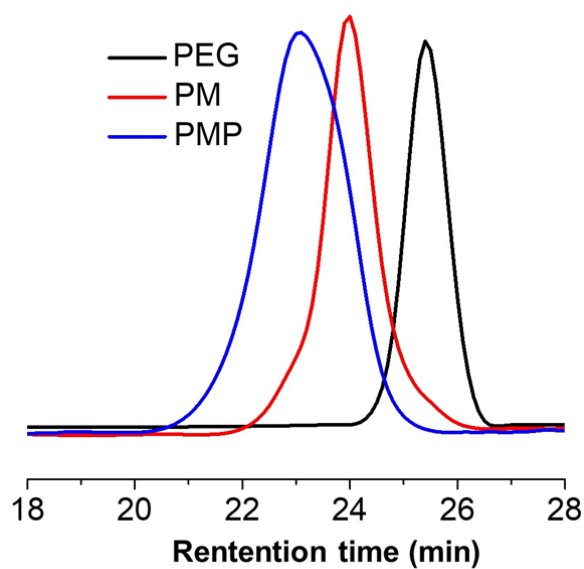
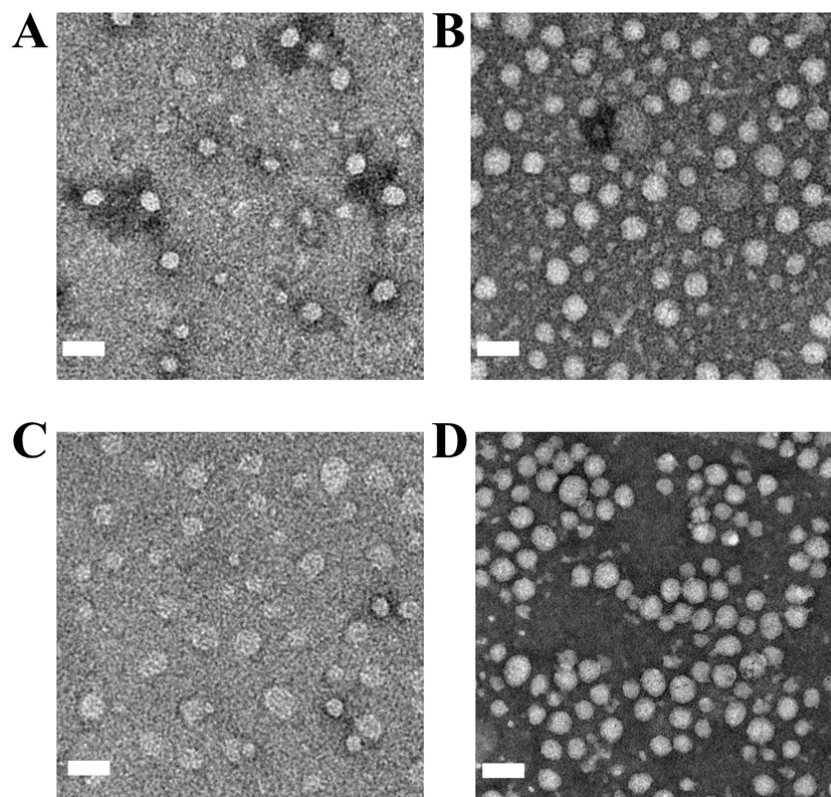


Supplementary Figure 1. High resolution mass spectrum (HRMS) (MALDI-TOF) spectrum of PTX-SS-N₃, calcd [M+Na]⁺ 1137.3443.



Supplementary Figure 2. Gel Permeation Chromatography (GPC) traces of PEG, PM and PMP.

