Supporting Information For

Synthesis, characterization and biological evaluation of mixed-ligand ruthenium(II) complexes forphotodynamic therapy

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Content

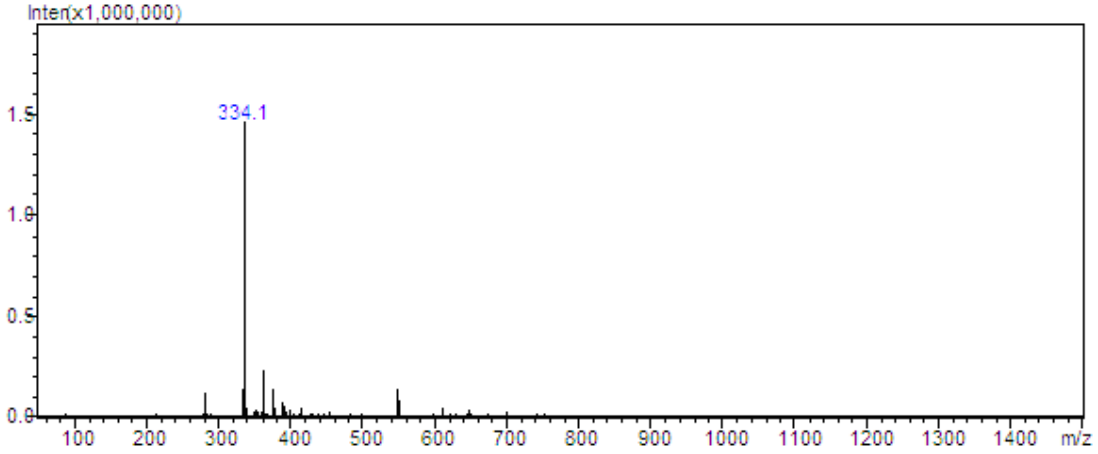

Figure S1 ES-MS ($CHCl_3$) spectrum of ligand dpe.

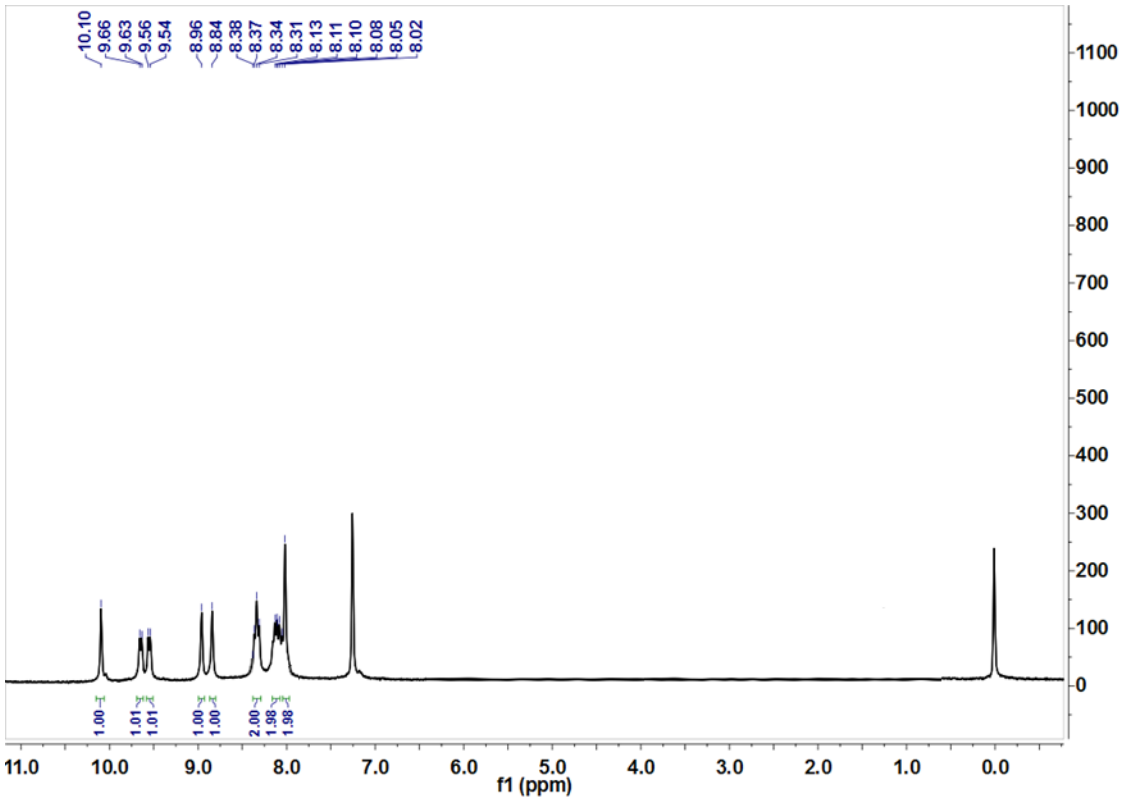

Figure S2 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of ligand dpe.

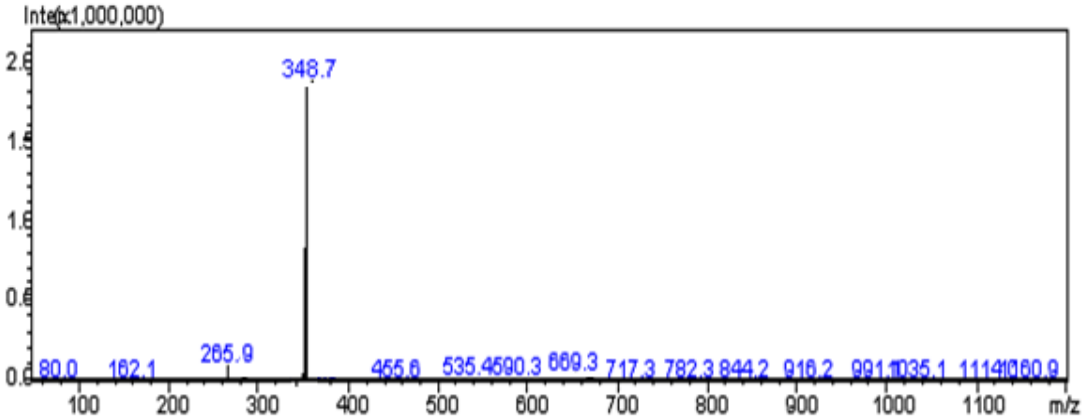

Figure S3 ES-MS (CH_3CN) spectrum of **Ru1**.

