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

$^{1}$H NMR

$^{13}$C NMR
(E)-1-(benzofuran-2-yl)-3-(piperidin-1-yl)prop-2-en-1-one (5)

$^1$HNMR

$^{13}$CNMR
(E)-2-[1-(benzofuran-2-yl)ethylidene]-N-(4-chlorophenyl)hydrazine-1-carboxamide (7)

$^1$HNMR

$^{13}$CNMR
(E)-2-(1-(benzofuran-2-yl)ethylidene)-N-(4-chlorophenyl)hydrazine-1-carbothioamide (8)

$^1$HNMR

$^{13}$CNMR
(E)-1-(benzofuran-2-yl)ethylidene]-2-((E)-3,4-dimethoxybenzylidene)hydrazine (9)

$^1$HNMR

$^{13}$CNMR
(E)-1-[1-(benzofuran-2-yl)ethylidene]-2-((E)-2-methoxybenzylidene)hydrazine (10)

$^1$HNMR

$^{13}$CNMR
(E)-1-[1-(benzofuran-2-yl)ethylidene]-2-((E)-4-hydroxybenzylidene)hydrazine (11)

$^1$HNMR

$^{13}$CNMR
(1E,2E)-1-[1-benzofuran-2-yl] ethyldene]-2-((E)-3-phenylallylidene)hydrazine (12)

$^1$HNMR

$^{13}$CNMR
Cytotoxic activity of some compounds against human cell line

| Comp. No. | Code. | In vitro Cytotoxicity IC50 (µM) |
|-----------|-------|-------------------------------|
|           |       | WI38  | HePG2 | PC3   | Hela  | MCF7 |
| 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 | 60.01±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.(µM) | 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  |
|       | 100 | 81.4 | 93.7 | 76.1 | 79.8 |
|-------|-----|------|------|------|------|
| 3.125 | 100 |      |      |      |      |
| 1.56  | 100 | 99.5 | 100  | 88.6 | 99.1 |

OE-B12

|       | 100 | 47.9 | 26.2 | 31.2 | 20.3 |
|-------|-----|------|------|------|------|
| Comp.9|     |      |      |      |      |
| 100   | 60.6| 36.8 | 44.8 | 28.2 | 38.2 |
| 50    | 59.2| 49.6 | 52.6 | 37.1 | 50.6 |
| 25    | 85.2| 60.5 | 60.2 | 50.4 | 64.2 |
| 12.5  | 99.7| 78.2 | 75.8 | 73.2 | 79.5 |
| 6.25  | 100 | 94.4 | 96.1 | 92.0 | 96.0 |
| 3.125 | 100 | 100  | 100  | 100  | 100  |
| 1.56  | 100 |      |      |      |      |

OE-E4

|       | 100 | 47.4 | 29.5 | 37.5 | 36.1 |
|-------|-----|------|------|------|------|
| Comp.3|     |      |      |      |      |
| 100   | 59.2| 42.8 | 59.5 | 50.7 | 47.6 |
| 50    | 71.8| 50.2 | 71.9 | 64.8 | 61.3 |
| 25    | 85.3| 76.1 | 92.8 | 75.9 | 72.4 |
| 12.5  | 97.0| 82.4 | 100  | 97.1 | 94.7 |
| 6.25  | 100 | 100  | 100  | 100  | 100  |
| 3.125 | 100 |      |      |      |      |
| 1.56  | 100 |      |      |      |      |

OE-B15

|       | 100 | 43.3 | 38.1 | 23.5 | 17.0 |
|-------|-----|------|------|------|------|
| Comp.10|      |      |      |      |      |
| 100   | 54.8| 50.2 | 37.0 | 25.8 | 58.0 |
| 50    | 71.7| 63.1 | 46.8 | 33.7 | 65.2 |
| 25    | 93.6| 72.7 | 59.1 | 48.1 | 79.3 |
| 12.5  | 100 | 91.9 | 78.2 | 63.5 | 94.7 |
| 6.25  | 100 | 100  | 96.3 | 85.9 | 100  |
| 3.125 | 100 |      |      |      |      |
| 1.56  | 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.(µM) | 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 |
| Value | OE-B12 | OE-E4 | OE-B15 |
|-------|--------|-------|--------|
|       | Comp.9 | Comp.3 | Comp.10 |
| 3.125 | 100    | 100   | 100    |
| 1.56  | 100    | 100   | 100    |
| OE-B12 | 100 | 99.5 | 100 |
|       | 100   | 100   | 100    |
|       | 81.4  | 93.7  | 76.1   |
|       | 93.7  | 76.1  | 79.8   |
|       | 94.4  | 96.1  | 92.0   |
|       | 96.1  | 96.1  | 96.0   |
|       | 99.5  | 100   | 100    |
|       | 99.1  | 100   | 100    |
| 100   | 47.9  | 37.5  | 23.5   |
| 50    | 47.4  | 37.5  | 17.0   |
| 25    | 47.3  | 37.5  | 17.0   |
| 12.5  | 47.2  | 37.5  | 17.0   |
| 6.25  | 47.1  | 37.5  | 17.0   |
| 3.125 | 47.0  | 37.5  | 17.0   |
| 1.56  | 47.0  | 37.5  | 17.0   |
Lab Report

| ser | compound      | PI3K-α IC50 ng/ml | SD. ± |
|-----|---------------|-------------------|-------|
|     | code          | conc              |       |
| 1   | OE-G12        | 2.21              | 0.11  |
| *** | LY294002      | 8.04              | 0.42  |

