Supporting Information

BODIPY-Based Fluorescent Surfactant for Cell Membrane Imaging and Photodynamic Therapy

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Synthesis of C8BCOOH.

2-octyl-pyrrole (1). Pyrrole (2.00 g, 29.8 mmol), Octanoyl chloride (7.80 g, 44.7 mmol), and zinc powder (3.88 g, 59.7 mmol) were mixed in 50 mL of toluene. This mixture was stirred at room temperature for 4 hours. The reaction solution was suspended with saturated $NaHCO_3$ solution and extracted with 30 mL ethyl acetate for three times. The mixed solution was washed with water, dried with anhydrous sodium sulfate. The solvent was evaporated *in vacuo* and the residue was dissolved in 150 mL of 2-propanol. $NaBH_4$ (4.00 g, 107.5 mmol) was added slowly at room temperature, and refluxed at 90 ^oC for 10 hours. The hot reaction solution was poured into 150 mL ice water and 10 % hydrochloric acid solution was added for acidification. The suspension was extracted thrice with 50 mL dichloromethane, and the mixed organic solution was washed with saturated saline solution, and the extracts were dried over anhydrous sodium sulfate. After evaporated, the residue was purified with chromatograph using dichloromethane/methanol (100:1 to 30:1) as eluent to afford **2-octyl-pyrrole** (1.98 g, 51 % yield). ^1H NMR (400 MHz, $CDCl_3$, ppm): δ 0.79 (t, 3H), 1.20-1.42 (m, 10H, CH_2), 1.53 (m, 2H), 2.50 (m, 2H), 5.83 (s, 1H), 6.04 (s, 1H), 6.56 (s, 1H), 7.79 (br s, 1H). ^{13}C NMR ($CDCl_3$, ppm): 14.1, 22.7, 27.8, 29.3, 29.4, 29.5, 29.7, 31.9, 104.8, 108.2, 116.0, 132.9. MS-ESI (m/z, $[M+H]^+$): calcd, 180.1; found, 180.2.

Fluorescent Surfactant C8BCOOH. 2-octyl-pyrrole (1.00 g, 5.6 mmol) and 4-formylbenzoic acid (0.21 g, 1.4 mmol) were mixed in 100 mL of anhydrous

dichloromethane, and 10 μL trifluoroacetic acid, triethylamine, and boron trifluoride diethyl etherate (BF_3-OEt_2) were added. After stirred at 25 °C overnight, *p*-chloranil (0.35 g, 1.4 mmol) was added, and stirred for 30 minutes. After the temperature was cooled to 0 °C, 5 mL of triethylamine and 6 mL of BF_3-OEt_2 were added, and the reaction was continued for 3 hours. The mixed solution was washed thrice with saturated sodium bicarbonate solution, and the aqueous phase was extracted with dichloromethane. The organic solvent was removed in vacuo. The residue was purified with chromatograph using dichloromethane/methanol (from 100:1 to 10:1) as the eluent to afford the final compound **C8BCOOH** (0.10 g, 13 % yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 0.88 (t, 6H), 1.28 (m, 20H), 1.60 (m, 4H), 2.34 (m, 2H), 6.55 (m, 2H), 7.07 (m, 2H), 7.55 (m, 2H), 7.92 (s, 2H); ^{13}C NMR (400 MHz, $CDCl_3$, ppm) δ 14.1, 23.4, 29.8, 31.0, 32.8, 33.1, 35.4, 45.9, 107.3, 115.2, 125.5, 128.2, 131.4, 137.5, 140.6, 143.7, 149.2, 180.9; HRMS-ESI (m/z, $[M-H]^-$): calcd, 535.3307; found, 535.3314. Anal. Calcd for $C_{32}H_{43}BF_2N_2O_2$-$C_4H_{10}O$: C, 70.81; H, 8.75; N, 4.59. Found: C, 70.64; H, 8.63; N, 4.67.

Additional Results.

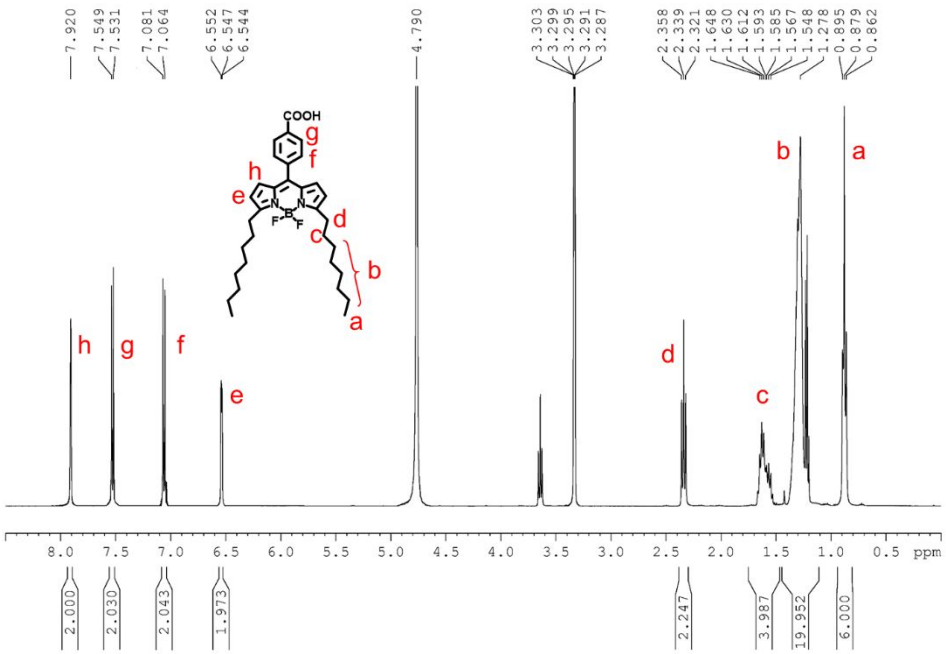

Figure S1. ^{1}H NMR spectrum of **C8BCOOH** in CD_3OD.

