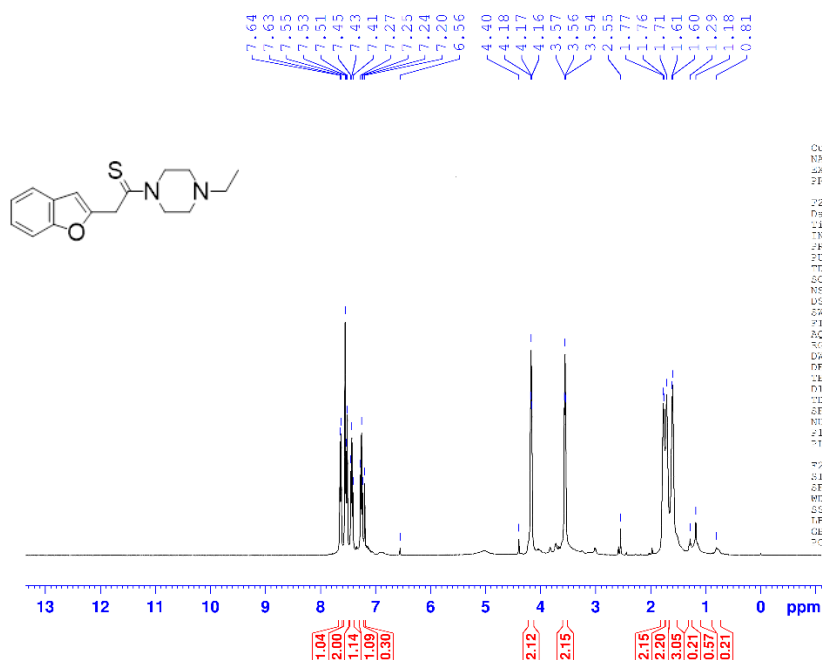


2-(benzofuran-2-yl)-1-(4-methylpiperazin-1-yl)ethanethione (3).

 ^1H NMR

Omar Elkholly-OE-E4-proton-CDCL3-D



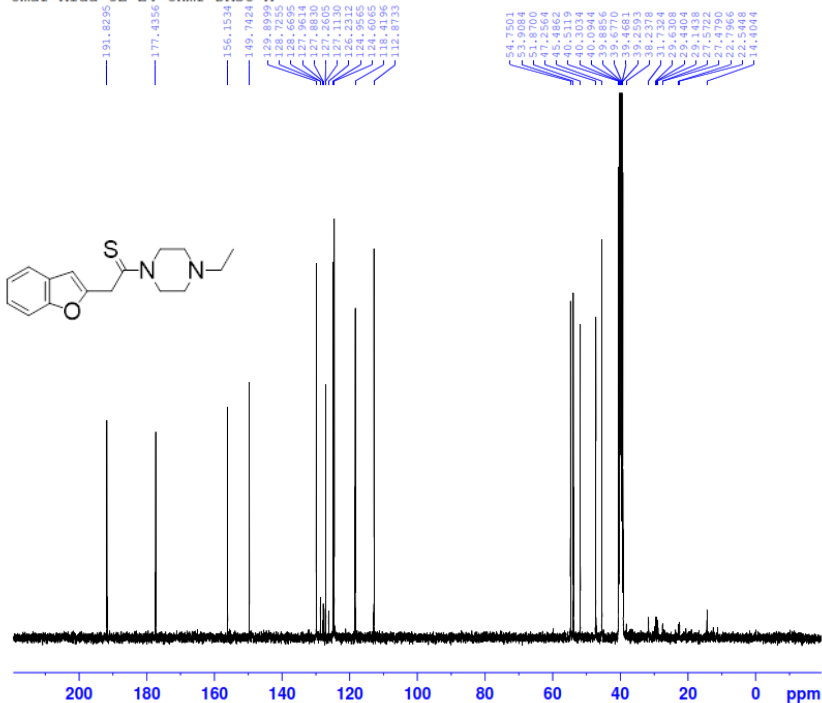
Current Data Parameters
NAME Omar Elkholly OE E4 prot
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200615
Time 12.50 h
INSTRUM spect
PROBHD z108618 0945 f
PULPROG zgpg30
TD 65536
SOLVENT CDCL3
NS 16
DS 4
SWH 8012.822 Hz
FIDRES 0.244532 Hz
AQ 4.083465 sec
RG 95.3
DA 62.400 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TDC 400.2024712 MHz
SFO1 400.2024712 MHz
NUC1 1H
F1 13.50 usec
F1M1 13.00000000 M

F2 - Processing parameters
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SF 400.20000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

