Supporting Information of

Improved anti-tumor activity of novel redox-responsive paclitaxel-encapsulated liposomes based on disulfide phosphatidylcholine

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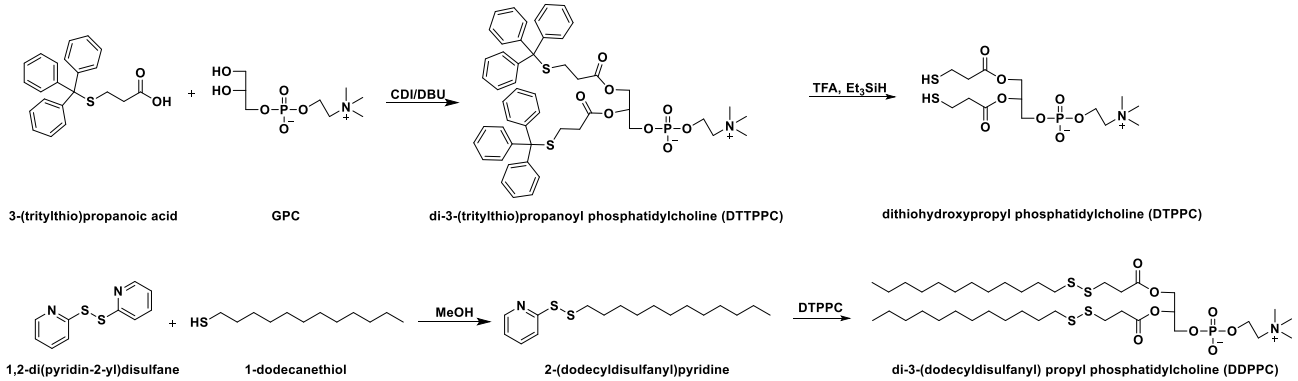
Scheme S1. Synthesis of SS-PC.



2.3. Critical aggregation concentration (CAC) and differential scanning calorimetry (DSC)

Critical aggregation concentration (CAC) of SS-PC was detected by pyrene fluorescence probe method [27]. SS-PC suspension (500 μg/mL) was 2-fold diluted to 0.49 μg/mL using Milli-Q water. Then, 10 mL of each sample was transferred into clean tubes with 0.04 mL of pyrene stock solution (6.08 mg/L). All the samples were vibrated for 4 h at 60 °C. Finally, the emission spectrum of each sample was detected with excitation wavelength of 334 nm by fluorescence spectrophotometer (Horiba Co., Kyoto, Japan). The peak intensity ratio of I_3 (384 nm)/I_1 (373 nm) (I_3/I_1) were recorded. The I_3/I_1 values were used to plot versus concentration in Log scale.

The phase transition temperature of SS-PC was detected by a differential scanning calorimeter (DSC, Gerätebau GmbH Thermal, Selb, Germany) using SS-PC sample (about 5 mg) with heating rate 5 °C/min from -40 °C to 80 °C.

The self-assembly ability of SS-PC was checked by measuring the critical aggregation concentration (CAC) using pyrene fluorescent probe method. As shown in Figure S7a, the CAC value was determined using the crossing point of the plot and was estimated to be 2.0 μg/mL, which indicated that SS-PC had great self-assembly ability due to its amphiphilic structure. The thermal performance of SS-PC was checked by differential scanning calorimetry (DSC). As shown in Figure S7b, the phase transition temperature (T_c) of SS-PC was detected as the peak of 37.8 °C.

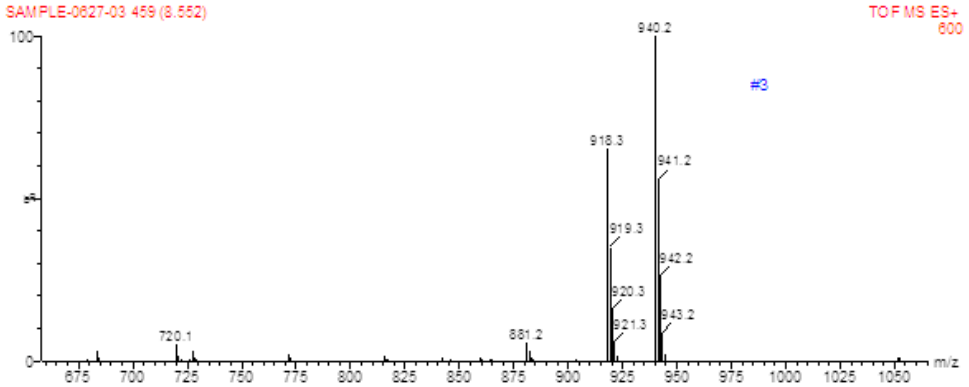


Figure S1. MS of di-3-(tritylthio)propanoyl phosphatidylcholine (DTTPPC), m/z $[M+H]^+$ calculated 918.3, found 918.3; $[M+Na]^+$ calculated 940.3, found 940.1.