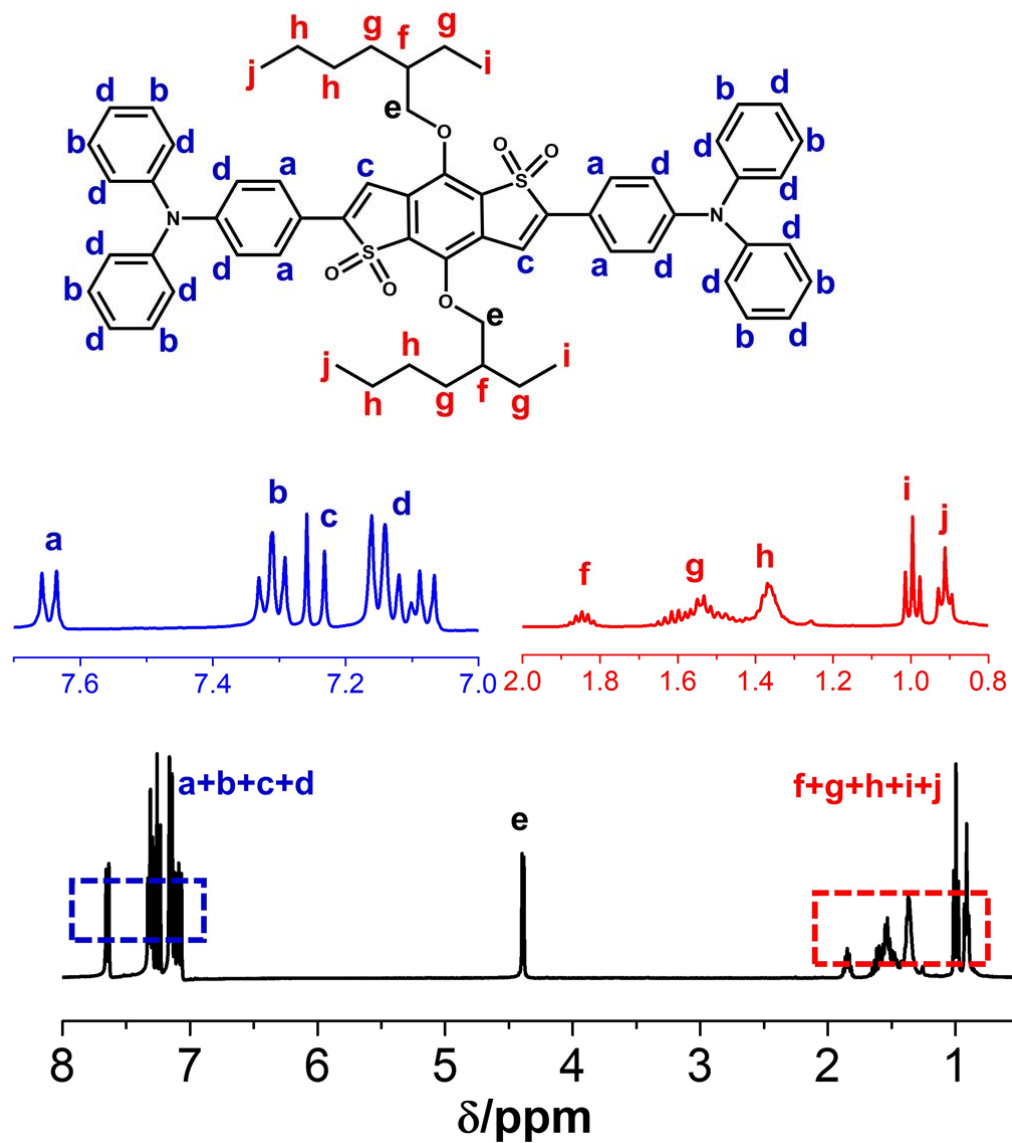


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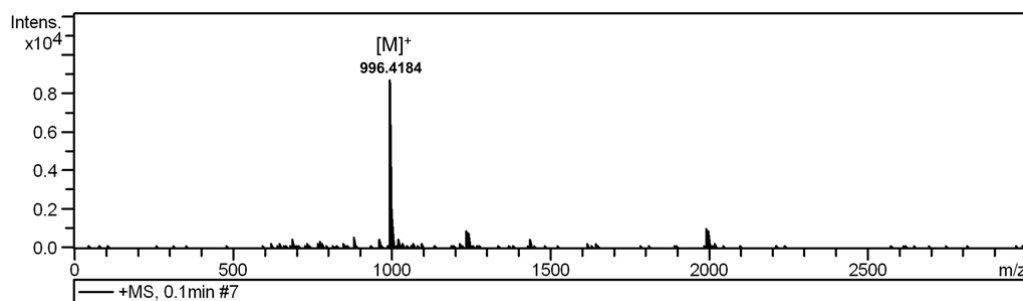
12 **Supplementary Figure 3.** The TEM image of **A)** PM, **B)** PMP, **C)** TB@PM and **D)** TB@PMP
 13 micelles, scale bar: 50 nm.

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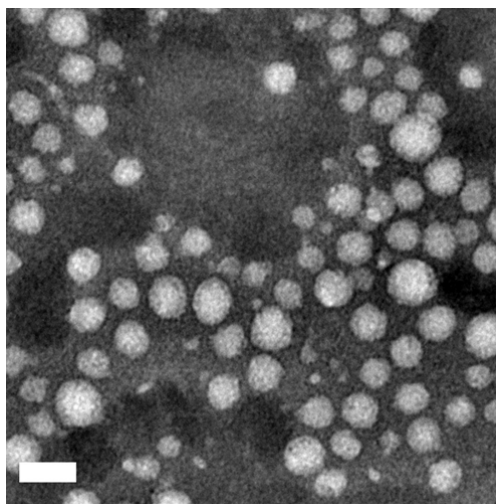


Supplementary Figure 4. Structure and ^1H NMR spectrum of TB.



Supplementary Figure 5. HRMS (MALDI-TOF) spectrum of TB, calcd $[\text{M}]^+$ 996.4200.

