



Supporting Information

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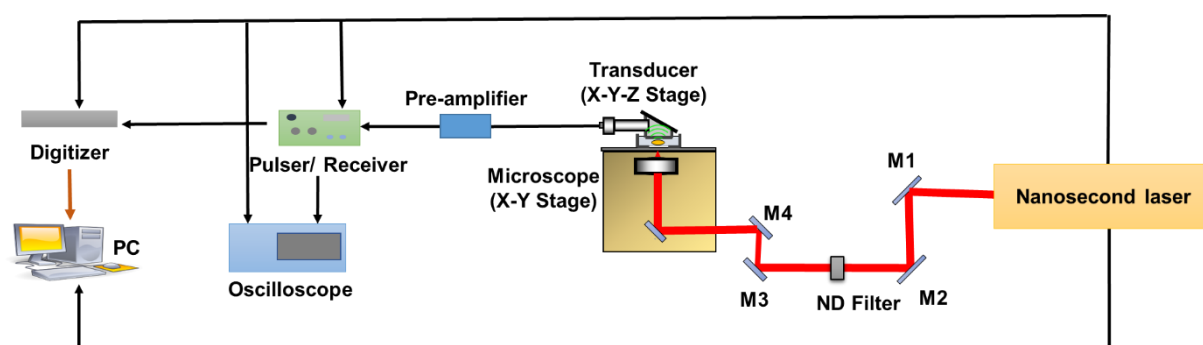
Functionalized NIR-II Semiconducting Polymer Nanoparticles
for Single-cell to Whole-Organ Imaging of PSMA-Positive
Prostate Cancer

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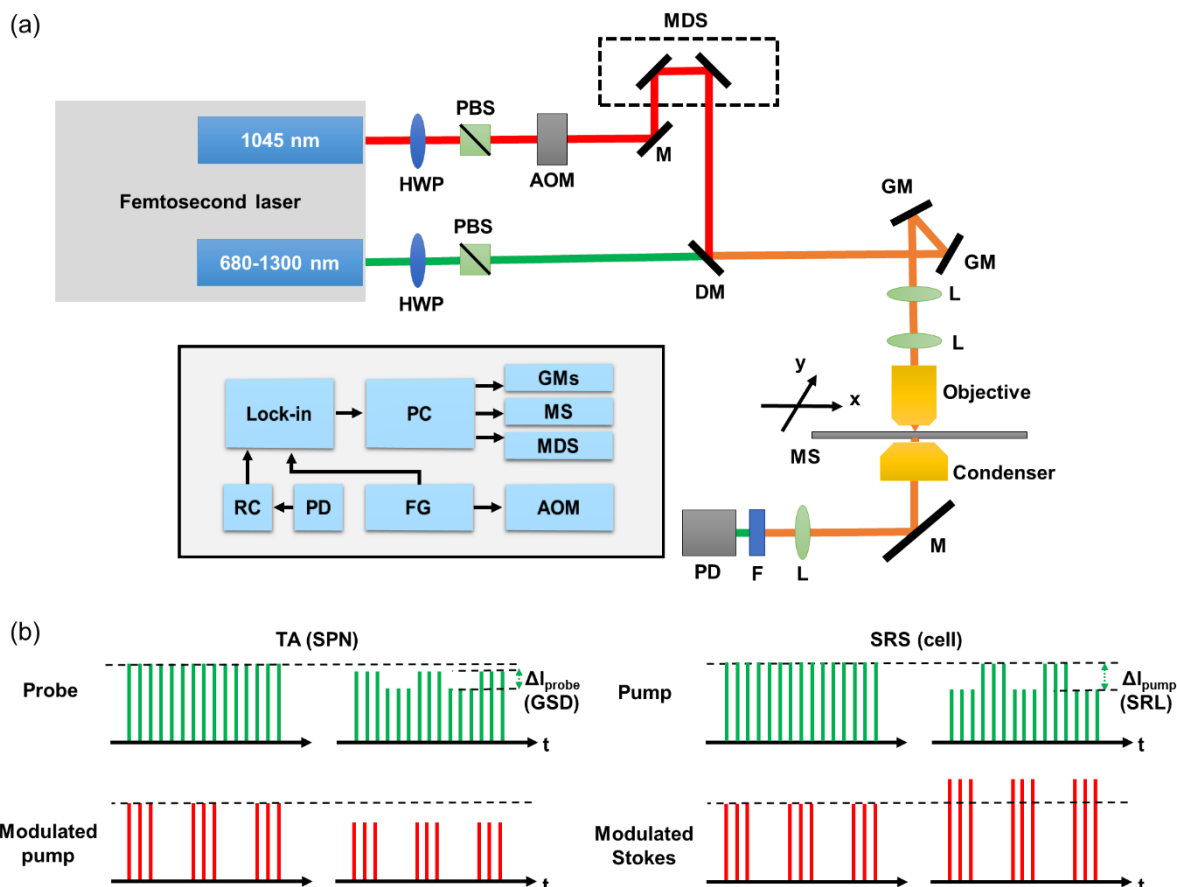
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Functionalized NIR-II Semiconducting Polymer Nanoparticles for Single-Cell to Whole-Organ Imaging of PSMA-Positive Prostate Cancer

