Supporting Information

Real-Time Imaging of Cancer Cell Generations and Monitoring Tumor Growth using a Nucleus-Targeted Red Fluorescent Probe

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Contents

Synthesis and Characterization of PTB

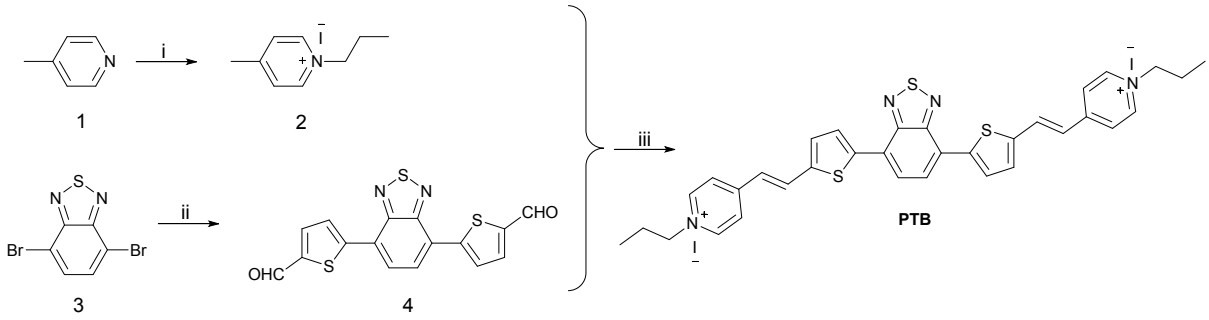
The detailed synthetic route for the compound is shown in Scheme S1, as follows:

Synthesis of 4-N-propylpyridium iodide (2):4-N-propylpyridium iodide was synthesized according to a previous report from the literature [S1].

Synthesis of 4,7-bis(5-formyl-2-thiophenyl)-2,1,3-benzothiadiazole (4): Compound 4 was synthesized according to a previous report from the literature [S2]. A 2 M Cs_2CO_3 (16.29 g, 50 mmol in 25 mL H_2O) solution in a 250 mL single port flask was degassed for over 20 min with N_2, Then, distilled toluene (75 mL) and Ethanol (50 mL), 5-formyl-2-thienylboronic acid (3.96 g, 25 mmol), 4,7-dibromo-2,1,3-benzothiadiazole (3 g, 10 mmol) and $PdCl_2(PPh_3)_2$ (352 mg, 0.5 mmol) were added to the flask, which was degassed twice again.After refluxing overnight, the mixture was poured into water and extracted with chloroform 3 times, and the organic solvents were removed by a rotary evaporator. The pure product was recrystallized from $CHCl_3$ to afford the product as a red solid (1.4 g, yield: 40%).^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ: 10.00 (s, 2H), 8.26 (d,2H), 8.06 (s, 2H), 7.87 (d, 2H).

Synthesis of **PTB**: To a solution of 4-N-propylpyridium iodide(2, 1.32 g, 5 mmol) were added4,7-bis(5-formyl-2-thiophenyl)-2,1,3-benzothiadiazole(4, 0.71 g, 2 mmol) and piperidine (0.43 g, 5mmol) in DCM/Ethanol (2/1, 75 mL). The reaction mixture was then stirred at room temperature for 24 h. The resulting mixture was filtered, and the collected solid was washed with DCM and Ethanol several times to afford the product as a dark brown solid (1.18 g, yield: 70%). ^{1}H NMR (400 MHz, DMSO-d_6, ppm) δ: 8.94-8.92 (d, 4H), 8.27-8.20 (dt, 10H), 7.61 (d, 2H), 7.29-7.25 (d, 2H), 4.47-4.43 (t, 4H), 1.98-1.89 (dt, 4H), 0.92-0.89 (t, 6H). ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ: 152.81, 151.83, 144.43, 142.91, 141.91, 134.04, 132.90, 129.12, 126.79,

125.29, 123.91, 122.70, 61.36, 24.38, 10.68.HRMS (MALDI-TOF): $[M-2I]^+$ calcd for $C_{34}H_{32}N_4S_3$, 592.180; found, 591.917.



Scheme S1. Synthetic route of **PTB**[a].

[a]Reagents: (i) iodopropyl, DCM; (ii) 5-formyl-2-thienylboronic acid, $PdCl_2(PPh_3)_2$, 2 M Cs_2CO_3, Toluene, Ethanol; (iii) DCM, EtOH, piperidine.

