

*Electronic Supplementary Information for*

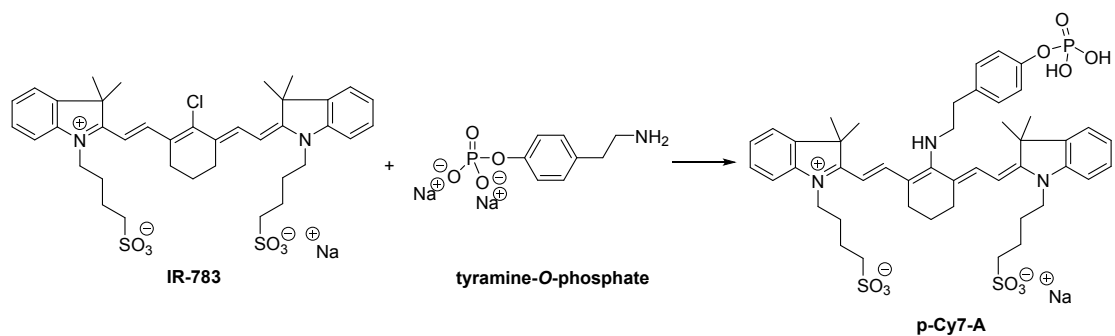
**Real-time monitoring and accurate diagnosis of drug-induced  
hepatotoxicity *in vivo* by ratio fluorescent and photoacoustic  
imagings of peroxynitrite**

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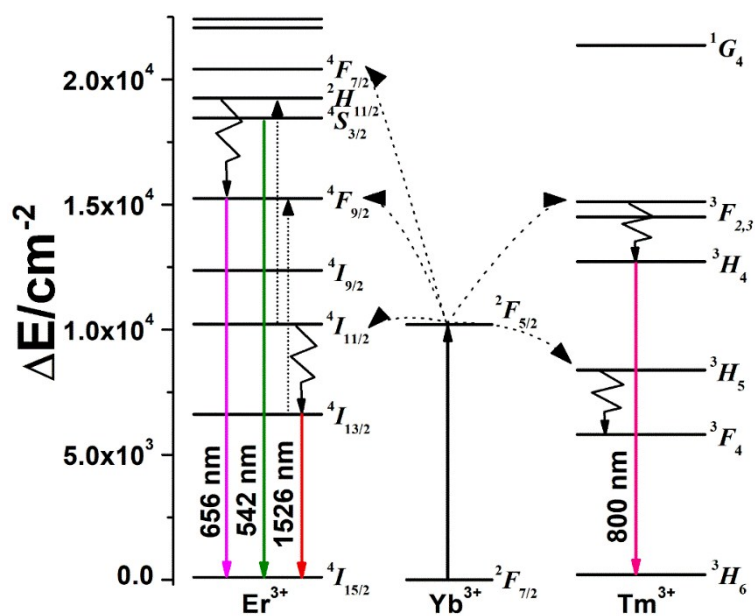
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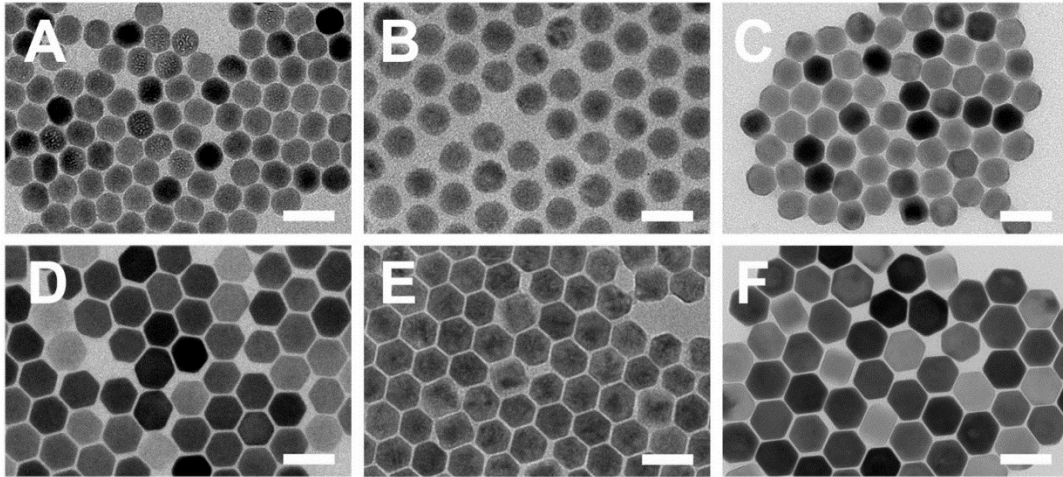
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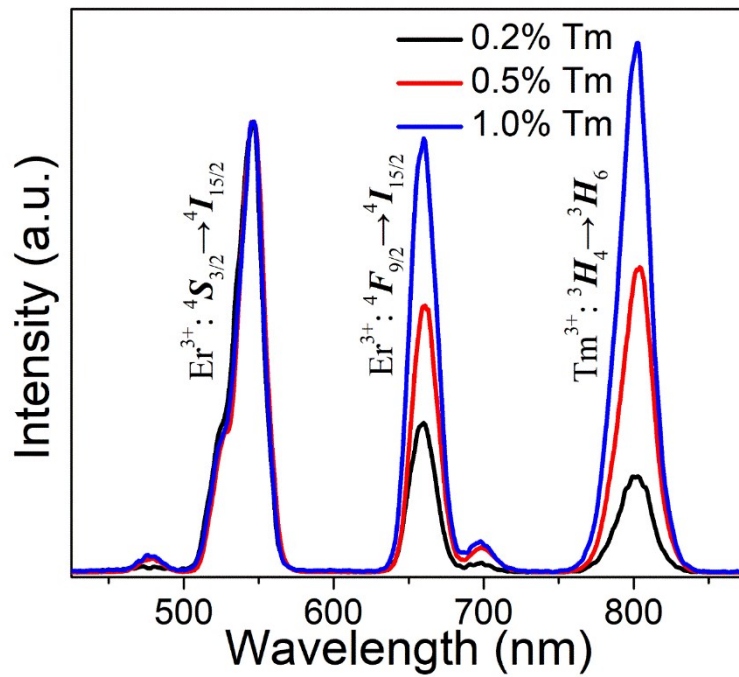
**Scheme S1.** The preparations of P-cy7



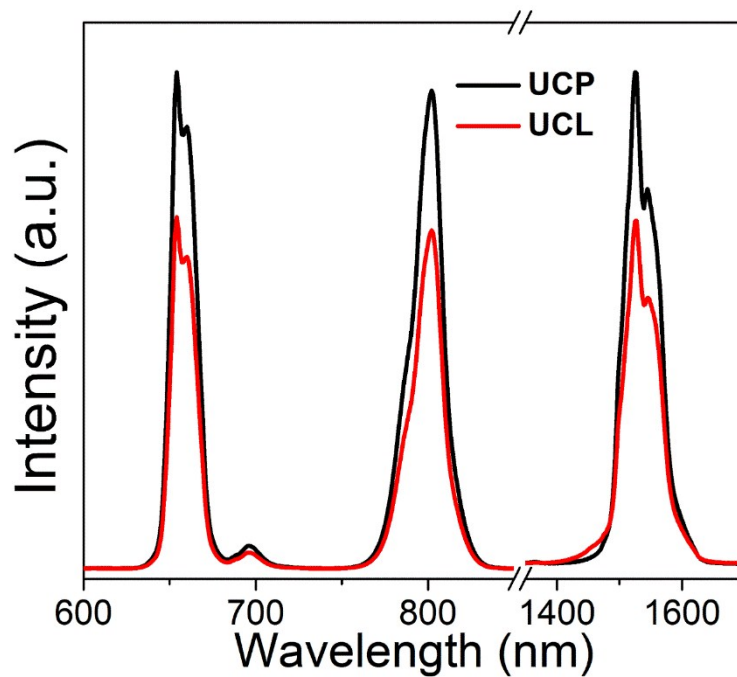
**Fig. S1** Energy transfer mechanism of UCP nanoparticles.



