

Electronic Supplementary Information

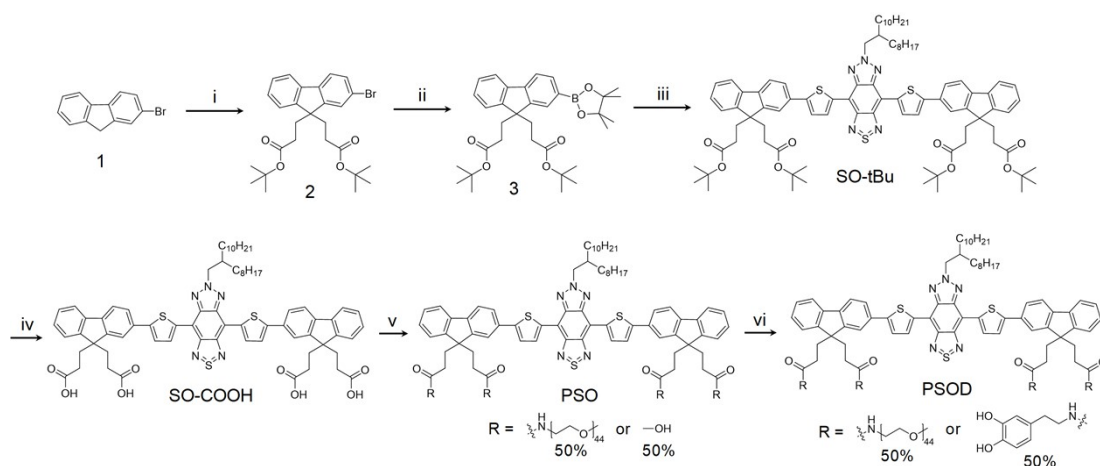
Iron-Chelated Semiconducting Oligomer Nanoparticles for NIR-II Fluorescence Imaging-Guided Enhanced Chemodynamic/Photothermal Combination Therapy

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1. Supporting figures



Scheme S1 Synthetic route of PSOD. Reagents and conditions: i) tert-butyl acrylate, tetrabutylammonium bromide, KOH, toluene, N₂, 25 °C, 12 h; ii) Pd(dppf)₂Cl₂, bis(pinacolato)diboron, KOAc, dimethylformamide (DMF), 90 °C, 12 h; iii) benzothiadiazolethiophenedibromide (TBZ-Br), methyltrioctylammonium chloride, K₂CO₃, Pd(PPh₃)₄, H₂O, toluene, 100 °C, 24 h; iv) trifluoroacetic acid (TFA), CH₂Cl₂, room temperature, 24 h; v) mPEG-NH₂, N,N'-diisopropylcarbodiimide (DIC), 4-dimethylaminopyridine (DMAP), tetrahydrofuran (THF), N₂, room temperature, 48 h; vi) 3-hydroxytyramine hydrochloride, DIC, DMAP, THF, N₂, room temperature, 24 h.

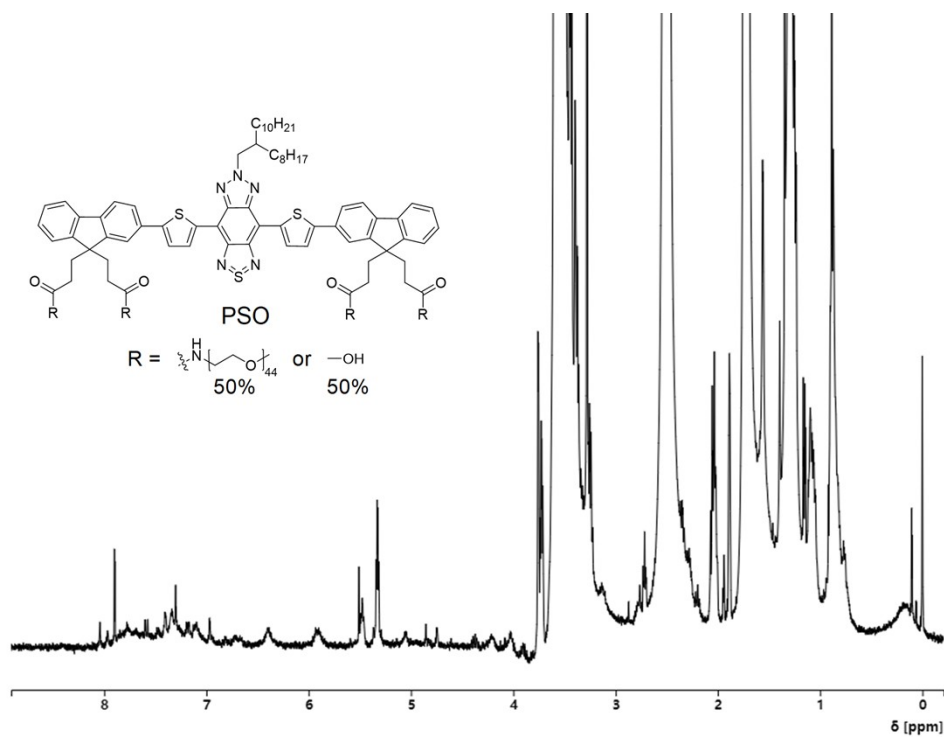


Fig. S1 ^1H NMR spectrum of PSO. THF- d_4 was used as the solvent.

