

Title	Isoquinolinequinone N-oxides as anticancer agents effective against drug resistant cell lines
Authors	Kruschel, Ryan D.;Buzid, Alyah;Khandavilli, Udaya Bhaskara Rao;Lawrence, Simon E.;Glennon, Jeremy D.;McCarthy, Florence O.
Publication date	2019-12-18
Original Citation	Kruschel, R. D., Buzid, A., Khandavilli, U. B. R., Lawrence, S. E., Glennon, J. D. and McCarthy, F. O. (2020) 'Isoquinolinequinone N- oxides as anticancer agents effective against drug resistant cell lines', Organic & Biomolecular Chemistry, 18(3), pp. 557-568. doi: 10.1039/C90B02441G
Type of publication	Article (peer-reviewed)
Link to publisher's version	https://pubs.rsc.org/en/content/articlehtml/2020/ob/c9ob02441g - 10.1039/C90B02441G
Rights	https://pubs.rsc.org/en/content/articlelanding/2020/0B/ C90B02441G
Download date	2025-01-18 06:12:25
Item downloaded from	https://hdl.handle.net/10468/9633



University College Cork, Ireland Coláiste na hOllscoile Corcaigh

Isoquinolinequinone *N*-oxides as Anticancer Agents Effective Against Drug Resistant Cell Lines

Ryan D. Kruschel,^a Alyah Buzid,^a Udaya B. Rao Khandavilli,^a Simon E. Lawrence,^a Jeremy D. Glennon ^a and Florence O. McCarthy *^a

^aSchool of Chemistry, Analytical and Biological Chemistry Research Facility, University College Cork, Cork T12 K8AF, Ireland; <u>f.mccarthy@ucc.ie</u>, <u>r.kruschel@umail.ucc.ie</u>

*Correspondence: f.mccarthy@ucc.ie; Tel.: 00353214901695

Supplementary Information

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¹H NMR of **5**



















¹H NMR of **13**



¹H NMR of **14**











Confirmation of regioisomer assignment of compound 15 and 16

- With respect to morpholino derivative 5 Crystal structure obtained
- On HMBC analysis, C(1)CH₃ is more downfield and correlated to the C(8) quinone



- C(6)H correlates to C(8) quinone confirmed using X-ray single crystal and HMBC



For the benzylamine isoquinolinequinone N-oxides 15 and 16:

- C(7) Regioisomer 15 Correlation of C(6)H with 181.0 ppm , which is the C(8) carbonyl
- C(6) Regioisomer 16 Correlation of C(7)H with 179.1 ppm, which is the C(5) carbonyl

C(7) Regioisomer 15

- Like morpholino derivative $\mathbf{5}$, C(1)CH₃ correlates to C(8) carbonyl



- C(6)H also correlates to the C(8) carbonyl carbon





C(6) Regioisomer 16





- C(7)H correlates to the C(5) carbonyl carbon

NCI60 One dose Screen

Developmental Therapeutics Program		NSC: D-805937 / 1	Conc: 1.00E-5 Molar	Test Date: Jul 30, 2018
One Dose Mean Graph		Experiment ID: 1807OS85		Report Date: Aug 15, 2018
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A539/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H522 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2	Growth Percent 100.95 92.07 99.76 104.65 95.78 121.04 94.97 111.00 108.94 114.63 106.68 95.16 104.05 85.24 93.64 106.14 109.65 96.44 108.56 117.31 97.14 104.37 100.32 106.04 95.78 99.21 112.74 99.46 88.01 59.02 107.89 112.80 104.87 109.99 84.05 99.88 95.42 94.82 113.49 87.86 110.24 95.06 102.86 117.36 101.11 105.62 110.66	Mean Growth	Percent - Growth Perc	
Mean Delta Range	102.02 43.00 67.26			
	150	100 50	0 -50	-100 -150

Developmental Therapeutics Program		NSC: D-802087 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 13, 2017
One Dose Mean Graph		Experiment ID: 1711OS00		Report Date: Dec 09, 2017
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
$\begin{array}{l} \textbf{Panel/Cell Line} \\ \begin{array}{l} \mbox{Leukemia} \\ \mbox{CCRF-CEM} \\ \mbox{HL-60(TB)} \\ \mbox{K-562} \\ \mbox{MOLT-4} \\ \mbox{RPMI-8226} \\ \mbox{SR} \\ \hline \mbox{Non-Small Cell Lung Cancer} \\ \mbox{A549/ATCC} \\ \mbox{EKVX} \\ \mbox{HOP-62} \\ \mbox{HOP-63} \\ \mbox{HOP-63} \\ \mbox{HOP-64} \\ \$	Growth Percent 107.91 107.98 102.23 109.73 100.34 91.64 104.42 92.63 105.81 153.93 103.02 88.36 88.40 85.93 94.68 95.75 106.43 96.43 89.36 104.47 86.95 105.41 87.73 89.29 99.34 100.82 88.81 106.56 87.97 65.07 104.02 104.51 88.54 112.95 85.62 113.96 88.95 81.66 94.70 81.33 97.60 110.99 96.34 94.51 100.26 84.06 105.35 89.50 108.54 76.13 97.72 100.80 81.39 95.01	Mean Growth	Percent - Growth Perc	zent
Mean Delta Range	97.34 32.27 88.86			
	150	100 50	0 -50	-100 -150

Developmental Ther	apeutics Program	NSC: D-802096 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 13, 2017
One Dose Me	One Dose Mean Graph		Experiment ID: 1711OS00	
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Per	cent
Leukemia CCBE-CEM	94 77			
HL-60(TB)	98.11			
K-562	95.02		•	
MOLT-4 BPMI-8226	89.48			
SR	76.67		_	
Non-Small Cell Lung Cancer	00.54			
A549/ATCC EKVX	99.51			
HOP-62	87.58			
HOP-92	95.47		_	
NCI-H226	98.04			
NCI-H23	87.21			
NCI-H460	81.26		-	
NCI-H522	98.52			
COLO 205	75.87			
HCC-2998	102.95			
HCT-116	93.50			
HC1-15 HT29	108 23			
KM12	78.30			
SW-620	99.40			
SF-268	91 43			
SF-295	93.82			
SF-539	98.10			
SNB-19 SNB-75	87.35 99.64			
U251	93.10			
Melanoma	00.00			
MALME-3M	86.82 67.09			
M14	93.21		•	
MDA-MB-435	105.17			
SK-MEL-2 SK-MEL-28	86.49			
SK-MEL-5	87.62		•	
UACC-257	88.79			
Ovarian Cancer	82.49			
IGROV1	74.41			
OVCAR-3	89.32			
OVCAR-4 OVCAR-5	05.00 78.47			
OVCAR-8	91.71			
NCI/ADR-RES	94.06		1	
Renal Cancer	85.14			
786-0	98.46			
	108.11			
CAKI-1	83.89			
RXF 393	95.16		•	
SN12C	90.14			
UO-31	78.45			
Prostate Cancer				
PC-3 DU-145	87.68			
Breast Cancer	32.35			
MCF7	89.63			
HS 578T	82.84 94 53			
BT-549	81.97			
T-47D	97.36			
	00.73			
Mean	90.65			
Delta Bange	23.56			
hange				
		100		
	150	100 50	0 -50	-100 -150

Developmental Ther	apeutics Program	NSC: D-802085 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 13, 2017
One Dose Mea	an Graph	Experiment ID: 1711	DS00	Report Date: Dec 09, 2017
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H227 NCI-H226 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-288 SF-295 SF-539 SNB-19 SNB-75 UZ51 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28	Growth Percent 89.13 81.85 69.13 75.86 88.37 54.14 102.99 71.46 91.25 116.91 93.86 71.98 92.47 67.11 78.81 78.53 96.24 76.01 73.33 91.98 83.04 105.64 78.79 87.20 96.87 93.18 88.86 98.95 61.73 -1.94 66.89 103.42 72.85 108.08 98.95 61.73 -1.94 66.89 103.42 72.85 108.08 51.38 103.66 65.83 66.68 44.09 64.56 81.65 97.80 81.69 91.42 84.72 124.21 76.02 81.47 94.51 88.57 119.31 74.16 75.57 95.84 76.05 70.25 115.78 89.98 82.21 53.91 82.60	Mean Growth	Percent - Growth Perc	
Delta Range	84.54 126.15 150	100 50	0 -50	-100 -150
			- 00	

Developmental Thera	apeutics Program	NSC: D-805938 / 1	Conc: 1.00E-5 Molar	Test Date: Jul 30, 2018
One Dose Mean Graph		Experiment ID: 1807OS85		Report Date: Aug 15, 2018
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H228 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2	77.28 24.48 64.35 79.78 75.84 86.52 58.13 79.31 79.90 103.63 86.34 31.82 81.47 30.36 64.28 30.94 69.61 25.31 36.77 19.77 62.36 48.20 73.51 78.29 82.79 82.79 82.79 82.79 82.79 82.79 82.79 82.79 82.79 82.79 82.79 82.79 82.79 82.79 82.71 38.67 71.14 35.32 -26.62 31.35 -66.76 52.12 91.34 -90.93 53.38 97.31 38.74			
	150	100 50	0 -50	-100 -150

Developmental Ther	apeutics Program	NSC: D-805936 / 1	Conc: 1.00E-5 Molar	Test Date: Jul 30, 2018
One Dose Mean Graph		Experiment ID: 1807	OS85	Report Date: Aug 15, 2018
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H23 NCI-H23 NCI-H23 NCI-H23 NCI-H23 NCI-H23 NCI-H23 NCI-H23 NCI-H522 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-289 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-62 Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-4 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468	Growth Percent 97.32 61.86 97.38 99.30 93.72 107.41 98.61 100.32 133.48 118.36 107.37 88.98 96.22 88.64 102.22 56.47 100.68 67.43 87.91 68.20 96.92 92.12 95.25 95.79 106.93 101.01 118.94 100.97 82.82 37.03 87.84 56.610 99.42 113.22 70.79 87.47 55.65 96.17 13.17 73.77 118.24 102.81 137.72 100.82 92.36 97.87 91.37	Mean Growth	Percent - Growth Perc	
	150	100 50	0 -50	-100 -150

Developmental Therapeutics Program		NSC: D-802086 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 13, 2017
One Dose Mea	One Dose Mean Graph		DS00	Report Date: Dec 09, 2017
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	ent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H230 NCI-H226 NCI-H220 NCI-H322M NCI-H322M NCI-H322M NCI-H322 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-62 OVarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-5 OVCAR-5 SK-OV-3 Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-470 MDA-MB-468 Mean Delta Range	25.55 -30.91 21.02 13.63 41.11 27.00 18.20 17.04 87.10 86.90 70.96 5.25 51.44 11.73 21.97 -11.84 21.83 1.86 11.57 6.01 37.07 16.68 33.01 30.10 7.13 41.70 100.34 20.13 6.45 -75.42 14.03 -76.51 27.25 56.42 -96.47 -7.87 -10.78 18.01 -12.75 -57.33 61.54 4.60 3.37 109.28 51.64 88.63 36.90 51.77 52.43 8.24 86.60 46.08 16.07 38.03 -30.15 14.77 76.03 50.93 13.72 -21.25 21.80 118.27 205.75			
	150	100 50	u -50	-100 -150

Developmental Therapeutics Program		NSC: D-805945 / 1	Conc: 1.00E-5 Molar	Test Date: Jul 30, 2018
One Dose Mean Graph		Experiment ID: 1807OS85		Report Date: Aug 15, 2018
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H227 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-268 SF-268 SF-275 U251 Meianoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-	81.55 29.00 71.03 95.57 76.14 95.54 55.31 84.00 97.91 105.98 82.06 40.04 71.89 28.19 23.28 8.07 50.06 15.97 49.07 16.54 61.25 42.47 89.16 86.40 83.76 81.46 147.19 64.01 34.36 -46.20 23.96 -17.34 70.72 96.28 -47.90 49.34 27.26 70.19 7.04 25.95 96.12 34.98 70.58 119.55 97.87 102.68 74.40 39.98 133.46 90.75 61.91 <th></th> <th></th> <th>-100 -150</th>			-100 -150
	150	100 50	U -5U	-100 -150