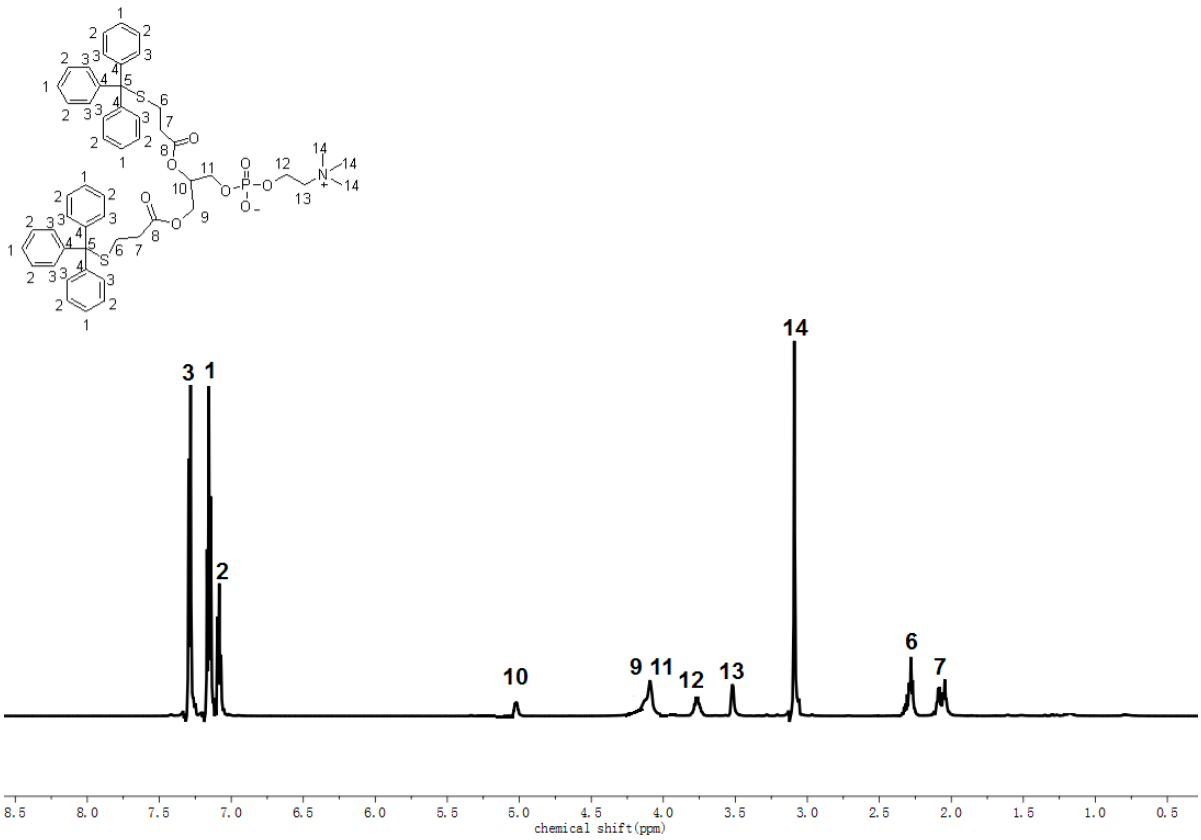


Figure S2. ^{1}H-NMR of di-3-(tritylthio)propanoyl phosphatidylcholine (300 MHz, $CDCl_3$, TMS): δ 2.10 (4H, q, J=7.0 Hz), 2.46 (4H, m), 2.71 (4H, m), 3.05 (4H, q, J=8.0 Hz), 3.09 (9H, s), 3.68 (2H, t, J=5.5 Hz), 3.97 (3H, m), 4.07 (2H, m), 4.19 (2H, m), 5.08 (2H, m), 5.23 (4H, d, J=6.5 Hz), 5.45 (4H, d, J=4.5 Hz), 6.95 6.99 (2H, s), 7.37 (2H, s), 7.40 (2H, d, J=2.0 Hz), 7.98 (2H, q, J=6.0 Hz).

