

Supporting Information for

**A two-photon AIE fluorophore as a photosensitizer for highly efficient
mitochondria-targeted photodynamic therapy**

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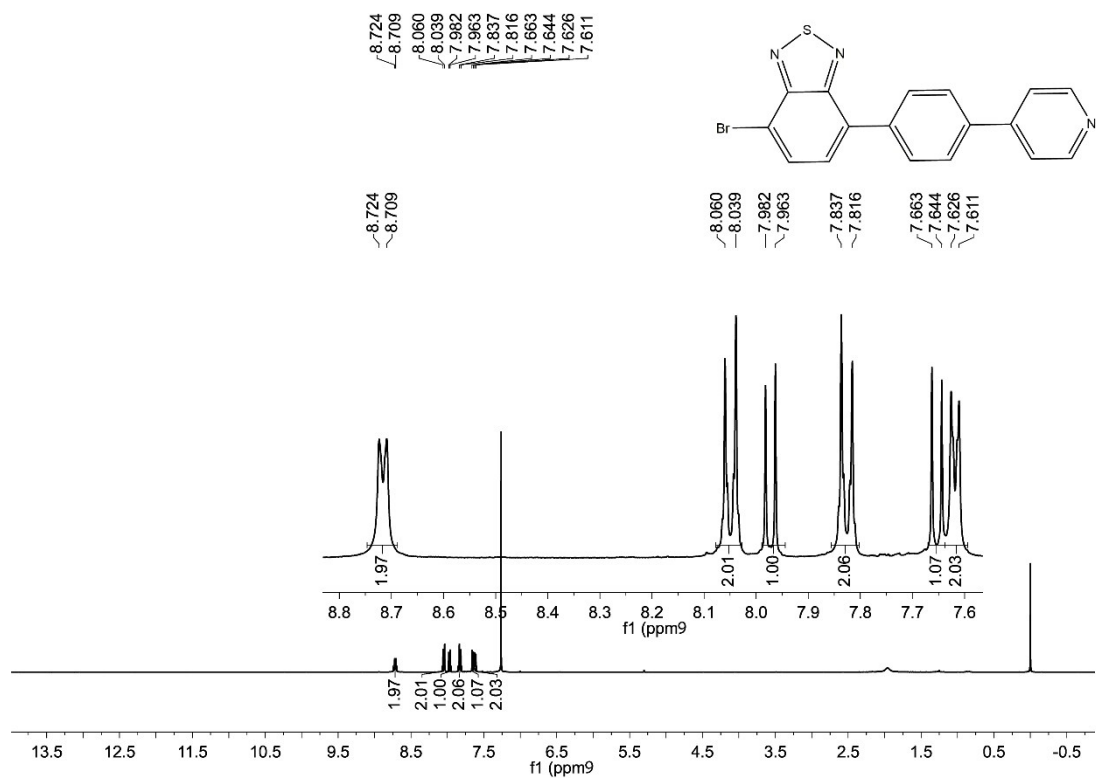


Figure S1. ¹H NMR spectrum of compound **1** in CDCl₃.

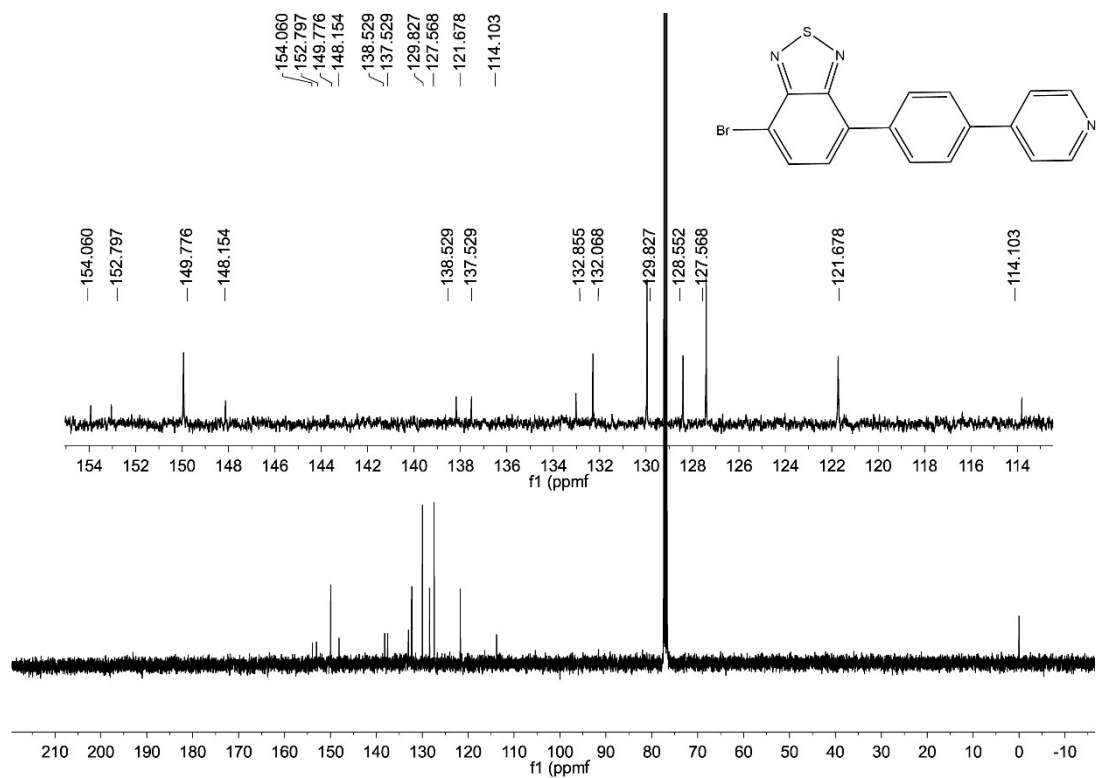


Figure S2. ¹³C NMR spectrum of compound **1** in CDCl₃.

