Supplementary Materials

Polypeptide micelles with dual pH activable dyes for sensing cells and cancer imaging

Ping Gong[†], Yueting Yang[†], Huqiang Yi, Shengtao Fang, Pengfei Zhang, Zonghai Sheng, Guanhui Gao, Duyang Gao, and Lintao Cai*

Guangdong Key Laboratory of Nanomedicine, Shenzhen Key Laboratory of Cancer Nanotechnology, Institute of Biomedicine and Biotechnology, Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, Shenzhen 518055, PR China.

Corresponding author: Shenzhen Institutes of Advanced Technology, Chinese Academy of Science, Shenzhen 518055, China.

Address correspondence: Tel: 86-755-86392210; Fax: 86-755-86392299; E-mail: lt.cai@siat.ac.cn (Lintao Cai).

Characterization of the Molecular Weight of PEG-PLL-PLLeu

The apparent molecular weight and polydispersity of each PEG-PLL-PLLeu was determined by gel permeation chromatography (VE2001 GPCmax, Malven Company) at 40°C and 2xPLgel 5 μ m MIXED-C 300x7.5mm column was used. Freeze-dried samples were dissolved in DMF and filtered on 0.45 μ m filters, before being injected in the apparatus. A calibration based on polyethylene glycol (PEG) standards (K=14.1×10⁻⁵ dL/g and α =0.7 at 40°C. in DMF) was employed on order to calculate the molecular weight from times of elution measured by the instrument. Flow rate was 1.0 mL/min, concentration of sample was 3.0-4.0 mg/mL and injection volume was 200 uL.

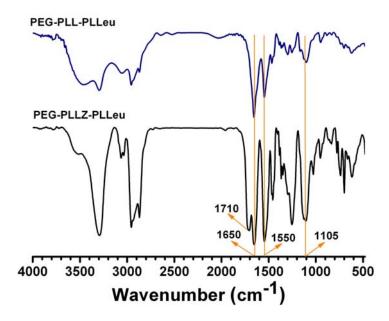


Fig. S1. FT-IR spectrum of PEG-PLLZ-PLLeu and PEG-PLL-PLLeu copolymers

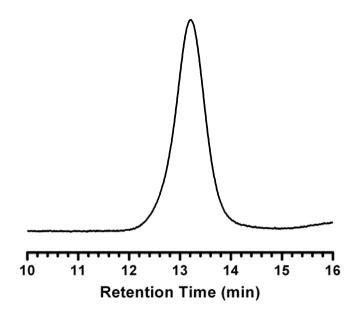


Fig. S2. Gel permeation chromatography (GPC) of PEG-PLL-PLLeu.

$$H_2N$$
 S_S H_1O $Rhodamine B$ N S_S NH_2

Fig. S3. Synthesis of rhodamine B-cystamine (RBLC)

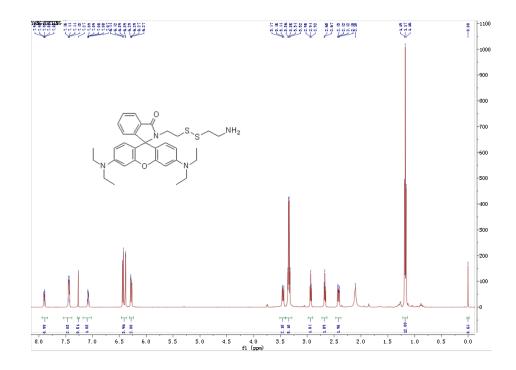


Fig. S4. Rhodamine B-cystamine (RBLC) was confirmed by HRMS. ¹H NMR (400 MHz, *d*₆ -DMSO, TMS) δ 1.17 (t, J = 7.05 Hz, 12H, *CH3*CH2), 2. 42 (t, J =8 Hz, 2H, CH2*CH*2S-), 2.67 (t, J = 6.05 Hz, 2H, -S*CH*2CH2), 2.94 (t, J = 6.05 Hz, 2H, -S*CH*2*CH*2), 3.34 (q, J=7.05 Hz, 8H, CH3*CH*2), 3.45 (t, J = 8 Hz, 2H, *CH*2CH2S-), 6.28 (dd, J = 8.9 Hz, 2.5 Hz, 2H, Xanthene-*H*), 6.39 (d, J = 2.5 Hz, 2H, Xanthene-*H*), 6.43 (d, J = 8.85 Hz, 2H, Xanthene-*H*), 7.07-7.10 (m, 1H, Ar-*H*), 7.41-7.47 (m, 2H, Ar-*H*), 7.88-7.91 (m, 1H, Ar-*H*).

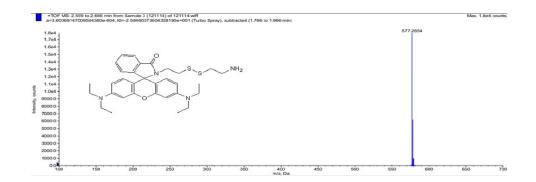


Fig. S5. Mass spectrum of RBLC. HRMS (EI) $m/z C_{32}H_{39}N_4O_2S_2^+(M^+)$: 577.2666. Found 577.2654.

Table S1. Encapsulation efficiency (EE) and drug loading efficiency (LE) of RBLC

PEG-PLL-PLLeu-FITC/RBLC feed molar	EE of RBLC (%)	LE of RBLC (%)
ratio		
13.5	66.5	4.7
5.4	53.4	8.9