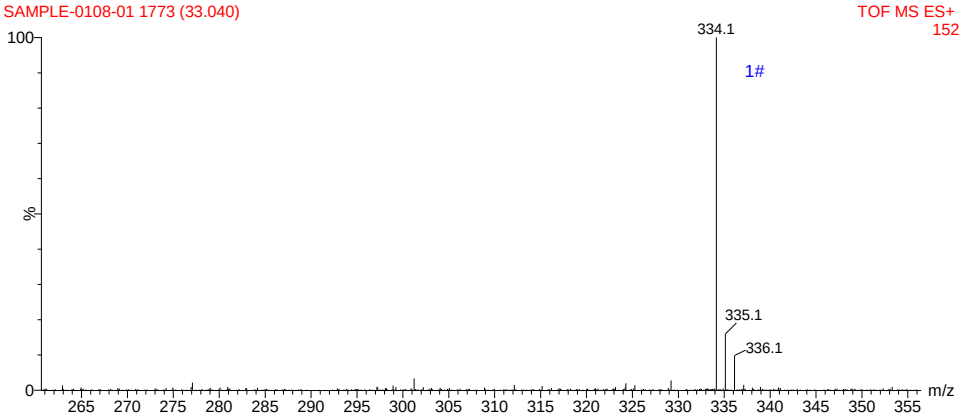


Figure S3. MS of 2-(dodecyldisulfanyl)pyridine, m/z $[M+Na]^+$ calculated 334.2, found 334.1.

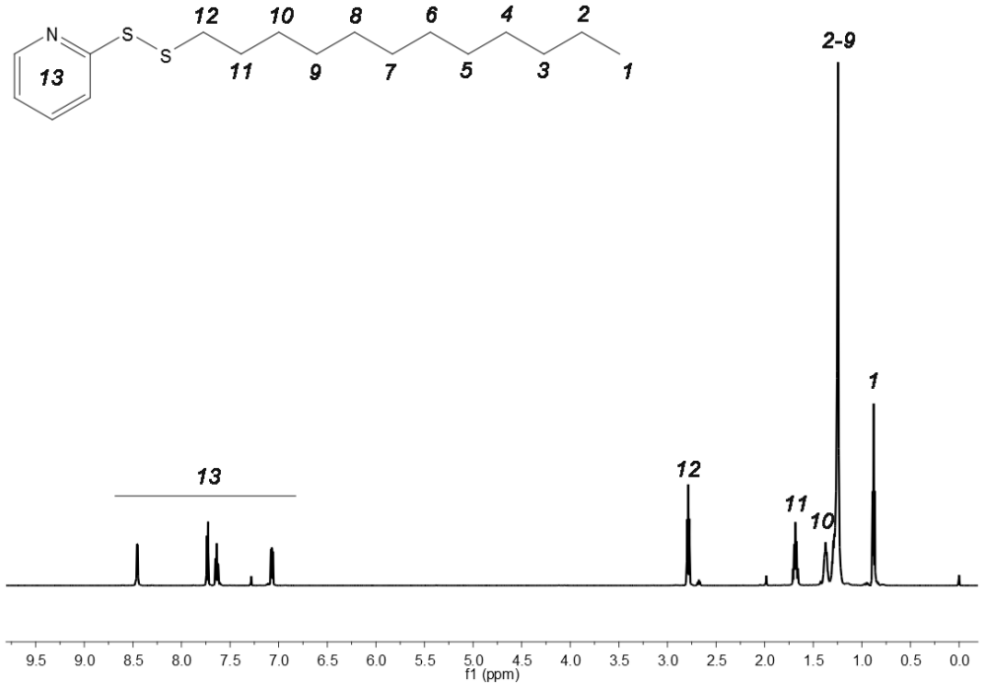


Figure S4. ^{1}H NMR of 2-(dodecyldisulfanyl)pyridine (300 MHz, $CDCl_3$, TMS): δ 0.88 (3H, s), 1.24 (14H, s), 1.37(2H, s), 1.68 (2H, t, J=4.5 Hz), 2.79 (2H, t, J=4.5 Hz), 7.07-8.46 (4H, m).

