Supplementary Information

Self-assembled BODIPY derivative with A-D-A structure as organic nanoparticles for photodynamic/photothermal cancer therapy

Guojing Li [1], Mengqian Yang [1], Qilong Sha [1], Li Li [1], Xiaogang Luo [1,3], Fengshou Wu [1,2]*

[1] Faculty of Resources and Environmental Engineering, Guizhou Institute of Technology, \linebreak Guiyang 550003, China

[2] State Key Laboratory of Environmental Geochemistry, Institute of Geochemistry, Chinese Academy of Sciences, Guiyang 550081, China.

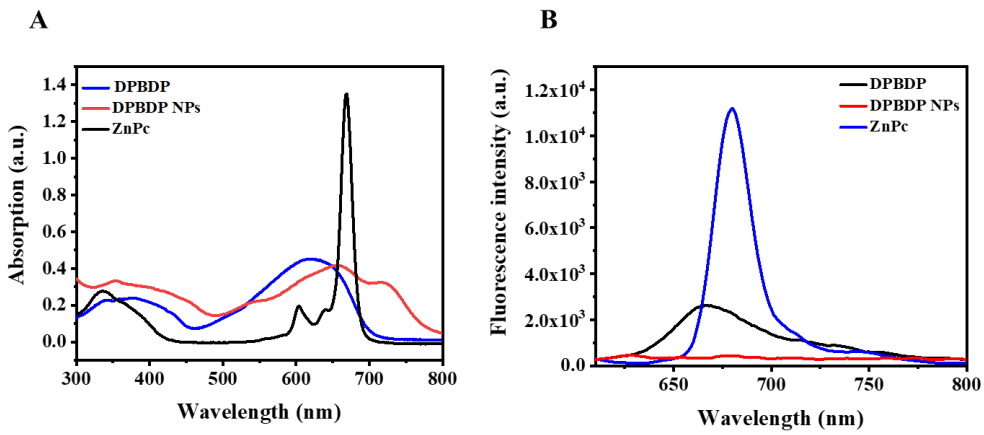

Figure S1. (A) Absorption spectrum of DPBDP in THF, DPBDP NPs in deionized water and ZnPc in toluene at the same concentration; (B) The fluorescence spectra of the same concentration of DPBDP, DPBDP NPs, and ZnPc.

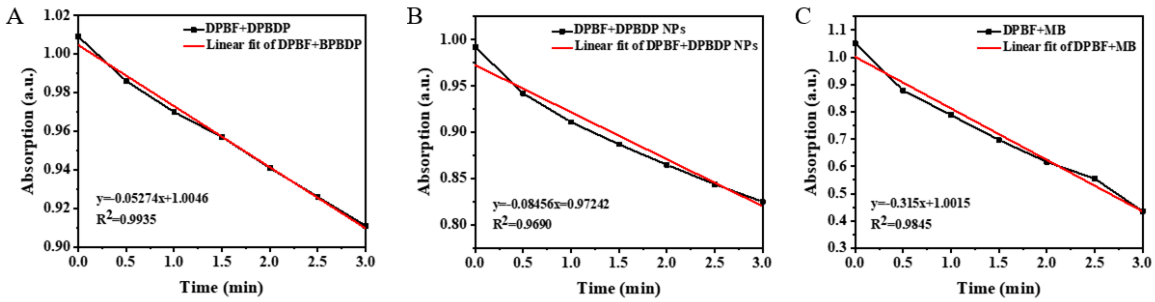

Figure S2. The fitting curve of absorbance with time (A) DPBF+DPBDP; (B) DPBF+DPBDP NPs; (C) DPBF+MB

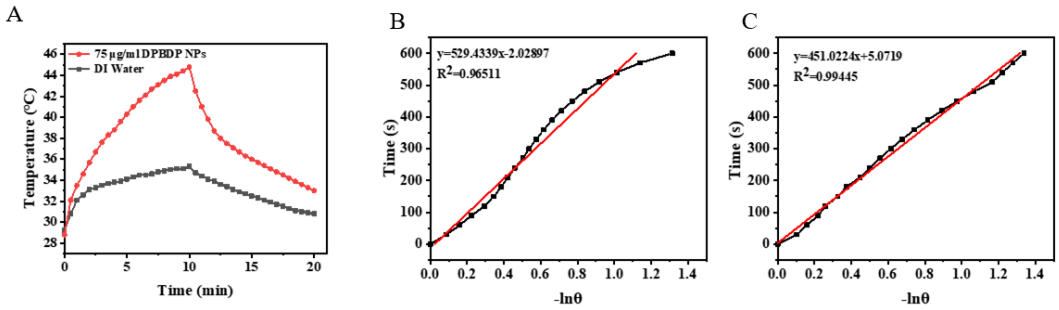

Figure S3. (A) Photothermal curves of DPBDP NPs (75 μg/mL) and deionized water under laser irradiation (690 nm, 1.5 W/cm^2, 10 min) followed by naturally cooling; -lnθ curve fitting of cooling time to temperature driving force in cooling phase of DPBDP NPs (75μg/mL) (B) and DI water (C).

