Supporting Information

A phosphorescent iridium probe for sensing polarity in endoplasmic reticulum and in vivo

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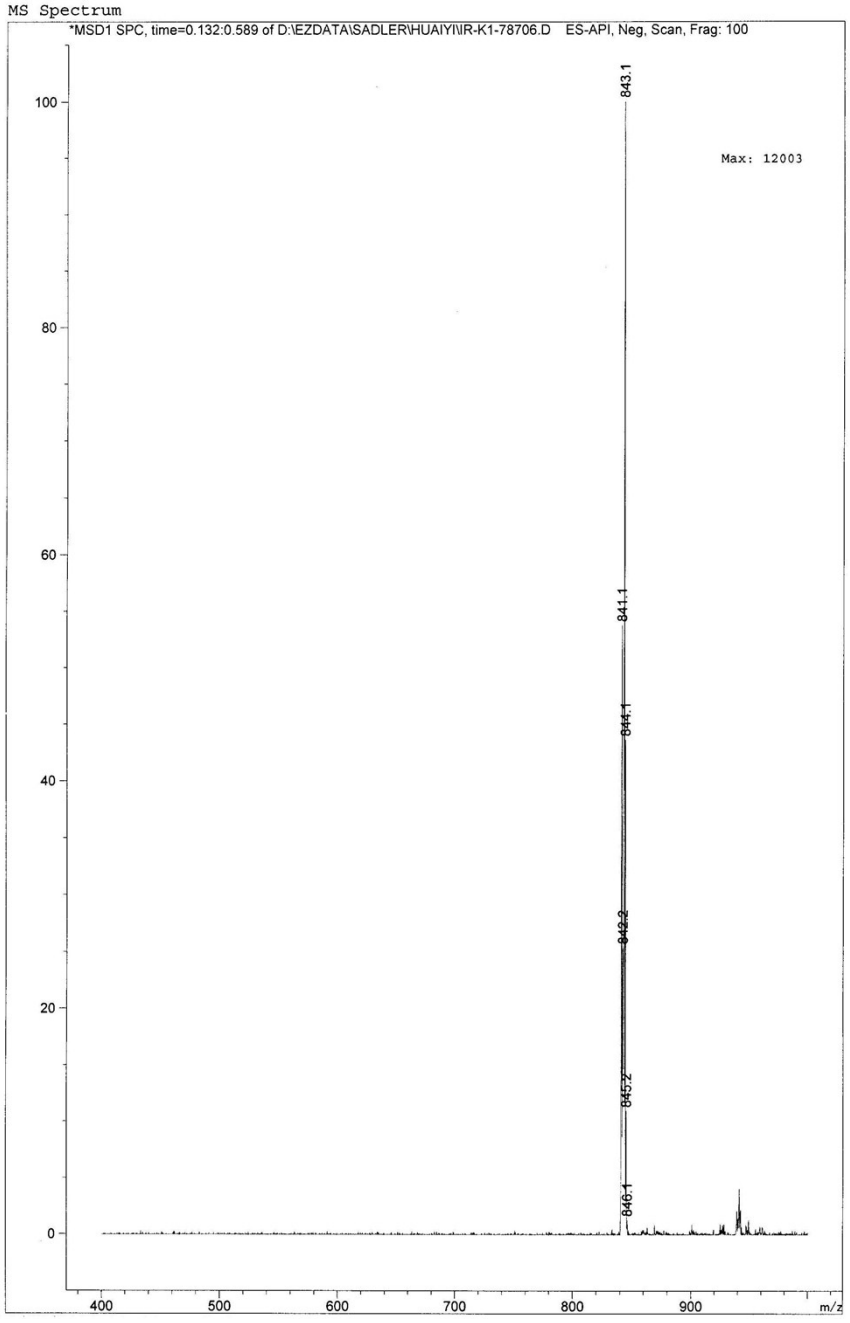

Fig. S1. The ESI-MS of complex **1** (CH_3OH, negative mode).

