

Supporting Information

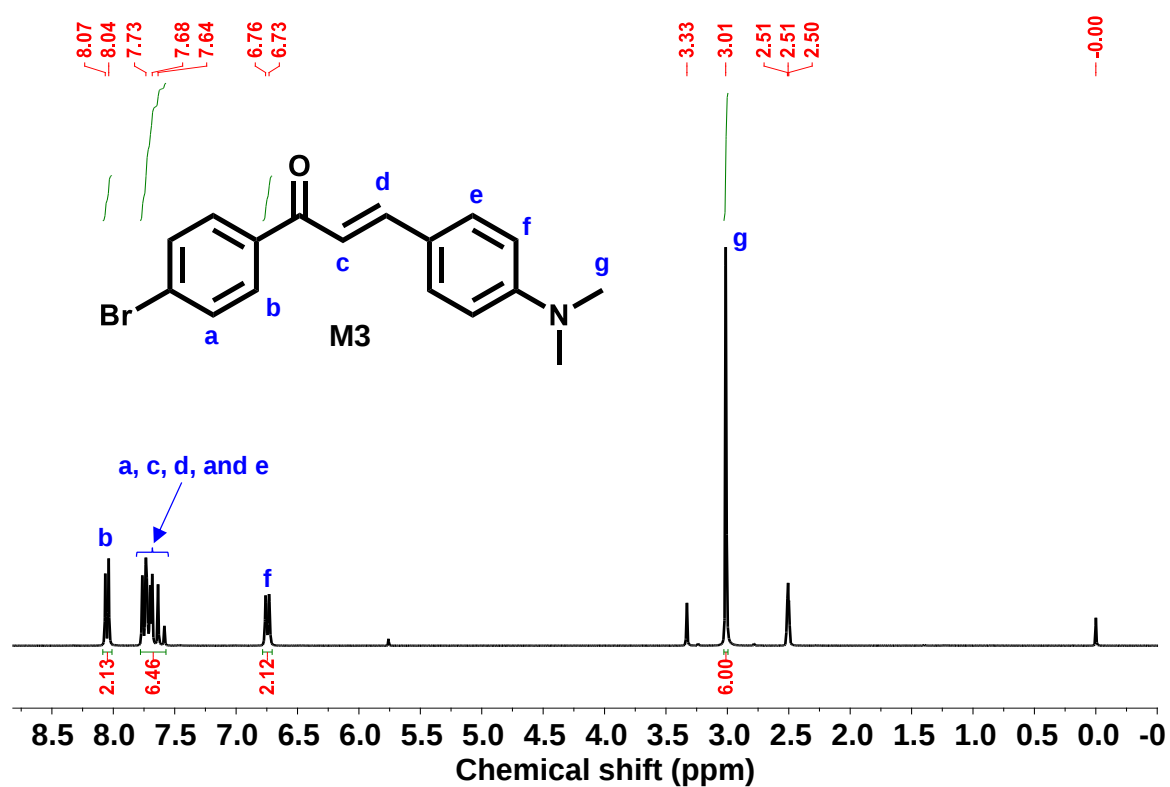
Nanoparticles Destabilizing the Cell Membranes Triggered by NIR Light for Cancer Imaging and Photo-Immunotherapy

*Dongsheng Tang^{1,2}, Minhui Cui^{1,2}, Bin Wang^{1,2}, Ganghao Liang^{1,2}, Hanchen Zhang^{1,2},
Haihua Xiao^{1,2*}*

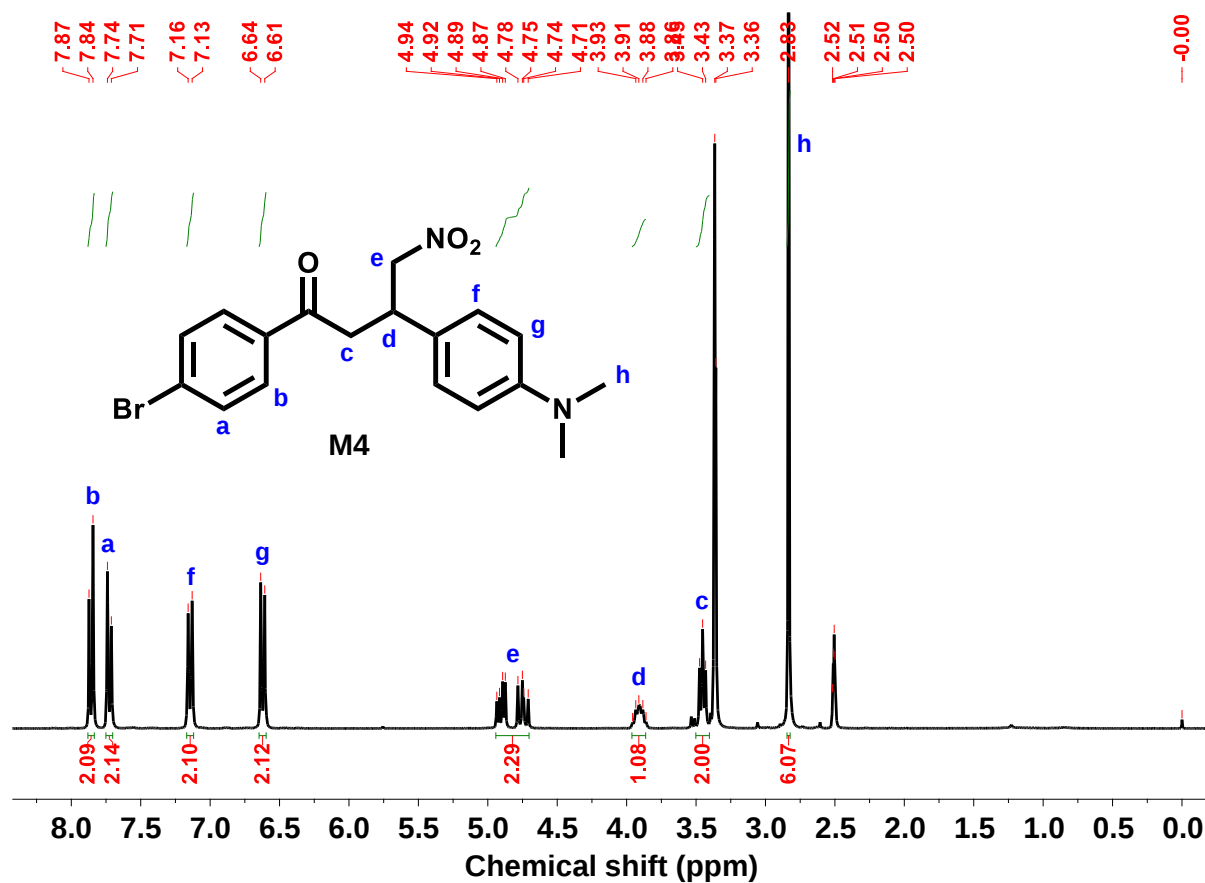
¹Beijing National Laboratory for Molecular Sciences, Laboratory of Polymer Physics and Chemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, P. R. China

