

Supplementary information

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Copies of ^1H , ^{13}C NMR and LC-MS of isoindole-thiazole derivatives Fig. S1-S6

NCI protocols for compound 3

Fig.S7-S8, Table S1

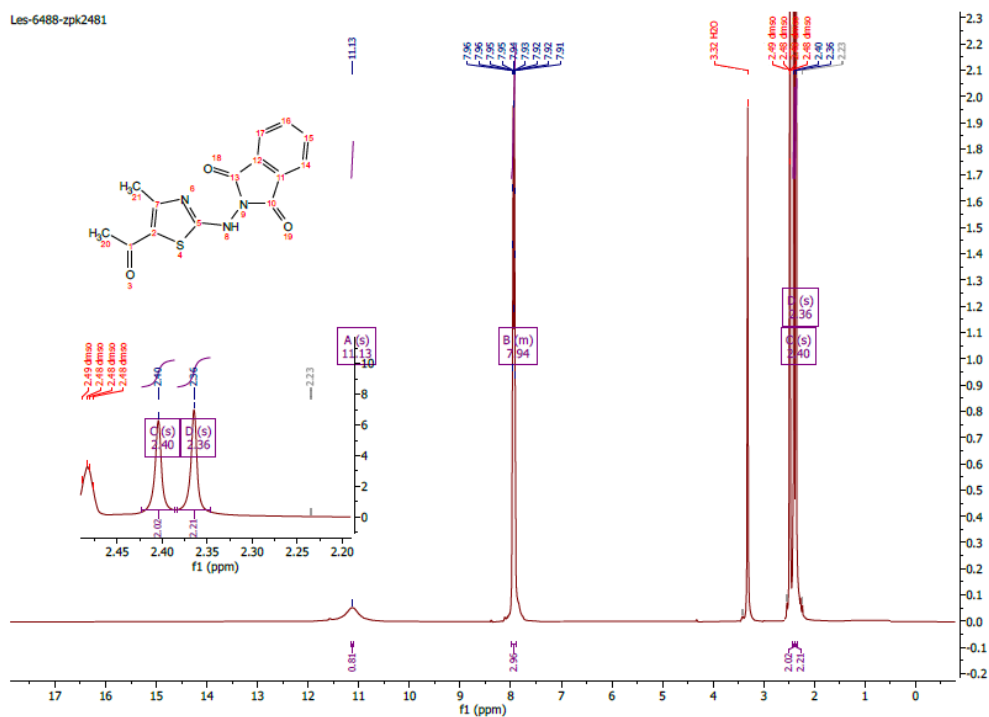


Figure S1. ^1H NMR spectrum of compound **2** (DMSO- d_6).

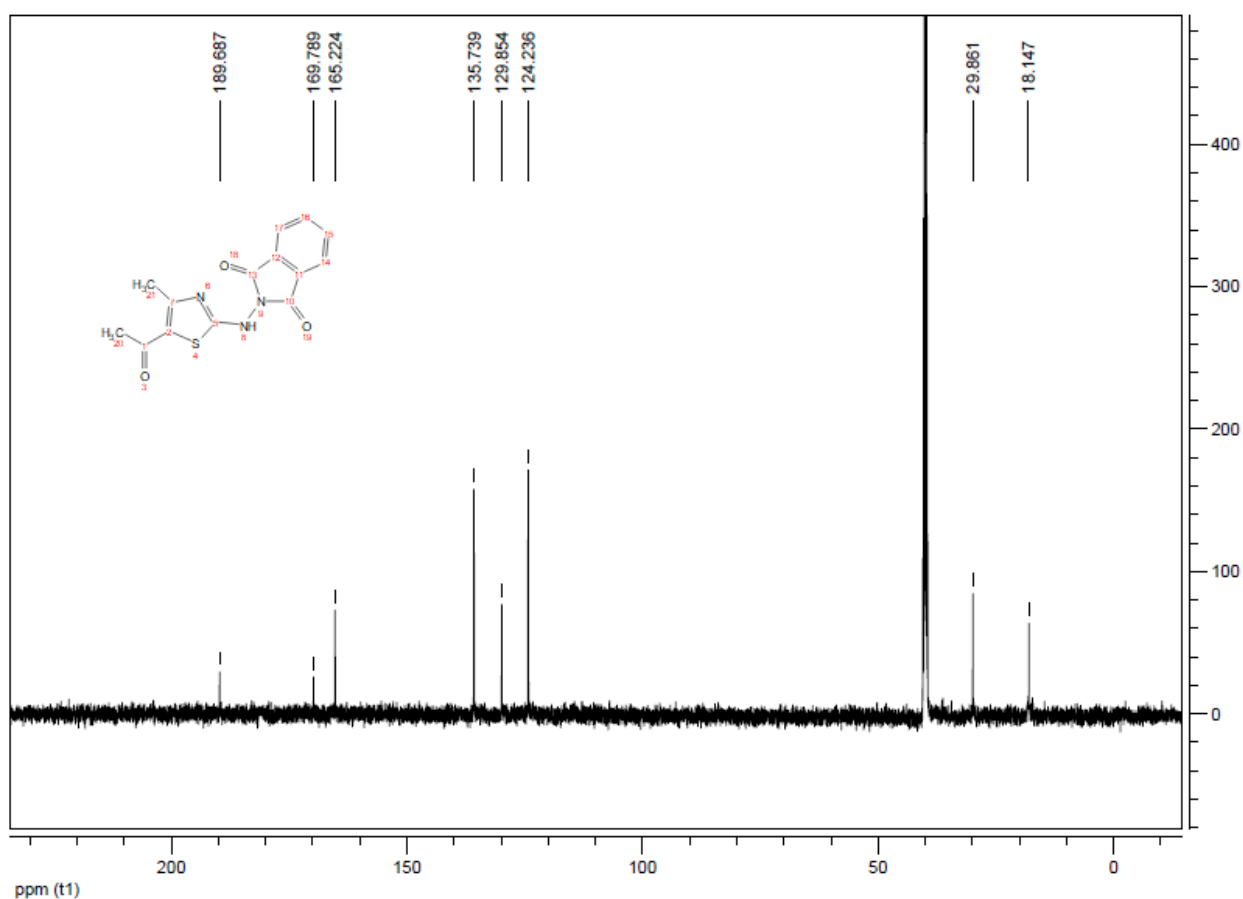


Figure S2. ^{13}C NMR spectrum of compound **2** (DMSO- d_6).

