Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary data:

Table S1 Crystal data and structure refinement parameters for complexes **2** and **4**.

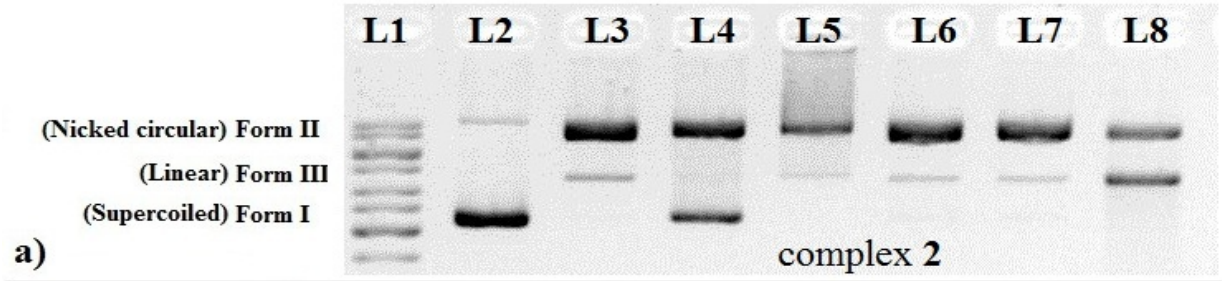
Compound	**2**	**4**
Empirical formula	$Cu(C_9H_9BrNO)_2$	$Ni(H_2O)_4(C_9H_9NO)^{2+}\cdot 2Br^-$
Formula weight	517.70	584.94
Crystal system	Monoclinic	Monoclinic
Space group	$P2_{1/c}$	$P2_{1/c}$
Unit cell dimensions		
a (Å)	10.2397(8)	11.2099 (2)
b (Å)	10.0932(6)	7.3582 (2)
c (Å)	8.7855(6)	13.2536 (3)
α (º)	90.00°	90.00°
β (º)	102.225 (7)°	93.857 (2)°
γ (º)	90.00°	90.00°
V (Å^3)	887.40 (11)	1090.74 (4)
Z	2	2
F(000)	510	588
D_x (Mg m^{-3})	1.937	1.781
T (K)	100	100
Absorption coefficient, μ	5.75	5.90
θ ranges (º)	2.9-27.6	4.0-76.6
Reflections collected	5938	5502
Independent reflections	2059	2268
Data/Restraints/Parameters	2059/0/142	2268/4/150
Range of *h, k, l*	-13/10, -13/12, -10/11	-14/9, -7/9, -13/16
Goodness-of-fit on F^2	1.01	1.05
$R[F^2 > 2\sigma(F^2)]$	0.028	0.030
$wR(F^2)$	0.066	0.087

Table S2 Selected bond lengths (Å) and bond angles (º) for complexes **2** and **4**.

