Electronic Supplementary Information

Colorimetric chemosensor for heptanal with selectivity over formaldehyde and acetaldehyde through synergistic interaction of hydrophobic interactions and oxime formation

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Determination of the optimal ratio of DA-A and DA-B

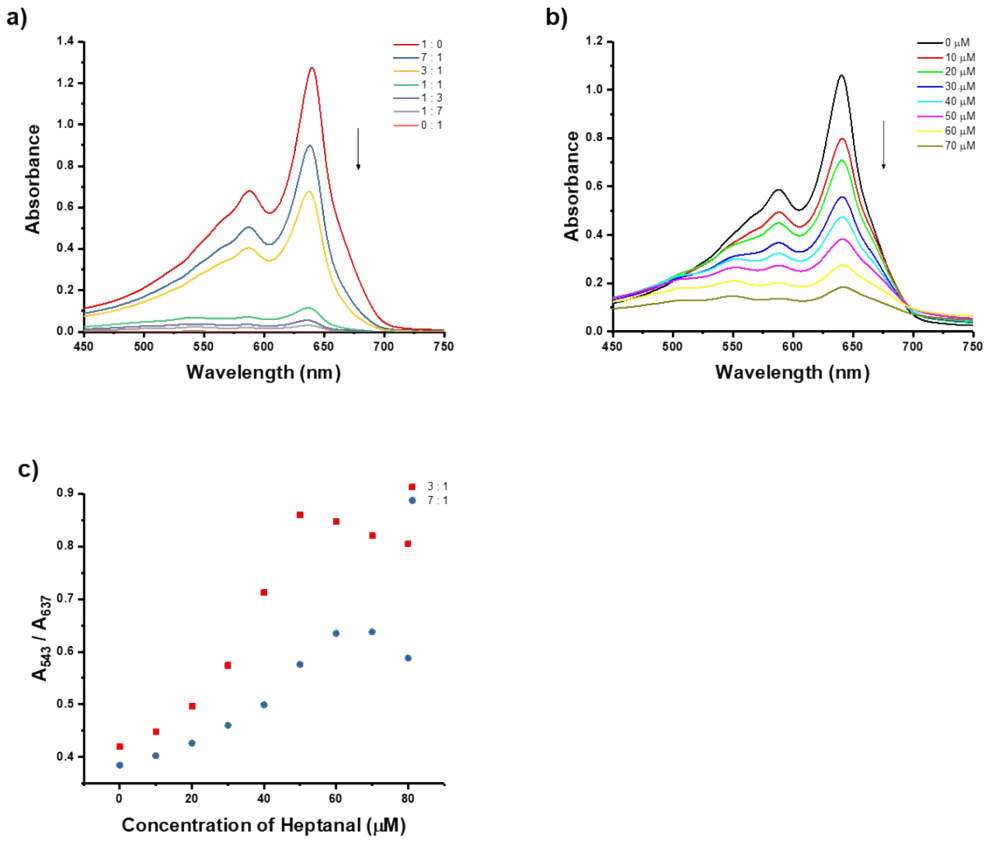

Fig. S1 a) UV-Vis spectra of PDA liposomes (100 μM) composed with various ratio of **DA-A** and **DA-B** (1:0, 7:1, 3:1, 1:1, 1:3, 1:7, and 0:1) in the acetate buffer (20 mM, pH 4.0); b) UV-Vis spectra obtained 2 h after the addition of heptanal solutions (0, 10, 20, 30, 40, 50, 60, and 70 μM in 0.1 % MeOH) to the acetate buffer (20 mM, pH 4.0) containing PDA liposomes (100 μM) composed with 1:0 ratio of **DA-A** and **DA-B**; c) Plot of the absorbance ratio at 543 and 637 nm in PDA liposomes (100 μM) composed with 3:1 and 7:1 ratio of **DA-A** and **DA-B** *versus* heptanal concentrations.

Investigation of temperature parameter in PDA liposome

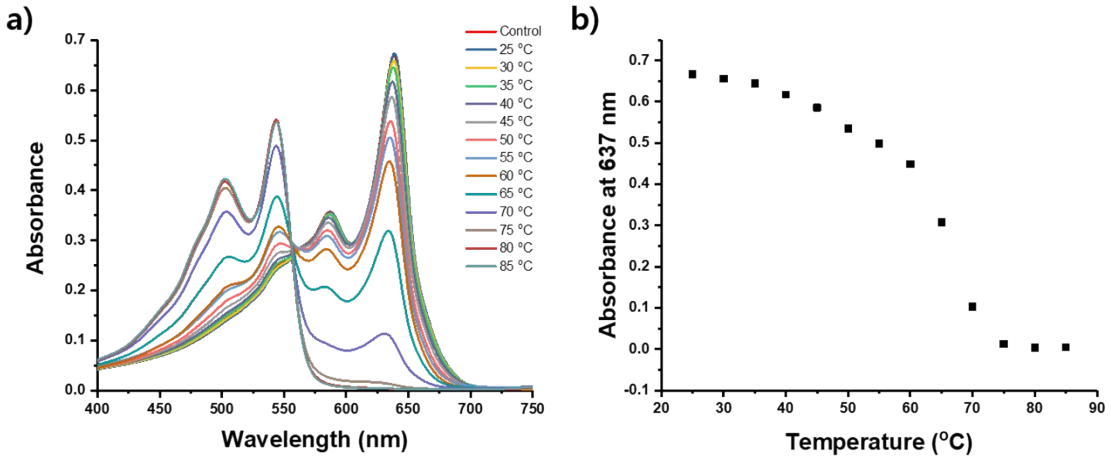

Fig. S2 a) UV-Vis spectra of PDA liposomes (100 µM) in acetate buffer (20 mM, pH 4.0) obtained after incubation for 20 min at various temperatures; b) Plot of absorbance at 637 nm for various temperatures.