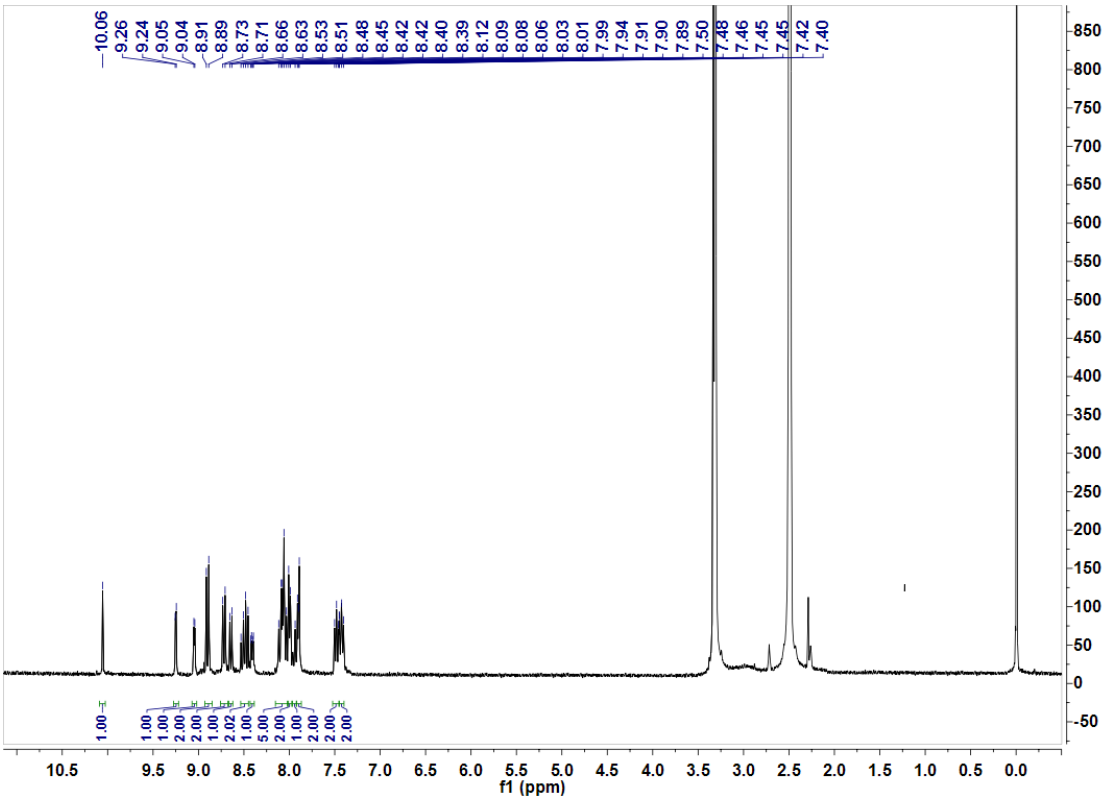

Figure S4 ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of **Ru1**.

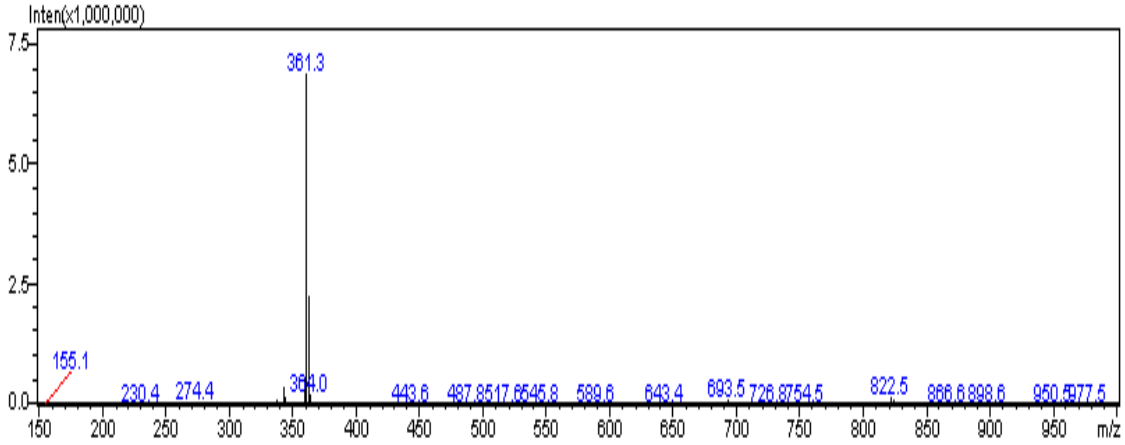

Figure S5 ES-MS (CH_3CN) spectrum of **Ru2**.