22

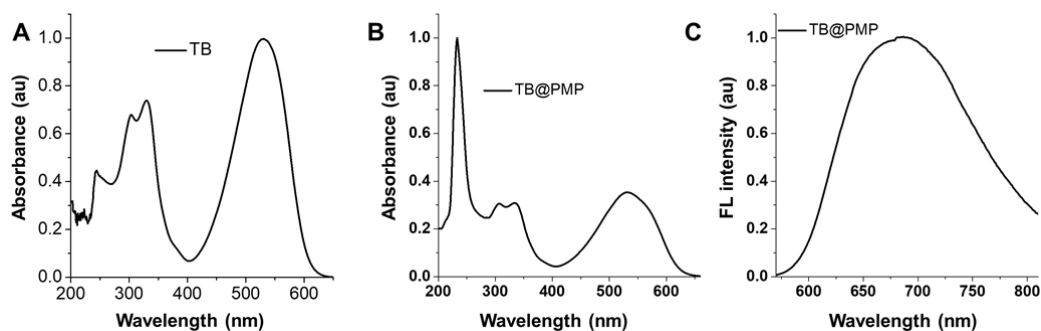


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24 **Supplementary Figure 6.** The TEM image of TB@PMP micelles after 7 days storage at room
25 temperature, scale bar: 50 nm.

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27

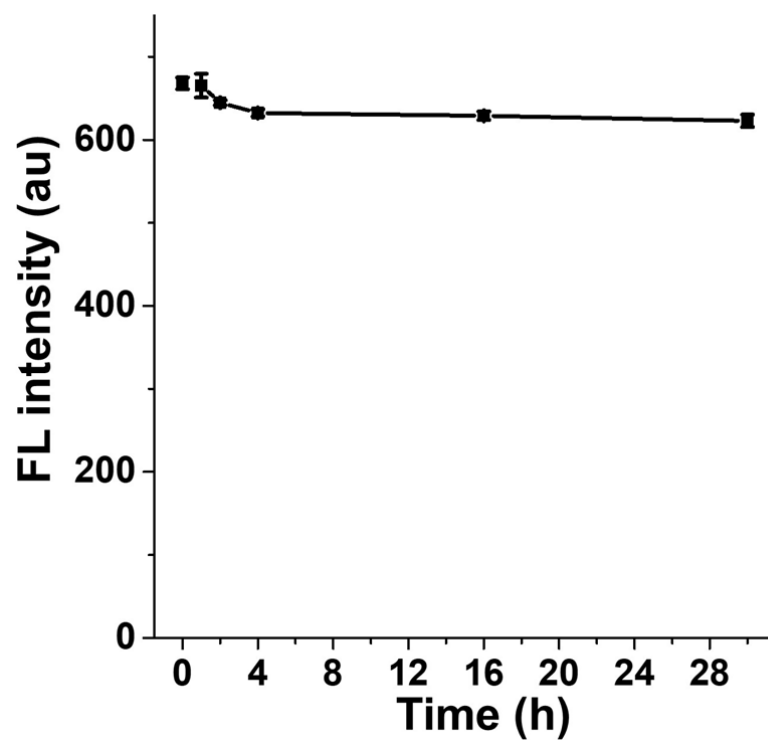


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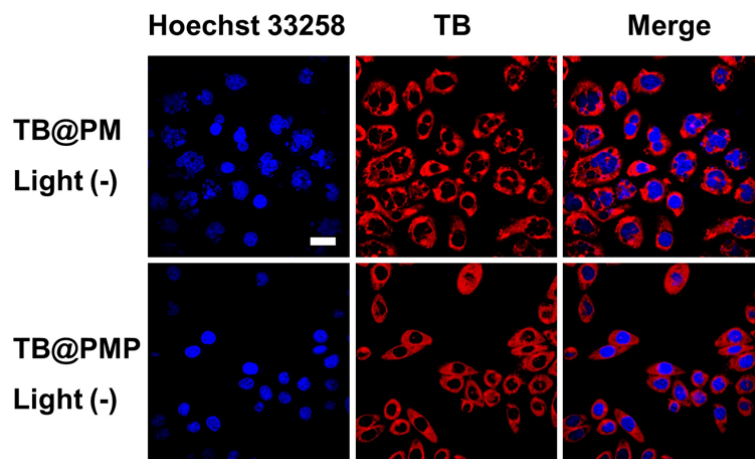
29 **Supplementary Figure 7.** **A)** Absorption spectrum of TB (2.8×10^{-6} M) in THF; **B)** Absorption of
30 TB@PMP micelles ($30 \mu\text{g mL}^{-1}$) in aqueous solution; **C)** FL spectra (Ex: 530 nm) of TB@PMP
31 micelles ($30 \mu\text{g mL}^{-1}$) in aqueous solution.