Estimation of limit of detection for heptanal using PDA liposome

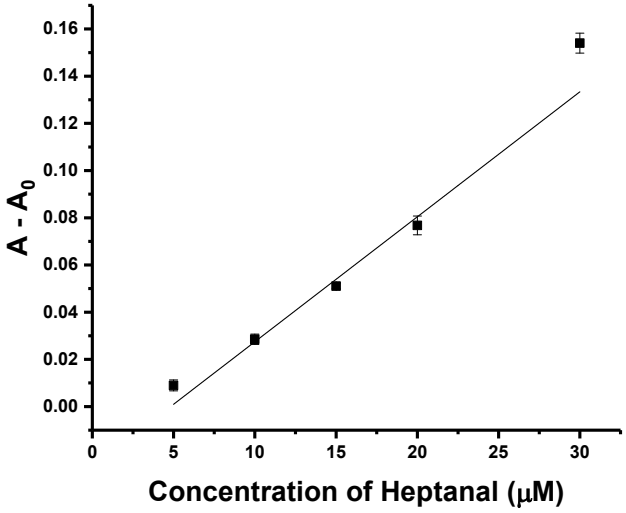

Fig. S3 Plot of absorbance ratio at 543 and 637 nm against heptanal concentrations (5, 10, 15, 20, and 30 μM in 0.1 % MeOH) where A and A_0 means absorbance ratio at 543 and 637 nm in the presence and absence of heptanal, respectively.

Intercept = -0.0255

Slope = 0.0053

R^2 = 0.9436

Limit of detection (LOD) = 4.8 μM

Dynamic light scattering (DLS) of PDA liposome

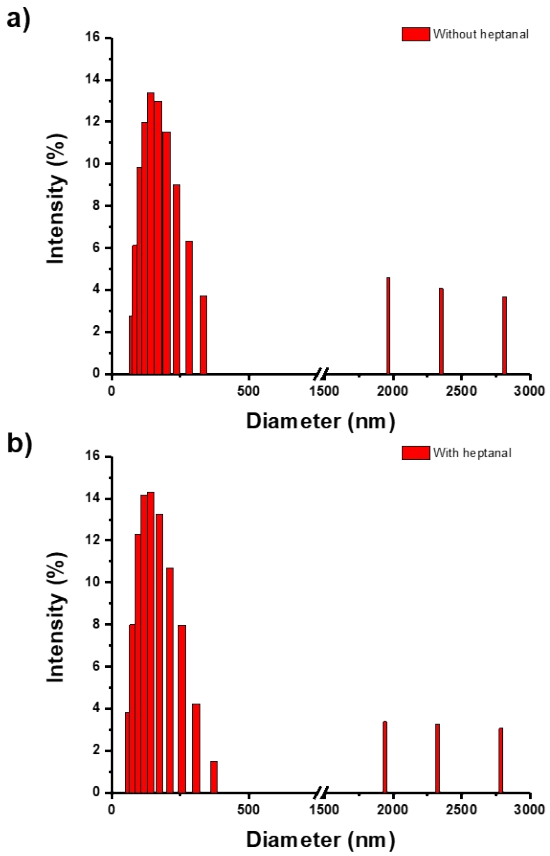

Fig. S4 The size distribution of PDA liposomes (100 µM) obtained after 2h incubation in the a) absence and b) presence of heptanal (50 µM in 0.1 % MeOH).

Raman spectra of PDA liposome

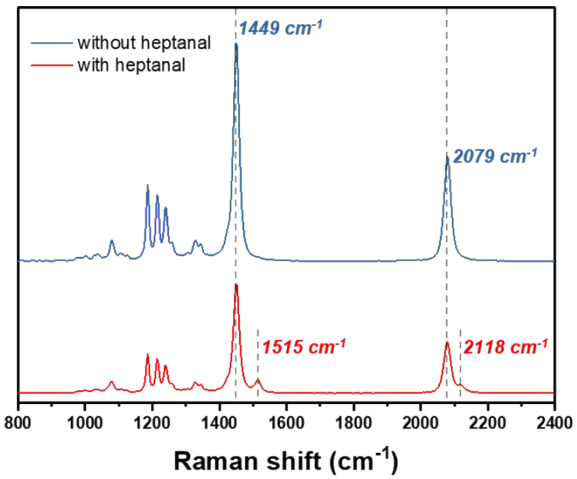

Fig. S5 Raman spectra of PDA liposomes (500 µM) 2h after incubation in the absence and presence of heptanal (250 µM).

