Supporting Information

to

Base-triggerable lauryl sarcosinate-dodecyl sulfate catanionic liposomes. Structure, biophysical characterization, and drug entrapment/release studies

Chinapaka Ravindar,[#] S. Thirupathi Reddy,[#] D. Sivaramakrishna,[#] Deepthi Priyanka Damera Musti J. Swamy*

School of Chemistry, University of Hyderabad, Hyderabad 500 046, India.

Running title: 'Base-triggerable' lauryl sarcosinate-dodecyl sulfate catanionic liposomes

*Corresponding author:

Prof. Musti J. Swamy, School of Chemistry, University of Hyderabad, Hyderabad - 500 046, India, Tel: +91-40-2301-1071; E-mail: mjswamy@uohyd.ac.in, mjswamy1@gmail.com; Website: http://chemistry.uohyd.ac.in/~mjs/

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) of the LS-DS complex. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. [U(eq) = ⅓ $\sum_i \sum_j U_{ij}\, a_{i*}\, a_{j*}\, a_i\, a_j \cos(a\mathrm{i}, a\mathrm{j})$].

Atom	X	Y	Z	U (eq)
S(1)	5765(1)	7507(1)	10492(1)	44(1)
O(1)	5729(1)	8619(3)	10762(1)	71(1)
O(2)	5780(1)	5654(3)	10554(1)	76(1)
O(3)	5448(1)	7940(3)	10221(1)	74(1)
O(4)	6223(1)	8097(3)	10394(1)	62(1)
O(5)	5453(1)	4224(3)	9727(1)	56(1)
O(6)	6052(1)	2527(3)	9778(1)	48(1)
N(1)	5183(1)	3016(4)	10272(1)	43(1)
C(1)	6364(1)	7304(5)	10111(1)	61(1)
C(2)	6778(1)	8156(5)	10044(1)	60(1)
C(3)	6952(1)	7457(4)	9747(1)	58(1)
C(4)	7378(1)	8255(5)	9678(1)	58(1)
C(5)	7547(1)	7576(5)	9378(1)	59(1)
C(6)	7972(1)	8376(5)	9305(1)	61(1)
C(7)	8140(1)	7675(5)	9006(1)	63(1)
C(8)	8568(1)	8441(5)	8931(1)	67(1)
C(9)	8735(1)	7687(5)	8636(1)	73(1)
C(10)	9164(1)	8378(6)	8558(1)	90(1)
C(11)	9327(2)	7553(8)	8270(1)	124(2)
C(12)	9739(2)	8240(9)	8176(1)	168(3)
C(13)	5001(1)	2073(4)	10539(1)	58(1)
C(14)	5566(1)	2177(4)	10161(1)	46(1)
C(15)	5679(1)	3115(4)	9866(1)	39(1)
C(16)	6167(1)	3255(4)	9477(1)	48(1)
C(17)	6599(1)	2513(4)	9414(1)	47(1)
C(18)	6733(1)	3236(5)	9103(1)	51(1)
C(19)	7174(1)	2586(4)	9028(1)	49(1)
C(20)	7313(1)	3365(4)	8722(1)	53(1)
C(21)	7749(1)	2661(5)	8641(1)	54(1)
C(22)	7896(1)	3443(5)	8339(1)	57(1)
C(23)	8331(1)	2720(5)	8258(1)	59(1)
C(24)	8476(1)	3498(5)	7956(1)	65(1)
C(25)	8911(1)	2792(6)	7877(1)	73(1)
C(26)	9054(1)	3603(7)	7576(1)	99(2)
C(27)	9486(2)	2945(9)	7495(1)	157(3)

Table S2. Bond lengths and bond angles of the LS-DS complex.

