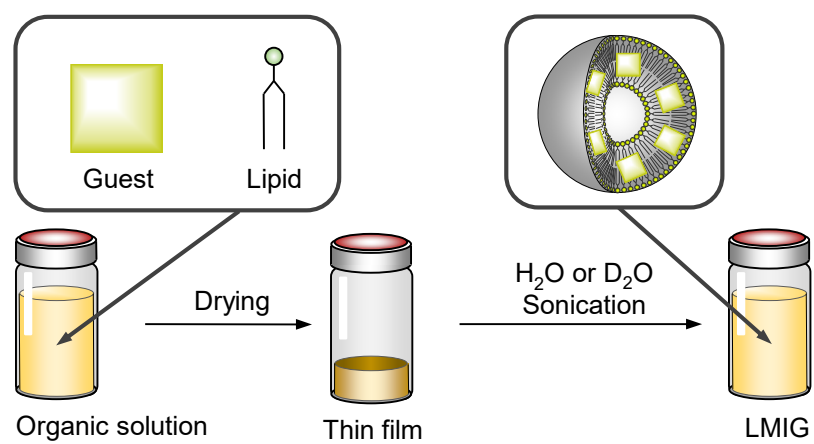


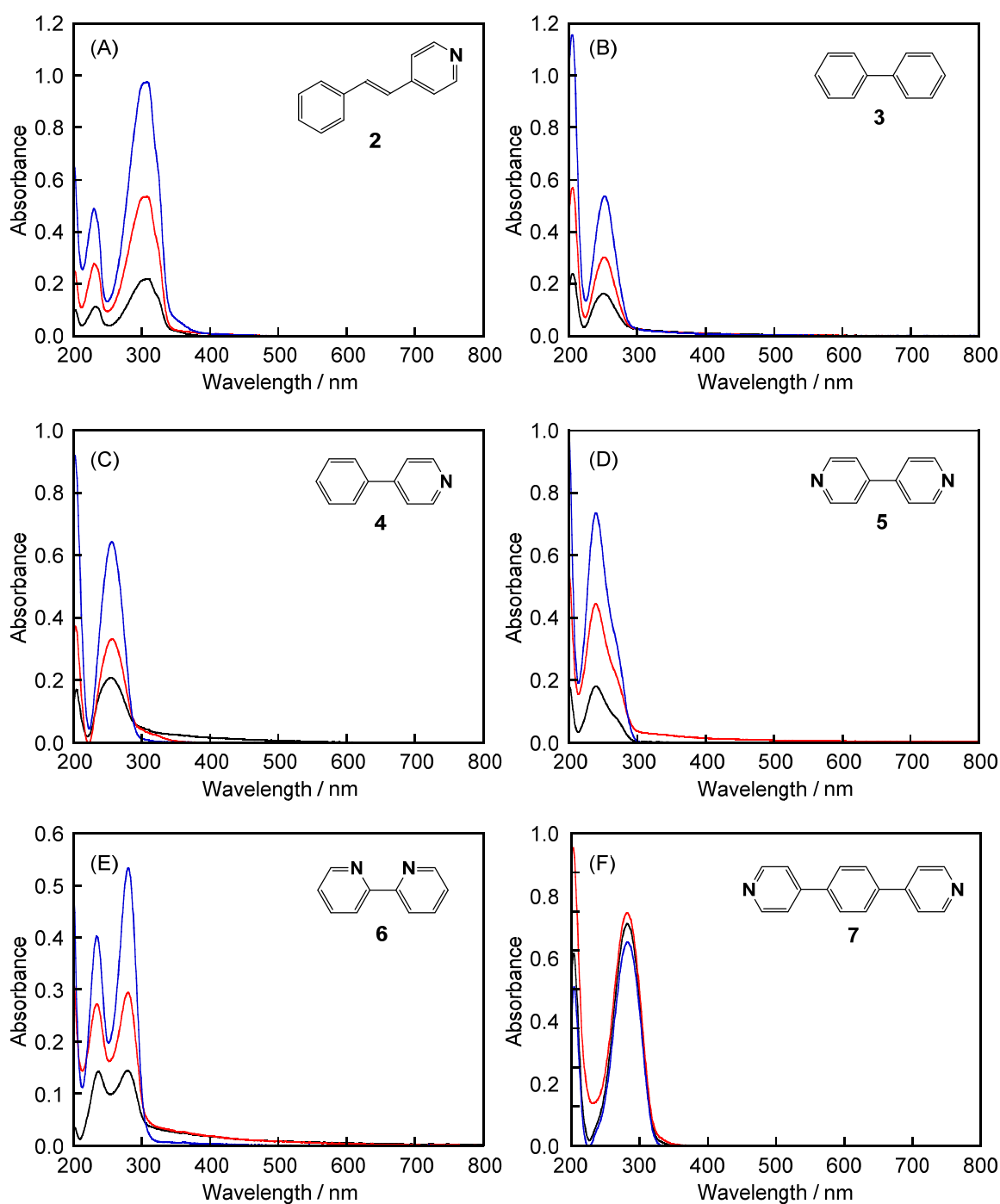
## Electronic Supplementary Information

### **Formation of lipid membrane-incorporated