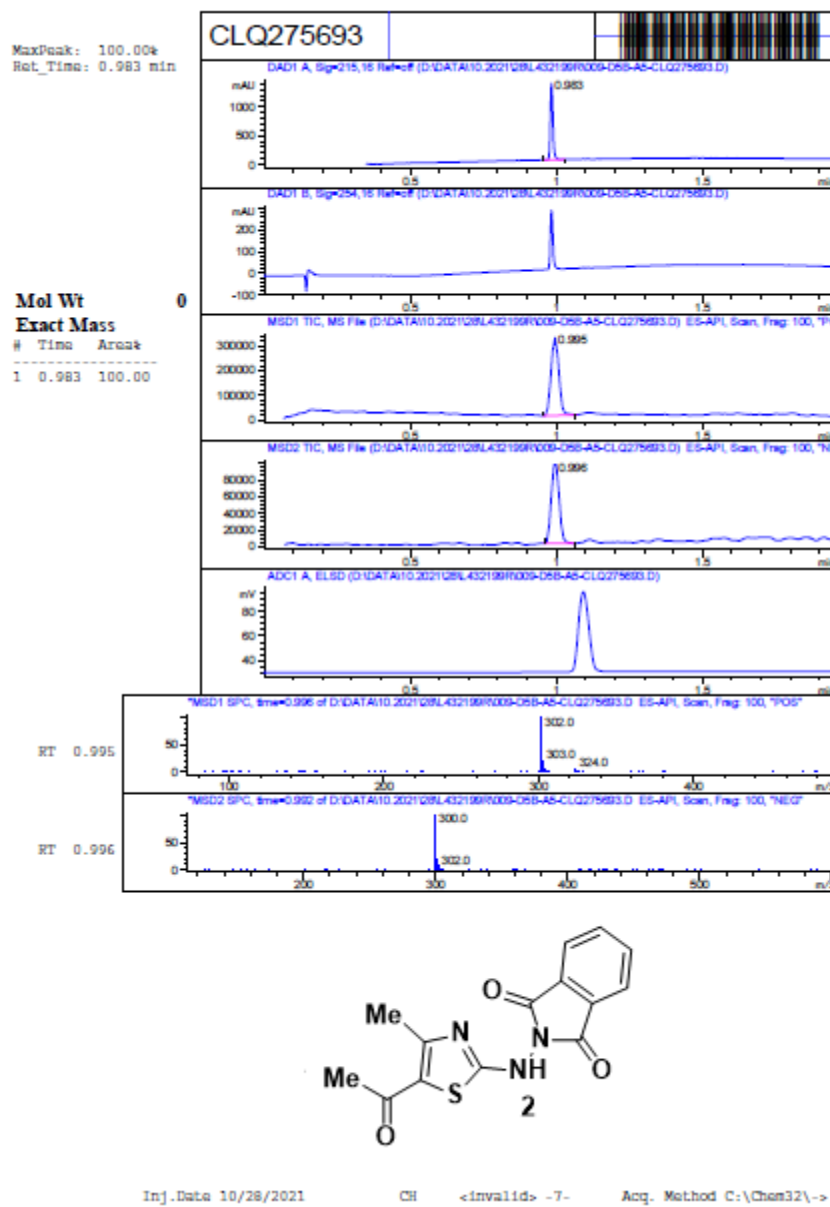


Figure S3. LCMS spectrum of compound 2.

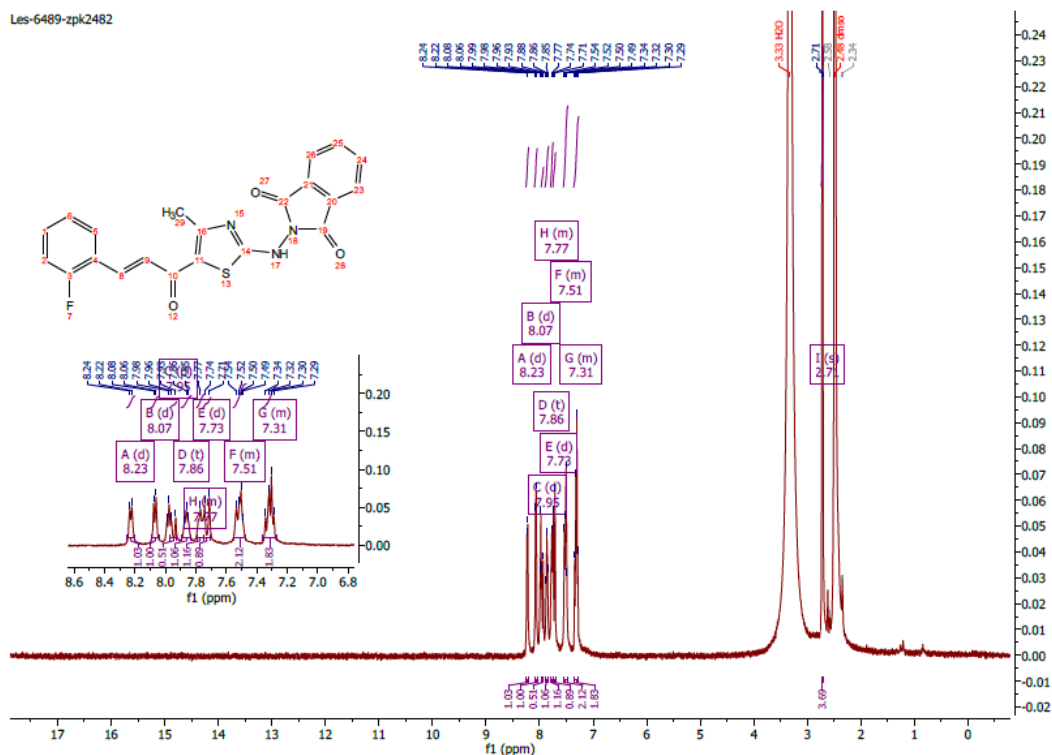


Figure S4. ^1H NMR spectrum of compound **3** (DMSO- d_6).

