

## **Electronic Supporting Information (ESI)**

**Triphenylstannyl((arylimino)methyl)benzoates with selective potency that induce G1 and G2/M cell cycle arrest and trigger apoptosis via ROS in human cervical cancer cells**

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15. **Figure S13.** The data indicated in the histogram refers to the percentage of cells in each phase of the cell cycle.

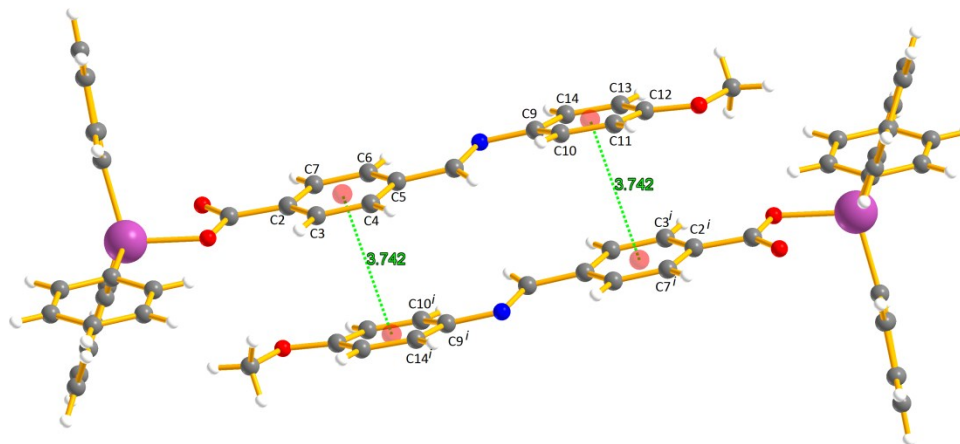
**Table S1.** Crystal data and structure refinement details for pro-ligands **HL<sup>3</sup>**, **HL<sup>5</sup>** and **HL<sup>6</sup>**

	<b>HL<sup>3</sup></b>	<b>HL<sup>5</sup></b>	<b>HL<sup>6</sup></b>
Empirical formula	C <sub>15</sub> H <sub>13</sub> N <sub>1</sub> O <sub>2</sub>	C <sub>15</sub> H <sub>13</sub> N <sub>1</sub> O <sub>3</sub>	C <sub>16</sub> H <sub>15</sub> N <sub>1</sub> O <sub>3</sub>
Formula weight	239.26	255.26	269.29
Temperature (K)	298(2)	296(2)	298(2)
Crystal system	Monoclinic	Orthorhombic	Triclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> 2 <sub>1</sub> <i>ca</i>	<i>P</i> $\bar{1}$
<i>a</i> (Å)	24.5835(17)	6.1246(5)	4.8722(6)
<i>b</i> (Å)	7.2032(5)	57.377(4)	7.6353(8)
<i>c</i> (Å)	14.2362(10)	7.2367(4)	19.256(2)
∠ (°)	90	90	92.857(9)
∠ (°)	105.711(7)	90	96.511(9)
∠ (°)	90	90	104.261(10)
<i>V</i> (Å <sup>3</sup> )	2426.8(3)	2543.1(3)	687.53(14)
<i>Z</i>	8	8	2
<i>D</i> <sub>calc</sub> (g/cm <sup>3</sup> )	1.310	1.333	1.301
∠ (mm <sup>-1</sup> )	0.087	0.094	0.090
<i>F</i> (000)	1008	1072	284
Reflections measured	11916	13265	5200
Independent reflections ( <i>R</i> <sub>int</sub> )	5568 (0.0329)	4431 (0.1330)	3103 (0.0312)
Reflection with <i>I</i> > 2σ( <i>I</i> )	2802	3727	1618
Number of parameters	331	337	184
<i>R</i> 1 <sup>a</sup> (□□□□□□□□)	0.0610	0.1665	0.0857
<i>wR</i> 2 <sup>b</sup> (□□□□□□□□)	0.1371	0.4128	0.2099
GOF ( <i>F</i> <sup>2</sup> )	1.014	1.687	1.039

