

Cytotoxic effects of gold(I) complexes against colon, cervical and osteo carcinoma cell lines: A mechanistic approach

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Supplementary materials

Table 1S. Mid FT-IR frequencies (cm⁻¹) of free ligand and Au(I) complexes (**0-2**).

Ligand/ Complex	Stretch NH							Stretch C=S
[Au(Ipr)Cl]	-	3073	1109	2960	1366	1258	1462	-
Tu	3405, 3274	-	-	-	-	1616	1468	1080
1	3471, 3369	3166	1059	2963, 2869	1466	1630	1466	842
Me₂Tu	3267	-	-	-	1444	1525	-	1040
2	3377	3162	1133	2931, 2873	1371	1571	1462	985

Table 2S. ¹H NMR chemical shifts (ppm) for free ligands and gold(I) complexes (**0-2**) in CDCl₃.

Ligand/complex	H-3	H-4	H-5	H-6	H-7	H-8	H-9	N-H
[Au(Ipr)Cl](0)	7.39 d	7.55 t	2.46 m	1.33 d	1.21 d	7.98 s	-	-
1	7.36 d	7.62 t	2.49 m	1.30 d	1.24 d	6.91 s	-	7.28
2	7.35 d	7.52 t	2.50 m	1.26 d	1.21 d	7.84 s	2.80 s	8.16
Tu	-	-	-	-	-	-	-	6.81
Me₂Tu	-	-	-	-	-	-	2.81 s	6.62

Table 3S. ¹³C NMR chemical shifts (ppm) for free ligands and gold(I) complexes (**0-2**) in CDCl₃.

Ligand/ Complex	C1	C2	C3	C4	C5	C6	C7	C8	Au=C	C=S	C11
[Au(Ipr)Cl](0)	145.5	133.9	123.0	130.7	28.8	24.5	24.0	124.2	175.3	-	-
1	145.3	133.1	123.7	129.8	28.1	23.8	23.3	-	180.7	177.0	-
2	145.9	133.3	124.0	131.1	28.8	24.5	23.9	124.4	181.1	176.4	32.3
Tu	-	-	-	-	-	-	-	-	-	185.5	-
Me₂Tu	-	-	-	-	-	-	-	-	-	182.3	30.8

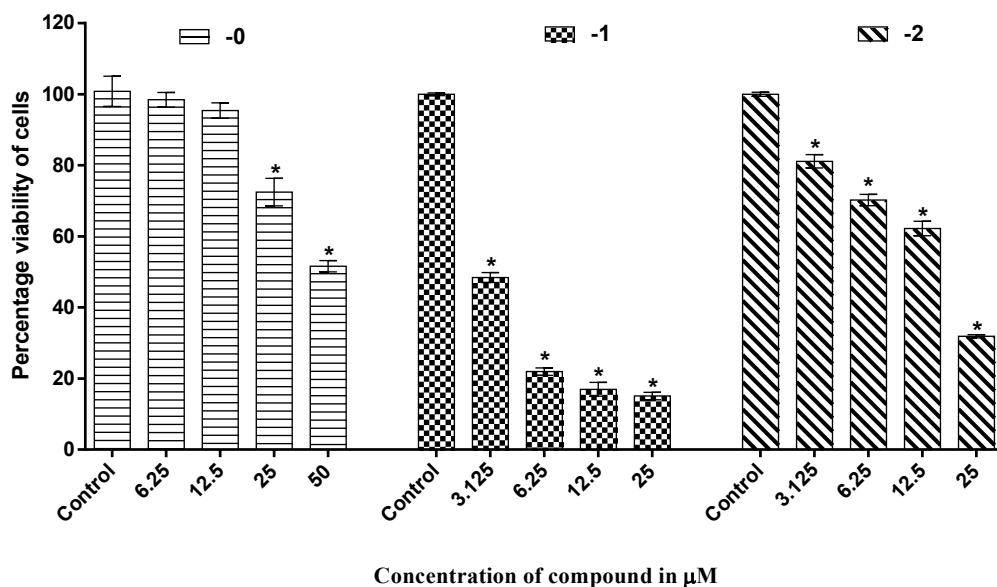
Table 4S. Selected bond lengths and bond angles for complexes **1** and **2**.

Bond Length (Å)		Bond Angles (°)	
Complex 1			
Au1—S1	2.3024(13)	C1—Au1—S1	177.12 (12)
Au1—C1	1.995 (4)	C28—S1—Au1	103.6 (2)
S1—C28	1.706 (6)	N3—C28—N4	118.6 (6)
N3—C28	1.320 (9)	S1—C28— N3	123.0 (4)
N4—C28	1.321 (7)	S1—C28— N4	118.40 (4)
Complex 2			
Au1—S1	2.2977(7)	C4—Au1—S1	176.40 (7)
Au1—C4	2.007 (2)	Au1—S1—C1	105.79 (10)
S1—C1	1.724 (3)	N1—C1—N2	119.20 (3)
N1—C1	1.326 (4)	S1—C1— N1	122.40 (2)
N2—C1	1.322 (4)	S1—C1— N2	118.40 (2)

Table 5S. Summary of crystal data and details of the structure refinement for complex **1** and **2**.