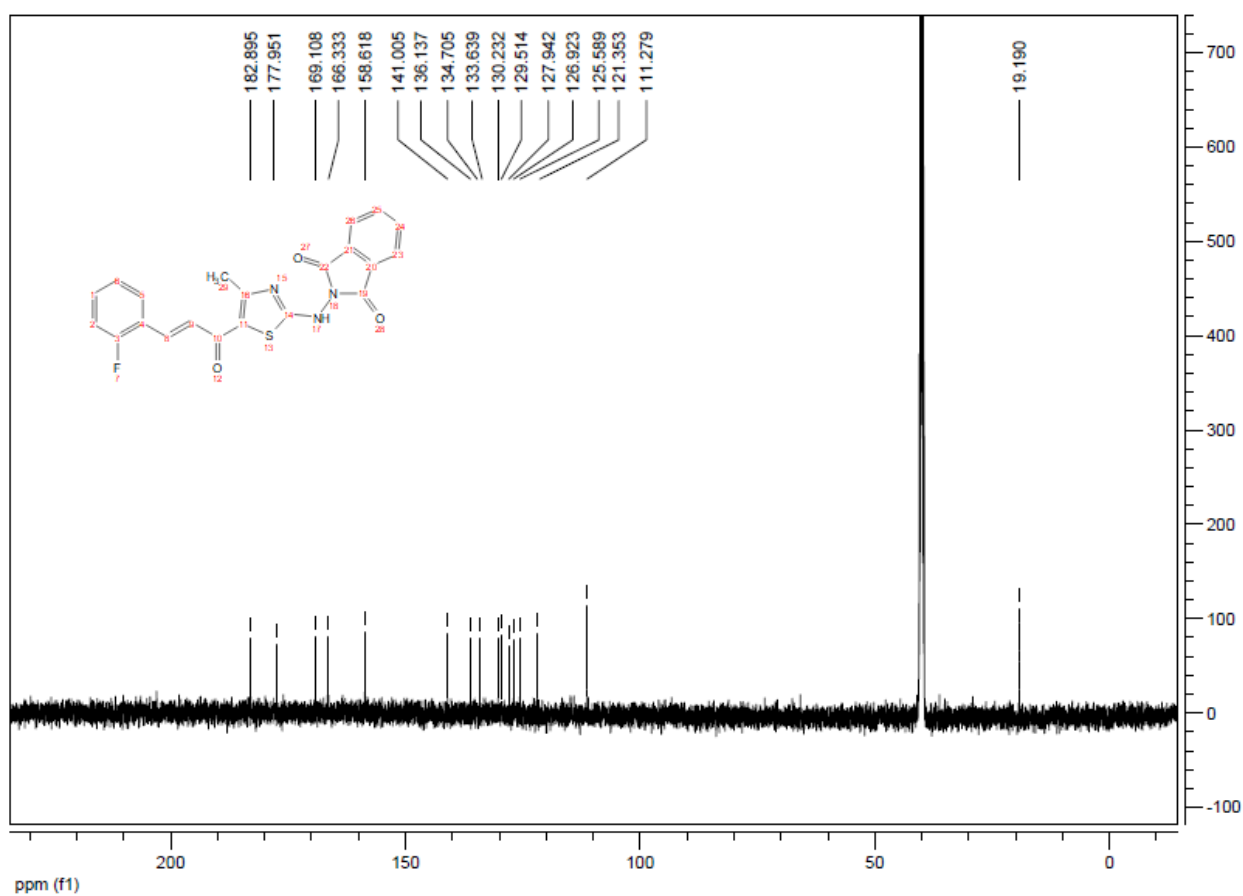


Figure S5. ^{13}C NMR spectrum of compound **3** (DMSO- d_6).