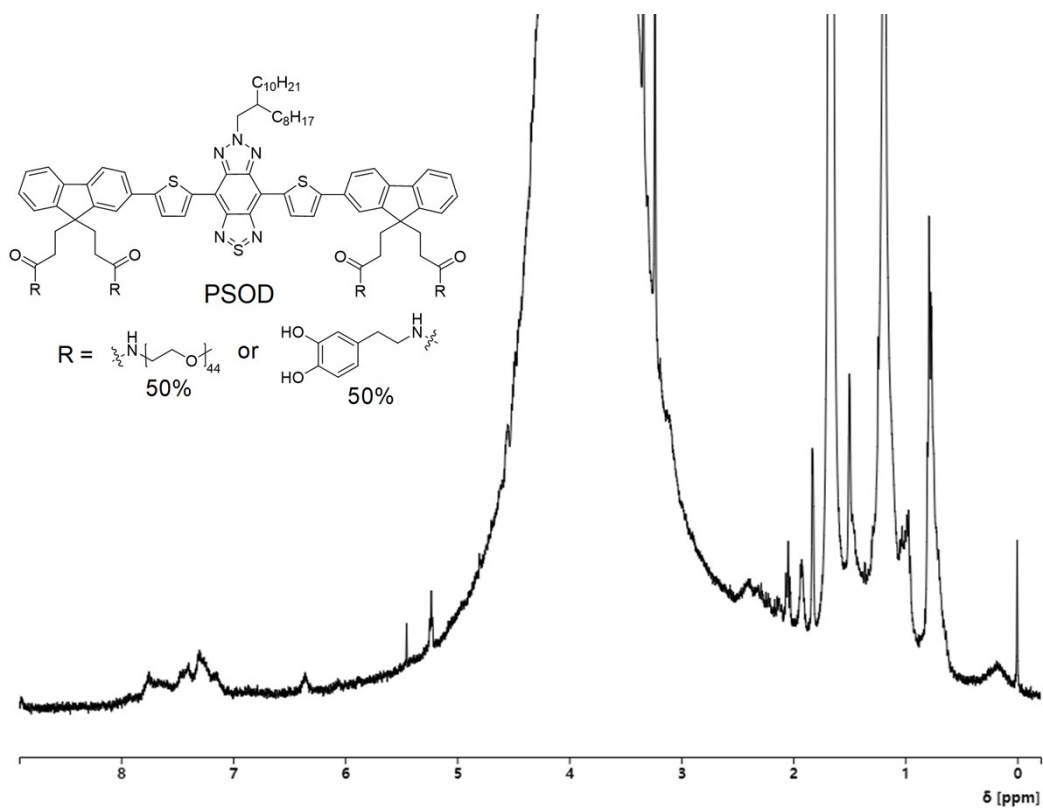


Fig. S2 ^1H NMR spectrum of PSOD. THF- d_4 was used as the solvent.

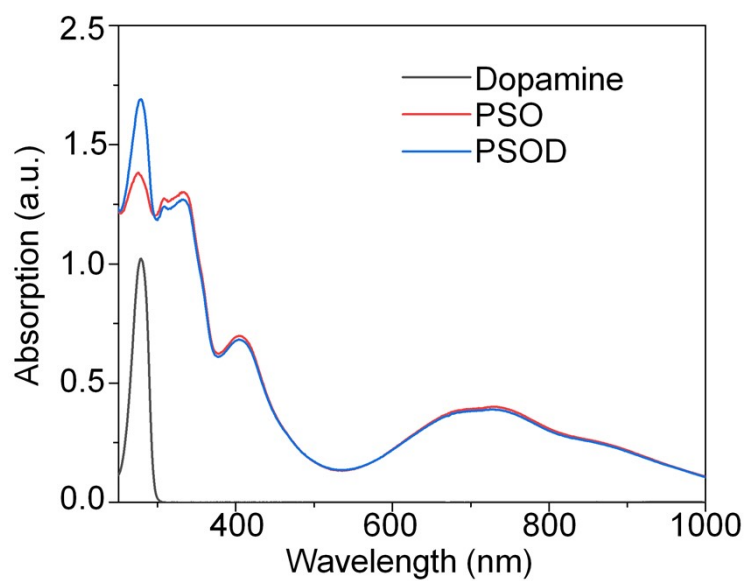


Fig. S3 Absorption spectra of dopamine, PSO and PSOD in water.