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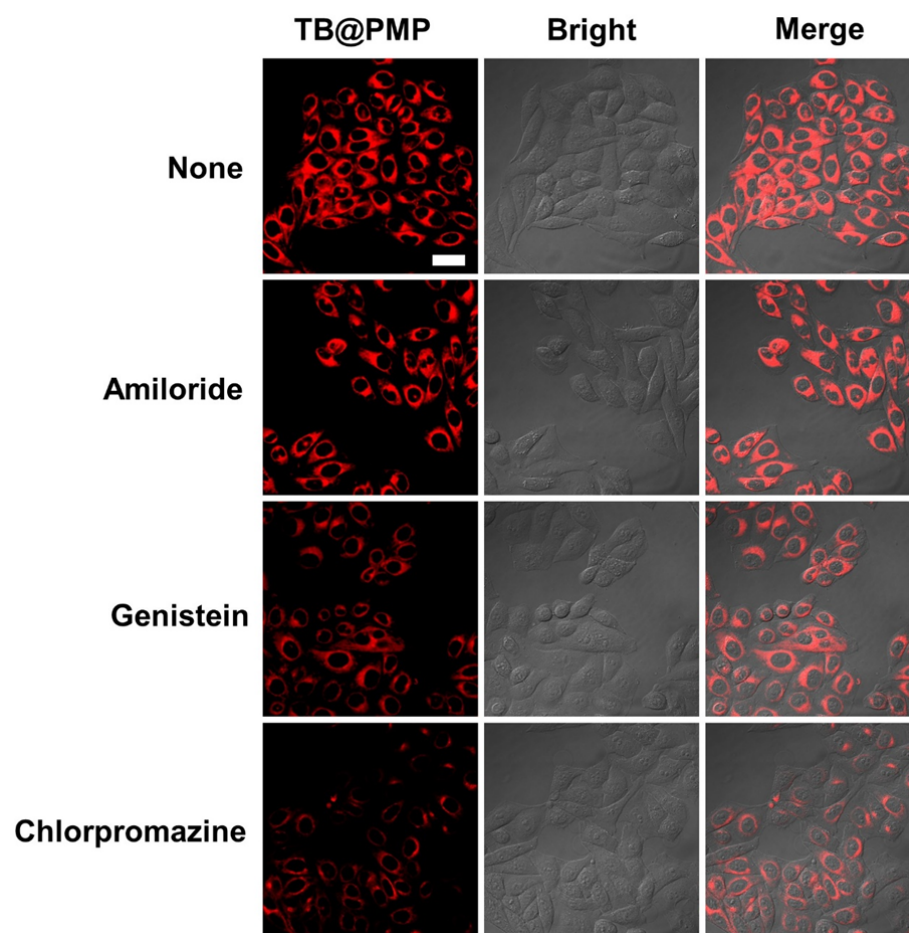
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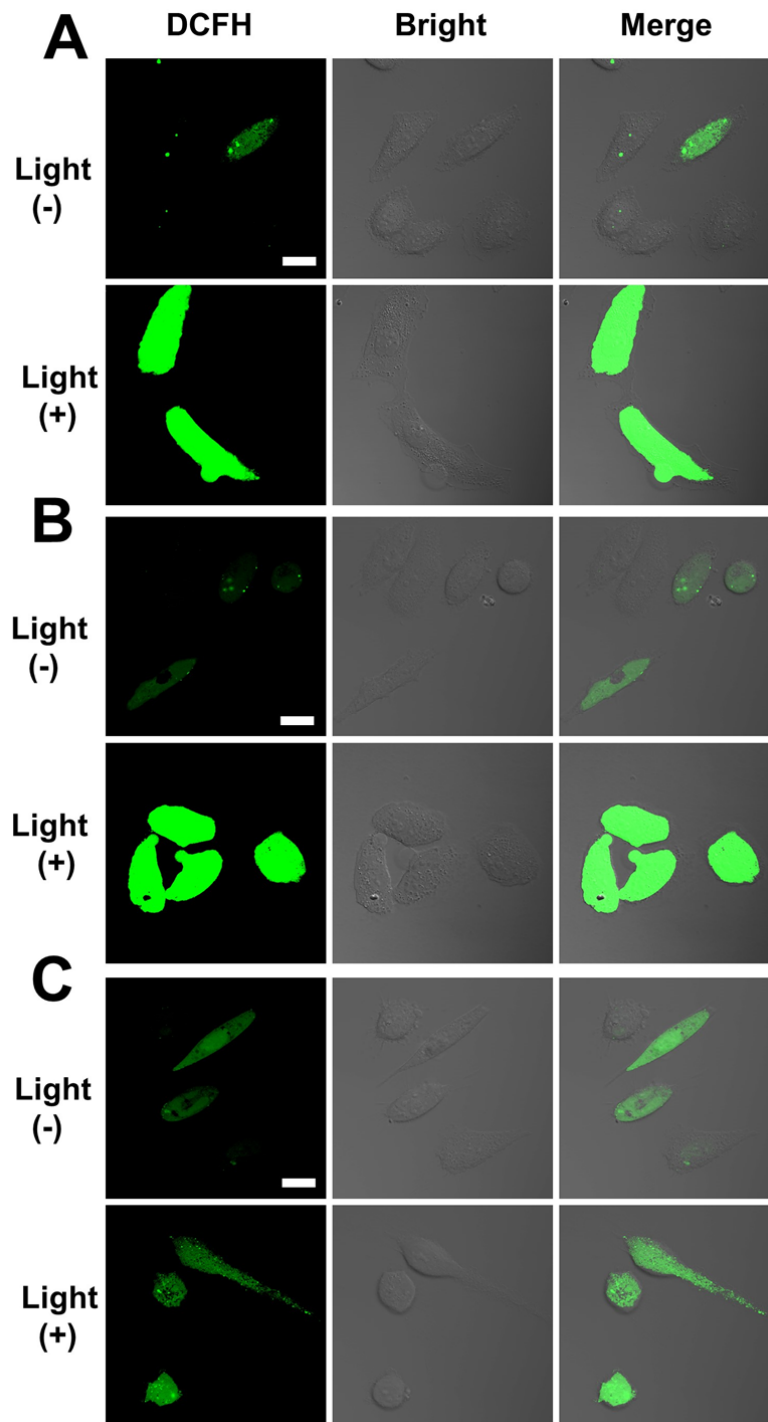
Supplementary Figure 8. Fluorescence intensity of 630 nm of TB@PMP micelles ($30 \mu\text{g mL}^{-1}$) in aqueous solution with 10 mM DTT (Ex: 530 nm).



