Supporting information for

Visible-light Excitation of BODIPYs Enables Self-promoted Radical Arylation at their 3, 5-positions with Diazonium Salts

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1. General information

Reagents and solvents were used as received from commercial suppliers (Energy Chemicals, Shanghai, China) unless noted otherwise. The light source is optical parallel reactor (WP-TEC-1020SL, WATTCAS, Shanghai, China). All reactions were performed in oven-dried or flame-dried glassware unless stated otherwise and were monitored by TLC using 0.25 mm silica gel plates with UV indicator (60F-254). ^{1}H and ^{13}C NMR spectra were recorded on a 300, 400 or 500 MHz NMR spectrometer at room temperature. Chemical shifts (δ) are given in ppm relative to $CDCl_3$ (7.26 ppm for ^{1}H and 77 ppm for ^{13}C) or to internal TMS. High-resolution mass spectra (HRMS) were obtained using APCI-TOF and ESI-TOF in positive mode.

UV-visible absorption and fluorescence emission spectra were recorded on commercial spectrophotometers (Shimadzu UV-2450 and Edinburgh FS5 spectrometers, 190-900 nm scan range) at room temperature (10 mm quartz cuvette). Relative fluorescence quantum efficiencies of BODIPY derivatives were obtained by comparing the areas under the corrected emission spectrum of the test sample in various solvents with Cresly Violet perchlorate (Φ = 0.54 in methanol)[1] and Rhodamine B (Φ = 0.49 in Ethanol)[2] and 1,7-diphenyl-3,5-di(4-methoxyphenyl) -azadipyrromethene (Φ = 0.36 in chloroform).[3] Non-degassed, spectroscopic grade solvents and a 10 mm quartz cuvette were used. Dilute solutions (0.01<A<0.05) were used to minimize the reabsorption effects. Quantum yields were determined using the following equation:

$$\Phi_X = \Phi_S (I_X/I_S) (A_S/A_X) (n_X/n_S)^2$$

Where Φ_S stands for the reported quantum yield of the standard, I stands for the integrated emission spectra, A stands for the absorbance at the excitation wavelength and *n* stands for the refractive index of the solvent being used. X subscript stands for the test sample, and S subscript stands for the standard.

Cyclic voltammograms of 2 mM **1a** were measured in dichloromethane solution, containing 0.1 M $TBAPF_6$ as the supporting electrolyte, glassy carbon electrode as a working electrode, Pt wire as a counter electrode, and saturated calomel electrode (SCE) as reference electrode at 100 mV s^{-1} of scaning rate at room temperature.

Crystals of compounds **3n, 4b** and **5a** suitable for X-ray analysis were obtained *via* the slow diffusion of petroleum ether into their dichloromethane solutions. The vial containing this solution was placed, loosely capped, to promote the crystallization. A suitable crystal was chosen and mounted on a glass fiber using grease. Data were collected using a diffractometer equipped with a graphite crystal monochromator situated in the incident beam for data collection at room temperature. Cell parameters were retrieved using SMART software and refined using SAINT on all observed reflections. The determination of unit cell parameters and data collections were performed with Mo *Kα* radiation (λ) at 0.71073 Å. Data reduction was performed using the SAINT software which corrects for Lp and decay. The structure was solved by the direct method using the SHELXS-97 program and refined by least squares method on F^2, SHELXL-2018/3, incorporated in SHELXTL V5.10. CCDC-1907874 (**3n)** CCDC-1907883 (**4b**) and CCDC-1907884 (**5a**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

2. Determination of excited state reduction potential of BODIPY 1a

Excited state reduction potential of BODIPY **1a** was estimated to be - 0.58 V vs. SCE according to the following equations:[4]

$E_{1/2}$ (**1a**$^{+\cdot}$/**1a***) = $E^{ox} - E_{0,0}$

where E^{ox} was obtained from its cyclic voltammetry spectrum (Figure S1); $E_{0,0}$ was caculated from its photoluminescence maximum (526 nm as shown in Figure S2) using the equation $E_{0,0} = hc / \lambda_{max}$ =1240 nm / λ_{max}.

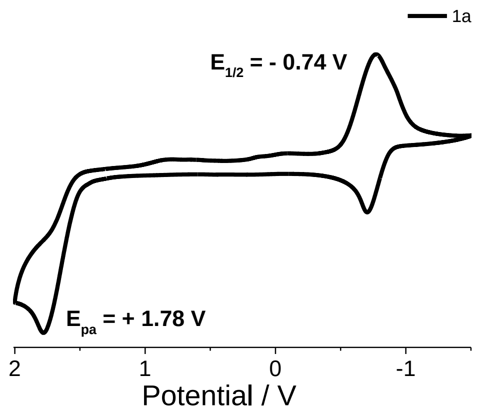


Figure S1. Cyclic voltammetry of BODIPY **1a** (2 mM in dichloromethane). E^{ox} = +1.78 V vs. SCE)

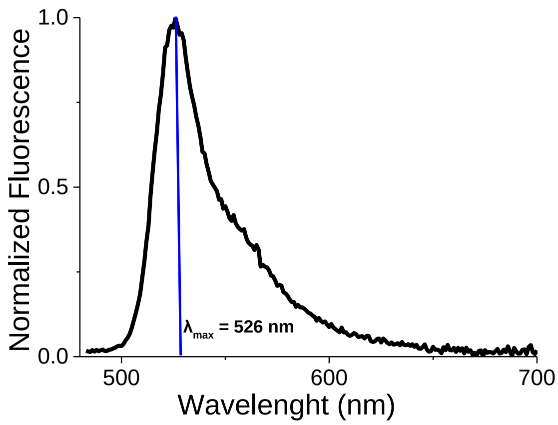


Figure S2. Fluorescence of BODIPY **1a** in dichloromethane

3. Synthesis and characterization

BODIPYs **1a-f** were synthesized by following the procedures described in our previous paper.[5] Diazonium salts **2a-j** were synthesized according to literature.[6]

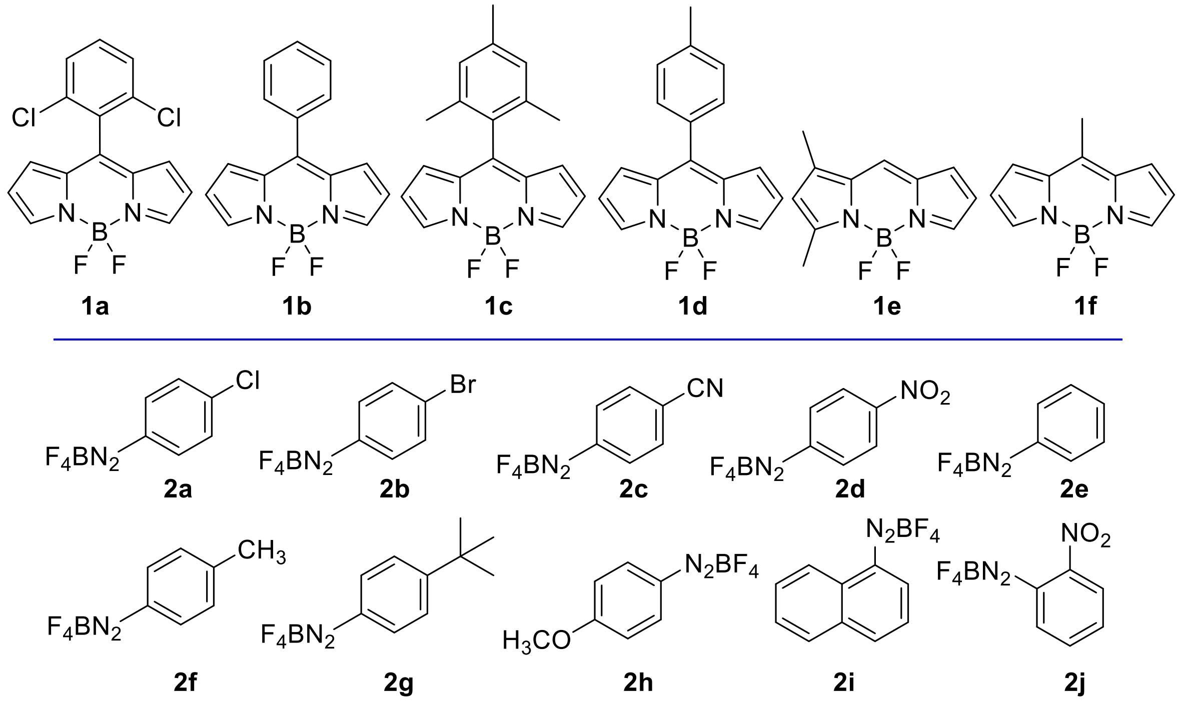
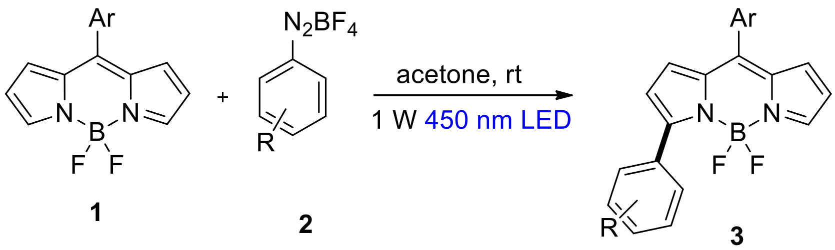


Figure S3. Chemical structure of BODIPYs **1a-f** and diazonium salts **2a-j.**

General radical C–H monoarylation procedure:



General radical mono-arylation procedure of BODIPYs: To 2.0 ml acetone in a 10 ml reaction tube were added BODIPY **1** (0.1 mmol) and diazonium salt **2** (0.12 mmol). The mixture was irradiated with 1 W blue LED at room temperature for 1 h, and TLC was used to follow the reaction. Upon the completion of the reaction, the mixture was poured into aqueous $NaHCO_3$ and was extracted with dichloromethane (30 mL × 3). Organic layers were combined, dried over anhydrous Na_2SO_4, and organic solvent was removed under vacuum. The crude product was purified by column chromatography (eluent, petroleum ether/dichloromethane: 2:1-1:1, v/v) on silica to afford the desired BODIPYs **3** as red solids.

BODIPY **3a:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2a** (27 mg, 0.12 mmol) for 1 h affords **3a** in 52% (24 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.95 (d, *J* = 7.7 Hz, 2H), 7.87 (s, 1H), 7.52 - 7.41 (m, 5H), 6.74 (d, *J* = 4.2 Hz, 1H), 6.65 (d, *J* = 3.7 Hz, 2H), 6.51 (d, *J* = 3.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 159.82, 144.07, 139.15, 137.08, 136.64, 135.45, 134.06, 131.67, 131.36, 130.99, 130.41, 128.86, 128.64, 128.38, 121.39, 119.06. HRMS calcd. For $C_{21}H_{12}BCl_3FN_2$ $[M-F]^+$: 427.0143, found 427.0167.

Synthesis of 3a at 1 mmol scale: To 4.0 ml acetone in a 10 ml reaction tube were added BODIPY **1a** (1 mmol, 340 mg) and diazonium salt **2** (1.2 mmol, 270 mg). The mixture was irradiated with 1 W blue LED at room temperature for 2 h, and TLC was used to follow the reaction. Upon the completion of the reaction, the mixture was poured into aqueous $NaHCO_3$ and was extracted with dichloromethane (30 mL × 3). Organic layers were combined, dried over anhydrous Na_2SO_4, and organic solvent was removed under vacuum. The crude product was purified by column chromatography (eluent, petroleum ether/dichloromethane: 2:1, v/v) on silica to afford the desired BODIPYs **3a** in 46% (205 mg) as orange solid.

BODIPY **3b:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2b** (34 mg, 0.12 mmol) for 1 h affords **3b** in 47% (23 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.87 (d, *J* = 8.2 Hz, 3H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 7.9 Hz, 2H), 7.45 - 7.42 (m, 1H), 6.74 (d, *J* = 4.2 Hz, 1H), 6.65 - 6.64 (m, 2H), 6.51 (d, *J* = 3.1 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 159.83, 144.16, 139.20, 137.15, 135.51, 134.12, 131.82, 131.68, 131.36, 131.18, 130.96, 130.89, 128.72, 128.39, 125.16, 121.33, 119.09. HRMS calcd. For $C_{21}H_{13}BCl_3F_2N_2$ $[M+H]^+$: 490.9695, found 490.9703.

BODIPY **3c:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2c** (30 mg, 0.12 mmol) for 1 h affords **3c** in 54% (34 mg) isolated yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.10 (d, *J* = 8.5 Hz, 2H), 7.95 (s, 1H), 7.79 (d, *J* = 8.5 Hz, 2H), 7.59 - 7.40 (m, 3H), 6.74 (t, *J* = 4.5 Hz, 2H), 6.67 (d, *J* = 4.0 Hz, 1H), 6.56 (d, *J* = 3.0 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 157.46, 146.09, 140.32, 137.03, 136.35, 135.31, 134.92, 132.28, 131.64, 131.48, 131.13, 130.59, 130.28, 130.22, 130.17, 128.54, 121.12, 120.12, 118.83, 113.39. HRMS calcd. For $C_{22}H_{12}BCl_2FN_3$ $[M-F]^+$: 418.0485 found 418.0509.

BODIPY **3d:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2d** (29 mg, 0.12 mmol) for 1 h affords **3d** in 42% (19 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$)

δ: 8.34 (d, *J* = 8.7 Hz, 2H), 8.15 (d, *J* = 8.7 Hz, 2H), 7.96 (s, 1H), 7.52 (d, *J* = 7.1 Hz, 2H), 7.46 - 7.46 (m, 1H), 6.75 (t, *J* = 4.0 Hz, 2H), 6.70 (d, *J* = 4.3 Hz, 1H), 6.57 (d, *J* = 4.1 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 156.73, 148.32, 146.42, 140.40, 138.27, 137.05, 135.39, 134.97, 131.59, 131.33, 130.48, 130.37, 128.46, 123.70, 121.08, 120.26, 105.12. HRMS calcd. For $C_{21}H_{12}BCl_2FN_3O_2$ [M-F] $^+$: 483.0384, found 483.0382.

BODIPY **3e:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2e** (25 mg, 0.12 mmol) for 12 h affords **3e** in 40% (16 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.00 (d, *J* = 6.6 Hz, 2H), 7.85 (s, 1H), 7.50 - 7.48 (m, 5H), 7.45 - 7.41 (m, 1H), 6.75 (d, *J* = 3.6 Hz, 1H), 6.68 (d, *J* = 4.0 Hz, 1H), 6.62 (d, *J* = 2.6 Hz, 1H), 6.49 (d, *J* = 2.1 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ:161.76, 143.35, 138.85, 137.15, 135.55, 133.77, 131.95, 131.78, 131.28, 131.13, 130.47, 129.69, 128.53, 128.36, 128.07, 121.83, 118.66. HRMS calcd. For $C_{21}H_{13}BCl_2FN_2$ [M-F] $^+$: 393.0533, found 393.0552.

BODIPY **3f:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2f** (26 mg, 0.12 mmol) for 1 h affords **3f** in 45% (20 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.92 (d, *J* = 8.0 Hz, 2H), 7.82 (s, 1H), 7.48 (d, *J* = 7.7 Hz, 2H), 7.43 - 7.41 (m, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 6.74 (d, *J* = 4.4 Hz, 1H), 6.69 (d, *J* = 4.4 Hz, 1H), 6.59 (d, *J* = 4.0 Hz, 1H), 6.46 (d, *J* = 3.6 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 162.20, 142.63, 141.07, 138.25, 137.27, 135.56, 133.55, 131.84, 131.22, 129.70, 129.35, 129.03, 128.33, 127.49, 121.91, 118.30 21.72. HRMS calcd. For $C_{22}H_{15}BCl_2FN_2$ [M-F] $^+$: 407.0689, found 407.0672.

