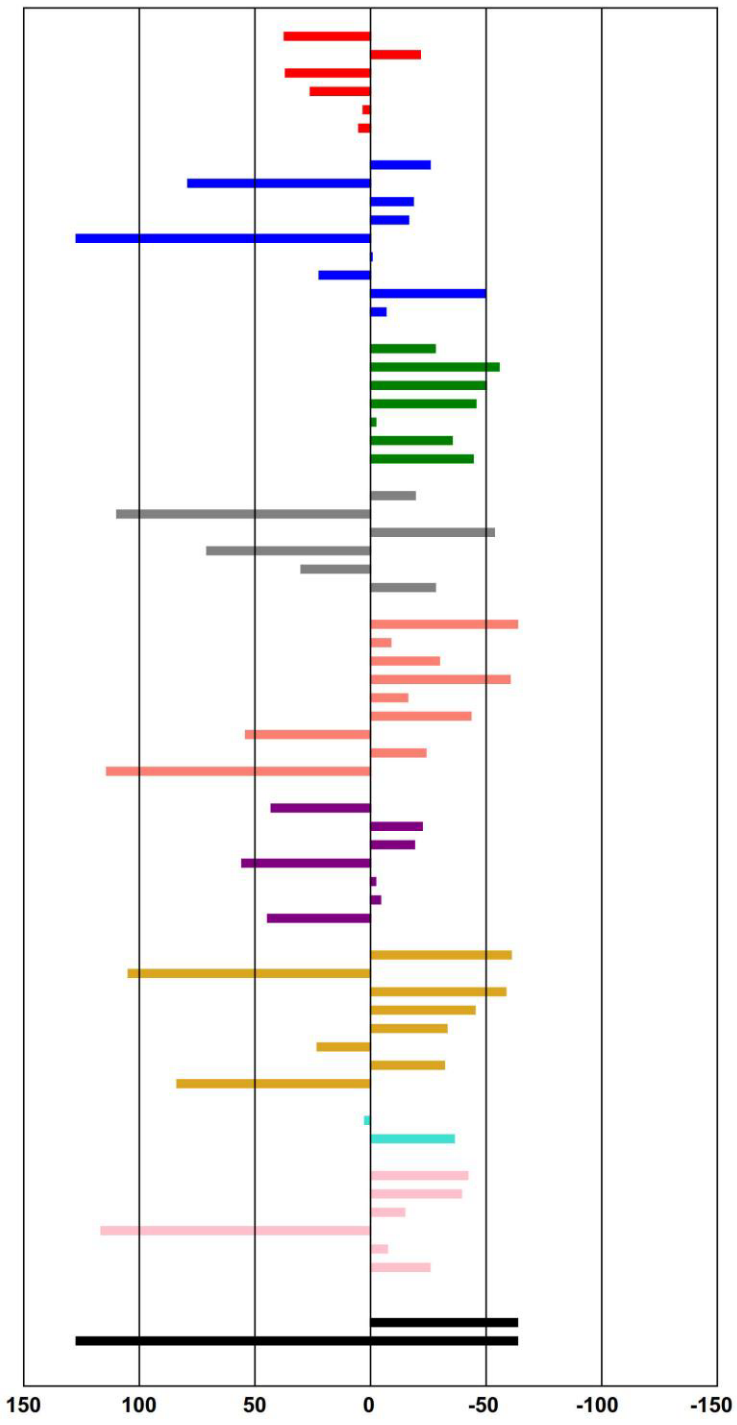

Figure S19. Anticancer screening data of compound 1 at a 5-dose assay

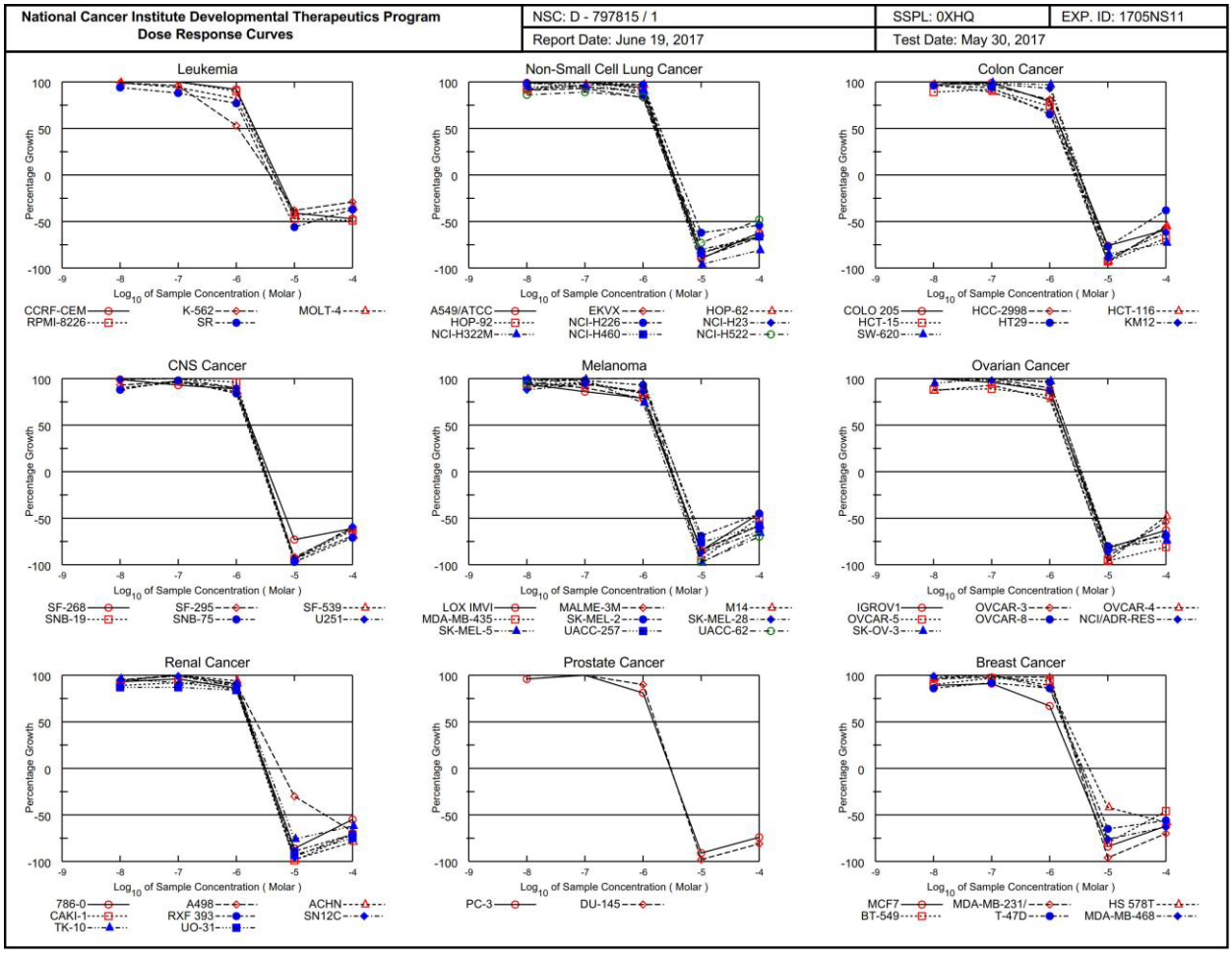

Figure S20. Anticancer screening data of compound 3 at a 5-dose assay

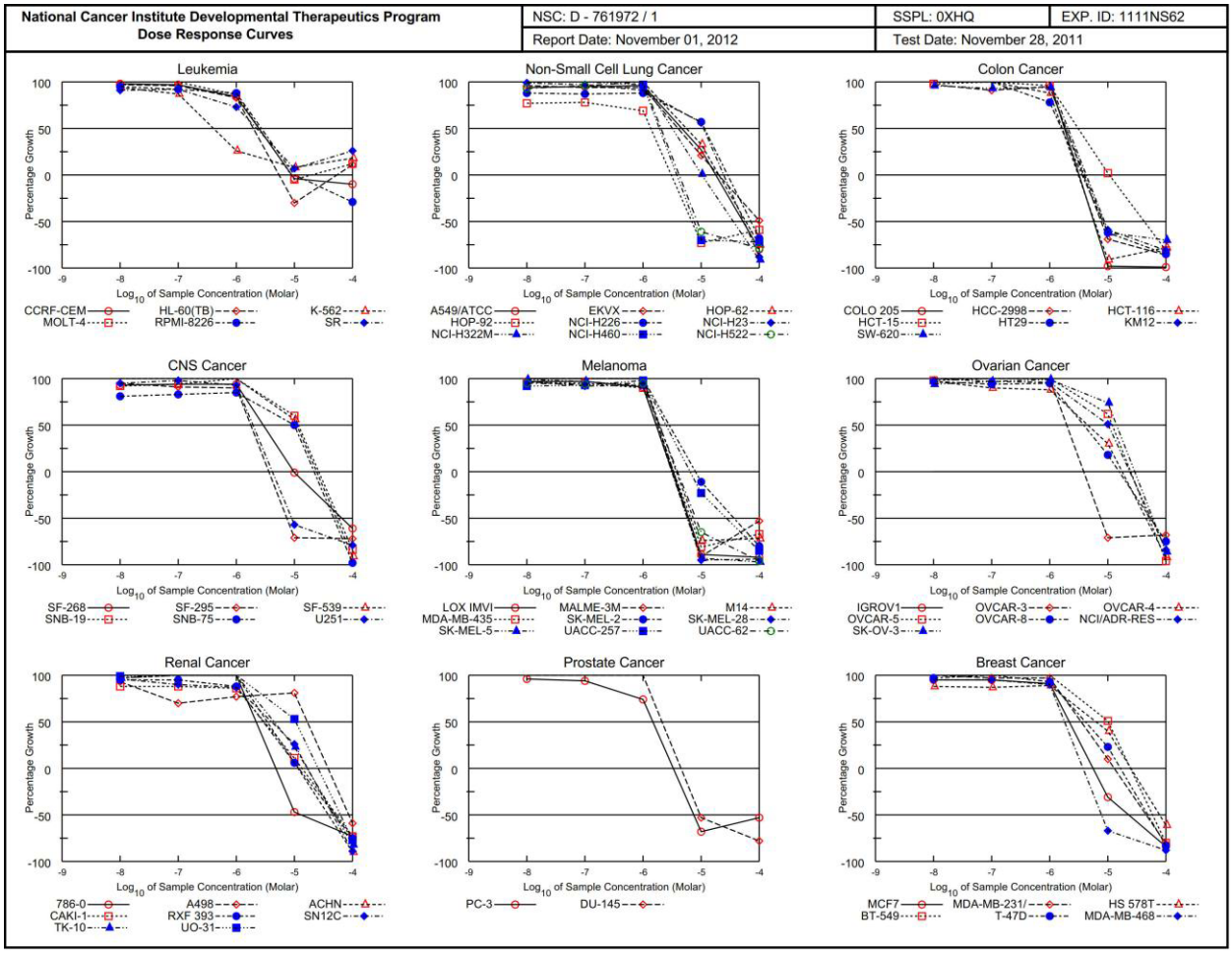

Figure S21. Anticancer screening data of compound 4 at a 5-dose assay

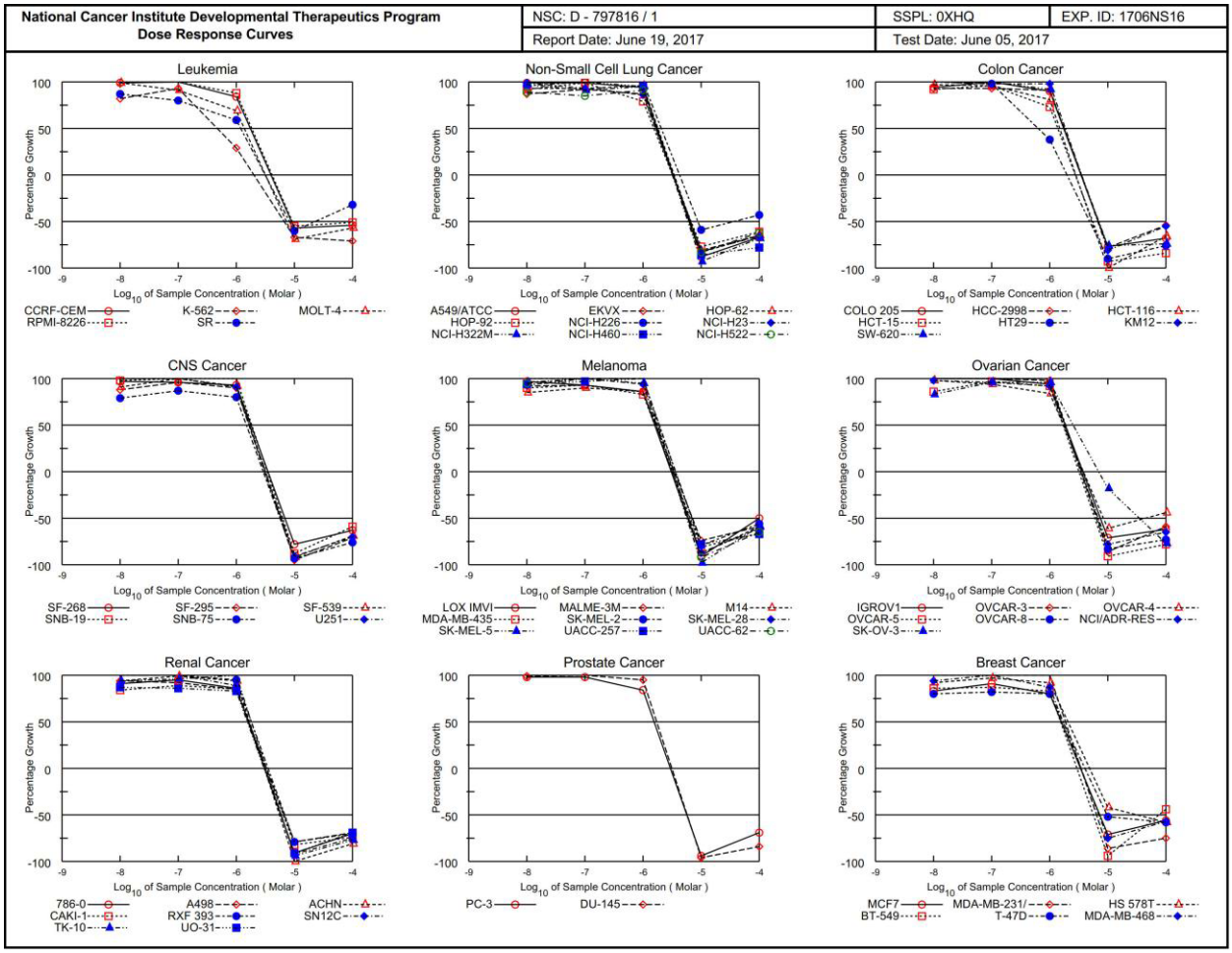