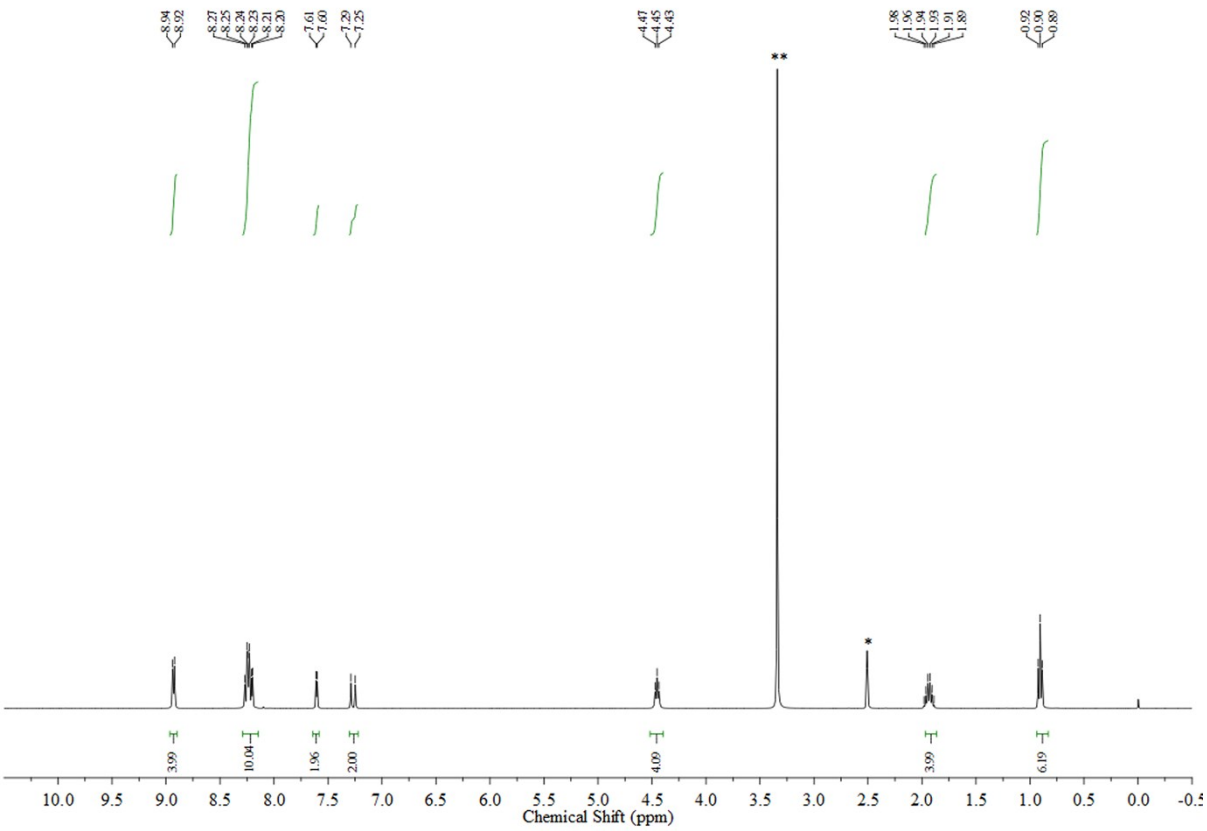


Fig. S1. ^{1}H NMR spectra of **PTB**.