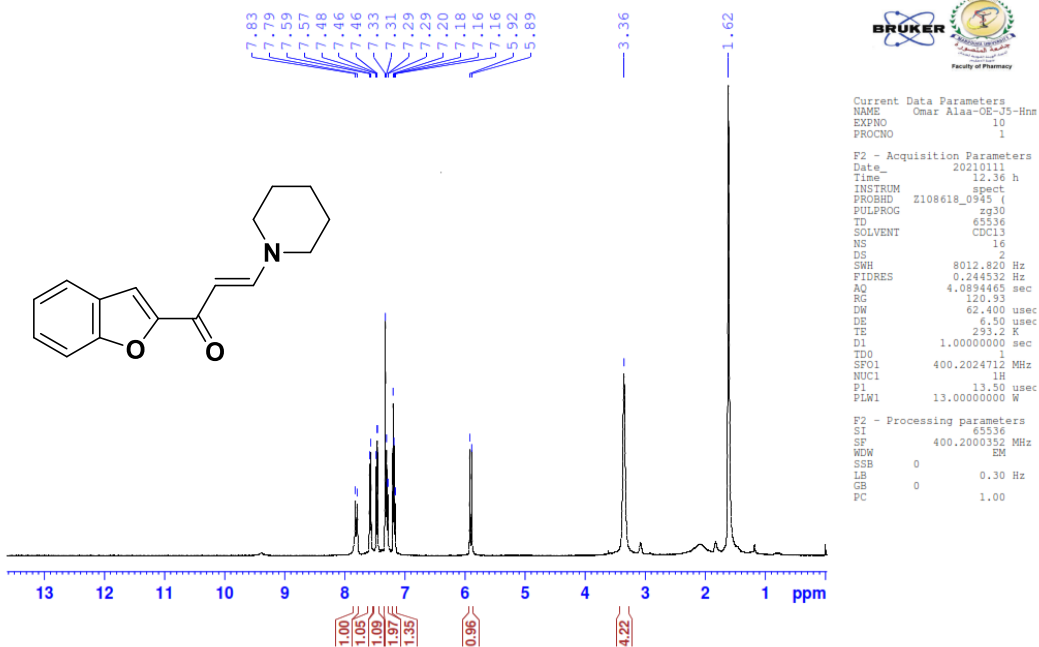
 ^{13}C NMR

Omar Alaa-OE E4-Cnmr-DMSO-A

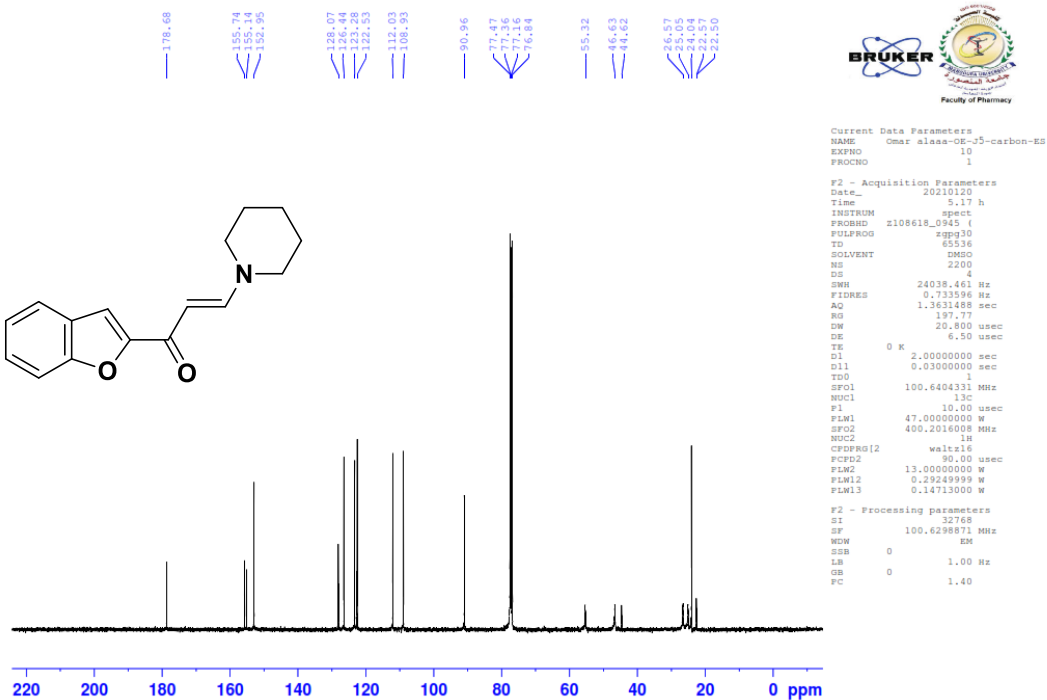


(E)-1-(benzofuran-2-yl)-3-(piperidin-1-yl)prop-2-en-1-one (5)¹HNMR

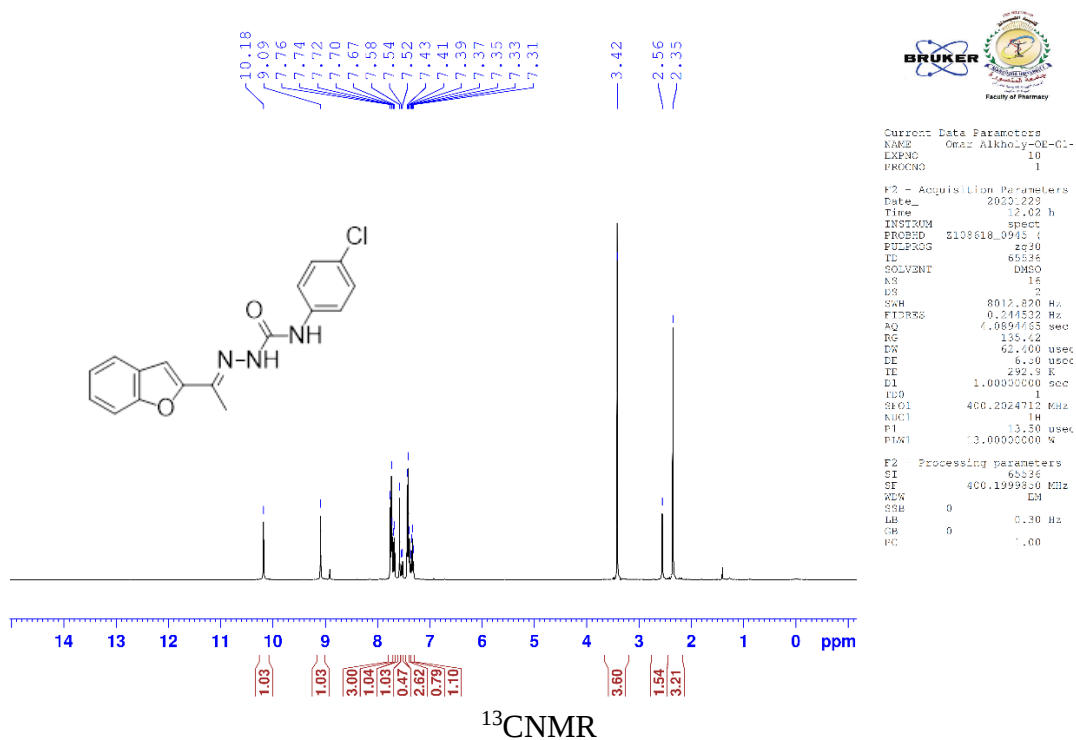
