Supporting information

A PEGylated conjugated-BODIPY oligomer for NIR-II imaging-guided photothermal therapy

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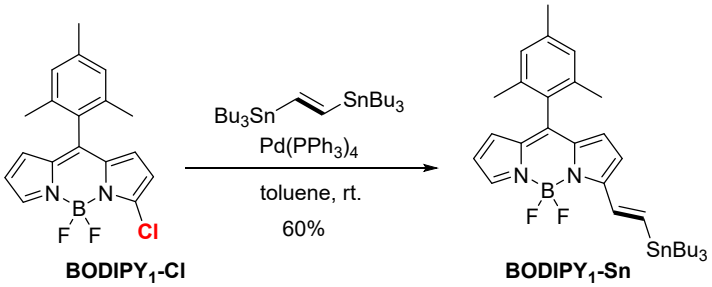
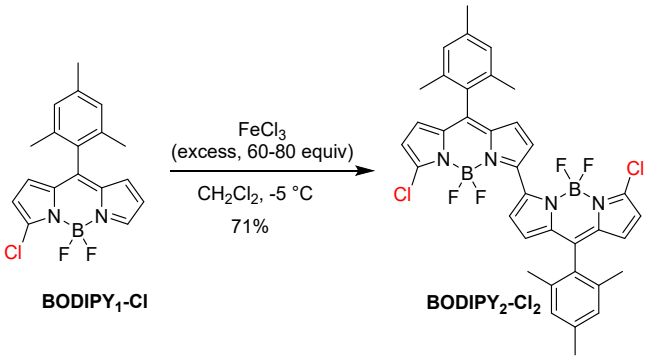
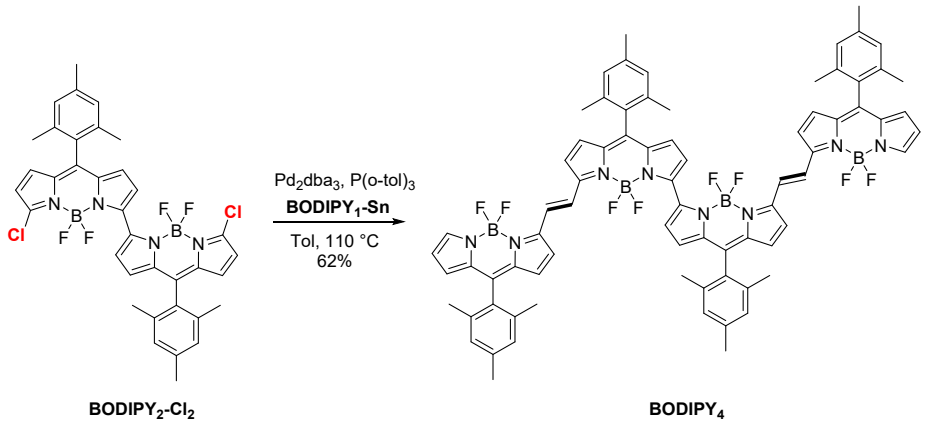
[†]Yuan Wang, Tongtong Shan contributed equally to this work.



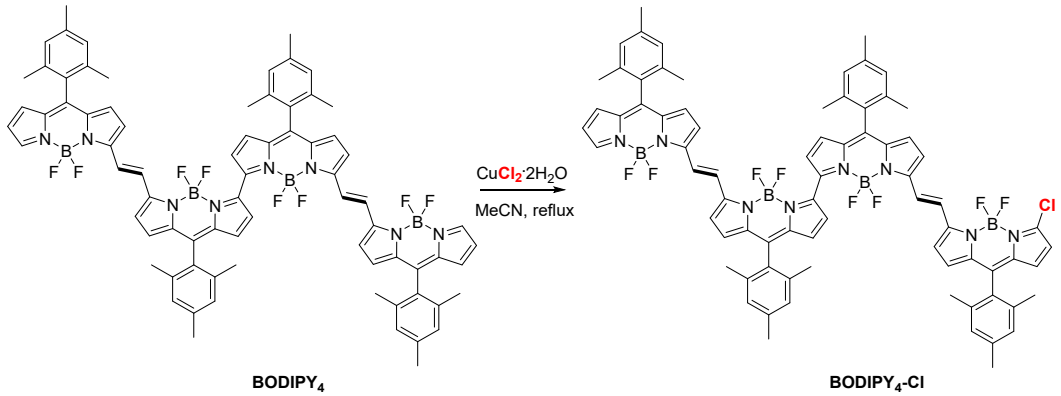
Scheme S1. Synthesis of $BODIPY_1$-Sn.