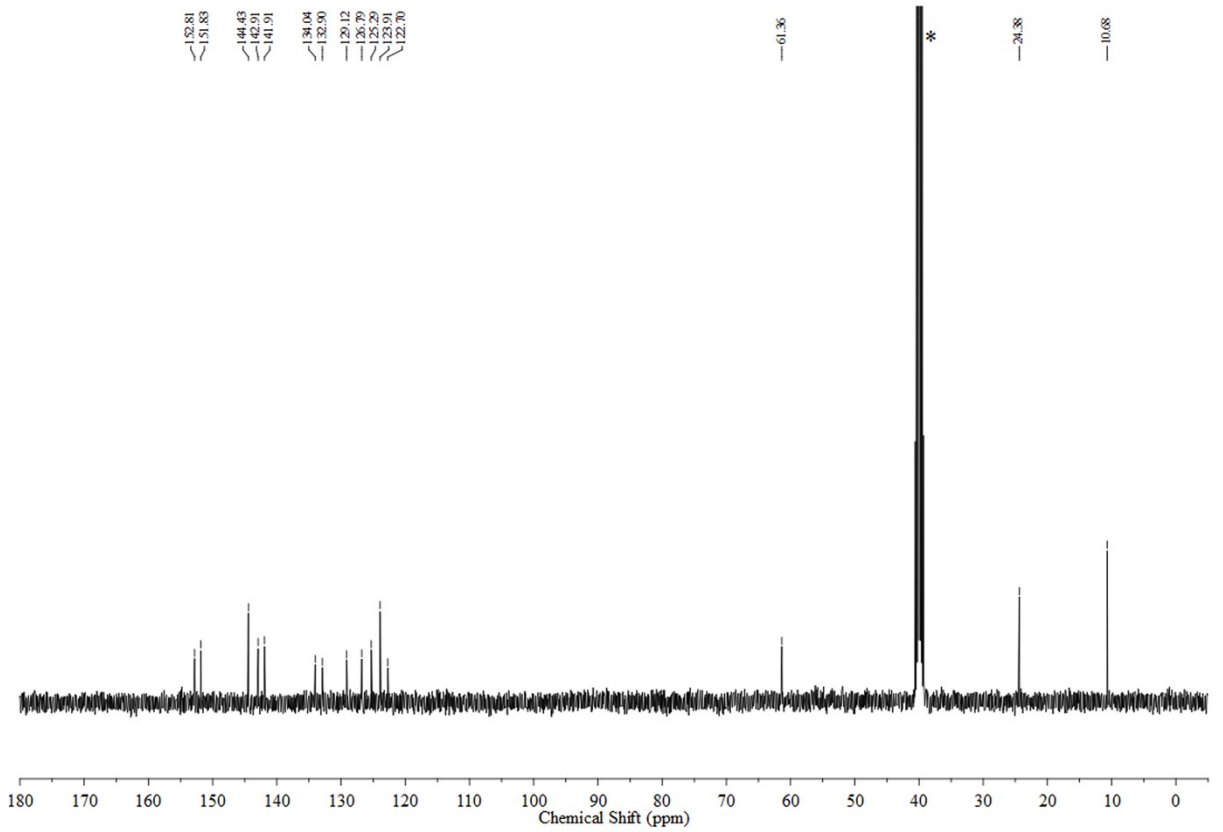


Fig. S2. ^{13}C NMR spectra of **PTB**.

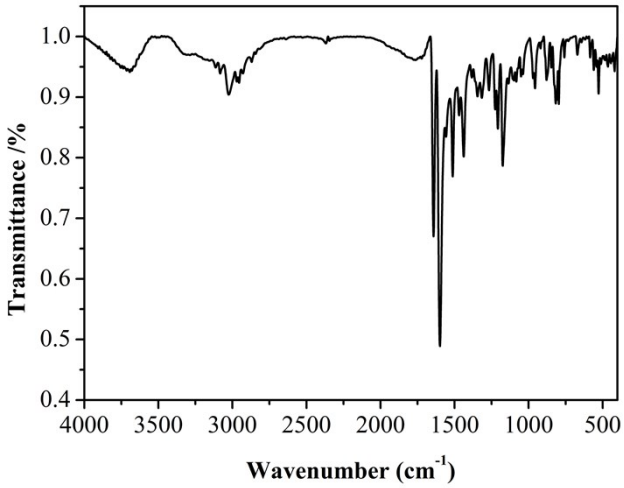


Fig. S3. IR spectra of **PTB**.