Supplementary Figure 9. Confocal images of HeLa cells incubated with TB@PMP and TB@PMP micelles ($250 \mu\text{g mL}^{-1}$) for 4 h in dark, respectively. Scale bar: $20 \mu\text{m}$.



Supplementary Figure 10. Confocal laser scanning microscopy images of HeLa cells after incubation with TB@PMP micelles ($250 \mu\text{g mL}^{-1}$) containing different endocytosis inhibitor: none, Amiloride, genistein, and chlorpromazine. Scale bar: $20 \mu\text{m}$.

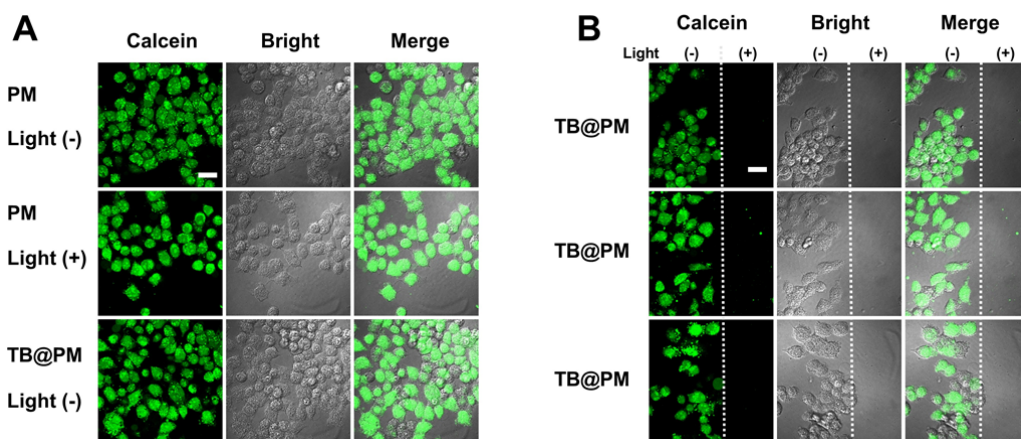


48

49 **Supplementary Figure 11.** Detection of intracellular ROS production by DCFH-DA in HeLa
 50 cells after incubation with TB@PM micelles (A), TB@PMP micelles (B) and Ce6@PMP micelles
 51 (C) respectively, without or with light irradiation (white light, 100 mW cm⁻², 3 min) (the
 52 parameters of green light channel of all samples were adjusted to a high level compared to Figure
 53 3C and D). Scale bar: 20 μm.

54

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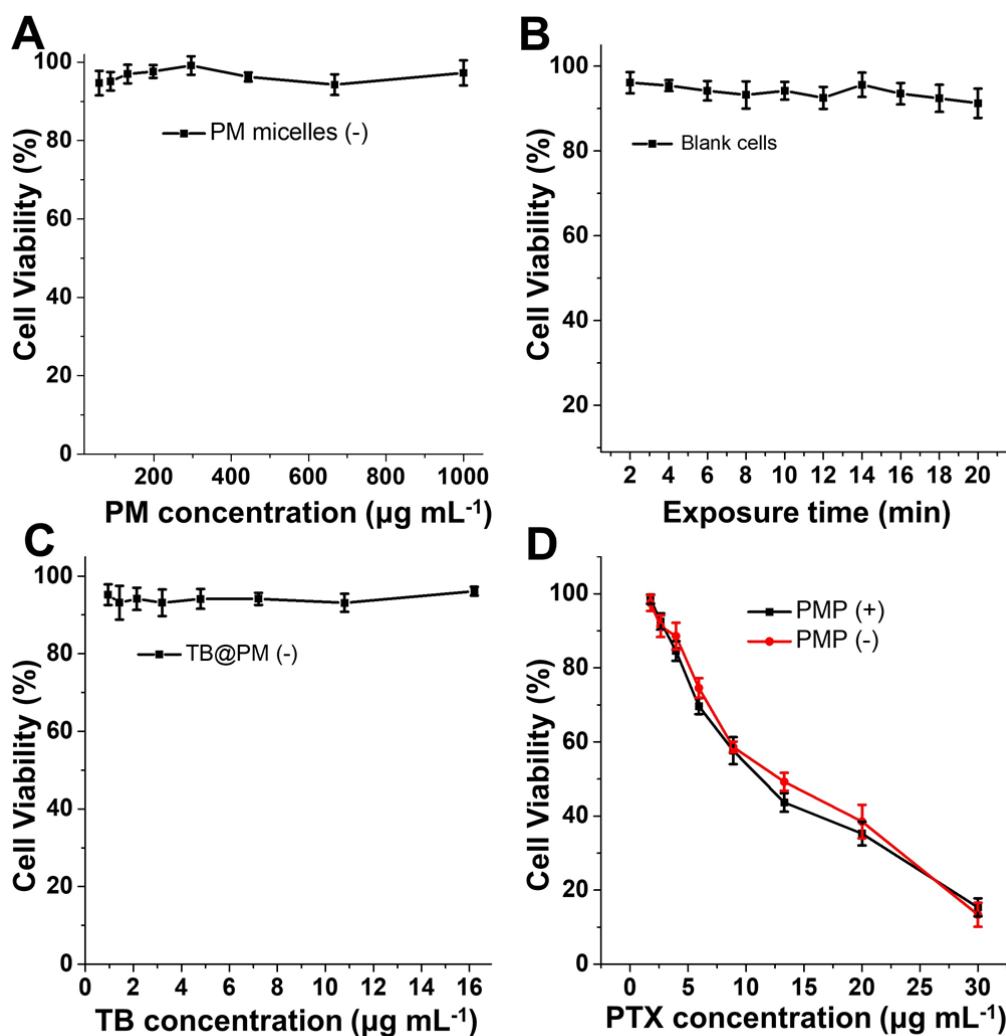


