Supporting Information

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

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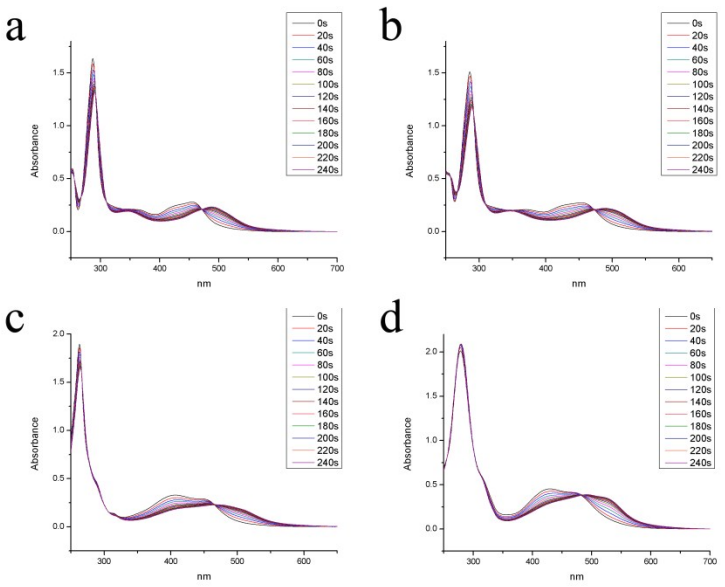


Fig. S1 a-d: absorption spectra changes of **1**, **2, 3** and **4**(30μM) in H_2O upon irradiation (470nm)

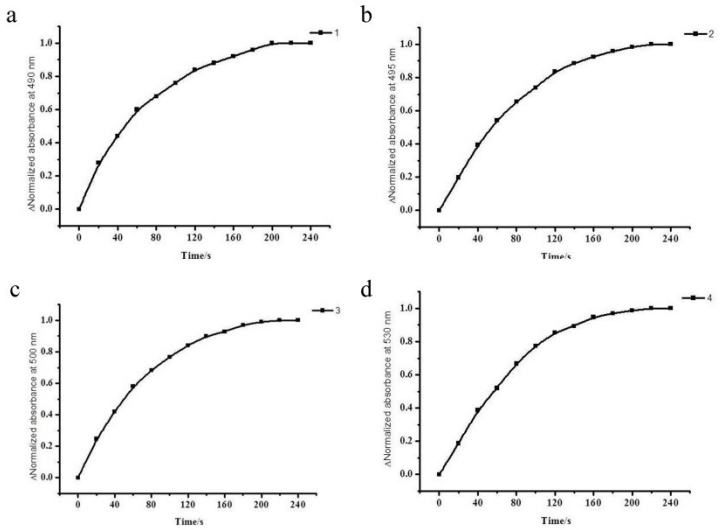
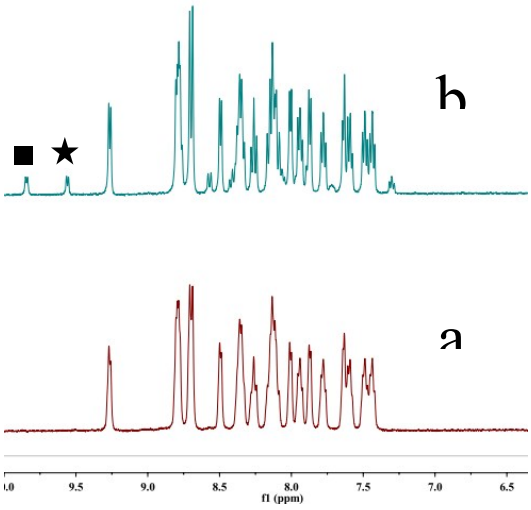


Fig. S2 a-d: absorbance changes at 490 nm for **1**, 495 nm for **2**, 500 nm for **3**, 530 nm for **4** with different irradiation times.



1

Fig. S3 ^{1}H NMR spectra changes of **1** in Ar-saturated D_2O: (a) before irradiation, (b) irradiation for 5 min (λ_{irr}=470 nm).Twonew peaks appeared at 9.56 ppm and 9.85 ppm, which was consistent with previous reports.[6] The H labeled with★was assigned to bis-aquatedcomplex, and mono-aquated complex was labeled by ■.

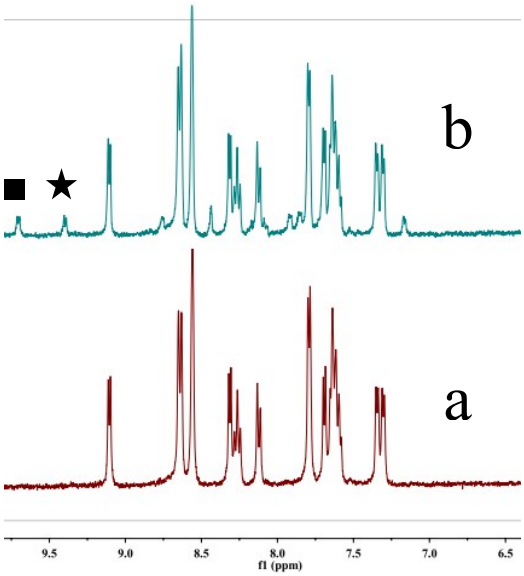


Fig. S4 ^{1}H NMR spectra changes of **2** in Ar-saturated D_2O: (a) before irradiation, (b) irradiation for 5 min (λ_{irr}=470 nm). Similar with complex **1**, two new peaks were assigned to bis-aquated (★) and mono-aquated (■) complex, respectively.