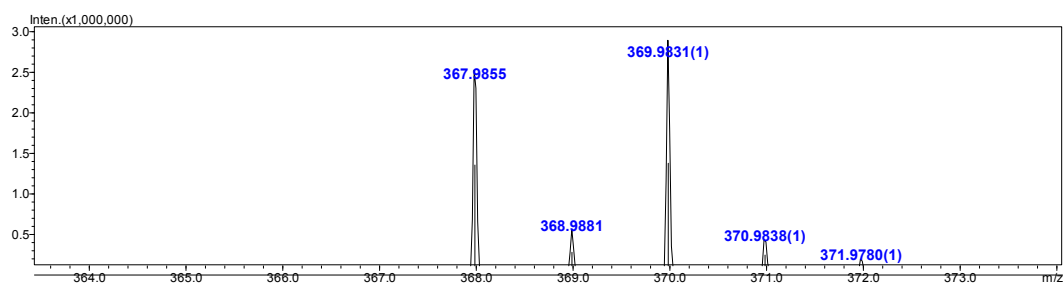


Figure S3. HRMS spectrum of compound 1.

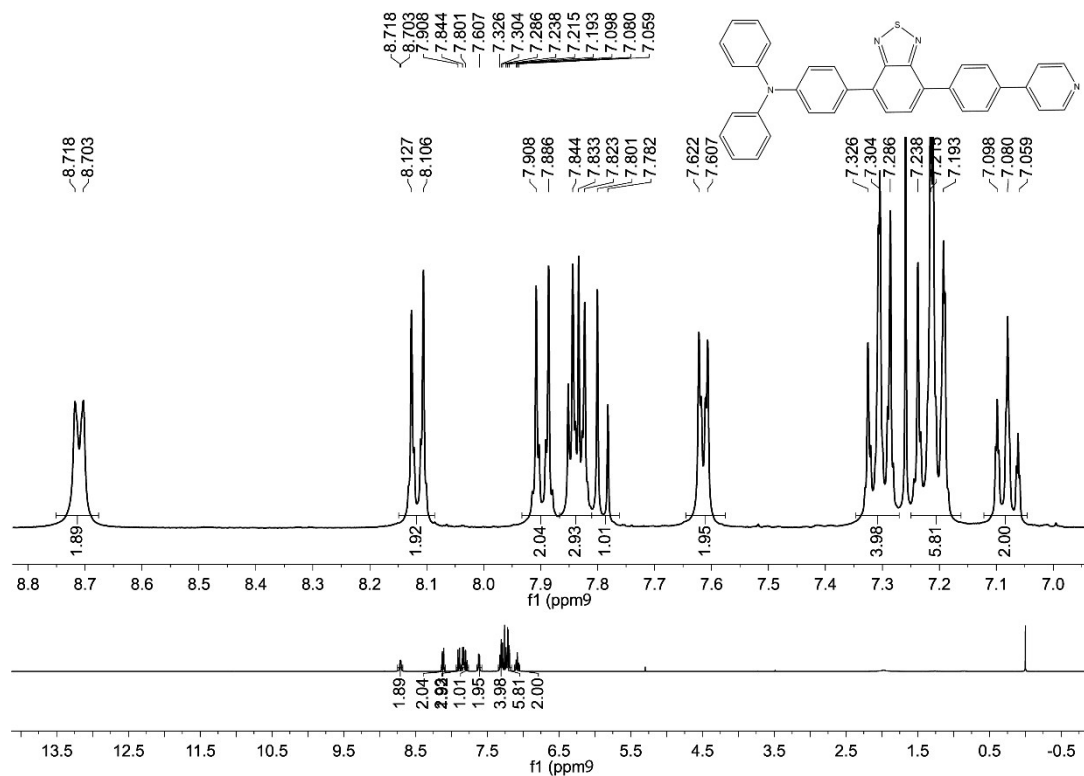


Figure S4. ¹H NMR spectrum of compound 2 in CDCl₃.

