Supporting Information

Supramolecular Switch for the Regulation of Antibacterial Efficacy of Near-Infrared Photosensitizer

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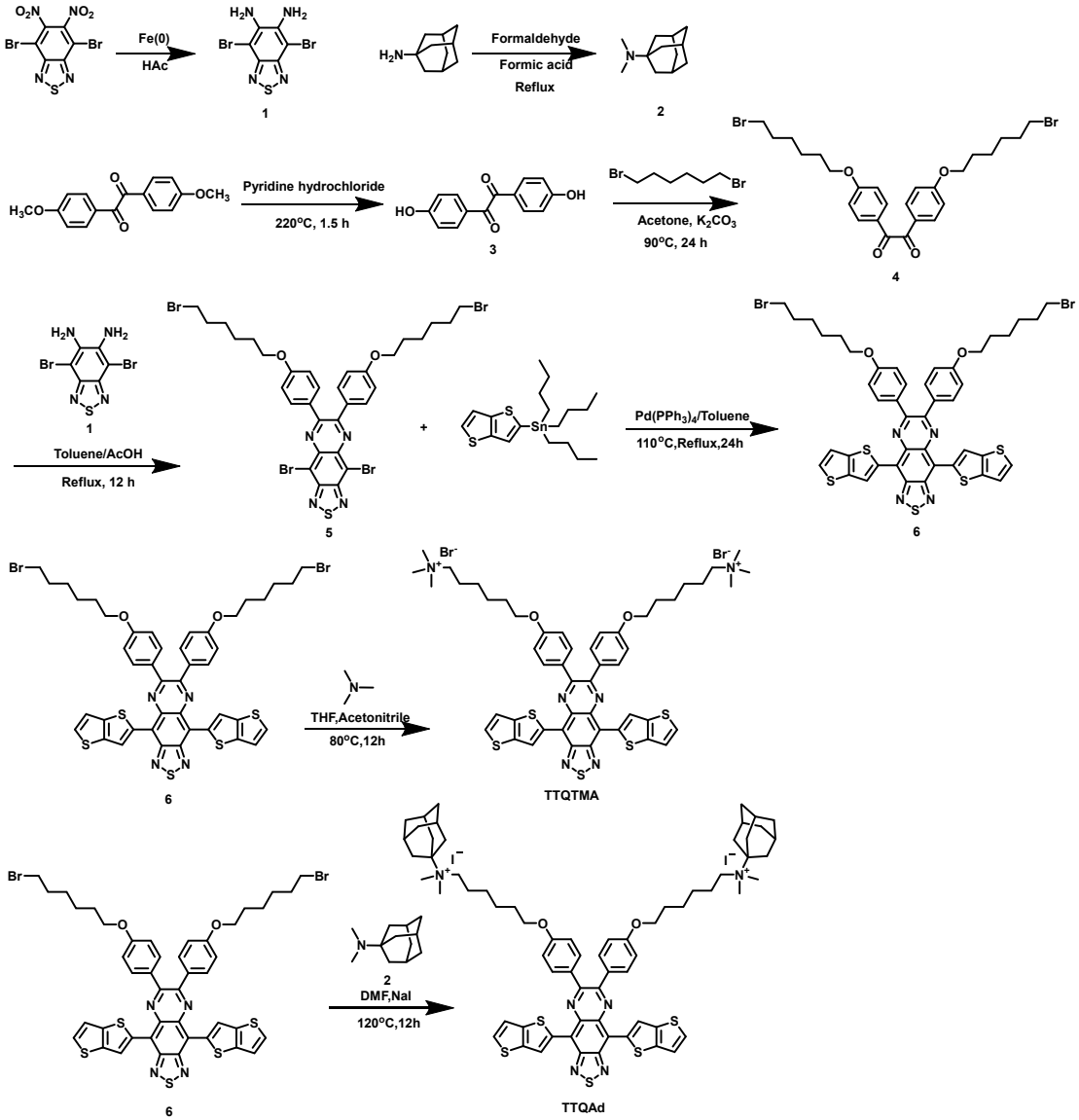

Scheme S1. The synthetic routes of TTQAd and TTQTMA.

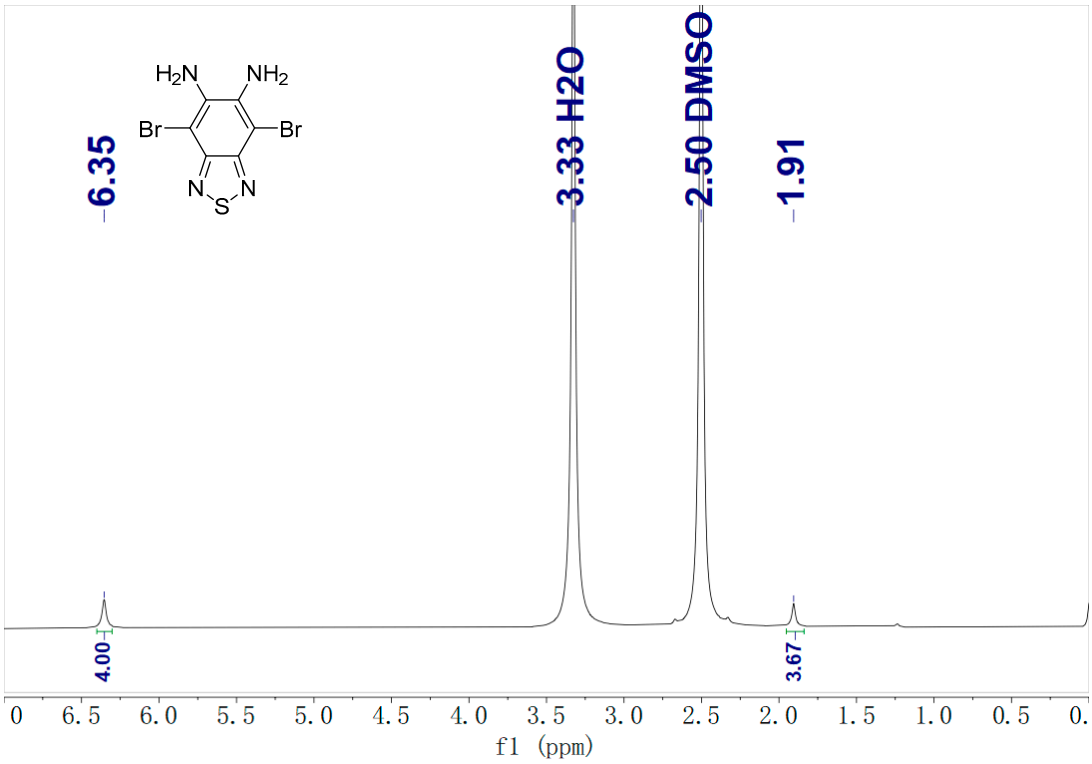

Figure S1. ^{1}H NMR spectrum of 4,7-dibromo-2,1,3-benzothiadiazole-5,6-diamine (1) in DMSO.

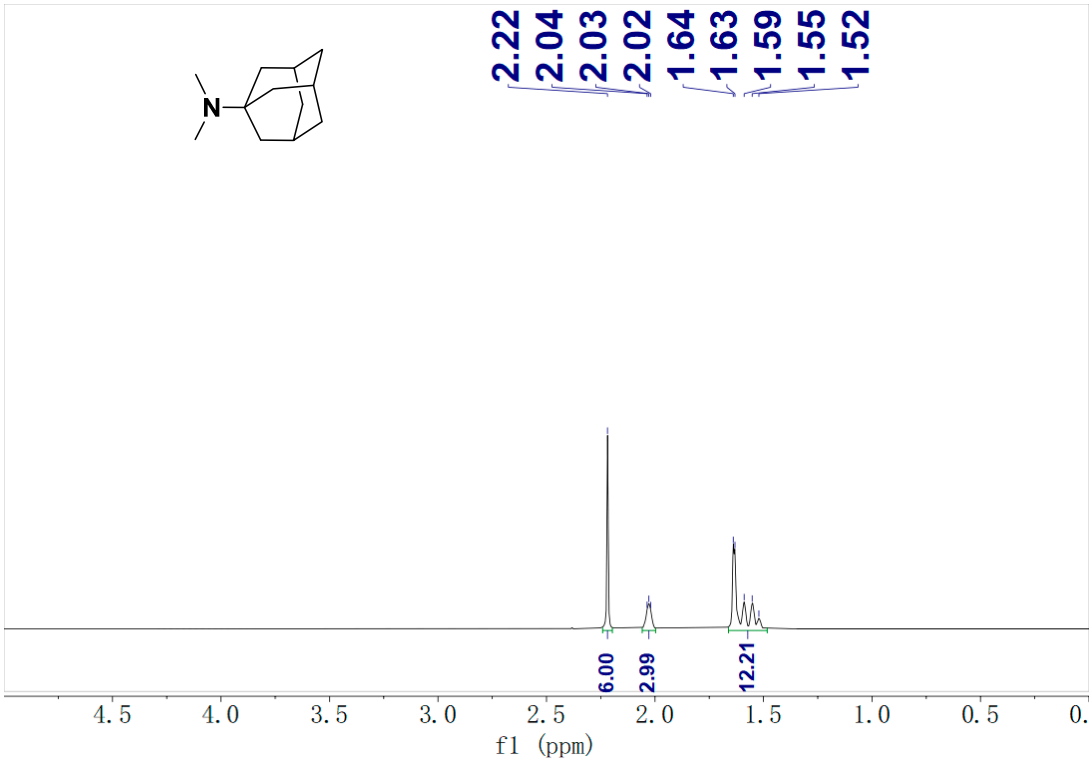

Figure S2. ^{1}H NMR spectrum of dimethyl-1-adamantylamine (2) in $CDCl_3$.

