Supporting Information

Molecular Engineering of a Commercially Available NIR-II Fluorescent Cyanine Dye for Improved Tumor Targeting and Imaging

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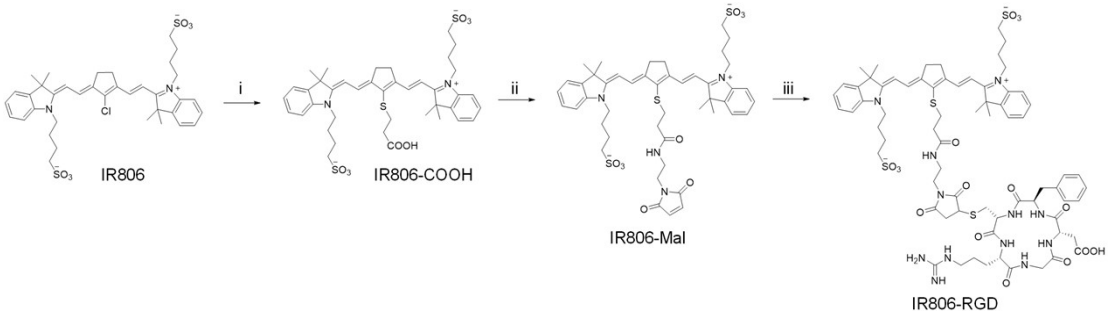
Supporting figures



Scheme S1. Synthetic route of IR806-RGD. Reagents and conditons: i) mercaptopropionic acid, methanol, trimethylamine, room temperature, 24 h; ii) 1-[Bis(dimethylamino)methylene]-1H-1,2,3-triazolo[4,5-b]pyridinium 3-oxide hexafluorophosphate (HATU), N-Hydroxybenzotriazole, N,N-dimethylformamide (DMF), N,N-diisopropylethylamine (DIPEA), N-(2-Aminoethyl)maleimide, room temperature, 24 h; iii) cRGDyC, PBS (pH 7.4), room temperature, 12 h.

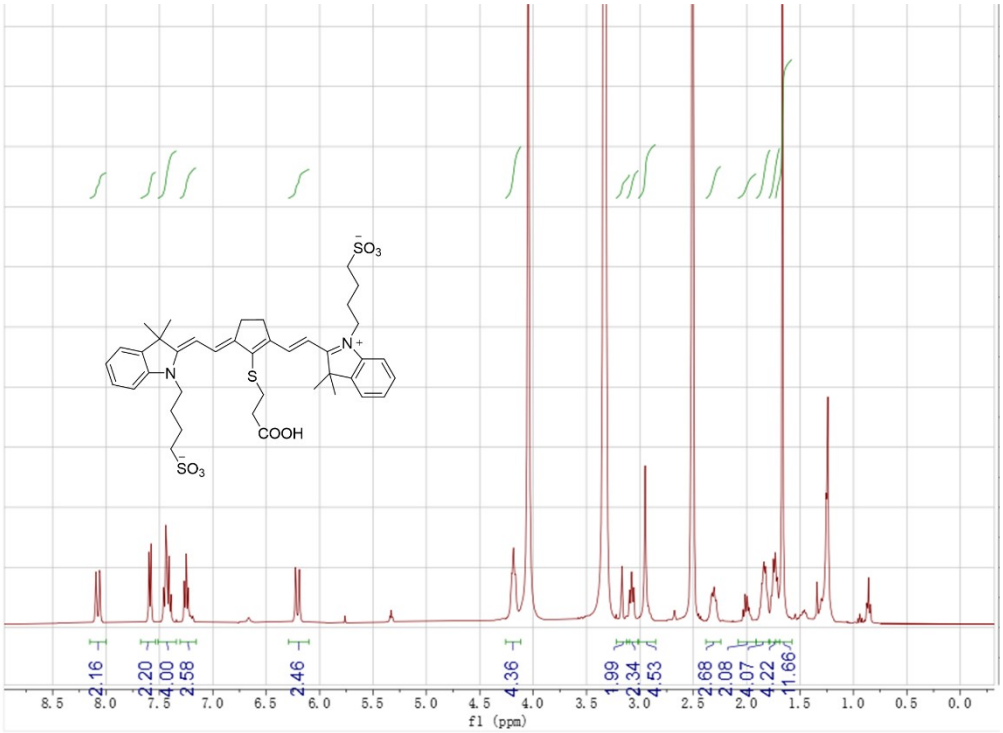


Figure S1. ^{1}H NMR spectrum of IR806-COOH. DMSO-d_6 was used as the solvent.

