Supporting Information

A nuclear permeable Ru(II)-based photoactivated chemotherapeutic agent towards a series of cancer cells: in vitro and in vivo studies

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Fig. S1 a-d: absorption spectra changes of 1, 2, 3 and 4(30μM) in H₂O upon irradiation (470nm)

Fig. S2 a-d: absorbance changes at 490 nm for 1, 495 nm for 2, 500 nm for 3, 530 nm for 4 with different irradiation times.
Fig. S3 $^1$H NMR spectra changes of 1 in Ar-saturated D$_2$O: (a) before irradiation, (b) irradiation for 5 min ($\lambda_{irr}$=470 nm). Two new peaks appeared at 9.56 ppm and 9.85 ppm, which was consistent with previous reports. The H labeled with $\star$ was assigned to bis-aquated complex, and mono-aquated complex was labeled by $\Box$.  

Fig. S4 $^1$H NMR spectra changes of 2 in Ar-saturated D$_2$O: (a) before irradiation, (b) irradiation for 5 min ($\lambda_{irr}$=470 nm). Similar with complex 1, two new peaks were assigned to bis-aquated ($\star$) and mono-aquated ($\Box$) complex, respectively.  

Fig. S5 $^1$H NMR spectra changes of 3 in Ar-saturated D$_2$O: (a) before irradiation, (b) irradiation for 5 min ($\lambda_{irr}$=470 nm). Similar with complex 1, two new peaks were assigned to bis-aquated ($\star$) and mono-aquated ($\Box$) complex, respectively.
Fig. S6 $^1$H NMR spectra changes of 4 in Ar-saturated D$_2$O: (a) before irradiation, (b) irradiation for 5 min ($\lambda_{irr}$=470 nm). Only one new mono-aquated peak was observed (labeled by ■), which was also consistent with its relatively low photo-induced ligand dissociation quantum yield.
Fig. S7 HR ESI-MS spectra of 1 before (top) and after 470 nm light irradiation (bottom) in CH$_3$CN.
**Fig. S8** HR ESI-MS spectra of 2 before (top) and after 470 nm light irradiation (bottom) in CH$_3$CN.
Fig. S9 HR ESI-MS spectra of 3 before (top) and after 470 nm light irradiation (bottom) in CH$_3$CN.
Fig. S10 HR ESI-MS spectra of 4 before (top) and after 470 nm light irradiation (bottom) in CH₃CN.

Fig. S11 TEM images of SKOV-3 cells incubated with control (a), 1(b), 2(c), 3 (d) and stained with osmium tetroxide, (The white arrows indicated the accumulated Ru complex, n=nucleus, nu=nucleolus, m=mitochondria ).
Fig. S12 The percentage of apoptotic SKOV-3 cells analyzed by flow cytometry. (1) Dark control, with no complex added; (2-4) SKOV-3 cells incubated with complex 1-3 (100nM) for 4 h, respectively, cell medium discarded and added with fresh medium, then irradiated for 0.5 h (470nm LED, 22.5mW/cm²), and incubated for more 10 h in the dark.

![Flow Cytometry Images](image)

Fig. S13 Solid tumors extracted from mice treated after 12 days.

![Tumor Images](image)

Fig. S14 H&E staining images of important organs of different groups: PBS+light, Ru+Light, Ru+dark groups after 12 days treatment.
Fig. S15 Partial MTT assays of different cells. (a) SKOV-3 Cell viabilities treated with complex 4; (b) A549 and Hela cell viabilities treated with complex 4; (c) A549 DDP and SKOV-3 DDP cells viabilities treated with complex 4; (d) Cell viabilities treated with complex 3 upon irradiation for 30 min using 470 nm LED (22.5 mW/cm²).

Fig. S16 MTT assays of normal L-02 cells. Cells treated with complex 4 upon irradiation for 30 min using 470 nm LED (22.5 mW/cm²) or in the dark.
**Fig. S17** MTT assays of SKOV-3 cells under hypoxia condition. Cells treated with complex 4 upon irradiation for 30 min using 470 nm LED (22.5 mW/cm²) or in the dark.

**Fig. S18** MTT assays of 4T1 cells. Cells treated with complex 4 upon irradiation for 30 min using 470 nm LED (22.5 mW/cm²) or in the dark.

**Fig. S19** Caspase levels of SKOV-3 cells relative to the control.
Fig. S20 HPLC of 1.

Fig. S21 HPLC of 2.

Fig. S22 HPLC of 3.
Fig. S23 HPLC of 4.