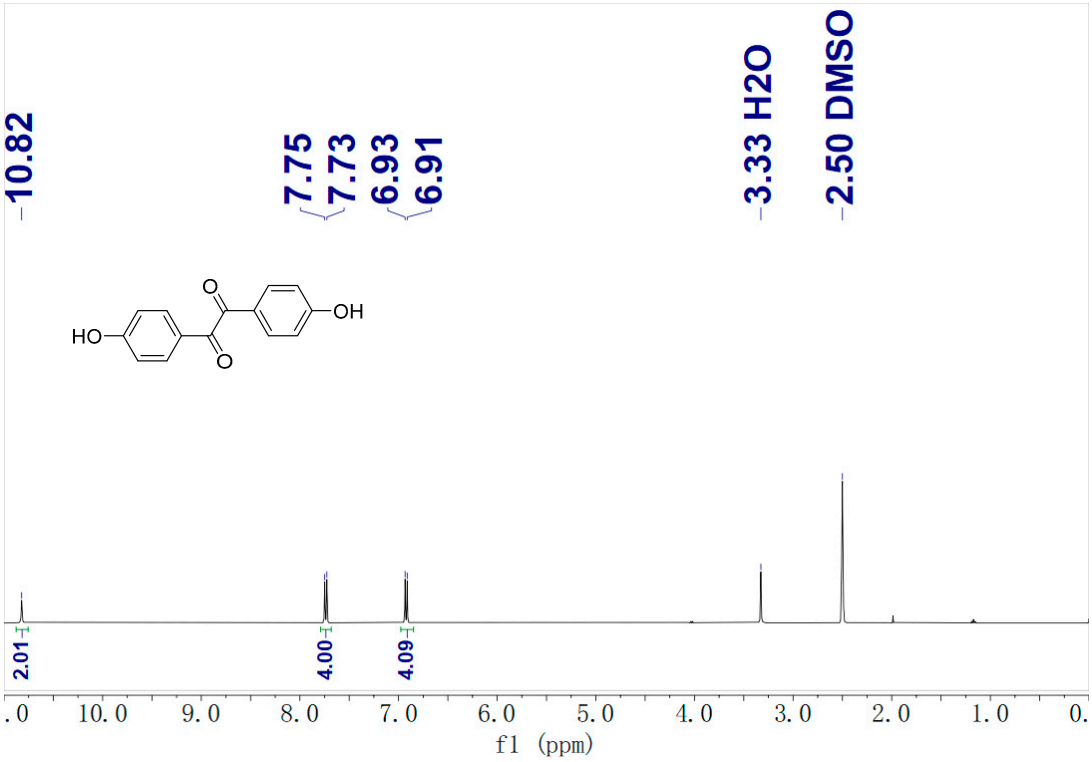

Figure S3. [1]H NMR spectrum of 4,4'-dihydroxy-benzil (3) in DMSO.

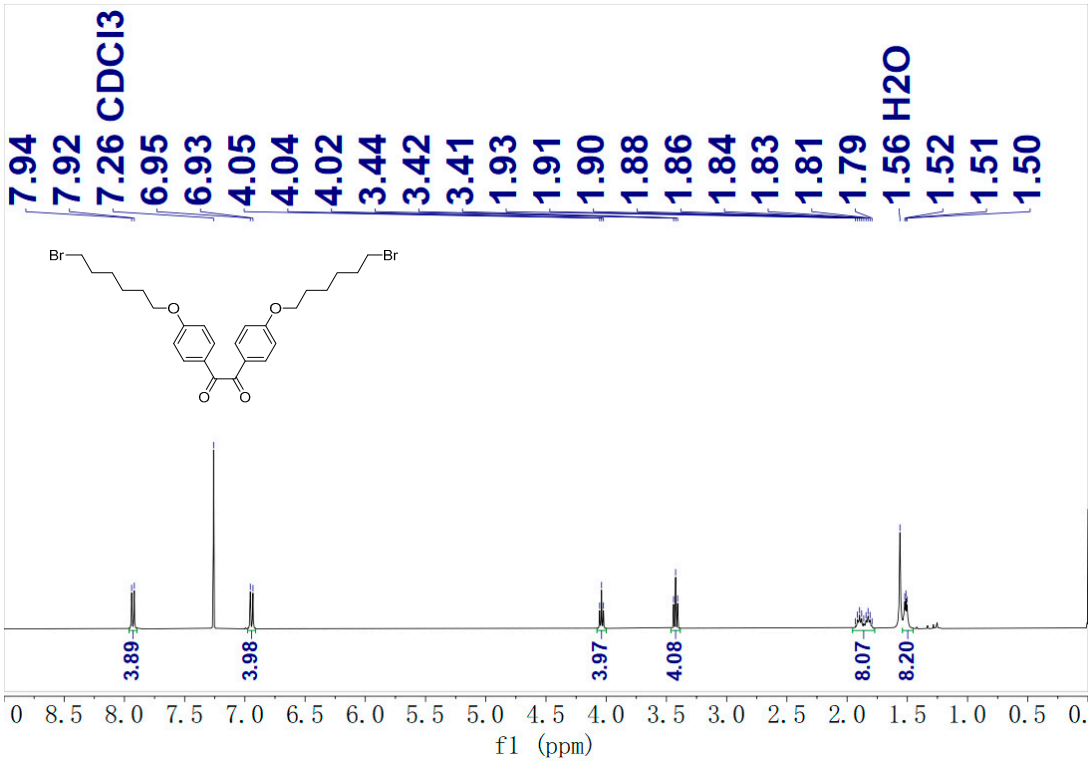

Figure S4. [1]H NMR spectrum of compound 4 in DMSO.

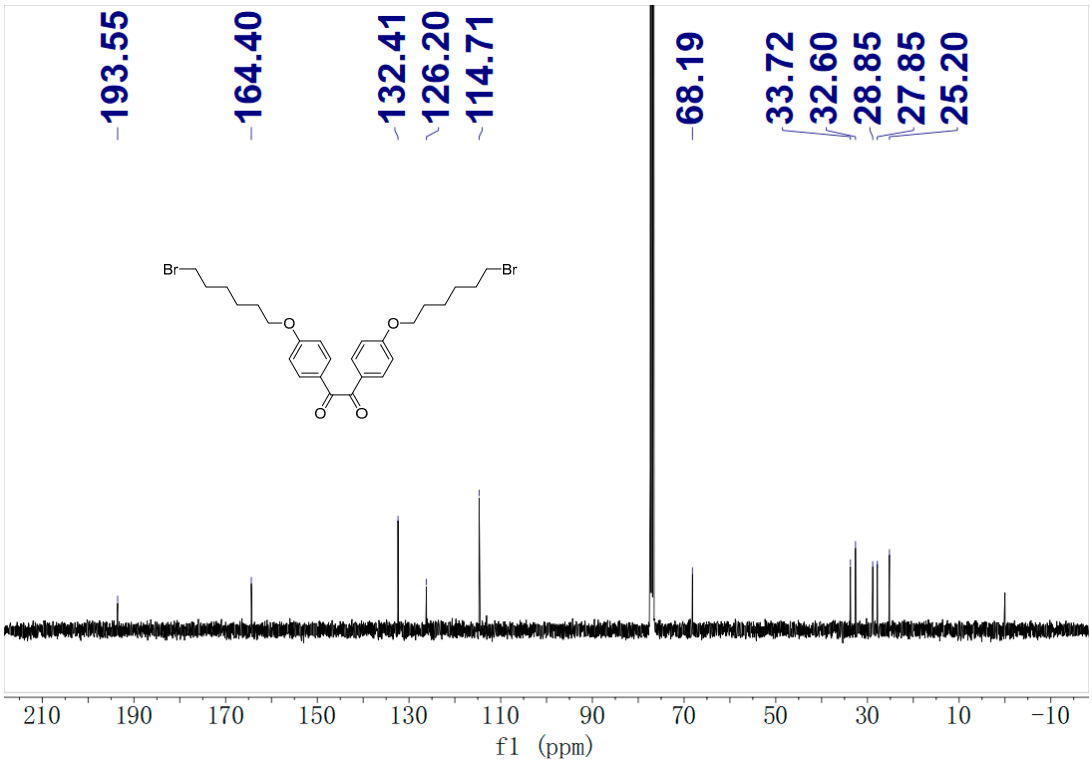

Figure S5. ^{13}C NMR spectrum of compound 4 in DMSO.

