

Figure S1. <sup>1</sup>H NMR spectra of S1.

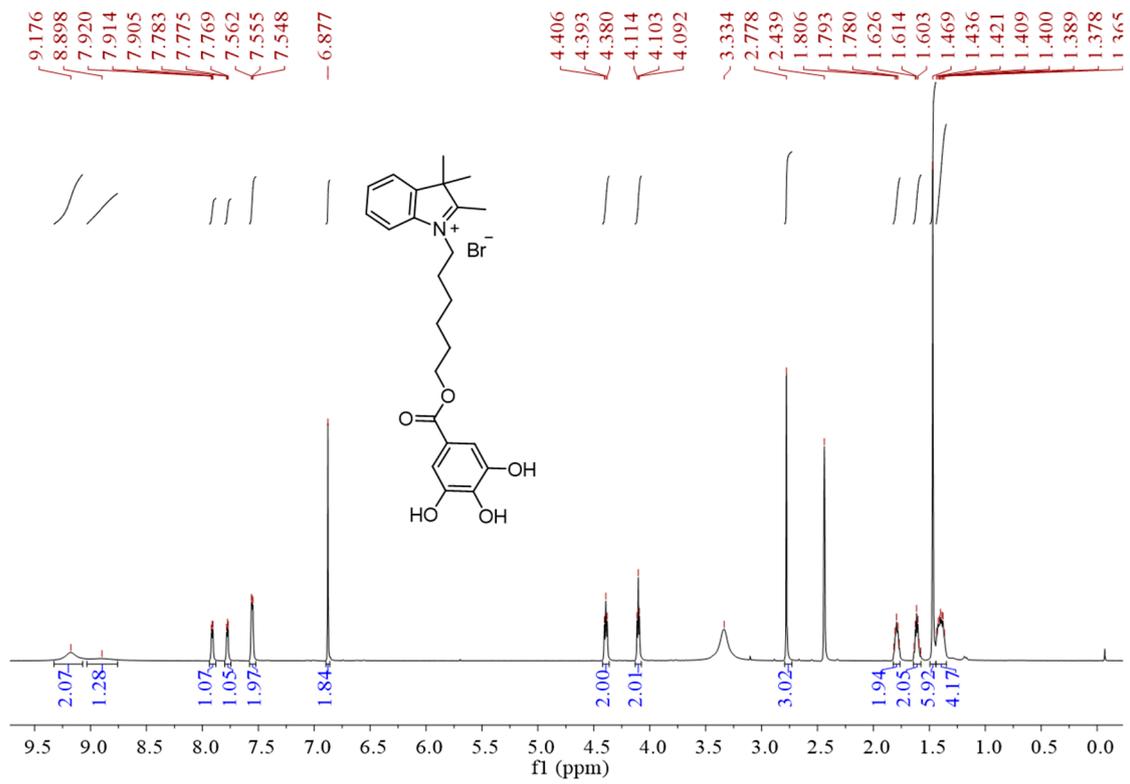
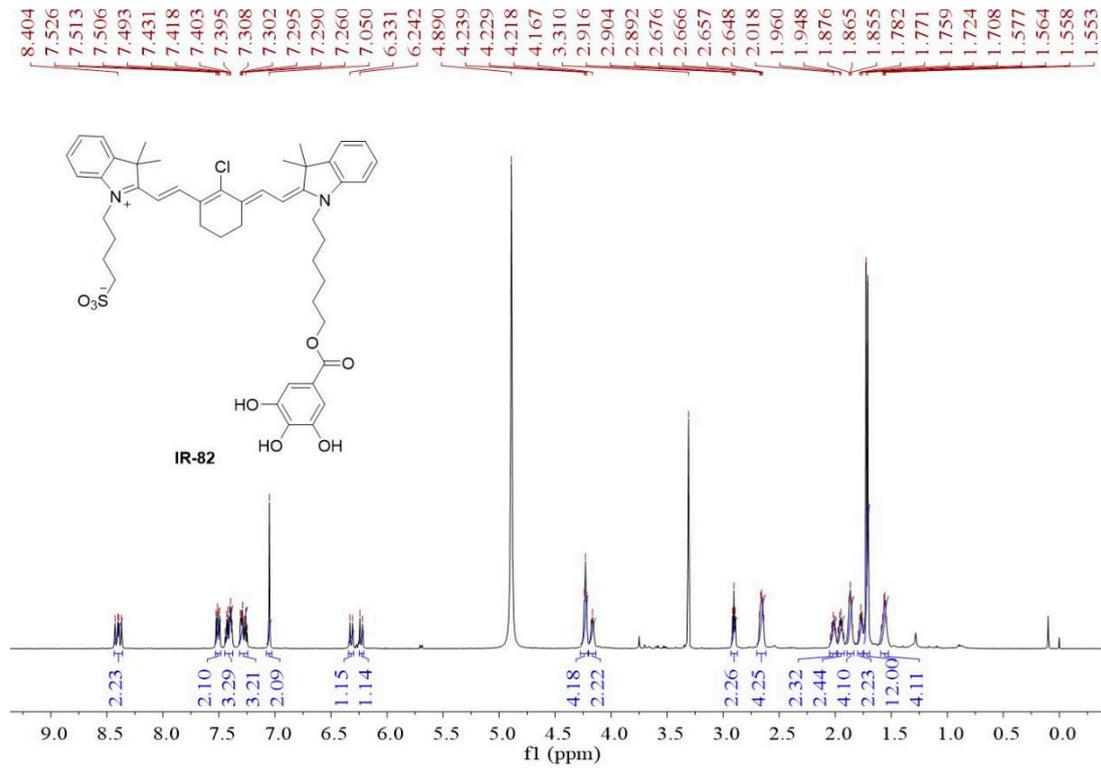