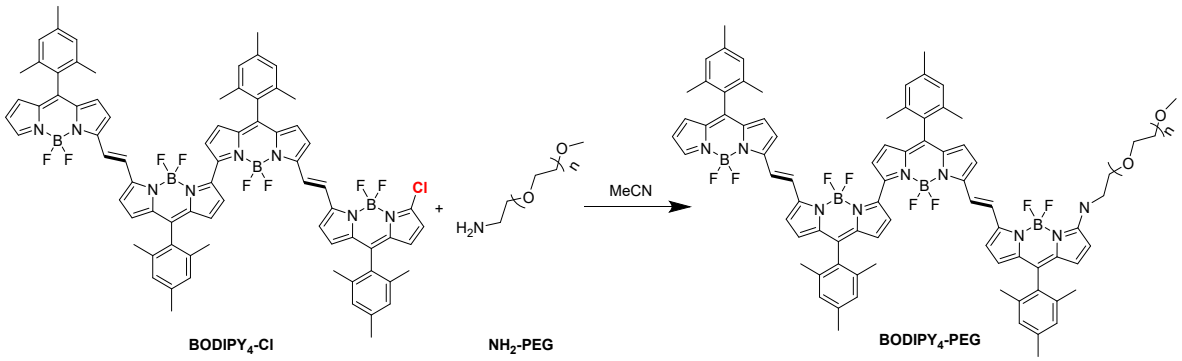
Scheme S2. Synthesis of $BODIPY_2$-Cl_2.



Scheme S3. Synthesis of $BODIPY_4$.



Scheme S4. Synthesis of $BODIPY_4$-Cl.



Scheme S5. Synthesis of $BODIPY_4$-PEG.

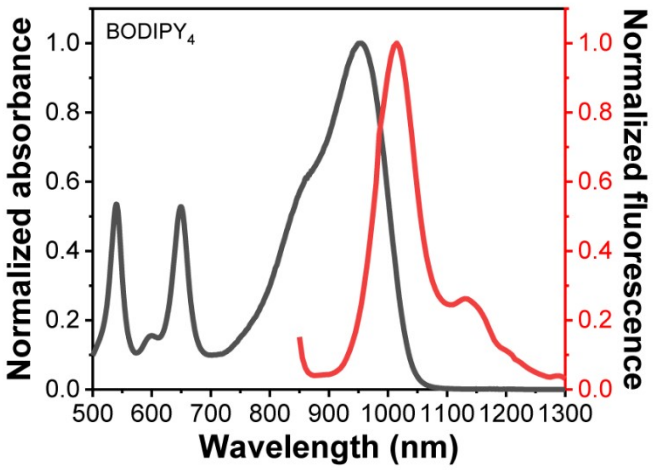


Fig. S1. Absorbance and emission spectra of $BODIPY_4$.

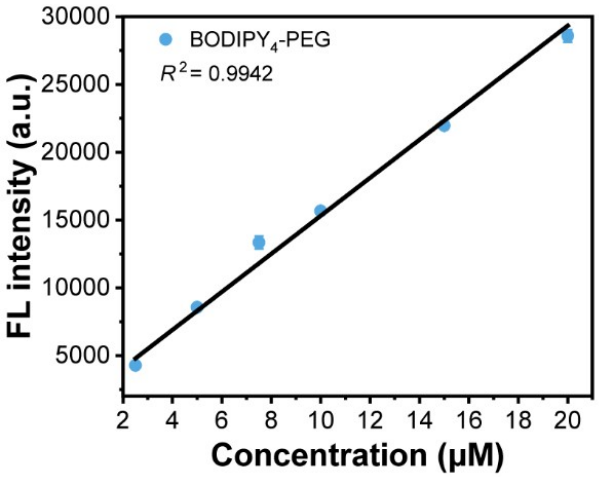


Fig. S2. The linear relationship between concentration and fluorescence intensity of $BODIPY_4$-PEG.

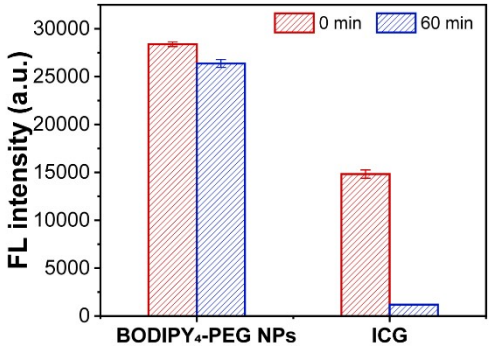


Fig. S3. Photostability of $BODIPY_4$-PEG and ICG.