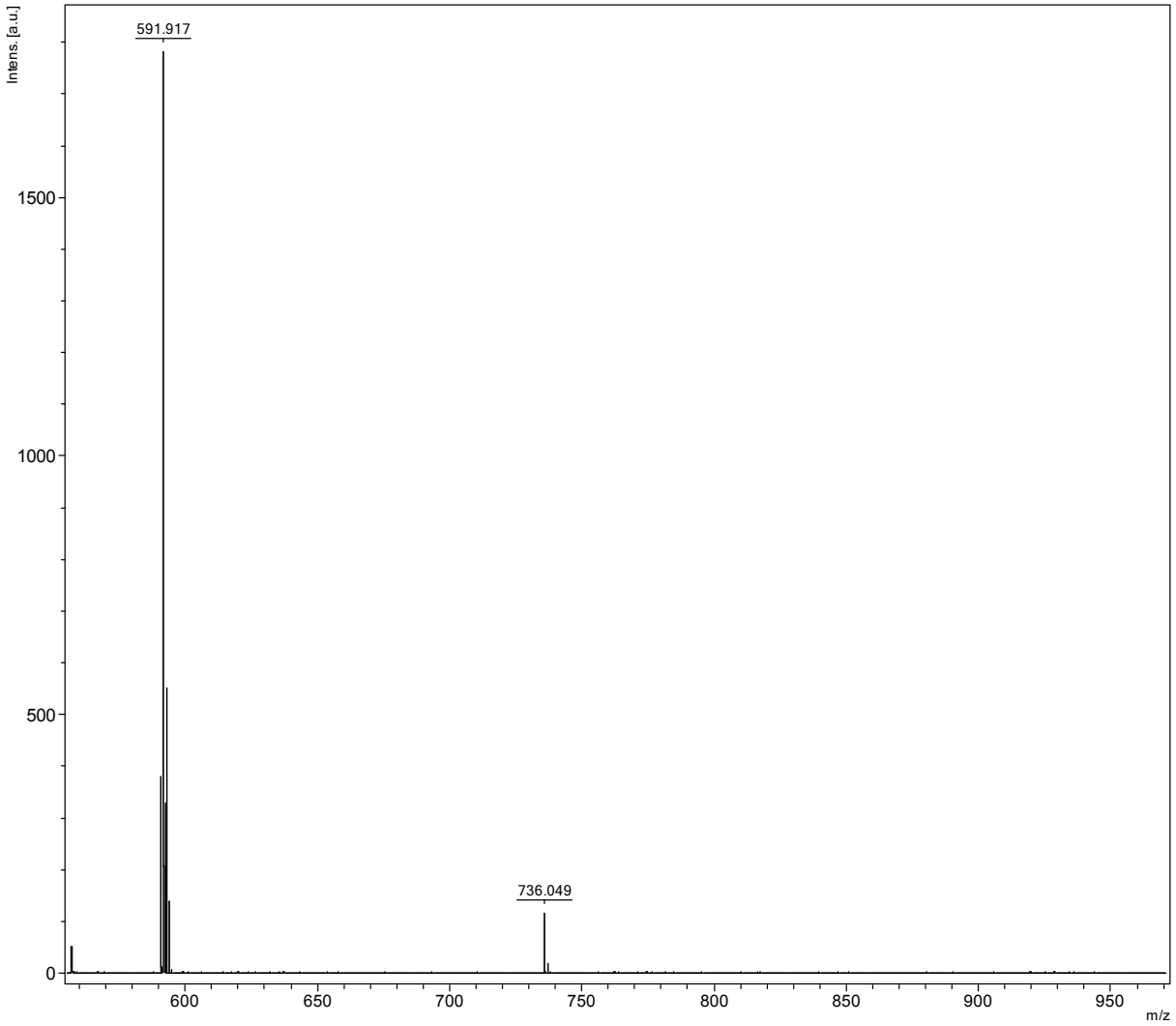


Fig. S4. HRMS of **PTB**.

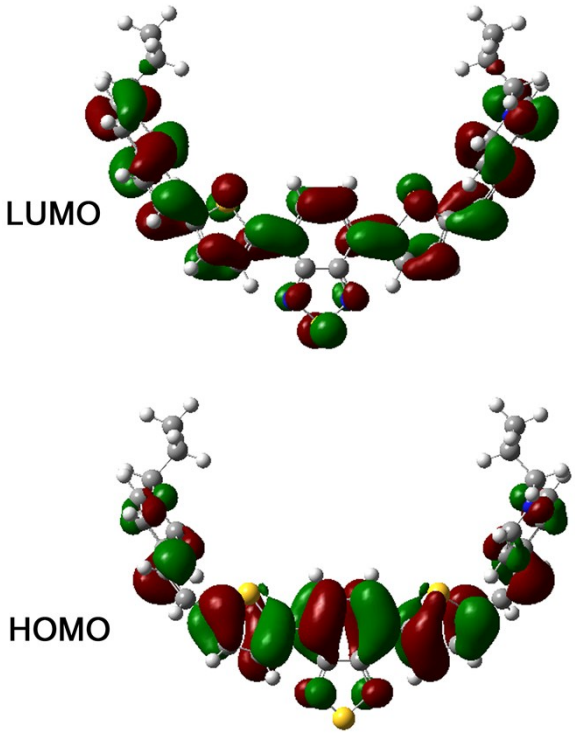


Fig. S5. Molecular orbital amplitude plot of HOMO and LUMO energy level of **PTB** calculated by B3LYP/6-31G (d) basis set.

