

A high water-soluble triblock conjugated polymer for *in vivo* NIR-II imaging and photothermal therapy of cancer

Xiaomei Lu,^{*,#,a} Pengcheng Yuan,^{#,b} Wansu Zhang,^b Qi Wu,^a Xiaoxiao Wang,^a Meng Zhao,^a Pengfei Sun,^{*,b} Wei Huang,^c and Quli Fan^{*,b}

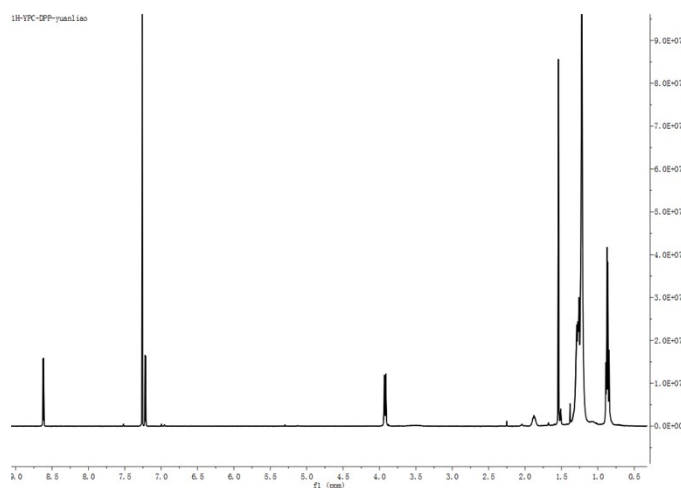


Fig. S1 ¹H-NMR spectra of DPP in CDCl₃.

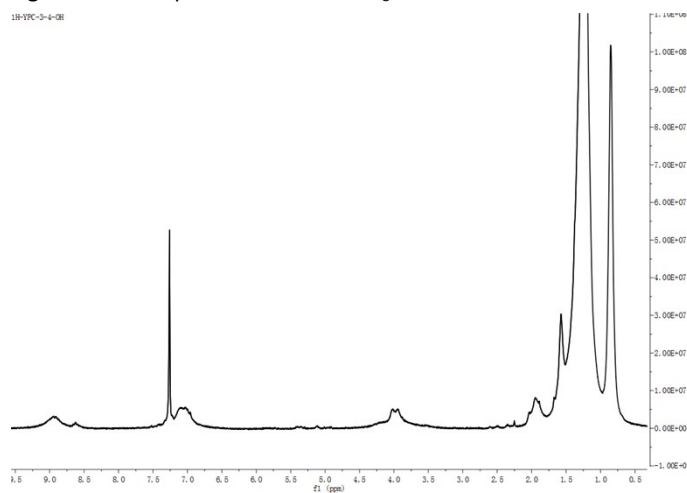


Fig. S2 ¹H-NMR spectra of DPP-OH in CDCl₃.

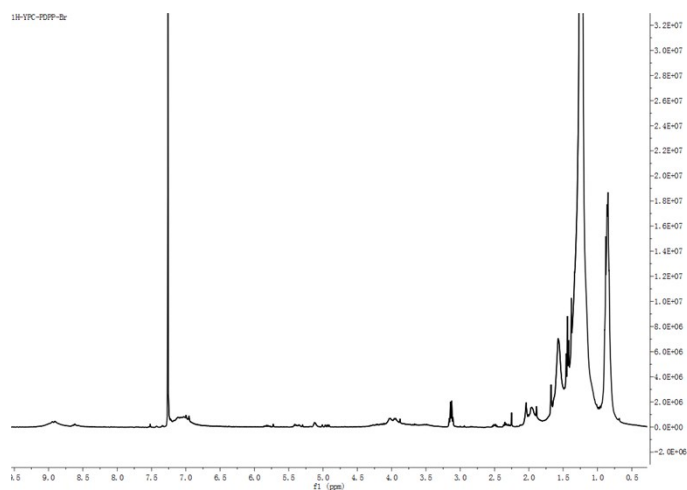


Fig. S3 ¹H-NMR spectra of DPP-Br in CDCl₃.

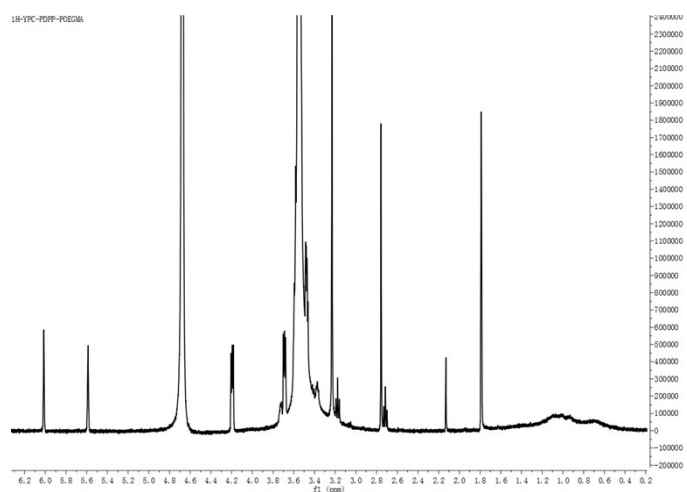


Fig. S4 ¹H-NMR spectra of POEGMA-*b*-PDPP-*b*-POEGMA in D₂O.

