## **Supporting Information**

H. Surya Prakash Rao,<sup>a</sup>\* Avinash Desai,<sup>a</sup> Ivy Sarkar, <sup>b</sup> Monalisa Mohapatra,<sup>b</sup> Ashok Kumar Mishra<sup>b</sup>\*

<sup>a</sup> Department of Chemistry, Pondicherry University, Pondicherry – 605 014 INDIA

<sup>b</sup> Department of Chemistry, Indian Institute of Technology Madras, Chennai - 600 036 INDIA



Figure S1: Normalized absorption spectra of (a) Cum and (b) Cum-Chl (except water) at 2.5  $\mu$ M in solvents of different polarity.



Figure S2: Normalized fluorescence spectra of (a) Cum and (b) Cum-Chl (longer wavelength excitation) (except water) at 2.5  $\mu$ M in solvents of different polarity.



Figure S3: Blue shift of  $\lambda_{em, max}$  of (a) Cum and Cum-Chl monomer in NaDC medium at  $\lambda_{ex}$  440 nm.



Figure S4: Blue shift of  $\lambda_{em, max}$  of (a) Cum and Cum-Chl monomer in NaC medium at  $\lambda_{ex}$  440 nm.



Figure S5: Fluorescence spectra of (a) Cum and (b) Cum-Chl at  $\lambda_{ex}$  440 nm in DMPC liposome and water at 21°C.



Figure S6: Drop in fluorescence anisotropy ( $r_{ss}$ ) of Cum with temperature ( $\lambda_{ex}$  440 nm,  $\lambda_{em}$  480 nm), inset shows its derivative plot.



Figure S7: Derivative plot of fluorescence intensity of H-aggregates of Cum-Chl (2.5  $\mu$ M) in DMPC liposome with temperature at  $\lambda_{ex}$  440 nm.



Figure S8; <sup>1</sup>H NMR (400 MHz, CDCl3) spectrum of 3-Cholesterylpropanenitrile 4



Figure S9; <sup>13</sup>C NMR (100 MHz, CDCl3) spectrum of 3-Cholesterylpropanenitrile 4



Figure S10; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of Ethyl 5-(3-cholesteryl)-3-oxopentanoate 5



Figure S11; <sup>13</sup>C NMR (100 MHz, CDCl3) spectrum of Ethyl 5-(3-cholesteryl)-3-oxopentanoate 5



Figure S12; HRMS Spectrum of Ethyl 5-(3-cholesteryl)-3-oxopentanoate 5



Figure S13; <sup>1</sup>H NMR (400 MHz, CDCl3) spectrum of 7-(Diethylamino)-3-(3-cholesteryl)propanoyl)-2H-chromen-2-one 2



Figure S14; <sup>13</sup>C NMR (100 MHz, CDCl3) spectrum of 7-(Diethylamino)-3-(3-cholesteryl)propanoyl)-2H-chromen-2-one 2



Figure S15; HRMS Spectrum of 7-(Diethylamino)-3-(3-cholesteryl)propanoyl)-2H-chromen-2one 2