**Table S2.** Crystal data and structure refinement details for triphenyltin compounds **5**, **7-11**

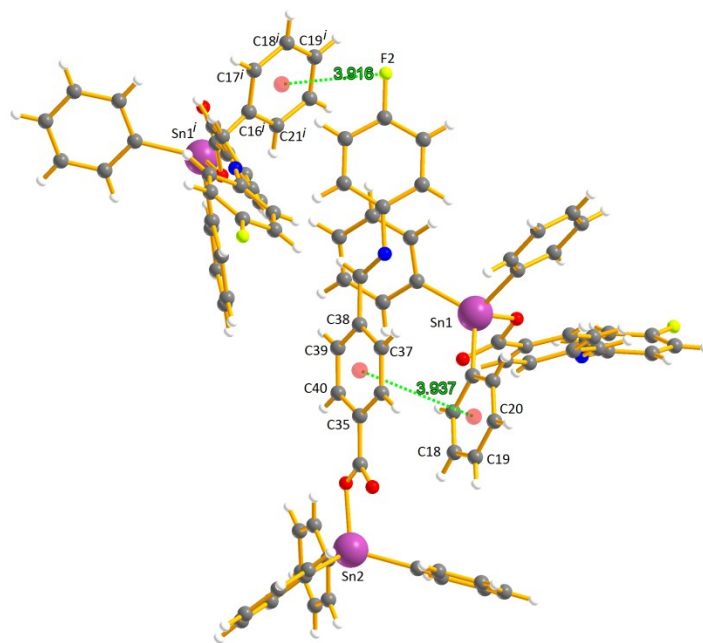
	<b>5</b>	<b>7</b>	<b>8</b>	<b>9</b>	<b>10</b>	<b>11</b>
Empirical formula	C <sub>33</sub> H <sub>27</sub> NO <sub>3</sub> Sn	C <sub>32</sub> H <sub>24</sub> FNO <sub>2</sub> Sn	C <sub>34</sub> H <sub>30</sub> N <sub>2</sub> O <sub>2</sub> Sn	C <sub>26</sub> H <sub>22</sub> O <sub>4</sub> Sn	C <sub>32</sub> H <sub>25</sub> NO <sub>2</sub> Sn	C <sub>32</sub> H <sub>24</sub> FNO <sub>2</sub> Sn
Formula weight	604.24	592.21	617.29	517.12	574.22	592.21
Temperature (K)	298(2)	296(2)	296(2)	296(2)	296(2)	296(2)
Crystal system	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	<i>Pbca</i>	<i>Pca2</i> <sub>1</sub>	<i>P2</i> <sub>1</sub> / <i>n</i>	<i>P2</i> <sub>1</sub> / <i>n</i>	<i>P</i> <sub>1</sub> <sup>1</sup>	<i>P2</i> <sub>1</sub> / <i>c</i>
<i>a</i> (Å)	8.3521(3)	19.5733(7)	11.7022(6)	10.5925(2)	9.6664(3)	26.2984(8)
<i>b</i> (Å)	17.4627(6)	14.9548(5)	10.3673(6)	19.0045(4)	14.5629(6)	9.5246(4)
<i>c</i> (Å)	38.415(3)	18.3132(6)	48.186(2)	11.3877(3)	19.7869(7)	21.8019(8)
□ (°)	90	90	90	90	101.707(3)	90
□ (°)	90	90	92.817(4)	96.160(2)	94.317(4)	92.563(3)
□ (°)	90	90	90	90	96.279(3)	90
<i>V</i> (Å <sup>3</sup> )	5602.8(5)	5360.5(3)	5838.8(5)	2279.17(9)	2697.49(17)	5455.5(3)
<i>Z</i>	8	8	8	4	4	8
<i>D</i> <sub>calc</sub> (g/cm <sup>3</sup> )	1.433	1.468	1.404	1.507	1.414	1.442
<i>μ</i> (mm <sup>-1</sup> )	0.946	0.989	0.908	1.150	0.975	0.972
<i>F</i> (000)	2448	2384	2512	1040	1160	2384
Reflections measured	20102	14398	22687	9877	23758	33258
Independent reflections ( <i>R</i> <sub>int</sub> )	6563 (0.0366)	8091 (0.0220)	13233 (0.0965)	5183 (0.0163)	11011 (0.0271)	12601 (0.0318)
Reflection with <i>I</i> > 2σ( <i>I</i> )	5411	6716	7477	4426	8792	9989
Number of parameters	4832	668	707	286	649	667
<i>RI</i> <sup>a</sup> ( <i>I</i> ≥ 2σ)	0.0618	0.0312	0.1246	0.0246	0.0391	0.0532
<i>wR2</i> <sup>b</sup> ( <i>I</i> ≥ 2σ)	0.1003	0.0646	0.2046	0.0536	0.0771	0.0981
GOF ( <i>F</i> <sup>2</sup> )	1.159	1.079	1.154	1.068	1.055	1.159

<sup>a</sup>  $RI = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ . <sup>b</sup>  $wR2 = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$