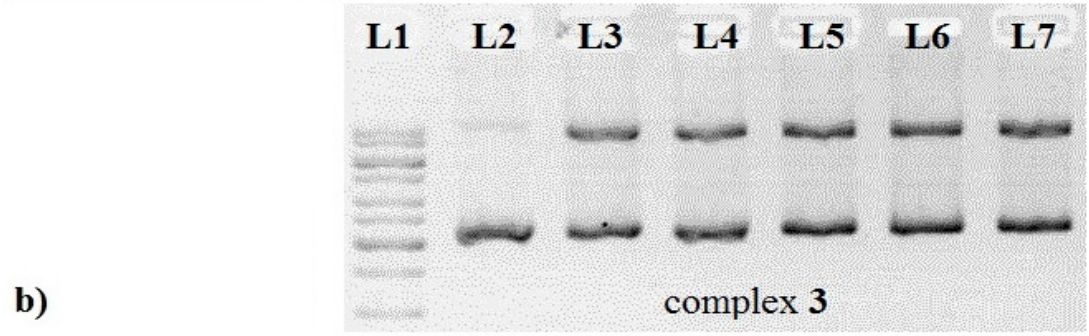
2		**4**	
Cu1-O1	1.8962 (18)	Ni1-N1	2.0778 (18)
Cu1-N1	2.008 (2)	Ni1-O1W	2.0790 (18)
O1-C1	1.312 (3)	Ni1-O2W	2.0879 (18)
N1-C7	1.296 (3)	O1-C7	1.361 (3)
N1-C8	1.472 (3)	O1-C8	1.433 (3)
Br1-C9	1.958 (3)	N1-C1	1.277 (3)
		N1-C9	1.473 (3)
O1-Cu1-O1	180.00	O1W-Ni1-O1W	180.00
O1-Cu1-N1	91.30 (8)	O1W-Ni1-O2W	93.24 (7)
O1-Cu1-N1	88.70 (8)	O1W-Ni1-O2W	86.76 (7)
N1-Cu1-N1	180.00	O2W-Ni1-O2W	180.00
C1-O1-Cu1	130.37 (16)	N1-Ni1-N1	180.00
C7-N1-Cu1	124.82 (17)	N1-Ni1-O1W	88.51 (7)
C8-N1-Cu1	119.76 (17)	N1-Ni1-O1W	91.49 (7)
		N1-Ni1-O2W	90.81 (7)
		N1-Ni1-O2W	89.19 (7)
		C7-O1-C8	118.24 (17)
		O1-C8-C9	112.4 (2)
		N1-C9-C8	112.4 (2)
		C5-C6-C7	121.1 (2)

Table S3 Hydrogen bond distances (Å) of complex **4**.

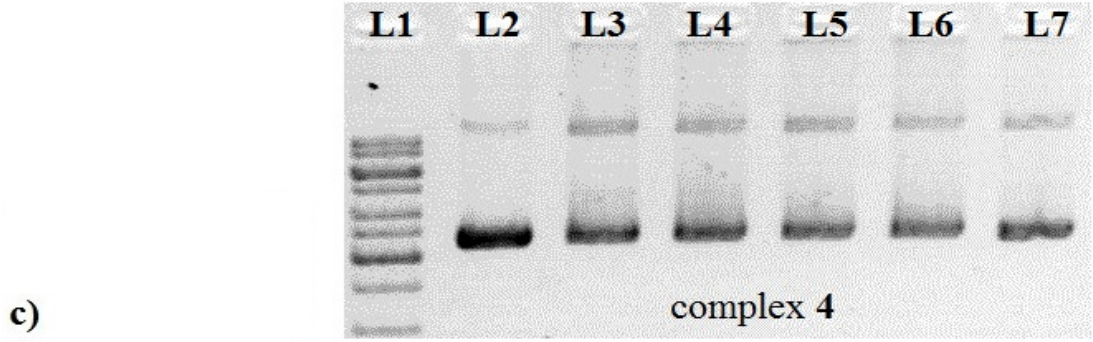
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H11···Br1	0.84 (1)	2.48 (1)	3.3134 (16)	175 (4)
O1W—H12···Br1	0.85 (1)	2.51 (2)	3.3141 (17)	158 (4)
O2W—H21···Br1	0.85 (1)	2.45 (2)	3.2721 (19)	165 (5)
O2W—H22···Br1	0.85 (1)	2.46 (1)	2.2973 (18)	168 (4)



Form/%	Form II	5.7	80.1	53.1	90.3	89.2	88.7	50.9
	Form III	-	19.9	6.8	9.7	10.8	11.3	49.1
	Form I	94.3	-	40.1	-	-	-	-