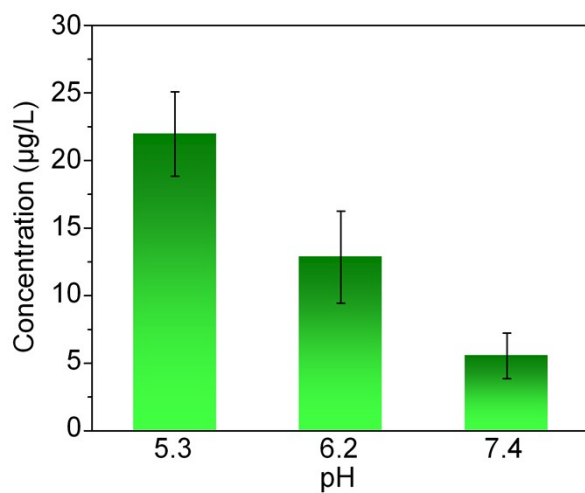


Fig. S4. Concentration of Fe³⁺ ion in DHA@FePSOD solution under different pH.

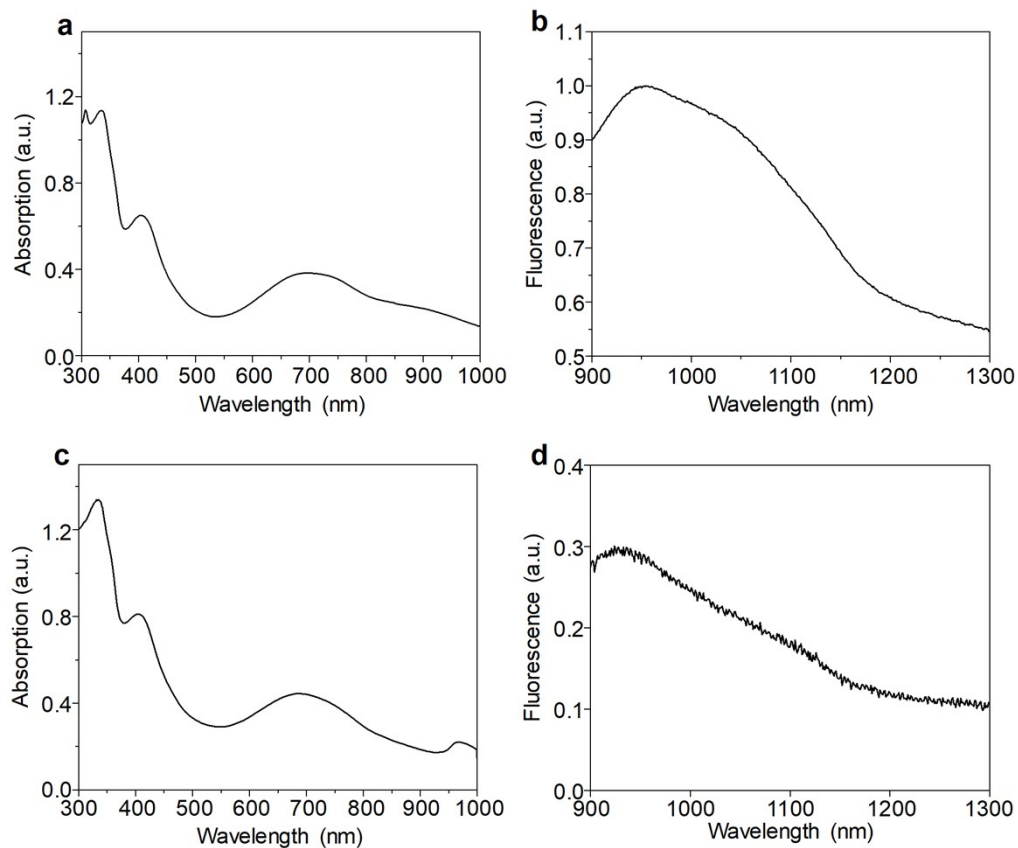


Fig. S5 Absorption (a) and emission (b) spectra of PSOD in PBS (pH 7.4). Absorption (c) and emission (d) spectra of FePSOD in PBS (pH 7.4).