Complex	1	2
Empirical formula	C ₂₈ H ₄₀ AuF ₆ N ₄ PS	C ₃₀ H ₄₄ AuF ₆ N ₄ PS
Formula weight	806.63	834.69
Crystal symmetry	Monoclinic	Monoclinic
Space group	P 2 ₁ /n	P 2 ₁ /c
Crystal color	Colorless	Colorless
Crystal size / mm	0.65 × 0.39 × 0.20	0.40 × 0.32 × 0.20
Wavelength/Å	0.71073	0.71073
Temperature/K	298	173
a (Å)	9.2495(8)	8.6566 (2)
b (Å)	15.474(14)	23.5651 (9)
c (Å)	23.370(2)	17.3653 (5)
β (°)	96.419(2)	98.966 (2)
Cell volume (Å ³)	3324.0(5)	3499.1 (2)
<i>D</i> _x (g m ⁻³)	1.612	1.686
<i>μ</i> (mm ⁻¹)	4.594	4.37
<i>Z</i>	4	4
<i>θ</i> range (°)	1.754 - 28.296	1.468 - 25.642
<i>h, k, l</i> limits	-7:12, -20:20, -31:31	-10:10, -28:28, -21:21
<i>Reflns: Total, uniq., Rint</i>	23485, 8236, 0.0320	47989, 6605, 0.0417
<i>Data/restraints/parameters</i>	8236 / 66 / 396	6605 / 2 / 449
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.051, 0.160, 1.07	0.020, 0.047, 1.01
<i>Δρ</i> _{max} , <i>Δρ</i> _{min} (e Å ⁻³)	2.09, -3.31	0.90, -0.58

MG-63



MG-63

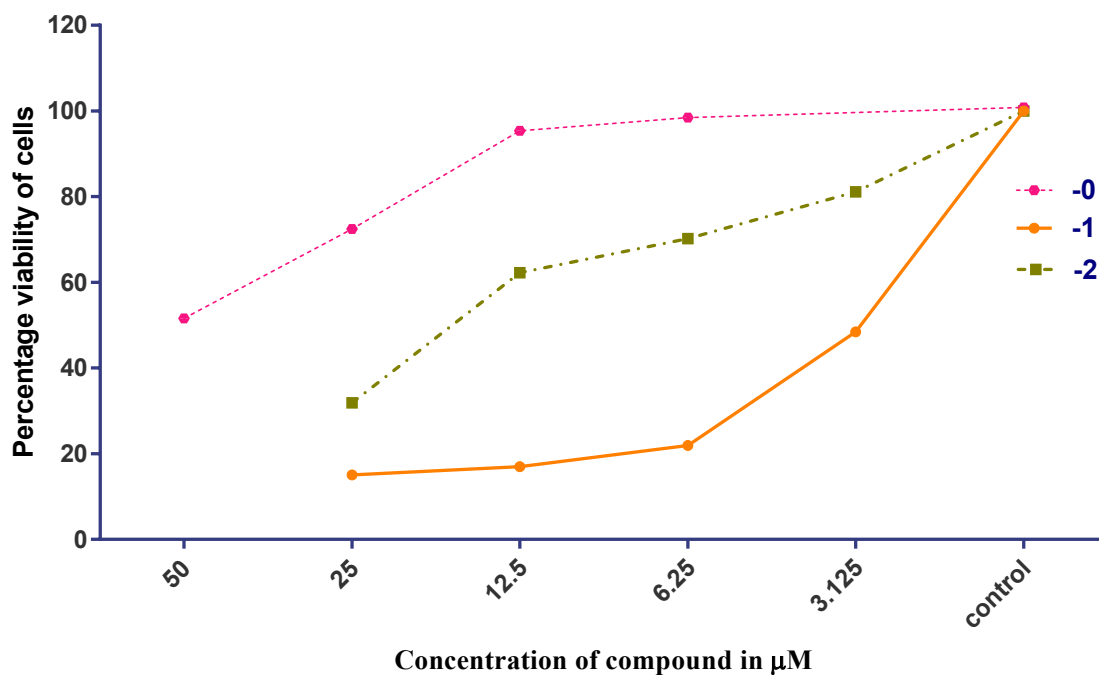


Fig. 1S Graph of cytotoxic effect of series complexes (*0-2*) concentrations on cell viability of MG-63 cell line. "*" represents a statistically significant difference between the various concentrations and respective control groups of the gold complexes. For the comparison of significance between groups, Sidak's multiple comparison test was used according to the GraphPad Prism v6.05. The values having $p < 0.05$ are considered significant.