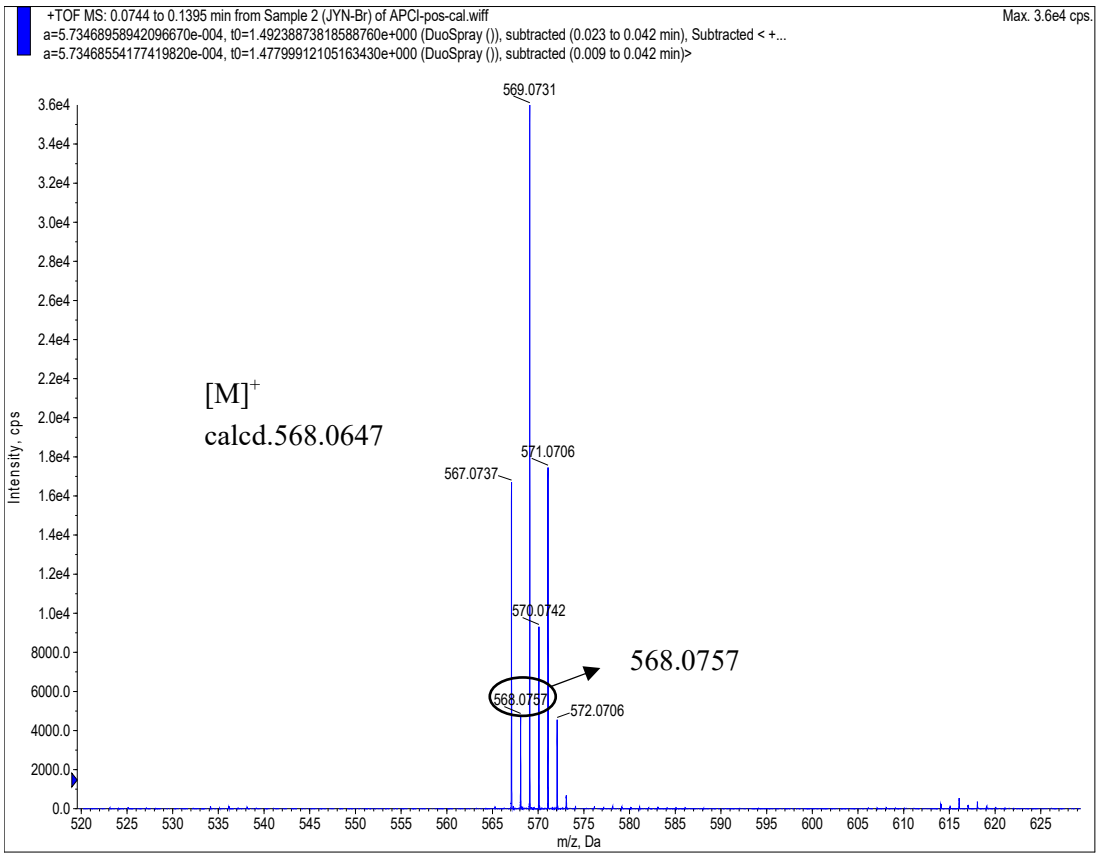

Figure S6. HRMS of Compound 4.

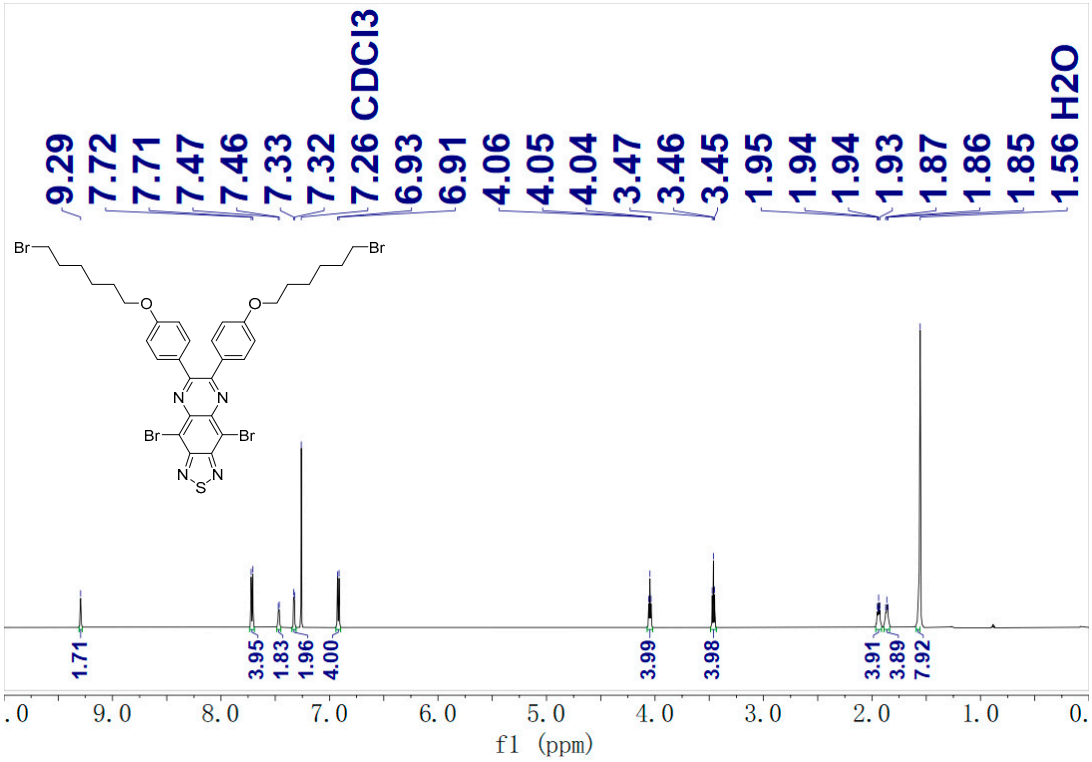

Figure S7. ^{1}H NMR spectrum of compound 5 in $CDCl_3$.

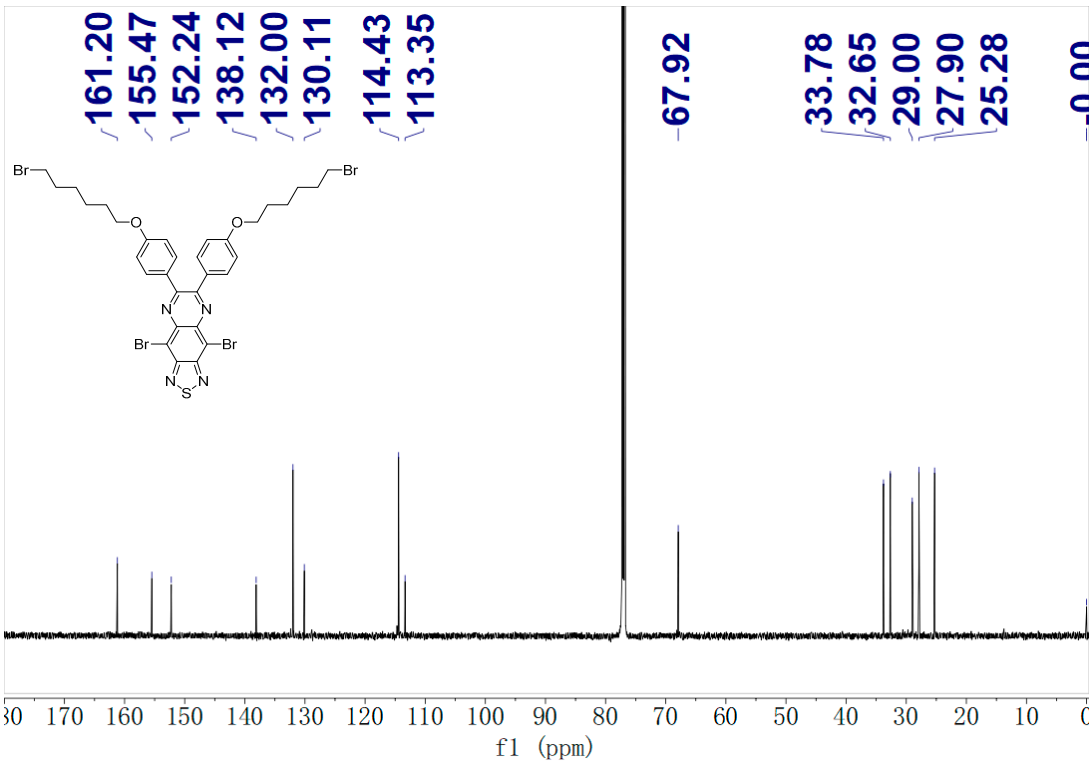

Figure S8. ^{13}C NMR spectrum of compound 5 in $CDCl_3$.

