Electronic Supplementary Material (ESI) for Dalton Transactions.

Biocompatible hypocrellin A-Fe(III) nanoparticles exhibiting efficient photo-activated CDT *in vitro* and *in vivo*

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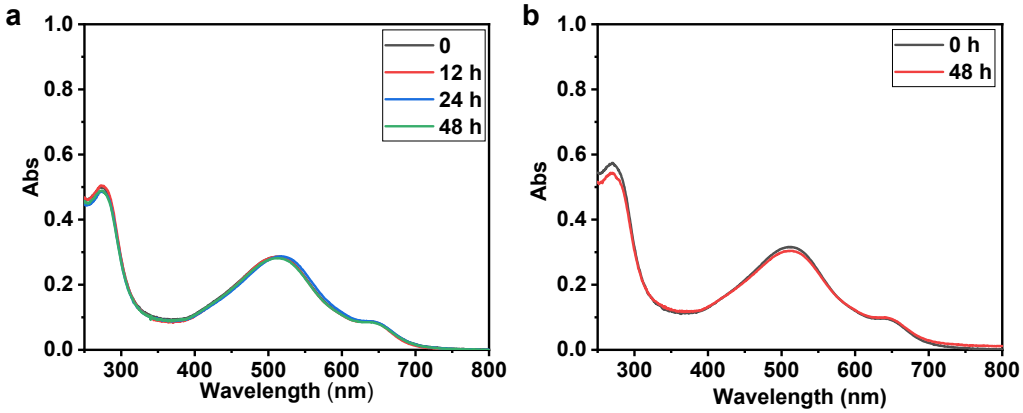

Fig. S1 (a) UV-vis absorption spectral changes of HA-Fe(III) NPs (20 μg/mL) in H_2O (containing 1% DMSO) over 48 h in the dark. (b) UV-vis absorption spectra of HA-Fe(III) NPs (the mother solution (5 mg/mL in DMSO) was diluted into 20 μg/mL in H_2O) before and after 48 h.

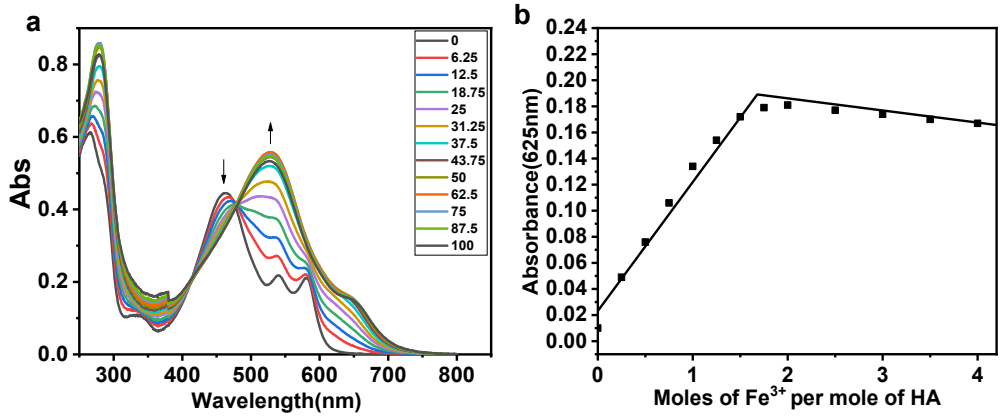

Fig. S2 (a) Absorption spectral changes of HA (25 μM) in ethanol upon addition of $FeCl_3$ (μM); (b) mole ratio plot for Fe^{3+}-HA in ethanol obtained by plotting the absorbance at 625 nm as a function of the mole ratio of Fe^{3+} to HA.

