

Supplementary Information

Fluorescent sensor for water based on photo-induced electron transfer and Förster resonance energy transfer: anthracene-(aminomethyl)phenylboronic acid ester-BODIPY structure

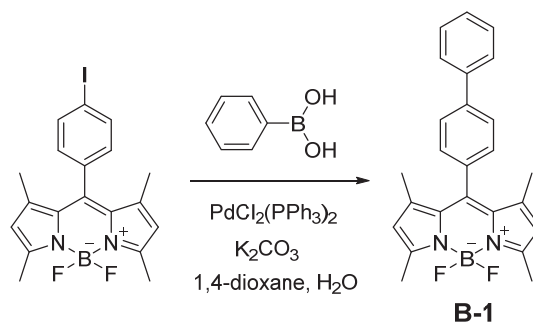
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Synthesis of 10-([1,1'-Biphenyl]-4-yl)-5,5-difluoro-1,3,7,9-tetramethyl-5H-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinine (B-1)

A solution of 5,5-difluoro-10-(4-iodophenyl)-1,3,7,9-tetramethyl-5H-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinine (0.050 g, 0.11 mmol), phenylboronic acid (0.016 g, 0.13 mmol), PdCl₂(PPh₃)₂ (0.017 g, 0.024 mmol), and K₂CO₃ (0.061 g, 0.44 mmol) in 1,4-dioxane (9 mL) and water (0.44 mL) was refluxed for 12 h under a nitrogen atmosphere. After concentrating under reduced pressure, the resulting residue was dissolved in dichloromethane, and washed with water. The dichloromethane extract was dried over Na₂SO₄, filtrated, and evaporated under reduced pressure. The residue was chromatographed on silica gel (dichloromethane-hexane = 2 : 1 as eluent) to give **B-1** (0.027 g, 61 % yield) as an orange solid; ¹H NMR (400 MHz, CDCl₃): δ = 1.45 (s, 6H), 2.57 (s, 6H), 5.99 (s, 2H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.40 (t, 1H), 7.40 (t, 2H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.75 (d, *J* = 8.3 Hz, 2H) ppm; HRMS (ESI): *m/z* (%):[M+Na⁺] Calcd for C₂₅H₂₃N₂BF₂Na, 423.18146; found 423.18143.



