Supporting Information

Enhancing Hydrophilicity of Photoacoustic Probes for Effective Ratiometric Imaging of Hydrogen Peroxide

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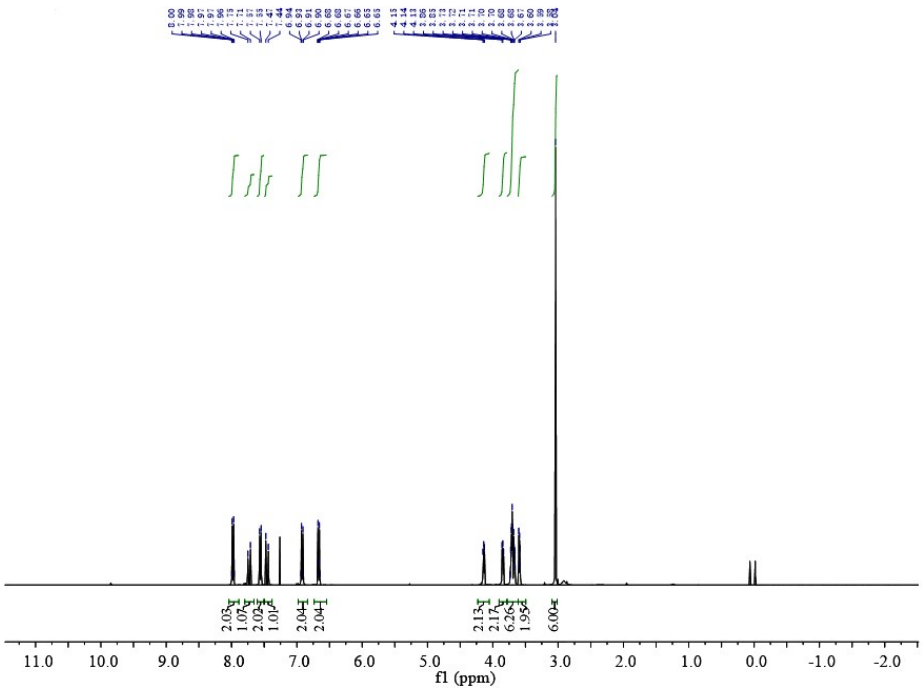

Figure S1. ^{1}H-NMR spectrum of compound 2a in $CDCl_3$.

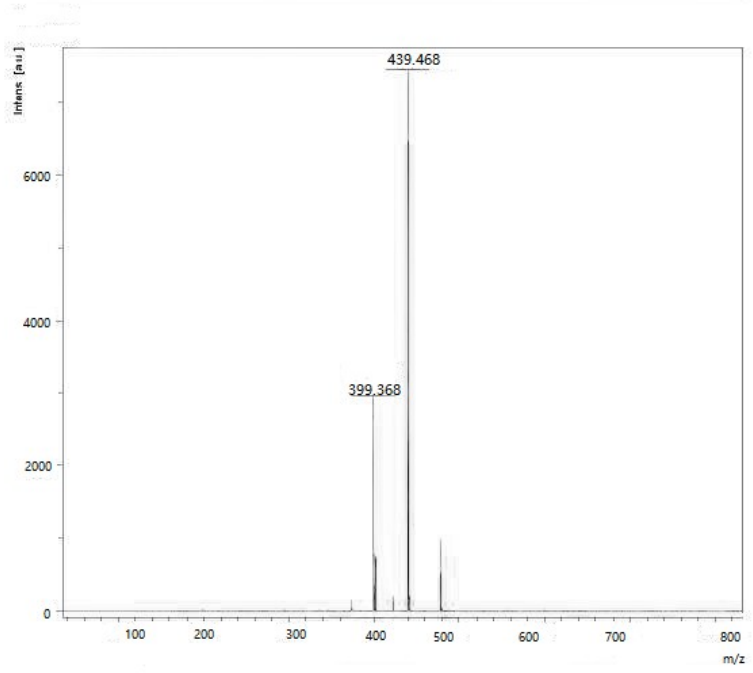

Figure S2. MALDI-TOF-MS of compound 2a.

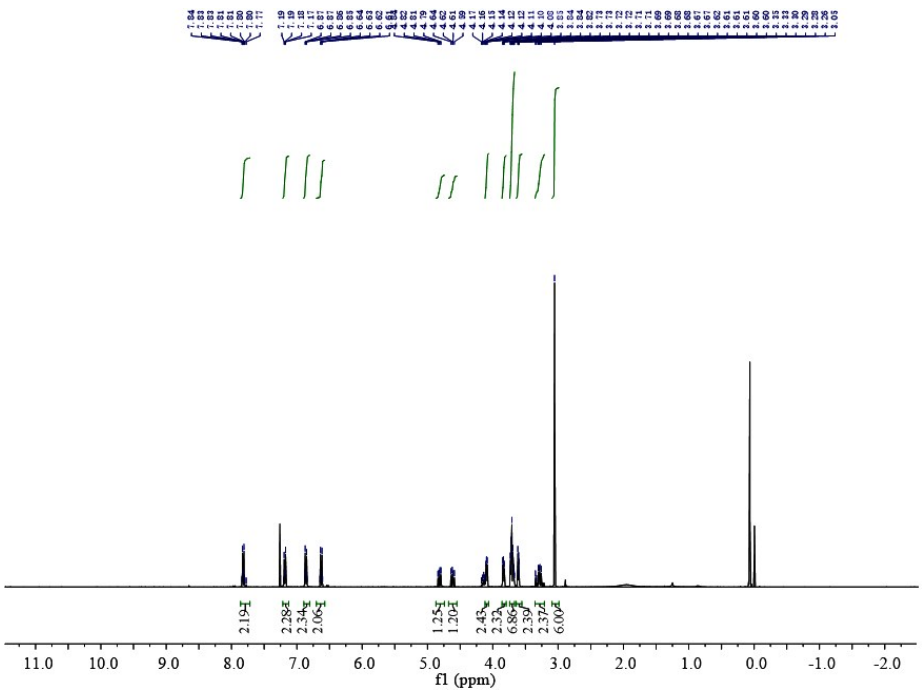

Figure S3. ^{1}H-NMR spectrum of compound 3a in $CDCl_3$.

