Supporting Information

A Superior Fluorescent Probe for Detection of Cardiolipin

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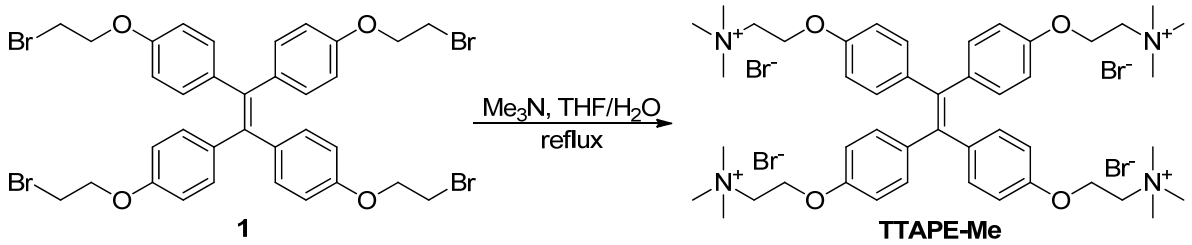
Experimental section

Synthesis of 1,1,2,2-Tetrakis[4-(2-trimethylammonioethoxy)-phenyl]ethene Tetrabromide (TTAPE-Me): Compound 1 was synthesized according to previous publications.[1] Quaternization of 1 with an excess amount of trimethylamine generated TTAPE-Me. Pale yellow powder; 85% yield. ^{1}H NMR (400 MHz, D2O), δ (ppm): 7.09 (d, 8H), 6.83 (d, 8H), 4.46 (t, 8H), 3.80 (t, 8H), 3.25 (s, 36H). ^{13}C NMR (100 MHz, D2O), δ (ppm): 155.4, 139.2, 137.4, 132.3, 113.7, 64.8, 61.6, 53.7. MS (TOF), m/e 855.6561 ([M–2Br–3CH3]$^{+}$, calcd. 855.6725).



Scheme S1. Synthetic route of TTAPE-Me.