²University of Chinese Academy of Sciences, Beijing 100049, P. R. China

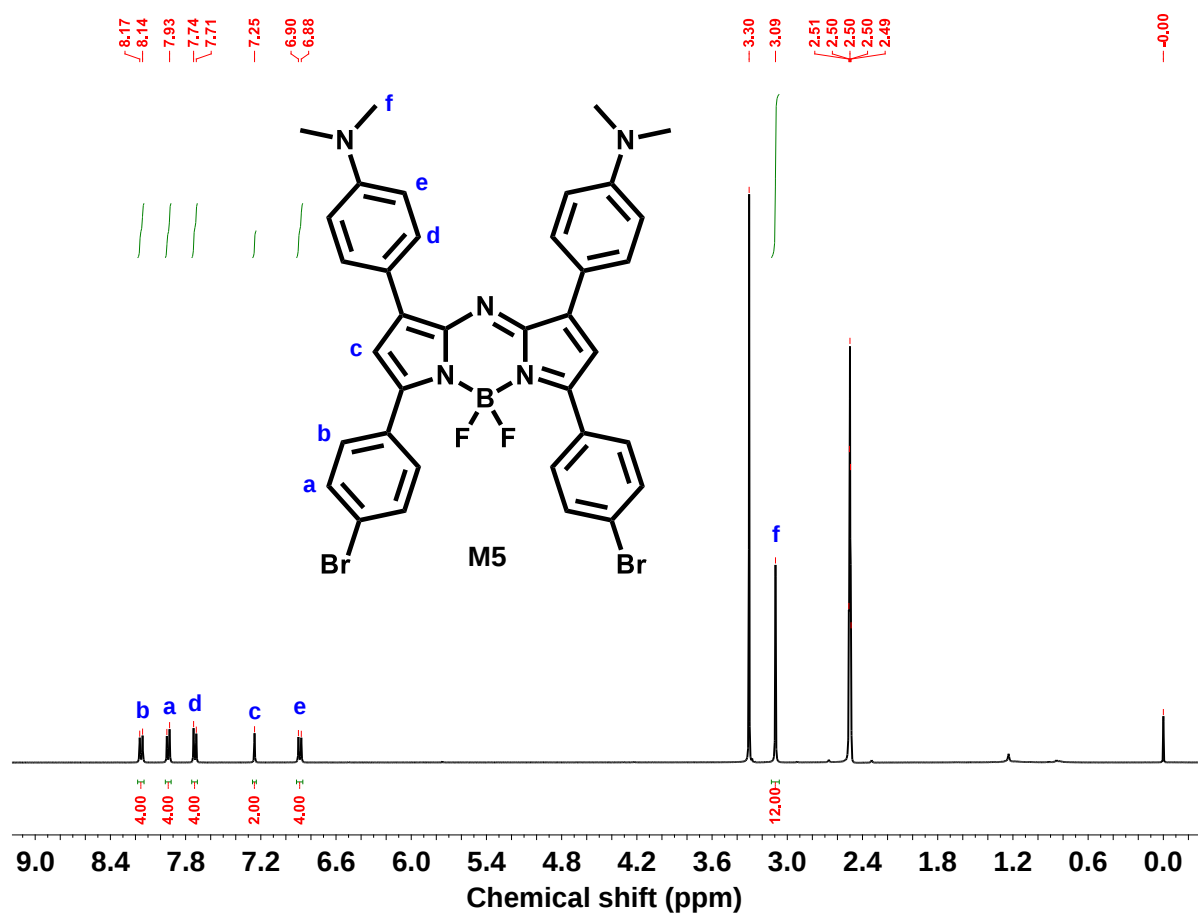
E-mail: hhxiao@iccas.ac.cn



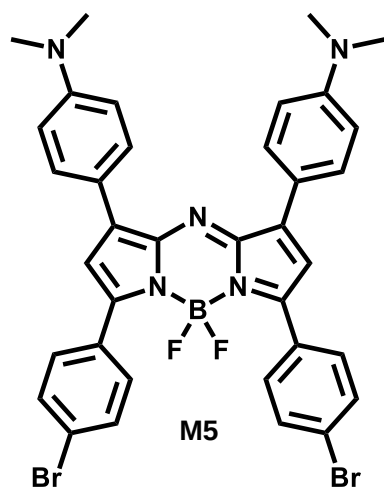
Supplementary Fig. 1. ¹H NMR spectrum of M3 in DMSO-*d*₆. ¹H NMR chemical shift was assigned (a-g).



Supplementary Fig. 2. ^1H NMR spectrum of M4 in $\text{DMSO-}d_6$. ^1H NMR chemical shift was assigned (a-h).



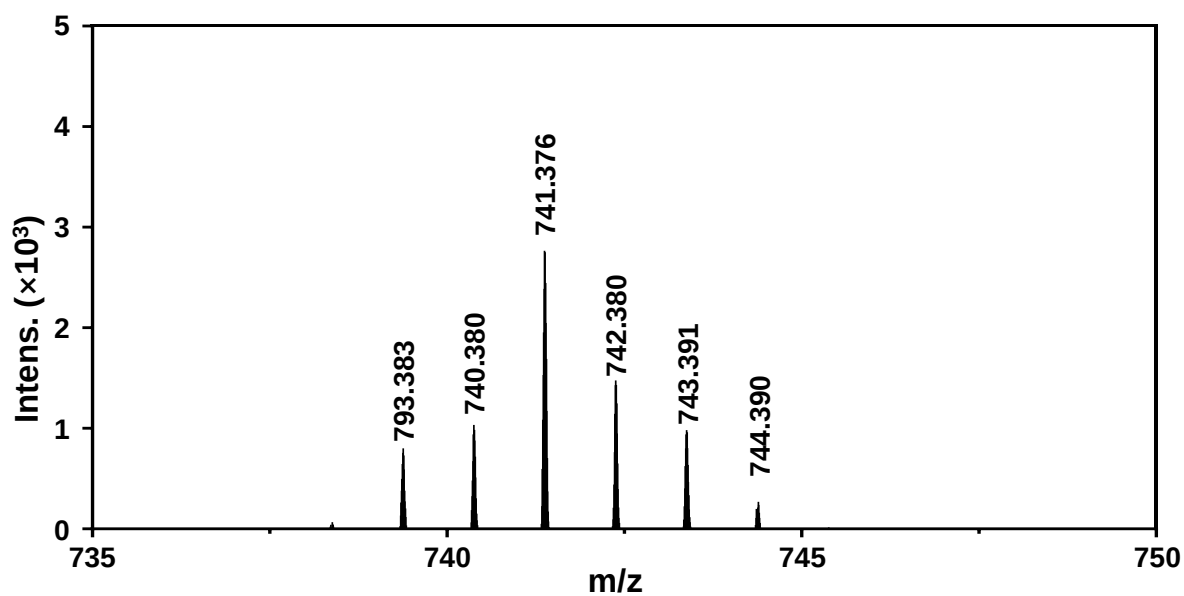
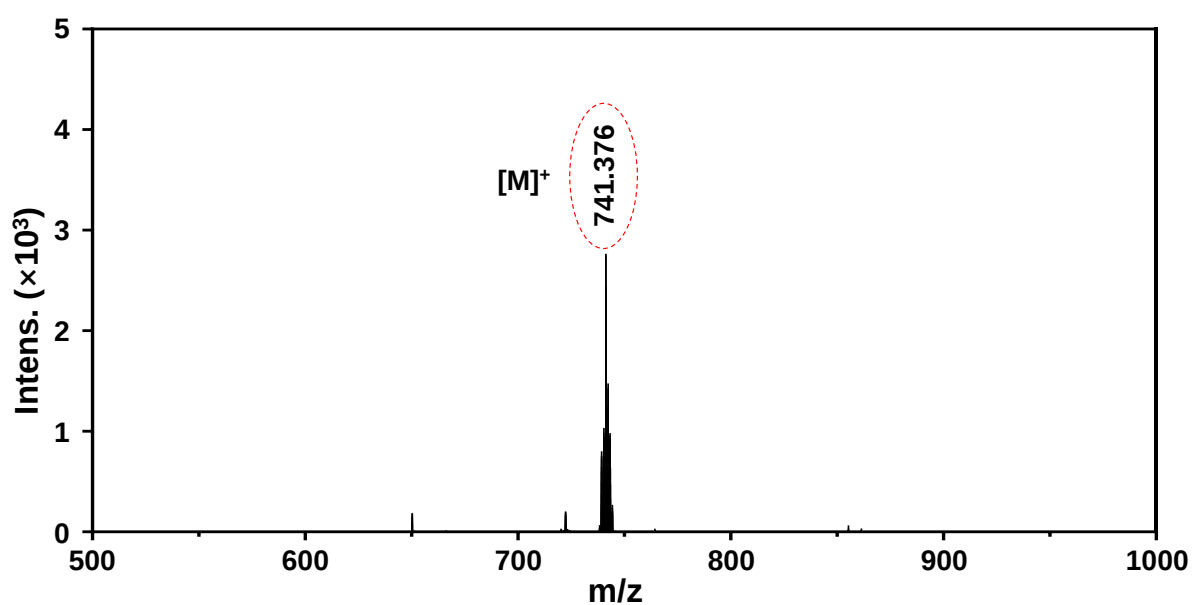
Supplementary Fig. 3. ^1H NMR spectrum of M5 in $\text{DMSO-}d_6$. ^1H NMR chemical shift was assigned (a-f).



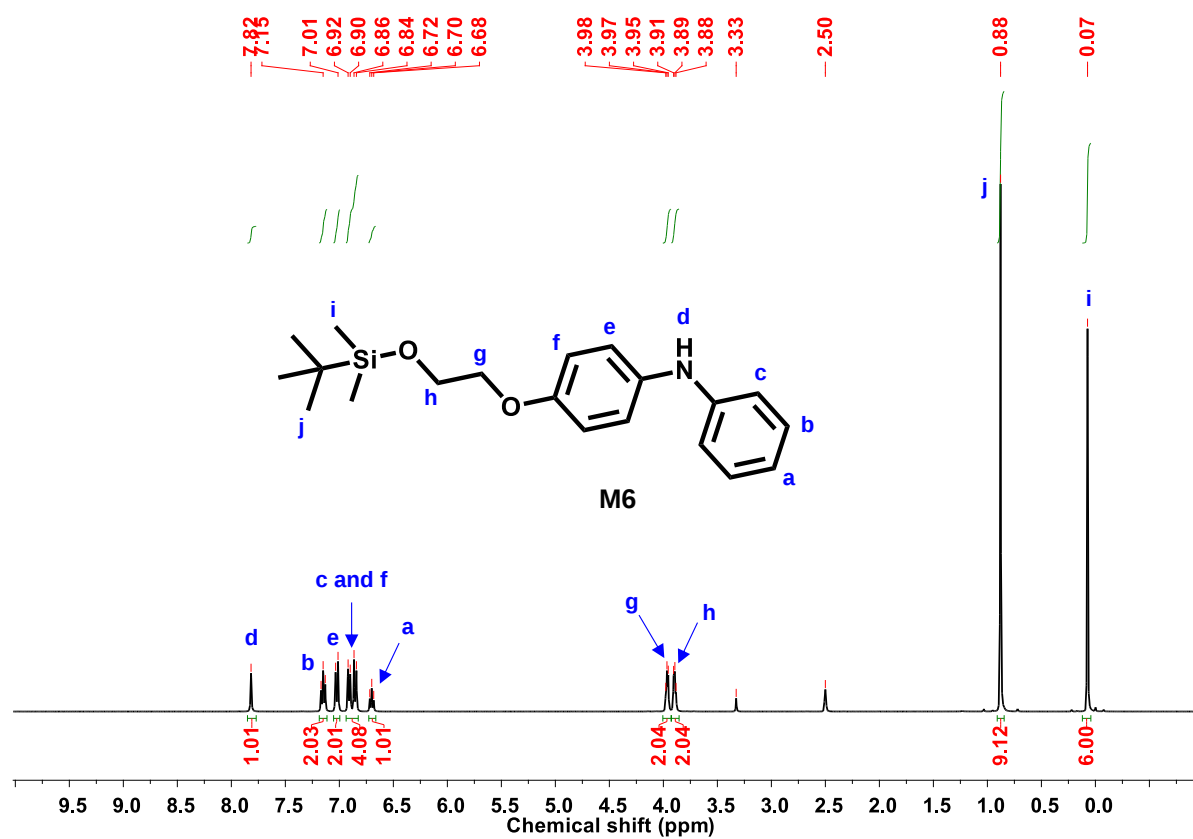
Chemical Formula: $C_{36}H_{30}BBr_2F_2N_5$