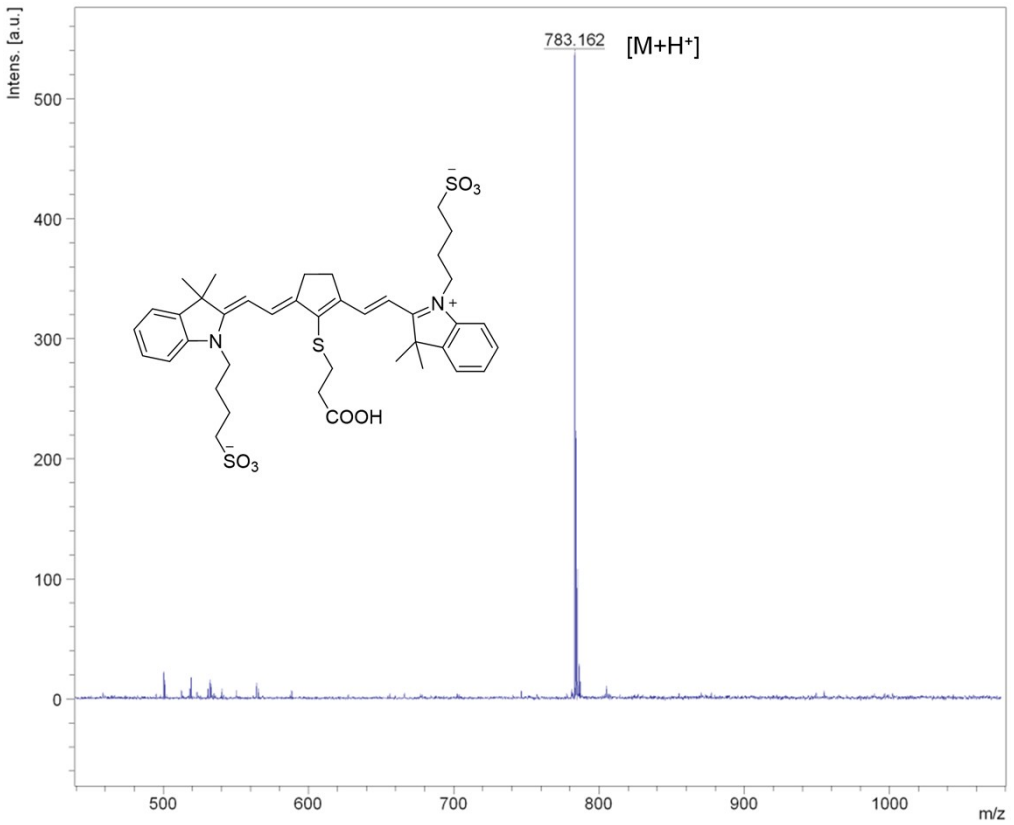


Figure S2. MALDI-TOF MS of IR806-COOH.