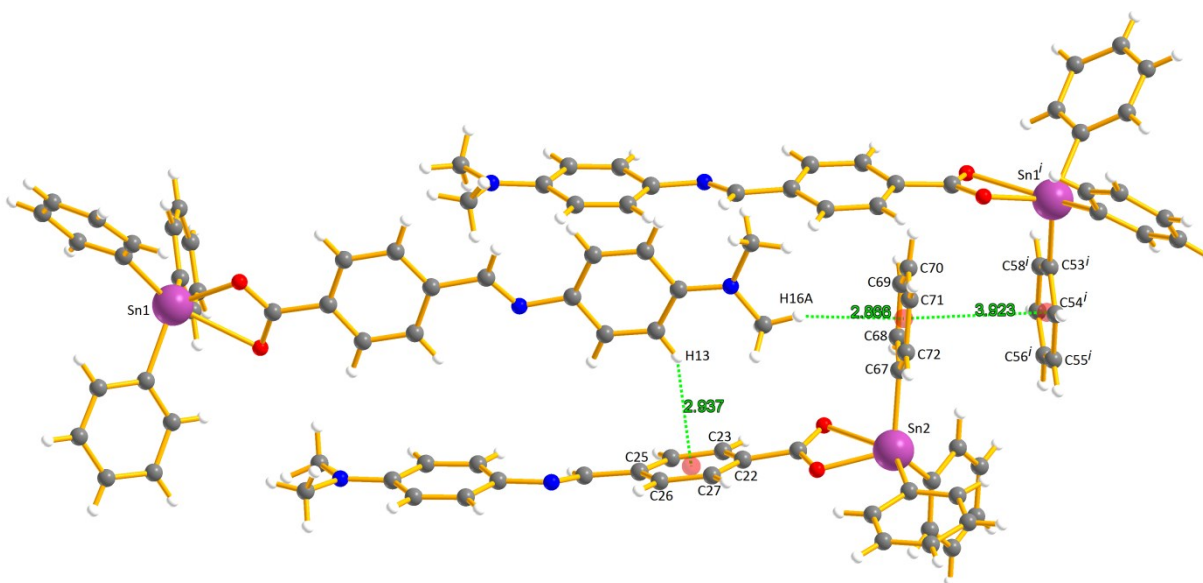


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**Figure S1.**  $\pi \cdots \pi$  and C-H $\cdots\pi$  interactions in the structures of compounds **5**. Symmetry code to generate equivalent atoms: *i*) 1-x, 1-y, 2-z.

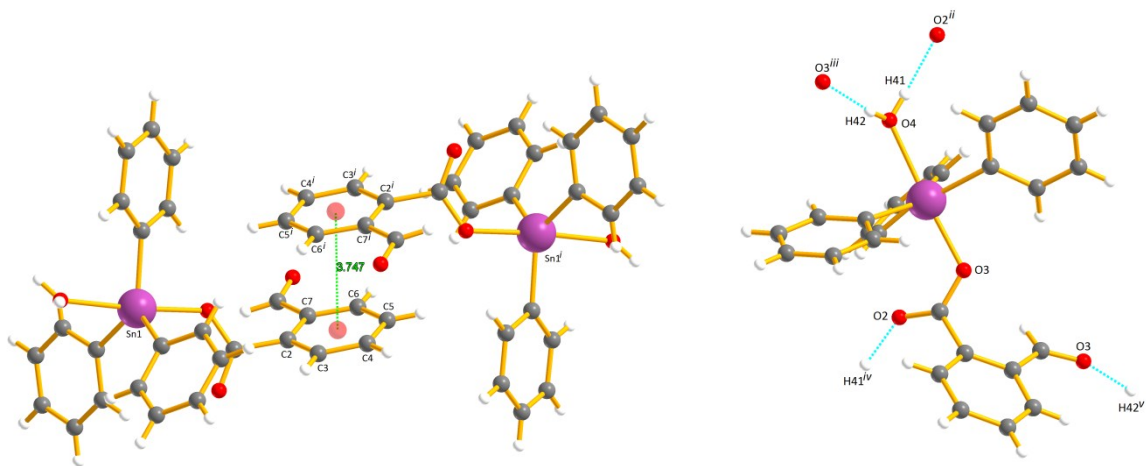


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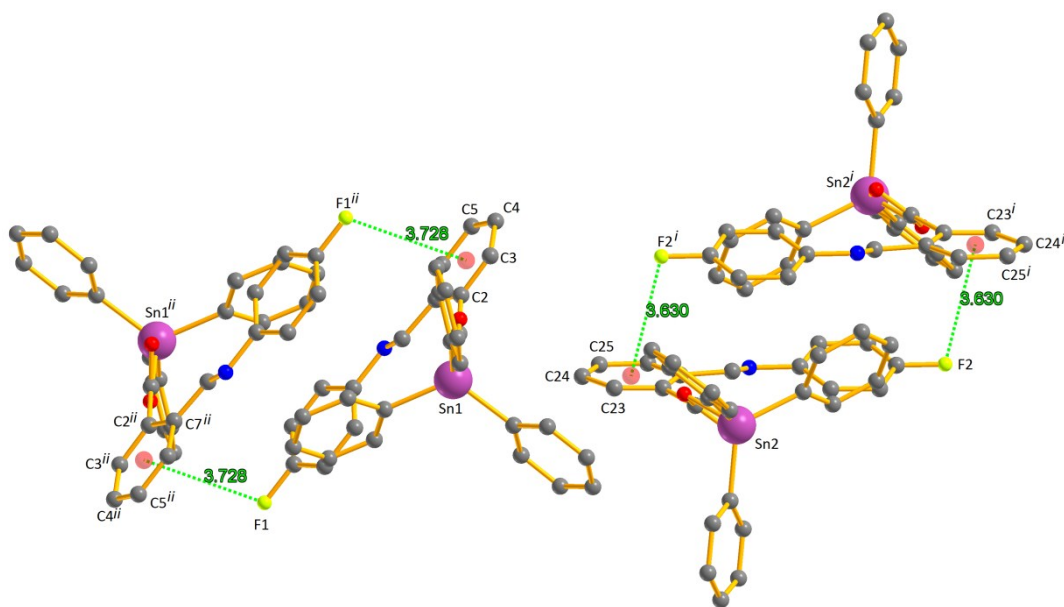
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**Figure S2.**  $\pi \cdots \pi$  and C-H $\cdots$  $\pi$  interactions in the structures of compounds **7** and **8**. Symmetry code to generate equivalent atoms: *i*) -x,1-y,-1/2+z (**7**); *i*) 1/2-x,-1/2+y,1.5-z (**8**).