Calculation: $[M]^+$ m/z 741.091

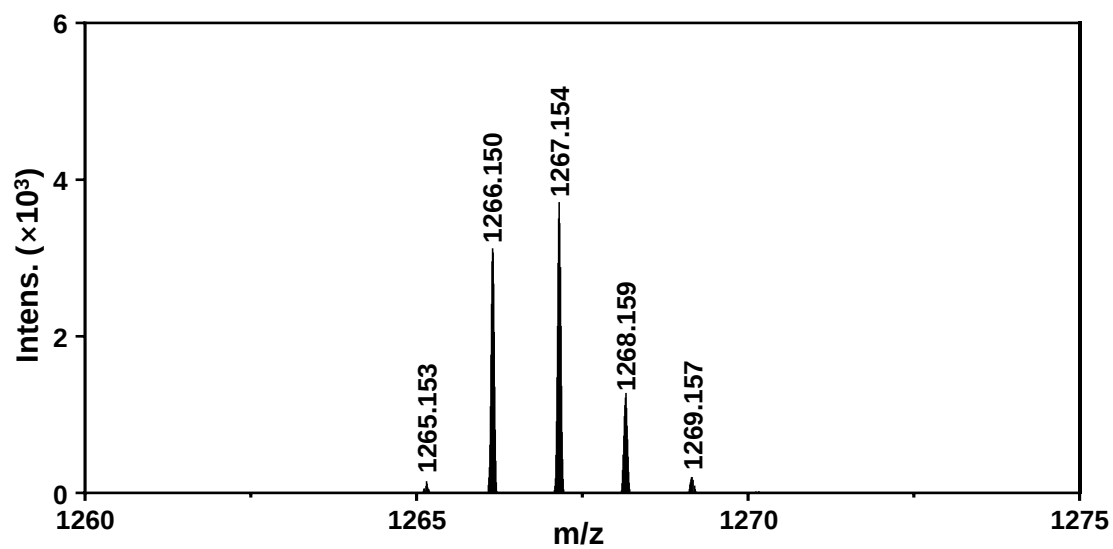
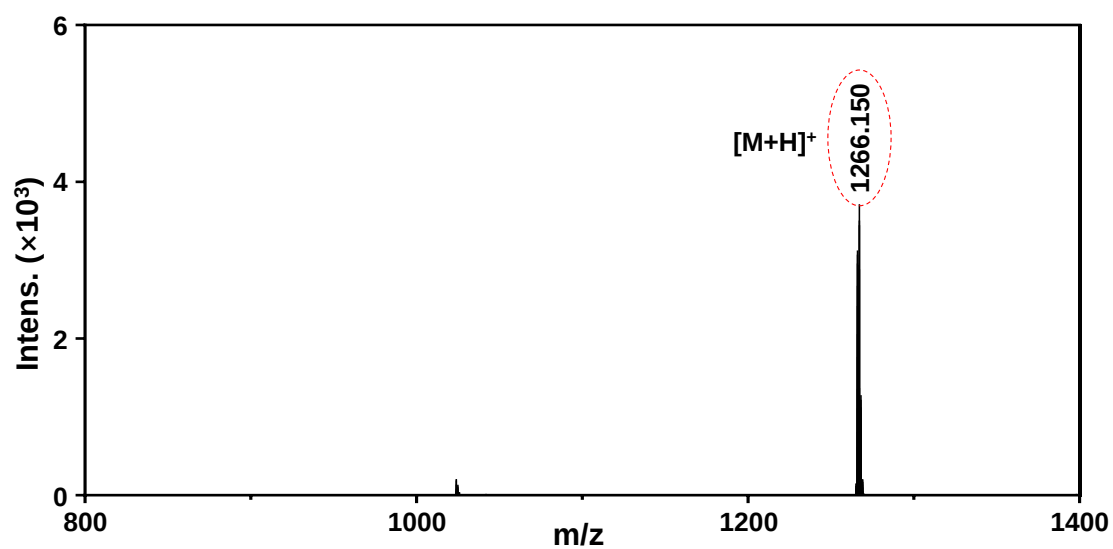
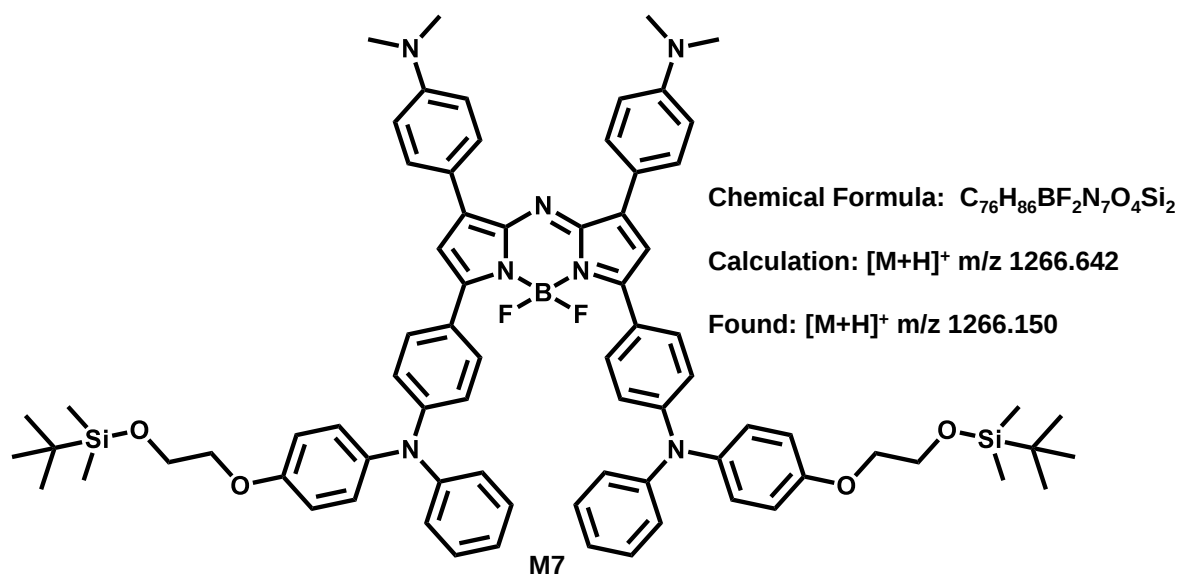
Found: $[M]^+$ m/z 741.376



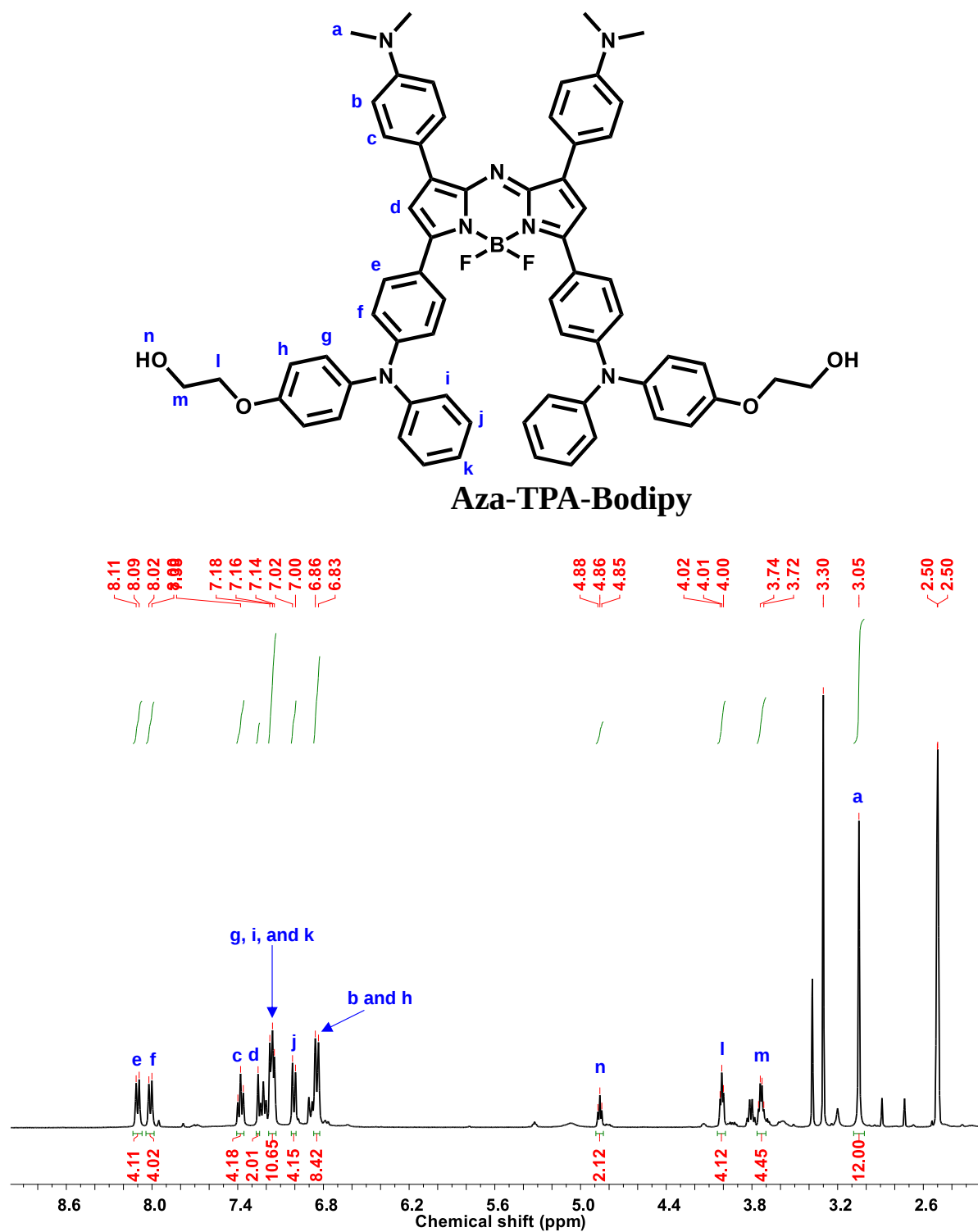
Supplementary Fig. 4. MALDI-TOF-MS spectrum of M5.



