Supporting Information:

# High Singlet Oxygen Yield Photosensitizer based Polypeptide Nanoparticles for low-Power Near Infrared Light Imaging–guided Photodynamic Therapy

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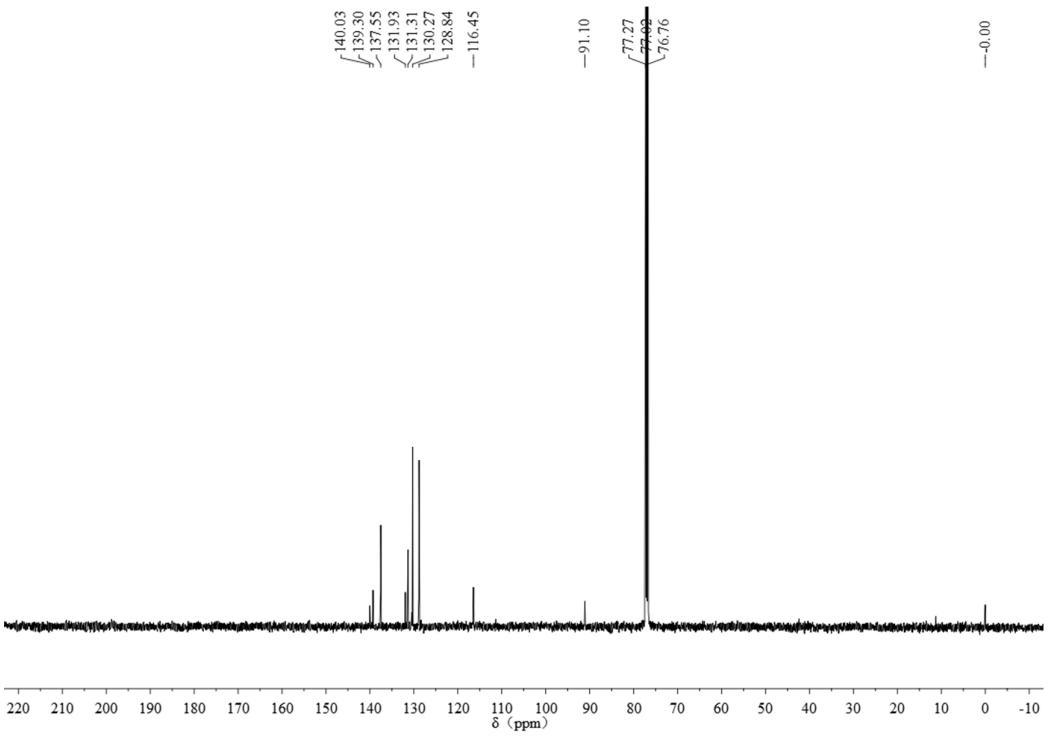