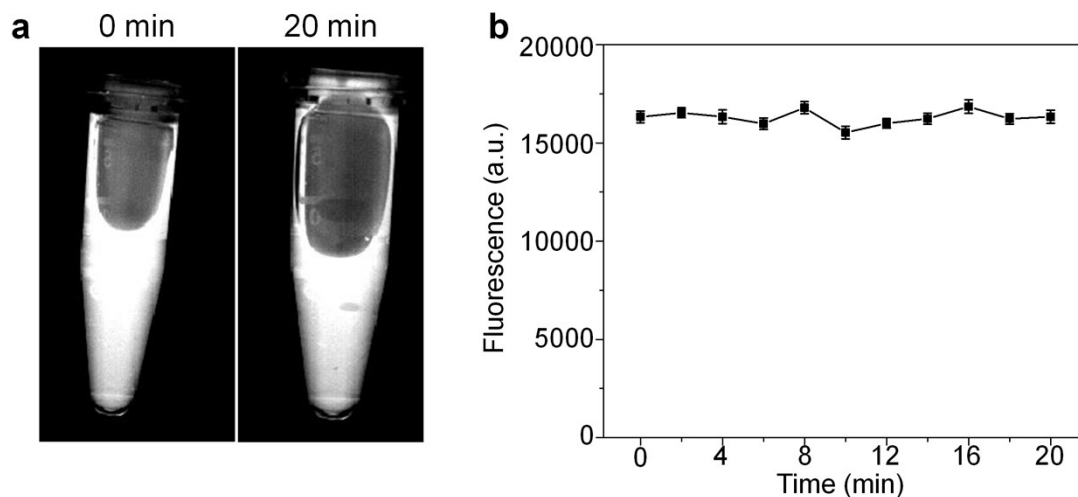


Fig. S6 (a) NIR-II fluorescence images of DHA@FePSOD solution before and after 20 min continuous laser irradiation (808 nm, 1 W/cm²). (b) NIR-II fluorescence intensity changes of DHA@FePSOD under continuous laser irradiation (808 nm, 1 W/cm²) for 20 min. The error bars represent standard deviations of three separate measurements.

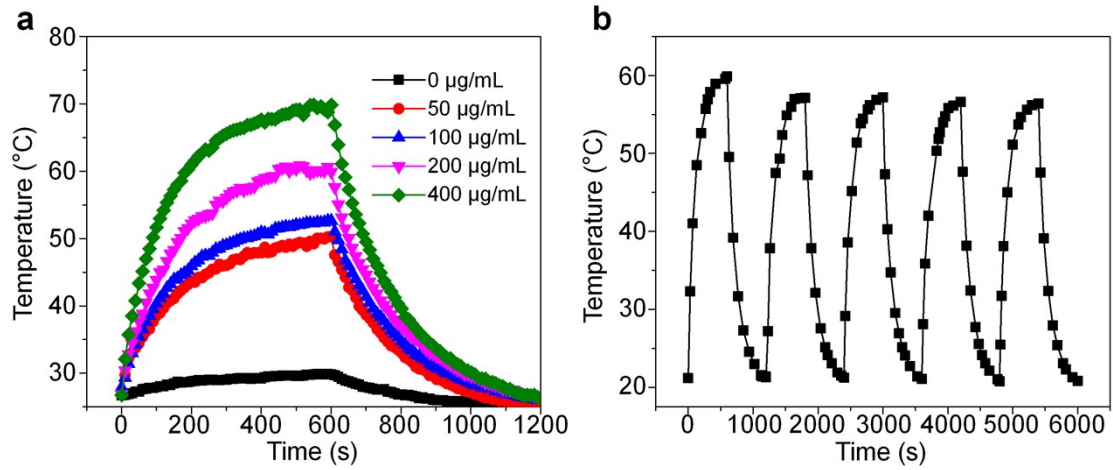


Fig. S7 (a) Heating and natural cooling curves of FePSOD with different concentrations under 808 nm laser irradiation (1 W/cm^2 , 10 min). (b) Thermal stability of FePSOD under heating and natural cooling cycles.

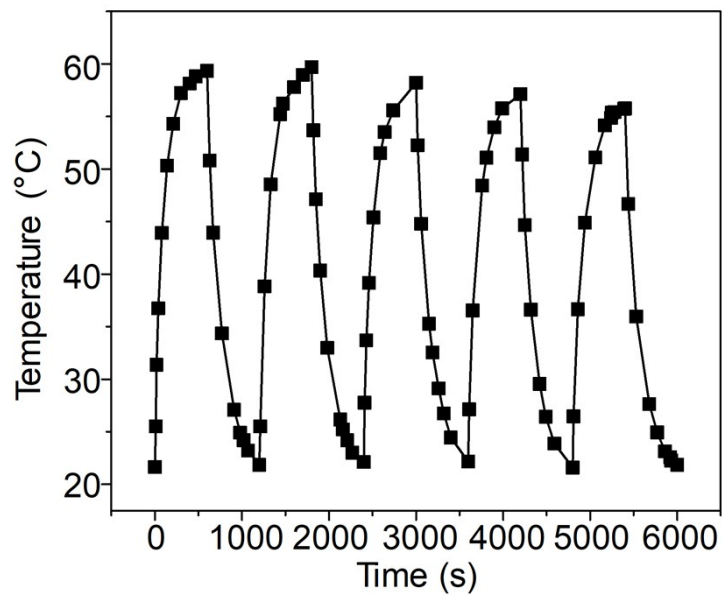


Fig. S8 Thermal stability of DHA@FePSOD under heating and natural cooling cycles.