Selectivity test for mimic serum

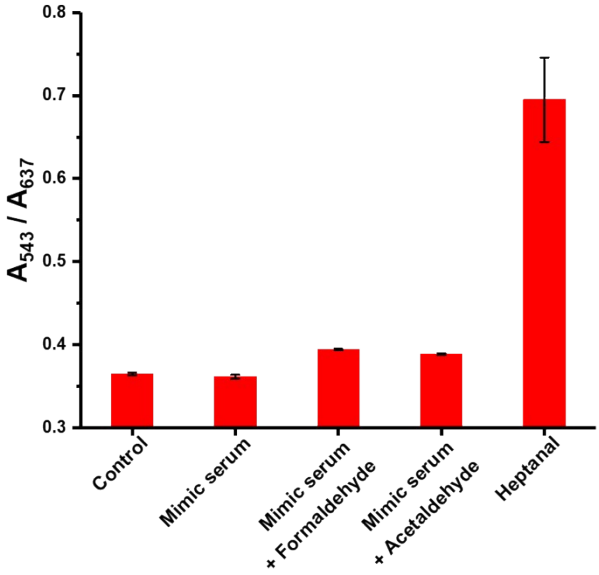

Fig. S6 Plot of the absorbance ratio at 543 and 637 nm obtained 2 h after the addition of mimic serum (combination of glucose, urea, proline, and NaCl, 500 μM), mimic serum with aldehydes (formaldehyde and acetaldehyde, 500 μM), and heptanal (50 μM) to the acetate buffer containing the PDA liposomes (100 μM).

Characterization of compounds

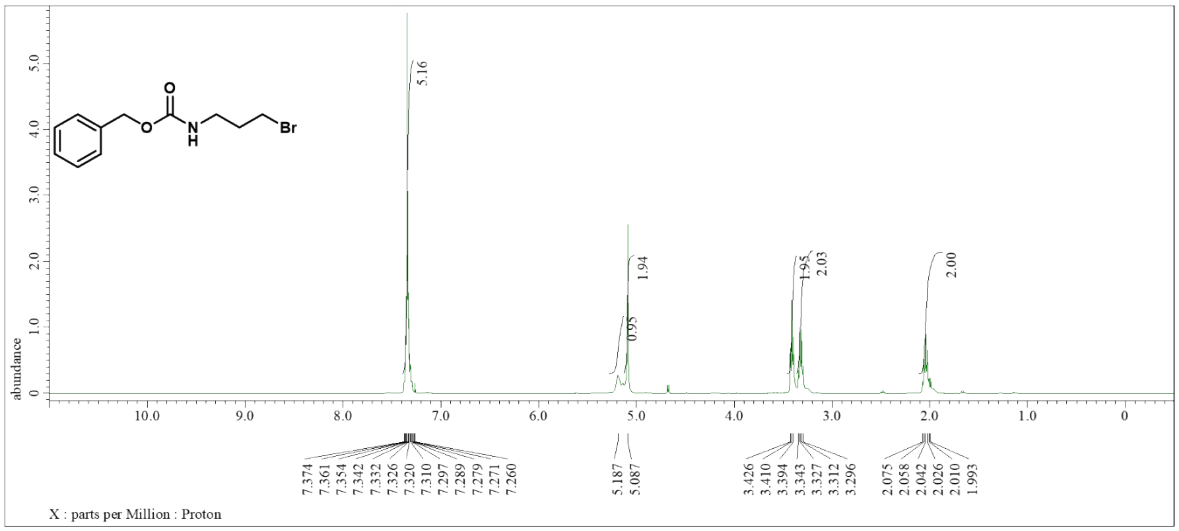

Fig. S7 ^{1}H-NMR spectrum of compound **7** in $CDCl_3$.

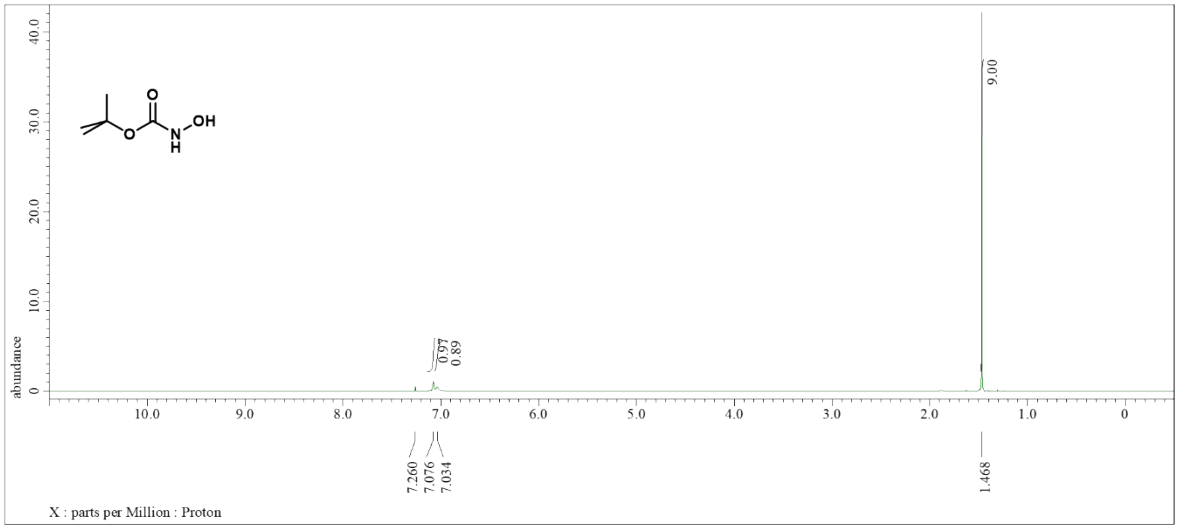

Fig. S8 ^{1}H-NMR spectrum of compound **6** in $CDCl_3$.