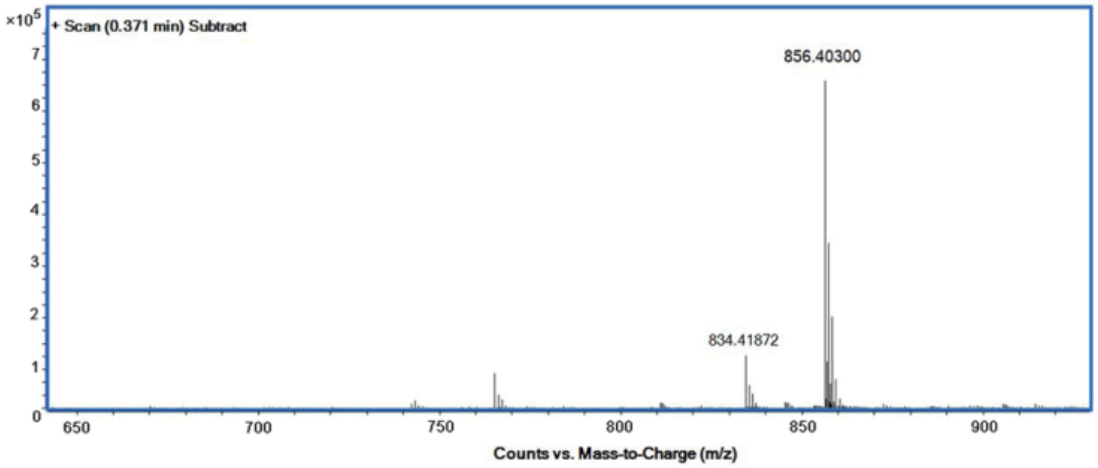


Figure S5. HRMS of SS-PC, calculated of $[M+H]^+$ 834.42, found 834.42, calculated of $[M+Na]^+$ 856.41, found 856.40.

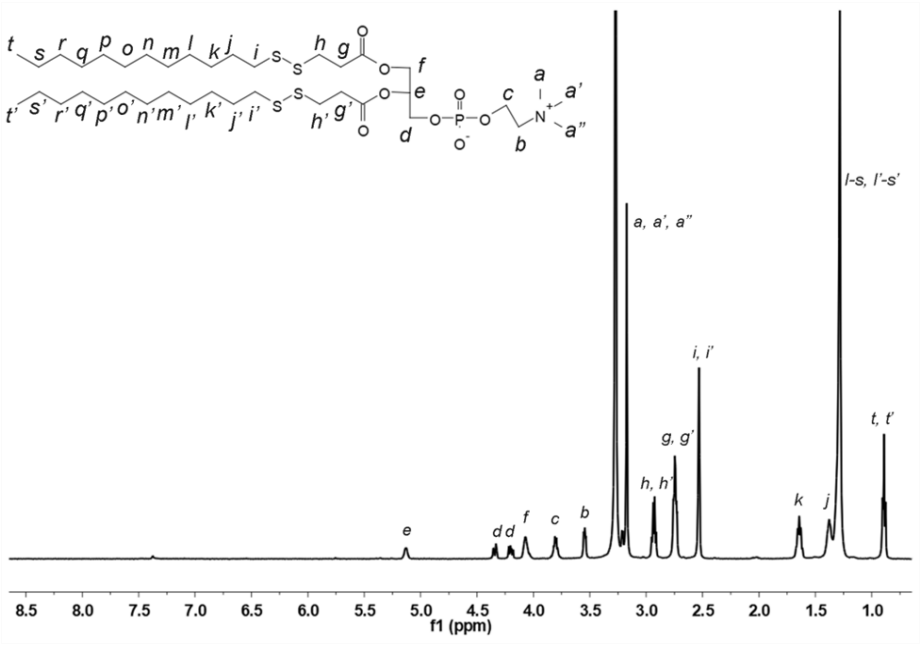


Figure S6. ^{1}H-NMR of SS-PC (300 MHz, $CDCl_3$, TMS): δ 0.89 (6H, t, J=4.5 Hz), 1.28 (32H, s), 1.38 (4H, s), 1.64 (4H, t, J=4.5 Hz), 2.53 (4H, s), 2.75 (4H, s), 2.93 (4H, d, J=6.0 Hz), 3.17 (9H, s), 3.54 (2H, s), 3.80 (2H, s), 4.07 (2H, s), 4.33 (1H, t, J=6.0 Hz), 4.41 (1H, t, J=6.0 Hz), 5.13 (1H, s).