BODIPY **3g:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2g** (30 mg, 0.12 mmol) for 1 h affords **3c** in 49% (28 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.97 (d, *J* = 8.3 Hz, 2H), 7.82 (s, 1H), 7.53 - 7.48 (m, 4H), 744 - 7.41 (m, 1H), 6.74 (d, *J* = 4.3 Hz, 1H), 6.70 (d, *J* = 4.4 Hz, 1H), 6.59 (d, *J* = 4.0 Hz, 1H), 6.47 (d, *J* = 2.8 Hz, 1H), 1.37 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ:162.40, 154.21, 142.75, 138.86, 137.61, 135.86, 133.77, 132.11, 131.53, 129.83, 129.19, 128.61, 127.71, 125.89, 122.25, 118.57, 35.36, 31.58. HRMS calcd. For $C_{25}H_{21}BCl_2FN_2$ [M-F] $^+$:449.1159, found 449.1142.

BODIPY **3h:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2h** (27 mg, 0.12 mmol) for 1 h affords **3h** in 30% (14 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.04 (d, *J* = 7.0 Hz, 2H), 7.80 (s, 1H), 7.49 - 7.47 (m, 2H), 7.43 - 7.41 (m, 1H), 7.03

(d, J = 8.9 Hz, 2H), 6.73 (d, J = 9.5 Hz, 1H), 6.71 (d, J = 9.5 Hz, 1H), 6.56 (s, 1H), 6.46 (s, 1H), 3.88 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 162.08, 161.75, 141.83, 137.49, 135.61, 133.31, 131.92, 131.7, 131.42, 131.17, 128.32, 126.85, 124.20, 121.92, 117.98, 114.14, 55.53. HRMS calcd. For $C_{22}H_{15}BCl_2FN_2O$ [M-F] $^+$: 423.0639, found 423.0663.

BODIPY **3i:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2i** (30 mg, 0.12 mmol) for 1 h affords **3i** in 35% (16 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.55 (s, 1H), 8.11 - 8.09 (m, 1H), 7.98 - 7.94 (m, 2H), 7.89 - 7.86 (m, 2H), 7.57 - 7.49 (m, 4H), 7.43 - 7.41 (m, 1H) 6.81 (d, J = 4.4 Hz, 1H), 6.78 (d, J = 4.5 Hz, 1H), 6.63 (d, J = 4.0 Hz, 1H), 6.49 (d, J = 3.0 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 161.64, 143.32, 138.64, 137.39, 135.57, 134.13, 133.85, 133.07, 131.82, 131.28, 131.13, 130.32, 129.31, 128.36, 128.14, 128.00, 127.84, 127.64, 126.68, 126.53, 126.48, 126.42, 122.18, 118.64. HRMS $C_{25}H_{15}BCl_2FN_2$ [M-F] $^+$: 443.0689, found 443.0705.

BODIPY **3j:** BODIPY **1b** (28 mg, 0.1 mmol) and diazonium salt **2c** (30 mg, 0.12 mmol) for 1 h affords **3j** in 41% (15 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.05 (d, J = 8.5 Hz, 2H), 7.92 (s, 1H), 7.76 (d, J = 8.5 Hz, 2H), 7.60 - 7.55 (m, 5H), 6.99 (d, J = 4.0 Hz, 1H), 6.96 (d, J = 4.0 Hz, 1H), 6.68 (d, J = 4.0 Hz, 1H), 6.59 (d, J = 3.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 156.31, 147.07, 144.76, 137.35, 136.79, 134.97, 133.90, 132.31, 132.18, 131.71, 130.95, 130.69, 130.10, 130.07, 130.04, 128.65, 120.43, 119.47, 118.81, 113.08. HRMS $C_{22}H_{14}BFN_3$ [M-F] $^+$: 350.1265, found 350.1269.

BODIPY **3k:** BODIPY **1c** (31 mg, 0.1 mmol) and diazonium salt **2c** (30 mg, 0.12 mmol) for 1 h affords **3k** in 50% (21 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.06 (d, J = 8.0 Hz, 2H), 7.89 (s, 1H), 7.76 (d, J = 8.5 Hz, 2H), 6.98 (s, 2H), 6.72 (t, J = 4.4 Hz, 2H), 6.61 (d, J = 4.5 Hz, 1H), 6.51 (d, J = 4.0 Hz, 1H), 2.38 (s, 3H), 2.14 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 156.25, 147.31, 144.87, 139.16, 137.68, 136.71, 136.56, 135.40, 132.17, 130.73, 130.36, 130.04, 129.77, 128.39, 120.41, 119.51, 118.82, 113.03, 21.29, 20.18. HRMS $C_{25}H_{20}BFN_3$ [M-F] $^+$: 392.1734, found 392.1730.

BODIPY **3l:** BODIPY **1d** (30 mg, 0.1 mmol) and diazonium salt **2c** (30 mg, 0.12 mmol) for 1 h affords **3l** in 37% (15 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.04 (d, J = 8.1 Hz, 2H), 7.90 (s, 1H), 7.76 (d, J =8.2 Hz, 2H), 7.57 (d, J = 8.4 Hz, 2H), 7.08 (d, J = 8.4 Hz, 2H), 7.02 – 7.00 (m, 2H), 6.68 (d, J = 4.3 Hz, 1H), 6.60 (d, J

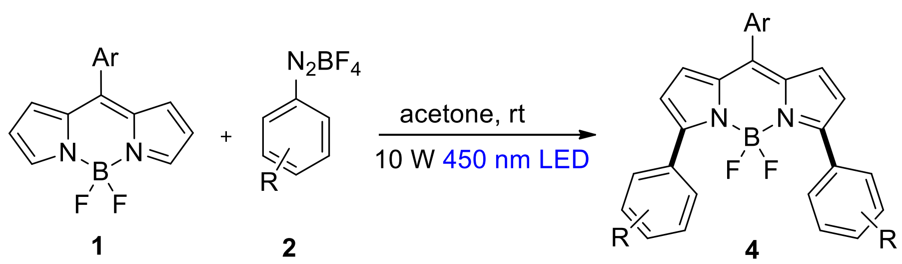
= 2.1 Hz, 1H), 3.93 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 162.27, 155.57, 147.15, 144.07, 137.26, 136.94, 134.82, 132.63, 132.15, 131.45, 130.04, 126.39, 120.18, 119.22, 118.85, 114.26, 112.92, 55.71. HRMS $C_{23}H_{16}BFN_2O$ [M-F] $^+$: 380.1370, found 380.1360.

BODIPY **3m:** BODIPY **1e** (22 mg, 0.1 mmol) and diazonium salt **2c** (26 mg, 0.12 mmol) for 1 h affords **3m** in 48% (16 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.99 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.5 Hz, 2H), 7.26 (s, 1H), 6.99 (d, *J* = 4.0 Hz, 1H), 6.58 (d, *J* = 4.0 Hz, 1H), 6.20 (s, 1H), 2.57 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 164.06, 151.79, 145.80, 137.64, 136.67, 135.16, 132.07, 129.81, 129.78, 129.75, 127.22, 124.42, 122.24, 119.06, 118.52, 112.10, 15.48, 11.56. HRMS $C_{18}H_{14}BFN_3$ [M-F] $^+$: 302.1265, found 302.1270.

BODIPY **3n:** BODIPY **1c** (31 mg, 0.1 mmol) and diazonium salt **2j** (29 mg, 0.12 mmol) for 1 h affords **3n** in 38% (17 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.21 (d, *J* = 8.5 Hz, 1H), 7.75 - 7.70 (m, 3H), 7.66 - 7.63 (m, 1H), 6.98 (s, 2H), 6.76 (d, *J* = 4.0 Hz, 1H), 6.66 (d, *J* = 4.0 Hz, 1H), 6.44 (d, *J* = 4.2 Hz, 1H), 6.42 (d, *J* = 3.6 Hz, 1H), 2.38 (s, 3H), 2.17 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 154.41, 148.60, 147.30, 144.09, 139.03, 136.64, 136.26, 135.31, 132.85, 132.13, 130.48, 129.94, 129.87, 128.34, 128.04, 124.67, 119.94, 118.75, 21.28, 20.17. HRMS $C_{24}H_{20}BFN_3O_2$ [M-F] $^+$: 412.1633, found 412.1630.

BODIPY **3o:** BODIPY **1f** (21 mg, 0.1 mmol) and diazonium salt **2a** (27 mg, 0.12 mmol) for 1 h affords **3o** in 42% (13 mg) isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.88 - 7.83 (m, 2H), 7.77 (s, 1H), 7.47 - 7.41 (m, 2H), 7.37 (d, *J* = 4.3 Hz, 1H), 7.25 (s, 1H), 6.65 (d, *J* = 4.2 Hz, 1H), 6.53 (d, *J* = 3.4 Hz, 1H), 2.64 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 157.99, 144.28, 142.55, 137.68, 136.22, 135.13, 130.96, 130.92, 130.89, 129.07, 128.83, 127.14, 120.23, 118.16, 16.32. HRMS $C_{16}H_{13}BClF_2N_2$ [M+H] $^+$: 317.0828, found 317.08255.

General radical C–H diarylation procedure:



General radical dis-arylation procedure of BODIPYs: To 2.0 ml acetone in a 10 ml reaction tube were added BODIPY **1** (0.1 mmol) and diazonium salt **2** (0.4 mmol). The mixture was irradiated with 10 W blue LED at room temperature around 3h, and TLC was used to follow the reaction. Upon the completion of the reaction, the mixture was poured into aqueous $NaHCO_3$ and was extracted with dichloromethane (30 mL × 3). Organic layers were combined, dried over anhydrous Na_2SO_4, and organic solvent was removed under vacuum. The crude product was purified by column chromatography (eluent, petroleum ether/dichloromethane: 2:1-1:1, v/v) on silica to afford the desired BODIPYs **4** as dark red solids.

BODIPY **4a:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2a** (90 mg, 0.4 mmol) for 3 h affords **4a** in 68% (38mg) isolated yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.6 Hz, 4H), 7.53 - 7.50 (m, 2H), 7.47 - 7.40 (m, 5H), 6.68 (d, *J* = 4.0 Hz, 2H), 6.60 (d, *J* = 4.0 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 158.67, 136.28, 135.76, 131.32, 131.02, 130.96, 130.91, 130.80, 129.49, 128.79, 128.40, 127.91, 127.58, 121.46. HRMS calcd. For $C_{27}H_{15}BCl_4FN_2$ [M-F] $^+$: 537.0066, found 537.0052.

Synthesis of 4a at 1 mmol scale: To 4.0 ml acetone in a 10 ml reaction tube were added BODIPY **1a** (1 mmol, 340 mg) and diazonium salt **2** (4 mmol, 900 mg). The mixture was irradiated with 10 W blue LED at room temperature for 6 h, and TLC was used to follow the reaction. Upon the completion of the reaction, the mixture was poured into aqueous $NaHCO_3$ and was extracted with dichloromethane (30 mL × 3). Organic layers were combined, dried over anhydrous Na_2SO_4, and organic solvent was removed under vacuum. The crude product was purified by column chromatography (eluent, petroleum ether/dichloromethane: 2:1, v/v) on silica to afford the desired BODIPYs **4a** in 52% (289 mg) as red solid.

BODIPY **4b:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2b** (136 mg, 0.6 mmol) for 24 h affords **4b** in 68% (44 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.78 (d, *J* = 8.5 Hz, 4H), 7.57 (d, *J* = 8.6 Hz, 4H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.46 - 7.43 (m, 1H), 6.68 (d, *J* = 4.3 Hz, 2H), 6.60 (d, *J* = 4.3 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 158.70, 137.74, 136.33, 135.71, 131.86, 131.74, 131.33, 131.23, 131.1, 129.54, 128.40, 124.79, 121.49. HRMS calcd. For $C_{27}H_{15}BBr_2Cl_2F_2N_2Na$ [M+Na] $^+$: 666.8932, found 666.8939.

BODIPY **4c:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2c** (93 mg, 0.4 mmol) for 3 h affords **4a** in 67% (36 mg) isolated yield. ^{1}H NMR (300 MHz, $CDCl_3$)

δ: 8.01 (d, *J* = 8.0 Hz, 4H), 7.74 (d, *J* = 8.0 Hz, 4H), 7.56 - 7.48 (m, 3H), 6.77 (d, *J* = 4.0 Hz, 2H), 6.67 (d, *J* = 4.0 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 157.94, 139.53, 136.90, 136.36, 135.59, 132.20, 131.65, 131.44, 130.32, 130.17, 128.52, 121.99, 118.61, 113.46.HRMS calcd. For $C_{29}H_{15}BCl_2FN_4$ [M-F] $^+$: 519.0751, found 519.0763.

BODIPY **4d:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2d** (95 mg, 0.4 mmol) for 3 h affords **4d** in 61% (35 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.30 (d, *J* = 8.8 Hz, 4H), 8.06 (d, *J* = 8.8 Hz, 4H), 7.56 - 7.54 (m, 2H), 7.49 - 7.48 (m, 1H), 6.80 (d, *J* = 4.3 Hz, 2H), 6.71 (d, *J* = 4.3 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 157.61, 148.39, 139.87, 138.12, 137.03, 135.51, 131.74, 131.28, 130.54, 130.50, 128.54, 123.69, 122.18. HRMS calcd. For $C_{27}H_{15}BCl_2FN_4O_4$ [M-F] $^+$: 559.0547, found 559.0547.

BODIPY **4e:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2e** (84 mg, 0.4 mmol) for 36h affords **4e** in 65% (26 mg) isolated yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.91 (d, *J* = 5.0 Hz, 4H), 7.53 - 7.42 (m, 9H), 6.66 (d, *J* = 4.0 Hz, 2H), 6.61 (d, *J* = 4.0 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 159.92, 137.29, 136.08, 135.82, 132.50, 132.12, 131.15, 129.86, 129.65, 129.16, 128.39, 128.34, 121.54. HRMS calcd. For $C_{27}H_{17}BCl_2FN_2$ [M-F] $^+$: 469.0846, found 469.0863.

BODIPY **4f:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2f** (84 mg, 0.4 mmol) for 3 h affords **4f** in 58% (30 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.84 (d, *J* = 8.0 Hz, 4H), 7.50 - 7.48 (m, 2H), 7.43 - 7.39 (m, 1H), 7.24 (d, *J* = 7.8 Hz, 4H), 6.62 (d, *J* = 4.2 Hz, 2H), 6.59 (d, *J* = 4.0 Hz, 2H), 2.39 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 159.82, 140.12, 136.44, 135.97, 135.86, 132.24, 131.08, 129.74, 129.61, 129.21, 128.87, 128.30, 121.34, 21.66. HRMS calcd. For $C_{29}H_{21}BCl_2FN_2$ [M-F] $^+$: 497.1159, found 497.1159.

BODIPY **4g:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2g** (124 mg, 0.5 mmol) for 3 h affords **4g** in 42% (25 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.89 (d, *J* = 8.4 Hz, 4H), 7.51 - 7.45 (m, 6H), 7.43 - 7.40 (m, 1H), 6.63 - 6.61 (m, 4H), 1.35 (s, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 159.73, 153.01, 136.33, 136.04, 135.88, 132.29, 131.07, 129.66, 129.43, 128.79, 128.30, 125.49, 121.52, 34.98, 31.36. HRMS calcd. For $C_{35}H_{33}BCl_2FN_2$[M-F] $^+$: 581.2098, found 581.2070.

BODIPY **4h**: BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2h** (89 mg, 0.4 mmol) for 3h affords **4h** in 41% (22 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$)

δ: 7.93 (d, J = 7.1 Hz, 4H), 7.49 (d, J = 8.5 Hz, 2H), 7.42 - 7.39 (m, 1H), 6.97 (d, J = 8.9 Hz, 4H), 6.61-6.59 (m, 4H), 3.86 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 161.04, 159.19, 135.94, 135.48, 132.30, 131.39, 131.34, 131.01, 128.60, 128.29, 125.13, 121.06, 113.98, 55.09. HRMS calcd. For $C_{29}H_{21}BCl_2FN_2O_2$ [M-F] $^+$: 529.1057, found 529.1080.