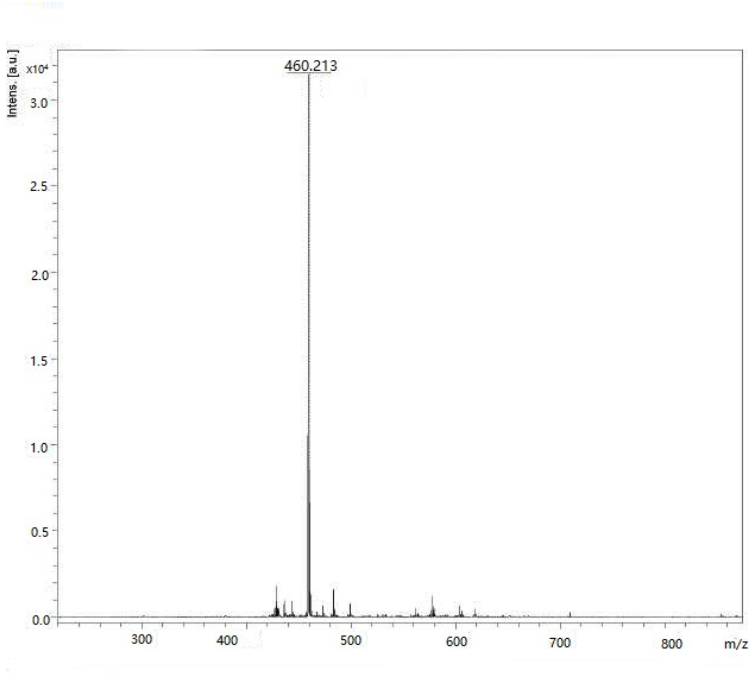

Figure S4. MALDI-TOF-MS of compound 3a.

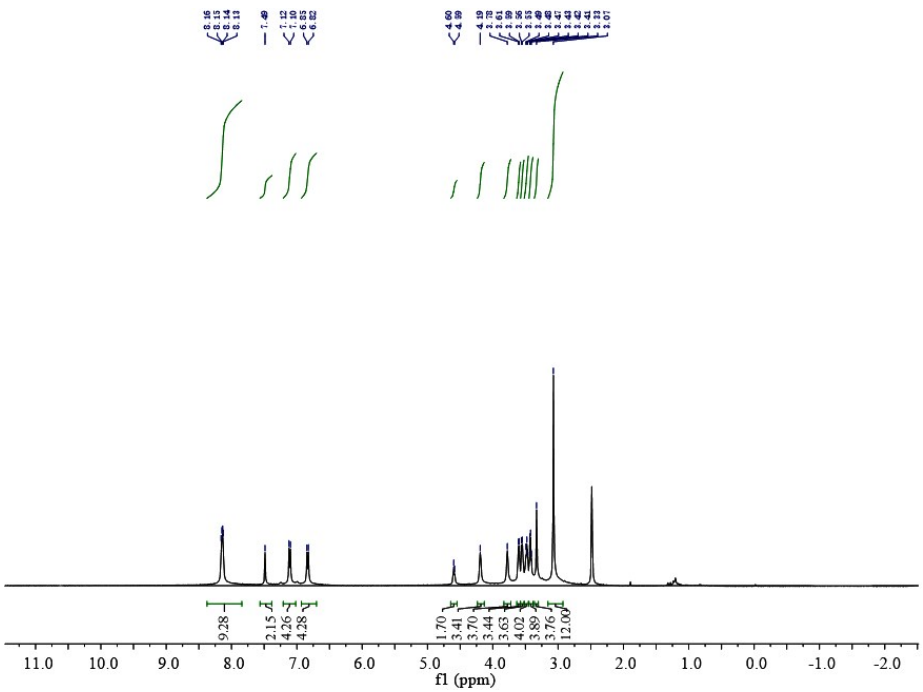

Figure S5. [1]H-NMR spectrum of compound 4a in DMSO-d6.

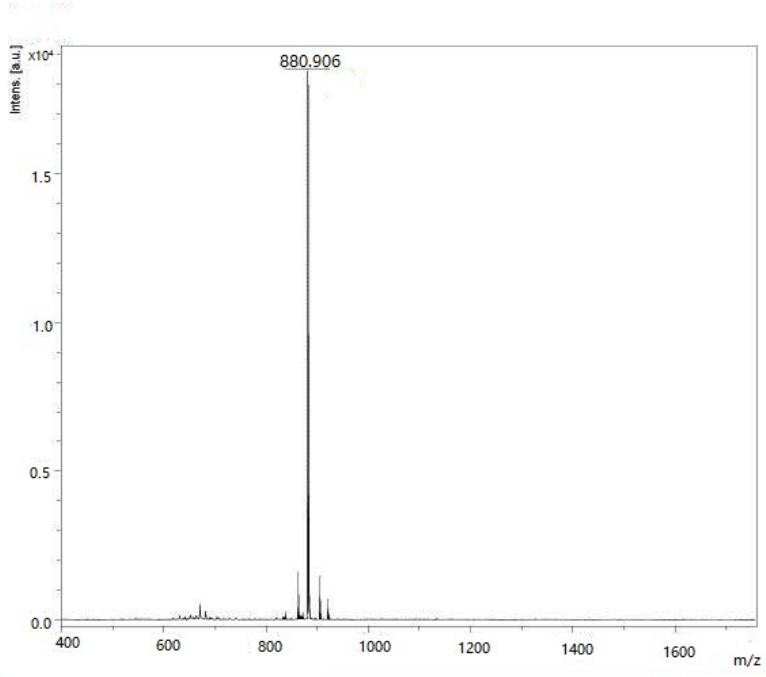

Figure S6. MALDI-TOF-MS of compound 4a.