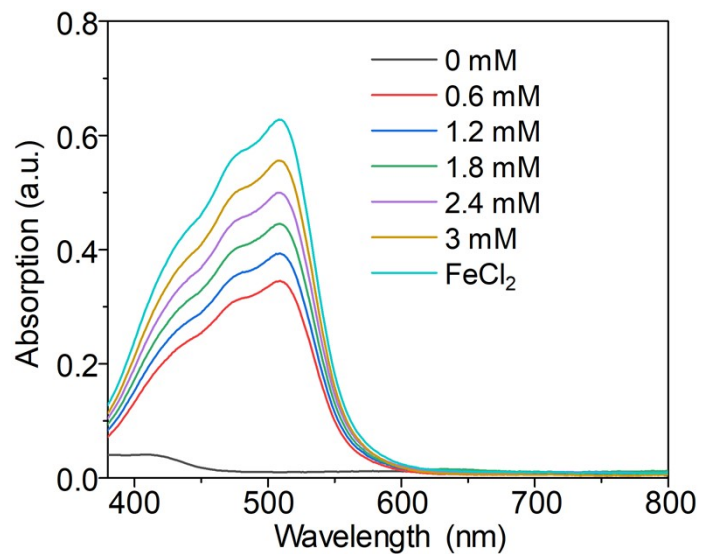


Fig. S9 Absorption of 1,10-phenanthroline under treatment of FePSOD (200 $\mu\text{g/mL}$) and different concentrations of GSH.

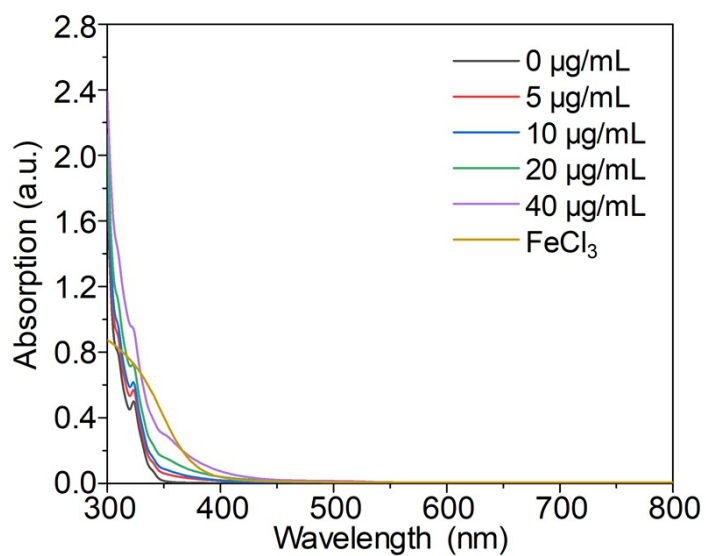


Fig. S10. Absorption spectra of Fe^{3+} ion and 1,10-phenanthroline incubated Fe^{3+} under different concentrations.