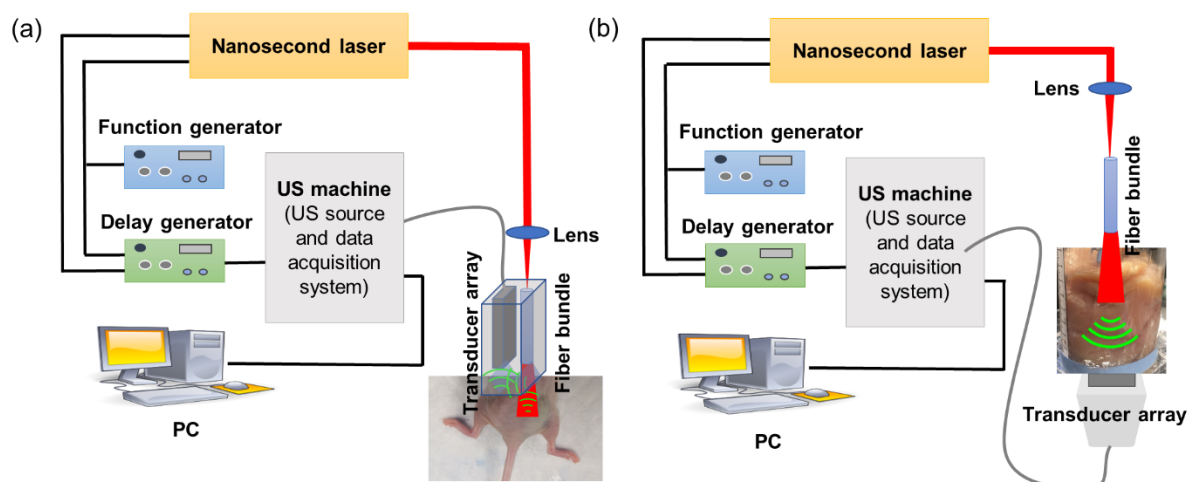
Jiayingzi Wu, Hyeon Jeong Lee, Liyan You, Xuyi Luo, Tsukasa Hasegawa, Peng Lin, Timothy Ratliff, Minoru Ashizawa, Jianguo Mei*, Ji-Xin Cheng*



Scheme S1: PA spectroscopy setup. M1, M2, M3, M4: mirrors.



Scheme S2: A multimodal TA/SRS microscope. TA: transient absorption. SRS: stimulated Raman scattering. a) Layout of the system. HWP: half-wave plate; PBS: polarization beam splitter; AOM: acousto-optic modulator; L: lens; M: mirror; DM: dichroic mirror; F: filter; GM: galvo mirror; PD: photodiode; PC: personal computer; MS: motorized stage; MDS: motorized delay stage; RC: resonant circuit; FG: function generator. b) Detection schemes of TA and SRS processes. GSD: ground-state depletion signal; SRL: stimulated Raman loss signal. In the TA process, the modulated 1045-nm laser beam is acting as the pump beam, and the other laser beam is acting as the probe beam. GSD signal is detected, when the absorption of the pump beam causes the less photons in the probe beam being absorbed. In the SRS process, the other laser beam is acting as the pump beam and the modulated 1045-nm laser beam is acting as the Stokes beam. SRL signal is detected, when the frequency difference between the pump and Stokes matches the vibrational transition of the chemical bond of interest.



