Supporting information

Highly Efficient Near-Infrared BODIPY Phototherapeutic Nanoparticles for Cancer Treatment

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Materials and apparatus

2,4-dimethyl-pyrrole, 4-diethylaminobenzaldehyde, and N-bromosuccinimide were purchased from Tokyo Chemical Industry Co., Ltd. (Shanghai, China). 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT), DCFH-DA (2, 7-dichlorofluorescein diacetate) Detection Kit, Live-Dead Cell Staining Kit, and Annexin V-FITC Apoptosis Detection Kit were obtained from Jiangsu KeyGEN BioTECH Corp., Ltd. The other common chemicals were obtained from local commercial suppliers.

The NMR spectra were measured on Bruker 400 NMR spectrometer by employing $CDCl_3$ as the deuterated solvent. The absorption and emission spectra were taken on a Shimadzu UV-2450 PC UV/Vis spectrophotometer and a PerkinElmer LS-55 fluorescence spectrophotometer, respectively. Size and size distribution (DLS) of the nanoparticles were recorded on Malvern Zeta-sizer Nano. TEM images were collected

on a JEOL JEM-1011 electron microscope. Confocal laser scanning microscopy (CLSM) images were photoed by using Zeiss LSM 700 camera. Flow analysis of the cells was analyzed by Guava easyCyte 6-2L Base System (Merck Millipore, USA).

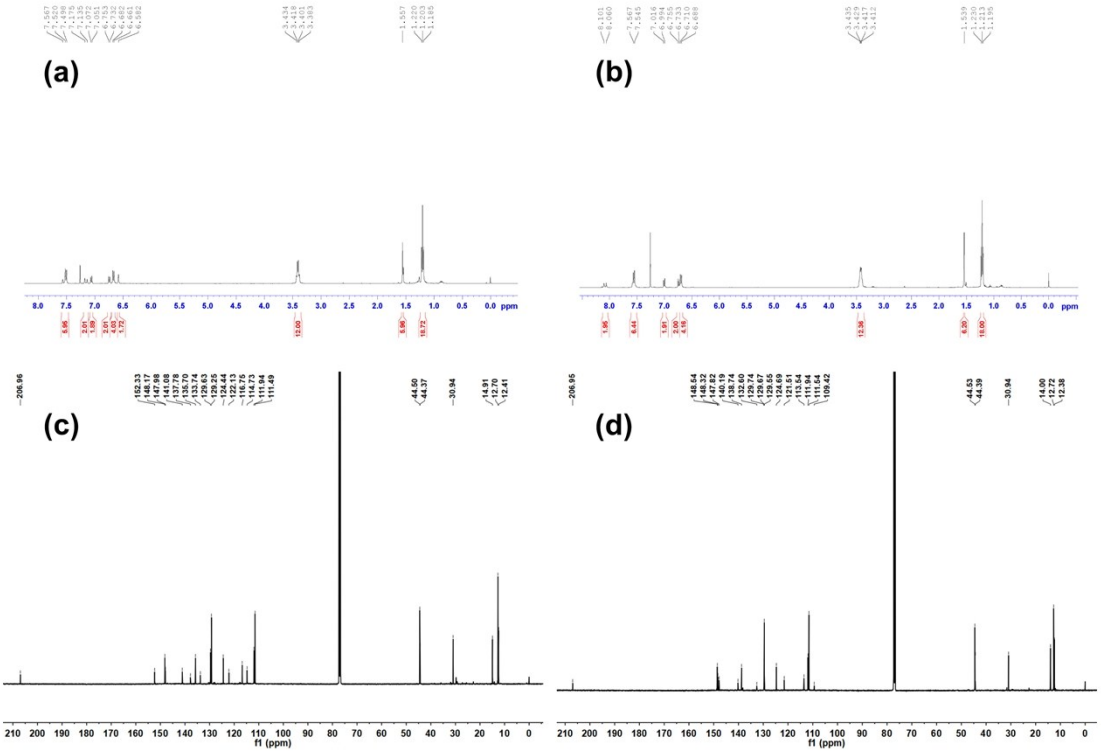

Fig. S1 ^{1}H NMR spectra of (a) NBP and (b) NBB; ^{13}C NMR spectra of (c) NBP and (d) NBB. Solvent: $CDCl_3$.