BODIPY**4i:** BODIPY **1a** (34 mg, 0.1 mmol) and diazonium salt **2i** (250 mg, 1 mmol) for 24 h affords **4i** in 49% (28 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.43 (s, 2H), 8.05 (d, J = 8.5 Hz, 2H), 7.91-7.87 (m, 4H), 7.83 (d, J = 7.5 Hz, 2H), 7.54 - 7.47 (m, 7H), 6.75 (d, J = 4.0 Hz, 2H), 6.72 (d, J = 3.6 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 159.84, 136.38, 135.87, 138.88, 133.06, 132.21, 131.20, 129.98, 129.89, 129.16, 128.37, 127.98, 127.78, 127.25, 126.78, 126.74, 126.43, 121.96. HRMS calcd. For $C_{35}H_{21}BCl_2FN_2$ [M-F] $^+$: 569.1159, found 569.1181.

BODIPY **4j:** BODIPY **1b** (28 mg, 0.1 mmol) and diazonium salt **2c** (93 mg, 0.4 mmol) for 3 h affords **4j** in 45% (21 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (d, J = 8.3 Hz, 4H), 7.73 (d, J = 8.3 Hz, 4H), 7.65 - 7.56 (m, 5H), 6.70 (d, J = 4.2Hz, 2H), 6.69 (d, J = 4.3 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 156.96, 146.46, 137.20, 136.71, 133.89, 132.18, 132.12, 130.95, 130.74, 130.12, 128.68, 121.42, 118.68, 113.24. HRMS calcd. For $C_{29}H_{17}BFN_4$ [M-F] $^+$: 451.1530, found 451.1533.

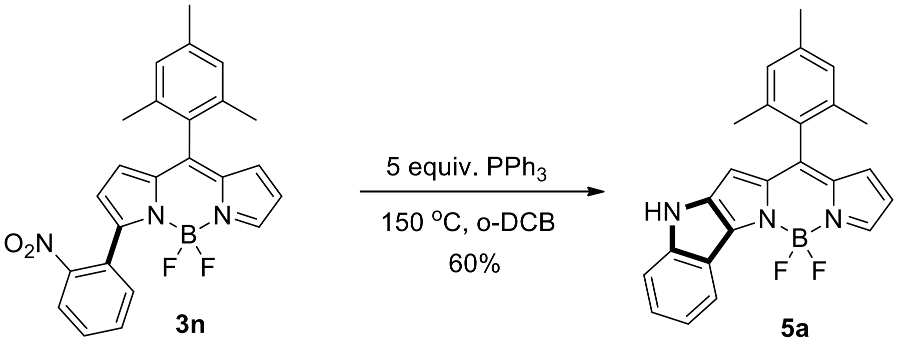
BODIPY **4k:** BODIPY **1c** (31 mg, 0.1 mmol) and diazonium salt **2c** (93 mg, 0.4 mmol) for 3 h affords **4k** in 36% (18 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.98 (d, J = 8.5 Hz, 4H), 7.73 (d, J = 8.5 Hz, 4H), 7.00 (s, 2H), 6.75 (d, J = 4.5 Hz, 2H), 6.62 (d, J = 4.5 Hz, 2H), 2.39 (s, 3H), 2.19 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 156.87, 146.61, 139.29, 137.50, 136.68, 136.64, 132.17, 130.65, 130.08, 129.75, 128.46, 121.42, 118.70, 113.16, 21.30, 20.25. HRMS calcd. For $C_{32}H_{23}BFN_4$ [M-F] $^+$: 493.2000, found 493.2008.

BODIPY **4l:** BODIPY **1d** (30 mg, 0.1 mmol) and diazonium salt **2c** (93 mg, 0.4mmol) for 3 h affords **4l** in 28% (14 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.95 (d, J = 8.3 Hz, 4H), 7.72 (d, J = 8.4Hz, 4H), 7.58 (d, J = 8.6 Hz, 2H), 7.09 (d, J = 8.6 Hz, 2H), 7.04 (d, J = 4.2 Hz, 2H), 6.69 (d, J = 4.1 Hz, 2H), 3.94 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 162.26, 156.26, 146.59, 137.08, 136.75, 132.69, 132.16, 131.95, 130.09, 126.33, 121.22, 118.59, 114.29, 113.04, 55.83. HRMS calcd. For $C_{30}H_{19}BFN_4O$ [M-F] $^+$: 481.1636, found 481.1631.

BODIPY **4n:** BODIPY **1c** (31 mg, 0.1 mmol) and diazonium salt **2j** (94 mg, 0.4 mmol) for 3 h affords **4n** in 41% (23 mg) isolated yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.07 (d, *J* = 8.0 Hz, 2H), 7.63 - 7.59 (m, 4H), 7.54 - 7.50 (m, 2H), 7.00 (s, 2H), 6.73 (d, *J* = 4.1 Hz, 2H), 6.37 (d, *J* = 4.1 Hz, 2H), 2.39 (s, 3H), 2.24 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ: 154.12, 148.31, 146.61, 139.02, 136.84, 136.08, 132.81, 132.23, 130.24, 129.89, 128.34, 127.96, 124.55, 120.22, 21.32, 20.27. HRMS calcd. For $C_{30}H_{23}BFN_4O_4$ [M-F] $^+$: 533.1796, found 533.1795.

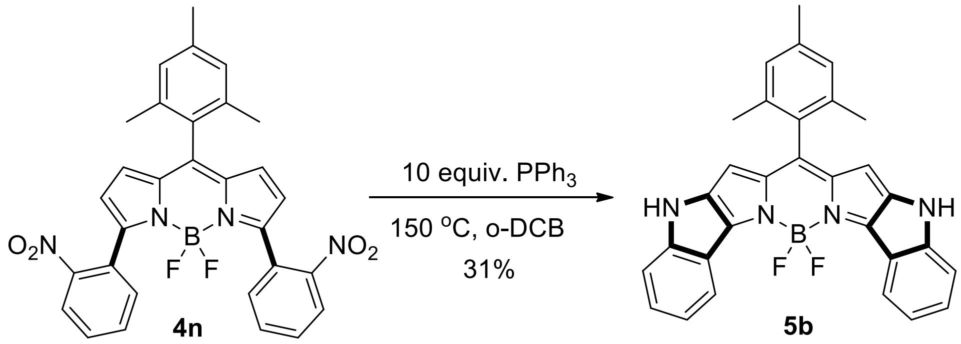
BODIPY **4o:** BODIPY **1f** (21 mg, 0.1 mmol) and diazonium salt **2a** (90 mg, 0.4 mmol) for 3 h affords **4o** in 51% (22 mg) isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79 - 7.74 (m, 4H), 7.41 - 7.36 (m, 4H), 7.33 (d, *J* = 4.2 Hz, 2H), 6.61 (d, *J* = 4.1 Hz, 2H), 2.66 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 157.19, 142.55, 137.01, 135.96, 131.19, 130.95, 130.91, 130.87, 128.78, 127.88, 120.51, 16.27. HRMS $C_{22}H_{16}BCl_2F_2N_2$ [M+H] $^+$: 427.0752, found 427.07405.

Indole-Fused BODIPY 5a:



BODIPY **5a:** In the experimental procedure in the reference. BODIPY **3n** (0.15 mmol, 65 mg), PPh_3 (0.75 mmol, 197 mg), 2.0 mL ortho-dichlorobenzene (o-DCB) were added as solvent in a 10 mL Schlenk reaction tube, and heated at 150 °C under argon gas protection for 24 h, **5a** was isolated with 60% (36 mg). ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.18 (d, *J* = 7.8 Hz, 1H), 7.75 (s, 1H), 7.36 - 7.32 (m, 2H), 7.13 - 7.10 (m, 2H), 6.95 (s, 2H), 6.44 (d, *J* = 3.4 Hz, 1H), 6.36 (d, *J* = 1.8 Hz, 1H), 5.95 (brs, 1H), 2.37 (s, 3H), 2.13 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 150.76, 150.33, 144.12, 140.56, 140.06, 139.80, 138.58, 136.89, 135.36, 130.98, 130.49, 128.18, 126.24, 125.08, 121.18, 116.66, 114.63, 114.60, 112.22, 103.77, 21.27, 20.15. HRMS calcd. For $C_{24}H_{20}BFN_3$ [M-F] $^+$: 380.1734, found 380.1726.

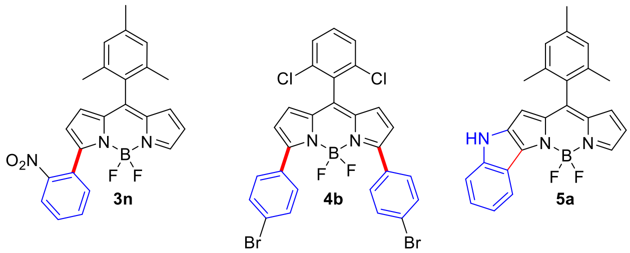
Indole-Fused BODIPY 5b:



BODIPY **5b:** BODIPY **4n** (0.1 mmol, 55 mg), PPh_3 (1.0 mmol, 262 mg), 2.0 mL o-DCB were added as solvent in a 10 mL Schlenk reaction tube, and heated at 150 °C under argon gas protection for 36 h, **5b** was isolated with 31% (15 mg). ^{1}H NMR (500 MHz, *d6*-DMSO) δ: 10.59 (s, 2H), 7.99 (d, *J* = 7.6 Hz, 2H), 7.38 - 7.35 (m, 2H), 7.30 (d, *J* = 8.2 Hz, 2H) 7.12 (t, *J* = 7.5 Hz, 2H), 7.07 (s, 2H), 5.93 (s, 2H), 2.34 (s, 3H), 2.15 (s, 6H). ^{13}C NMR (126 MHz, DMSO) δ: 149.09, 145.56, 141.07, 139.73, 139.34, 137.92, 136.20, 130.28, 129.09, 128.01, 122.71, 119.66, 113.56, 112.64, 101.74, 20.7, 19.69. HRMS calcd. For $C_{30}H_{23}BFN_4$ [M-F]$^{+}$: 469.2000, found 469.1992.

4. Crystal data

Table S1. Selected Geometrical Parameters of 3n, 4b and 5a obtained from crystallography



	3n	4b	5a
B-N bond length (Å)	1.5459 (26) 1.5581 (26)	1.5596 (63) 1.5643 (62)	1.5166 (41) 1.5354 (40)
dihedral angles between *meso*-mesityl group and dipyyrin core (deg)	83.919 (42)	82.906 (145)	86.766 (72)
dihedral angles of two pyrrole rings in dipyyrin core (deg)	5.936 (53)	5.169 (136)	10.658 (122)
dihedral angles between α-aryl group and dipyyrin core (deg)	58.937 (62) /	36.828 (169) 41.219 (169)	4.038 (77) /
the average and maximum deviations of the eleven atoms from the mean plane of dipyrrin (C_9N_2) core and indole(Å)	/	/	0.113/0.2838
the interplanar distance of two adjacent molecules(Å)	6.1417	2.1049	5.6697

Table S2. Crystal experimental details.

	3n	**4b**	**5a**
Crystal data			
Chemical formula	$C_{24}H_{20}BF_2N_2O_3$	$C_{27}H_{15}BBr_2Cl_2F_2N_2$	$C_{24}H_{20}BF_2N_3$
M_r	431.24	646.94	339.27
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$	Orthorhombic, $P2_12_12_1$
Temperature (K)	300(2)	300(2)	298.15
a, b, c (Å)	12.9718(5), 14.7930(6), 12.7375(18)	12.998(2), 11.2288(14), 18.281(3)	10.0602(6), 11.9480(8), 17.5342(11)
α, β, γ (°)	90, 117.8580(10), 90	90, 104.899(5), 90	90, 90, 90
V (Å^3)	2160.96(14)	2578.4(6)	2107.6(2)
Z	4	4	4
$D_{cale.}$ (Mg·m^{-3})	1.326	1.667	1.258
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.097	3.386	0.087
Crystal size (mm)	0.20 × 0.21 × 0.20	0.21 × 0.21 × 0.2	0.22 × 0.21 × 0.21
Diffractometer	Bruker APEX-II CCD	Bruker APEX-II CCD	Bruker APEX-II CCD
Absorption coefficient (mm^{-1})	0.097	3.386	0.087
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	42127, 4966, 3824	66241, 5909, 3916	52266, 4827, 3428
R_{int}	0.0725	0.1528	0.0632
θ_{max} [°]	27.528	27.495	27.57
θ_{min} [°]	3.277	2.866	2.88
R_1 [$I \geqslant \sigma(I)$]	0.0528	0.0947	0.0599
wR_2	0.1534	0.2282	0.1525
No. of reflections	3824	3916	5041
No. of parameters	292	325	281
Wavelength	0.71073	0.710760	0.71073
Largest diff. peak/hole (eA^{-3})	0.254, -0.241	0.883, -0.728	0.1756, -0.1693
Parameter	292	325	274

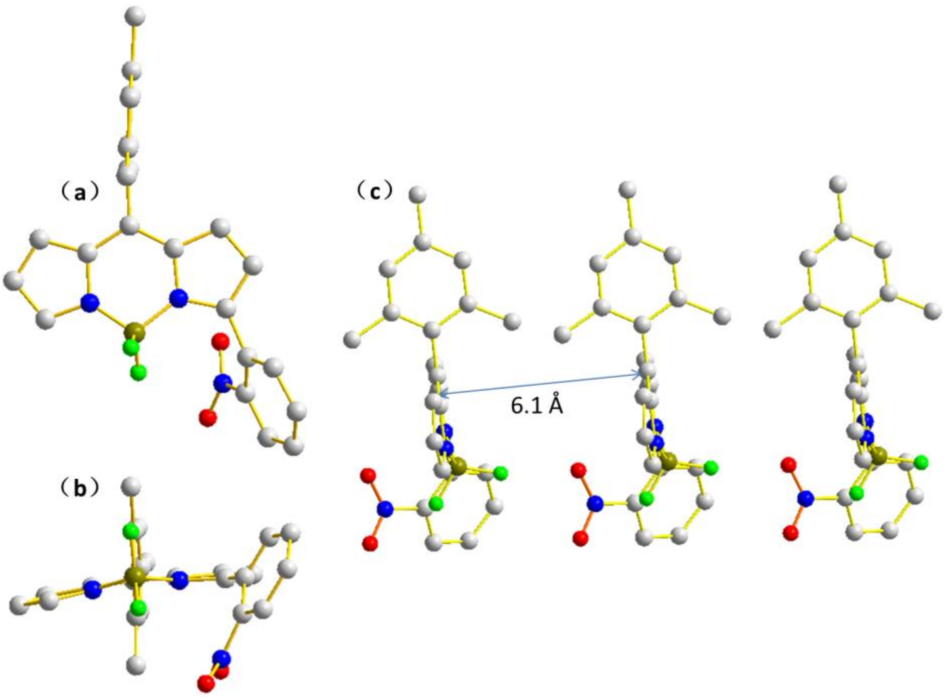


Figure S4. Top (a) and front (b) views of X-Ray structures of BODIPY **3n**, and Crystal packing (c).C, light gray; N, blue; B, dark yellow; F, bright green; O, red. Hydrogen atoms have removed for clarity.