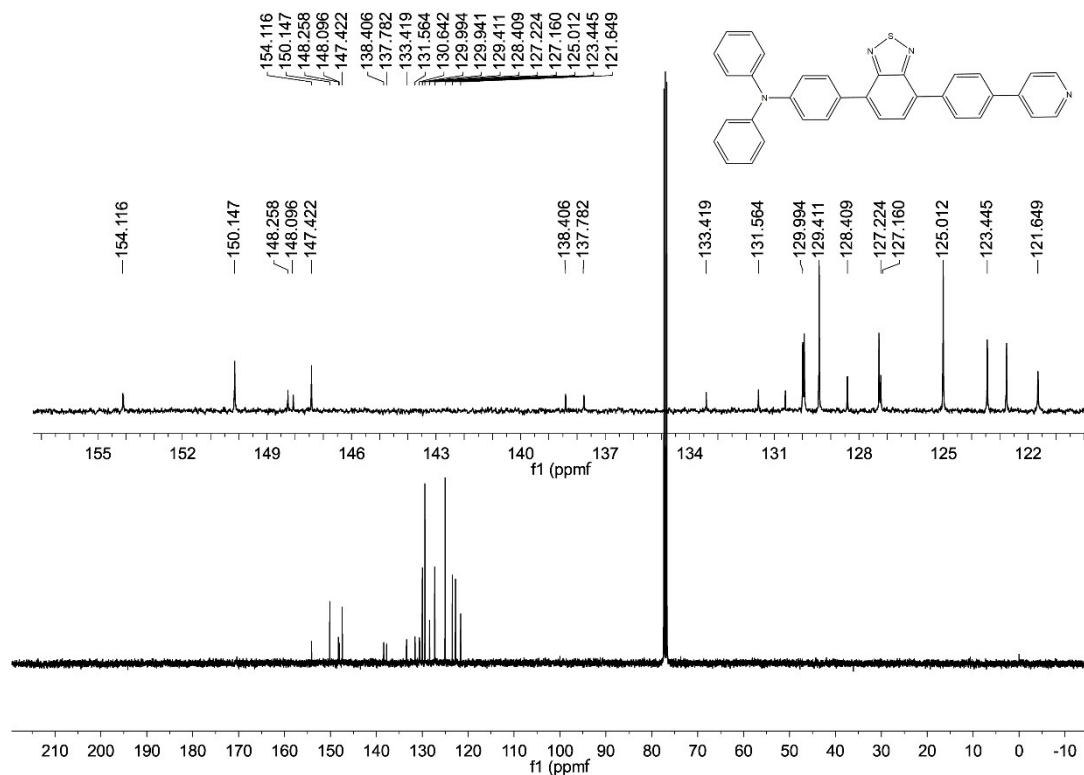


Figure S5. ¹³C NMR spectrum spectrum of compound **2** in CDCl₃.

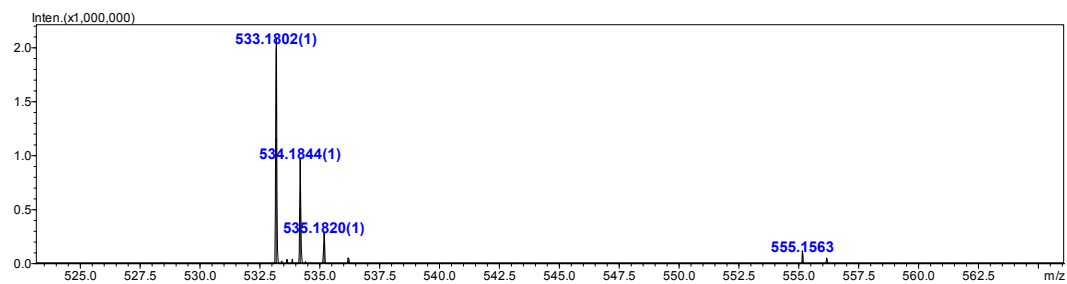


Figure S6. HRMS spectrum of compound **2**.

