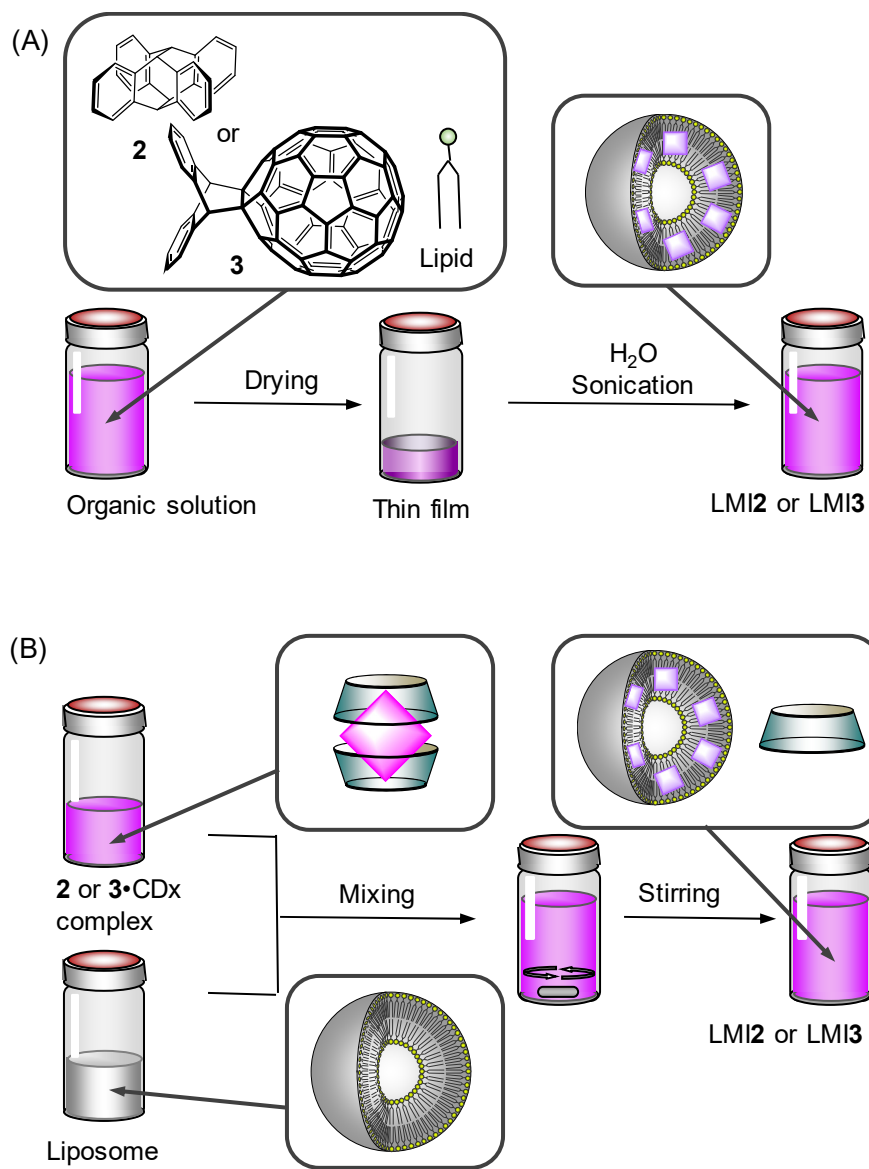


## **Electronic Supplementary Information**

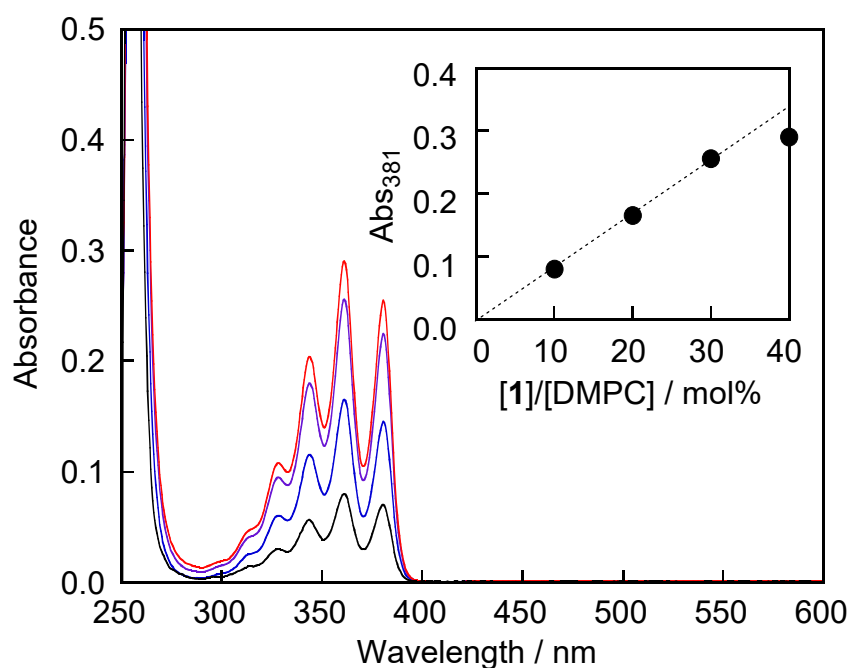
### **Incorporation of large guest molecules in liposomes via chemical reactions in lipid membranes**