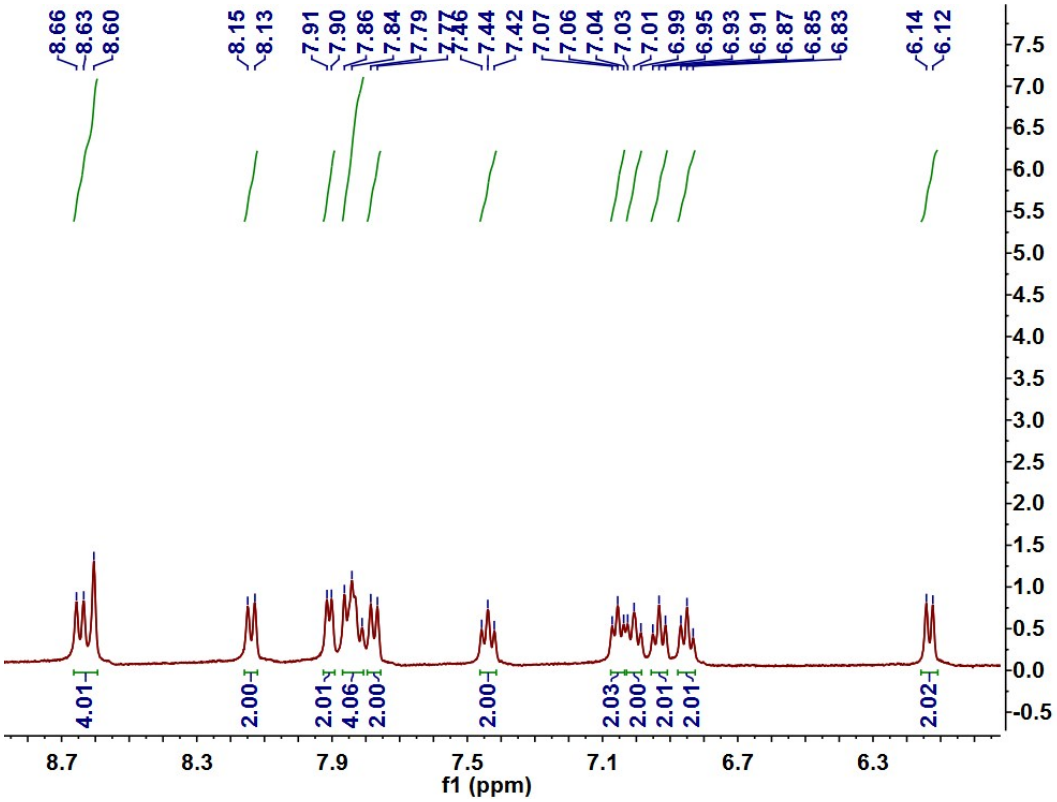

Fig. S2. The 400 MHz ^{1}H NMR spectrum of complex **1** in the DMSO-d^{6} solution.