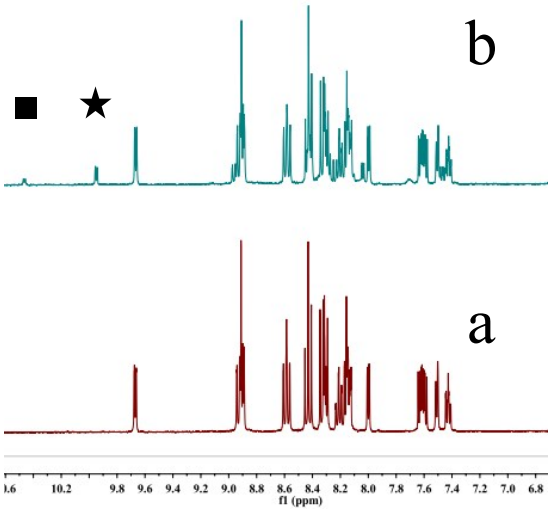


Fig. S5 ^{1}H NMR spectra changes of **3** in Ar-saturated D_2O: (a) before irradiation, (b) irradiation for 5 min (λ_{irr}=470 nm). Similar with complex **1**, two new peaks were assigned to bis-aquated (★) and mono-aquated (■) complex, respectively.

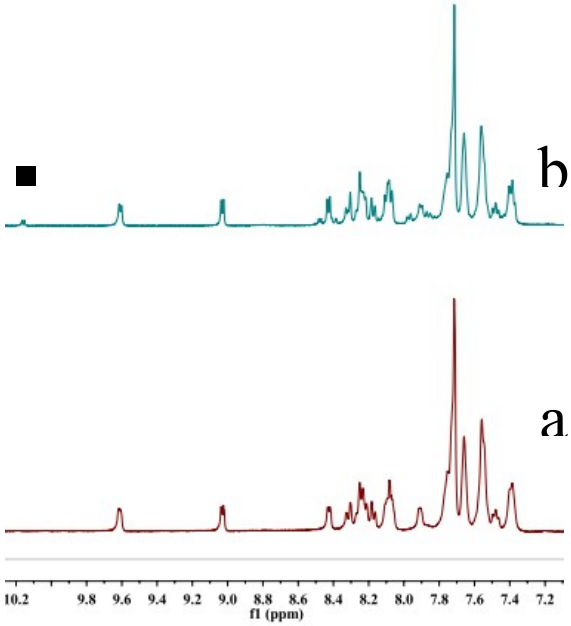
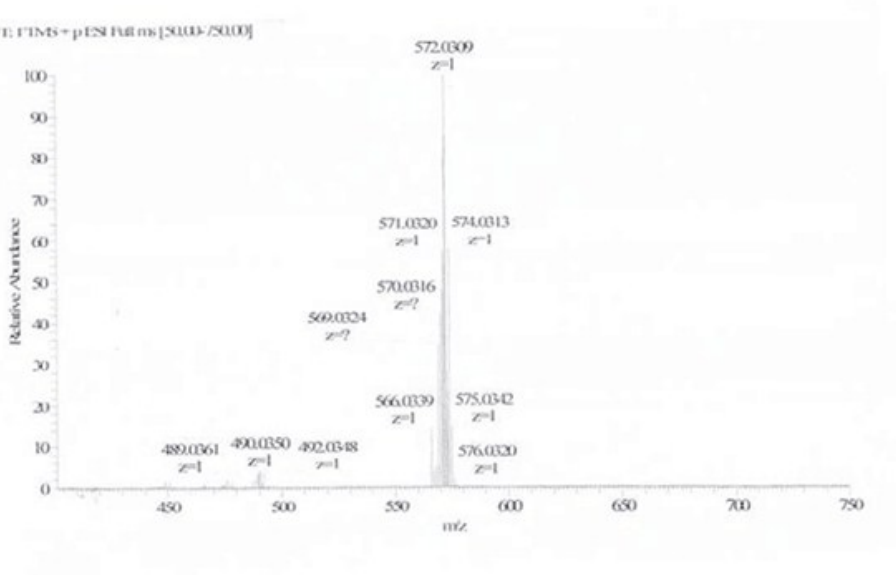


Fig. S6 ^{1}H NMR spectra changes of **4** in Ar-saturated D_2O: (a) before irradiation, (b) irradiation for 5 min (λ_{irr}=470 nm). Only one new mono-aquated peak was observed (labeled by ■), which was also consistent with its relatively low photo-induced ligand dissociation quantum yield.