**Figure S1.** $^{13}C$ NMR spectrum of **2a** in $CDCl_3$.

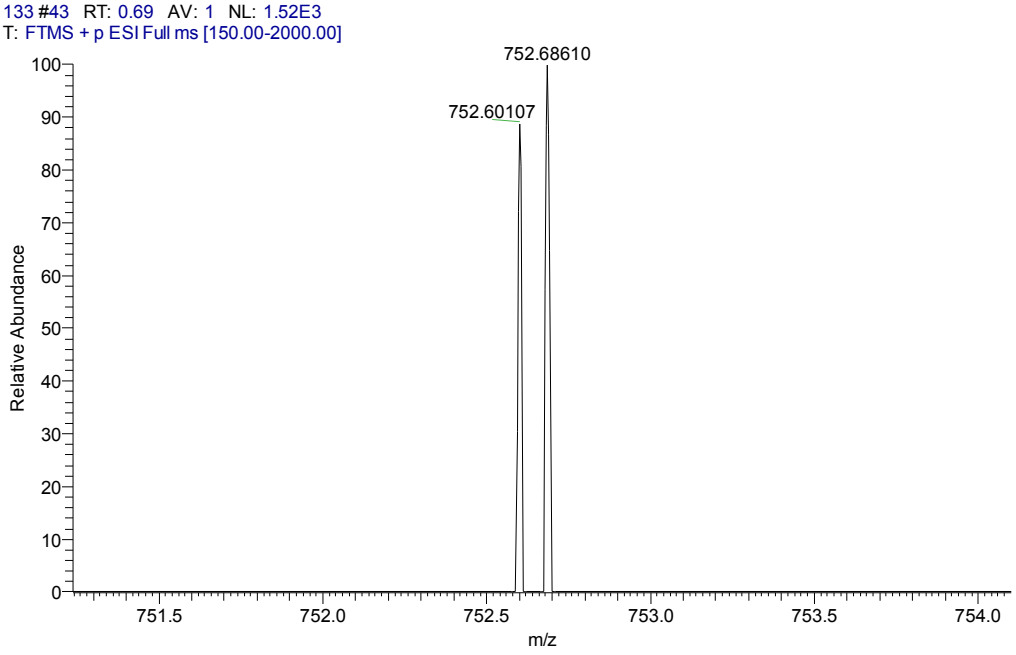


**Figure S2.** HRMS of **2a.**

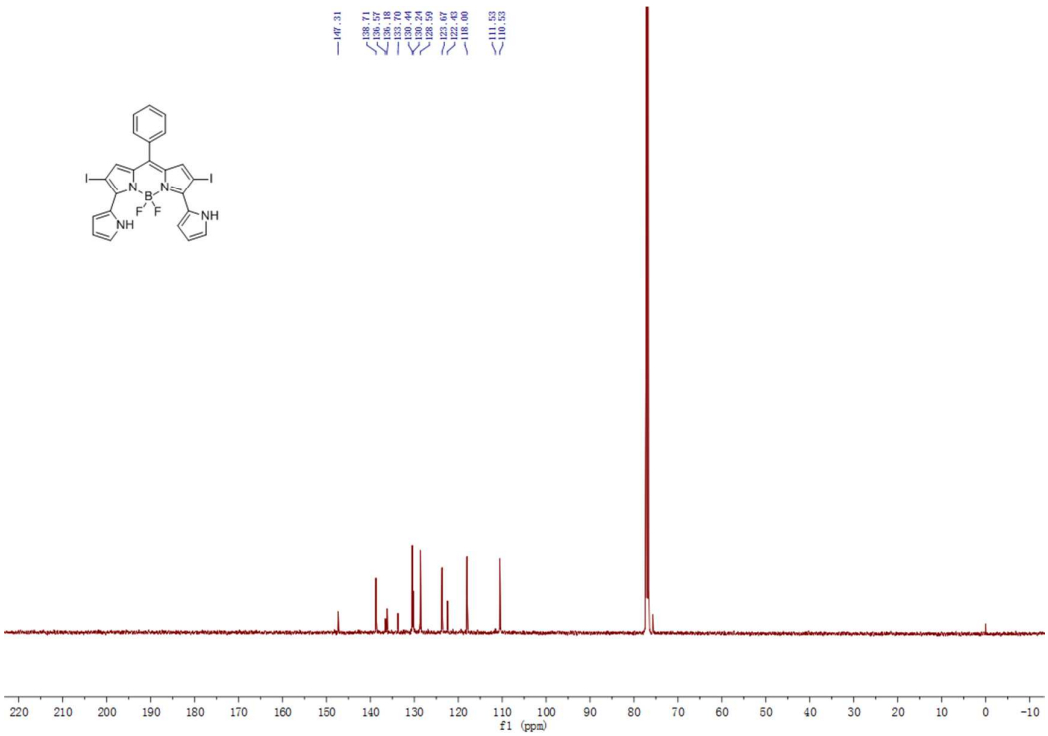


**Figure S3.** $^{13}C$ NMR spectrum of BDPI in $CDCl_3$.

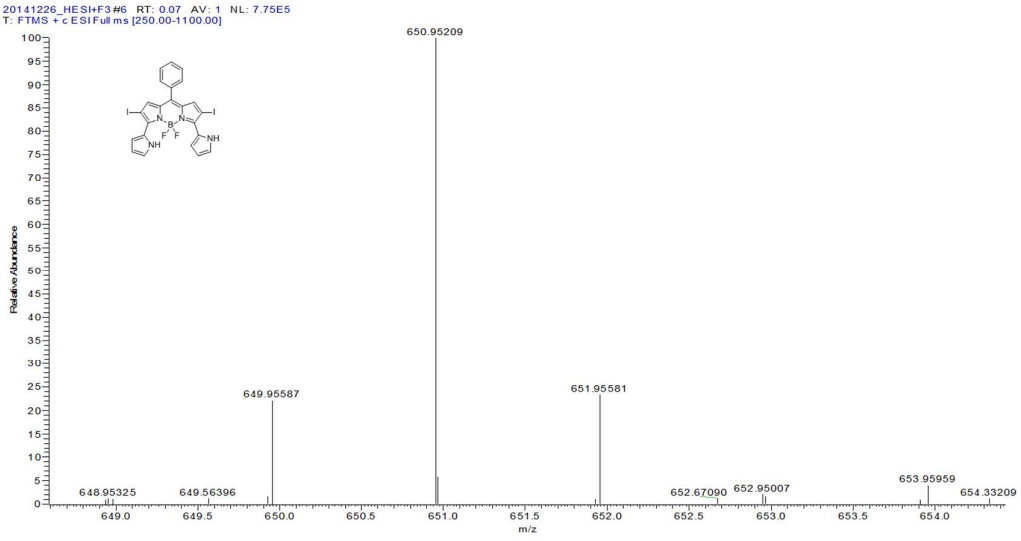