Omar Alaa-OE-J5-Hnmr-OE

¹³CNMR

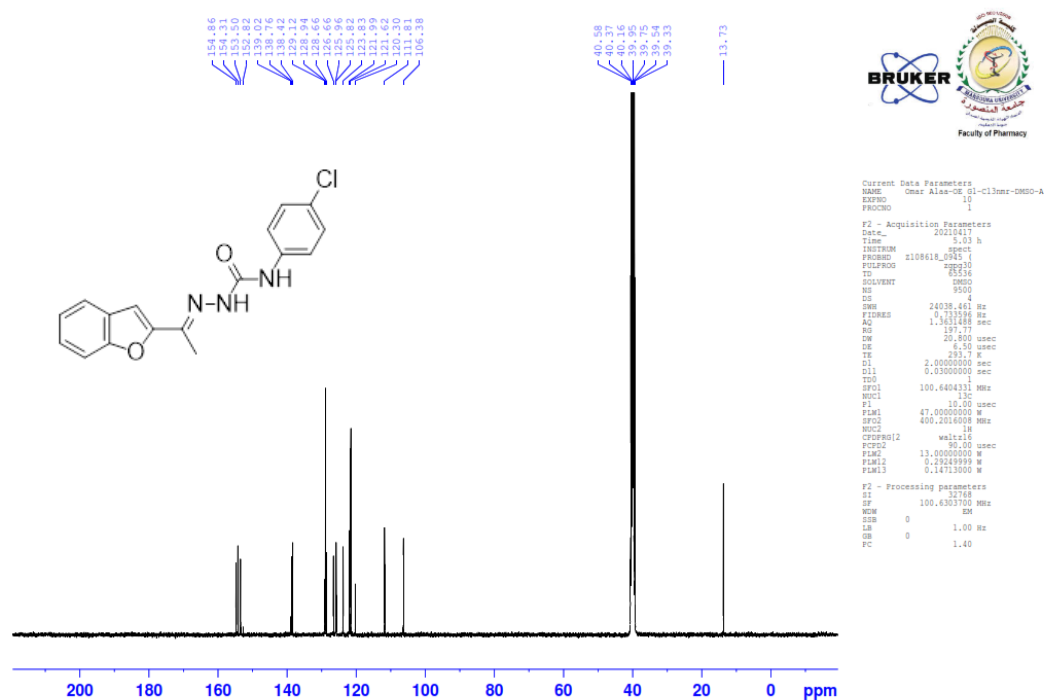
Omar alaaa-OE-J5-carbon

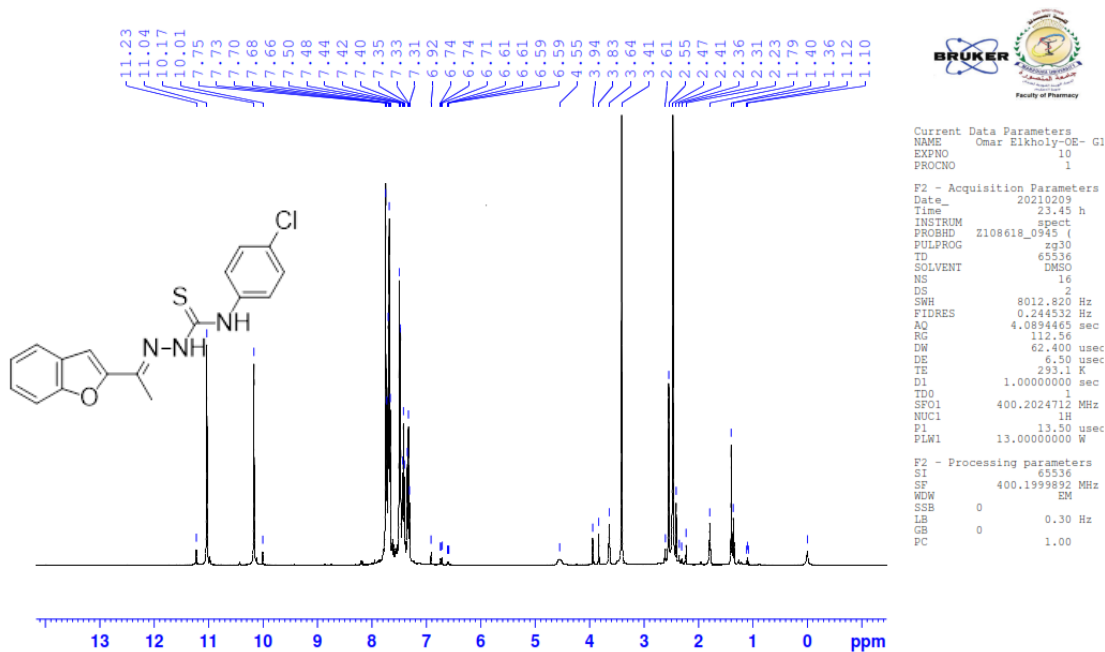


(E)-2-[1-(benzofuran-2-yl)ethylidene]-N-(4-chlorophenyl)hydrazine-1-carboxamide
(7)
¹HNMR