The calculation of fluorescence quantum yield

The fluorescence quantum yields of DPBDP and DPBDP NPs were calculated using the following equation with zinc phthalocyanine (ZnPc) as a reference.

$$\varphi_f = \varphi_f^R \frac{I_f}{I_f^R} \frac{A^R}{A} (\frac{n}{n^R})^2$$

φ_f^R is the fluorescence quantum yield of ZnPc (0.30, in toluene); The letters *S* and *R* represent the samples and ZnPc respectively; *A* is the absorbance; *I* is the integrated fluorescence intensity, and the samples and ZnPc were excited at the same wavelength for measuring *I*; *n* is the solvent's refractive index.

Singlet oxygen detection

The experiments were performed with 50 μM DPBF in MeOH/H2O (1:1), followed by the addition of photosensitizer (0.5 μM). The cuvette was irradiated under 635 nm laser at 0.05 W/cm^2. The change of absorbance at 414 nm was recorded every 30 seconds. The $^1O_2$ yields of DPBDP and DPBDP NPs were calculated by the following equation.

$$\Phi_{\Delta}^{S} = \Phi_{\Delta}^{R} \frac{k^{S} F^{R}}{k^{R} F^{S}}$$

Φ_{Δ}^{R} is the singlet oxygen quantum yield of MB (Φ_{Δ}^{R} = 0.52). The letters *S* and *R* represent the samples and MB respectively; *k* is the slope of the curve of DPBF absorbance (414 nm) versus irradiation time. *F* is the absorption correction factor (F=1–10^{-OD}). *OD* is the corresponding absorbance of samples at 690 nm.