Bond lengths (Å)		Bond angles (degrees)	
S(1)-O(1)	1.419(2)	O(1)-S(1)-O(2)	116.07(15)
S(1)-O(2)	1.417(2)	O(1)-S(1)-O(3)	112.47(15)
S(1)-O(3)	1.439(2)	O(1)-S(1)-O(4)	101.68(13)
S(1)-O(4)	1.577(2)	O(2)-S(1)-O(3)	111.67(16)
O(5)-C(15)	1.190(3)	O(2)-S(1)-O(4)	108.34(14)
O(6)-C(15)	1.321(3)	O(3)-S(1)-O(4)	105.48(14)
O(6)-C(16)	1.456(3)	O(4)-C(1)-C(2)	109.1(3)
N(1)-C(14)	1.460(4)	O(5)-C(15)-O(6)	124.8(3)
N(1)-C(13)	1.488(4)	O(5)-C(15)-C(14)	123.6(3)
C(1)-O(4)	1.438(3)	O(6)-C(15)-C(14)	111.6(2)
C(1)-C(2)	1.479(4)	O(6)-C(16)-C(17)	109.2(2)
C(2)-C(3)	1.508(4)	C(15)-O(6)-C(16)	115.3(2)
C(3)-C(4)	1.498(4)	C(14)-N(1)-C(13)	115.1(2)
C(4)-C(5)	1.507(4)	N(1)-C(14)-C(15)	109.5(2)
C(5)-C(6)	1.501(4)	C(1)-O(4)-S(1)	117.85(19)
C(6)-C(7)	1.507(4)	C(1)-C(2)-C(3)	113.8(3)
C(7)-C(8)	1.501(4)	C(2)-C(3)-C(4)	115.1(3)
C(8)-C(9)	1.507(4)	C(3)-C(4)-C(5)	115.0(3)
C(9)-C(10)	1.489(5)	C(4)-C(5)-C(6)	115.5(3)
C(10)-C(11)	1.496(5)	C(5)-C(6)-C(7)	115.0(3)
C(11)-C(12)	1.461(6)	C(6)-C(7)-C(8)	115.9(3)
C(14)-C(15)	1.500(4)	C(7)-C(8)-C(9)	114.9(3)
C(16)-C(17)	1.491(4)	C(8)-C(9)-C(10)	116.6(3)
C(17)-C(18)	1.514(4)	C(9)-C(10)-C(11)	115.1(4)
C(18)-C(19)	1.507(4)	C(10)-C(11)-C(12)	117.1(5)
C(19)-C(20)	1.515(4)	C(16)-C(17)-C(18)	111.0(2)
C(20)-C(21)	1.516(4)	C(17)-C(18)-C(19)	114.2(2)
C(21)-C(22)	1.511(4)	C(18)-C(19)-C(20)	113.8(3)
C(22)-C(23)	1.516(4)	C(19)-C(20)-C(21)	113.8(3)
C(23)-C(24)	1.510(4)	C(22)-C(21)-C(20)	114.6(3)
C(24)-C(25)	1.510(4)	C(21)-C(22)-C(23)	114.2(3)
C(25)-C(26)	1.514(5)	C(22)-C(23)-C(24)	114.0(3)
C(26)-C(27)	1.493(6)	C(23)-C(24)-C(25)	114.0(3)
		C(24)-C(25)-C(26)	113.3(3)
		C(25)-C(26)-C(27)	114.4(4)

Table S3. Torsion angles (degrees) of the LS-DS complex.

S1	O4	C1	C2	174.7(2)
O1	S1	O4	C1	-176.6(2)
O2	S1	O4	C1	60.6(2)
O3	S1	O4	C1	-59.1(2)
C3	C2	C1	O4	-178.7(3)
C16	O6	C15	O5	-3.6(4)
O5	C15	C14	N1	-8.4(4)
O6	C15	C14	N1	173.1(2)
C16	O6	C15	C14	174.9(2)
C18	C17	C16	O6	-179.9(2)
C15	O6	C16	C17	178.4(2)
C13	N1	C14	C15	172.5(2)
C1	C2	C3	C4	-178.3(3)
C3	C4	C5	C6	179.5(3)
C4	C5	C6	C7	179.5(3)
C5	C4	C3	C2	-179.0(3)
C5	C6	C7	C8	-179.2(3)
C9	C8	C7	C6	178.5(3)
C7	C8	C9	C10	-178.5(3)
C8	C9	C10	C11	177.9(4)
C9	C10	C11	C12	177.5(4)
C16	C17	C18	C19	178.3(2)
C17	C18	C19	C20	-178.0(2)
C21	C20	C19	C18	-178.0(3)
C19	C20	C21	C22	-179.1(3)
C23	C22	C21	C20	-179.6(3)
C21	C22	C23	C24	179.7(3)
C25	C24	C23	C22	179.4(3)
C23	C24	C25	C26	-179.3(3)
C24	C25	C26	C27	179.3(4)