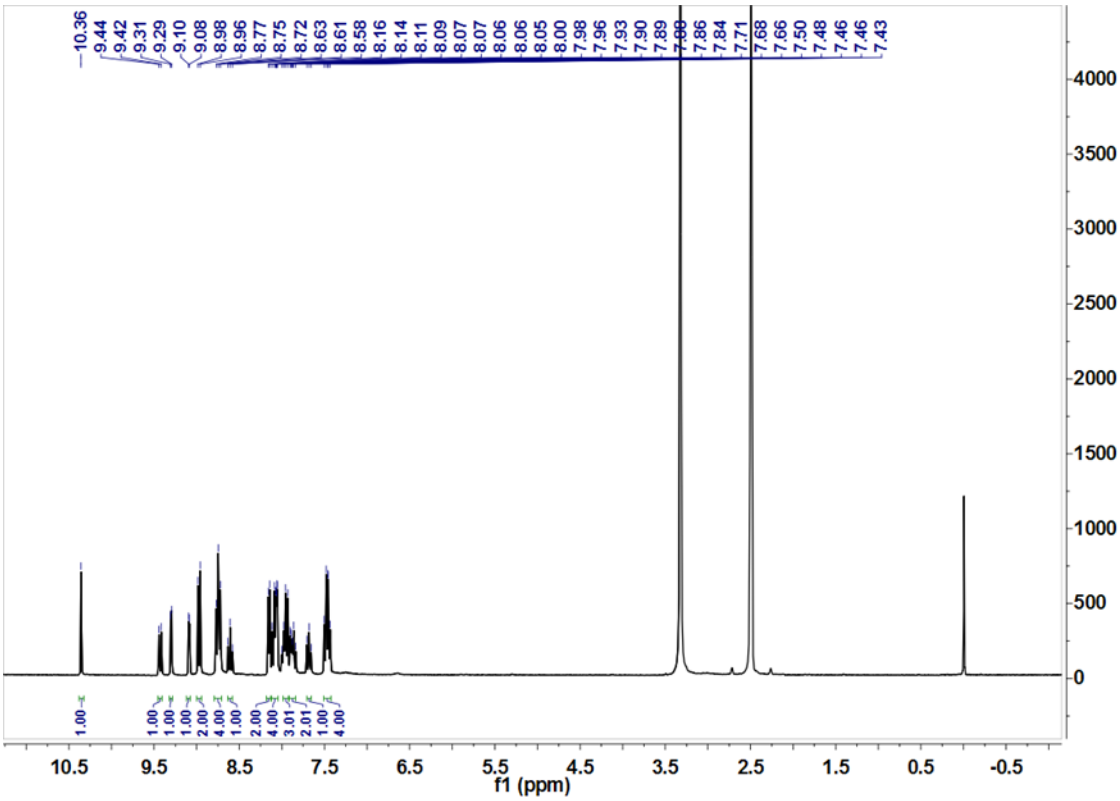

Figure S6 ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of **Ru2**.

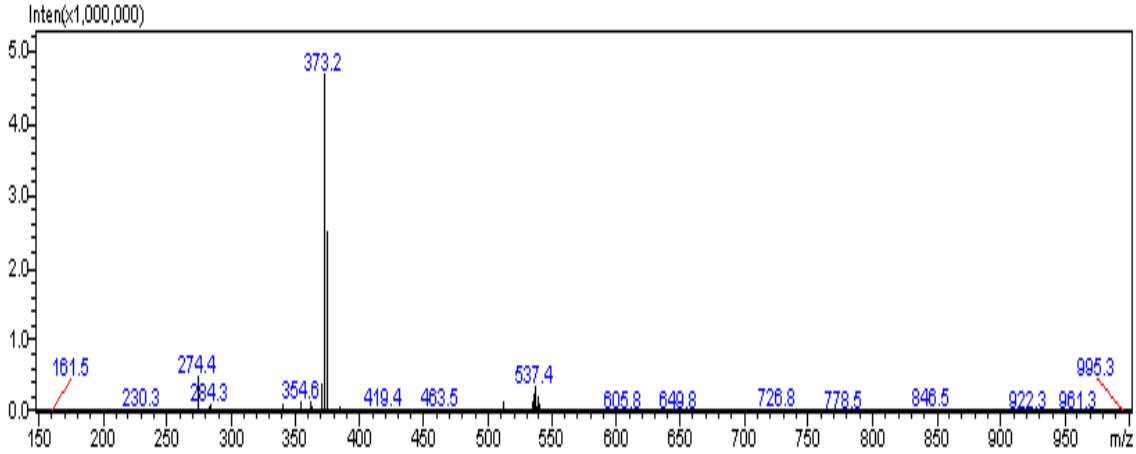

Figure S7 ES-MS (CH_3CN) spectrum of **Ru3**.