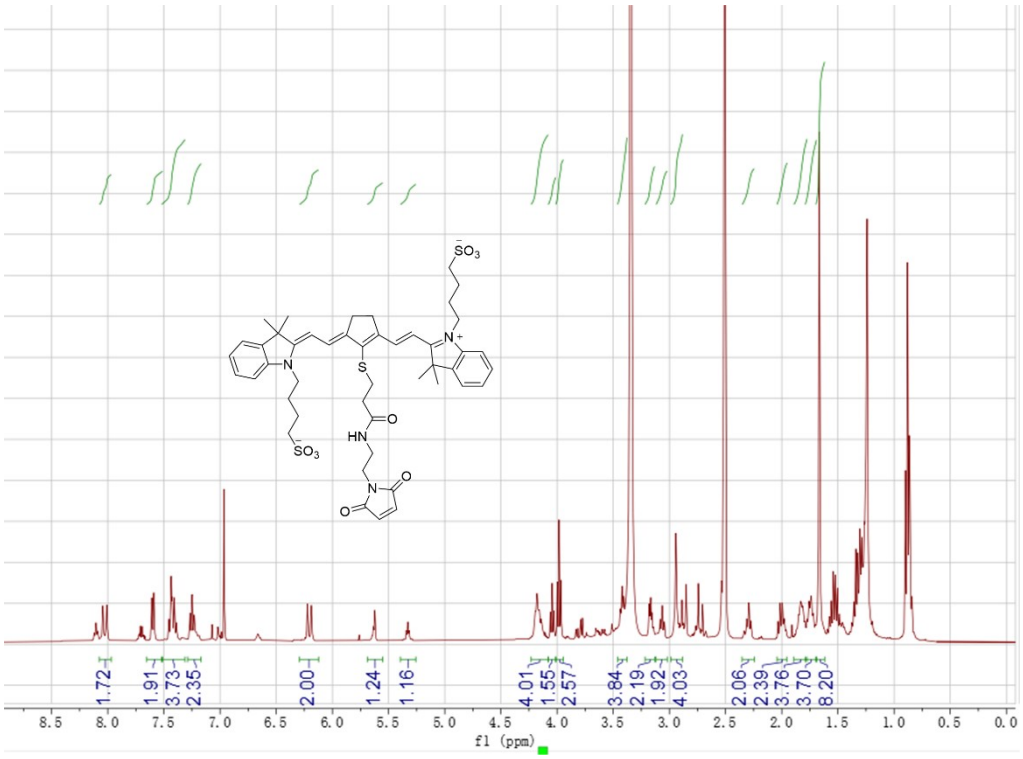


Figure S3. ^{1}H NMR spectrum of IR806-Mal. DMSO-d_6 was used as the solvent.