1



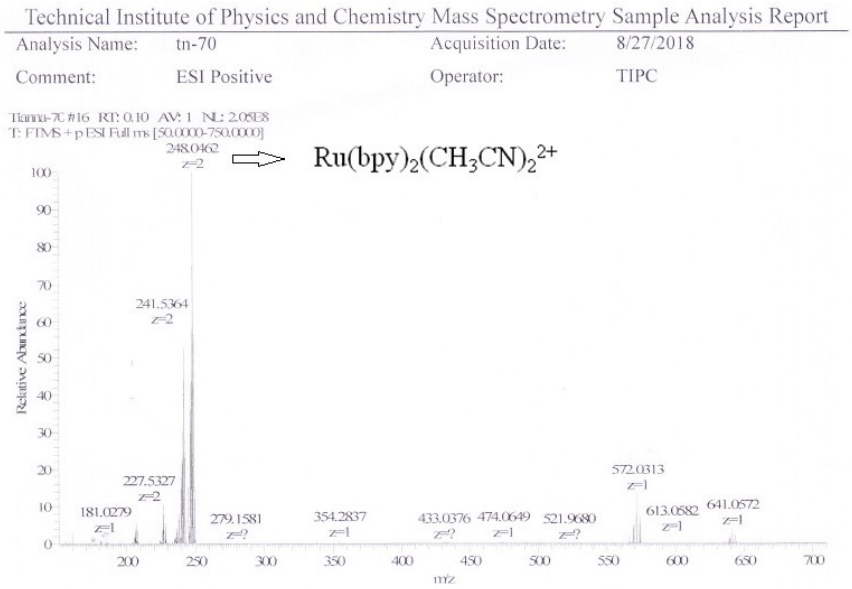
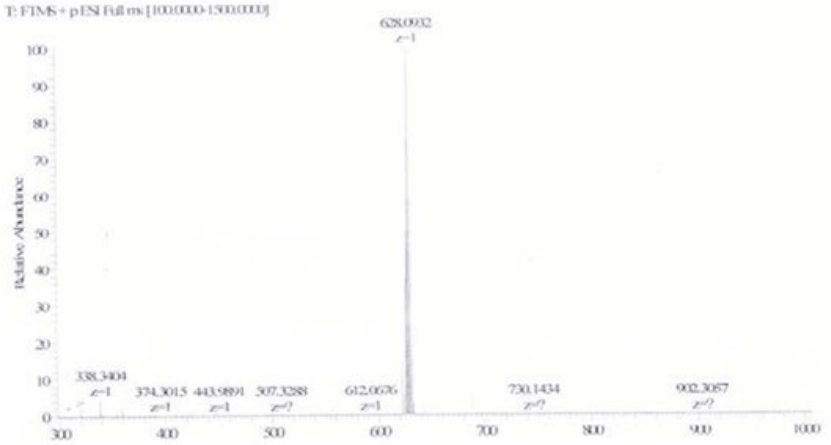


Fig. S7 HR ESI-MS spectra of **1** before (top) and after 470 nm light irradiation (bottom) in CH_3CN.

2



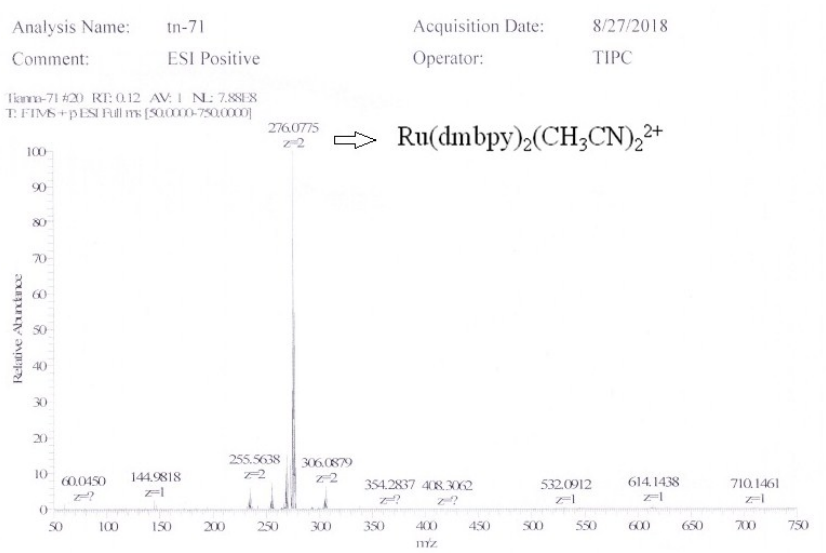
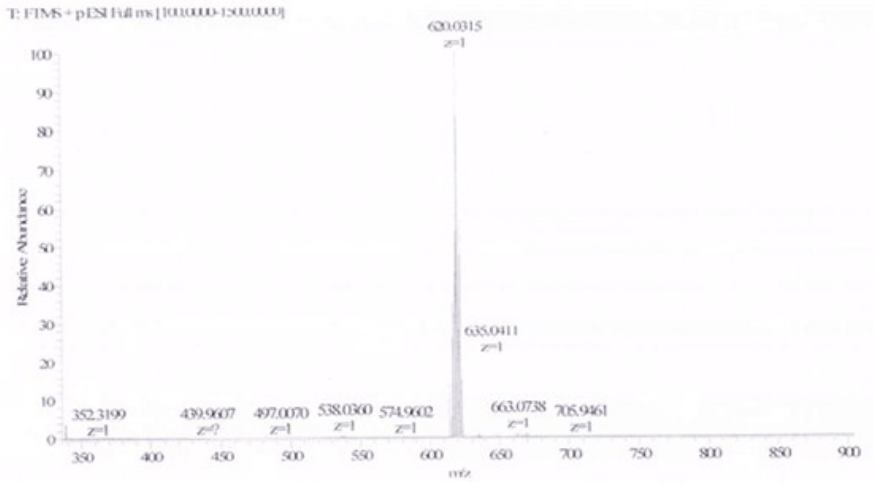