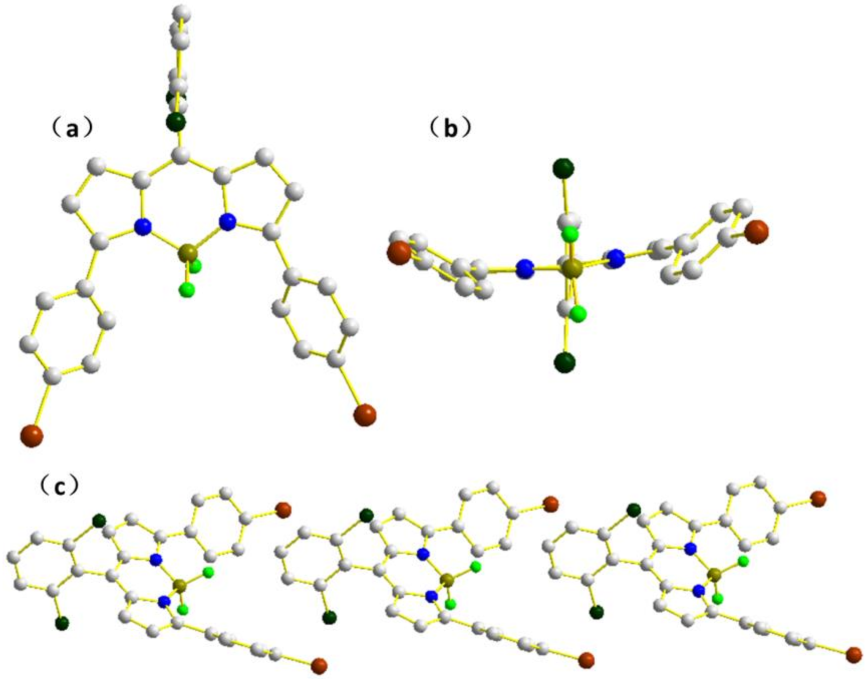


Figure S5. Top (a) and front (b) views of X-Ray structures of BODIPY **4b**, and Crystal packing (c).C, light gray; N, blue; B, dark yellow; F, bright green; O, red; Cl, dark green; Br, Green. Hydrogen atoms have removed for clarity.

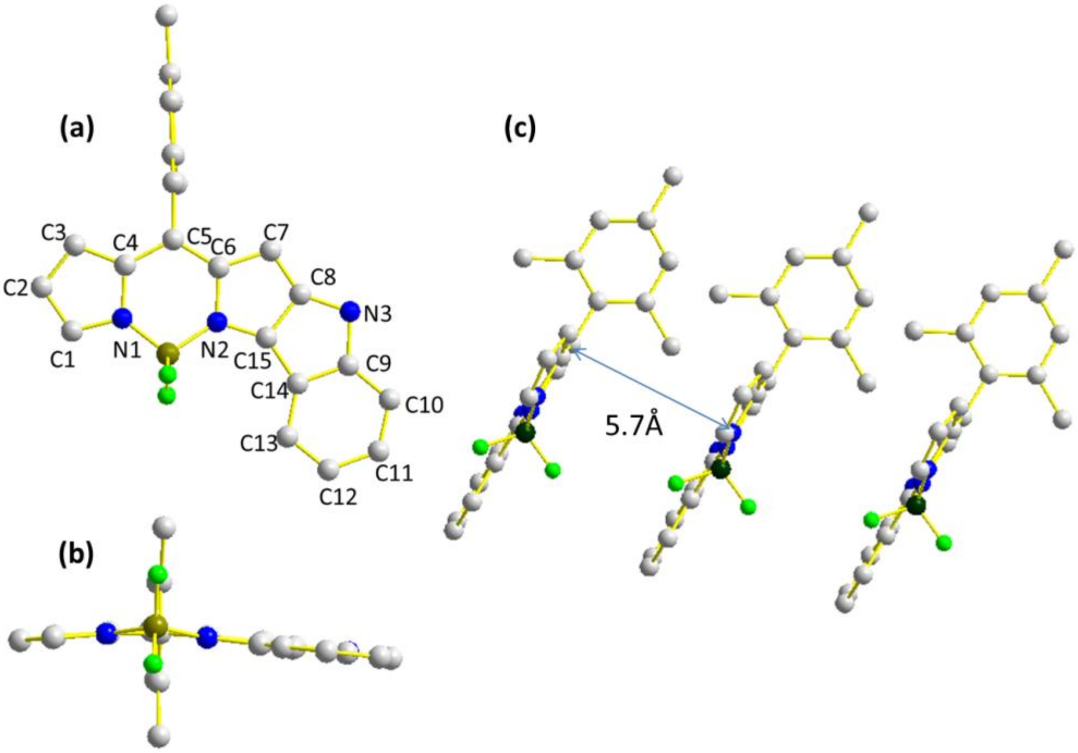


Figure S6. Top (a) and front (b) views of X-Ray structures of BODIPY **5a**, and Crystal packing (c).C, light gray; N, blue; B, dark yellow; F, bright green. Hydrogen atoms have removed for clarity.

5. Mechanism studies

5.1 Stern-Volmer emission quenching

Steady-state emission spectra were recorded using Edinburgh FS5 spectrometers. To a degassed acetonitrile solution of BODIPY **1a** (9×10^{-6} M) was added various amount of 4-chlorophenyl diazonium salt **2a**. The emission spectra of **1a** was then collected under excitation at 480 nm as shown in Figure S7a.

The emission intensity of **1a** at 526 nm was used to determine the Stern-Volmer quenching values (Figure S7b). The Stern-Volmer plot, as shown in Figure S5b, shows a linear correlation between the amounts of **2a** and the ratio I_0/I.[7,8]

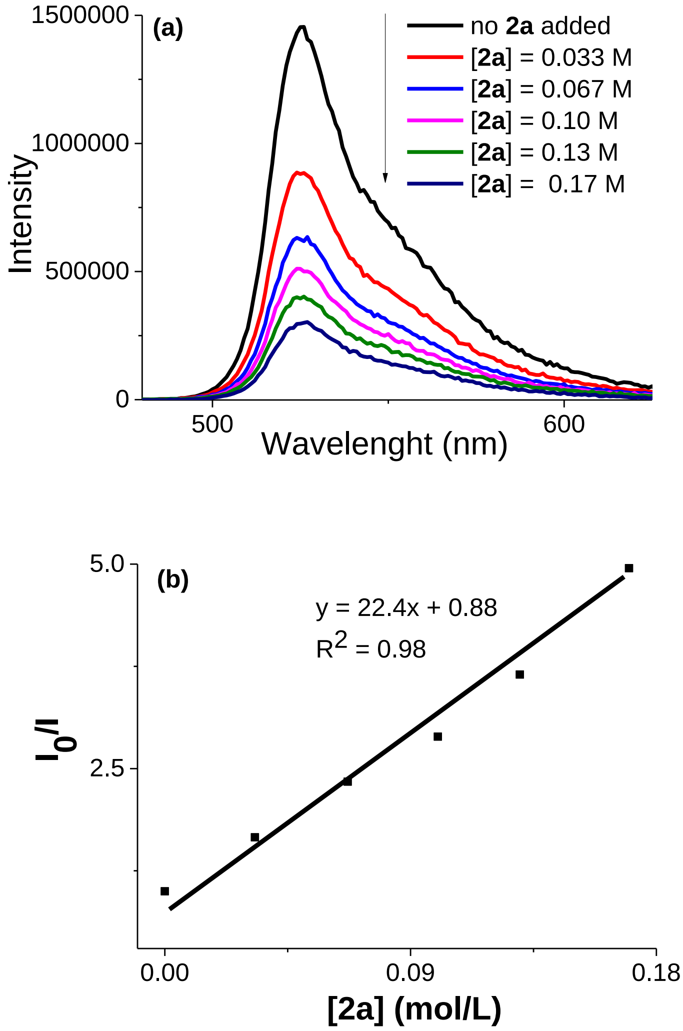
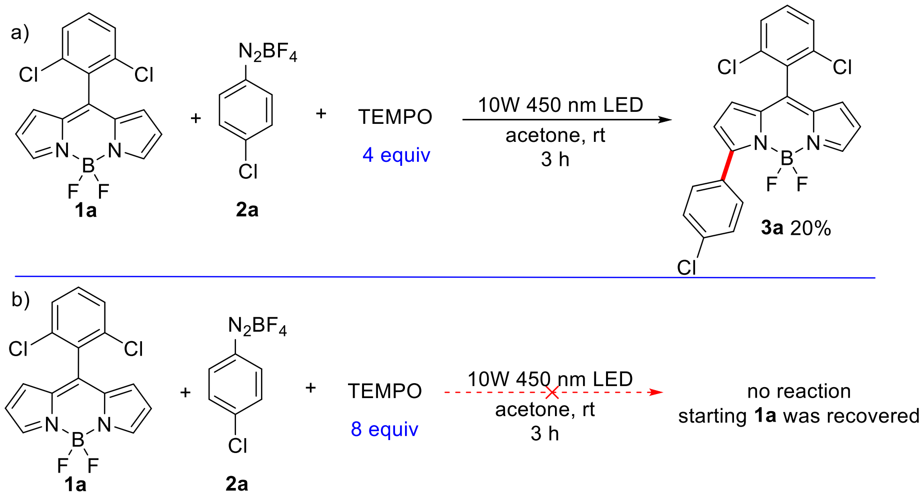


Figure S7. (a) The emission spectra of BODIPY **1a** (9×10^{-6} M) in acetonitrile at 25 °C with increasing amounts of 4-chlorophenyl diazonium salt **2a** (0 – 0.17 M) under excitation at 480 nm. (b) The Stern–Volmer plot of **1a** vs. [**2a**].

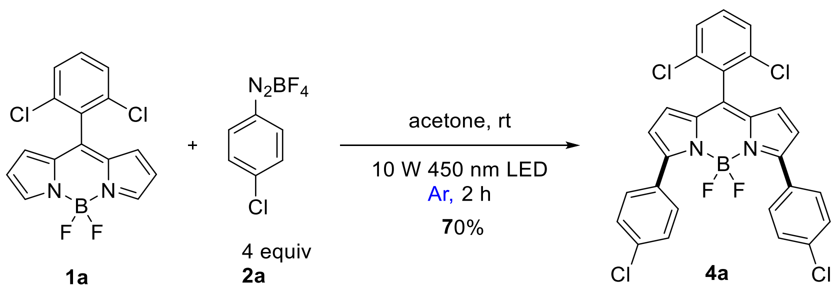
5.2 The influence of TEMPO to radical arylation reaction

When the radical scavenger TEMPO were added into the standard reaction between the aryl diazonium salt **2a** and BODIPY **1a**, the reaction was significantly inhibited. As shown in Scheme S1a, 4.0 equiv of TEMPO (62 mg, 0.4 mmol) were combined with the diazonium salt **2a** (90 mg, 0.4 mmol) in 2.0 mL acetone, followed by addition of BODIPY **1a** (34 mg, 0.1 mmol) under standard diarylation reaction condition, this reaction only gave **3a** in 20% yield with no formation of diarylated **4a**. Increasing the amount of TEMPO to 8 equiv (Scheme S1b), no desired arylated BODIPYs were dectected and most of BODIPY **1a** was recovered.



Scheme S1. The influence of TEMPO to this radical arylation reaction

5.3 Synthesis of 4a under Ar



Scheme S2. Synthesis of **4a** under Ar

The reaction between **1a** and **2a** under Ar was studied (Scheme S1). This reaction gave similar result to the standard reaction under air, indicating that O_2 is not involved in this arylation reaction.

6. Photophysical data

Table S3. Photophysical properties of BODIPYs 3 and 4 at room temperature in dichloromethane

dyes	λ_{abs}^{max}(nm)	λ_{em}^{max}(nm)	ε ($cm^{-1}M^{-1}$)	Φ^{a}	Stokes-shift (cm^{-1})
1c[b]	500	515	77300	0.99	480
3a	544	567	51400	0.66	750
3b	544	568	59170	0.99	764
3c	543	567	56200	0.67	800
3d	546	570	50883	0.71	770
3e	540	565	52600	0.68	820
3f	546	567	47864	0.72	650
3g	547	566	50403	0.67	630
3h	557	584	74300	0.53	850
3i	553	582	67100	0.56	920
3j	529	555	55200	0.08	890
3k	529	555	72800	0.77	890
3l	527	548	45751	0.21	770
3m	523	551	57200	0.82	990
3n	511	526	80500	0.01	560
3o	522	544	67000	0.87	775
4a	575	613	59100	0.99	1120
4b	575	610	49878	0.99	1000
4c	569	611	42200	0.99	1210
4d	578	619	43451	0.99	1180
4e	568	604	48800	0.99	1050
4f	577	613	47622	0.86	1010
4g	580	615	46154	0.81	990
4h	596	637	73500	0.85	1080
4i	590	633	51900	0.84	1170
4j	557	597	58100	0.99	1200
4k	559	595	49696	0.99	1100

4l	552	590	34091	0.99	1190
4n	523	554	82400	< 0.01	1090
4o	548	586	56400	0.89	1180
5a	596	628	31100	0.17	860
5b	680	698	59850	0.31	380
6[c]	607	622	145500	0.71	394

[a] The fluorescence quantum yields of **4a-l** and **5a** were calculated using Cresyl Violet perchlorate (ϕ = 0.54 in methanol) as the reference. The fluorescence quantum yields of **3a-n** were calculated using Rhodamine B (ϕ = 0.49 in ethanol) as the reference. The fluorescence quantum yields of **5b** were calculated using 1, 7-diphenyl-3, 5-di(4-methoxyphenyl) -azadipyrromethene (ϕ = 0.36 in chloroform) as the reference. The standard errors are less than 10%.[b] Date from ref 9. [c] Date from ref 10

7. Absorption and emission spectra of all BODIPYs recorded in dichloromethane at room temperature

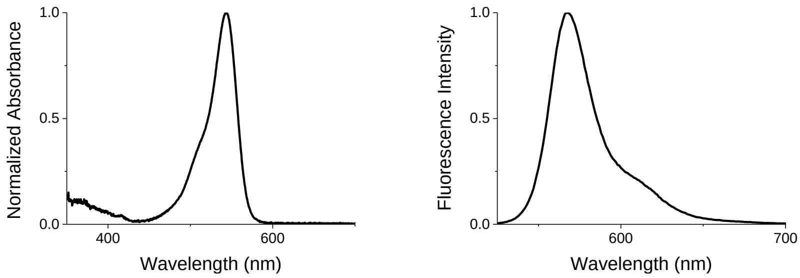


Figure S8: Absorption (left) and emission (right) spectra of compound **3a** recorded in dichloromethane (Excited at 520 nm)

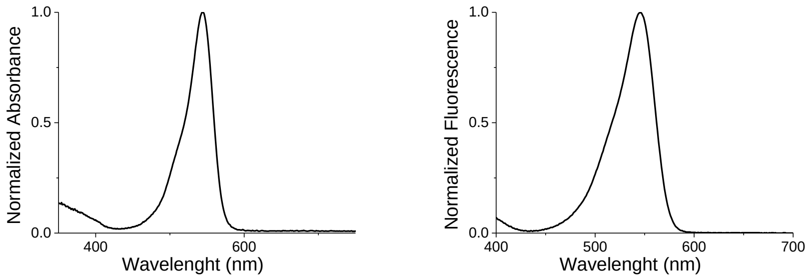


Figure S9: Absorption (left) and emission (right) spectra of compound **3b** recorded in dichloromethane (Excited at 510 nm)

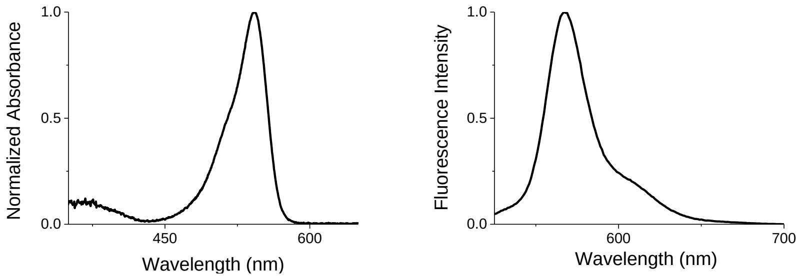


Figure S10: Absorption (left) and emission (right) spectra of compound **3c** recorded in dichloromethane (Excited at 520 nm).

