Supporting Information

Antitumor Properties and Mechanisms of Mitochondria-Targeted Ag(I) and Au(I) Complexes Containing N-heterocyclic Carbenes Derived from Cyclophanes

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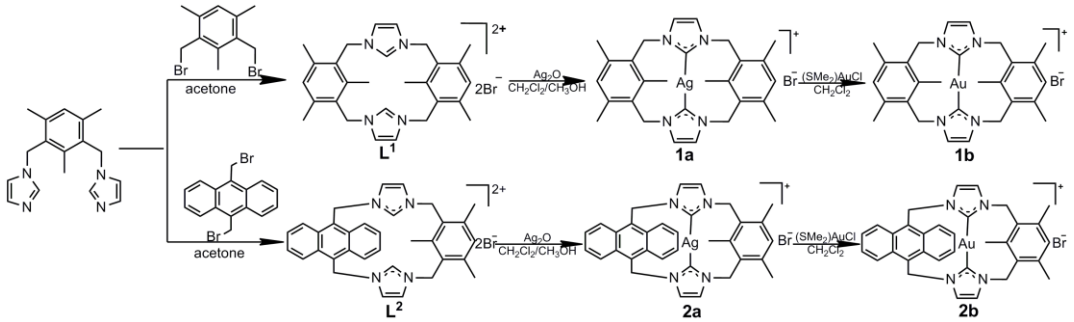

Scheme S1. Synthesis of NHC complexes **1a-b** and **2a-b.**

Table S1. Crystallographic data of complexes **1a'**, **1b'** and ligands $\mathbf{L^{1\prime}}$, $\mathbf{L^{2\prime}}$.

Compound	**1a'**	**1b'**	$\mathbf{L^{1\prime}}$	$\mathbf{L^{2\prime}}$
CDCC no.	980884	980885	980882	980883
Empirical formula	$C_{28}H_{32}AgF_6N_4P{\bullet}CH_3CN$	$C_{28}H_{32}AuF_6N_4P{\bullet}CH_3CN$	$C_{28}H_{34}F_{12}N_4P_2$	$C_{33}H_{32}F_{12}N_4P_2{\bullet}3CH_3CN$
Molecular weight	717.46	807.57	716.53	897.73
Description	Block, colourless	Block, colourless	Block, colourless	Block, colourless
Temperature (K)	293(2)	150(2)	150(2)	150(2)
Crystal size (mm)	0.50 × 0.40 × 0.40	0.20 × 0.16 × 0.14	0.18 × 0.14 × 0.13	0.23× 0.19 × 0.17
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic
Space group	Ibam	Ibam	P21/c	P21/n
a (Å)	17.9559(7)	18.7883(10)	8.6600(5)	12.9199(9)
b (Å)	18.8882(7)	17.8671(8)	19.8775(10)	15.8918(8)
c (Å)	17.9394(7)	18.1775(7)	11.7276(5)	20.2181(11)
α (°)	90.00	90.00	90.00	90.00
β (°)	90.00	90.00	130.999(3)	95.307(2)
γ (°)	90.00	90.00	90.00	90.00
Volume, Å	6084.2(4)	6102.0(5)	1523.61(13)	4133.4(4)
Z	8	8	2	4
Absorption coefficient (mm^{-1})	0.781	4.940	0.244	0.198
F(000)	2920	3184	736	1848
θ range (deg)	3.13-27.48	3.12-27.47	3.08/27.47	3.01-27.48
Completeness to θ_{max}	0.986	0.987	0.974	0.965
Density (calcd) (mg/m^{-3})	1.567	1.758	1.562	1.443
Reflections collected/unique	12864/3565	11507/3570	10629/3398	13658
Final R indices[I > 2σ(I)]	R1=0.0474	R1=0.0547	R1=0.0683	R1=0.1126
	wR2=0.1359	wR2=0.1377	wR2=0.1537	wR2=0.2048
R indices (all data)	R1=0.0504	R1=0.0616,	R1=0.0535	R1=0.0727
	wR2=0.1423	wR2=0.1432	wR2=0.1428	wR2=0.1815
GOF	1.132	1.035	1.050	1.068

Table S2. Selected bond lengths (Å) and bond angles (deg) of **1a'** and **1b'**.