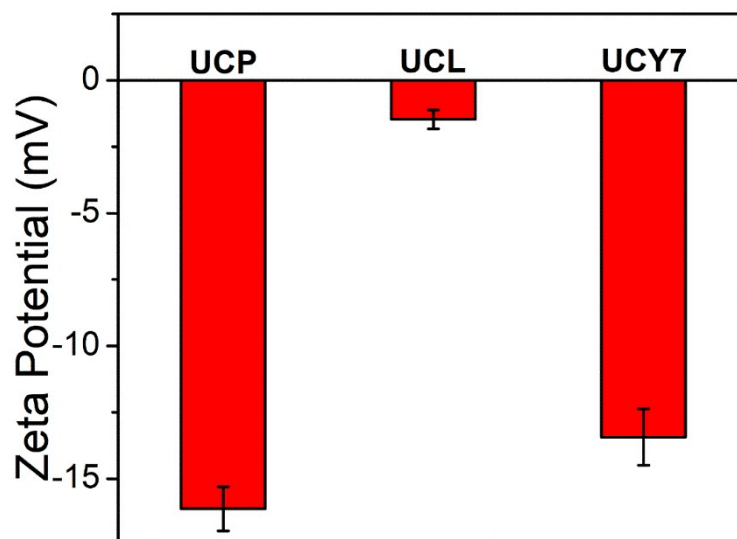
**Fig. S2** TEM images of NaYF<sub>4</sub>:20%Yb,2%Er,x%Tm: x = 0.2 (A), 0.5 (B) and 1.0 (C), and NaYF<sub>4</sub>:20%Yb,2%Er,x%Tm@NaYF<sub>4</sub>: x = 0.2 (D), 0.5 (E) and 1.0 (F), scale bars, 50 nm.



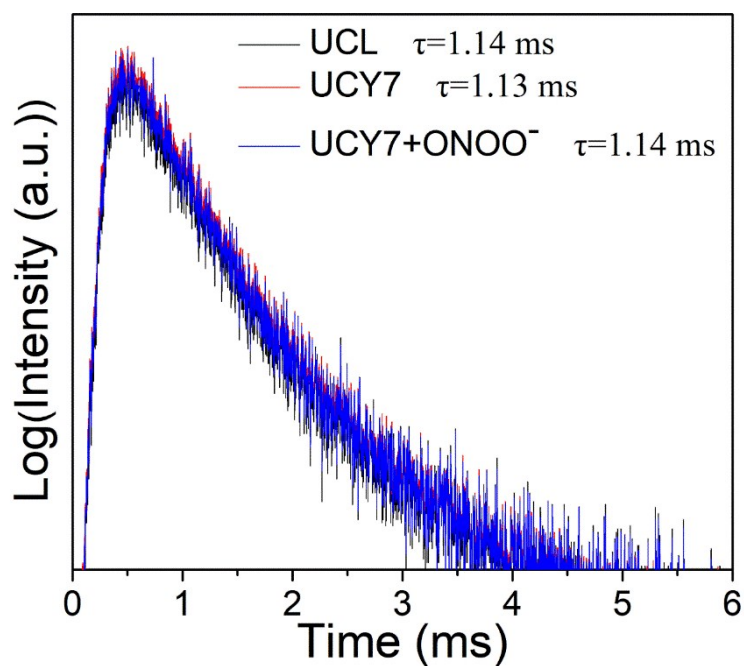
**Fig. S3** Luminescence emission spectra of NaYF<sub>4</sub>:20%Yb,2%Er,x%Tm (x = 0.2, 0.5% and 1%).



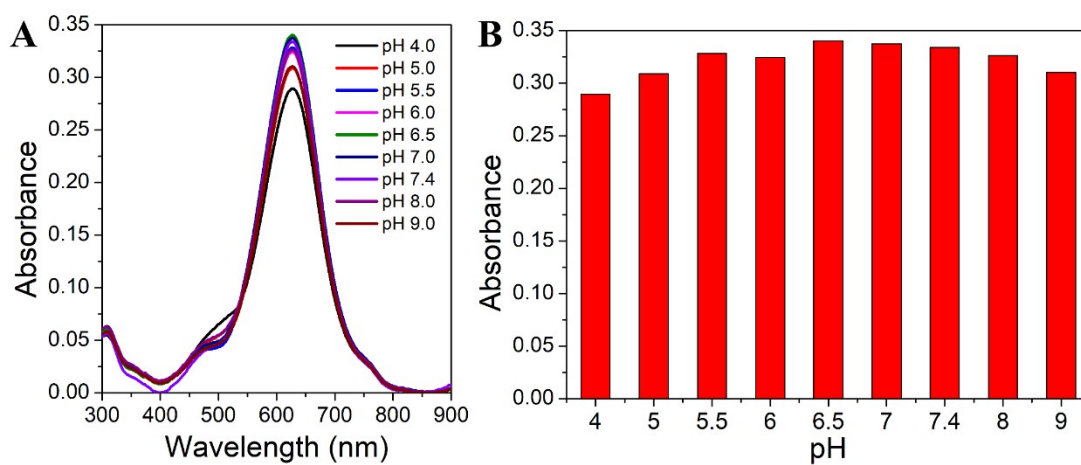
**Fig. S4** Luminescence emission spectra of UCP and UCL.



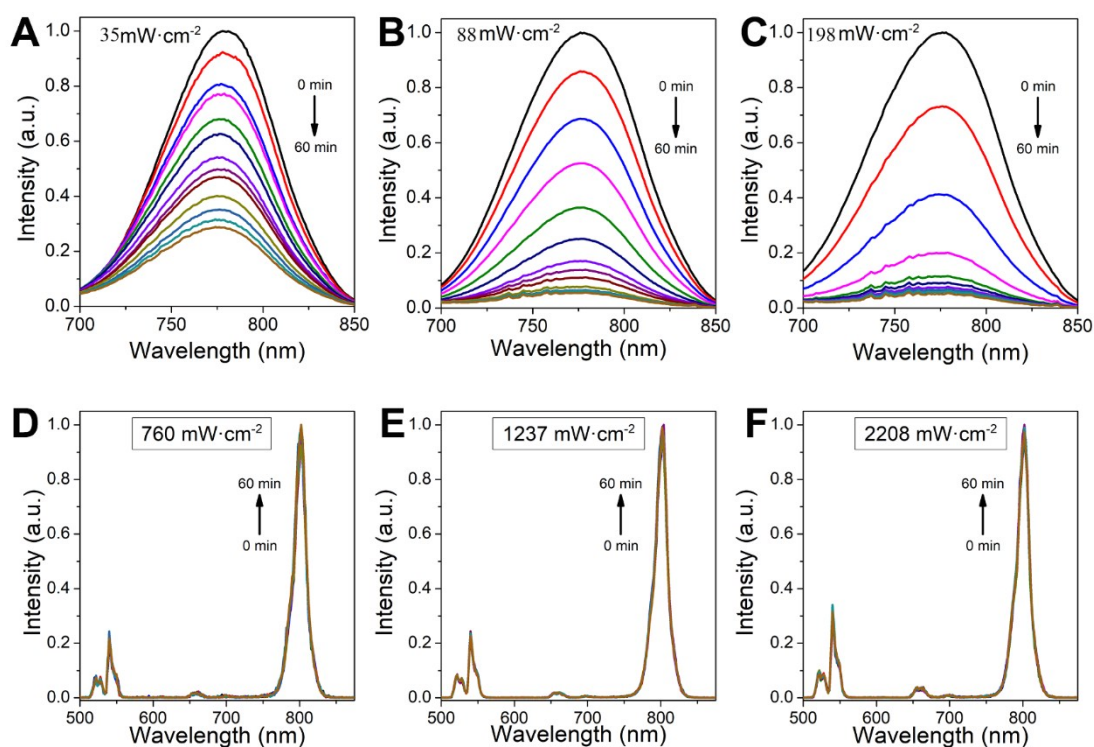
**Fig. S5** Zeta potentials of UCP, UCL and UCY7.



