Electronic Supplementary Information

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

Chikako Komeda, Atsushi Ikeda,* Jun-ichi Kikuchi, Norihiro Ishida-Kitagawa, Hisashi Tatebe, Kazuhiro Shiozaki and Motofusa Akiyama

aGraduate School of Materials Science, Nara Institute of Science and Technology, 8916-5 Takayama, Ikoma, Nara 630-0192, Japan.
bGraduate School of Biological Sciences, Nara Institute of Science and Technology, 8916-5 Takayama, Ikoma, Nara 630-0192, Japan.
cDepartment of Applied Chemistry, Faculty of Science and Engineering, Chuo University, 1-13-27 Kasuga, Bunkyo-ku, Tokyo 113-8551, Japan.
**Experimental Section**

**Materials:** $\gamma$-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 2, $^{S1}$$^{31}$ 3$^{24}$ and C$_{60}$-derivative 4$^{S2}$ were prepared according to the method described previously.

**$^1$H NMR spectroscopy:** $^1$H NMR spectra were recorded on a JEOL JNM-ECP 400 M spectrometer in CDCl$_3$, 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**


**Fig. S1** Positive ion MALDI-TOF mass spectrum of 3
**Fig. S2** Fluorescence spectral change ($\lambda_{ex} = 488$ 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 C$_{60}$-4\*CDx complex (red line).
Fig. S3  UV-vis absorption spectra of the C$_{60}$-4•γ-CDx complex (black line) and LMIC$_{60}$-4 (red line) ([C$_{60}$-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 LMIC_{60}-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 LMIC_{60}-4 (A) before the photoirradiation and (B) after the photoirradiation for 5 min.
Fig. S6 (A) Partial $^1$H NMR spectra of 3 in LMIC$_{60}$-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 LMIC$_{60}$-4.