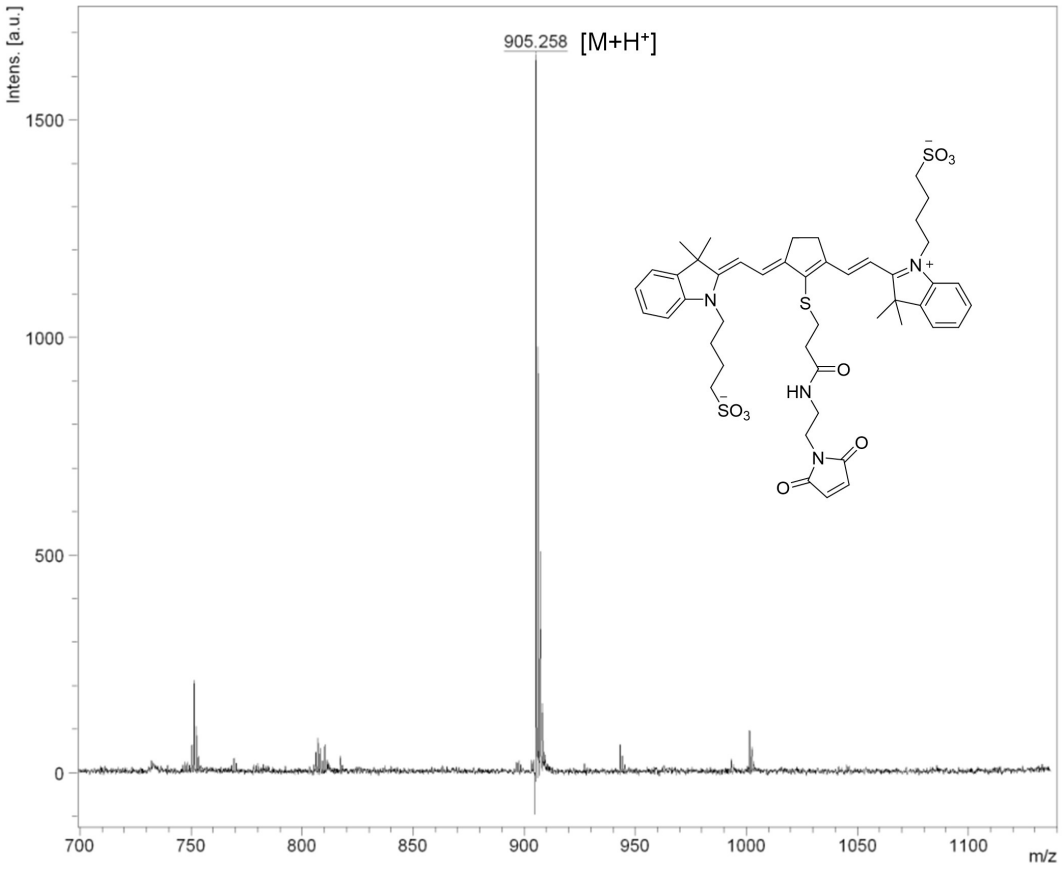


Figure S4. MALDI-TOF MS of IR806-Mal.

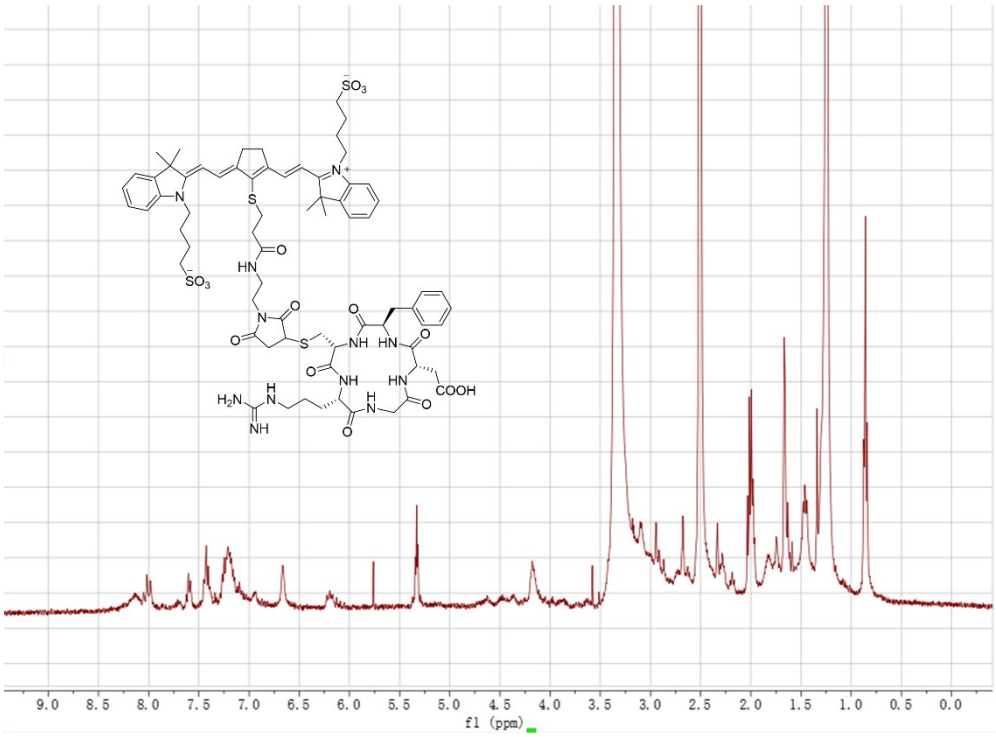


Figure S5. ^{1}H NMR spectrum of IR806-RGD. DMSO-d_6 was used as the solvent.