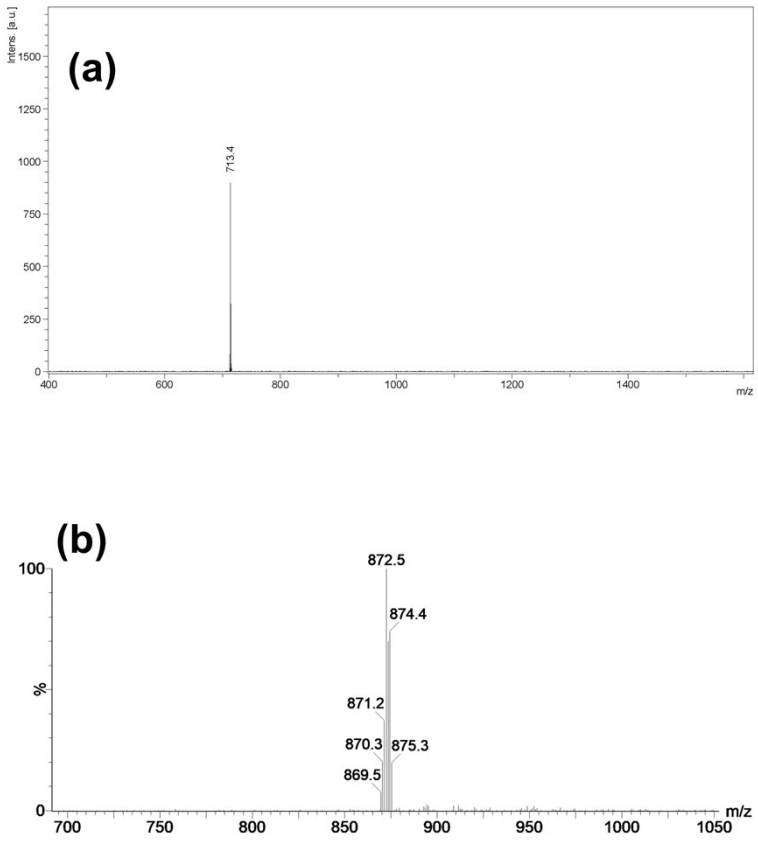

Fig. S2 MS spectra of (a) NBP and (b) NBB in CH_2Cl_2.

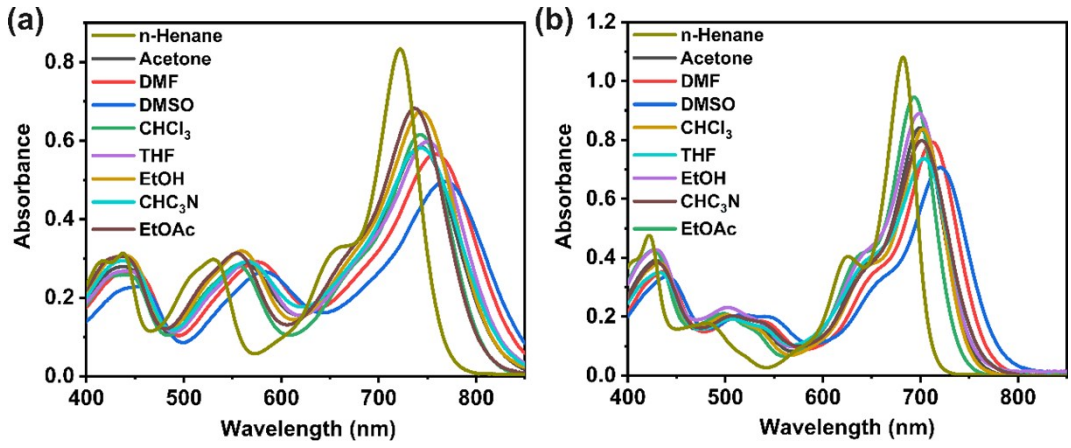

Fig. S3 Absorption spectra of NBB (a) and NBP (b) in different solutions.

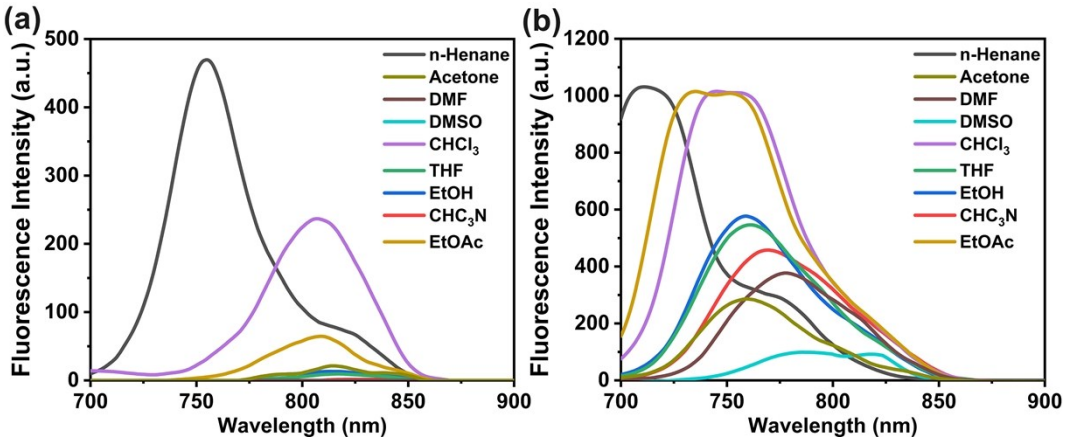

Fig. S4 Fluorescence spectra of NBB (a) and NBP (b) in different solutions.