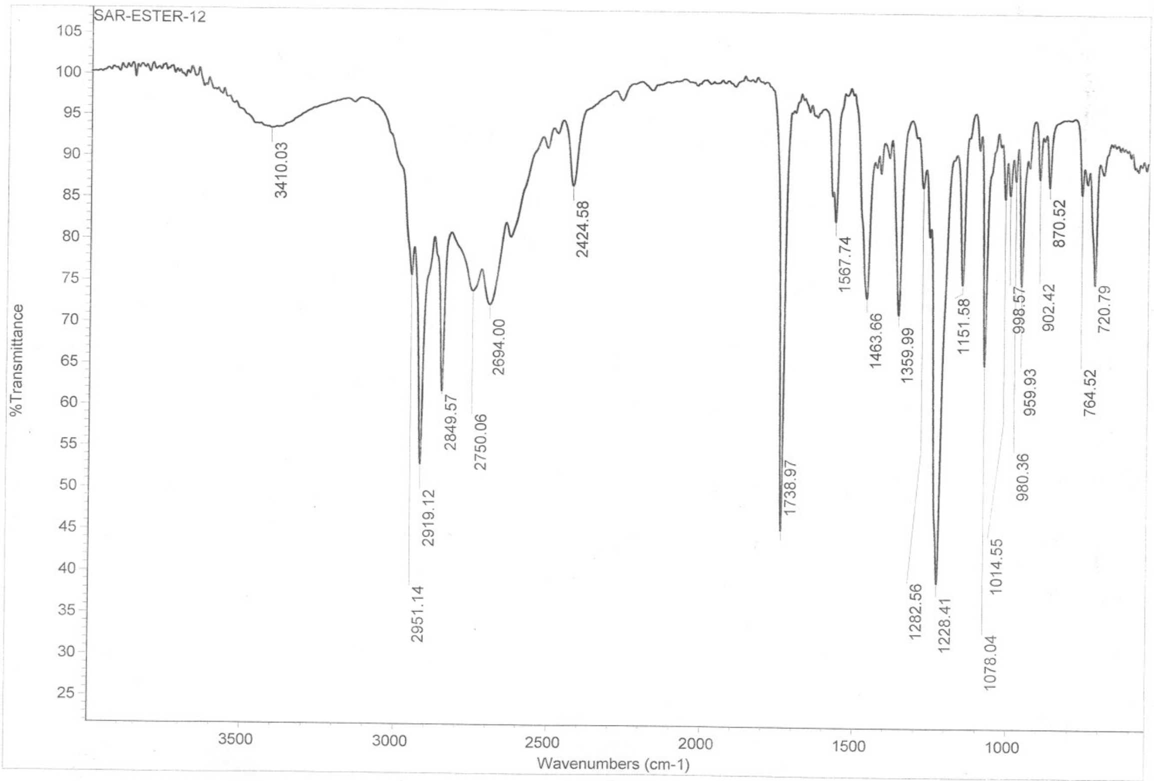

Fig. S1. FTIR spectrum of lauryl sarcosinate hydrochloride (KBr pellet), recorded at room temperature.