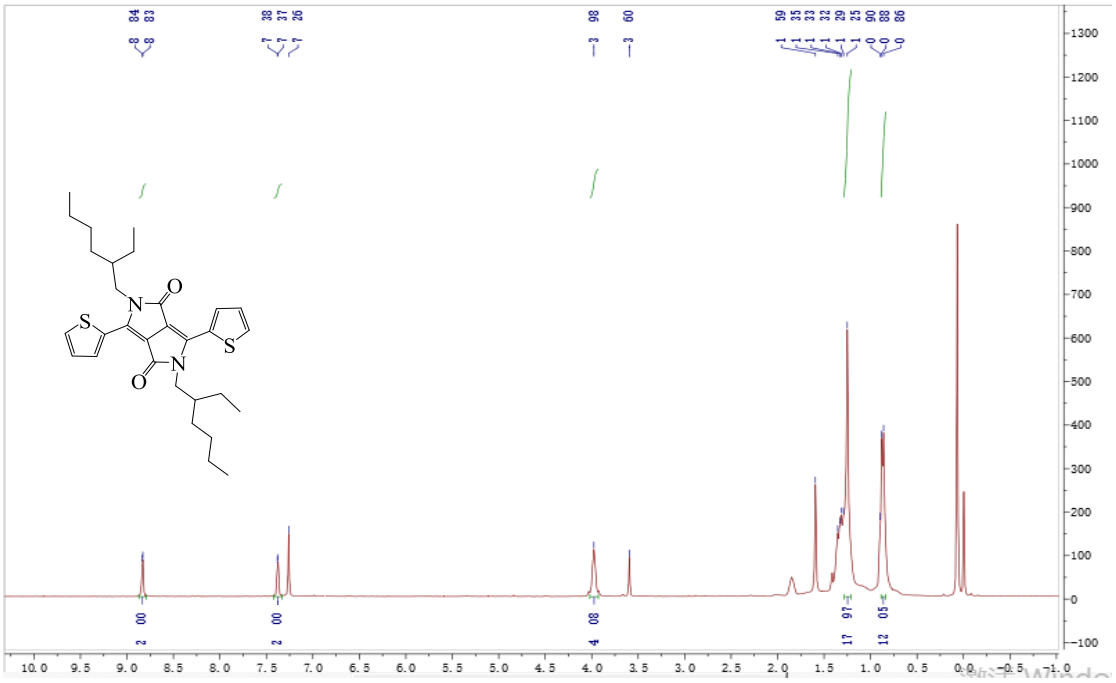

Figure S4. ^{1}H NMR spectrum of compound 1a

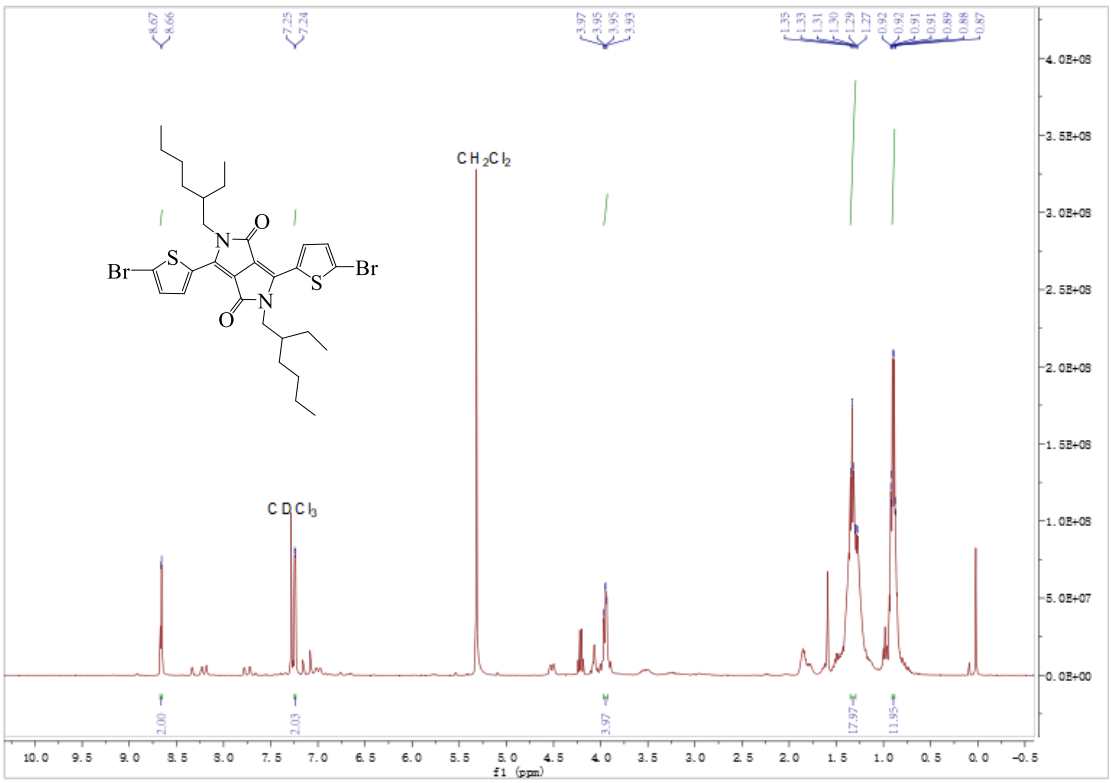

Figure S5. ^{1}H NMR spectrum of compound 2a