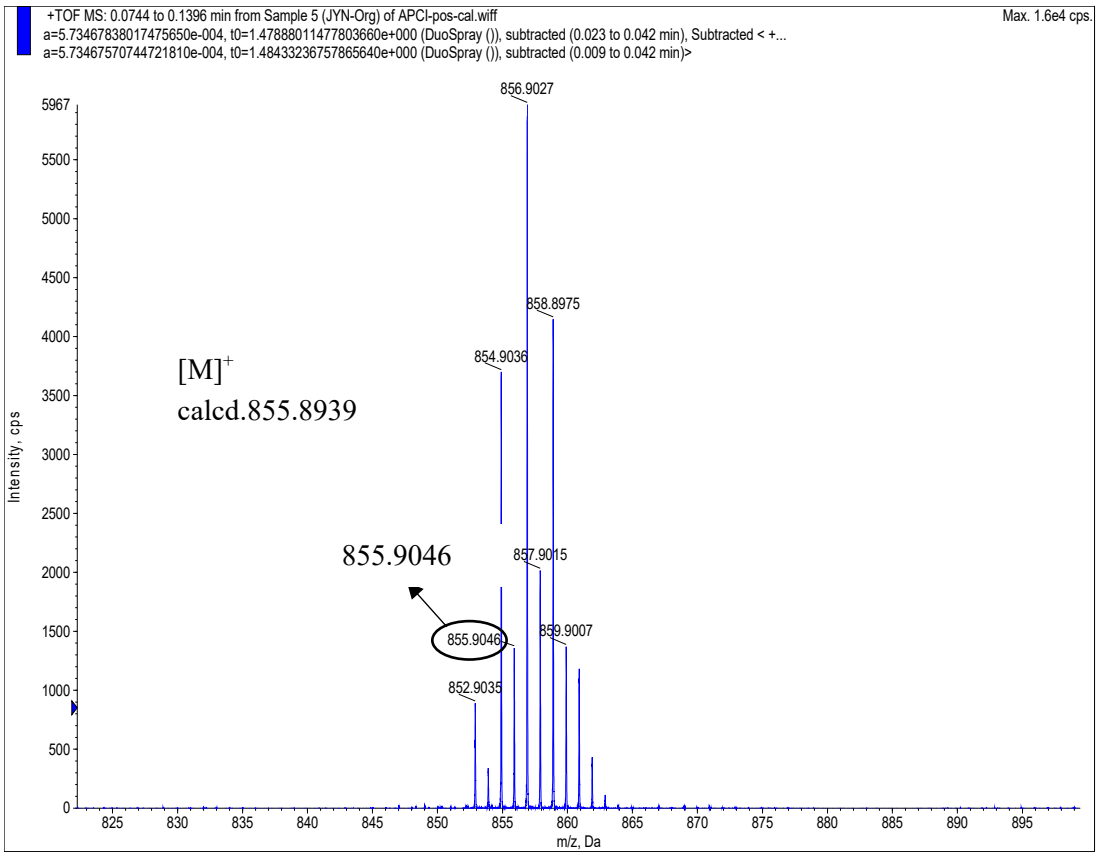

Figure S9. HRMS of compound 5.

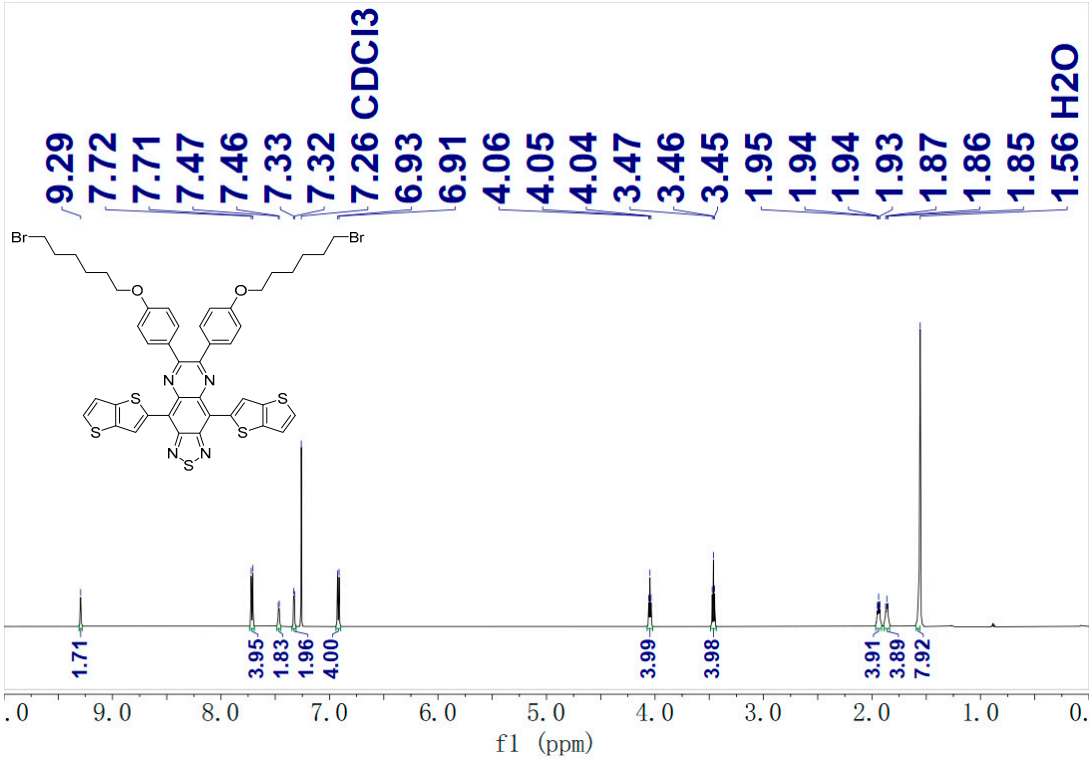

Figure S10. ^{1}H NMR spectrum of compound 6 in $CDCl_3$.

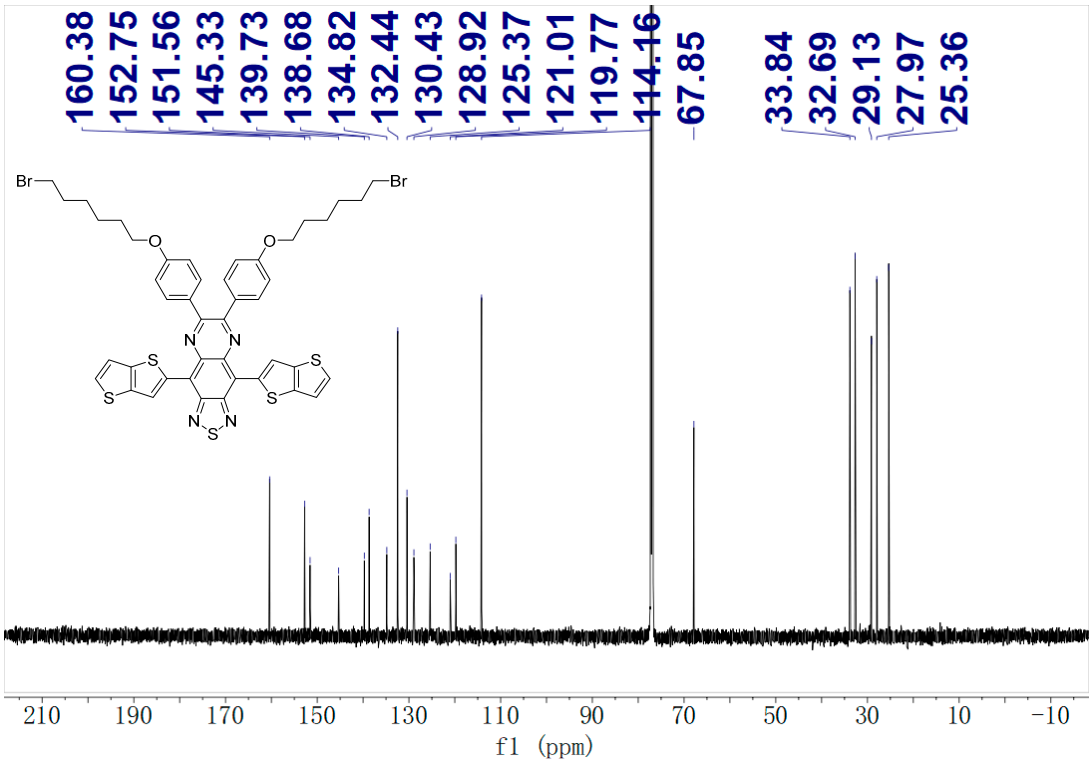

Figure S11. ^{13}C NMR spectrum of compound 6 in $CDCl_3$.

