

Electronic Supplementary Information

Fluorescent monofunctional platinum complex derived from NBD visualizes its distribution behavior in tumour cells

Shengde Wu, Xiaoyong Wang,* Chengcheng Zhu, Yajie Song, Jing Wang, Yizhi Li and Zijian Guo*

Contents

Fig. S1. ESI-MS spectra of complexes **1** and **2** in methanol (positive mode).

Fig. S2. Excitation (Ex) and emission (Em) spectra of complex **1** and ligand L.

Fig. S3. Time-dependent ESI-MS spectra of complex **2** in water (positive mode).

Scheme S1. Proposed reactions of complex **2** in water.

Fig. S4. Time-dependent ^1H NMR spectra for the reaction between complex **1** and 5'-GMP.

Fig. S5. Circular dichroism spectra of CT-DNA after incubation with complex **1**.

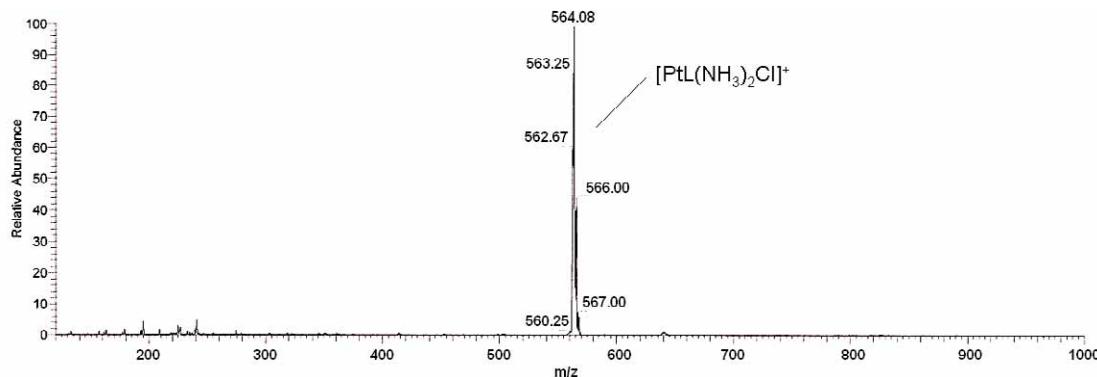
Fig. S6. Fluorescence spectra of complex **1** after incubation with CT-DNA.

Fig. S7. Confocal microscope images of HeLa cells in the presence of complex **1** determined at different incubation time.

Fig. S8. Close-up confocal microscope images of HeLa cells treated with complex **1** for 17 h.

Fig. S9. Time-dependent confocal microscope image of **1**-treated HeLa cells in PBS buffer after elimination of the complex.

Fig. S10. Confocal microscope images ($\lambda_{\text{ex}} = 488$ nm) of HeLa cells after treatment with ligand L (10 μM) for different time.