Developmental Ther	apeutics Program	NSC: D-802088 / 1	Conc: 1.00E-5 Molar	Test Date: Nov 13, 2017	
One Dose Mea	an Graph	Experiment ID: 1711	Report Date: Dec 09, 2017		
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Perc	cent	
Panel/Cell Line Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H227 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M SCIO COS Calco Cal	Growth Percent 80.19 52.37 75.62 88.15 91.91 66.92 91.26 65.76 100.80 145.57 102.53 59.71 72.51 55.37 87.52 6.73 74.05 28.28 69.14 27.39 71.55 64.32 79.31 82.66 89.46 87.46 106.13 83.56 57.18 -13.21 62.86 49.93 78.22 95.18 48.50 48.40 68.44 63.43 5.12 35.43 89.07 61.71 91.69 103.28 89.94 129.42 85.47 73.03 96.27 55.87 75.17 84.27 55.87 75.17 84.27 55.87 75.17 84.27 55.87 70.84 100.76 91.43 80.56 28.85 72.76 85.97 15.87 100.76 91.43 80.56 28.85 72.76 85.97 15.87 100.76 91.43 80.56 28.85 72.76 85.97 15.87 100.76	Mean Growth	Percent - Growth Perc	Sent	
-	150	100 50	0 -50	-100 -150	

Developmental Ther	apeutics Program	NSC: D-815388/1	Conc: 1.00E-5 Molar	Test Date: May 20, 2019		
One Dose Mea	an Graph	Experiment ID: 19050	Report Date: Jun 10, 2019			
Panel/Cell Line	Growth Percent	Mean Growth I	Percent - Growth Perc	cent		
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M COLO 205 HCC-2998 HCT-116 HCT-116 HCT-15 HT29 KM12 SW-620 CNS Cancer SF-288 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-62 Ovcarian Cancer IGROV1 OVCAR-5 OVCAR-5 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer 786-0 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-468 Mean Deita Range	98.80 128.76 99.61 111.12 109.52 84.32 107.15 97.80 92.68 109.62 96.53 99.00 95.67 89.23 59.66 107.53 85.18 83.03 84.28 77.69 95.65 91.84 92.69 101.02 96.45 115.97 97.30 90.83 32.69 95.59 104.32 86.76 107.69 96.48 85.30 94.11 91.35 71.39 75.60 116.41 91.31 107.68 105.91 101.29 103.97 102.34 102.					
	150	100 50	0 -50	-100 -150		

Developmental Ther	apeutics Program	NSC: D-815386/1	Conc: 1.00E-5 Molar	Test Date: May 20, 2019		
One Dose Mea	an Graph	Experiment ID: 19050	Report Date: Jun 10, 2019			
Panel/Cell Line	Growth Percent	Mean Growth I	Percent - Growth Perc	ent		
Leukemia CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A549/ATCC EKVX HOP-62 HOP-92 NCI-H322M NCI-H322M NCI-H322M NCI-H322M NCI-H322M COLO 205 HCC-2998 HCT-116 HT29 KM12 SW-620 CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251 Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-27 UACC-62 OVCAR-4 OVCAR-5 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3 Renal Cancer 786-0 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31 Prostate Cancer PC-3 DU-145 Breast Cancer MCF7 MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-231/ATCC HS 578T BT-549 T-47D MDA-MB-231/ATCC	6.23 -31.40 1.96 -36.17 -0.20 4.44 -4.94 -54.91 2.96 -27.19 -50.03 -5.71 -13.14 -26.11 -37.16 -34.51 -12.58 -68.48 5.35 -10.54 -27.89 -4.22 -84.02 -90.23 -11.40 -71.47 -9.66 -28.17 -96.92 -80.15 -89.56 -29.63 14.12 -98.45 -89.56 -29.50 -56.64 -35.41 -95.01 -63.34 -29.50 3.56 -25.34 -89.10 18.07 -13.60 4.06 -92.72 -62.07 -62.07 <					
Deita Deita Range	63.35 116.52 150	100 50	0 -50	-100 -150		

NCI60 – Five Dose Data





National Cancer Institute Developmental Therapeutics Program In-Vitro Testing Results											n				
NSC : D - 805	939 / 1				Experiment ID : 1809NS03						Test	Гуре : 08	Units : M	lolar	
Report Date :	October	r 18, 20 <i>1</i>	18		Tes	t Date	: Septe	mber 17,	2018			QNS :		MC :	
COMI : RK CH	10.0.2				Sta	in Rea	gent : S	RB Dual-	Pass F	Related	I	SSPL	: 0Y2V		
						Lo	og10 Con	centration				-1			
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	o Optica -6.0	l Densiti -5.0	es -4.0	-8.0	-7.0	ercent G -6.0	Frowth -5.0	-4.0	GI50	TGI	LC50
CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.555 0.925 0.278 0.645 0.838 0.345	2.485 3.282 2.640 2.975 2.851 1.836	2.576 3.219 2.781 3.012 2.887 1.871	1.164 3.192 2.715 2.966 2.838 1.878	0.753 3.233 2.516 2.415 2.622 1.571	0.546 0.508 0.326 0.401 0.554 0.318	0.521 0.577 0.274 0.561 0.644 0.330	105 97 106 102 102 102	32 96 103 100 99 103	10 98 95 76 89 82	-2 -45 2 -38 -34 -8	-6 -38 -2 -13 -23 -4	5.59E-8 2.16E-6 3.04E-6 1.69E-6 2.07E-6 2.28E-6	7.30E-6 4.84E-6 3.60E-5 4.65E-6 5.29E-6 8.19E-6	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H227 NCI-H322M NCI-H460 NCI-H522	Cancer 0.431 0.872 0.326 0.922 1.257 0.664 0.681 0.353 0.827	2.311 2.152 1.375 1.477 2.301 2.229 2.241 3.149 2.555	2.240 2.054 1.291 1.383 2.163 2.066 2.137 3.196 2.456	2.229 1.953 1.296 1.360 2.069 2.074 2.137 3.184 2.334	2.199 1.999 0.785 1.400 2.026 1.843 2.136 3.149 2.247	0.523 0.558 0.068 0.699 0.232 0.371 0.015 0.300 0.304	0.134 0.207 0.043 0.069 0.385 0.345 0.345 0.123 0.117	96 92 83 87 90 93 102 94	96 84 92 79 78 90 93 101 87	94 88 44 86 74 75 93 100 82	5 -36 -79 -24 -82 -44 -98 -15 -63	-69 -76 -87 -93 -69 -48 -99 -65 -86	3.12E-6 2.02E-6 7.44E-7 2.12E-6 1.63E-6 1.63E-6 1.68E-6 2.72E-6 1.66E-6	1.16E-5 5.12E-6 2.27E-6 6.03E-6 2.98E-6 4.27E-6 3.08E-6 7.40E-6 3.67E-6	5.53E-5 2.22E-5 5.79E-6 2.38E-5 6.26E-6 > 1.00E-4 5.62E-6 4.99E-5 8.11E-6
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.375 1.137 0.201 0.362 0.256 0.576 0.290	2.012 3.308 2.397 2.375 1.988 2.845 1.997	1.989 3.252 2.353 2.285 2.047 2.820 2.057	1.976 3.161 2.262 2.266 1.951 2.818 1.901	1.759 3.062 1.275 1.793 1.884 2.602 1.557	0.089 0.109 0.187 0.125 0.202 0.333 0.130	0.095 0.056 0.057 0.151 0.200 0.084 0.119	99 97 98 96 103 99 104	98 93 94 95 98 99 94	85 89 49 71 94 89 74	-76 -90 -7 -66 -21 -42 -55	-75 -95 -72 -58 -22 -86 -59	1.64E-6 1.64E-6 9.45E-7 1.43E-6 2.41E-6 1.99E-6 1.54E-6	3.35E-6 3.13E-6 7.50E-6 3.31E-6 6.54E-6 4.77E-6 3.74E-6	6.85E-6 5.95E-6 4.60E-5 7.69E-6 > 1.00E-4 1.51E-5 9.09E-6
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.781 1.102 1.016 0.588 0.854 0.520	2.278 3.203 2.836 2.250 1.672 2.449	2.195 3.083 2.769 2.244 1.581 2.390	2.153 3.096 2.792 2.215 1.555 2.336	2.070 3.110 2.855 2.048 1.634 2.070	0.548 0.146 0.008 0.112 0.022 0.013	0.191 0.132 0.011 0.055 0.028 0.022	94 94 96 100 89 97	92 95 98 86 94	86 96 101 88 95 80	-30 -87 -99 -81 -97 -98	-76 -88 -99 -91 -97 -96	2.05E-6 1.78E-6 1.80E-6 1.68E-6 1.72E-6 1.48E-6	5.52E-6 3.34E-6 3.20E-6 3.31E-6 3.12E-6 2.83E-6	2.76E-5 6.28E-6 5.68E-6 6.55E-6 5.67E-6 5.40E-6
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.758 0.842 0.458 0.666 1.247 0.839 1.028 0.764 0.978	3.337 1.822 2.172 2.990 2.886 2.540 3.204 2.132 2.861	3.279 1.797 2.140 2.981 2.888 2.611 3.187 2.082 2.961	3.275 1.786 2.179 3.016 2.832 2.609 3.095 2.009 2.913	2.681 1.658 2.058 2.920 2.770 2.630 2.313 1.856 2.602	0.154 0.040 0.090 0.479 0.135 0.046 0.210 0.155	0.251 0.114 0.110 0.553 0.095 0.037 0.270 0.344	98 97 98 100 100 104 99 96 105	98 96 100 101 97 104 95 91 103	75 83 93 97 93 105 59 80 86	-80 -95 -80 -90 -62 -84 -96 -73 -84	-67 -87 -76 -82 -56 -89 -96 -65 -65	1.44E-6 1.53E-6 1.78E-6 1.79E-6 1.96E-6 1.96E-6 1.14E-6 1.57E-6 1.63E-6	3.04E-6 2.92E-6 3.45E-6 3.31E-6 3.69E-6 3.60E-6 2.41E-6 3.34E-6 3.21E-6	6.42E-6 5.57E-6 6.69E-6 6.13E-6 8.41E-6 6.62E-6 5.07E-6 7.11E-6 6.30E-6
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.412 0.511 0.631 0.576 0.342 0.682 0.558	1.984 1.863 1.631 1.648 1.768 2.396 1.690	1.937 1.895 1.572 1.636 1.757 2.392 1.694	1.900 1.846 1.550 1.594 1.730 2.321 1.681	1.690 0.521 1.257 1.615 0.458 2.142 1.656	0.214 0.341 0.019 0.038 0.068 0.611 0.359	0.112 0.094 0.009 0.069 0.030 0.586 0.002	97 102 94 99 99 100 100	95 99 92 95 97 96 99	81 1 63 97 8 85 97	-48 -33 -97 -93 -80 -10 -36	-73 -82 -99 -88 -91 -14 -100	1.74E-6 3.14E-7 1.20E-6 1.76E-6 3.39E-7 2.33E-6 2.26E-6	4.24E-6 1.05E-6 2.47E-6 3.23E-6 1.24E-6 7.78E-6 5.38E-6	1.18E-5 2.22E-5 5.08E-6 5.91E-6 4.54E-6 > 1.00E-4 1.67E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.670 1.579 0.355 0.878 1.198 0.754 0.792 0.771	2.699 2.461 1.655 2.444 1.965 2.932 2.121 2.208	2.631 2.454 1.670 2.376 1.945 2.901 2.089 2.097	2.641 2.354 1.634 2.337 1.816 2.970 2.013 1.989	2.627 2.388 1.619 2.344 1.772 2.657 2.104 2.029	0.328 1.724 0.101 0.382 0.143 0.074 0.694 0.172	0.201 0.034 0.003 0.051 0.115 0.062 0.050 0.006	97 99 101 96 97 99 98 92	97 88 98 93 81 102 92 85	96 92 97 94 75 87 99 87	-51 16 -72 -56 -88 -90 -12 -78	-70 -98 -99 -94 -90 -92 -94 -99	2.07E-6 3.58E-6 1.90E-6 1.95E-6 1.42E-6 1.62E-6 2.74E-6 1.69E-6	4.51E-6 1.39E-5 3.77E-6 4.20E-6 2.88E-6 3.10E-6 7.74E-6 3.39E-6	9.84E-6 3.81E-5 7.45E-6 9.05E-6 5.84E-6 5.93E-6 2.90E-5 6.80E-6
Prostate Cancer DU-145	0.477	1.878	1.929	1.941	1.912	0.003	0.001	104	105	102	-99	-100	1.82E-6	3.22E-6	5.69E-6
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.631 0.725 1.104 1.199 0.489 0.945	3.142 1.663 2.260 2.726 1.196 1.631	2.937 1.711 2.190 2.638 1.132 1.539	2.922 1.653 2.199 2.636 1.116 1.517	2.493 1.604 2.225 2.650 1.026 1.283	0.295 0.665 1.032 0.045 0.429 0.337	0.317 0.549 1.009 0.046 0.299 0.276	92 105 94 94 91 86	91 99 95 94 89 83	74 94 97 95 76 49	-53 -8 -7 -96 -12 -64	-50 -24 -9 -96 -39 -71	1.55E-6 2.68E-6 2.84E-6 1.72E-6 1.97E-6 9.46E-7	3.82E-6 8.28E-6 8.64E-6 3.14E-6 7.26E-6 2.71E-6	> 1.00E-4 > 1.00E-4 5.73E-6 > 1.00E-4 7.48E-6