Figure S2.  $^1\text{H}$  NMR spectra of key intermediates S2.



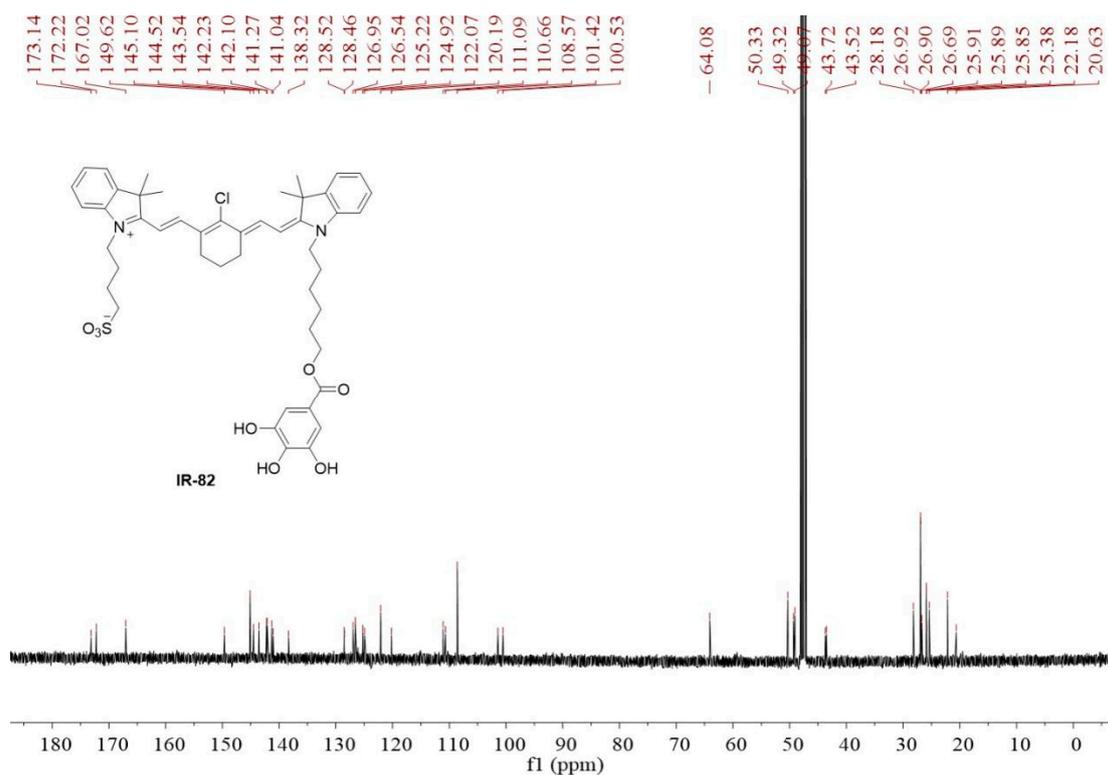


Figure S4.  $^{13}\text{C}$  NMR spectra of IR-82.