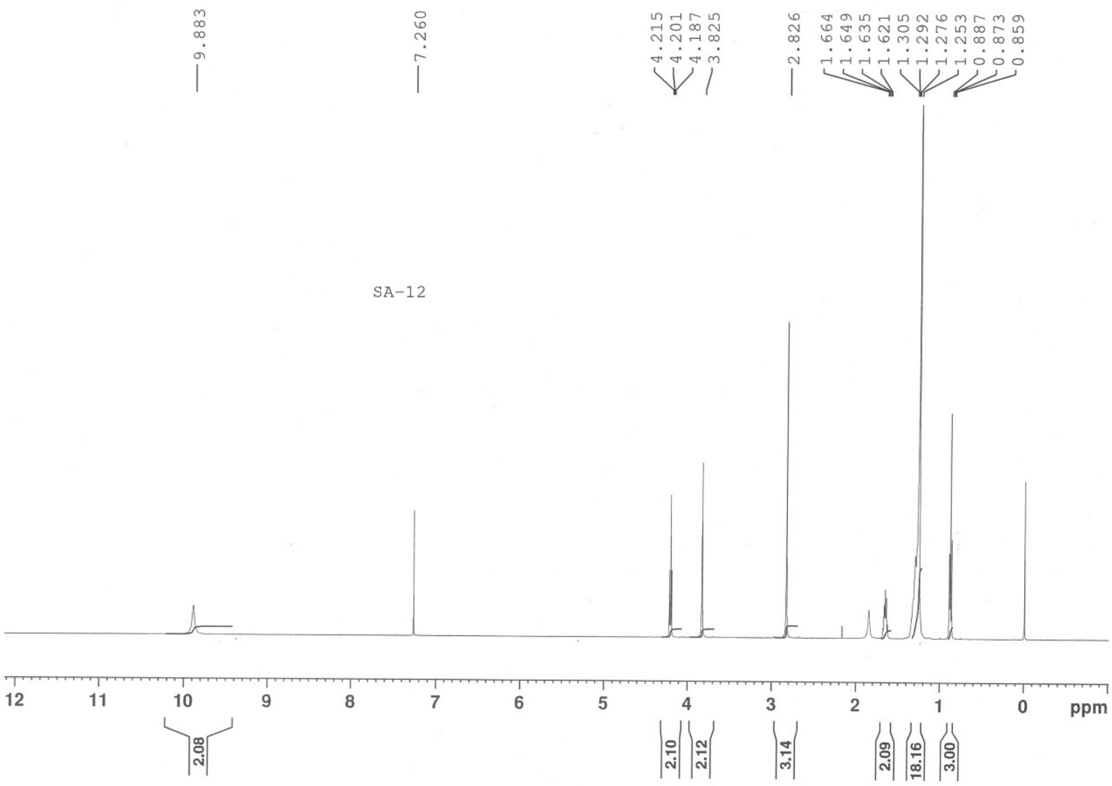

Fig. S2. [1]H-NMR spectrum of lauryl sarcosinate hydrochloride recorded at room temperature (solvent: $CDCl_3$).

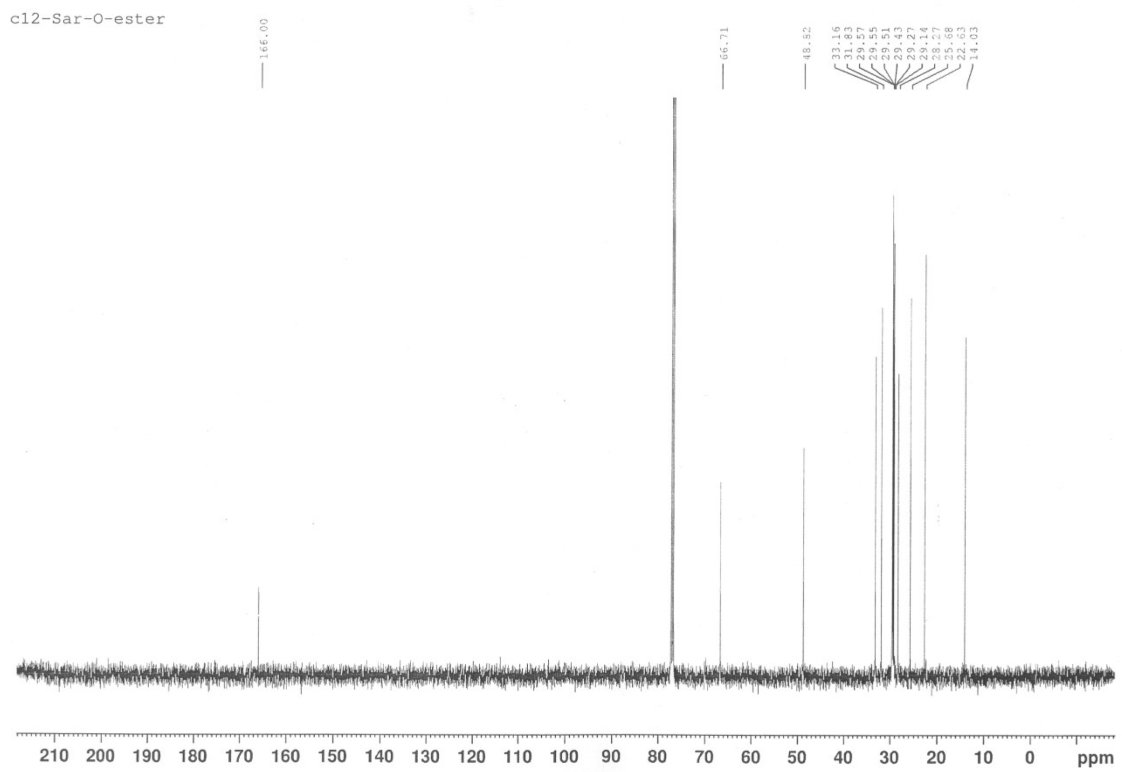

Fig. S3. ^{13}C-NMR spectrum of lauryl sarcosinate hydrochloride recorded at room temperature (solvent: $CDCl_3$).