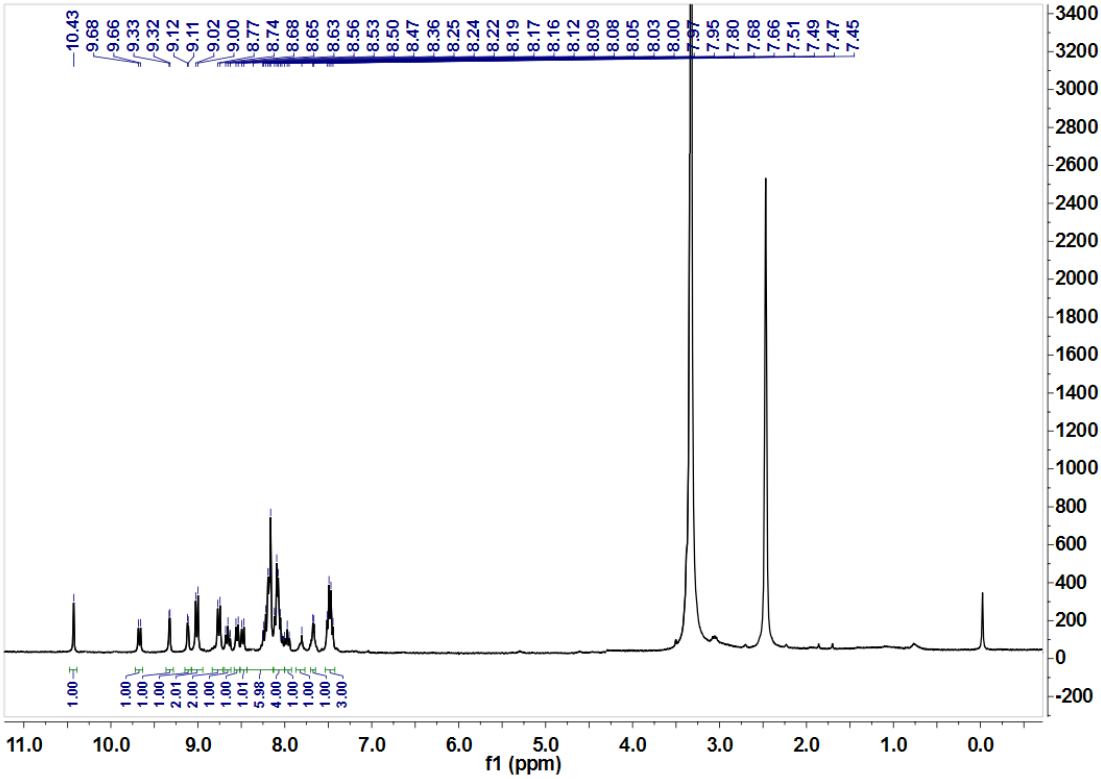

Figure S8 ^{1}H NMR spectrum (300 MHz, DMSO-d_6) of **Ru3**.

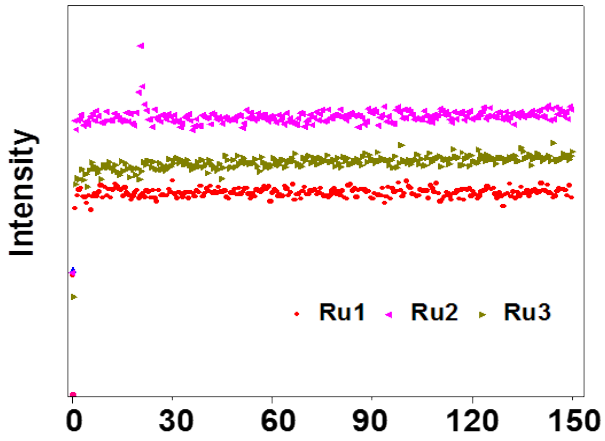

Figure S9 Photostability of **Ru1-Ru3** under continuous irradiation.

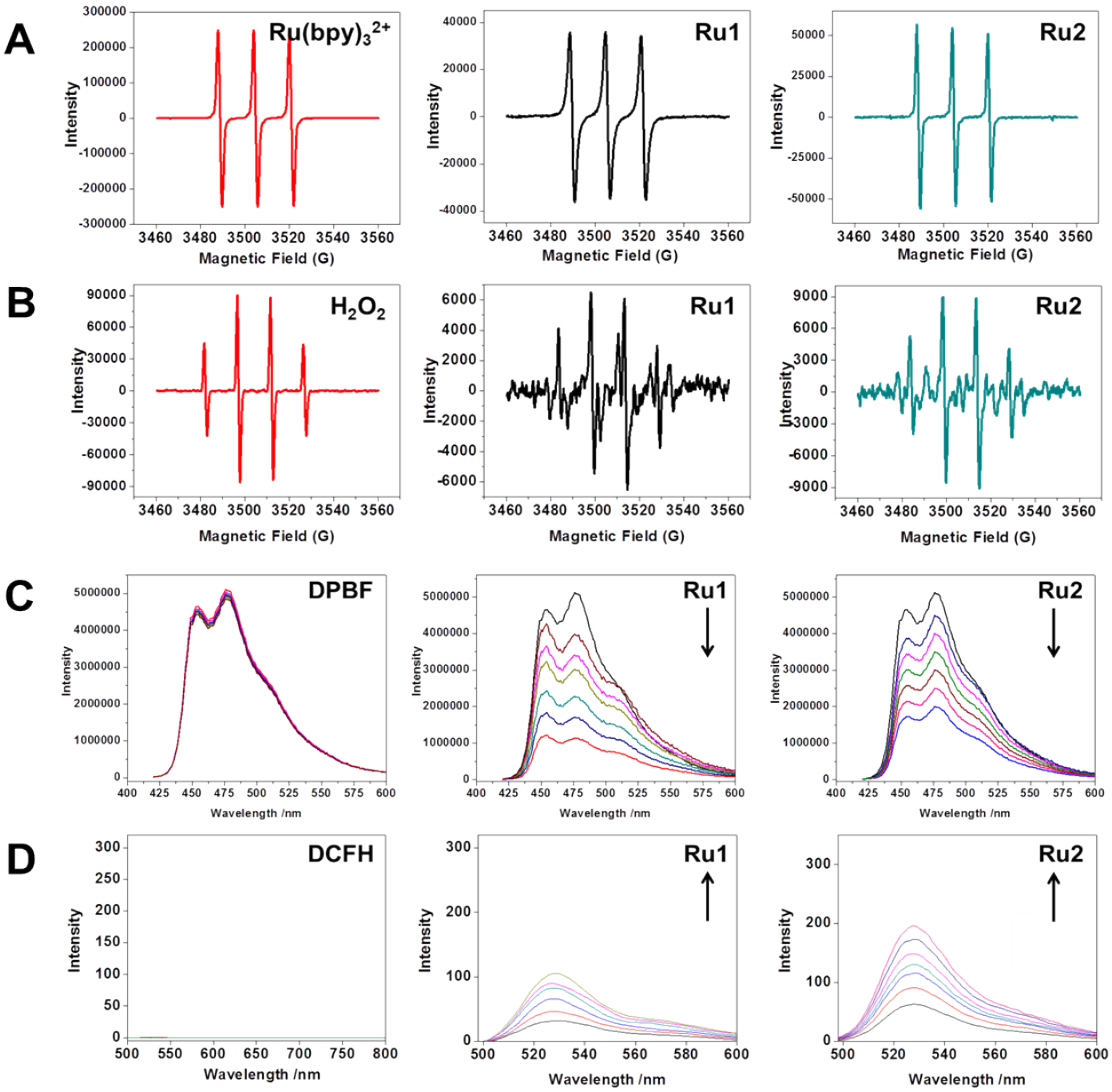

Figure S10 (A) ESR signals of $[Ru(bpy)_3]^{2+}$ and **Ru1** and **Ru2** trapped by TEMP. (B) ESR signals of H_2O_2 and **Ru1** and **Ru2**trapped by DMPO. (C) Emission spectra of DPBF–**Ru1** and DPBF–**Ru2**. (D) Emission spectra changes of DCFH–**Ru1** and DCFH–**Ru2**.