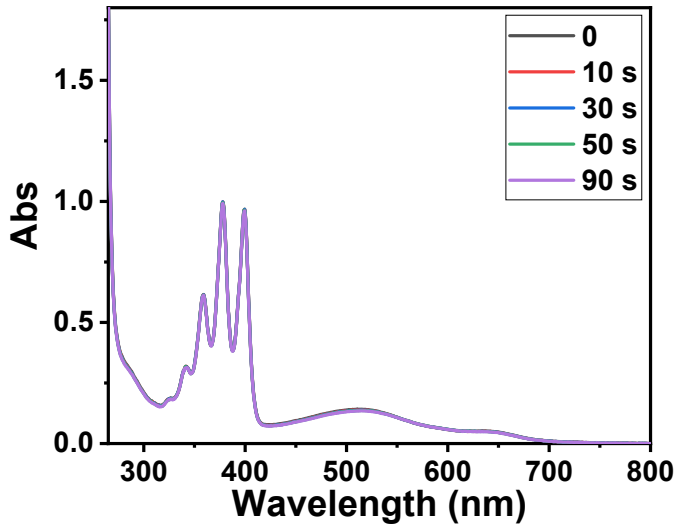

Fig.S3 Degradation of ABDA in the presence of HA-Fe(III) NPs (10 μg/mL) upon 600 nm irradiation (22.5 mW/cm^2) with different times.

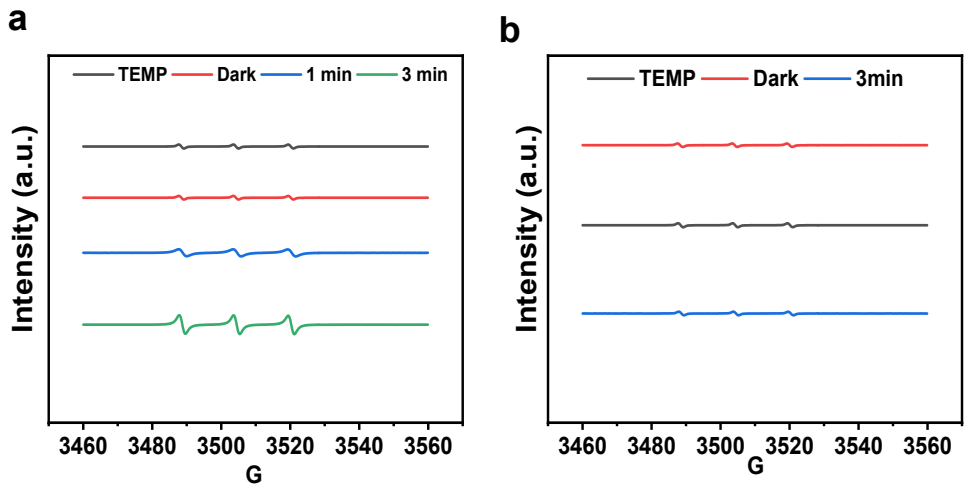

Fig S4 EPR spectra of HA (0.2 mM) (a) or HA-Fe(III) NPs (with the same absorbance as HA at 600 nm) (b) in air-saturated DMSO (containing 20 mM TEMP) in the dark or upon irradiation (600 nm, 22.5 mW cm^{-2}).