Figure S22. Anticancer screening data of compound 6 at a 5-dose assay

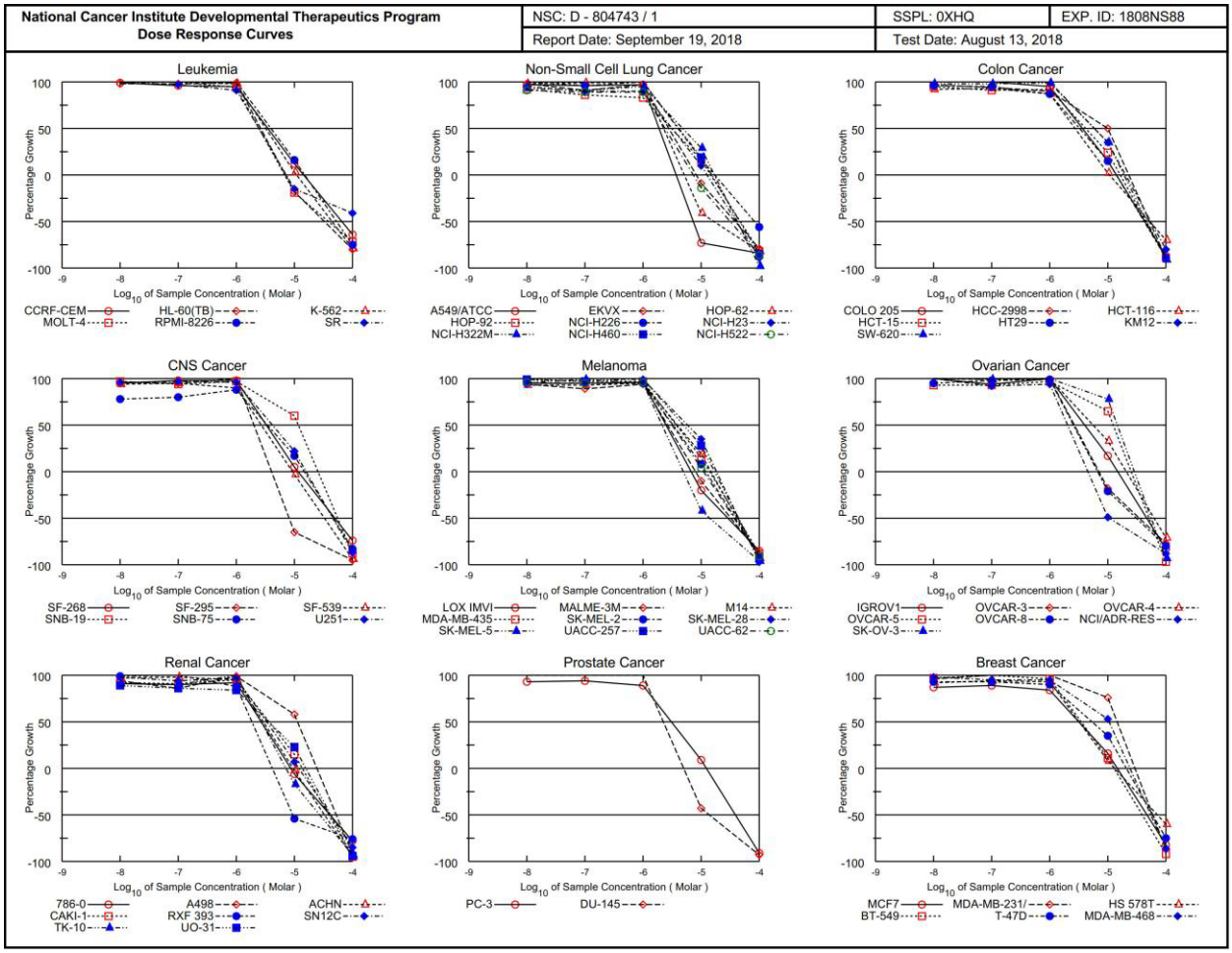

Figure S23. Anticancer screening data of compound 7 at a 5-dose assay

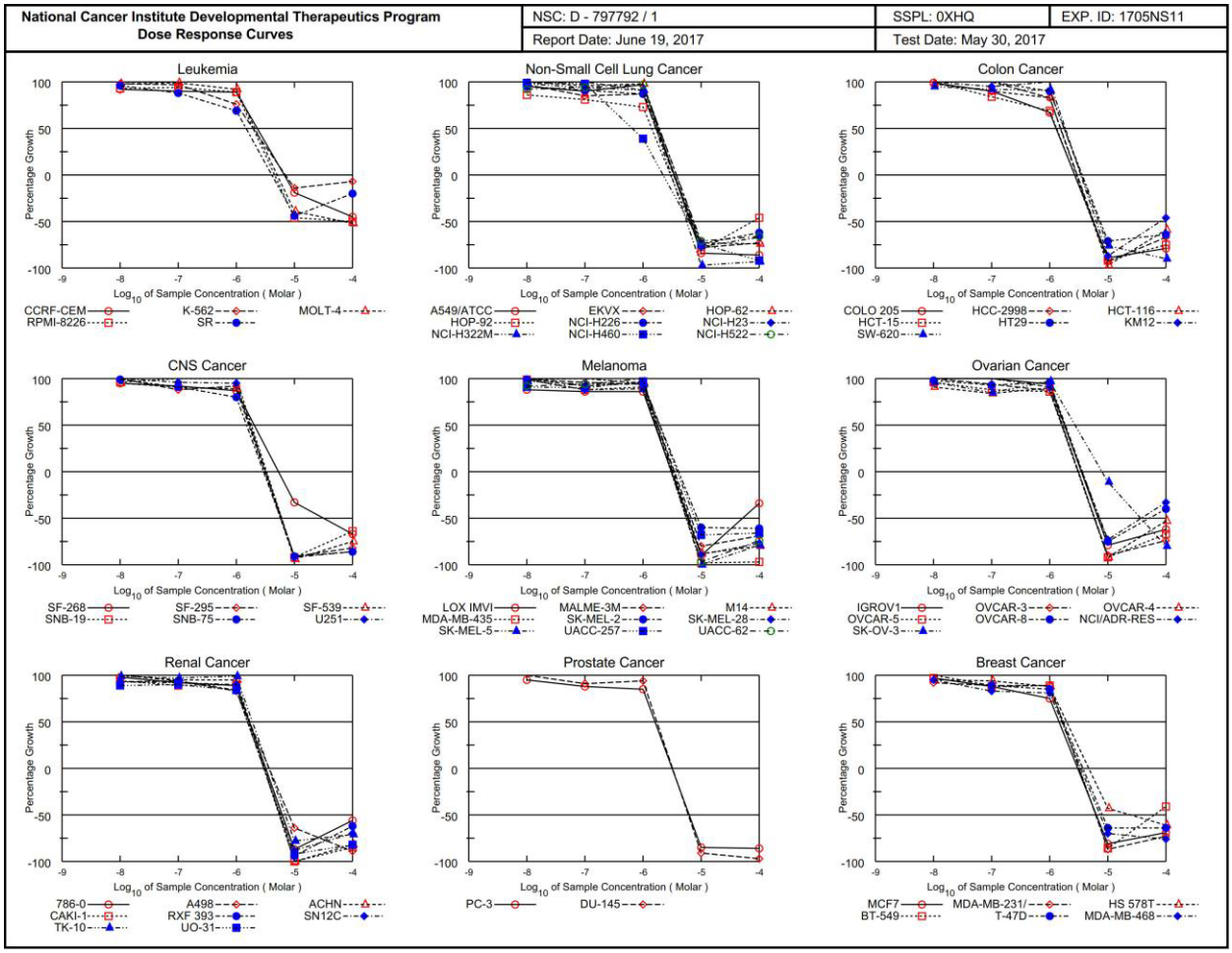

Figure S24. Anticancer screening data of compound 8 at a 5-dose assay

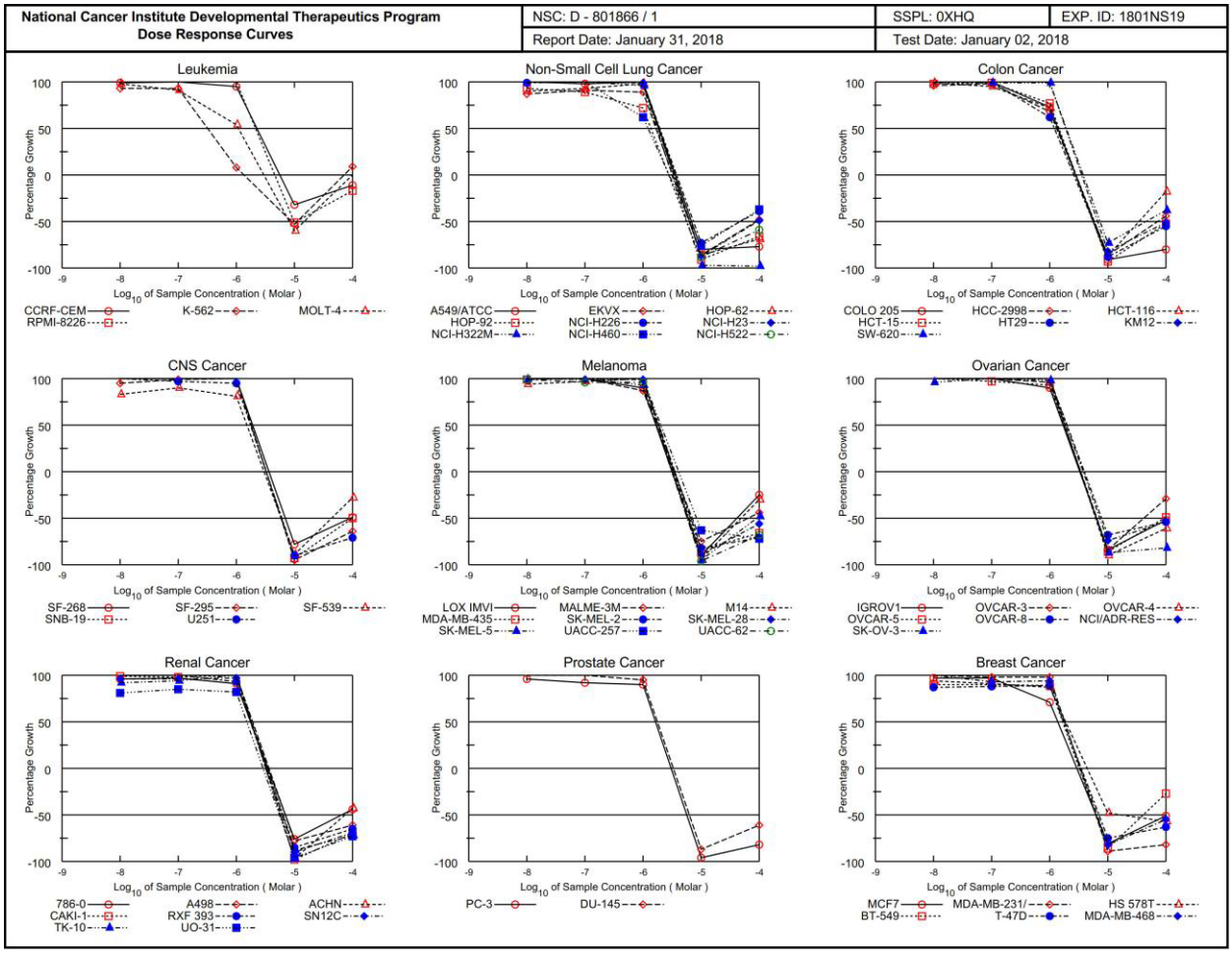