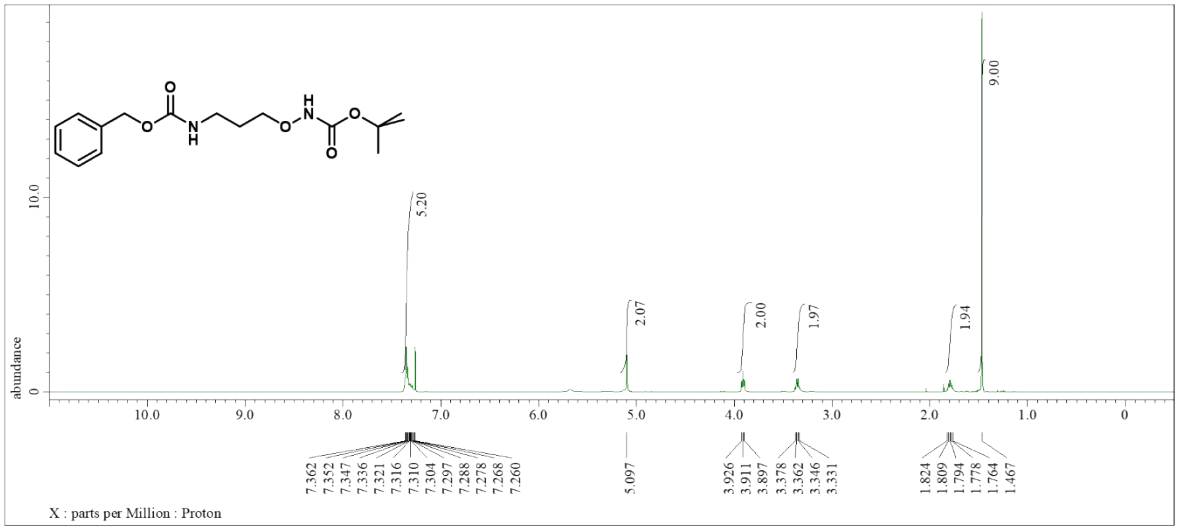

Fig. S9 ^{1}H-NMR spectrum of compound **5** in $CDCl_3$.

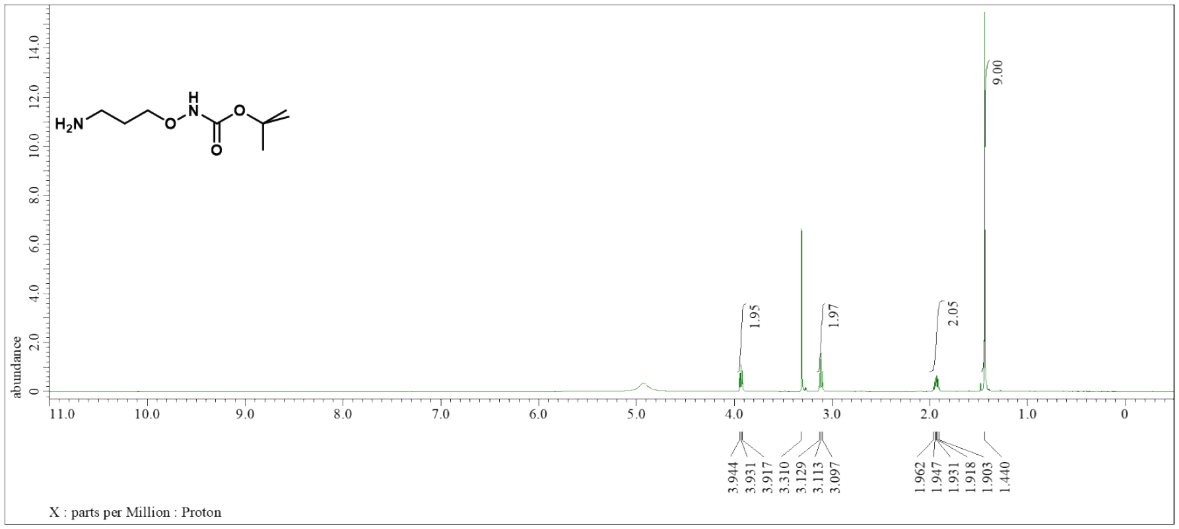

Fig. S10 ^{1}H-NMR spectrum of compound **4** in CD_3OD.