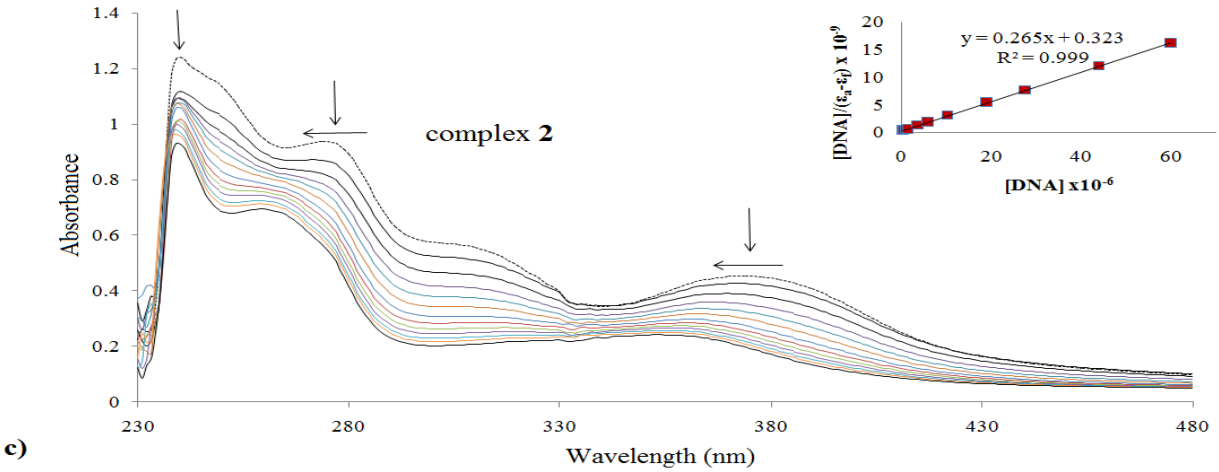


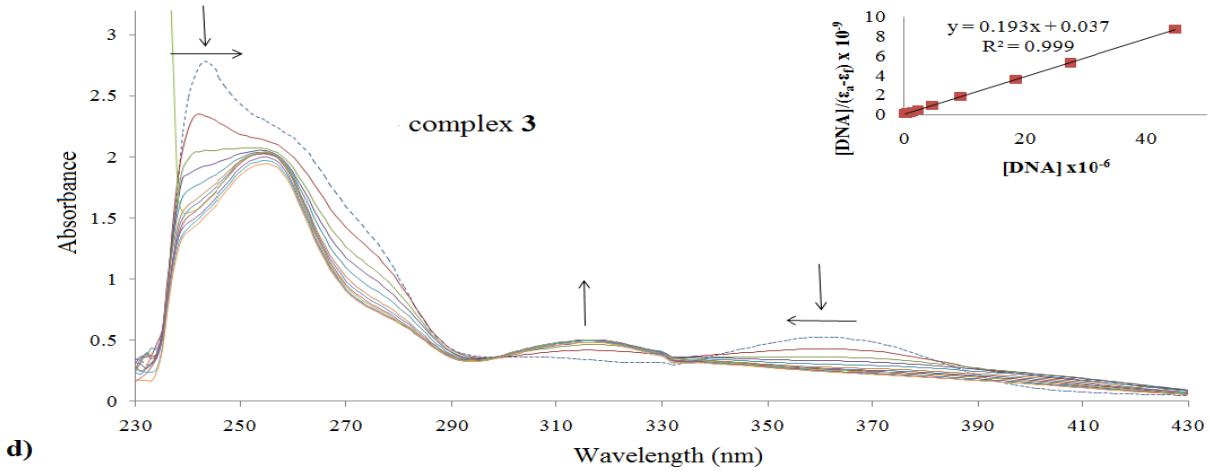
Form/%	Form II	83.6	57.5	61.4	61.8	61.9	57.1
	Form III	-	-	-	-	-	-
	Form I	16.4	42.6	38.6	38.2	38.1	42.9



Form/%	Form II	87.5	77.8	79.1	76.9	80.6	82.3
	Form III	-	-	-	-	-	-
	Form I	12.5	22.2	20.9	23.1	19.4	17.7