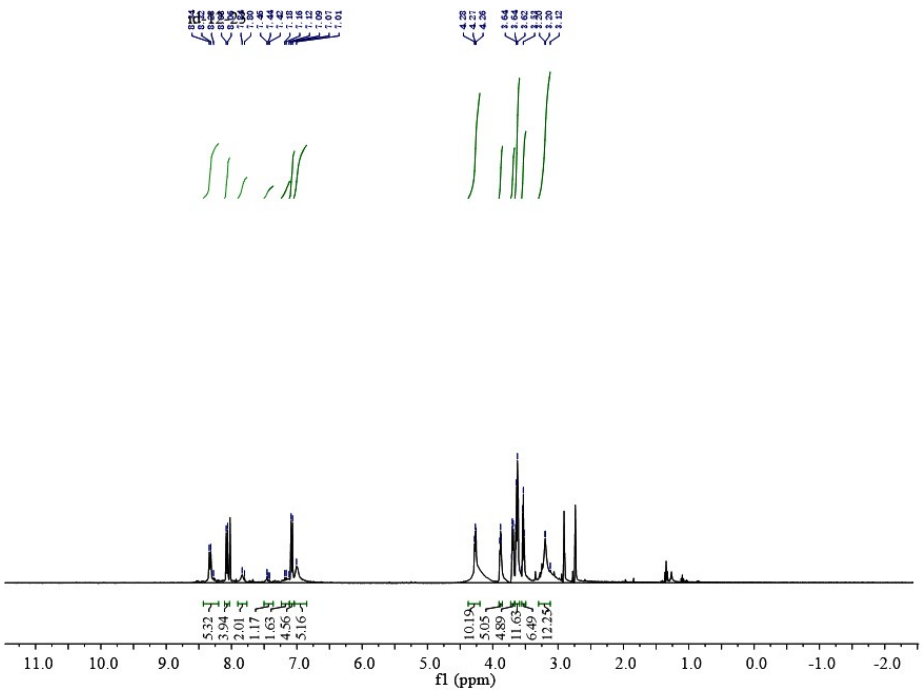

Figure S7. ^{1}H NMR spectrum of compound 5a in DMF-d7.

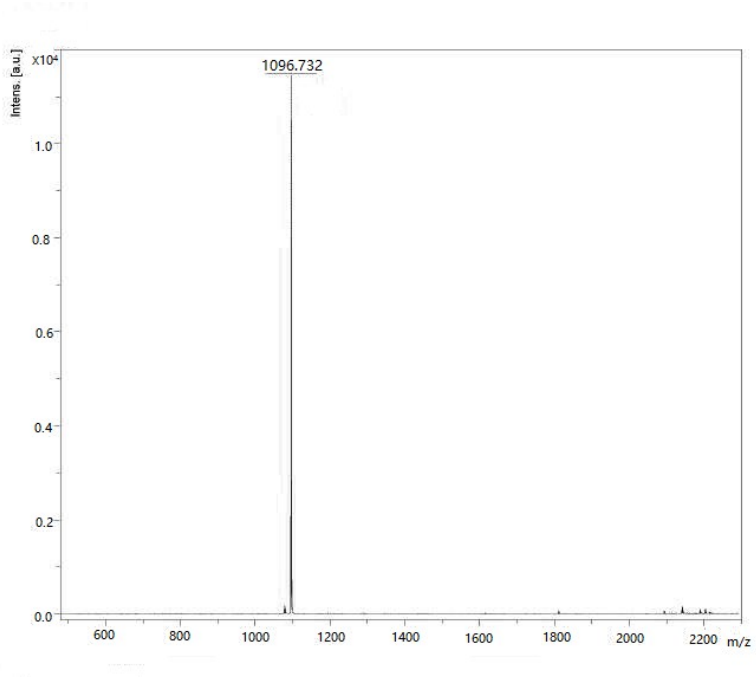

Figure S8. MALDI-TOF-MS of compound 5a.

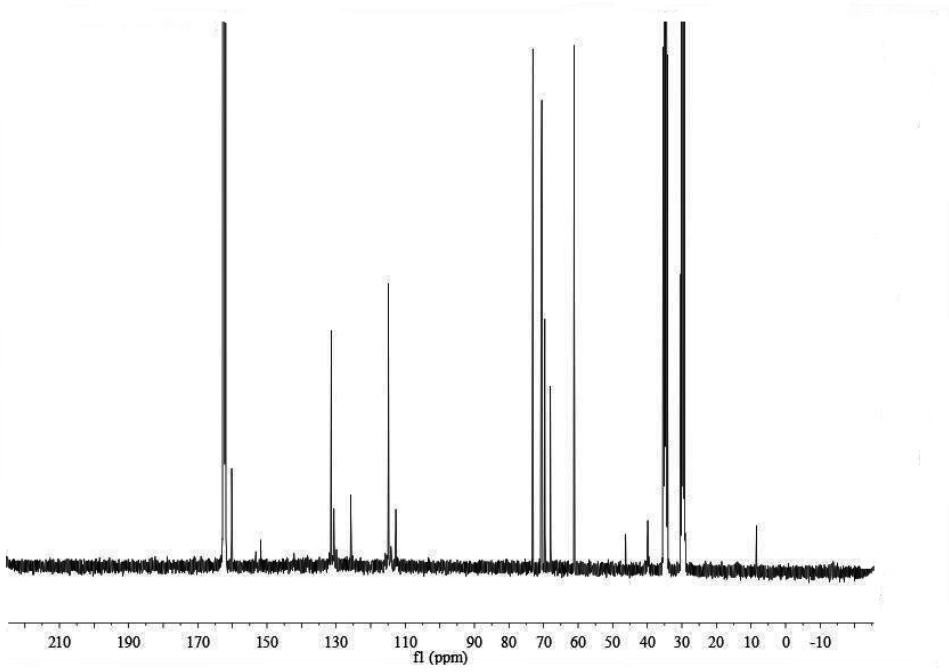

Figure S9. ^{13}C NMR spectrum of compound 5a in DMF-d7.