Fig. S8 HR ESI-MS spectra of **2** before (top) and after 470 nm light irradiation (bottom) in CH_3CN.

3



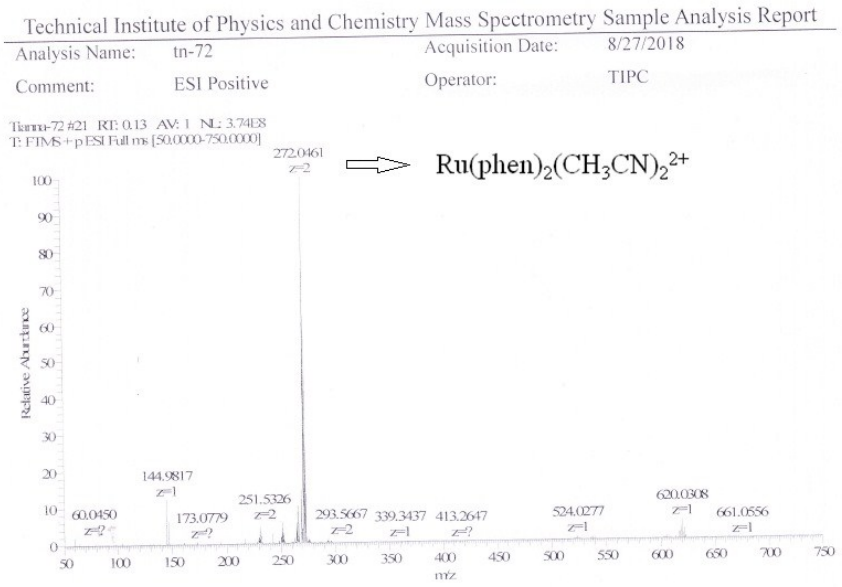
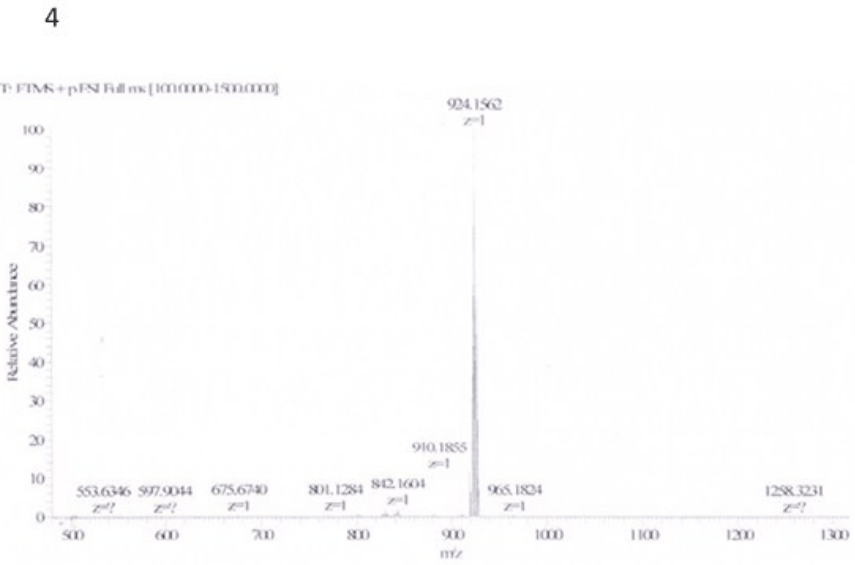


Fig. S9 HR ESI-MS spectra of **3** before (top) and after 470 nm light irradiation (bottom) in CH_3CN.