Fig. S1 Electrophoresis result of incubating pBR322 with radical scavengers and 160 μM of **2** (a), **3** (b), and **4** (c) in TN buffer (5 mM Tris, 50 mM NaCl) pH 7.5 at 37 ºC for 24 h. For gel a) Lane 1, Gene Ruler™ 1 kb DNA ladder; lane 2, DNA alone; lane 3, DNA+ **2**; lane 4, DNA+ 1 mM neocuprione+ **2**; lane 5, DNA+ 2 mM thiourea+ **2**; lane 6, DNA+ 2 mM sodium azide+ **2**; lane 7, DNA+ 0.5 mM DMSO+ **2**; lane 8, DNA+ 1 mM tiron+ **2**. For gels b) and c) Lane 1, Gene Ruler™ 1 kb DNA ladder; lane 2, DNA alone; lane 3, DNA+ **3** or **4**; lane 4, DNA+ 2 mM thiourea+ **3** or **4**; lane 5, DNA+ 2 mM sodium azide+ **3** or **4**; lane 6, DNA+ 0.5 mM DMSO+ **3** or **4**; lane 7, DNA+ 1 mM tiron+ **3** or **4**.





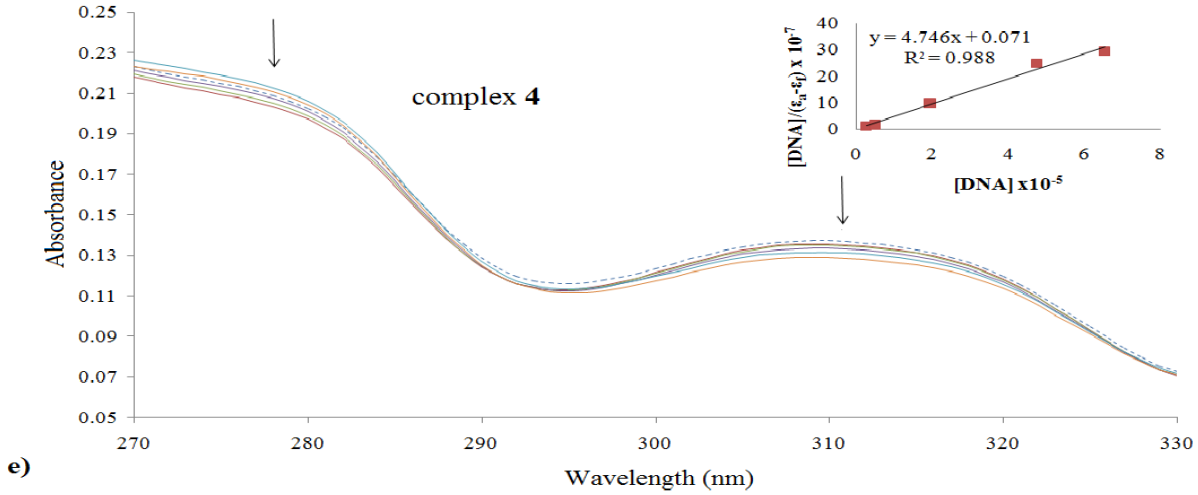


Fig. S2 UV-Vis absorption spectra of complexes **2** (c), **3** (d), and **4** (e) in TN buffer pH 7.5, in the absence (dashed line) and presence (solid line) of CT-DNA with increasing concentrations. Arrows show the change in absorbance with increasing DNA concentration. The insets represent the K_b calculation plots for the spectra changes at 373 nm, 361 nm, and 309 nm of complexes **2**, **3**, and **4** respectively.