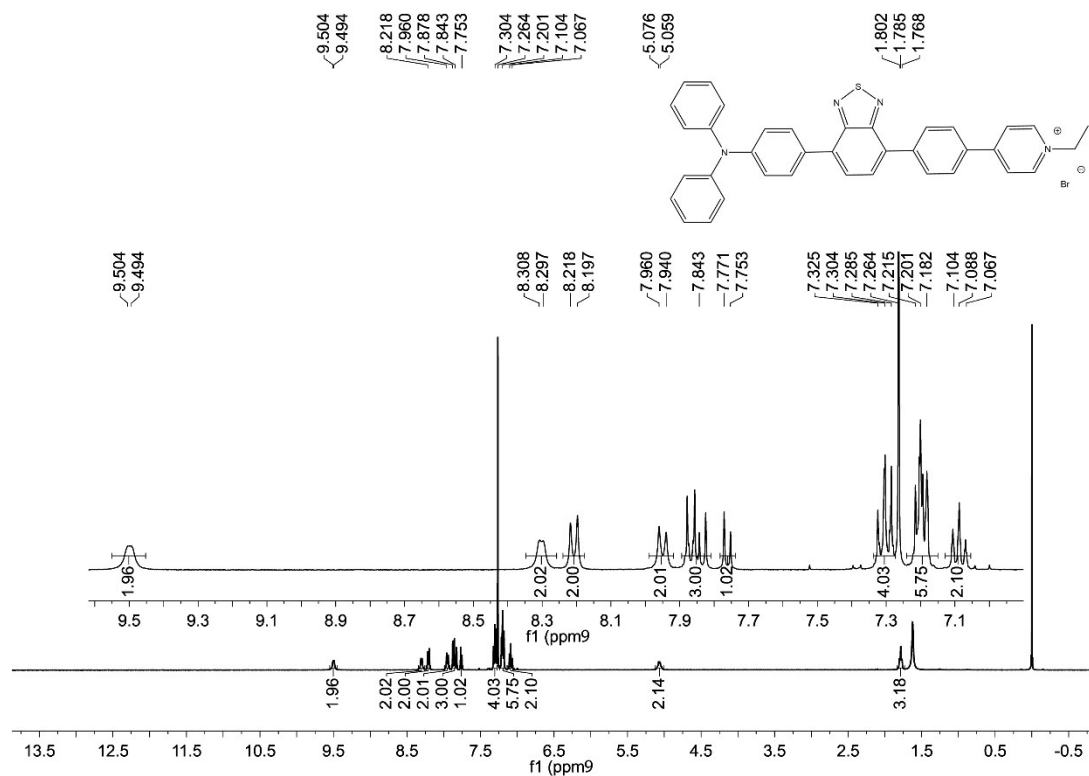


Figure S7. ¹H NMR spectrum of TBBP in CDCl₃

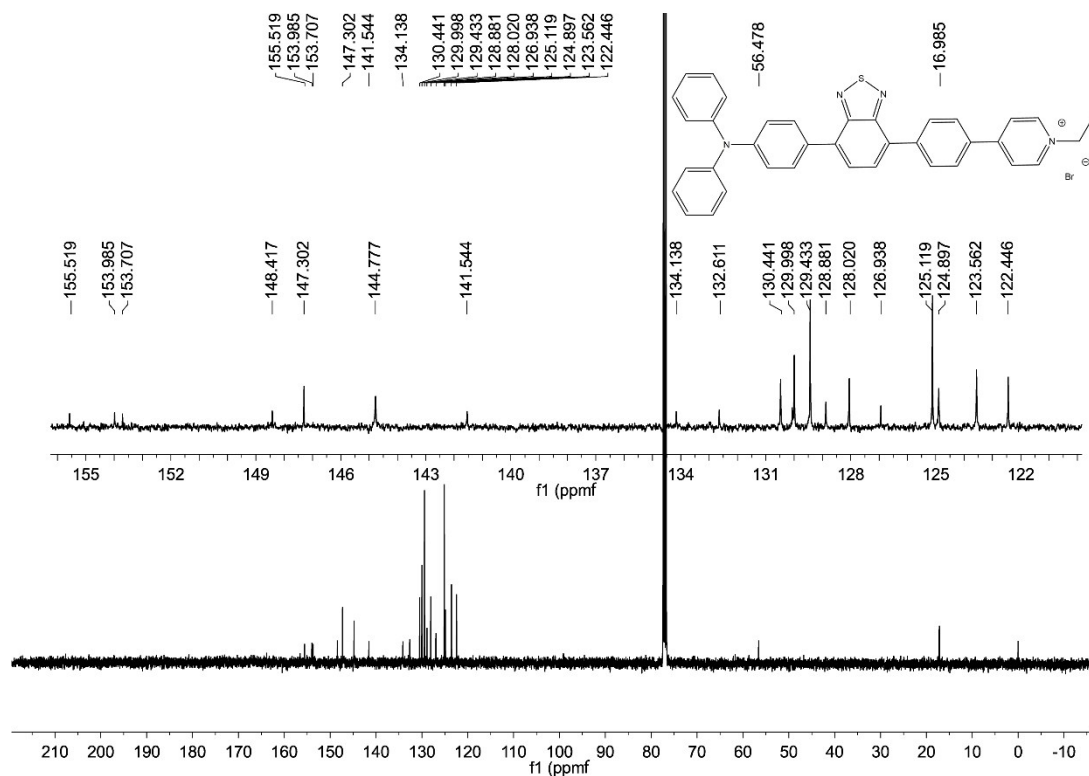


Figure S8. ¹³C NMR spectrum of compound TBBP in CDCl₃.

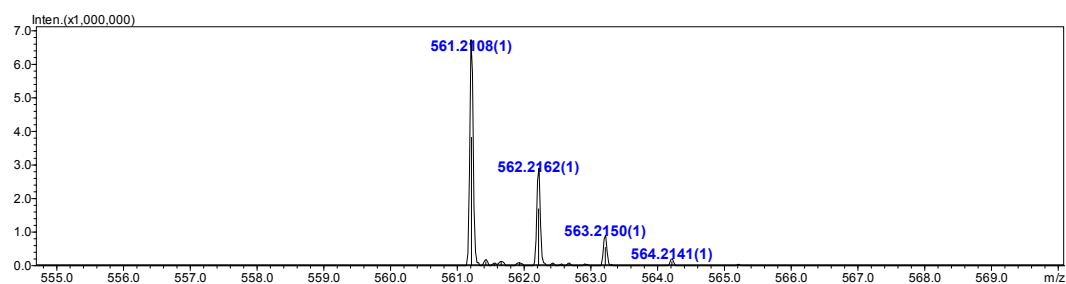


Figure S9. HRMS spectrum of compound **TBBP**.

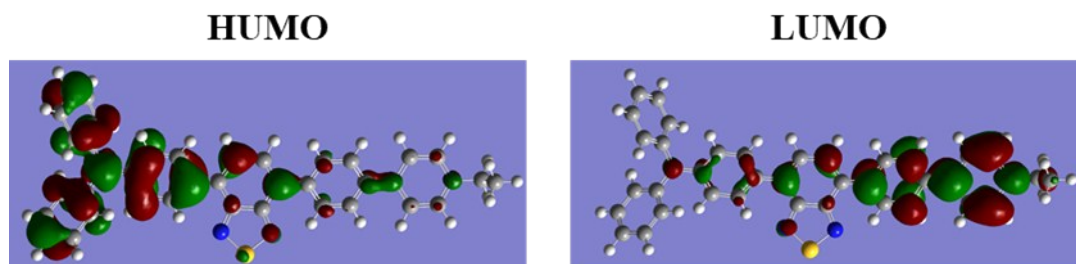


Figure S10. Molecular orbital amplitude plots of HOMO and LUMO of **TBBP**.