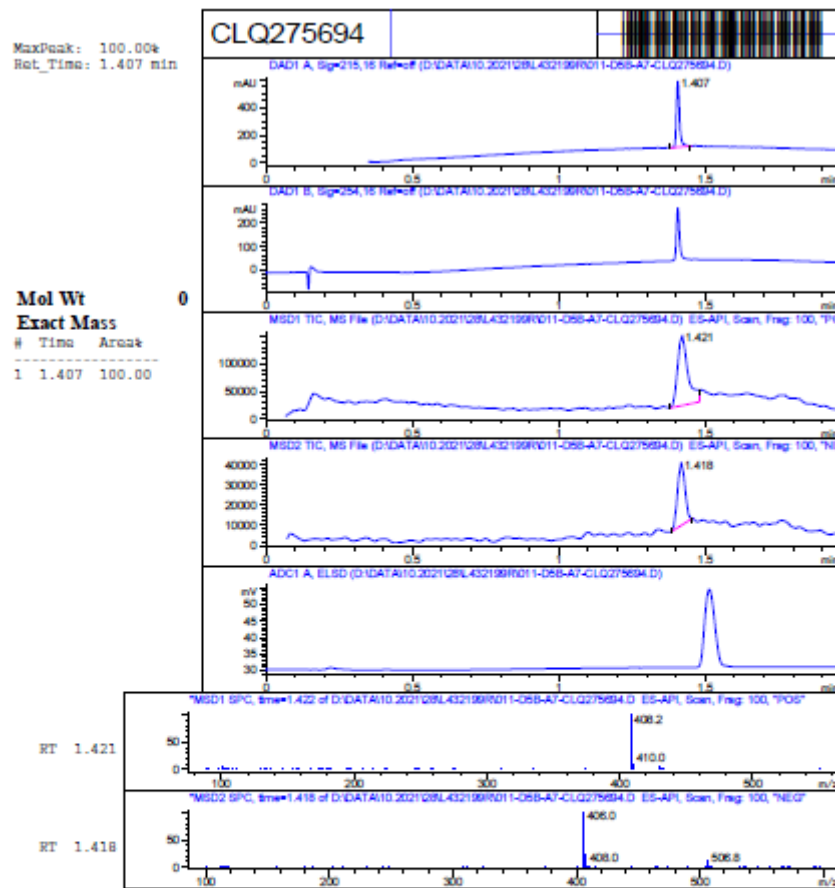


Figure S6. LCMS spectrum of compound 3.

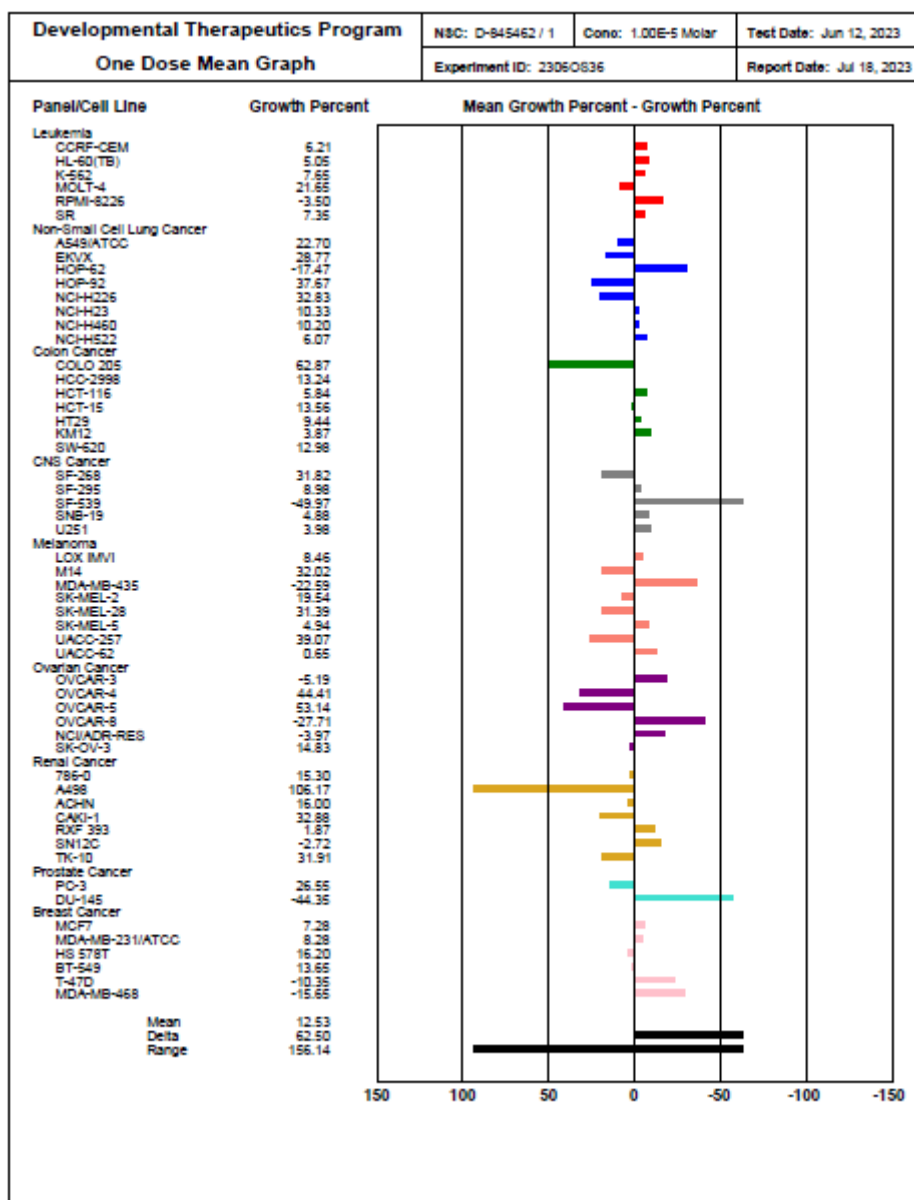


Figure S7. NCI-60 cell lines screening protocol in concentration 10 μ M for compound 3.