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

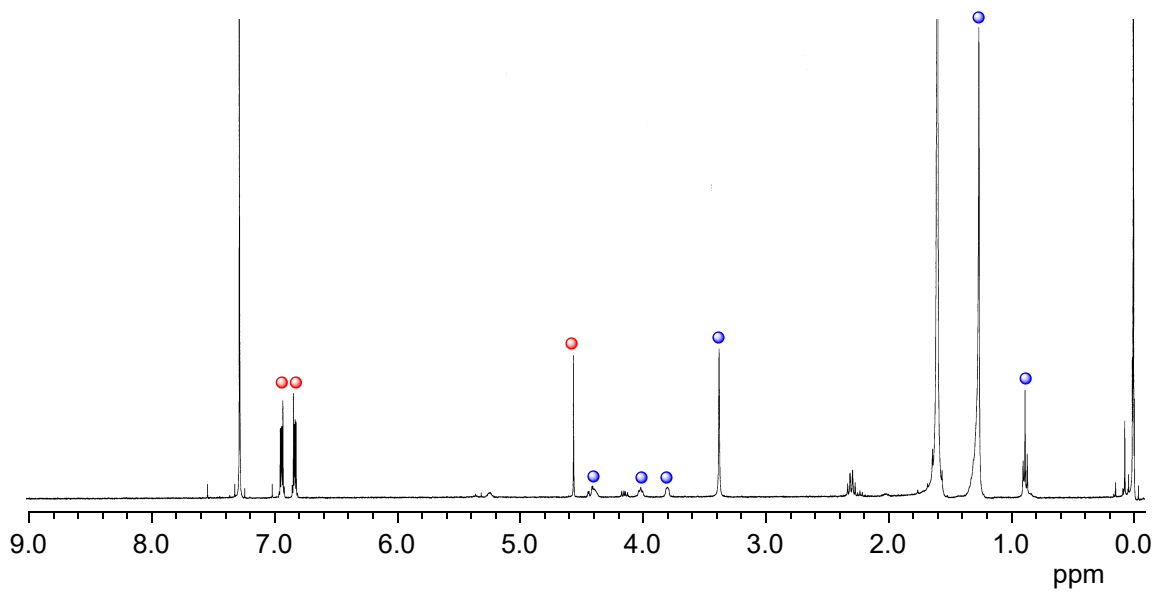
*Department of Applied Chemistry, Graduate School of Engineering, Hiroshima  
University, 1-4-1 Kagamiyama, Higashi-Hiroshima 739-8527, Japan*