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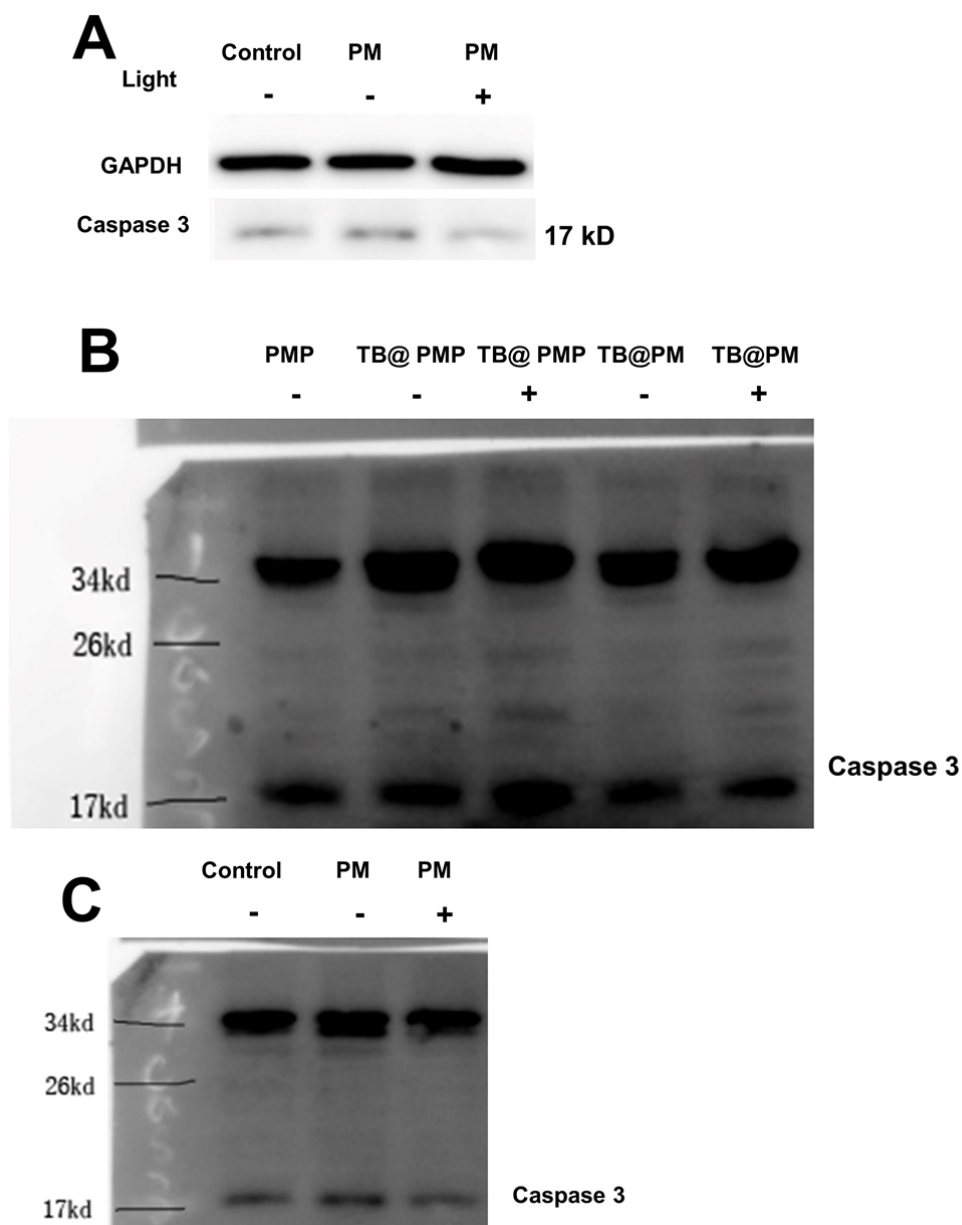
57 **Supplementary Figure 12. A) and B)** PM, TB@PM micelles were without or with light
 58 irradiation (white light, 100 mW cm⁻², 20 min) incubated with HeLa cells for 12 h. The cells on
 59 the left of the dotted white line were without light irradiation, and the right ones were with light
 60 irradiation. Scale bar: 20 μm.

