Electronic Supplementary Information

A photo-triggerable drug carrier based on cleavage of PEG lipids by photosensitiser-generated reactive singlet oxygen

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Experimental Section

Materials: γ-CDx and **1** were purchased from Wako Pure Chemical Industries Ltd. (Tokyo, Japan) and NOF Corp. (Tokyo, Japan), respectively. Compound **5** was purchased from Avanti Polar Lipids Inc (Alabama, USA).

Compounds $\mathbf{2}^{S1}$, $\mathbf{3}^{24}$ and C_{60} -derivative $\mathbf{4}^{S2}$ were prepared according to the method described previously.

¹**H NMR spectroscopy:** ¹H NMR spectra were recorded on a JEOL JNM-ECP 400 M spectrometer in CDCl₃, and the chemical shifts were expressed with reference to tetramethylsilane (TMS) as the internal standard.

Mass spectroscopy: The MALDI-TOF mass spectrum was recorded on an Autoflex II spectrometer from Bruker Daltonics using 1,8-dihydroxy-9(10H)-anthracenone (dithranol) as a matrix. The EI mass spectra were recorded on a JEOL JMS-700 mass spectrometer.

References

- S1 Y. Murakami, A. Nakano and H. Ikeda, J. Org. Chem., 1982, 47, 2137–2144.
- S2 A. M. Cassell, W. A. Scrivens and J. M. Tour, Angew. Chem. Int. Ed., 1998, 31, 1528–1531.



Fig. S1 Positive ion MALDI-TOF mass spectrum of 3



Fig. S2 Fluorescence spectral change ($\lambda_{ex} = 488 \text{ nm}$) of the liposome 1, 2 and 3 {1:2:3 = 5:95:15 (mol/mol/mol)} containing 5 (0.25 mol%) before (black line) and after the exchange reaction with the C₆₀-4• γ -CDx complex (red line).



Fig. S3 UV-vis absorption spectra of the C₆₀-4• γ -CDx complex (black line) and LMIC₆₀-4 (red line) ([C₆₀-4] = 0.01 mM, 1 mm cell).



Fig. S4 EI mass spectra of (A and C) two cholesterol-related compounds separated from the photolysates of 3 in LMIC₆₀-4 by column chromatography on silica; commercial (B) cholesterol and (D) cholesterol formate as reference standards.



Fig. S5 Positive ion MALDI-TOF mass spectrum of C_{60} -4 in LMIC₆₀-4 (A) before the photoirradiation and (B) after the photoirradiation for 5 min.



Fig. S6 (A) Partial ¹H NMR spectra of 3 in LMIC₆₀-4 before (black line) and after photoirradiation for 0.5 (blue line), 1 (green line), 1.5 (orange line), 3 (red line) and 5 (purple line) min. (B) Time-dependent photocleavage of 3 in LMIC₆₀-4.