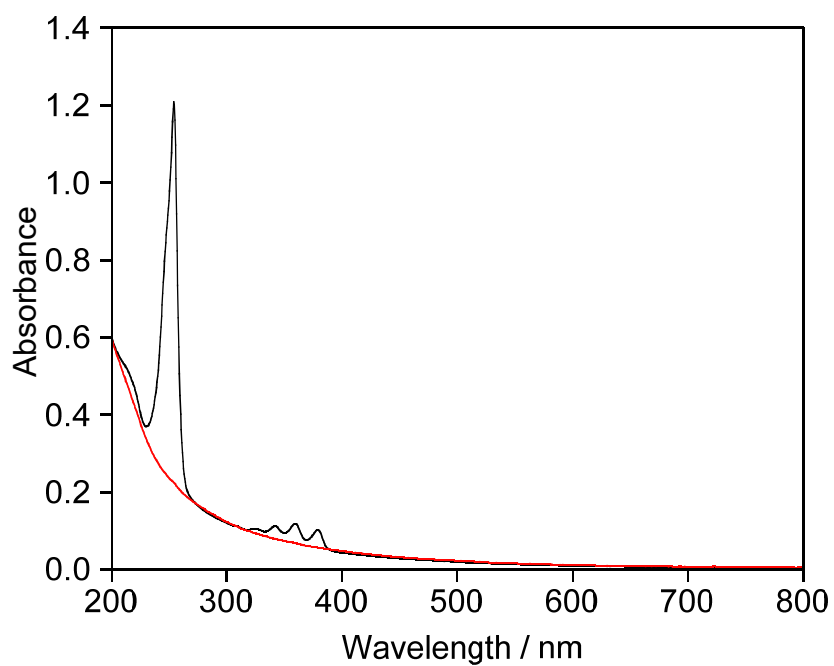
**Scheme S1** (A) Premixing method and (B) exchange method for preparation of LMI2 and LMI3.



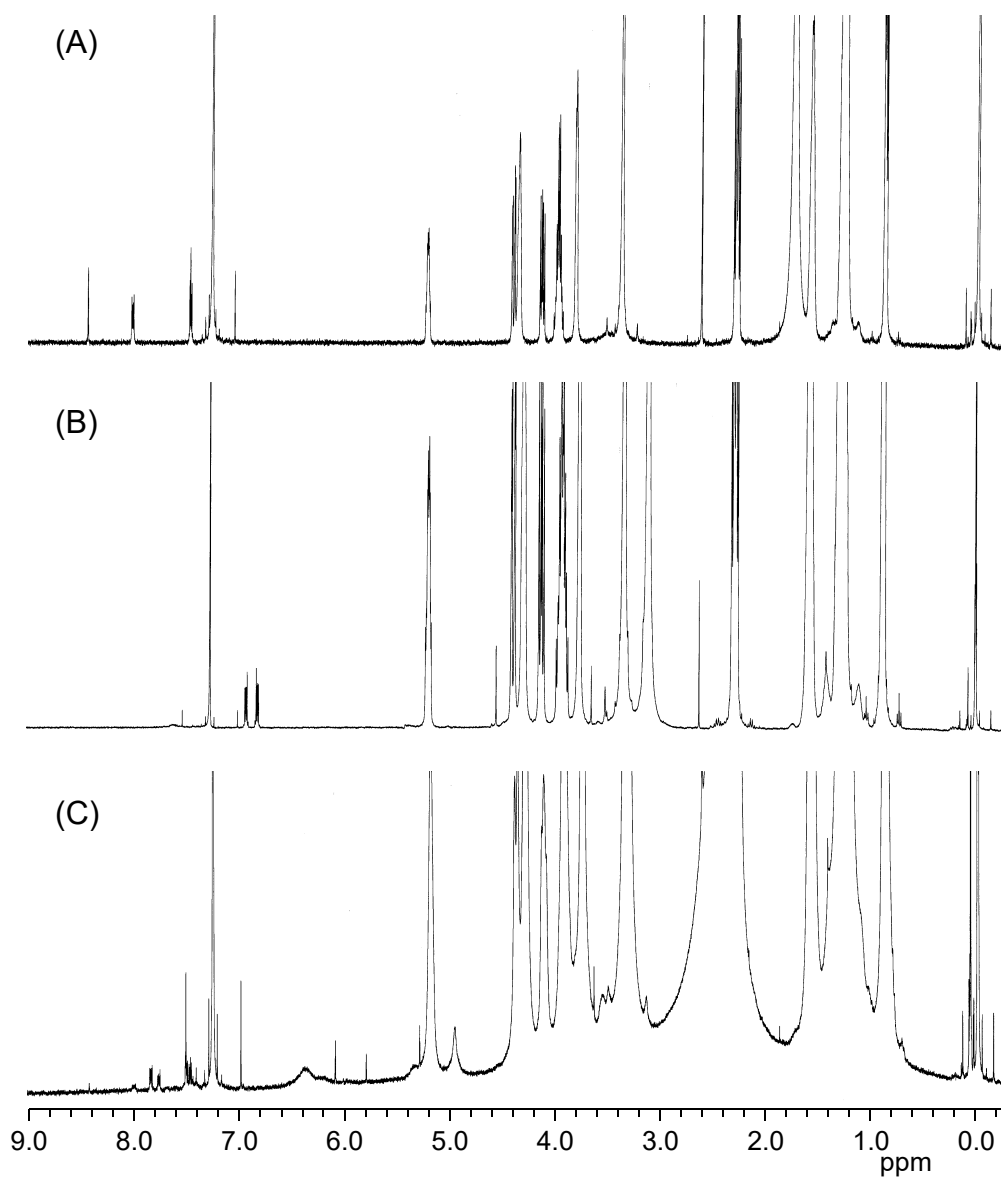
**Fig. S1** UV-vis absorption spectra of LMI1 prepared using premixing method.  $[1]/[DMPC]$  = (a) 10.0 (black line), (b) 20.0 (blue line), (c) 30.0 (purple line), and (d) 40.0 (red line) mol%. All absorption spectra were obtained by subtracting light scattering by DMPC liposomes and were recorded at 25 °C (1 mm cell).  $[DMPC] = 2.0$  mM. Inset: absorbance (Abs) at 381 nm versus  $[1]/[DMPC]$ . Dashed line shows extrapolated absorbances, corresponding to 50% solubility of **1** in water.