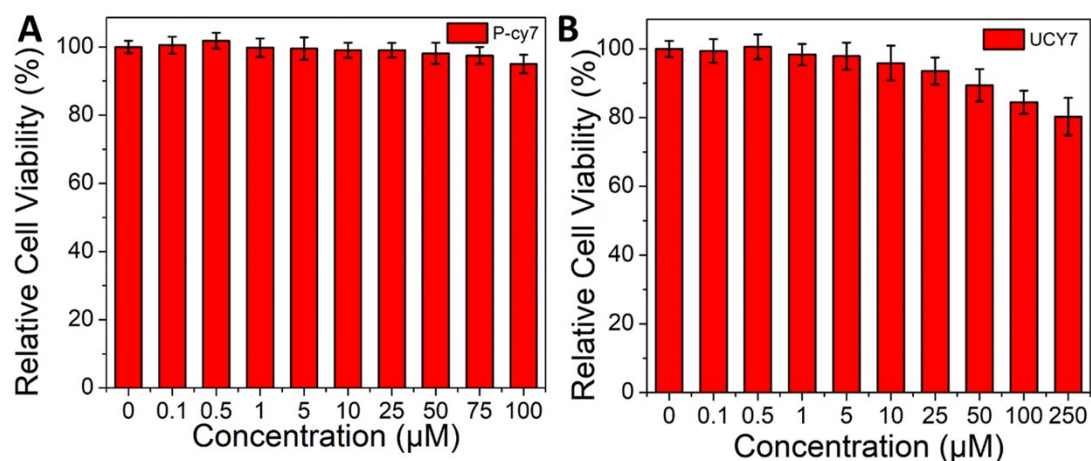
**Fig. S6** Lifetime decay curves at 1525 nm of UCL, UCY7 and UCY7+ONOO<sup>-</sup>.



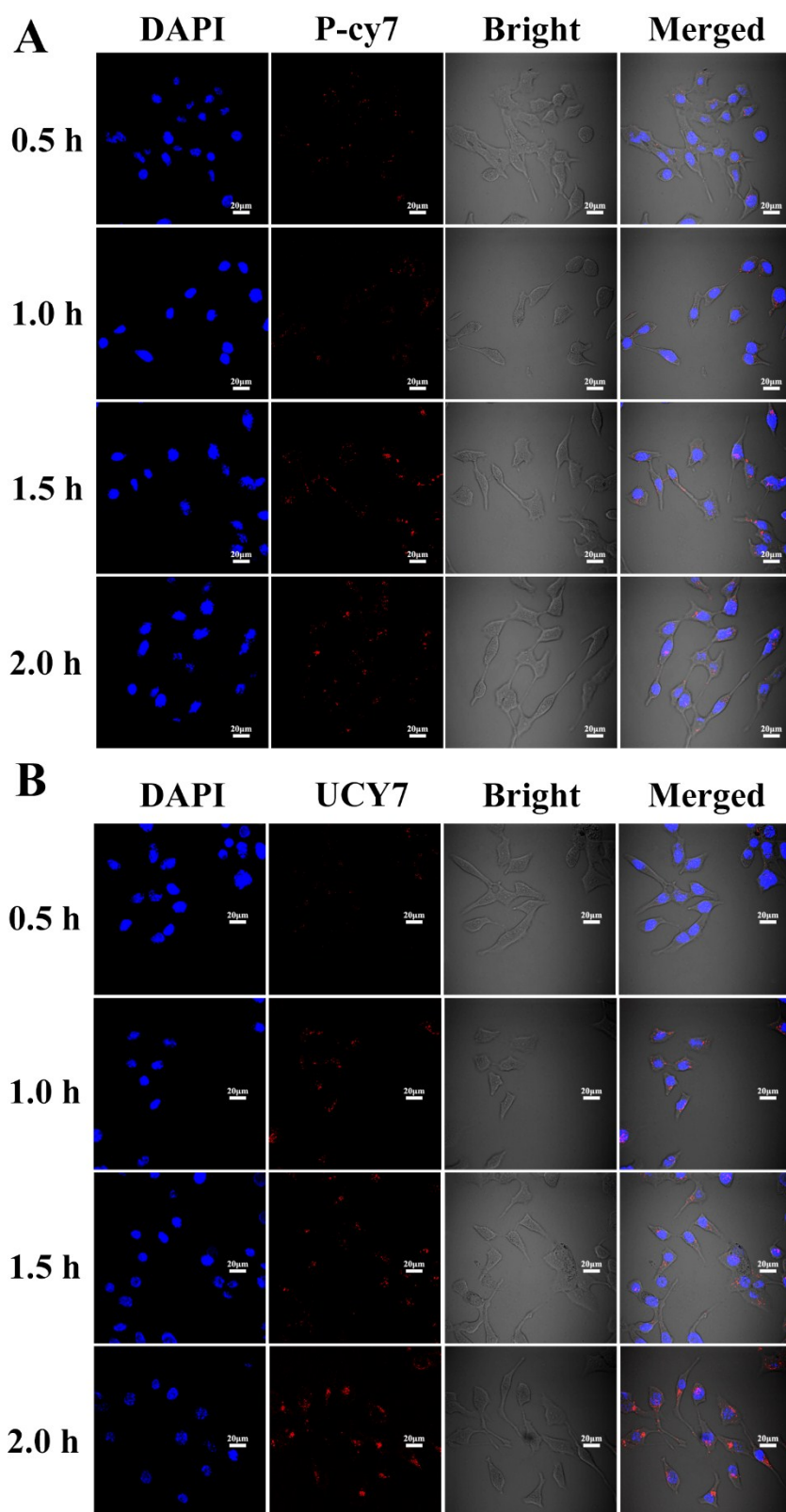
**Fig. S7** (A) UV-vis absorption spectra of UCY7 (0.1 mM) in different pH Tris-HCl solutions.