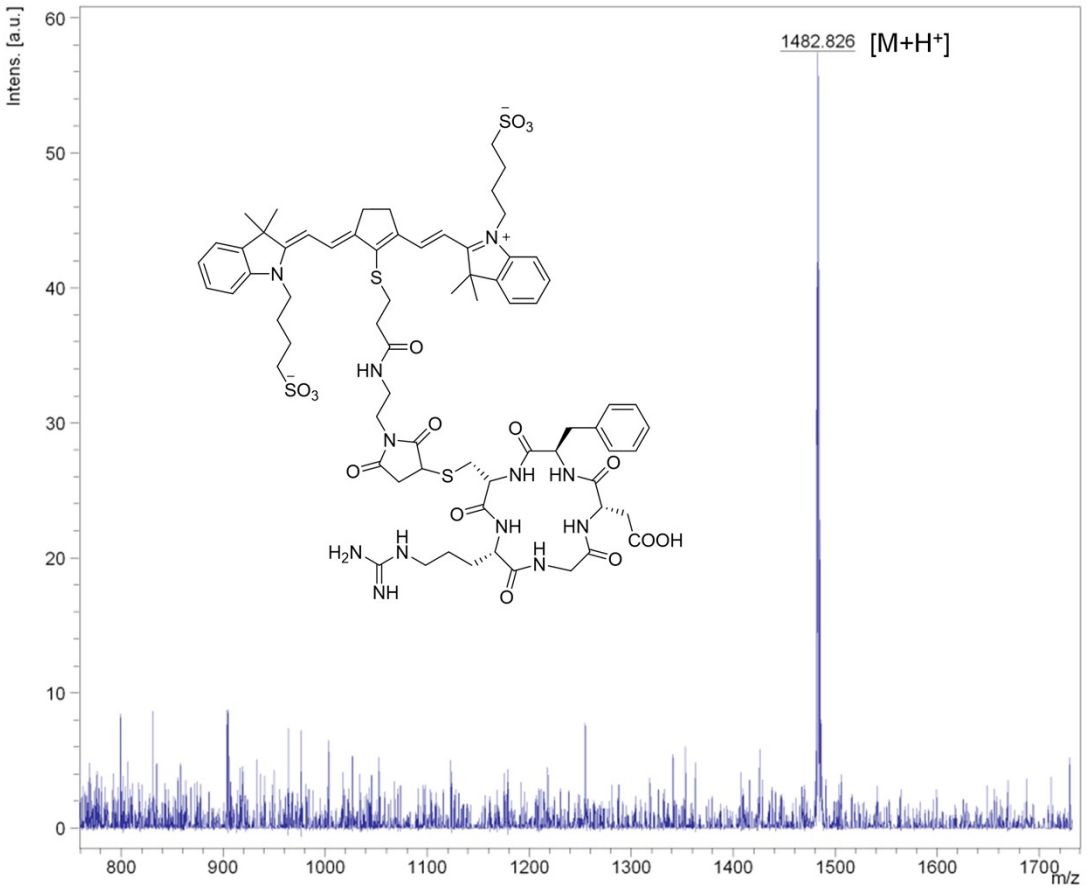


Figure S6. MALDI-TOF MS of IR806-RGD.

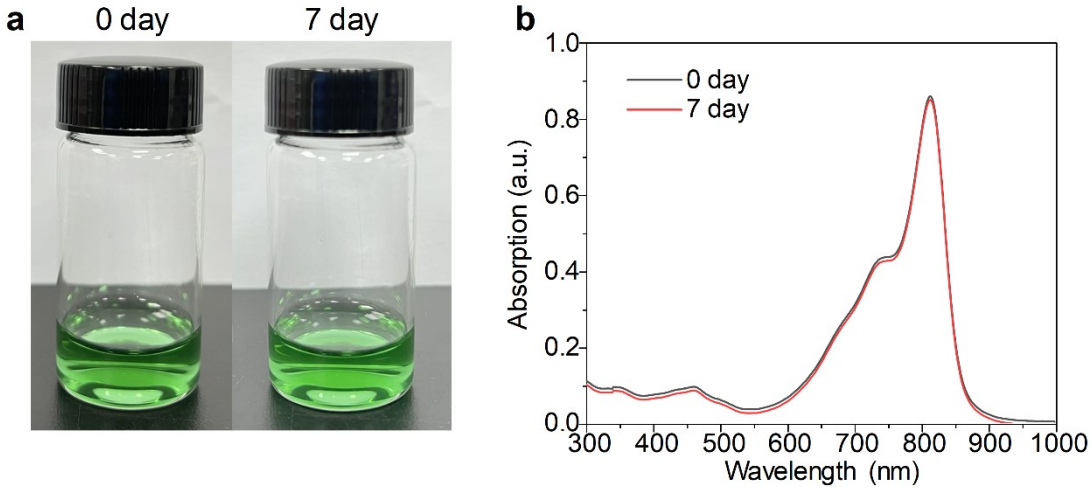


Figure S7. (a) Images of PBS solution (pH 7.4) of IR806-RGD before and after 7 day's storage under 4 °C. (b) Absorption spectra of IR806-RGD solution before and after 7 day's storage under 4 °C.