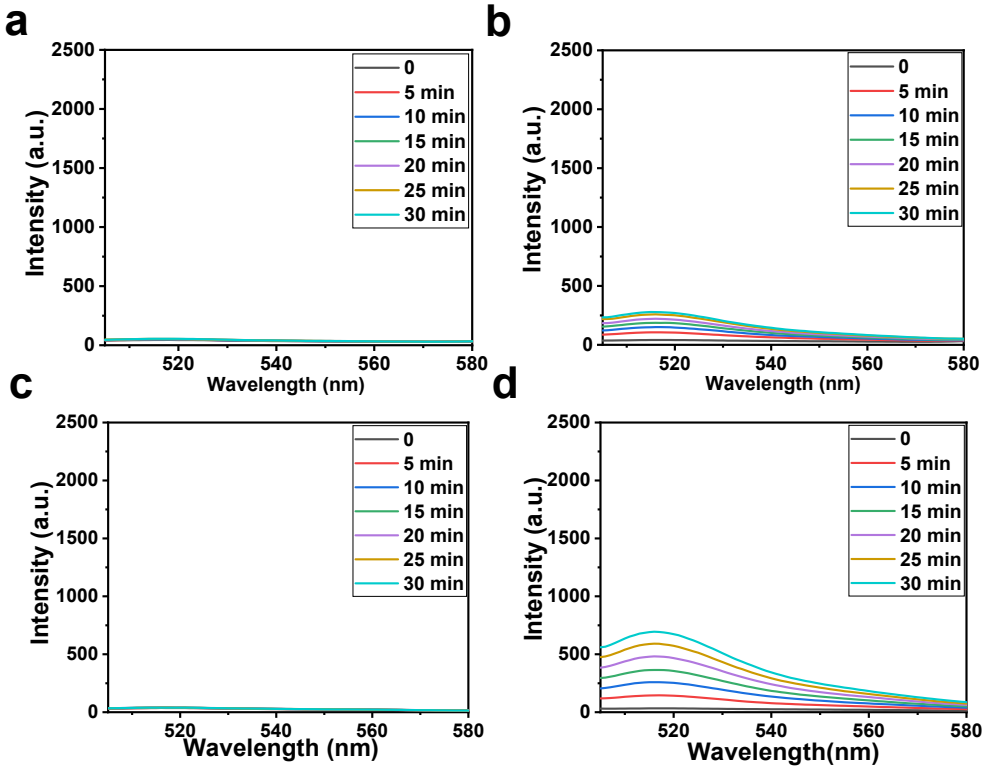

Fig.S5 Photoinduced •OH generation ability of HA and HA-Fe(III) NPs (the absorbance at 600 nm was adjusted to the same as that of HA) using HPF (10 μM) as a •OH fluorescence probe in PBS. (a) HA + Dark; (b) HA + Light (600 nm LED, 22.5 mW cm^{-2}); (c) HA-Fe(III) NPs + Dark; (d) HA-Fe(III) NPs + Light (600 LED, 22.5 mW cm^{-2}). The fluorescence spectra were recorded using excitation wavelength of 490 nm.

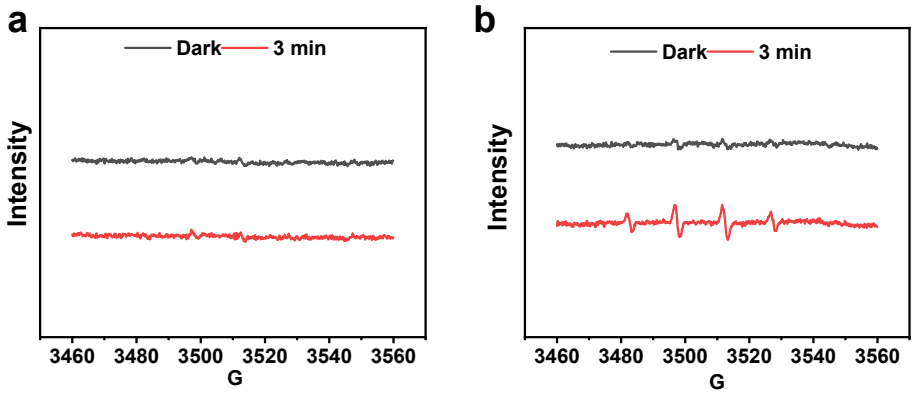

Fig. S6 EPR spectra of HA (0.3 mM) (a) or HA-Fe(III) NPs (with the same absorbance as HA at 600 nm) (b) in air-saturated PBS (containing 20 mM DMPO) in the dark or upon irradiation (600 nm, 22.5 mW cm^{-2}).

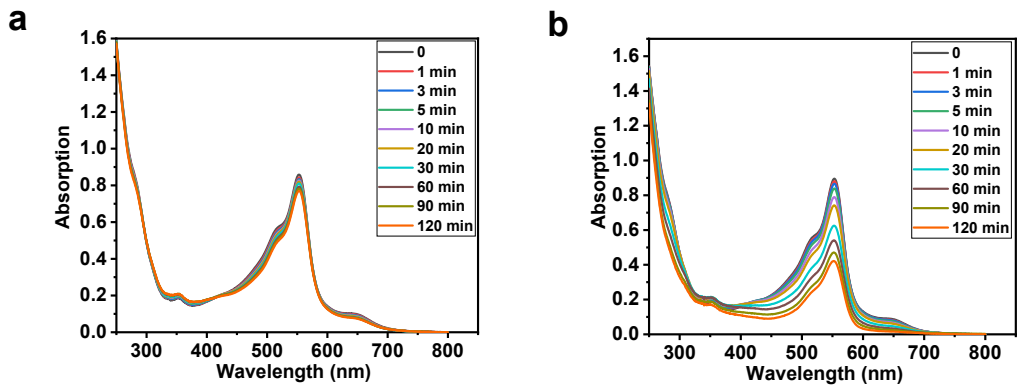

Fig. S7 UV-vis spectral changes of Rhodamine B (RhB) under different conditions. (a) HA-Fe(III) NPs (25 μg/mL) + RhB (40 μM) + H_2O_2 (8.8 mM) + dark; (b) HA-Fe(III) NPs (25 μg/mL) + RhB (40 μM) + H_2O_2 (8.8 mM) + Light (600 nm, 22.5 mW/cm^2).