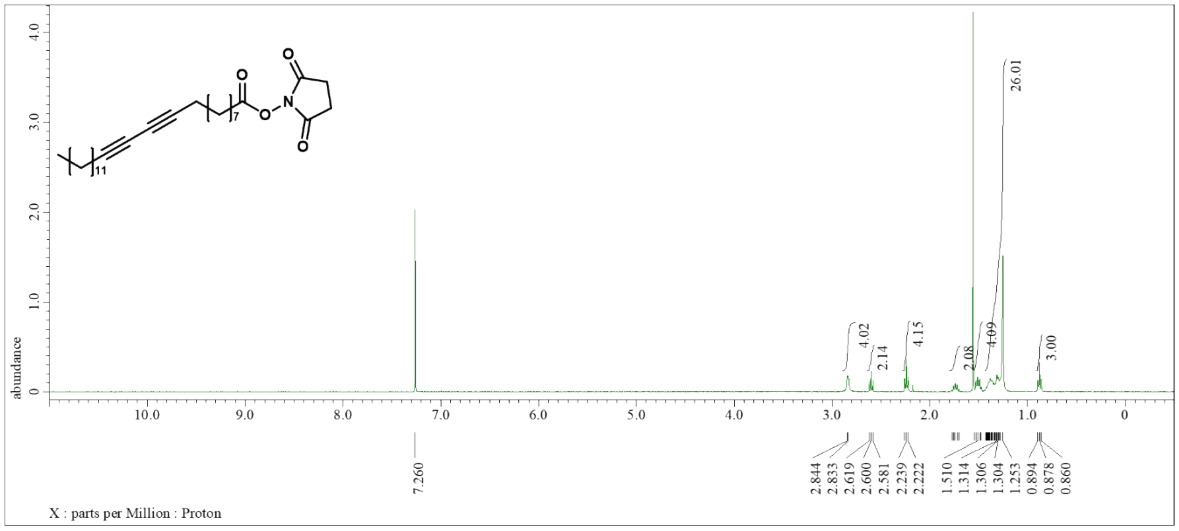

Fig. S11 ^{1}H-NMR spectrum of compound **3** in $CDCl_3$

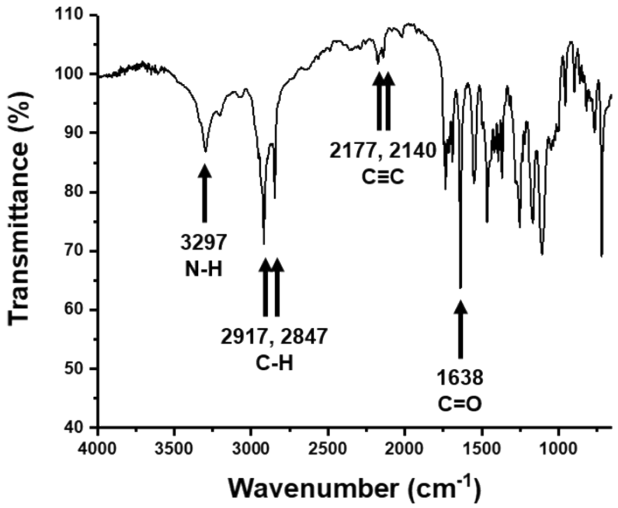

Fig. S12 FT-IR spectrum of compound **2**

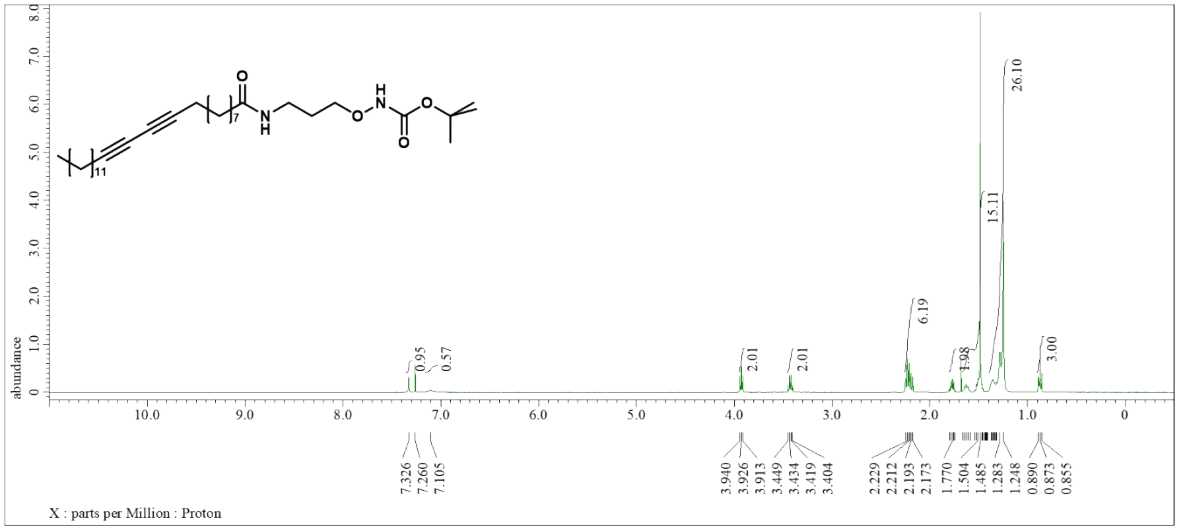

Fig. S13 ^{1}H-NMR spectrum of compound **2** in $CDCl_3$