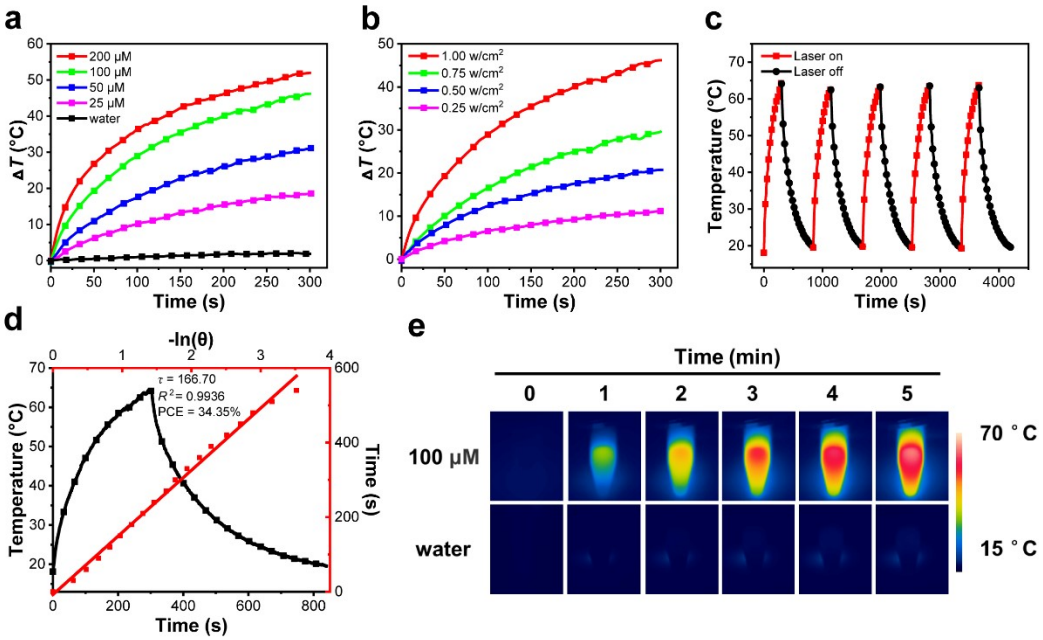


Fig. S4. Photothermal conversion curves of $BODIPY_4$-PEG NPs aqueous solution at various concentrations (a) and different power densities (b) (100 μM) under 808 nm laser irradiation for 5 min. (c) Photothermal stability of $BODIPY_4$-PEG. The heating and cooling cyclic curves of $BODIPY_4$-PEG (100 μM) under 808 nm laser irradiation (1.00 W cm^{-2}, 5 cycles). (d) The heating-cooling curve of $BODIPY_4$-PEG aqueous solution (100 μM) under 808 nm laser irradiation (1.00 W cm^{-2}) (heating time 5 min, cooling time 9 min) and the relationship between -Ln(θ) and cooling time calculated by the curve and formula. (e) Thermal images of $BODIPY_4$-PEG and water under 808 nm laser irradiation (1.00 W cm^{-2}, 5 min).