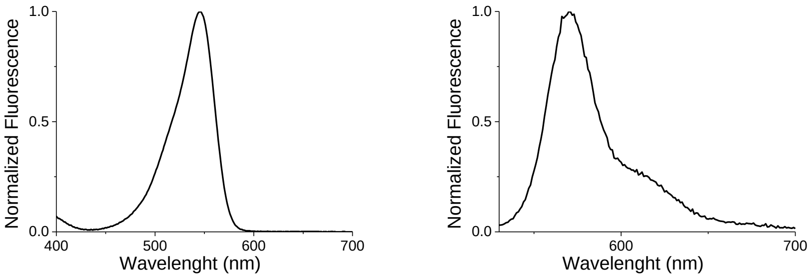


Figure S11: Absorption (left) and emission (right) spectra of compound **3d** recorded in dichloromethane (Excited at 510 nm)

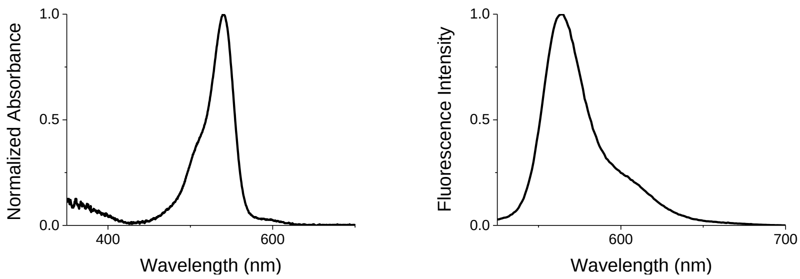


Figure S12: Absorption (left) and emission (right) spectra of compound **3e** recorded in dichloromethane (Excited at 520 nm)

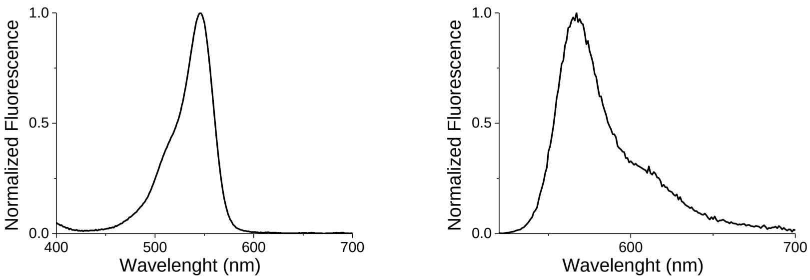


Figure S13: Absorption (left) and emission (right) spectra of compound **3f** recorded in dichloromethane (Excited at 510 nm)

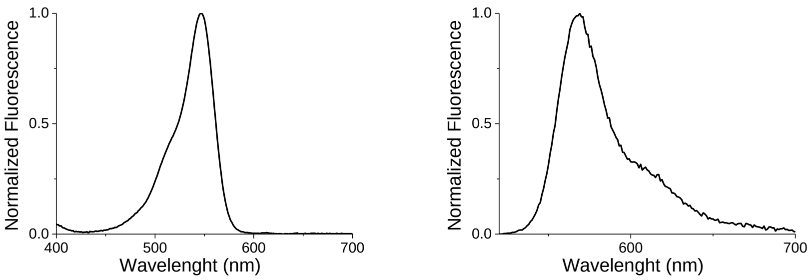


Figure S14: Absorption (left) and emission (right) spectra of compound **3g** recorded in dichloromethane (Excited at 510 nm)

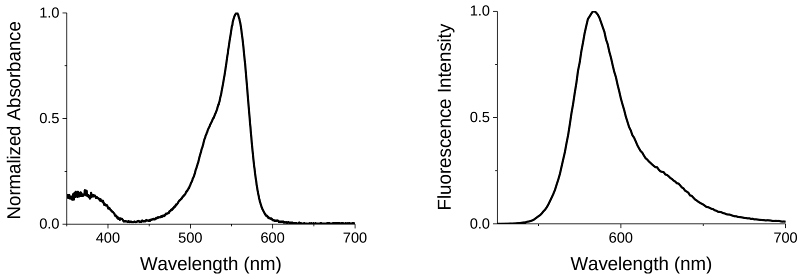


Figure S15: Absorption (left) and emission (right) spectra of compound **3h** recorded in dichloromethane (Excited at 520 nm)

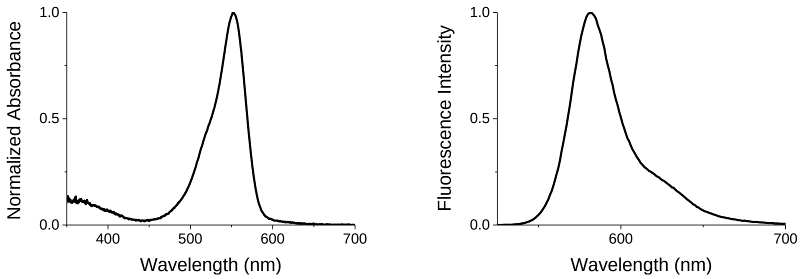


Figure S16: Absorption (left) and emission (right) spectra of compound **3i** recorded in dichloromethane (Excited at 520 nm)

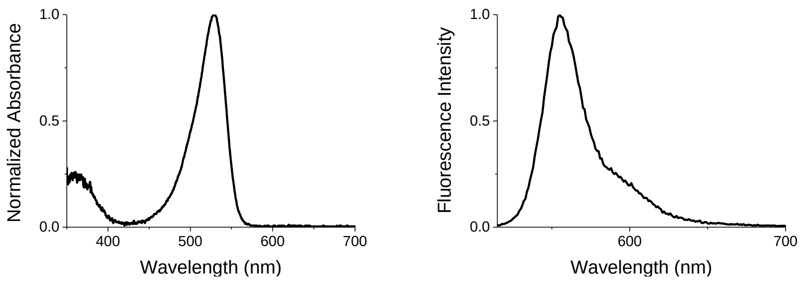


Figure S17: Absorption (left) and emission (right) spectra of compound **3j** recorded in dichloromethane (Excited at 500 nm)

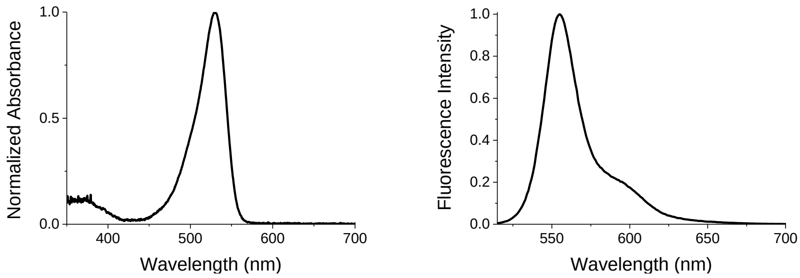


Figure S18: Absorption (left) and emission (right) spectra of compound **3k** recorded in dichloromethane (Excited at 510 nm)

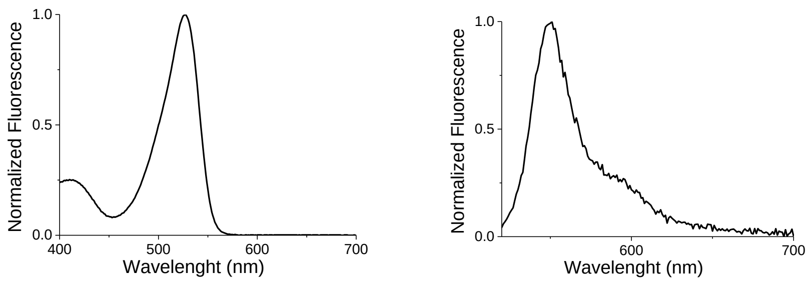


Figure S19: Absorption (left) and emission (right) spectra of compound **3l** recorded in dichloromethane (Excited at 510 nm)

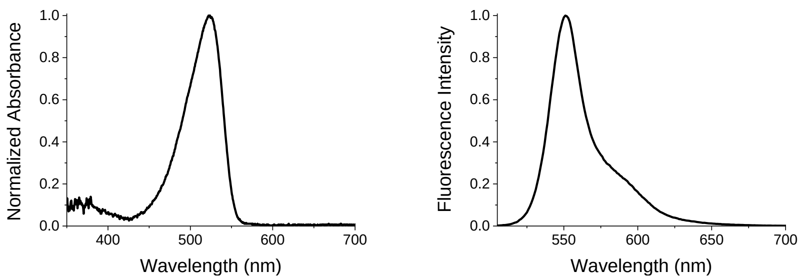


Figure S20: Absorption (left) and emission (right) spectra of compound **3m** recorded in dichloromethane (Excited at 500 nm)

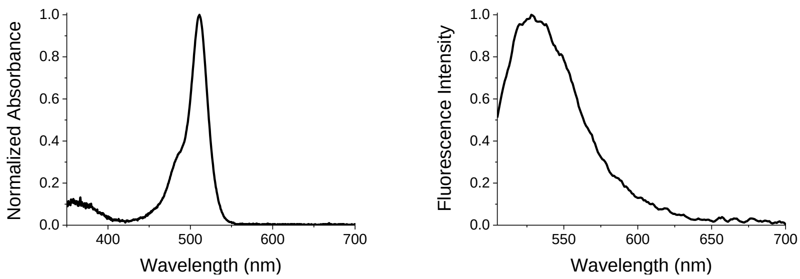


Figure S21: Absorption (left) and emission (right) spectra of compound **3n** recorded in dichloromethane (Excited at 500 nm)

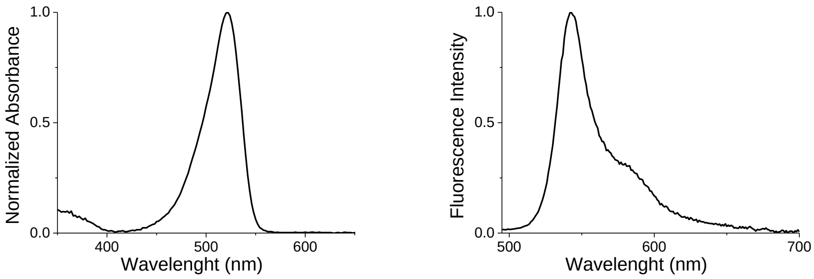


Figure S22: Absorption (left) and emission (right) spectra of compound **3o** recorded in dichloromethane (Excited at 490 nm)

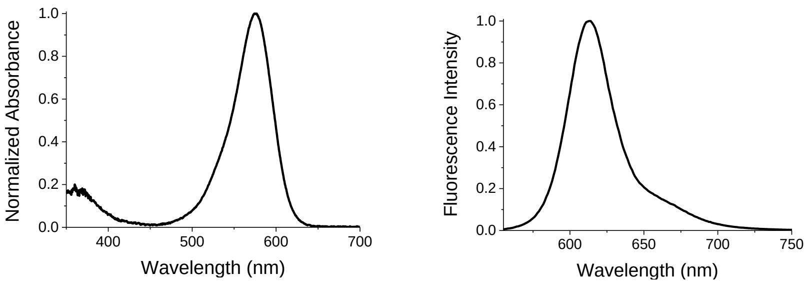


Figure S23: Absorption (left) and emission (right) spectra of compound **4a** recorded in dichloromethane (Excited at 550 nm)

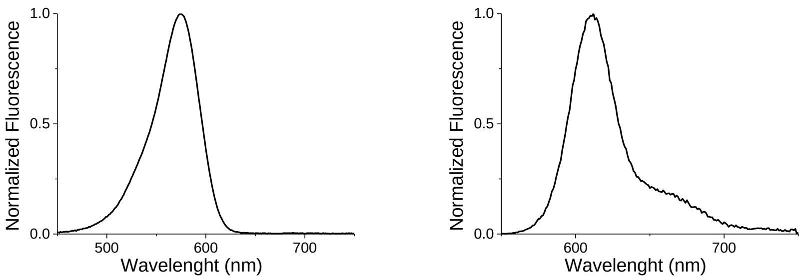


Figure S24: Absorption (left) and emission (right) spectra of compound **4b** recorded in dichloromethane (Excited at 540 nm)

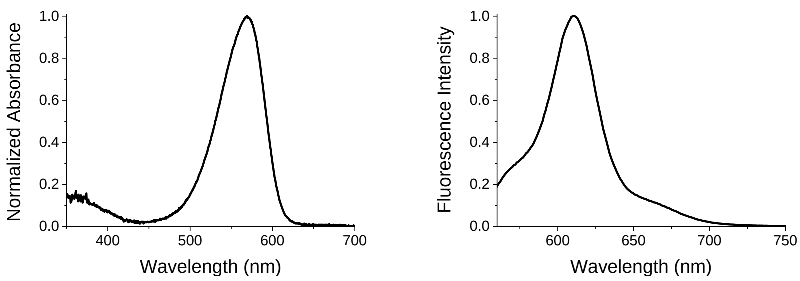


Figure S25: Absorption (left) and emission (right) spectra of compound **4c** recorded in dichloromethane (Excited at 550 nm)

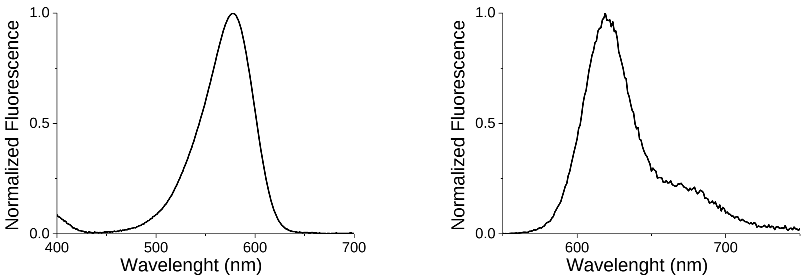


Figure S26: Absorption (left) and emission (right) spectra of compound **4d** recorded in dichloromethane (Excited at 540 nm)

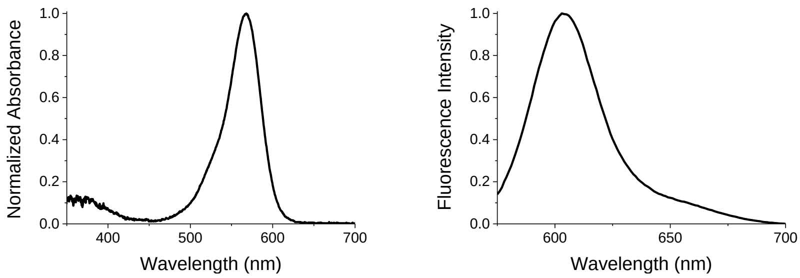


Figure S27: Absorption (left) and emission (right) spectra of compound **4e** recorded in dichloromethane (Excited at 550 nm)

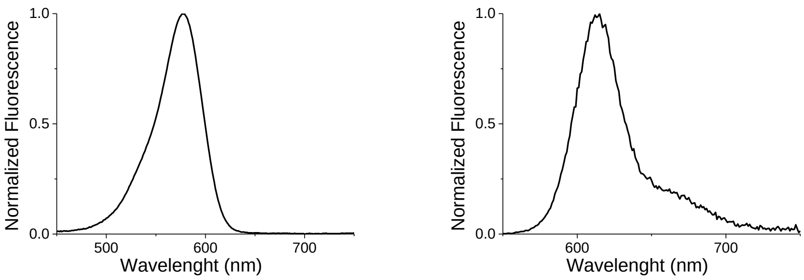


Figure S28: Absorption (left) and emission (right) spectra of compound **4f** recorded in dichloromethane (Excited at 540 nm)

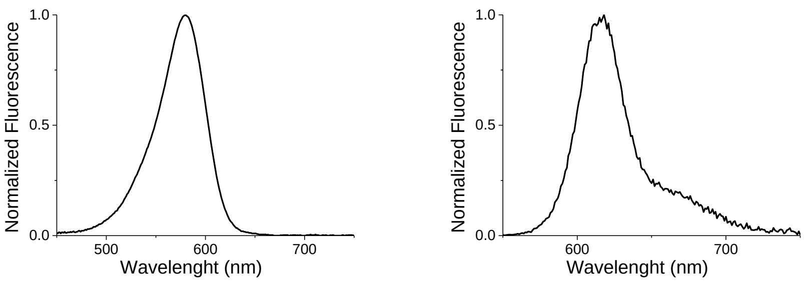


Figure S29: Absorption (left) and emission (right) spectra of compound **4g** recorded in dichloromethane (Excited at 540 nm)