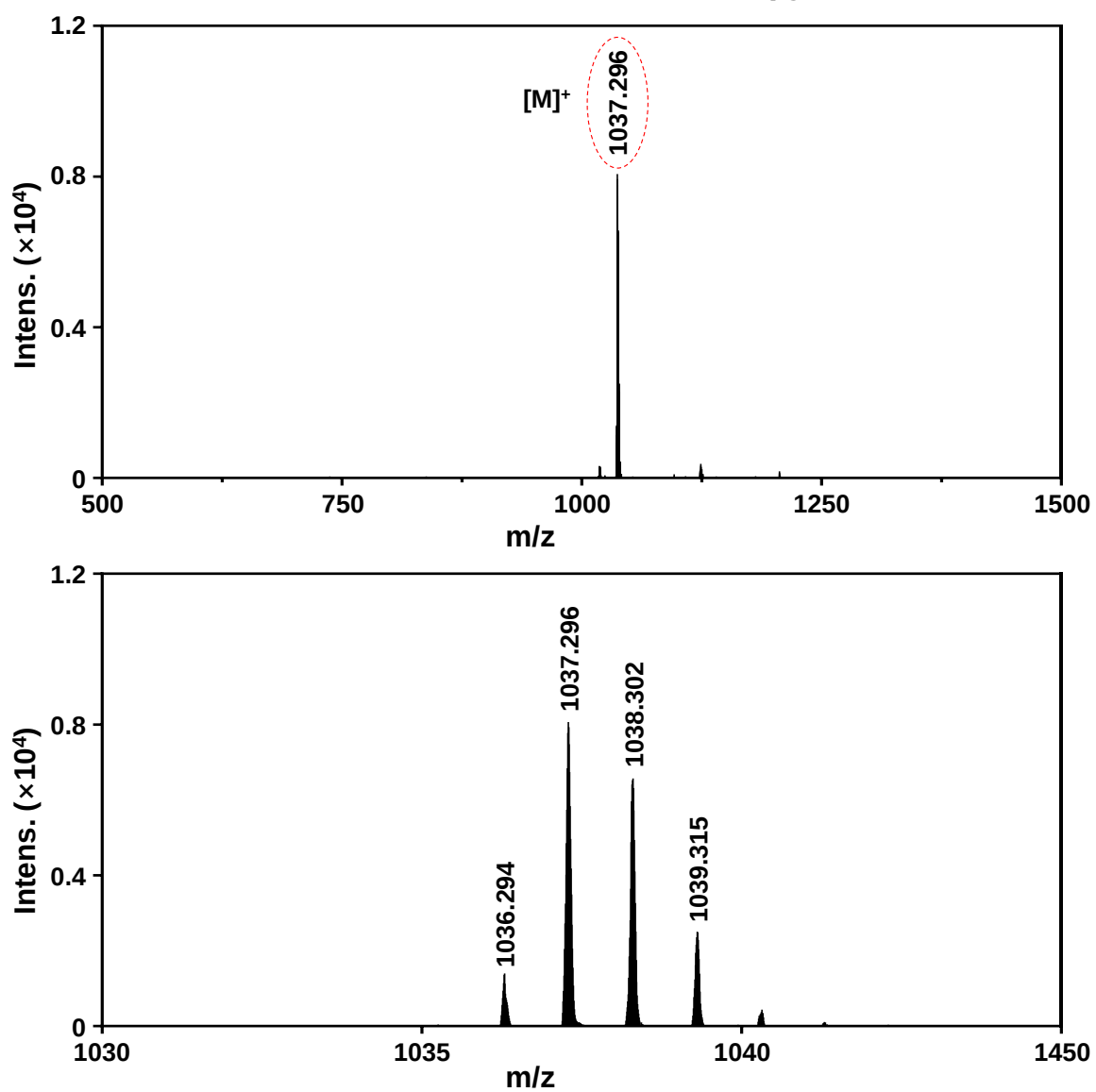
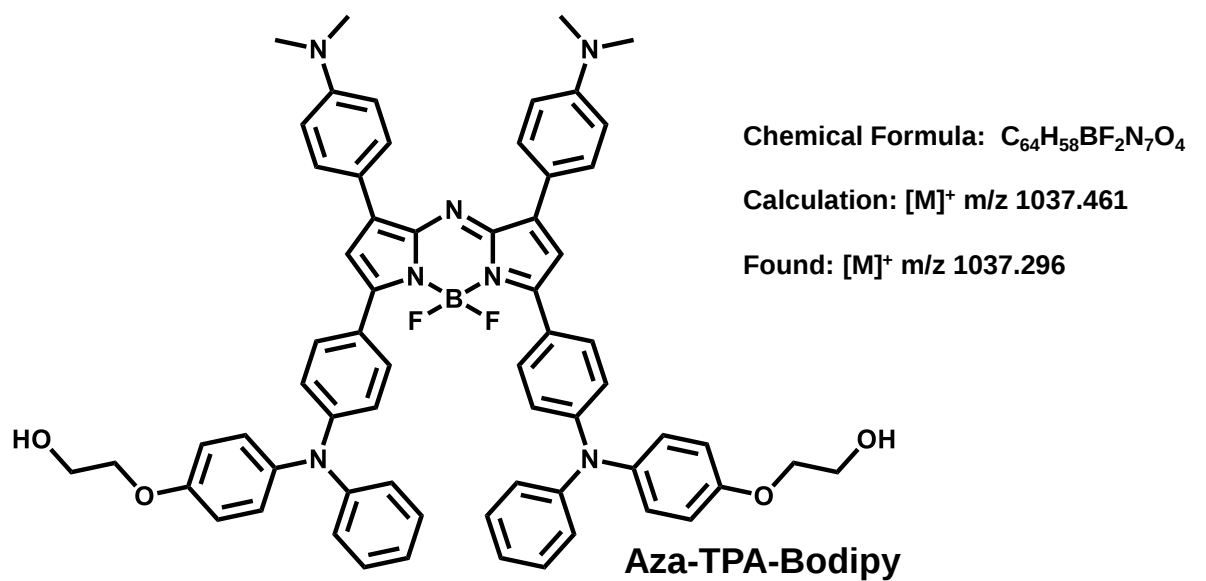
Supplementary Fig. 5. ^1H NMR spectrum of M6 in $\text{DMSO}-d_6$. ^1H NMR chemical shift was assigned (a-j).



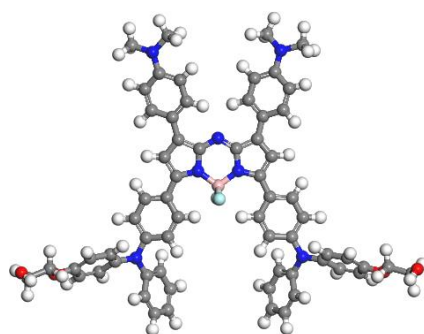
Supplementary Fig. 7. MALDI-TOF-MS spectrum of M7.



Supplementary Fig. 8. ¹H NMR spectrum of Aza-TPA-Bodipy in DMSO-*d*₆. ¹H NMR chemical shift was assigned (a-n).

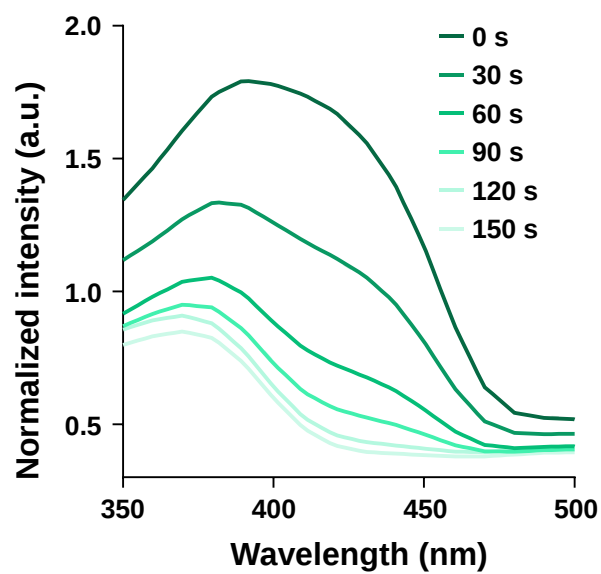


Supplementary Fig. 9. MALDI-TOF-MS spectrum of Aza-TPA-Bodipy.