small $\pi$ -molecules bearing hydrophilic groups**

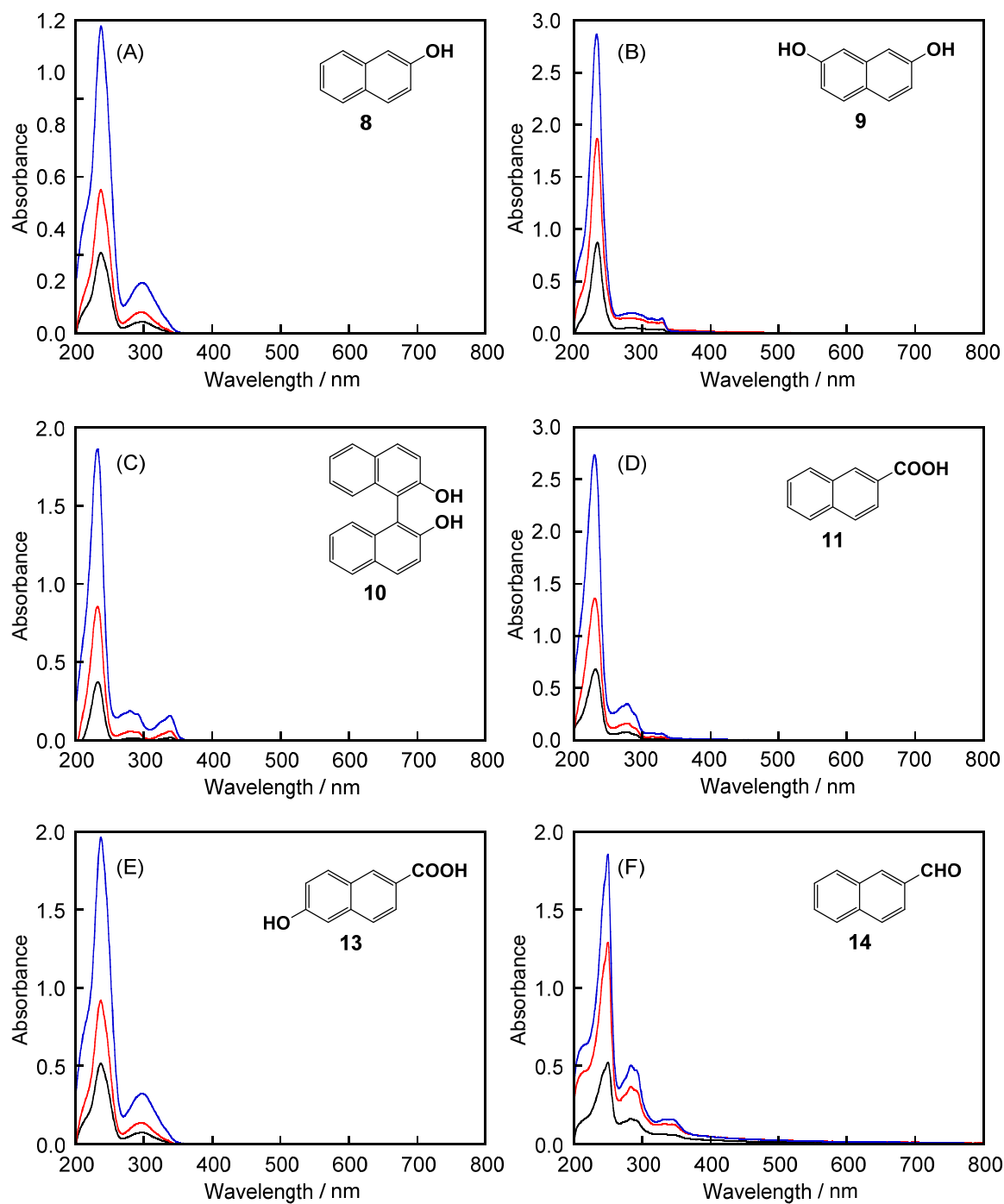
Atsushi Ikeda,\* Kengo Ashizawa, Yuki Tsuchiya, Masafumi Ueda and Kouta Sugikawa