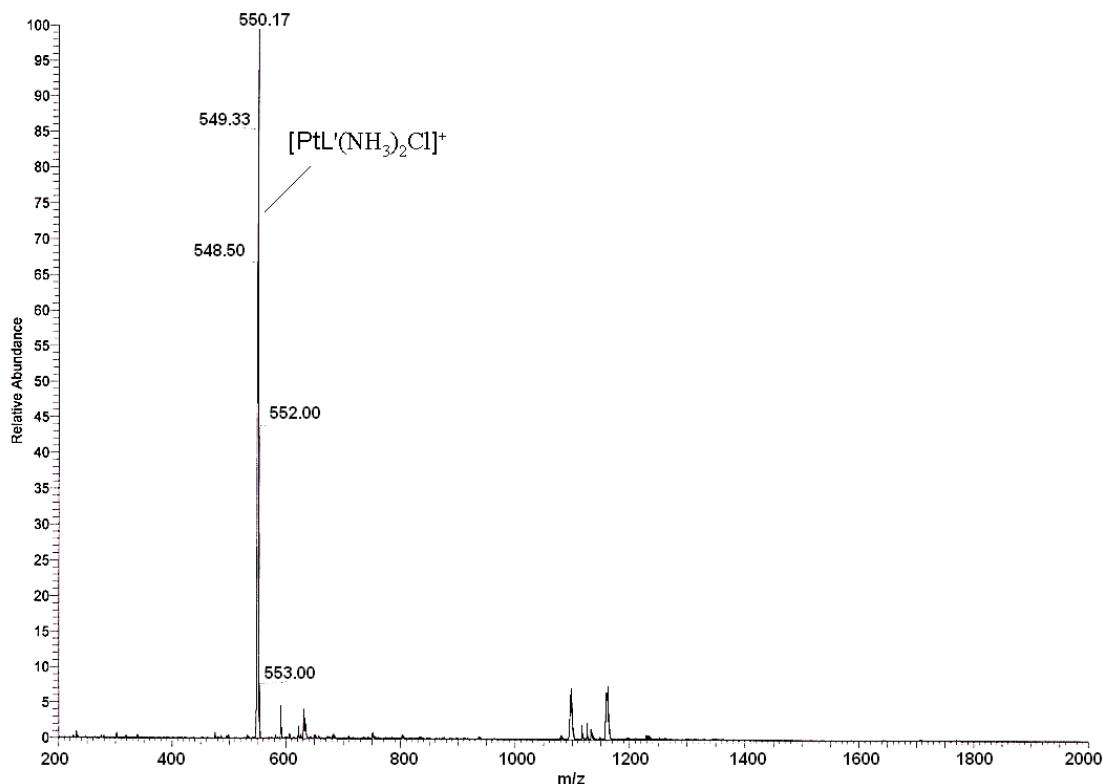


Fig. S1. ESI-MS spectra of complexes **1** and **2** in methanol (positive mode). Assignments: m/z 564.08, $[\text{PtL}(\text{NH}_3)_2\text{Cl}]^+$ ($\text{C}_{14}\text{H}_{19}\text{N}_7\text{O}_3\text{ClPt}$, calcd 563.09); m/z 550.17, $[\text{PtL}'(\text{NH}_3)_2\text{Cl}]^+$ ($\text{C}_{13}\text{H}_{17}\text{N}_7\text{O}_3\text{ClPt}$, calcd 549.07).

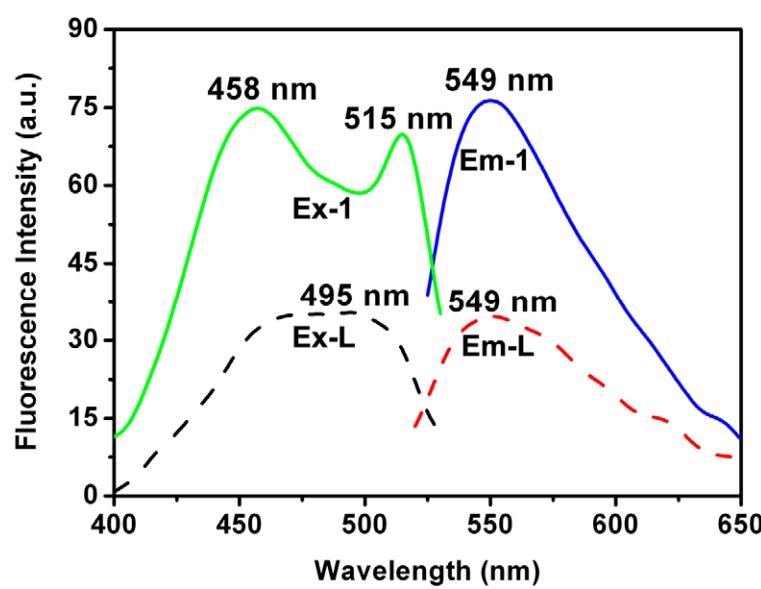


Fig. S2. Excitation (Ex) and emission (Em) spectra of complex **1** and ligand L (0.01 mM) in PBS buffer.