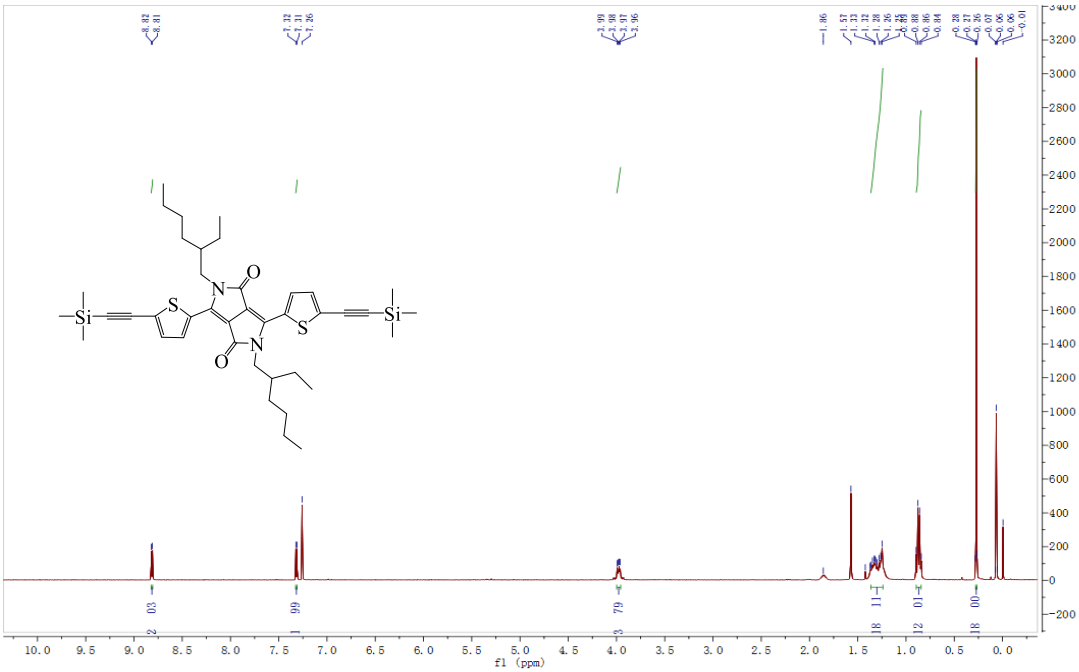

Figure S6. ^{1}H NMR spectrum of compound 3a

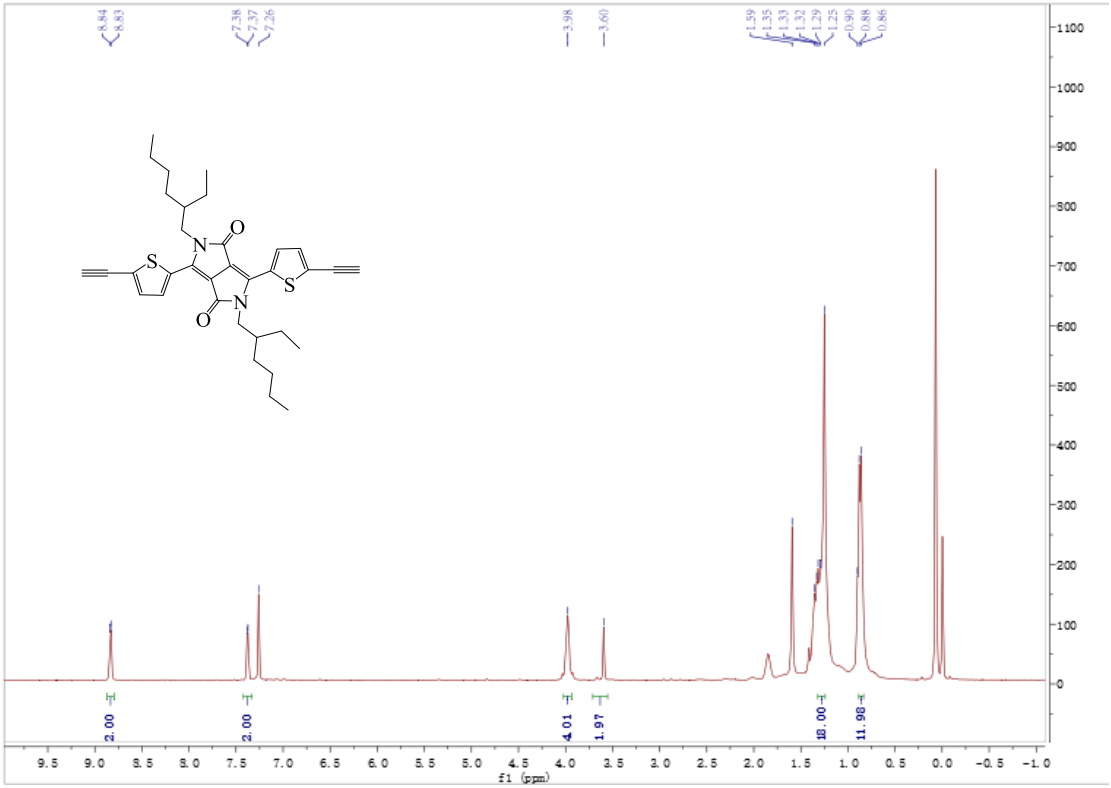