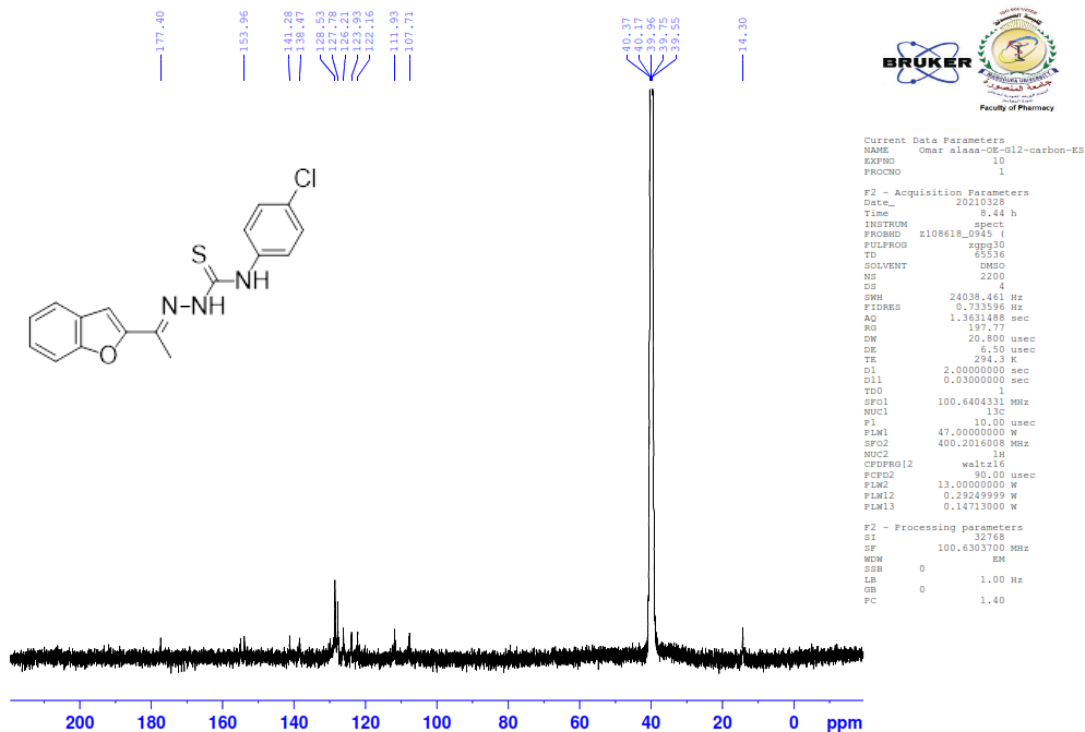


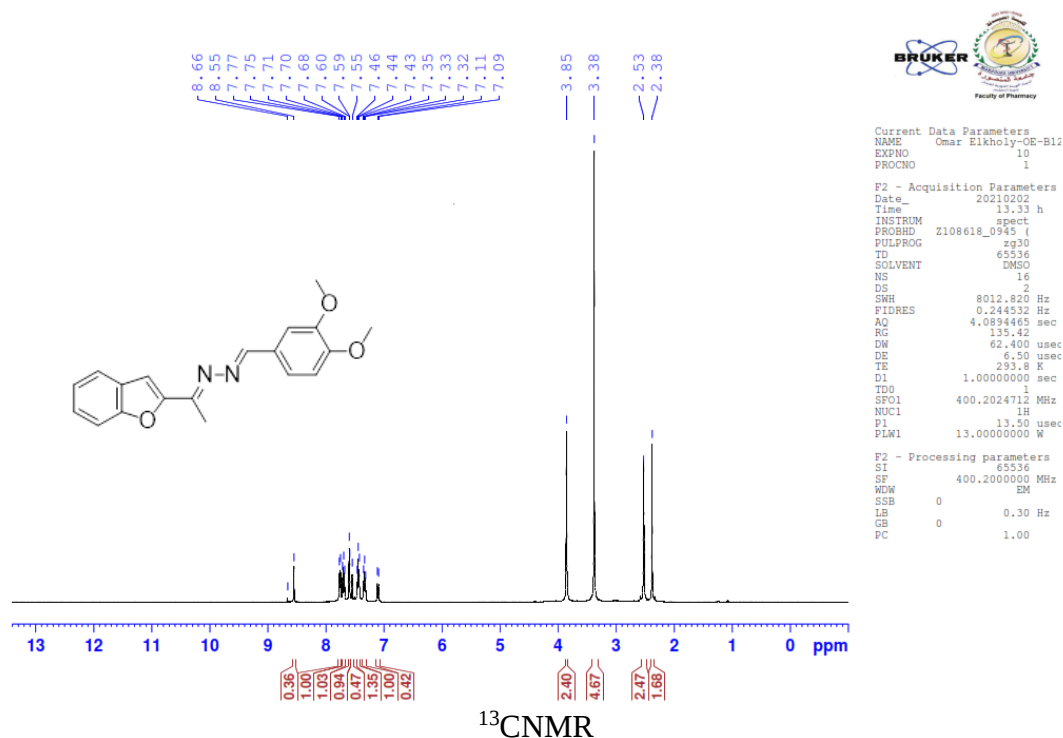
Omar Alaa-OE G1-Cl13nmr-DMSO-A



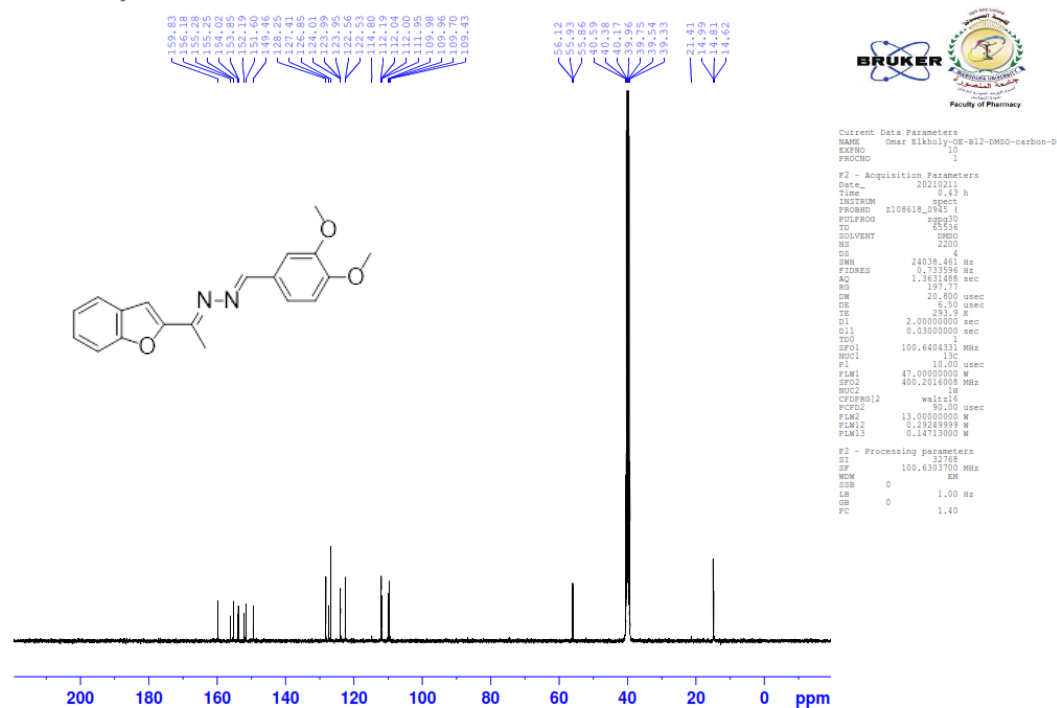
(E)-2-(1-(benzofuran-2-yl)ethylidene)-*N*-(4-chlorophenyl)hydrazine-1-carbothioamide**(8)**
¹HNMR¹³CNMR

Omar alaaa-OE-G12-carbon-ES

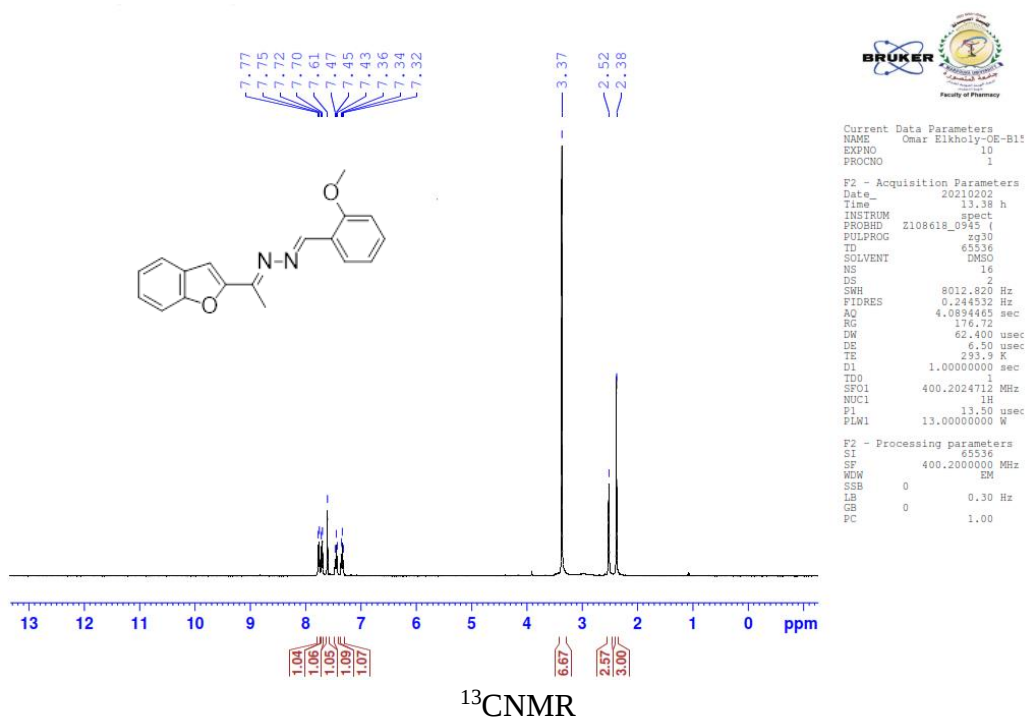


(E)-1-[1-(benzofuran-2-yl)ethylidene]-2-((*E*)-3,4-dimethoxybenzylidene)hydrazine (**9**)¹HNMR