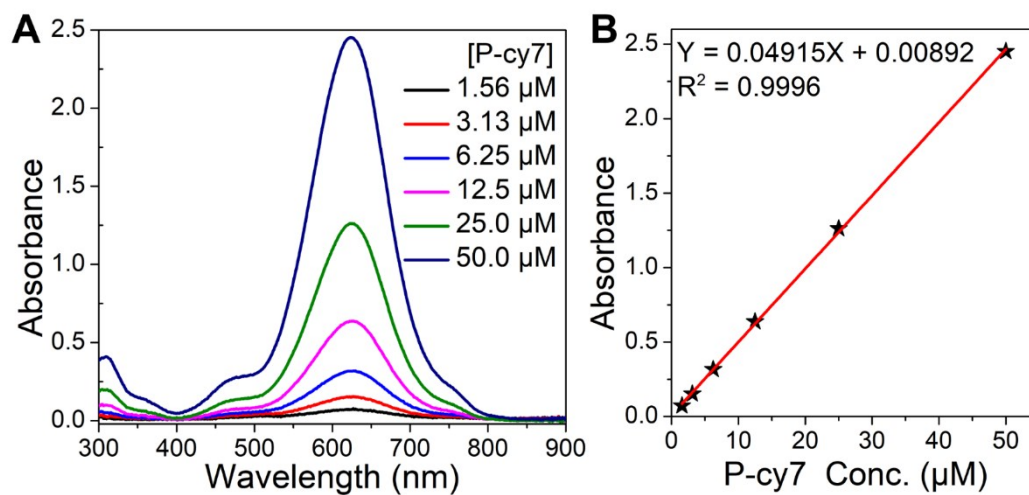
**Fig. S8** Emission spectra of P-cy7 (0.1 mM, Ex = 660 nm) and UCY7 (0.1 mM, Ex = 660 nm) in Tris-HCl (pH7.4) illuminated with corresponding laser at different power density.



**Fig. S9** Relative viabilities of HepG2 cells after incubation with various concentrations of P-cy7 (A) and UCY7 (B) in the dark for 24 h. Data are presented as means  $\pm$  s.d. (n = 5).

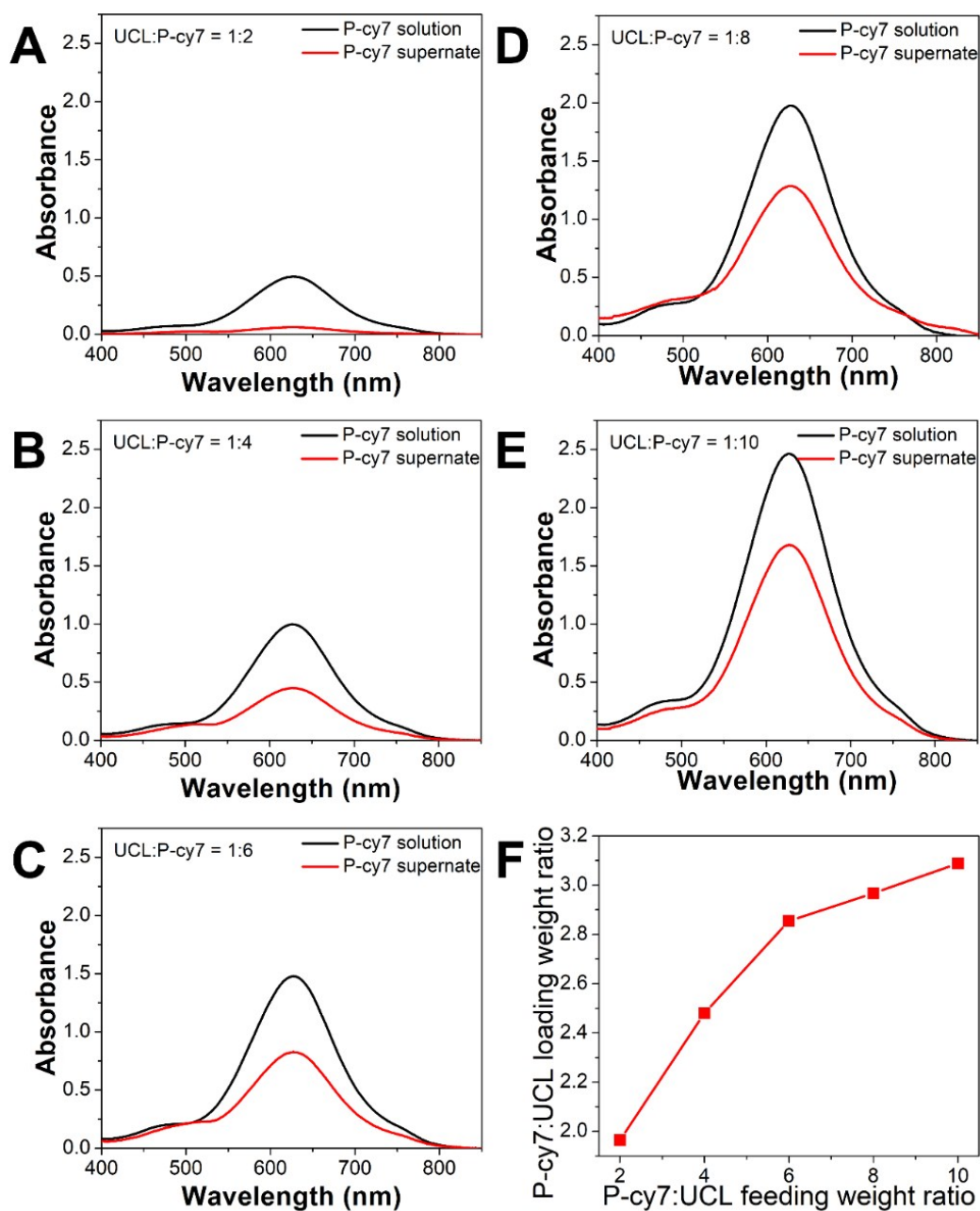


**Fig. S10** Confocal images of HepG2 cells treated with P-cy7 (A) and UCY7 (B) at different time points. Blue (Ex = 405 nm, Em = 460 ± 40 nm) and red (Ex = 633 nm, Em = 700 ± 50 nm) represent DAPI and P-cy7 / UCY7 fluorescence, respectively.

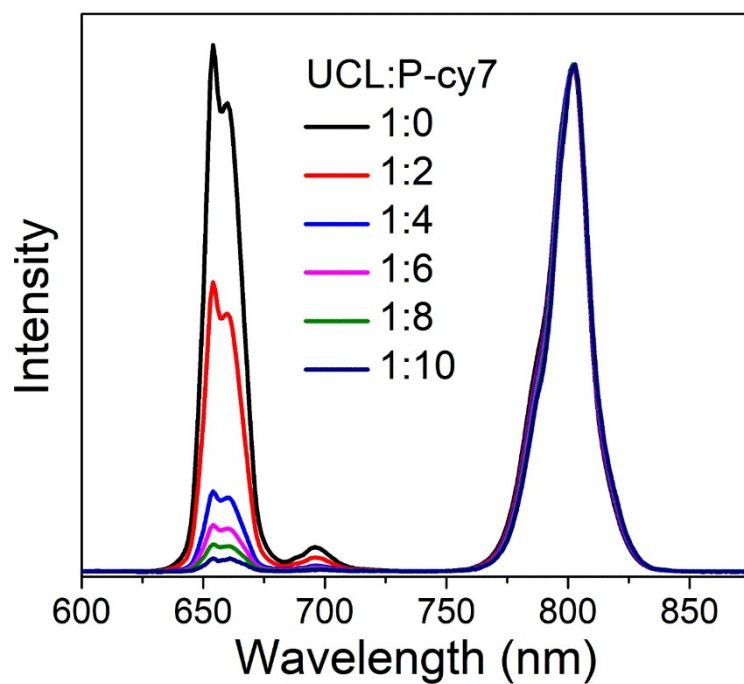


**Fig. S11** (A) UV-vis absorption spectra and (B) the standard curves for P-cy7 solution detected at 624 nm ( $Y = 0.04915X + 0.00892$ ).