Figure S25. Anticancer screening data of compound 9 at a 5-dose assay

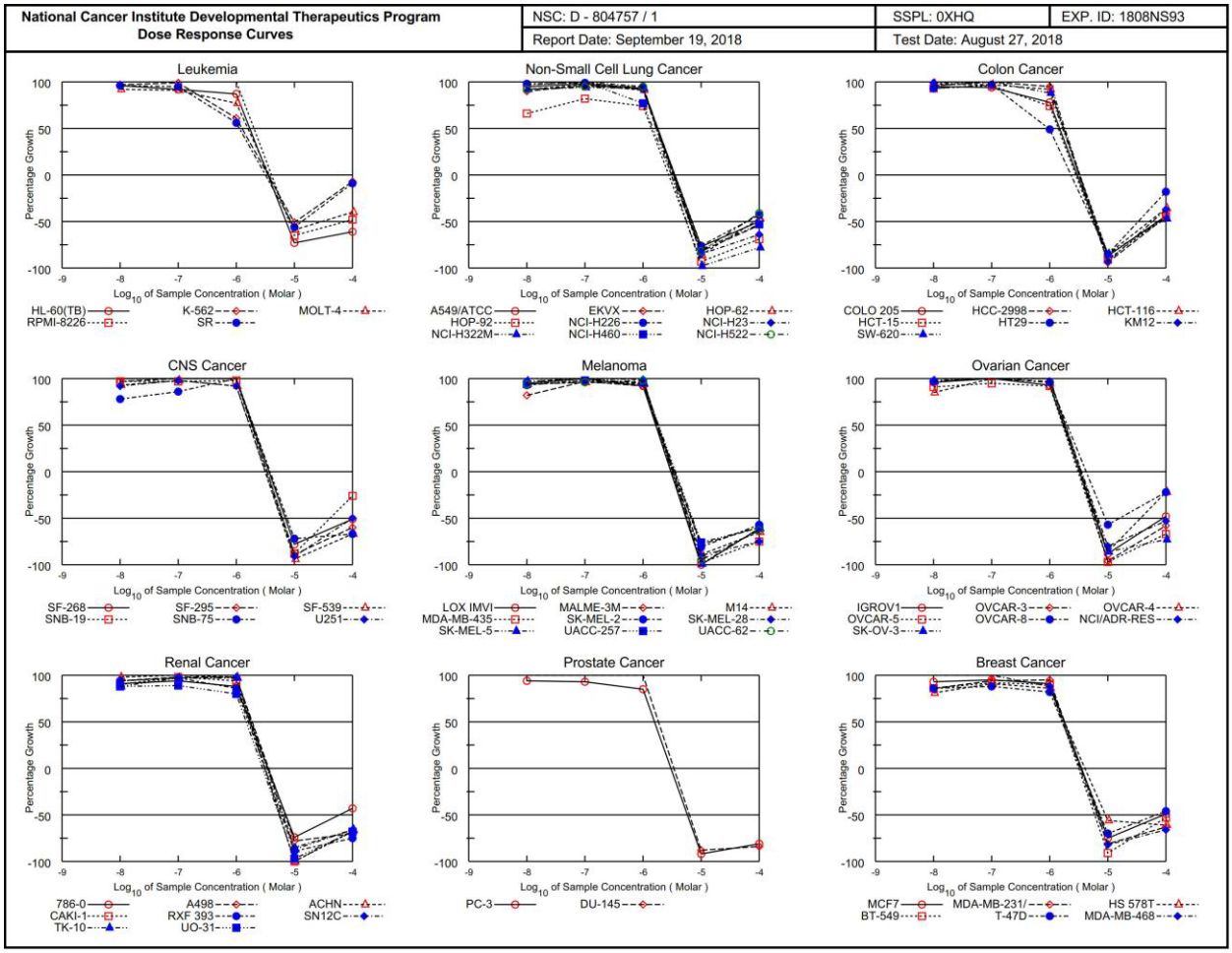

Figure S26. Anticancer screening data of compound 11 at a 5-dose assay

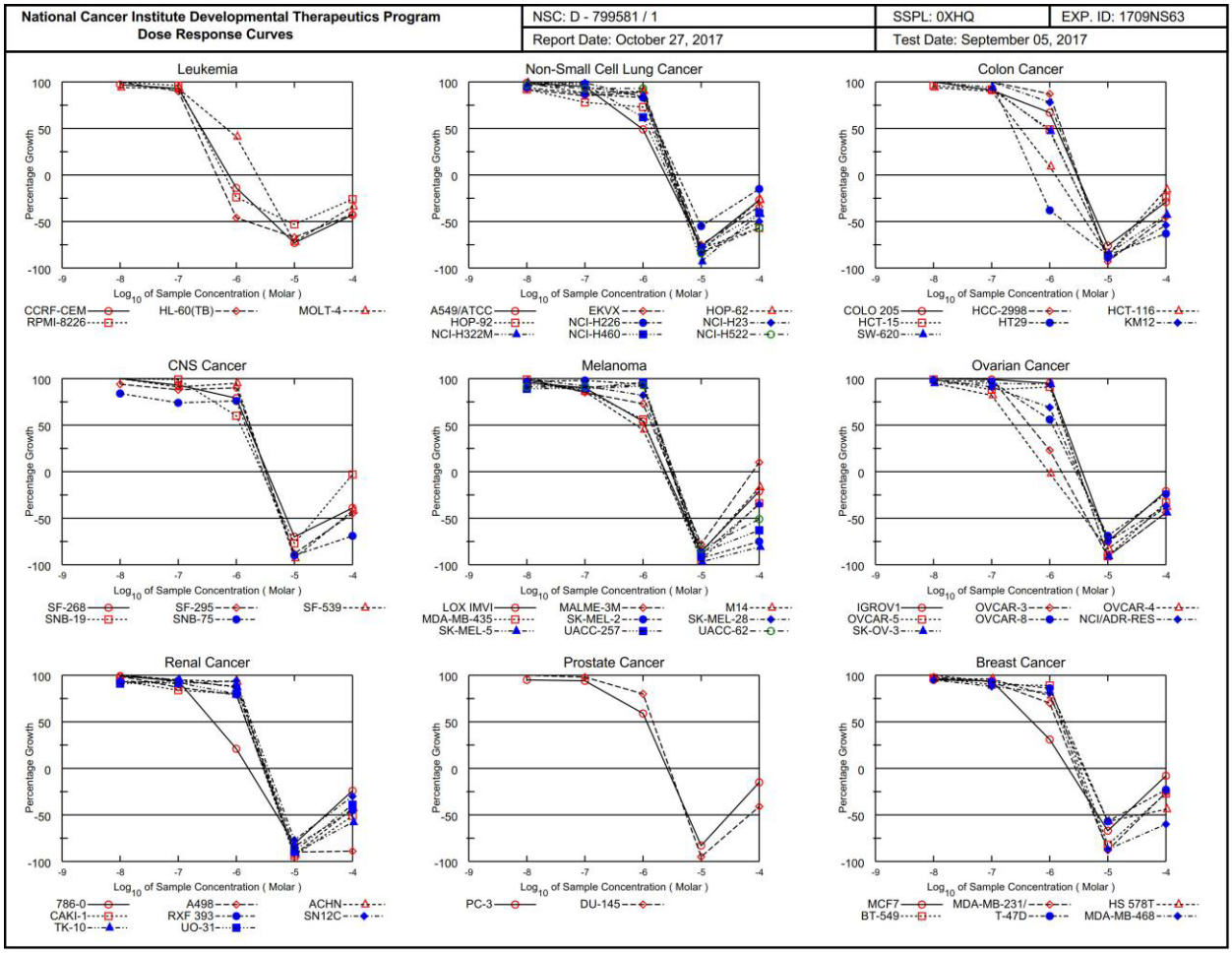

Figure S27. Anticancer screening data of compound 12 at a 5-dose assay

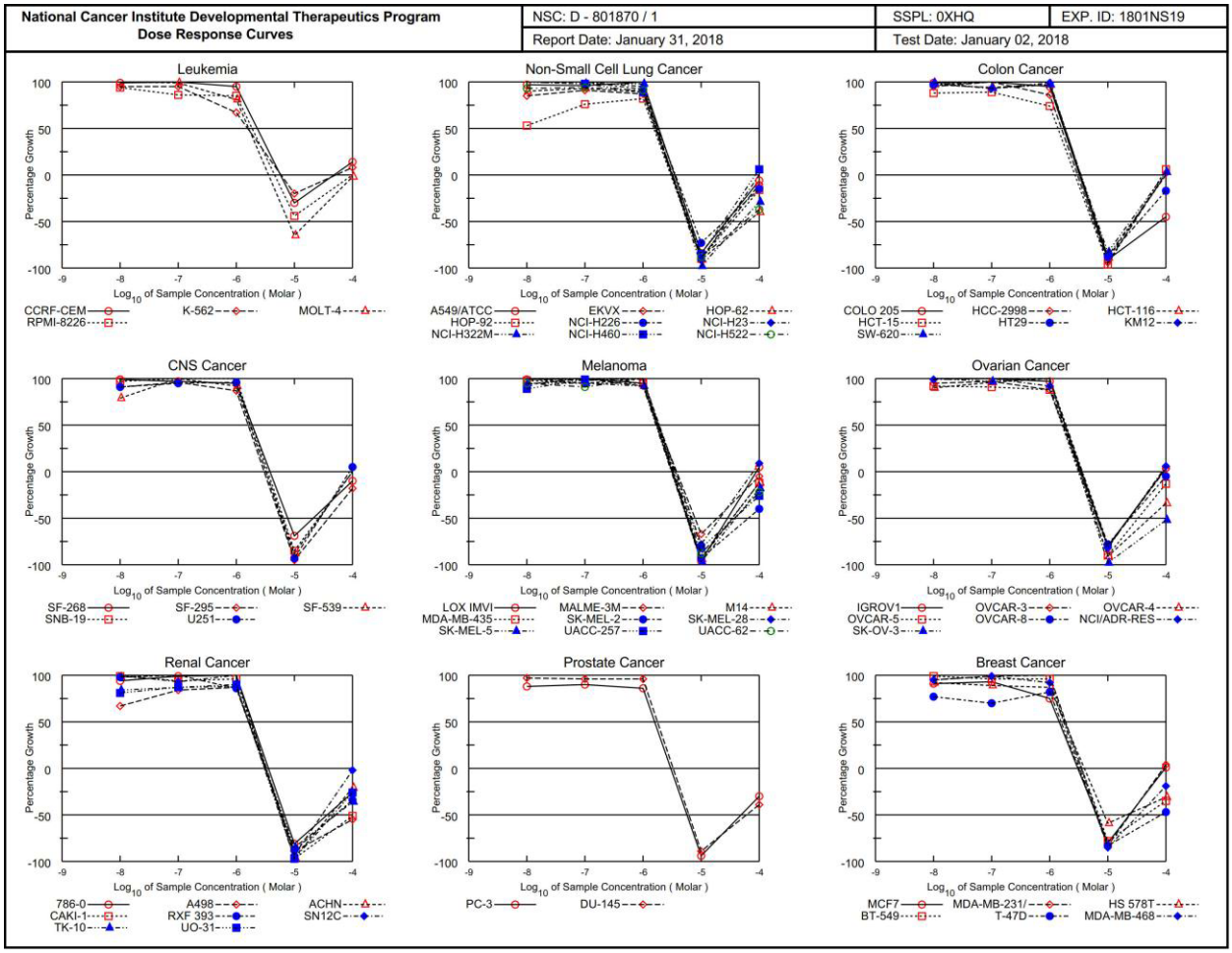