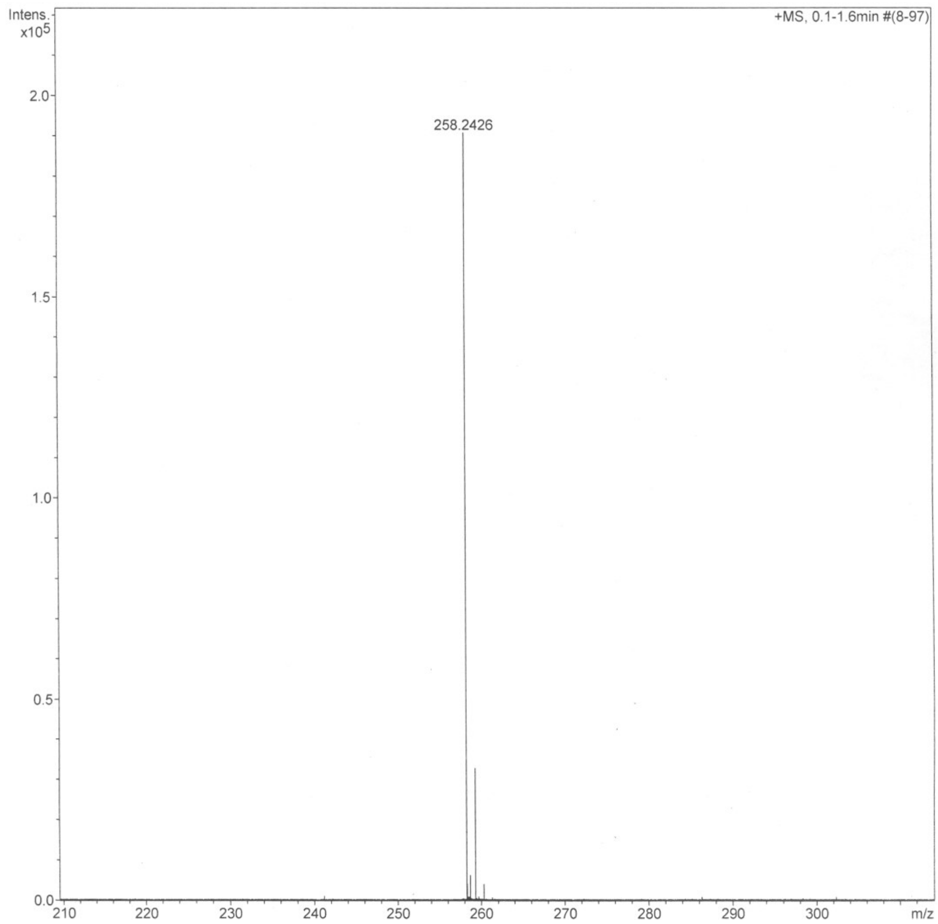

Fig. S4. ESI mass spectrum of lauryl sarcosinate hydrochloride. The molecular weight estimated from the molecular ion peak (m/z = 258.2426) very closely matches the formula weight of 258.2433 (lauryl sarcosinate cation, molecular formula $C_{15}H_{32}NO_2$).

