

Supporting Information for

Triphenylphosphonium-Functionalized Dimeric BODIPY-Based Nanoparticles for Mitochondria- Targeting Photodynamic Therapy

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S1. NMR and HR-MS spectra of BODIPY dimers

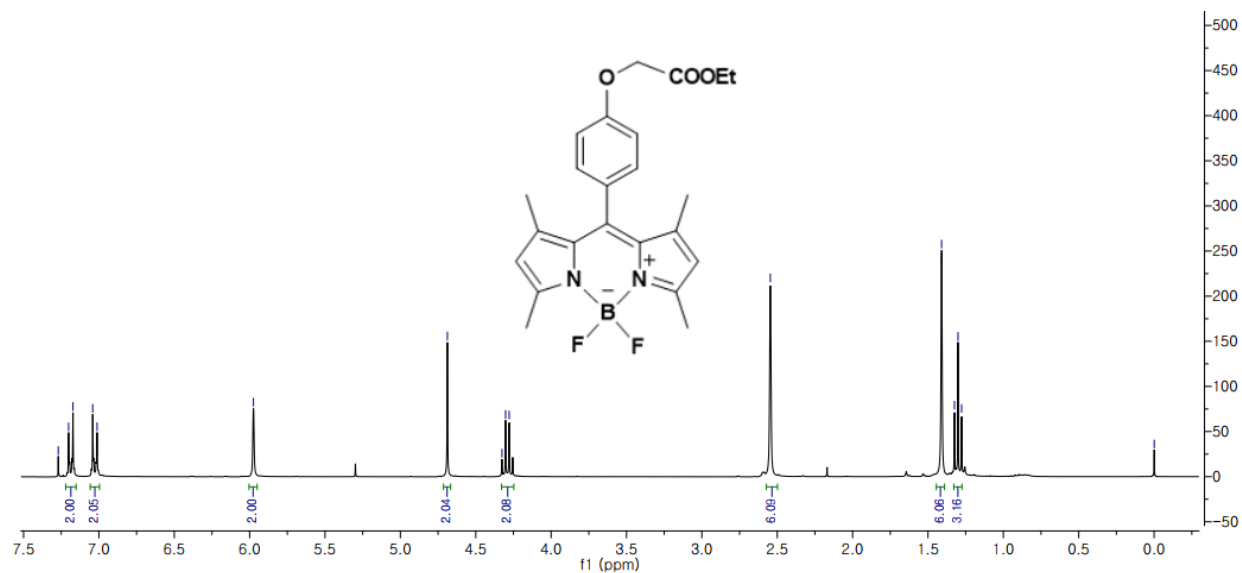


Figure S1. ¹H NMR spectrum of BODIPY 1 in CDCl₃ at 300 MHz.

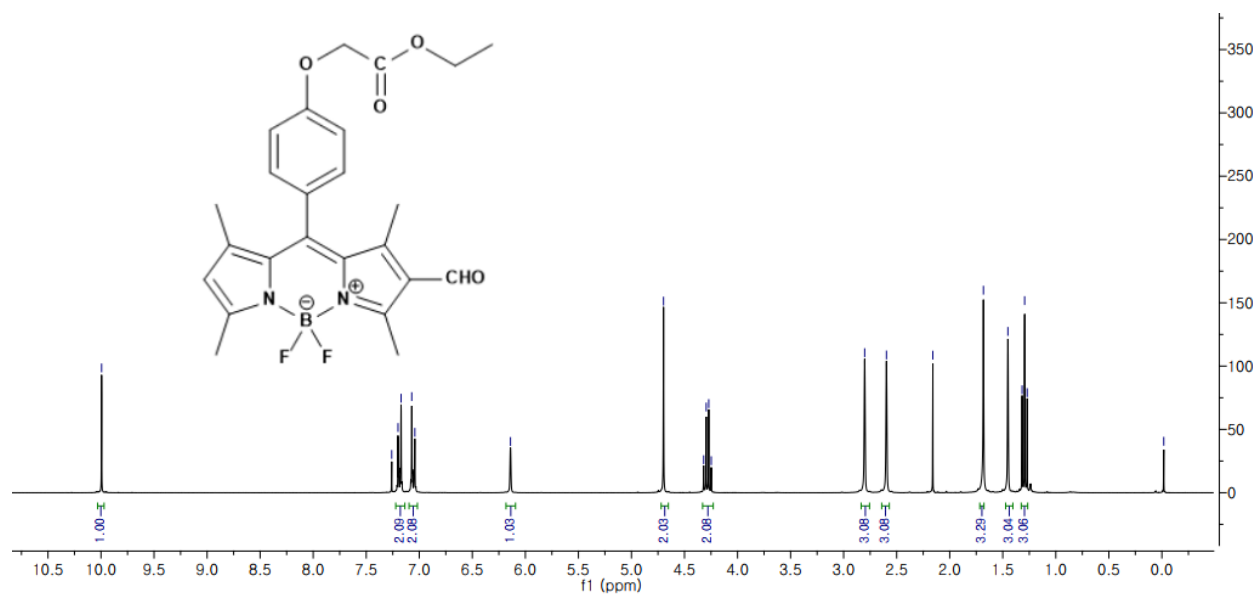


Figure S2. ¹H NMR spectrum of BODIPY 2 in CDCl₃ at 300 MHz.