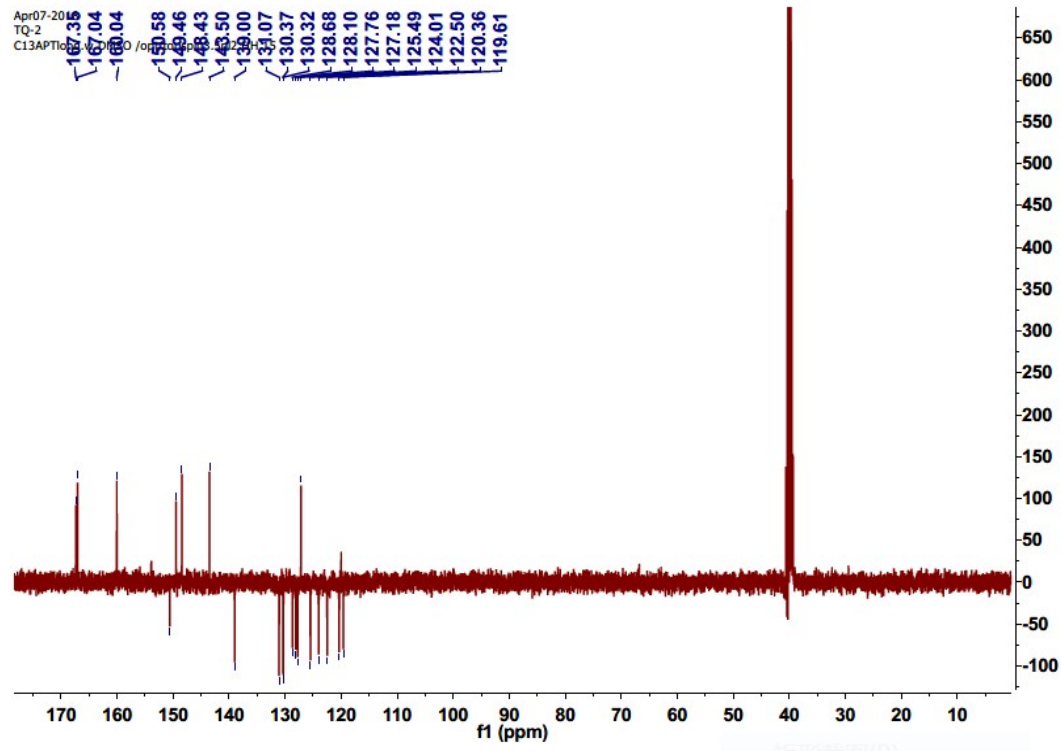

Fig. S3. The 101 MHz ^{13}C NMR spectrum of complex **1** in the DMSO-d^{6} solution.

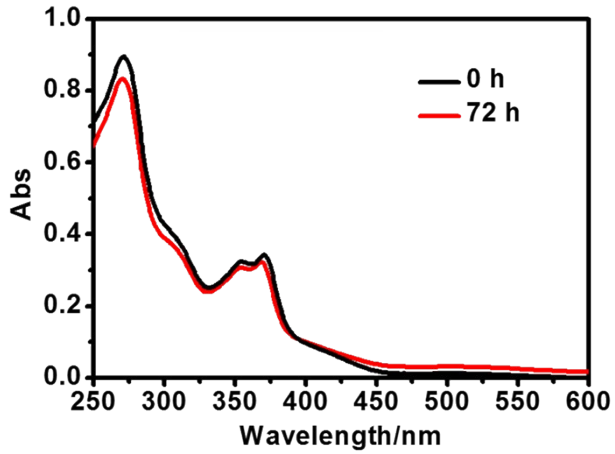

Fig. S4. The stability of **1** in the cell culture medium (RPMI-1640) for 72 h via UV-vis spectrophotometer.

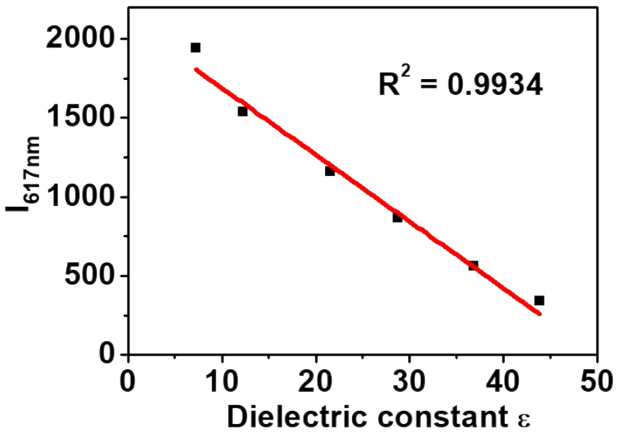

Fig. S5. The emission intensity at 617 nm of **1** as a function of dielectric constant ε.

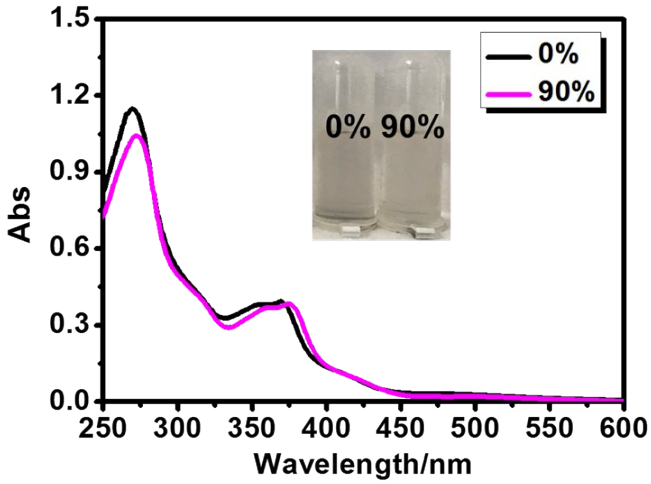

Fig. S6. The UV-vis absorbance of **1** in 0% and 90% 1,4-dioxane-water systems.