Scheme S1 Synthesis of **B-1**

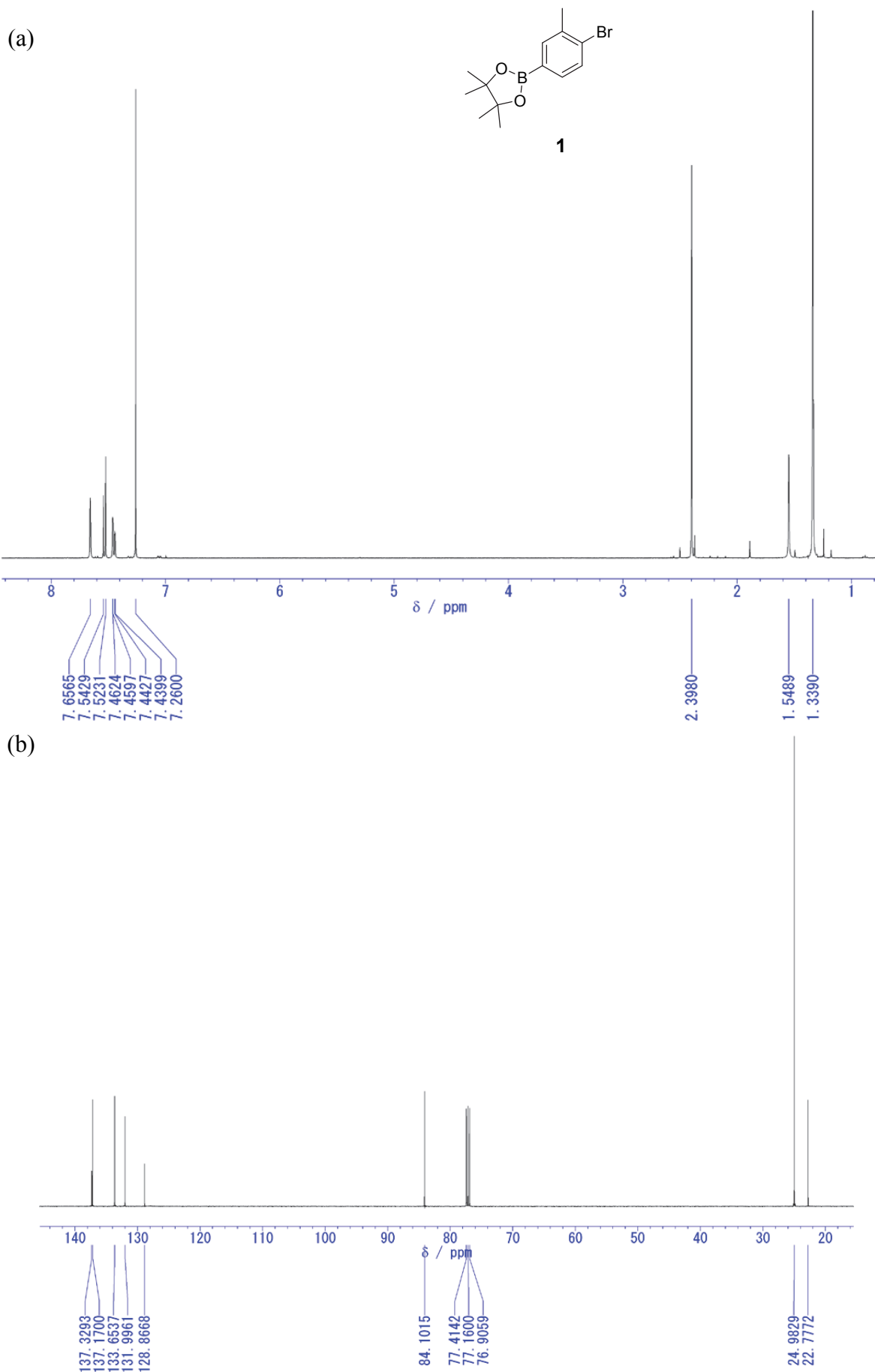


Fig. S1 (a) ^1H NMR (400 MHz) and (b) ^{13}C NMR (125 MHz) spectra of **1** in CDCl_3 .

