

Supporting Information (SI)

$\alpha\text{v}\beta\text{3}$ Integrin-targeted ICG-derivated theranostic probes for imaging-guided surgery and photothermal therapy of oral cancer

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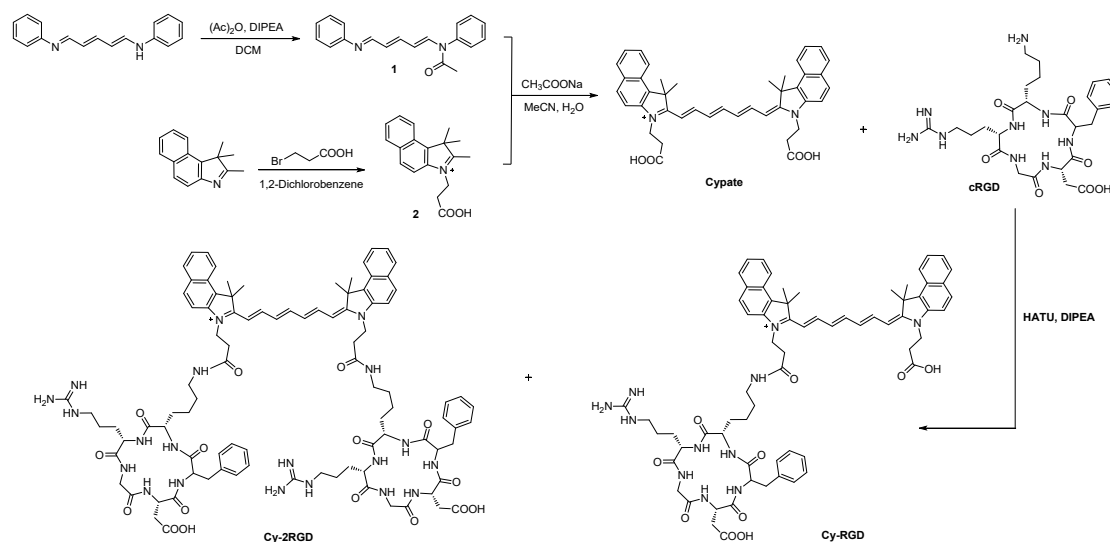
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Scheme S1. The synthetic route of probes Cy-RGD and Cy-2RGD.

