

Supplementary materials

New cobalt (II) Complexes with Imidazole Derivatives Developed as Effective Antimicrobial and Antitumor Species

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Table S1. Selected angles (°) in (1)-(3).

(1)			(2)			(3)					
O(3)	Co(1)	O(1)	106.14(11)	O(5)	Co(1)	O(1)	106.23(14)	N(3)	Co(1)	C(1A)	97.19(12)
N(3)	Co(1)	O(1)	92.87(12)	N(2)	Co(1)	O(1)	115.97(15)	N(2)	Co(1)	C(1A)	133.93(14)
N(3)	Co(1)	O(3)	113.21(12)	N(2)	Co(1)	O(5)	103.02(14)	N(2)	Co(1)	N(3)	99.81(13)
N(1)	Co(1)	O(1)	111.55(13)	N(1)	Co(1)	O(1)	114.02(16)	O(1)	Co(1)	C(1A)	114.13(12)
N(1)	Co(1)	O(3)	120.51(12)	N(1)	Co(1)	O(5)	100.37(15)	O(1)	Co(1)	N(3)	103.37(12)
N(1)	Co(1)	N(3)	109.05(13)	N(1)	Co(1)	N(2)	114.77(17)	O(1)	Co(1)	N(2)	103.02(13)
								O(3)	Co(1)	C(1A)	29.67(11)
								O(3)	Co(1)	N(3)	102.88(12)
								O(3)	Co(1)	N(2)	104.44(13)
								O(3)	Co(1)	O(1)	137.73(11)
								O(4)	Co(1)	C(1A)	29.19(11)
								O(4)	Co(1)	N(3)	89.35(11)
								O(4)	Co(1)	N(2)	162.65(12)
								O(4)	Co(1)	O(1)	88.97(10)
								O(4)	Co(1)	O(3)	58.86(10)
								O(2)	Co(1)	C(1A)	85.25(11)
								O(2)	Co(1)	N(3)	160.44(12)
								O(2)	Co(1)	N(2)	92.16(12)
								O(2)	Co(1)	O(1)	58.53(10)
								O(2)	Co(1)	O(3)	88.86(10)
								O(2)	Co(1)	O(4)	83.37(10)

	N(11) Co(3)	N(10)	105.42(14)
	O(12) Co(3)	N(10)	103.76(14)
	O(12) Co(3)	N(11)	102.41(13)
	O(9) Co(3)	N(10)	97.40(13)
	O(9) Co(3)	N(11)	104.84(14)
	O(9) Co(3)	O(12)	139.35(15)
	N(7) Co(2)	N(6)	100.31(14)
	O(5) Co(2)	N(6)	102.57(13)
	O(5) Co(2)	N(7)	110.79(14)
	O(7) Co(2)	N(6)	110.42(13)
	O(7) Co(2)	N(7)	100.76(13)
	O(7) Co(2)	O(5)	128.74(13)

Table S2. Continuous Shape Measures for the coordination polyhedron around the Co(II) atom.

Geometry	Co1 (compound 1)	Co1 (compound 2)	Co3 (compound 3)
PP-5	30.990	34.297	30.063
vOC-5	7.796	8.032	4.109
TBPY-5	3.318	3.020	5.782
SPY-5	5.643	5.918	3.225
JTBPY-5	4.249	3.820	6.493

Geometry	Co1 (compound 3)
HP-6	29.330
PPY-6	23.830
OC-6	4.345
TPR-6	12.152
JPPY-6	26.949