Scheme S3: PA tomography setup with (a) reflection-mode or (b) transmission-mode detection. *In vivo* PA imaging and *ex vivo* imaging of organs and tumors were carried out with a reflection-mode detection. Imaging depth evaluation in chicken-breast tissue was carried out with a transmission-mode detection.

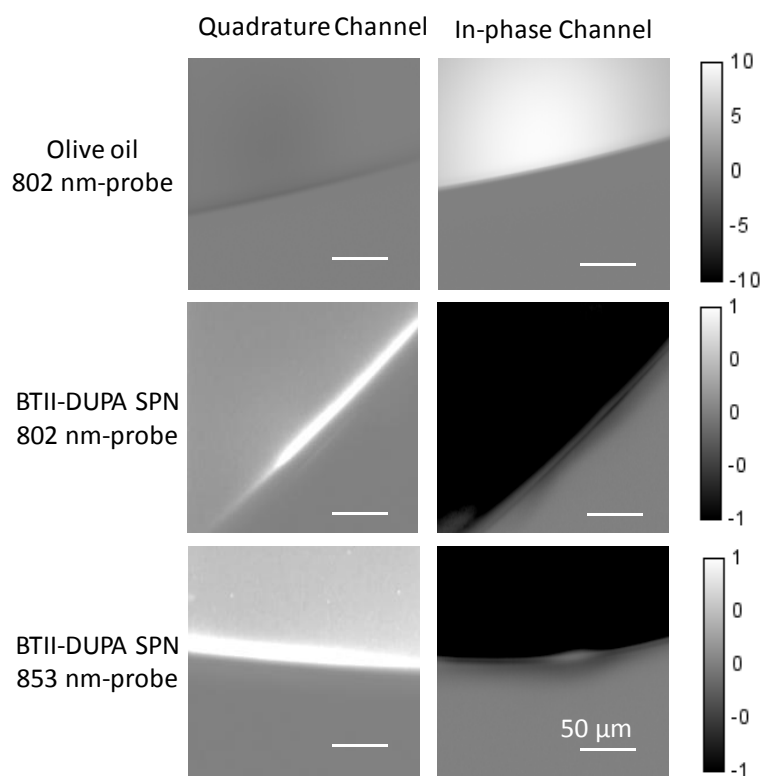


Figure S1. In-phase and quadrature-channel TA images of BTII-DUPA SPN and olive oil (a representative of C-H bonds). When imaging of olive oil, the power of pump beam was 100 mW at 1045 nm and the probe beam was 20 mW at 802 nm. When imaging of BTII-DUPA SPN, the power of pump beam was 10 mW at 1045 nm and the probe beam was 10 mW at 802 nm or 853 nm.

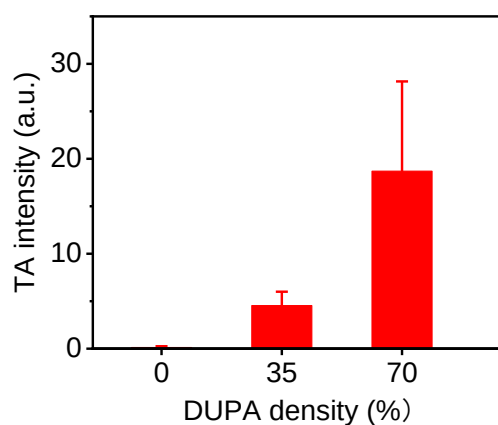


Figure S2. Quantification of TA intensity in LNCaP cells treated with different BTII-DUPA SPNs which have different DUPA functionalities (0%, 35% and 70%), respectively. Error bars represent for standard deviations.