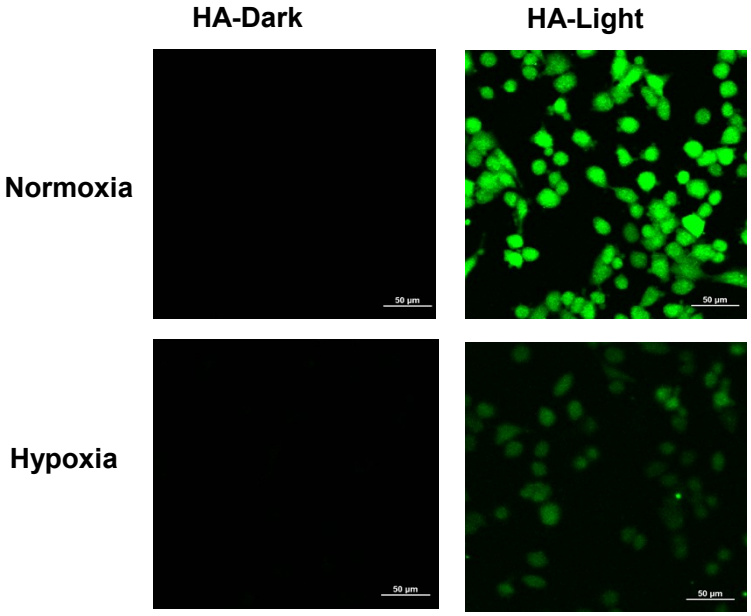

Fig. S8 Confocal fluorescence images of A549 intracellular ROS levels. Cells were treated with HA (0.14 μM) under normoxia (21% O_2) or hypoxia (3% O_2). The light groups were irradiated by 600 nm LED for 30 min (22.5 mW cm^{-2}). DCFH-DA was used as the ROS probe. Scale bars: 50 μm.

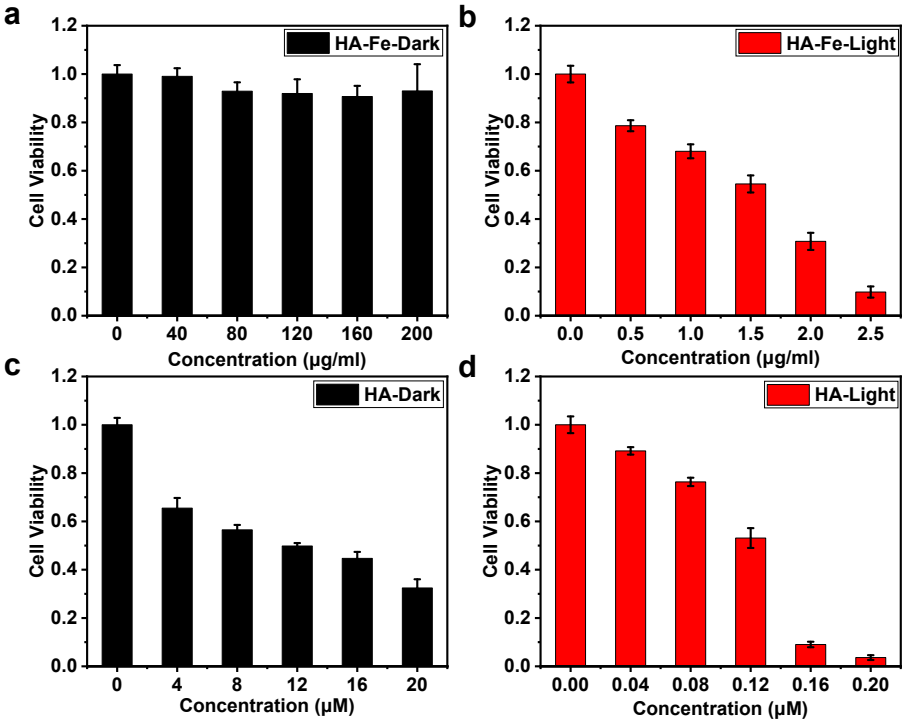

Fig. S9 Cell viability of cisplatin-resistant A549 cells treated by HA-Fe(III) NPs or HA in the dark or under light irradiation for 30 min (600 nm, 22.5 mW cm^{-2}).