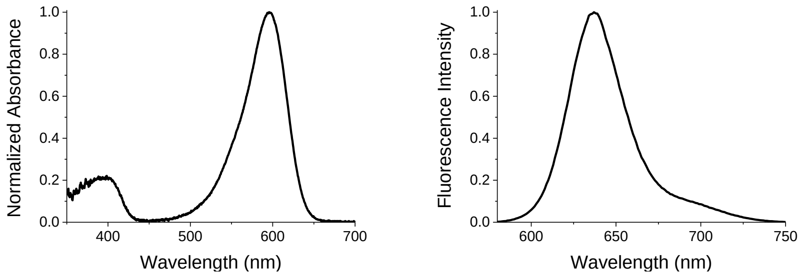


Figure S30: Absorption (left) and emission (right) spectra of compound **4h** recorded in dichloromethane (Excited at 570 nm)

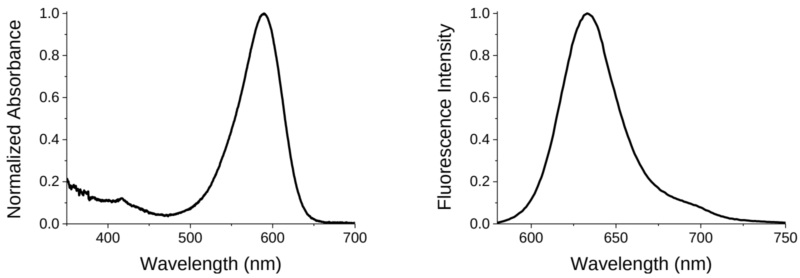


Figure S31: Absorption (left) and emission (right) spectra of compound **4i** recorded in dichloromethane (Excited at 570 nm)

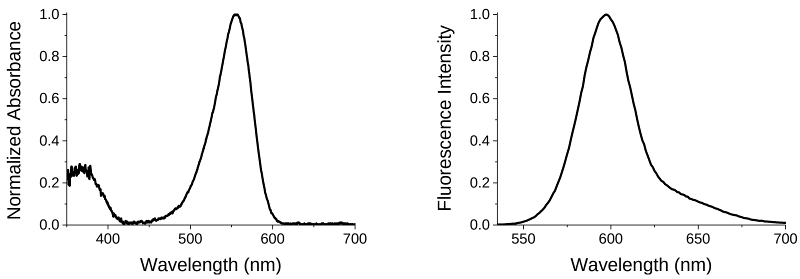


Figure S32: Absorption (left) and emission (right) spectra of compound **4j** recorded in dichloromethane (Excited at 530 nm)

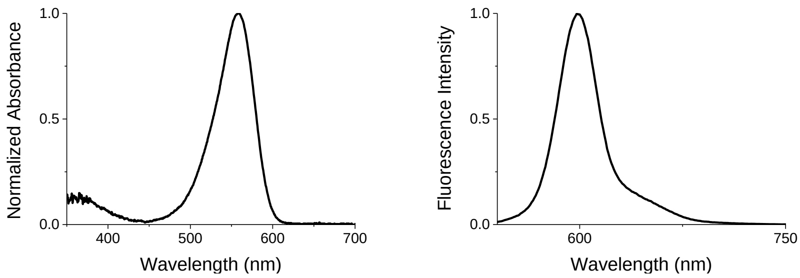


Figure S33: Absorption (left) and emission (right) spectra of compound **4k** recorded in dichloromethane (Excited at 530 nm)

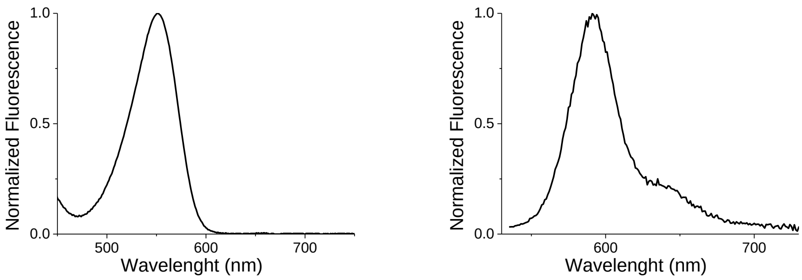


Figure S34: Absorption (left) and emission (right) spectra of compound **4l** recorded in dichloromethane (Excited at 530 nm)

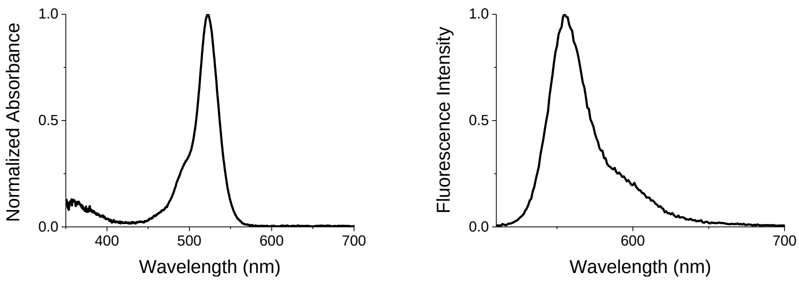


Figure S35: Absorption (left) and emission (right) spectra of compound**4n** recorded in dichloromethane (Excited at 500 nm)

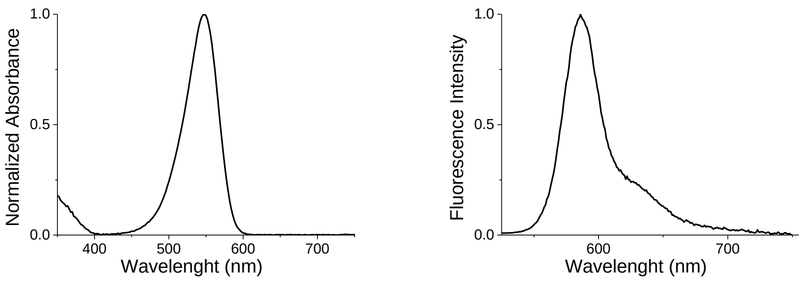


Figure S36: Absorption (left) and emission (right) spectra of compound **4o** recorded in dichloromethane (Excited at 520 nm)

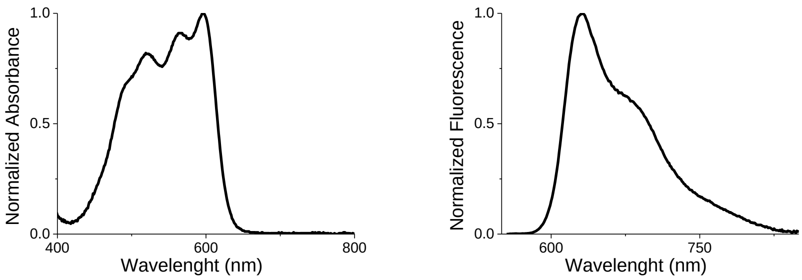


Figure S37: Absorption (left) and emission (right) spectra of compound **5a** recorded in dichloromethane (Excited at 550 nm)

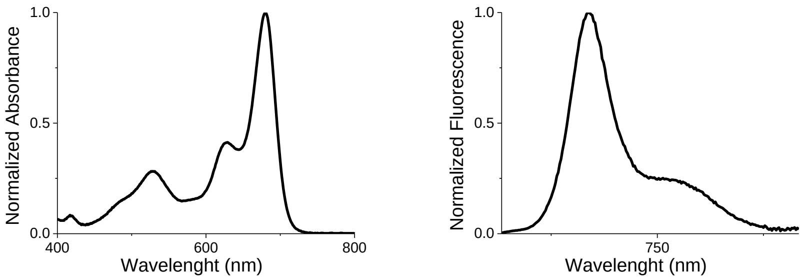


Figure S38: Absorption (left) and emission (right) spectra of compound **5b** recorded in dichloromethane (Excited at 635 nm)

8. Cellular studies

Cell Culture

The HeLa cells were cultured in a Roswell Park Memorial Institute 1640 medium (RPMI-1640, Gibco, America) with 10% fetal bovine serum (FBS, Lonsera, Shanghai, China) at 37 °C with 5% CO_2.

Cytotoxicity Determined by the CCK-8 Method

The HeLa cells were plated at 5000 cells per well in a 96-well plate in a 1640 medium and allowed to grow for 24 h. A gradient concentration of **5b** from 1 to 100 μM in a fresh medium was added as a replacement, and the cells were incubated for 24 h at 37 °C with 5% CO_2. The working solutions were then removed, and the cells were washed with PBS buffer two times. A total of 10 μL of CCK-8 (Cell Counting Kit-8, BIOMIKY) was added into each well, and the cells were further incubated at 37 °C for 1 h in a 10% CO_2 humidified atmosphere. The plate was then shaken for 5 min, and the absorbance was measured at 450 nm using a microplate reader.

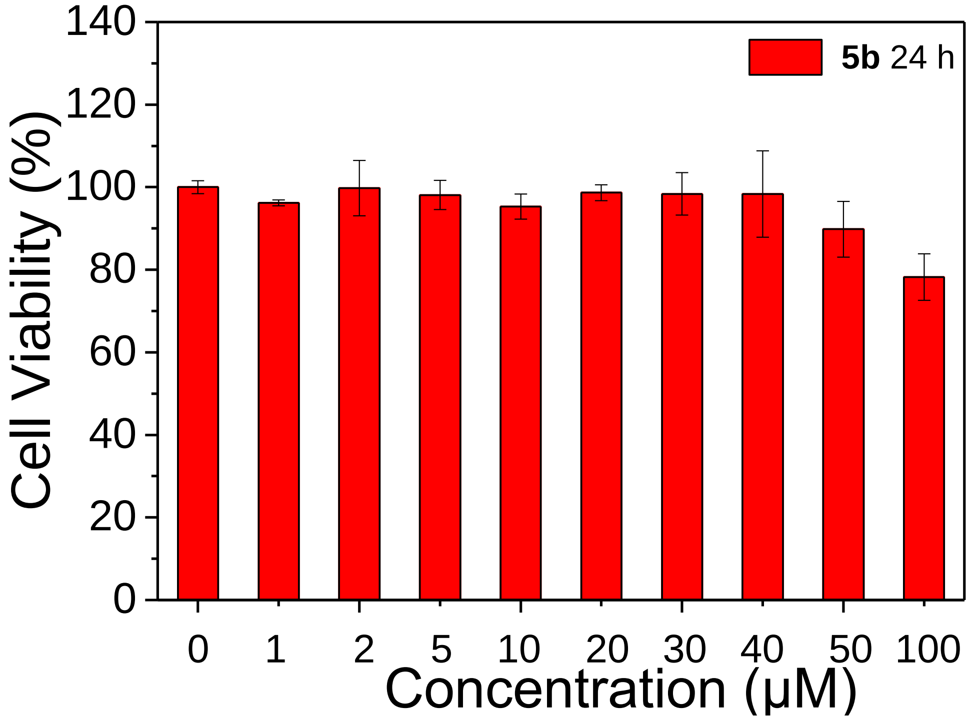


Figure S39. Viability of HeLa cells treated with 0, 1, 2, 5, 10, 20, 30, 40, 50 and 100 μM **5b** for 24 h.

Cell Incubation and Imaging

A total of 30000 HeLa cells were seeded into a glass bottom dish with the same procedure above. A solution of **5b** solution in RPMI-1640 medium (containing 1% DMSO, 5 μM) was added to the above cells and incubated for another 15 min at 37 °C with 5% CO_2. The working solutions were then removed, and the cells were then washed with PBS two times and fixed by 4% formaldehyde for 20 min. The organelle tracer DAPI (1.67 μg/mL) was added subsequently and incubated for 20 min to stain the nucleus. The above solution in dish was removed, and the cells were washed with PBS buffer two times before imaging using a confocal fluorescence microscope (Leica Microsystems SP8 MP).

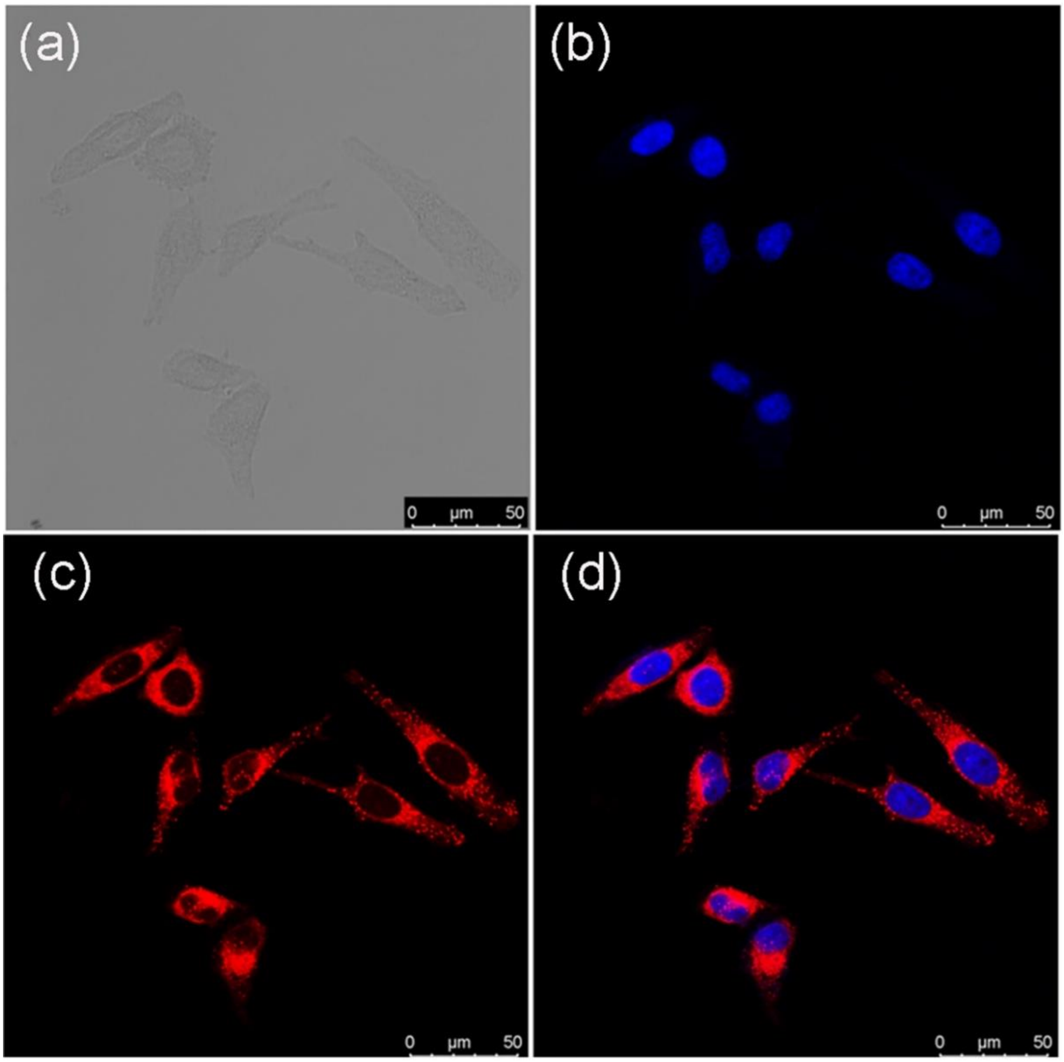
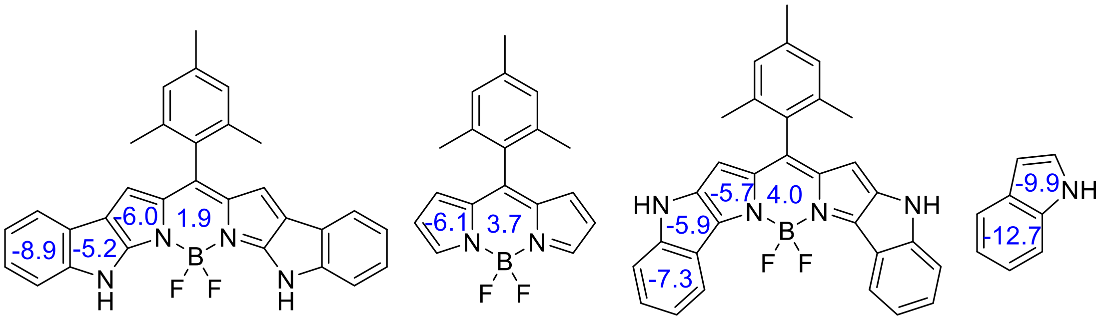


Figure S40. Confocal fluorescence images of HeLa cells stained with **5b** (5 uM) and DAPI. (a) Bright field. (b) DAPI fluorescence. (c) **5b** fluorescence after incubation for 15 min, using excitation wavelengths of 638 nm, and recording over the 650-760 nm spectral regions. (d) merged images of parts b and c.

