Supplementary Materials

Structural characterization of new zinc(II) complexes with N_2O_2 chelating thiosemicarbazidato ligand; Investigation of the relationship between their DNA interaction and *in vitro* antiproliferative activity on human cancer cells

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Table S1. Hydrogen-bond parameters for **Zn1** (Å, º).

D-H· · ·A	D-H	H···A	D···A	D-H···A
C15—H15···F1^{i}	0.93	2.53	3.434 (8)	166

Symmetry code: (i) −x+3/2, y+1/2, −z+1/2.

Table S2. Selected SC pBR322 DNA cleavage data in the presence of varying concentrations of complex **Zn 1** in Fig. 4A.

Lane no.	**Reaction conditions**	**Form I (%)**	**Form II (%)**
1	DNA	79.3	20.7
2	DNA+ Zn 1 (50 μM)	70.5	29.5
3	DNA+ Zn 1 (100 μM)	69.5	30.5
4	DNA+ Zn 1 (200 μM)	66.8	33.2
5	DNA+ Zn 1 (500 μM)	66.5	33.5
6	DNA+ Zn 1 (2000 μM)	64.8	35.2
7	DNA+ Zn 1 (3000 μM)	62.6	37.4

Table S3. Selected SC pBR322 DNA cleavage data in the presence of varying concentrations of complex **Zn 2** in Fig. 4B.

Lane no.	**Reaction conditions**	**Form I (%)**	**Form II (%)**
1	DNA	55.8	44.2
2	DNA+ Zn 2 (50 μM)	53.3	46.7
3	DNA+ Zn 2 (100 μM)	51.6	48.4
4	DNA+ Zn 2 (200 μM)	51.8	48.2
5	DNA+ Zn 2 (500 μM)	49.7	50.3
6	DNA+ Zn 2 (2000 μM)	45.7	54.3
7	DNA+ Zn 2 (3000 μM)	41.9	58.1

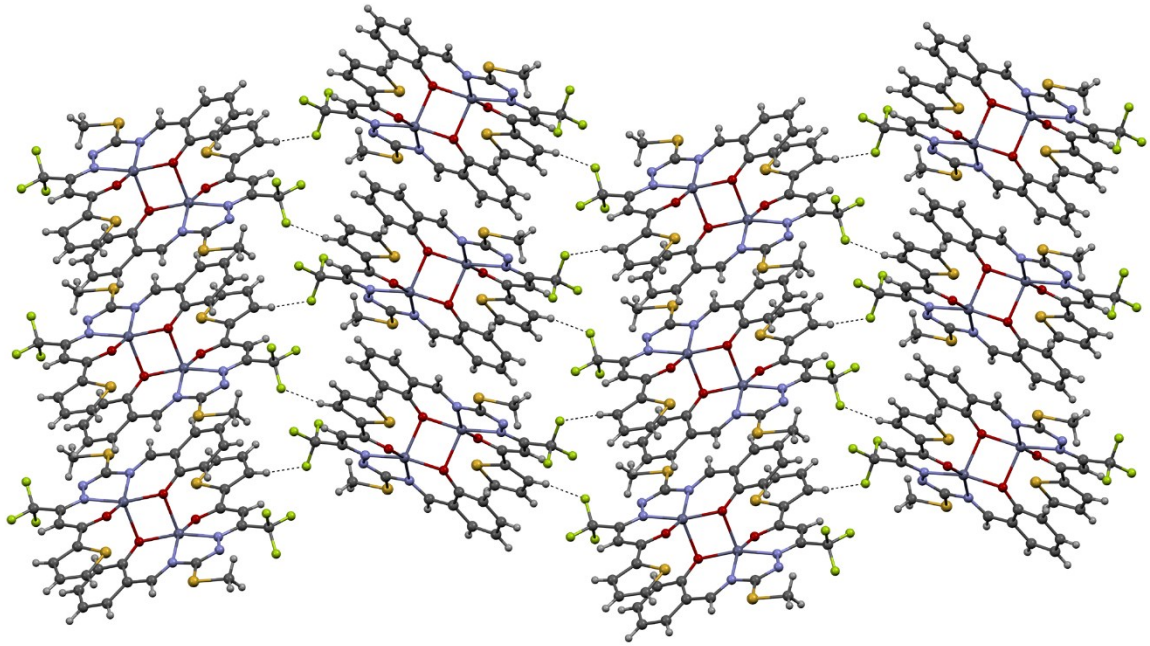

Figure S1. An infinite 2D layer in **Zn1**.