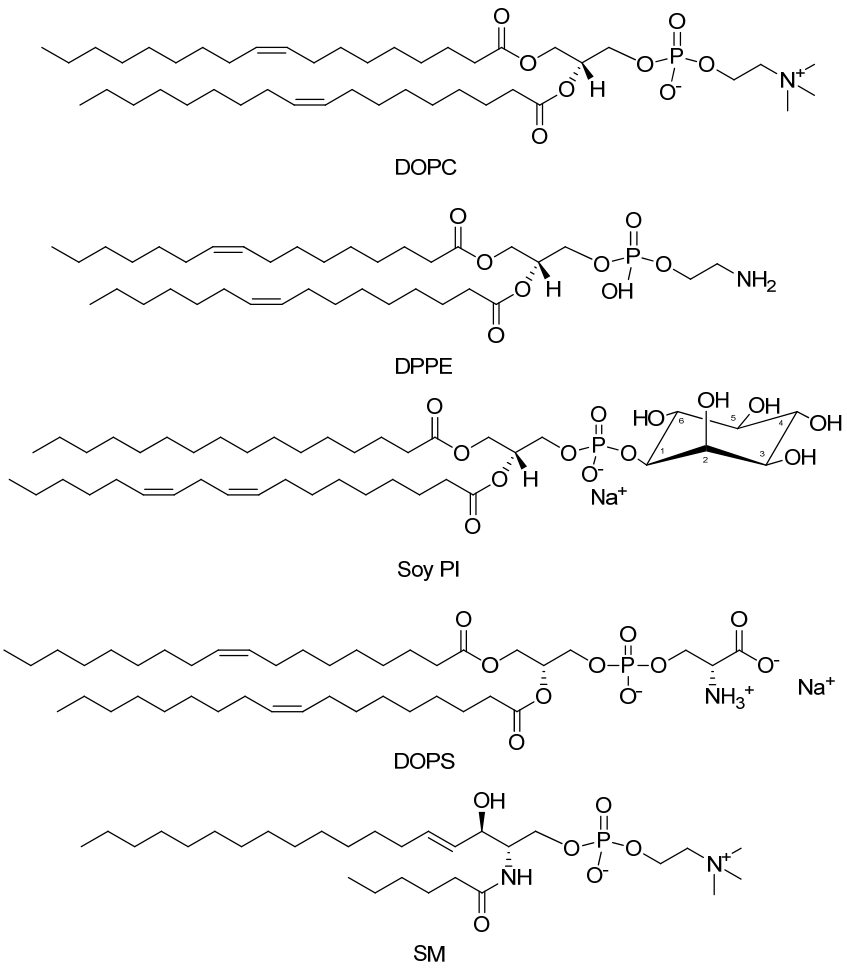


Chart S1. Chemical structures of DOPC (1,2-dioleoyl-*sn*-glycero-4-phosphocholine), DPPE (1,2-dipalmitoleoyl-*sn*-glycero-3-phosphoethanolamine), soy PI (L-α-phosphatidylinositol (Soy) (sodium salt)), DOPS (1,2-dioleoyl-*sn*-glycero-3-phospho-L-serine (sodium salt)), and SM (*N*-hexanoyl-D-sphingomyelin).

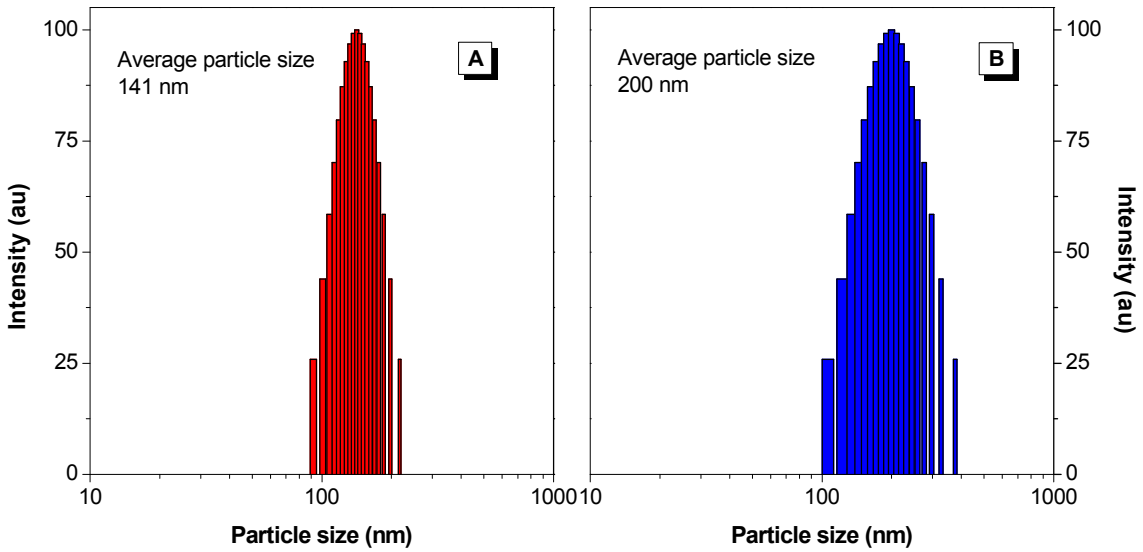


Figure S1. Particle analysis of (A) CL-containing and (B) CL-free vesicles. CL-containing and CL-free LUVs are composed of TOCL/DOPC (50 mol % TOCL) and pure DOPC, respectively, in a 25 mM HEPES buffer at pH 7.4 (vesicles for Figure 1–3). $[lipid]_{total}$ = 22 μM.