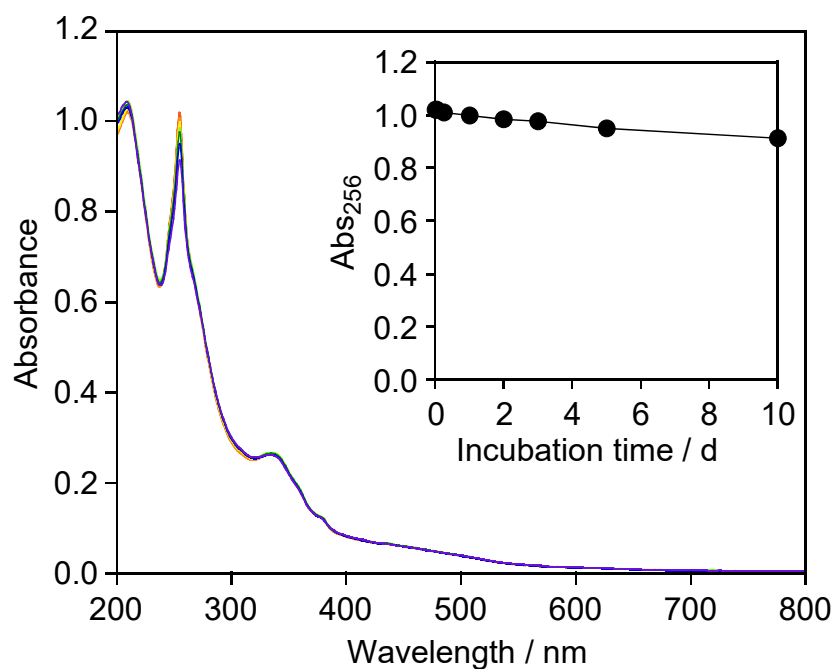
**Fig. S2**  $^1\text{H}$  NMR spectrum of LMI1 in water after 12 h photoirradiation and centrifugation (●: 2, ●: DMPC). Initial concentration:  $[\mathbf{1}]/[\text{DMPC}] = 1.4 \text{ mol}\%$ ,  $[\text{DMPC}] = 4.0 \text{ mM}$ .