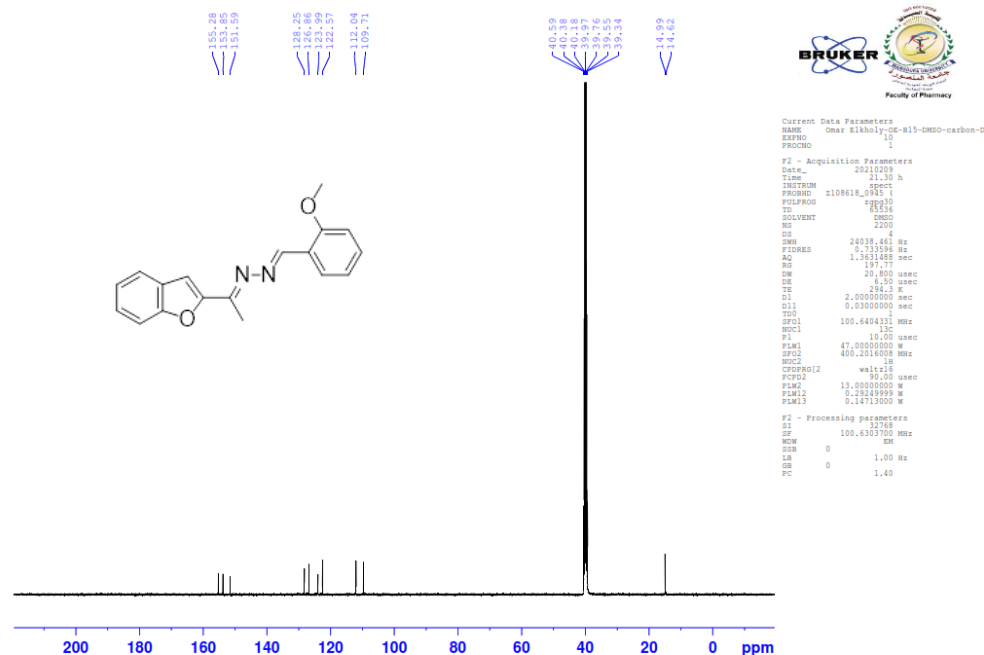
Omar Elkholy-OE-B12-DMSO-carbon-D

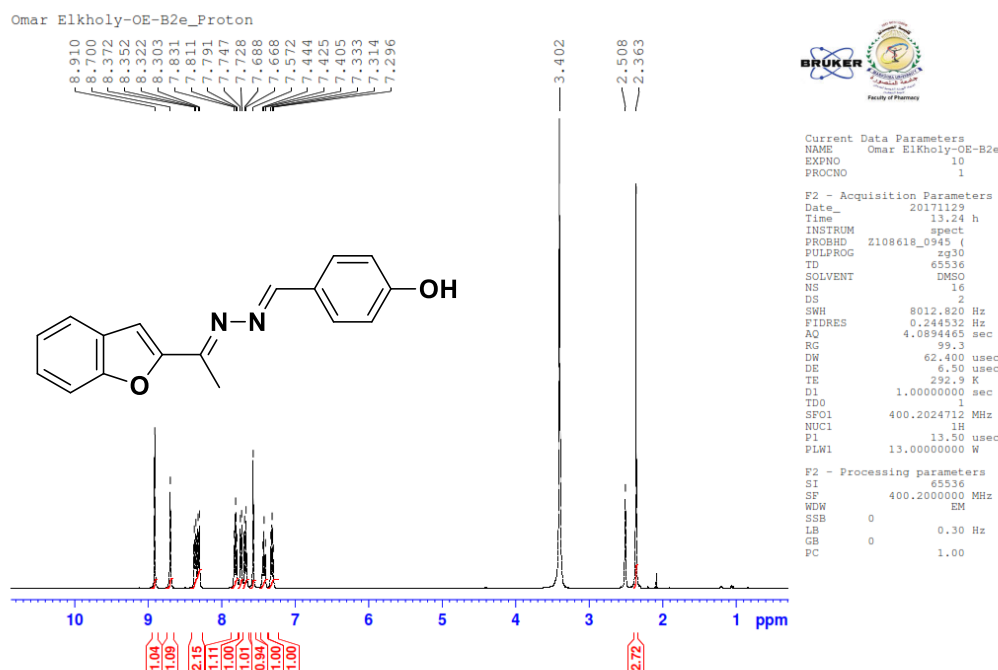
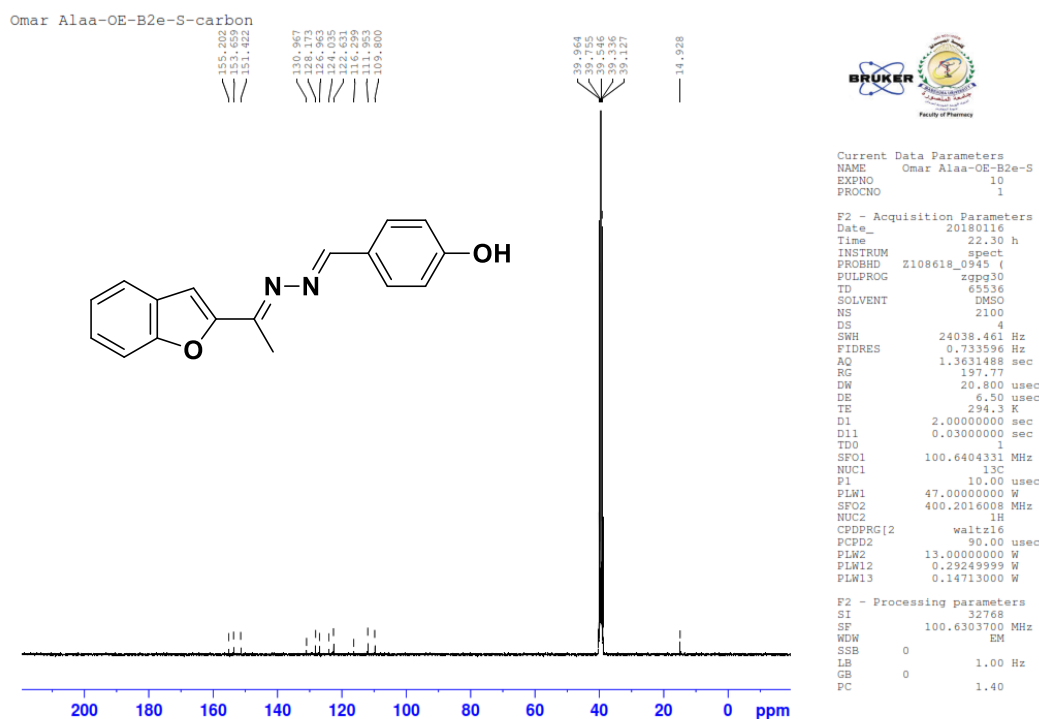


(E)-1-[1-(benzofuran-2-yl)ethylidene]-2-((E)-2-methoxybenzylidene)hydrazine
(10)
¹HNMR



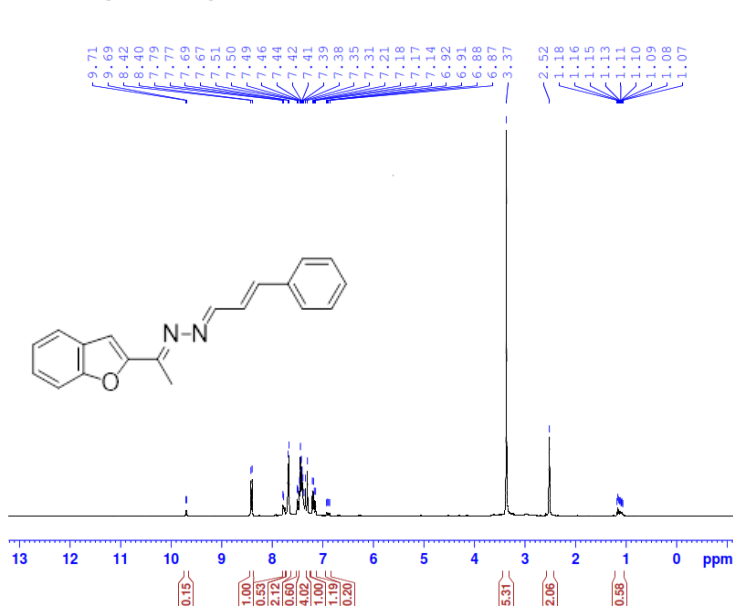
Omar Elkholy-OE-B15-DMSO-carbon-D



(E)-1-[1-(benzofuran-2-yl)ethylidene]-2-((E)-4-hydroxybenzylidene)hydrazine (11)¹HNMR¹³CNMR

(1E,2E)-1-[1-benzofuran-2-yl] ethylidene]-2-((E)-3-phenylallylidene)hydrazine (12)**¹HNMR**