Mean of effective endpoints across 59 cell lines for compound 3 as Log₁₀ Concentration (SD)

GI₅₀ -5.8 (±0.26); TGI -5.37 (±0.24); LC₅₀ -4.82 (±0.41)





National Cancer Institute Developmental Therapeutics Program In-Vitro Testing Results																
NSC : D - 802		Experiment ID : 1801NS19						Test	Гуре : 08	Units : N	lolar					
Report Date :	Februar	ry 02, 20)18		Tes	t Date	: Janua	ıry 02, 20	18			QNS	QNS :		MC :	
COMI : AGS	1.1.7.1				Sta	in Rea	gent : S	RB Dual	Pass I	Related		SSPL	: 0Y2V			
	Time			Mear	Optica	Lo I Densiti	og10 Cor es	centration	P	ercent G	irowth	•				
Panel/Cell Line Leukemia	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	
CCRF-CEM K-562 MOLT-4 RPMI-8226	0.289 0.074 0.476 0.592	1.705 0.882 2.189 2.130	1.732 0.919 2.264 2.134	1.758 0.907 2.254 2.224	1.654 0.880 2.144 2.125	0.321 0.116 0.487 0.630	0.284 0.102 0.391 0.392	102 104 104 100	104 103 104 106	96 100 97 100	2 5 1 2	-2 3 -18 -34	3.11E-6 3.36E-6 3.09E-6 3.24E-6	3.68E-5 > 1.00E-4 1.08E-5 1.17E-5	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4	
Non-Small Cell Lun A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H228 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.319 0.408 0.856 1.068 0.617 0.479 0.544 0.160 0.913	1.621 1.173 1.965 1.524 1.238 1.855 1.409 1.514 2.105	1.616 1.063 1.896 1.471 1.254 1.883 1.452 1.465 1.995	1.626 1.157 1.901 1.479 1.244 1.916 1.468 1.658 2.017	1.612 1.101 1.914 1.537 1.205 1.603 1.444 1.387 1.996	0.251 0.270 0.895 0.726 0.745 0.323 0.576 0.214 0.685	0.108 0.100 0.013 0.188 0.246 0.280 0.006 0.059 0.204	100 86 94 88 103 102 105 96 91	100 98 94 90 101 104 107 111 93	99 91 95 103 95 82 104 91 91	-21 -34 -32 21 -33 4 4 -25	-66 -76 -98 -82 -60 -42 -99 -63 -78	2.56E-6 2.12E-6 3.12E-6 2.46E-6 4.01E-6 1.89E-6 3.45E-6 2.94E-6 2.25E-6	6.64E-6 5.35E-6 1.08E-5 5.78E-6 1.80E-5 5.19E-6 1.09E-5 1.15E-5 6.09E-6	4.35E-5 2.44E-5 3.35E-5 2.27E-5 7.49E-5 > 1.00E-4 3.34E-5 6.37E-5 2.98E-5	
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.426 0.576 0.234 0.247 0.221 0.408 0.273	1.092 2.115 1.855 1.404 1.239 1.831 1.897	1.122 2.133 1.873 1.403 1.326 1.963 2.004	1.108 2.136 1.772 1.463 1.315 1.936 1.968	0.994 2.182 1.747 1.362 1.291 1.626 1.959	0.141 0.607 0.198 0.226 0.196 0.543 0.312	0.054 0.091 0.014 0.013 0.143 0.141 0.053	104 101 100 109 109 107	102 101 95 105 107 107 104	85 104 93 96 105 86 104	-67 2 -15 -9 -12 9 2	-87 -84 -94 -95 -35 -65 -81	1.70E-6 3.40E-6 2.50E-6 2.76E-6 2.97E-6 2.93E-6 3.39E-6	3.63E-6 1.05E-5 7.22E-6 8.26E-6 7.96E-6 1.34E-5 1.07E-5	7.73E-6 4.00E-5 2.75E-5 3.01E-5 > 1.00E-4 6.22E-5 4.28E-5	
CNS Cancer SF-268 SF-295 SF-539 SNB-19 U251	0.510 0.542 0.664 0.431 0.289	1.729 2.092 2.045 1.469 1.344	1.731 2.140 1.951 1.526 1.269	1.715 2.201 2.031 1.502 1.352	1.677 2.020 2.053 1.469 1.294	0.643 0.566 0.593 0.416 0.266	0.142 0.029 0.017 0.004 0.025	100 103 93 105 93	99 107 99 103 101	96 95 101 100 95	11 2 -11 -4 -8	-72 -95 -97 -99 -91	3.46E-6 3.04E-6 2.85E-6 3.04E-6 2.74E-6	1.35E-5 1.04E-5 8.02E-6 9.23E-6 8.34E-6	5.41E-5 3.43E-5 2.84E-5 3.06E-5 3.19E-5	
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-28 SK-MEL-5 UACC-257 UACC-62	0.315 0.432 0.362 0.513 1.130 0.633 0.716 1.049 1.056	2.204 0.902 1.264 2.161 2.075 1.768 2.965 2.162 2.718	2.211 0.922 1.268 2.162 2.088 1.694 2.952 2.101 2.696	2.166 0.938 1.298 2.229 2.086 1.921 2.940 2.092 2.540	1.839 0.802 1.197 2.190 2.054 1.931 2.488 1.998 2.271	0.352 0.025 0.206 0.048 0.890 0.973 0.041 0.168 0.176	0.139 0.008 0.029 0.019 0.039 0.014 0.009 0.048	100 104 100 100 101 93 99 95 99	98 108 104 104 101 113 99 94 89	81 79 93 102 98 114 79 85 73	2 -94 -91 -21 30 -94 -84 -83	-56 -98 -92 -96 -82 -94 -98 -99 -99	2.45E-6 1.47E-6 2.06E-6 1.86E-6 2.52E-6 5.79E-6 1.47E-6 1.62E-6 1.41E-6	1.08E-5 2.85E-6 4.81E-6 3.38E-6 6.63E-6 1.74E-5 2.85E-6 3.19E-6 2.93E-6	7.91E-5 5.55E-6 1.38E-5 6.15E-6 2.95E-5 4.42E-5 5.54E-6 6.30E-6 6.12E-6	
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.426 0.434 0.753 0.588 0.444 0.407 0.819	1.584 1.580 1.696 1.394 1.735 1.409 1.515	1.567 1.718 1.663 1.411 1.765 1.416 1.467	1.574 1.701 1.728 1.422 1.739 1.443 1.504	1.428 1.478 1.536 1.480 1.650 1.400 1.459	0.294 0.329 0.066 0.514 0.377 0.368 1.091	0.120 0.044 0.021 0.094 0.202 0.350 0.008	99 112 97 102 102 101 93	99 110 103 104 100 103 98	87 91 83 111 93 99 92	-31 -24 -91 -13 -15 -10 39	-72 -90 -97 -84 -55 -14 -99	2.05E-6 2.27E-6 1.55E-6 3.11E-6 2.51E-6 2.83E-6 6.20E-6	5.45E-6 6.16E-6 2.99E-6 7.91E-6 7.24E-6 8.16E-6 1.92E-5	2.92E-5 2.46E-5 5.80E-6 3.34E-5 7.68E-5 > 1.00E-4 4.41E-5	
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.554 1.381 0.419 0.532 1.040 0.569 0.742 0.737	2.000 2.098 1.401 1.741 1.684 1.838 1.485 2.138	1.951 1.971 1.531 1.714 1.663 1.738 1.440 1.969	2.014 1.927 1.506 1.681 1.756 1.654 1.510 2.021	1.970 2.000 1.380 1.636 1.677 1.502 1.687 1.844	0.932 1.600 0.419 0.973 1.026 0.209 1.118 0.781	0.012 0.024 0.020 0.011 0.110 0.060 0.019 0.004	97 82 113 98 97 92 94 88	101 76 111 95 111 85 103 92	98 86 98 91 99 74 127 79	26 31 36 -1 -63 51 3	-98 -95 -95 -89 -89 -89 -98	4.65E-6 4.48E-6 3.08E-6 5.66E-6 3.08E-6 1.49E-6 1.01E-5 2.41E-6	1.63E-5 1.73E-5 9.97E-6 1.87E-5 9.69E-6 3.45E-6 2.19E-5 1.07E-5	4.11E-5 4.22E-5 3.35E-5 4.40E-5 3.57E-5 8.00E-6 4.78E-5 3.30E-5	
Prostate Cancer PC-3 DU-145	0.442 0.292	1.815 1.087	1.748 1.159	1.819 1.322	1.624 1.202	0.487 0.388	0.089 0.018	95 109	100 130	86 114	3 12	-80 -94	2.73E-6 4.26E-6	1.09E-5 1.30E-5	4.37E-5 3.85E-5	
MDA-MB-231/ATC MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.278 C 0.485 1.070 1.061 0.737 0.726	1.615 1.227 2.082 2.154 1.337 1.339	1.585 1.235 2.137 2.103 1.315 1.318	1.458 1.181 2.116 2.096 1.361 1.309	1.136 1.056 2.150 2.080 1.346 1.066	0.112 0.455 1.594 1.307 0.416 0.214	0.093 0.049 1.093 0.025 0.327 0.086	98 101 105 95 96 96	88 94 103 95 104 95	64 77 107 93 101 55	-60 -6 52 22 -44 -71	-67 -90 2 -98 -56 -88	1.30E-6 2.11E-6 1.08E-5 4.08E-6 2.26E-6 1.10E-6	3.29E-6 8.40E-6 > 1.00E-4 1.54E-5 5.00E-6 2.75E-6	8.32E-6 3.33E-5 > 1.00E-4 4.01E-5 3.37E-5 6.87E-6	







GI₅₀ -5.56 (±0.19); TGI -5.05 (±0.32); LC₅₀ -4.5 (±0.36)