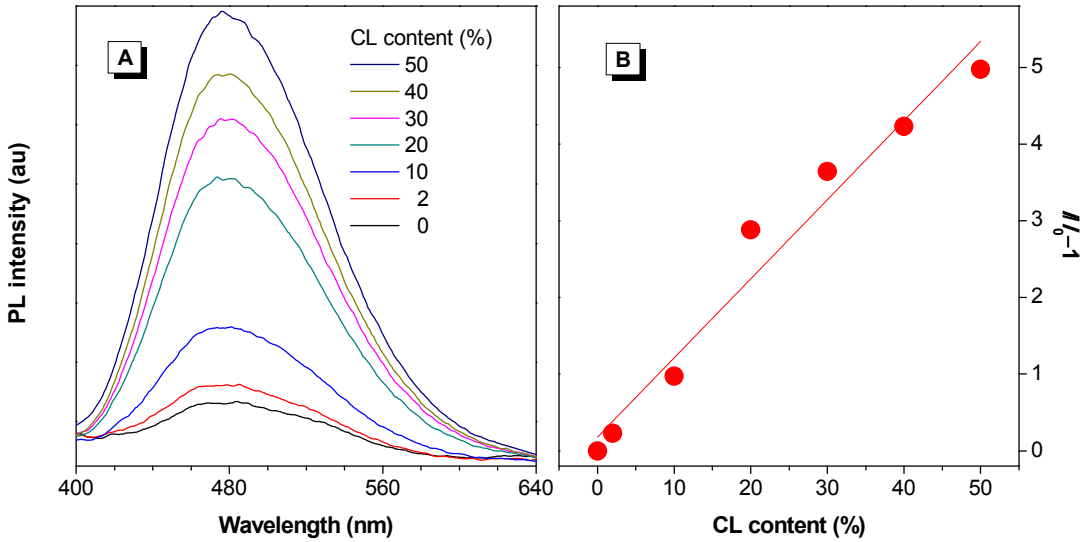


Figure S2. (A) Emission spectra of TTAPE-Me in the presence of LUVs with different CL content (2–50 mol % TOCL). (B) Plot of the fluorescence enhancement at 480 nm versus CL content. [dye] = 10 μM; $[lipid]_{total}$ = 22 μM; λ_{ex}= 350 nm.

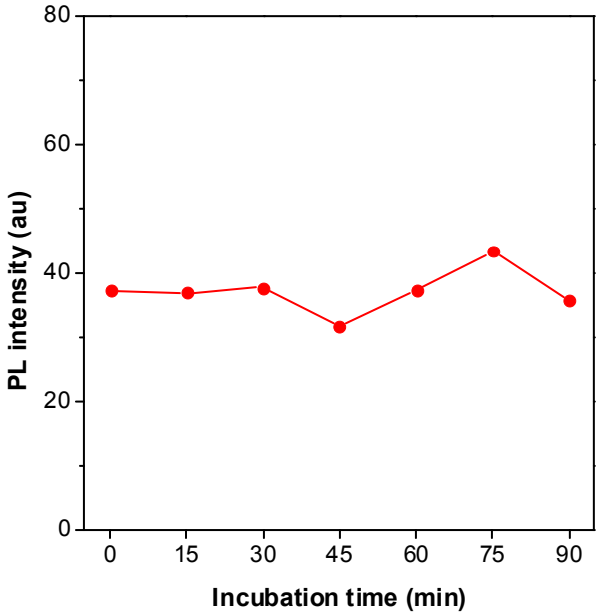


Figure S3. Changes with time in fluorescence intensity of TTAPE-Me (10 μM) upon addition to CL-containing LUVs ($[lipid]_{total}$ = 22 μM, 50 mol % of TOCL).

