

Supporting Information

Unraveling the Impact of Hydroxylation on Interactions of Bile Acid Cationic Lipids with Model Membranes by In-depth Calorimetry Studies

Manish Singh and Avinash Bajaj*

^aThe Laboratory of Nanotechnology and Chemical Biology, Regional Centre for Biotechnology,
180 Udyog Vihar, Phase I, Gurgaon-122016, Haryana, India.

Corresponding author: Avinash Bajaj

E-mail: bajaj@rcb.res.in

Table S1. Thermodynamic characterization of phase transition exhibited by DPPC liposomes doped with cationic bile acids **LCA-TMA**, **DCA-TMA**, **CDCA-TMA**, **CA-TMA** as determined from differential scanning calorimetry.

Amphiphile	Doping (%)	T_m (°C)	ΔH_c (Kcal/mol)	ΔS (Cal/K.mol)	FWHM ($\Delta T_{1/2}$)	ΔH_{vH} (Kcal/mol)	CU
DPPC	100	35.67					
		41.38	8.85	28.2	0.77	882.52	99.71
LCA-TMA	5 mol%	40.74	7.70	24.6	1.63	415.64	53.97
	10 mol%	39.59	7.83	25.1	2.82	238.60	30.47
	20 mol%	39.02	8.05	25.8	3.899	172.27	31.40
	30 mol%	37.31	8.41	27.1	4.84	137.06	16.29
	50 mol%	36.42	8.79	28.4	5.81	113.67	12.93
CDCA-TMA	5 mol%	40.59	7.87	25.2	1.83	368.77	46.85
	10 mol%	39.59	8.07	25.8	3.00	224.21	27.78
	20 mol%	35.48	6.85	25.9	5.78	113.45	16.56
		39.06	1.00		2.24	299.71	299.71
	30 mol%	32.99	6.99	30.1	7.00	92.23	13.19
	50 mol%	37.22	2.14		3.26	203.64	95.16
DCA-TMA	5 mol%	40.77	7.44	23.7	1.60	422.31	56.76
	10 mol%	39.69	7.73	24.7	2.90	232.18	30.03
	20 mol%	35.08	8.60	27.9	1.68	388.97	45.22
	30 mol%	34.64	9.57	31.1	1.33	488.44	51.03
	50 mol%	34.36	11.0	35.8	1.65	393.99	35.81
CA-TMA	5 mol%	41.26	7.98	25.4	1.72	394.91	49.48
	10 mol%	41.05	8.33	26.5	2.13	318.07	38.18
	20 mol%	39.09	8.88	278.5	2.30	291.09	32.78
	30 mol%	37.66	10.04	32.3	1.46	455.60	45.37
	50 mol%	37.33	11.43	36.8	1.09	609.15	53.29

Table S2. Thermodynamic characterization of phase transition exhibited by DPPC liposomes doped with cationic bile acids **LCA-DME**, **CDCA-DME**, **DCA-DME**, **CA-DME** as determined from differential scanning calorimetry.

Amphiphile	Doping (%)	T_m (°C)	ΔH_c (Kcal/mol)	ΔS (Cal/K.mol)	FWHM ($\Delta T_{1/2}$)	ΔH_{vh} (Kcal/mol)	CU
DPPC	100	35.67					
		41.38	8.85	28.2	0.77	882.52	99.71
LCA-DME	5 mol%	40.92	7.43	23.7	1.583	371.08	49.94
	10 mol%	40.32	8.48	27.1	2.20	307.73	36.28
	20 mol%	38.75	8.00	25.7	4.31	155.32	19.41
	30 mol%	37.41	8.34	26.3	5.85	113.48	13.60
	50 mol%	33.16	10.05	32.0	8.11	79.73	7.93
CDCA-DME	5 mol%	40.49	7.5	23.9	1.76	385.23	51.36
	10 mol%	39.23	8.02	25.0	3.53	190.21	23.71
	20 mol%	33.80	6.23	28.0	5.89	110.16	17.68
		38.43	2.22		3.26	204.95	91.99
	30 mol%	30.72	4.20	30.3	2.22	286.17	68.13
		35.80	5.08		5.28	124.45	24.49
50 mol%	30.09	4.51	33.6	5.39	117.50	26.05	
DCA-DME	5 mol%	34.10	4.79		3.24	200.59	41.87
		40.52	8.29	26.0	1.75	385.43	46.49
		39.42	8.44	27.0	3.24	207.32	24.56
		34.93	10.08	32.0	1.11	585.05	58.04
		34.76	10.62	34.0	1.19	545.10	51.32
CA-DME	5 mol%	34.49	11.06	36.0	1.06	610.85	55.23
		40.86	8.46	26.9	1.58	429.46	50.76
		39.89	8.27	26.9	1.72	392.40	47.44
		37.89	8.65	27.8	1.42	463.39	54.26
		36.99	9.92	32.0	1.34	494.81	49.88
50 mol%	36.34	10.38	33.6	1.19	553.59	53.33	