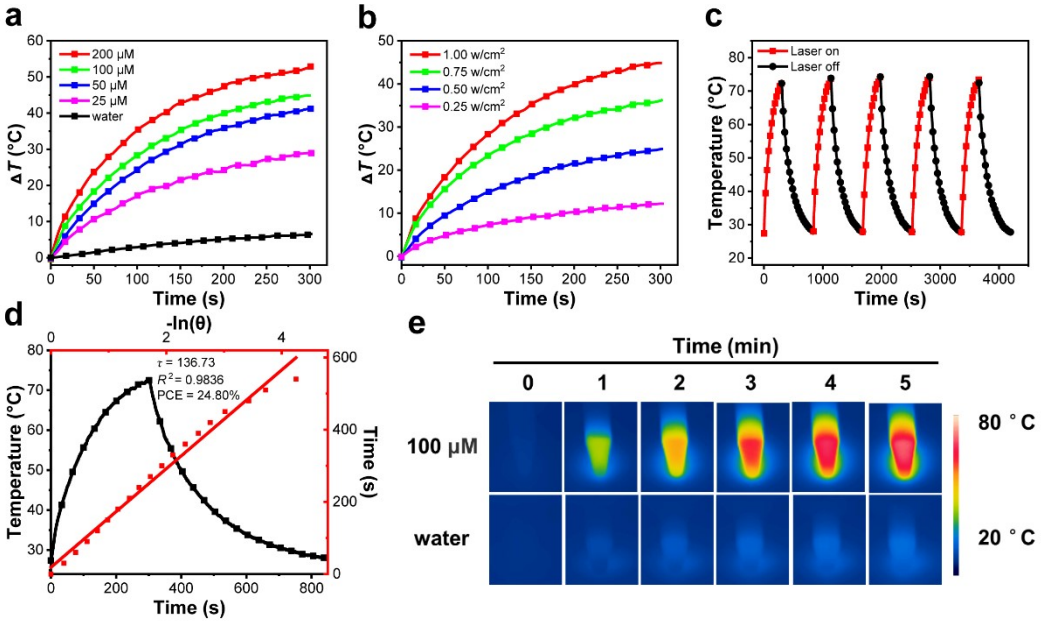


Fig. S5. Photothermal conversion curves of $BODIPY_4$-PEG NPs aqueous solution at various concentrations (a) and different power densities (b) (100 μM) under 1064 nm laser irradiation for 5 min. (c) Photothermal stability of $BODIPY_4$-PEG. The heating and cooling cyclic curves of $BODIPY_4$-PEG (100 μM) under 1064 nm laser irradiation (1.00 W cm^{-2}, 5 cycles). (d) The heating-cooling curve of $BODIPY_4$-PEG aqueous solution (100 μM) under 1064 nm laser irradiation (1.00 W cm^{-2}) (heating time 5 min, cooling time 9 min) and the relationship between -Ln(θ) and cooling time calculated by the curve and formula. (e) Thermal images of $BODIPY_4$-PEG NPs and water under 1064 nm laser irradiation (1.00 W cm^{-2}, 5 min).

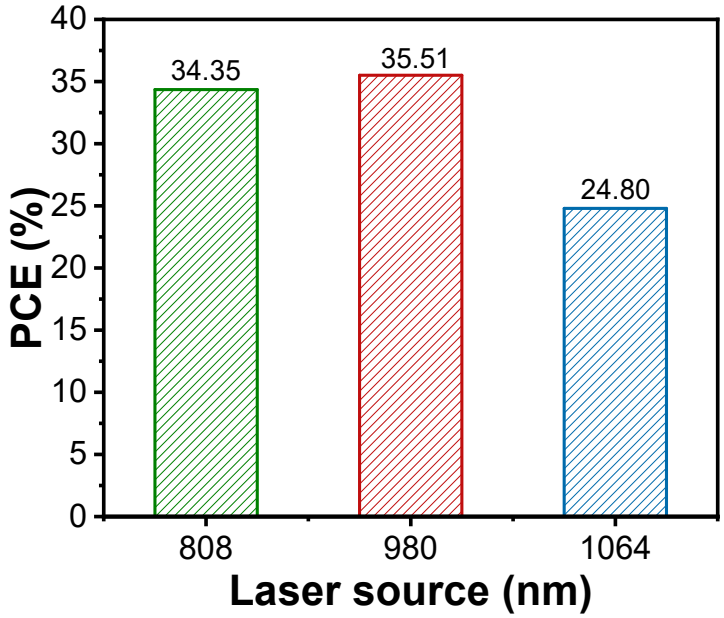


Fig. S6. Summary of PCEs of $BODIPY_4$-PEG under different laser sources.

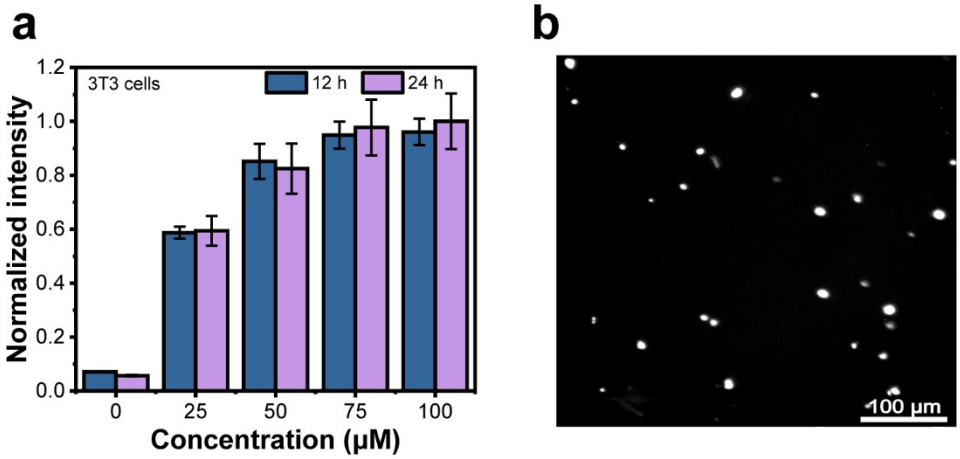


Fig. S7. (a) Quantitative statistic of 3T3 cells' uptake intensity after coincubation with $BODIPY_4$-PEG for 12 h or 24 h. (c) Photograph of 4T1 cells after co-incubating with $BODIPY_4$-PEG for 24 h (808 nm, 1000 LP, 1000 ms).

