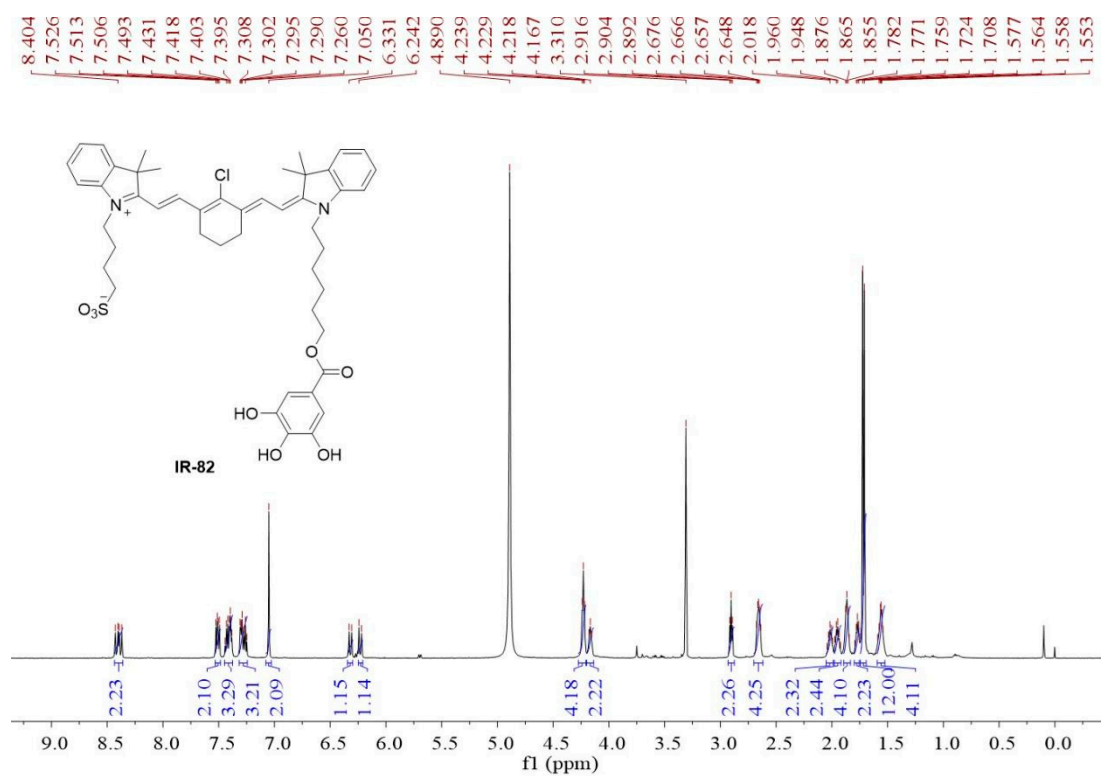


**Figure S1.** <sup>1</sup>H NMR spectra of S1.





**Figure S3.