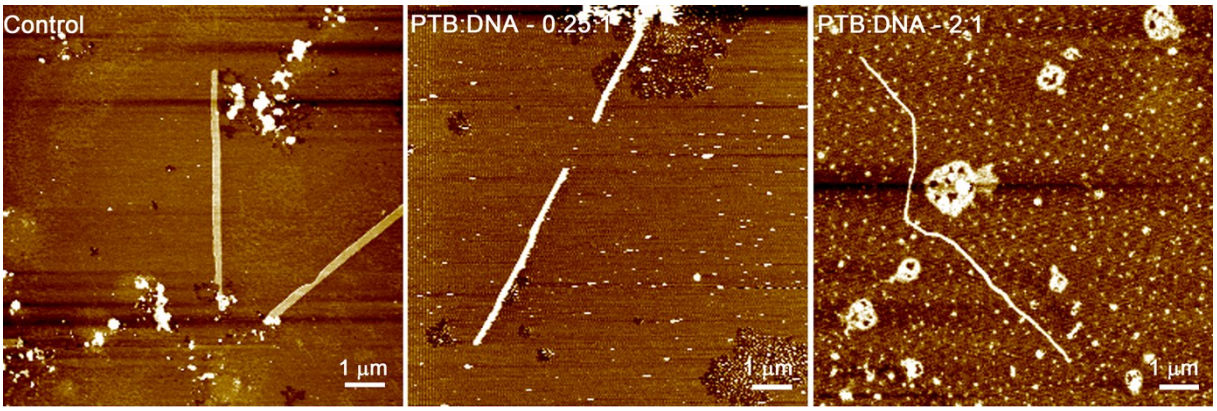


Fig. S6. AFM imags of DNA (1 ng/µL) with different **PTB** concentration ranges from 0 to 2 ng/µL.

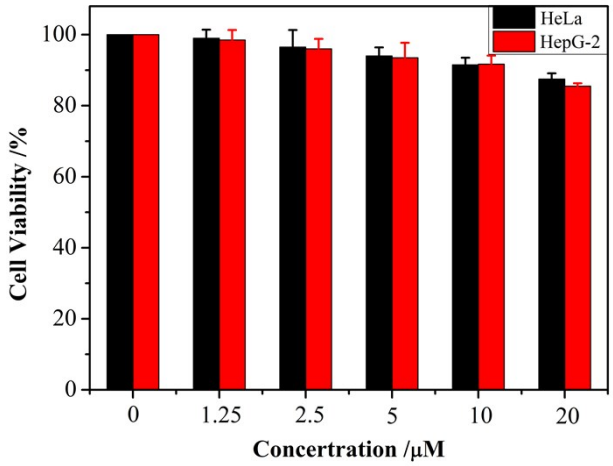


Fig. S7. Metabolic viability of HeLa cells and HePG-2 cells after incubation with **PTB** at different concentrations.