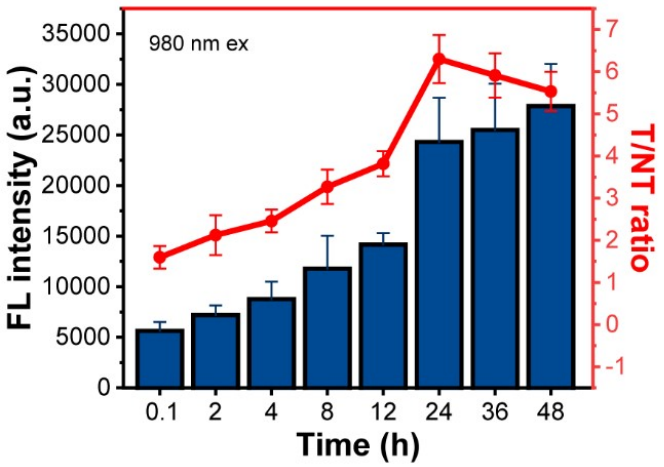


Fig. S8. Quantitative statistics of fluorescence intensity at 4T1 tumor sites.

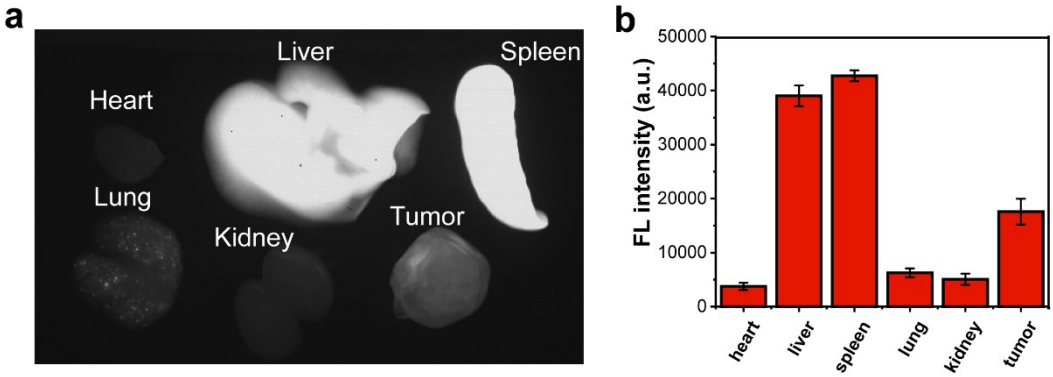


Fig. S9. (a) NIR-II fluorescence image of major organs and tumor resected at 48 h post-injection of $BODIPY_4$-PEG. (d) Quantitative statistics of fluorescence intensity of major organs and tumors (n = 3).

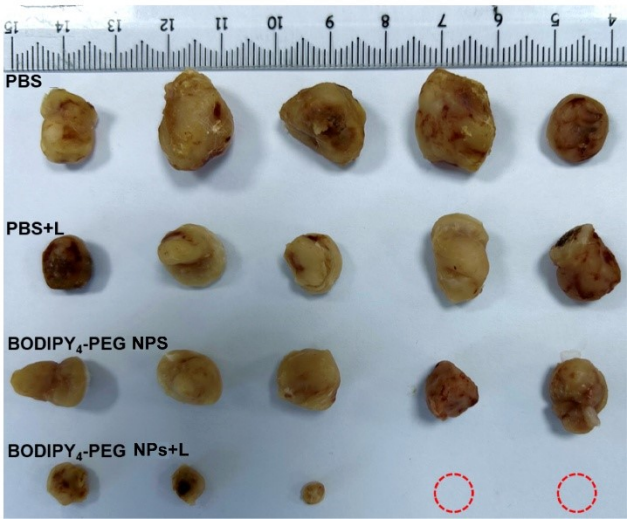


Fig. S10. Photographs of the 4T1 tumors excised from the mice after the four treatments with PBS, PBS+L, BODIPY$_4$-PEG NPs, and BODIPY$_4$-PEG NPs+L as indicated.

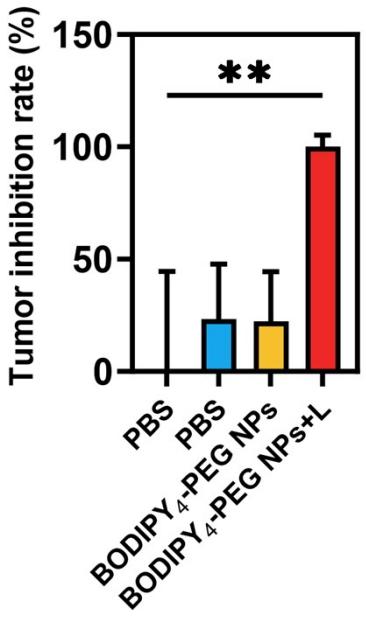


Fig. S11. Curves of tumor inhibition rates for different experimental groups (n = 5, mean ± SEM) and n represented independent experiments. **P < 0.01.