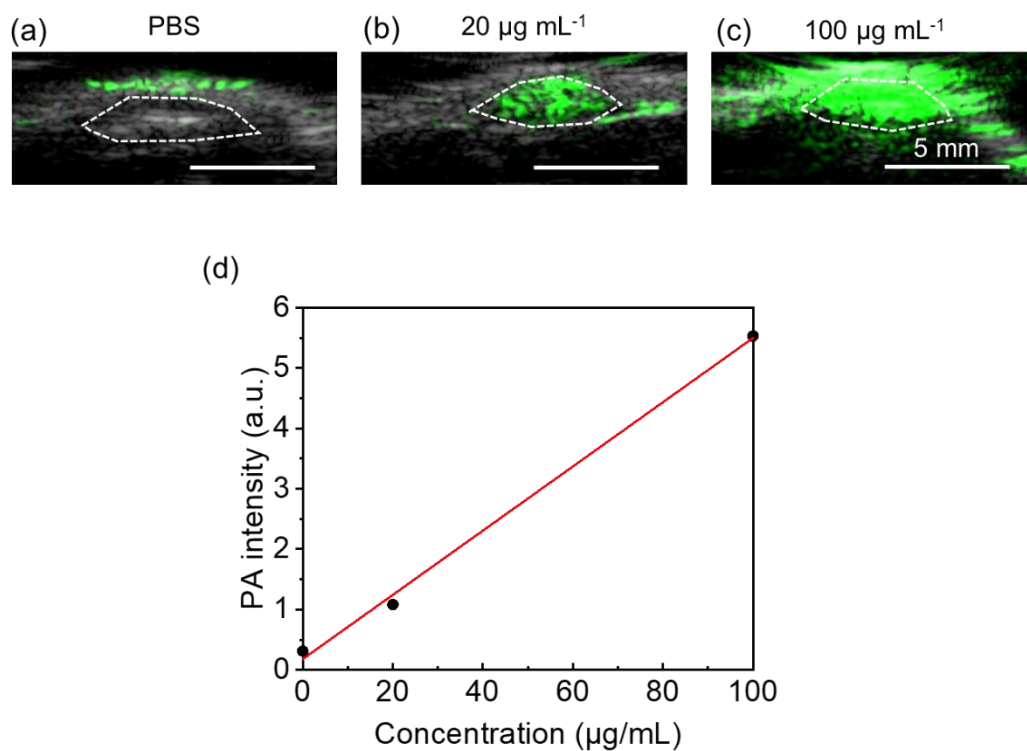


Figure S3. PA/US imaging of mouse skin with subcutaneous injection of 50 μl Marigel containing (a) PBS, (b) 20 $\mu\text{g mL}^{-1}$ BTII-DUPA SPN and (c) 100 $\mu\text{g mL}^{-1}$ BTII-DUPA SPN, respectively. (d) PA intensity as a function of BTII-DUPA SPN concentration and the corresponding linear fitting curve ($R > 0.99$)

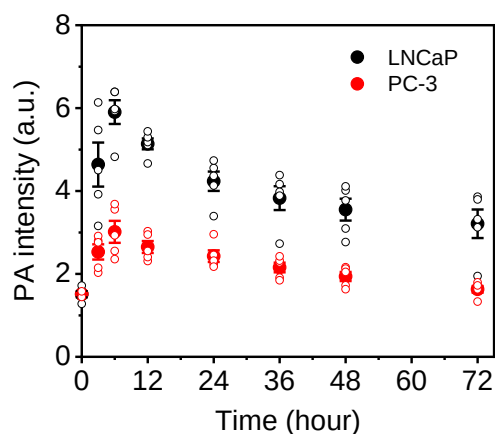


Figure S4. PA signal intensity in LNCaP and PC-3 tumors as a function over time. The data of 5 independent measurements are indicated by open circles. The averaged PA intensities from the 5 measurements are indicated by solid circles. Error represent for standard error of mean.