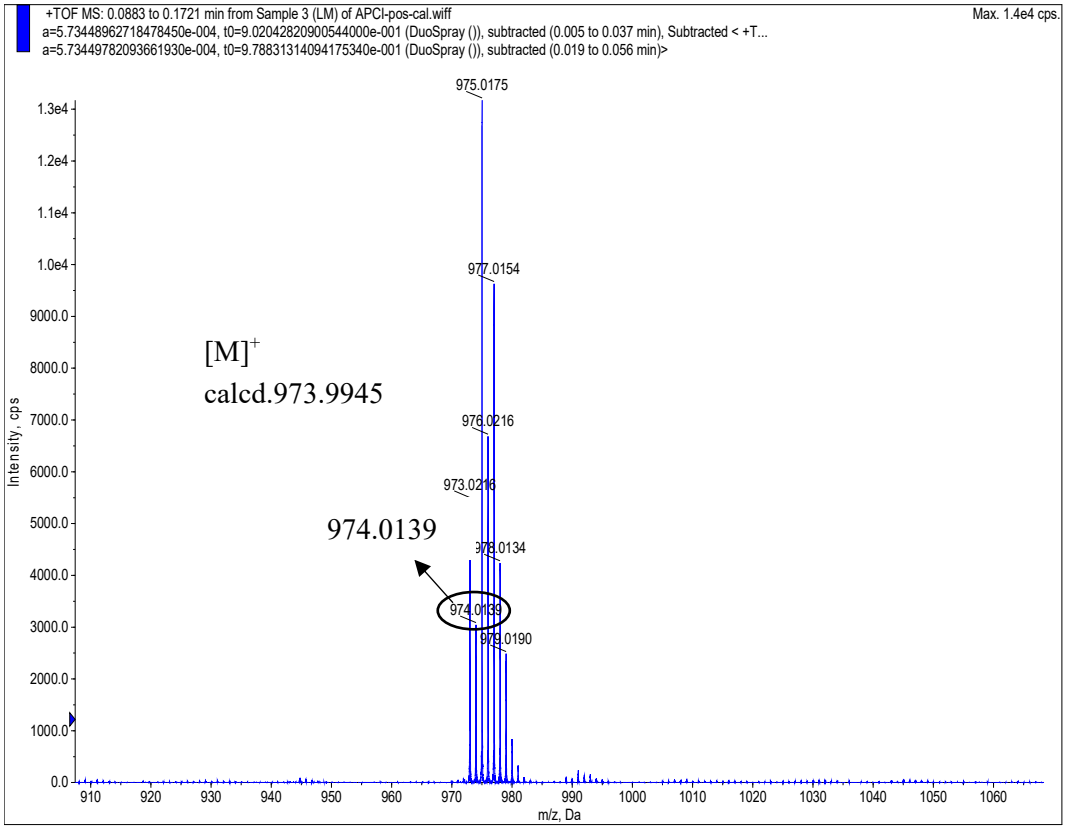

Figure S12. HRMS of compound 6.

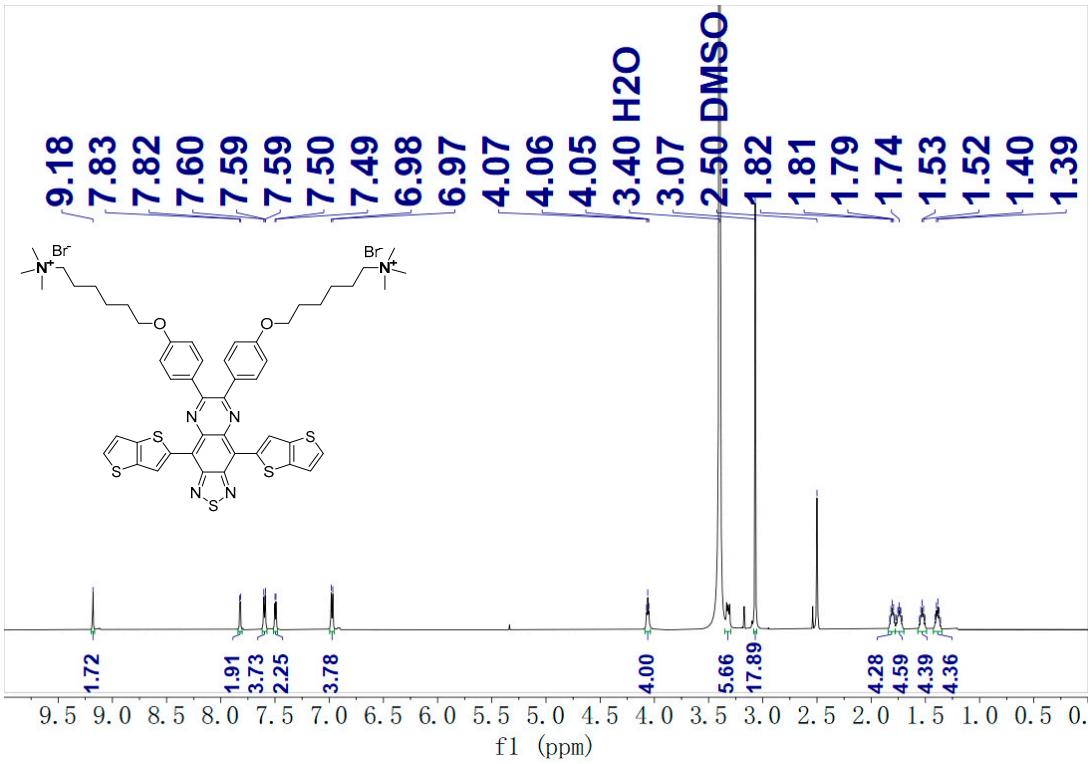

Figure S13. ^{1}H NMR spectrum of TTQTMA in DMSO.

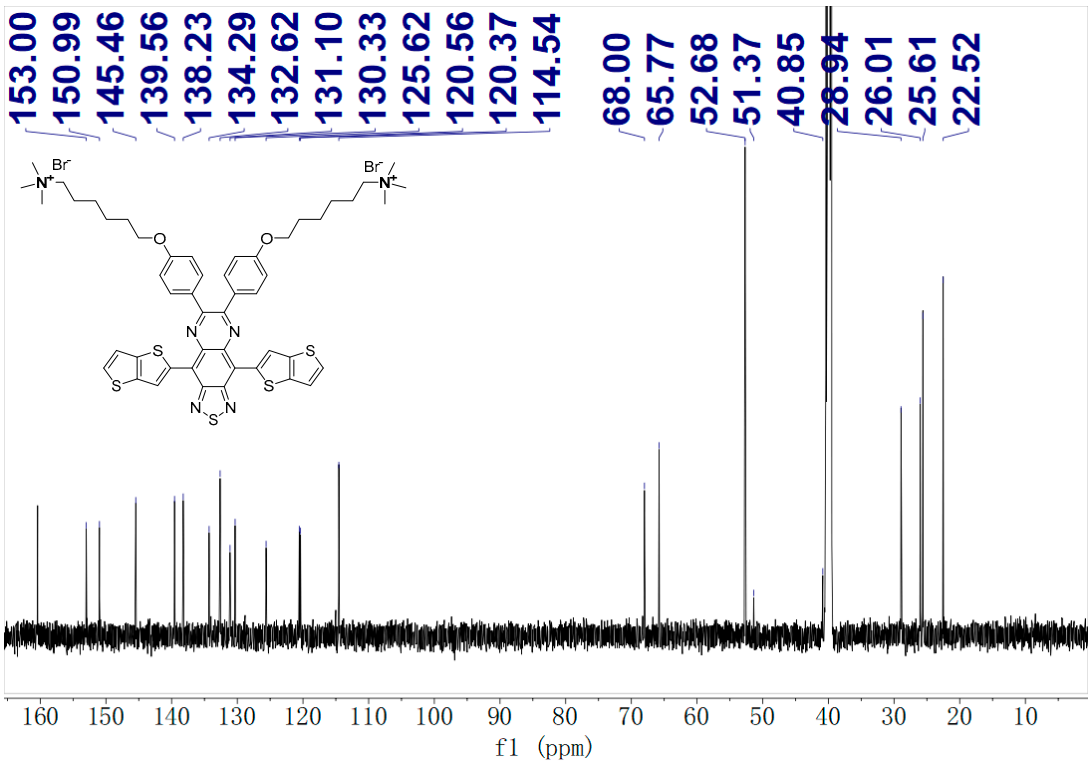

Figure S14. ^{13}C NMR spectrum of TTQTMA in DMSO.

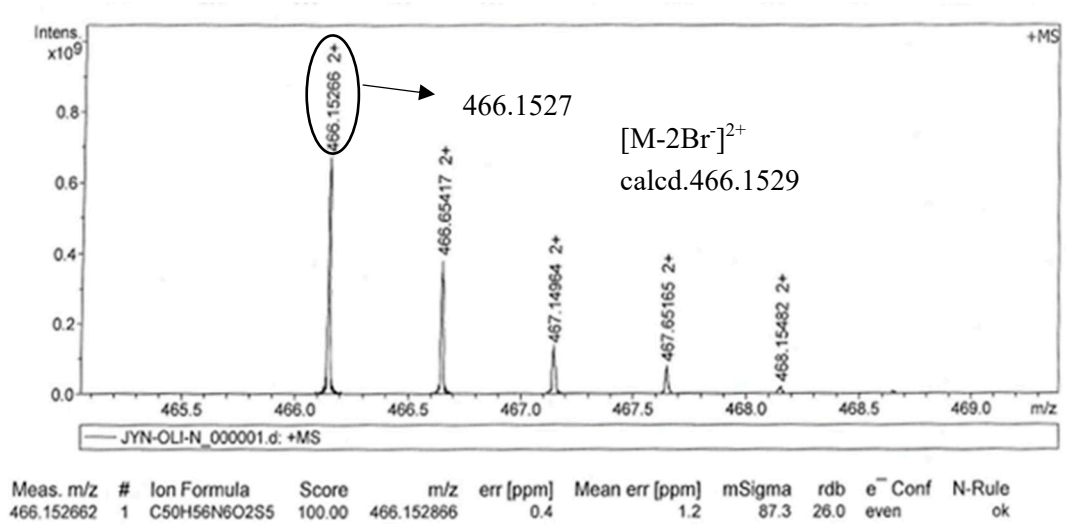

Figure S15. HRMS of TTQTMA.