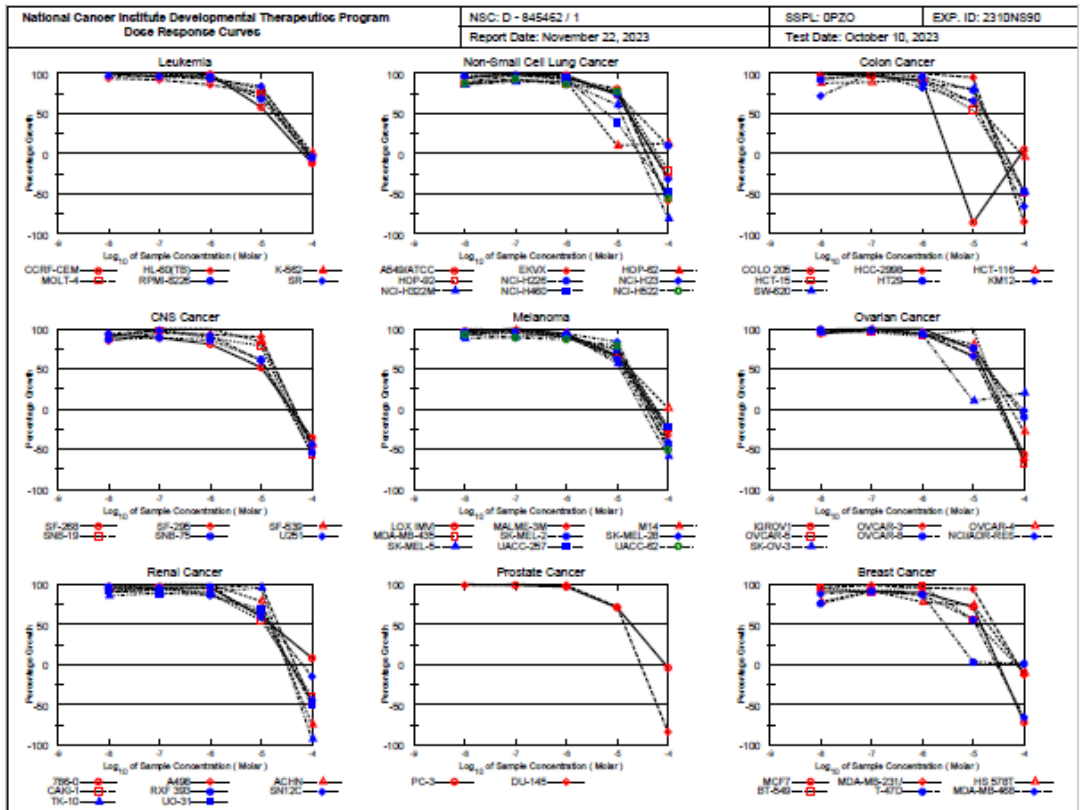


Figure S8b. NCI-60 cell lines screening protocol concentrations ranging from 10^{-4} to 10^{-8} M for compound 3.

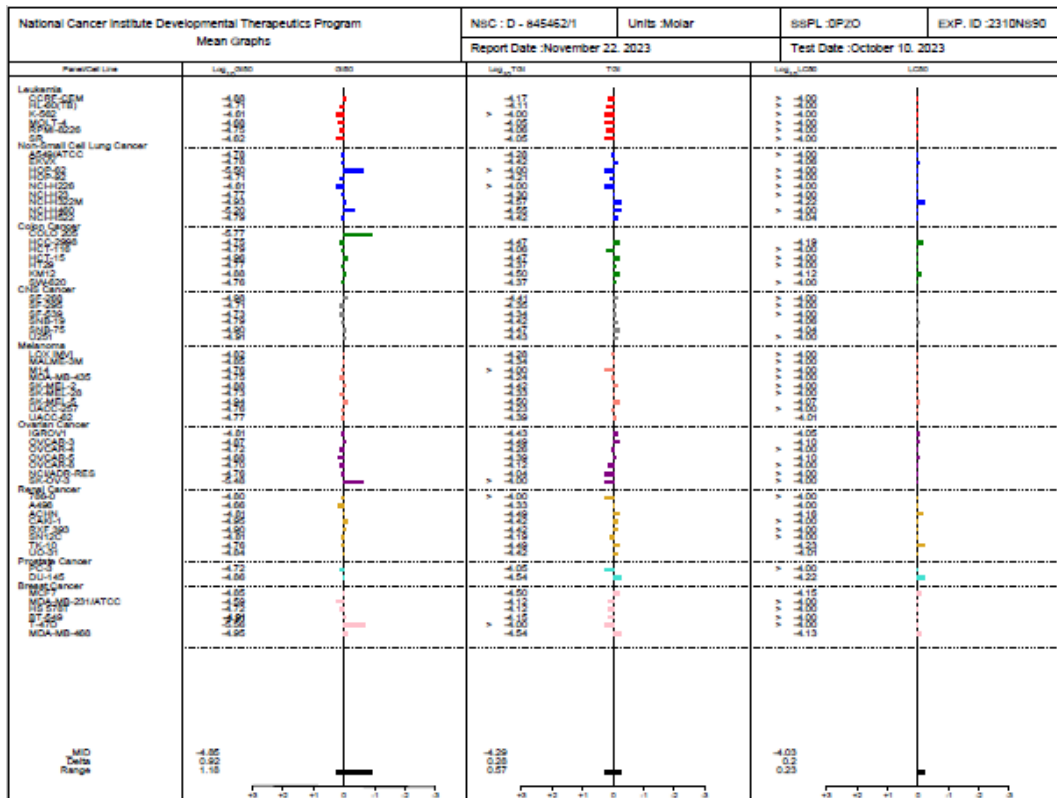


Figure S8c. NCI-60 cell lines screening protocol concentrations ranging from 10^{-4} to 10^{-8} M for compound 3.