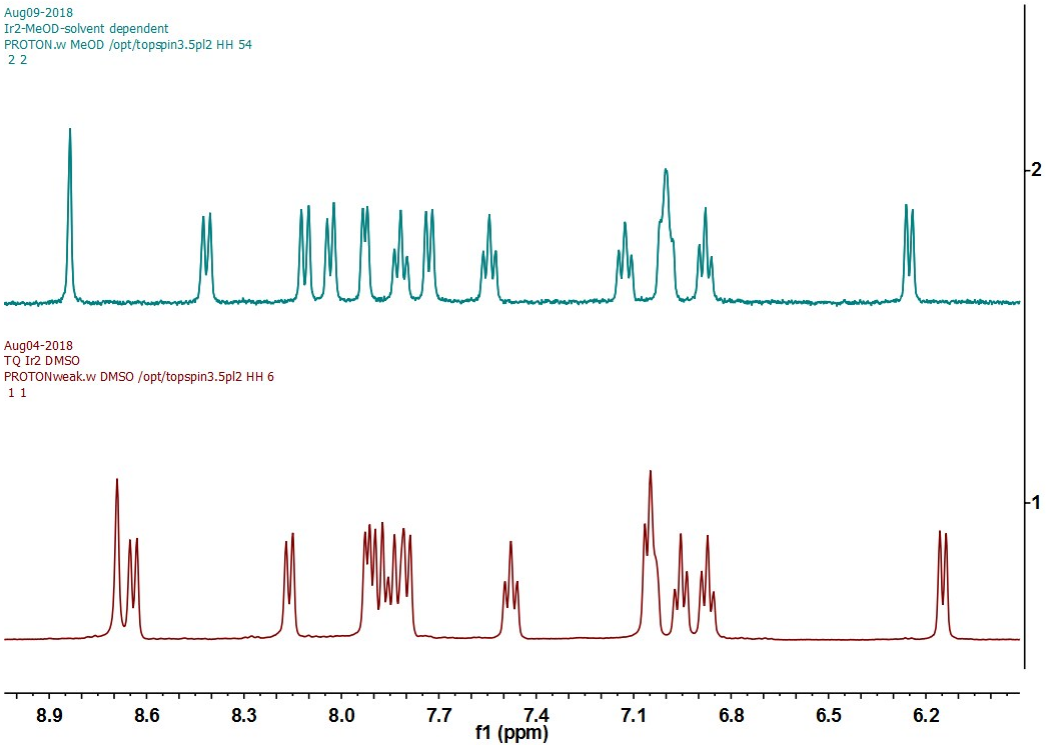

Fig. S7. The ^{1}H NMR spectra of **1** in DMSO-d^{6} and MeOD solution, respectively.

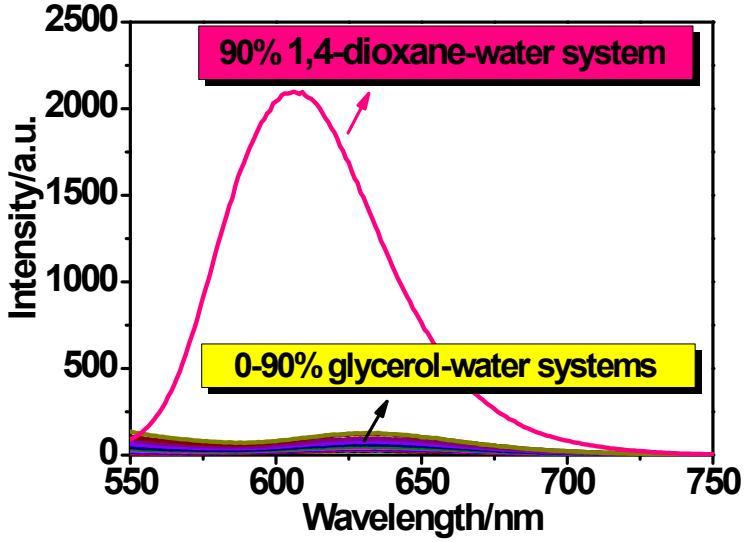

Fig. S8. The emission spectra of **1** in various proportional glycerol-water systems (0%-90%), compare to the emission spectra in 90% 1,4-dioxane-water system. The wavelength of excitation was 405 nm.