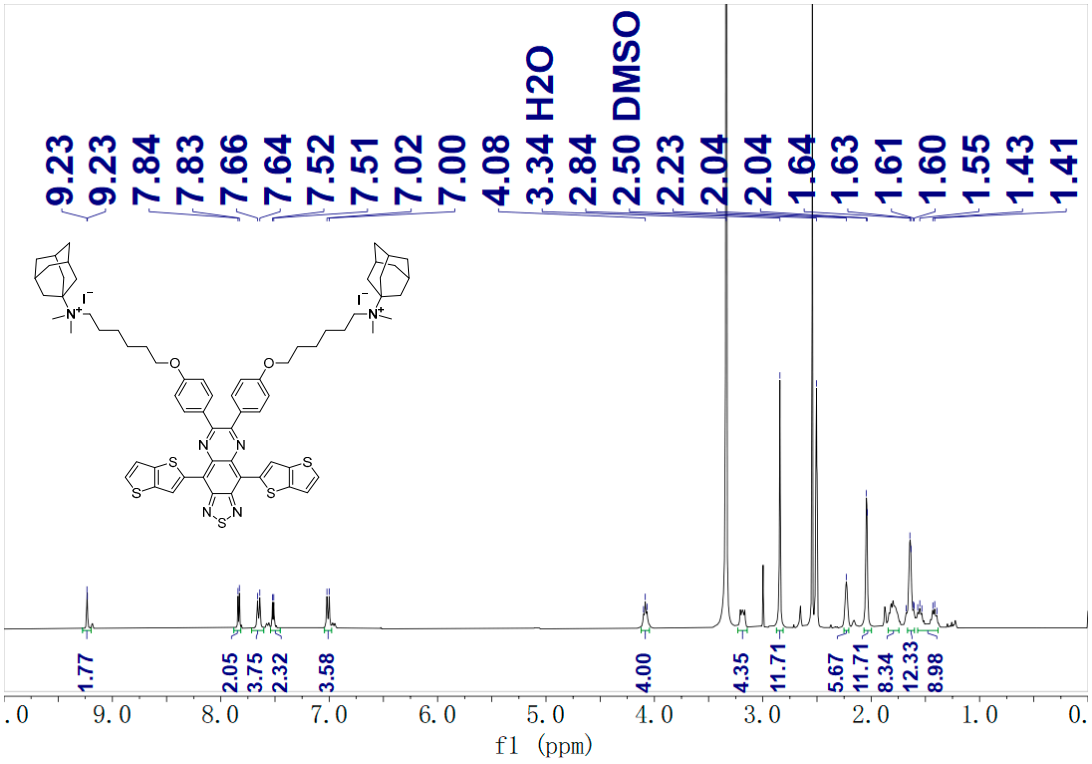

Figure S16. ^{1}H NMR spectrum of TTQAd in DMSO.

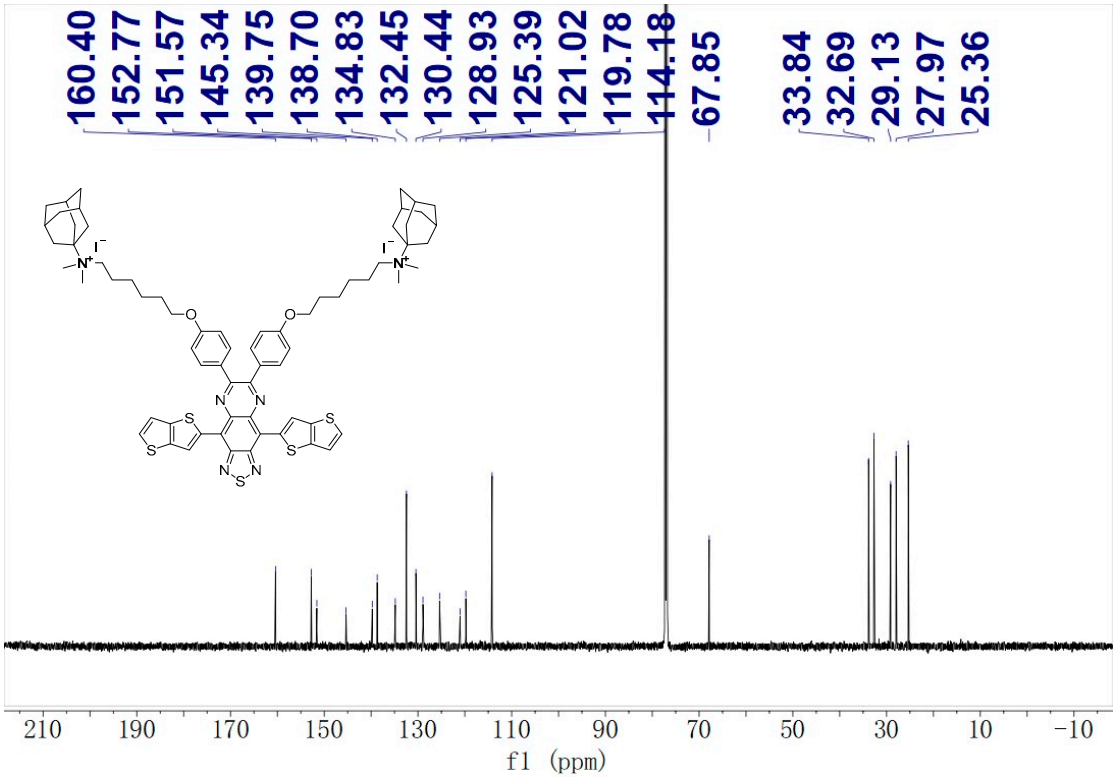

Figure S17. ^{13}C NMR spectrum of TTQAd in DMSO.

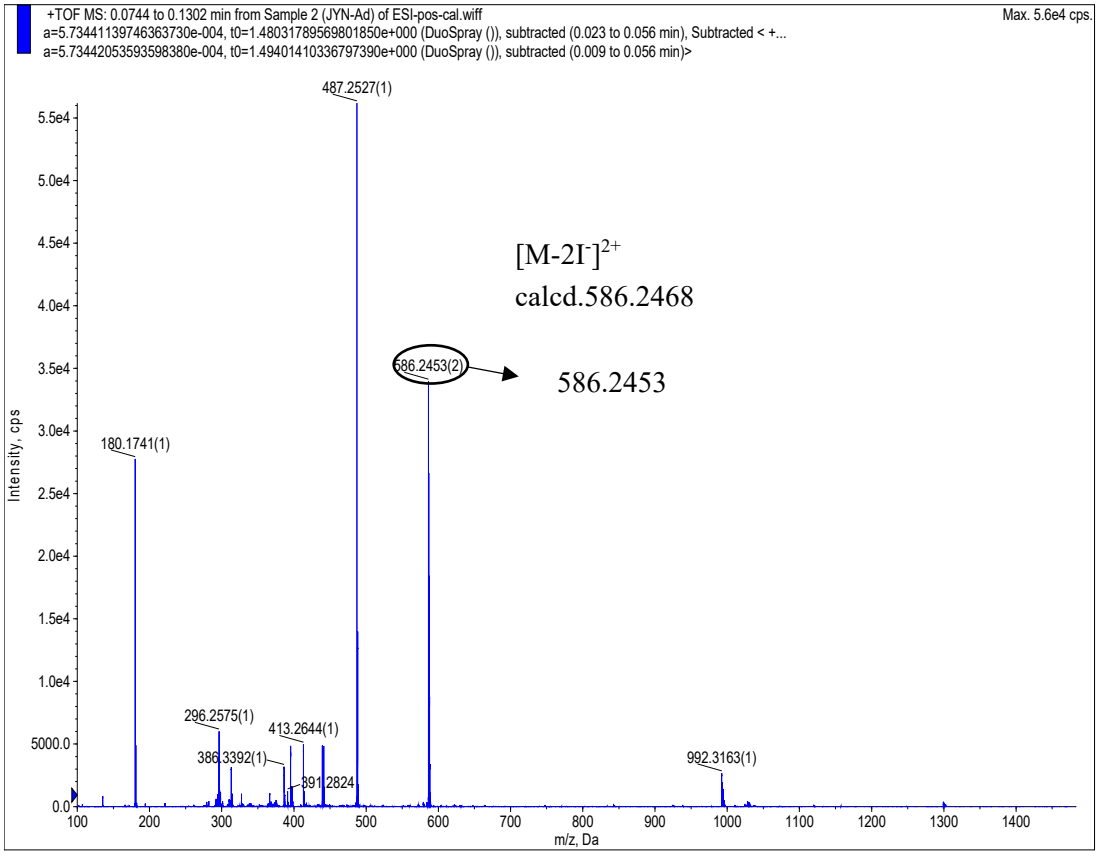

Figure S18. HRMS of TTQAd.