Omar Elkholly-OE-B18-WH-proton



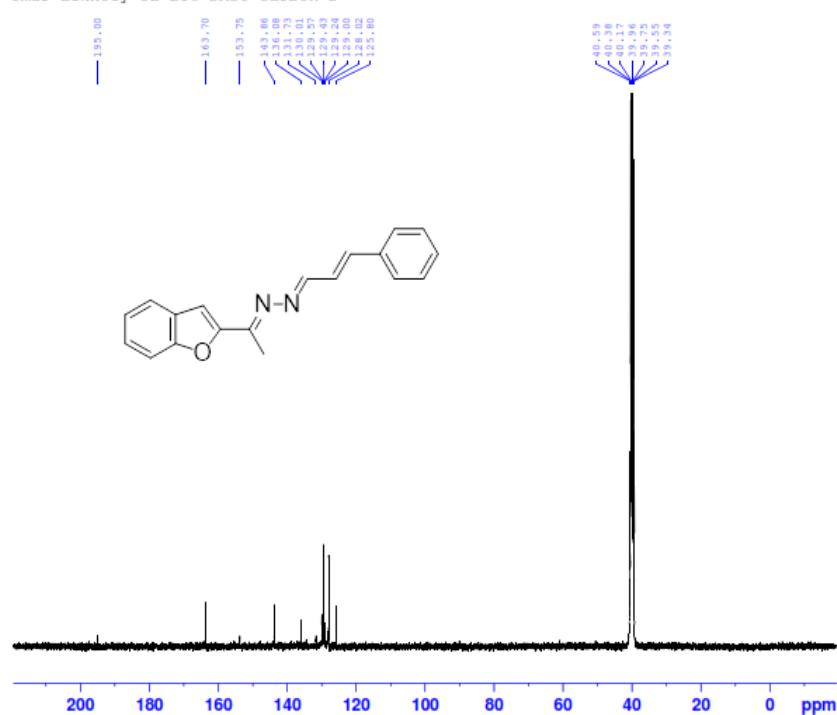
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NAME Omar Elkholly-OE-B18
EXPNO 10
PROCNO 1

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Time 13:42 h
INSTRUM spect
PROBHD 1108618_0945 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 176.72
DW 62.400 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec
TDO 400.2024712 MHz
NUC1 1H
P1 13.50 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³CNMR

Omar Elkholly-OE-B18-DMSO-carbon-D



Current Data Parameters
NAME Omar Elkholly-OE-B18-DMSO-carbon-D
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210209
Time 23:40 h
INSTRUM spect
PROBHD 1108618_0945 ()
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2200
DS 4
SWH 24019.461 Hz
FIDRES 0.733384 Hz
AQ 1.3431488 sec
RG 197.77
DW 20.800 usec
DE 6.30 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 100.6404331 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.00000000 W
SFO2 400.2014608 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.39048999 W
PLW13 0.14713000 W

F2 - Processing parameters
SI 32768
SF 100.6303700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Cytotoxic activity of some compounds against human cell line

Comp. No.	Code.	In vitro Cytotoxicity IC50 (μM) •				
		WI38	HePG2	PC3	Hela	MCF7
••	DOX	6.72±0.5	4.50±0.2	8.87±0.6	5.57±0.4	4.17±0.2
7	OE-G1	>100	81.59±3.9	93.86±4.7	66.05±3.2	76.91±3.8
12	OE-B18	56.45±3.2	62.04±3.2	74.38±3.9	39.82±2.7	68.36±3.6
5	OE-J5	63.97±3.1	12.61±1.0	41.52±2.6	28.33±2.2	19.92±1.5
8	OE-G12	48.18±2.8	9.73±0.7	17.49±1.3	7.94±0.5	11.58±0.9
9	OE-B12	82.31±4.3	26.40±2.1	32.10±2.2	17.02±1.4	28.10±2.3
3	OE-E4	78.52±3.8	34.82±2.5	65.01±3.2	51.37±3.1	45.07±2.9
10	OE-B15	67.74±3.4	50.97±3.0	24.76±1.9	13.82±1.0	62.83±3.3
11	OE-B2e	43.25±2.9	84.92±3.2	>100	89.31±3.2	>100

• IC50 (μM) : 1 – 10 (very strong). 11 – 20 (strong). 21 – 50 (moderate). 51 – 100 (weak)

and above 100 (non-cytotoxic)

•• DOX : Doxorubicin

Average of Relative viability of cells (%)

Conc.(μ M)	WI38	HePG2	PC3	Hela	MCF7
OE-G1					
Comp.7					
100	55.5	48.1	50.9	42.9	47.8
50	76.2	60.2	64.8	56.3	58.0
25	89.3	72.5	76.5	68.4	70.2
12.5	100	87.4	93.6	80.7	88.9
6.25	100	99.7	100	93.8	97.6
3.125	100	100	100	100	100
1.56	100	100	100	100	100
OE-B18					
Comp.12					
100	41.0	39.4	47.3	34.1	43.2
50	52.5	54.0	55.0	41.8	57.1
25	61.9	70.5	71.7	59.2	70.2
12.5	78.1	91.3	86.6	72.3	81.8
6.25	91.3	100	98.4	86.6	94.7
3.125	100	100	100	100	100
1.56	100	100	100	100	100
OE-J5					
Comp.5					
100	38.2	15.3	32.9	26.3	20.4
50	57.1	24.0	47.8	38.1	32.5
25	72.3	37.2	58.1	51.4	41.8
12.5	91.8	42.3	67.2	62.9	54.9
6.25	100	65.0	92.7	79.3	72.1
3.125	100	76.8	100	96.6	96.2
1.56	100	100	100	100	100
OE-G12					
Comp.8					
100	36.4	13.2	19.3	8.2	13.7
50	48.2	20.8	27.1	16.0	21.2
25	62.7	29.1	39.2	24.5	28.3
12.5	75.6	24.9	51.6	32.8	42.9
6.25	89.3	67.3	72.9	53.7	65.7

3.125	100	81.4	93.7	76.1	79.8
1.56	100	99.5	100	88.6	99.1
OE-B12					
Comp.9					
100	47.9	26.2	31.2	20.3	25.3
50	60.6	36.8	44.8	28.2	38.2
25	74.5	49.6	52.6	37.1	50.6
12.5	85.2	60.5	60.2	50.4	64.2
6.25	99.7	78.2	75.8	73.2	79.5
3.125	100	94.4	96.1	92.0	96.0
1.56	100	100	100	100	100
OE-E4					
Comp.3					
100	47.4	29.5	37.5	36.1	33.9
50	59.2	42.8	59.5	50.7	47.6
25	71.8	50.2	71.9	64.8	61.3
12.5	85.3	76.1	92.8	75.9	72.4
6.25	97.0	82.4	100	97.1	94.7
3.125	100	100	100	100	100
1.56	100	100	100	100	100
OE-B15					
Comp.10					
100	43.3	38.1	23.5	17.0	40.4
50	54.8	50.2	37.0	25.8	58.0
25	71.7	63.1	46.8	33.7	65.2
12.5	93.6	72.7	59.1	48.1	79.3
6.25	100	91.9	78.2	63.5	94.7
3.125	100	100	96.3	85.9	100
1.56	100	100	100	100	100