** <sup>1</sup>H NMR spectra of IR-82.

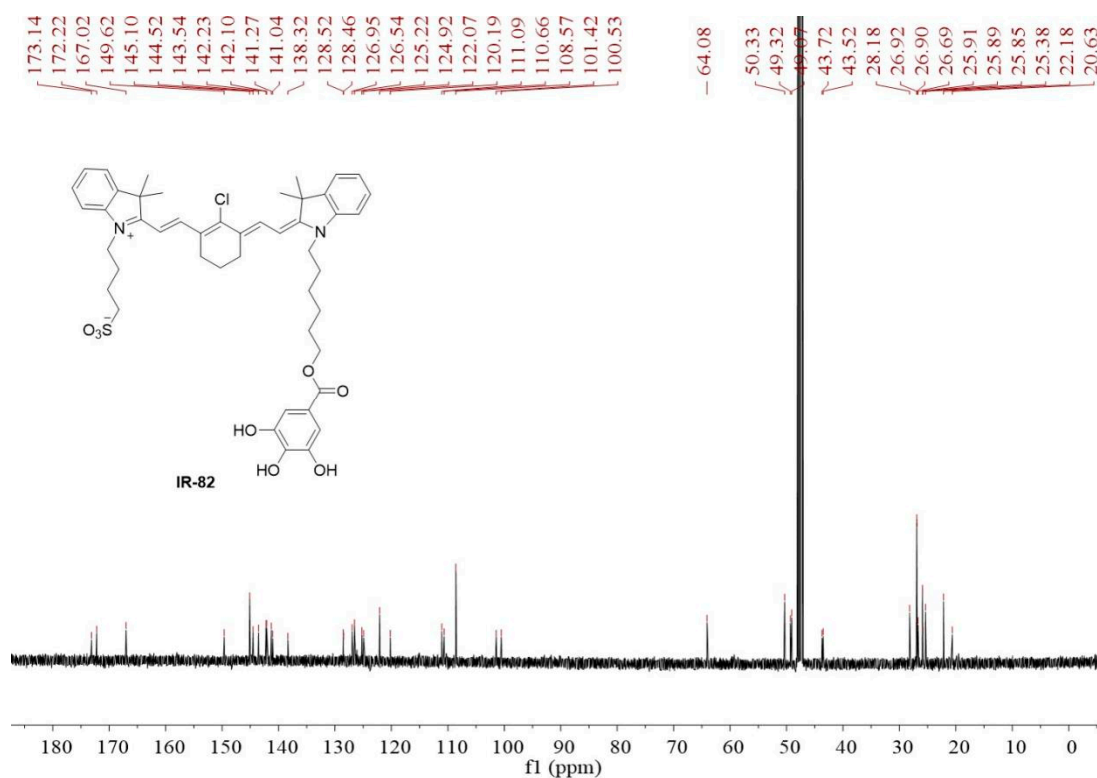


Figure S4. <sup>13</sup>C NMR spectra of IR-82.