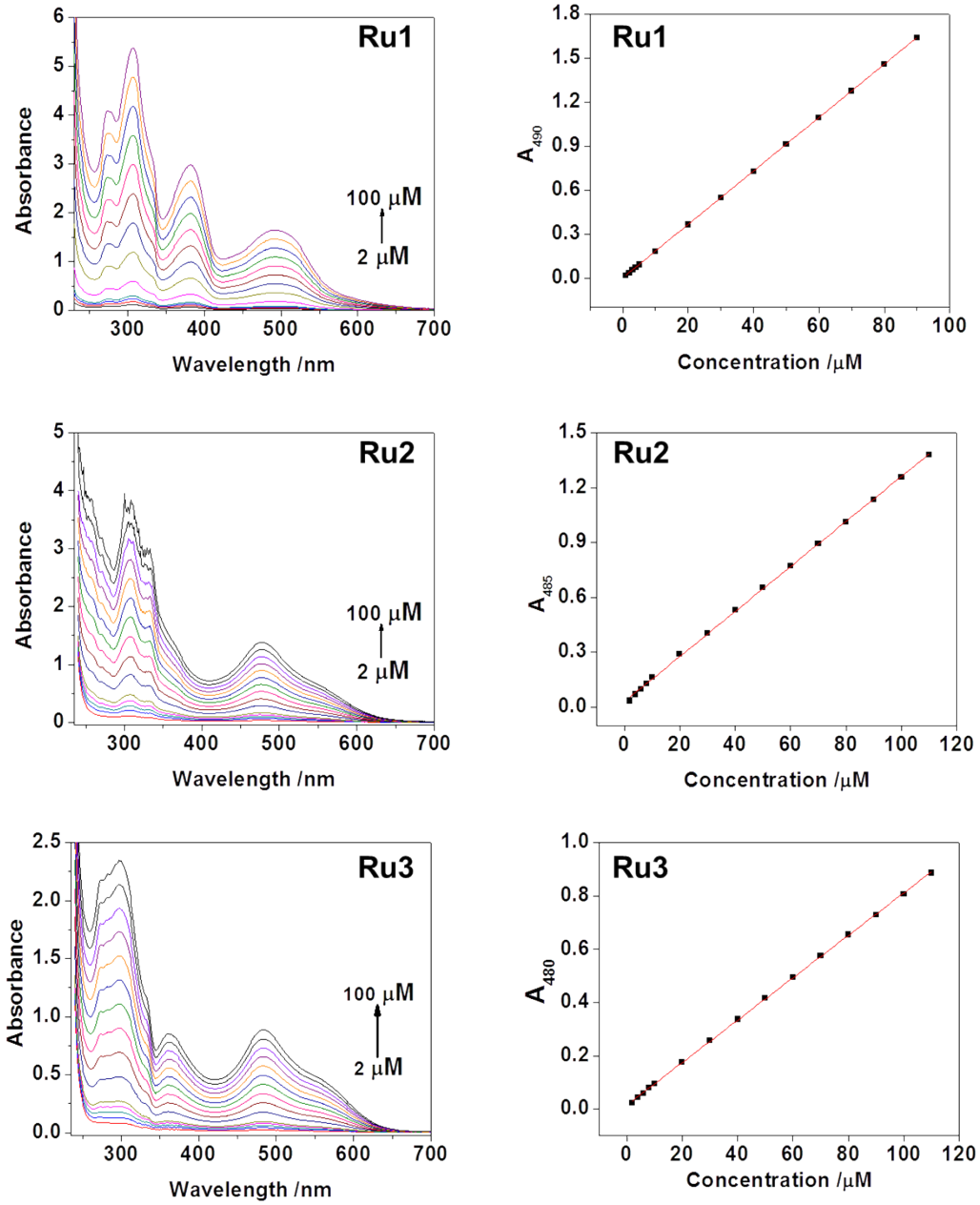

Figure S11 UV-visspectra of **Ru1-Ru3** by gradually increasing concentration in Tris-HCl buffer (5 mM Tris, 50 mM NaCl, pH = 7.4).

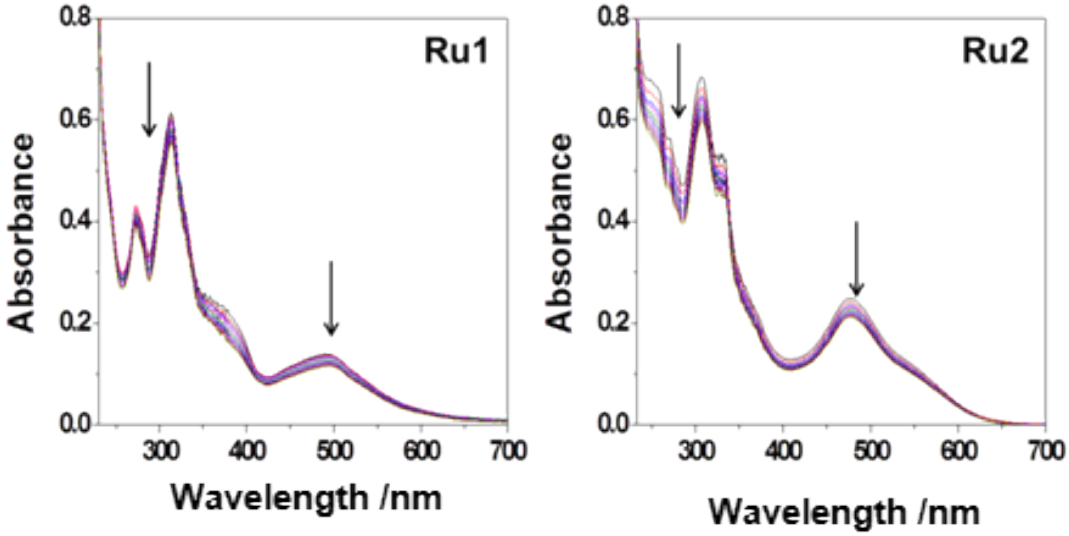

Figure S12 Changes in UV–Vis spectra of **Ru1** and **Ru2** upon adding CT–DNA;