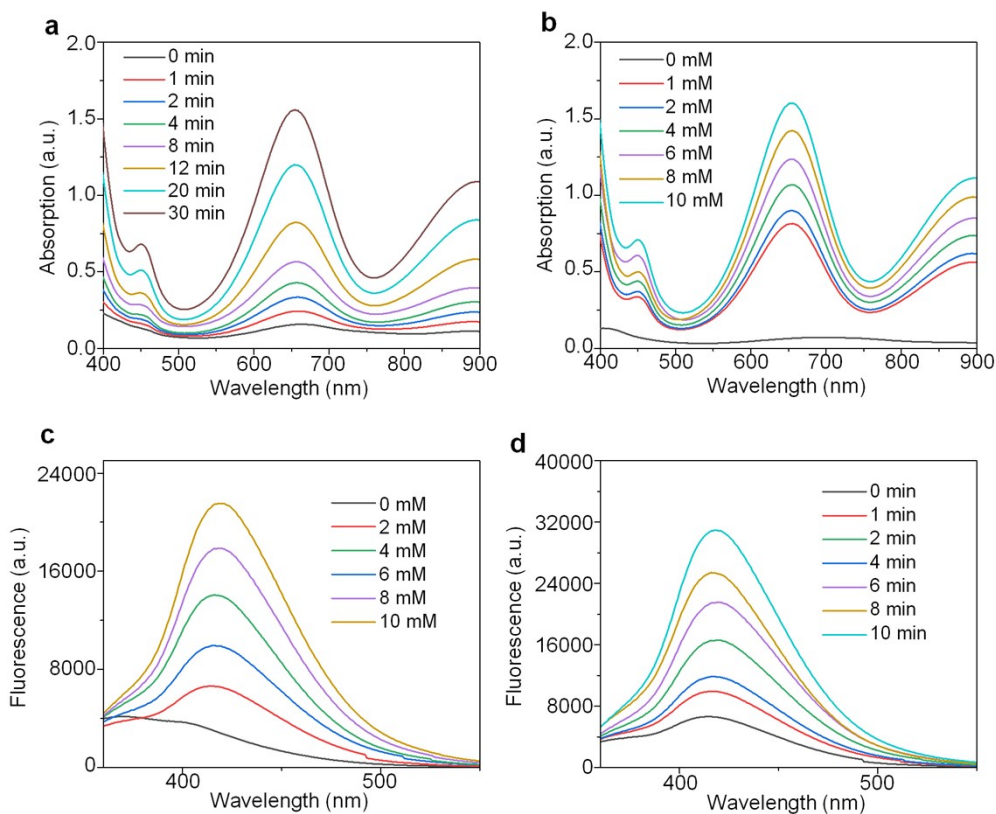


Fig. S11 (a) Absorption spectra of TMB under treatment of FePSOD (100 μg/mL), GSH (3 mM) and H₂O₂ (10 mM) at different incubation time. (b) Absorption spectra of TMB under treatment of FePSOD (100 μg/mL), GSH (3 mM) and different concentrations of H₂O₂. (c) Fluorescence spectra of 1,4-dicarboxybenzene under treatment of FePSOD (100 μg/mL), GSH (3 mM) and different concentrations of H₂O₂. (d) Fluorescence spectra of 1,4-dicarboxybenzene under treatment of FePSOD (100 μg/mL), GSH (3 mM) and H₂O₂ (10 mM) at different incubation time.

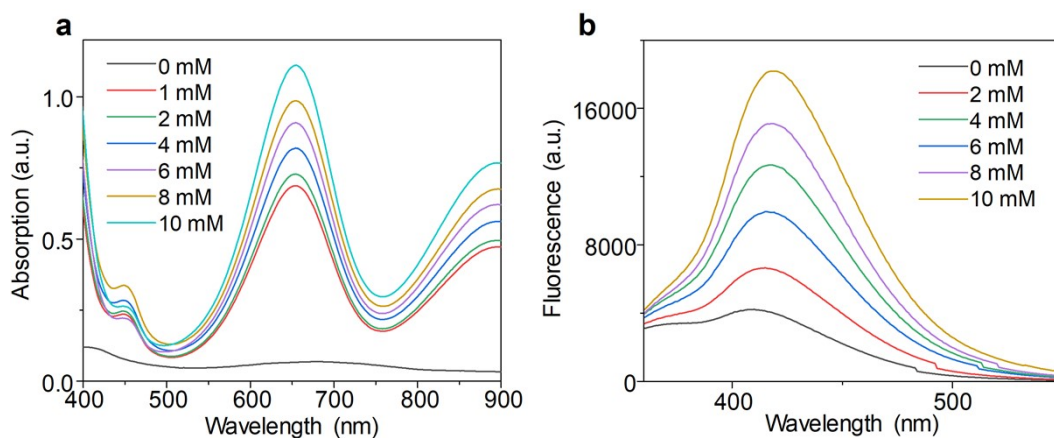


Fig. S12 (a) Absorption spectra of TMB under treatment of DHA@FePSOD (2 mg/mL), GSH (3 mM) and different concentrations of H₂O₂. (b) Fluorescence spectra of 1,4-dicarboxybenzene under treatment of DHA@FePSOD (2 mg/mL), GSH (3 mM) and different concentrations of H₂O₂.