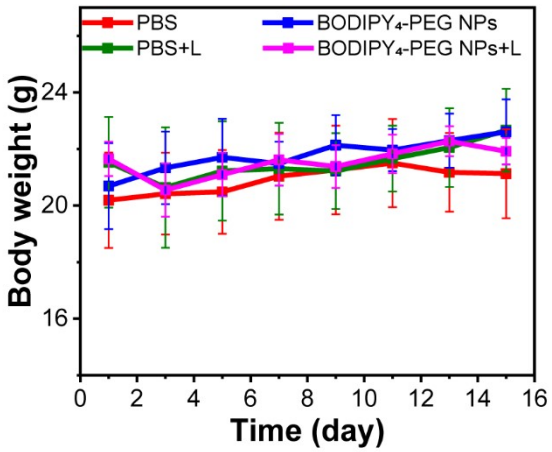


Fig. S12. Variation curve of body weights of mice under the four treatments (n = 5, mean ± SEM).

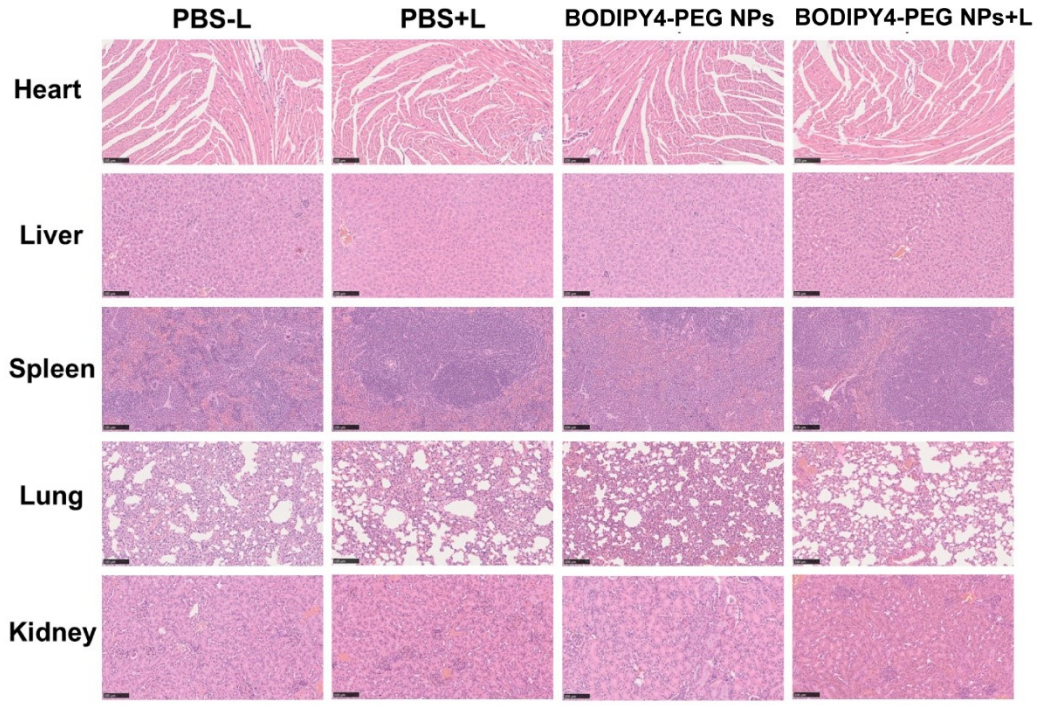


Fig. S13. H&E staining images of the main organs including the heart, liver, spleen, lung, and kidney of mice in different treatment groups. Scale bar: 100 μm.