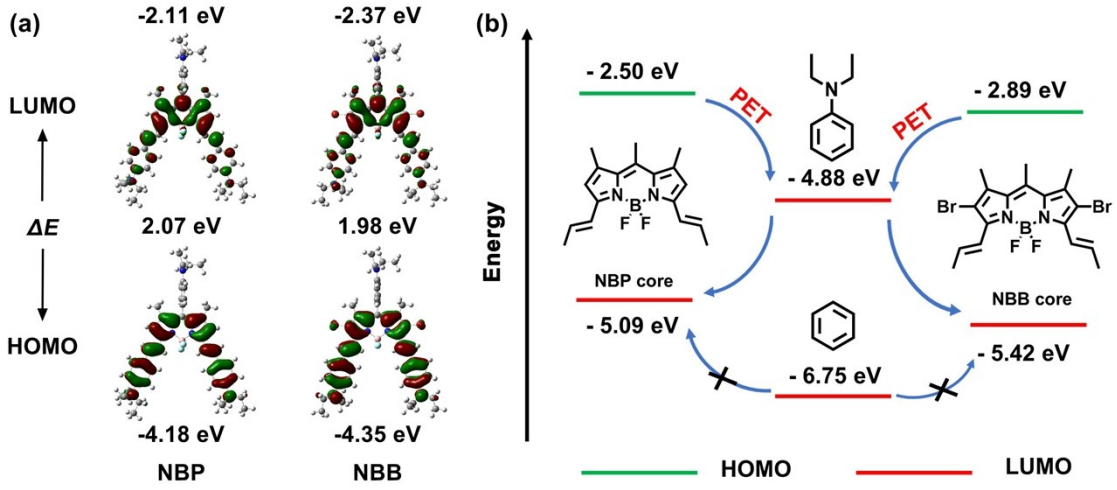

Fig. S5 (a) Electron density contours and orbital energies calculated for the HOMO and LUMO of NBP and NBB. (b) HOMO and LUMO energy levels of the NBP core, NBB core, diethylaminobenzene moiety, and benzene unit, respectively.

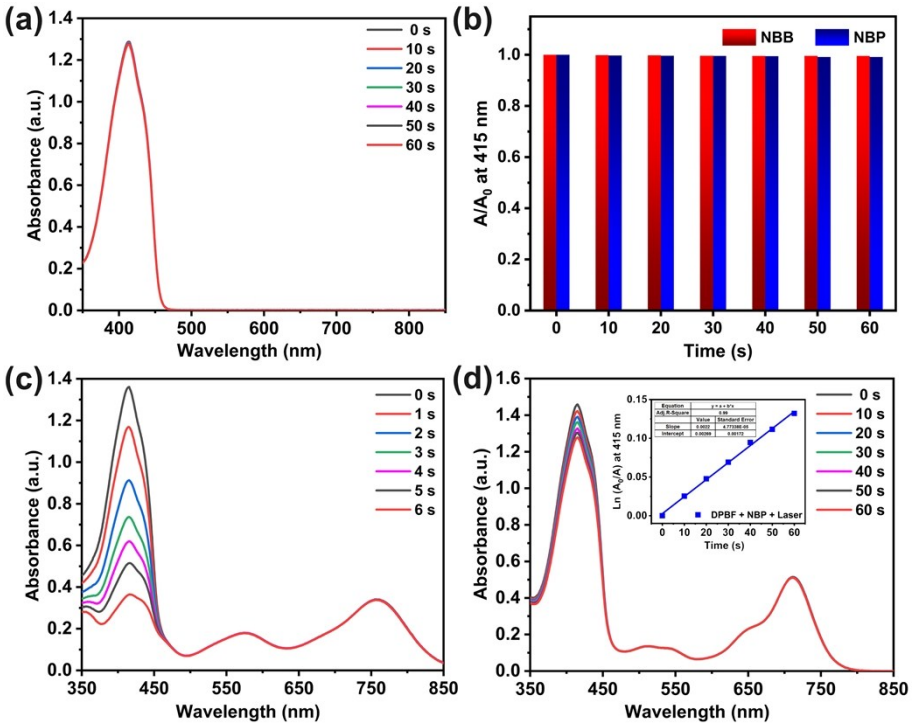

Fig. S6 (a) Absorption of DPBF upon irradiation, (b) DPBF with NBB or NBP without irradiation, (c) DPBF with NBB, and (d) DPBF with NBP in DMF. Laser irradiation, 808 nm, 0.48 W cm^{-2}.

