Electronic Supplementary Information

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

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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. \([\text{I}]/[\text{DMPC}]\) = (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 \([\text{I}]/[\text{DMPC}]\). Dashed line shows extrapolated absorbances, corresponding to 50% solubility of 1 in water.
**Fig. S2** $^1$H NMR spectrum of LMI in water after 12 h photoirradiation and centrifugation ($●$: 2, $●$: DMPC). Initial concentration: [I]/[DMPC] = 1.4 mol%, [DMPC] = 4.0 mM.
Fig. S3  UV-vis absorption spectrum of LMI\textbf{I} in water before (black line) and after 12 h photoirradiation and centrifugation. Initial concentration (red line): $[1]/[\text{DMPC}] = 1.4$ mol\%, $[\text{DMPC}] = 4.0$ mM.
Fig. S4  Complete $^1$H NMR spectra of (A) LMII, (B) LMII after photoirradiation at 365 nm for 3 h (1.5 W m$^{-2}$) and (C) LMIC$_{60}$–1 after heating at 55 °C for 18 h. All spectra were obtained using CDCl$_3$ solutions of freeze-dried samples.
Fig. S5 Changes in absorption at $\lambda_{\text{max}}$ of LMI$_{3-4}$ 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, [I] = 0.056 mM, [C$_{60}$] = 0.056 mM before heating at 55 °C for 18 h). Inset shows change in absorption of LMI$_{3-4}$ at 254 nm.
Fig. S6  $^1$H NMR spectra of (A) 2·β-CDx, (B) 2·DMe-β-CDx, (C) 2·TMe-β-CDx and (D) 2·γ-CDx mixtures ([2] = 7.0 mM, [CDx] = 14.0 mM) in D$_2$O at 25 °C (○: free CDx, ●: CDx complexed with 2, •: CDx aggregated with 2).
Fig. S7 ¹H NMR spectrum of 3·γ-CDx mixture ([3] = 3.4 mM, [γ-CDx] = 13.9 mM) in D₂O at 25 °C (○: free γ-CDx, ●: γ-CDx complexed with 3, ●: γ-CDx aggregated with 3).