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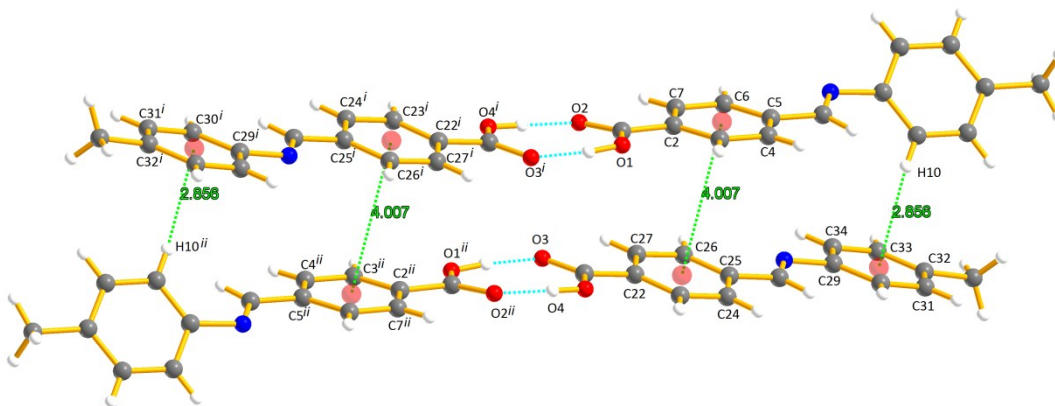
**Figure S3.**  $\pi \cdots \pi$  and hydrogen-bond interactions in the structure of compound **9**:  $d_{O4 \cdots O2} = 2.687(2) \text{ \AA}$ ,  $\angle_{O4-H41 \cdots O2} = 168(2)^\circ$ ;  $d_{O4 \cdots O3} = 2.772(3) \text{ \AA}$ ,  $\angle_{O4-H42 \cdots O3} = 172(2)^\circ$ . Symmetry code to generate equivalent atoms: *i*)  $2-x, 2-y, 1-z$ ; *ii*)  $-1/2+x, 1.5-y, -1/2+z$ ; *iii*)  $-1+x, y, z$ ; *iv*)  $1/2+x, 1.5-y, 1/2+z$ ; *v*)  $1+x, y, z$ .



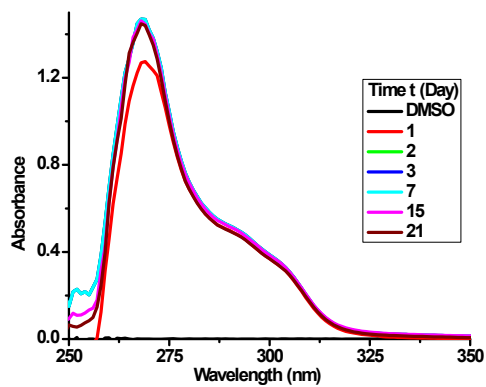
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**Figure S4.**  $F \cdots \pi$  interactions in the structure of compound **11**. Symmetry code to generate equivalent atoms: *i*)  $2-x, 1-y, 1-z$ ; *ii*)  $1-x, -y, 1-z$ .

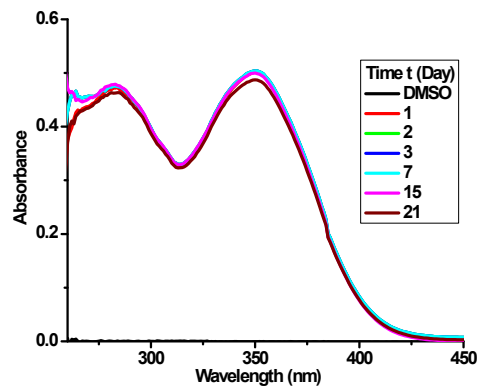




**Figure S5.**  $\pi \cdots \pi$  and C–H $\cdots\pi$  interactions in the structure of compound **HL**<sup>3</sup>. Symmetry code to generate equivalent atoms: *i*) 2-x,1-y,1-z; *ii*) 2-x,1-y,1-z.