Figure S28. Anticancer screening data of compound 14 at a 5-dose assay

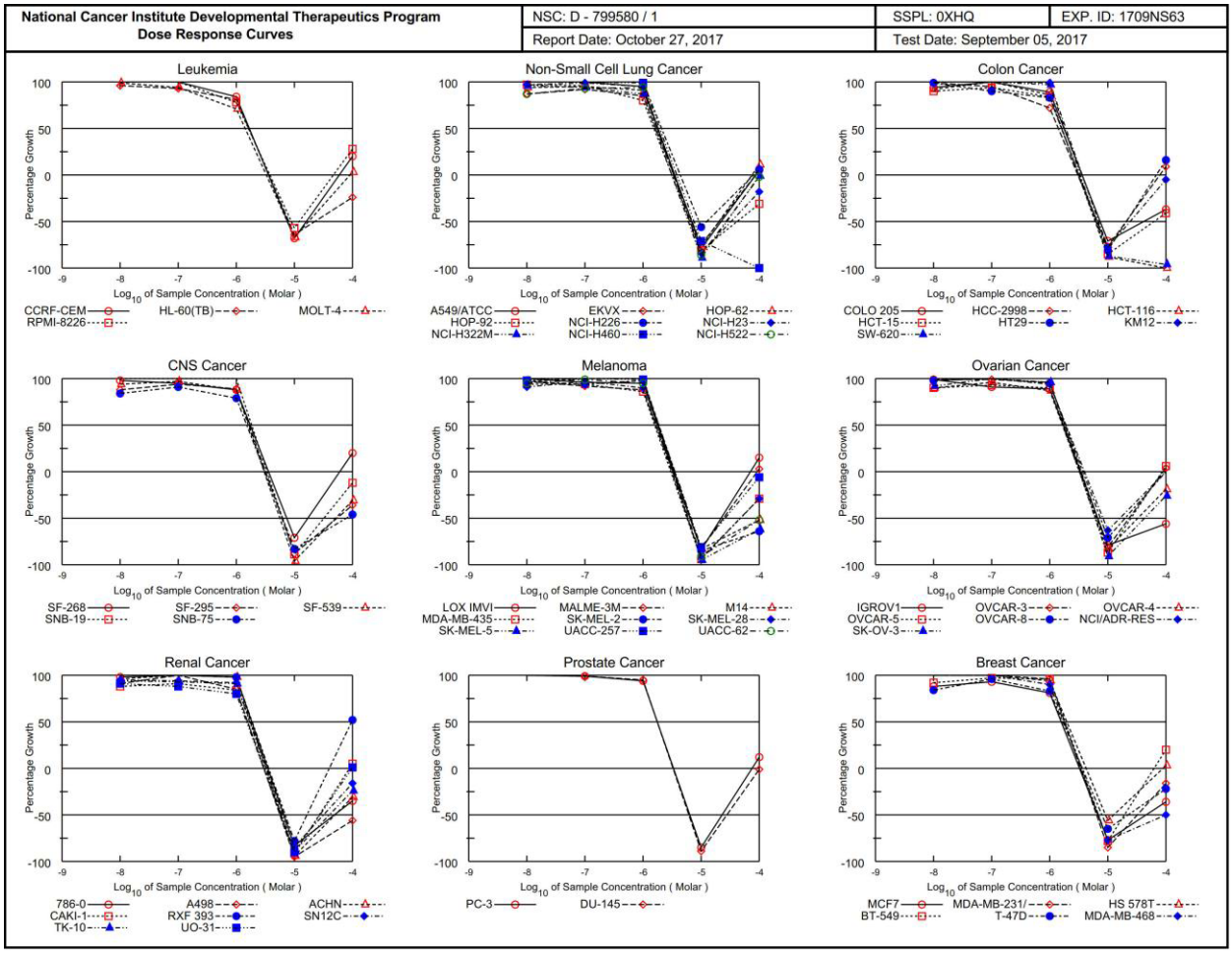

Figure S29. Anticancer screening data of compound 15 at a 5-dose assay

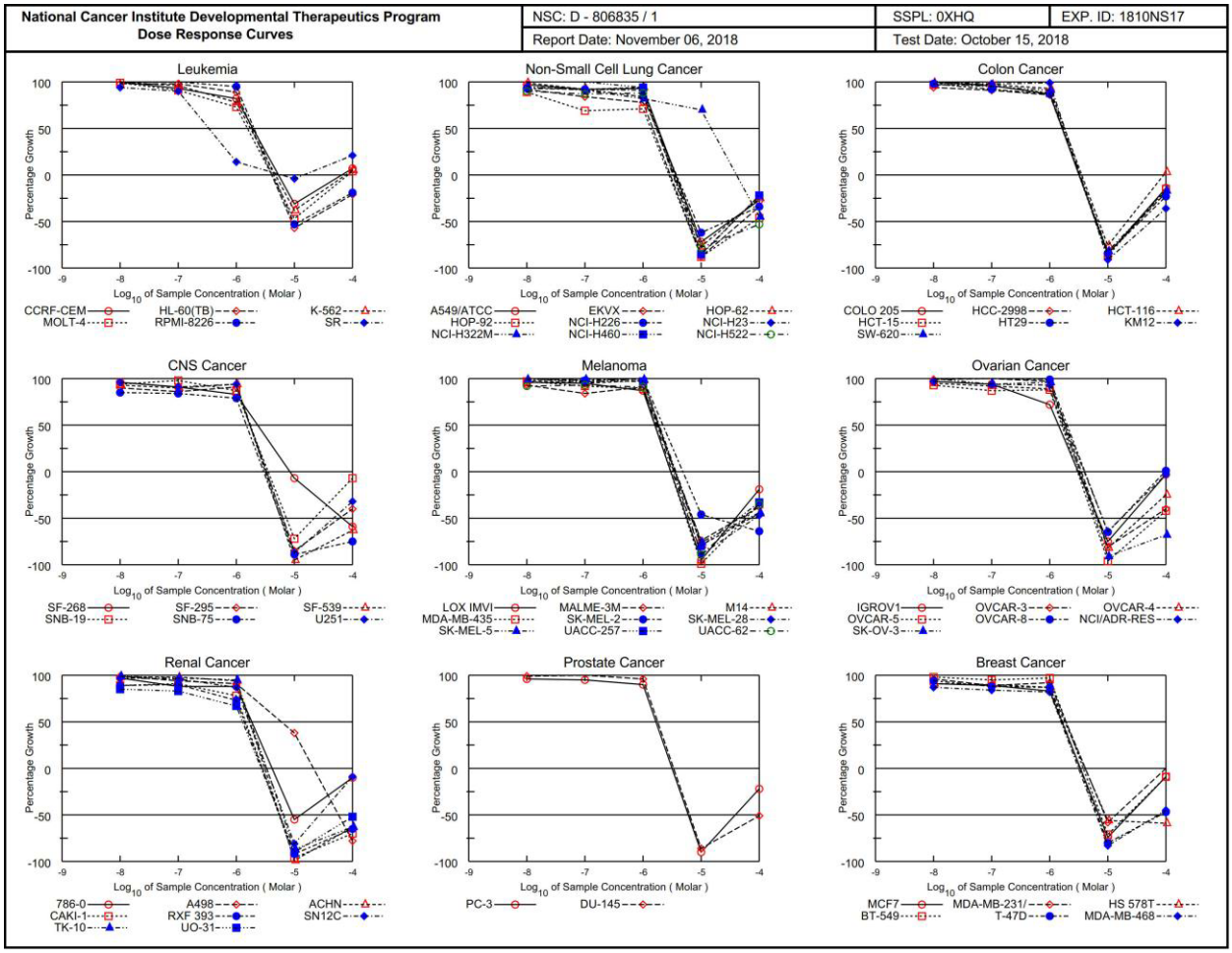

Figure S30. Anticancer screening data of compound 16 at a 5-dose assay

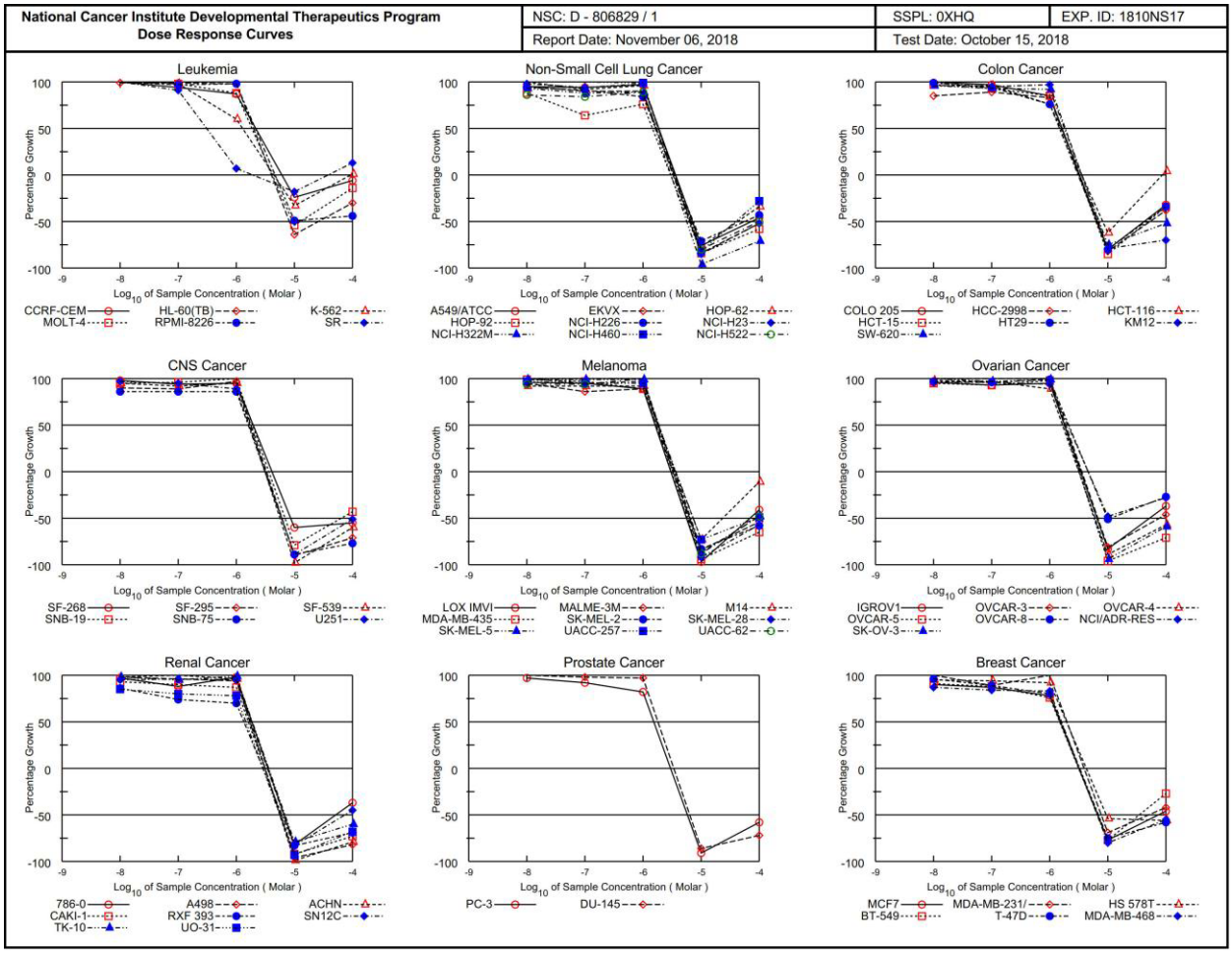

Figure S31. Anticancer screening data of compound 19 at a 5-dose assay