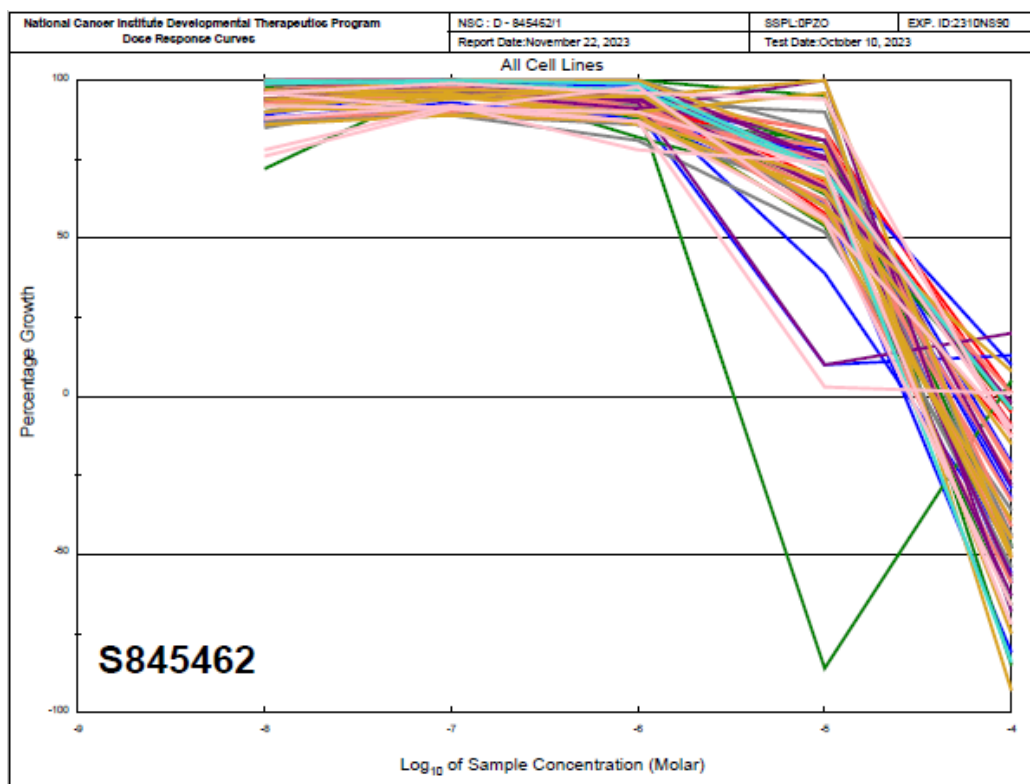


Figure S8d. NCI-60 cell lines screening protocol concentrations ranging from 10^{-4} to 10^{-8} M for compound **3**.

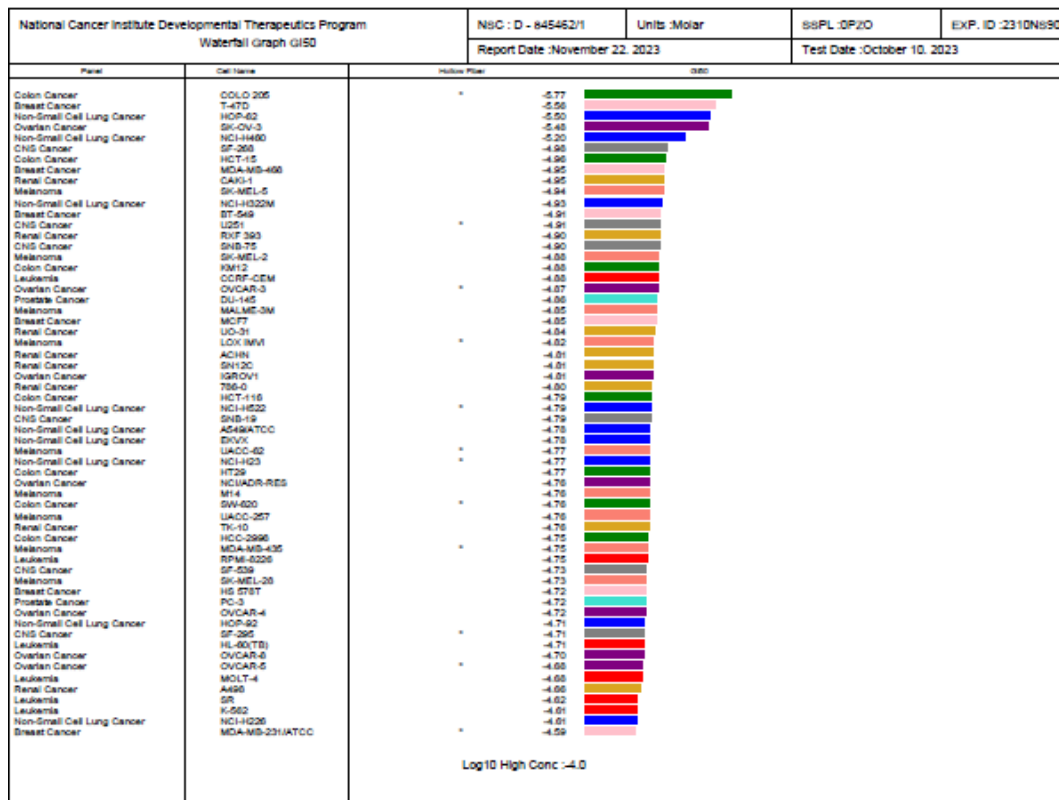


Figure S8e. NCI-60 cell lines screening protocol concentrations ranging from 10^{-4} to 10^{-8} M for compound **3**.