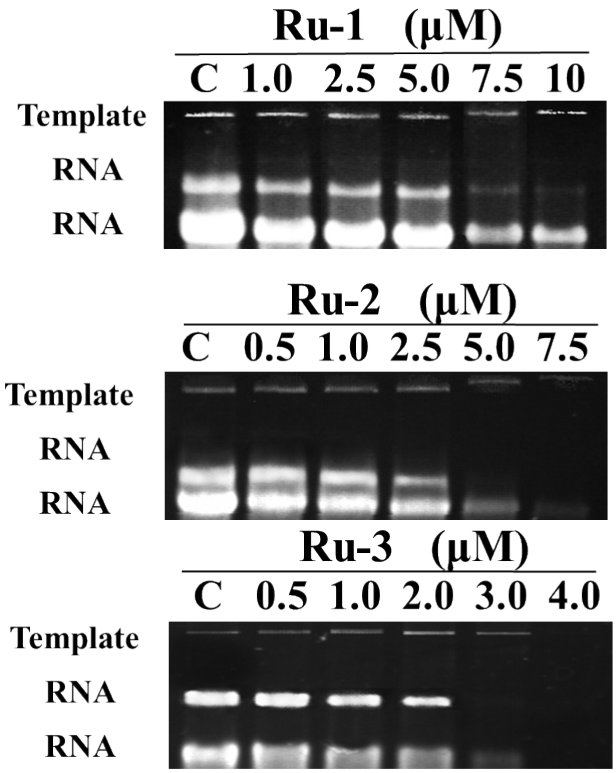

Figure S13 Ru(II) complexes inhibited RNA production during DNA transcription.

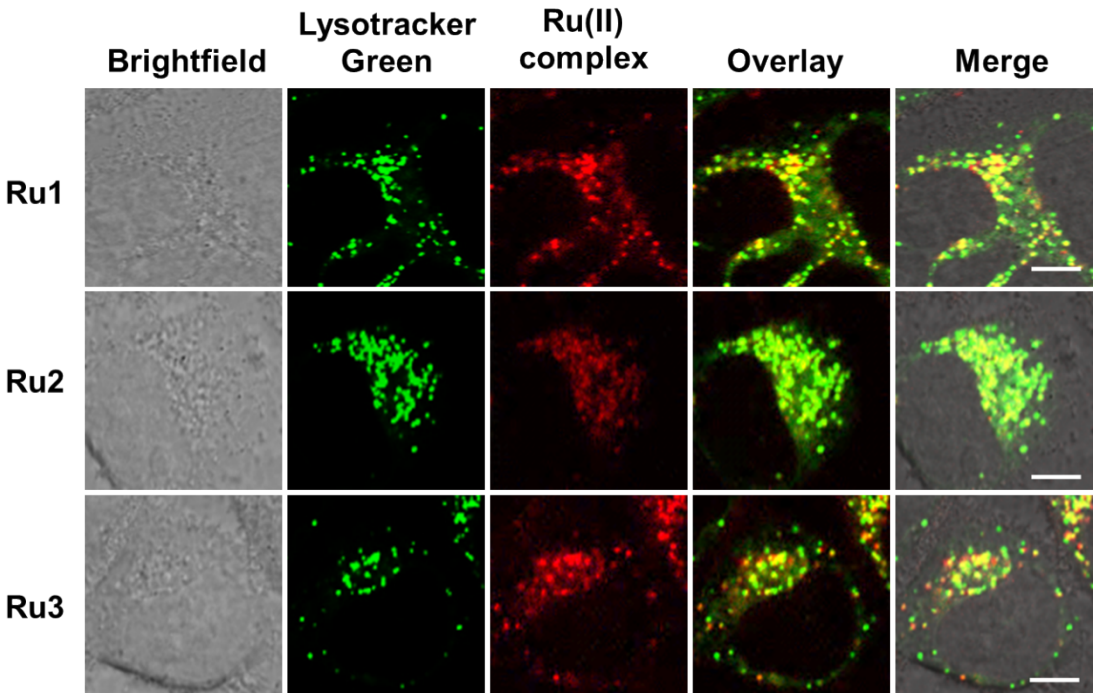

Figure S14 Colocalization images of **Ru1–Ru3** with lysosome dye. Scale bars = 5 μm.