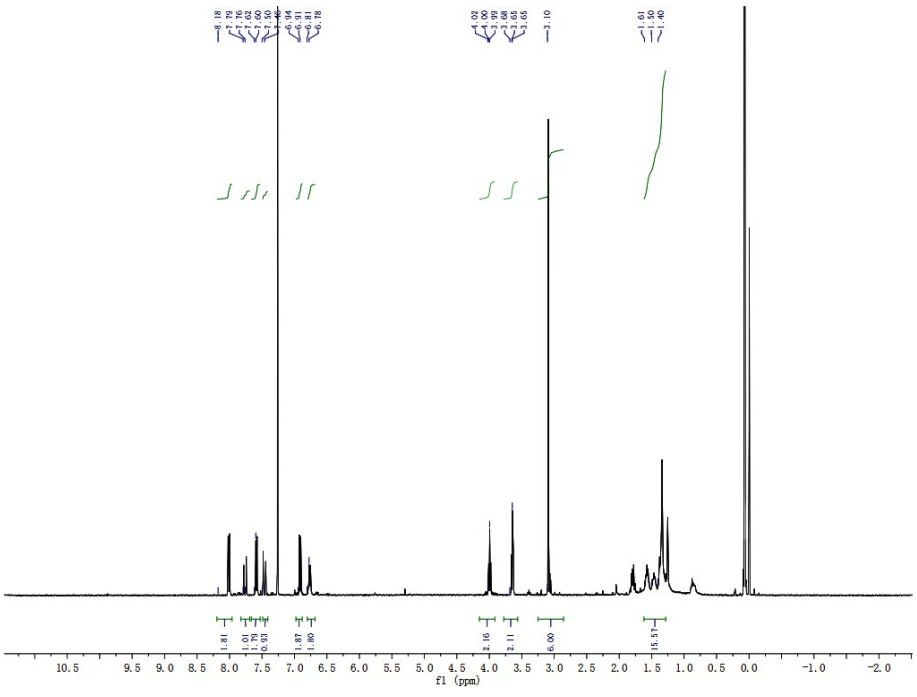

Figure S10. ^{1}H NMR spectrum of compound 2b in $CDCl_3$.

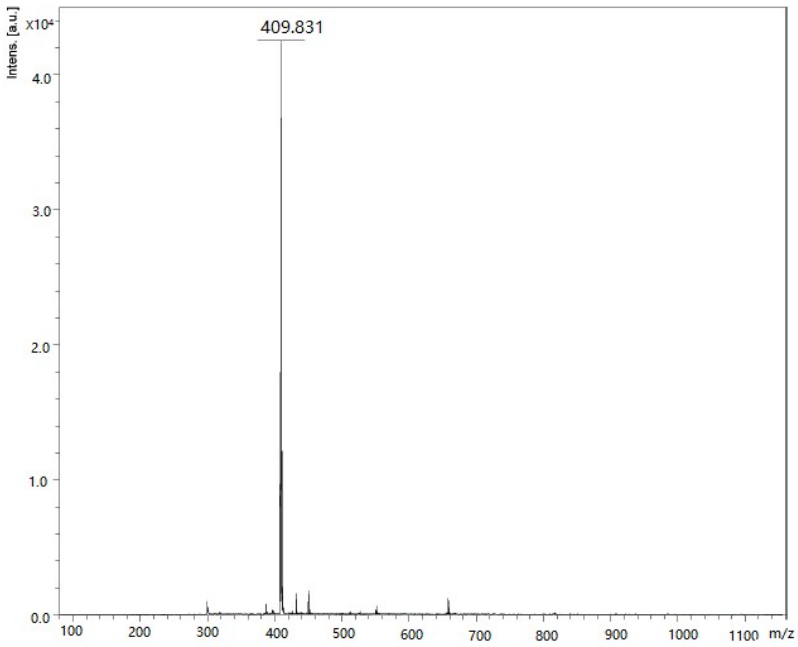

Figure S11. MALDI-TOF-MS of compound 2b.

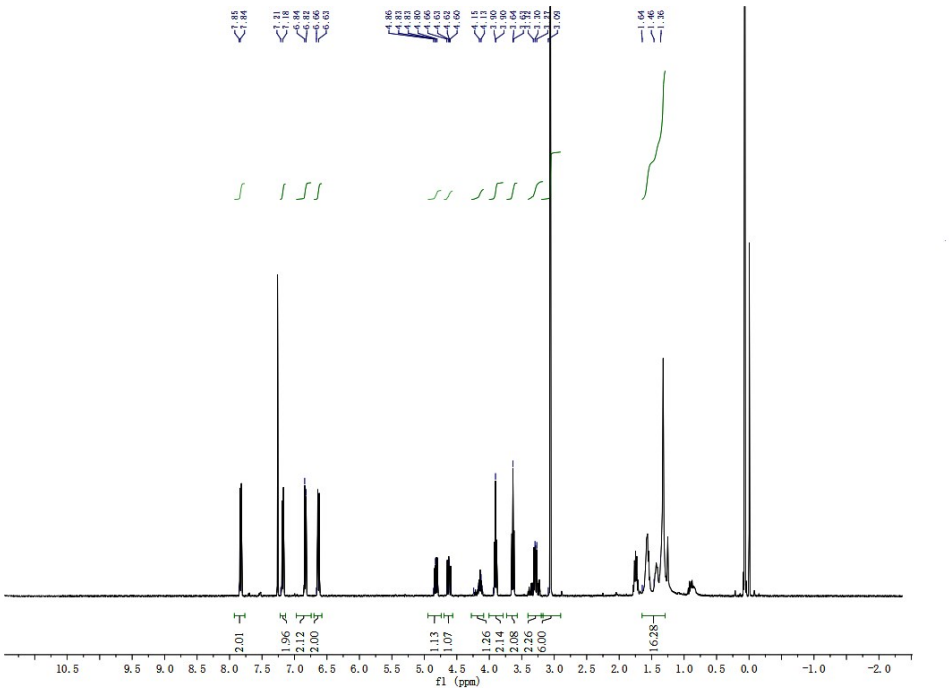

Figure S12. ^{1}H NMR spectrum of compound 3b in $CDCl_3$.

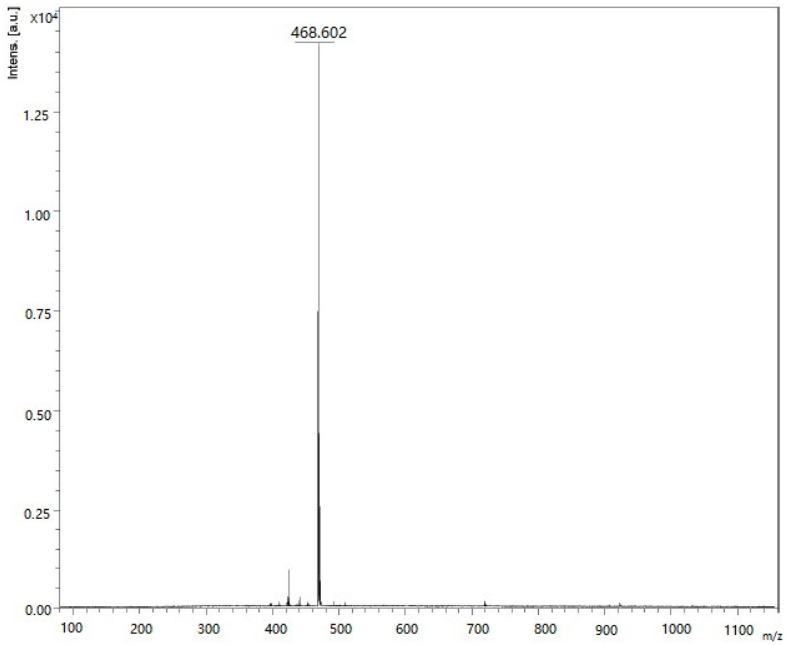

Figure S13. MALDI-TOF-MS of compound 3b.