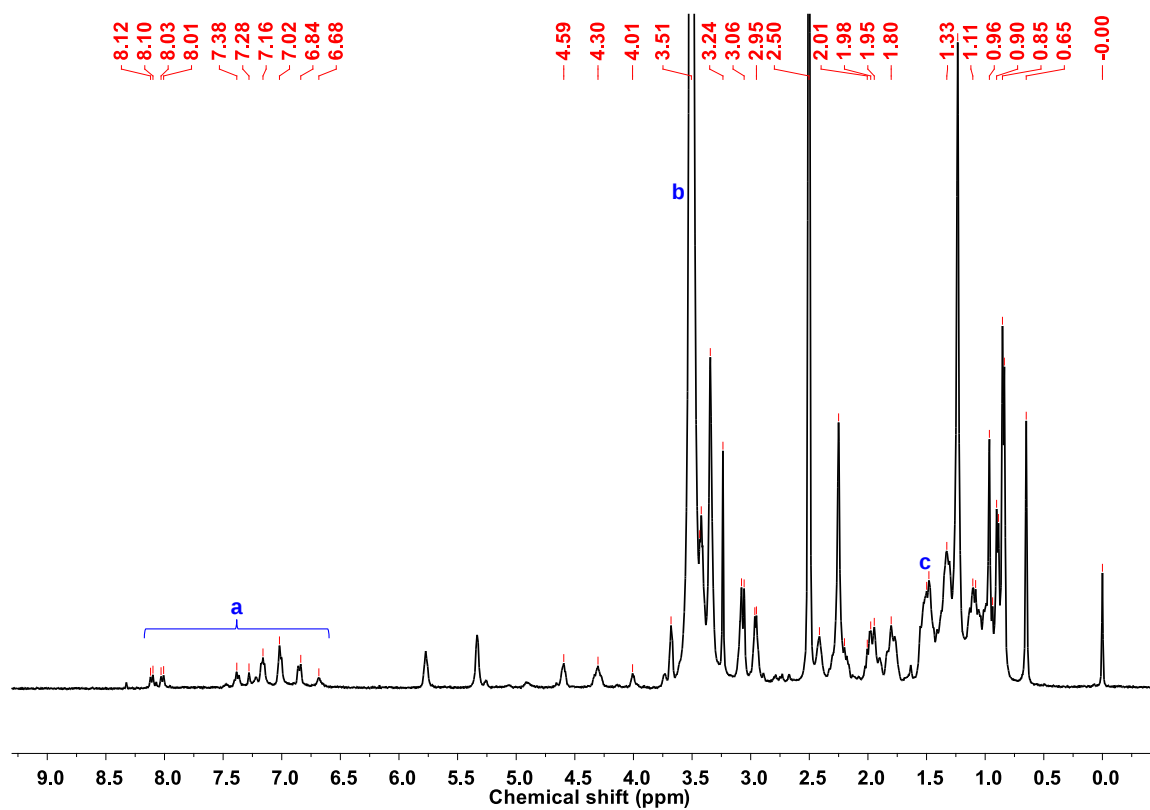
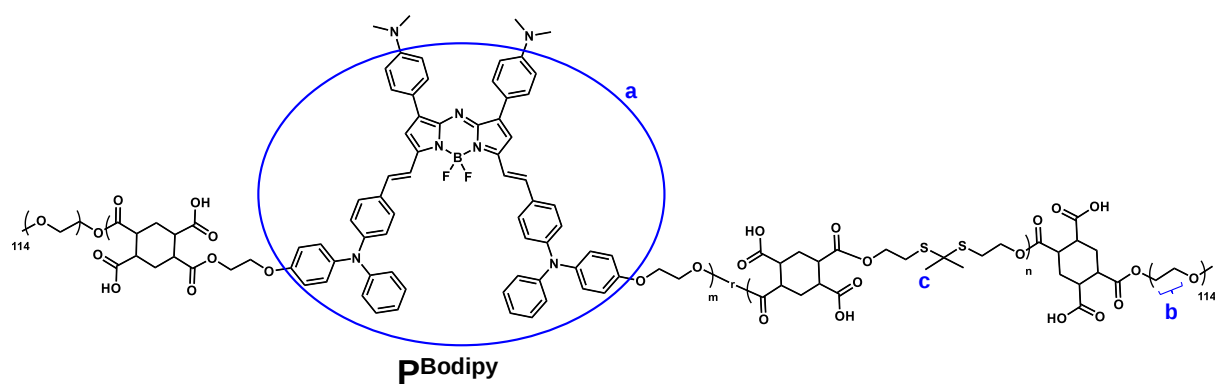


S₀ optimized geometry

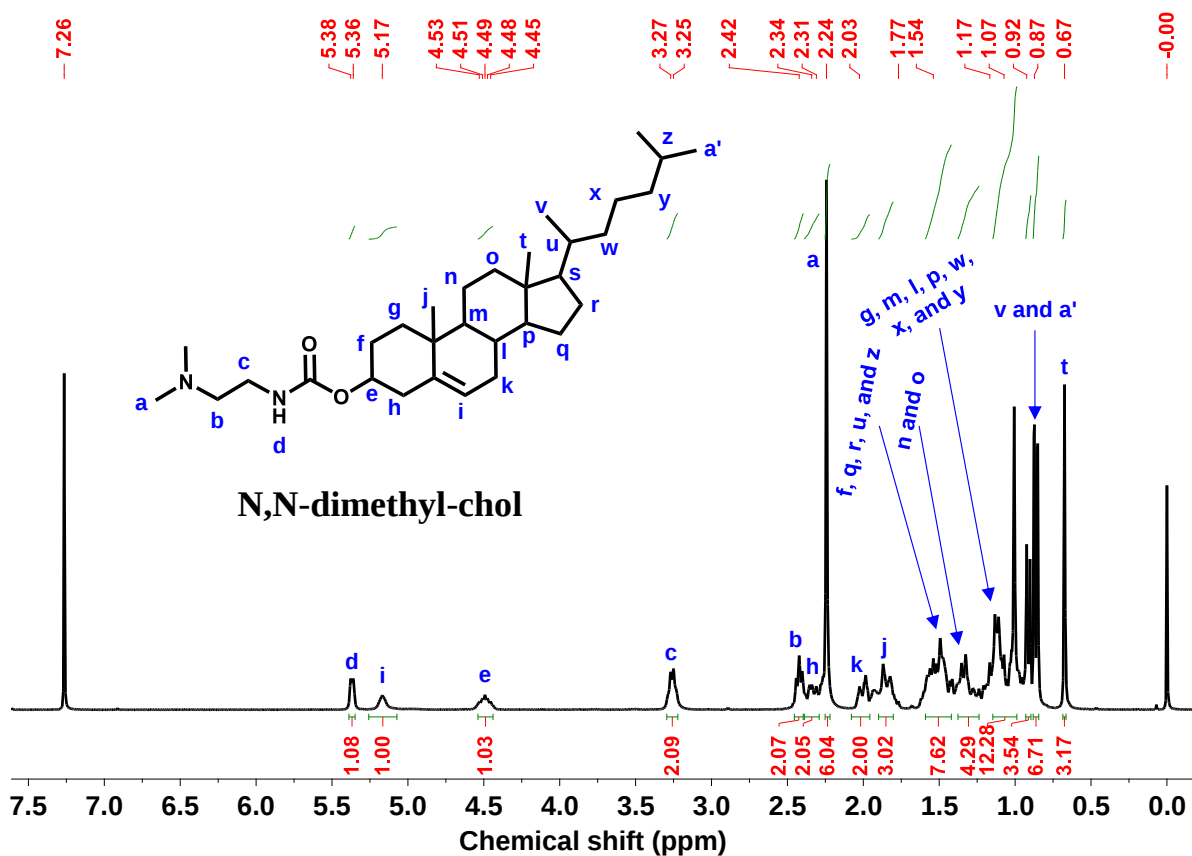
Supplementary Fig. 10. The optimized structures of Aza-TPA-Bodipy.



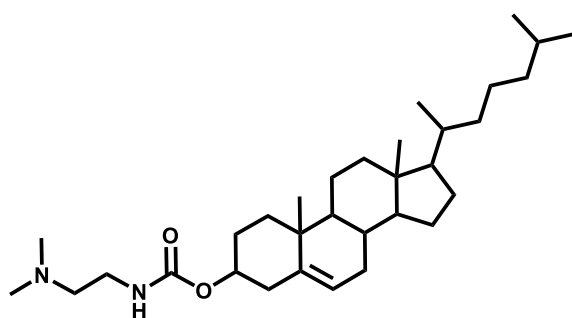
Supplementary Fig. 11. Absorbance change of Aza-TPA-Bodipy after 808 nm light irradiation (1.0 W cm^{-2}).



Supplementary Fig. 12. ^1H NMR spectrum of pBodipy in $\text{DMSO-}d_6$. ^1H NMR chemical shift was assigned (a-c).



Supplementary Fig. 13. ^1H NMR spectrum of N,N-dimethyl-chol in CDCl_3 . ^1H NMR chemical shift was assigned (a-a').