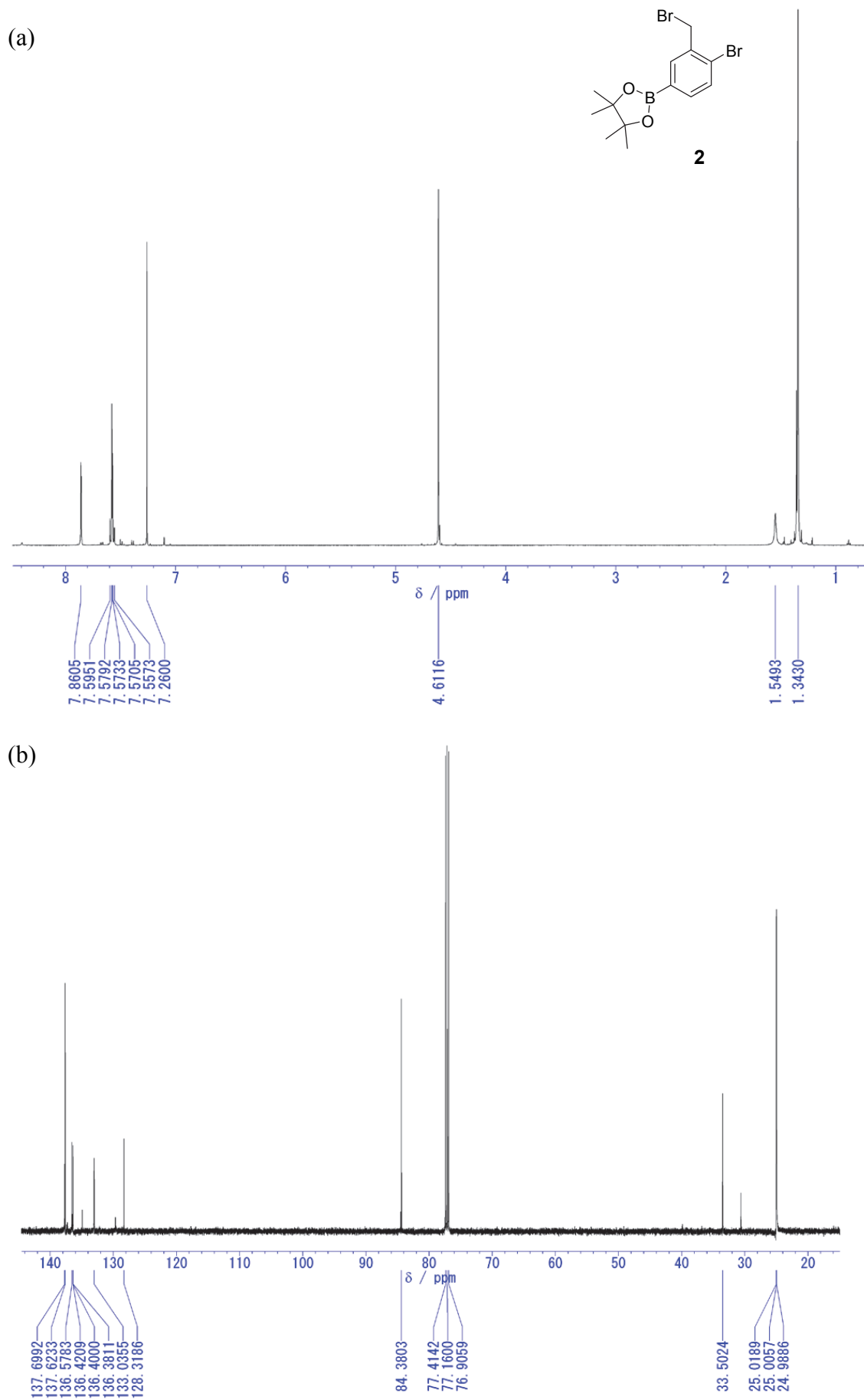


Fig. S2 (a) ^1H NMR (500 MHz) and (b) ^{13}C NMR (125 MHz) spectra of **2** in CDCl_3 .