Cytotoxic activity of some compounds against human cell line

Comp. No.	Code.	In vitro Cytotoxicity IC50 (μM) •				
		WI38	HePG2	PC3	Hela	MCF7
••	DOX	6.72±0.5	4.50±0.2	8.87±0.6	5.57±0.4	4.17±0.2
7	OE-G1	>100	81.59±3.9	93.86±4.7	66.05±3.2	76.91±3.8
12	OE-B18	56.45±3.2	62.04±3.2	74.38±3.9	39.82±2.7	68.36±3.6
5	OE-J5	63.97±3.1	12.61±1.0	41.52±2.6	28.33±2.2	19.92±1.5
8	OE-G12	48.18±2.8	9.73±0.7	17.49±1.3	7.94±0.5	11.58±0.9
9	OE-B12	82.31±4.3	26.40±2.1	32.10±2.2	17.02±1.4	28.10±2.3
3	OE-E4	78.52±3.8	34.82±2.5	65.01±3.2	51.37±3.1	45.07±2.9
10	OE-B15	67.74±3.4	50.97±3.0	24.76±1.9	13.82±1.0	62.83±3.3
11	OE-B2e	43.25±2.9	84.92±3.2	>100	89.31±3.2	>100

• IC50 (μM) : 1 – 10 (very strong). 11 – 20 (strong). 21 – 50 (moderate). 51 – 100 (weak)

and above 100 (non-cytotoxic)

•• DOX : Doxorubicin

Average of Relative viability of cells (%)

Conc.(μ M)	WI38	HePG2	PC3	Hela	MCF7
OE-G1					
Comp.7					
100	55.5	48.1	50.9	42.9	47.8
50	76.2	60.2	64.8	56.3	58.0
25	89.3	72.5	76.5	68.4	70.2
12.5	100	87.4	93.6	80.7	88.9
6.25	100	99.7	100	93.8	97.6
3.125	100	100	100	100	100
1.56	100	100	100	100	100
OE-B18					
Comp.12					
100	41.0	39.4	47.3	34.1	43.2
50	52.5	54.0	55.0	41.8	57.1
25	61.9	70.5	71.7	59.2	70.2
12.5	78.1	91.3	86.6	72.3	81.8
6.25	91.3	100	98.4	86.6	94.7
3.125	100	100	100	100	100
1.56	100	100	100	100	100
OE-J5					
Comp.5					
100	38.2	15.3	32.9	26.3	20.4
50	57.1	24.0	47.8	38.1	32.5
25	72.3	37.2	58.1	51.4	41.8
12.5	91.8	42.3	67.2	62.9	54.9
6.25	100	65.0	92.7	79.3	72.1
3.125	100	76.8	100	96.6	96.2
1.56	100	100	100	100	100
OE-G12					
Comp.8					
100	36.4	13.2	19.3	8.2	13.7
50	48.2	20.8	27.1	16.0	21.2
25	62.7	29.1	39.2	24.5	28.3
12.5	75.6	24.9	51.6	32.8	42.9
6.25	89.3	67.3	72.9	53.7	65.7

3.125	100	81.4	93.7	76.1	79.8
1.56	100	99.5	100	88.6	99.1
OE-B12					
Comp.9					
100	47.9	26.2	31.2	20.3	25.3
50	60.6	36.8	44.8	28.2	38.2
25	74.5	49.6	52.6	37.1	50.6
12.5	85.2	60.5	60.2	50.4	64.2
6.25	99.7	78.2	75.8	73.2	79.5
3.125	100	94.4	96.1	92.0	96.0
1.56	100	100	100	100	100
OE-E4					
Comp.3					
100	47.4	29.5	37.5	36.1	33.9
50	59.2	42.8	59.5	50.7	47.6
25	71.8	50.2	71.9	64.8	61.3
12.5	85.3	76.1	92.8	75.9	72.4
6.25	97.0	82.4	100	97.1	94.7
3.125	100	100	100	100	100
1.56	100	100	100	100	100
OE-B15					
Comp.10					
100	43.3	38.1	23.5	17.0	40.4
50	54.8	50.2	37.0	25.8	58.0
25	71.7	63.1	46.8	33.7	65.2
12.5	93.6	72.7	59.1	48.1	79.3
6.25	100	91.9	78.2	63.5	94.7
3.125	100	100	96.3	85.9	100
1.56	100	100	100	100	100

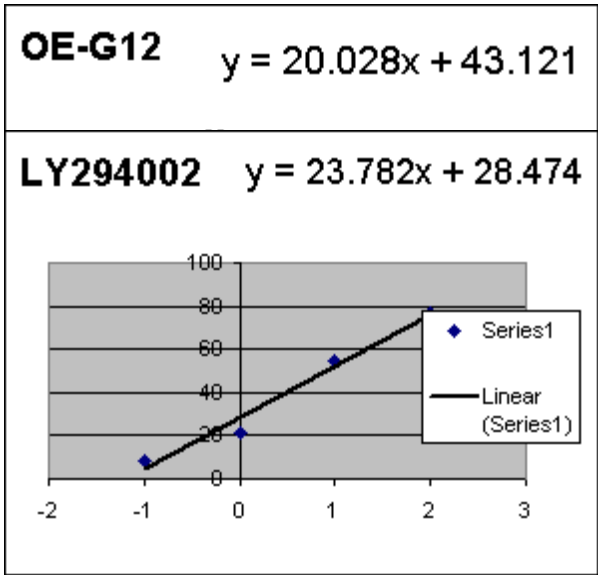
Researcher : Dr.Omar elkholy email: dr.kholy93@gmail.com mob. 01278084495
Date : 23-03-2021
Assay : PI3K- α assay
Samples : 01 sample .
Reference : ---
Cell lines : ---
Kit used : ---
Solvent : DMSO
Assay samples : ---

Lab Report

ser	compound			PI3K- α IC50 ng/ml	SD. $\pm$
	code	M.W	conc		
1	OE-G12			2.21	0.11
***	LY294002			8.04	0.42

Detailed results:

PI3K-α													
code	IC50	conc	log	%inh	T2	T1	ΔT	RFU2	RFU1	ΔRFU	slope	K.Activity	EC
OE-G12		100	2	80.7	30	0	30	19.26	0	19.26	3.33333	23.112023	120
		10	1	67	30	0	30	32.98	0	32.98	3.33333	39.57604	120
		1	0	42.7	30	0	30	57.31	0	57.31	3.33333	68.772069	120
		0.1	-1	22.1	30	0	30	77.91	0	77.91	3.33333	93.492093	120
	EC			0	30	0	30	100	0	100	3.33333	120	120
code	IC50	conc	log	%inh	T2	T1	ΔT	RFU2	RFU1	ΔRFU	slope	K.Activity	EC
LY294002		100	2	76.7	30	0	30	23.26	0	23.26	3.33333	27.912028	120
		10	1	54.8	30	0	30	45.18	0	45.18	3.33333	54.216054	120
		1	0	21.2	30	0	30	78.76	0	78.76	3.33333	94.512095	120
		0.1	-1	8.66	30	0	30	91.34	0	91.34	3.33333	109.60811	120
	EC			0	30	0	30	100	0	100	3.33333	120	120