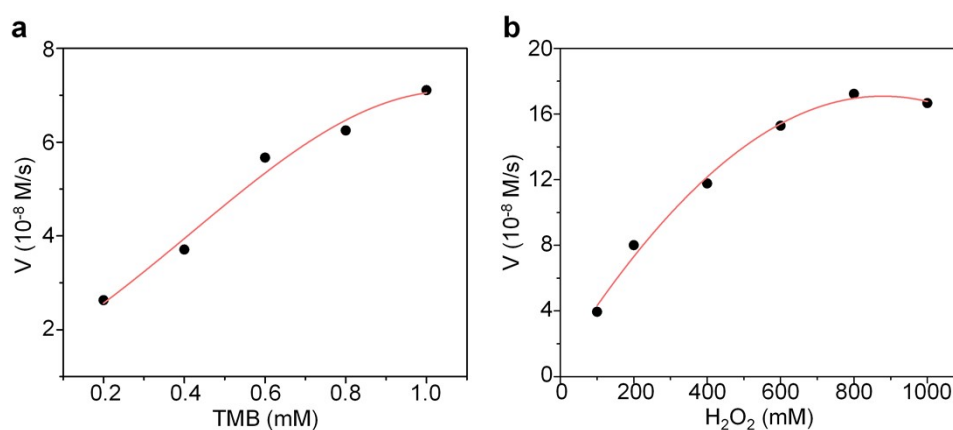


Fig. S13. (a) Michaelis-Menten curve of hydroxyl radical generation velocities versus TMB (a) or H₂O₂ (b) in the presence of DHA@FePSOD.

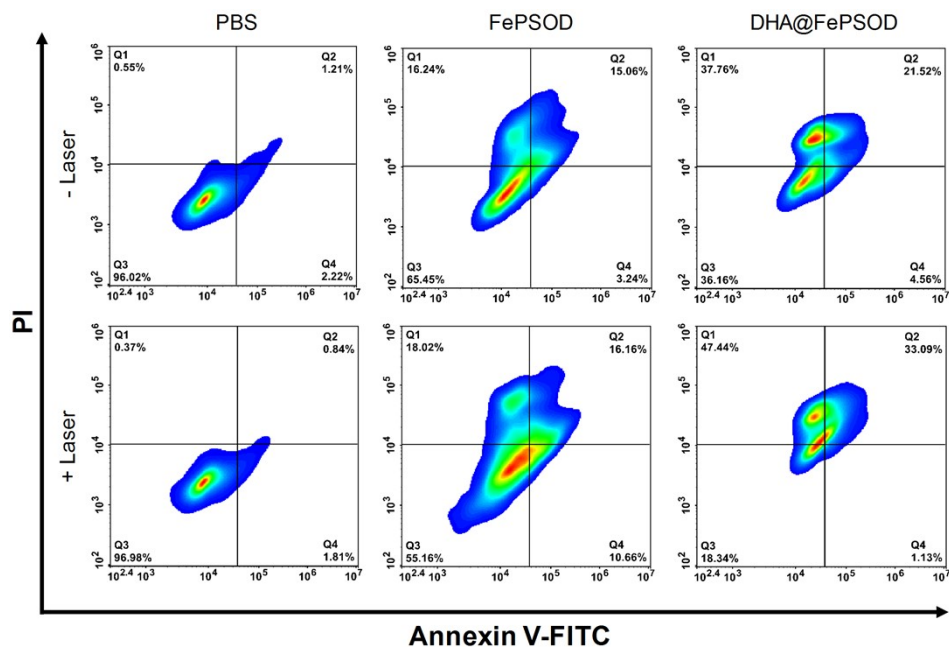


Fig. S14 Flow cytometry analysis of viability of 4T1 cells under different treatments.

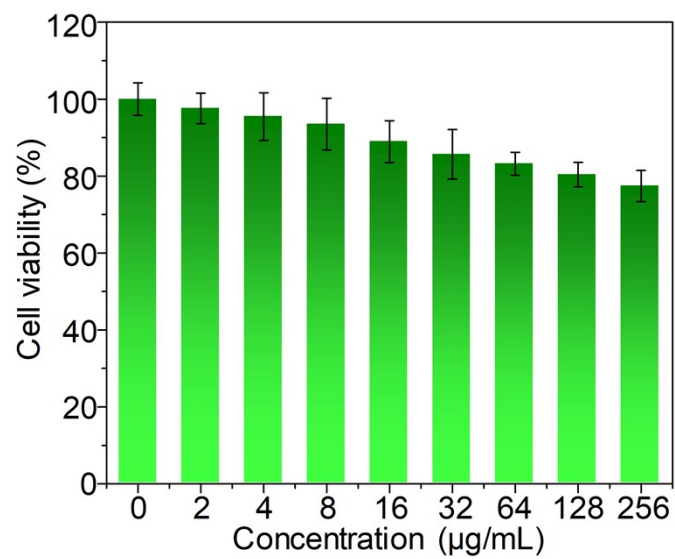


Fig. S15. Viability of NIH-3T3 cells treated with different concentrations of DHA@FePSOD without laser irradiation.