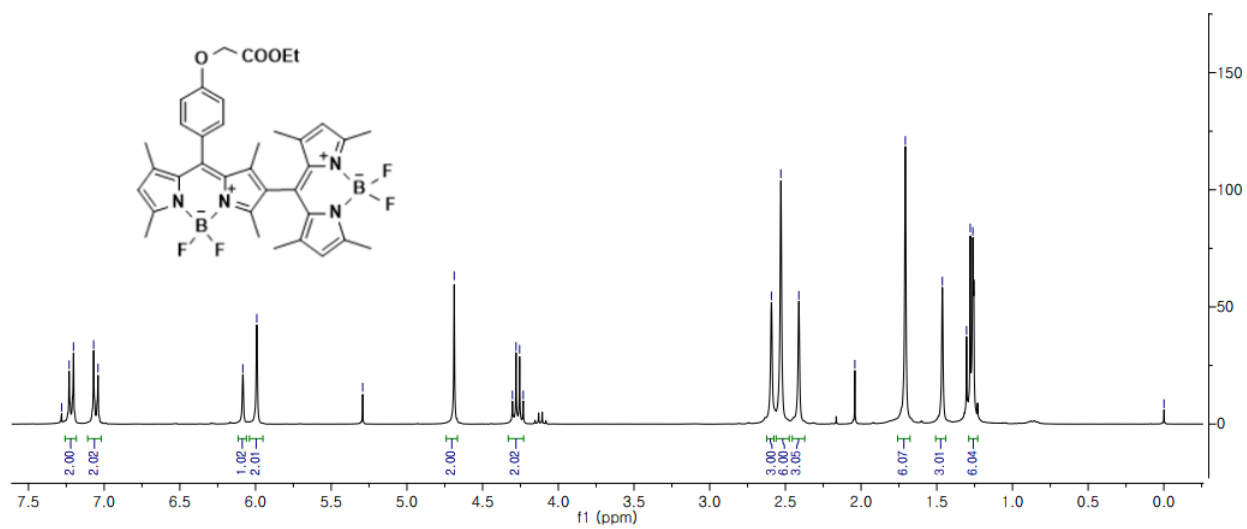


Figure S3. ^1H NMR spectrum of BODIPY **3a** in CDCl_3 at 300 MHz.

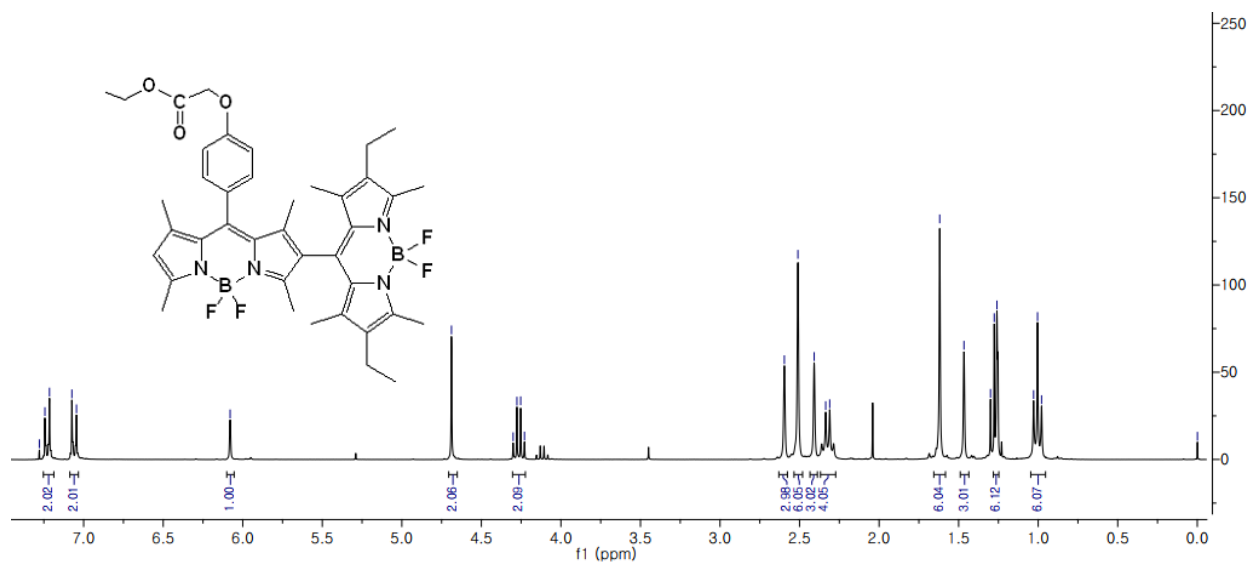


Figure S4. ^1H NMR spectrum of BODIPY **3b** in CDCl_3 at 300 MHz.