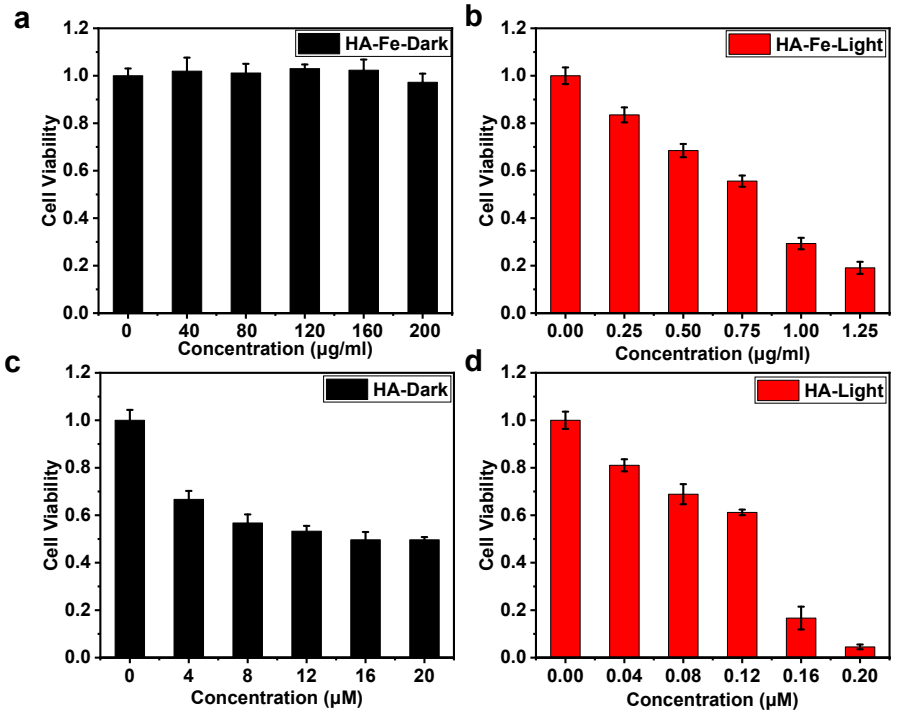

Fig. S10 Cell viability of SKOV-3 cells incubated with HA-Fe(III) NPs or HA in the dark or under light irradiation for 30 min (600 nm, 22.5 mW cm^{-2}).