**Figure S4.** HRMS of BDPI.

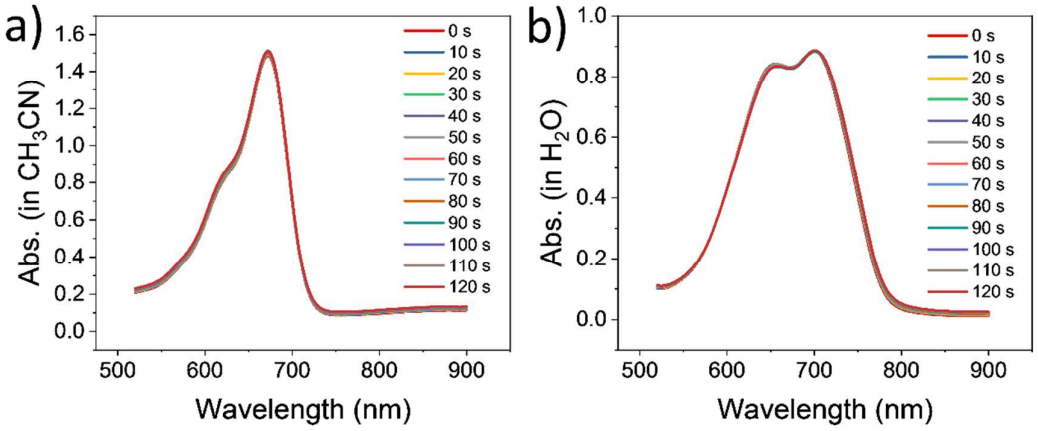


**Figure S5.** Absorption spectra changes of BDPI upon irradiation (recorded at 10 s interval) in $CH_3CN$ (a) and $H_2O$ (b). Irradiation: 635 nm laser with 0.5 mW/cm$^2$.