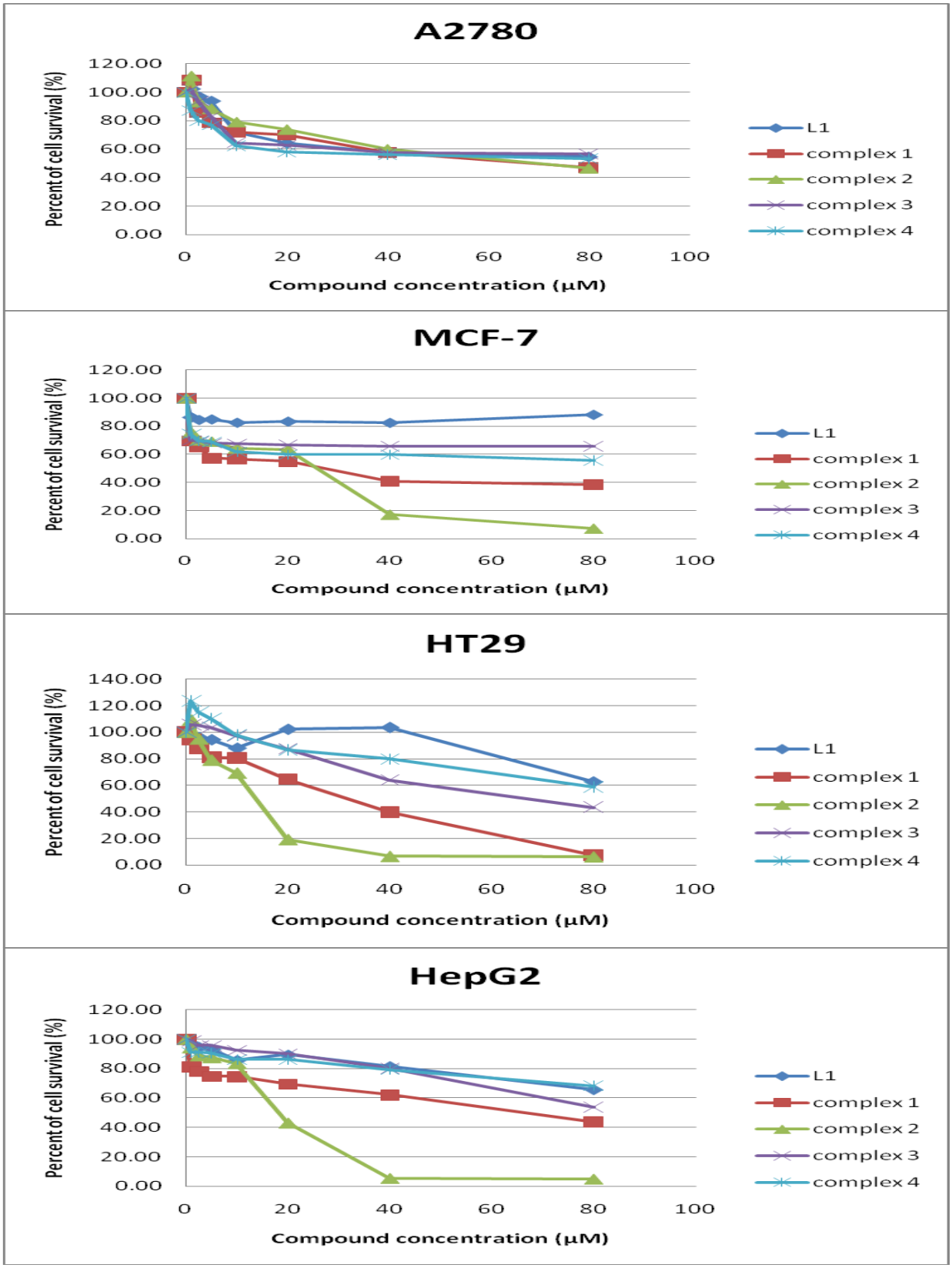


Fig. S3 A2780, MCF-7, HT29, and HepG2 cells survival in the presence of increasing concentration of **L1** and complexes **1-4**