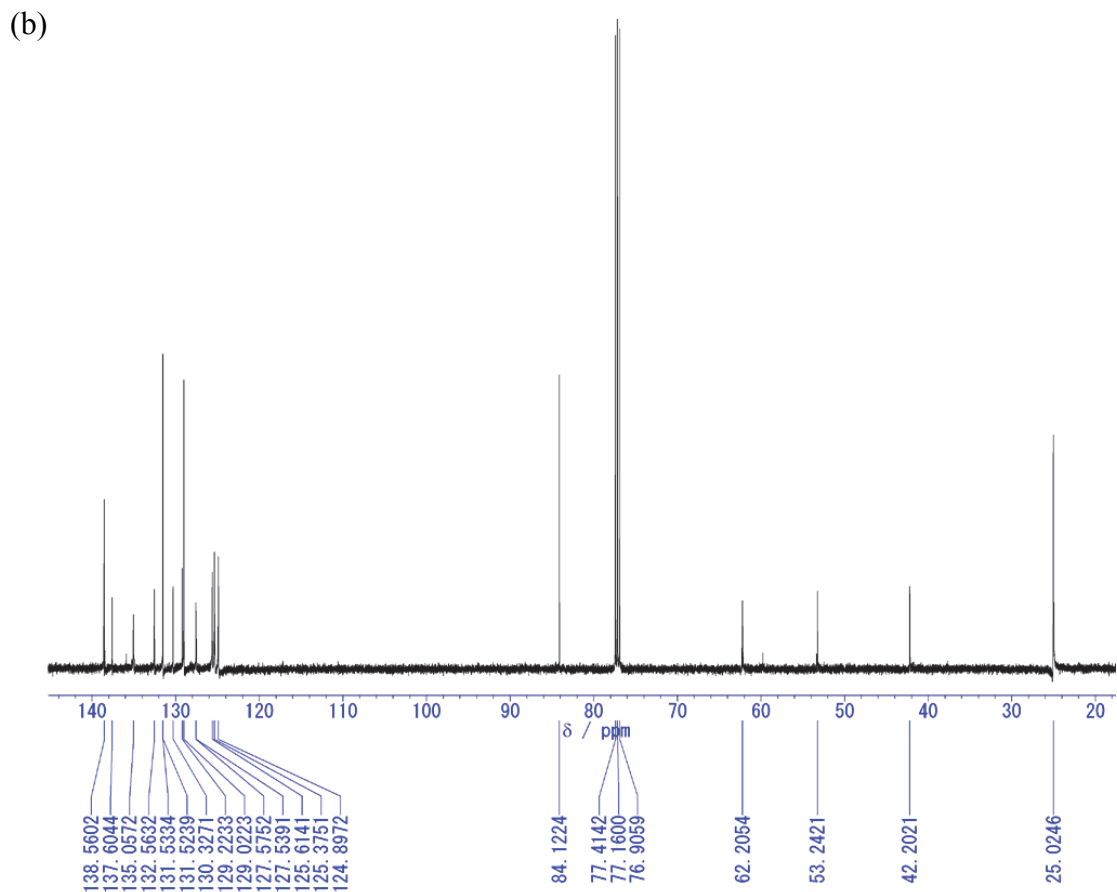
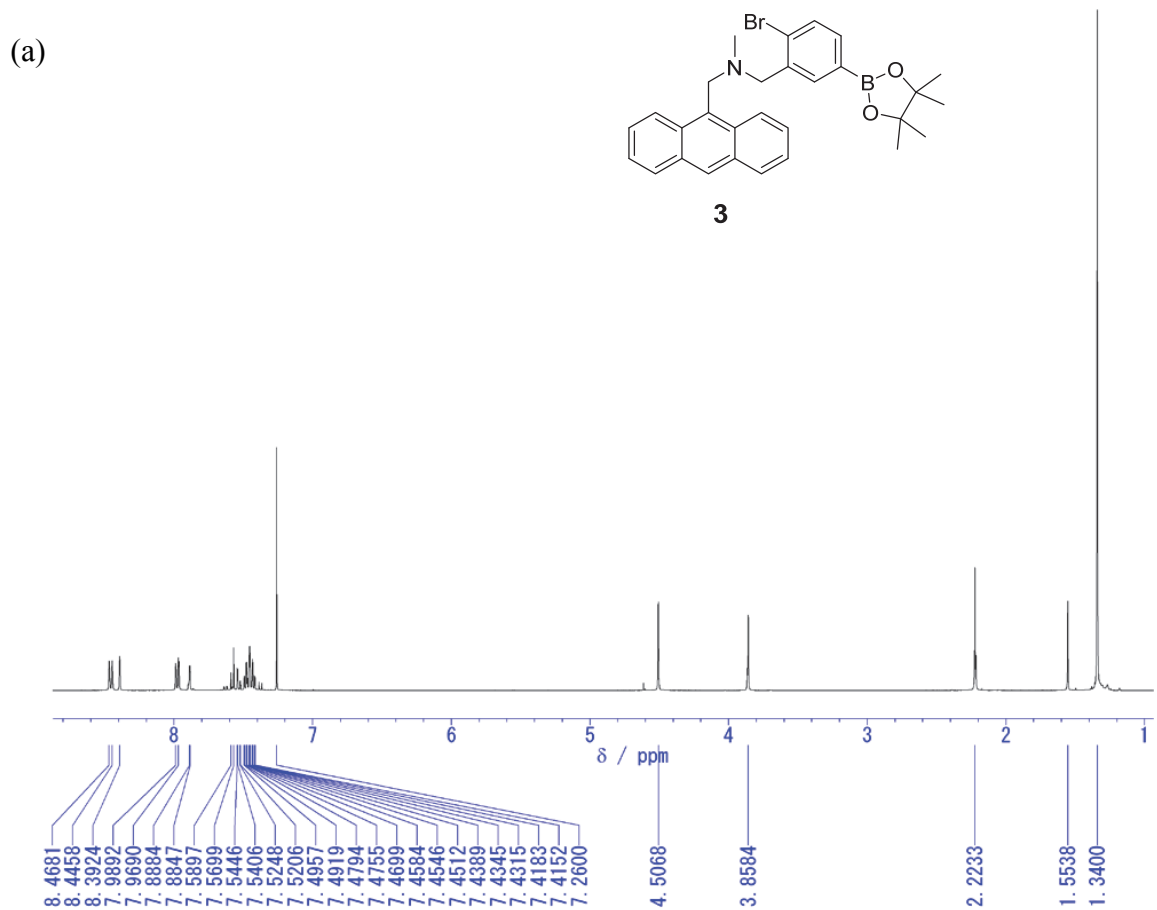


Fig. S3 (a) ^1H HMR (400 MHz) and (b) ^{13}C HMR (125 MHz) spectra of **3** in CDCl_3 .