National Cancer Institute Developmental Therapeutics Program Waterfall Graph T01			NsC : D - 845462/1	Units :Molar	SSPL :DP20	EXP. ID :2310N690
			Report Date :November 22, 2023		Test Date :October 10, 2023	
Panel	Cell Name	HalfLog P50	TS			
Non-Small Cell Lung Cancer	NCI-H322M	-4.57				
Non-Small Cell Lung Cancer	NCI-H460	-4.55				
Breast Cancer	MDA-MB-468	-4.54				
Prostate Cancer	DU-145	-4.54				
Melanoma	SK-MEL-5	-4.50				
Colon Cancer	KM12	-4.50				
Breast Cancer	MCF7	-4.50				
Renal Cancer	TK-10	-4.49				
Renal Cancer	ACHN	-4.49				
Ovarian Cancer	OVCA9-3	-4.49	*			
Colon Cancer	HCC-9598	-4.47				
Colon Cancer	HCT-15	-4.47				
CNS Cancer	SNB-75	-4.47				
Ovarian Cancer	IGROV1	-4.43				
CNS Cancer	U251	-4.43	*			
Renal Cancer	RFP-393	-4.42				
Renal Cancer	UC-291	-4.42				
CNS Cancer	SNB-19	-4.42				
Melanoma	SK-MEL-2	-4.42				
Non-Small Cell Lung Cancer	NCI-H522	-4.42	*			
Non-Small Cell Lung Cancer	DRXV	-4.42				
Renal Cancer	CAOS-1	-4.42				
CNS Cancer	SP-203	-4.41				
Ovarian Cancer	OVCA9-5	-4.39	*			
Melanoma	UACC-62	-4.37	*			
Colon Cancer	HT29	-4.37				
Colon Cancer	SW-620	-4.37	*			
CNS Cancer	SP-295	-4.35	*			
CNS Cancer	SP-539	-4.34	*			
Melanoma	MALME-3M	-4.34				
Renal Cancer	A498	-4.33				
Melanoma	SK-MEL-28	-4.33	*			
Non-Small Cell Lung Cancer	NCI-H23	-4.30	*			
Non-Small Cell Lung Cancer	A549ATCC	-4.28	*			
Melanoma	LOX IMVI	-4.28	*			
Ovarian Cancer	OVCA9-4	-4.24	*			
Melanoma	MDA-MB-435	-4.24	*			
Melanoma	UACC-257	-4.23	*			
Non-Small Cell Lung Cancer	HOP-62	-4.21	*			
Renal Cancer	SN12C	-4.19	*			
Leukemia	CCRF-CEM	-4.17	*			
Breast Cancer	BT-549	-4.15	*			
Breast Cancer	HS 578T	-4.12	*			
Breast Cancer	MDA-MB-231ATCC	-4.12	*			
Ovarian Cancer	OVCA9-8	-4.12	*			
Leukemia	HL-60(TB)	-4.11	*			
Leukemia	RPMI-8226	-4.06	*			
Colon Cancer	HCT-116	-4.05	*			
Prostate Cancer	PC-3	-4.05	*			
Leukemia	MOLT-4	-4.05	*			
Leukemia	SR	-4.05	*			
Ovarian Cancer	NCIADR-RES	-4.04	*			
Leukemia	K-562	> -4.00	*			
Non-Small Cell Lung Cancer	HOP-62	> -4.00	*			
Non-Small Cell Lung Cancer	NCI-H226	> -4.00	*			
Melanoma	M14	> -4.00	*			
Ovarian Cancer	SK-OV-3	> -4.00	*			
Renal Cancer	786-O	> -4.00	*			
Breast Cancer	T-47D	> -4.00	*			

Log10 High Conc : -4.0

Figure S8f. NCI-60 cell lines screening protocol concentrations ranging from 10^{-4} to 10^{-8} M for compound **3**.

National Cancer Institute Developmental Therapeutics Program Waterfall Graph LC50			NsC : D - 845462/1	Units :Molar	SSPL :DP20	EXP. ID :2310N690
			Report Date :November 22, 2023		Test Date :October 10, 2023	
Panel	Cell Name	HalfLog P50	LC50			
Renal Cancer	TK-10	-4.23				
Non-Small Cell Lung Cancer	NCI-H322M	-4.22				
Prostate Cancer	DU-145	-4.22				
Colon Cancer	NCI-D2998	-4.18				
Renal Cancer	ACHN	-4.15				
Breast Cancer	MCF7	-4.15				
Breast Cancer	MDA-MB-468	-4.15				
Colon Cancer	KM12	-4.12				
Ovarian Cancer	OVCA9-5	-4.10	*			
Ovarian Cancer	OVCA9-3	-4.10	*			
Melanoma	SK-MEL-5	-4.07	*			
Non-Small Cell Lung Cancer	DRXV	-4.06	*			
CNS Cancer	SNB-19	-4.06	*			
Ovarian Cancer	IGROV1	-4.05	*			
Non-Small Cell Lung Cancer	NCI-H522	-4.04	*			
CNS Cancer	SNB-75	-4.04	*			
Renal Cancer	UC-291	-4.01	*			
Melanoma	UACC-62	-4.00	*			
Renal Cancer	A498	-4.00	*			
Leukemia	CCRF-CEM	> -4.00	*			
Leukemia	HL-60(TB)	> -4.00	*			
Leukemia	K-562	> -4.00	*			
Leukemia	MOLT-4	> -4.00	*			
Leukemia	RPMI-8226	> -4.00	*			
Leukemia	SR	> -4.00	*			
Non-Small Cell Lung Cancer	A549ATCC	> -4.00	*			
Non-Small Cell Lung Cancer	HOP-62	> -4.00	*			
Non-Small Cell Lung Cancer	HOP-62	> -4.00	*			
Non-Small Cell Lung Cancer	NCI-H226	> -4.00	*			
Non-Small Cell Lung Cancer	NCI-H23	> -4.00	*			
Non-Small Cell Lung Cancer	NCI-H460	> -4.00	*			
Colon Cancer	HCT-116	> -4.00	*			
Colon Cancer	HCT-15	> -4.00	*			
Colon Cancer	HT29	> -4.00	*			
Colon Cancer	SW-620	> -4.00	*			
CNS Cancer	SP-203	> -4.00	*			
CNS Cancer	SP-295	> -4.00	*			
CNS Cancer	SP-539	> -4.00	*			
CNS Cancer	U251	> -4.00	*			
Melanoma	LOX IMVI	> -4.00	*			
Melanoma	MALME-3M	> -4.00	*			
Melanoma	M14	> -4.00	*			
Melanoma	MDA-MB-435	> -4.00	*			
Melanoma	SK-MEL-2	> -4.00	*			
Melanoma	SK-MEL-28	> -4.00	*			
Melanoma	UACC-257	> -4.00	*			
Ovarian Cancer	OVCA9-4	> -4.00	*			
Ovarian Cancer	OVCA9-8	> -4.00	*			
Ovarian Cancer	NCIADR-RES	> -4.00	*			
Ovarian Cancer	SK-OV-3	> -4.00	*			
Renal Cancer	786-O	> -4.00	*			
Renal Cancer	CAOS-1	> -4.00	*			
Renal Cancer	RFP-393	> -4.00	*			
Renal Cancer	SN12C	> -4.00	*			
Prostate Cancer	PC-3	> -4.00	*			
Breast Cancer	MDA-MB-231ATCC	> -4.00	*			
Breast Cancer	HS 578T	> -4.00	*			
Breast Cancer	BT-549	> -4.00	*			
Breast Cancer	T-47D	> -4.00	*			

Log10 High Conc : -4.0

Figure S8g. NCI-60 cell lines screening protocol concentrations ranging from 10^{-4} to 10^{-8} M for compound **3**.