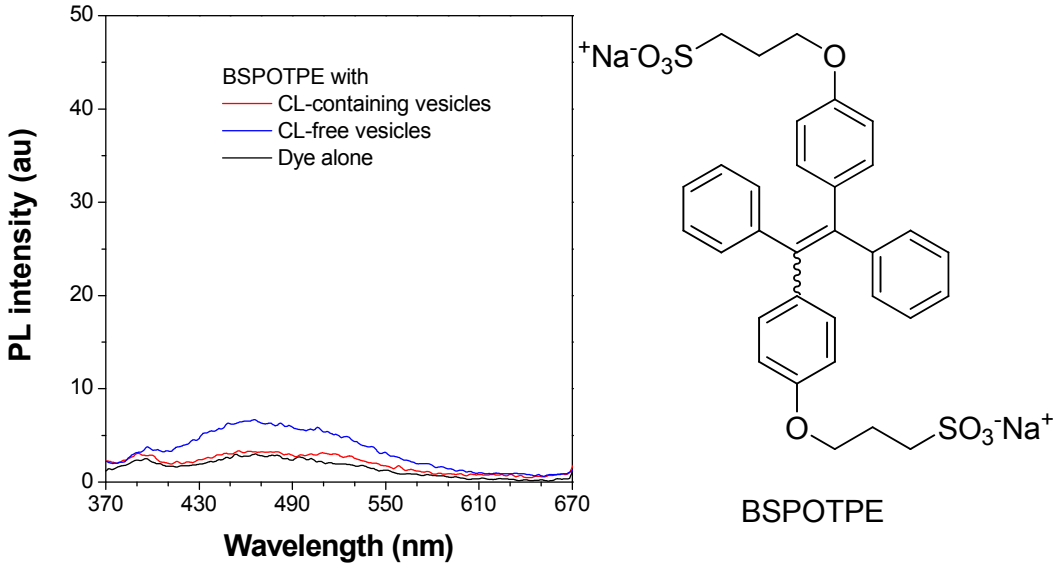


Figure S4. Emission spectra of BSPOTPE alone and with added CL-containing and CL-free LUVs. CL-containing and CL-free LUVs are composed of TOCL/DOPC (50 mol % TOCL) and pure DOPC, respectively, in a 25 mM HEPES buffer at pH 7.4. [dye] = 10 μM; $[lipid]_{total}$ = 22 μM; λ_{ex} = 350 nm.

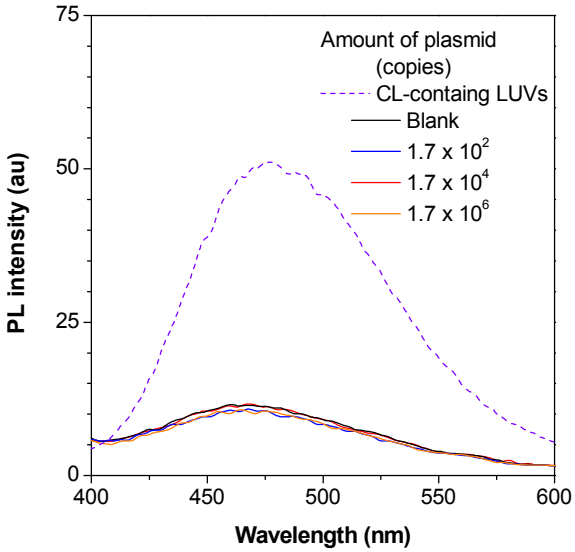


Figure S5. Emission spectra of TTAPE-Me in the presence of different amount of DNA (pUC 18 DNA, 2686 bp) in 25 mM HEPES buffer, pH 7.4. The one of TTAPE-Me with CL-containing LUVs composed of TOCL/DOPC (50 mol % TOCL; 22 μM) is shown for comparison (purple dash line). [dye] = 10 μM; λ_{ex} = 350 nm.