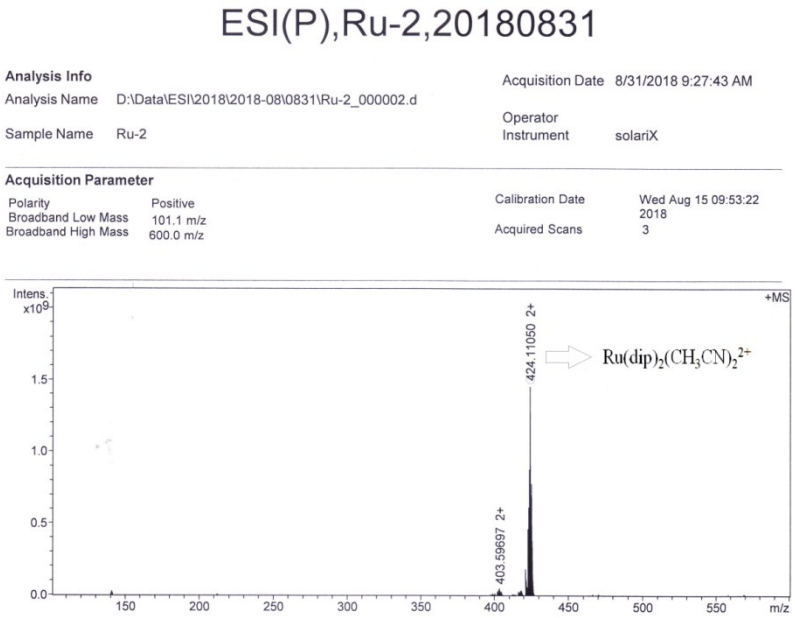


Fig. S10 HR ESI-MS spectra of **4** before (top) and after 470 nm light irradiation (bottom) in CH_3CN.

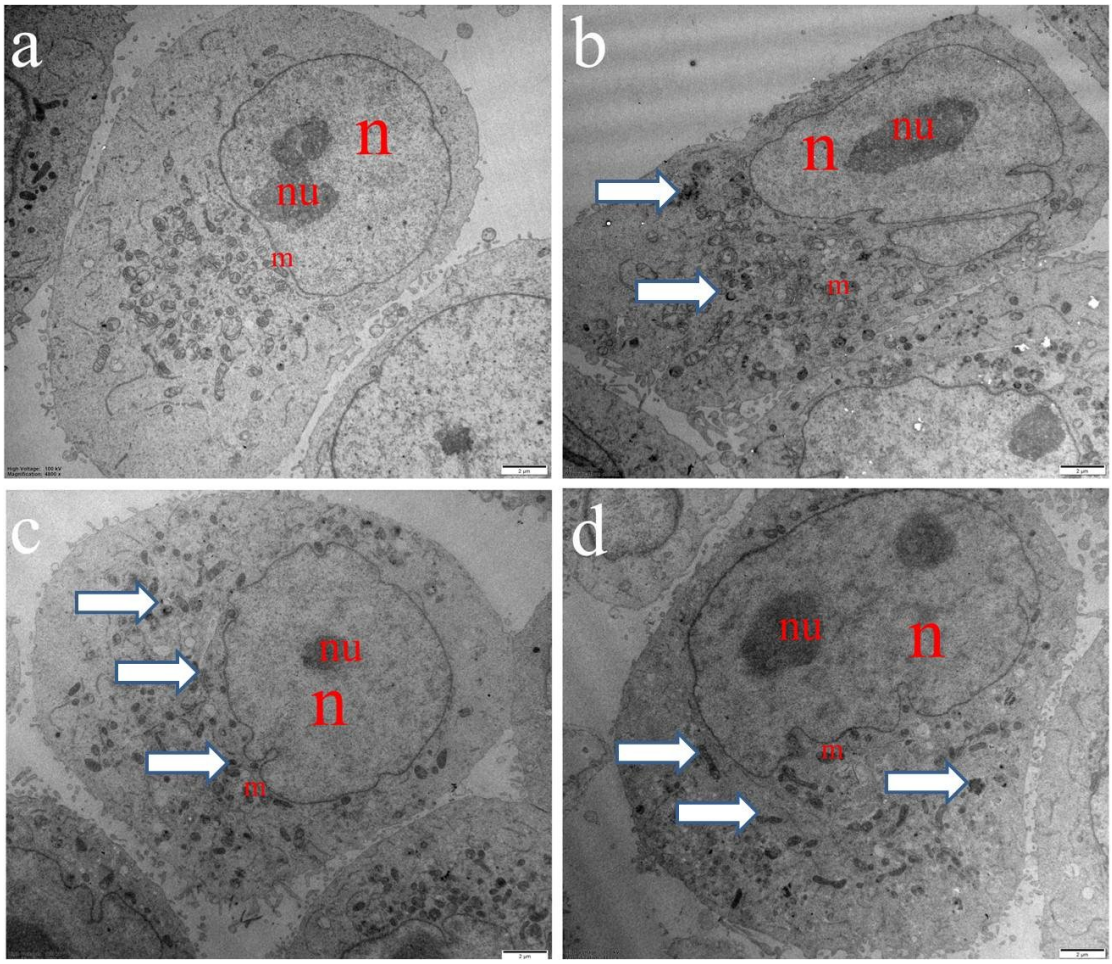


Fig. S11 TEM images of SKOV-3 cells incubated with control (a), **1**(b), **2**(c), **3** (d) and stained with osmium tetroxide, (The white arrows indicated the accumulated Ru complex, n=nucleus, nu=nucleolus, m=mitochondria).