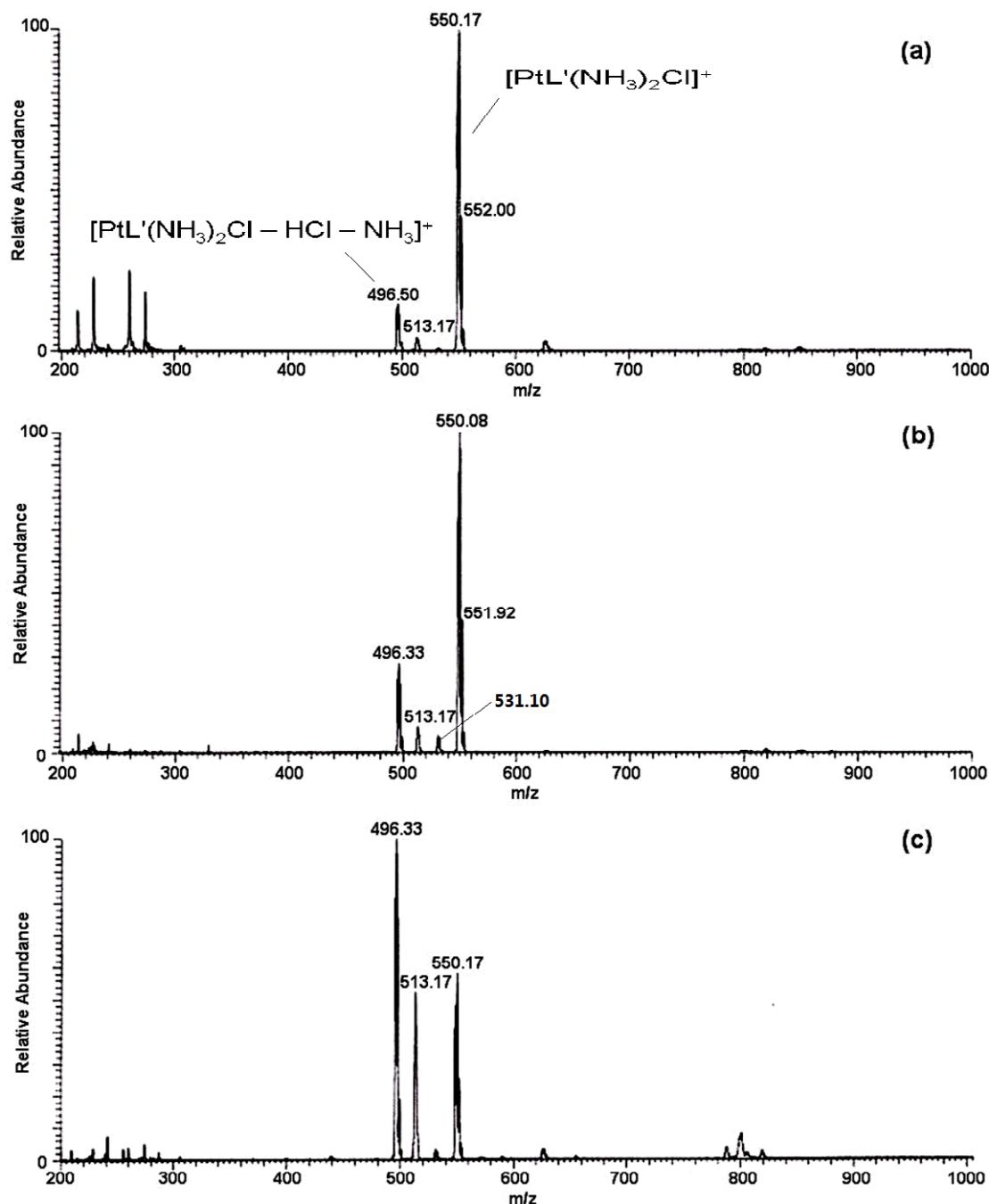