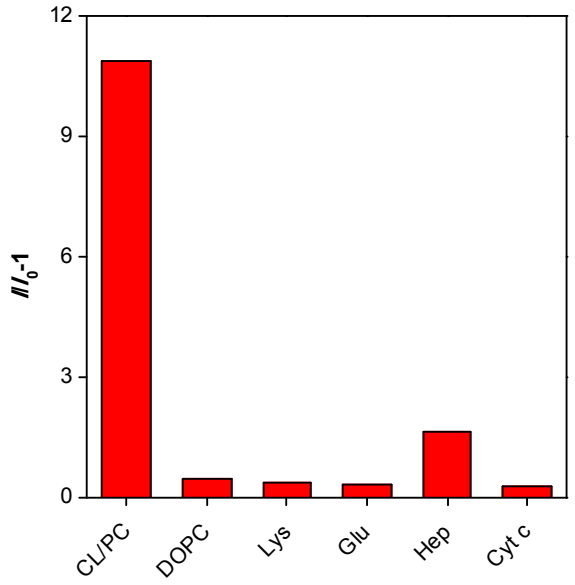


Figure S6. Change in fluorescence intensity of TTAPE-Me (10 μM) with different charged biomolecules ($[lipid]_{total}$ = 22 μM; left to right: LUVs of TOCL:DOPC (50 mol % TOCL), LUVs of pure DOPC, 22 μM lysine, 22 μM glutamic acid, 22 μM heparin, and 22 μM cytochrome *c*) in 25 mM HEPES buffer, pH 7.4, λ_{ex} = 350 nm, λ_{em} = 480 nm.

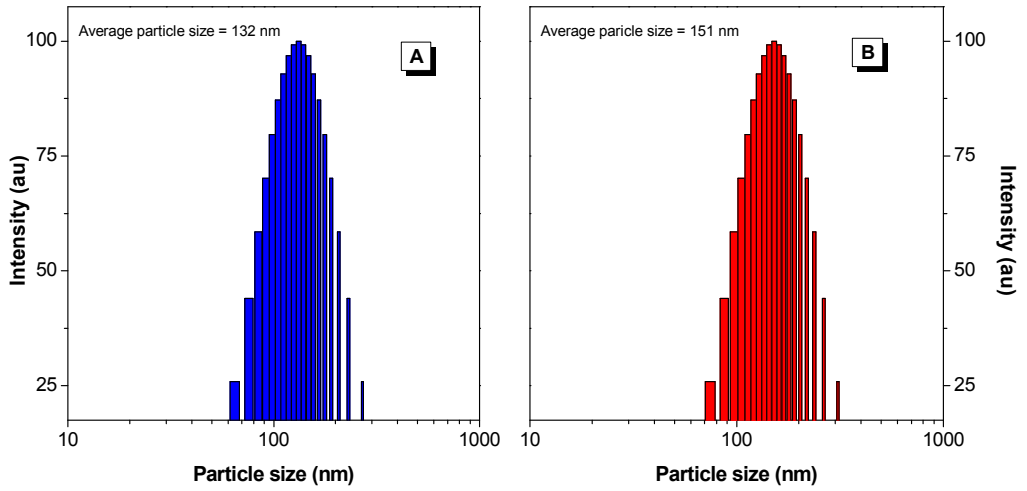


Figure S7. Particle analysis of the all-component LUVs (A) with (17 mol % TOCL, 39.5 mol % DOPC, 38.8 mol % DPPE, 1.7 mol % Soy PI, 1 mol % DOPS & 2 mol % SM) and (B) without TOCL (56.5 mol % DOPC, 38.8 mol % DPPE, 1.7 mol % Soy PI, 1 mol % DOPS & 2 mol % SM) in a 25 mM HEPES buffer at pH 7.4. Emission spectra of TTAPE-Me an NAO with these LUVs are shown in Figures 4C and 4D, respectively.

REFERENCES

(1) Hong,Y.; Häußler, M.; Lam, J. W. Y.; Li, Z.; Sin, K. K.; Dong, Y.; Tong, H.; Liu, J.; Qin, A.; Renneberg R.; Tang, B. Z. *Eur. J. Chem* **2008**, *14*, 6428.