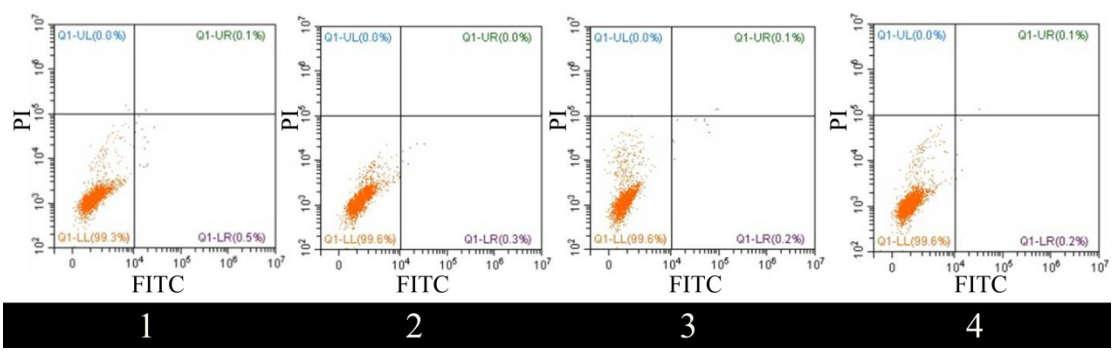


Fig. S12 The percentage of apoptotic SKOV-3 cells analyzed by flow cytometry. (1) Dark control, with no complex added; (2-4) SKOV-3 cells incubated with complex **1-3**(100nM) for 4 h, respectively, cell medium discarded and added with fresh medium, then irradiated for 0.5 h (470nm LED, 22.5mW/cm^2), and incubated for more 10 h in the dark.

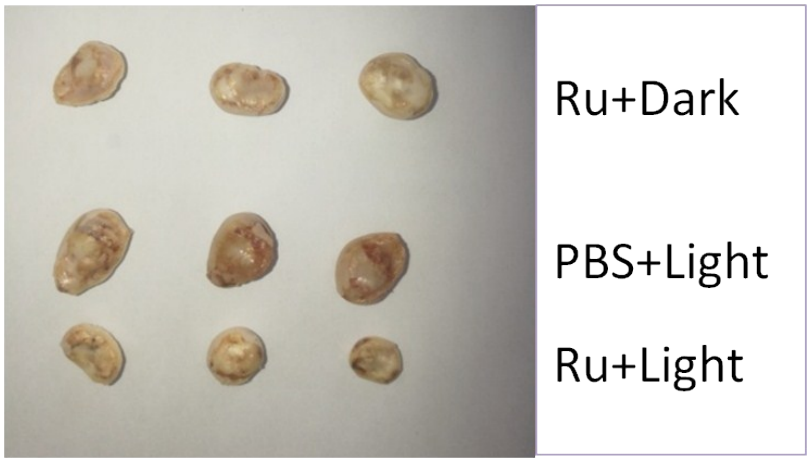


Fig. S13 Solid tumors extracted from mice treated after 12 days.

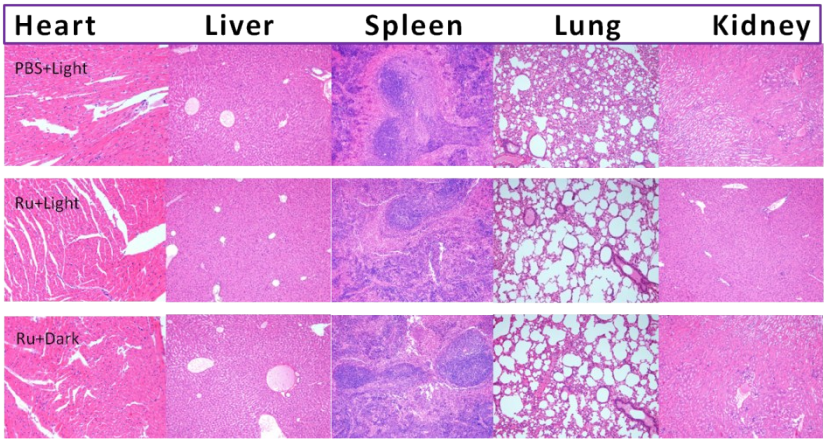


Fig. S14 H&E staining images of important organs of different groups: PBS+light, Ru+Light, Ru+dark groups after12 days treatment.