Geometry	Co2 (compound 3)
SP-4	30.034
T-4	0.905
SS-4	5.744
vTBPY-4	2.774

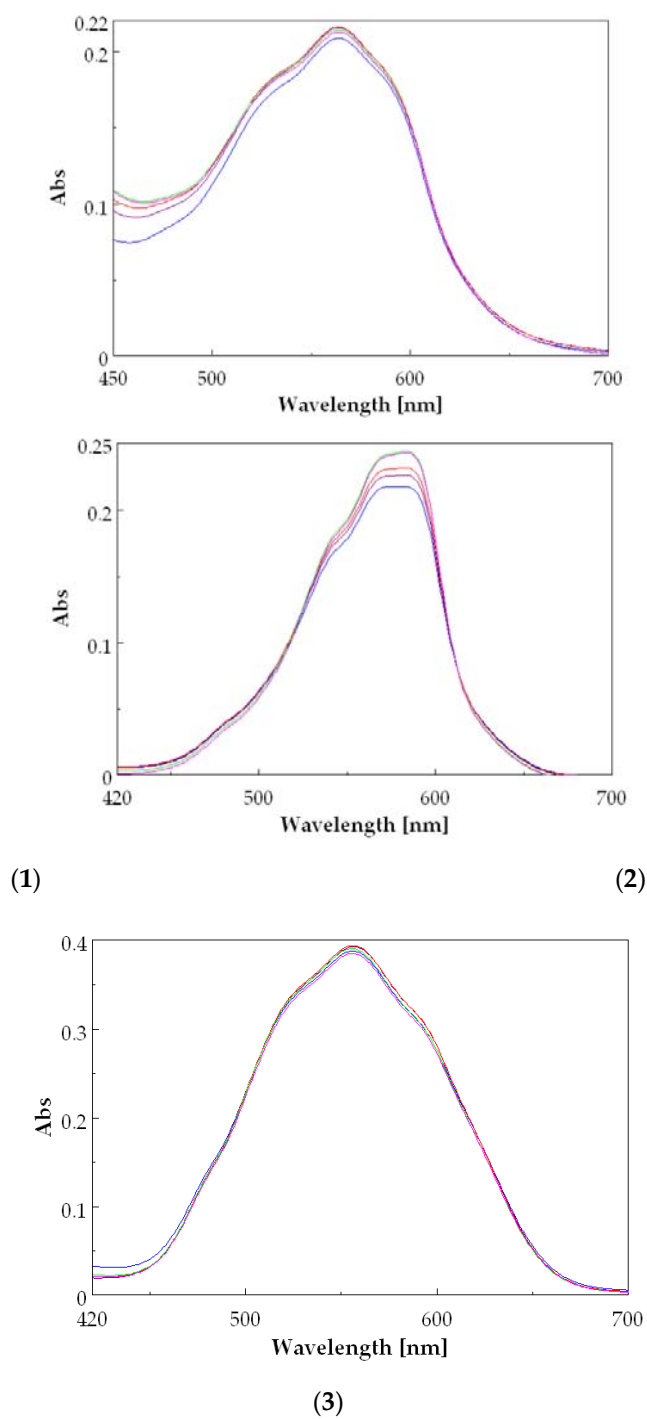


Figure S1. UV-Vis spectra in DMSO solution of complexes (1)-(3): (blue – 0 min, purple – 6 h, red – 12 h, green – 24 h, magenta -48h).

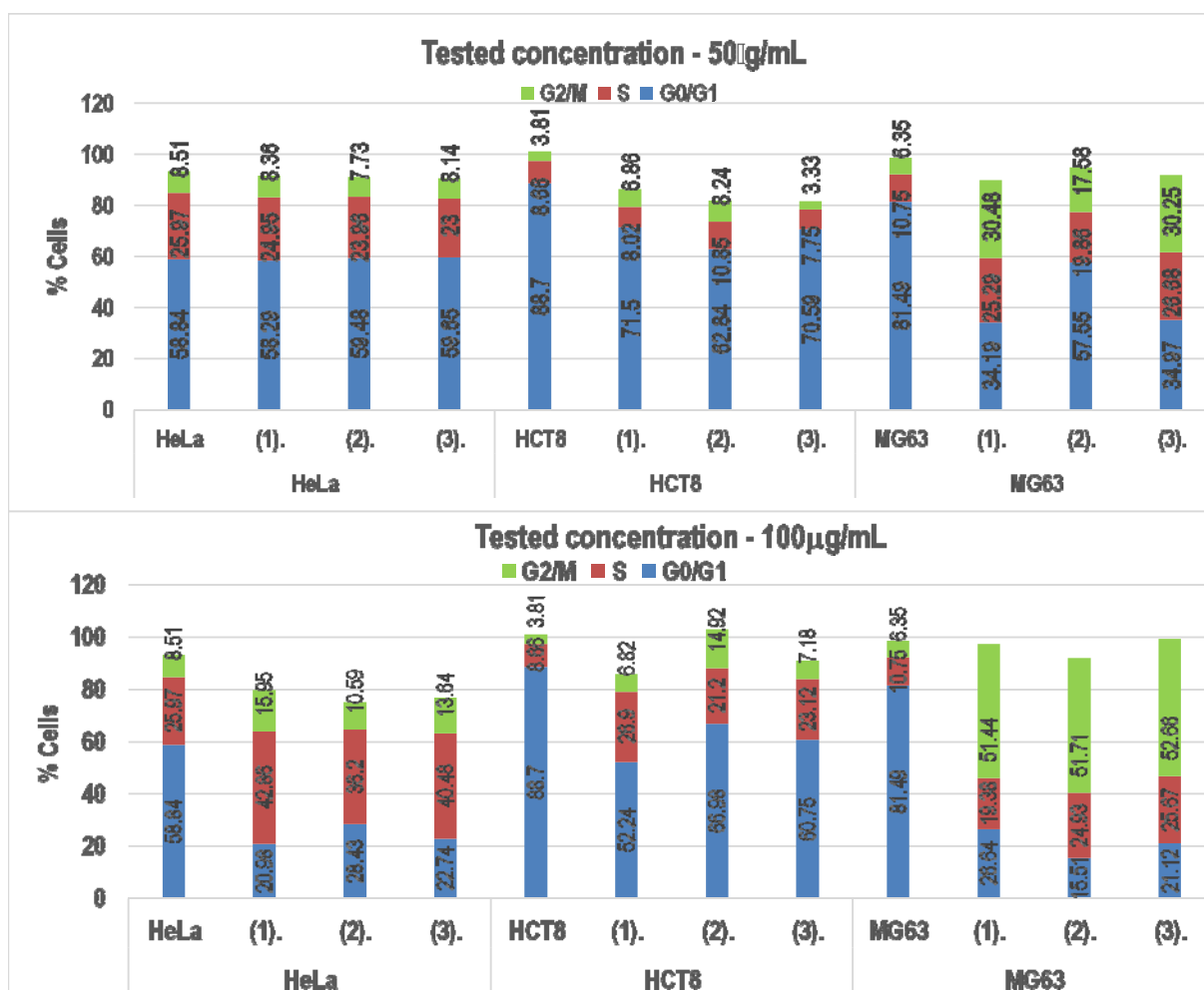


Figure S2. Effect of complexes (1) - (3) on cell cycle phases in HeLa, HCT8 and MG63 cells. The results are presented as percent of cells in different phases of the cell cycle.