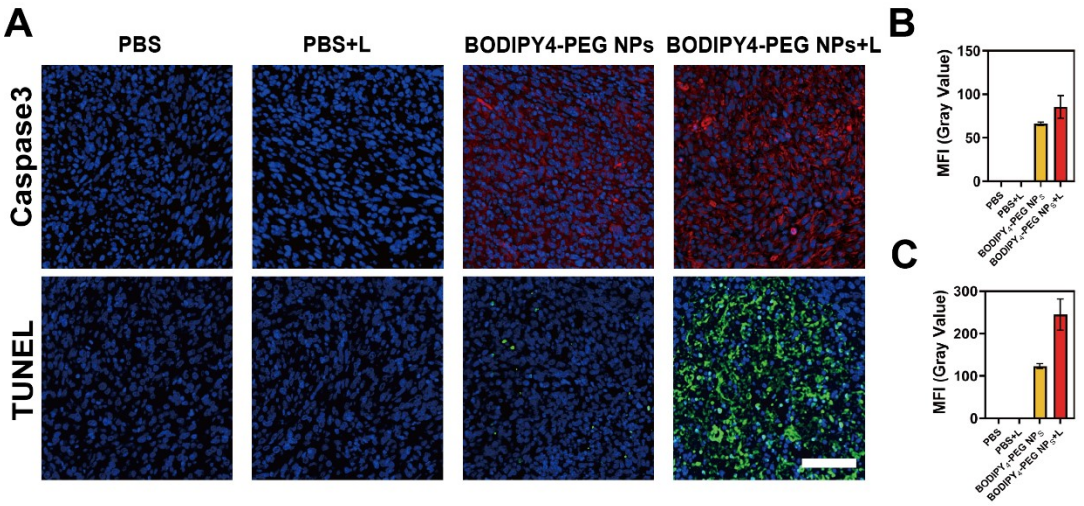


Fig. S14. Immunofluorescence staining experiments. (A) The staining results of Caspase-3 and TUNEL, as well as the quantification of their fluorescence intensities (B) and (C). Scale bar:100 μm.

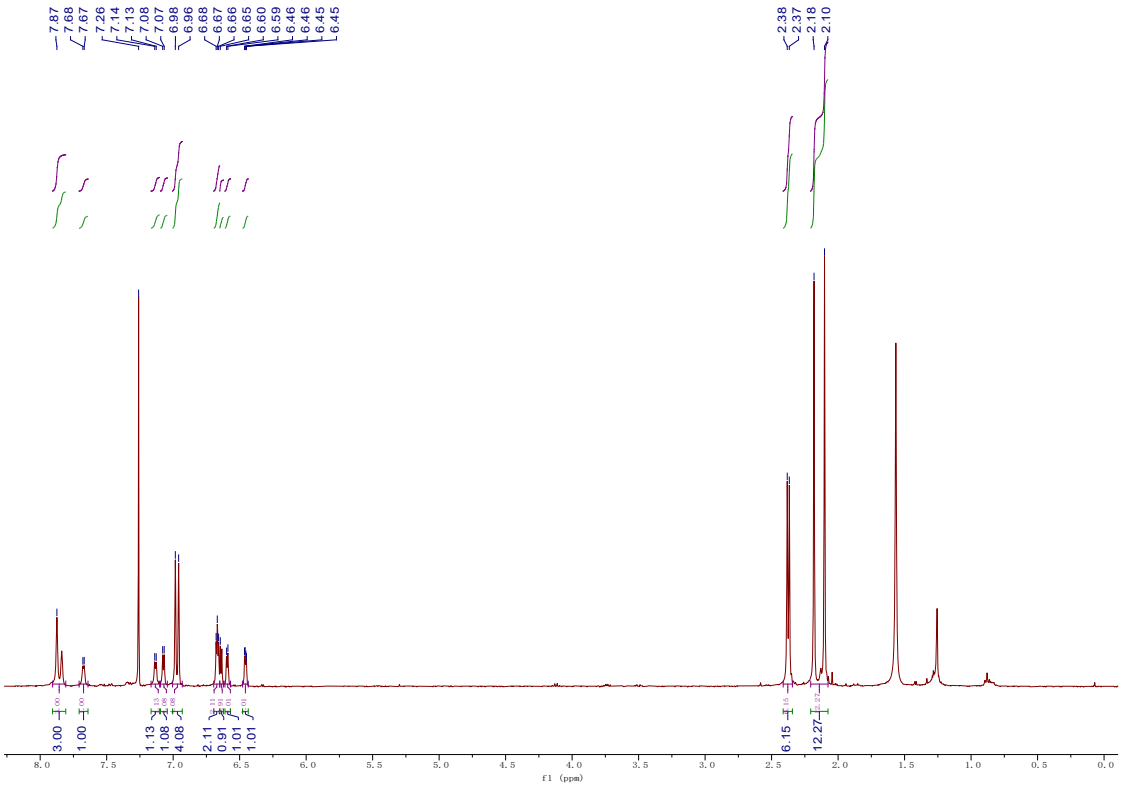


Fig. S15. ^{1}H NMR spectrum of $BODIPY_4$ in $CDCl_3$.