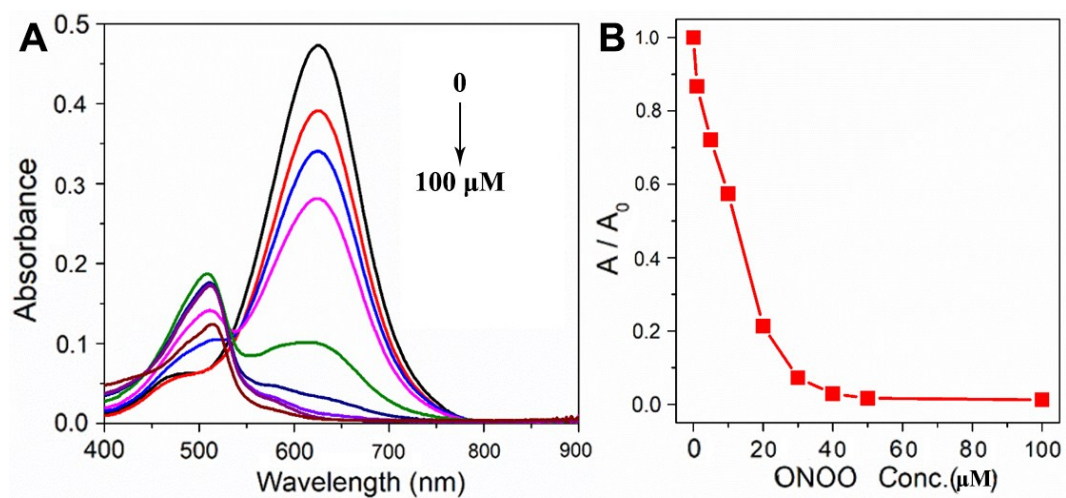




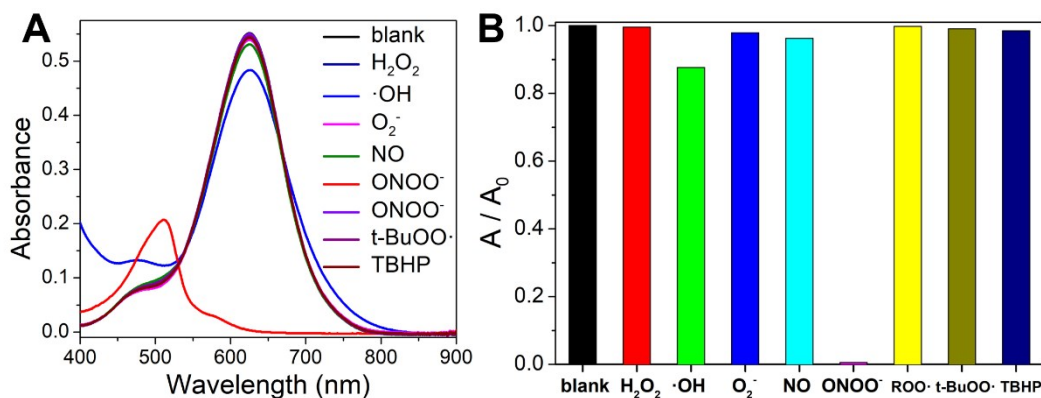
**Fig. S12** UCL:P-cy7 loading weight ratios and loading efficiency with different feeding weight ratios. UCL: 0.1 mM; P-cy7:  $n \times 0.1$  mM ( $n=2, 4, 6, 8, 10$ ); The solution (P-cy7 solution and P-cy7 supernate) was diluted 20 times before the test.



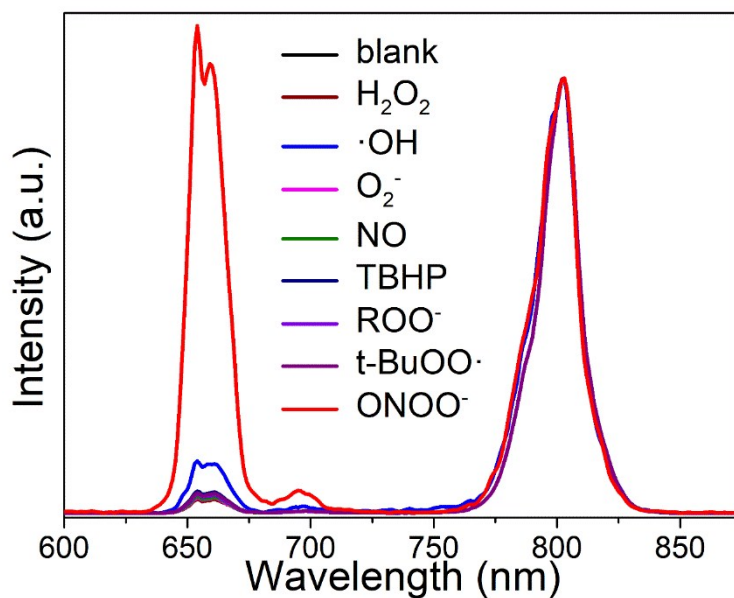
**Fig. S13** Emission spectra of UCL with different concentration of P-cy7. UCL: 0.1 mM; P-cy7:  $n \times 0.1$  mM ( $n=0, 2, 4, 6, 8, 10$ ).



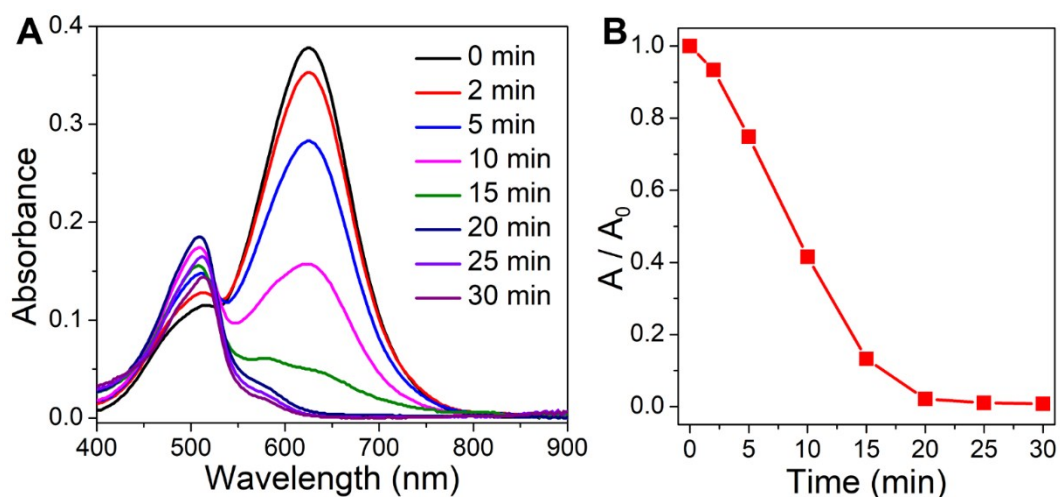
**Fig. S14** (A) UV-vis absorption spectra of UCY7 (0.1 mM) and (B) the ratio of  $A/A_0$  at 624 nm against the concentration of  $\text{ONOO}^-$