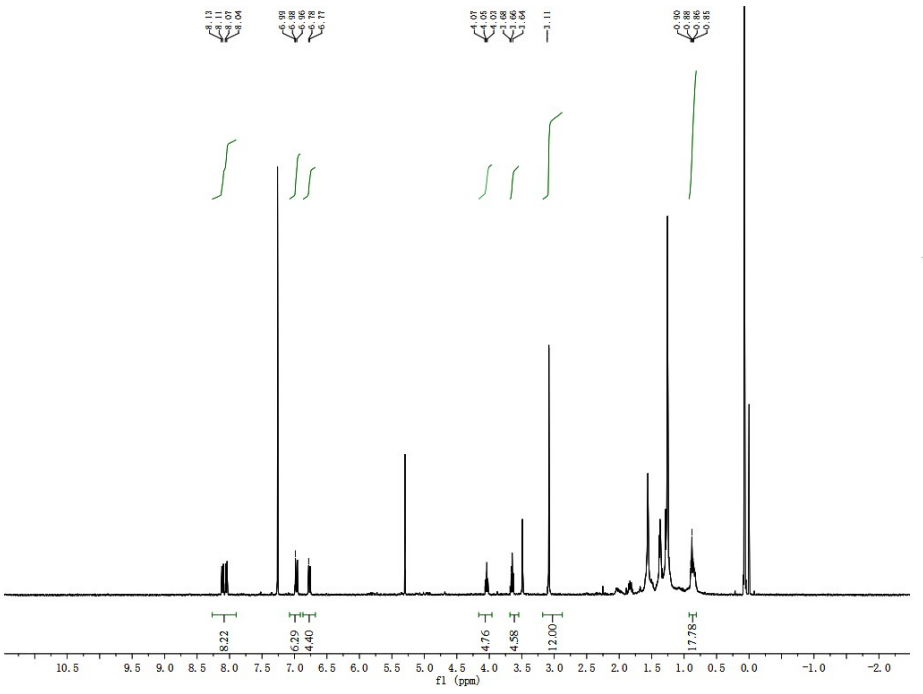

Figure S14. ^{1}H NMR spectrum of compound 4b in $CDCl_3$.

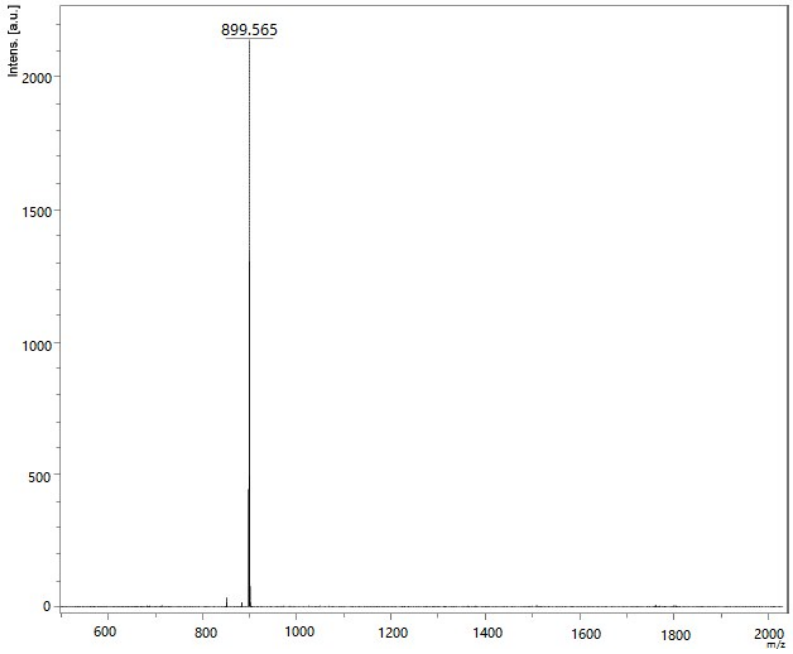

Figure S15. MALDI-TOF-MS of compound 4b.

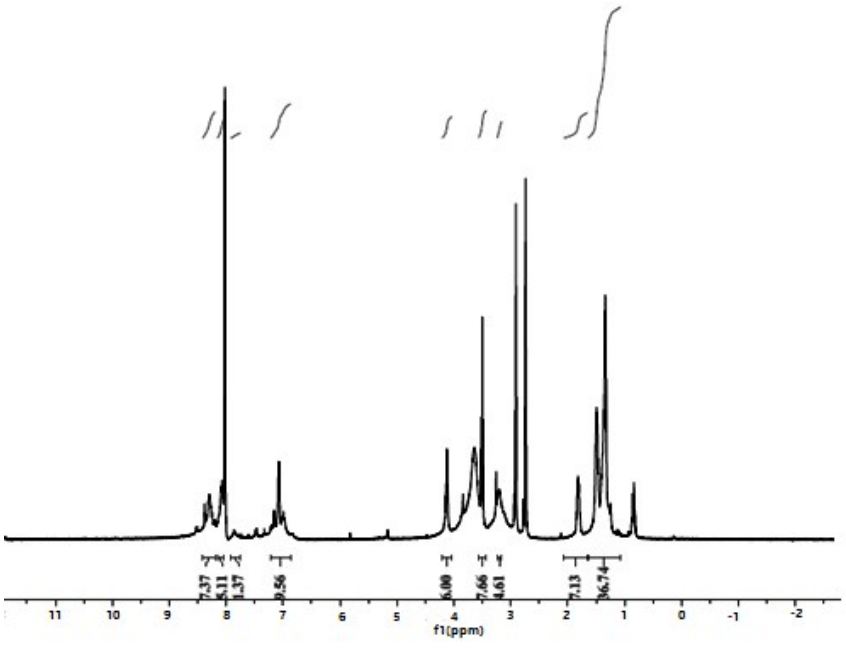

Figure S16. ^{1}H NMR spectrum of compound 5b in DMF-d7.