Figure S7. ^{1}H NMR spectrum of compound 4a

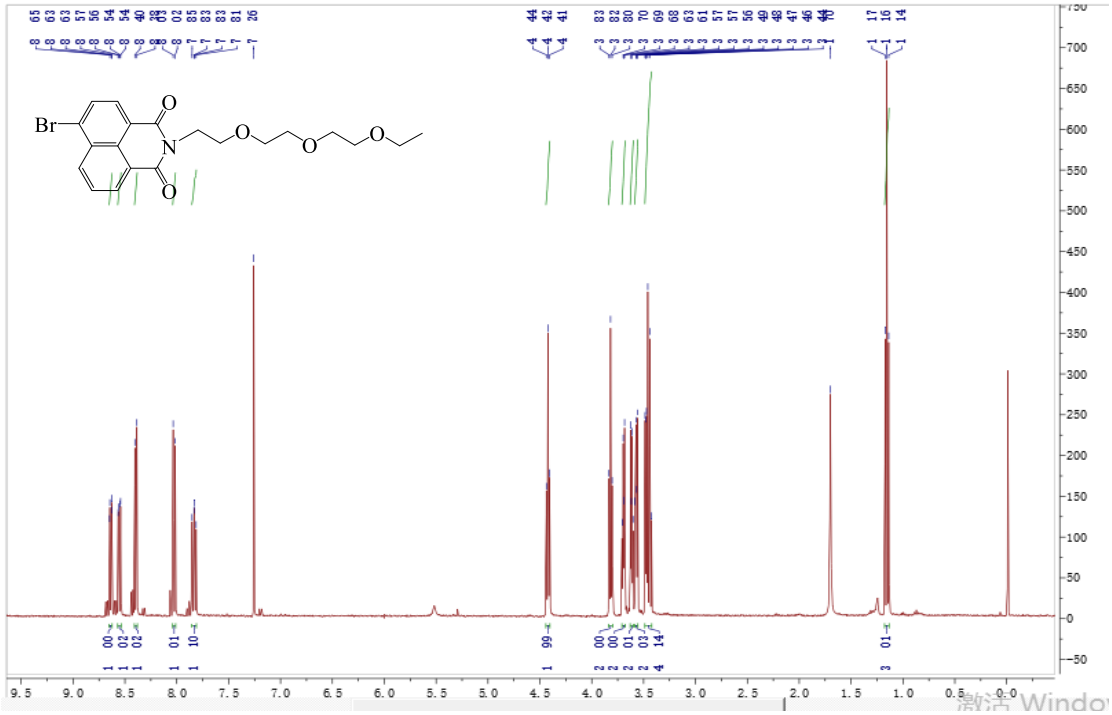

Figure S8. ^{1}H NMR spectrum of compound 4b

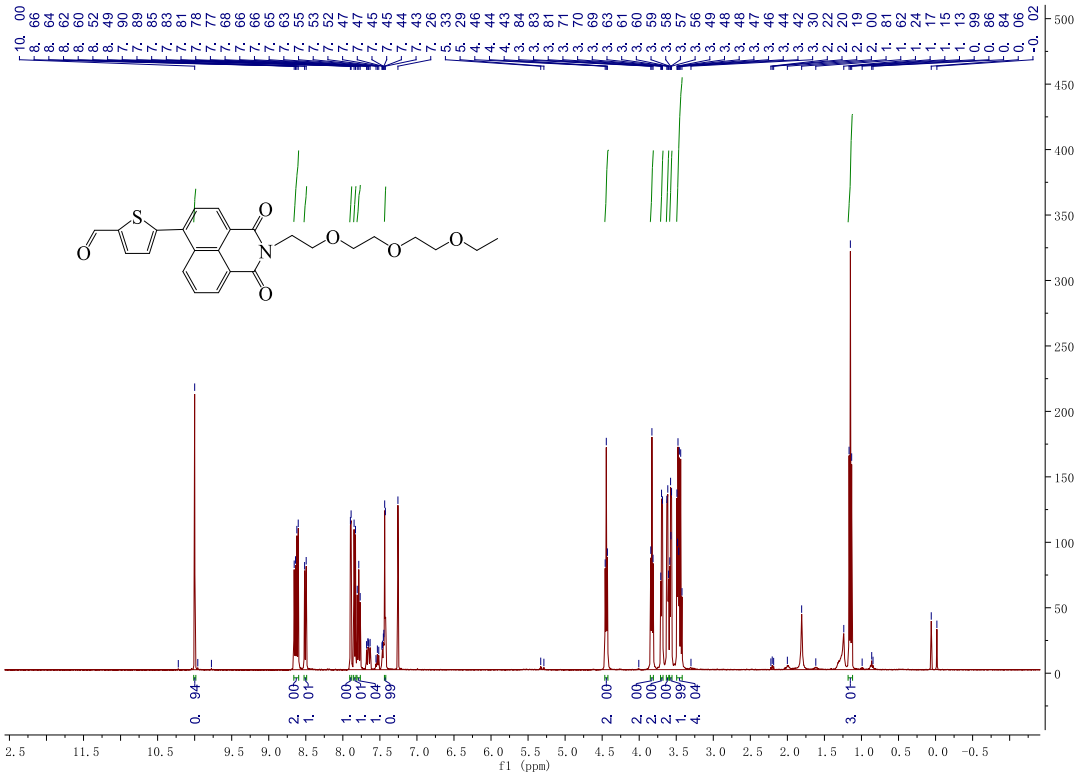