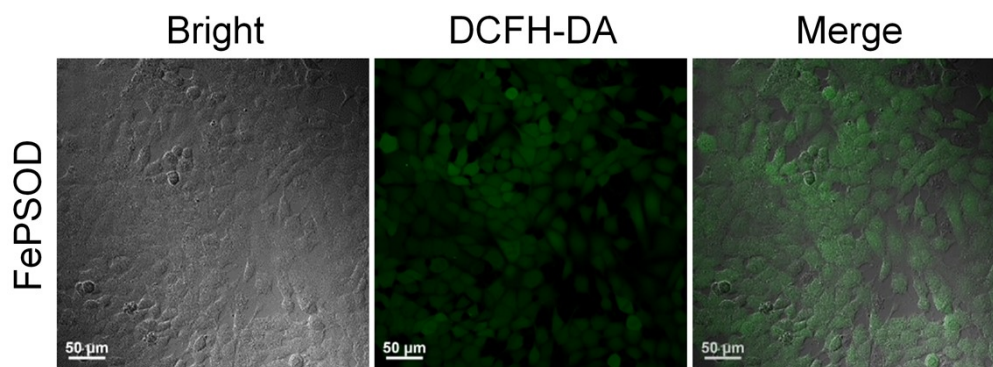


Fig. S16 Confocal fluorescence images of DCFH-DA-treated 4T1 cells incubated with FePSOD.

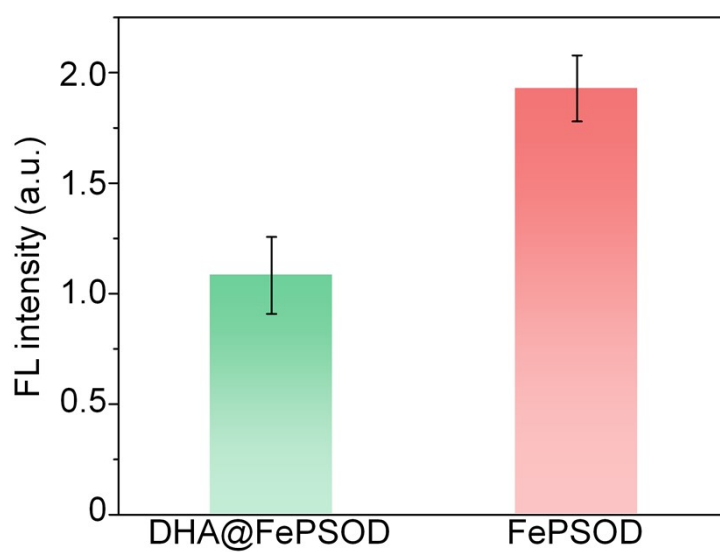


Fig. S17. Quantification of green fluorescence intensities from DCFH-DA-treated 4T1 cells incubated with FePSOD or DHA@FePSOD.

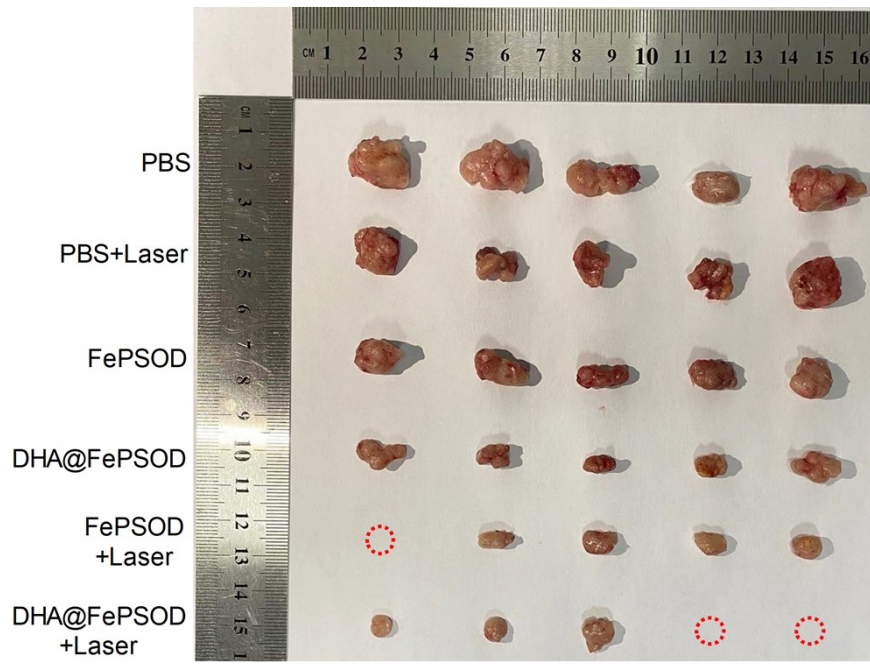


Fig. S18 Images of tumor resected from different treatment groups at $t = 16$ day.