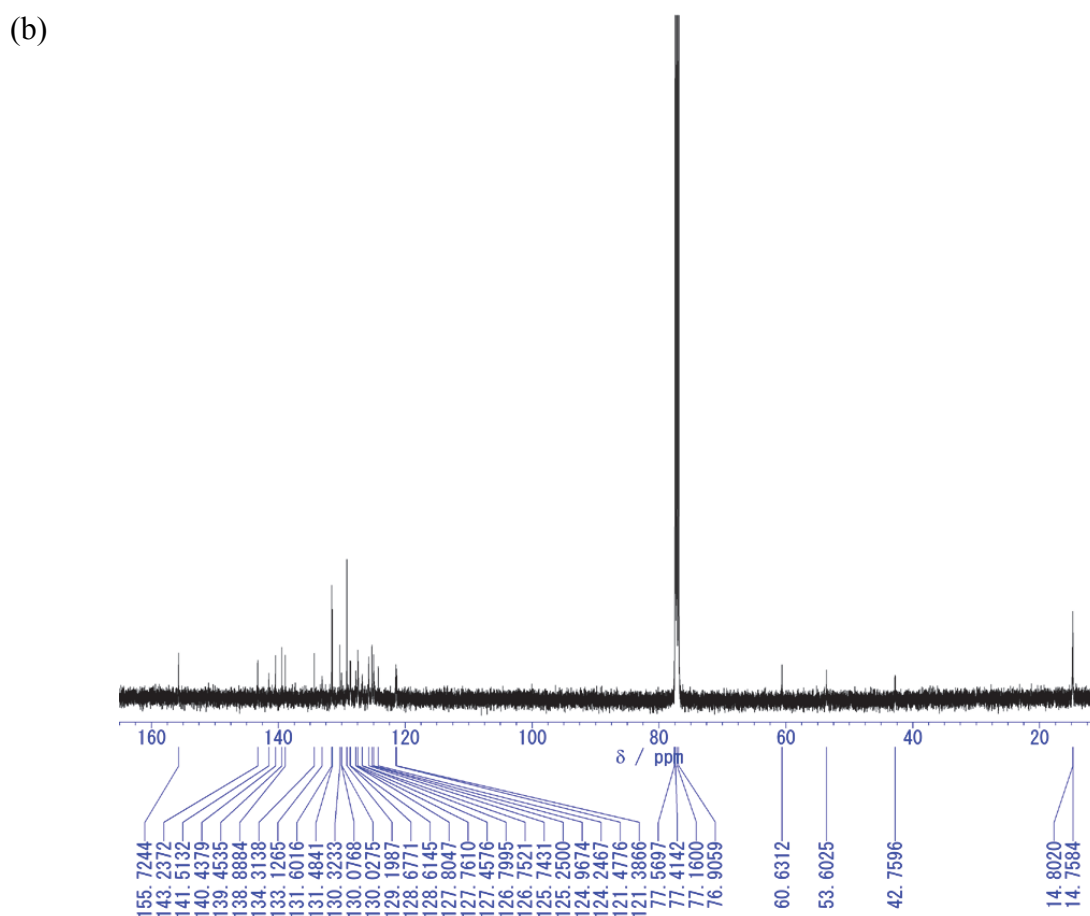
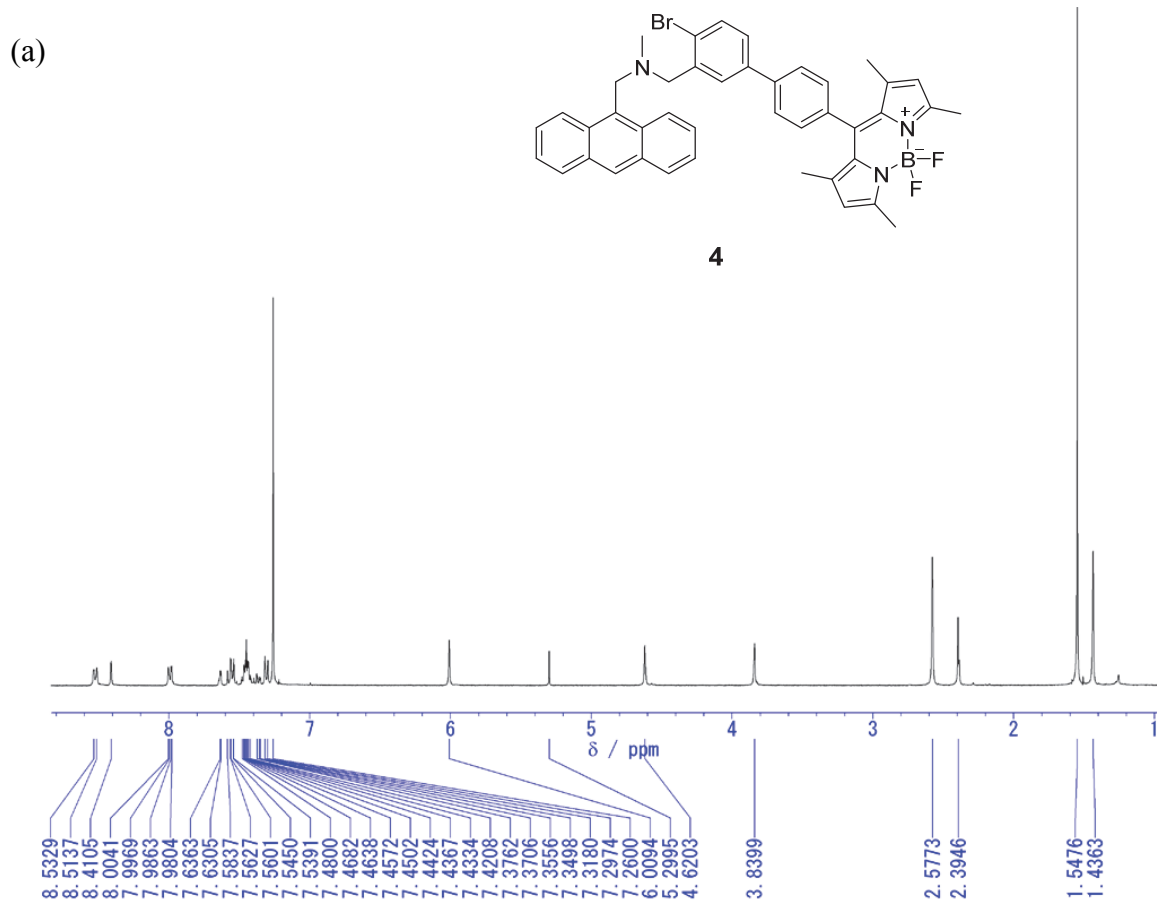