Figure S9. ^{1}H NMR spectrum of compound 5b

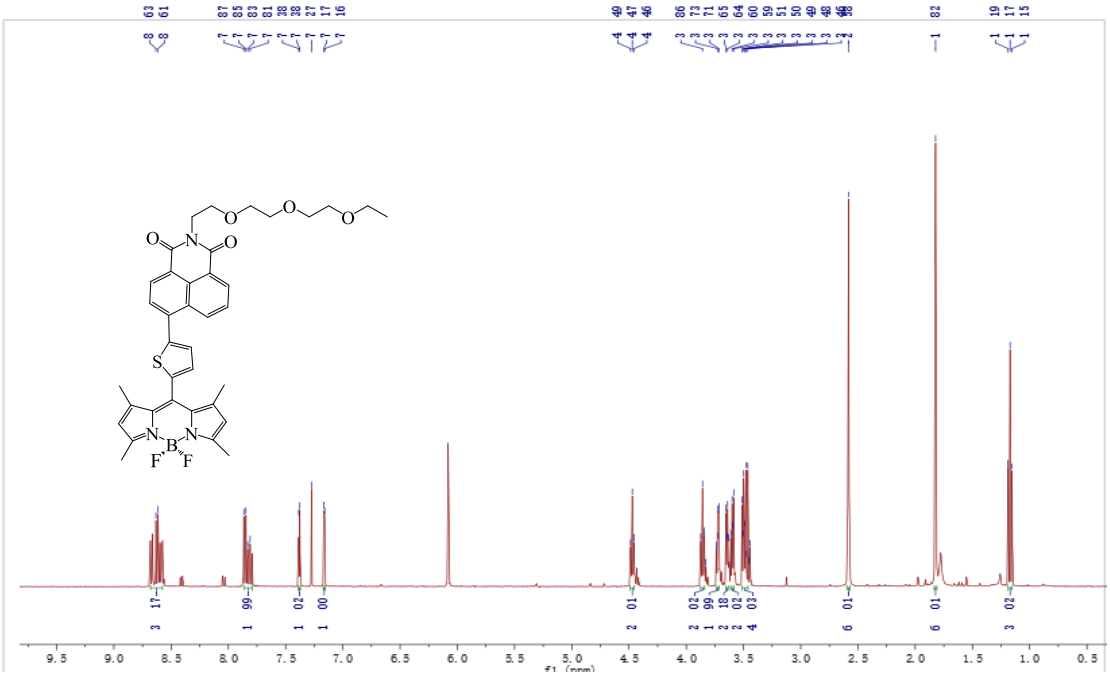

Figure S10. ^{1}H NMR spectrum of compound 6b

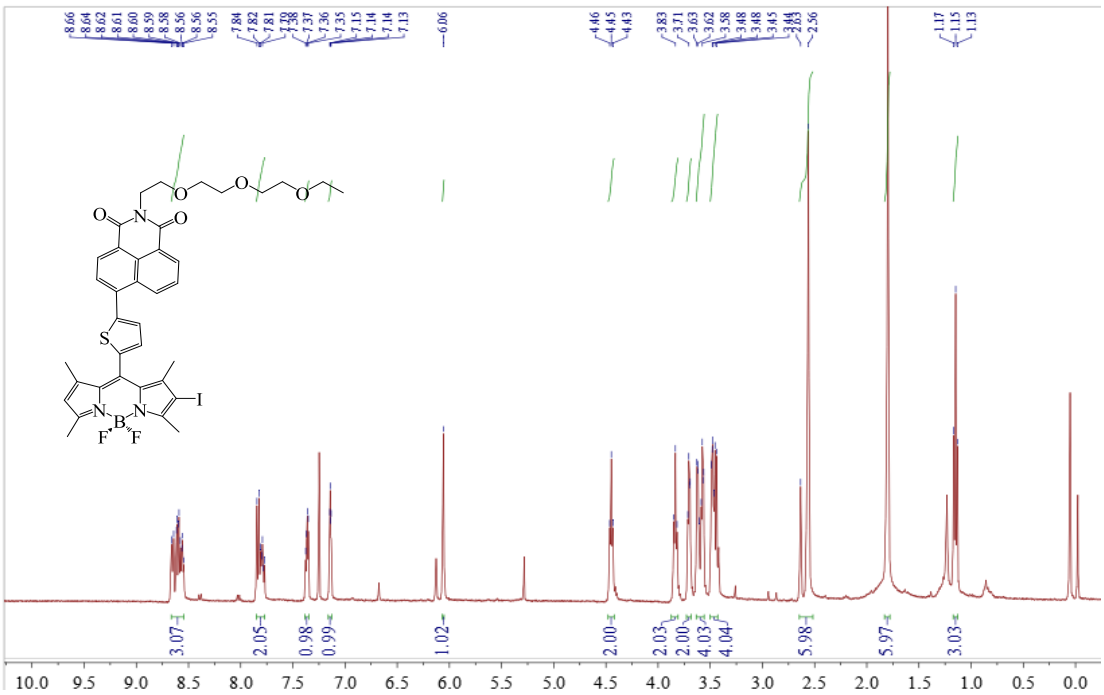