National Cancer Institute Developmental Therapeutics Program In-Vitro Testing Results															
NSC : D - 805946 / 1						Experiment ID : 1809NS03						Test	Туре : 08	Units : M	lolar
Report Date :	Octobe	r 18, 20′	18		Tes	t Date	: Septe	mber 17,	2018			QNS	:	MC :	
COMI : RK LE	I 1-007				Sta	in Rea	gent : S	RB Dual-	Pass I	Related	I	SSPL	: 0Y2V		
						Lo	og10 Cor	ncentration				-1			
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mear -7.0	o Optica -6.0	l Densiti -5.0	es -4.0	-8.0	P -7.0	ercent G -6.0	Frowth -5.0	-4.0	GI50	TGI	LC50
CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.555 0.925 0.278 0.645 0.838 0.345	2.485 3.282 2.640 2.975 2.851 1.836	2.507 3.170 2.623 2.932 2.782 1.772	2.558 3.242 2.709 3.041 2.866 1.822	2.277 3.216 2.421 2.803 2.561 1.667	0.683 0.455 0.367 0.444 0.843 0.461	0.487 0.493 0.239 0.317 0.469 0.318	101 95 99 98 97 96	104 98 103 103 101 99	89 97 91 93 86 89	7 -51 4 -31 8	-12 -47 -14 -51 -44 -8	2.98E-6 2.08E-6 2.94E-6 2.21E-6 2.61E-6 3.00E-6	2.23E-5 4.54E-6 1.63E-5 5.60E-6 1.01E-5 3.14E-5	 > 1.00E-4 > 1.00E-4 9.05E-5 > 1.00E-4 > 1.00E-4
Non-Small Cell Lung A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H227 NCI-H322M NCI-H460 NCI-H522	Cancer 0.431 0.872 0.326 0.922 1.257 0.664 0.681 0.353 0.827	2.311 2.152 1.375 1.477 2.301 2.229 2.241 3.149 2.555	2.236 1.902 1.249 2.119 2.157 2.153 3.156 2.380	2.318 2.044 1.336 1.486 2.226 2.169 2.206 3.200 2.474	2.101 2.011 1.236 1.533 2.207 1.952 2.106 2.805 2.371	0.389 0.590 0.452 0.699 1.252 0.514 0.621 0.400 0.728	0.178 0.254 0.211 0.383 0.552 0.357 0.414 0.195 0.294	96 80 88 77 83 95 94 100 90	100 92 96 102 93 96 98 102 95	89 89 87 110 91 82 91 88 89	-10 -32 12 -24 -23 -9 2 -12	-59 -71 -35 -59 -56 -46 -39 -45 -65	2.47E-6 2.09E-6 3.10E-6 2.80E-6 2.03E-6 2.59E-6 2.59E-6 2.45E-6	7.94E-6 5.41E-6 1.79E-5 6.61E-6 9.90E-6 8.15E-6 1.09E-5 7.62E-6	6.61E-5 2.87E-5 > 1.00E-4 5.65E-5 7.78E-5 > 1.00E-4 > 1.00E-4 > 1.00E-4 5.29E-5
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.375 1.137 0.201 0.362 0.256 0.576 0.290	2.012 3.308 2.397 2.375 1.988 2.845 1.997	2.005 3.244 2.310 2.261 1.866 2.708 1.937	2.025 3.312 2.249 2.238 2.083 2.759 1.958	1.185 3.290 2.038 1.921 1.482 2.430 1.953	0.125 1.015 0.197 0.210 0.261 0.568 0.317	0.075 0.151 0.017 0.065 0.178 0.244 0.114	100 97 96 94 93 94 96	101 100 93 93 106 96 98	49 99 84 77 71 82 97	-67 -11 -2 -42 -1 2	-80 -87 -92 -82 -31 -58 -61	9.77E-7 2.80E-6 2.47E-6 1.70E-6 1.97E-6 2.40E-6 3.12E-6	2.67E-6 7.98E-6 9.48E-6 4.44E-6 1.02E-5 9.60E-6 1.06E-5	7.19E-6 3.28E-5 3.42E-5 1.57E-5 > 1.00E-4 7.31E-5 6.70E-5
CNS Cancer SF-268 SF-295 SF-539 SNB-19 SNB-75 U251	0.781 1.102 1.016 0.588 0.854 0.520	2.278 3.203 2.836 2.250 1.672 2.449	2.165 3.080 2.742 2.217 1.552 2.288	2.180 3.181 2.767 2.360 1.603 2.354	2.154 3.099 2.823 2.200 1.612 2.302	0.771 0.952 0.632 0.673 0.988 0.437	0.624 0.468 0.006 0.025 0.013 0.170	92 94 95 98 85 92	93 99 96 107 91 95	92 95 99 97 93 92	-1 -14 -38 5 16 -16	-20 -58 -99 -96 -99 -67	2.81E-6 2.60E-6 2.29E-6 3.25E-6 3.62E-6 2.46E-6	9.69E-6 7.49E-6 5.30E-6 1.12E-5 1.39E-5 7.11E-6	> 1.00E-4 6.74E-5 1.58E-5 3.52E-5 3.78E-5 4.60E-5
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UACC-62	0.758 0.842 0.458 0.666 1.247 0.839 1.028 0.764 0.978	3.337 1.822 2.172 2.990 2.886 2.540 3.204 2.132 2.861	3.255 1.692 2.061 2.966 2.853 2.543 3.140 2.047 2.918	3.272 1.815 2.167 3.062 2.933 2.718 3.118 2.095 3.044	3.031 1.204 2.051 2.982 2.685 2.582 2.432 1.869 2.727	0.770 0.020 0.217 0.050 1.221 1.241 0.028 0.359 0.239	0.296 0.049 0.058 0.331 0.465 0.019 0.204 0.292	97 87 94 99 98 100 97 94 103	97 99 100 103 103 110 96 97 110	88 37 93 100 88 102 65 81 93	-98 -53 -92 -2 24 -97 -53 -76	-61 -100 -89 -91 -73 -45 -98 -73 -70	2.72E-6 6.17E-7 1.97E-6 1.81E-6 2.63E-6 4.63E-6 1.23E-6 1.70E-6 1.80E-6	1.02E-5 1.88E-6 4.35E-6 3.30E-6 9.48E-6 2.22E-5 2.50E-6 4.02E-6 3.56E-6	6.62E-5 4.43E-6 9.58E-6 6.01E-6 4.69E-5 > 1.00E-4 5.10E-6 9.49E-6 7.05E-6
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES SK-OV-3	0.412 0.511 0.631 0.576 0.342 0.682 0.558	1.984 1.863 1.631 1.648 1.768 2.396 1.690	1.970 1.838 1.573 1.550 1.774 2.388 1.624	1.855 1.936 1.595 1.590 1.774 2.451 1.648	1.640 0.985 1.214 1.689 1.506 2.241 1.599	0.236 0.373 0.030 0.421 0.325 0.648 0.550	0.182 0.121 0.006 0.073 0.013 0.693 0.081	99 98 94 91 100 100 94	92 105 96 95 100 103 96	78 35 58 104 82 91 92	-43 -27 -95 -27 -5 -5 -2	-56 -76 -99 -87 -96 1 -85	1.71E-6 6.13E-7 1.13E-6 2.58E-6 2.32E-6 2.67E-6 2.81E-6	4.42E-6 3.67E-6 2.40E-6 6.22E-6 8.73E-6 9.63E-6	3.52E-5 2.93E-5 5.07E-6 2.41E-5 3.10E-5 > 1.00E-4 3.78E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C TK-10 UO-31	0.670 1.579 0.355 0.878 1.198 0.754 0.792 0.771	2.699 2.461 1.655 2.444 1.965 2.932 2.121 2.208	2.596 2.380 1.618 2.343 1.876 2.882 2.033 2.081	2.610 2.380 1.662 2.350 1.899 2.865 2.096 2.164	2.615 2.471 1.504 2.126 1.882 2.711 2.215 2.102	0.972 1.803 0.360 1.100 1.075 0.515 1.050 0.777	0.504 0.036 0.013 0.201 0.301 0.077 0.380 0.019	95 91 97 94 88 98 93 91	96 91 101 94 91 97 98 97	96 101 88 80 89 90 107 93	15 25 14 -10 -32 19	-25 -98 -96 -77 -75 -90 -52 -98	3.68E-6 4.72E-6 2.73E-6 2.84E-6 2.47E-6 2.13E-6 4.48E-6 2.90E-6	2.37E-5 1.61E-5 1.01E-5 1.43E-5 7.88E-6 5.48E-6 1.87E-5 1.01E-5	> 1.00E-4 4.09E-5 3.32E-5 5.04E-5 4.12E-5 2.06E-5 9.35E-5 3.27E-5
Prostate Cancer DU-145	0.477	1.878	1.894	1.988	1.926	0.550	0.005	101	108	103	5	-99	3.50E-6	1.12E-5	3.39E-5
Breast Cancer MCF7 MDA-MB-231/ATC0 HS 578T BT-549 T-47D MDA-MB-468	0.631 C 0.725 1.104 1.199 0.489 0.945	3.142 1.663 2.260 2.726 1.196 1.631	2.862 1.713 2.180 2.589 1.051 1.598	2.928 1.719 2.272 2.635 1.090 1.585	2.653 1.636 2.280 2.600 1.056 1.391	0.250 0.721 1.573 1.576 0.343 0.326	0.265 0.734 1.063 0.046 0.217 0.141	89 105 93 91 80 95	91 106 101 94 85 93	81 97 102 92 80 65	-60 41 25 -30 -66	-58 1 -4 -96 -56 -85	1.65E-6 3.03E-6 7.00E-6 4.19E-6 1.88E-6 1.30E-6	3.73E-6 8.24E-5 1.60E-5 5.35E-6 3.15E-6	8.44E-6 > 1.00E-4 > 1.00E-4 4.15E-5 5.99E-5 7.61E-6







GI₅₀ -5.62 (±0.19); TGI -5.09 (±0.3); LC₅₀ -4.42 (±0.41)