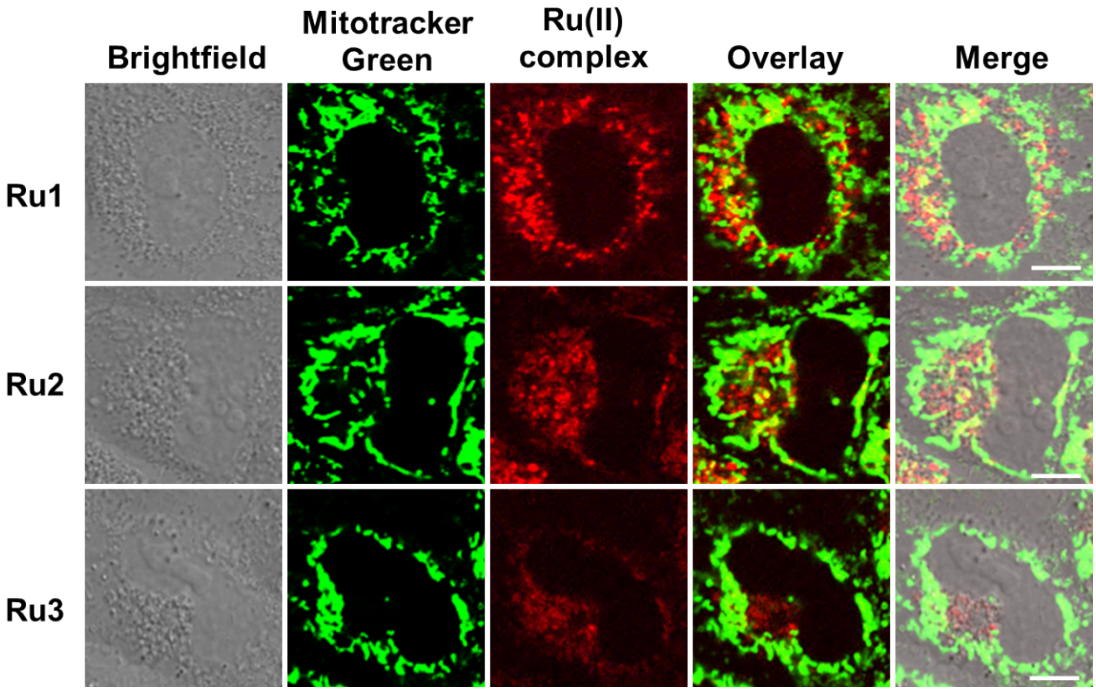

Figure S15 Colocalization images of **Ru1–Ru3** with mitochondria dye. Scale bars = 5 μm.

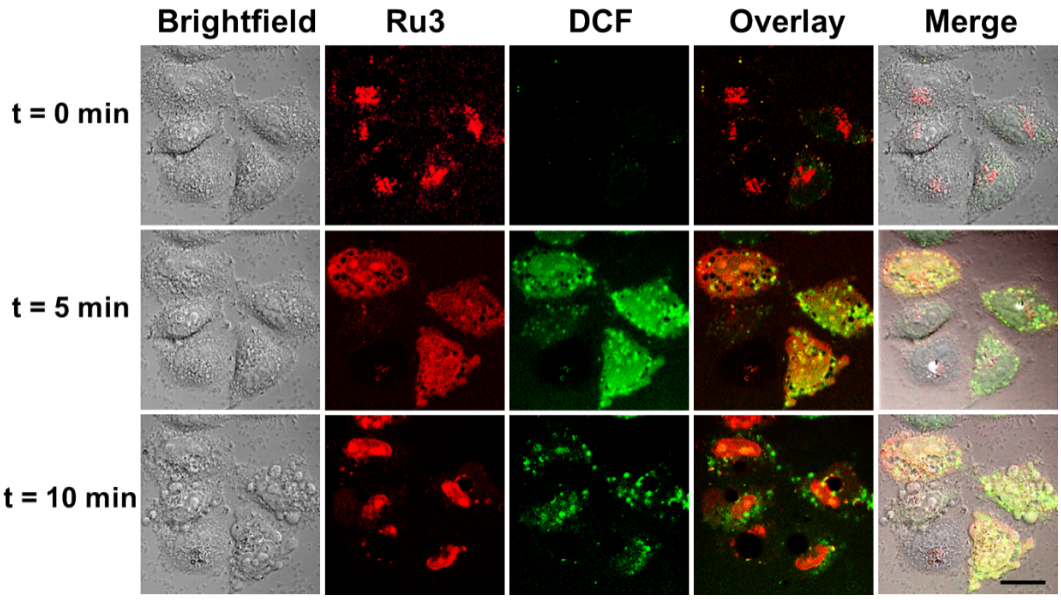

Figure S16 Morphology changes and cellular ROS generation within HepG2 cells incubated with **Ru3** (2.0 μM) at different time. Scale bars = 10 μm.

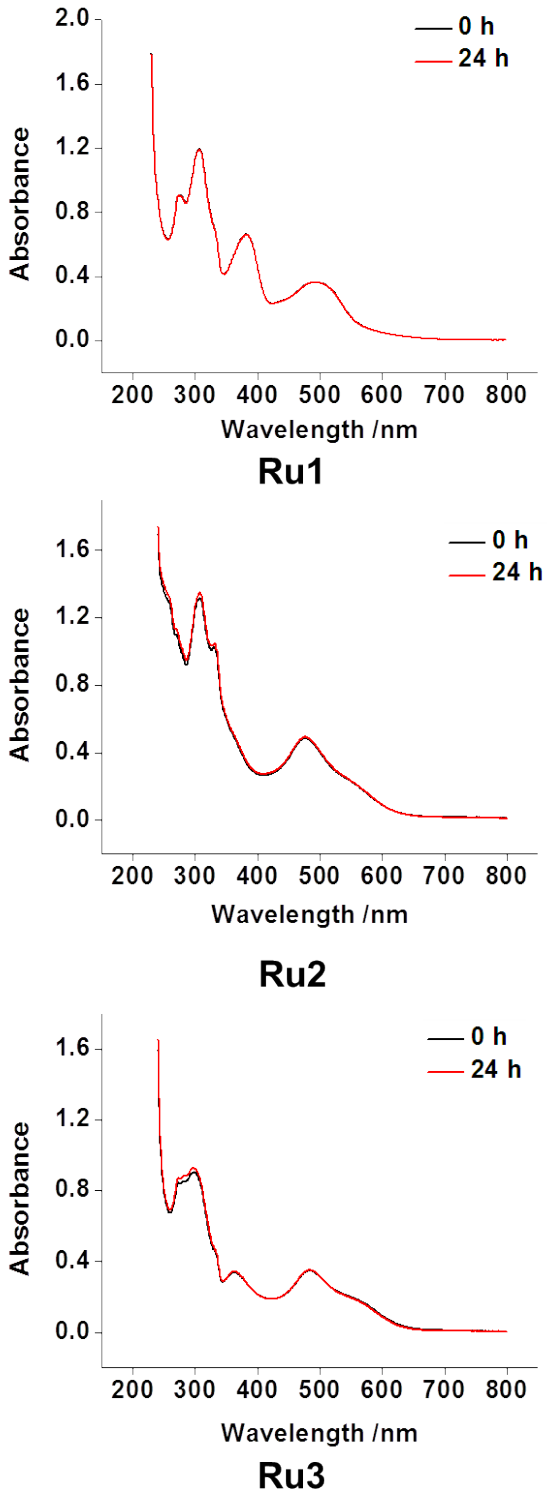

Figure S17 Photostability of **Ru1-3** (10 μM) detected by UV-Vis spectra in Tris-HCl buffer (5 mM Tris, 50 mM NaCl, pH = 7.4).