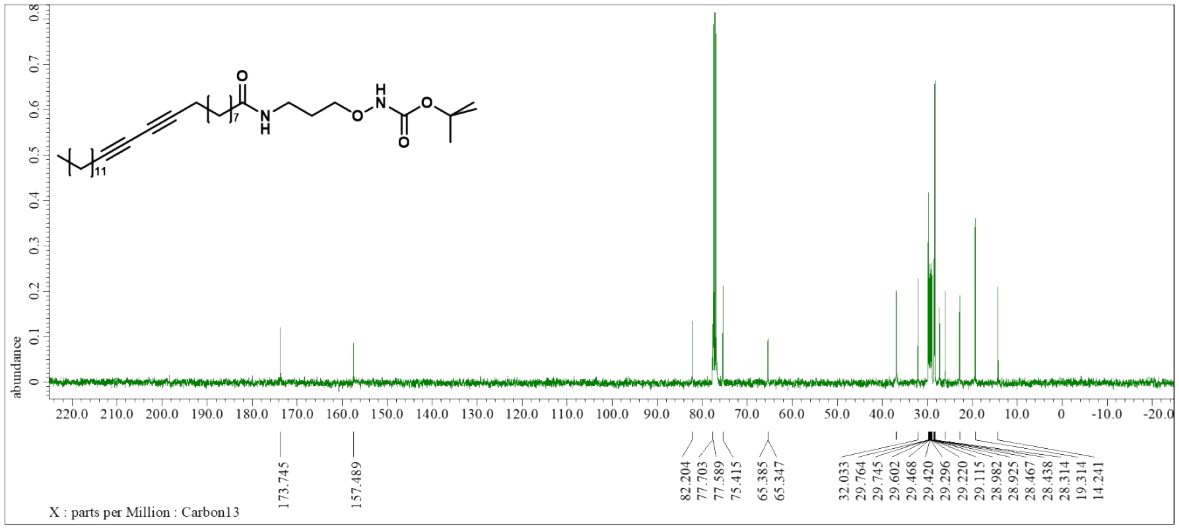

Fig. S14 ^{13}C-NMR spectrum of compound **2** in $CDCl_3$

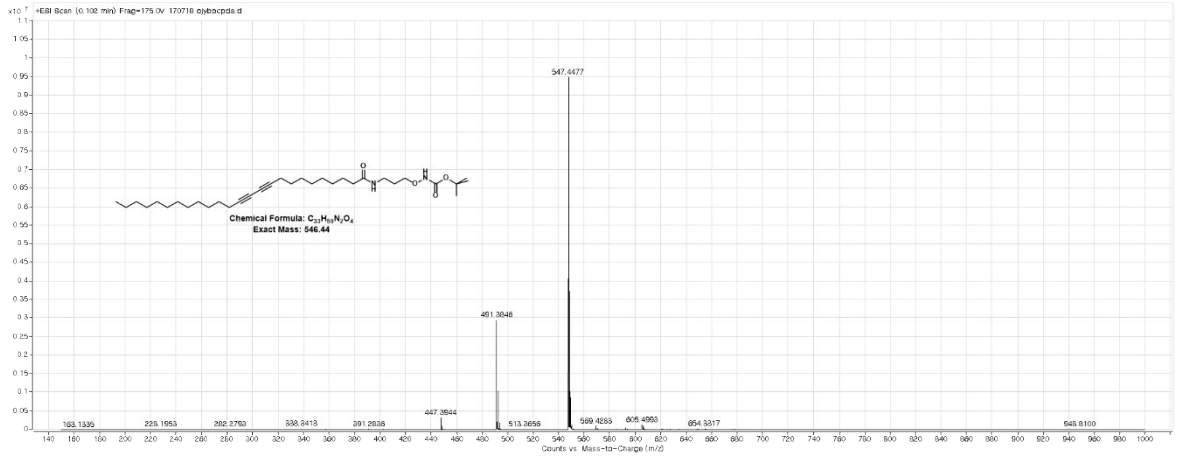

Fig. S15 ESI-MS spectrum of compound **2**

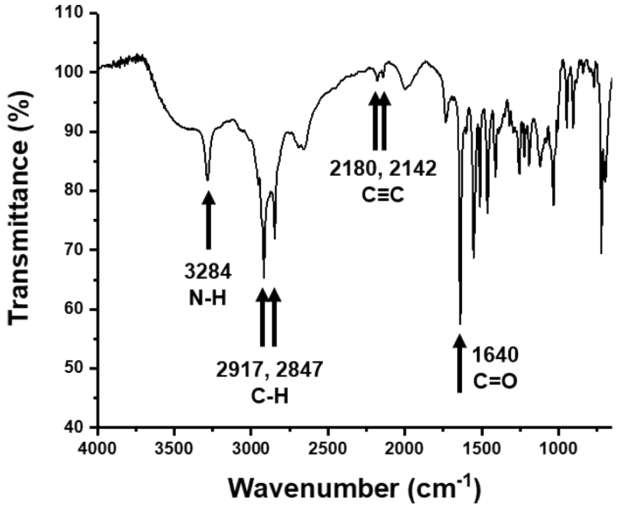

Fig. S16 FT-IR spectrum of compound **DA-A**