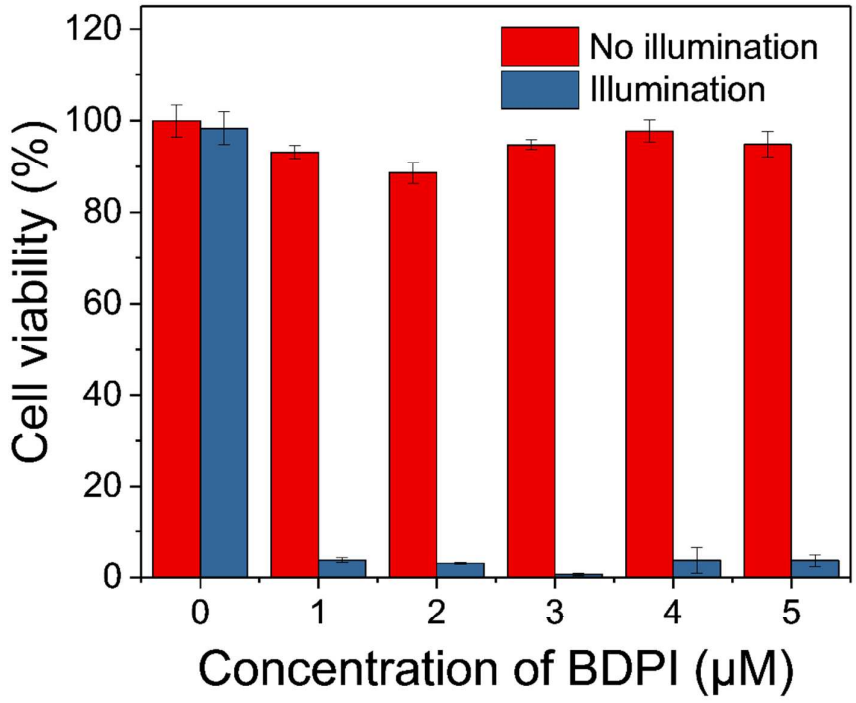


**Figure S6.** Cell viability of EMT6 cells after incubation with BDPI (1-5 μM) upon 20 mW/cm$^2$ (irradiation for 10 min) which is the output power density we used before.

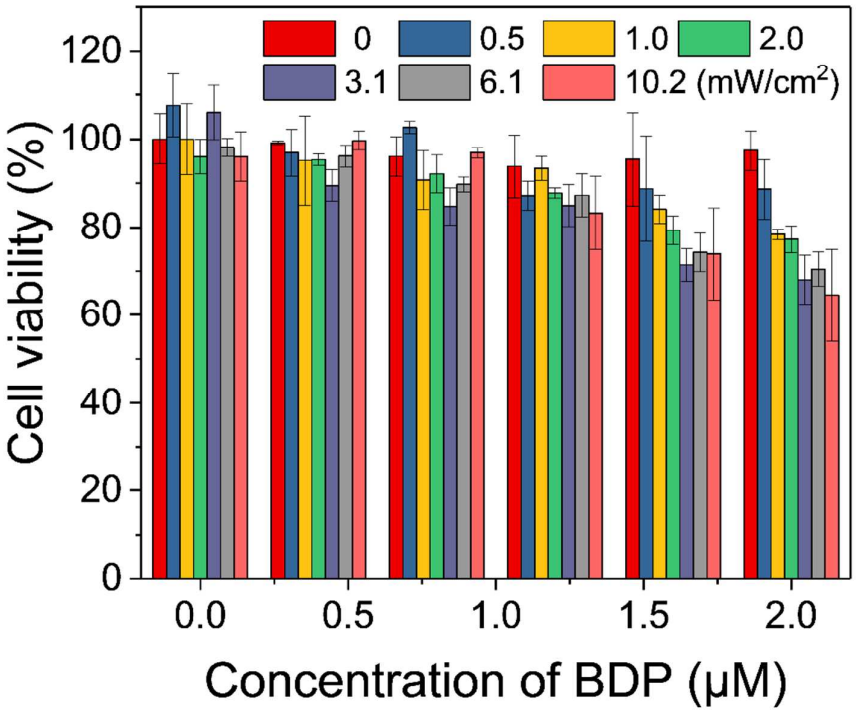


**Figure S7.** Cell viability of EMT6 cells after incubation with BDPBr (0.4-2.0 μM) upon different low power density (irradiation for just 5 min) which is applied in this manuscript.