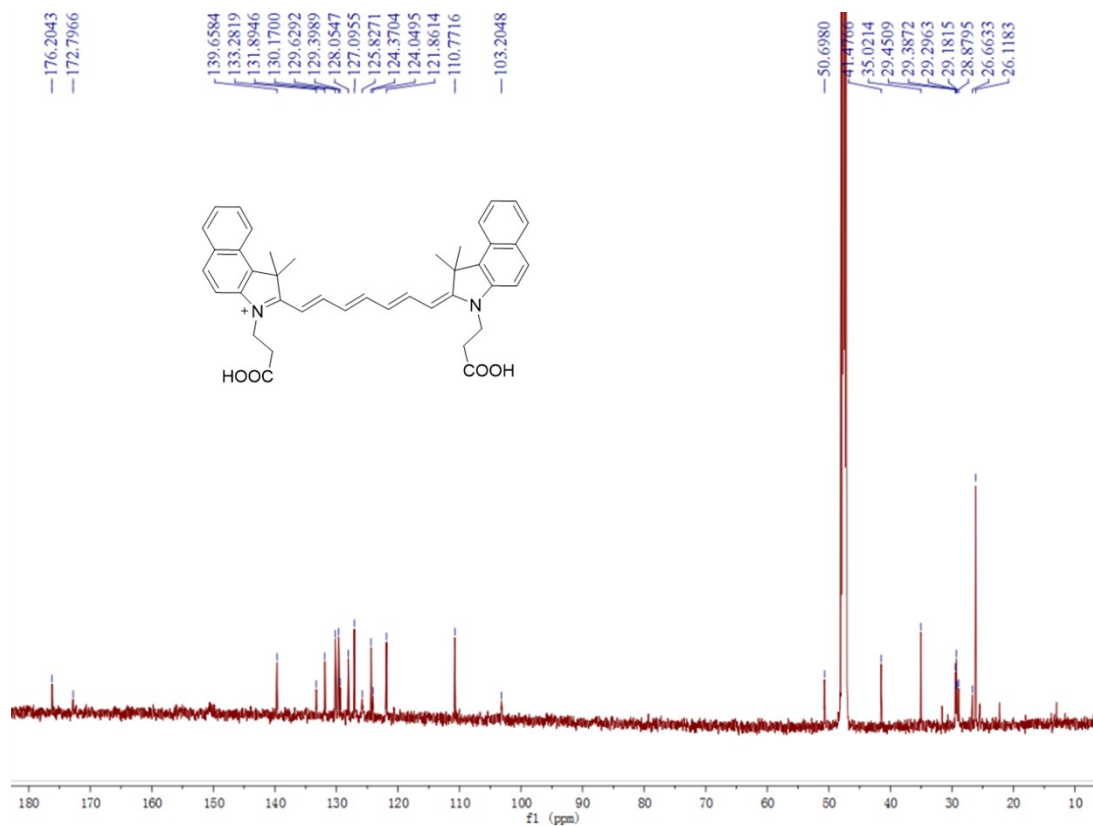
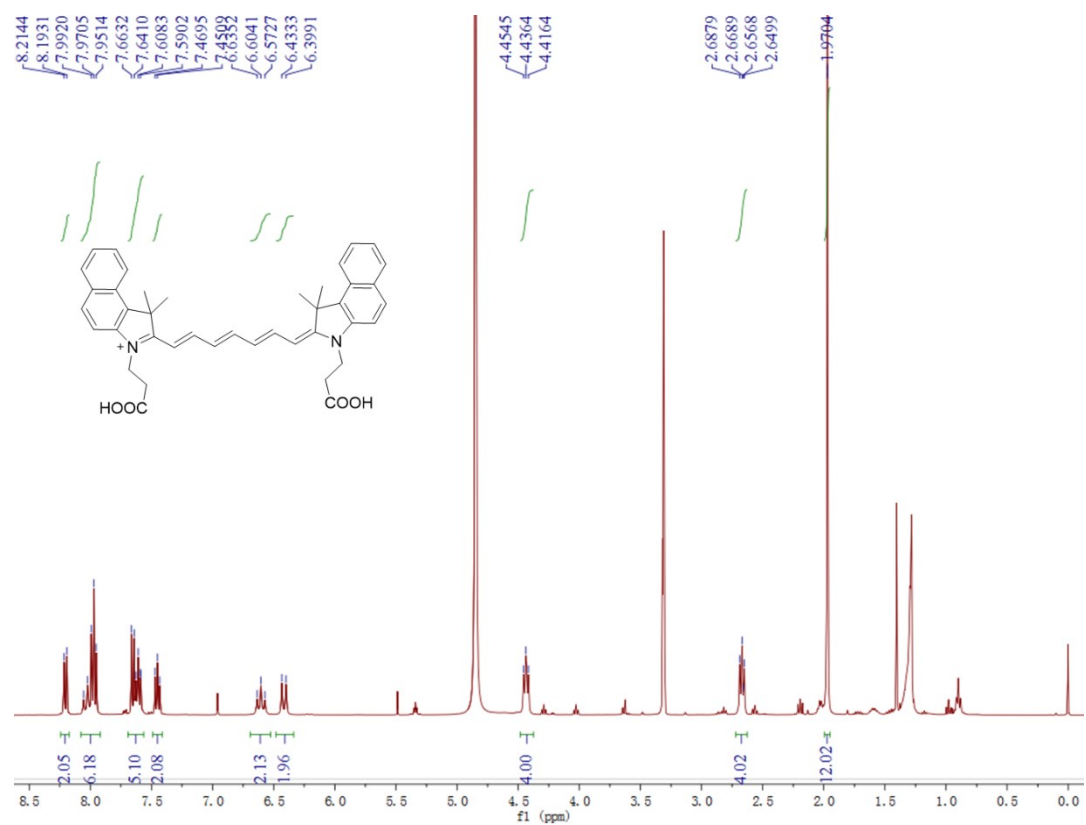


Figure S1. ¹H and ¹³C NMR spectra of compound cypate.