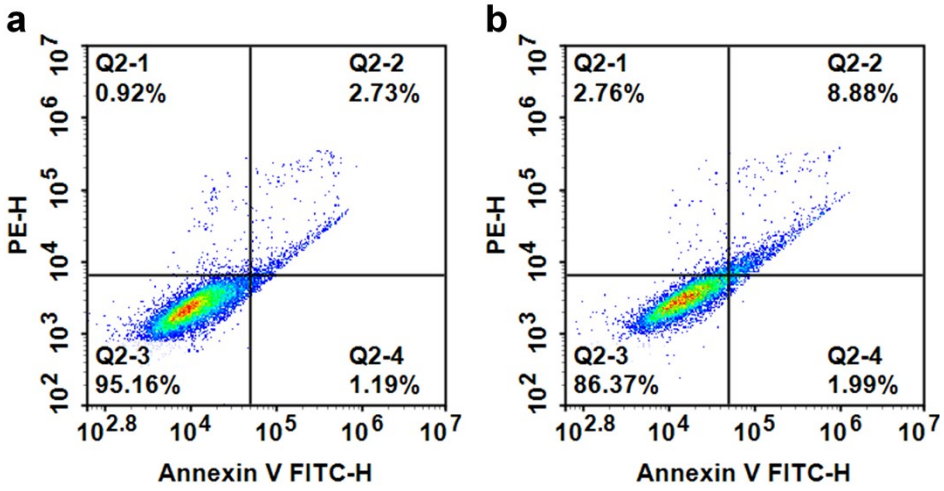


Figure S8. Flow cytometry analysis for viability of 4T1 cells treated with PBS (a) or IR806-RGD (b).

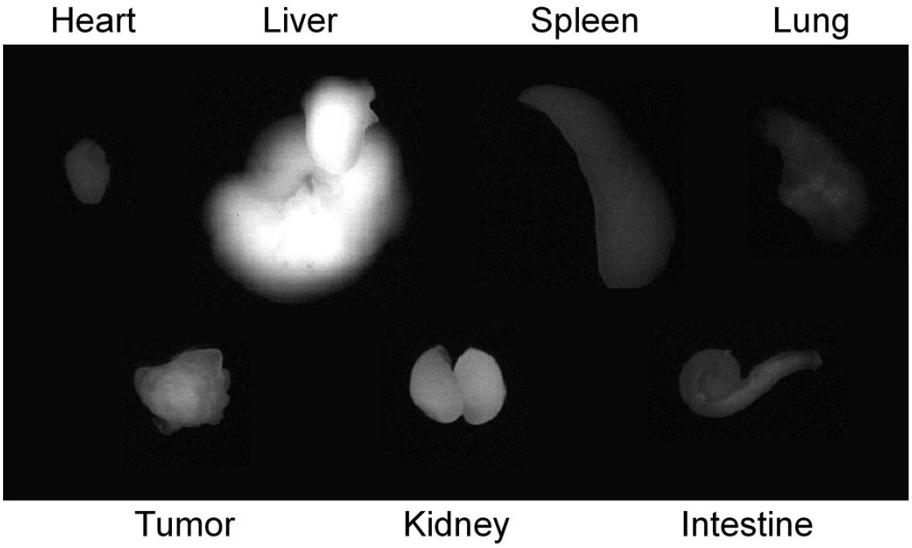


Figure S9. Ex vivo NIR-II fluorescence image of major organs and tumor resected from IR806-injected mice at t = 24 h post-injection.