Figure S11. ^{1}H NMR spectrum of compound 7b

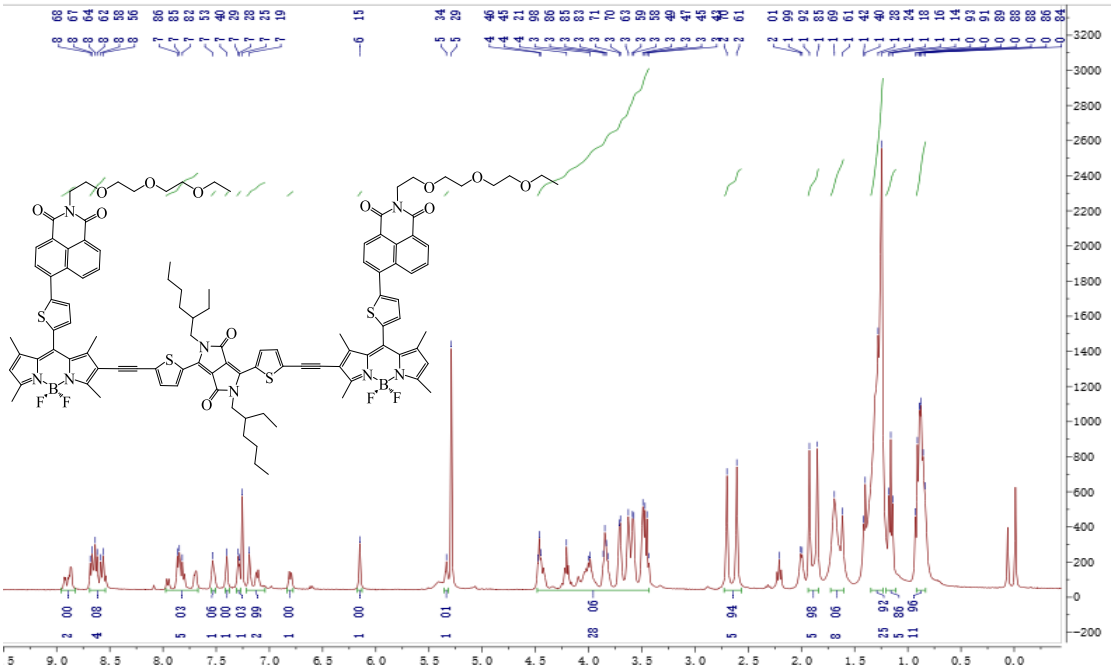

Figure S12. ^{1}H NMR spectrum of compound DPBDP