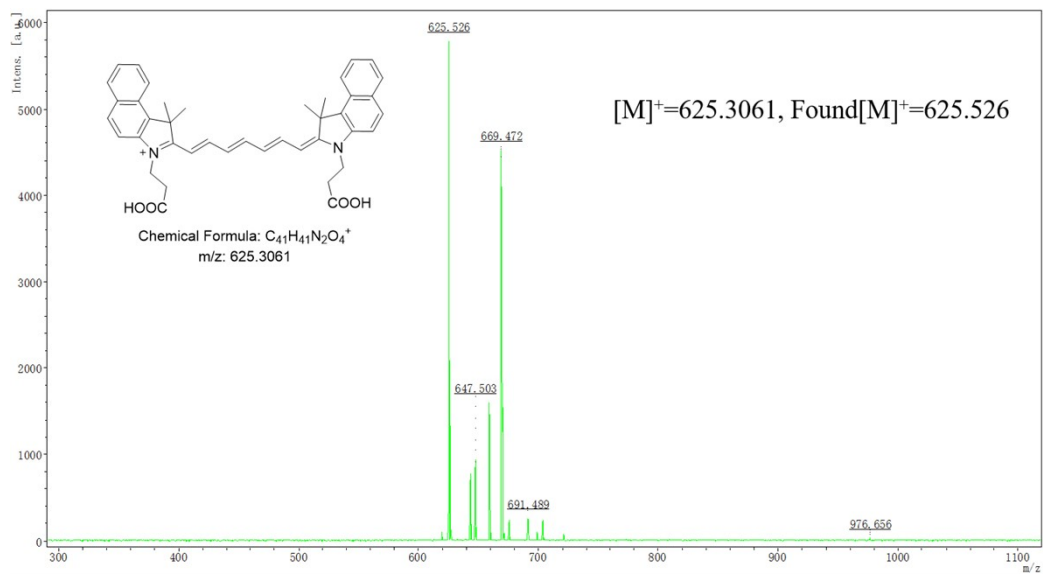


Figure S2. MALDI-TOF/MS spectrum of compound cypate.

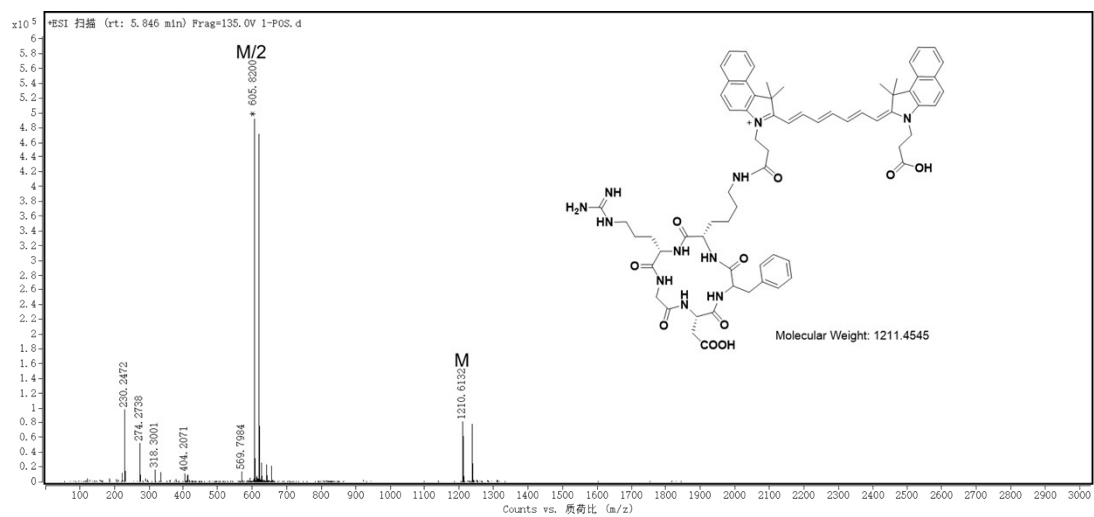


Figure S3. MALDI-TOF/MS spectrum of compound Cy-RGD.