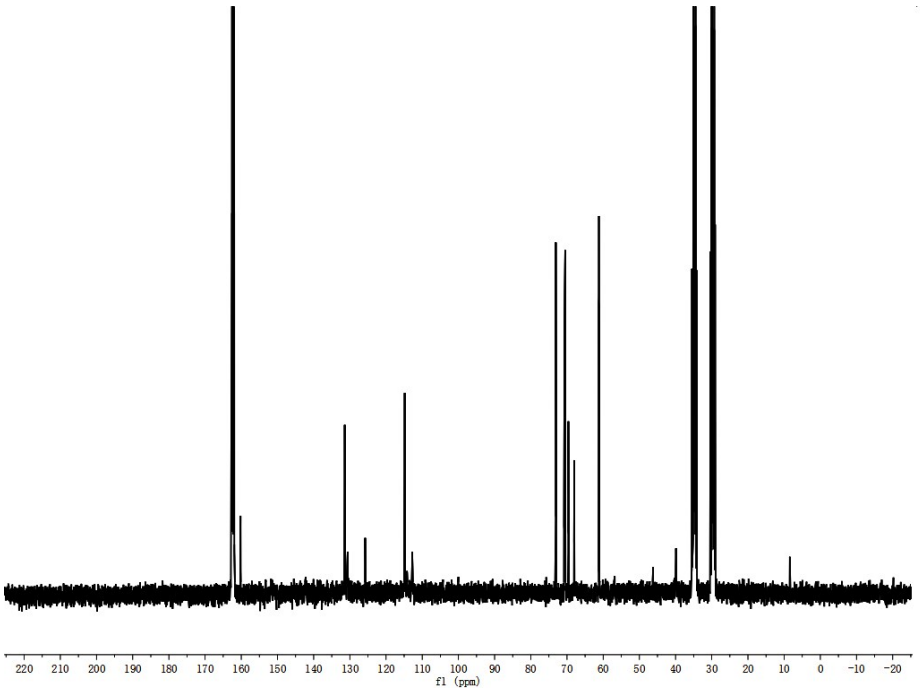

Figure S17. ^{13}C NMR spectrum of compound 5b in DMF-d7.

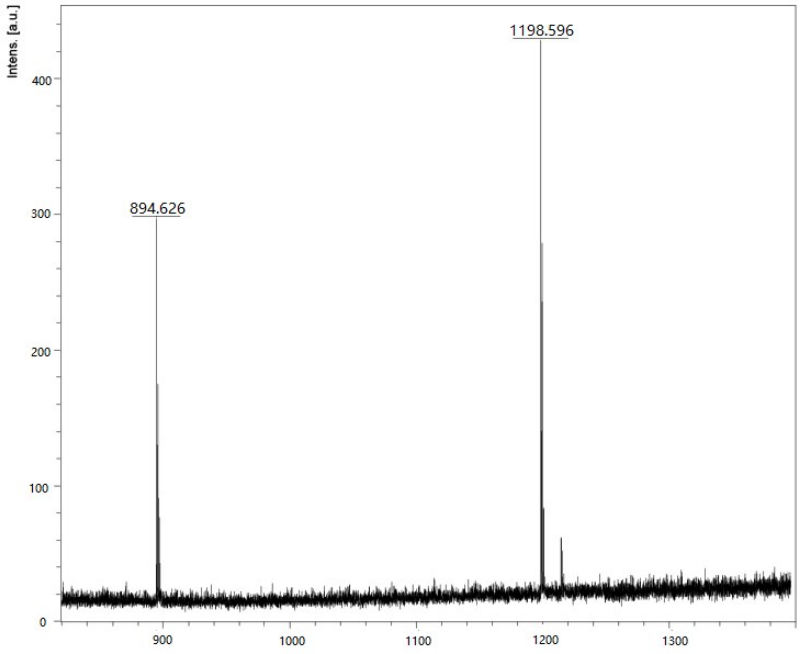

Figure S18. MALDI-TOF-MS of the Alk-Aza-BODIPY-BAPE probe in THF treated by H_2O_2.

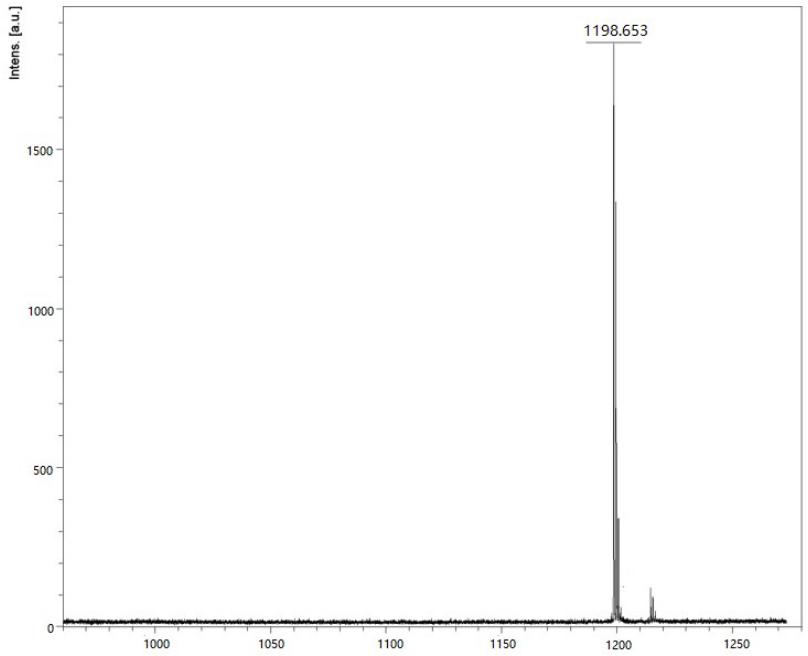

Figure S19. MALDI-TOF-MS of the Alk-Aza-BODIPY-BAPE probe in THF treated by $ONOO^-$.