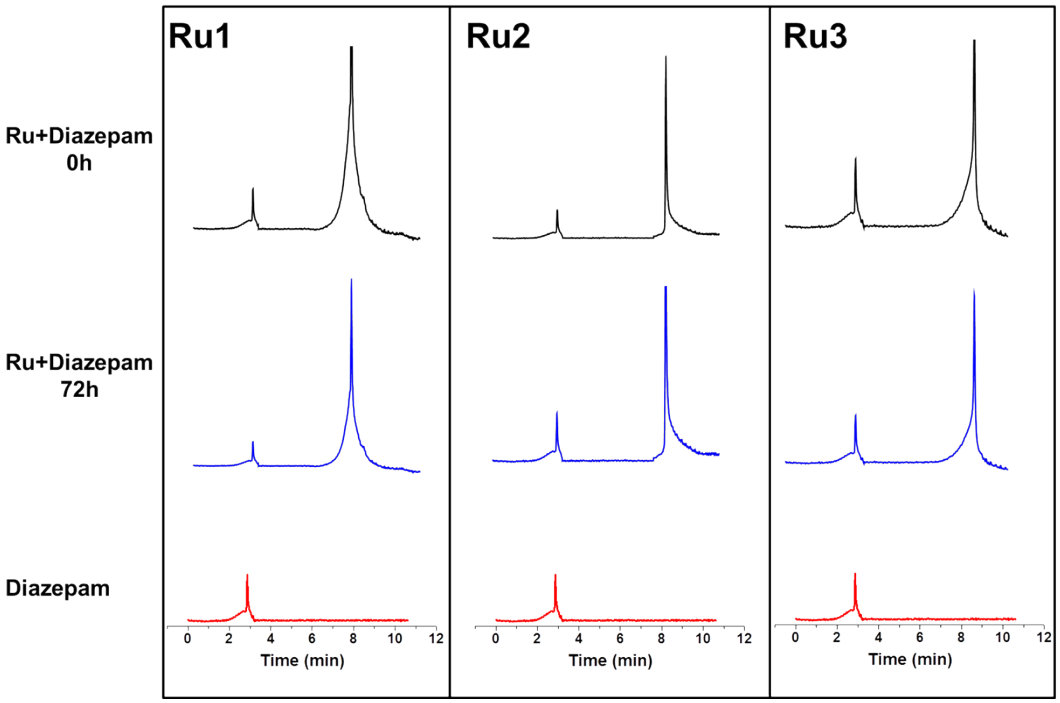

Figure S18 Plasma stability of **Ru1-Ru3** (10 μM) detected by HPLC.

Table S1. The crystal data and structure detail of **Ru1**.

	Ru1
Empirical formula	$C_{37}H_{25}Cl_2N_9O_8Ru$
Formula weight	895.63
Crystal system	Triclinic
Space group	P-1
a/ Å	9.0843(17)
b/ Å	10.6661(19)
c/ Å	22.980(4)
α [◦]	94.141(3)
β [◦]	98.605(3)
γ [◦]	107.719(3)
V [Å^3]	2080.7(6)
Temperature / K	173(2)
Z	2
Data / restraints / parameters	8831 / 18 / 514
R_1 [$I > 2\sigma(I)$]	0.0493
Final $wR(F2)$ values ($I > 2\sigma(I)$)	0.1348
Final R_1 values (all data)	0.0628
wR_2 (all data)	0.1422

Table S2 Selected bond lengths (Å) and angles (°) for **Ru1**.

Complex	**Ru1**	
Bond length (Å)	Ru(1)-N(2)	2.026(3)
	Ru(1)-N(4)	2.080(3)
	Ru(1)-N(6)	2.056(3)
	Ru(1)-N(7)	1.964(3)
	Ru(1)-N(8)	2.079(3)
	Ru(1)-N(9)	2.105(3)
Bond angles (º)	N(7)-Ru(1)-N(2)	92.45(11)
	N(7)-Ru(1)-N(6)	79.69(13)
	N(2)-Ru(1)-N(6)	91.97(11)
	N(7)-Ru(1)-N(8)	79.40(13)
	N(2)-Ru(1)-N(8)	92.03(12)
	N(6)-Ru(1)-N(8)	158.86(13)
	N(7)-Ru(1)-N(4)	170.84(11)
	N(2)-Ru(1)-N(4)	78.57(11)
	N(6)-Ru(1)-N(4)	98.60(11)
	N(8)-Ru(1)-N(4)	102.53(11)
	N(7)-Ru(1)-N(9)	90.69(11)
	N(2)-Ru(1)-N(9)	176.30(10)
	N(6)-Ru(1)-N(9)	90.52(11)
	N(8)-Ru(1)-N(9)	86.63(12)
	N(4)-Ru(1)-N(9)	98.35(11)

Table S3. Photophysical properties of **Ru1-Ru3** in CH_3CN.

Complex	Absorption		Emission		
	λ /nm (logε_{max})		λ /nm	Φ /%	τ_{em}/ ns
Ru1	310 (4.91)	494 (4.18)	675	0.97	43
Ru2	305 (4.95)	481 (4.26)	705	0.86	57
Ru3	308 (4.89)	485 (4.28)	710	1.02	50