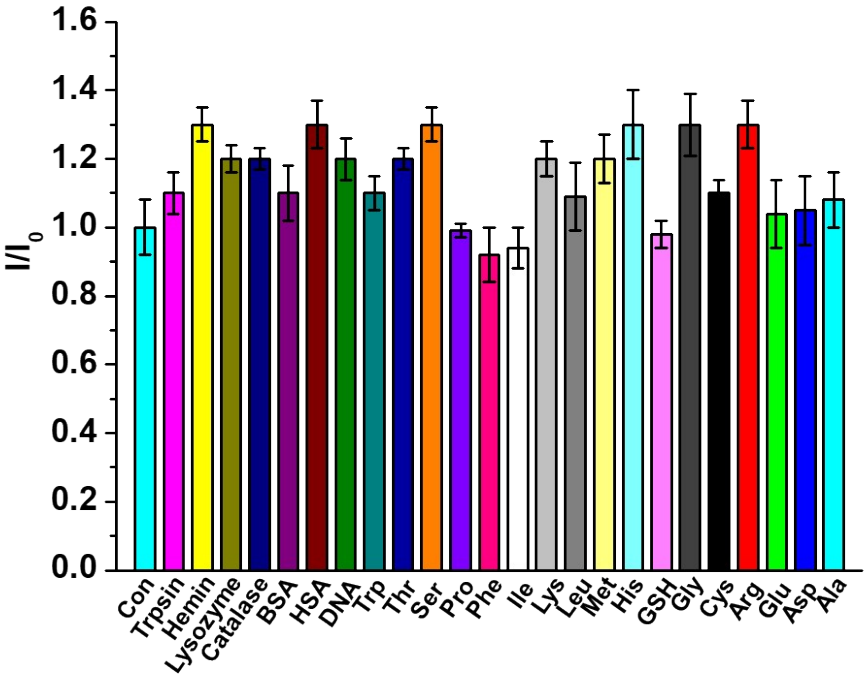

Fig. S9. The emission intensity I/I_0 at 600 nm of **1** in the absence of (I_0) and in the presence of kinds of biological molecules (I). The wavelength of excitation was 405 nm.

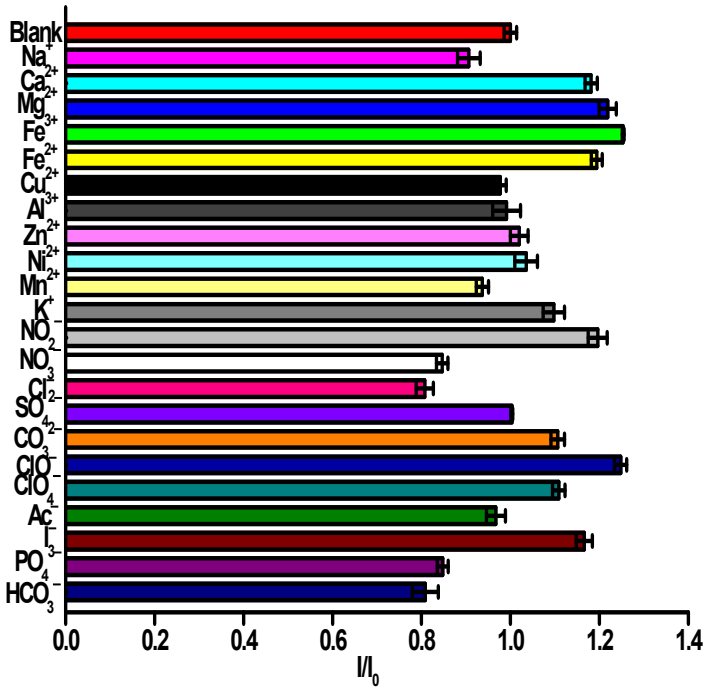

Fig. S10. The emission intensity I/I_0 at 600 nm of **1** in the absence of (I_0) and in the presence of kinds of common metal ions and anions (I). The wavelength of excitation was 405 nm.