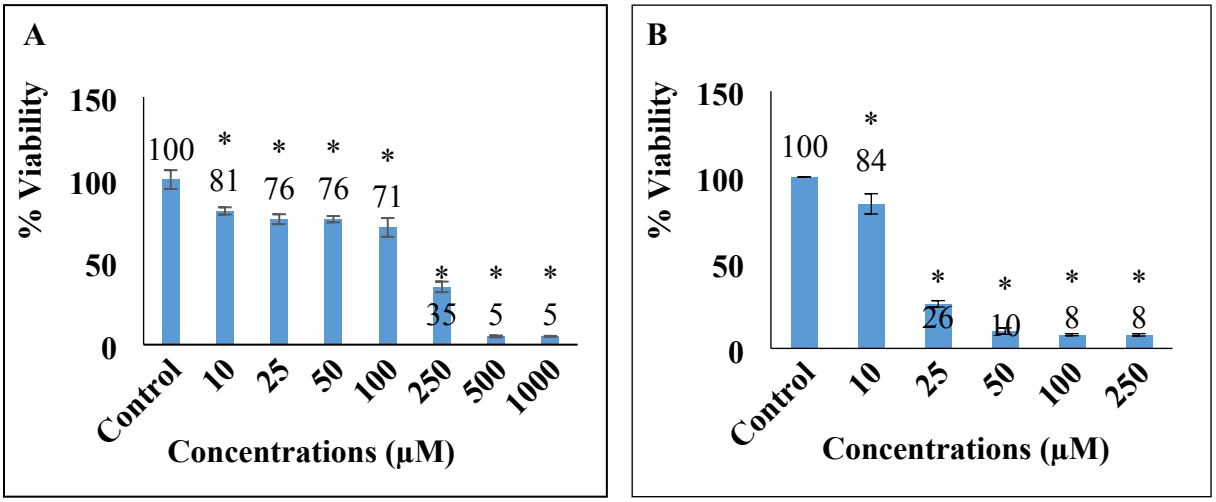

Figure S2. The effects of complex **Zn1** (A) and complex **Zn2** (B) on viability of HT-29 cell line for 24 h. Results are represented as mean of four experiments ± standard deviation. *p< 0.05 compared to control.

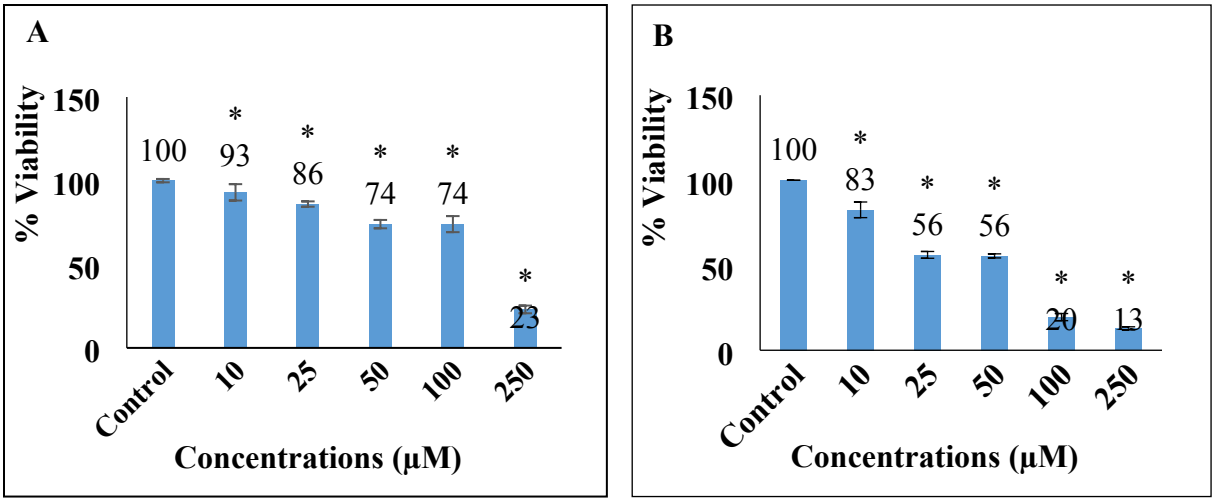

Figure S3. The effects of complex **Zn1** (A) and complex **Zn2** (B) on viability of HeLa cell line for 24 h. Results are represented as mean of four experiments ± standard deviation. *p< 0.05 compared to control.