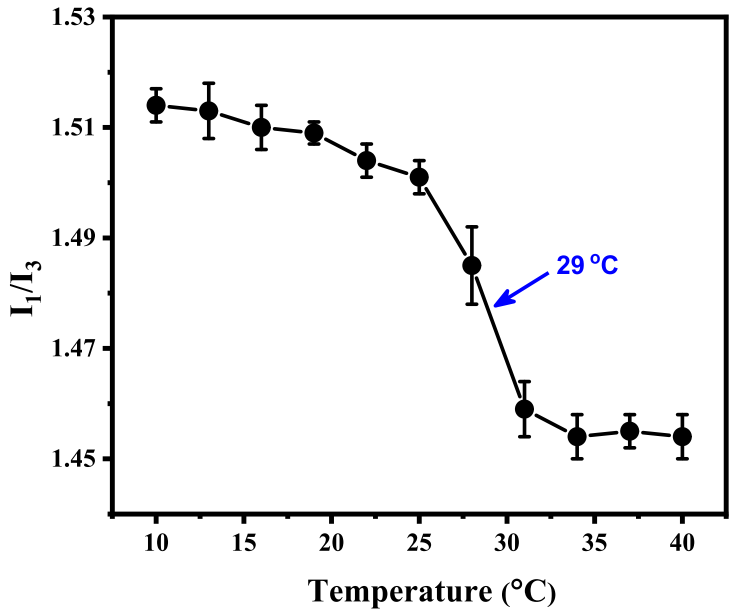

Fig. S5. Temperature dependence polarity ratio (I_1/I_3) of pyrene probe in LS-DS liposomes suspended in 20 mM sodium phosphate buffer pH 7.

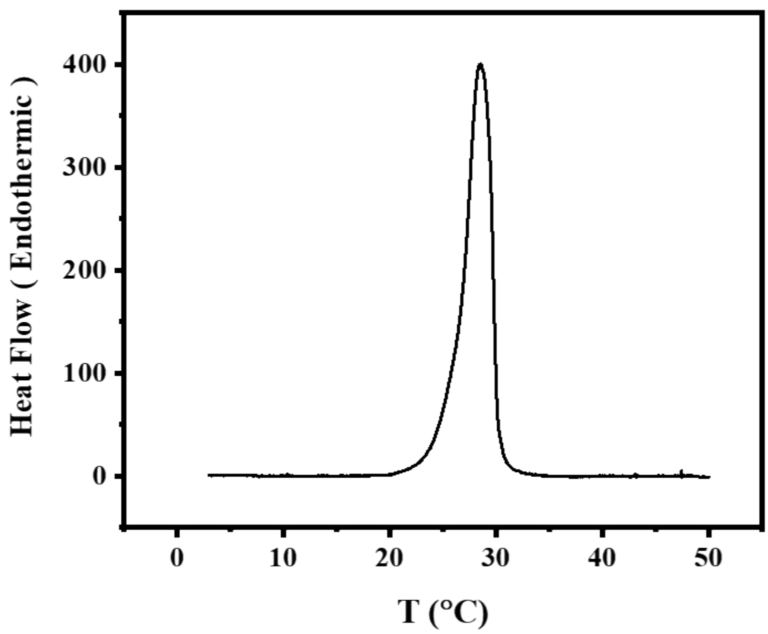

Fig. S6. DSC thermogram of LS-DS liposomes suspended in water.

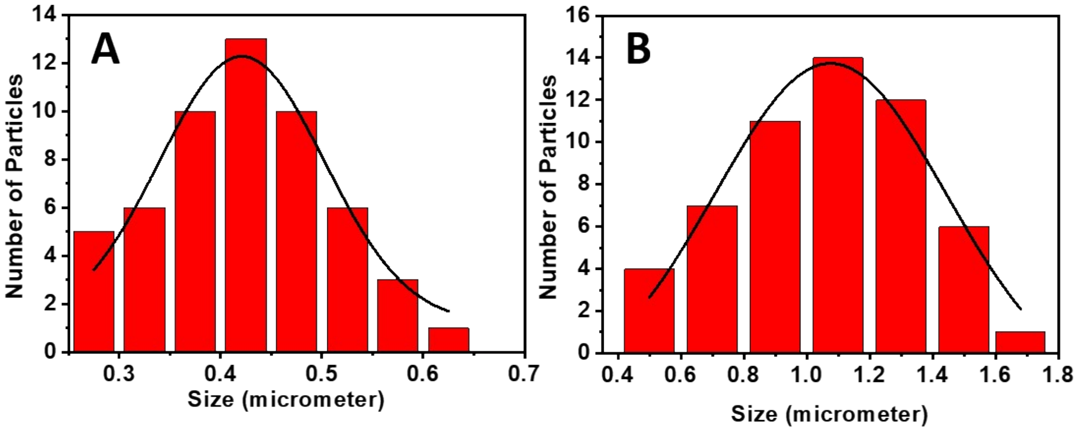

Fig. S7. Size distribution of (**A**) LS-DS vesicles and (**B**) LS-DS-R6G vesicles, obtained from AFM studies. The black solid lines correspond to Gaussian fits of the experimental data.