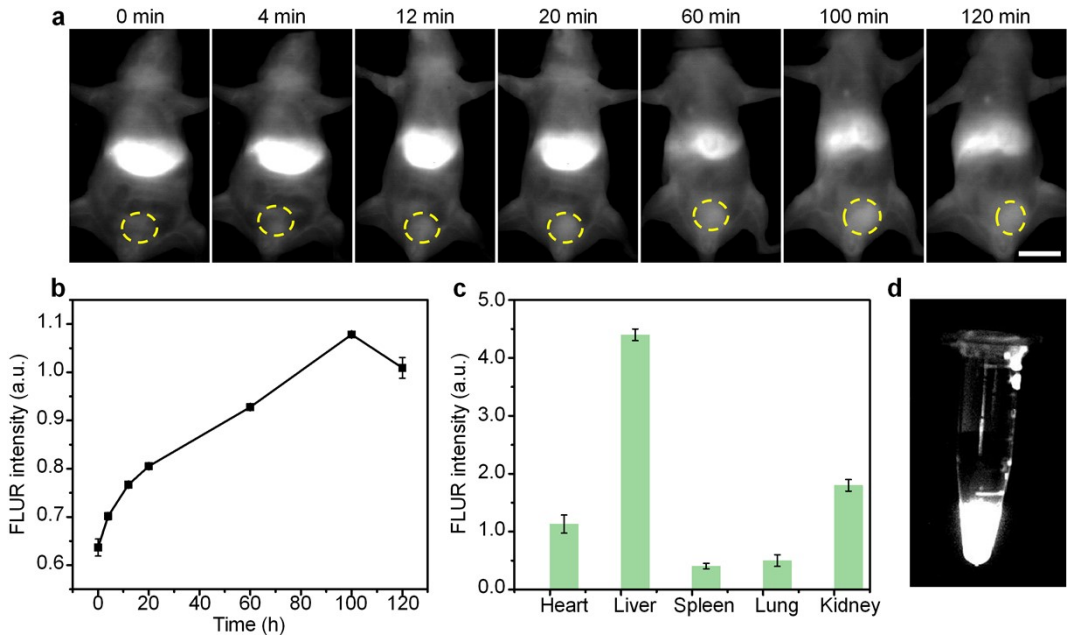


Figure S10. (a) NIR-II fluorescence images of mice i.v. injected with IR806-RGD at different time points. The yellow circles indicate the location of bladder. The scale bar represents 5 mm. The excitation wavelength was 808 nm with a 980 nm long-pass filter. The exposure time was 50 ms, and the laser power was 1.5 W/cm^2. (b) NIR-II fluorescence intensities of bladder as a function of post-injection time. (c) NIR-II fluorescence intensities of major organs resected from mice at t = 120 min post-injection. (d) NIR-II fluorescence image of urine collected from IR806-RGD-injected mice.

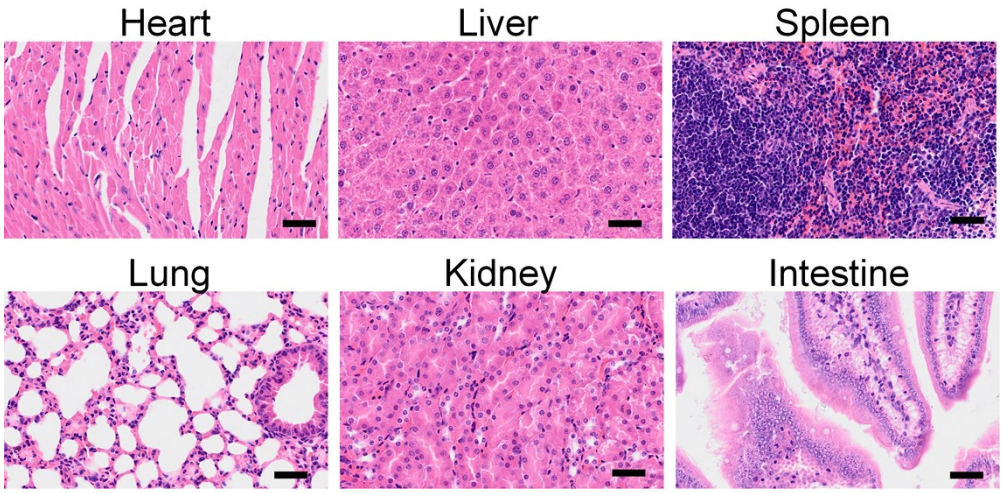


Figure S11. H&E staining of major organs collected from IR806-RGD injected mice. The scale bars represent 50 μm.