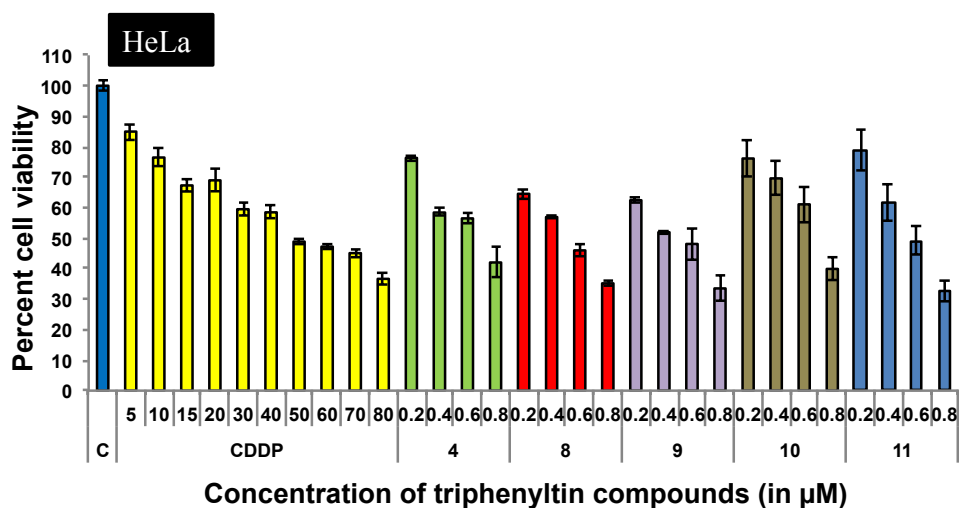
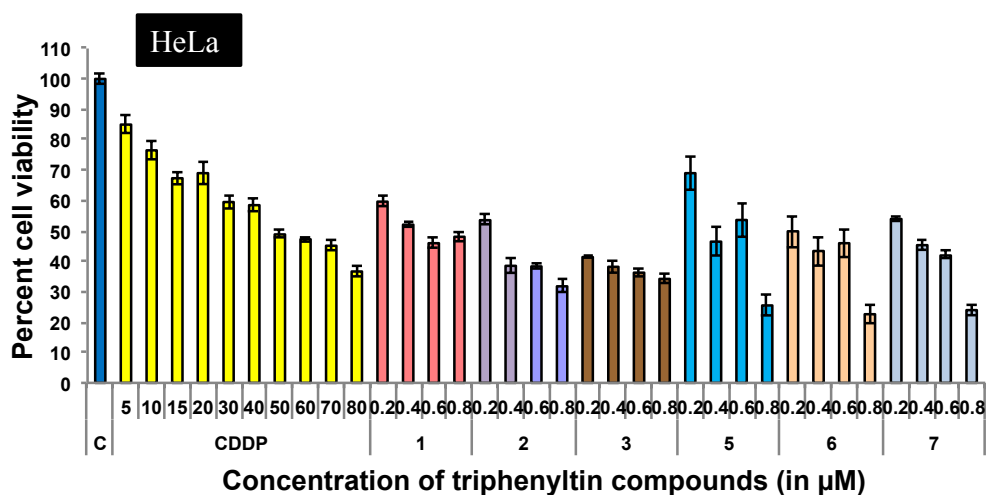


**Compound 1**

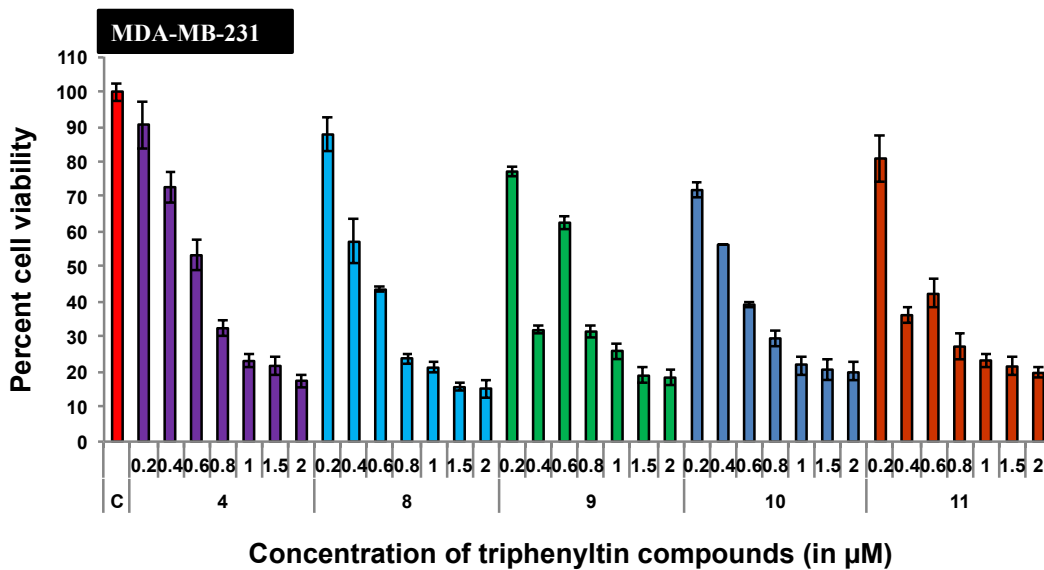
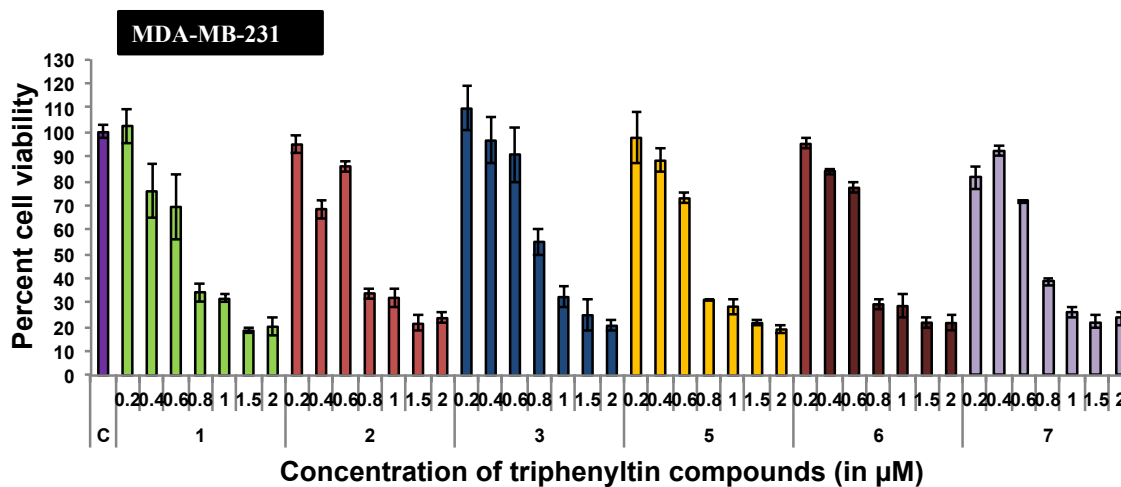