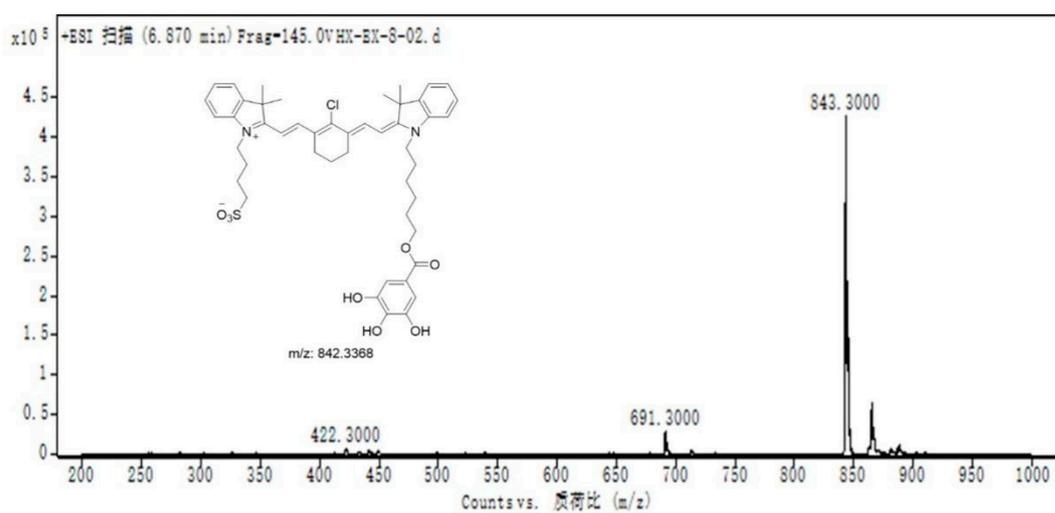
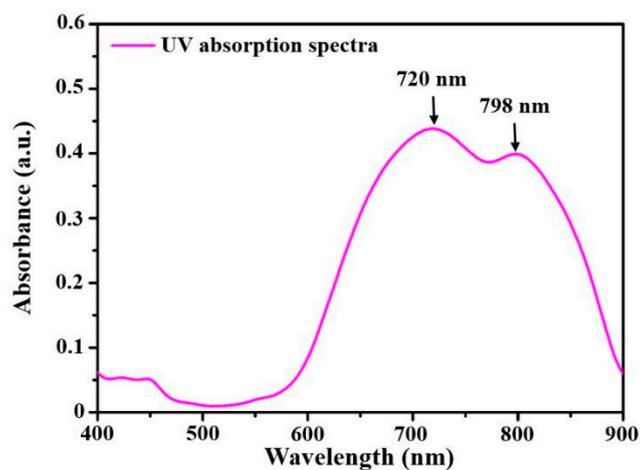
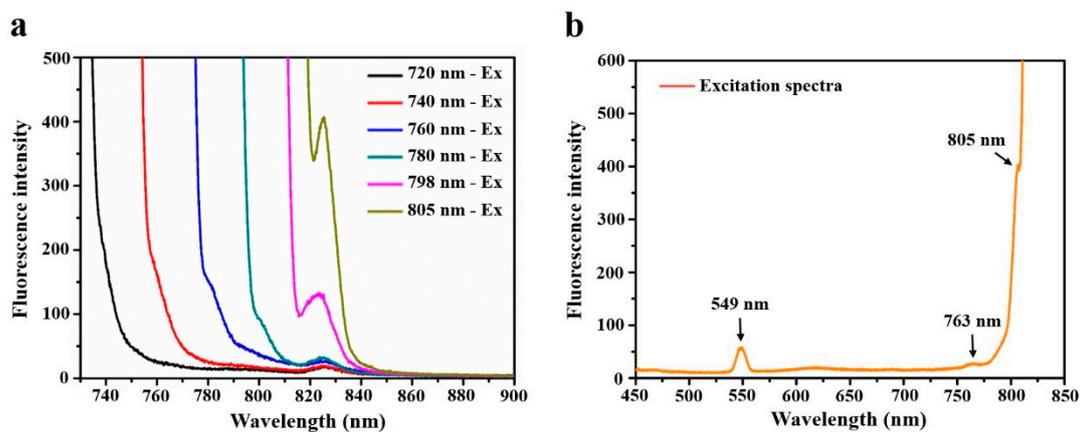


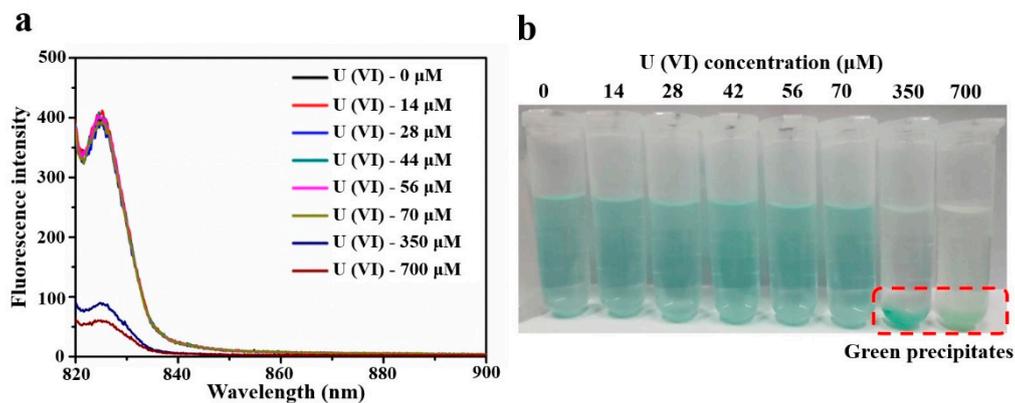
Figure S5. HRMS spectra of IR-82.