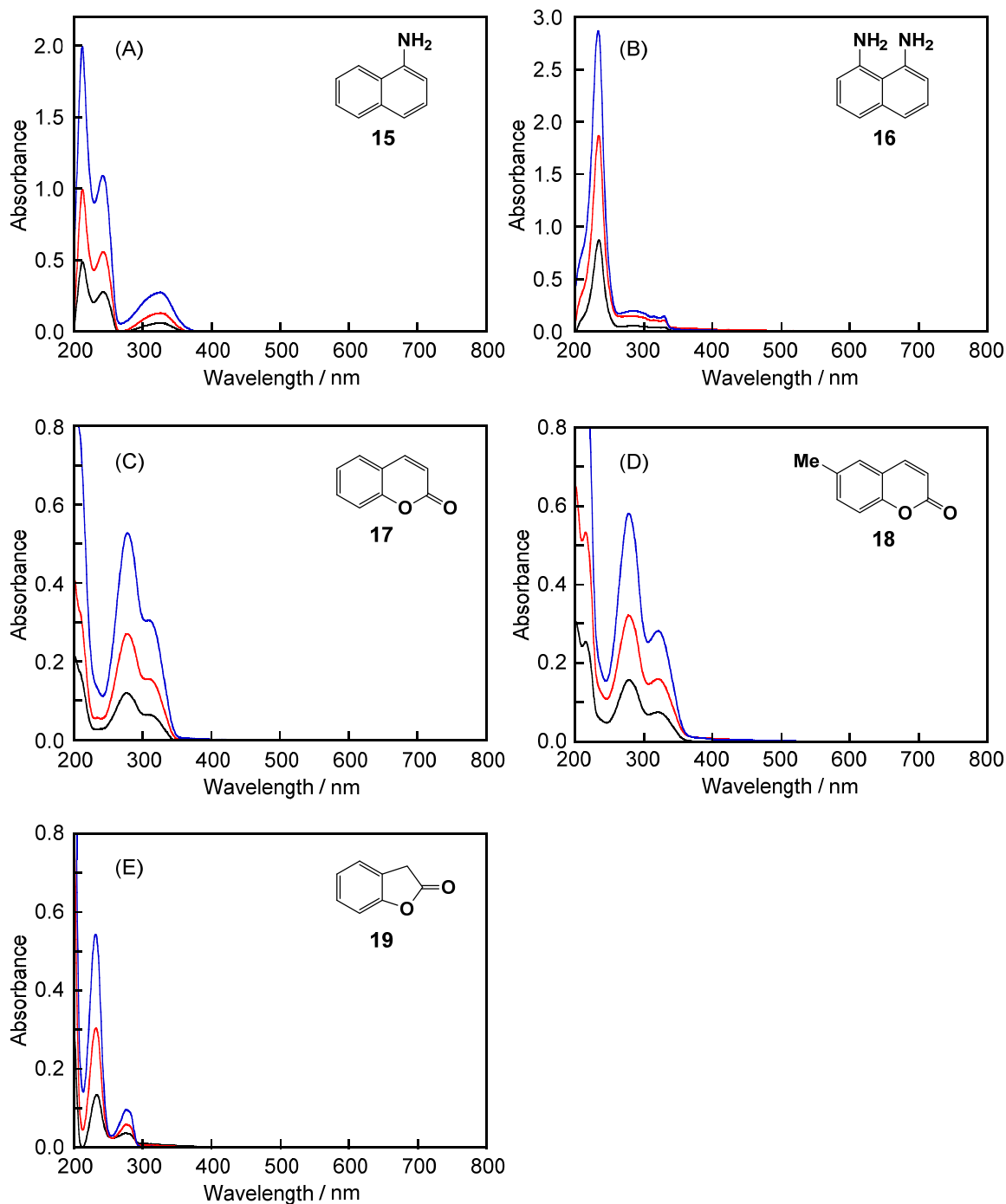
**Scheme S1.** The premixing method for the preparation of LMIGs.



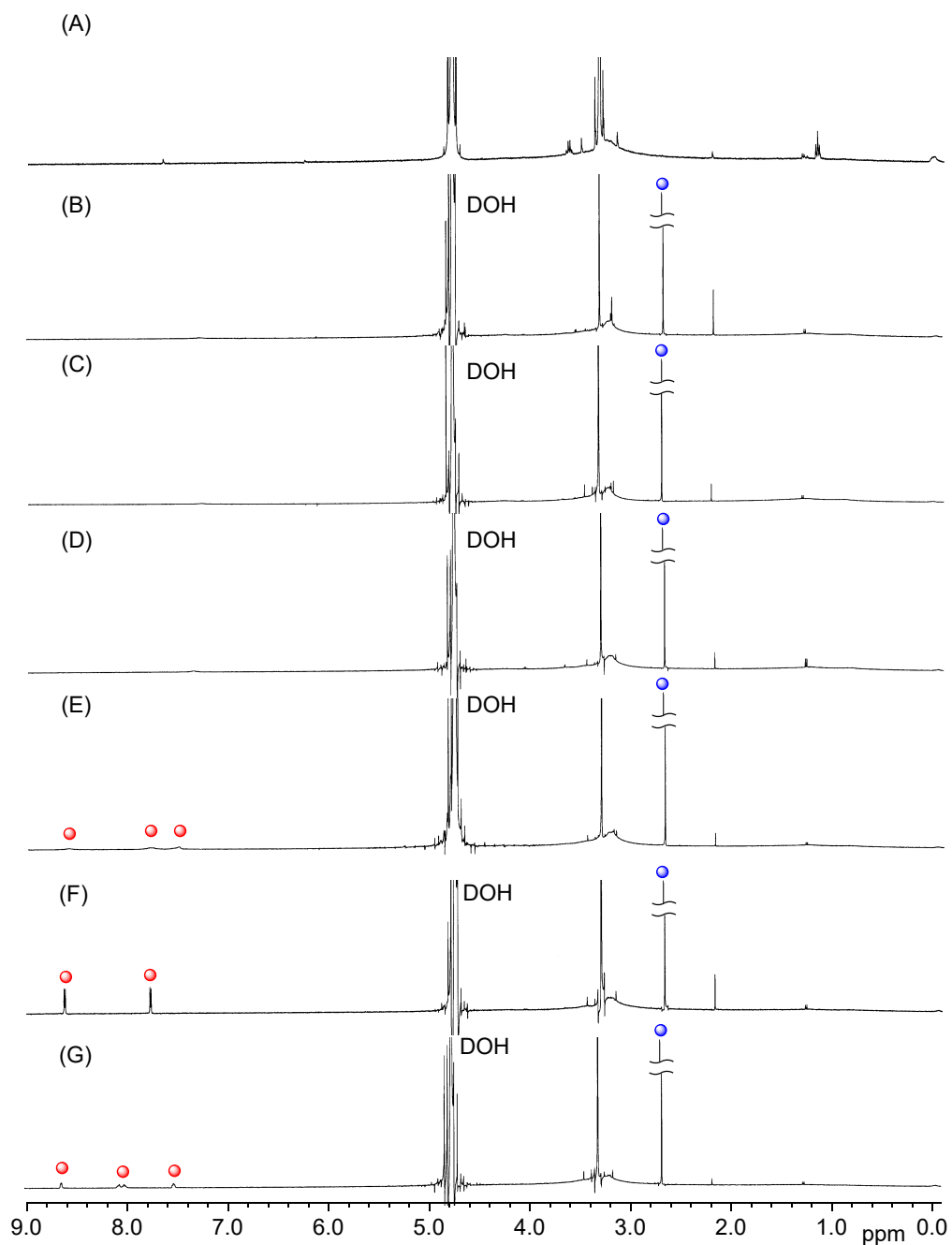
**Fig. S1** UV-vis absorption spectra of (A) LMI2, (B) LMI3, (C) LMI4, (D) LMI5, (E) LMI6 and (F) LMI7 prepared by the premixing method. [2–7]/[DMPC] = (a) 2.5 (black line), (b) 5.0 (red line) and (c) 20.0 (blue line) mol%. All of the absorption spectra were obtained by subtracting the light scattering from the DMPC liposomes and were measured at 25 °C (1 mm cell). [DMPC] = 4.0 mM.