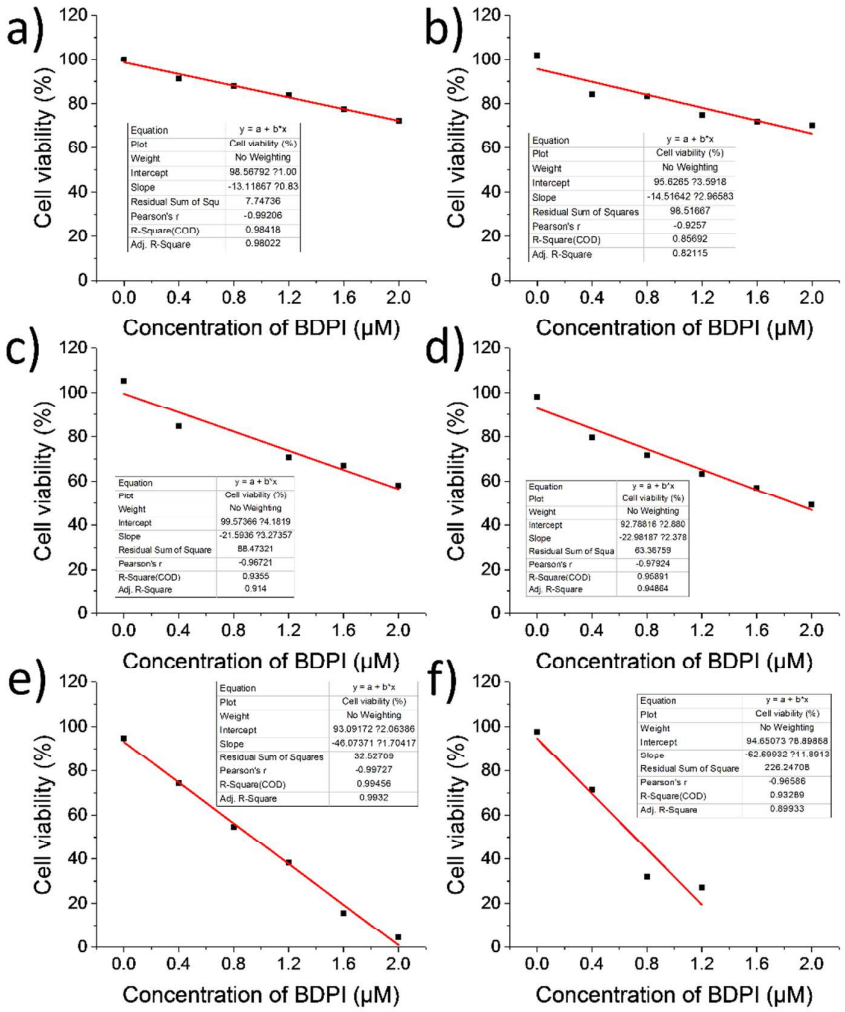


**Figure S8.** Each fitting line of the conclusion of BDPI upon low power density to evaluate the IC50 value: 3.70 μM (2.40 μg/mL, 0.5 mW/cm$^2$, a), 3.14 μM (2.04 μg/mL, 1.0 mW/cm$^2$, b), 2.30 μM (1.50 μg/mL, 2.0 mW/cm$^2$, c), 1.86 μM (1.21 μg/mL, 3.0 mW/cm$^2$, d), 0.93 μM (0.60 μg/mL, 6.1 mW/cm$^2$, e) and 0.71 μM (0.46 μg/mL, 10.2 mW/cm$^2$, f).