**Compound 5**

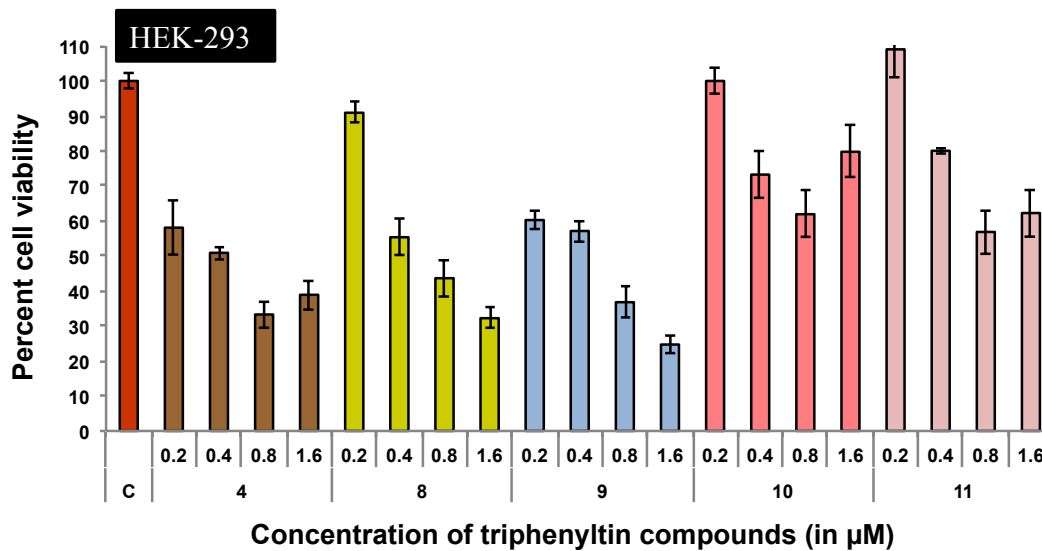
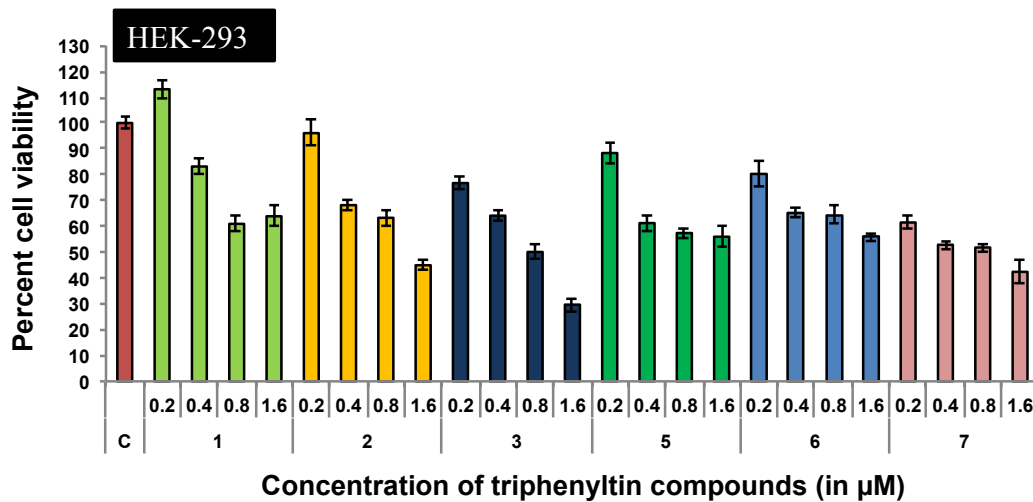
**Figure S6.** Uv-Vis absorption spectra over time for triphenyltin(IV) compounds **1** and **5** in DMSO.