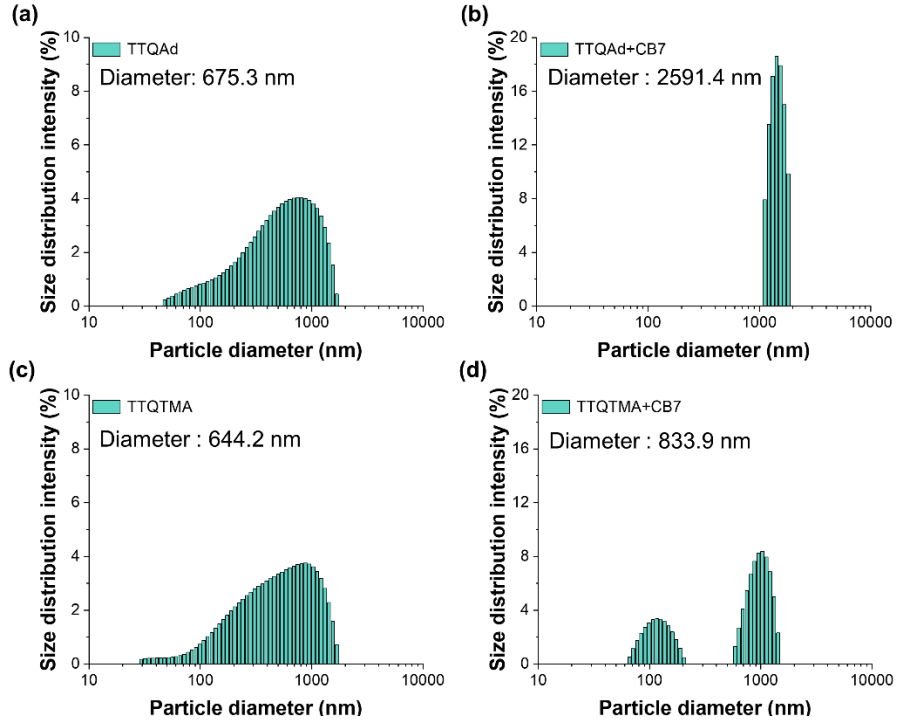

Figure S19. The hydrodynamic diameter histogram of TTQAd and TTQTMA before and after the addition of CB7. (TTQAd/TTQTMA: CB7= 1:2).

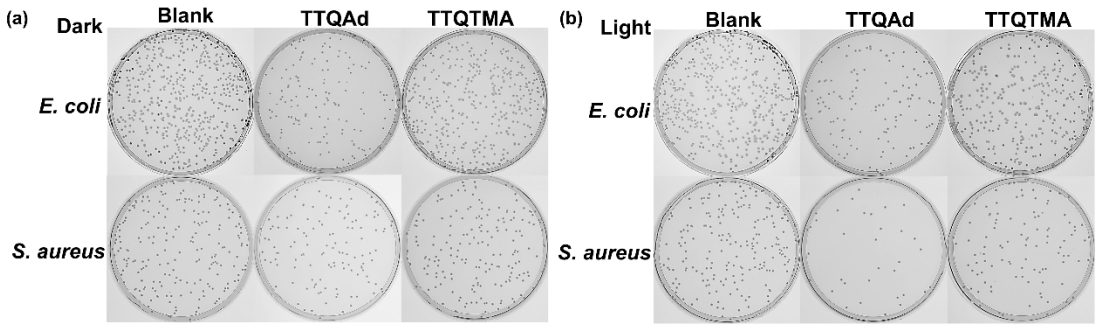

Figure S20. (a) The photographs of plate counting assay of *E. coli* and *S. aureus* treated with TTQAd/TTQTMA (20 μM) in the dark. (b) The photographs of plate counting assay of *E. coli* and *S. aureus* treated with TTQAd/TTQTMA (20 μM) followed by 808 nm laser irradiation (0.5 W cm^{-2}, 10 min).

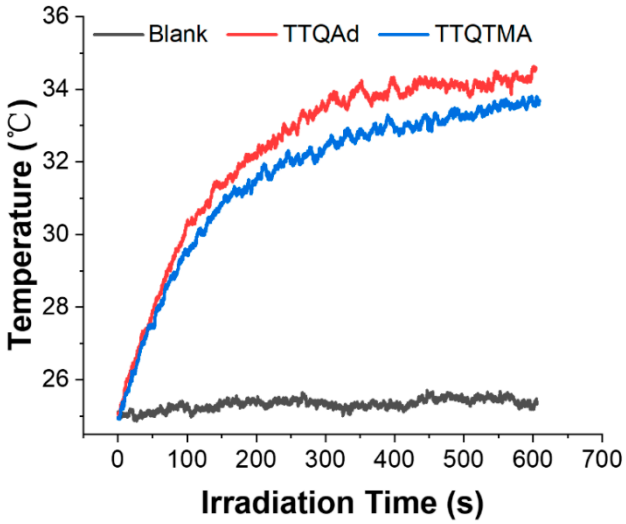

Figure S21. Photothermal conversion of TTQAd and TTQTMA in PBS (20 μM) under 808 nm laser irradiation (0.5 W cm^{-2}, 10 min).

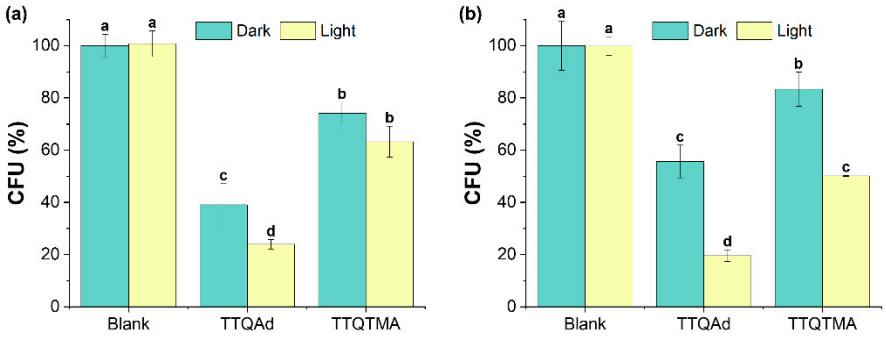

Figure S22. Bacterial viabilities of *E. coli* (a) and *S. aureus* (b) treated with TTQAd/TTQTMA (20 μM) with/without 808 nm laser irradiation (0.5 W cm^{-2}, 10 min). Different letters (a, b, c, d) in the bar graphs represent significant difference at $p < 0.05$ levels.

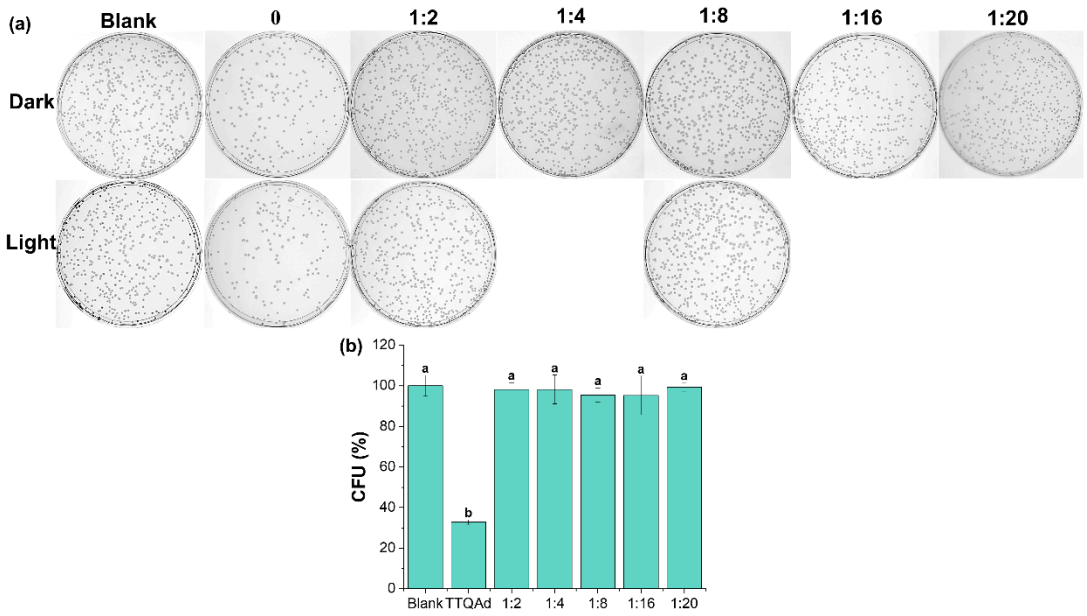

Figure S23. Photographs of *E. coli* colonies on agar plates (a) and bacterial viabilities of *E. coli* (b) treated with TTQAd before and after the addition of different amounts of CB7 with/without 808 nm laser irradiation (0.5 W cm^{-2}). [TTQAd] = 20 μM, [CB7] = 0, 40, 80, 160, 320, 400 μM. Different letters (a, b, c, d) represent significant difference at $p < 0.05$ levels.