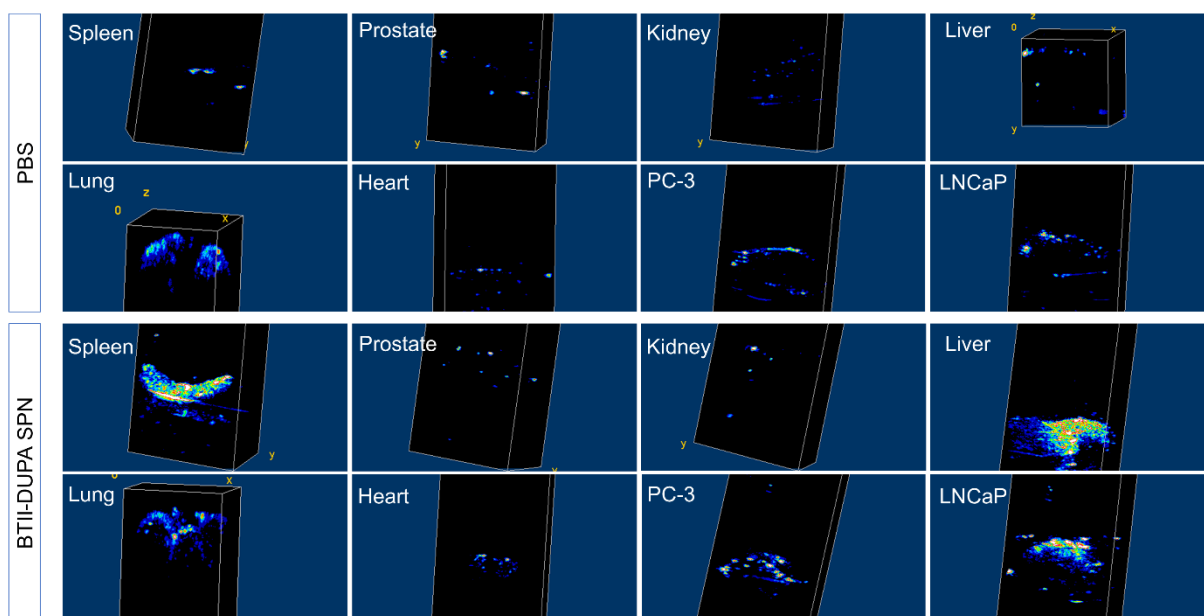


Figure S5. *Ex vivo* PA imaging of PC-3 tumor, LNCaP tumor and major organs 72 h after intravenous injection of PBS (200 μL) or BTII-DUPA SPN solution (200 μL , 800 $\mu\text{g mL}^{-1}$).

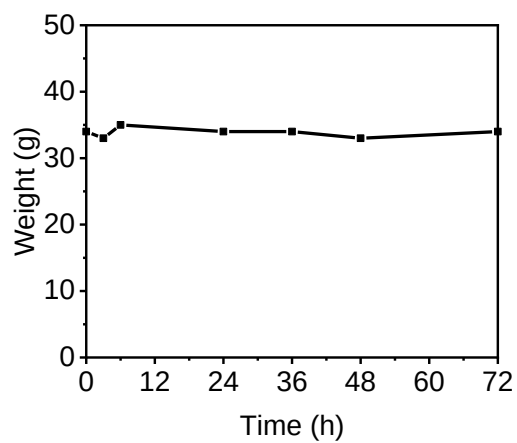
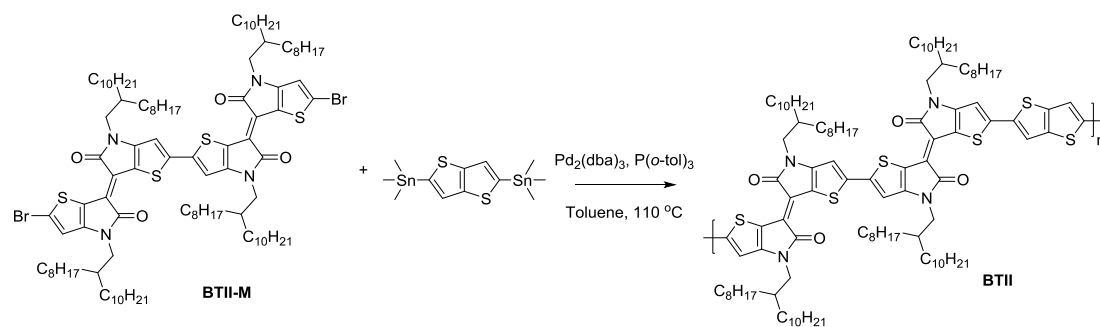


Figure S6. Body weight data of LNCaP- and PC-3- tumor-bearing mice after intravenous administration of BTII-DUPA SPN (200 μL , 800 $\mu\text{g mL}^{-1}$).