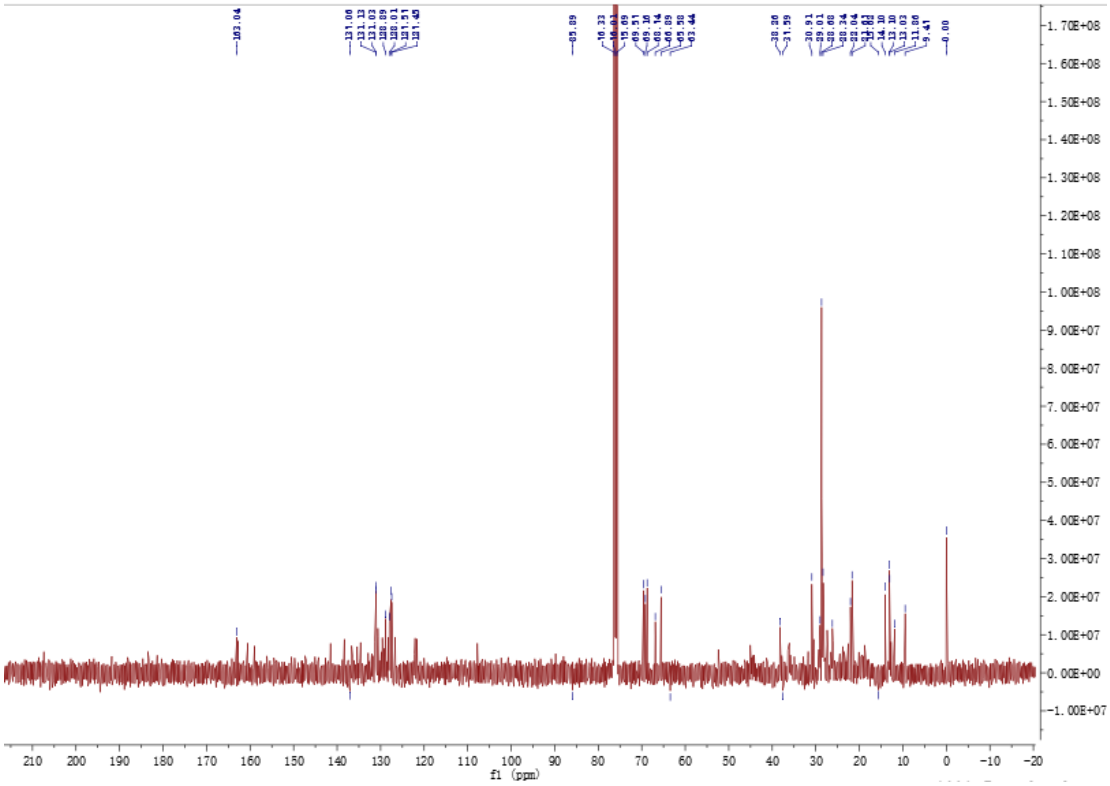

Figure S13. ^{13}C NMR spectrum of compound DPBDP

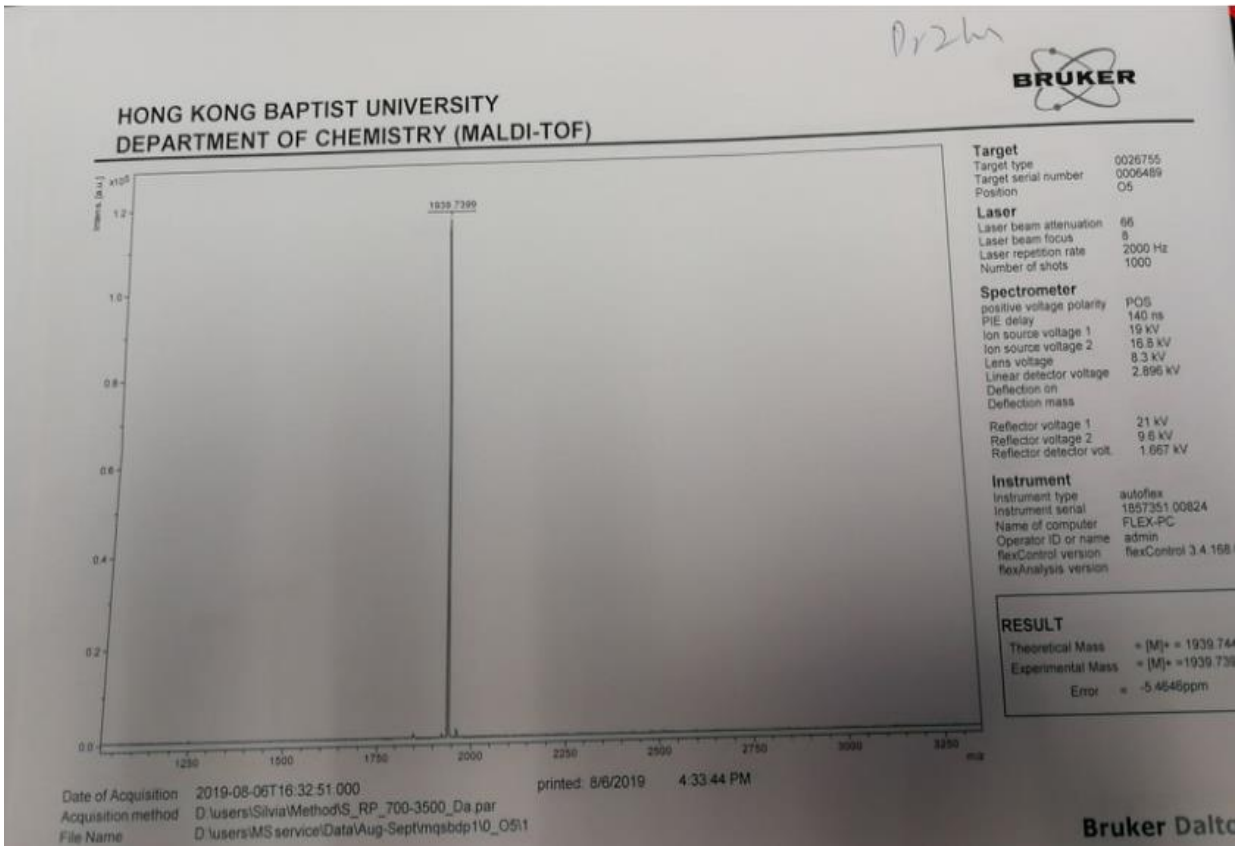

Figure S14. MALDI-TOF spectrum of compound DPBDP