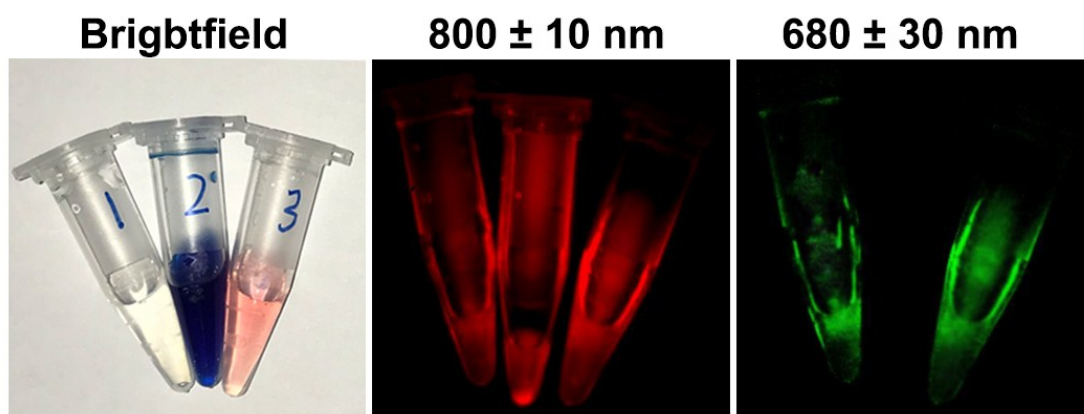
**Fig. S15** (A) UV-vis absorption spectra and the ratio of  $A_{656}/A_{800}$  of UCY7 (0.1 mM) in the presence of different biological species. H<sub>2</sub>O<sub>2</sub>: 200  $\mu$ M; ·OH: 200  $\mu$ M; O<sub>2</sub><sup>·-</sup>:200  $\mu$ M; NO: 200  $\mu$ M; ROO<sup>·</sup>: 200  $\mu$ M; t-BuOO<sup>·</sup>: 200  $\mu$ M; TBHP: 200  $\mu$ M; ONOO<sup>·</sup>: 50  $\mu$ M.



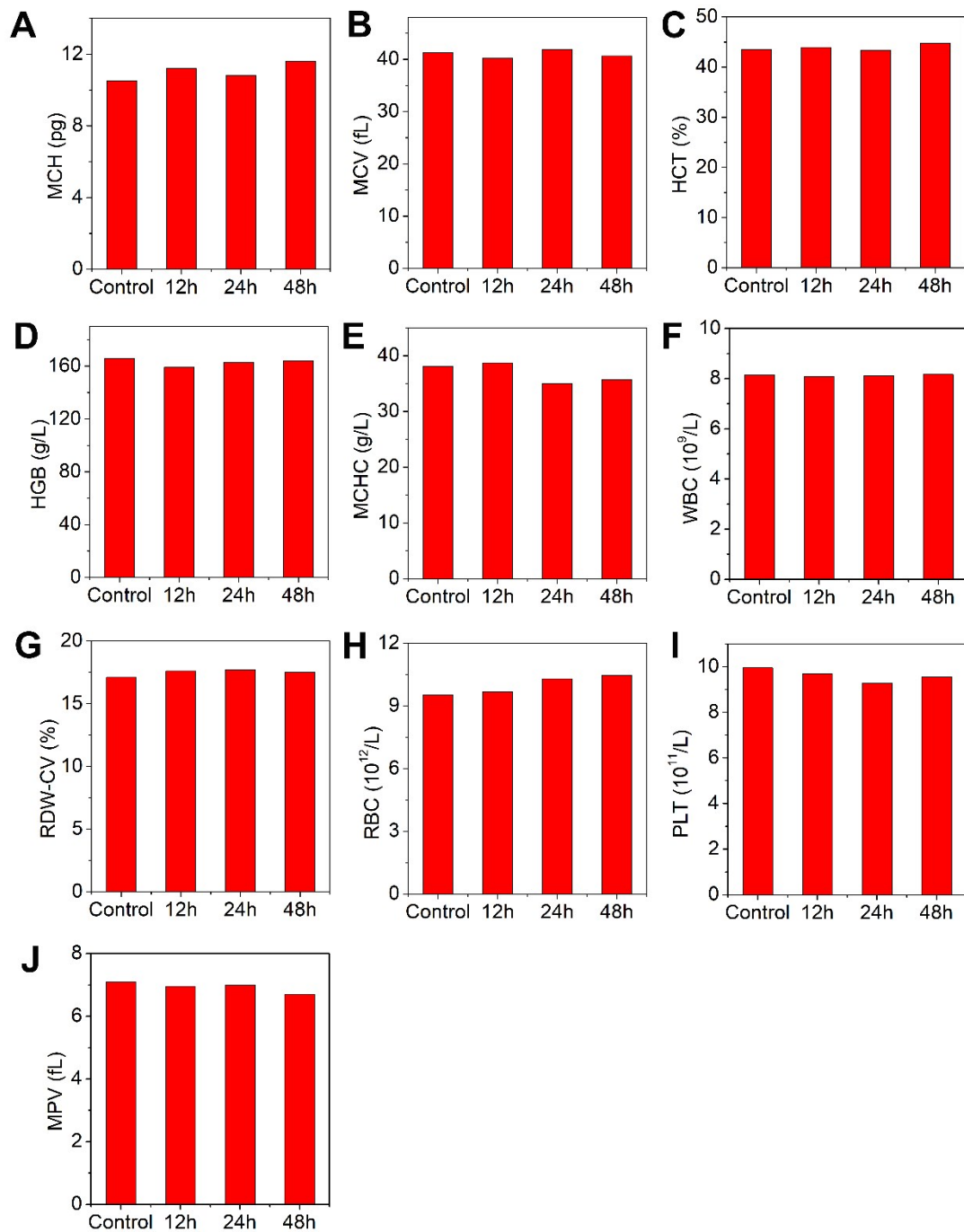
**Fig. S16** Fluorescence emission spectra of UCY7 (0.1 mM) in the presence of different biological species. H<sub>2</sub>O<sub>2</sub>: 200  $\mu$ M; ·OH: 200  $\mu$ M; O<sub>2</sub><sup>·-</sup>:200  $\mu$ M; NO: 200  $\mu$ M; ROO<sup>·</sup>: 200  $\mu$ M; t-BuOO<sup>·</sup>: 200  $\mu$ M; TBHP: 200  $\mu$ M; ONOO<sup>·</sup>: 50  $\mu$ M.



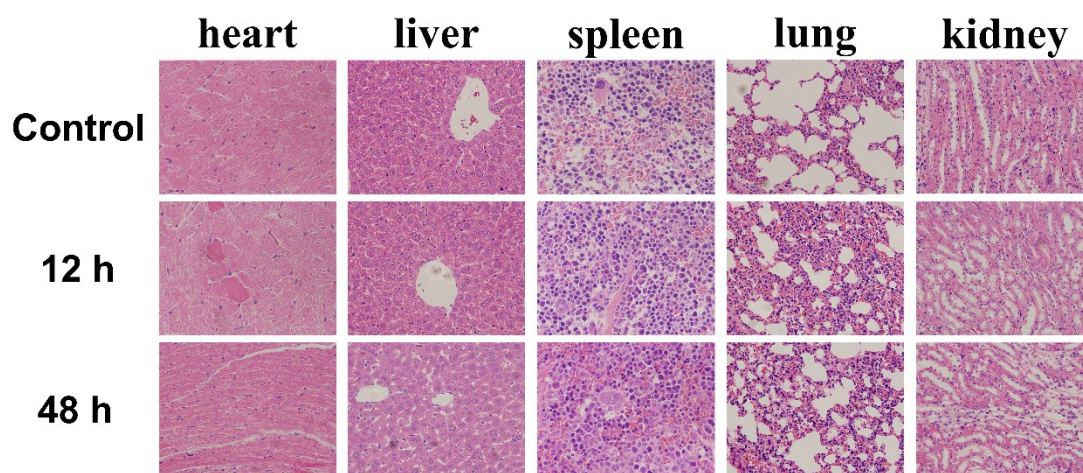
**Fig. S17** (A) UV-vis absorption spectra and (B) the ratio of  $A/A_0$  at 624 nm over time (0-30 min), UCY7: 0.1 mM, ONOO<sup>-</sup>: 50  $\mu$ M.