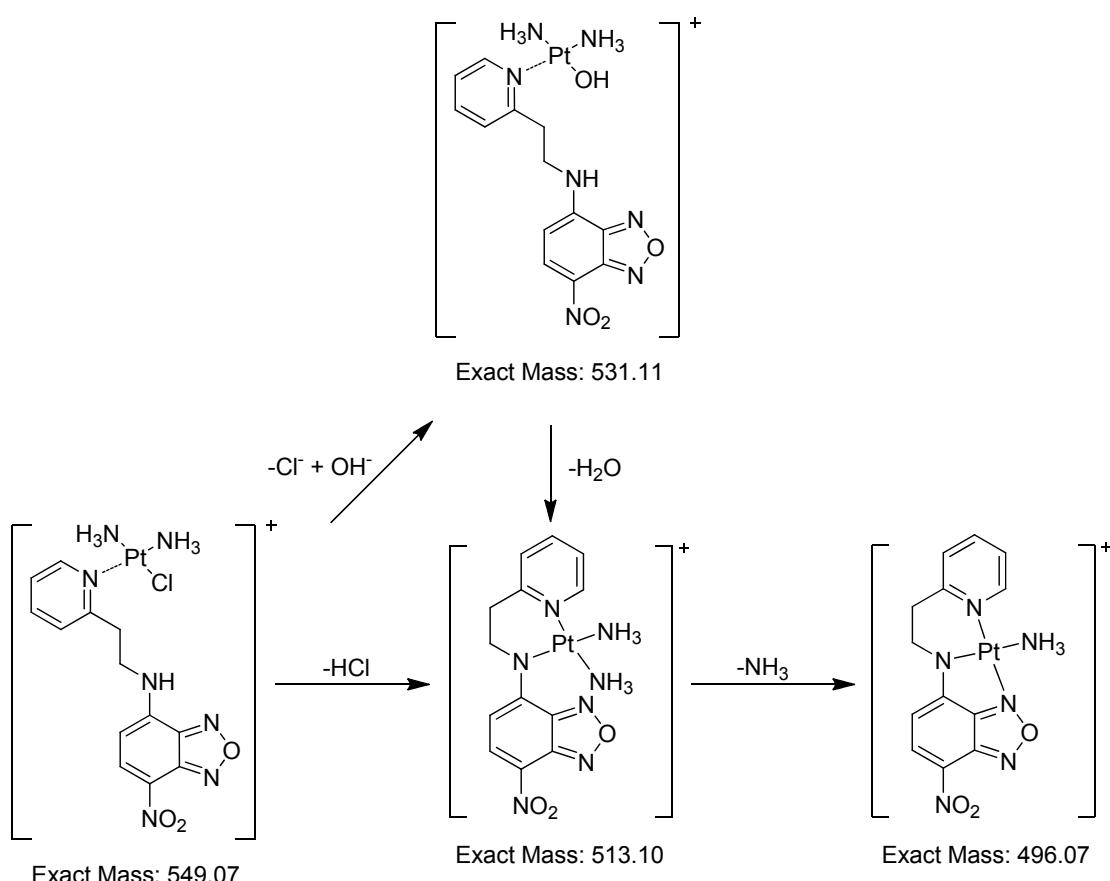