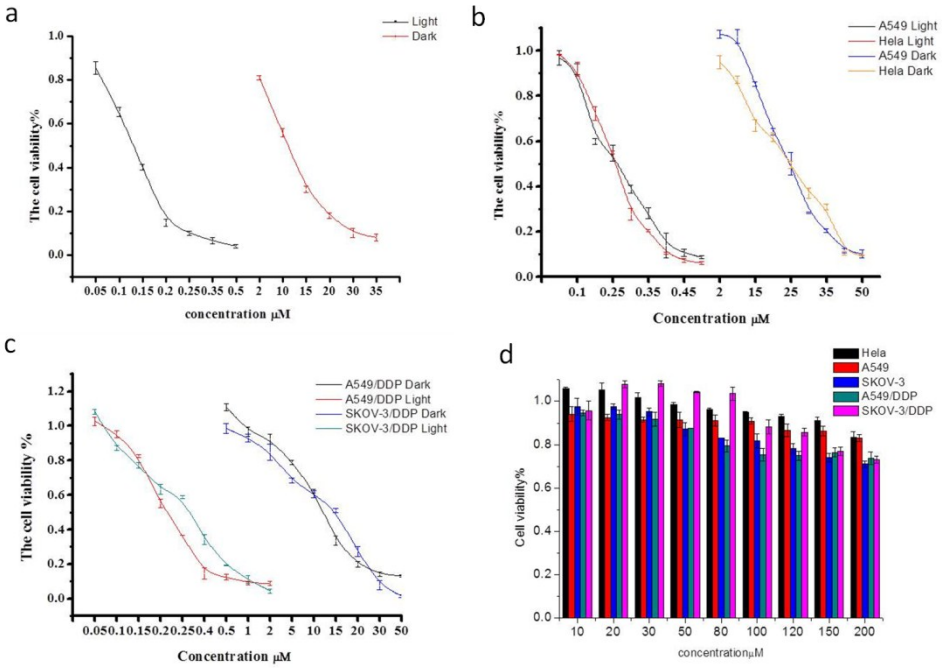


Fig. S15 Partial MTT assays of different cells. (a) SKOV-3 Cell viabilities treated with complex **4**; (b) A549 and Hela cell viabilities treated with complex **4**; (c) A549 DDP and SKOV-3 DDP cells viabilities treated with complex **4**; (d) Cell viabilities treated with complex **3** upon irradiation for 30 min using 470 nm LED (22.5 mW/cm^2).

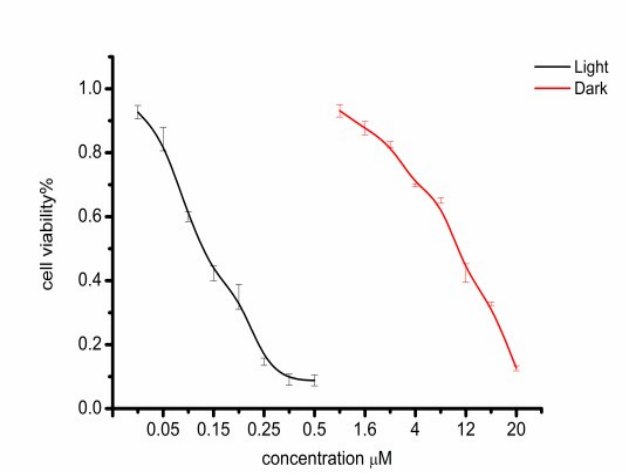


Fig. S16 MTT assays of normal L-02 cells. Cells treated with complex **4** upon irradiation for 30 min using 470 nm LED (22.5 mW/cm^2) or in the dark.

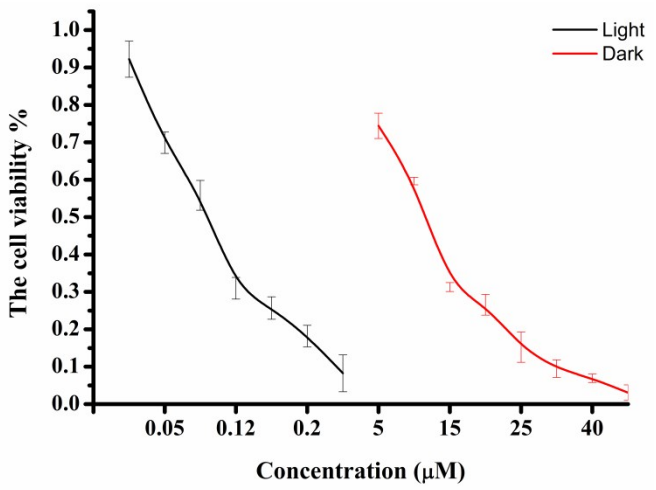


Fig. S17 MTT assays of SKOV-3 cells under hypoxia condition. Cells treated with complex **4** upon irradiation for 30 min using 470 nm LED (22.5 mW/cm^2) or in the dark.

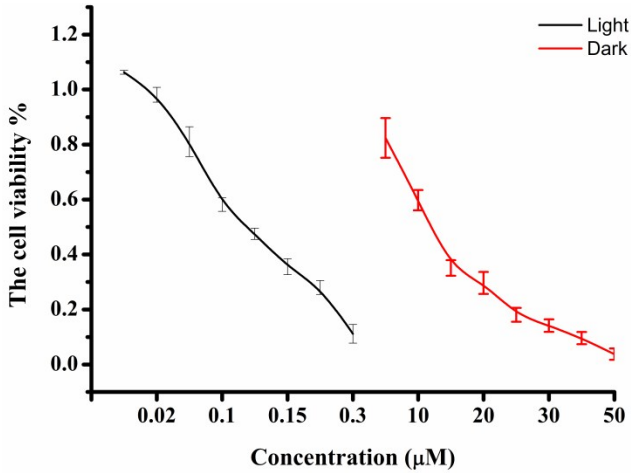


Fig. S18 MTT assays of 4T1 cells. Cells treated with complex **4** upon irradiation for 30 min using 470 nm LED (22.5 mW/cm^2) or in the dark.