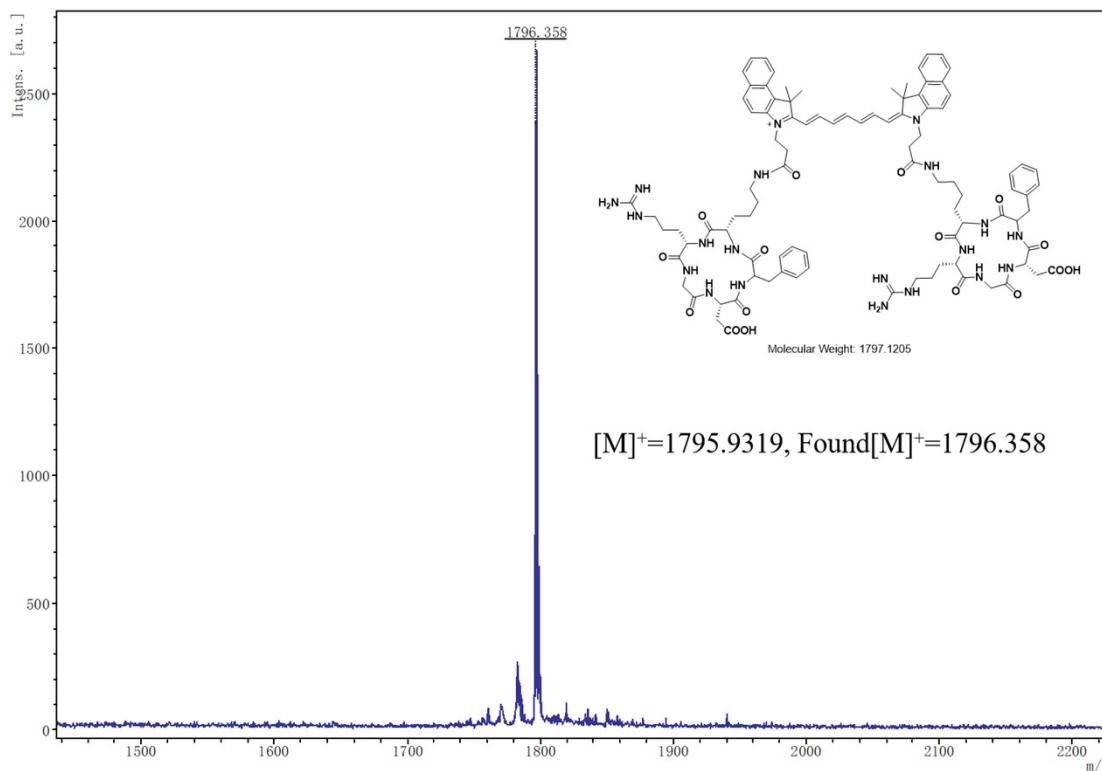


Figure S4. MALDI-TOF/MS spectrum of compound Cy-2RGD.

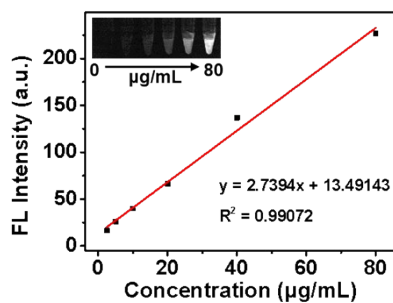


Figure S5. NIR fluorescence images of Cy-2RGD with different concentrations at 1000 nm.

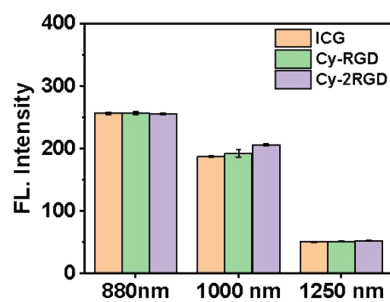


Figure S6. Quantitative fluorescence intensity of ICG, Cy-RGD, and Cy-2RGD with various long-pass filters in Fig.

1(d).

	Cy-RGD	Cy-2RGD
QY(θ)	2.0%	2.4%

Table S1. Quantum yields of Cy-RGD and Cy-2RGD in PBS buffer. ICG was chosen as the reference ($\Phi = 2.5\%$). All the measurements were performed at room temperature.