Fig. S3. Time-dependent ESI-MS spectra of complex 2 in water determined at 1 h (a), 6 h (b), and 96 h (c) after preparation (positive mode). Assignments: m/z 496.33, $[\text{PtL}'(\text{NH}_3)]^+$ ($\text{C}_{13}\text{H}_{13}\text{N}_6\text{O}_3\text{Pt}$, 496.07); 513.17, $[\text{PtL}'(\text{NH}_3)_2]^+$ ($\text{C}_{13}\text{H}_{16}\text{N}_7\text{O}_3\text{Pt}$, calcd 513.1); 531.10, $[\text{PtL}'(\text{NH}_3)_2(\text{OH})]^+$ ($\text{C}_{13}\text{H}_{18}\text{N}_7\text{O}_4\text{Pt}$, calcd 531.11); 550.17, $[\text{PtL}'(\text{NH}_3)_2\text{Cl}]^+$ ($\text{C}_{13}\text{H}_{17}\text{N}_7\text{O}_3\text{ClPt}$, calcd 549.07).



Scheme S1. Proposed reactions of complex **2** in water.

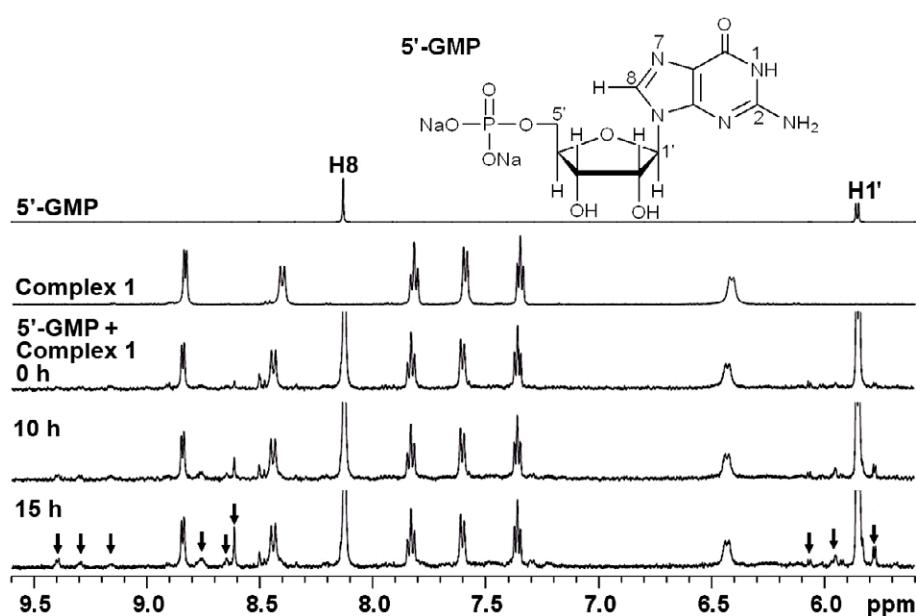


Fig. S4. ¹H NMR spectra of 5'-GMP (2.05 mg, 5.0 mmol), complex **1** (3.12 mg, 5.0 mmol), and their mixture (1:1) in aromatic region after incubation for 0, 10, and 15 h (D_2O , 298 K), respectively. Arrows indicate the reaction products.

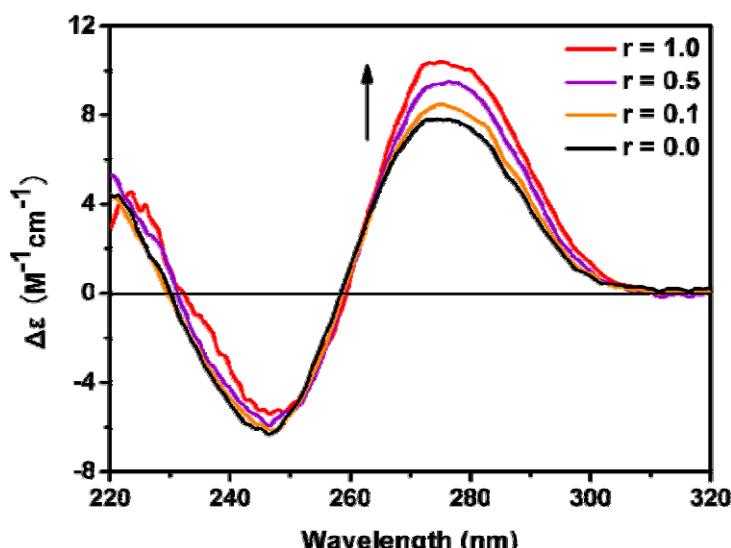


Fig. S5. Circular dichroism spectra of CT-DNA (0.1 mM) after 24 h incubation at 37 °C with complex **1** in different [complex]/[DNA] ratios (r) in PBS buffer. The baseline was corrected using PBS.