61

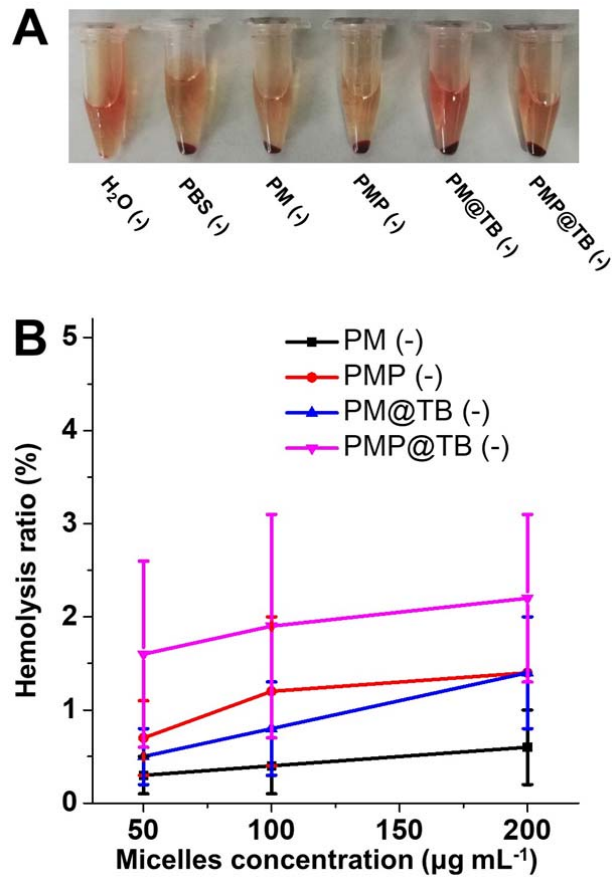
62



Supplementary Figure 13. CCK-8 assay of **A)** PM (-), **B)** different times at a power density of 100 mW cm^{-2} , **C)** TB@PM (-), and **D)** PMP (-), PMP (+) (white light, 100 mW cm^{-2} , 10 min) in HeLa cells after incubation for 48 h.



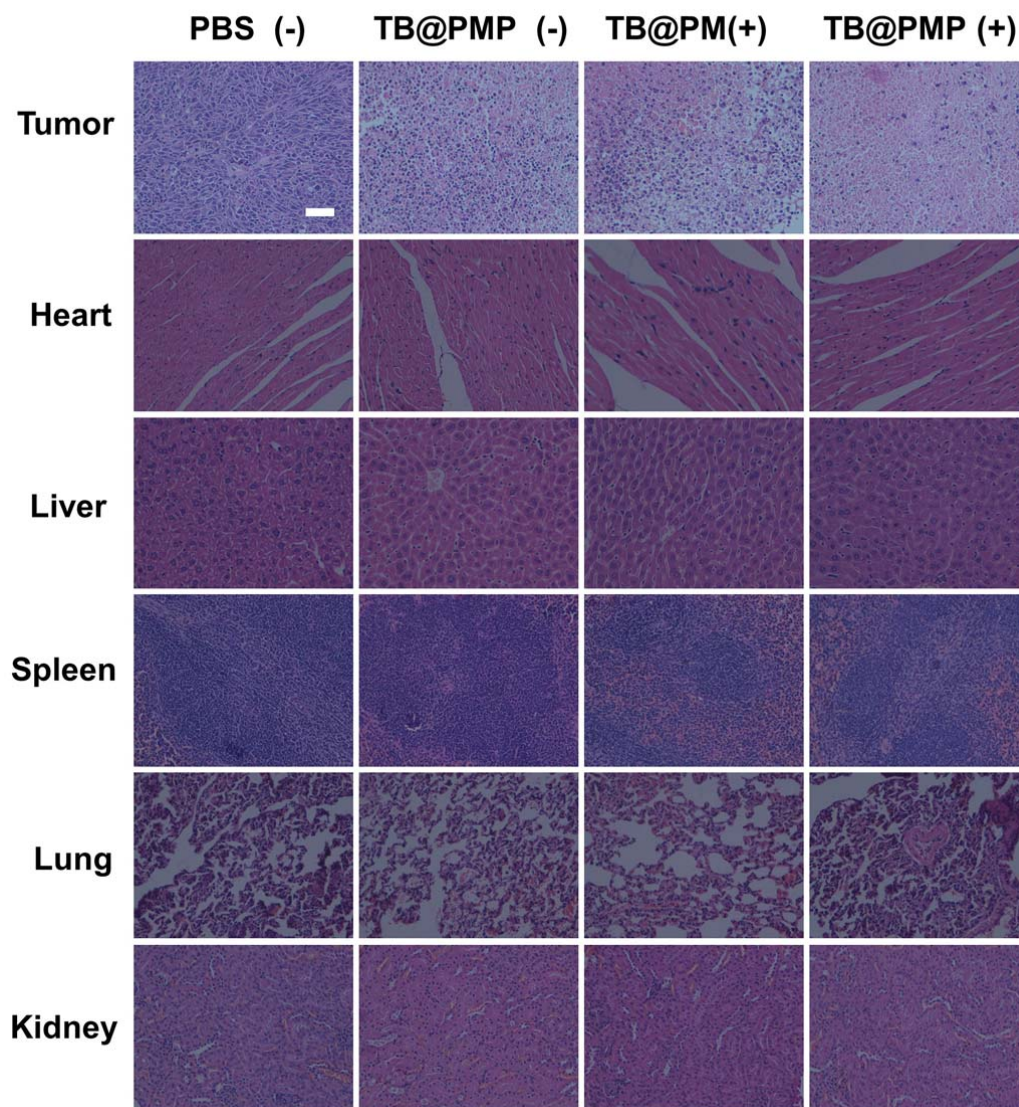
Supplementary Figure 14. A) Expressions of caspase 3 in HeLa cells of control group (-), PM (-), PM (+) (white light, 100 mW cm⁻², 10 min), GAPDH was used as a control; **B** and **C)** original blot images of caspase 3 in HeLa cells of Figure 5F and Supplementary Figure 14A, respectively.