		Natio	onal (Canc	er Ir	nstitu In-	ite Do Vitro	evelop Testir	men ng R	ital T esult	hera s	peuti	cs Prograr	n	
NSC : D - 815	5386 / 1				Exp	erimer	nt ID:1	906NS30)			Test	Туре : 08	Units : N	lolar
Report Date :	July 28,	2019			Tes	t Date	: June	24, 2019				QNS :		MC :	
COMI : RK 6.4	4.7				Sta	n Rea	gent : S	RB Dual-	Pass F	Related		SSP	L : 0Y2V		
					1	Lo	og10 Cor	ncentration				1		-	
Panel/Cell Line	Time Zero	Ctrl	-8.0	Mean -7.0	Optica -6.0	Densiti -5.0	es -4.0	-8.0	-7.0	ercent G -6.0	rowth -5.0	-4.0	GI50	TGI	LC50
CCRF-CEM HL-60(TB) K-562 MOLT-4 RPMI-8226 SR	0.555 0.970 0.175 0.690 0.896 0.401	2.338 3.133 1.369 2.474 2.775 1.135	2.392 3.065 1.308 2.574 2.781 1.120	2.432 3.081 1.181 2.525 2.774 1.109	1.336 1.247 0.594 1.687 2.203 0.824	0.359 0.578 0.140 0.341 0.563 0.336	0.357 0.503 0.150 0.470 0.555 0.367	103 97 95 106 100 98	105 98 84 103 100 96	44 13 35 56 70 58	-35 -40 -20 -51 -37 -16	-36 -48 -14 -32 -38 -8	7.93E-7 3.64E-7 4.97E-7 1.14E-6 1.52E-6 1.27E-6	3.58E-6 1.74E-6 4.30E-6 3.35E-6 4.48E-6 6.01E-6	> 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4 > 1.00E-4
Non-Small Cell Lun; A549/ATCC EKVX HOP-62 HOP-92 NCI-H226 NCI-H226 NCI-H228 NCI-H322M NCI-H460 NCI-H522	g Cancer 0.290 0.554 0.711 1.036 1.126 0.613 0.743 0.287 0.820	1.919 1.867 1.813 1.609 2.385 1.868 1.960 2.764 2.272	1.913 1.788 1.706 1.553 2.357 1.800 1.952 2.847 2.117	1.834 1.756 1.662 1.582 2.309 1.717 1.849 2.801 2.005	1.336 1.352 1.668 1.639 2.316 1.126 1.380 1.325 1.690	0.167 0.067 0.148 0.559 0.474 0.113 0.625 0.133 0.294	0.142 0.047 0.110 0.614 0.316 0.110 0.015 0.055 0.281	100 94 90 98 95 99 103 89	95 92 86 95 94 88 91 101 82	64 61 87 105 95 41 52 42 60	-43 -88 -79 -46 -58 -82 -16 -54 -64	-51 -92 -85 -41 -72 -82 -98 -81 -66	1.36E-6 1.67E-6 2.31E-6 1.96E-6 6.40E-7 1.08E-6 7.31E-7 1.20E-6	3.99E-6 2.56E-6 3.34E-6 4.96E-6 4.17E-6 2.16E-6 5.84E-6 2.74E-6 3.04E-6	7.54E-5 5.55E-6 6.67E-6 > 1.00E-4 8.87E-6 5.52E-6 2.60E-5 9.16E-6 7.68E-6
Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-15 HT29 KM12 SW-620	0.585 0.932 0.244 0.278 0.208 0.579 0.258	2.203 2.543 2.059 2.113 1.712 2.965 1.891	2.229 2.462 2.024 2.060 1.717 2.950 1.836	2.115 2.425 1.968 1.885 1.761 2.834 1.829	0.533 1.325 0.283 0.877 0.364 1.530 0.539	0.146 0.107 0.072 0.069 0.178 0.410 0.080	0.110 0.045 0.044 0.047 0.150 0.162 0.070	102 95 98 97 100 99 97	95 93 95 88 103 95 96	-9 24 2 33 10 40 17	-75 -89 -70 -75 -15 -29 -69	-81 -95 -82 -83 -28 -72 -73	2.70E-7 4.21E-7 3.05E-7 4.83E-7 3.74E-7 6.53E-7 3.85E-7	8.21E-7 1.64E-6 1.07E-6 2.01E-6 2.60E-6 3.77E-6 1.58E-6	4.17E-6 4.55E-6 5.22E-6 5.84E-6 > 1.00E-4 3.05E-5 6.00E-6
CNS Cancer SF-268 SF-295 SF-539 SNB-75 U251	0.838 0.781 1.054 1.027 0.272	2.441 2.926 2.819 1.811 1.582	2.244 2.904 2.745 1.679 1.550	2.221 2.764 2.732 1.656 1.475	1.930 1.980 2.089 1.820 1.157	0.515 0.049 0.013 0.019 0.082	0.295 0.060 0.004 0.025 0.071	88 99 96 83 98	86 92 95 80 92	68 56 59 101 68	-39 -94 -99 -98 -70	-65 -92 -100 -98 -74	1.48E-6 1.09E-6 1.13E-6 1.81E-6 1.34E-6	4.35E-6 2.36E-6 2.36E-6 3.22E-6 3.10E-6	2.72E-5 5.10E-6 4.90E-6 5.73E-6 7.15E-6
Melanoma LOX IMVI MALME-3M M14 MDA-MB-435 SK-MEL-2 SK-MEL-28 SK-MEL-28 UACC-257 UACC-62	0.496 0.763 0.430 0.512 1.127 0.772 0.784 0.739 0.975	2.775 1.675 1.807 2.664 2.562 1.914 3.159 1.905 2.652	2.644 1.672 1.840 2.692 2.536 1.979 3.121 1.816 2.555	2.429 1.371 1.940 2.765 2.466 2.042 3.004 1.746 2.401	1.002 0.280 0.988 0.170 2.016 1.942 0.657 0.796 1.227	0.054 0.013 0.113 0.061 0.221 0.390 0.020 0.139 0.193	0.031 0.015 0.104 0.036 0.233 0.027 0.007 0.115 0.143	94 100 102 101 98 106 98 92 94	85 67 110 105 93 111 93 86 85	22 -63 41 -67 62 102 -16 5 15	-89 -98 -74 -88 -80 -50 -98 -81 -80	-94 -98 -76 -93 -79 -97 -97 -84 -85	3.60E-7 1.34E-7 7.29E-7 2.08E-7 1.21E-6 2.41E-6 2.49E-7 2.79E-7 3.16E-7	1.58E-6 3.26E-7 2.26E-6 4.08E-7 2.72E-6 4.72E-6 7.12E-7 1.14E-6 1.44E-6	4.45E-6 7.89E-7 6.19E-6 7.98E-7 6.12E-6 1.02E-5 2.60E-6 4.33E-6 4.82E-6
Ovarian Cancer IGROV1 OVCAR-3 OVCAR-4 OVCAR-5 OVCAR-8 NCI/ADR-RES	0.547 0.469 0.560 0.600 0.444 0.563	2.134 1.531 1.500 1.584 2.368 2.074	2.177 1.602 1.496 1.569 2.252 2.091	2.020 1.511 1.384 1.522 2.151 1.970	1.188 0.410 0.676 1.334 1.063 1.076	0.144 0.070 0.031 0.046 0.256 0.387	0.206 0.048 0.018 0.118 0.075 0.266	103 107 100 98 94 101	93 98 88 94 89 93	40 -13 12 75 32 34	-74 -85 -94 -92 -42 -31	-62 -90 -97 -80 -83 -53	6.56E-7 2.72E-7 3.16E-7 1.40E-6 4.84E-7 5.35E-7	2.26E-6 7.70E-7 1.30E-6 2.80E-6 2.70E-6 3.31E-6	6.19E-6 3.28E-6 3.83E-6 5.58E-6 1.53E-5 7.38E-5
Renal Cancer 786-0 A498 ACHN CAKI-1 RXF 393 SN12C UO-31	0.921 1.553 0.354 0.772 0.883 0.558 0.542	2.757 2.098 1.569 2.673 1.677 1.964 1.595	2.719 2.041 1.597 2.506 1.668 1.894 1.465	2.670 1.921 1.521 2.258 1.589 1.858 1.465	2.556 1.957 1.065 1.716 1.429 0.881 1.239	0.762 0.073 0.008 0.475 0.193 0.034 0.015	0.222 0.010 0.228 0.117 0.018 0.033 -0.001	98 90 102 91 99 95 88	95 68 96 78 89 92 88	89 74 58 50 69 23 66	-17 -95 -98 -39 -78 -94 -97	-76 -99 -36 -85 -98 -94 -100	2.33E-6 1.39E-6 9.72E-7 1.34E-6 4.08E-7 1.26E-6	6.88E-6 2.74E-6 2.37E-6 3.66E-6 2.94E-6 1.57E-6 2.54E-6	3.61E-5 5.40E-6 1.77E-5 6.43E-6 4.21E-6 5.13E-6
Prostate Cancer PC-3 DU-145	0.573 0.410	1.664 1.710	1.551 1.774	1.511 1.764	0.819 1.359	0.497 0.014	0.420 0.017	90 105	86 104	23 73	-13 -97	-27 -96	3.69E-7 1.37E-6	4.26E-6 2.69E-6	> 1.00E-4 5.31E-6
Breast Cancer MCF7 MDA-MB-231/ATC HS 578T BT-549 T-47D MDA-MB-468	0.467 C 0.775 0.869 1.031 0.723 0.732	2.487 1.855 1.941 2.013 1.736 1.442	2.350 1.871 1.911 1.927 1.680 1.390	2.268 1.727 1.861 1.897 1.629 1.319	0.497 1.024 1.679 1.790 0.889 0.758	0.170 0.617 0.730 0.213 0.317 0.137	0.154 0.636 0.709 0.184 0.308 0.106	93 102 97 91 94 93	89 88 93 88 89 83	1 23 76 77 16 4	-64 -20 -16 -79 -56 -81	-67 -18 -18 -82 -57 -86	2.80E-7 3.85E-7 1.90E-6 1.49E-6 3.46E-7 2.59E-7	1.05E-6 3.38E-6 6.68E-6 3.12E-6 1.68E-6 1.10E-6	6.18E-6 > 1.00E-4 > 1.00E-4 6.50E-6 8.21E-6 4.28E-6







GI₅₀ -6.15 (±0.34); TGI -5.63 (±0.31); LC₅₀ -4.95 (±0.6)

Calculation of Mean ${\rm GI}_{\rm 50}$ and Trends

Mean Gl₅₀ was calculated from 53 human cancer cell lines that were common across the four compounds **3,11,15** and **16**. Conditional formatting was applied to the Gl₅₀ values per compound row with the colour green representing more un-responsive cell lines and red representing more-responsive cell lines.

\sim				
	3	11	15	18
CCRF-CEM	0.0559	3.11	2.98	0.793
K-562	3.04	3.36	2.94	0.497
MOLT-4	1.69	3.09	2.21	1.14
RPMI-8226	2.07	3.24	2.61	1.52
A549/ATCC	3.12	2.56	2.47	1.36
EKVX	2.02	2.12	2.09	1.18
HOP-62	0.744	3.12	3.1	1.67
HOP-92	2.12	2.46	2.8	2.31
NCI-H226	1.42	4.01	2.81	1.96
NCI-H23	1.63	1.89	2.03	0.64
NCI-H322M	1.68	3 45	2 59	1.08
NCI-H460	2 72	2 94	2.33	0.731
NCI-H522	1.66	2.54	2.74	1.2
COLO-205	1.00	1 7	0.077	0.27
	1.04	2.4	0.977	0.27
HCT 116	1.04	5.4 2 F	2.0	0.421
	0.945	2.5	2.47	0.305
HCI-15	1.43	2.76	1.7	0.483
H1-29	2.41	2.97	1.97	0.374
KM12	1.99	2.93	2.4	0.653
SW-620	1.54	3.39	3.12	0.385
SF-268	2.05	3.46	2.81	1.48
SF-295	1.78	3.04	2.6	1.09
SF-539	1.8	2.85	2.29	1.13
U251	1.48	2.74	2.46	1.34
LOX IMVI	1.44	2.45	2.72	0.36
MALME-3M	1.53	1.47	0.617	0.134
M14	1.78	2.06	1.97	0.729
MDA-MB-435	1.79	1.86	1.81	0.208
SK-MEL-2	1.89	2.52	2.63	1.21
SK-MEL-28	1.96	5.79	4.63	2.21
SK-MEL-5	1.14	1.47	1.23	0.249
UACC-257	1.57	1.62	1.7	0.279
UACC-62	1.63	1.41	1.8	0.316
IGROV1	1.74	2.05	1.71	0.656
OVCAR-3	0.314	2.27	0.613	0.272
OVCAR-4	1.2	1.55	1.13	0.316
OVCAR-5	1.76	3.11	2.58	1.4
OVCAR-8	0.339	2.51	2.32	0.484
NCI-ADR/RES	2.33	2.83	2.67	0.535
786-0	2.07	4 65	3.68	2 33
A498	3 58	4 48	4 72	1 39
	19	3.08	2 73	1 13
CAKI-1	1.9	5.66	2.75	0.972
	1.55	2.09	2.04	1 24
SN12C	1.42	1.40	2.47	0.409
JIO 21	1.02	1.49	2.15	0.406
00-31	1.09	2.41	2.9	1.20
DU-145	1.82	4.26	3.5	1.37
	1.55	1.3	1.65	0.29
MDA-MB-	2.68	2.11	3.03	0.385
231/ATCC			_	
HS 578T	2.84	10.8	7	1.9
BT-549	1.72	4.08	4.19	1.49
T-47D	1.97	2.26	1.88	0.346
MDA-MB-468	0.946	1.1	1.3	0.259
Mean GI ₅₀	1.75	2.93	2.52	0.91

Mean LC₅₀ was calculated from 50 human cancer cell lines that were common across the four compounds **3,11,15** and **16**. Conditional formatting was applied to the GI₅₀ values per compound row with the colour green representing more un-responsive cell lines and red representing more-responsive cell lines.