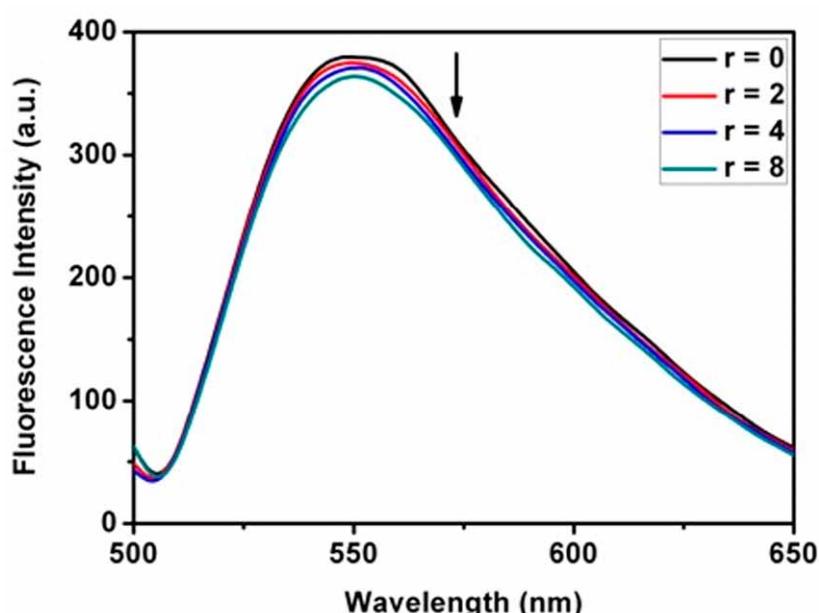


Fig. S6. Fluorescence spectra of complex **1** (50 μ M) after incubation for 24 h with CT-DNA in different [DNA]/[1] ratios (r) in PBS buffer.