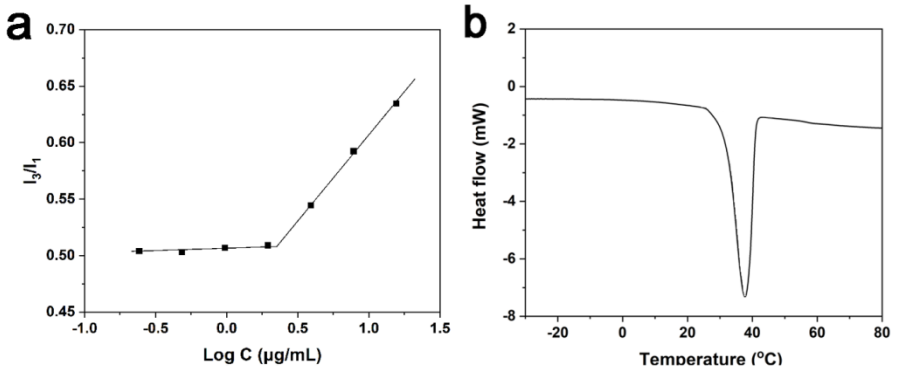


Figure S7. (a) CAC of SS-PC was determined using the crossing point of the plot and was estimated to be 2.0 μg/mL; (b) DSC curve of SS-PC, the phase transition temperature (T_c) of SS-PC was detected as the peak temperature of 37.8 °C.

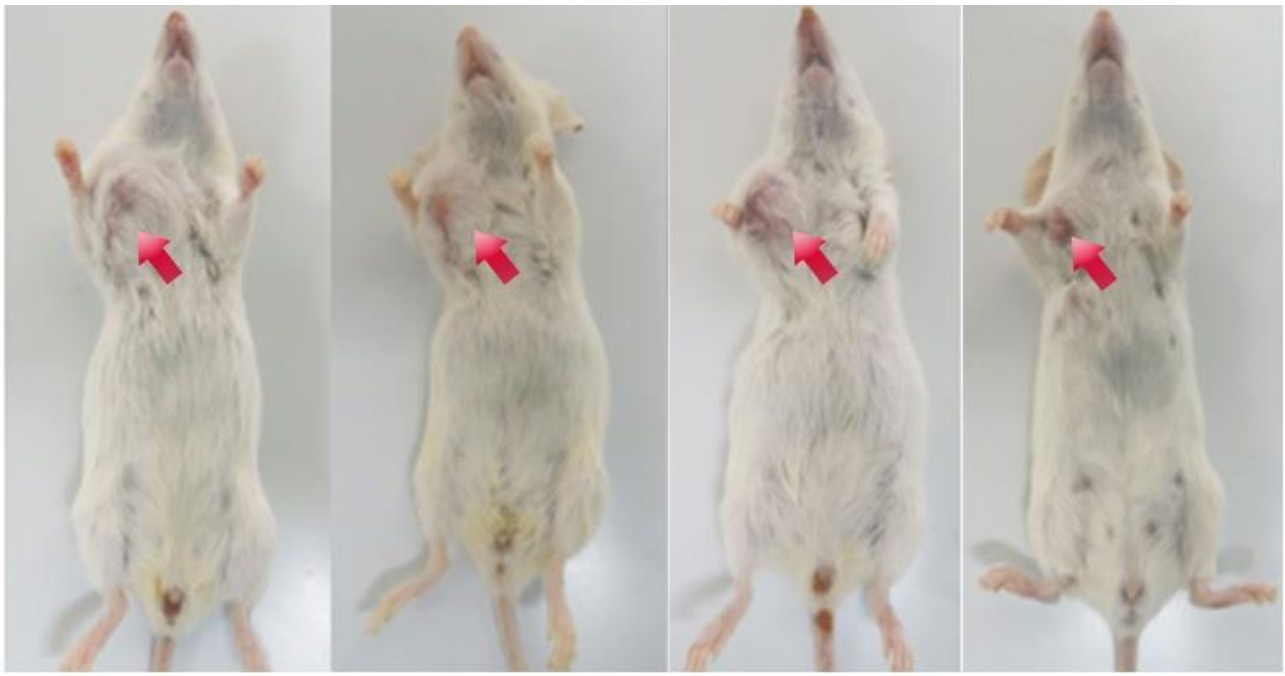


Figure S8. The photos of tumor-bearing mice after 21 days treatment in *in vivo* anti-tumor efficiency test.