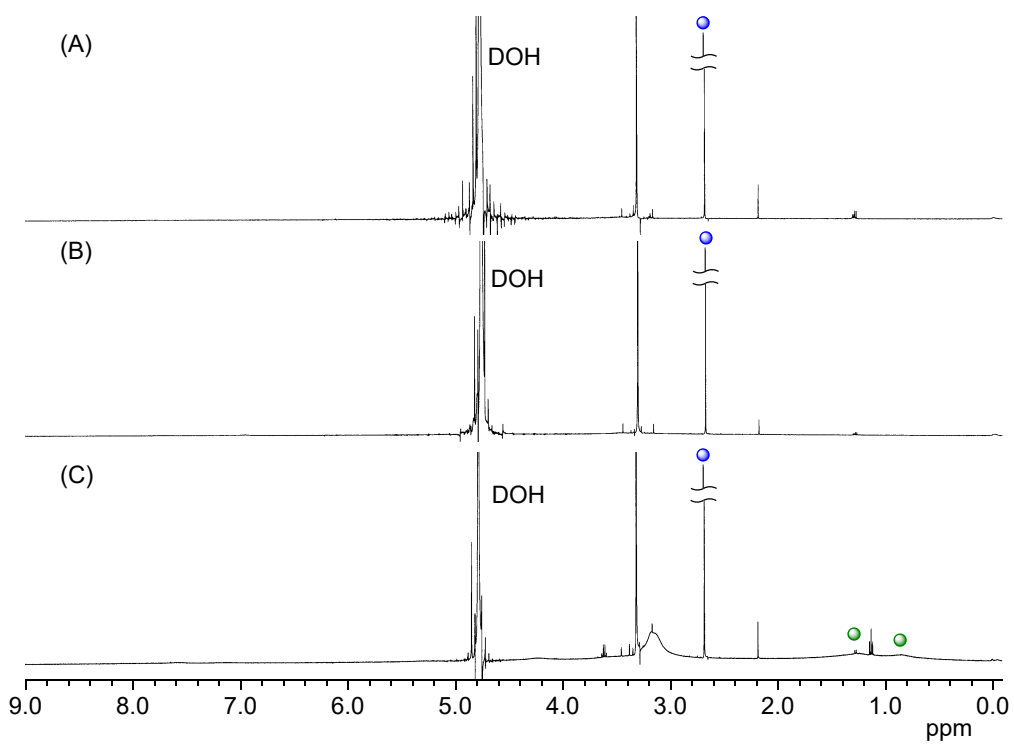
**Fig. S2** UV-vis absorption spectra of (A) LMI8, (B) LMI9, (C) LMI10, (D) LMI11, (E) LMI13 and (F) LMI14 prepared by the premixing method. [8–11, 13 or 14]/[DMPC] = (a) 2.5 (black line), (b) 5.0 (red line) and (c) 20.0 (blue line) mol%. All of the absorption spectra were obtained by subtracting the light scattering from the DMPC liposomes and were measured at 25 °C (1 mm cell). [DMPC] = 4.0 mM for 8, 9, 11, 13 or 14, [DMPC] = 2.0 mM for 10.