Scheme S4. Synthetic routes for BTII

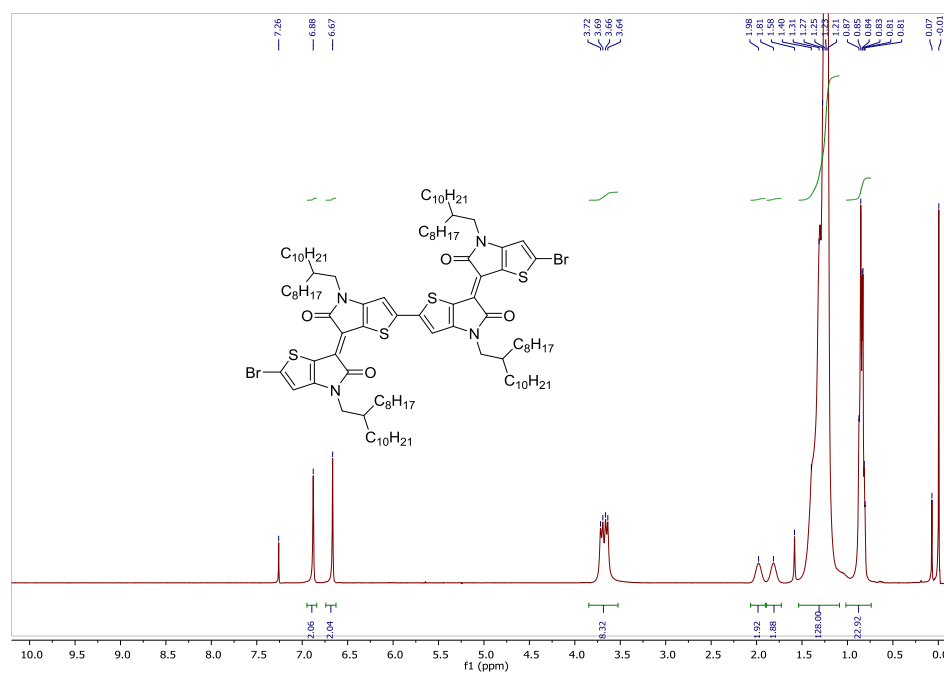


Figure S7. ^1H NMR spectrum of BTII-M.