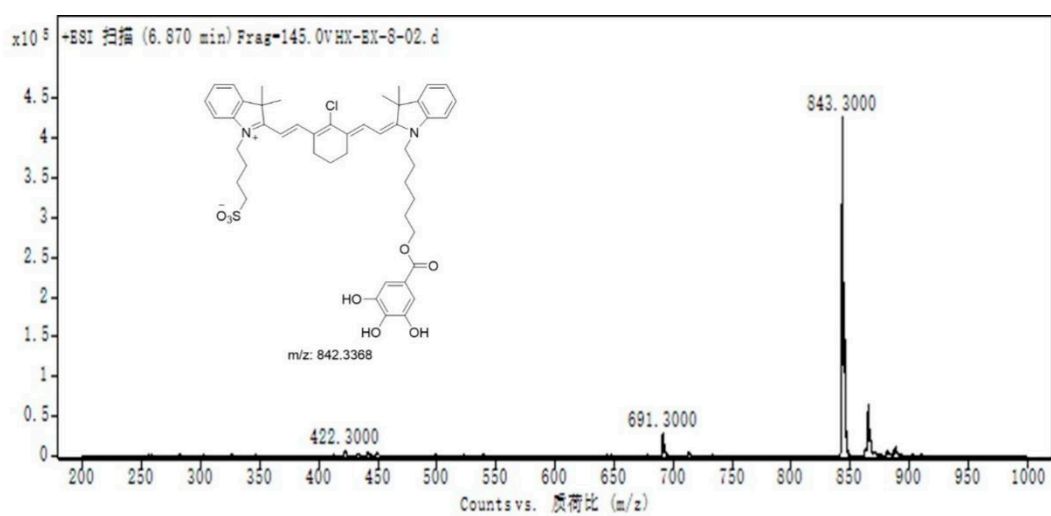
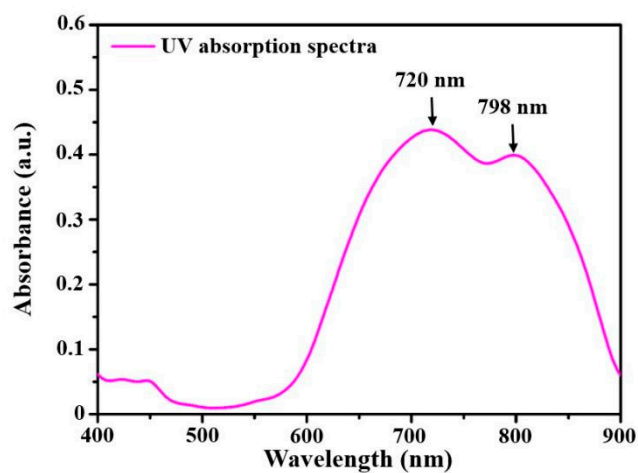
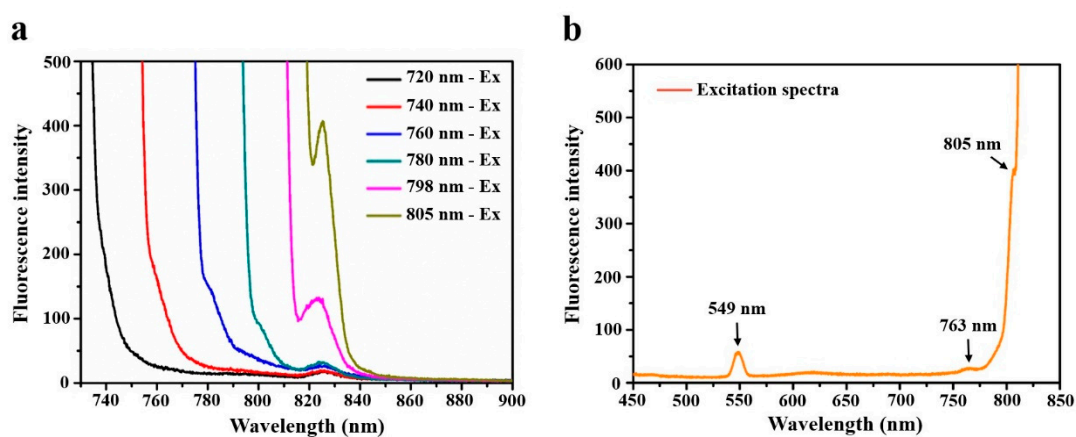


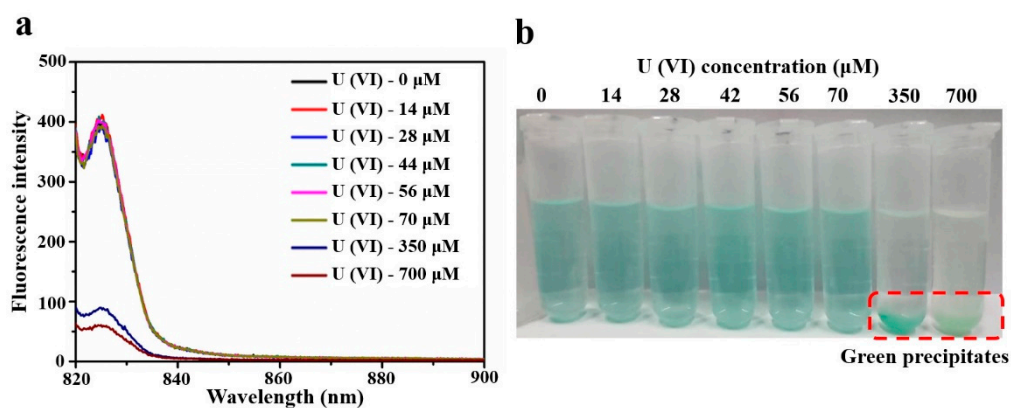
Figure S5. HRMS spectra of IR-82.