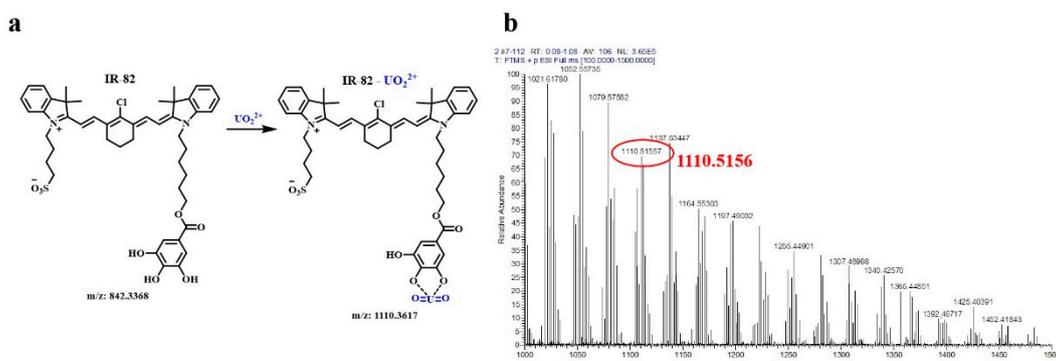
**Figure S6.** Ultraviolet absorption spectra of cyanine molecule IR-82 (10  $\mu$ M) in 0.02 M Tris-HCl solution (pH = 7.4).



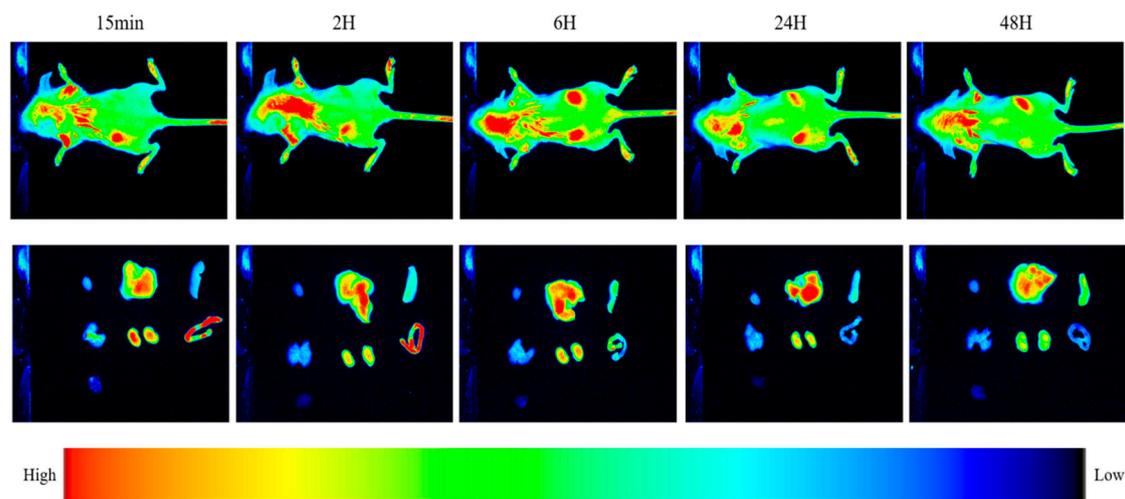
**Figure S7.** (a) Fluorescence emission spectra of IR-82 (10  $\mu$ M) at different excitation wavelengths. (b) Fluorescence excitation spectra of IR-82 at 825 nm fluorescence emission. The maximum fluorescence excitation wavelength of cyanine molecule IR-82 is 805 nm, and the maximum fluorescence emission wavelength is 825 nm.



**Figure S8.** Fluorescence response of IR-82 (10 μM) toward different concentrations of UO<sub>2</sub><sup>2+</sup> (a) and corresponding mixture solution (b). When the concentration of UO<sub>2</sub><sup>2+</sup> increased to 350 μM and 700 μM, the generated green precipitates by IR-82 and UO<sub>2</sub><sup>2+</sup> could be clearly observed by naked eyes.



**Figure S9.** (a) The possible chelation form of IR-82 toward UO<sub>2</sub><sup>2+</sup>. (b) HRMS spectra of IR-82 and UO<sub>2</sub><sup>2+</sup> mixture solution.



**Figure S10.** IR-82 metabolism in mice. (a) In vivo and ex vivo NIR fluorescence images of normal BALB/c mice taken at 15 min, 2 h, 6 h, 24 h and 48 h after IR-82 was administered via i.p. injection.