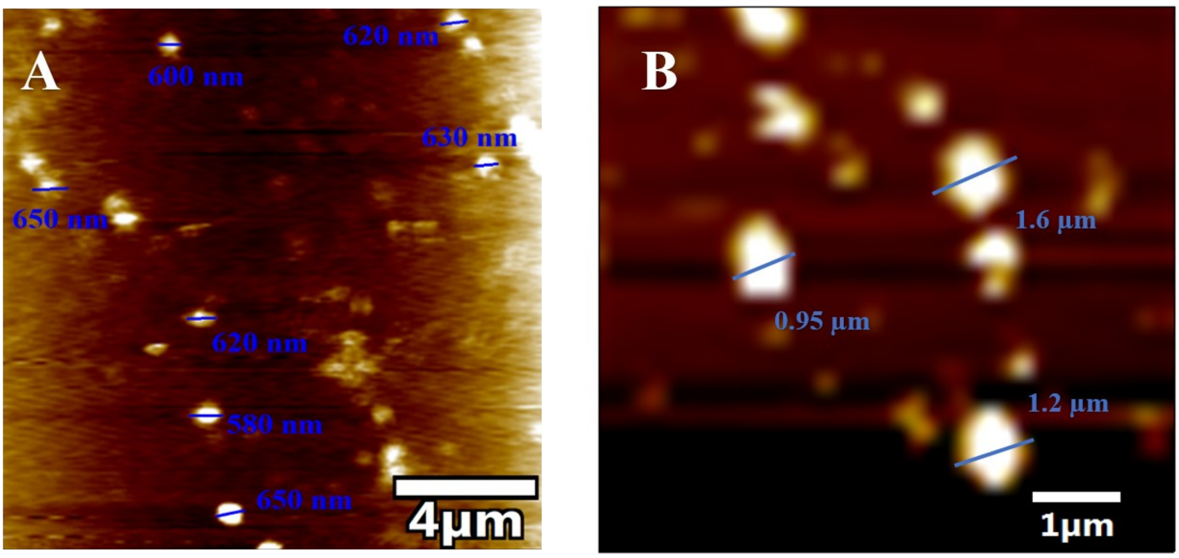

Fig. S8. AFM images of (**A**) LS-DS vesicles and (**B**) LS-DS-R6G vesicles in the hydrated state at pH 7.0. Images were obtained using a liquid cell.

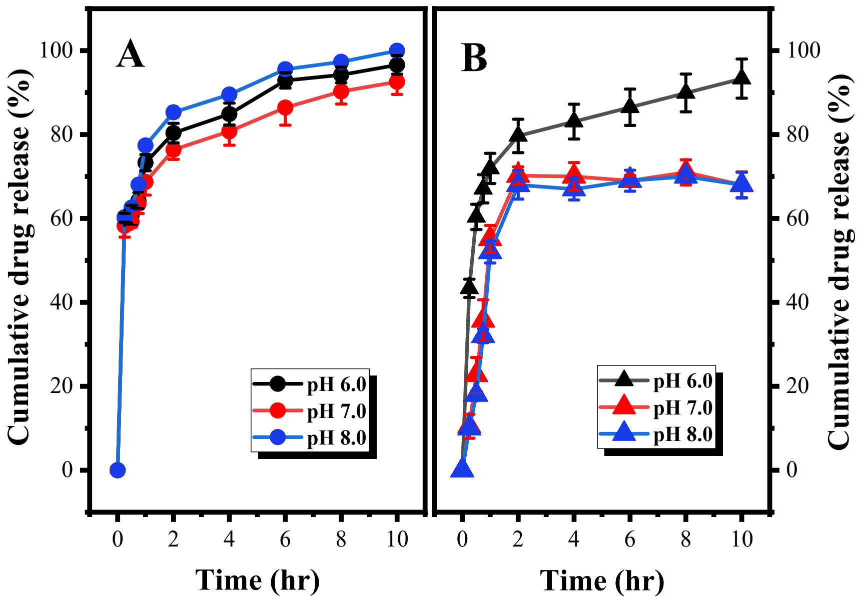

Figure S9. Release profiles of (**A**) free 5-FU and (**B**) free R6G at pH 6.0, pH 7.0 and 8.0.