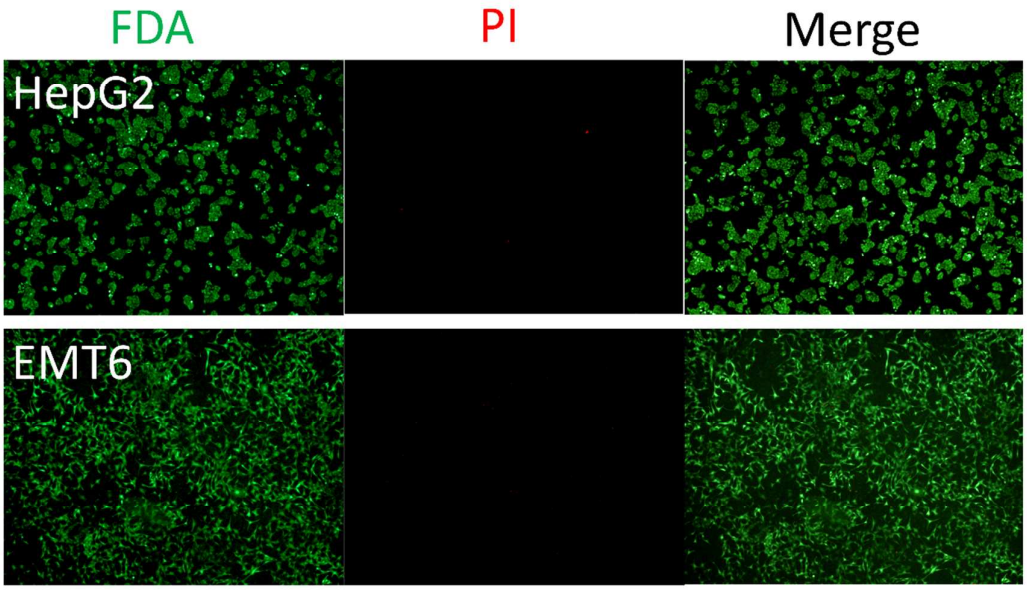


**Figure S9.** Fluorescence imaging of dead/alive staining of HepG2 or EMT6 cancer cells without illumination (magnification ×4).

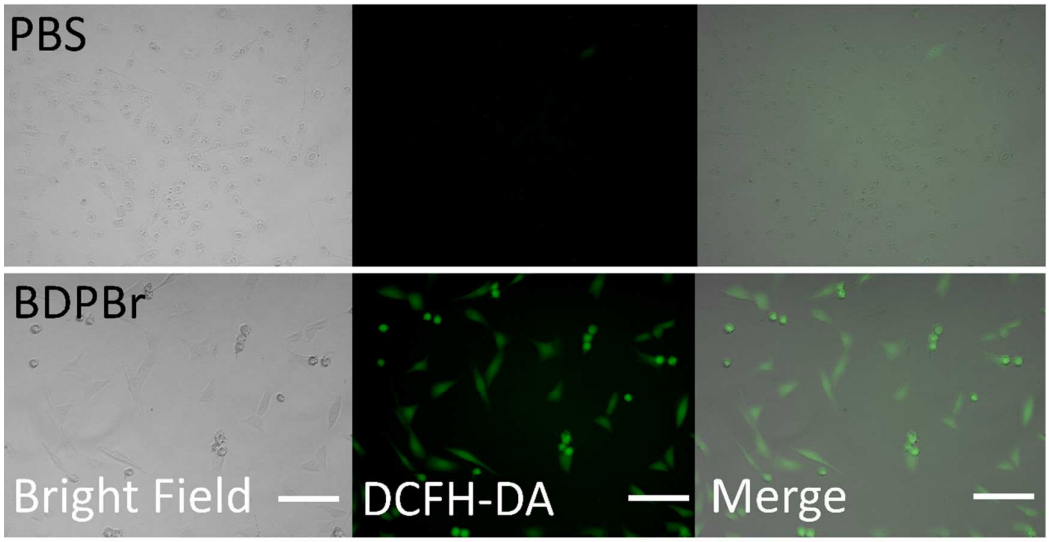


**Figure S10.** Intracellular ROS generation of EMT6 cell after incubation with PBS and BDPBr under NIR illumination. The scale bars are 50 μm.