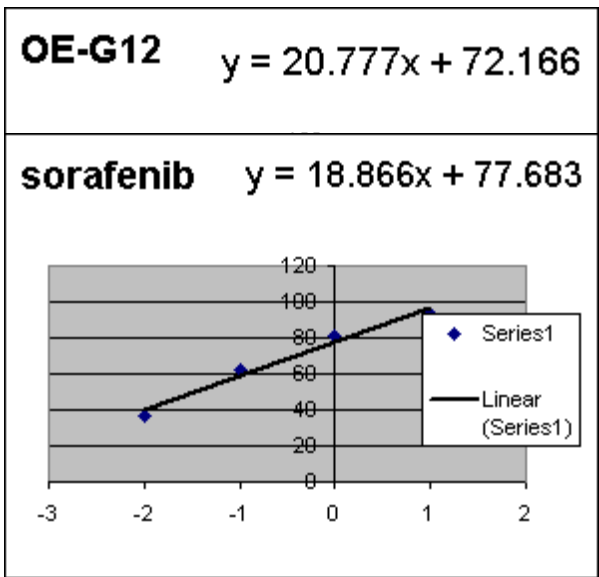
Researcher : Dr.Omar elkholy email: dr.kholy93@gmail.com mob. 01278084495
Date : 23-03-2021
Assay : VEGFR2 assay
Samples : 01 sample .
Reference : ---
Cell lines : ---
Kit used : ---
Solvent : DMSO
Assay samples : ---

Lab Report

ser	compound		conc	VEGFR2	SD. ±
	code	M.W		IC50 ng/ml	
1	OE-G12			86	4
***	Sorafenib			34	1

Detailed results:

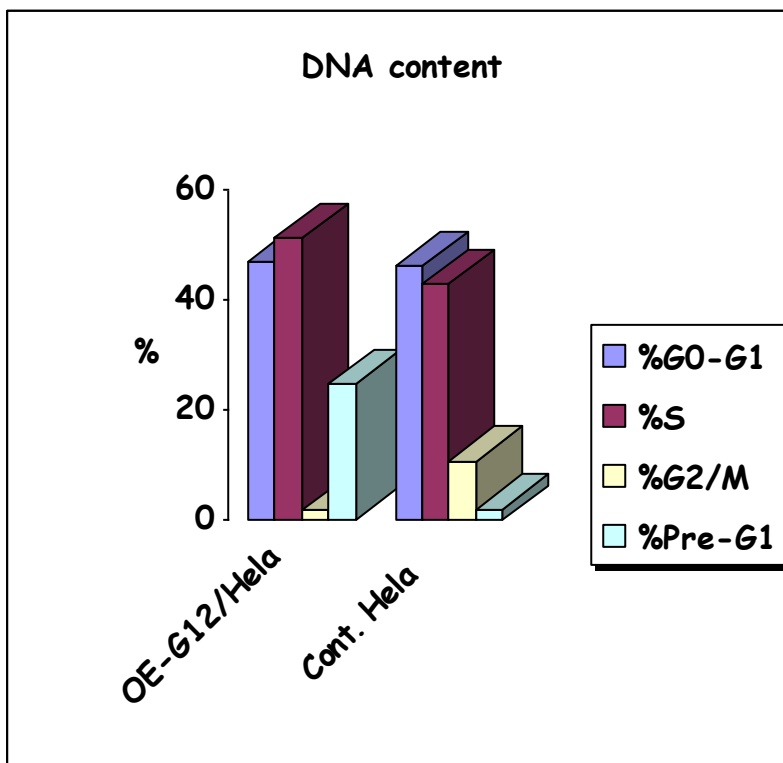
vegfr2													
code	IC50	conc	log	%inh	T2	T1	ΔT	RFU2	RFU1	ΔRFU	slope	K.Activity	EC
OE-G12		10	1	90.4	30	0	30	9.59	0	9.59	3.33333	11.508012	120
		1	0	75.3	30	0	30	24.71	0	24.71	3.33333	29.65203	120
		0.1	-1	52.7	30	0	30	47.26	0	47.26	3.33333	56.712057	120
		0.01	-2	28.7	30	0	30	71.33	0	71.33	3.33333	85.596086	120
EC				0	30	0	30	100	0	100	3.33333	120	120
code	IC50	conc	log	%inh	T2	T1	ΔT	RFU2	RFU1	ΔRFU	slope	K.Activity	EC
sorafenib		10	1	93.1	30	0	30	6.88	0	6.88	3.33333	8.2560083	120
		1	0	81.4	30	0	30	18.64	0	18.64	3.33333	22.368022	120
		0.1	-1	61.7	30	0	30	38.25	0	38.25	3.33333	45.900046	120
		0.01	-2	36.8	30	0	30	63.23	0	63.23	3.33333	75.876076	120
EC				0	30	0	30	100	0	100	3.33333	120	120



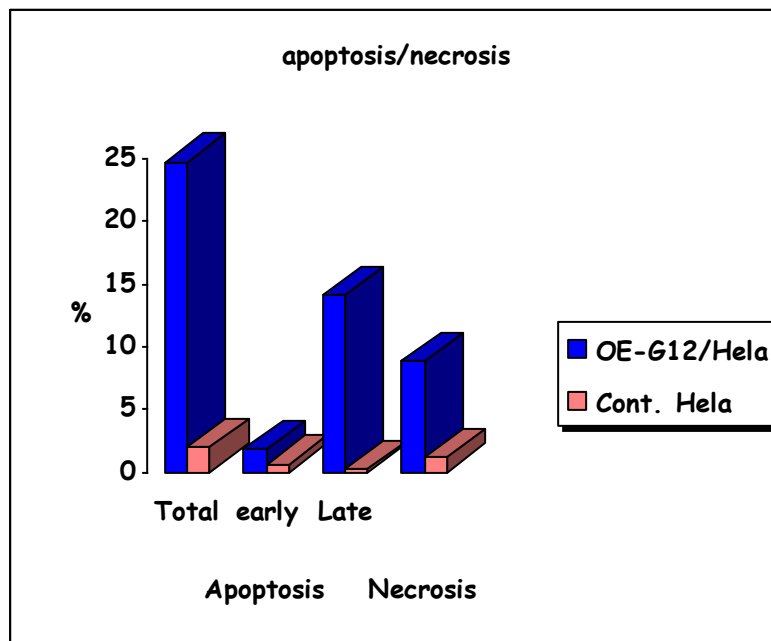
Researcher : Dr.Omar El-Khouly email : dr.kholy93@gmail.com mob. 01278084495
Assay : Cell Cycle Analysis
Samples : 02 samples
cell line : ---
Ref. : ---
Date : 23-03-2021
Reader : BD FACSCalibur
Kit used : ab139418_Propidium Iodide Flow Cytometry Kit/BD
Solvent : DMSO
Assay samples : Cell culture

Lab Report

Ser	Sample data		Results DNA content				
	code	IC50 uM	%G0-G1	%S	%G2/M	%Pre-G1	Comment
1	OE-G12/Hela		47.06	51.23	1.71	24.71	cell growth arrest@G1/S phase
2	Cont. Hela		46.26	42.99	10.75	1.95	---



s	code	conc	Apoptosis			Necrosis
			Total	Early	Late	
1	OE-G12/Hela		24.71	1.79	14.11	8.81
2	Cont. Hela		1.95	0.63	0.17	1.15



Detailed results