Fig. S4 (a) ^1H HMR (400 MHz) and (b) ^{13}C HMR (125 MHz) spectra of **4** in CDCl_3 .

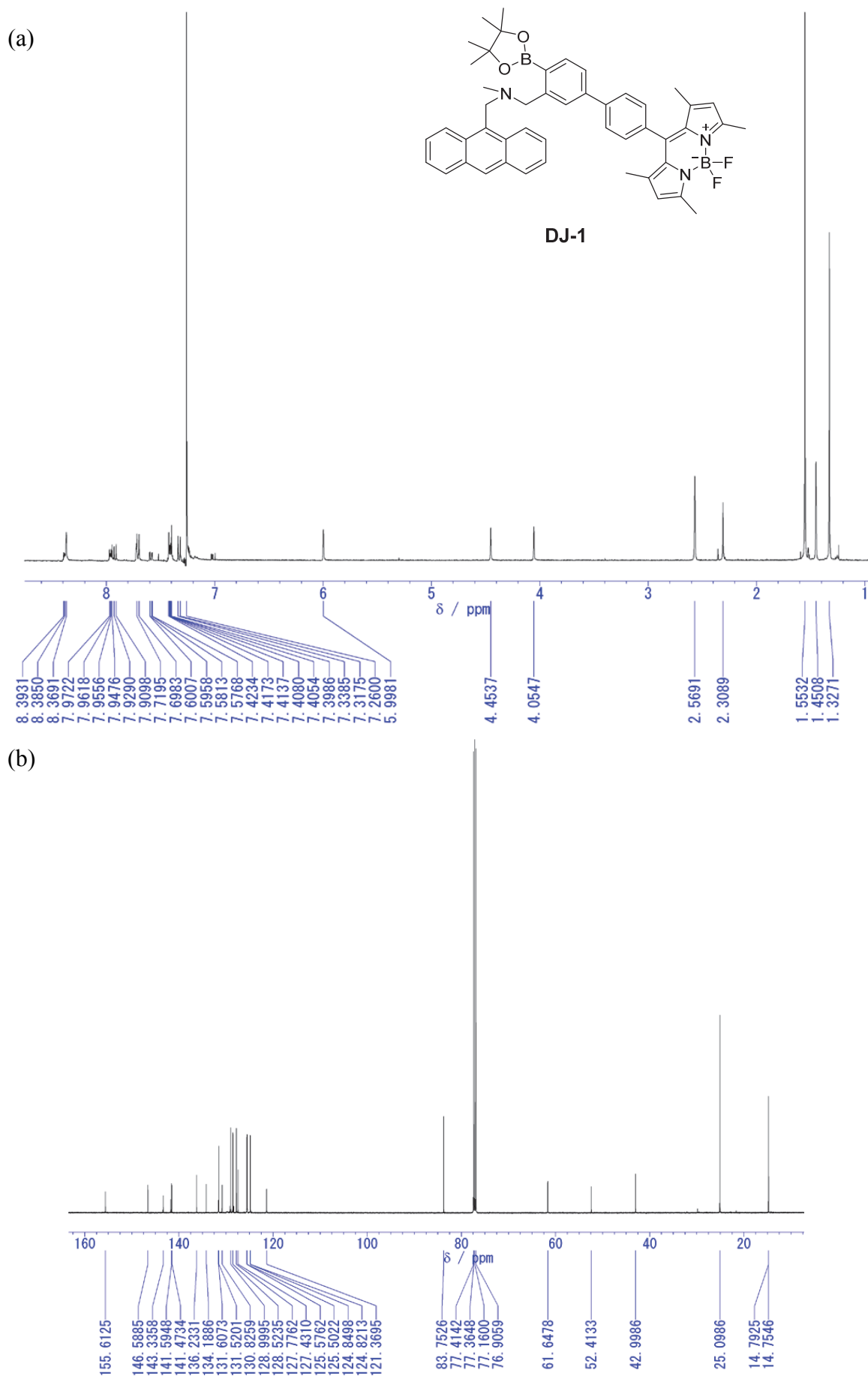


Fig. S5 (a) ^1H NMR (400 MHz) and (b) ^{13}C NMR (125 MHz) spectra of **DJ-1** in CDCl_3 .