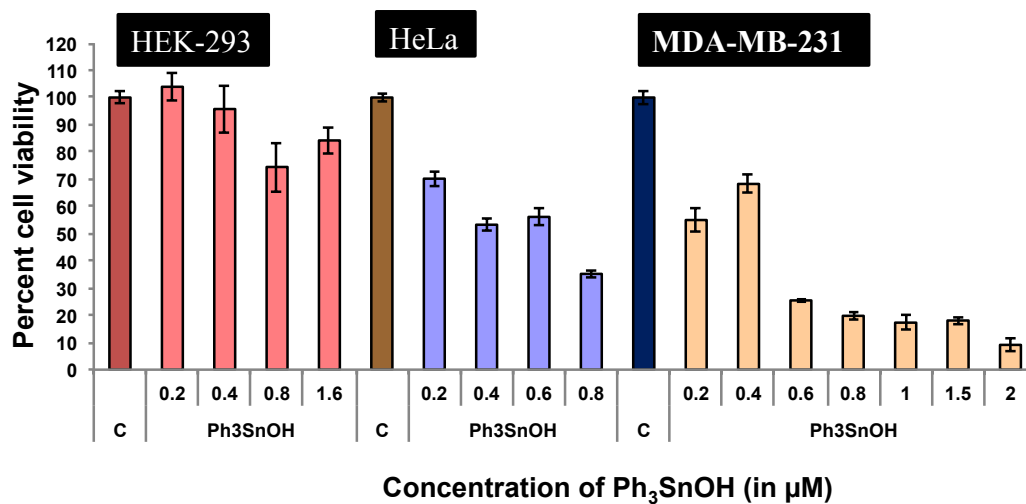
**Figure S7.** Bar representations of dose dependent cytotoxic effects of compounds 1-11 on HeLa cells by MTT assay after incubation with various concentrations of compounds for 24 h. Bars represent  $\pm$  SEM (n = 3).



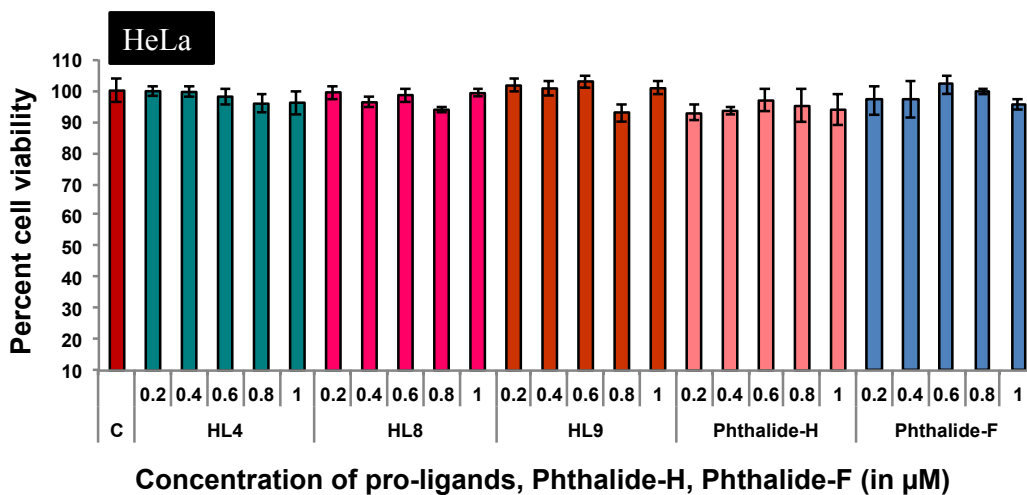
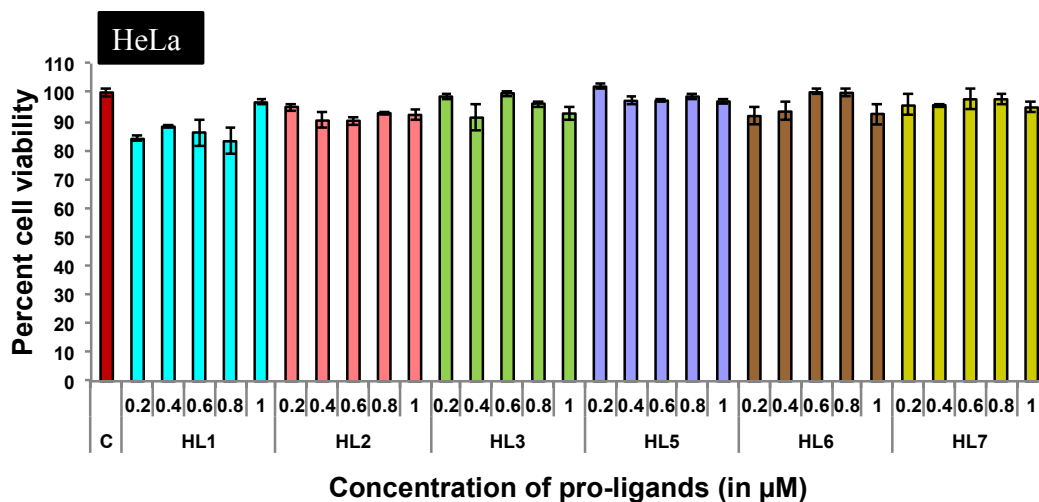
**Figure S8.** Bar representations of dose dependent cytotoxic effects of compounds 1-11 on MDA-MB-231 cells by MTT assay after incubation with various concentrations of compounds for 24 h. Bars represent  $\pm$  SEM (n = 3).