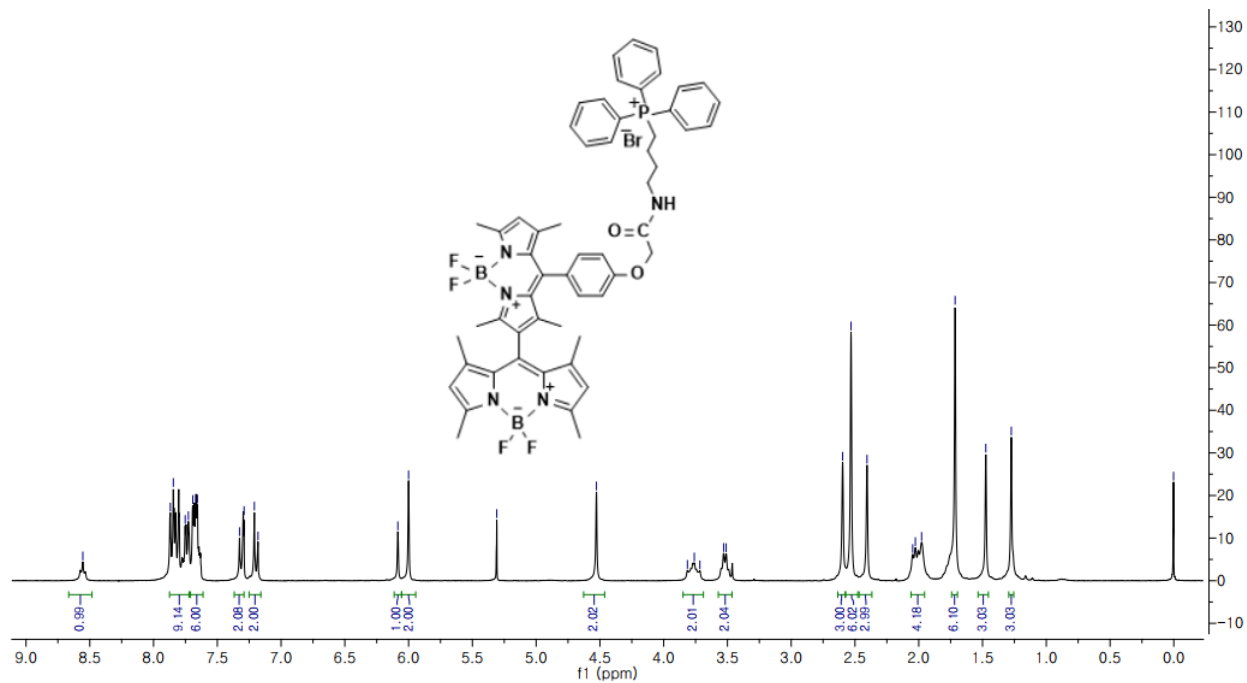


Figure S5. ¹H NMR spectrum of BODIPY BTTP in CDCl₃ at 300 MHz.

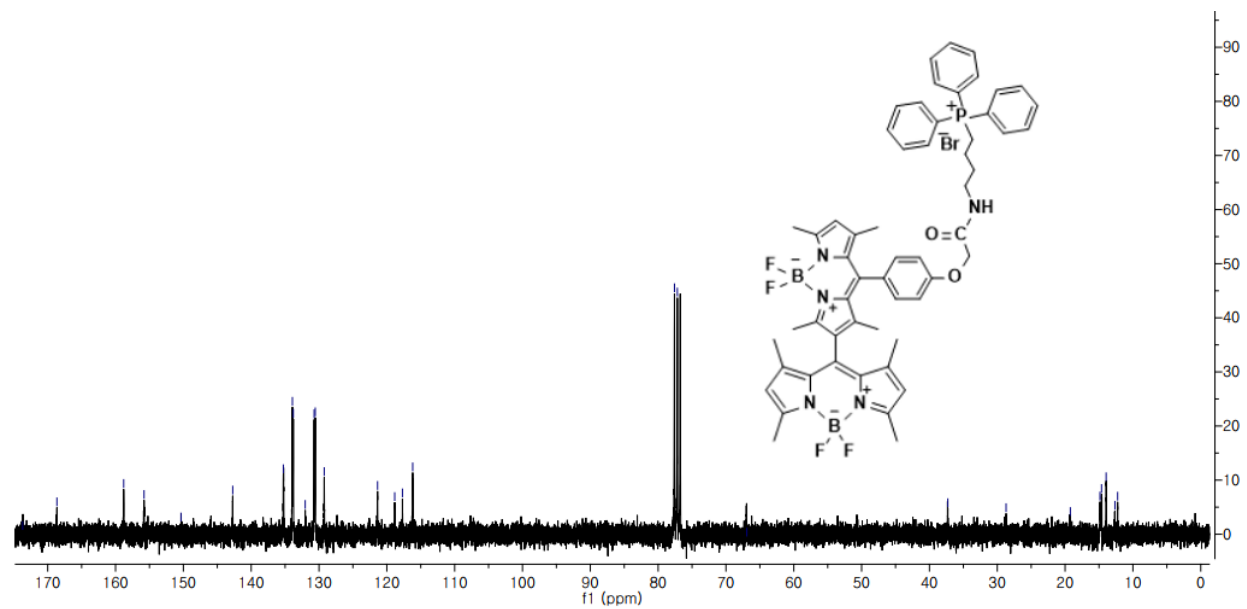


Figure S6. ¹³C NMR spectrum of BODIPY BTTP in CDCl₃ at 75.4 MHz.