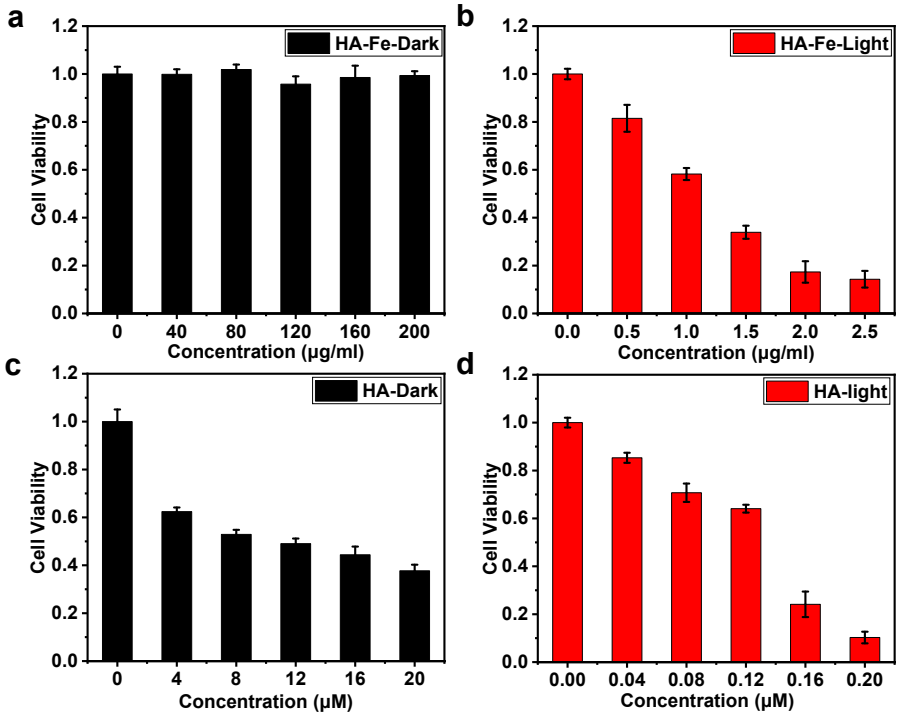

Fig. S11 Cell viability of A549 cells incubated with HA-Fe(III) NPs or HA in the dark or under light irradiation for 30 min (600 nm, 22.5 mW cm^{-2}).

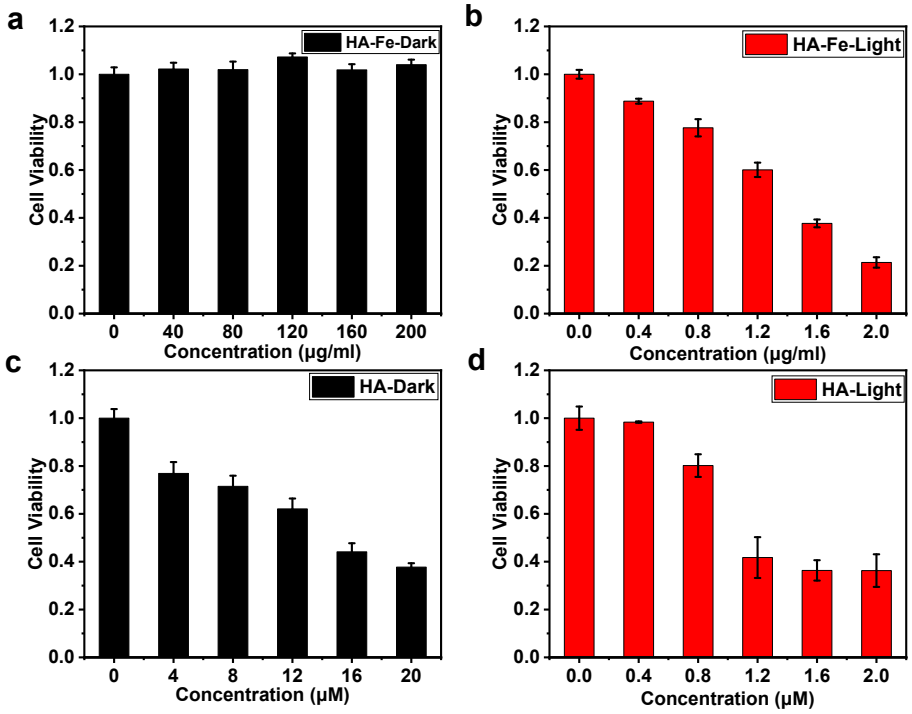

Fig. S12 Cell viability of A549 cells (in hypoxia, 3% O_2) incubated with HA-Fe(III) NPs or HA in the dark or under light irradiation for 30 min (600 nm, 22.5 mW cm^{-2}).

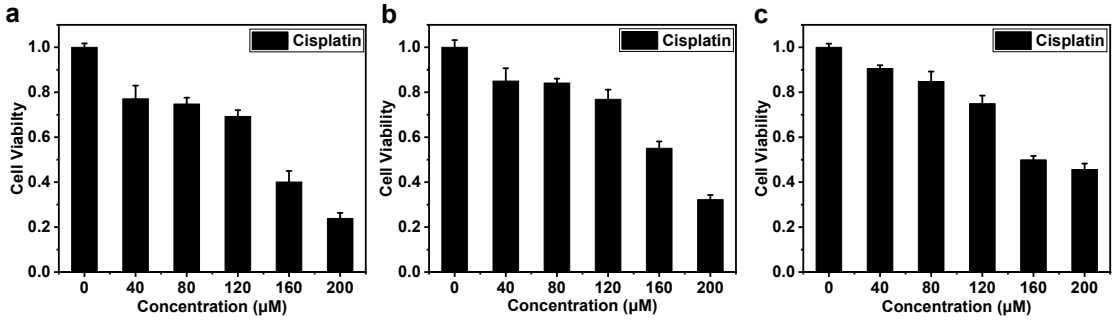

Fig. S13 Cytotoxicity of cisplatin towards A549 (left), cis-A549 (middle) and SKOV3 cells (right).