	-			
	3	11	15	16
	100	100	100	100
N-302	100	100	100	100
RPIVII-8226	100	100	100	100
A549/ATCC	55.3	43.5	66.1	75.4
EKVX	22.2	24.4	28.7	5.55
HOP-62	5.79	33.5	100	6.67
HOP-92	23.8	22.7	56.5	100
NCI-H226	6.26	74.9	//.8	8.87
NCI-H23	100	100	100	5.52
NCI-H322M	5.62	33.4	100	26
NCI-H460	49.9	63.7	100	9.16
NCI-H522	8.11	29.8	52.9	7.68
COLO-205	6.85	7.73	7.19	4.17
HCC-2998	5.95	40	32.8	4.55
HCT-116	46	27.5	34.2	5.22
HCT-15	7.69	30.1	15.7	5.84
HT-29	100	100	100	100
KM12	15.1	62.2	73.1	30.5
SW-620	9.09	42.8	67	6
SF-268	27.6	54.1	100	27.2
SF-295	6.28	34.3	67.4	5.1
SF-539	5.68	28.4	15.8	4.9
U251	5.4	31.9	46	7.15
LOX IMVI	6.42	79.1	66.2	4.45
MALME-3M	5.57	5.55	4.43	0.789
M14	6.69	13.8	9.58	6.19
MDA-MB-435	6.13	6.15	6.01	0.798
SK-MEL-2	8.41	29.5	46.9	6.12
SK-MEL-28	6.62	44.2	100	10.2
SK-MEL-5	5.07	5.54	5.1	2.6
UACC-257	/.11	6.3	9.49	4.33
UACC-62	6.3	6.12	7.05	4.82
IGROV1	11.8	29.2	35.2	6.19
OVCAR-3	22.2	24.6	29.3	3.28
OVCAR-4	5.08	5.8	5.07	3.83
OVCAR-5	5.91	33.4	24.1	5.58
	4.54	76.8	31	15.3
NCI-ADR/RES	100	100	100	73.8
780-0	9.84	41.1	100	50.1
A490	0.05	42.2	40.9	J.4
	9.05	44	50.4	17.7 C 42
NAF 393	5.04	55.7	41.2	0.45
JIO 21	5.95	0 22	20.0	4.21 E 12
DIL-145	5.60	38 5	32.7	5.15
MDA-MB-	5.05	50.5	55.5	5.51
231/ATCC	100	33.3	100	100
HS 578T	100	100	100	100
BT-549	5.73	40.1	41.5	6.5
T-47D	100	33.7	59.9	8.21
MDA-MB-468	7.48	6.87	7.61	4.28
Mean LCso	28.3	42.14	52.99	23.86

COMPARE Analysis

Correlation of 15 - Tetrangulol



Tetrangulol

	NSC:S80	SEED 5946 Endpt:GI50 Expld:AVGDATA hiConc:-4.0 vectorld: 252406 count expts: 1
	NSC:S19	
		correlation: 0.687
		compareResultId: 6870704
Leukemia	5 50 4 50	
CCRF-CEM	-5.53 -4.52	
K-562	-5.53 -4.73	-
MOLT-4	-5.66 -5.26	Ð
RPMI-8226	-5.58 -4.54	
SR	-5.52 -5.87	
	-5.61-5.29	
EKVX	-5.68 -5.15	
HOP-62	-5.51 -4.79	E
HOP-92	-5.55 -4.00	E
NCI-H226	-5.55 -5.02	E E
NCI-H23	-5.69 -5.40	
NCI-H460	-5.56 -6.18	
NCI-H522	-5.61 -6.02	
Colon		
COLO205	-6.01 -5.49	
HCC-2998	-5.55 -5.29	P
HCI-116 HCT-15	-5.61 -4.95	
HT29	-5.71 -5.09	
KM12	-5.62 -5.41	-
SW-620	-5.50 -4.76	E
CNS		
SF-268	-5.55 -5.25	
SF-295 SE-539	-5.58 -4.70	-0
SNB-19	-5.49 -4.70	É
SNB-75	-5.44 -4.72	
U251	-5.61 -4.68	-1
Melanoma		
LOXIMVI MALME-3M	-5.57 -6.25	
M14	-5.71 -6.17	
MDA-MB-435	-5.74 -6.75	—
SK-MEL-2	-5.58 -4.99	E
SK-MEL-28	-5.33 -4.00	
SK-MEL-5	-5.91 -6.48	
UACC-62	-5.75 -5.81	
Ovarian		
IGROV1	-5.77 -5.66	₽
OVCAR-3	-6.21 -6.40	
OVCAR-4	-5.95 -5.34	
OVCAR-5	-5.59 -4.29	
NCI/ADR-RES	-5.57 -5.22	d
SK-OV-3	-5.55 -4.08	e
Renal		
786-0	-5.43 -5.13	<u> </u>
A498	-5.33 -4.00	
CAKI-1	-5.55 -4.00	
RXF393	-5.61 -4.00	
SN12C	-5.67 -4.14	—— þ
TK-10	-5.35 -4.26	
UO-31	-5.54 -4.00	E
Prostate	4 70	
DU-145	-5.46 -5.34	
Breast		
MCF7	-5.78 -5.48	=
MDA-MB-231/ATCC	-5.52 -4.76	
HS578T	-5.16 -4.39	
MDA-N RT-549	-6.72 -5 38 -4 98	
T-47D	-5.73 -5.29	
summary		
MG-MID	-5.62 -5.14	
Delta	0.47 1.14	
Range	1.06 3.80 -	
	L1	
	3	2 1 0 -1 -2 -3

Correlation of 15 - (1S,3S)-austrocortirubin



07 Endpt:GI50 Expl vectorid: 239782 or GDATA hiCa -4.0 correlation: 0.681 compareResultId: 6870705 Small Cell Lung DMS114 -5.84 -5.80 DMS273 Leukemia _ CCRF-CEM HL-60(TB) -5.53 **-5.24** -5.68 **-5.79** -5.53 **-5.37** -5.66 **-5.11** -5.58 **-5.09** K-562 C MOLT-4 RPMI-8226 -SR -5.52 **-5.53** Non-SmallCellLung . -5.61 **-5.53** -5.68 **-5.09** A549/ATCC EKVX -5.51 **-5.07** -5.55 **-5.02** HOP-62 HOP-92 -5.55 **-4.62** -5.69 **-5.62** -5.59 **-5.54** NCI-H226 NCI-H23 NCI-H322M NCI-H460 NCI-H522 -5.56 **-5.78** -5.61 **-5.34** LXFL529 -5.42 Colon _ -6.01 **-5.75** COLO205 _ DLD-1 -5.88 HCC-2998 -5.55 **-5.43** -5.61 **-5.58** -5.77 **-5.40** HCT-116 Ь HCT-15 HT29 KM12 -5.71**-5.57** -5.62 **-5.38** KM20L2 -4.00 SW-620 -5.50 **-5.41** CNS _ SF-268 -5.55 <mark>-5.28</mark> -5.58 **-5.46** -5.64 **-5.51** -5.49 **-5.31** SF-295 SF-539 SNB-19 SNB-75 -5.44 **-5.03** -**5.42** SNB-78 U251 -5.61 **-5.33** XF498 -5.54 Melanoma LOXIMVI MALME-3M -5.57 **-5.60** -6.21 **-5.99** -5.71 **-5.58** -5.74 **-5.73** M14 MDA-MB-435 **-6.53** -5.58 **-5.47** M19-MEL SK-MEL-2 -5.33 **-5.15** -5.91 **-5.88** -5.77 **-5.70** SK-MEL-28 SK-MEL-5 UACC-257 Þ UACC-62 -5.75 **-5.83** Ovarian ____ IGROV1 OVCAR-3 -5.77 **-5.34** -6.21 **-6.07** Ь -5.95 **-5.43** -5.59 **-4.90** OVCAR-4 OVCAR-5 OVCAR-8 -5.64 **-5.39** -5.57 **-5.42** -5.55 **-4.85** NCI/ADR-RES SK-OV-3 Renal 786-0 -5.43 **-5.11** -5.33 **-5.12** -5.56 **-5.29** -5.55 **-4.76** A498 ACHN CAKI-1 RXF393 -5.61 **-5.28** -5.67 -5.44 -5.35 -4.63 -5.54 -4.94 RXF-631 SN12C TK-10 UO-31 -F Prostate PC-3 -5.47 DU-145 -5.46 **-5.39** Breast MCF7 -5.78 <mark>-5.31</mark> Ь MDA-MB-231/ATCC -5.52 **-5.11** Ð -5.32 -5.11 -5.16 -4.74 -5.73 -5.38 -5.11 -5.73 -5.16 HS578T MDA-N BT-549 T-47D Mux. summary _____ MG-MID ~uta -5.88 **-5.67** -5.62**-5.38** 0.47**1.38** 1.06**2.53** Delta Range

Developmental Therapeutics Program Mean Graph Selected Data Vectors

Correlation of 15 – NSC 331757

Developmental Therapeutics Program Mean Graph Selected Data Vectors

----SEED----NSC:S805946 Endpt:GI50 Expld:1809NS03 hiConc:-4.0 vectorId: 829235 count expts: 1

. . .



	100.000	vectorid: 419150 count expts: 4
		correlation: 0.653
Small Cell Lung		compareResultid: 6870763
DMS114	-4.94	
DMS273	-4.66	-
Leukemia		
CCRF-CEM	-5.53 -4.66	9
HL-60(TB)	-5.68 -4.87	_ _
K-562	-5.53 -4.74	
MOLT-4	-5.66 -4.78	₽ -
RPMI-8226	-5.58 -4./3	
Non-SmallCellLung	-0.02 -0.00	
A549/ATCC	-5.61 -4.66	
EKVX	-5.68 -4.67	-
HOP-18	-4.07	
HOP-62	-5.51 -4.57	4
HOP-92	-5.55 -4.61	Ę
NCI-H226	-5.55 -4.65	F
NCI-H23	-5.69 -4.72	P
NCI-H322M	-5.59 -4.68	E
NCI-H460	-5.56 -4.78	4-
NCI-H522	-5.61-4.72	
Colon	-4.81	7
COL 0205	-6.01-5.08	
DLD-1	-4.76	-
HCC-2998	-5.55 -4.74	d
HCT-116	-5.61 -4.73	4
HCT-15	-5.77 -4.75	
HT29	-5.71 -4.85	₽-
KM12	-5.62 -4.81	-
KM20L2	-4.74	r
SW-620	-5.50 -4.87	9
CNS		
SF-268	-5.55 -4.63	E .
SF-293 SE-530	-5.56 -4.07	
SNB-19	-5.49 -4.67	-
SNB-75	-5.44 -4.32	
SNB-78	-4.52	
U251	-5.61 -4.70	
XF498	-4.59	_
Melanoma		
LOXIMVI	-5.57 -4.80	G
MALME-3M	-6.21 -4.89	
M14	-5.71 -4.74	
M19-MEL	-4.78	1
SK-MEL-28	-5.30 -4.71	
SK-MEL-5	-5.91 -4.84	
UACC-257	-5.77 -4.93	—
UACC-62	-5.75 -4.69	
Ovarian		
IGROV1	-5.77 -4.60	
OVCAR-3	-6.21 -5.11	
OVCAR-4	-5.95 -4.82	
OVCAR-5	-5.59 -4.72	E.
OVCAR-8	-5.64 -4.65	
Benal	-5.55 -4.40	
786-0	-5 43 -4.73	
A498	-5.33 -4.69	
ACHN	-5.56 -4.74	d-
CAKI-1	-5.55 -4.59	Ę
RXF393	-5.61 -4.71	4
RXF-631	-4.62	-
SN12C	-5.67 -4.74	f
TK-10	-5.35 -4.62	크
UO-31	-5.54 -4.70	4
summary	-5.62 4 74	
NIG-WID Delta	-0.02-4./1	
Range	1.061.04	
	1	
	1	0 -1