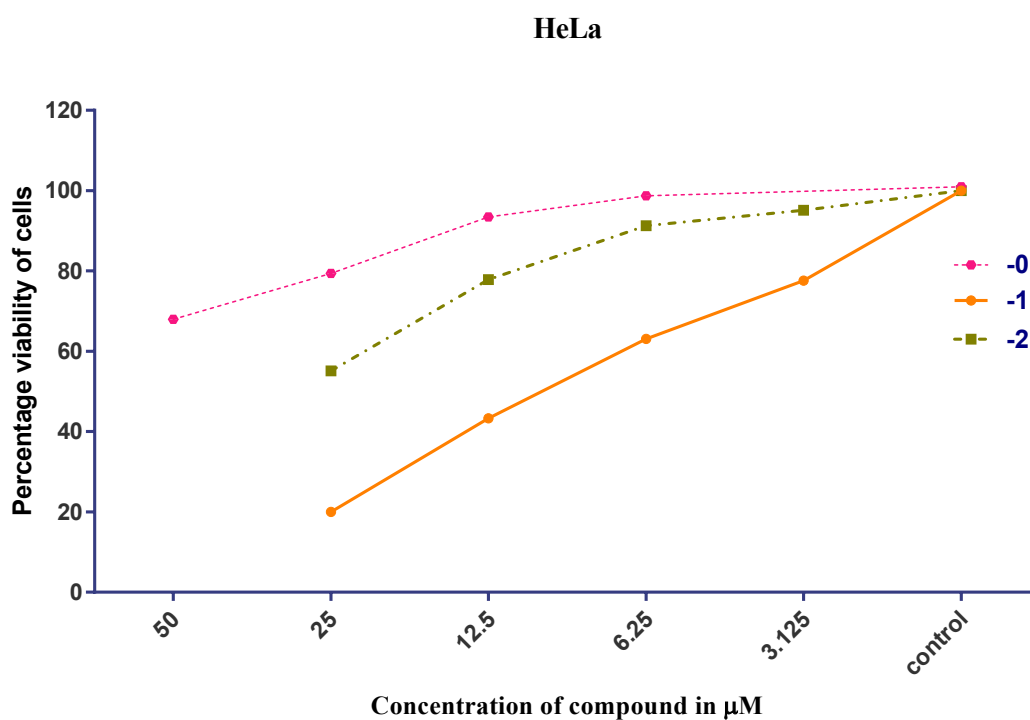
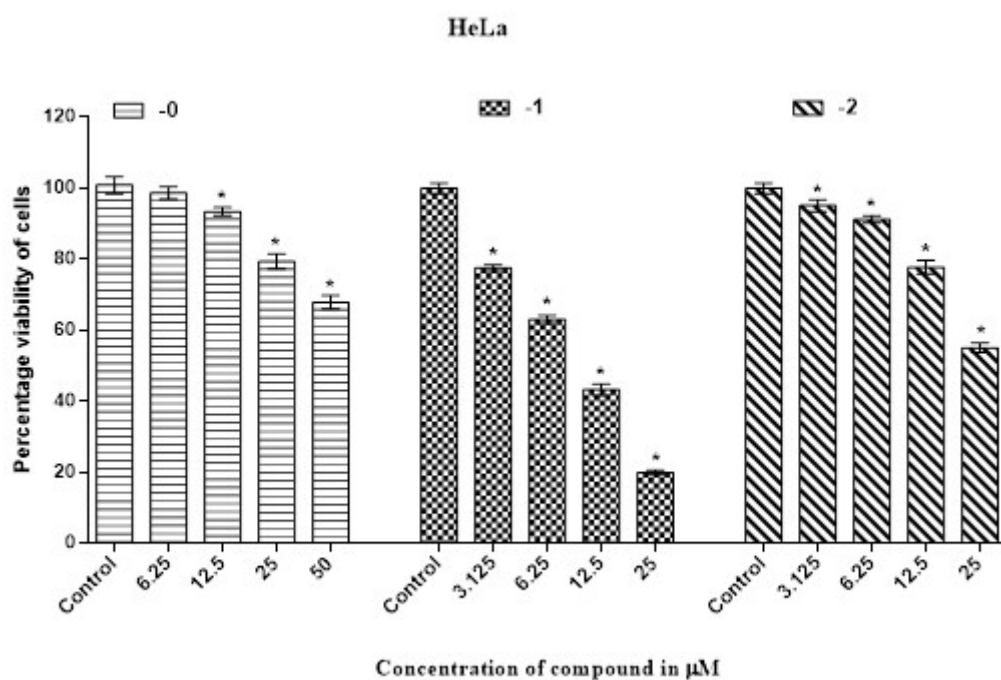


Fig. 2S In vitro cytotoxic effect of series complexes (**0-2**) concentrations on cell viability of HeLa cell line. "*" represents a statistically significant difference between the various concentrations and respective control groups of the gold complexes. For the comparison of significance between groups, Sidak's multiple comparison test was used according to the GraphPad Prism v6.05. The values having $p < 0.05$ are considered significant.