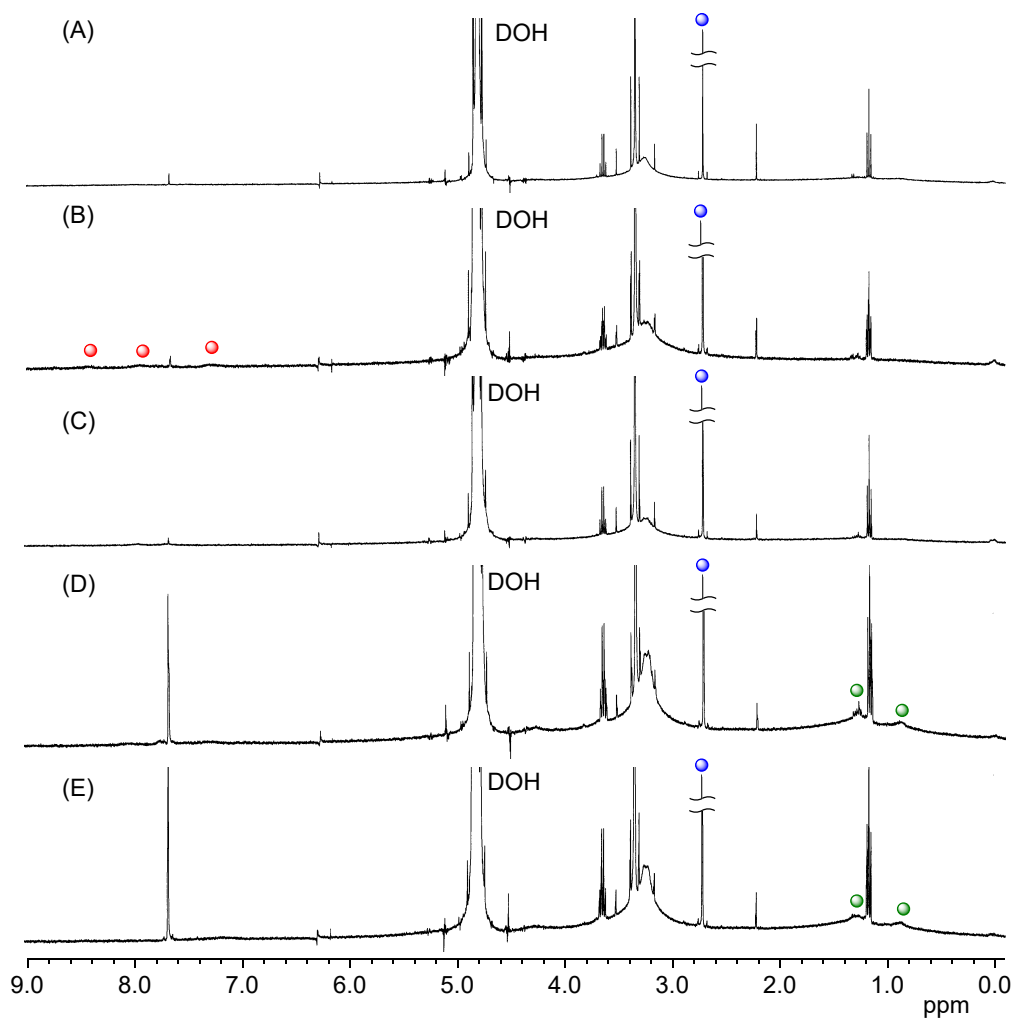
**Fig. S3** UV-vis absorption spectra of (A) LMI15, (B) LMI16, (C) LMI17, (D) LMI18 and (E) LMI19 prepared by the premixing method. [15–19]/[DMPC] = (a) 2.5 (black line), (b) 5.0 (red line) and (c) 20.0 (blue line) mol%. All of the absorption spectra were obtained by subtracting the light scattering from the DMPC liposomes and were measured at 25 °C (1 mm cell). [DMPC] = 4.0 mM.



**Fig. S4** <sup>1</sup>H NMR spectra of (A) DMPC liposome, (B) LMI1, (C) LMI2, (D) LMI3, (E) LMI4, (F) LMI5 and (G) LMI6 in D<sub>2</sub>O at 25 °C (●: free guest molecule and ●: DMSO). [1–6]/[DMPC] = 10.0 mol%, [DMPC] = 4.0 mM, [DMSO] = 0.4 mM.