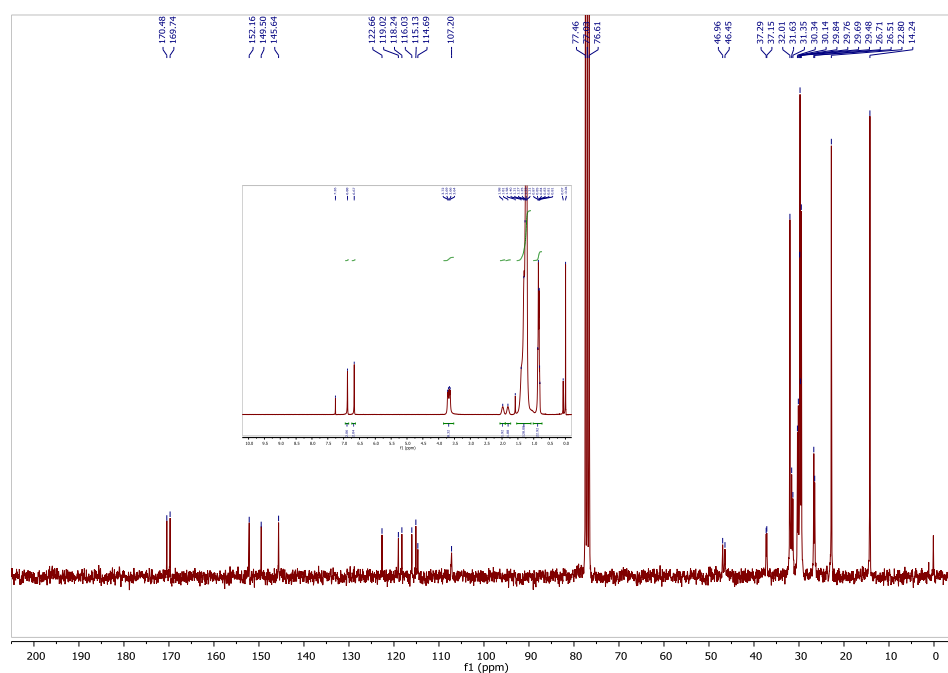
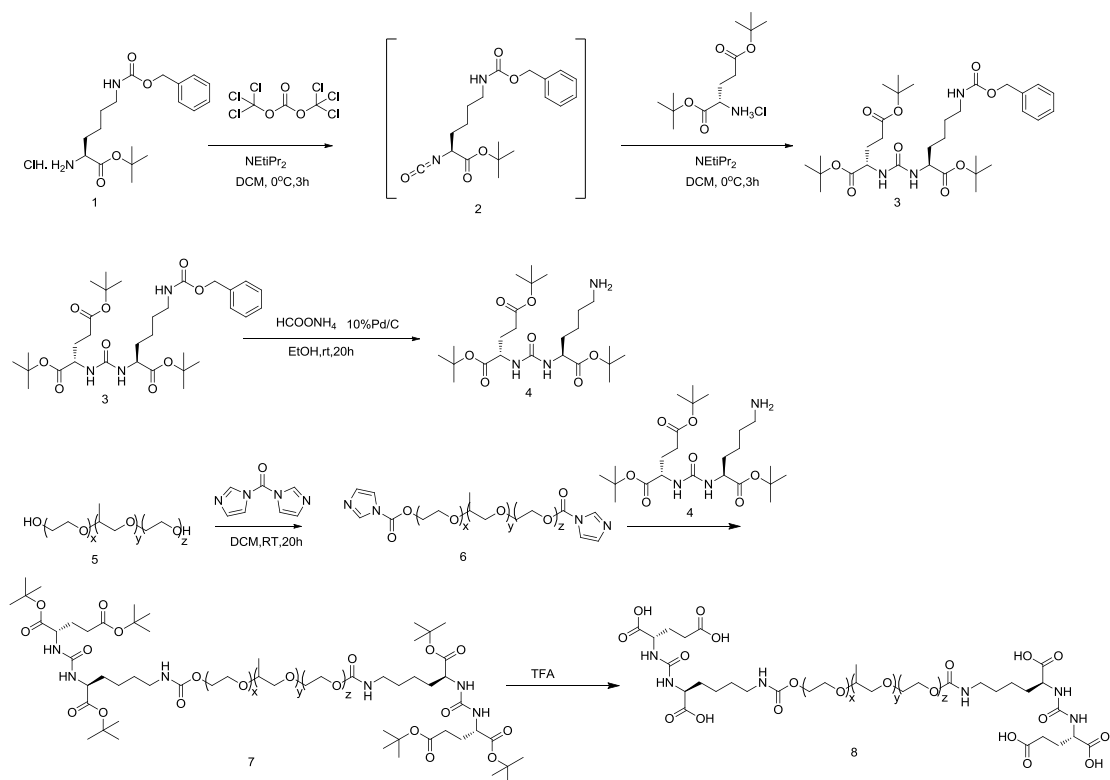


Figure S8. ^{13}C NMR spectrum of BTII-M.



Scheme S5. Synthetic routes for DUPA-F127-DUPA (Compound 8).