9. DFT caclulations

The ground state geometry was optimized by using DFT method at B3LYP/6-31G(d) level. The same method was used for vibrational analysis to verify that the optimized structures correspond to local minima on the energy surface. TD-DFT computations were used the optimized ground state geometries under the B3LYP/6-31+G(d,p) theoretical level. NICS(0) values were calculated at the GIAO-B3lyp/6-31+G(d,p) level. The calculated molecules in dichloromethane were done using the Self-Consistent Reaction Field (SCRF) method and Polarizable Continuum Model (PCM). All of the calculations were carried out by the methods implemented in Gaussian 09 package.[11]



6 **1c** **5b** **indole**

Figure S41. NICS(0) values (ppm) for BODIPY **1c**, **5b**, **6** and indole, calculated at the B3LYP/6-31+G(d,p)//B3LYP/6- 31G(d) level.

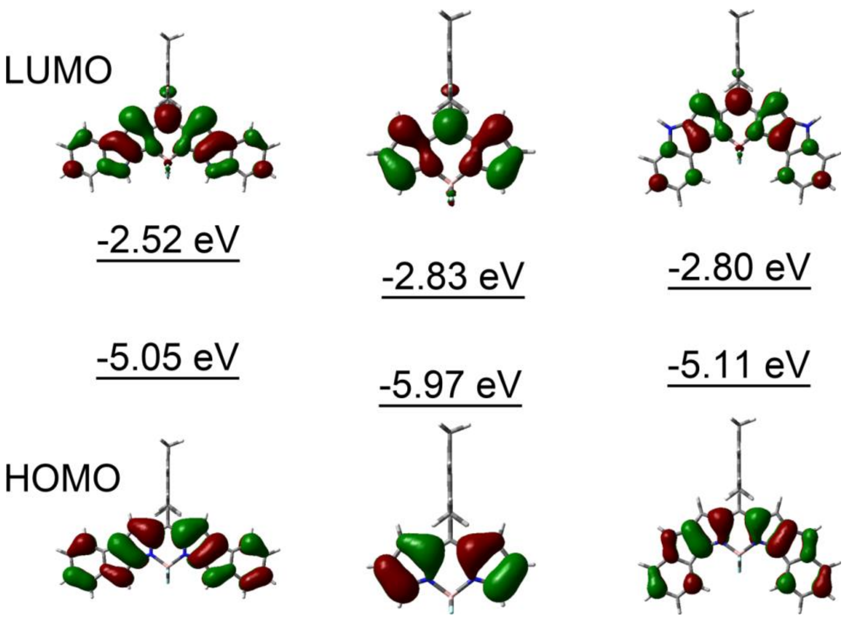


Figure S42. HOMO-LUMO energy levels and the interfacial plots of the orbitals for BODIPYs **6** , **1c** and **5b**.

Table S4. Selected electronic excitation energies (eV) and oscillator strengths (*f*), configurations of the low-lying excited states of the BODIPYs **5a**, **5b** and **6** calculated by TDDFT/B3LYP/6-31+G(d,p), based on the optimized ground state geometries. The TDDFT of all the molecules in dichloromethane were using the Self Consistent Reaction Field (SCRF) method and the Polarizable Continuum Model (PCM).

	Electronic transition	TD//B3LYP/6-31+G(d, p)				
		Energy/ eV [a]		*f* [b]	Composition [c]	CI [d]
5a	S0→S1	2.2748 eV	545.02 nm	0.1247	HOMO → LUMO	0.5211
					HOMO -1 → LUMO	0.4770
	S0→S2	2.5938 eV	478.00 nm	0.7752	HOMO -1 → LUMO	0.5197
					HOMO → LUMO	0.4791
	S0→S3	2.8954 eV	428.21 nm	0.0008	HOMO -2 → LUMO	0.7044
5b	S0→S1	2.0450 eV	606.28 nm	0.3906	HOMO → LUMO	0.6334
					HOMO -1 → LUMO	0.3196
	S0→S2	2.3642 eV	524.43 nm	0.6487	HOMO -1 → LUMO	0.6293
					HOMO → LUMO	0.3231
	S0→S3	2.3733 eV	522.40 nm	0.0165	HOMO -2 → LUMO	0.7044
6	S0→S1	2.3550 eV	526.47 nm	1.3813	HOMO → LUMO	0.7048
	S0→S2	2.7635 eV	448.65 nm	0.0136	HOMO -1 → LUMO	0.7008
	S0→S3	2.9071 eV	426.49 nm	0.0121	HOMO -2 → LUMO	0.7032

[a] Only the selected low-lying excited states are presented. [b] Oscillator strength. [c] Only the main configurations are presented. [d] The CI coefficients are in absolute values.

Table S5. DFT optimized coordinates for BODIPY 1c, 5a, 5b and 6.

Compound 1c

B	-3.11783200	0.00333200	0.02600800
C	-2.55387500	2.53514800	-0.03174400
C	-1.42551200	3.37944400	-0.03878000
C	-0.30836500	2.55296400	-0.02331100
C	-0.77791800	1.21373400	-0.00801900
C	-0.07600800	-0.00014900	-0.00275200
C	-0.78068300	-1.21244500	-0.00751600
C	-0.31424200	-2.55276600	-0.02217900
C	-1.43330200	-3.37666300	-0.03731200
C	-2.55970600	-2.52975800	-0.03068200
C	1.42032700	-0.00159800	0.00137600
C	2.11518600	-0.00411600	1.22923700
C	3.51373100	-0.00908300	1.20748100
C	4.23693800	-0.00870100	0.01084300
C	3.52176900	-0.01027100	-1.19059700
C	2.12335400	-0.00530800	-1.22182800
C	1.38137700	-0.00564800	2.55201400
C	5.74758400	0.01761200	0.01591000
C	1.39883800	-0.00800900	-2.54974800
F	-3.86242500	0.00440400	1.20147400
F	-3.96064500	0.00410200	-1.07982800
N	-2.17423900	1.24622000	-0.01307300
N	-2.17708000	-1.24170100	-0.01259600
H	-1.44656400	4.46029700	-0.05487600
H	0.73219300	2.84693200	-0.02545600
H	0.72562000	-2.84922200	-0.02414100
H	-1.45682700	-4.45747300	-0.05292100
H	-3.60876500	-2.79506100	-0.03793600
H	4.05068800	-0.01471900	2.15372700
H	4.06509300	-0.01686100	-2.13319600
H	2.08776500	-0.00634000	3.38691300
H	0.73681200	-0.88638700	2.65535100
H	0.73686500	0.87493400	2.65689500
H	6.15947500	-0.47619400	-0.87031800
H	6.15351600	-0.47732100	0.90426500
H	6.12416100	1.04914500	0.01785400
H	0.75511100	-0.88886800	-2.65698900
H	2.11114200	-0.00936600	-3.37959900
H	0.75510900	0.87247400	-2.66000500
H	-3.60232500	2.80287300	-0.03909900

Compound 5a

C	-1.25871113	1.82832048	-0.11993197
C	-0.03017072	-0.26111966	0.04402414
C	-1.24712192	0.42138956	-0.01552071
C	-2.33433482	2.73068904	-0.30137463
C	-1.78630302	4.00829073	-0.40992394
C	-0.39387286	3.86318869	-0.28729549
N	1.18592087	0.44175904	0.01818799
N	-0.07504532	2.56485695	-0.11555158
B	1.32832745	1.97875280	0.20456552
F	2.28870896	2.48629280	-0.66868996
C	0.22230186	-1.67273884	0.06671383
C	1.59840225	-1.79481038	0.04457831
C	2.16544133	-0.48456516	0.01070467
F	1.68004295	2.27096030	1.52331316
H	-0.53805248	-2.43995488	0.07894686
H	-3.37779074	2.45267837	-0.35858958
H	-2.31363674	4.93931483	-0.56636480
H	0.37768124	4.62123884	-0.31276179
C	-2.53964957	-0.33315347	-0.00237666
C	-3.10104886	-0.79131678	-1.21266689
C	-3.19113861	-0.57596623	1.22578922
C	-4.31419113	-1.48768805	-1.16948176
C	-4.40115861	-1.27714773	1.21758206
C	-4.98257361	-1.73873783	0.03231480
H	-4.74632712	-1.84252768	-2.10282802
H	-4.90117346	-1.46755430	2.16505802
C	-2.42016498	-0.54784493	-2.54146507
H	-2.26248119	0.52142759	-2.72383596
H	-1.43489026	-1.02666655	-2.58336423
H	-3.02205169	-0.94470832	-3.36394350
C	-2.60424576	-0.10023941	2.53619680
H	-1.61121015	-0.52991173	2.71294798
H	-2.48613827	0.98946802	2.55268067
H	-3.24749780	-0.38228406	3.37463178
C	-6.30694766	-2.46591851	0.05014356
H	-7.14649170	-1.75835789	0.02876233
H	-6.41411441	-3.12429144	-0.81798269
H	-6.41856511	-3.07165071	0.95571826
C	3.58893824	-0.60926668	-0.02399435
C	4.66508189	0.29049036	-0.08839388
C	3.83401991	-2.02164970	-0.00176585
C	5.95841099	-0.21719300	-0.11247217
H	4.47275734	1.35721685	-0.13167112
C	5.13623701	-2.52387740	-0.02705725

C	6.18593160	-1.60745255	-0.07924221
H	6.80443232	0.46159662	-0.16197835
H	5.32536577	-3.59294603	-0.00926297
H	7.20672271	-1.97896255	-0.09981217
N	2.62866220	-2.71552484	0.03943326
H	2.53750228	-3.71990022	0.04421794

Compound 5b

C	-0.76339082	1.20903079	0.04207435
C	-0.74142308	-1.22218160	0.04185521
C	-1.45461452	-0.01291422	0.04274172
C	-1.27855709	2.54003165	-0.05661241
C	-0.16204081	3.35939535	-0.08711511
C	0.99958474	2.53968882	-0.00624558
N	0.66007117	-1.22682842	0.07666897
N	0.63780334	1.23899526	0.07701957
B	1.52821869	0.01397963	0.40926348
F	2.69098966	0.02457999	-0.36819465
C	-1.23245288	-2.56226468	-0.05703743
C	-0.10131916	-3.36130442	-0.08775165
C	1.04527196	-2.52074294	-0.00691247
F	1.86787388	0.01681336	1.76460823
H	-2.27457184	-2.84099368	-0.11406377
H	-2.32554866	2.79982586	-0.11371734
C	-2.95155188	-0.02652404	0.00702236
C	-3.62826456	-0.03320270	-1.23103637
C	-3.67739988	-0.03818271	1.21711821
C	-5.02738929	-0.05043475	-1.23310008
C	-5.07508955	-0.05538437	1.16423577
C	-5.77057021	-0.05824166	-0.04886764
H	-5.54876456	-0.05939734	-2.18815110
H	-5.63383907	-0.06825071	2.09788909
C	-2.87384543	-0.02659105	-2.54218508
H	-2.23541829	0.85967754	-2.63478785
H	-2.21930101	-0.90102769	-2.63488332
H	-3.56678986	-0.03279036	-3.38851602
C	-2.97371295	-0.03660056	2.55606976
H	-2.32447967	-0.91243602	2.67104994
H	-2.33721692	0.84797157	2.67512735
H	-3.69791018	-0.04371002	3.37579466
C	-7.28130807	-0.04508632	-0.07852826
H	-7.66801636	0.98270019	-0.06727432
H	-7.66824412	-0.52712768	-0.98236431
H	-7.70340123	-0.55900311	0.79147163

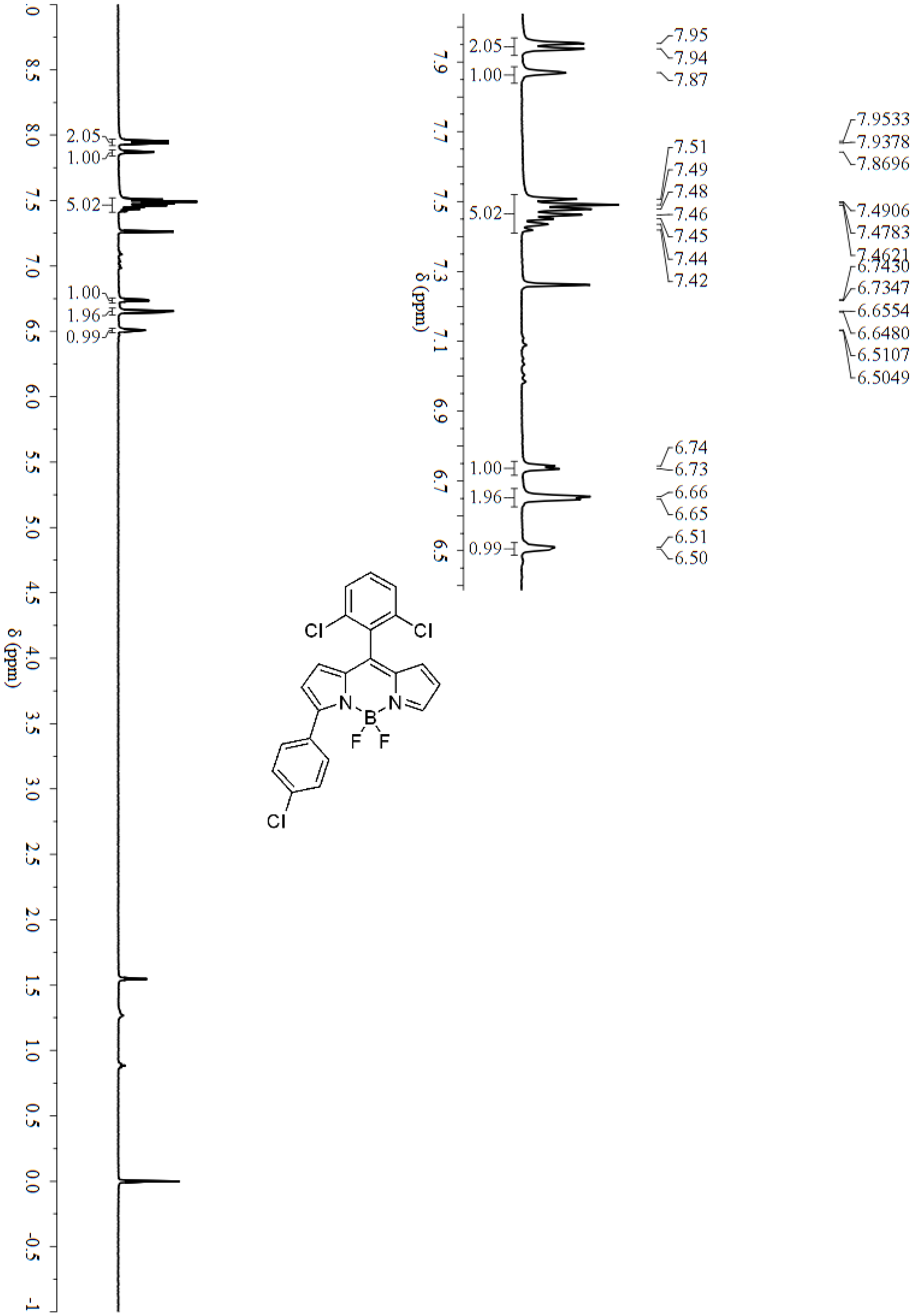
C	2.21350593	-3.34358760	-0.05014103
C	3.59836096	-3.11097415	-0.03427750
C	1.71427884	-4.68461528	-0.15090388
C	4.46005214	-4.19957687	-0.10129706
H	3.97167889	-2.09366942	0.01614505
C	2.58632176	-5.77267226	-0.21801258
C	3.95610767	-5.51248047	-0.18913007
H	5.53405211	-4.03932616	-0.09030031
H	2.20979434	-6.78864660	-0.29214225
H	4.65090393	-6.34626997	-0.24057001
N	0.32353846	-4.67429554	-0.17068270
H	-0.26115666	-5.49062920	-0.26350213
C	2.15278311	3.38352486	-0.04910333
C	3.54166880	3.17621070	-0.03282527
C	1.62933183	4.71529785	-0.14984130
C	4.38340386	4.28034171	-0.09951977
H	3.93361614	2.16594328	0.01775247
C	2.48141589	5.81902655	-0.21667369
C	3.85569224	5.58387182	-0.18745931
H	5.46013727	4.13964103	-0.08821294
H	2.08644370	6.82794907	-0.29077698
H	4.53519430	6.43018124	-0.23868406
N	0.23902664	4.67986047	-0.16992702
H	-0.36020221	5.48568267	-0.26211817