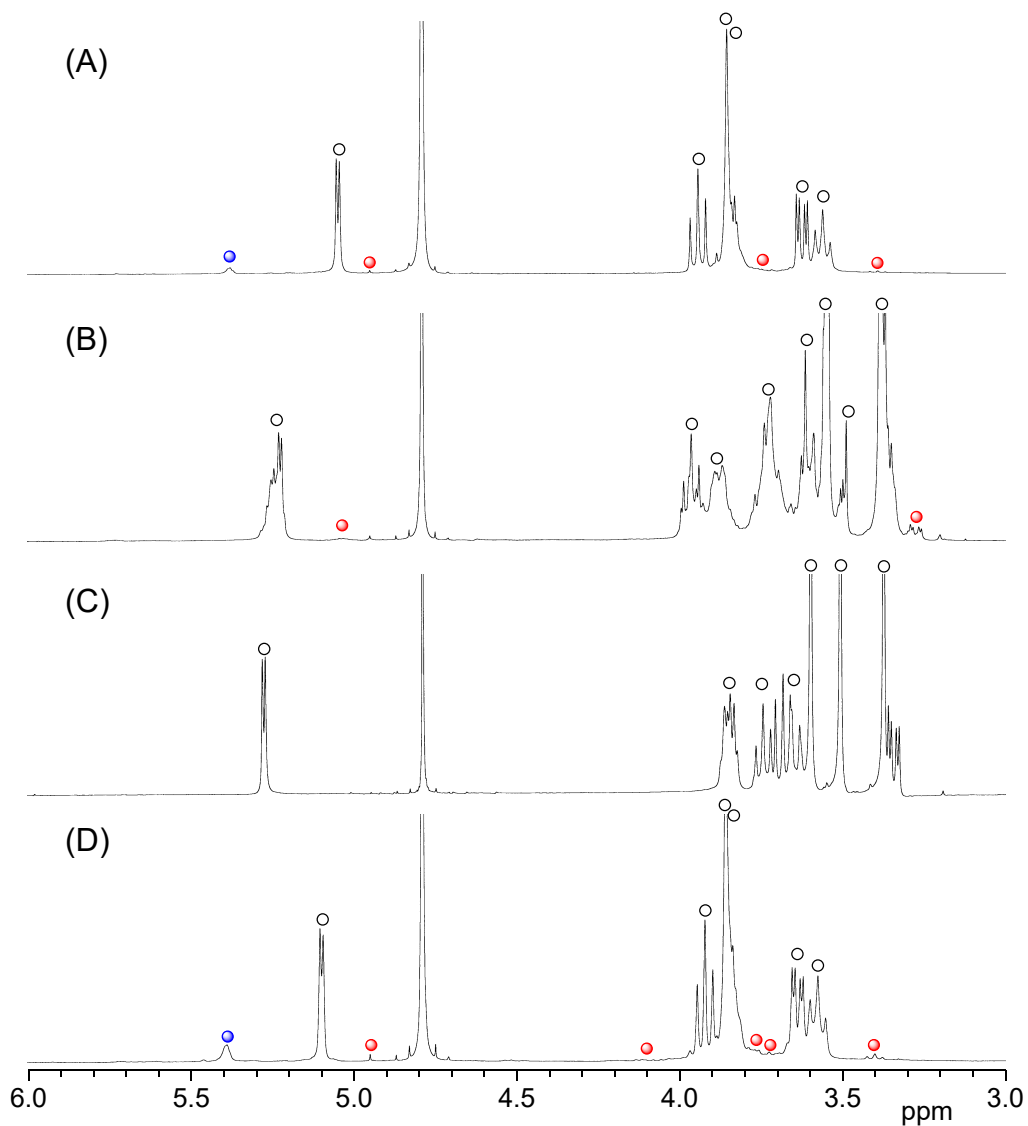
**Fig. S3** UV-vis absorption spectrum of LMI1 in water before (black line) and after 12 h photoirradiation and centrifugation. Initial concentration (red line):  $[1]/[DMPC] = 1.4$  mol%,  $[DMPC] = 4.0$  mM.