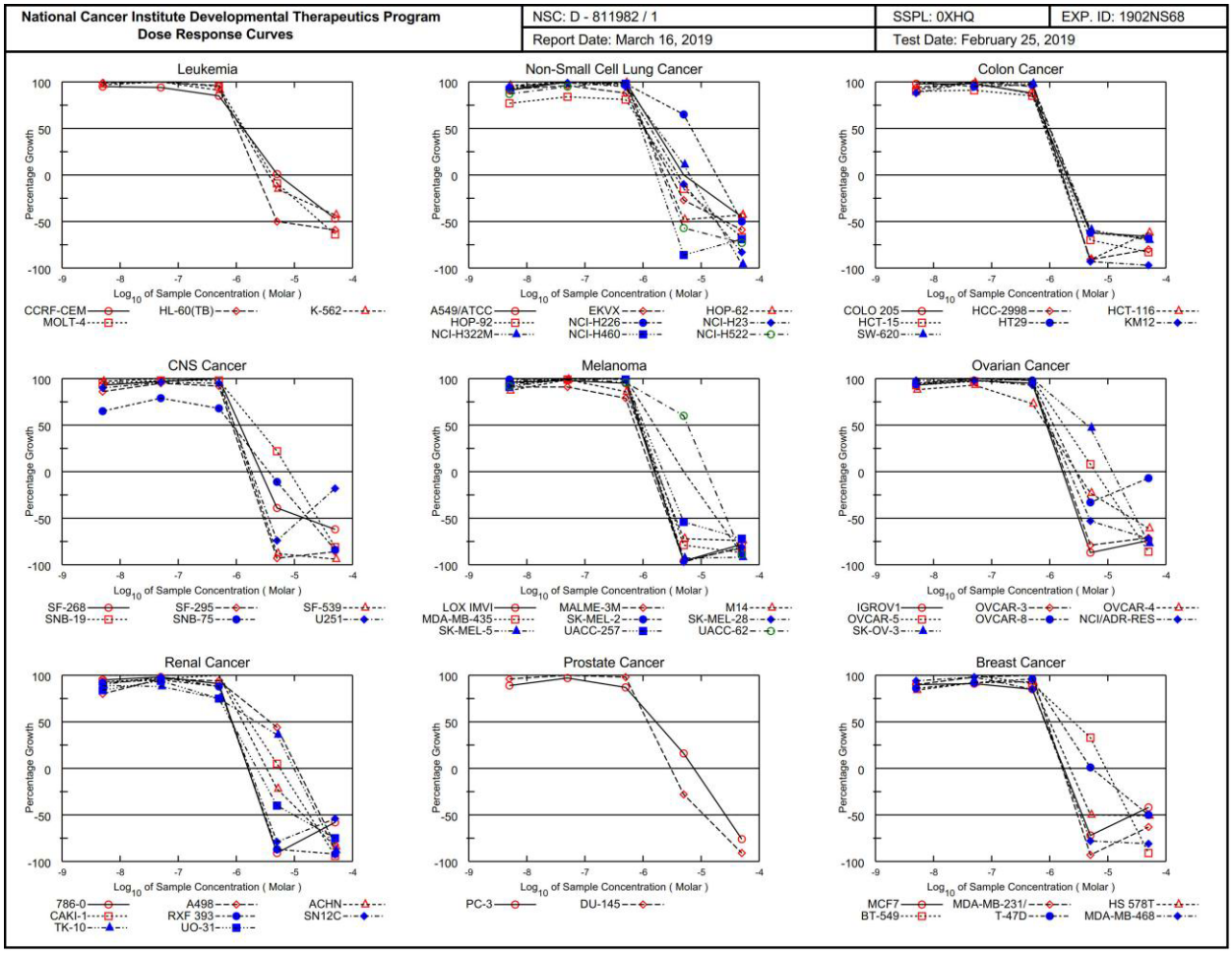

Figure S32. Anticancer screening data of compound 20 at a 5-dose assay

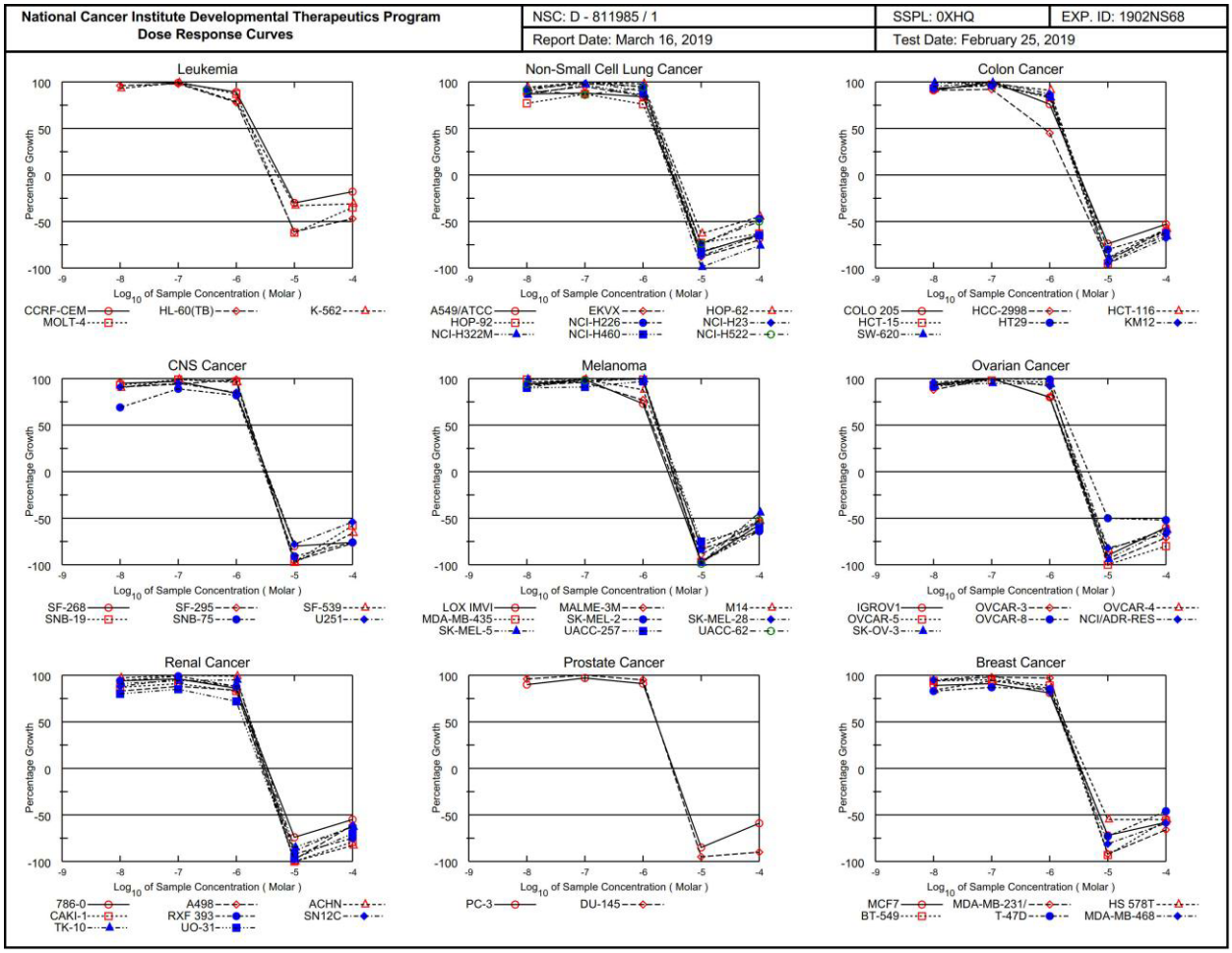

Table S1. Influence of compounds 1, 3, 4, 6, 7-9, 11, 12, 14-16, 19, 20 and standard drugs doxorubicin (DRB) and 5-fluorouracil (5-FU) on the growth of individual tumor cell panel.