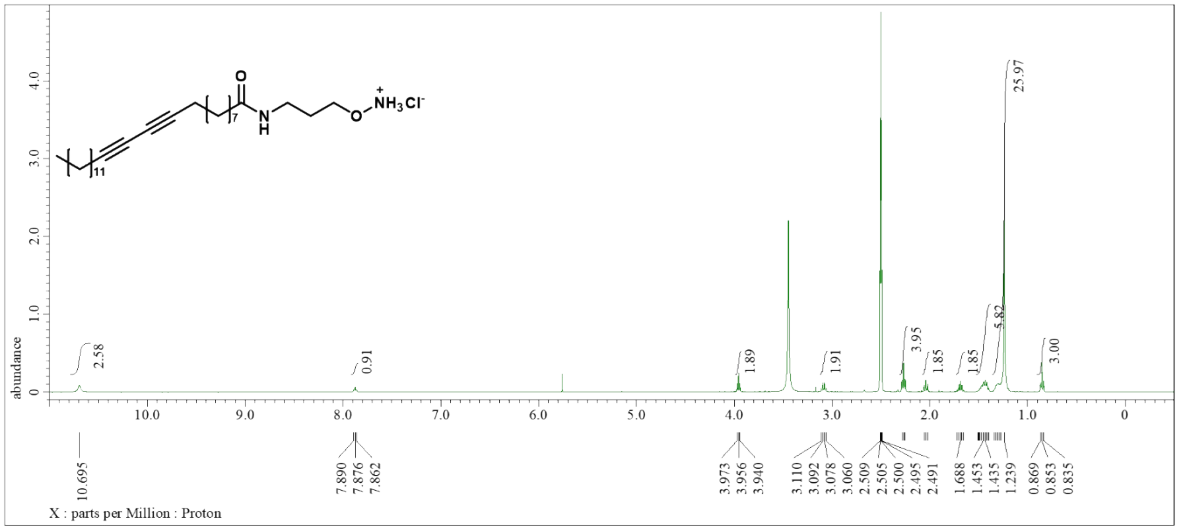

Fig. S17 ^{1}H-NMR spectrum of compound **DA-A** in DMSO-d_6

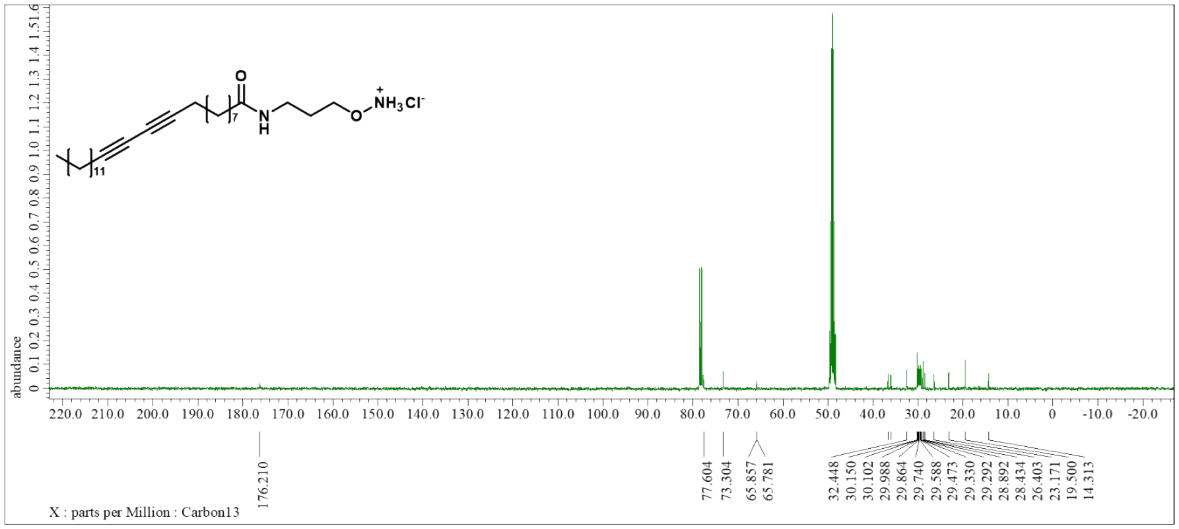

Fig. S18 ^{13}C-NMR spectrum of compound **DA-A** in DMSO-d_6 : $CDCl_3$ = 1 : 1

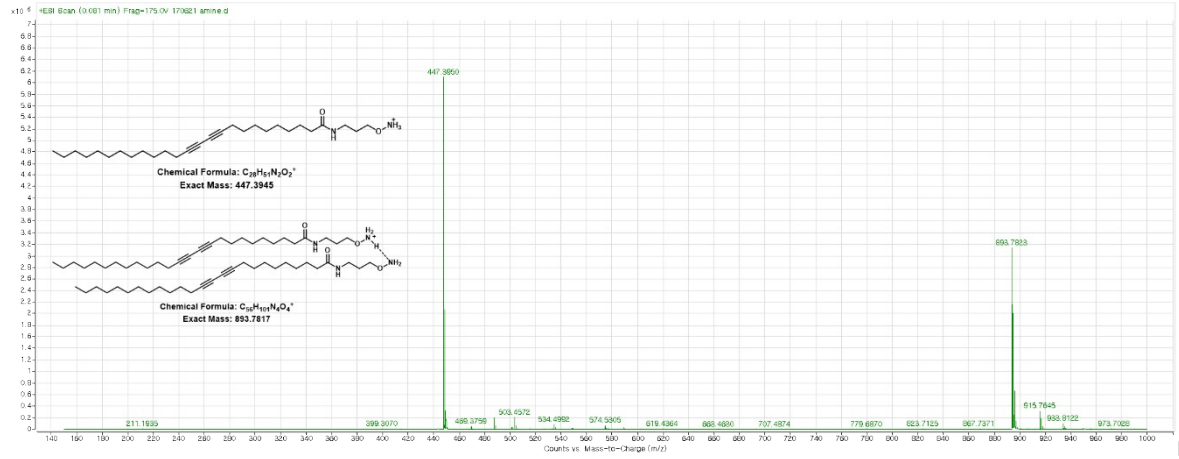