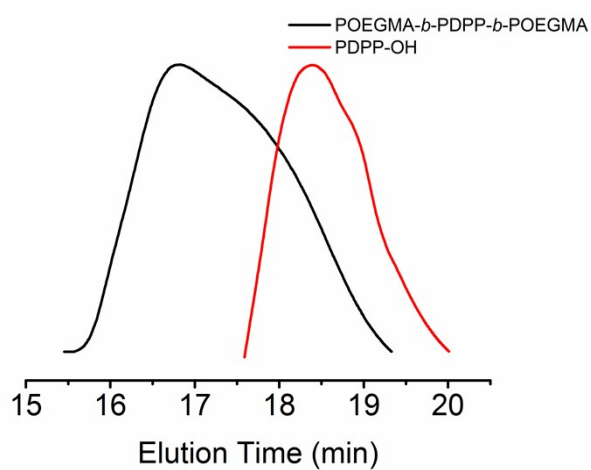


Fig. S5 GPC of PDPP-OH, POEGMA-*b*-PDPP-*b*-POEG.

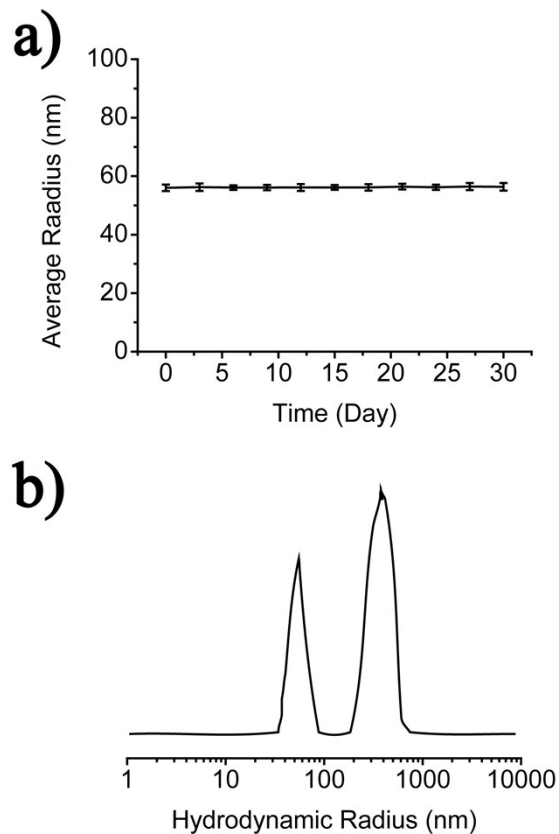


Fig. S6 (a) Average hydrodynamic radius of the *POEGMA-b-PDPP-b-POEGMA* stored in PBS for different time periods (0-30 days). (b) Representative DLS of *encapsulated nanomaterials* (PDPP-DSPE-PEG NPs) 30 days post preparation in PBS (pH = 7.4).

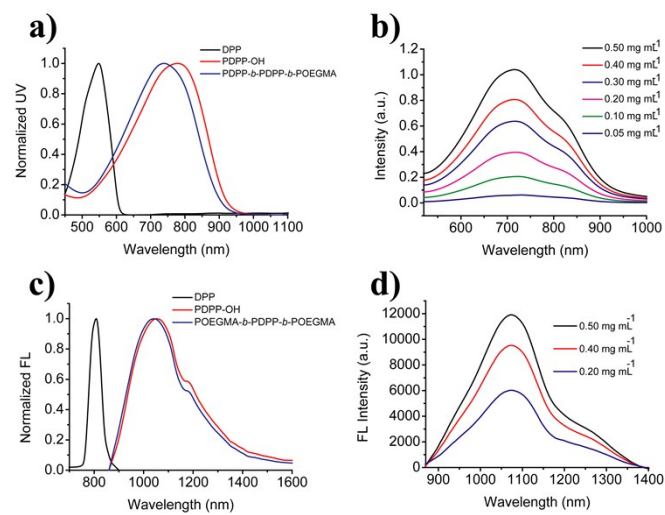


Fig. S7 UV and FL Spectra. (a) Normalized UV/vis/NIR spectra of PDPP, PDPP-OH, POEGMA-*b*-PDPP-*b*-POEGMA in DCM. (b) Normalized UV/vis/NIR spectra of PDPP, PDPP-OH, POEGMA-*b*-PDPP-*b*-POEGMA in H₂O. (c) FL spectra of PDPP, PDPP-OH, POEGMA-*b*-PDPP-*b*-POEGMA in DCM. (d) FL spectra of POEGMA-*b*-PDPP-*b*-POEGMA in H₂O.