Panel/cell line	GI_{50}[a], μM															
	1	3	4	6	7	8	9	11	12	14	15	16	19	20	DRB	5-FU
Leukemia																
CCRF-CEM	2.07	2.41	1.74	3.52	2.32	2.27	NT	0.25	2.28	1.67	1.93	2.14	1.31	2.12	0.08	9.97
HL-60(TB)	NT	1.95	NT	2.63	NT	NT	1.70	0.20	NT	1.64	1.85	1.98	1.03	1.58	0.19	2.30
K-562	1.08	0.40	0.47	3.18	1.96	0.32	1.25	NT	1.57	NT	1.75	1.28	1.22	1.80	NT	3.58
MOLT-4	1.79	2.50	1.37	2.46	2.10	1.09	1.59	0.67	1.62	1.42	1.55	1.84	1.35	1.78	0.03	0.35
RPMI-8226	1.94	2.71	1.85	3.91	1.94	2.26	2.06	0.24	1.86	1.60	2.03	2.12	NT	NT	0.08	0.04
SR	1.59	2.22	1.18	2.42	1.49	NT	1.14	NT	NT	NT	0.34	0.31	NT	NT	0.03	NT
MG_MID	1.69	2.03	1.32	3.02	1.96	1.48	1.55	0.34	1.83	1.58	1.57	1.61	1.23	1.82	0.08	3.25
NSC lung cancer																
A549/ATCC	1.73	4.62	1.74	1.89	1.81	2.02	1.79	0.96	1.87	1.81	1.83	1.86	1.59	1.60	0.06	0.18
EKVX	1.55	4.04	1.66	2.77	1.68	1.66	1.74	1.73	1.62	1.66	1.48	1.70	1.08	1.60	0.41	NT
HOP-62	1.81	5.89	1.81	2.30	1.91	1.82	1.70	1.71	1.65	1.76	1.81	1.84	1.08	1.98	0.07	0.39
HOP-92	1.73	1.36	1.52	3.10	1.41	1.37	1.39	1.42	1.54	1.54	1.35	1.45	1.04	1.48	0.10	77.9
NCI-H226	1.98	1.13	2.07	4.00	1.70	1.97	1.79	1.74	1.81	2.10	1.71	1.66	6.72	1.85	0.05	54.7
NCI-H23	1.71	1.11	1.65	3.15	1.76	1.83	1.78	1.60	1.75	1.76	1.70	1.82	1.34	1.77	0.15	0.33
NCI-H322M	1.63	3.69	1.73	4.78	1.64	1.73	1.68	1.55	1.76	1.72	14.9	1.62	1.74	1.57	NT	NT
NCI-H460	1.63	1.92	1.78	4.17	0.65	1.22	1.48	1.21	1.68	1.94	1.77	1.85	0.91	1.71	0.02	0.05
NCI-H522	1.65	2.04	1.71	2.38	1.90	1.93	1.80	1.75	1.70	1.75	1.69	1.70	1.04	1.83	0.03	7.27
MG_MID	1.71	2.87	1.74	3.17	1.49	1.73	1.68	1.52	1.71	1.78	3.14	1.72	1.84	1.71	0.11	20.12
Colon Cancer																
COLO 205	1.54	1.83	1.74	3.63	1.28	1.38	1.48	1.31	1.75	1.75	1.63	1.62	0.90	1.49	0.18	0.15
HCC-2998	1.51	1.89	1.75	10.1	1.54	1.31	1.74	1.61	1.58	1.40	1.63	1.58	0.87	0.79	0.26	0.05
HCT-116	1.29	1.64	1.49	2.73	1.52	1.37	1.73	0.31	1.79	1.60	1.80	1.54	0.81	1.69	0.08	0.22
HCT-15	1.39	3.06	1.39	4.21	1.31	1.44	1.40	0.97	1.38	1.59	1.65	1.61	0.84	1.53	6.46	0.11
HT29	1.27	1.59	0.63	3.25	1.78	1.20	0.94	0.24	1.93	1.59	1.64	1.48	0.99	1.63	0.12	0.17
KM12	1.73	2.07	1.84	6.09	1.86	1.93	1.92	1.47	1.84	1.89	1.82	1.86	0.91	1.60	0.27	0.21
SW-620	1.81	1.91	1.79	5.76	1.75	1.92	1.66	0.85	1.83	1.80	1.73	1.78	1.01	1.56	0.09	0.92
MG_MID	1.51	1.99	1.52	5.11	1.58	1.51	1.55	0.96	1.73	1.66	1.70	1.64	0.90	1.47	1.06	0.26
CNS cancer																
SF-268	1.74	2.90	1.79	3.27	2.04	1.91	1.97	1.56	1.88	1.73	2.32	1.95	1.22	1.61	0.10	1.62
SF-295	1.66	1.77	1.64	2.00	1.70	1.81	1.87	1.67	1.60	1.65	1.71	1.78	0.85	1.78	0.10	NT
SF-539	1.58	11.0	1.69	2.69	1.64	1.52	1.69	1.73	1.70	1.61	1.71	1.71	0.95	1.73	0.12	0.06
SNB-19	1.75	11.7	1.86	11.6	1.85	1.93	1.81	1.17	2.04	1.85	1.72	1.91	2.14	1.75	0.04	3.81
SNB-75	1.54	9.84	1.49	3.43	1.50	NT	1.98	1.43	NT	1.52	1.48	1.61	0.85	1.53	0.07	78.7
U251	1.65	1.94	1.67	4.17	1.74	1.76	1.69	NT	1.75	NT	1.74	1.66	0.92	1.64	0.04	0.92
MG_MID	1.65	6.53	1.69	4.53	1.58	1.79	1.83	1.51	1.79	1.67	1.78	1.77	1.15	1.67	0.08	17.02
Melanoma																
LOX IMVI	1.51	1.68	1.59	2.49	1.60	1.67	1.65	1.07	1.72	1.78	1.60	1.63	0.86	1.37	0.07	0.24
MALME-3M	1.50	2.02	1.68	2.64	1.79	1.70	1.77	1.42	1.84	1.66	1.77	1.68	0.73	1.46	0.12	0.05
M14	1.58	2.04	1.61	3.91	1.77	1.89	1.73	0.74	1.83	1.94	1.87	1.80	0.85	1.69	0.18	0.98
MDA-MB-435	1.56	1.71	1.59	3.76	1.65	1.87	1.85	1.10	1.73	1.58	1.61	1.64	0.95	1.78	0.25	0.07
SK-MEL-2	1.84	3.25	1.90	3.31	1.95	2.01	1.81	1.72	1.84	1.84	2.19	1.88	1.73	1.92	0.17	56.7
SK-MEL-28	1.62	1.70	1.75	5.87	1.66	1.81	1.81	1.55	2.15	1.66	1.84	1.77	0.95	1.82	0.21	1.03
SK-MEL-5	1.38	1.68	1.70	2.14	1.69	1.70	1.70	1.67	1.67	1.85	1.90	1.82	0.91	1.72	0.08	0.46
UACC-257	1.95	2.49	1.95	5.24	1.92	2.19	1.86	1.78	1.97	1.87	1.85	1.85	1.07	1.82	0.14	3.55
UACC-62	1.82	1.92	1.85	3.13	1.79	1.73	1.77	1.76	2.05	1.74	1.68	1.84	5.82	1.78	0.12	0.52
MG_MID	1.64	2.05	1.74	3.61	1.76	1.84	1.77	1.42	1.87	1.77	1.81	1.77	1.54	1.71	0.15	7.07
Ovarian Cancer																
IGROV1	1.65	NT	1.85	4.08	1.79	1.69	1.73	1.83	1.84	1.70	1.41	1.79	0.89	1.50	0.17	1.22
OVCAR-3	1.66	1.96	1.83	2.69	1.62	1.79	1.91	0.46	1.67	1.81	1.84	1.88	0.93	1.48	0.39	0.01
OVCAR-4	1.45	4.48	1.72	5.63	1.65	1.86	1.99	0.24	1.86	1.66	1.69	1.66	0.86	1.53	0.37	4.43
OVCAR-5	1.51	11.9	1.69	1.24	1.60	1.75	1.67	1.69	1.64	1.68	1.61	1.77	1.76	1.71	0.41	10.9
OVCAR-8	1.83	3.83	1.96	2.55	1.87	1.99	2.01	1.12	1.91	1.86	1.99	2.12	1.16	2.13	0.10	1.74
NCI/ADR-RES	1.63	10.2	1.76	2.02	1.78	1.98	1.84	1.35	1.74	1.91	1.89	2.05	0.99	1.74	7.16	0.31
SK-OV-3	1.83	14.1	2.54	14.5	2.73	1.81	1.89	1.73	1.87	1.77	1.76	1.79	4.42	1.72	0.22	21.8
MG_MID	1.65	7.75	1.91	4.67	1.86	1.84	1.86	1.20	1.79	1.77	1.74	1.86	1.57	1.69	1.26	5.77
Renal Cancer																
786-0	1.62	2.25	1.60	2.66	1.66	1.76	1.71	0.40	1.92	1.85	1.85	1.84	0.84	1.68	0.13	0.72
A498	2.17	16.7	1.63	11.4	1.68	2.03	1.87	1.49	1.63	1.56	5.99	1.71	3.83	1.54	0.10	0.35
ACHN	1.70	3.44	1.69	2.93	1.71	1.84	1.76	1.71	1.98	1.77	1.68	1.72	1.42	1.76	0.08	0.27
CAKI-1	1.55	3.05	1.62	3.70	1.62	1.81	1.69	1.49	1.74	1.56	1.45	1.61	1.69	1.52	0.95	0.07
RXF 393	1.68	2.88	1.81	1.84	1.56	1.74	1.61	1.67	1.62	NT	1.38	1.35	0.83	1.62	0.10	2.61

SN12C	1.62	4.02	1.64	3.34	1.68	1.79	1.83	1.81	1.88	1.73	1.67	1.79	0.84	1.64	0.07	0.49
TK-10	1.76	4.64	1.84	2.66	1.89	1.88	1.81	1.61	1.66	1.69	1.77	1.88	2.21	1.78	NT	1.12
UO-31	1.56	10.5	1.54	3.59	1.56	1.52	1.47	1.50	1.64	1.50	1.29	1.46	0.82	1.34	0.49	1.42
MG_MID	1.71	5.94	1.47	4.01	1.67	1.79	1.72	1.46	1.76	1.66	2.13	1.67	1.56	1.61	0.27	0.88
Prostate cancer																
PC-3	2.94	1.48	1.55	3.05	1.61	1.65	1.58	1.16	1.58	1.76	1.66	1.53	1.65	1.70	0.32	2.36
DU-145	3.02	2.30	1.72	2.25	1.74	1.77	1.98	1.48	1.77	1.76	1.79	1.81	1.21	1.72	0.11	0.36
MG_MID	2.98	1.89	1.64	2.65	1.67	1.71	1.78	1.32	1.67	1.76	1.72	1.67	1.43	1.71	0.21	1.36
Breast cancer																
MCF7	1.29	2.16	1.58	3.14	1.44	1.37	1.77	0.49	1.45	1.56	1.62	1.51	0.83	1.60	0.03	0.07
MDA-MB-31/ATCC	1.77	3.50	1.88	14.5	1.66	1.81	1.80	1.34	1.88	1.80	1.91	1.98	0.96	1.77	0.51	6.60
HS 578T	1.99	6.16	2.05	3.20	1.96	1.87	1.79	1.61	1.79	1.96	1.82	1.94	0.99	1.80	0.33	9.77
BT-549	1.79	1.01	1.55	3.46	1.68	1.68	1.66	1.69	1.84	1.84	1.90	1.48	2.56	1.64	0.23	10.6
T-47D	1.73	4.08	1.68	5.38	1.71	1.72	1.63	1.80	1.57	1.67	1.67	1.55	1.51	1.67	0.06	8.12
MDA-MB-468	1.66	1.79	1.70	10.4	1.61	1.78	1.68	1.52	1.74	1.74	1.56	1.59	0.82	1.58	0.05	NT
MG_MID	1.71	3.12	1.74	6.68	1.68	1.71	1.72	1.41	1.71	1.76	1.75	1.67	1.28	1.68	0.19	7.03
MG_MID$_{60}$	1.70	3.83	1.65	4.21	1.68	1.73	1.75	1.29	1.77	1.72	1.99	1.72	1.42	1.66	0.38	6.97

[a]GI_{50} was the drug concentration resulting in a 50% reduction in the net protein increase (as measured by SRB staining) in control cells during the drug incubation, determined at five concentration levels (100, 10, 1.0, 0.1 and 0.01 µM).