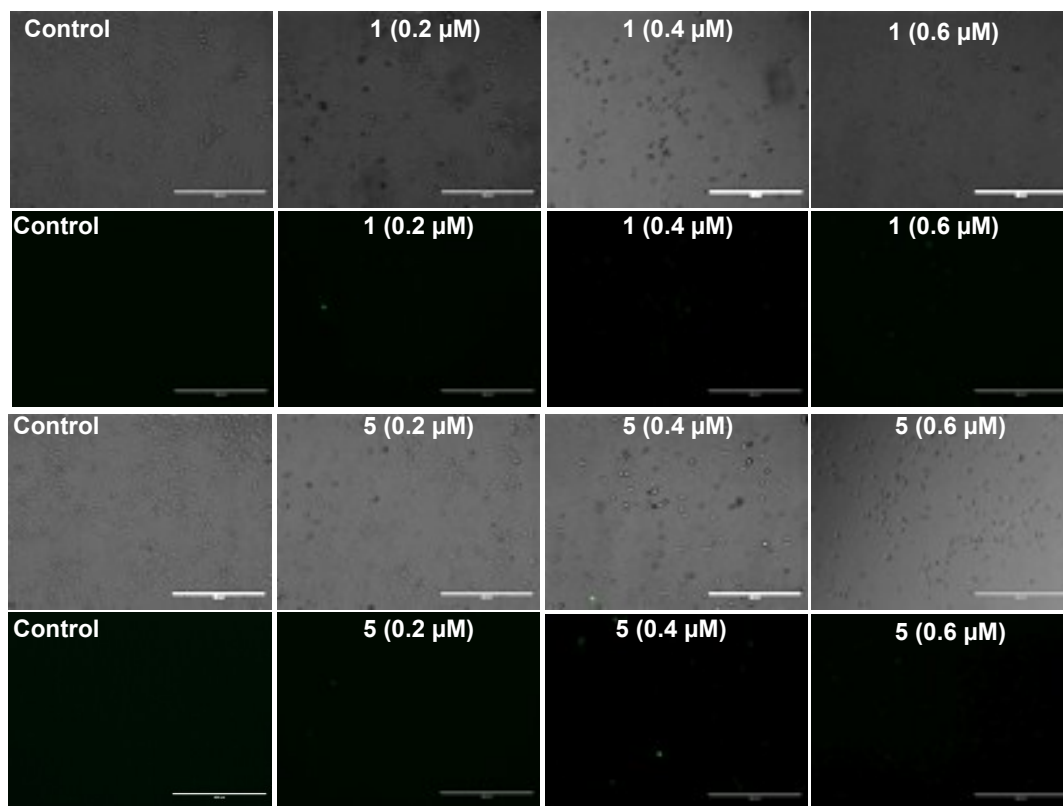
**Figure S9.** Bar representations of dose dependent cytotoxic effects of compounds **1-11** on HEK-293 cells by MTT assay after incubation with various concentrations of compounds for 24 h. Bars represent  $\pm$  SEM (n = 3).



**Figure S10.** Bar representations of dose dependent cytotoxic effects of Ph<sub>3</sub>SnOH on normal cells HEK-293 and cancer cells HeLa and MDA-MB-231 by MTT assay after incubation with various concentrations of compounds for 24 h. Bars represent  $\pm$  SEM (n = 3).

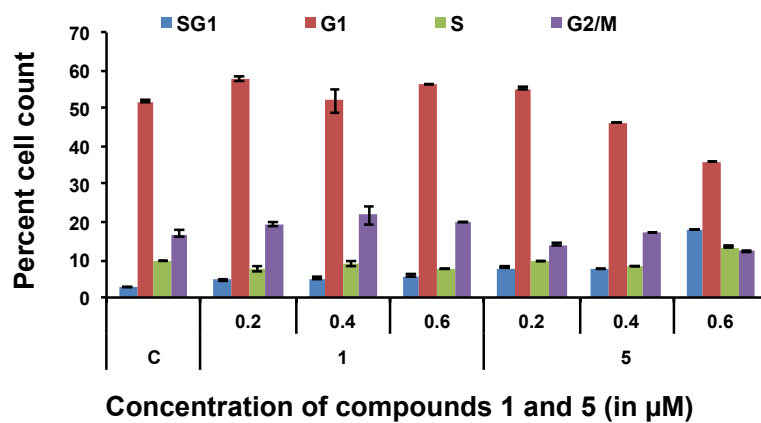


**Figure S11.** Bar representations of dose dependent cytotoxic effects of Pro-ligands HL<sup>1</sup>-HL<sup>9</sup>, Phthalide-H and Phthalide-F on HeLa cells by MTT assay after incubation with various concentrations of compounds for 24 h. Bars represent  $\pm$  SEM (n = 3).



**Figure S12.** Dose-dependent generations of ROS through DCFH-DA fluorescence staining dye after 24h treatment with  $\text{IC}_{50}$  concentrations of **1** and **5** in HEK 293 cells detected by measuring the fluorescence intensity viewed through fluorescence microscope.





**Figure S13.** The data indicated in the histogram refers to the percentage of cells in each phase of the cell cycle.