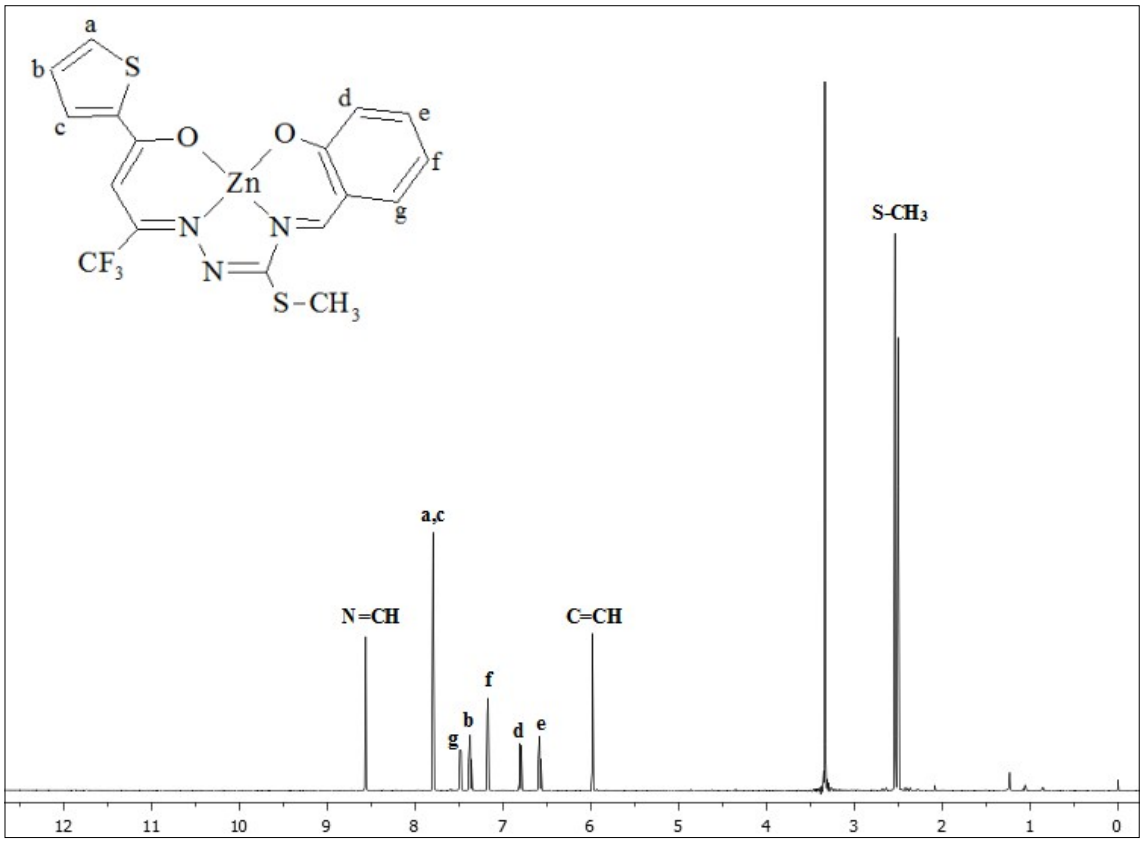

Figure S4. ^{1}H NMR spectrum of complex **Zn1** in DMSO-d_6.