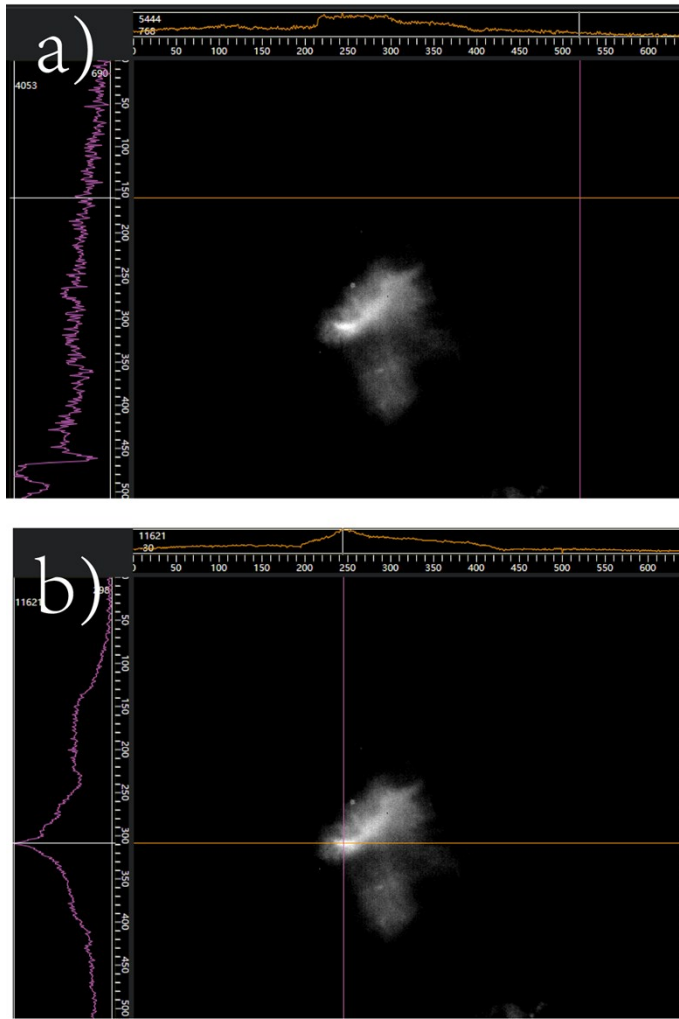


Fig. S8 Signal-to-background ratio (SBR) of Hep G2 tumor from mice injected with POEGMA-*b*-PDPP-*b*-POEGMA.

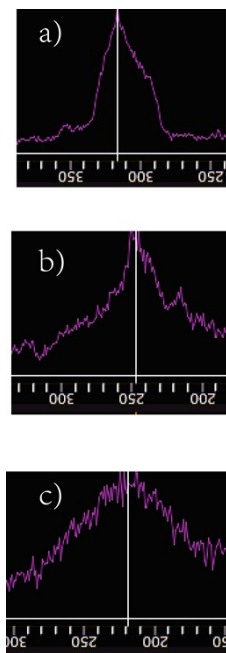


Fig. S9 Signal-to-background ratio (SBR) of NIR-II images from meat injected with POEGMA-*b*-PDPP-*b*-POEGMA at different depth (3mm, 5mm, 7mm).

Quantum yield test. The fluorescence quantum yield of POEGMA-*b*-PDPP-*b*-POEGMA was measured in a similar way to previous method. ¹ A home build setup was used to measure the fluorescence spectra in the region of 900-1600 nm using an array detector (Princeton OMA-V) and a spectrometer (Acton SP2300i) under an 808 nm diode laser excitation (RMPC lasers, 160 mW). During emission measurements, one 850-nm (Thorlabs), one 1000-nm (Thorlabs), one 1100-nm (Omega), and one 1300-nm (Omega) short-pass filter were used as excitation filters and one 900-nm long-pass filter (Thorlabs) was used as emission filter. The obtained emission spectra were further corrected by the detector sensitivity profile and the absorbance features of the filter. The fluorescence quantum yield was determined against the reference fluorophore IR1061 with a known quantum yield of 0.50% (Φ_{st}) in aqueous solution. All samples were measured at 25 °C, and reference fluorophore IR1061 was used with optical density (OD) of 0.08 at 808 nm. Their NIR-II fluorescence emission intensities were measured under the same 808 nm excitation. The intensity read out from the InGaAs camera was a spectrally integrated total emission intensity in the 900-1400 nm region. Using the measured optical density (OD) at 808 nm and spectrally integrated fluorescence intensity (F), the quantum yield of the test sample can be calculated according to the following equation:

$$\begin{aligned}\Phi_x(\lambda) &= \Phi_{st}(\lambda) \times \frac{F_x}{F_{st}} \times \frac{A_{st}(\lambda)}{A_x(\lambda)} \\ &= \Phi_{st}(\lambda) \times \frac{F_x}{F_{st}} \times \frac{1 - 10^{-OD_{st}(\lambda)}}{1 - 10^{-OD_x(\lambda)}}\end{aligned}$$

References

- 1 S. Diao, G. Hong, J. T. Robinson, L. Jiao, A. L. Antaris, J. Z. Wu, C. L. Choi, H. J. Dai, *J. Am. Chem. Soc.*, 2012, **134**, 16971.