Table S2. Influence of compounds 1, 3, 4, 6, 7-9, 11, 12, 14-16, 19, 20 on the growth of individual tumor cell panel.

Panel/cell line	TGI[a], μM													
	1	3	4	6	7	8	9	11	12	14	15	16	19	20
Leukemia														
CCRF-CEM	4.91	8.96	3.93	14.5	6.73	5.63	NT	0.74	NT	NT	NT	6.06	5.26	5.56
HL-60(TB)	NT	NT	NT	7.02	NT	NT	3.50	0.46	NT	3.63	4.06	4.02	2.27	3.62
K-562	3.79	>100	2.02	10.8	7.00	NT	3.50	NT	NT	NT	NT	NT	3.63	5.04
MOLT-4	4.50	NT	3.15	6.80	5.04	NT	3.70	2.30	3.59	NT	NT	4.16	4.07	3.86
RPMI-8226	4.51	10.1	4.15	14.9	4.58	4.73	4.10	0.63	4.54	NT	4.42	4.63	NT	NT
SR	3.79	>100	3.13	7.17	4.12	NT	3.16	NT	NT	NT	NT	NT	NT	NT
MG_MID	4.30	54.76	3.28	10.19	5.49	5.18	3.59	1.03	4.06	3.63	4.24	4.72	3.81	4.52
NSC lung cancer														
A549/ATCC	3.24	17.8	3.28	3.71	3.43	3.73	3.52	2.45	3.50	NT	3.66	3.62	5.11	3.18
EKVX	3.03	20.1	3.29	8.27	3.37	3.21	3.38	3.49	3.11	NT	2.96	3.29	2.94	3.10
HOP-62	3.42	20.4	3.49	5.16	3.75	3.41	3.25	3.34	3.13	NT	3.56	3.59	2.36	4.04
HOP-92	3.33	30.7	3.19	14.6	2.96	2.77	2.77	3.01	3.01	3.14	2.80	2.97	3.46	3.21
NCI-H226	4.09	28.5	4.25	16.9	3.47	3.81	3.54	4.01	3.63	NT	3.77	3.47	18.3	3.66
NCI-H23	3.39	24.6	3.26	12.5	3.50	3.40	3.37	3.17	NT	3.39	3.27	3.42	4.00	3.32
NCI-H322M	3.03	10.3	3.19	16.9	3.03	3.14	3.07	2.79	3.16	3.11	4.05	3.01	6.38	2.91
NCI-H460	3.21	3.80	3.35	15.2	2.20	2.81	3.09	2.77	NT	3.82	3.37	3.50	1.71	3.33
NCI-H522	3.42	4.19	3.32	7.31	3.77	3.50	3.44	3.35	3.23	3.33	3.38	3.36	2.17	3.63
MG_MID	3.35	17.82	3.40	11.17	3.28	3.30	3.27	3.15	3.25	3.36	3.42	3.36	5.16	3.38
Colon Cancer														
COLO 205	3.24	3.25	3.46	13.9	2.68	2.79	2.97	2.94	3.24	3.59	3.19	3.26	1.94	3.23
HCC-2998	2.93	3.81	3.46	23.0	2.97	2.76	3.19	3.05	NT	NT	3.21	3.18	1.62	2.14
HCT-116	2.63	3.11	2.81	10.6	2.88	2.82	3.31	1.25	3.33	3.11	NT	NT	1.54	3.21
HCT-15	2.77	1.04	2.75	16.4	2.68	2.84	2.81	2.32	NT	3.15	3.20	3.17	1.76	2.92
HT29	2.85	3.62	1.97	13.8	3.63	2.58	2.31	0.54	3.50	NT	3.23	3.08	2.04	3.28
KM12	3.24	4.26	3.51	20.3	3.44	3.60	3.42	2.91	3.41	3.63	3.33	3.57	1.65	3.02
SW-620	3.41	4.00	3.54	18.8	3.49	3.75	3.23	2.26	NT	3.37	3.36	3.54	2.11	3.04
MG_MID	3.01	3.30	3.07	16.69	3.11	3.02	3.03	2.18	3.37	3.37	3.25	3.30	1.80	2.98
CNS cancer														
SF-268	3.54	9.77	3.50	11.6	5.31	3.64	3.71	3.39	3.79	NT	8.44	4.12	2.69	3.25
SF-295	3.13	3.62	3.06	4.04	3.19	3.26	3.42	3.21	3.01	3.17	3.30	3.29	1.58	3.21
SF-539	3.01	2.41	3.16	9.26	3.07	2.99	3.13	3.19	NT	3.01	3.15	3.11	1.73	3.13
SNB-19	3.20	2.61	3.43	25.3	3.35	3.44	3.36	2.72	3.68	3.40	3.54	3.62	8.11	3.17
SNB-75	2.91	2.17	2.90	14.8	2.94	NT	3.84	2.87	NT	3.09	2.94	3.10	3.62	2.97
U251	3.09	4.18	3.15	15.9	3.23	3.26	3.17	NT	NT	NT	3.29	3.17	1.82	3.32
MG_MID	3.15	4.13	3.20	13.48	3.51	3.31	3.44	3.08	3.49	3.17	4.11	3.40	3.26	3.18
Melanoma														
LOX IMVI	3.03	3.19	3.05	6.76	3.08	3.16	3.01	2.42	NT	NT	3.00	3.02	1.57	2.70
MALME-3M	3.05	3.56	3.44	8.01	3.47	3.46	3.48	NT	3.79	NT	3.56	3.26	1.42	2.91
M14	3.13	3.87	3.12	14.8	3.31	3.38	3.26	2.19	3.30	3.59	3.58	3.62	1.76	3.34
MDA-MB-435	2.95	3.36	3.21	14.0	3.02	3.49	3.28	2.36	3.19	3.00	2.97	3.07	1.81	3.20
SK-MEL-2	3.75	8.17	3.63	12.2	4.09	3.69	3.48	3.18	3.32	3.43	4.83	3.52	5.04	3.58
SK-MEL-28	3.15	3.14	3.30	18.4	3.18	3.35	3.32	3.03	NT	3.11	3.38	3.26	1.67	3.25
SK-MEL-5	2.70	3.14	3.09	4.94	3.06	3.14	3.08	3.07	3.08	3.32	3.68	3.39	1.65	3.19
UACC-257	3.73	6.47	3.70	17.0	3.89	4.29	3.63	3.34	3.65	3.54	3.54	3.68	2.21	3.65
UACC-62	3.25	3.93	3.35	10.9	3.21	3.16	3.22	3.39	3.64	3.23	3.20	3.39	12.6	3.17
MG_MID	3.19	4.31	3.32	11.89	3.37	3.46	3.30	2.87	3.42	3.32	3.53	3.36	3.30	3.22
Ovarian Cancer														
IGROV1	3.26	NT	3.72	14.8	3.48	3.28	3.27	3.61	NT	3.37	3.08	3.43	1.67	2.95
OVCAR-3	3.13	3.84	3.42	7.06	3.10	3.40	3.37	1.60	NT	NT	3.51	3.56	1.79	2.85
OVCAR-4	2.81	17.5	3.79	20.8	3.12	3.39	3.60	0.94	3.38	3.25	3.32	3.16	2.85	3.09
OVCAR-5	2.89	24.6	3.18	25.3	3.04	3.32	3.07	3.18	3.13	NT	3.01	3.21	6.15	3.06
OVCAR-8	3.51	15.6	3.61	6.66	3.66	3.94	4.25	2.80	3.65	NT	NT	4.57	2.80	4.61
NCI/ADR-RES	3.18	24.0	3.47	4.52	3.59	3.80	3.52	3.01	NT	NT	3.93	4.59	2.17	3.37
SK-OV-3	3.49	28.9	3.97	28.6	7.93	3.37	3.50	3.23	3.30	3.27	3.26	3.25	12.0	3.17
MG_MID	3.18	19.07	3.59	15.39	3.99	3.50	3.51	2.62	3.37	3.30	3.35	3.68	4.20	3.30
Renal Cancer														
786-0	3.16	4.84	3.06	8.59	3.21	3.51	3.48	1.60	3.59	3.48	4.14	3.51	1.58	3.44
A498	5.63	38.1	3.29	24.5	3.67	3.79	3.60	2.94	3.14	2.96	21.4	3.13	11.2	2.90
ACHN	3.09	11.5	3.06	9.56	3.08	3.26	3.14	3.16	3.45	3.24	3.07	3.10	3.40	3.14
CAKI-1	2.89	13.7	3.23	13.8	2.97	3.22	3.05	2.89	3.15	NT	2.82	3.06	5.58	2.85
RXF 393	3.18	11.7	3.51	4.15	2.98	3.32	3.10	3.27	3.13	NT	2.78	2.86	1.59	3.07

SN12C	3.03	16.8	3.11	12.0	3.20	3.31	3.44	3.55	3.37	3.33	3.30	3.41	1.67	3.15
TK-10	3.50	16.7	3.32	7.15	3.61	3.45	3.37	3.08	3.23	3.20	3.33	3.59	9.75	3.36
UO-31	2.99	25.5	2.99	15.7	3.00	2.89	2.82	2.96	3.04	NT	2.68	2.85	2.24	2.65
MG_MID	3.43	17.36	3.20	11.93	3.22	3.34	3.25	2.93	3.26	3.24	5.44	3.19	4.63	3.07
Prostate cancer														
PC-3	2.94	3.33	2.97	12.3	3.17	3.06	3.02	2.62	3.00	NT	3.16	2.98	7.48	3.28
DU-145	3.02	4.70	3.14	5.02	3.23	3.33	3.55	2.87	3.30	3.28	3.37	3.40	3.01	3.15
MG_MID	2.98	4.02	3.06	8.66	3.20	3.20	3.29	2.75	3.15	3.28	3.27	3.19	5.25	3.22
Breast cancer														
MCF7	2.77	5.54	3.39	14.5	3.01	2.92	3.54	2.06	NT	3.25	3.38	3.18	1.73	3.40
MDA-MB-31/ATCC	3.21	13.0	3.48	29.3	3.20	3.35	3.47	2.77	NT	3.40	4.12	3.91	1.71	3.27
HS 578T	4.79	24.7	4.86	13.2	4.69	4.39	4.04	3.78	3.94	NT	4.08	4.26	2.23	4.07
BT-549	3.46	24.5	2.96	12.7	3.24	3.23	3.14	3.32	3.56	NT	3.78	3.14	9.23	3.07
T-47D	3.71	16.3	4.03	20.9	3.69	3.47	3.46	4.02	3.15	3.64	3.31	3.26	5.15	3.45
MDA-MB-468	3.38	3.74	3.44	24.0	3.45	3.43	3.30	3.03	3.33	3.45	3.13	3.22	1.66	3.20
MG_MID	3.55	14.63	3.69	19.10	3.55	3.47	3.49	3.16	3.50	3.44	3.63	3.50	3.62	3.41
MG_MID_{60}	3.34	15.49	3.31	13.17	3.64	3.53	3.35	2.64	3.43	3.35	3.80	3.52	3.89	3.36

[a]TGI is a molar concentration of the compound leading to total inhibition

Table S3. Influence of compounds 1, 3, 4, 6, 7-9, 11, 12, 14-16, 19, 20 on the growth of individual tumor cell panel.