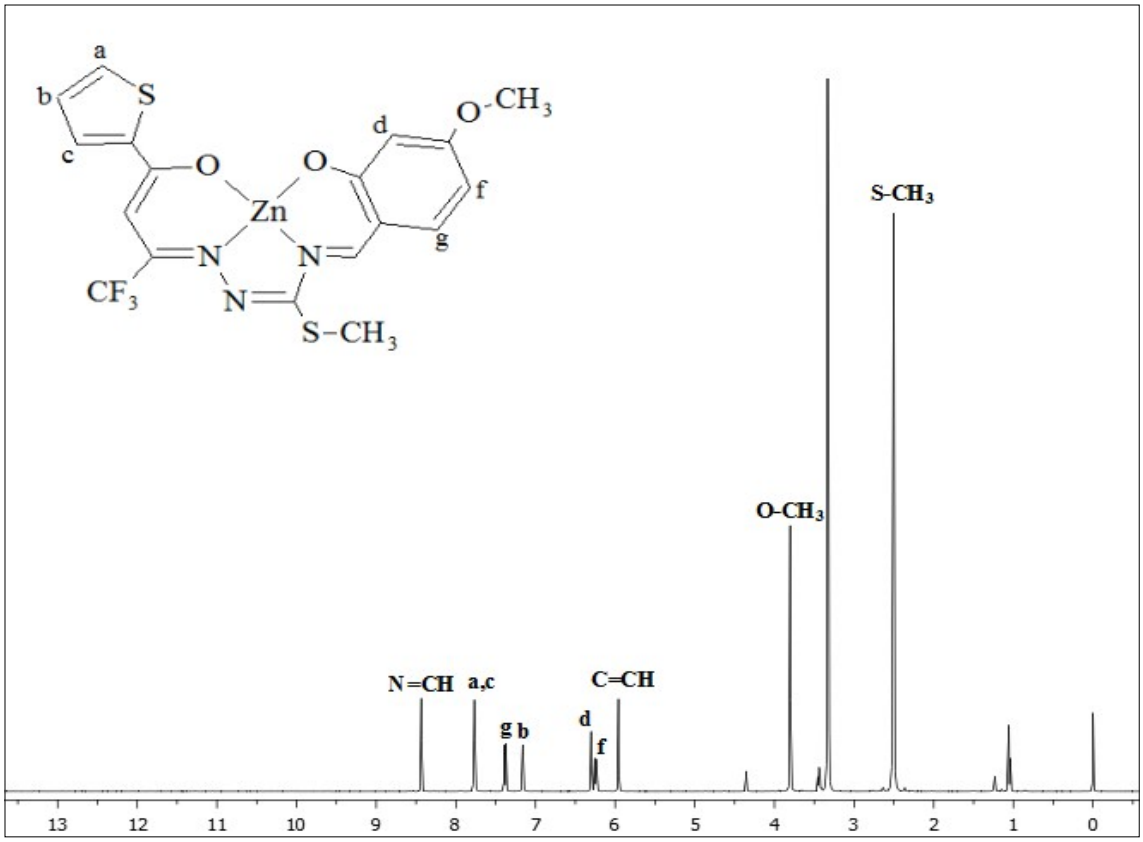

Figure S5. ^{1}H NMR spectrum of complex **Zn2** in DMSO-d_6.