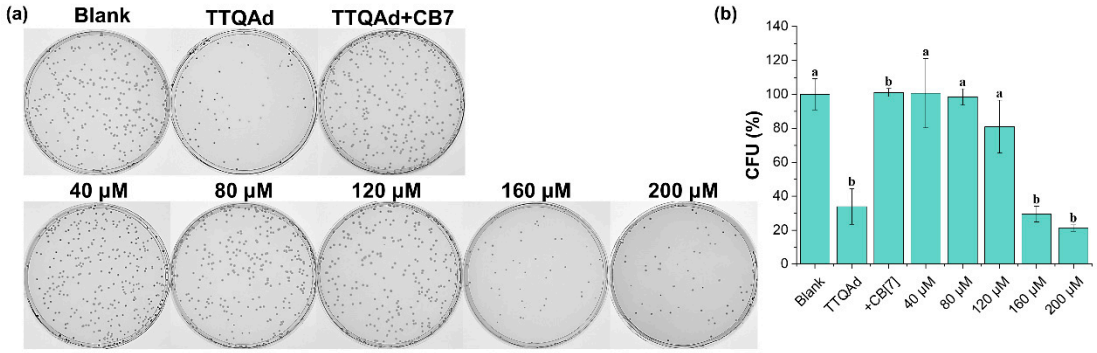

Figure S24. Photographs of *E. coli* colonies on agar plates (a) and bacterial viabilities of *E. coli* (b) treated with TTQAd-CB7 and different amounts of TMeAd. [TTQAd-CB7] = 20 μM, [TMeAd] = 0, 40, 80, 120, 160, 200 μM. Different letters (a, b) in the bar graph represent significant difference at $p < 0.05$ levels.

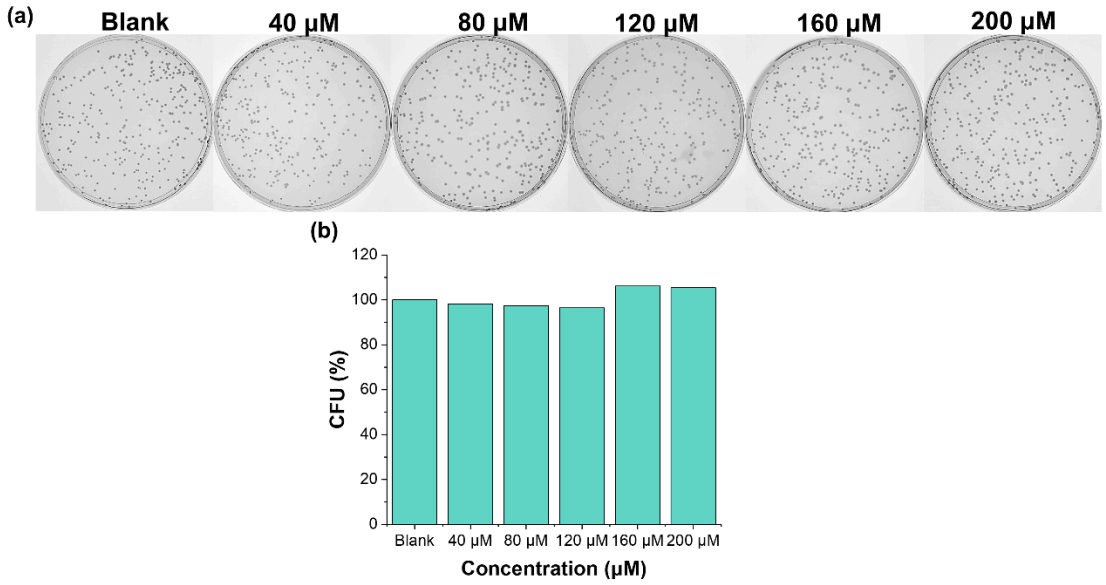

Figure S25. Photographs of *E. coli* colonies on agar plates (a) and bacterial viabilities of *E. coli* (b) treated with TMeAd. [TMeAd] = 0, 40, 80, 120, 160, 200 μM.

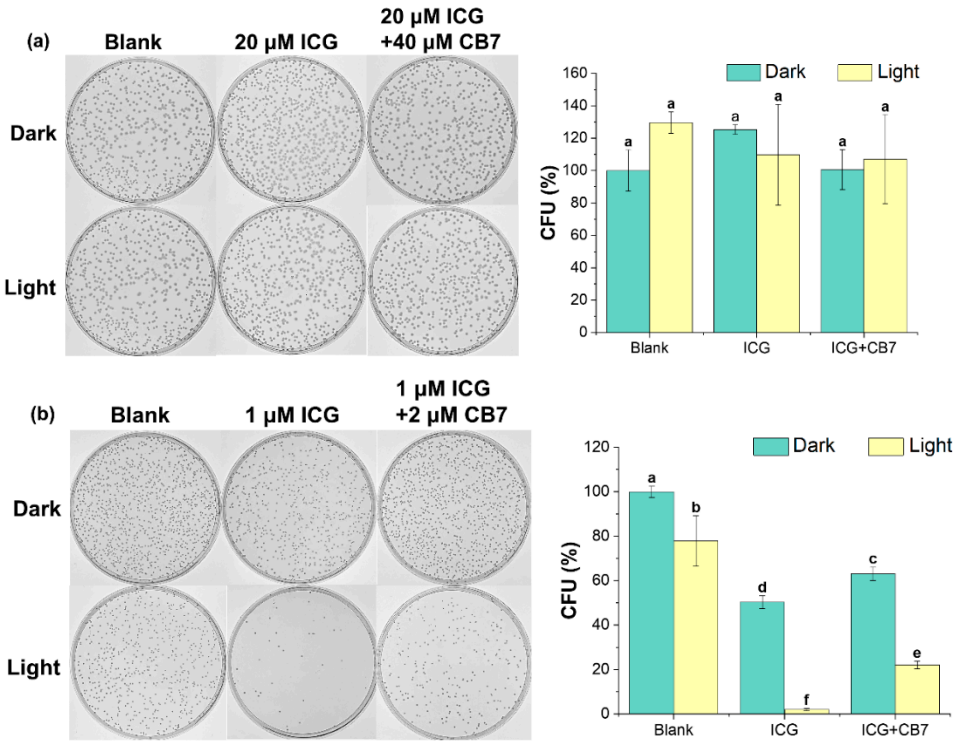

Figure S26. (a) Photographs of *E. coli* colonies on agar plates and bacterial viabilities of *E. coli* treated with ICG (20 μM) before and after the addition of CB7 (40 μM) with/without 808 nm laser irradiation (0.5 W cm^{-2}, 10 min); (b) Photographs of *S. aureus* colonies on agar plates and bacterial viabilities of *S. aureus* treated with ICG (1

μM) before and after the addition of CB7 (2 μM) with/without 808 nm laser irradiation (0.5 W cm^{-2}, 10 min); Different letters (a, b, c, d) in the bar graphs represent significant difference at $p < 0.05$ levels.

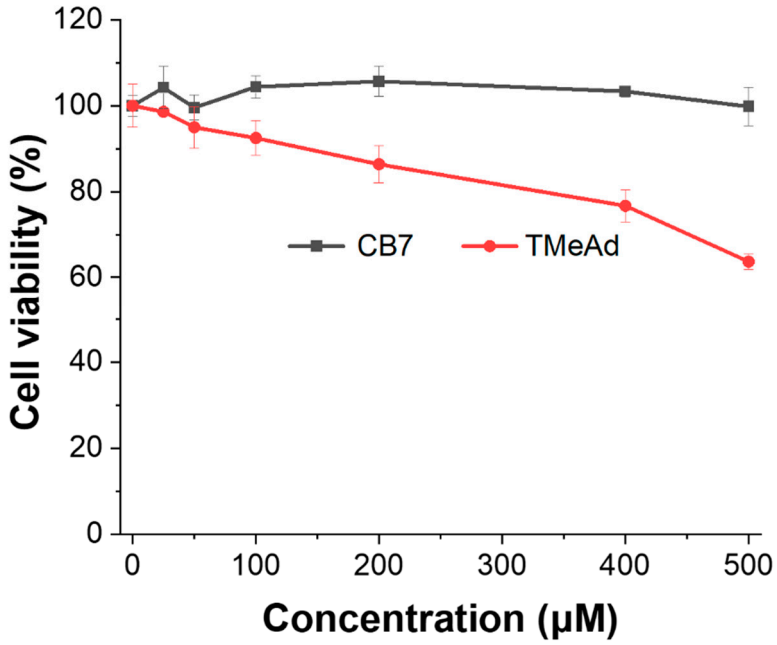

Figure S27. Cell viability after treating with CB7 and TMeAd at different concentrations in the absence of light.