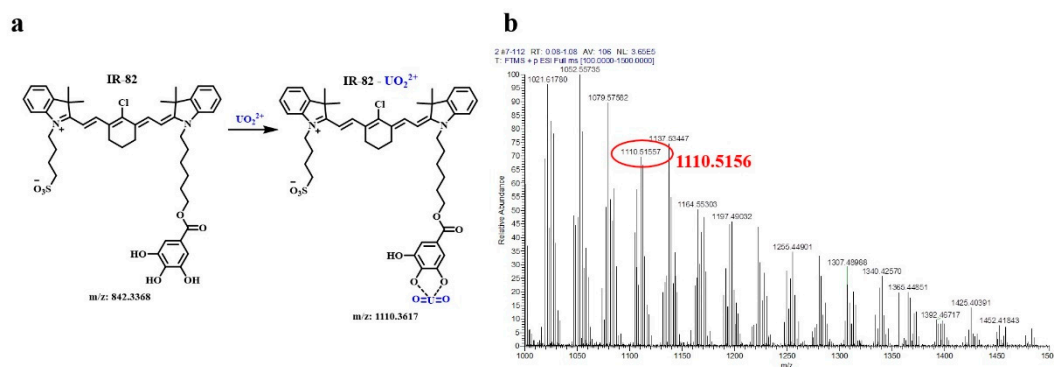
**Figure S6.** Ultraviolet absorption spectra of cyanine molecule IR-82 (10  $\mu$ M) in 0.02 M Tris-HCl solution (pH = 7.4).



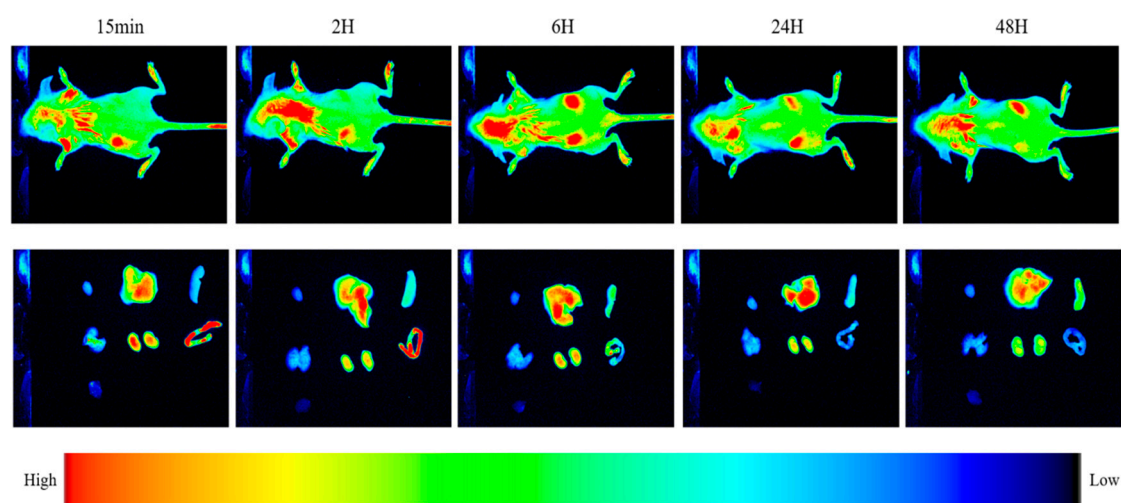
**Figure S7.** (a) Fluorescence emission spectra of IR-82 (10  $\mu$ M) at different excitation wavelengths. (b) Fluorescence excitation spectra of IR-82 at 825 nm fluorescence emission. The maximum fluorescence excitation wavelength of cyanine molecule IR-82 is 805 nm, and the maximum fluorescence emission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



**Figure S8.** Fluorescence response of IR-82 (10  $\mu\text{M}$ ) toward different concentrations of  $\text{UO}_2^{2+}$  (a) and corresponding mixture solution (b). When the concentration of  $\text{UO}_2^{2+}$  increased to 350  $\mu\text{M}$  and 700  $\mu\text{M}$ , the generated green precipitates by IR-82 and  $\text{UO}_2^{2+}$  could be clearly observed by naked eyes.



**Figure S9.** (a) The possible chelation form of IR-82 toward  $\text{UO}_2^{2+}$ . (b) HRMS spectra of IR-82 and  $\text{UO}_2^{2+}$  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 administrated via i.p. injection.