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: ---
### Detailed results:

#### PI3K-α

| code   | IC50 | conc | log | %inh | T2  | T1  | ΔT | RFU2 | RFU1 | ΔRFU | slope | K.Activity | EC |
|--------|------|------|-----|------|-----|-----|----|------|------|------|-------|------------|----|
| OE-G12 | 100  | 2    | 0.7 | 30   | 30  | 0   | 19.26 | 0   | 19.26 | 3.3333 | 23.112023 | 120 |
|        | 10   | 1    | 67  | 30   | 0   | 30  | 32.98 | 0   | 32.98 | 3.3333 | 39.57604   | 120 |
|        | 1    | 0    | 42.7| 30   | 0   | 30  | 57.31 | 0   | 57.31 | 3.3333 | 68.772069  | 120 |
|        | 0.1  | -1   | 22.1| 30   | 0   | 30  | 77.91 | 0   | 77.91 | 3.3333 | 93.492093  | 120 |
| EC     | 0    | 30   | 0   | 30   | 100 | 0   | 100  | 0   | 100   | 3.3333 | 120   | 120 |

#### OE-G12

- **Equation**: \( y = 20.028x + 43.121 \)

#### LY294002

| 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 | 3.3333 | 27.912028 | 120 |
|        | 10   | 1    | 54.8| 30   | 0   | 30  | 45.18 | 0   | 45.18 | 3.3333 | 54.216054 | 120 |
|        | 1    | 0    | 21.2| 30   | 0   | 30  | 78.76 | 0   | 78.76 | 3.3333 | 94.512095 | 120 |
|        | 0.1  | -1   | 8.66| 30   | 0   | 30  | 91.34 | 0   | 91.34 | 3.3333 | 109.60811 | 120 |
| EC     | 0    | 30   | 0   | 30   | 100 | 0   | 100  | 0   | 100   | 3.3333 | 120   | 120 |

#### LY294002

- **Equation**: \( y = 23.782x + 28.474 \)
**Lab Report**

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

**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**: ---
**Detailed results:**

### vegfr2

| code   | IC50  | conc | log | %inh | T2 | T1 | ΔT  | RFU2 | RFU1 | ΔRFU  | slope    | K.Activity | EC |
|--------|-------|------|-----|------|----|----|-----|------|------|-------|----------|------------|---|
| OE-G12 | 10    | 0    | 90.4| 30   | 30 | 9.59| 0   | 9.59 | 3.33333 | 11.508012 | 120 |
|        | 1     | 0    | 75.3| 30   | 30 | 24.71| 0   | 24.71| 3.33333 | 29.65203  | 120 |
|        | 0.1   | -1   | 52.7| 30   | 30 | 47.26| 0   | 47.26| 3.33333 | 56.712057 | 120 |
|        | 0.01  | -2   | 28.7| 30   | 30 | 71.33| 0   | 71.33| 3.33333 | 85.596086 | 120 |
| EC     | 0     | 30   | 0   | 30   | 100| 0   | 100 | 3.33333 | 120         | 120 |

### sorafenib

| code   | IC50  | conc | log | %inh | T2 | T1 | ΔT  | RFU2 | RFU1 | ΔRFU  | slope    | K.Activity | EC |
|--------|-------|------|-----|------|----|----|-----|------|------|-------|----------|------------|---|
| OE-G12 | 10    | 1    | 93.1| 30   | 30 | 6.88| 0   | 6.88 | 3.33333 | 8.2560083 | 120 |
|        | 1     | 0    | 81.4| 30   | 30 | 18.64| 0   | 18.64| 3.33333 | 22.368022 | 120 |
|        | 0.1   | -1   | 61.7| 30   | 30 | 38.25| 0   | 38.25| 3.33333 | 45.900046 | 120 |
|        | 0.01  | -2   | 36.8| 30   | 30 | 63.23| 0   | 63.23| 3.33333 | 75.876076 | 120 |
| EC     | 0     | 30   | 0   | 30   | 100| 0   | 100 | 3.33333 | 120         | 120 |

**OE-G12**

\[ y = 20.777x + 72.166 \]

**sorafenib**

\[ y = 18.866x + 77.683 \]
## Lab Report

| Ser | Sample data       | Results DNA content | Comment                  |
|-----|-------------------|---------------------|--------------------------|
|     | code              | IC50 uM             | %G0-G1 | %S  | %G2/M | %Pre-G1 |                   |
| 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  |         |                   |

**DNA content**

- %G0-G1
- %S
- %G2/M
- %Pre-G1

**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

**Researcher:** Dr. Omar El-Khouly  
**email:** dr.kholy93@gmail.com  
**mob.:** 01278084495

**Assay:** Cell Cycle Analysis  
**Samples:** 02 samples  
**cell line:** ---
| 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     |

![Apoptosis/Necrosis Bar Chart](chart.png)
Detailed results

Date: 31 mar 2021
Sample: Hela

Diploid 100%

- % pre G: 1.95%
- % DIP G1: 46.26%
- % DIP G2/M: 10.75%
- % DIPS: 42.99%

CV: 5.88

Aggregates: 2.41%
Cell debris: 2.19%