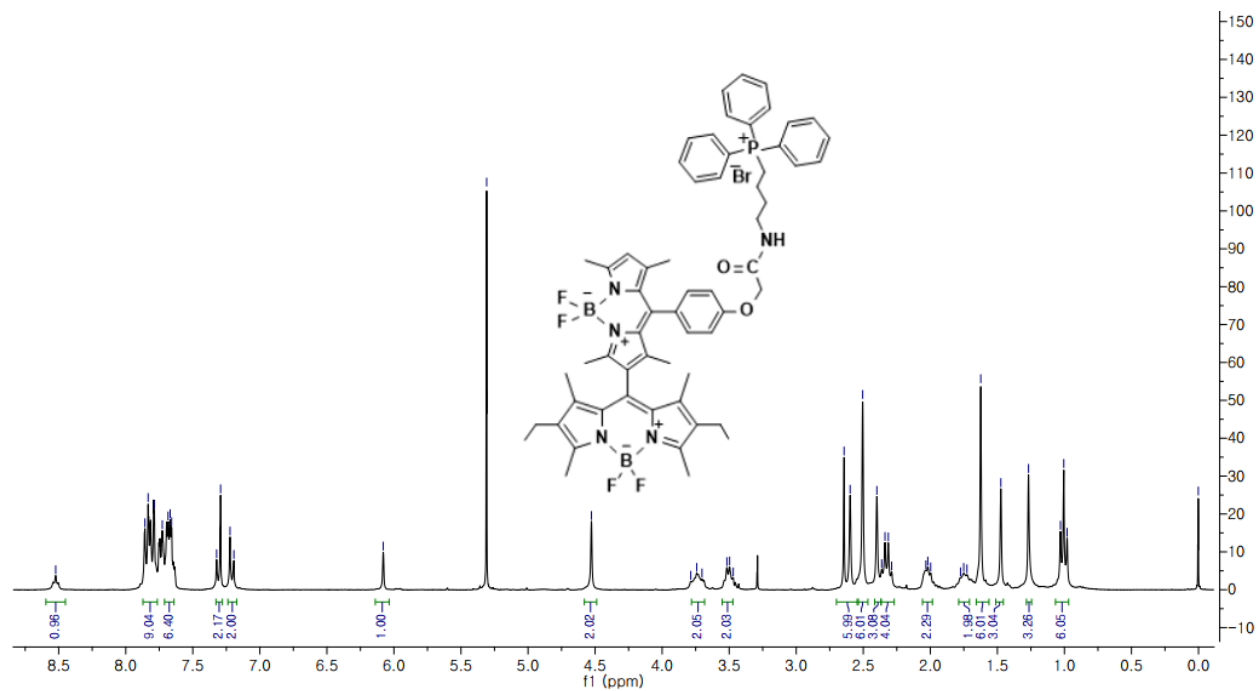


Figure S7. ^1H NMR spectrum of BODIPY BeTPP in CDCl_3 at 300 MHz.

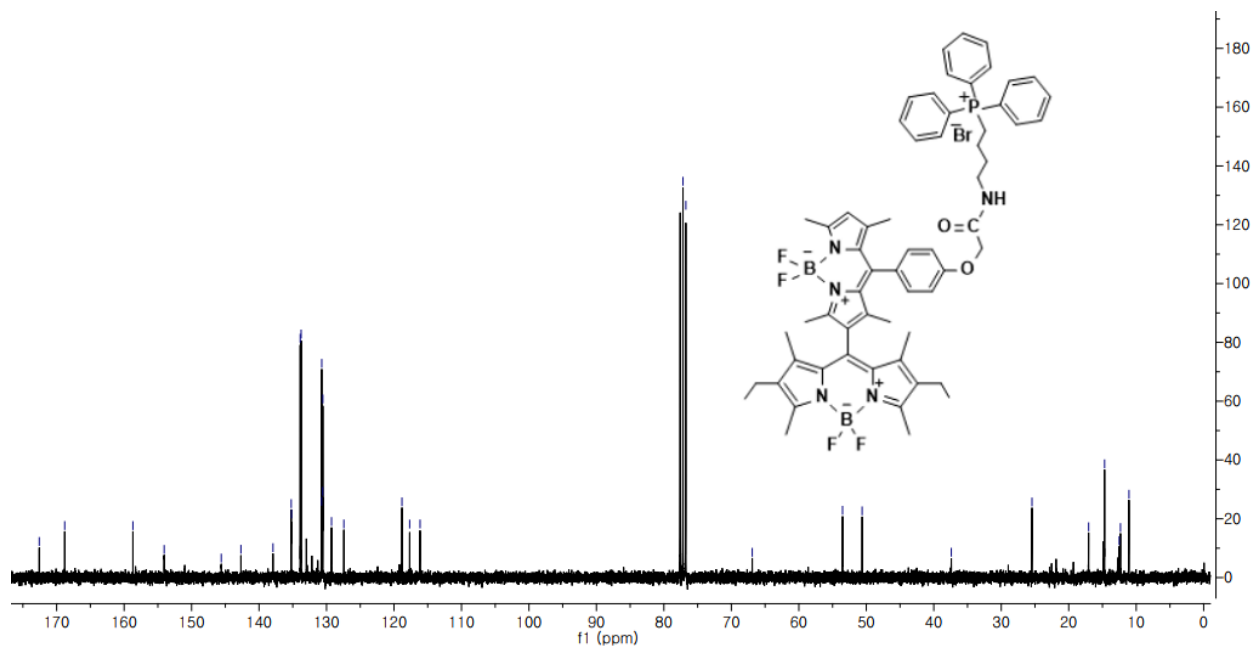


Figure S8. ^{13}C NMR spectrum of BODIPY BeTPP in CDCl_3 at 75.4 MHz.