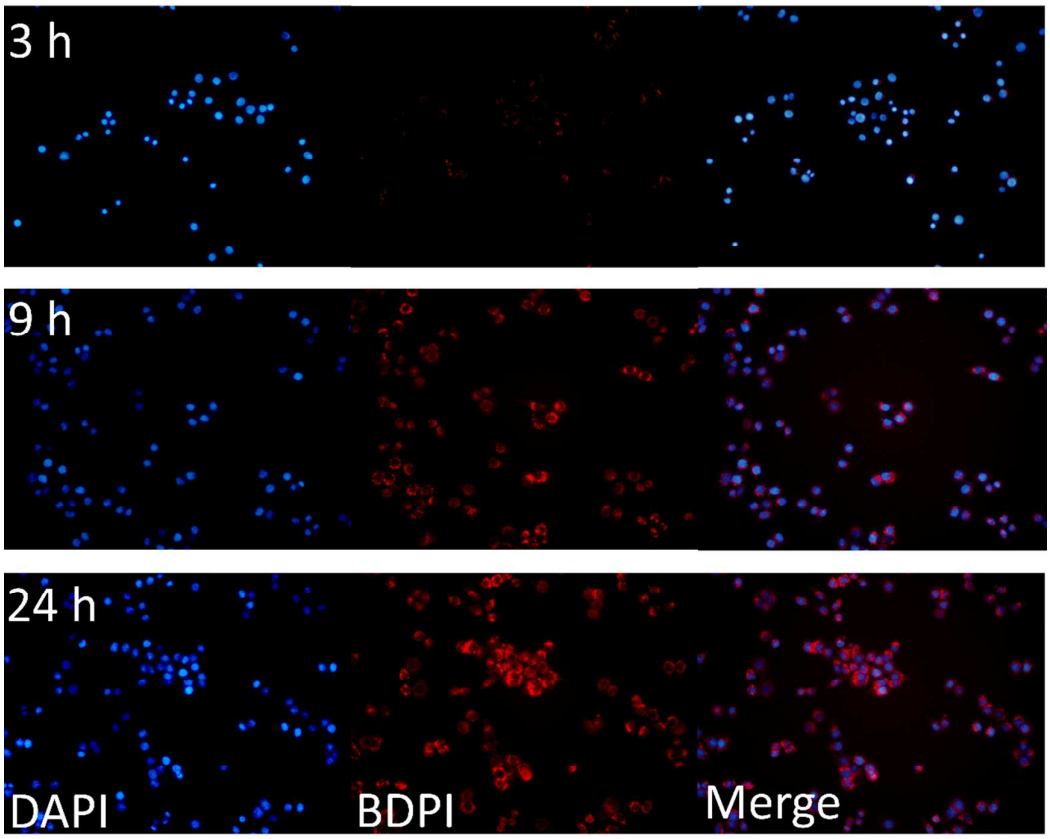


**Figure S11.** Cellular uptake fluorescence images of HepG2 cells at predominant time points after PBDPI NPs feeding (magnification ×20).

**Table S1.** Irradiation output power *in vivo* in previous PDT researches.

| PSs | Dosage (mg/kg) | Lamp wavelength (nm) | Power density (mW/cm2) | Irradiation time (min) | Energy density (J/cm$^2$) | References |
|---|---|---|---|---|---|---|
| PpIX | 3 | 661 | 20 | 30 | 36 | [1] |
| PpIX | 10 | 635 | 5 | 30 | 9 | [2] |
| Ce6 | 2.5 | 660 | 500 | 30 | 900 | [3] |
| BDP | 0.375 | 670-800 | 12 | 30 | 21.6 | [4] |
| BDP | 5 | 660 | 35 | 20 | 42 | [5] |
| TPZ | 2 | 660 | 220 | 10 | 132 | [6] |

**References:**

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