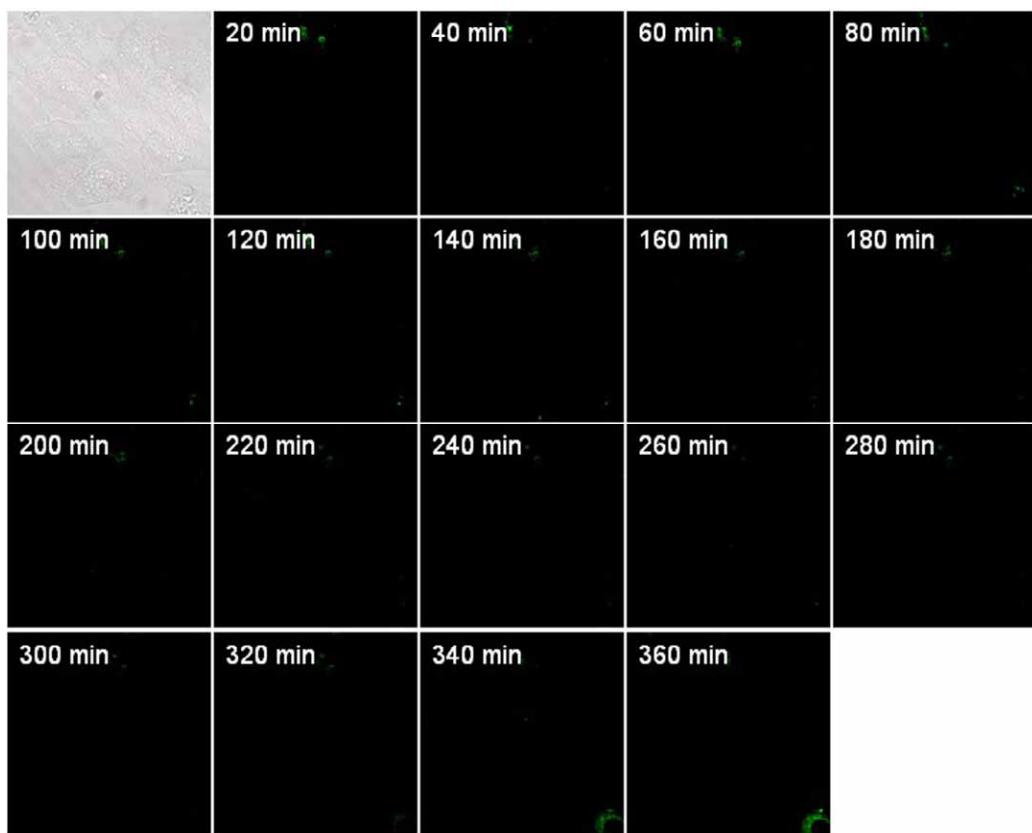


Fig. S7. Confocal microscope images of HeLa cells in the presence of complex 1 determined at different incubation time.

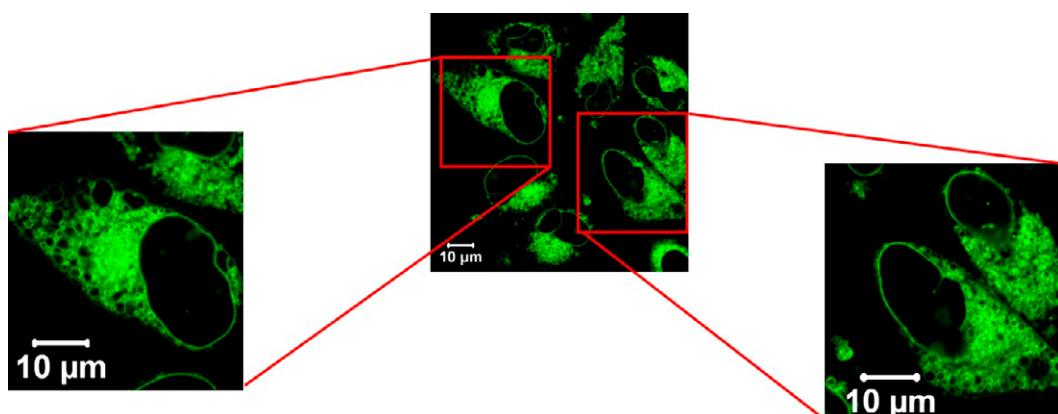


Fig. S8. Close-up confocal microscope images of HeLa cells treated with complex 1 for 17 h.