N,N-dimethyl-chol

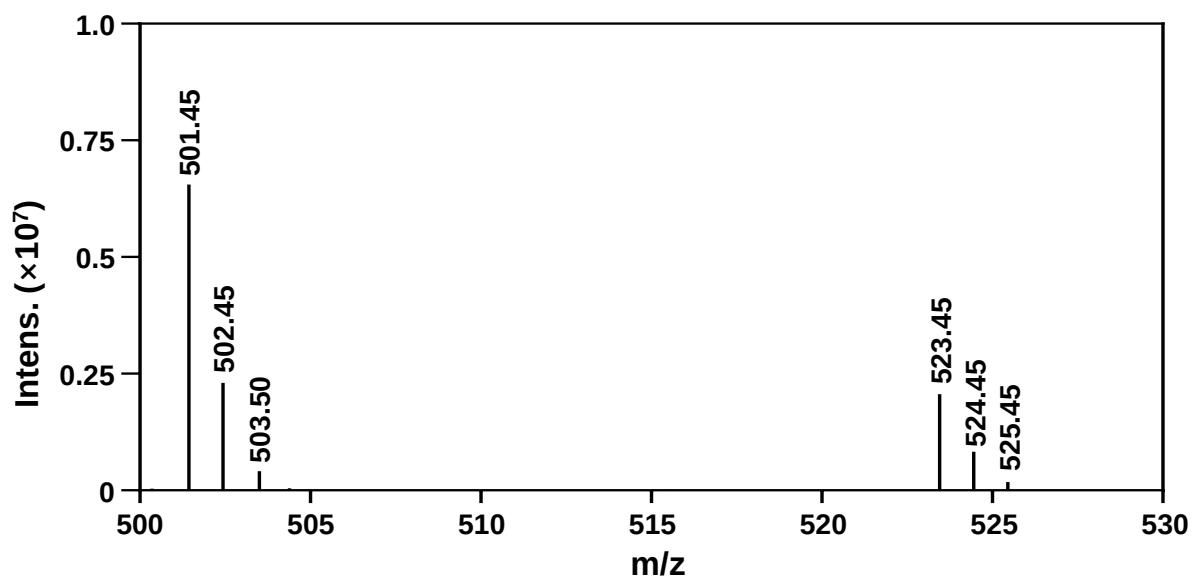
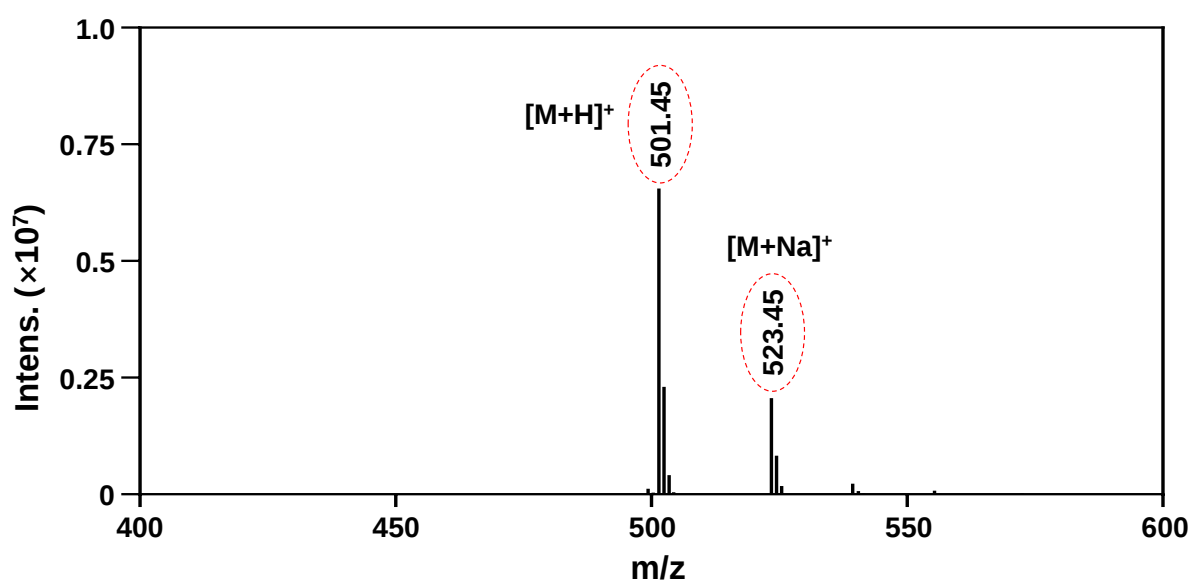
Chemical Formula: $C_{32}H_{56}N_2O_2$