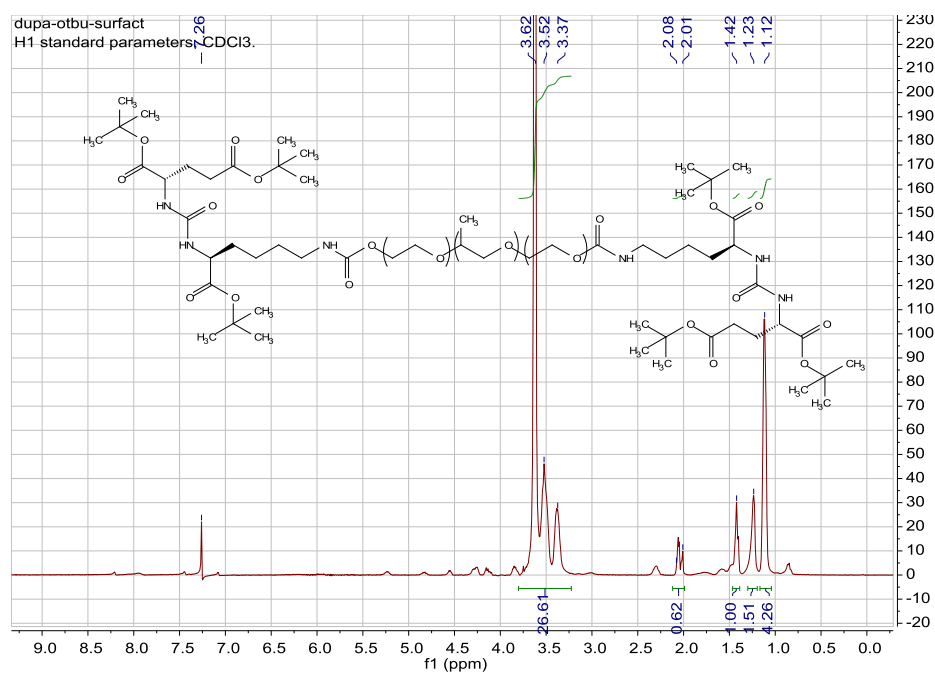


Figure S9. ^1H NMR spectrum of compound 7. (The peak at 1.42ppm is corresponding to the Boc H on DUPA, and this peak indicates the DUPA has been successfully added on the polymer.)

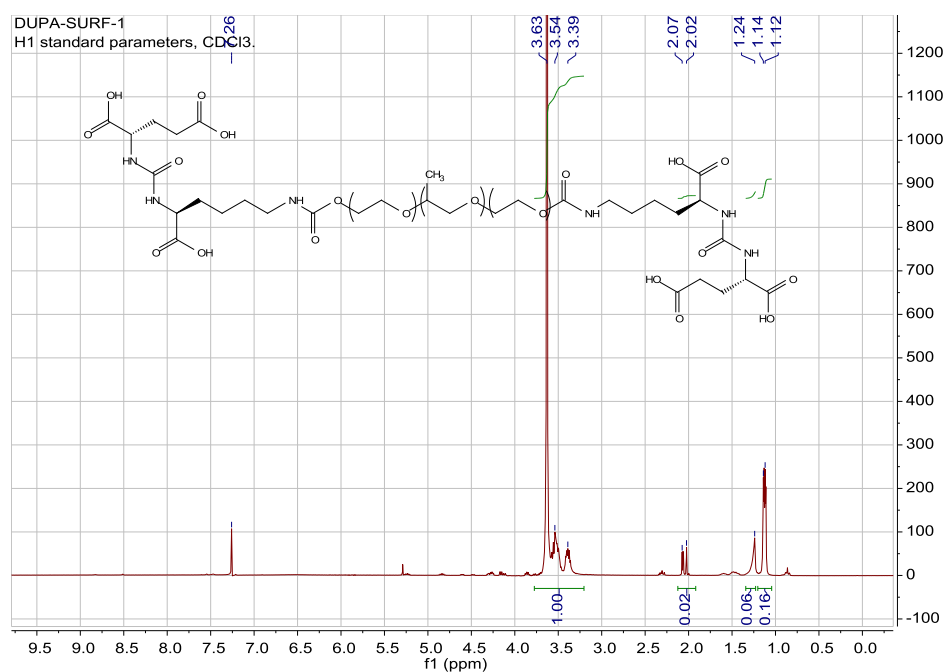


Figure S10. ^1H NMR spectrum of compound 8. (Compared with Figure S9, the peak at 1.42ppm disappears, this indicates the de-protect of DUPA.)