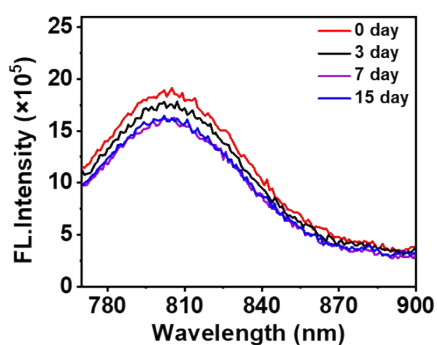


Figure S7. The stability of Cy-2RGD in PBS buffer at room temperature.

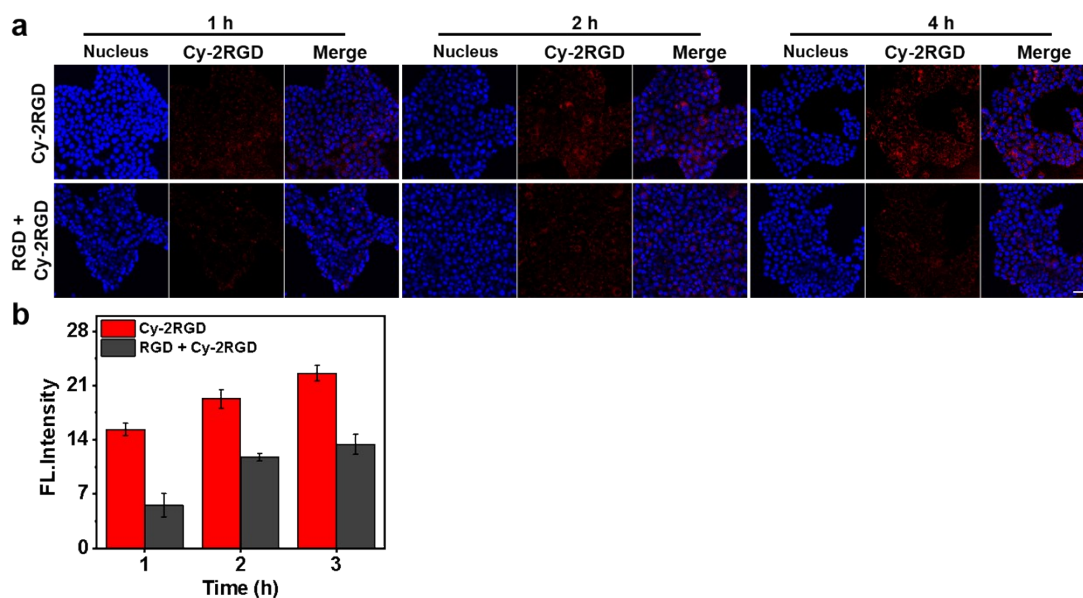


Figure S8. (a) Confocal fluorescence images of CAL-27 cells that were pretreated with or without RGD peptide ($5 \mu\text{g mL}^{-1}$, 4 h) for 4 h, then followed by incubating with Cy-2RGD ($10 \mu\text{g mL}^{-1}$) for different time points (1 h, 2 h, and 4 h) at 37°C , (b) Quantitative fluorescence intensities of (a). Scale bar: $40 \mu\text{m}$.

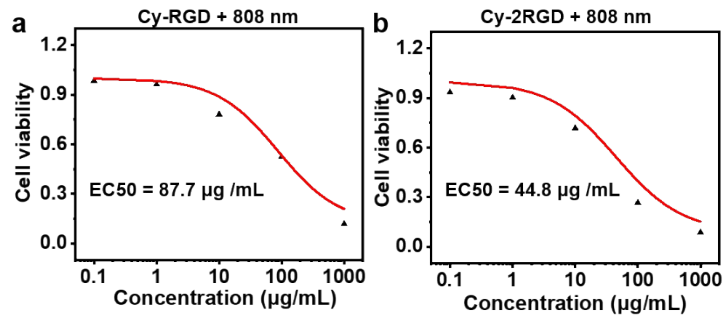


Fig S9. The fitted curve EC50 of Cy-RGD and Cy-2RGD under 808 nm laser irradiation.