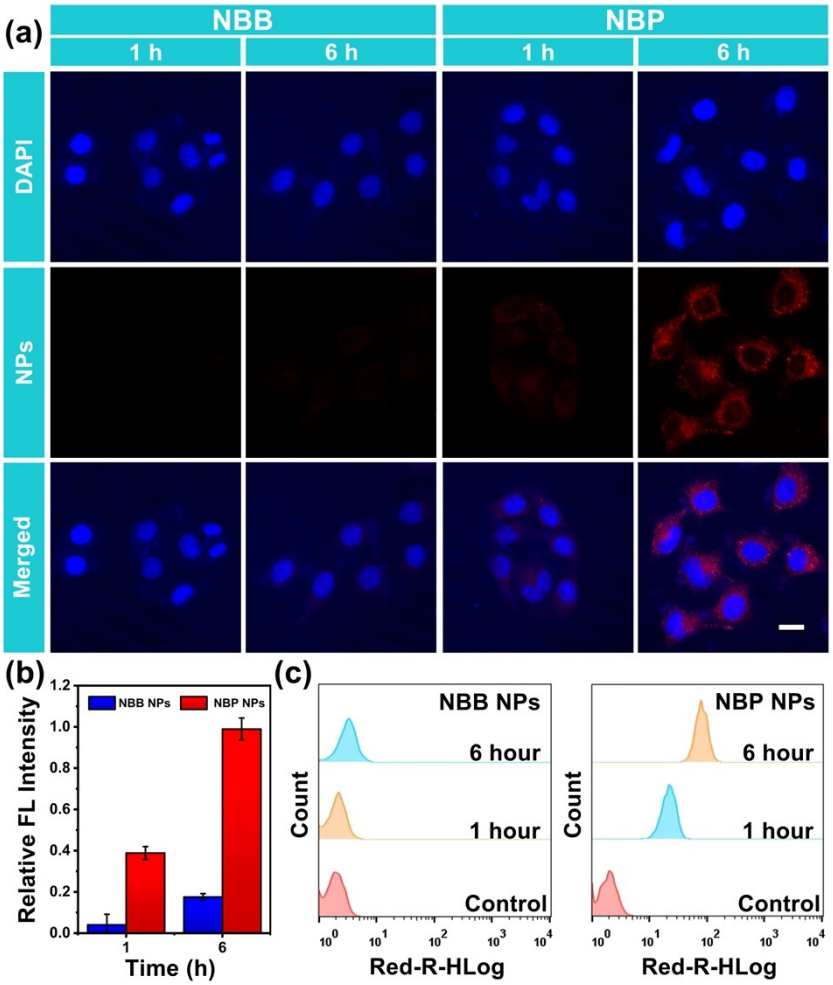

Fig. S7 CLSM images of HeLa cells incubated with NBB NPs and NBP NPs (10 μM) from 1 to 6 h. Scale bars: 20 μm. (b) Relative fluorescence intensity of HeLa cells loaded with NBB and NBP NPs for different periods. (c) Flow cytometry results of NBB and NBP NPs under the identical conditions as the CLSM images with a blank group as the control.

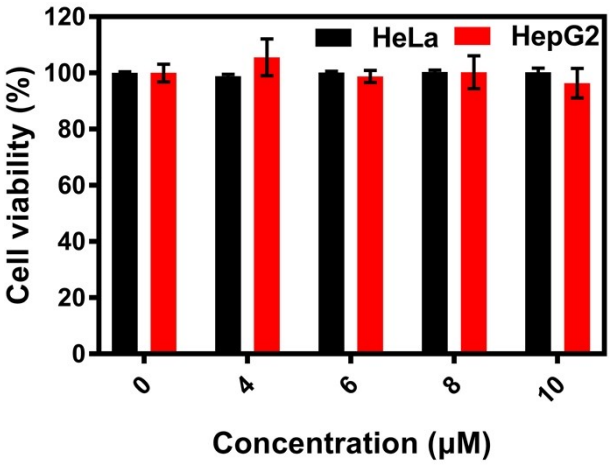

Fig. S8 Viability of HeLa and HepG2 cells incubated with various concentrations of NBP NPs, respectively.