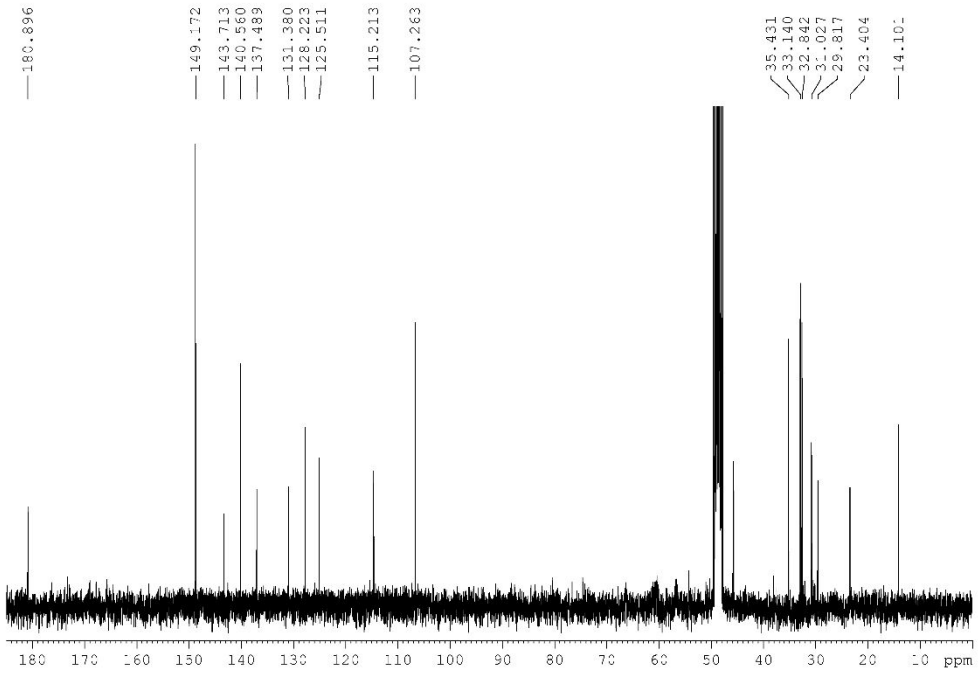

Figure S2. ^{13}C NMR spectrum of **C8BCOOH** in CD_3OD.

Table S1. The HOMO and LUMO levels of different moieties in BODIPY derivative.

	HOMO/eV	LUMO/eV
Benzene	-6.98	-0.26
Benzoic acid	-7.34	-1.57
BODIPY	-6.25	-3.14
C8-BODIPY	-5.78	-2.81

Table S2. The size and zeta-potential values of **C8BCOONa** with different concentrations.

$C_{C8BCOONa}$/μM	d/nm	ζ/mV
20	146.8	-35.3
50	132.7	-30.2
100	151.2	-33.4
1000	158.4	-31.6

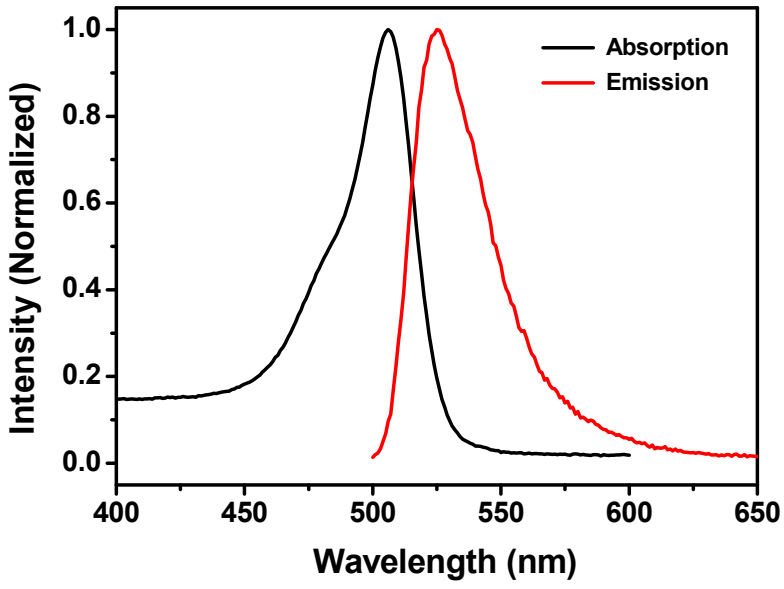

Figure S3. Normalized absorbance spectrum and fluorescence emission spectrum of C8BCOONa. The concentration is 2 μM.

Table S3. The size and ζ-potential values of DOPC vesicles with different C8BCOONa concentrations. The concentration of DOPC is 1 mM.

$C_{C8BCOONa}$/μM	d/nm	ζ/mV
0	193.8	-2.3
2	186.7	0.8
4	208.9	-3.3
6	204.3	-0.5
8	199.7	-1.6
10	204.6	-2.8
15	215.5	-1.2
20	209.2	-5.1
30	188.4	-0.4