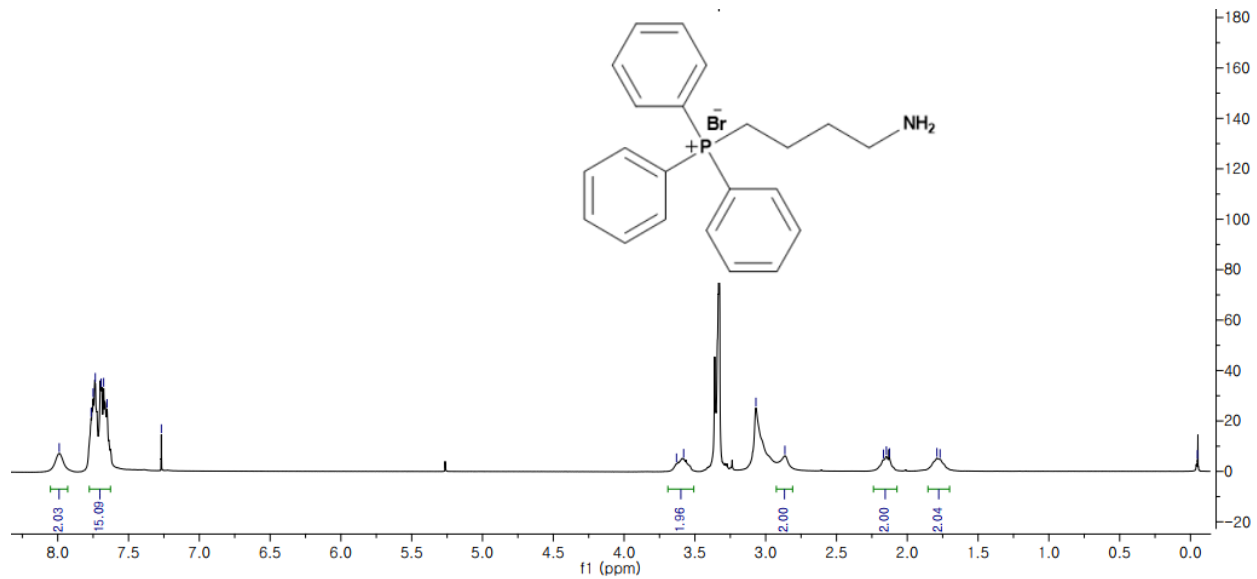


Figure S9. ^1H NMR spectrum of TPP-NH₂ in CDCl₃ at 300 MHz.

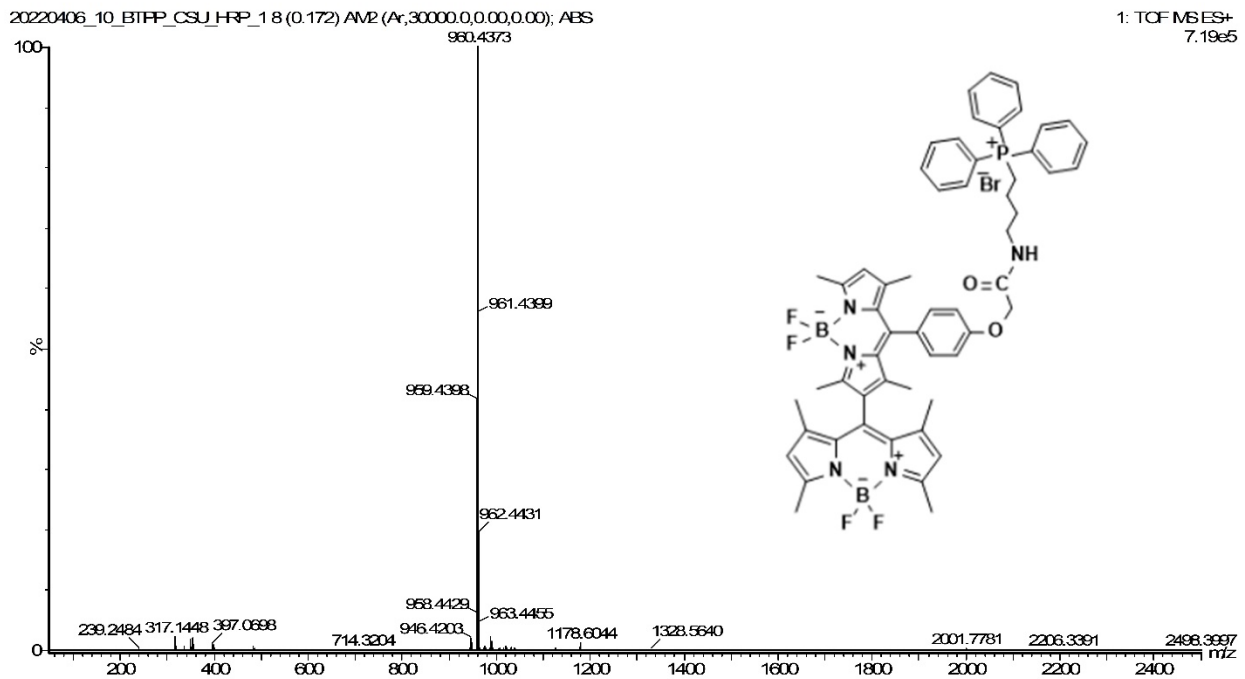


Figure S10. HR-MS spectrum of BODIPY BTTP.