Correlation of 16 – NSC658444



NSC 658444

	NSC:S8	15386 Endpt:GI5 vectorId: 191	SEED 0 Expld:AVGDATA hiConc:-4.0 4555 count expts: 1
	NSC:S6	58444 Endpt:GI5	ARGET 0 Expld:AVGDATA hlConc:-4.0 790 count expts: 2
		correl:	ation: 0.725
		compareR	autild: 6869704
CCRE-CEM	-6 10 -5 06		_
HL-60(TB)	-6.44 -5.58		
K-562	-6.30 -4.69		
MOLT-4	-5.95 -4.77		
RPMI-8226 SB	-5.82 -4.60 -5.90 -5.80		
Non-SmallCellLung			
A549/ATCC	-5.87 -4.78		
EKVX	-5.93 -4.71	_	
HOP-62 HOP-92	-5.78 -4.74 -5.64 -4.66		
NCI-H226	-5.71 -4.50		
NCI-H23	-6.19 -5.03		3
NCI-H322M	-5.97 -4.75	-	
NCI-H480 NCI-H522	-5.92 -4.74		
Colon			
COLO205	-6.57 -5.52		
HCC-2998	-6.38 -4.78	_	
HCT-15	-6.32 -5.06		====
HT29	-6.43 -5.44		
KM12	-6.18 -4.78	_]
SW-620	-6.42 -5.37		
SF-268	-5.83 -4.62	-	
SF-295	-5.96 -4.81		
SF-539	-5.95 -4.78	=	
SNB-19 SNB-75	-4.73 -5.74 -4.74		
U251	-5.87 -4.70		
Melanoma			
LOXIMVI	-6.44 -5.21		
MALME-3M M14	-6.14 -5.03		
MDA-MB-435	-6.68 -5.71		
SK-MEL-2	-5.92 -4.78		
SK-MEL-28	-5.66 -4.77		
UACC-257	-6.55 -5.14		
UACC-62	-6.50 -5.29		
Ovarian			1
IGROV1 OVCAR-3	-6.18 -4.83 -6.57 -5.59	_	
OVCAR-4	-6.50 -5.13		
OVCAR-5	-5.85 -4.73		
OVCAR-8	-6.32 -5.04		
NCI/ADR-RES SK-OV-3	-6.27 - 6.41 - 4.58		<u></u>
Renal			
786-0	-5.63 -4.79		
A498 ACHN	-5.86 -4.62 -5.95 -4.67		
CAKI-1	-6.01 -4.58		
RXF393	-5.87 -4.76		
SN12C	-6.39 -4.84	-	
IK-10 UO-31	-4.77 -5.90 -4.74		
Prostate			
PC-3	-6.43 -4.76	_	
DU-145 Breast	-5.86 -4.79	L	
MCF7	-6.55 -5.57		
MDA-MB-231/ATCC	-6.41 -4.58		
HS578T	-5.72 -4.59		
MDA-N RT-540	-5.83 -5.83		
T-47D	-6.46 -5.06		
summary			
MG-MID	-6.15 -4.97		
Range	1.24 1.30		
	1		
	1		
	1		

Correlation of 16 - (1S,3S)-austrocrotirubin



	Developmental Therapeutics Program Mean Graph Selected Data Vectors			
	Selected Data vectors			
	NSC:S8	15386 Endpt:GI5 vectorid: 191	SEED i0 Expld:AVGDATA hiConc:-4.0 4555 count expts: 1	
	NSC:86	8307 Endpt:Gl5 vectorid: 235	i0 Expld:AVGDATA hlConc:-4.0 9782 count expts: 5	
		correl	ation: 0.705 esultid: 6869705	
Small Cell Lung		comparent		
DMS114 DMS273	-5.84 -5.80			
Leukemia				
HL-60(TB)	-6.10 -5.24 -6.44 -5.79	t		
K-562	-6.30 -5.37	_		
RPMI-8226	-5.82 -5.09			
SR Non-SmallCelll ung	-5.90 -5.53		-	
A549/ATCC	-5.87 -5.53		-	
EKVX	-5.93 -5.09			
HOP-92	-5.64 -5.02			
NCI-H226	-5.71 -4.62		1	
NCI-H322M	-5.97 -5.54		-	
NCI-H460	-6.14 -5.78	_	_	
LXFL529	-5.92 - 5. 94 - 5.42			
Colon	8 67 6 76			
DLD-1	-6.57 - 6.75 - 5.88			
HCC-2998	-6.38 -5.43			
HCT-116 HCT-15	-6.32 -5.40			
HT29	-6.43 -5.57			
KM12 KM20L2	-6.18 -6.38 -4.00		1	
SW-620	-6.42 -5.41			
CNS SF-268	-5.83 -5.28			
SF-295	-5.96 -5.46			
SF-539 SNB-19	-5.95 -5.51 - 5.31			
SNB-75	-5.74 -5.03			
SNB-78 U251	-5.42 -5.87 -5.33			
XF498	-5.54		-	
Melanoma LOXIMVI	-6.44 -5.60		=	
MALME-3M	-6.87 -5.99			
M14 MDA-MB-435	-6.14 -5.58 -6.68 -5.73		-	
M19-MEL	-6.53			
SK-MEL-2 SK-MEL-28	-5.92 -5.47 -5.66 -5.15			
SK-MEL-5	-6.60 -5.88			
UACC-257 UACC-62	-6.55 -6.70 -6.50 -6.83			
Ovarian				
IGROV1 OVCAR-3	-6.18 -5.34 -6.57 -6.07			
OVCAR-4	-6.50 -5.43			
OVCAR-5 OVCAR-8	-5.85 -4.90 -6.32 -5.39			
NCI/ADR-RES	-6.27 -5.42			
SK-OV-3 Renal	-4.85			
786-0	-5.63 -5.11			
A498 ACHN	-5.86 -5.12 -5.95 -5.29			
CAKI-1	-6.01 -4.78	-6		
RXF393 RXF-631	-5.87 -5.28 -5.71		_	
SN12C	-6.39 -5.44			
TK-10 UO-31	-4.63 -5.90 -4.94			
Prostate			<u> </u>	
PC-3 DU-145	-6.43 -5.47 -5.86 -5.39			
Breast				
MCF7 MDA-MB-231/ATCC	-6.55 -6.31 -6.41 -5.11	_		
HS578T	-5.72 -4.74			
MDA-N BT-549	-5.73 -5.83 -5.11		-	
T-47D	-6.46 -5.16	_		
MDA-MB-468 summary	-6.59 -5.67			
MG-MID	-6.15 -5.38			
Delta Range	0.511.38 1.242.53			
	Ļ		Ļ,	
	2	1	-1 -2	

Correlation of 16 – Discorhabdin C-dienol.TFA



Discorhabdin C-dienol.TFA

	SEED NSC:S815386 Endpt:GI50 Expld:AVGDATA hiConc:-4.0
	vectorid: 1914555 count expts: 1 ————————————————————————————————————
	vectorid: 120131 count expts: 2
	correlation: 0.686 compareResultId: 6869707
Small Cell Lung	
DMS174	-5.99 -
Leukemia	
CCRF-CEM	-6.10 -5.71 E
HL-60(TB)	-6.44 -6.25
K-562 MOLT-4	-6.30 -0.64
RPMI-8226	-5.82 -5.72
Non-SmallCellLung	
A549/ATCC	-5.87 -5.50
EKVX	-5.93 -5.97
HOP-18	-4.97
HOP-62	-5.78 -4.75
HOP-92 NCLH226	-5.71-5.47
NCI-H23	-6.19 -6.10
NCI-H322M	-5.97 -5.88
NCI-H460	-6.14 -5.63 -
NCI-H522	-5.92 -6.55
Colon	
COLO205	-6.57 -6.94
DLD-1	-5.78
HCC-2998	-6.38 -6.93
HCT-15	-6.32 -5.94
HT29	-6.43 -6.51
KM12	-6.18 -5.74
KM20L2	-6.50
SW-620	-6.42 -6.27
CNS	
SF-268	-5.83 -6.01
SF-295	-5.96 -5.61
SF-539	-5.95 -5.89
SNB-19 SNB-75	-5.74 -5.00
SNB-78	-5.55 -
U251	-5.87 -5.85
XF498	-5.12
Melanoma	
LOXIMVI	-6.44 -6.13
M19-MEL	-6.42
SK-MEL-2	-5.92 -5.90
SK-MEL-5	-6.60 -5.97
UACC-257	-6.55 -6.21
UACC-62	-6.50 -6.07
Ovarian	
IGROV1	-6.18 -6.05
OVCAR-3	-6.57 - 5.99
OVCAR-4	-6.50 -5.83
OVCAR-5	-5.85 -5.58
NCI/ADB-RES	-0.32 -0.19
SK-OV-3	-4.88
Renal	
A498	-5.86 -5.00
CAKI-1	-6.01 -5.36 —
RXF393	-5.87 -5.59
SN12C	-6.39 -5.89
UU-31 Breast	-5.90 -4.90
MCF7	-6.55 -6.36
summary	
MG-MID	-6.15 -5.80
Delta	0.511.05
Range	1.24 2.19
	<u> </u>

Correlation of 16 – NSC331757



	NSC:S815386 Endpt: vectorid: 19	SEED I50 Expld:AVGDATA hiConc:-4.0
	NSC:S331757 Endpt:G	TARGET
	corre	elation: 0.672
Small Cell Lung	compare	ResultId: 6869805
DMS114	-4.94	<u> </u>
Leukemia	-4.66	
CCRF-CEM	-6.10 -4.66	E
HL-60(TB)	-6.44 -4.87	
K-562 MOLT-4	-6.30 -4.74 -5.95 -4.78	
RPMI-8226	-5.82 -4.73	-
SR	-5.90 -4.68	3
Non-SmallCellLung	-5 87 -4 66	
EKVX	-5.93 -4.67	-
HOP-18	-4.07	-
HOP-62	-5.78 -4.57	
NCI-H226	-5.71 -4.65	
NCI-H23	-6.19 -4.72	p
NCI-H322M	-5.97 -4.68	
NCI-H460 NCI-H522	-6.14 -4.78	₽- -{
LXFL529	-4.61	-
Colon		
COLO205	-6.57 -5.08	
HCC-2998	-6.38 -4.74	
HCT-116	-6.51 -4.73	
HCT-15	-6.32 -4.75	₽
HT29	-6.43 -4.85	
KM20L2	-0.10 -4.74	-
SW-620	-6.42 -4.87	
CNS		
SF-268 SF-295	-5.83 -4.63	-
SF-539	-5.95 -4.72	-
SNB-19	-4.67	1
SNB-75	-5.74 -4.32	
U251	-5.87 -4.70	
XF498	-4.59 -	-
Melanoma		<u> </u>
LOXIMVI MALME-3M	-6.44 -4.80 -6.87 -4.89	
M14	-6.14 -4.74	F
M19-MEL	-4.78	-
SK-MEL-2	-5.92 -4.71	
SK-MEL-5	-6.60 -4.84	
UACC-257	-6.55 -4.93	
UACC-62	-6.50 -4.69	P
IGROV1	-6.18 -4.60 -	-
OVCAR-3	-6.57 -5.11	
OVCAR-4	-6.50 -4.82	
OVCAR-5	-5.85 -4.72	<u>}</u>
SK-OV-3	-0.32 -4.60	-
Renal		
786-0	-5.63 -4.73	-
A498 ACHN	-5.95 -4.74	4
CAKI-1	-6.01 -4.59 E	4
RXF393	-5.87 -4.71	1
RXF-631	-4.62	1
TK-10	-0.53 -1.1-	-
UO-31	-5.90 -4.70	4
summary	C 4E 4 74	
MG-MID Delta	-5.1 3-4. 71 0.5 10.64	
Range	1.24 1.04	
	L	
	1	v