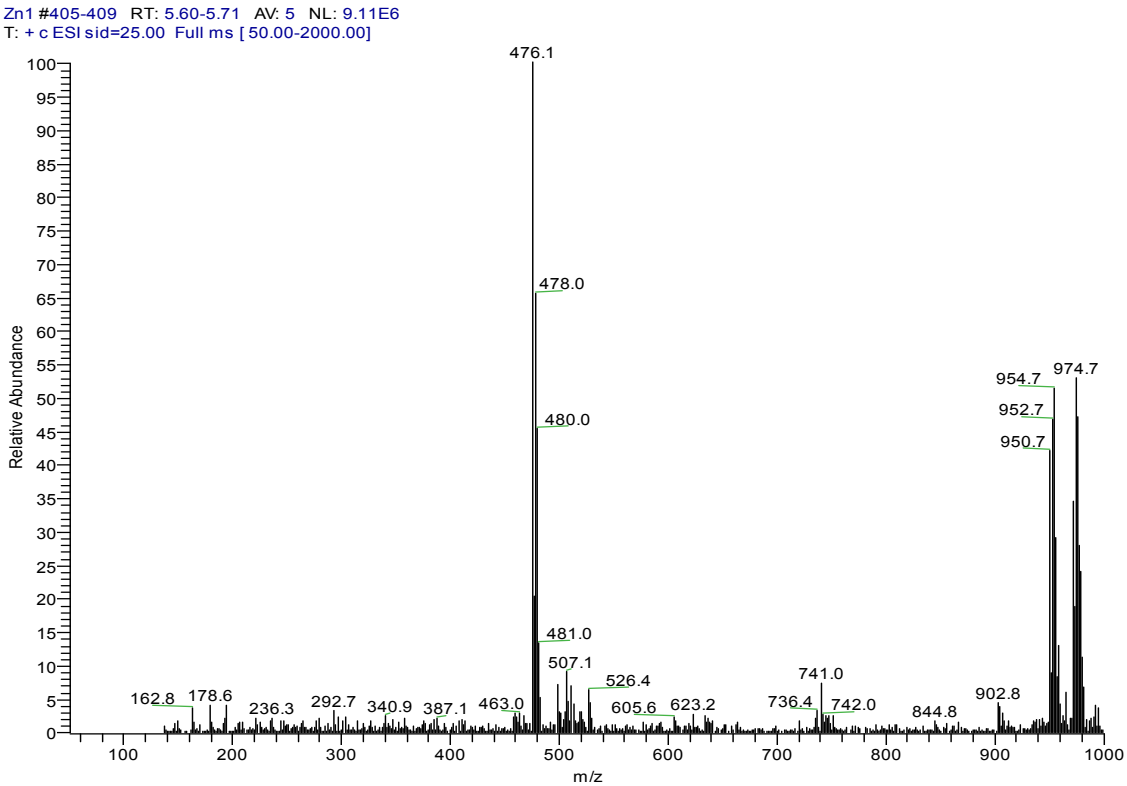

Figure S6. ESI-MS of complex **Zn1** in $CHCl_3$.

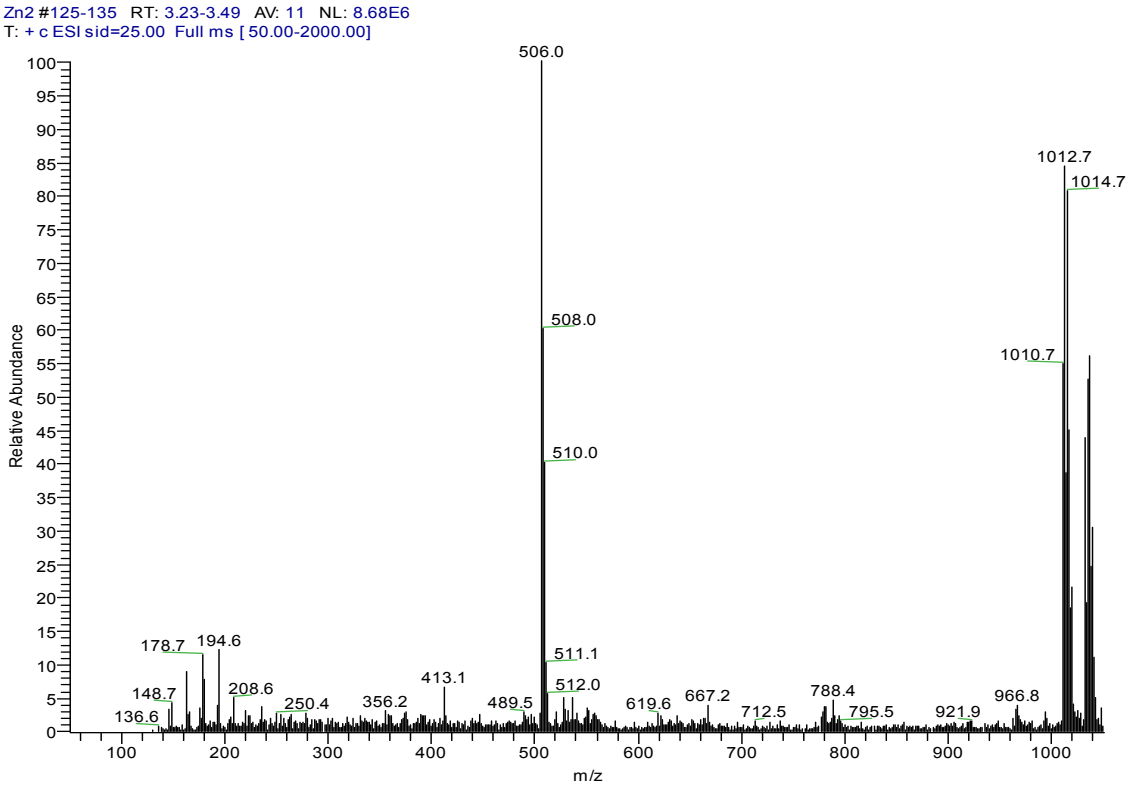

Figure S7. ESI-MS of complex **Zn2** in $CHCl_3$.