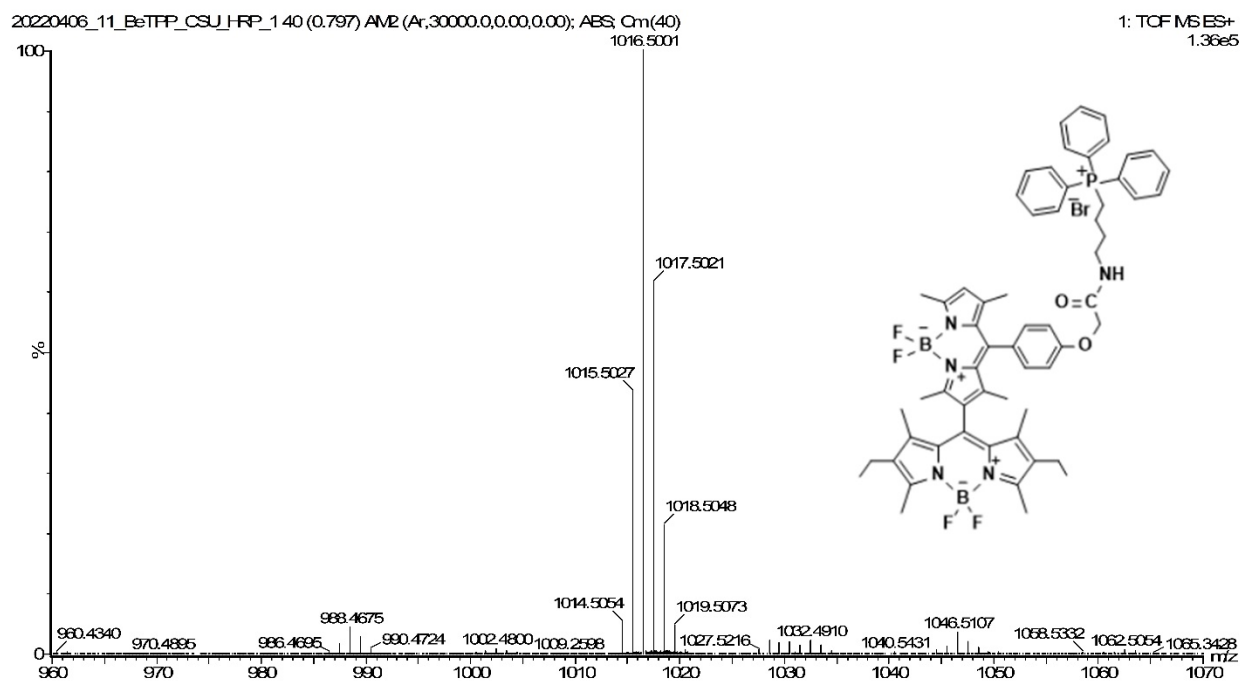


Figure S11. HR-MS spectrum of BODIPY BeTTP.

S2. Emission spectra of BODIPY dimers in different solvents

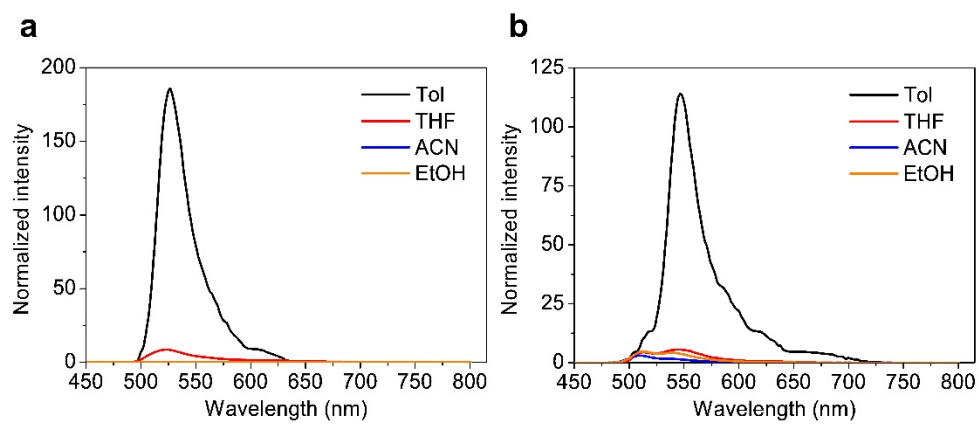


Figure S12. Fluorescence emission spectra of the BODIPY dimers, **BTPP** (a) and **BeTTP** (b) in various solvents. The fluorescence quenching appeared clearly up to the solvent polarity increase.