Complexes	**1a'**		**1b'**	
bond lengths (Å)	Ag1-C1	2.113(4)	Au1-C13	2.062(8)
	Ag1-C2	2.111(4)	Au1-C15	2.075(8)
bond angles (deg)	C2 - Ag1 - C1	178.04(18)	C13-Au1-C15	179.4(3)
	N1 - C1 - Ag1	127.65(18)	N1-C1-Au1	127.6(4)
	N2 - C2 - Ag1	127.97(18)	N2-C15-Au1	126.9(4)

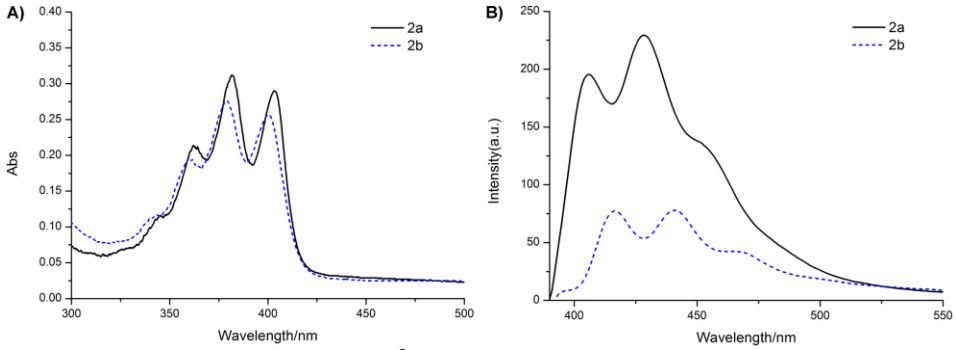

Fig. S1 (A) UV/Vis spectra of complexes **2a** and **2b** ($5*10^{-5}$ M) measured in CH_3OH at 298 K. (B) Emission spectra of complexes **2a** and **2b** ($5*10^{-5}$ M) measured in CH_3OH at 298 K. (λ_{ex} = 380 nm).

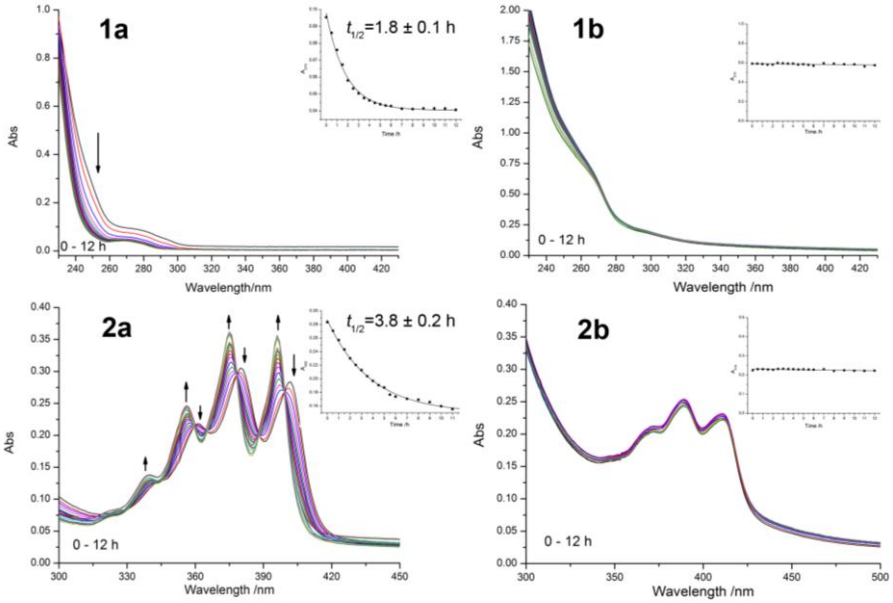

Fig. S2 Time-dependent UV/Vis absorption spectra of **1-2** ($5*10^{-5}$ M) measured in 100 mM NaCl solution. Insets: plots of the changes in absorbance at the indicated wavelengths against time. **1a**, 270 nm; **1b**, 270nm; **2a**, 402 nm; **2b**, 410 nm.