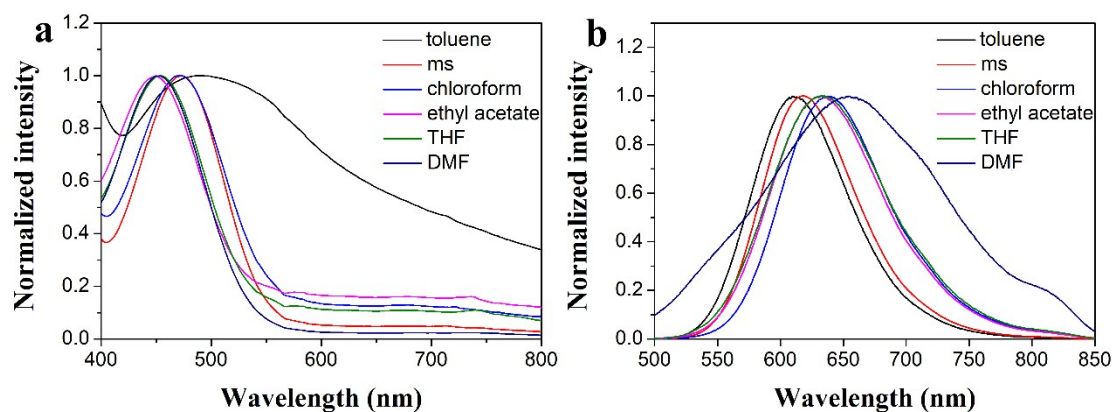


Figure S11. UV-Vis absorption (a) and emission spectra (b) of **TBBP**. ms: mixed solvents of

Toluene and CHCl_3 with volume ratio about 1:1.

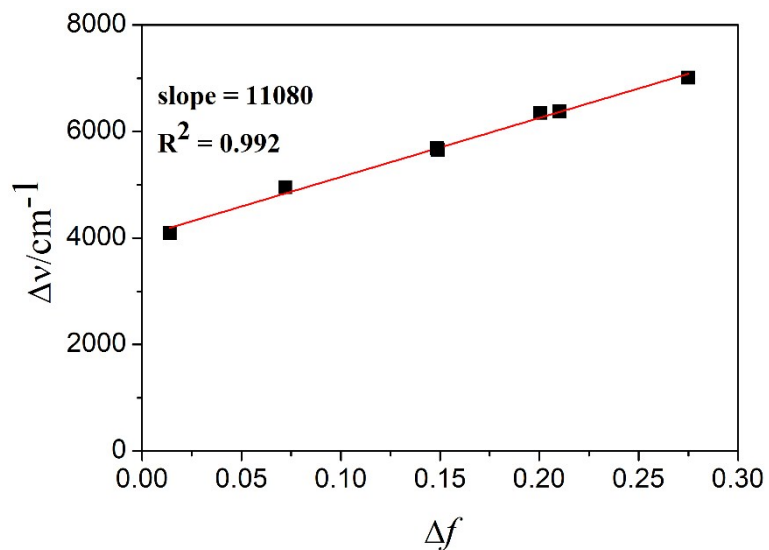


Figure S12. Plots of Stokes shift ($\Delta\nu$) versus the solvent polarity function (Δf) for **TBBP**.

Table S1. Solvent parameters.

solvent	ϵ	n	Δf
toluene	2.24	1.496	0.113098
ms	3.10	1.479	0.072100
chloroform	4.81	1.443	0.149202
ethyl acetate	6.02	1.370	0.200506
THF	7.58	1.405	0.210328
DMF	36.7	1.428	0.275158

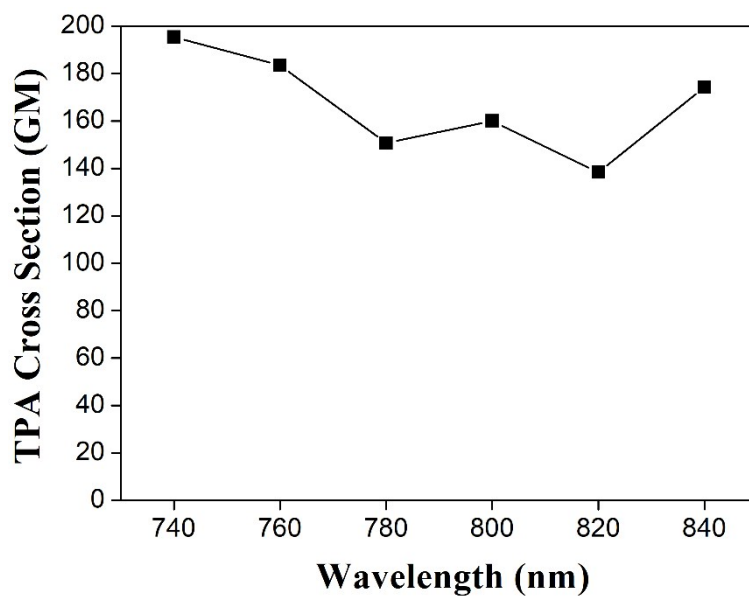


Figure S13. Two-photon absorption cross-section of **TBBP** in DMSO/water (1:9, v/v) for **TBBP**.