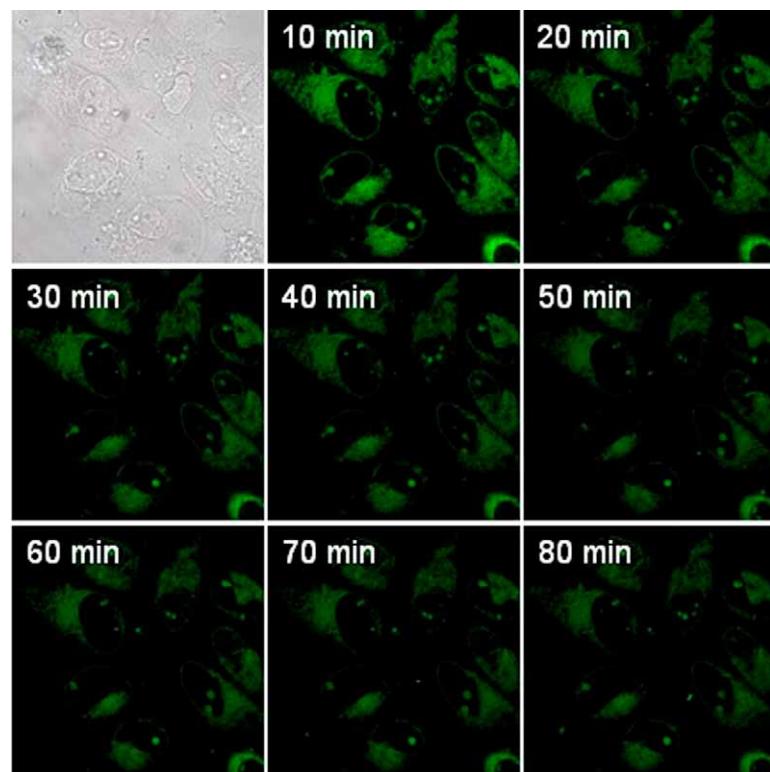


Fig. S9. Time-dependent confocal microscope images of **1**-treated HeLa cells in PBS buffer after elimination of the complex ($\lambda_{\text{ex}} = 488 \text{ nm}$).

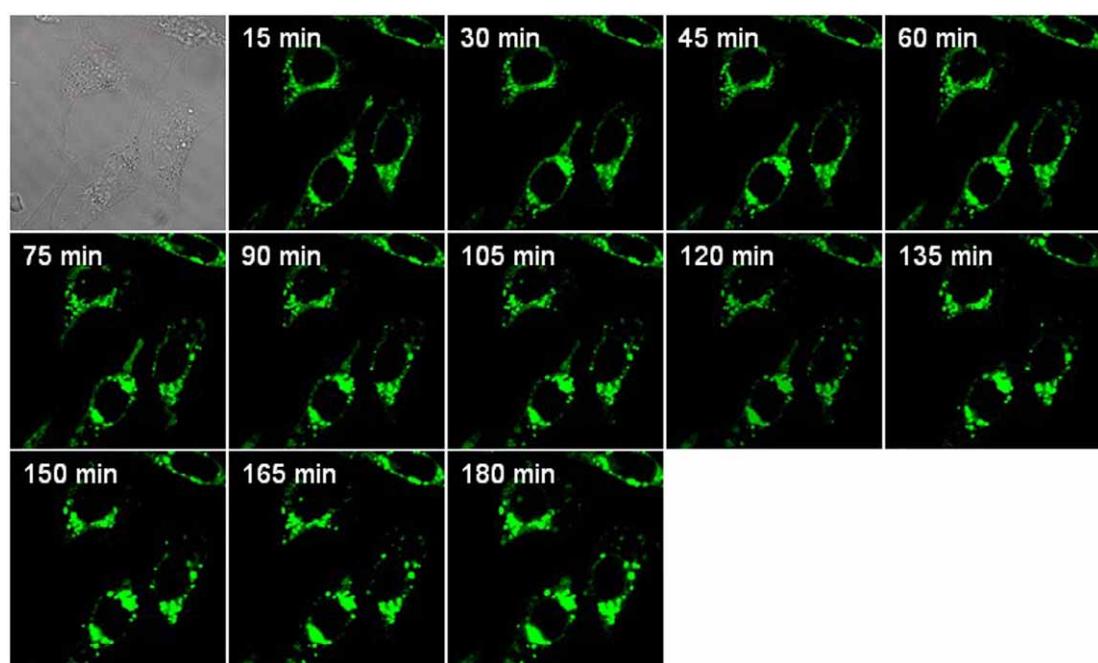


Fig. S10. Confocal microscope images ($\lambda_{\text{ex}} = 488 \text{ nm}$) of HeLa cells after treatment with ligand L (10 μM) for different time.