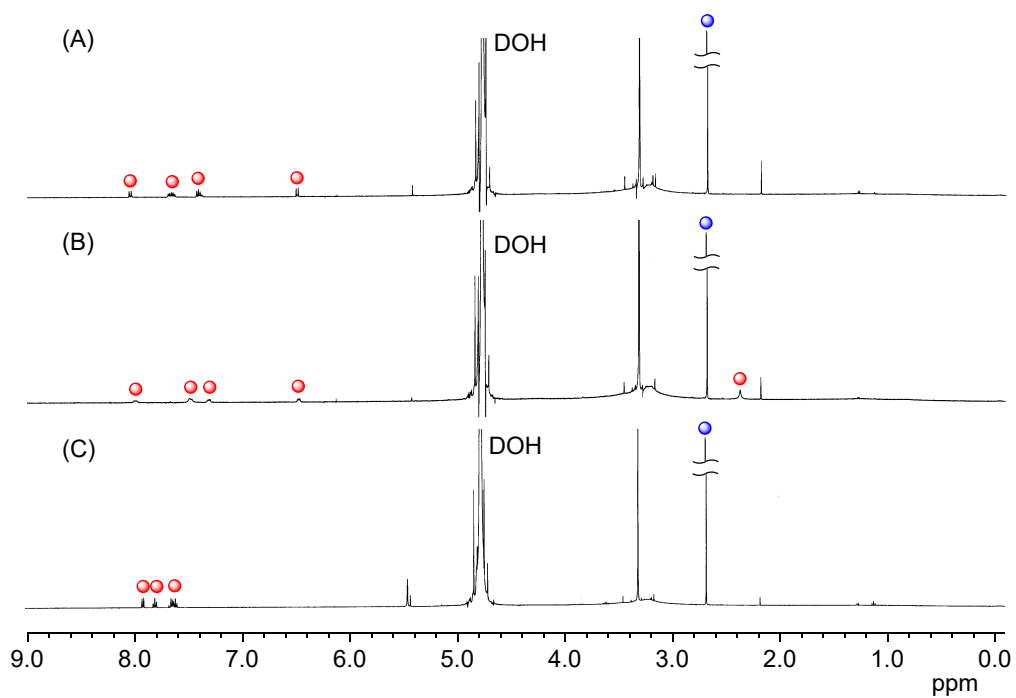


**Fig. S5** <sup>1</sup>H NMR spectra of (A) LMI8, (B) LMI9 and (C) LMI10 in D<sub>2</sub>O at 25 °C (●: free guest molecule, ●: DMPC lipid and ●: DMSO). [8–10]/[DMPC] = 10.0 mol%, [DMPC] = 4.0 mM, [DMSO] = 0.4 mM.

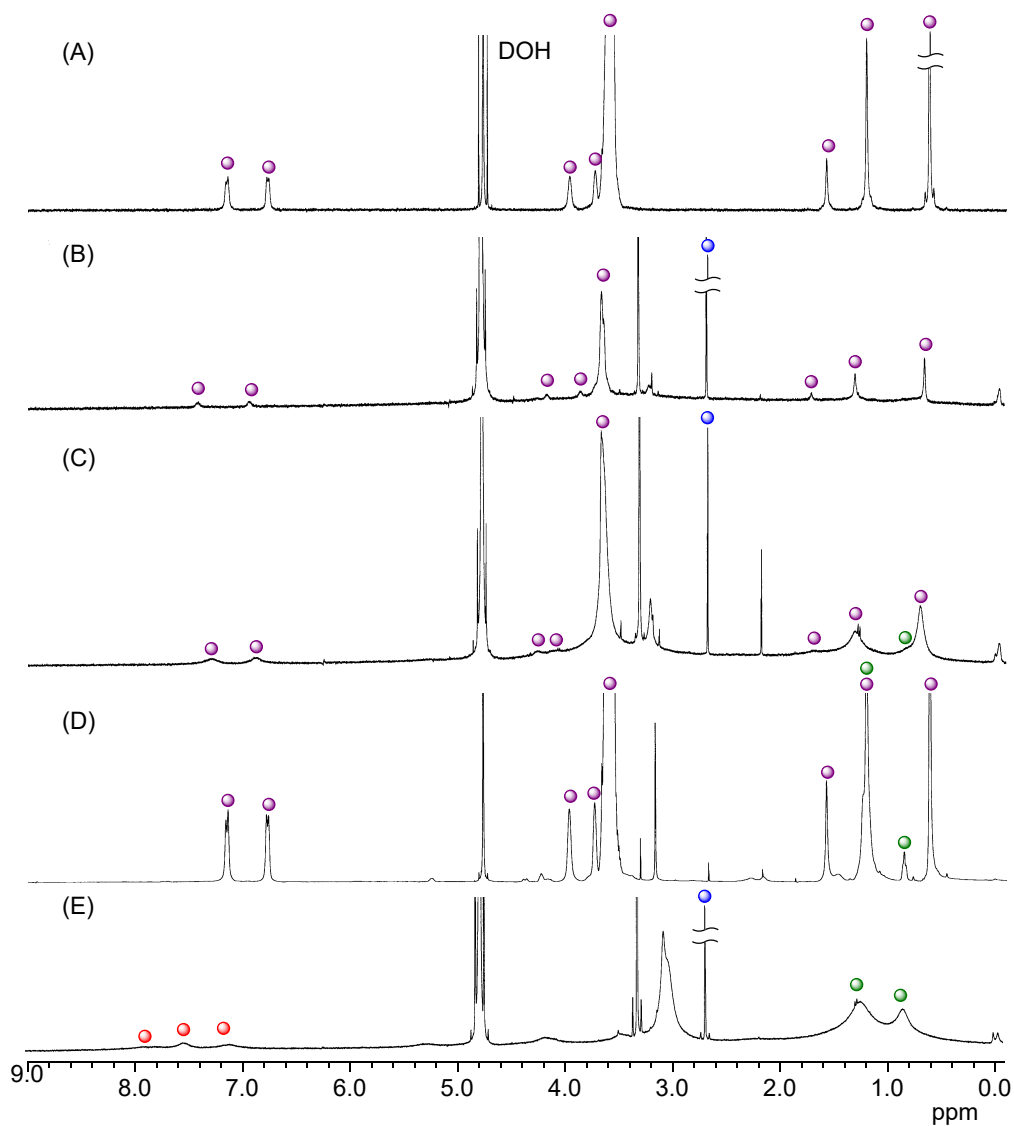


**Fig. S6**  $^1\text{H}$  NMR spectra of (A) LMI11, (B) LMI13, (C) LMI14, (D) LMI15 and (E) LMI16 in  $\text{D}_2\text{O}$  at 25 °C (●: free guest molecule, ●: DMPC lipid and ●: DMSO). [11 or 13–16]/[DMPC] = 10.0 mol%, [DMPC] = 4.0 mM, [DMSO] = 0.4 mM.