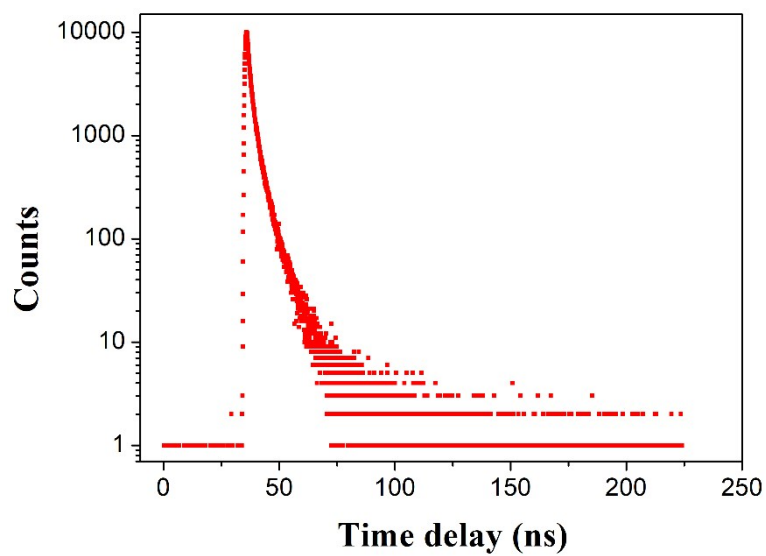


Figure S14. Fluorescence decay curves of **TBBP** in solid state.

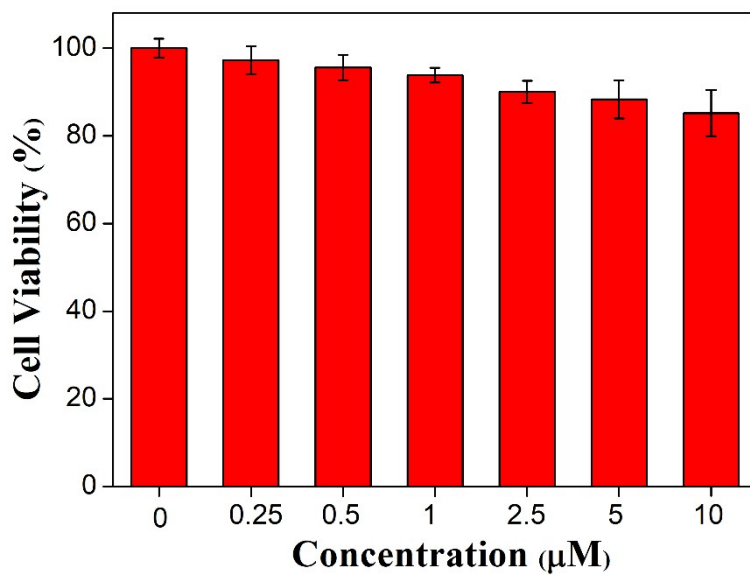


Figure S15. Cell viability assessed by MTT assay of HeLa cells incubated with different concentrations of **TBBP**.

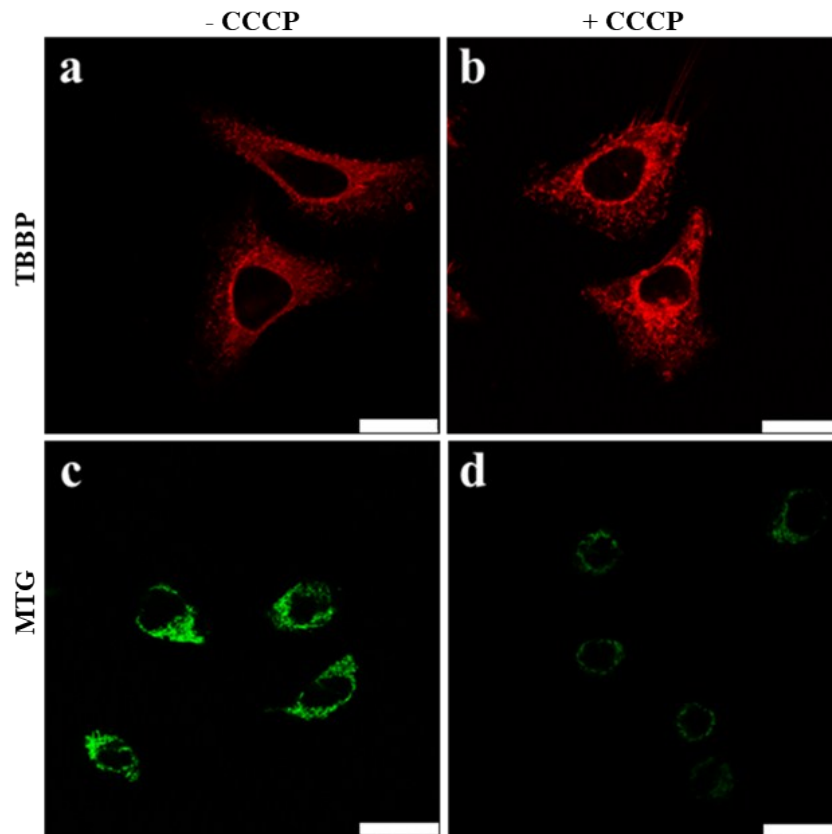


Figure S16. Confocal fluorescence images of CCCP (10 μ M) treated HeLa cells cultured with **TBBP** (4.0 μ M). Scale bar: 25 μ m

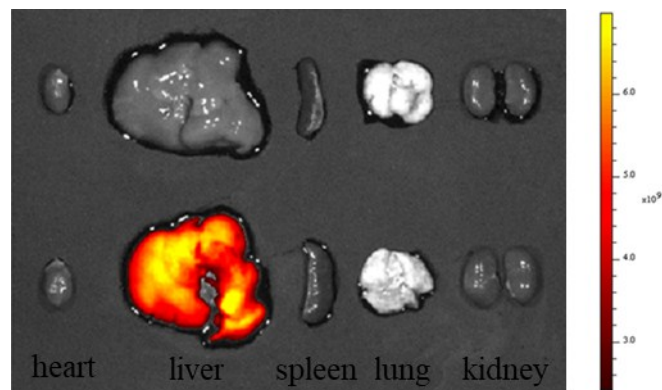


Figure S17. Ex vivo fluorescent images of mean organs from the mice administrated with AIEgen **TBBP**.