75

76 **Supplementary Figure 15. A)** Photographs of hemolysis assay after incubation with ultrapure
 77 water (positive control), PBS (negative control), and PM, PMP, TB@PM, and TB@PMP micelles
 78 for 3 h in dark. The presence of large amounts of hemoglobin in the supernatant is observed only
 79 in the positive control tub saline; **B)** The hemolysis ratio induced by PM, PMP, TB@PM, and
 80 TB@PMP micelles with different concentration incubated at 37 °C for 3 h in dark.

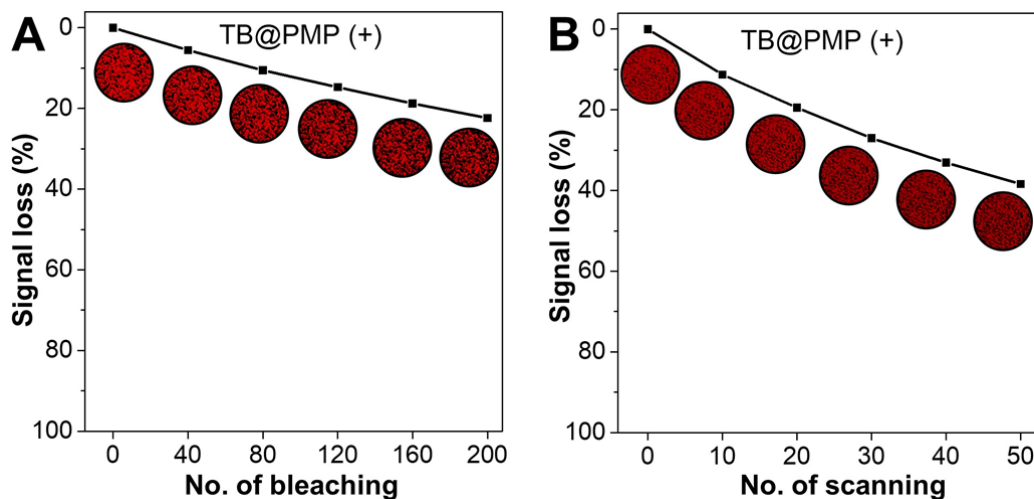
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82

83 **Supplementary Figure 16.** H&E staining images of the tumor organs obtained from the mice
84 after different treatments: intravenous injection of different samples: PBS, TB@PM, and
85 TB@PMP micelles and light irradiation treatment or not (532 nm, 250 mW cm⁻² for 30 min).
86 Scale bar: 100 μm.

87



88

89 **Supplementary Figure 17. A)** Signal loss (%) of fluorescent emission of tumor tissue treatment
 90 by TB@PMP (+) with increasing number of bleaching. Inset: Corresponding CLSM images of
 91 tumor tissue. 2.05 μ s per pixel, irradiation time: 6.201 s per bleaching; bleaching wavelength: 488
 92 nm; bleaching intensity: 50%; **B)** Signal loss (%) of fluorescent emission of tumor tissue treatment
 93 by TB@PMP (+) with increasing number of scans. Inset: CLSM images of tumor tissue; 4.01 μ s
 94 per pixel, irradiation time: 40.27 s per scan; scan wavelength: 488 nm; scan intensity: 8.6%.

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