S3. Emission spectra of BODIPY dimer-based NPs

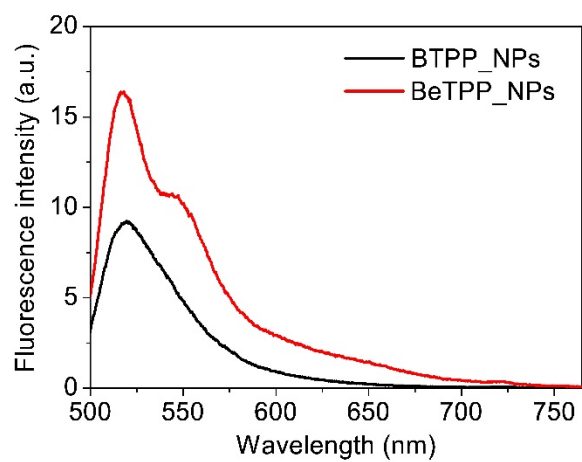


Figure S13. Fluorescence emission spectra of **BTTP** NPs and **BeTTP** NPs in aqueous media (3×10^{-6} M, $\lambda_{\text{ex}} = 480$ nm).

S4. Determination of the $^1\text{O}_2$ quantum yield of BODIPY dimers

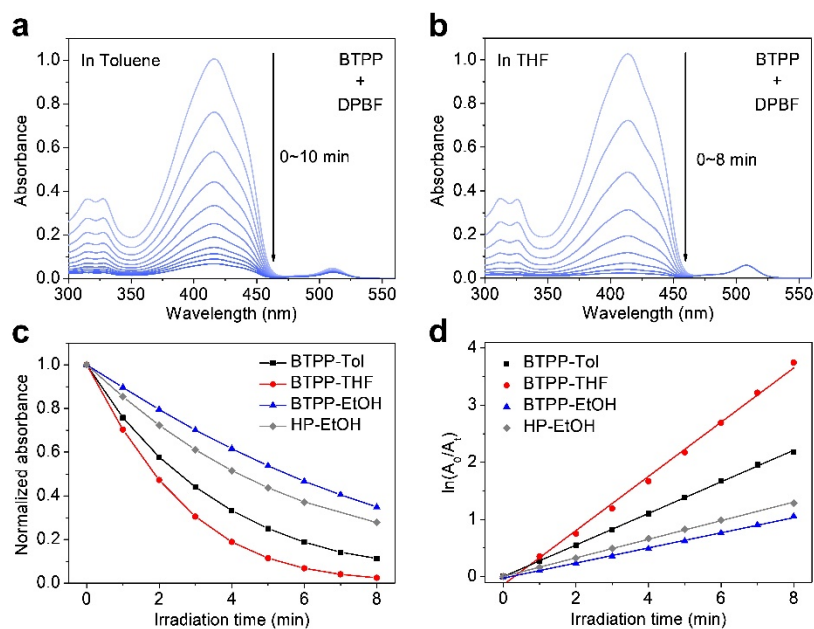


Figure S14. Absorption spectra of DPBF upon irradiation in the presence of **BTTP** in (a) toluene and (b) tetrahydrofuran (THF) under 520 nm for different times. (c) Plots of the change in absorbance of DPBF at 411 nm at different irradiation times using hematoporphyrin (HP) as the standard in EtOH at room temperature ($\Phi_{\Delta} = 0.53$). (d) $^1\text{O}_2$ assay using the absorbance attenuation of DPBF in the presence of **BTTP** in different solvents against HP as the standard in EtOH.

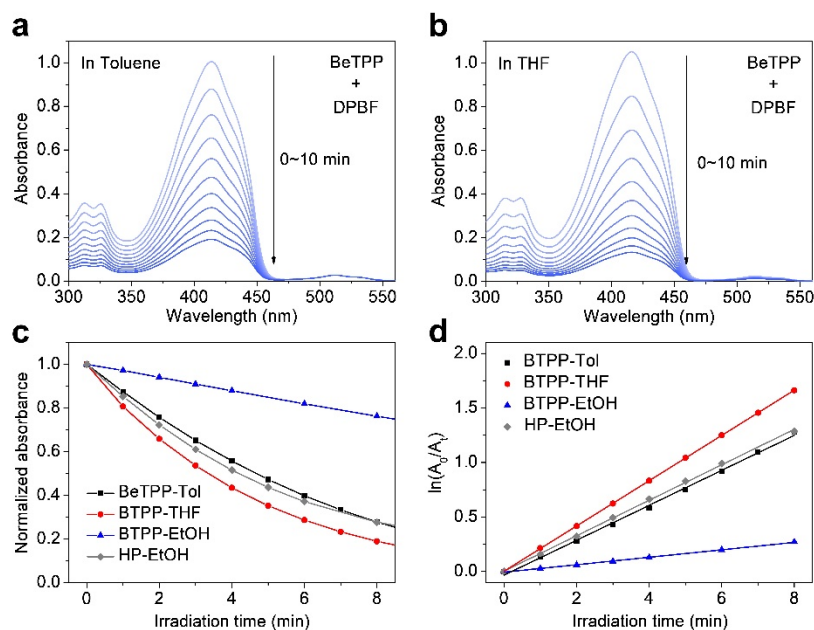


Figure S15. Absorption spectra of DPBF upon irradiation in the presence of **BeTTP** in (a) toluene and (b) tetrahydrofuran (THF) under 520 nm for different times. (c) Plots of the change in absorbance of DPBF at 411 nm at different irradiation times using hematoporphyrin (HP) as the standard in EtOH at room temperature ($\Phi_{\Delta} = 0.53$). (d) 1O_2 assay using the absorbance attenuation of DPBF in the presence of **BeTTP** in different solvents against HP as the standard in EtOH.