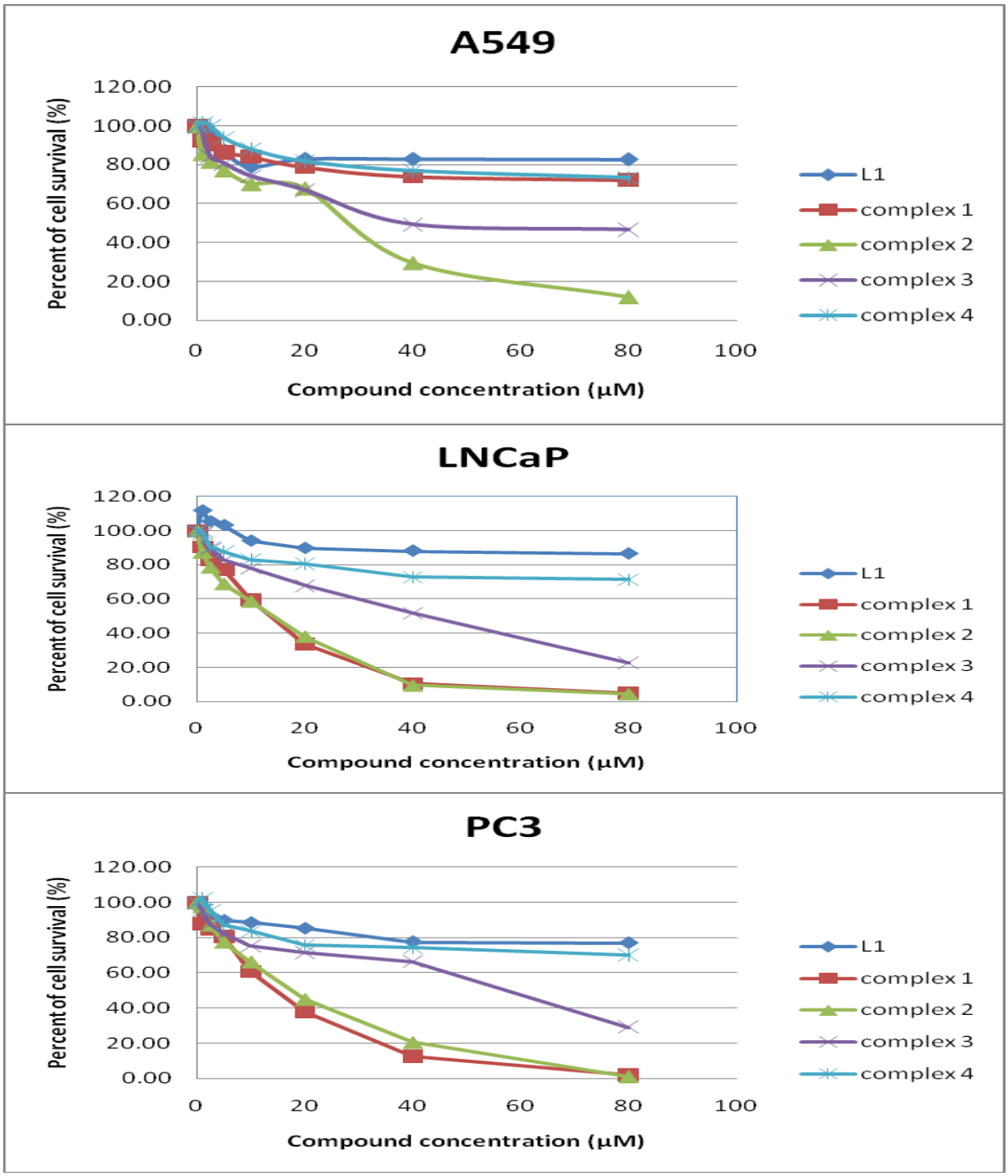


Fig. S4 A549, LNCaP, and PC3 cells survival in the presence of increasing concentration of **L1** and complexes **1-4**