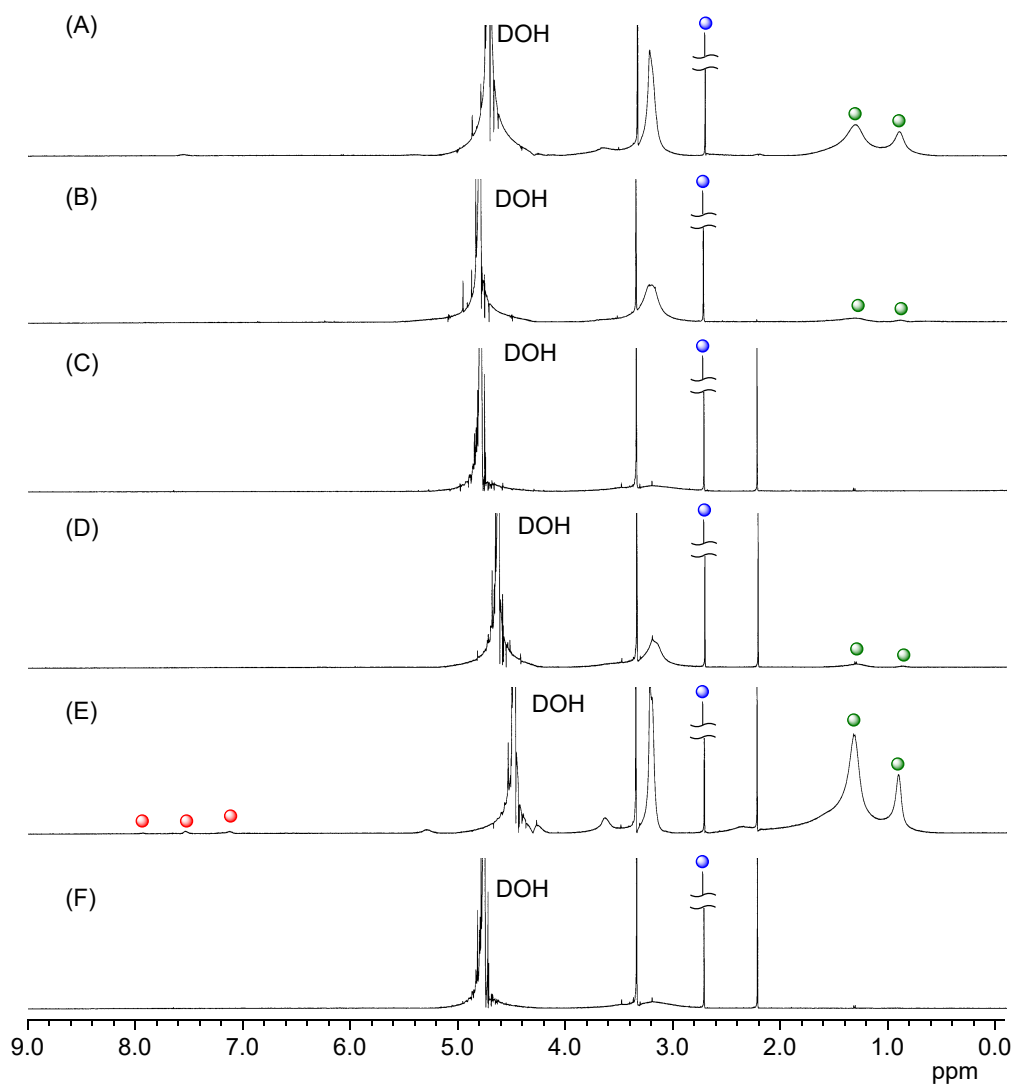




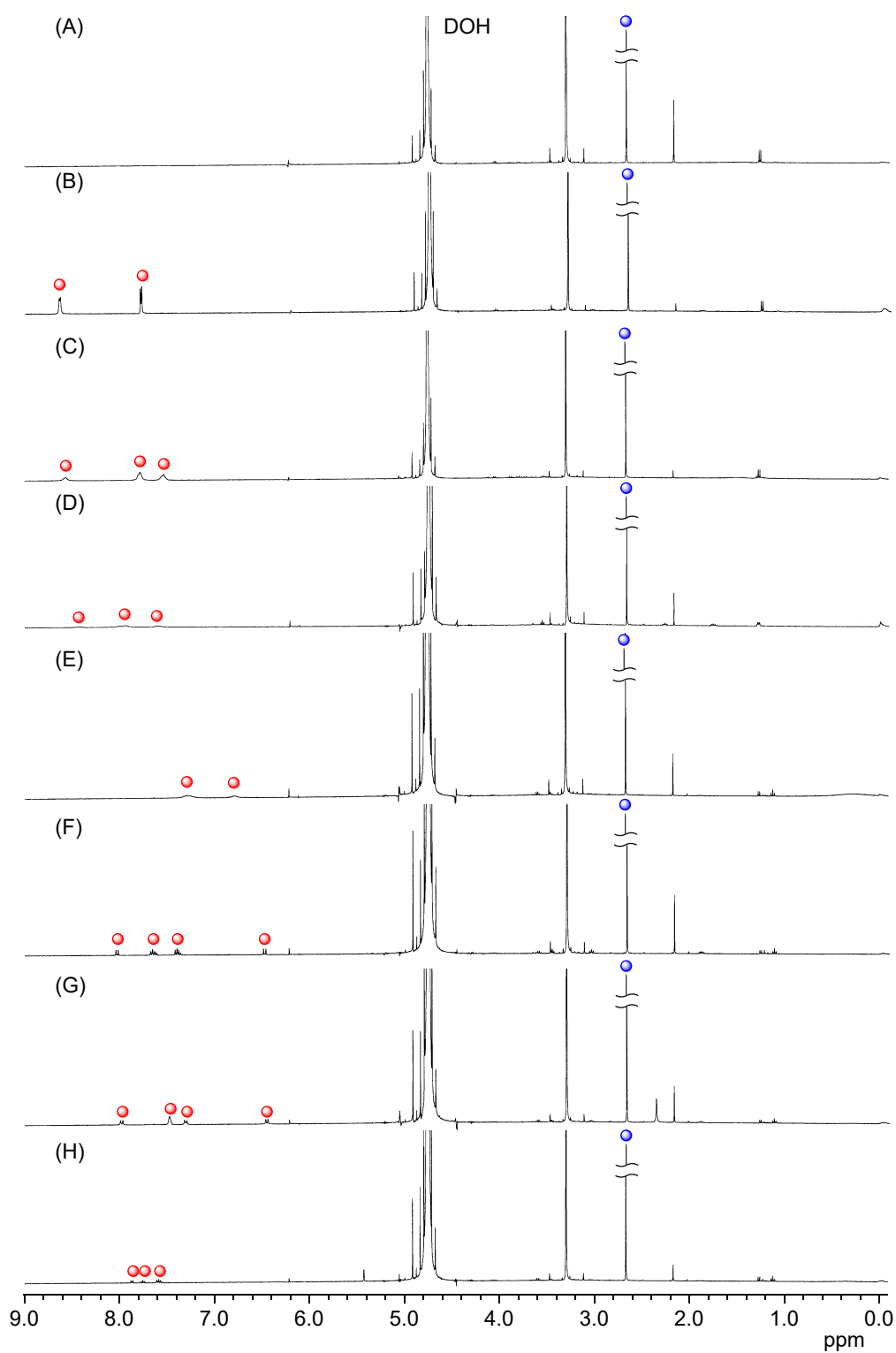
**Fig. S7**  $^1\text{H}$  NMR spectra of (A) LMI17, (B) LMI18 and (C) LMI19 in  $\text{D}_2\text{O}$  at 25  $^\circ\text{C}$  (●: free guest molecule and ●: DMSO).  $[\mathbf{17-19}]/[\text{DMPC}] = 10.0$  mol%,  $[\text{DMPC}] = 4.0$  mM,  $[\text{DMSO}] = 0.4$  mM.



**Fig. S8**  $^1\text{H}$  NMR spectra of (A) TX-100, DMPC TX-100 mixture with  $[\text{TX-100}]/[\text{DMPC}] =$  (B) 10.0, (C) 30.0 and (D) 1000 mol% and (E) LMI10 with  $[\mathbf{10}]/[\text{DMPC}] = 30.0$  mol% in  $\text{D}_2\text{O}$  at 25 °C (●: guest molecule, ●: TX-100 and ●: DMPC lipid in the small aggregates).  $[\text{DMPC}] = 4.0$  mM,  $[\text{DMSO}] = 0.4$  mM.



**Fig. S9**  $^1\text{H}$  NMR spectra of LMI10 consisting of DMPC in  $\text{D}_2\text{O}$  at (A) 30 °C and (B) 20 °C and LMI10 consisted of DPPC in  $\text{D}_2\text{O}$  at (C) 25 °C, (D) 37 °C, (E) 50 °C and then cooling at (F) 25 °C (●: guest molecule in the small aggregates, ●: DMPC lipid and ●: DMSO).  $[\mathbf{10}]/[\text{lipid}] = 10.0$  mol%,  $[\text{lipid}] = 4.0$  mM,  $[\text{DMSO}] = 0.4$  mM.



**Fig. S10** <sup>1</sup>H NMR spectra of (A) LMI4, (B) LMI5, (C) LMI6, (D) LMI11, (E) LMI16, (F) LMI17 (G) LMI18 and (H) LMI19 consisting of DPPC in D<sub>2</sub>O at 25 °C (●: free guest molecule and ●: DMSO). [4, 5, 6, 11, 16, 17, 18 or 19]/[DPPC] = 10.0 mol%, [DPPC] = 4.0 mM, [DMSO] = 0.4 mM.