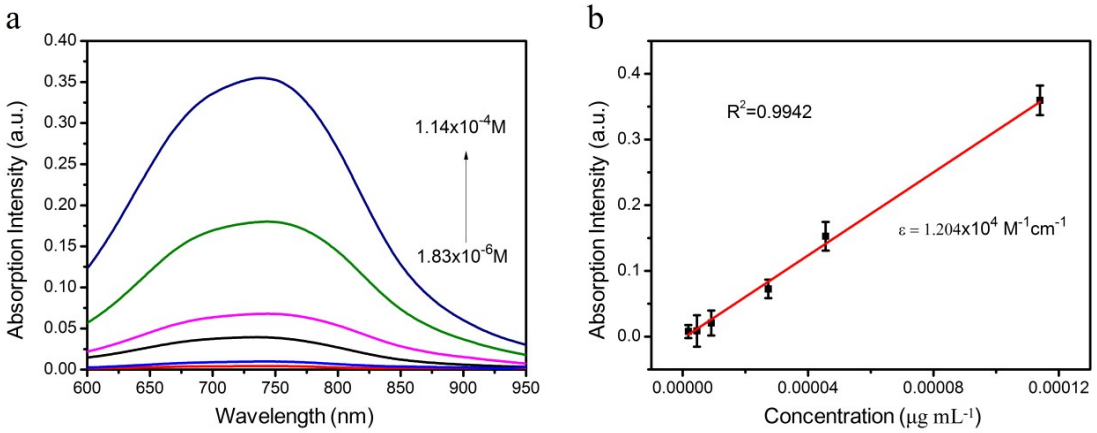

Figure S20. a) Absorption spectra of the OEG-Aza-BODIPY-BAPE probe with a series of concentrations in 1 × PBS (pH = 7.4). b) The plot of optical density at 720 nm versus concentration. The straight line is liner least-squares fit to the data.

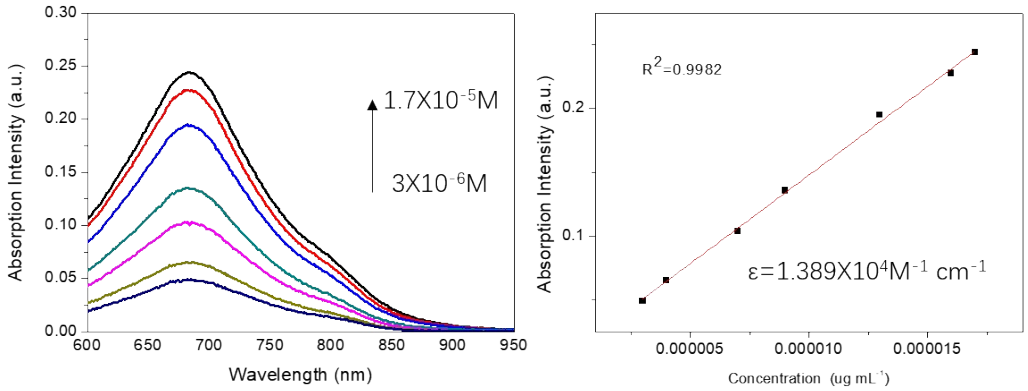

Figure S21. a) Absorption spectra of the Alk-Aza-BODIPY-BAPE probe with a series of concentrations in 1 × PBS (pH = 7.4). b) The plot of optical density at 700 nm versus concentration. The straight line is liner least-squares fit to the data.

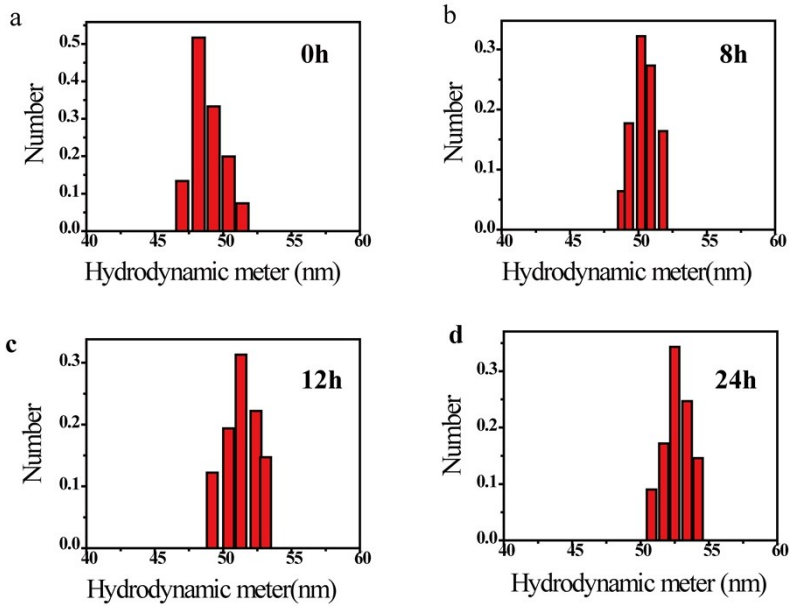

Figure S22. Hydrodynamic size change of OEG-Aza-BODIPY-BAPE NPs in PBS at different time.

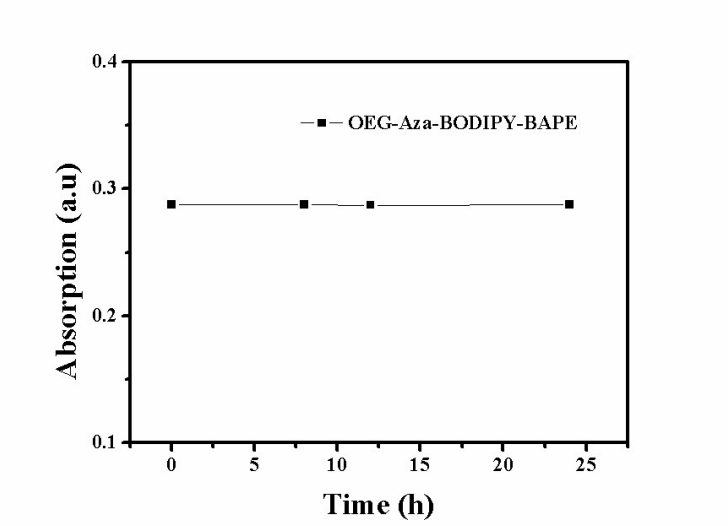

Figure S23. Absorption spectrum of OEG-Aza-BODIPY-BAPE in H_2O with 24 h.