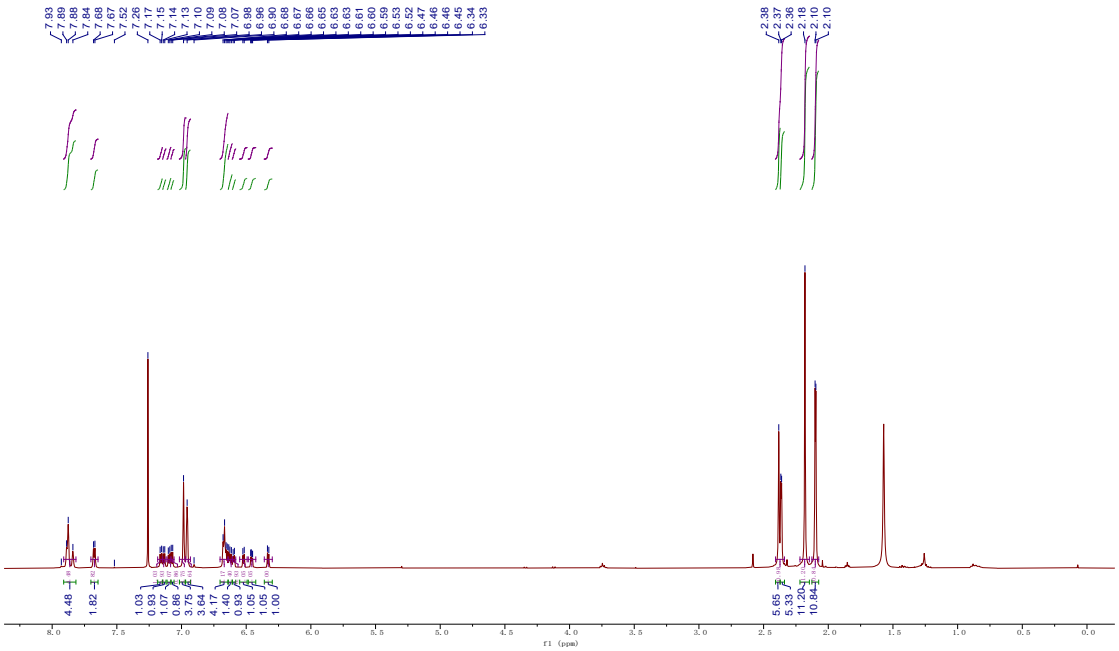


Fig. S16. ^{1}H NMR spectrum of $BODIPY_4$-Cl in $CDCl_3$.

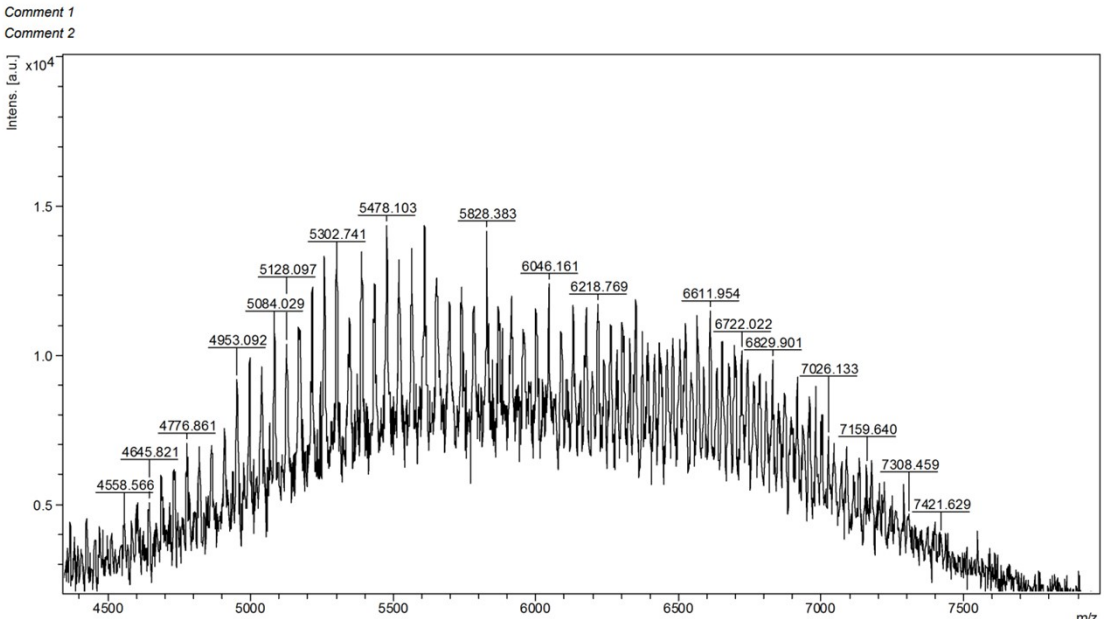


Fig. S17. The MALDI-TOF-MS of $BODIPY_4$-PEG.