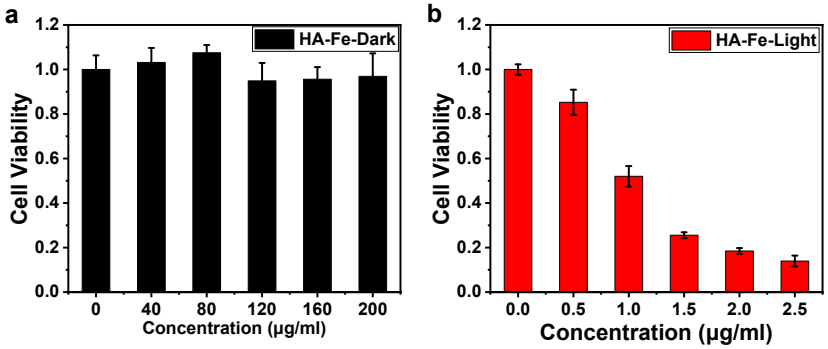

Fig. S14 Cell viability of ISOE80 cells incubated with HA-Fe(III) NPs in the dark or under light irradiation for 30 min (600 nm, 22.5 mW cm^{-2}).

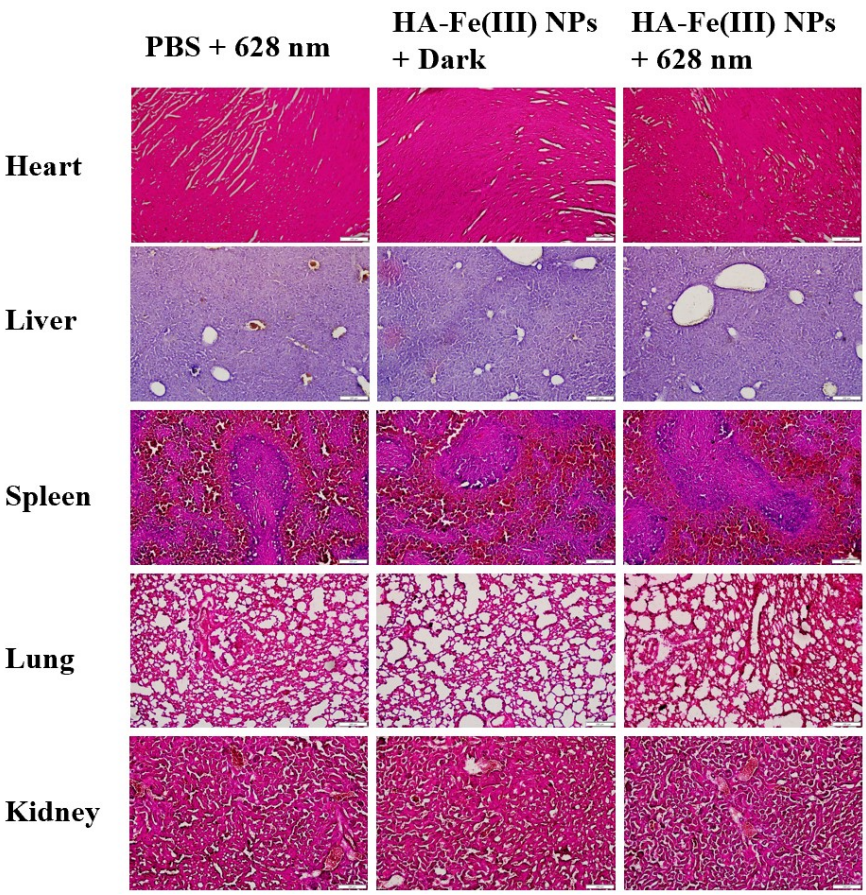

Fig. S15 Histological analysis of the organs acquired from the mice bearing 4T1 tumors on the 14th day after various treatments. Scale bars: 200 μm.