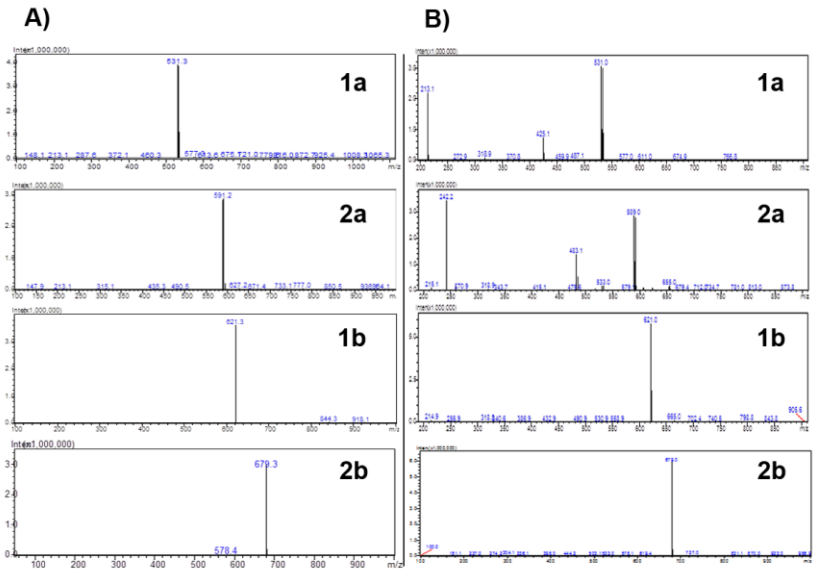

Fig. S3 ESI-MS spectra of complexes in H_2O (0.25%DMSO for: A) 0 h and B) 48 h.

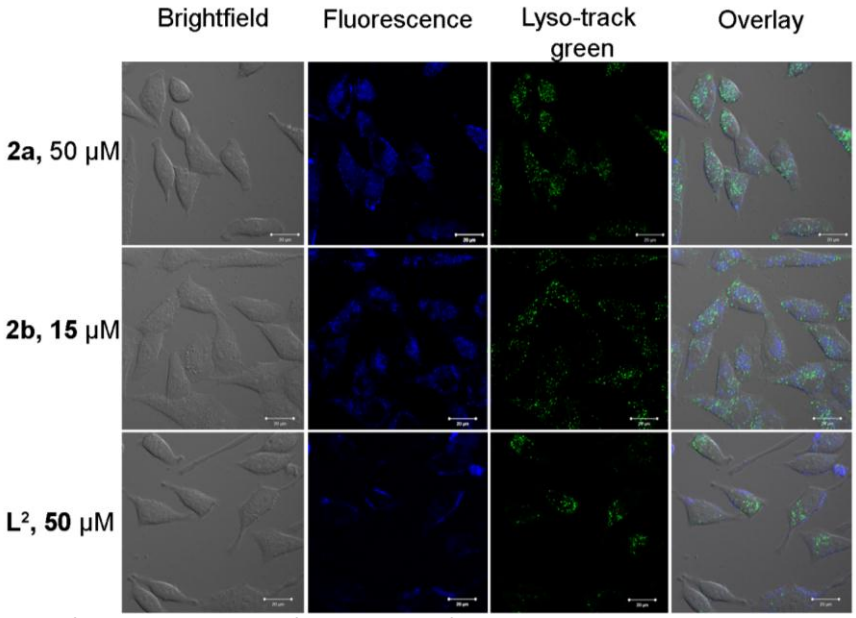

Fig. S4 Determination of intercellular localization of compound by confocal microscopy (63 × oil-immersion objective lens). **2a**, **2b** and $\mathbf{L}^2$ were excited at 405 nm (blue). Lyso-tracker green was excited at 488 nm (green).

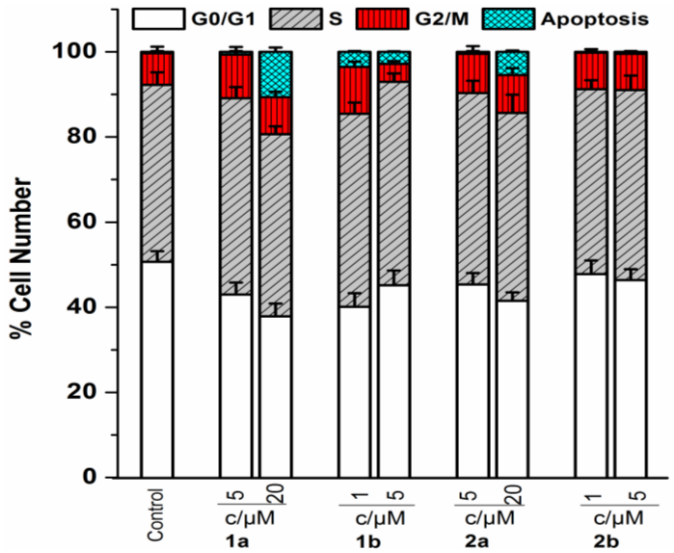

Fig. S5 Cell-cycle analysis of HeLa cells treated with DMSO alone or **1-2** at different concentrations for 24 h before exposure to PI and analysis by flow cytometry. Cell populations were determined and are expressed as the percentage of cells in the indicated cell-cycle phases.