Correlation of $\mathbf{3}$ – 2-Deoxyuridine



2-deoxyuridine

	NSC:S8	SE 5939 Endpt:GI50 F	ED xpld:1809NS03 hiConc:-4.0
	100.000	vectorld: 64258	GET—
	NSC:S2	3615 Endpt:GI50 E vectorid: 13160	xpld:AVGDATA hlConc:-3.0 0 count expts: 1
		correlatio	on: 0.711
Leukemia		compareResu	ultid: 6880852
CCRF-CEM	-7.25 -4.02		
HL-60(TB)	-5.67 -3.00	d	
K-562	-5.52 -3.00		
MOLT-4	-5.77 -3.26	- H-	-
SR	-5.64 -3.00	q	
Non-SmallCellLung			
A549/ATCC	-5.51 -3.00	4	
ERVX HOR 63	-5.69 -3.00	j	
HOP-92	-5.67 -3.00	L L	
NCI-H226	-5.85 -3.00		
NCI-H23	-5.79 -3.00		
NCI-H322M	-5.77 -3.00		
NCI-H460	-5.57 -3.00		
NCI-H522	-5.78 -3.00	1	
Colon			
COLO205	-5.79 -3.00	1	
HCC-2998	-5.78 -3.00	L	
HCT-116	-6.03 -3.00	L L	
HC1-13	-5.65 -5.00	Ľ	
KM12	-5.70 -3.00	с г	
SW-620	-5.81 -3.00	-	
CNS			
SF-268	-5.69 -3.00	c	
SF-295	-5.75 -3.00	e e	
SF-539	-5.75 -3.00	¢	
SNB-19	-5.78 -3.00	1	
SNB-75	-5.76 -3.00	[
U251	-5.83 -3.00	1	
	E 94 9 00		
MALME-3M	-5.81 -3.00	ľ	
M14	-5.75 -3.00		
MDA-MB-435	-5.75 -3.00		
SK-MEL-2	-5.72 -3.00	c	
SK-MEL-28	-5.71 -3.00	G	
SK-MEL-5	-5.94 -3.00	þ	
UACC-257	-5.80 -3.00	1	
UACC-62	-5.79 -3.00		
Ovarian			
OVCAR-3	-5.76 -5.00		_
OVCAR-4	-5.92 -3.00	5	
OVCAR-5	-5.75 -3.00	L. L.	
OVCAR-8	-6.47 -3.00		
NCI/ADR-RES	-5.63 -3.00	c	
SK-OV-3	-5.65 -3.00	C	
Renal			
786-0	-5.68 -3.00		
A498	-5.45 -3.00		
ACHN	-5.72 -3.00	4	
CAKI-1	-5.71-3.00	4	
SN12C	-5.79 -3.00	ľ	
TK-10	-5.56 -3.00	_	
UO-31	-5.77 -3.00		
Prostate			
PC-3	-3.00		
DU-145	-5.74 -3.00	E	
Breast			
MCF7	-5.81 -3.00		
MDA-MB-231/ATCC	-5.57 -3.00	9	
HS578T	-5.55 -3.00	4	
T-47D	-5.76 -3.00	1	
summarv _	-5.71-3.00		
MG-MID	-5.80 -3.02		
Delta	0.350.02		I
Range	1.81 <mark>1.02</mark>		1
	1		
	2	1 0	-1 -2
	1	Ó	-1

Correlation of 3- Nelarabine

		NSC:S8	 05939 Endpt:GI5 vectorld: 642	SEED 0 Expld:1809NS03 hiConc:-4.0 2587 count expts: 1
\searrow		NSC:S7	55985 Endpt:GI5	ARGET
Õ			vectorid: 310	Jose count expts: 1
N			correl compareR	ation: 0.675 esultId: 6880853
	Leukemia			
<pre></pre>	CCRF-CEM	-7.25 -5.72	_	
$N^{-}N^{-}NH_{2}$	HL-60(TB)	-5.67 -4.00	L.	
HO	K-562 MOLT-4	-5.32 -4.00		
	RPMI-8226	-5.68 -4.00		
	SR	-5.64 -4.00	0	
	Non-SmallCellLung			
OH	A549/ATCC	-5.51 -4.00		
Nelarahine	EKVX	-5.69 -4.00	6	
Neidrabille	HOP-62	-6.13 -4.00	_	
	NCI-H226	-5.85 -4.00		
	NCI-H23	-5.79 -4.00		
	NCI-H322M	-5.77 -4.00		
	NCI-H460	-5.57 -4.00		
	NCI-H522	-5.78 -4.00		
	Colon			
	COLO205	-5.79 -4.00		
	HCC-2998	-5.78 -4.00	1	
	HCT-116	-6.03 -4.00		
	HCT-15	-5.85 -4.00	_	u L
	H129 KM12	-0.02 -4.00	L.	
	SW-620	-5.81 -4.00		
	CNS			
	SF-268	-5.69 -4.00	6	
	SF-295	-5.75 -4.00	6	
	SF-539	-5.75 -4.00	E	
	SNB-19	-5.78 -4.00		
	SNB-75	-5.76 -4.00	1	
	U251	-5.83 -4.00		1
		-5.84 -4.00		
	MALME-3M	-5.81 -4.00		
	M14	-5.75 -4.00	E	
	MDA-MB-435	-5.75 -4.00	E	
	SK-MEL-2	-5.72 -4.00	E	
	SK-MEL-28	-5.71 -4.00	G	
	SK-MEL-5	-5.94 -4.00		
	UACC-257	-5.80 -4.00		
	UACC-62	-5.79 -4.00		
		-5 76 -4 00		
	OVCAR-3	-6.50 -4.00		
	OVCAR-4	-5.92 -4.00]
	OVCAR-5	-5.75 -4.00		
	OVCAR-8	-6.47 -4.00		
	NCI/ADR-RES	-5.63 -4.00	G	
	Renal			
	A498	-5.45 -4.00		
	ACHN	-5.72 -4.00	L.	
	RXF303	-5.71 -4.00		1
	SN12C	-5.79 -4.00		
	TK-10	-5.56 -4.00		
	UO-31	-5.77 -4.00		
	Prostate			
	PC-3	-4.00		
	DU-145	-5.74 -4.00	E	
	Breast	E 01 .4 00		
	MDA-MR-231/ATOC	-5.81 -4.00	_	
	HS578T	-5.55 -4 00		
	T-47D	-5.71 -4.00		
	MDA-MB-468	-6.02 -4.00		
	summary			
	MG-MID	-5.80 -4.04		
	Delta	0.35 <mark>0.04</mark>		
	Range	1.81 1.72		
		Ļ		
		2		
		2		 The second se Second second sec

Matrix COMPARE of 15 (NSC 805946) and 16 (NSC 815386)

Row Label	829235 4 NSC:S805946 Endpt:GI50 Expld:1809NS03 hiConc:-4.0 null	1914555 NSC:S815386 Endpt:GI50 Expld:AVGDATA hiConc:-4.0 null
829235 NSC:S805946 Endpt:GI50 Expld:1809NS03 hiConc:-4.0 null	correlation: 1.0 count cell lines: 59 seed stdDev: 0.185 target stdDev: 0.185 Select this result	correlation: 0.725 count cell lines: 56 seed stdDev: 0.185 target stdDev: 0.319 Select this result
1914555 NSC:S815386 Endpt:GI50 Expld:AVGDATA hiConc:-4.0 null	correlation: 0.725 count cell lines: 56 seed stdDev: 0.319 target stdDev: 0.185	correlation: 1.0 count cell lines: 57 seed stdDev: 0.319 target stdDev: 0.319 Select this result

Matrix COMPARE of 15 (NSC 805946) and 3 (NSC 805939)

Row Label		642587 NSC:S805939 Endpt:GI50 Expld:1809NS03 hiConc:-4.0 null
252406 NSC:S805946 Endpt:GI50 Expld:AVGDATA hiConc:-4.0 null	correlation: 1.0 count cell lines: 59 seed stdDev: 0.185 target stdDev: 0.185 Select this result	correlation: 0.291 count cell lines: 59 seed stdDev: 0.185 target stdDev: 0.263
642587 NSC:S805939 Endpt:GI50 Expld:1809NS03 hiConc:-4.0 null	correlation: 0.291 count cell lines: 59 seed stdDev: 0.263 target stdDev: 0.185 Select this result	correlation: 1.0 count cell lines: 59 seed stdDev: 0.263 target stdDev: 0.263 Select this result
Graph selected matrix COMPARE res	sults Select/Deselect All	

Matrix COMPARE of 16 (NSC 815386) and 3 (NSC 805939)

Row Label		1914555 NSC:S815386 Endpt:GI50 Expld:AVGDATA hiConc:-4.0 null
642587 NSC:S805939 Endpt:GI50 Expld:1809NS03 hiConc:-4.0 null	correlation: 1.0 count cell lines: 59 seed stdDev: 0.263 target stdDev: 0.263 Select this result	correlation: 0.2 count cell lines: 56 seed stdDev: 0.268 target stdDev: 0.319 Select this result
1914555 NSC:S815386 Endpt:GI50 Expld:AVGDATA hiConc:-4.0 null	correlation: 0.2 count cell lines: 56 seed stdDev: 0.319 target stdDev: 0.268 Select this result	correlation: 1.0 count cell lines: 57 seed stdDev: 0.319 target stdDev: 0.319 Select this result

Graph selected matrix COMPARE results Select/Deselect All

Electrochemical Graphs

CV of 2 mM **2**, 2 mM **3**, 2 mM **11**, 2 mM **15**, and 3 mM **16** obtained by a Pt electrode vs. Ag/Ag^+ using 0.1 M of tetrabutylammonium tetrafluoroborate in ACN, a scan rate of 100 mVs⁻¹.







Squarewave voltammetry (SWV) of 3 mM **2**, 2 mM **3**, 2 mM **11**, 3 mM **15**, and 3 mM **16** obtained by a Pt electrode vs. Ag/Ag^+ using 0.1 M of tetrabutylammonium tetrafluoroborate in ACN.





Adduct Binding Studies

Predicted adducts

Compounds **2**, **3**, **7** and **15** proposed adducts are shown. Compound **11** adducts are identical to compound **7** adducts due to loss of bromine. Compound **16** is opposite isomer to compound **15**, thus mass of adducts formed would be identical.



15-glu

LC/MS procedure and information

LC/MS : Acquity BSM, Acquity Sample Manager, Vion IMS QTof (SAA055K)
Column: Acquity UPLC-BEH-C18
Column Dimension : 2.1 mm x 50 mm
Column Particle Size : 1.7 μm
Mode: ESI ⁺
Mobile Phase: See Below
Gradient: See Below
Flow Rate: 0.600 mL/min
Sample Run Time: 5 minutes
Injection Volume: 1μL with a 2μL dilution

Mobile Phases and Gradients

Solvent A = Water + 0.1% Formic Acid

Solvent B = Acetonitrile + 0.1 % Formic Acid

Time (min)	Composition A (%)	Composition B (%)	Curve
0.00	98.0	2.0	Initial
0.50	98.0	2.0	6
2.00	50.0	50.0	6
4.00	5.0	95.0	6
4.10	98.0	2.0	6
5.00	98.0	2.0	6

Vion IMS QTof Source Parameters

Desolvation temperature:	450 °C	Cone gas:	50 L/hr
Desolvation gas:	800 L/hr	Capillary Voltage:	1.00 kV
Source Temperature:	120 °C	Scan Time:	0.200 s

LC/MS Results

Entry	Biological	Retention Time	Observed	Detector
	Nucleophile		mass	Response
			[m/z, (M+H⁺)]	
2	Cysteine	1.3	365.0798	20,237
	Glutathione	1.18	551.1445	10,072
	Serine	1.6	349.1026	20,342
3	Cysteine	1.39	381.0750	11,416
	Glutathione	1.14	567.1396	4154
	Serine	1.41	365.0981	1,017
7	Cysteine	1.88	470.1385	516
	Glutathione	1.83	656.2014	737
	Serine	N/A	N/A	N/A
11	Cysteine	1.88	470.1376	1,742
	Glutathione	1.83	656.2030	3,856
	Serine	N/A	N/A	N/A
15	Cysteine	1.72	486.1328	3,893
	Glutathione	1.68	672.1991	4,324
	Serine	N/A	N/A	N/A
16	Cysteine	1.78	486.1348	208
	Glutathione	1.76	672.1984	4,713
	Serine	N/A	N/A	N/A