Calculation: $[M+H]^+$ m/z 501.44

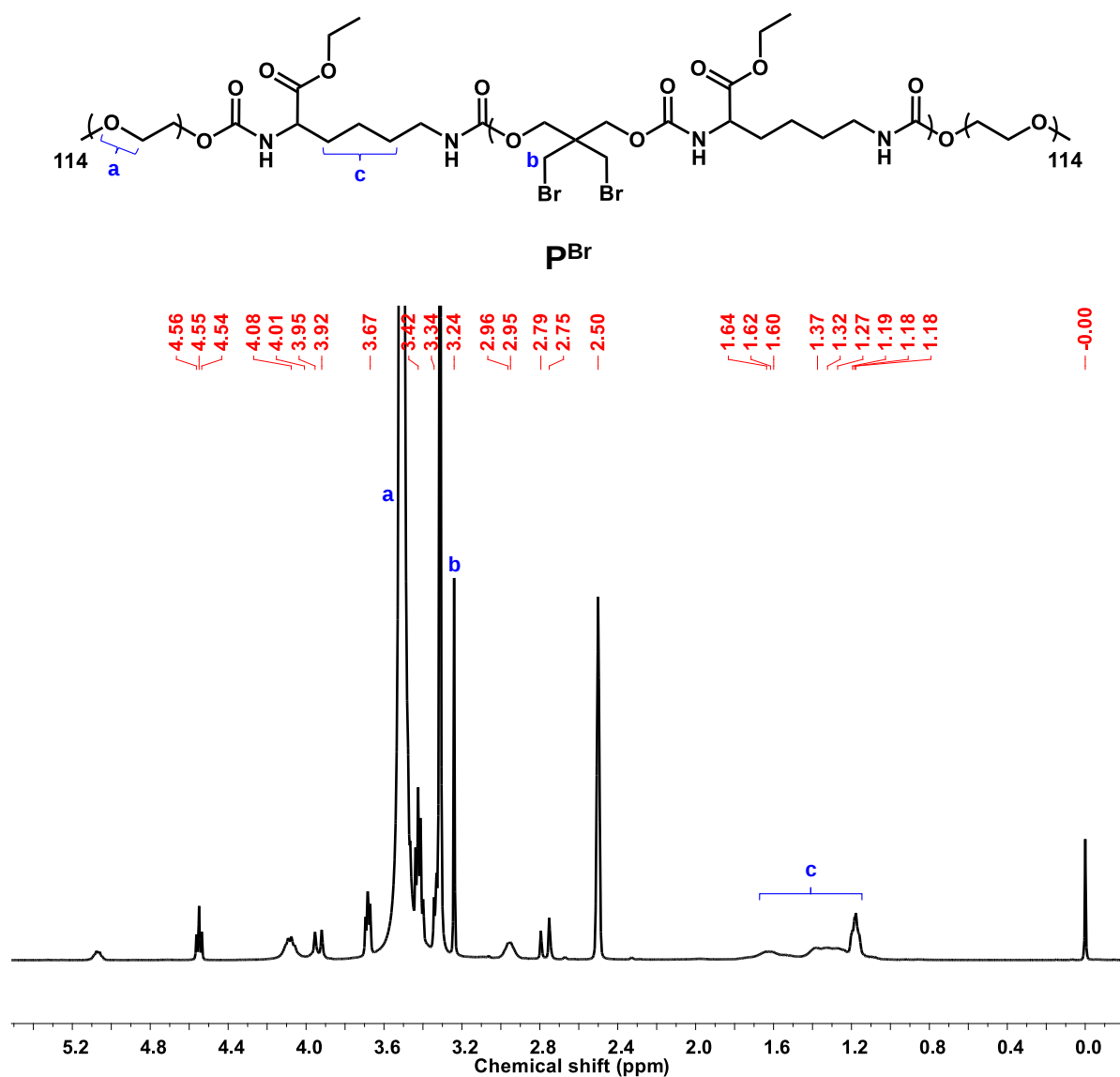
Found: $[M+H]^+$ m/z 501.45

Calculation: $[M+Na]^+$ m/z 523.42

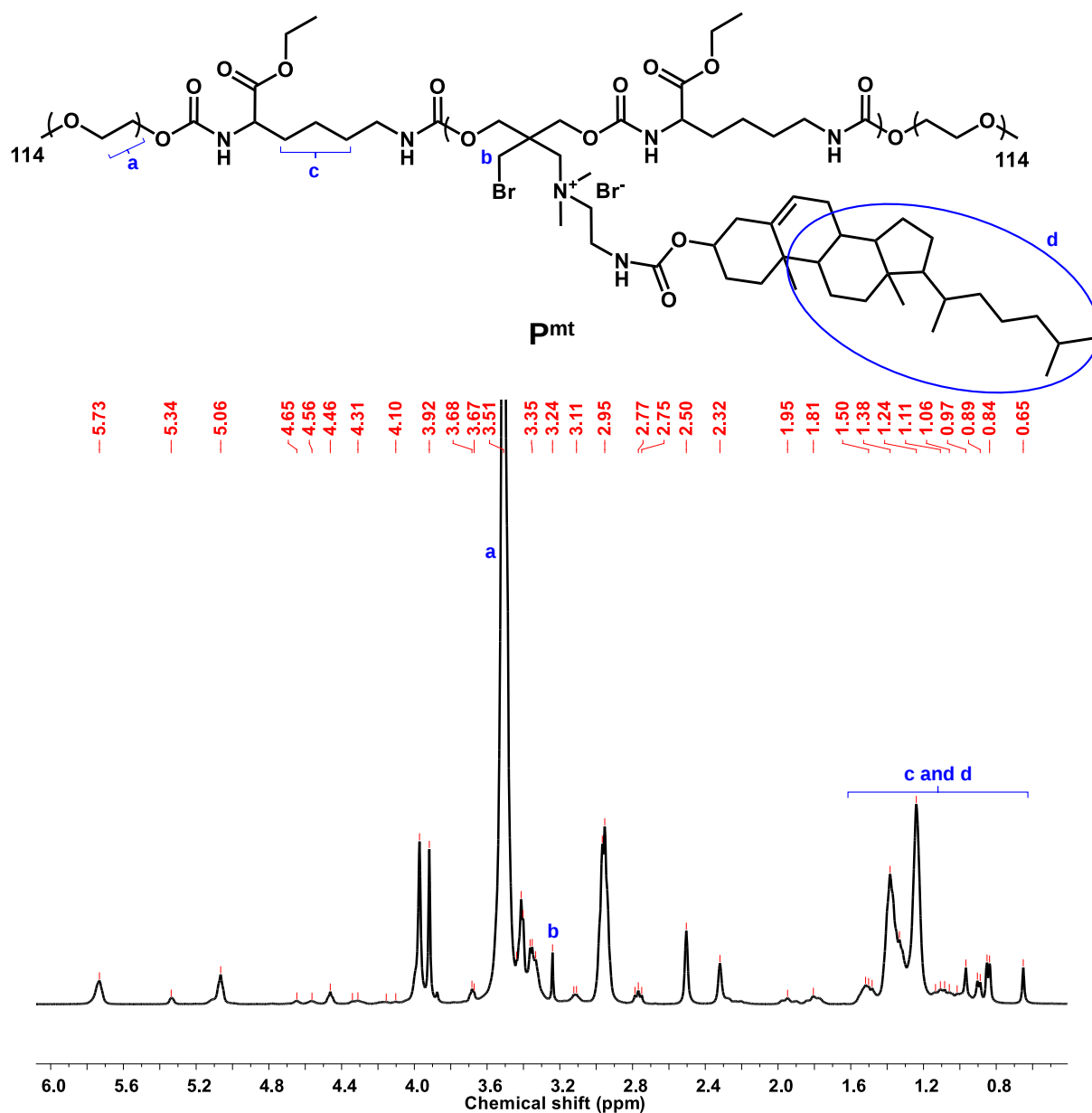
Found: $[M+Na]^+$ m/z 523.45



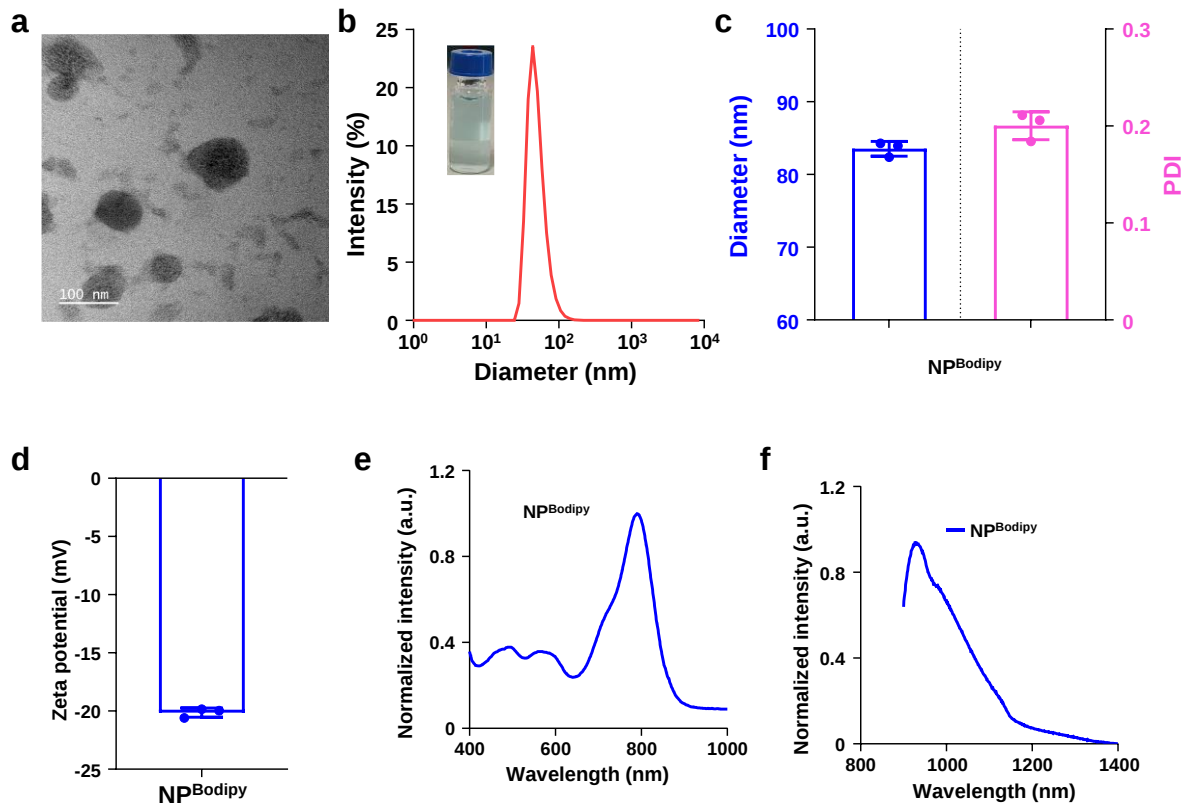
Supplementary Fig. 14. ESI-MS spectrum of N,N-dimethyl-chol.



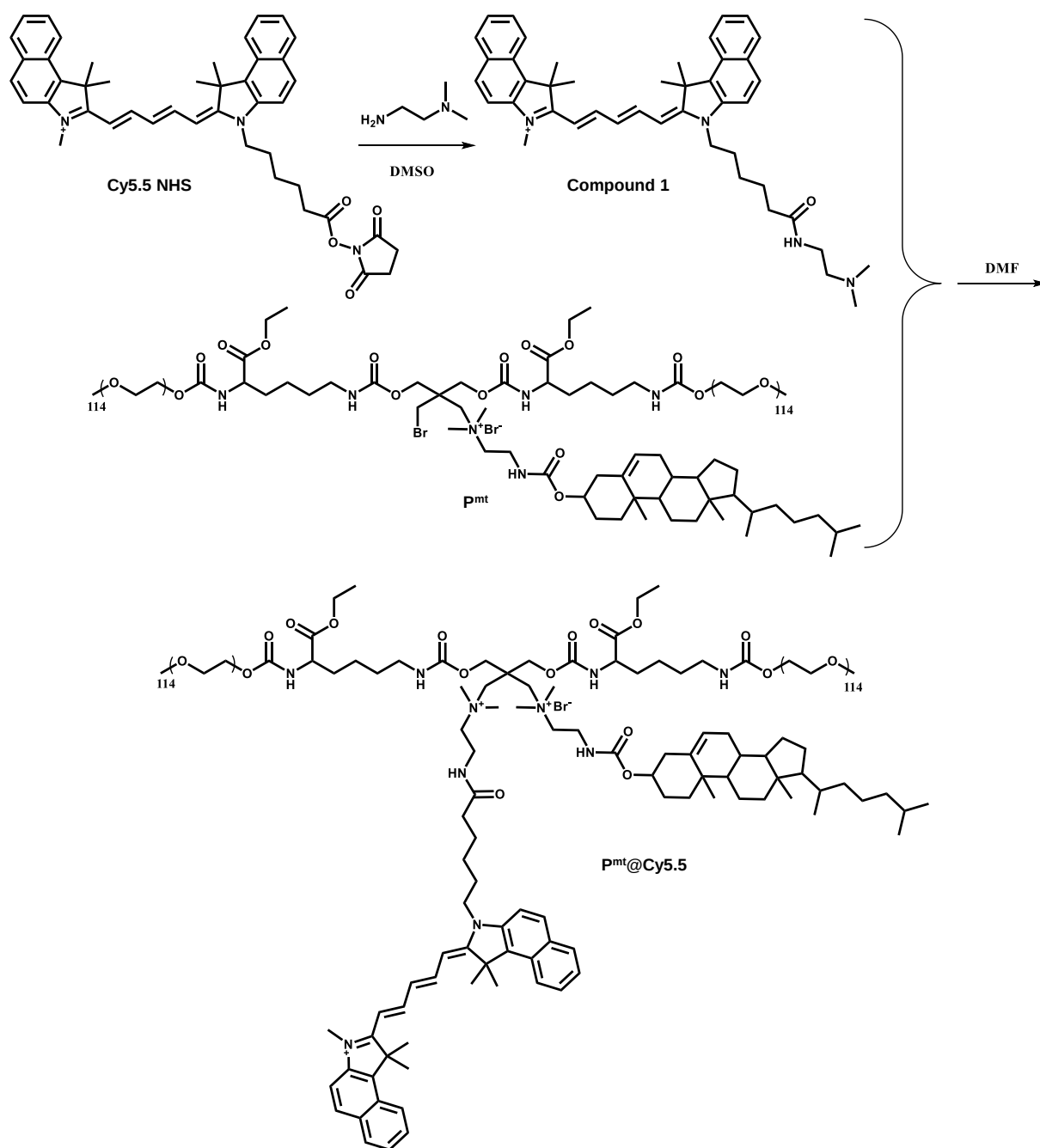
Supplementary Fig. 15. 1H NMR spectrum of P^{Br} in DMSO- d_6 . 1H NMR chemical shift was assigned (a-c).



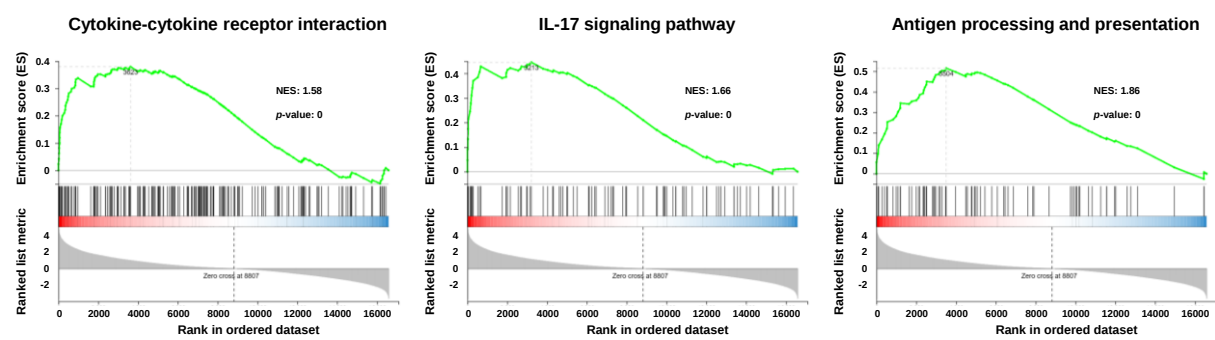
Supplementary Fig. 16. 1H NMR spectrum of P^{mt} in $DMSO-d_6$. 1H NMR chemical shift was assigned (a-d).