**Fig. S4** Complete  $^1\text{H}$  NMR spectra of (A) LMI1, (B) LMI1 after photoirradiation at 365 nm for 3 h ( $1.5 \text{ W m}^{-2}$ ) and (C) LMIC<sub>60-1</sub> after heating at 55 °C for 18 h. All spectra were obtained using  $\text{CDCl}_3$  solutions of freeze-dried samples.

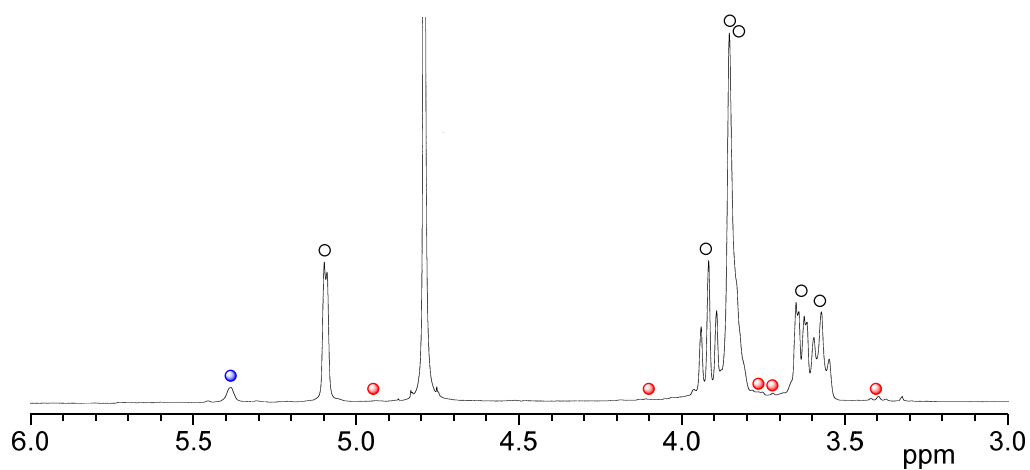


**Fig. S5** Changes in absorption at  $\lambda_{\max}$  of LMI3-4 kept at 25 °C for incubation times 0 (red line), 0.04 (orange line), 0.25 (yellowish orange line), 1 (yellow line), 2 (light-green line), 3 (green line), 5 (blue line) and 10 (purple line) d (initial concentrations: [DMPC] = 4.0 mM, [1] = 0.056 mM, [C<sub>60</sub>] = 0.056 mM before heating at 55 °C for 18 h). Inset shows change in absorption of LMI3-4 at 254 nm.



**Fig. S6**  $^1\text{H}$  NMR spectra of (A)  $2 \cdot \beta\text{-CDx}$ , (B)  $2 \cdot \text{DMe-}\beta\text{-CDx}$ , (C)  $2 \cdot \text{TMe-}\beta\text{-CDx}$  and (D)  $2 \cdot \gamma\text{-CDx}$  mixtures ( $[2] = 7.0 \text{ mM}$ ,  $[\text{CDx}] = 14.0 \text{ mM}$ ) in  $\text{D}_2\text{O}$  at  $25 \text{ }^\circ\text{C}$  ( $\circ$ : free CDx,  $\bullet$ : CDx complexed with **2**,  $\bullet$ : CDx aggregated with **2**).





**Fig. S7**  $^1\text{H}$  NMR spectrum of **3**· $\gamma$ -CDx mixture ( $[\mathbf{3}] = 3.4$  mM,  $[\gamma\text{-CDx}] = 13.9$  mM) in  $\text{D}_2\text{O}$  at  $25$  °C ( $\circ$ : free  $\gamma$ -CDx,  $\bullet$ :  $\gamma$ -CDx complexed with **3**,  $\bullet$ :  $\gamma$ -CDx aggregated with **3**).