Table S1. Influence of compound **3** on the growth of individual tumor cell lines.

Disease	Cell line	GI ₅₀ , μ M	SI (GI ₅₀)	TGI, μ M	SI (TGI)	LC ₅₀ , μ M
Leukemia	CCRF-CEM	13.2	1.19	67.8	0.74	>100.0
	HL-60(TB)	19.7	0.79	77.7	0.65	>100.0
	K-562	24.4	0.64	>100.0	-	>100.0
	MOLT-4	20.7	0.75	89.6	0.56	>100.0
	RPMI-8226	17.9	0.87	86.6	0.58	>100.0
	SR	24.2	0.64	90.0	0.56	>100.0
	MG_MID	20.01	0.78	85.28	0.59	>100.0
NSC lung cancer	A549/ATCC	16.7	0.94	52.1	0.97	>100.0
	EKVX	16.8	0.93	38.2	1.32	86.9
	HOP-62	3.18	4.94	>100.0	-	>100.0
	HOP-92	19.3	0.81	61.4	0.82	>100.0
	NCI-H226	24.6	0.63	>100.0	-	>100.0
	NCI-H23	16.8	0.93	50.0	1.01	>100.0
	NCI-H322M	11.9	1.32	26.8	1.89	60.4
	NCI-H460	6.25	2.51	28.1	1.80	>100.0
	NCI-H522	16.1	0.97	38.2	1.32	90.4
MG_MID	14.62	1.07	51.64	0.98	93.07	
Colon Cancer	COLO 205	1.70	9.24	No data	No data	No data
	HCC-2998	17.7	0.88	33.6	1.50	63.9
	HCT-116	16.1	0.97	87.0	0.58	>100.0
	HCT-15	10.9	1.44	33.8	1.49	>100.0
	HT29	17.0	0.92	42.3	1.19	>100.0
	KM12	13.1	1.2	31.5	1.60	75.5
	SW-620	17.4	0.90	42.4	1.19	>100.0
	MG_MID	13.41	1.17	45.1	1.12	89.9
CNS Cancer	SF-268	10.5	1.49	39.1	1.29	>100.0
	SF-295	19.6	0.80	45.0	1.12	>100.0
	SF-539	18.5	0.84	45.3	1.16	>100.0
	SNB-19	16.2	0.97	37.8	1.34	87.8
	SNB-75	12.6	1.24	34.1	1.48	91.9
	U251	12.4	1.26	37.5	1.35	>100.0
	MG_MID	14.96	1.05	39.8	1.27	96.61
Melanoma	LOX IMVI	15.2	1.03	52.6	0.96	>100.0
	MALME-3M	14.1	1.11	46.1	1.09	>100.0
	M14	17.4	0.90	>100.0	-	>100.0
	MDA-MB-435	17.8	0.88	57.7	0.87	>100.0
	SK-MEL-2	13.0	1.20	38.0	1.33	>100.0
	SK-MEL-28	18.6	0.84	46.8	1.08	>100.0
	SK-MEL-5	11.6	1.35	31.3	1.61	84.4
	UACC-257	17.5	0.89	58.6	0.86	>100.0
	UACC-62	16.8	0.93	40.7	1.24	98.7
MG_MID	15.77	0.99	52.42	0.96	98.12	
Ovarian Cancer	IGROV1	15.5	1.01	37.2	1.36	89.1
	OVCAR-3	13.4	1.17	32.5	1.55	79.1
	OVCAR-4	19.1	0.82	55.1	0.91	>100.0
	OVCAR-5	20.7	0.75	40.4	1.25	78.8
	OVCAR-8	20.0	0.78	75.8	0.66	>100.0
	NCI/ADR-RES	17.3	0.90	92.2	0.54	>100.0
	SK-OV-3	3.28	4.79	>100.0	-	>100.0
	MG_MID	15.61	1.00	55.53	0.91	92.42

	786-0	15.7	1.00	>100.0	-	>100.0
	A498	21.7	0.72	46.5	1.08	99.7
	ACHN	15.4	1.02	32.5	1.55	68.6
	CAKI-1	11.3	1.39	38.3	1.32	>100.0
Renal cancer	RXF 393	12.6	1.24	37.7	1.34	>100.0
	SN12C	15.5	1.01	65.2	0.77	>100.0
	TK-10	17.5	0.89	32.2	1.57	59.1
	UO-31	14.5	1.08	37.7	1.34	98.4
	MG_MID	15.52	1.01	48.76	1.03	90.72
	PC-3	19.1	0.82	88.8	0.57	>100.0
Prostate cancer	DU-145	13.9	1.13	28.9	1.75	60.4
	MG_MID	16.5	0.95	58.85	0.86	80.2
	MCF7	14.2	1.10	31.7	1.59	70.6
	MDA-MB-231/ATCC	25.7	0.61	75.7	0.66	>100.0
	HS 578T	19.1	0.82	75.2	0.67	>100.0
Breast Cancer	BT-549	12.3	1.27	71.5	0.70	>100.0
	T-47D	2.78	5.65	>100.0	-	>100.0
	MDA-MB-468	11.3	1.39	28.8	1.75	73.7
	MG_MID	14.23	1.10	63.81	0.79	90.71
	MG_MID	15.72		50.68		91.85