Panel/cell line	LC_{50}[a], μM													
	1	3	4	6	7	8	9	11	12	14	15	16	19	20
Leukemia														
CCRF-CEM	>100	>100	8.88	65.3	>100	>100	NT	NT	>100	NT	>100	>100	>50.0	>100
HL-60(TB)	NT	>100	NT	32.6	NT	NT	7.19	NT	NT	NT	NT	NT	5.00	NT
K-562	>100	>100	6.68	43.8	>100	NT	NT	NT	>100	NT	>100	>100	>50.0	>100
MOLT-4	>100	>100	7.25	38.2	74.8	NT	NT	NT	NT	NT	>100	NT	27.9	NT
RPMI-8226	>100	>100	9.27	52.9	96.8	NT	NT	NT	>100	NT	NT	>100	NT	NT
SR	NT	>100	NT	>100	>100	NT	NT	NT	NT	NT	>100	>100	NT	NT
MG_MID	>100	>100	8.02	55.47	94.32	>100	7.19	-	>100	-	>100	>100	33.22	>100
NSC lung cancer														
A549/ATCC	6.08	52.4	6.16	7.31	6.50	6.89	NT	NT	NT	NT	NT	NT	>50.0	6.34
EKVX	5.92	>100	6.53	38.4	6.77	NT	6.56	NT	NT	NT	NT	6.35	26.5	6.01
HOP-62	6.46	58.9	6.52	16.7	7.34	6.38	NT	NT	NT	NT	NT	NT	>50.0	NT
HOP-92	6.42	6.92	6.67	47.0	NT	5.61	5.52	6.42	NT	NT	NT	6.11	23.1	6.96
NCI-H226	8.43	71.8	NT	82.2	7.09	NT	NT	NT	NT	NT	NT	NT	49.9	NT
NCI-H23	6.68	54.5	6.47	40.0	6.95	NT	6.39	NT	NT	NT	NT	6.41	17.5	6.24
NCI-H322M	5.64	36.0	5.89	42.1	5.60	5.70	5.61	NT	NT	NT	>100	5.62	18.6	5.43
NCI-H460	6.30	7.56	6.30	46.2	6.12	NT	6.45	NT	NT	7.53	NT	NT	3.19	6.49
NCI-H522	NT	8.59	6.43	31.7	7.49	6.35	NT	6.40	NT	NT	6.78	6.64	4.54	NT
MG_MID	6.49	44.07	6.37	39.07	6.73	6.18	6.11	6.41	-	7.53	53.39	6.23	27.04	6.24
Colon Cancer														
COLO 205	6.82	5.77	6.86	43.0	5.61	5.64	NT	NT	NT	NT	NT	NT	4.17	6.96
HCC-2998	5.68	7.69	6.85	52.3	5.72	NT	NT	NT	NT	NT	NT	NT	3.02	4.97
HCT-116	5.38	5.92	5.31	52.9	5.47	NT	NT	NT	NT	6.05	NT	NT	2.93	6.08
HCT-15	5.52	42.3	5.52	45.4	5.47	5.59	NT	NT	NT	NT	NT	NT	3.69	5.56
HT29	NT	8.23	4.85	41.8	7.42	5.56	NT	1.75	NT	NT	NT	NT	4.22	6.59
KM12	6.09	8.78	6.68	55.1	NT	6.71	NT	5.78	NT	NT	NT	6.85	3.00	5.67
SW-620	6.44	8.35	7.03	47.0	6.95	NT	NT	NT	NT	6.31	NT	7.04	4.39	5.93
MG_MID	5.98	12.43	6.16	48.21	6.11	5.87	-	3.76	-	6.18	-	6.94	3.63	5.96
CNS cancer														
SF-268	7.19	65.6	6.84	49.6	31.5	NT	6.98	NT	NT	NT	67.9	8.68	14.8	6.56
SF-295	5.90	7.40	5.72	8.15	5.99	5.88	6.24	NT	NT	NT	NT	6.08	2.94	5.79
SF-539	5.72	52.7	5.90	33.0	5.78	NT	5.80	NT	NT	NT	5.79	5.66	3.17	5.67
SNB-19	5.86	58.1	6.31	55.2	6.07	NT	NT	NT	NT	NT	NT	NT	25.0	5.74
SNB-75	5.50	47.1	5.63	46.5	5.76	NT	7.44	5.72	NT	NT	5.85	5.97	17.1	5.77
U251	5.76	9.00	5.94	45.5	5.98	6.07	NT	NT	NT	NT	NT	6.07	NT	6.72
MG_MID	5.98	39.98	6.06	39.66	10.18	5.97	6.61	5.72	-	-	26.51	6.49	12.60	6.04
Melanoma														
LOX IMVI	NT	6.05	5.84	29.0	NT	NT	5.49	NT	NT	NT	NT	NT	2.86	5.31
MALME-3M	6.18	6.27	7.08	32.5	6.72	NT	6.84	NT	NT	NT	NT	6.34	2.74	5.82
M14	6.19	7.34	6.04	41.5	6.19	NT	6.12	NT	NT	6.65	NT	NT	3.64	6.62
MDA-MB-435	NT	6.59	6.49	43.0	5.55	6.51	5.81	NT	NT	NT	NT	5.75	3.45	5.76
SK-MEL-2	NT	36.7	6.91	38.9	8.57	6.80	6.69	5.87	NT	6.42	16.4	6.58	18.5	6.66
SK-MEL-28	6.13	5.78	6.22	44.0	6.07	6.18	6.11	NT	NT	NT	NT	5.97	2.94	5.80
SK-MEL-5	5.28	5.86	5.62	14.0	5.53	NT	5.56	5.64	NT	5.94	NT	NT	3.00	NT
UACC-257	7.14	27.6	7.01	43.8	7.77	8.38	7.09	6.25	NT	NT	NT	NT	4.68	7.14
UACC-62	5.80	8.07	6.06	37.0	5.77	5.76	5.85	6.52	NT	6.00	NT	NT	27.3	5.66
MG_MID	6.12	12.25	6.36	35.96	6.52	6.73	6.17	6.07	-	6.25	16.4	6.16	7.68	6.09
Ovarian Cancer														
IGROV1	6.44	NT	7.45	46.6	6.78	6.35	NT	NT	NT	6.69	NT	NT	3.14	5.80
OVCAR-3	5.91	7.52	6.39	34.8	5.94	NT	5.93	NT	NT	NT	NT	NT	3.44	5.46
OVCAR-4	NT	45.2	NT	63.1	5.88	6.17	NT	NT	NT	NT	NT	6.02	25.0	6.23
OVCAR-5	5.52	51.0	5.99	51.6	5.80	NT	5.65	NT	NT	NT	NT	5.81	20.9	5.57
OVCAR-8	6.73	54.1	6.67	30.8	NT	7.79	NT	NT	NT	NT	NT	NT	>50.0	10.0
NCI/ADR-RES	6.18	56.3	6.84	10.4	NT	7.30	6.73	NT	NT	NT	NT	>100	4.77	6.54
SK-OV-3	6.64	59.2	35.2	56.2	36.9	6.28	6.46	NT	5.82	NT	6.03	5.91	30.5	5.85
MG_MID	6.24	45.55	11.42	41.93	12.26	6.78	6.19	-	5.82	6.69	6.03	29.43	19.68	6.49
Renal Cancer														
786-0	6.19	12.7	5.85	40.9	6.18	NT	NT	NT	NT	NT	NT	NT	2.97	7.04
A498	33.0	86.7	6.63	52.7	8.00	7.08	6.93	5.81	6.04	5.60	57.6	5.74	27.7	5.44
ACHN	5.61	38.3	5.54	33.0	5.55	NT	5.62	NT	NT	NT	5.58	5.50	17.0	5.60
CAKI-1	5.40	53.6	6.43	39.3	5.45	5.73	5.53	5.60	5.71	NT	5.46	5.81	17.9	5.34
RXF 393	6.04	48.6	6.79	9.35	5.69	6.33	5.98	NT	NT	NT	5.59	6.05	3.07	5.81

SN12C	5.69	45.6	5.87	41.7	6.10	6.12	6.45	NT	NT	NT	NT	NT	3.34	6.03
TK-10	6.96	49.9	5.97	27.3	6.91	6.32	6.30	5.89	NT	NT	6.27	6.85	24.6	6.37
UO-31	5.74	62.1	5.79	42.1	5.77	5.52	5.42	NT	NT	NT	5.58	5.59	9.64	5.24
MG_MID	9.33	49.68	6.11	35.79	6.21	6.18	6.03	5.76	5.87	5.60	14.35	5.92	13.28	5.86
Prostate cancer														
PC-3	5.74	7.47	5.66	38.7	6.25	5.68	5.78	NT	NT	NT	NT	5.82	26.0	6.33
DU-145	5.58	9.61	5.75	13.8	6.00	6.26	6.38	NT	NT	NT	6.35	6.39	11.3	5.78
MG_MID	5.66	8.54	5.70	26.25	6.12	5.97	6.08	-	-	-	6.35	6.10	18.65	12.11
Breast cancer														
MCF7	5.94	22.7	7.28	46.7	6.30	6.22	NT	NT	NT	NT	NT	NT	NT	7.23
MDA-MB-31/ATCC	5.80	45.6	6.43	59.2	6.17	6.20	6.69	NT	NT	NT	NT	NT	3.04	6.02
HS 578T	31.0	77.4	32.6	71.2	2.44	15.9	9.11	NT	NT	NT	9.14	9.37	5.00	9.20
BT-549	NT	59.2	NT	39.0	NT	NT	5.96	NT	NT	NT	NT	NT	23.3	5.78
T-47D	7.96	48.6	9.66	59.5	7.99	7.00	NT	NT	NT	NT	NT	6.85	>50.0	NT
MDA-MB-468	6.88	7.81	6.98	55.1	7.39	6.60	6.50	6.01	NT	6.87	NT	6.51	3.36	6.47
MG_MID	11.52	43.55	12.59	55.12	6.06	8.38	7.06	6.01	-	6.87	9.14	7.57	16.94	6.94
MG_MID_{60}	7.16	32.0	7.64	41.94	17.17	6.51	6.43	5.62	5.84	6.52	18.9	9.35	16.97	

[a]LC_{50} is a parameter of cytotoxicity and reflects the molar concentration needed to kill 50% of the cells.