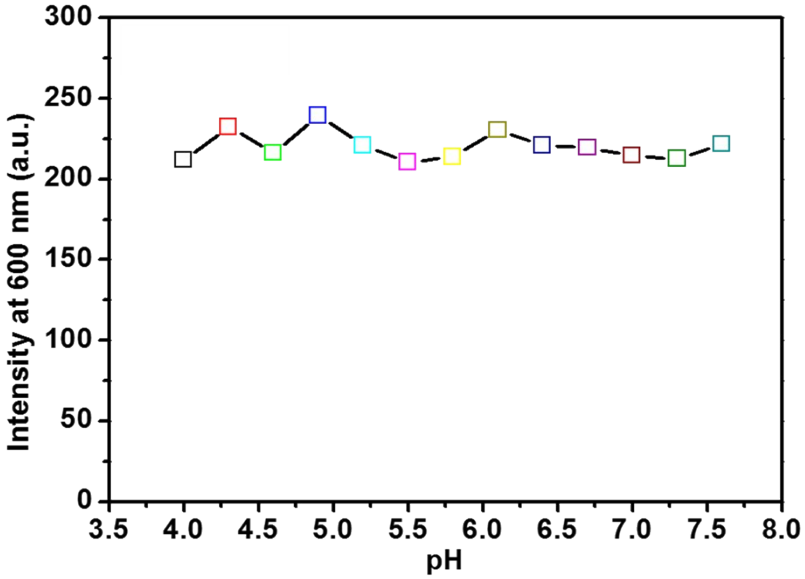

Fig. S11. The emission intensities at 600 nm of **1** in PBS solution with different pH values. The wavelength of excitation was 405 nm.

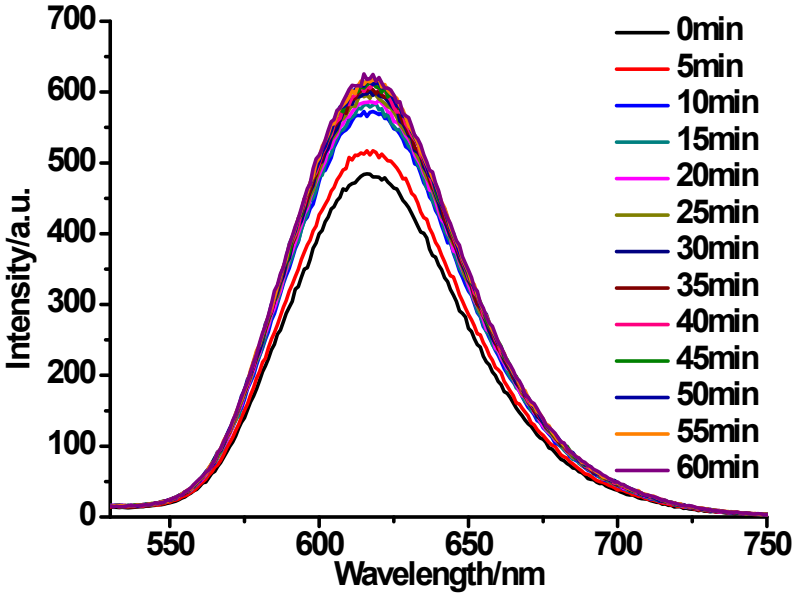

Fig. S12. The changes in emission intensity of **1** (10 μM) in 50% 1,4-dioxane-water system under 465 nm light irradiation for 60 minutes. The spectra were measured every 5 min. The power of the light was 6.5 mW/cm^2. The wavelength of excitation was 405 nm.

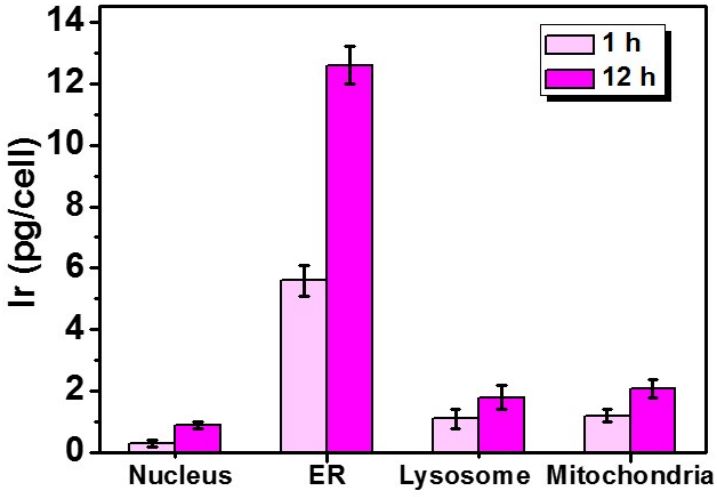

Fig. S13. Iridium concentrations determined in ER, lysosome, mitochondria and nucleus of the A549 cells with exposure to the iridium complex (10 μM) for 1 h and 12 h by ICP-MS.