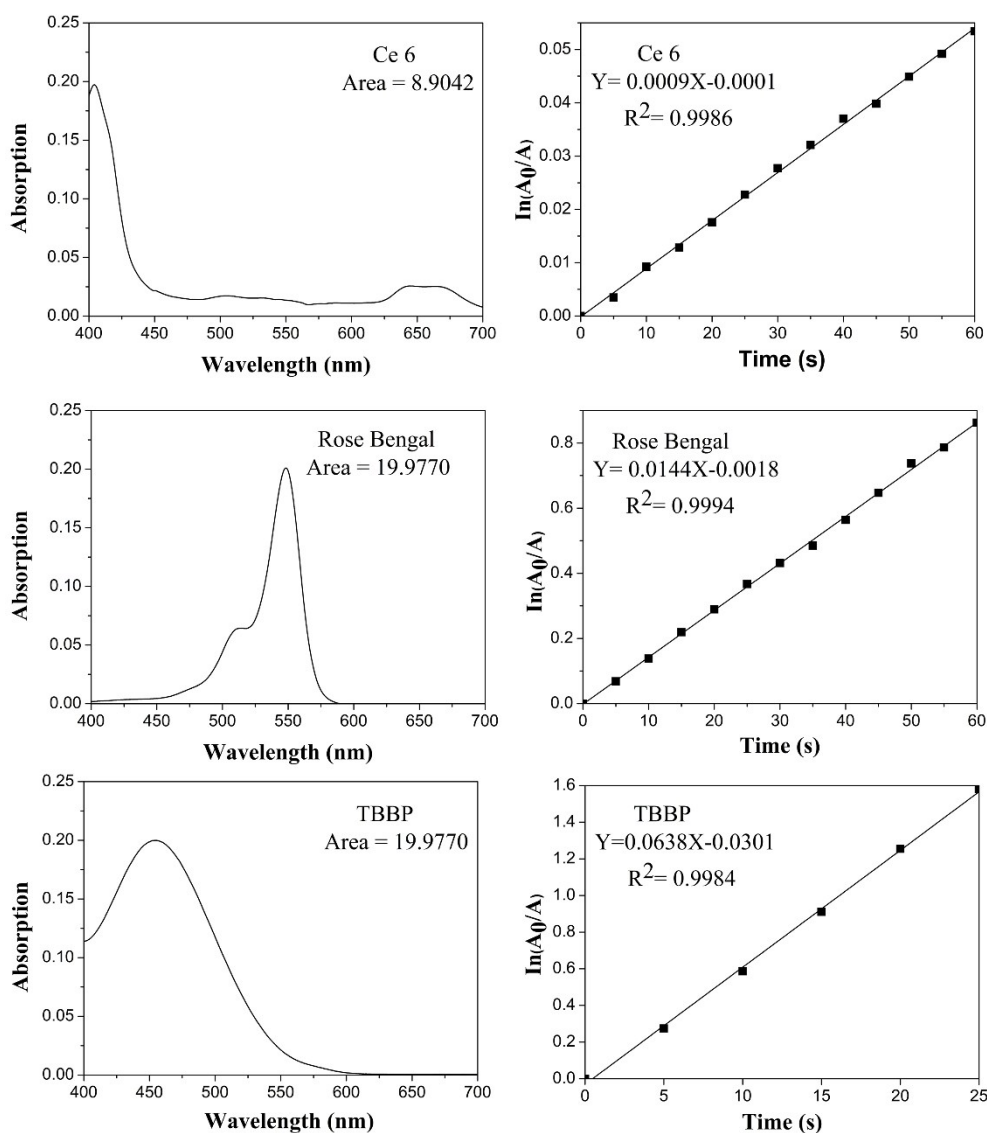


Figure S18. UV-vis spectra of ABDA in the presence of aggregates of **TBBP** under white light irradiation in water. Concentration: 10×10^{-6} M (**TBBP**) and 5×10^{-5} M (**ABDA**). The absorption peak area of **Ce6**, **Rose Bengal** and **TBBP**. The decomposition rate constants of ABDA by **Ce6**, **Rose Bengal** and **TBBP**.

Table S2. The 1O_2 quantum yields of **TBBP**, **RB** and **Ce6**

Compound	<i>A</i>	<i>K</i>	Φ
TBBP	19.977	0.0638	1.36
RB	8.1943	0.0144	0.75
Ce6	8.9042	0.0009	0.043