Fig. S19 ESI-MS spectrum of compound **DA-A**

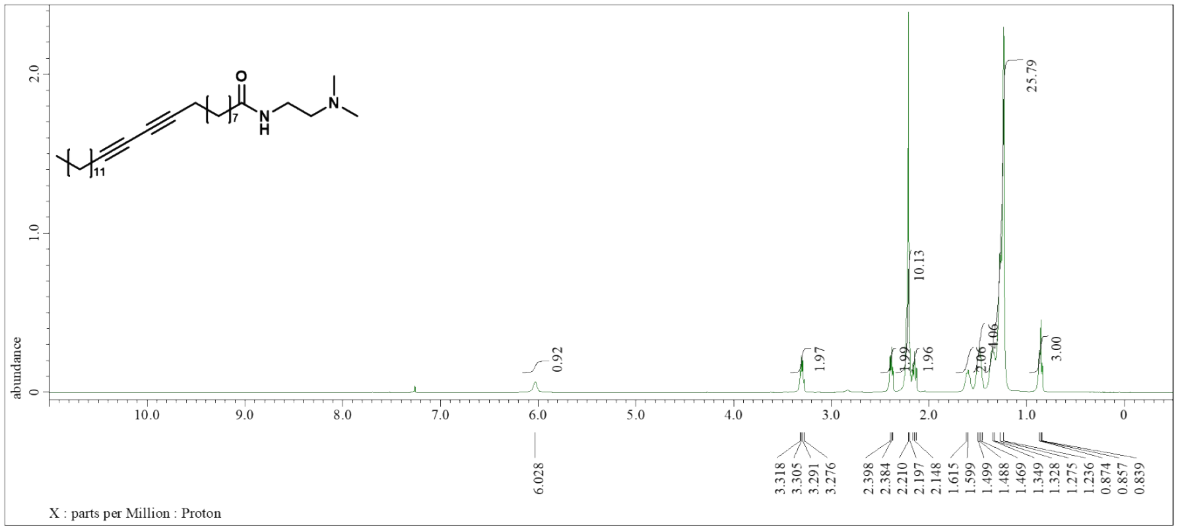

Fig. S20 ^{1}H-NMR spectrum of compound **9** in $CDCl_3$

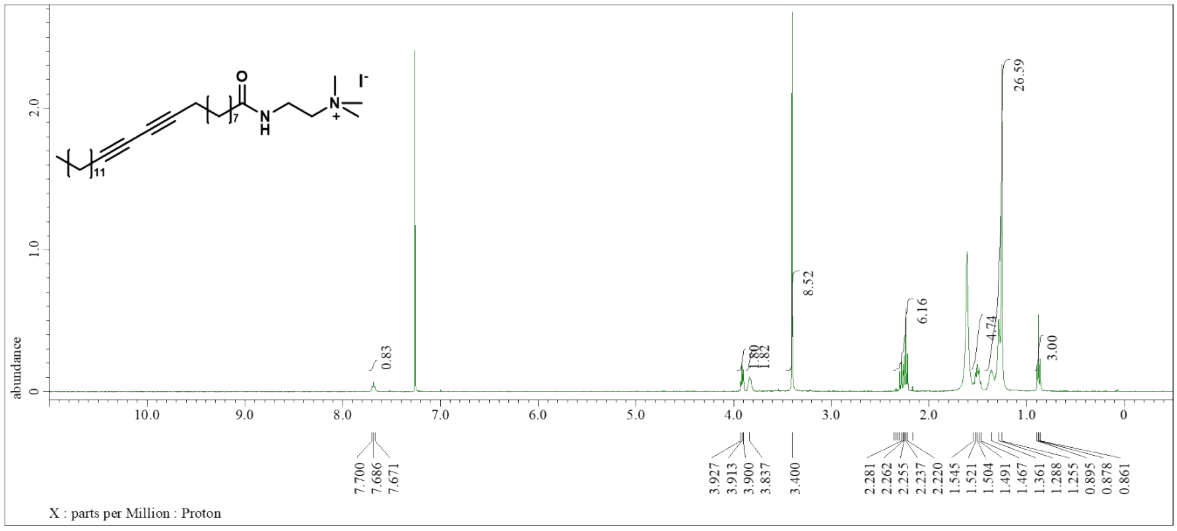

Fig. S21 ^{1}H-NMR spectrum of compound **DA-B** in $CDCl_3$