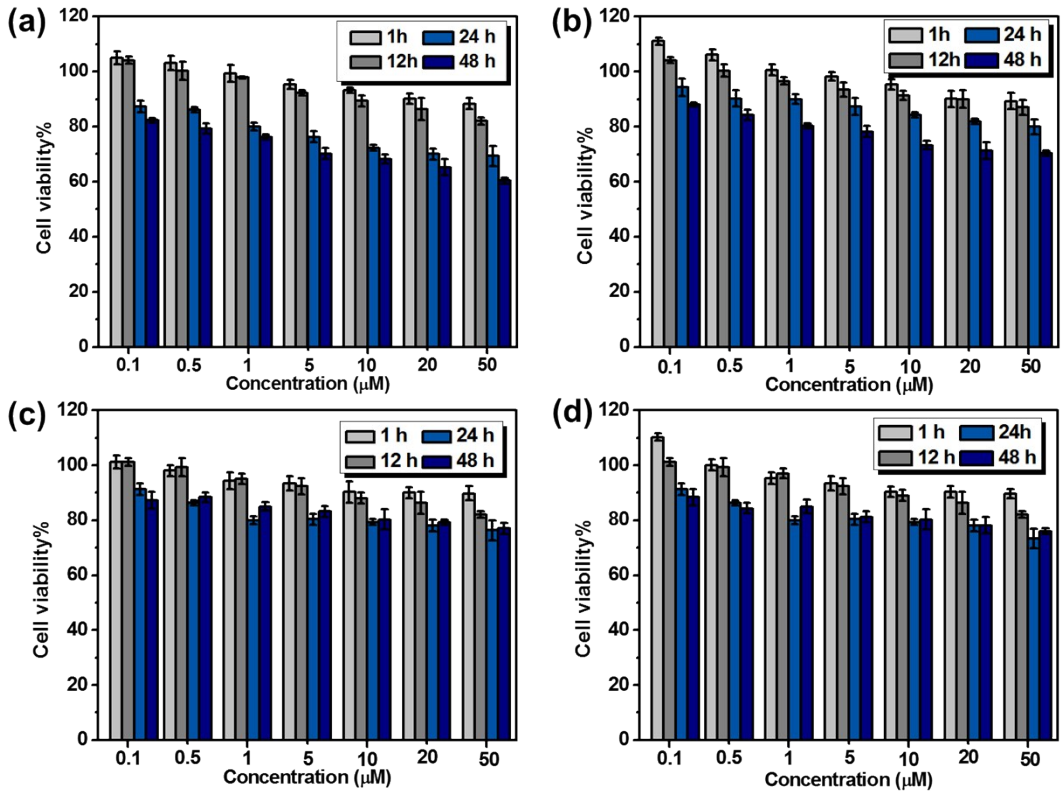

Fig. S14. The cell viabilities of A549, MRC-5, Hep-G2 and HL-7702 cells treated with **1** at different concentrations for 1 h, 12 h, 24 h and 48 h, respectively.

Table S1. Photophysical properties of **1** in different solvents (Polarity: water > methanol > acetonitrile > acetone > chloroform).

Solvents	Emission maximum (nm)	Quantum yield Φ
water	632	0.001
methanol	611	0.023
acetonitrile	594	0.064
acetone	588	0.201
chloroform	585	0.243

Table S2. The phosphorescence lifetimes of **1** in various 1,4-dioxane-water systems.

Percentage of 1,4-dioxane	Dielectric constant ε	Emission maximum (nm)	Lifetime τ (ns)
0%	79.6	627	53
10%	70.2	626	118
20%	62.1	624	170
30%	56.7	621	239
40%	43.8	621	368
50%	36.8	618	415
60%	28.7	614	580
70%	21.5	612	673
80%	12.2	606	759
90%	7.1	606	837