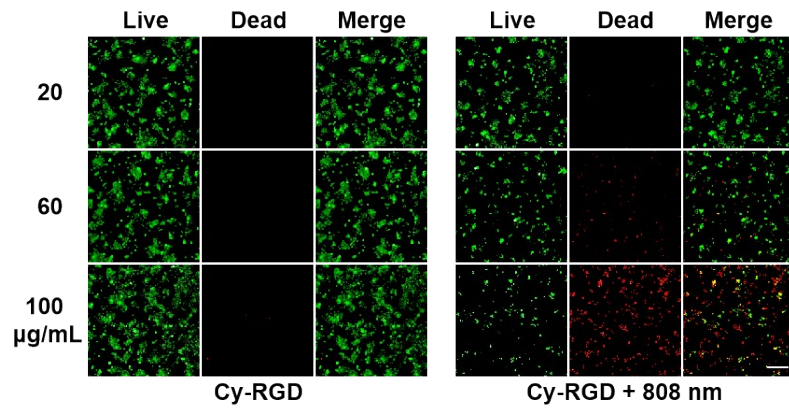


Fig S10. Live/dead fluorescence images of oral tumor cells treated with Cy-RGD for 24 h followed by 808 nm laser irradiation (1 W cm⁻², 5 min) or not.

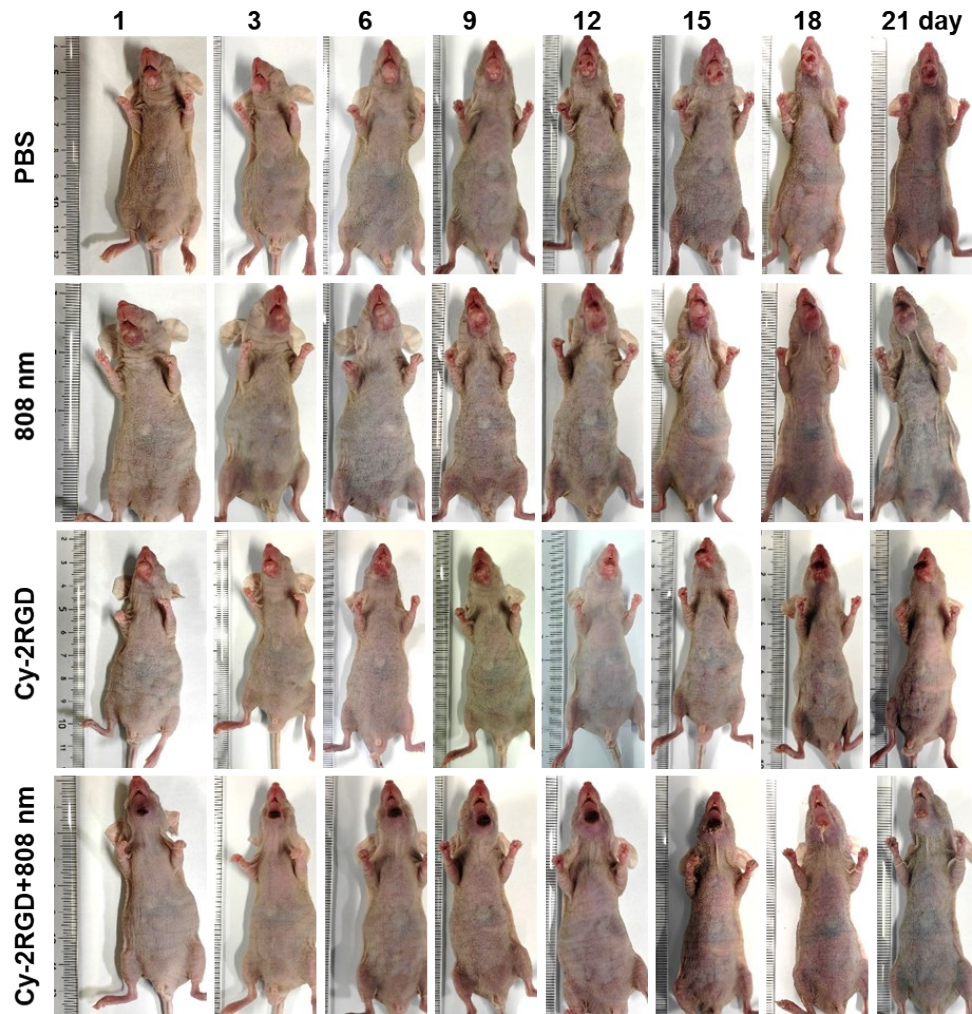


Figure S11. Images and representative mice captured on different days after each treatment.

