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## 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, °).

D-H···A	D-H	Н…А	D···A	D-H···A
$C15 - H15 \cdots F1^i$	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		70.2	20.7
1	DNA	/9.3	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.

DNA	55.8	44.2
DNA+ Zn 2 (50 μM)	53.3	46.7
DNA+ Zn 2 (100 µM)	51.6	48.4
DNA+ Zn 2 (200 µM)	51.8	48.2
DNA+ Zn 2 (500 µM)	49.7	50.3
DNA+ Zn 2 (2000 µM)	45.7	54.3
DNA+ Zn 2 (3000 µM)	41.9	58.1
	DNA DNA+ Zn 2 (50 μM) DNA+ Zn 2 (100 μM) DNA+ Zn 2 (200 μM) DNA+ Zn 2 (500 μM) DNA+ Zn 2 (2000 μM) DNA+ Zn 2 (3000 μM)	DNA55.8DNA+ Zn 2 (50 $\mu$ M)53.3DNA+ Zn 2 (100 $\mu$ M)51.6DNA+ Zn 2 (200 $\mu$ M)51.8DNA+ Zn 2 (500 $\mu$ M)49.7DNA+ Zn 2 (2000 $\mu$ M)45.7DNA+ Zn 2 (3000 $\mu$ M)41.9



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  $\pm$  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  $\pm$  standard deviation. \*p< 0.05 compared to control.



Figure S4. <sup>1</sup>H NMR spectrum of complex Zn1 in DMSO-d<sub>6</sub>.



Figure S5. <sup>1</sup>H NMR spectrum of complex Zn2 in DMSO-d<sub>6</sub>.



Figure S6. ESI-MS of complex Zn1 in CHCl<sub>3</sub>.



Figure S7. ESI-MS of complex Zn2 in CHCl<sub>3</sub>.