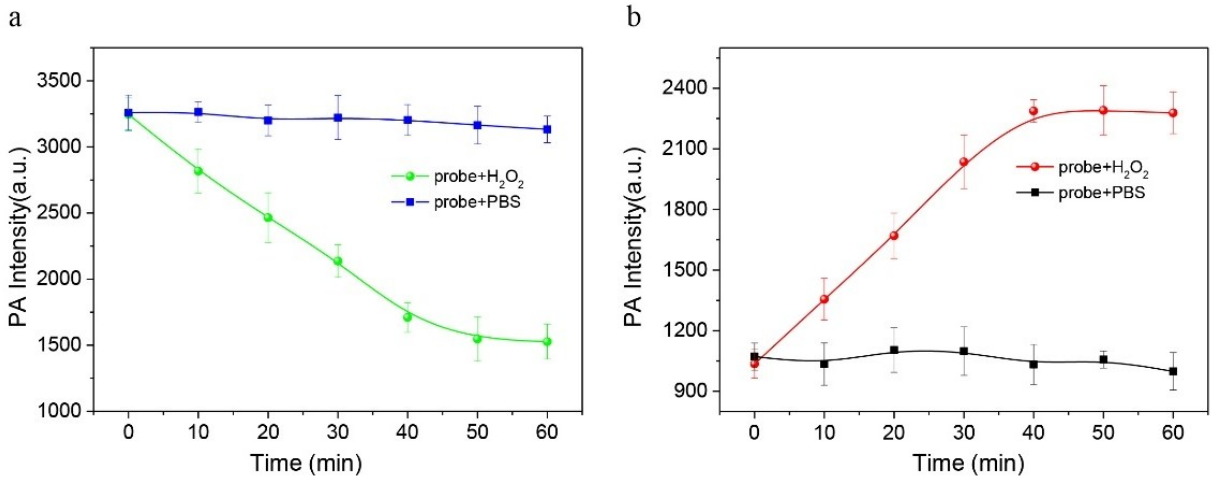

Figure S24. a) The PA intensity of the OEG-Aza-BODIPY-BAPE probe at 720 nm in the presence of H_2O_2 (green line) and PBS (blue line) in 1 × PBS (pH = 7.4). b) The PA intensity of the probe at 825 nm in the presence of H_2O_2 (red line) and PBS (black line) in 1 × PBS (pH = 7.4). Error bars were based on error of mean (n = 3).

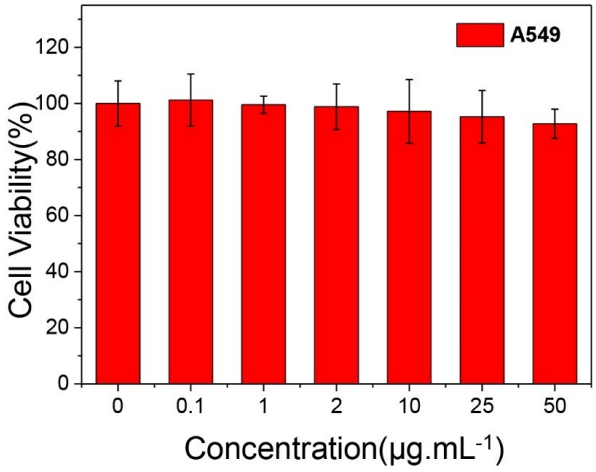

Figure S25. Cytotoxicity of A549 cells after incubation with the OEG-Aza-BODIPY-BAPE probe with different concentrations for 24 h.

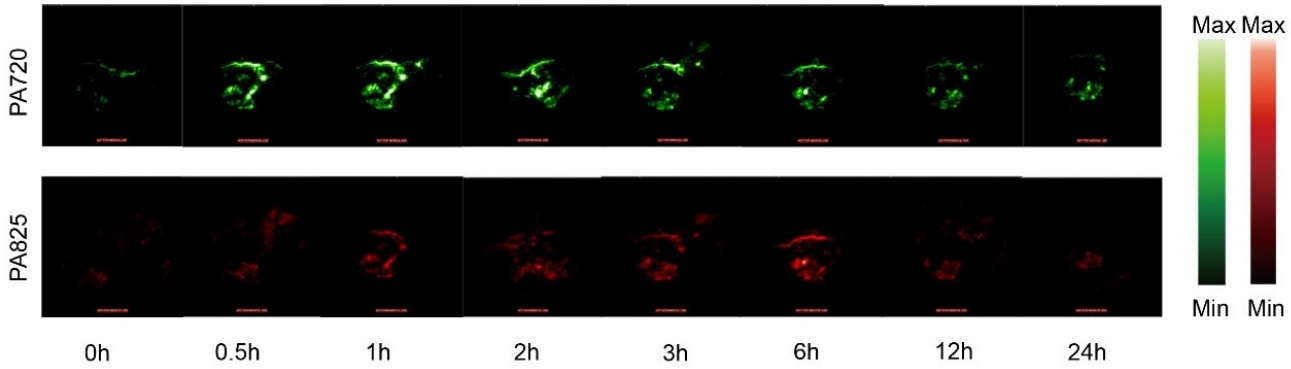

Figure S26. Representative PA images of tumor in a nude mice before and 0.5, 1, 2, 3, 6, 12, 24 h after the injection of the OEG-Aza-BODIPY-BAPE probe (200 μL, 100 μg mL^{-1}).

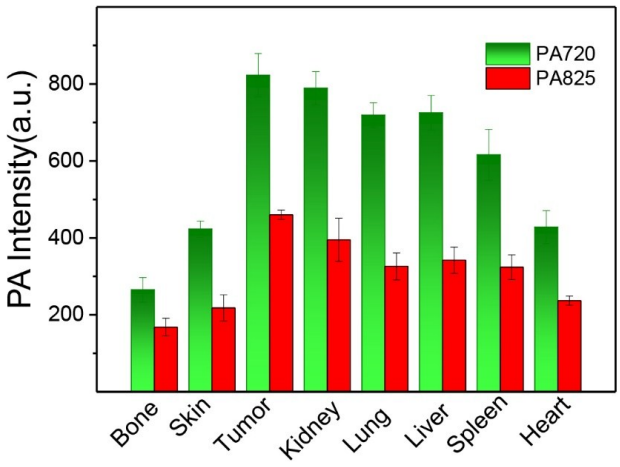

Figure S27. *Ex vivo* PA quantification of major organs of mice after systemic administration of the OEG-Aza-BODIPY-BAPE probe at 720 nm and 825 nm. Error bars were based on error of mean (n = 3).