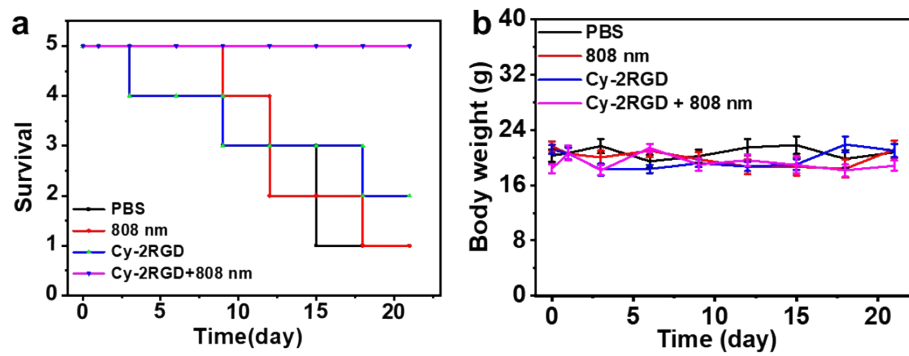


Figure S12. Survival curve (a) and body weight changes (b) of mice for each treatment group (n=5).

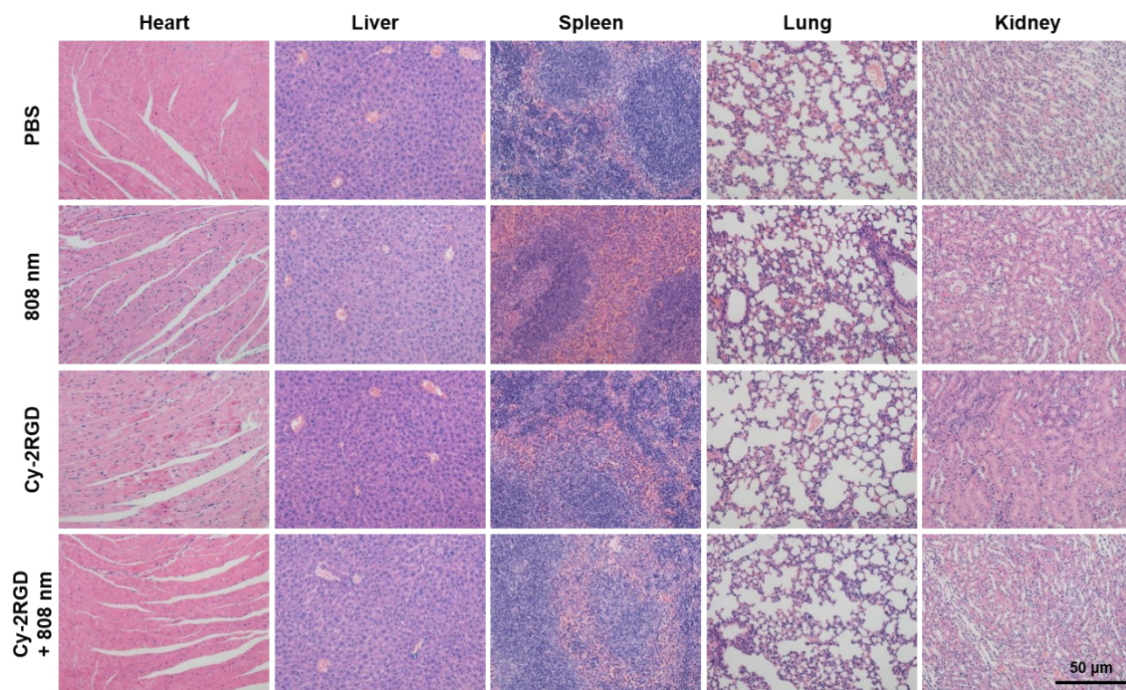


Figure S13. H&E staining graphs of major organs for representative mice with various treatments captured on 21 days. Scale bar: 50 μ m.



Supplementary video.mp4