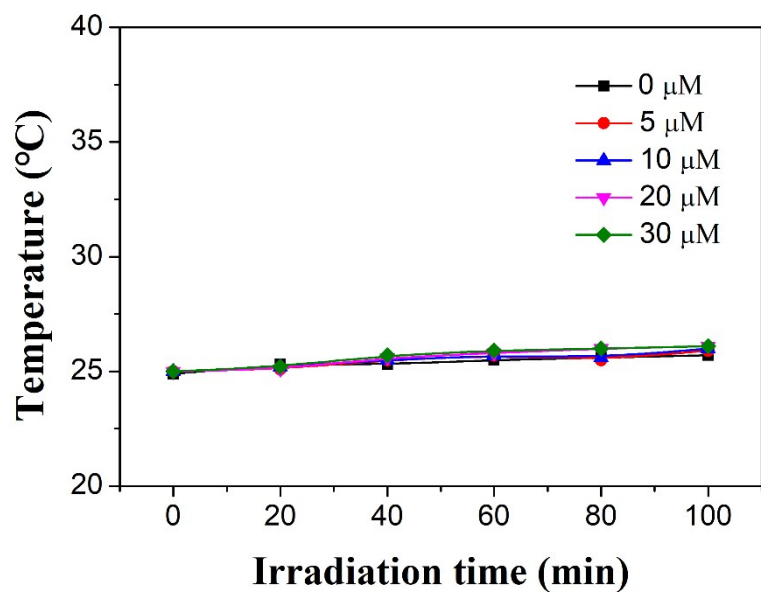


Figure S19. Photothermal conversion behaviors of the **TBBP** at different concentrations (5–30 μM) under white-light irradiation for different time.

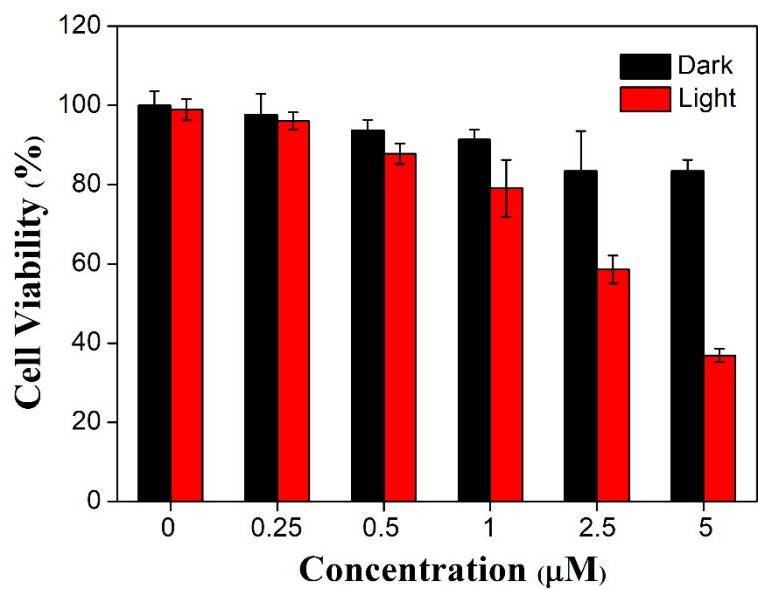


Figure S20. Cell viability of HeLa cells incubated with increasing concentrations of **Ce6** under dark or white light irradiation.

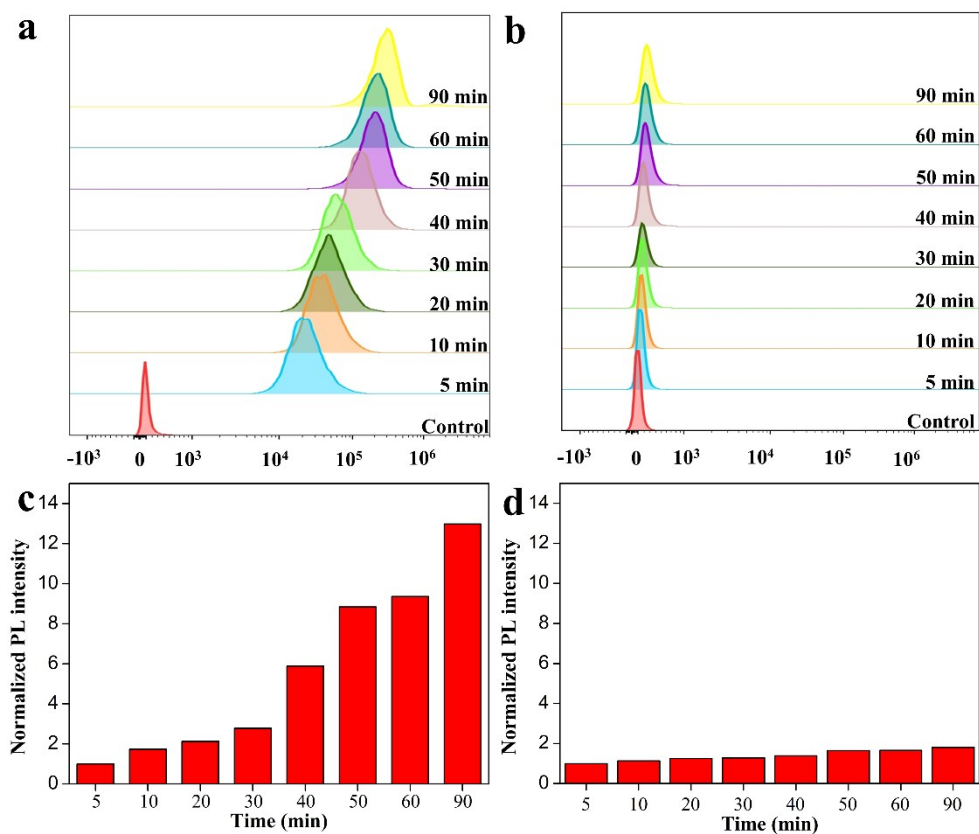


Figure S21. Flow cytometric analysis of HeLa cells treated with **TBBP** (a) and **Ce6** (b). The corresponding fluorescence intensity of HeLa cells treated with **TBBP** (c) and **Ce6** (d) after different treatments.

Movie of real-time dynamic change of **TBBP** (MOV).