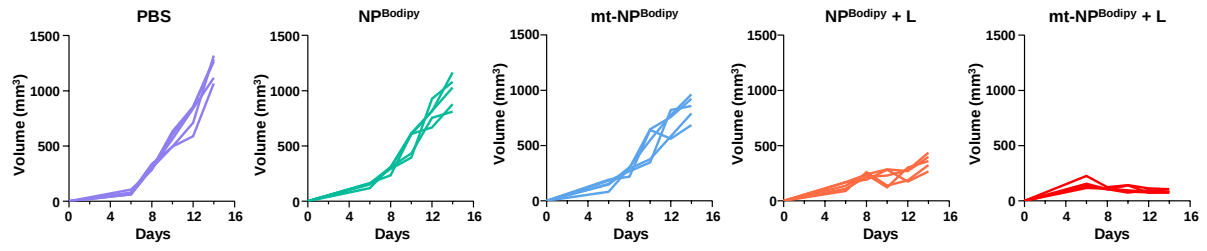
Supplementary Fig. 17. Characterization of NP^{Bodipy}. **a** The representative TEM of NP^{Bodipy} ($n = 3$ independent experiments). **b, c** Hydrodynamic diameters and PDI of NP^{Bodipy} ($n = 3$ independent samples, standard deviation for diameter and PDI are 1.02 and 0.014, respectively.). **d** Zeta potentials of mt-NP^{Bodipy} ($n = 3$ independent samples, standard deviation is 0.40). **e** Absorption spectra of NP^{Bodipy}. **f** PL spectra of NP^{Bodipy}. Data are presented as mean $\pm$ SD.



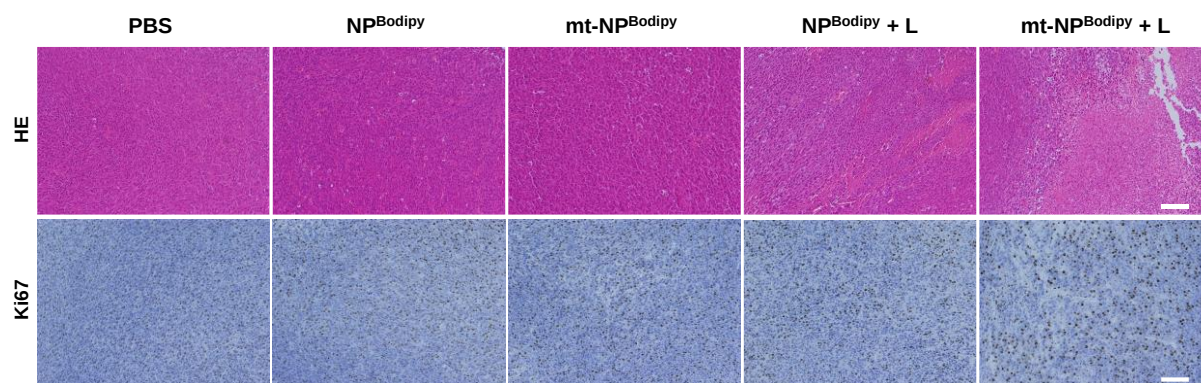
Supplementary Fig. 18. Synthetic route of Pmt@Cy5.5 .



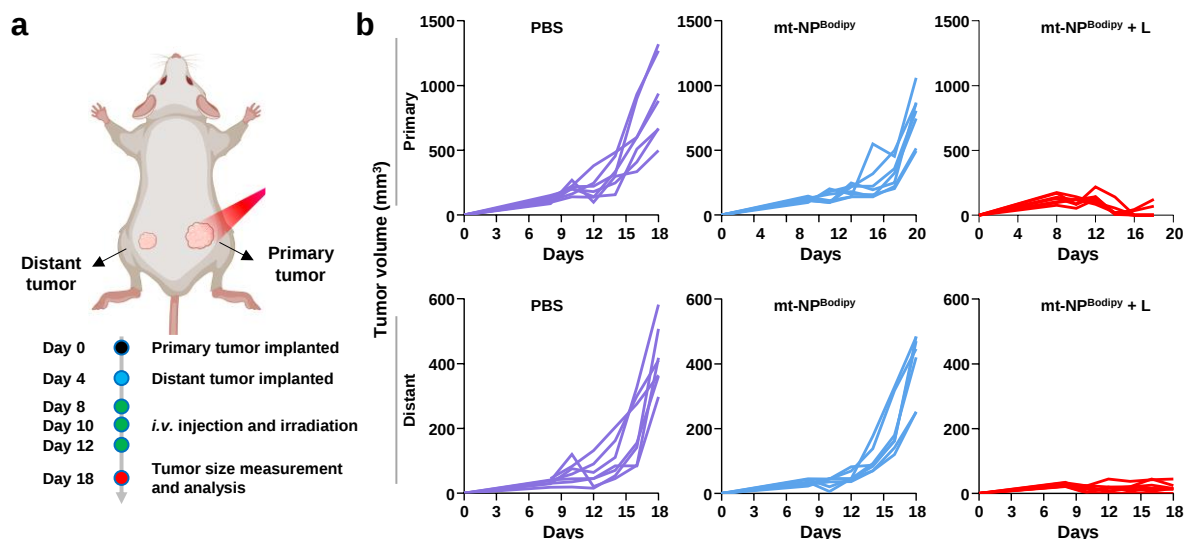
Supplementary Fig. 19. GSEA reveals positive enrichment of genes altered in mt-NP^{Bodipy} + L treatment cells.



Supplementary Fig. 20. Tumor growth inhibition curves ($n = 5$). This is the data of tumour value each mouse in Fig. 6f, and significant differences between $\text{mt-NP}^{\text{Bodipy}} + \text{L}$ and $\text{NP}^{\text{Bodipy}} + \text{L}$ have been annotated in the corresponding captions (**** $p < 0.0001$).

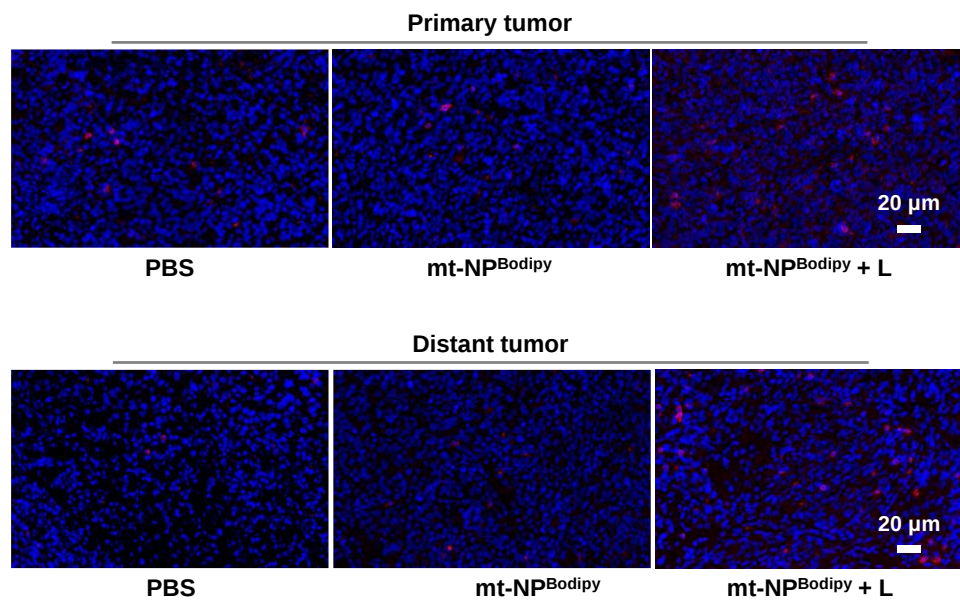


Supplementary Fig. 21. Hematoxylin and eosin (scale bar = 50 μ m) and Ki67 (scale bar = 100 μ m) staining of the tumor after the treatment. Experiment was repeated three times independently with similar results.

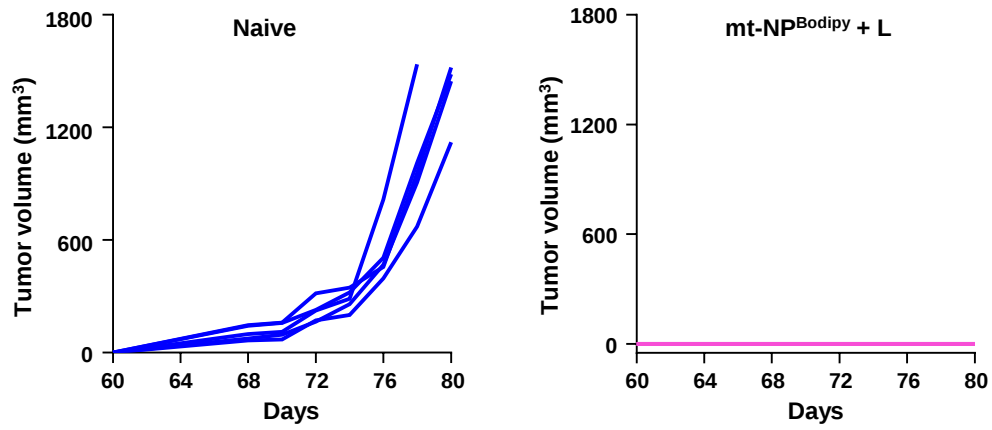


Supplementary Fig. 22. a Schematic treatment schedule. Figure created with Biorender.com.

b Individual and average tumor growth curves of primary and distant tumors ($n = 7$). This is the data of tumour value each mouse in Fig. 7b,c, and significant differences between mt-NP^{Bodipy} + L and mt-NP^{Bodipy} have been annotated in the corresponding captions ($****p < 0.0001$). Moreover, the significant differences between mt-NP^{Bodipy} + L and PBS have been annotated in the corresponding captions ($****p < 0.0001$).



Supplementary Fig. 23. a Representative immunofluorescent staining images of primary tumors and distant tumors. DAPI (blue) and CD8⁺ (red). Experiment was repeated three times independently with similar results.



Supplementary Fig. 24. Individual tumor growth curves of the treated mice ($n = 5$). This is the data of tumour value each mouse in Fig. 7i, and significant differences between mt-NP^{Bodipy} + L and naive have been annotated in the corresponding captions (**** $p < 0.0001$).