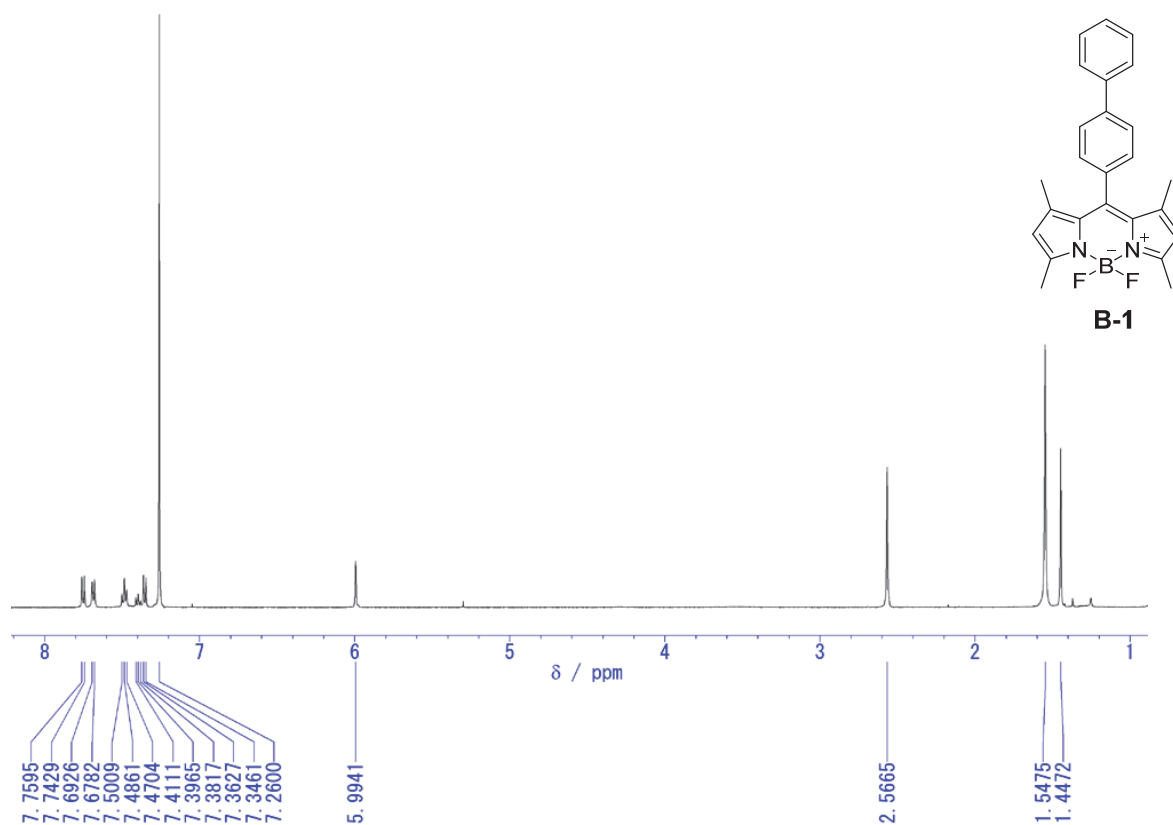


Fig. S6 ^1H NMR (400 MHz) spectrum of **B-1** in CDCl_3 .

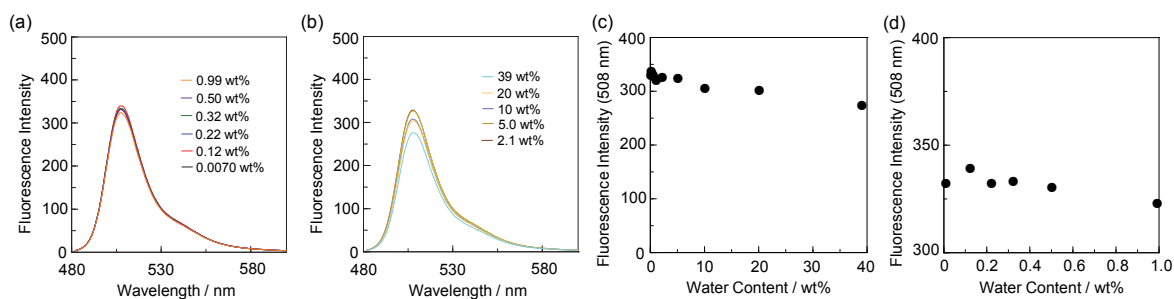


Fig. S7 Fluorescence spectra ($\lambda^{\text{ex}} = 472 \text{ nm}$) of **DJ-1** ($c = 4.0 \times 10^{-6} \text{ M}$) in acetonitrile containing (a) 0.007–0.99 wt% and (b) 2.1–39 wt% of water. Fluorescence peak intensity at 508 nm of **DJ-1** ($\lambda^{\text{ex}} = 472 \text{ nm}$) as a function of water content (c) below 40 wt% and (d) 1.0 wt% in acetonitrile.

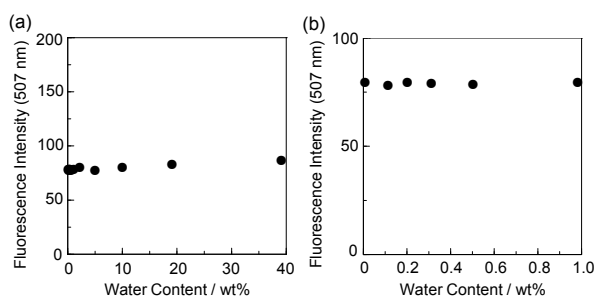


Fig. S8 Fluorescence peak intensity at 507 nm of **B-1** ($\lambda^{\text{ex}} = 367 \text{ nm}$) as a function of water content (a) below 40 wt% and (b) 1.0 wt% in acetonitrile.