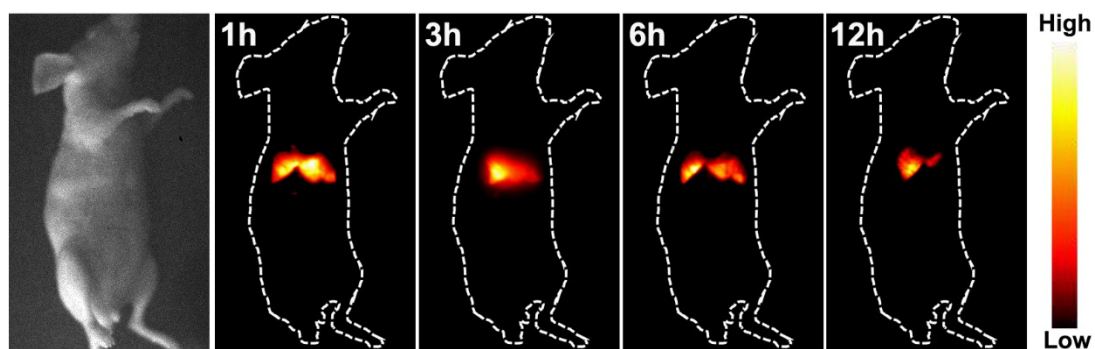
**Fig. S18** Brightfield (A) and luminescence images (B, C) of UCL, UCY7 and UCY7+ONOO<sup>-</sup> (Tube 1-3, respectively). Excitation: 980 nm (50 mW/cm<sup>2</sup>), exposure time: 10 ms, band pass filter 800 $\pm$ 10 nm and 680 $\pm$ 30 nm.



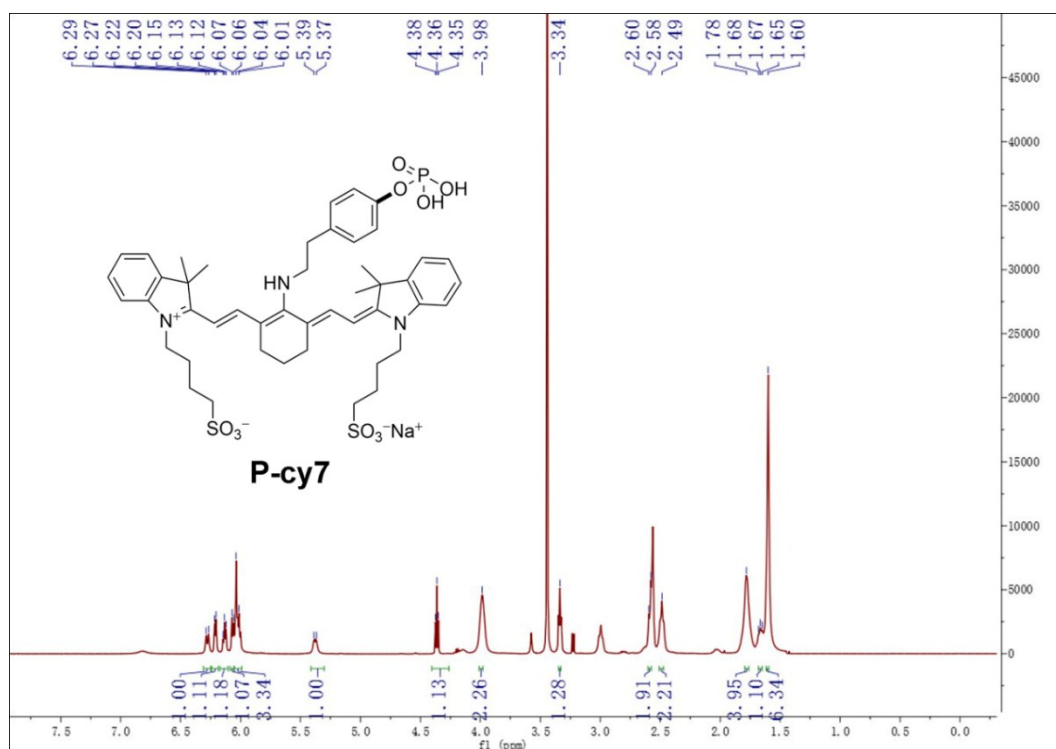
**Fig. S19** *In vivo* toxicology study and serum biochemistry results obtained from balb/c mice in 12, 24, 48 h of intravenous injection with UCY7; (A) mean corpuscular hemoglobin (MCH), (B) mean corpuscular volume (MCV), (C) hematocrit (HCT), (D) hemoglobin (HGB), (E) mean corpuscular hemoglobin concentration (MCHC), (F) white blood cells (WBC), (G) red cell distribution width-coefficient of variation, (H) red blood cells (RBC), (I) Platelets (PLT) and (J) mean platelet volume (MPV).



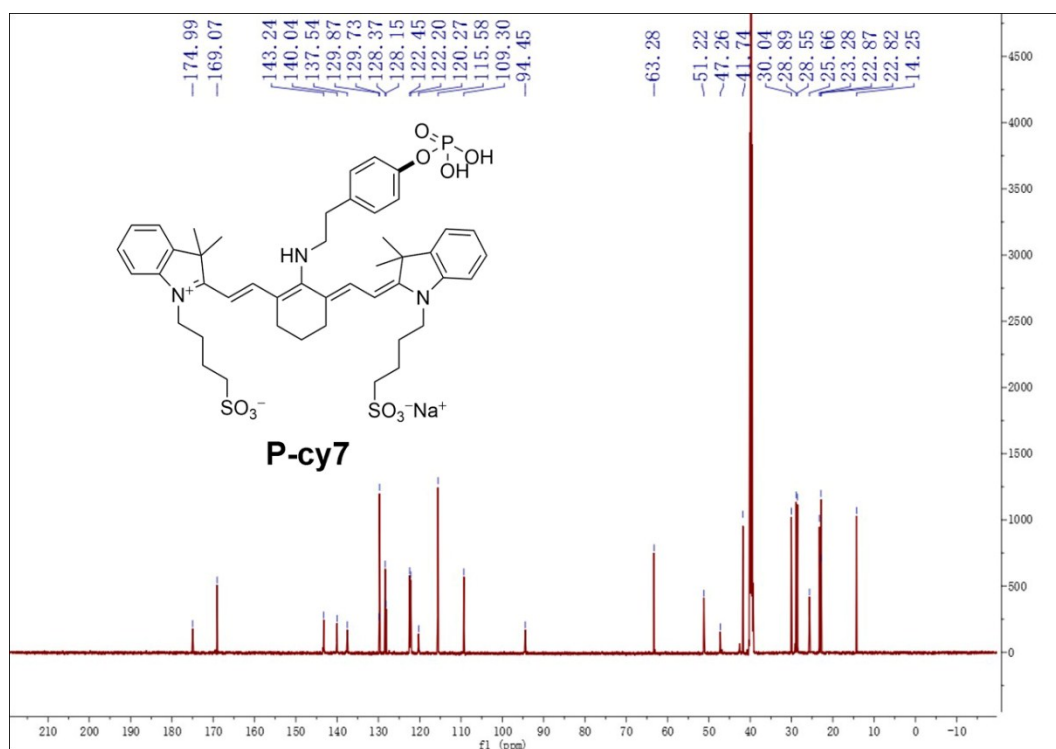
**Fig. S20** Representative histology of heart, spleen, lung and kidney of mice at 12 h and 48 h after intravenous nanoprobe.