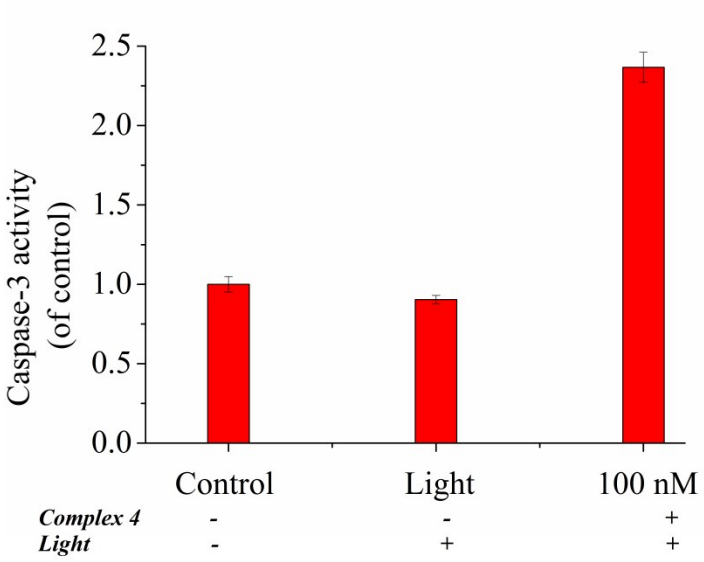


Fig. S19 Caspase levels of SKOV-3 cells relative to the control.

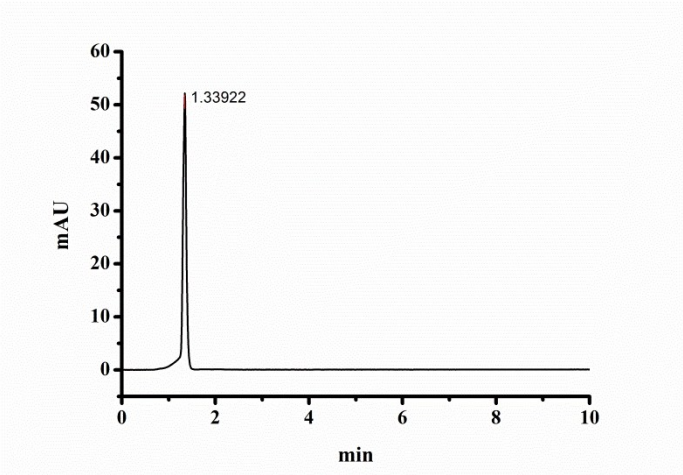


Fig. S20 HPLC of **1**.

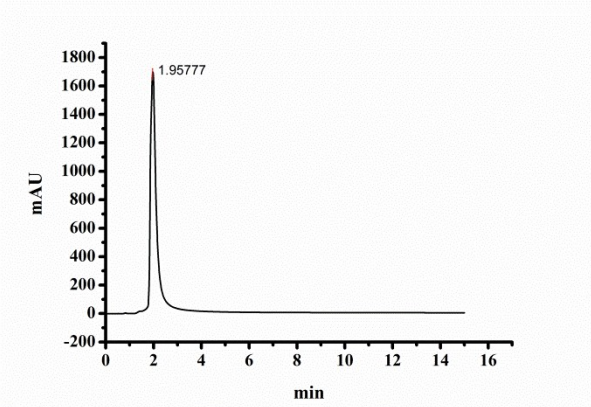


Fig. S21 HPLC of **2**.

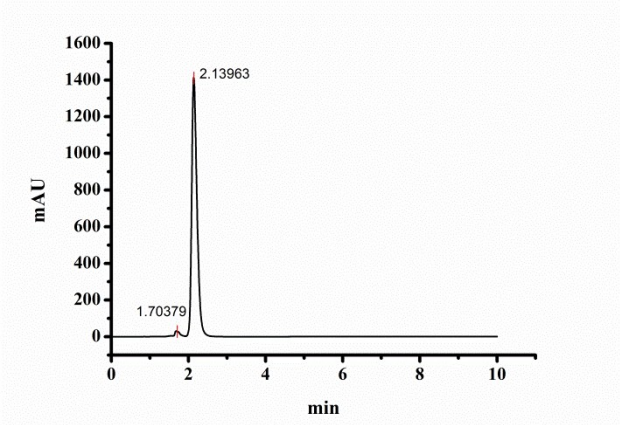


Fig. S22 HPLC of **3**.

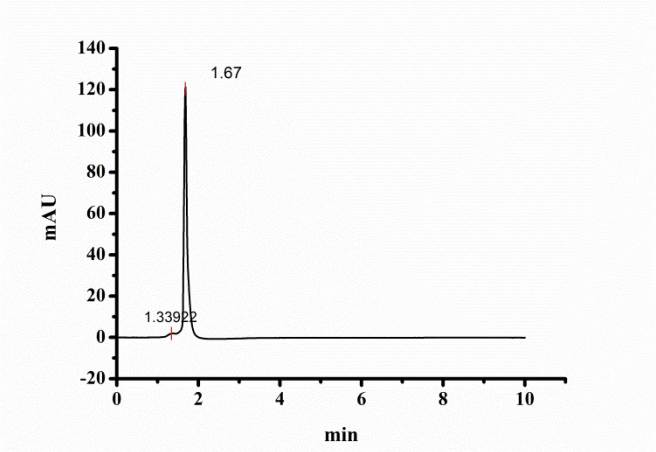


Fig. S23 HPLC of **4**.