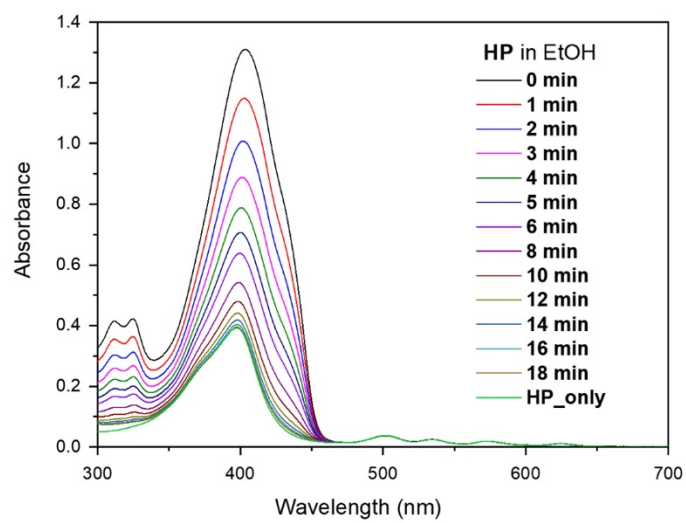


Figure S16. Absorption spectra of DPBF upon irradiation in the presence of HP in EtOH under 520 nm for different times.

S5. Theoretical characterization of the complete molecular structure

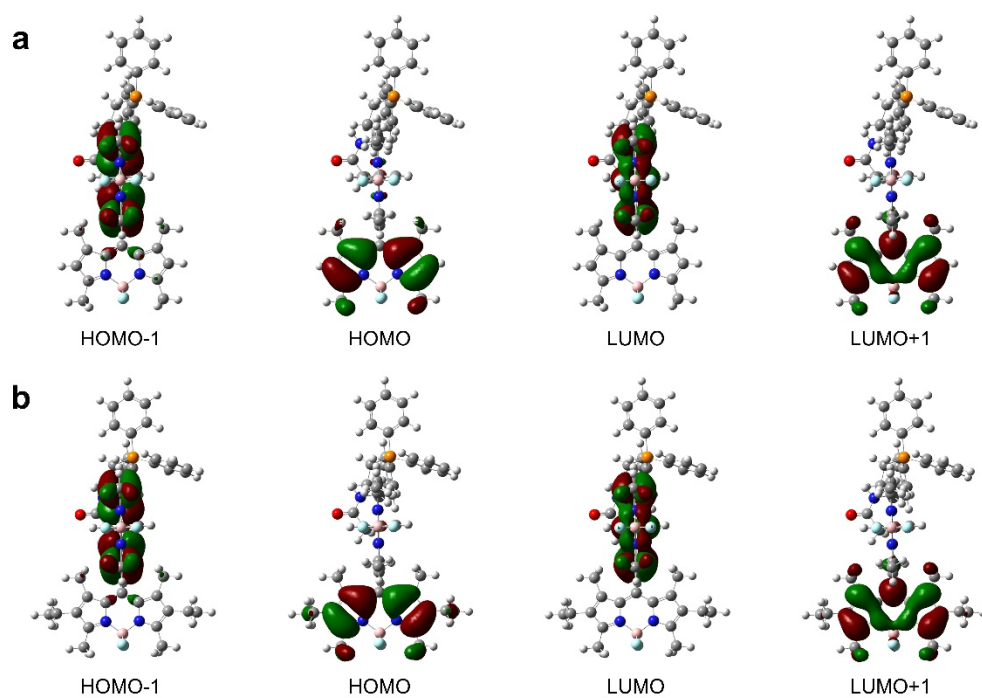


Figure S17. The frontier molecular orbitals of the **BTTP** (a) and **BeTPP** (b) for the complete structures.

Table S1. Transition energy (E), wavelength (λ), and oscillator strength (f) for the two lowest singlet excited states of BODIPY **BTTP** and **BeTTP**, and the contribution of frontier orbitals to each transition.

The calculations were carried out under methanol solvent.

	State	E (eV)	Wavelength (nm)	<i>f</i>	Major contributions to transition
	S ₁ (CT)	2.43	509.4	0.0059	HOMO → LUMO (99%)
BTTP	S ₂ (CT)	2.52	492.0	0.0001	HOMO-1 → LUMO+1 (97%)
	S ₃ (LE)	2.88	430.1	0.7578	HOMO-1 → LUMO (96%)
	S ₁ (CT)	2.30	539.2	0.0062	HOMO → LUMO (100%)
BeTTP	S ₂ (CT)	2.57	481.6	0.0023	HOMO-1 → LUMO+1 (97%)
	S ₃ (LE)	2.77	447.2	0.5372	HOMO → LUMO +1 (92%)