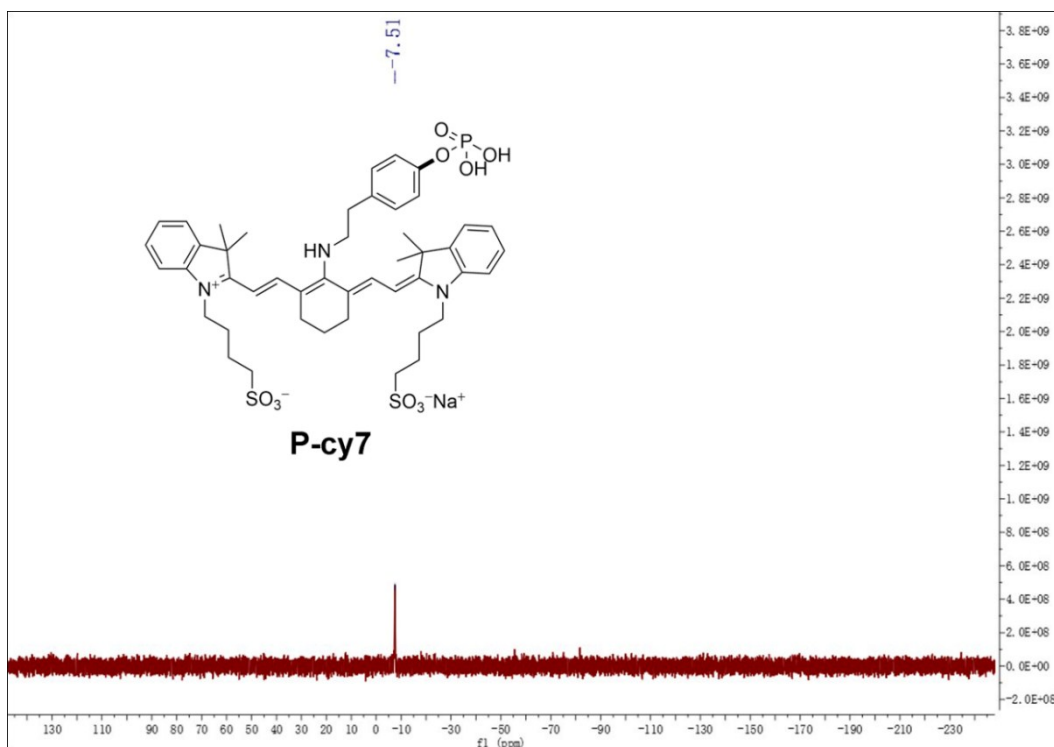
**Fig. S21** NIR-II FL bioimaging consequences for the abdomen (1200 nm long-pass filter) after intravenous injection with of UCY7 at different times under 980-nm excitation ( $P = 0.5 \text{ W} \cdot \text{cm}^{-2}$ ).



**Fig. S22** <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ(ppm): 6.28 (d, *J* = 8.3 Hz, 2H), 6.21 (d, *J* = 4.8 Hz, 2H), 6.13 (t, *J* = 5.0 Hz, 4H), 6.06 (d, *J* = 5.3 Hz, 2H), 6.02 (d, *J* = 9.5 Hz, 2H), 5.38 (d, *J* = 7.8 Hz, 2H), 4.36 (t, *J* = 5.2 Hz, 4H), 3.98 (s, 4H), 3.34 (s, 4H), 2.59 (d, *J* = 7.0 Hz, 4H), 2.49 (s, 4H), 1.78 (s, 8H), 1.67 -1.64 (m, 4H), 1.60 (s, 12H).

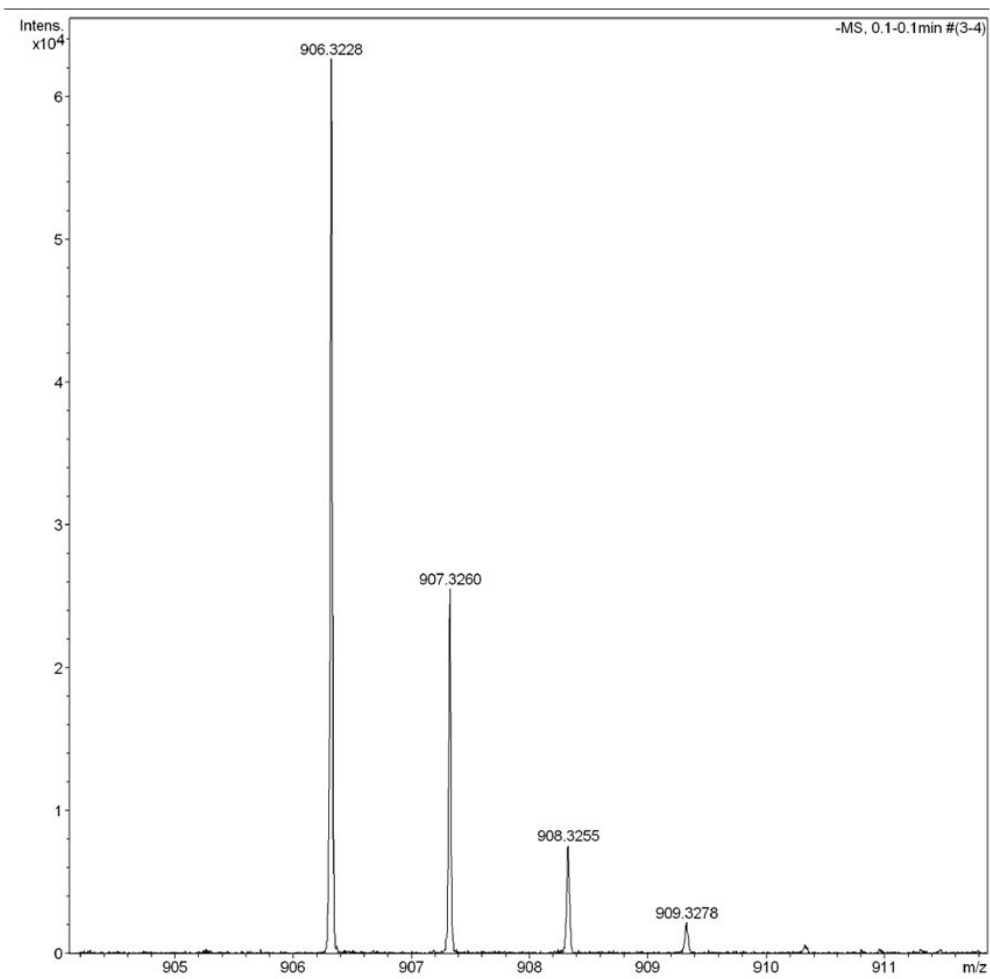


**Fig. S23** <sup>13</sup>C NMR (151 MHz, DMSO-d<sub>6</sub>) δ(ppm): 175.0, 169.1, 143.2, 140.0, 137.5, 129.8, 129.7, 128.3, 128.1, 122.4, 122.2, 120.3, 115.6, 109.3, 94.5, 63.3, 51.2, 47.3, 41.7, 30.0, 28.9, 28.6, 25.7, 23.3, 22.9, 22.8, 14.3.



**Fig. S24**  $^{31}\text{P}$  NMR(243 MHz,  $\text{DMSO-d}_6$ )  $\delta(\text{ppm}): -7.51$ .





**Fig. S25** Mass spectrum of probe P-cy7.