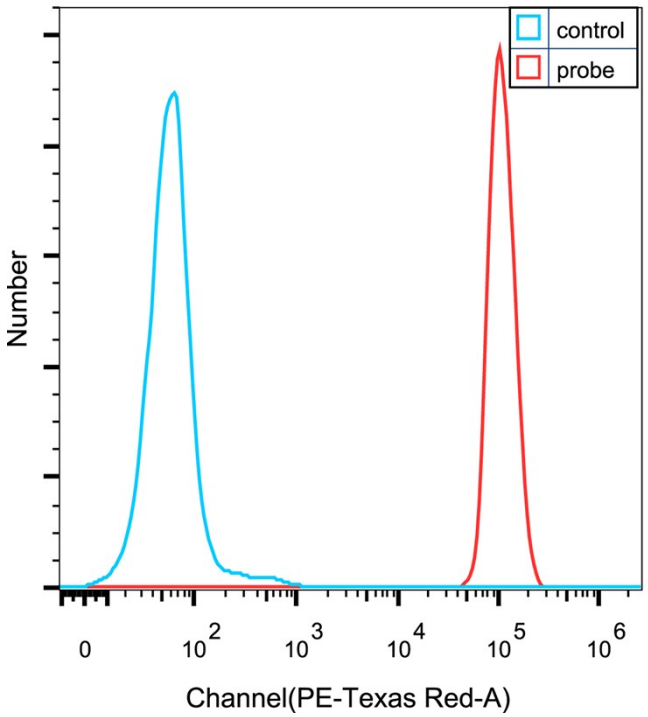


Fig. S8. Flow cytometry profiles of HeLa cells that were incubated with PBS or **PTB** at 37 °C for 4 h.

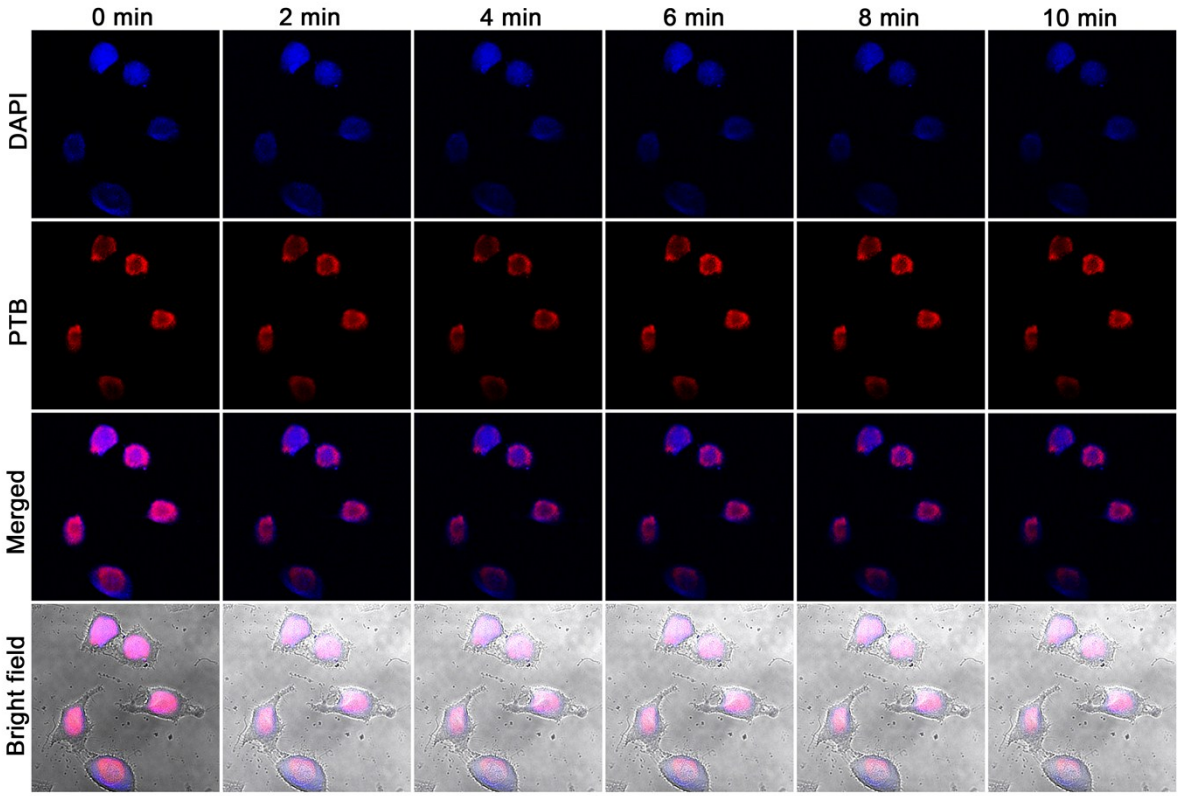


Fig. S9. Confocal microscopy images of HeLa cells of time-dependent laser irradiation. Concentration: 1 μM.

References

[S1] Y. Makoudi, M. E. Garah, F. Palmino, E. Duverger and F. Cherioux, J. Phys. Chem. C., 2009, **113**, 3713-3716.

[S2] B. Y. Fu, J. Baltazar, Z. K. Hu, A. T. Chien, S. Kumar, C. L. Henderson, D. M. Collard and E. Reichmanis, Chem. Mater. 2012, **24**, 4123-4133.