Compound 6

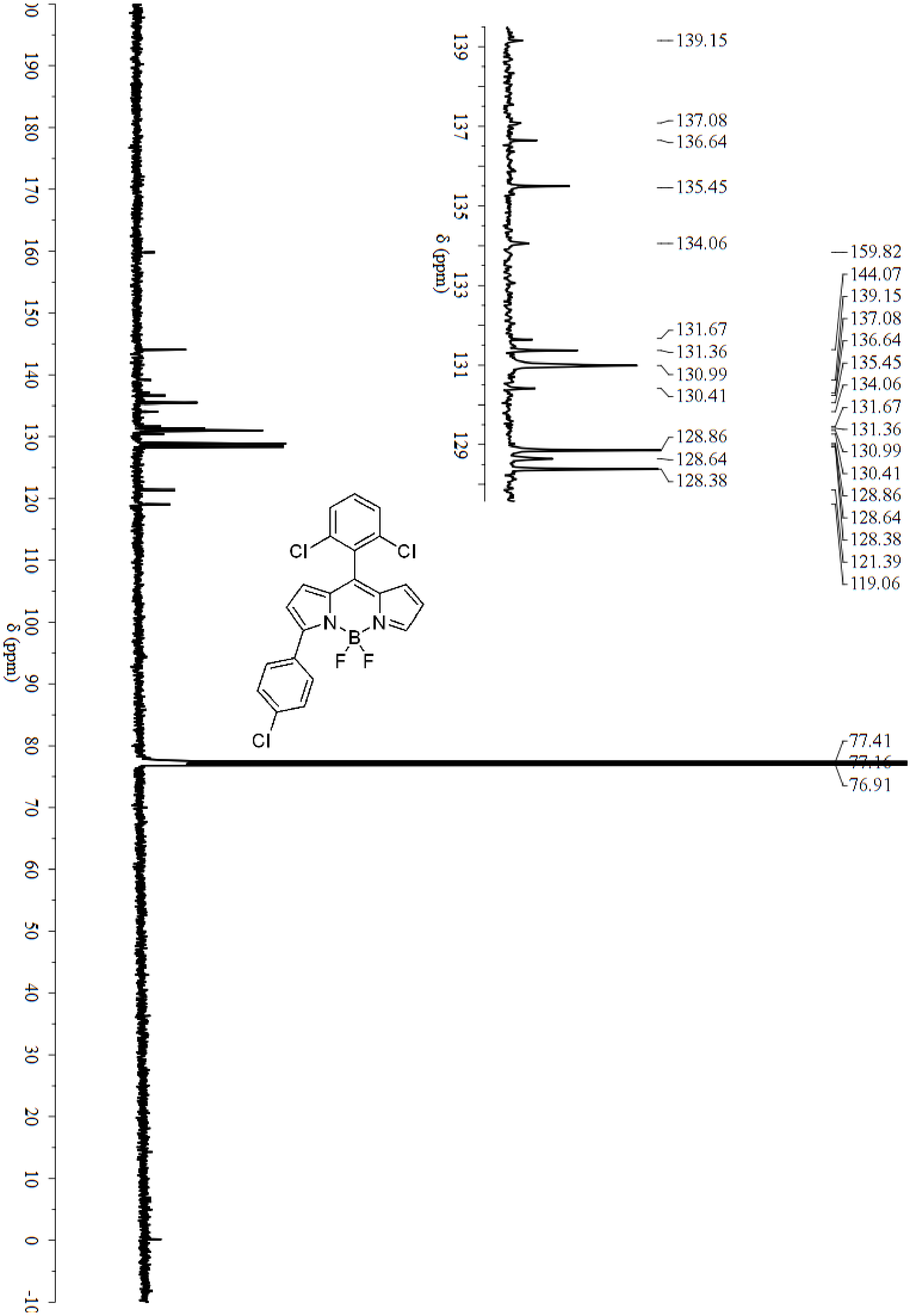
C	1.21368000	0.30668500	0.10494200
C	0.00047800	1.00878600	0.09886100
C	-1.21381400	0.30856700	0.10439900
N	1.22470200	-1.11038200	0.15360100
N	-1.22708800	-1.10847200	0.15335700
B	-0.00192200	-2.00377200	0.45501100
F	-0.00270800	-3.13386100	-0.36740400
F	-0.00235600	-2.40456300	1.79383400
C	-5.67361500	-3.14161400	-0.19328300
C	-4.58009900	-2.28805700	-0.10935100
C	-4.72069800	-0.86726900	-0.16119000
C	-5.99911800	-0.31767300	-0.29777500
C	-7.10154500	-1.17088600	-0.38139300
C	-6.93992800	-2.56323200	-0.33058900
H	-5.54999700	-4.21984000	-0.15401400
H	-6.13137400	0.75985800	-0.33911900
H	-8.09753000	-0.75071600	-0.48771700
H	-7.81139600	-3.20813900	-0.39833700

C	-3.37960400	-0.33005400	-0.05223700
C	-2.51622600	-1.45618100	0.05527300
N	-3.21754500	-2.61844500	0.03319000
H	-2.82965800	-3.55100000	0.03488700
C	-2.54901300	0.78818500	-0.01549900
H	-2.81789600	1.83311200	-0.08520000
C	5.66807800	-3.15048500	-0.19242400
C	4.57591300	-2.29520700	-0.10843500
C	4.71878600	-0.87462900	-0.15982000
C	5.99811300	-0.32703600	-0.29597400
C	7.09919400	-1.18198100	-0.37963000
C	6.93534100	-2.57408300	-0.32930000
H	5.54272800	-4.22852700	-0.15355800
H	6.13210000	0.75029400	-0.33697600
H	8.09587000	-0.76337000	-0.48562500
H	7.80579000	-3.22035900	-0.39709400
C	3.37851700	-0.33531100	-0.05107600
C	2.51332200	-1.46009800	0.05586300
N	3.21280100	-2.62346500	0.03368500
H	2.82343100	-3.55540000	0.03498600
C	2.54968000	0.78422700	-0.01427600
H	2.82021400	1.82874900	-0.08356700
C	0.00198500	2.50616000	0.05302100
C	0.00313500	3.17591200	-1.18863400
C	-0.00236400	3.23953000	1.25889700
C	0.00144500	4.57532500	-1.19878700
C	-0.00409500	4.63683600	1.19812600
C	0.00140500	5.32534000	-0.01908100
H	-0.00114800	5.09129000	-2.15678200
H	-0.01118000	5.20111700	2.12853100
C	0.00208600	2.41512500	-2.49614700
H	0.88190600	1.76750200	-2.58556600
H	-0.87884500	1.76900300	-2.58553500
H	0.00273800	3.10408000	-3.34574000
C	0.03147700	6.83566600	-0.05671700
H	1.06240500	7.21173700	-0.01473600
H	-0.41806400	7.22228600	-0.97719100
H	-0.50491500	7.26827900	0.79447900
C	-0.00893700	2.54440600	2.60232000
H	-0.89104800	1.90435500	2.72018200
H	0.86932400	1.90016600	2.72599500
H	-0.00983100	3.27382100	3.41742900

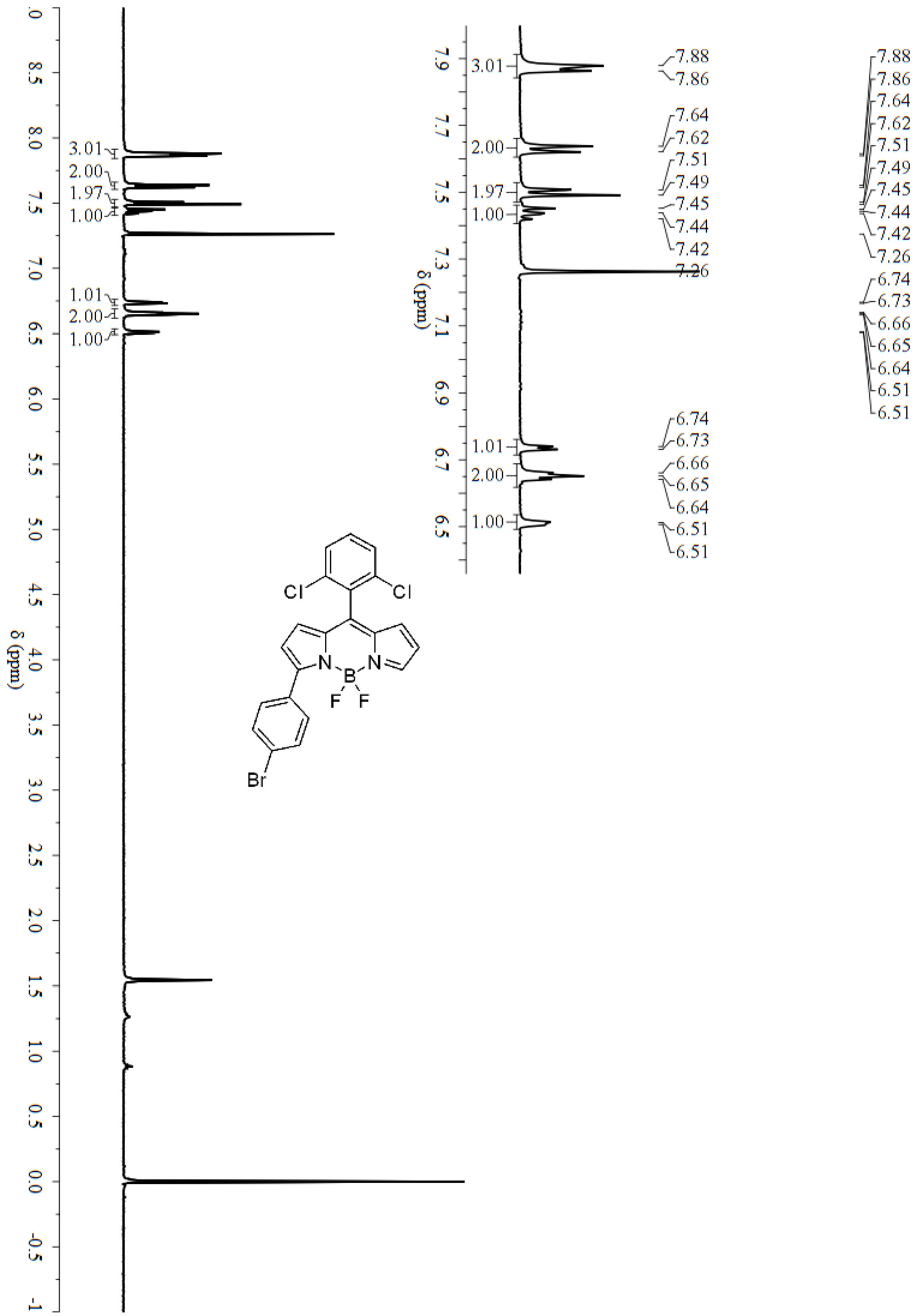
10. ^{1}H, ^{13}C NMR and HRMS spectra for all new compounds



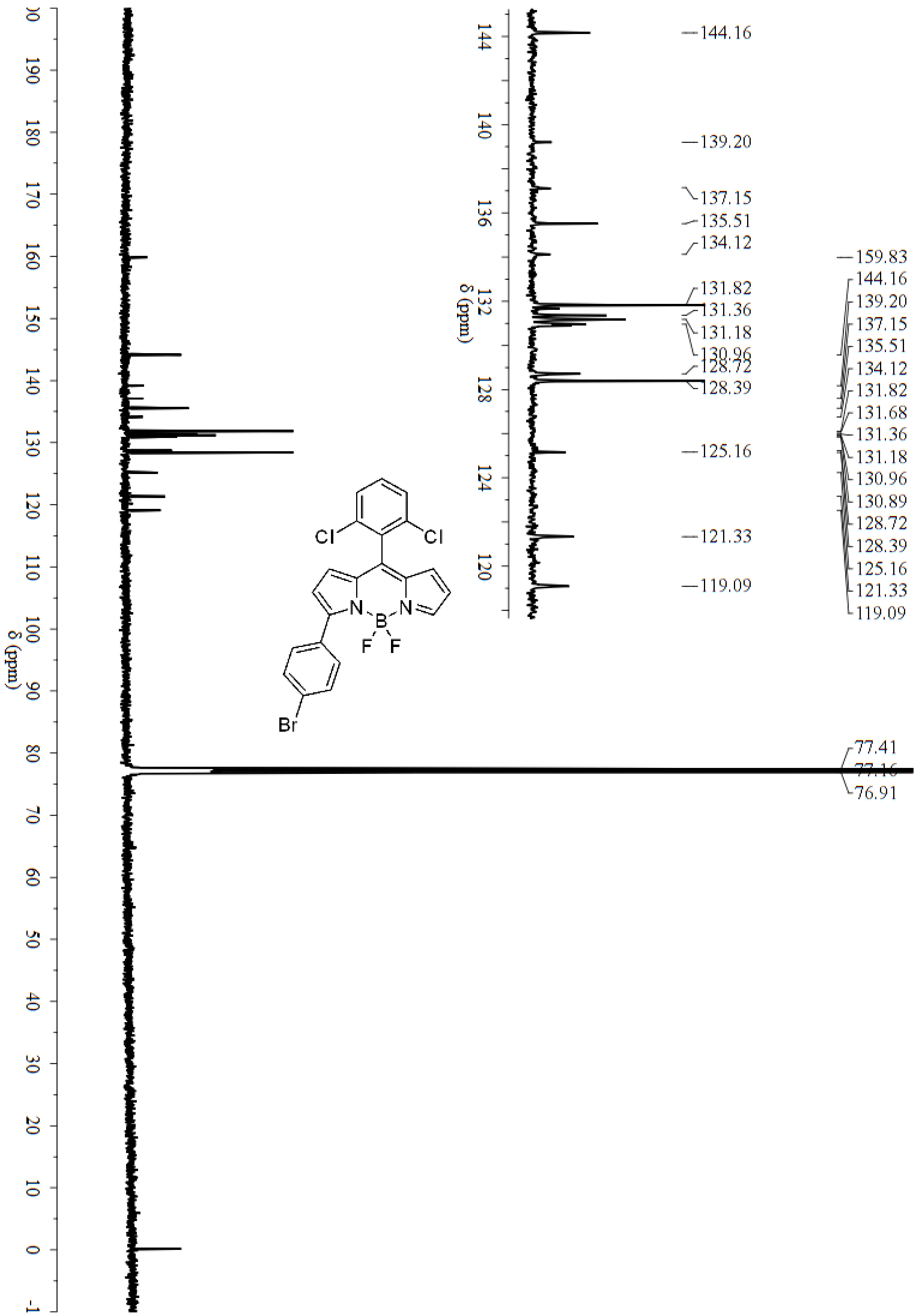
^{1}H NMR spectrum of **3a** in $CDCl_3$



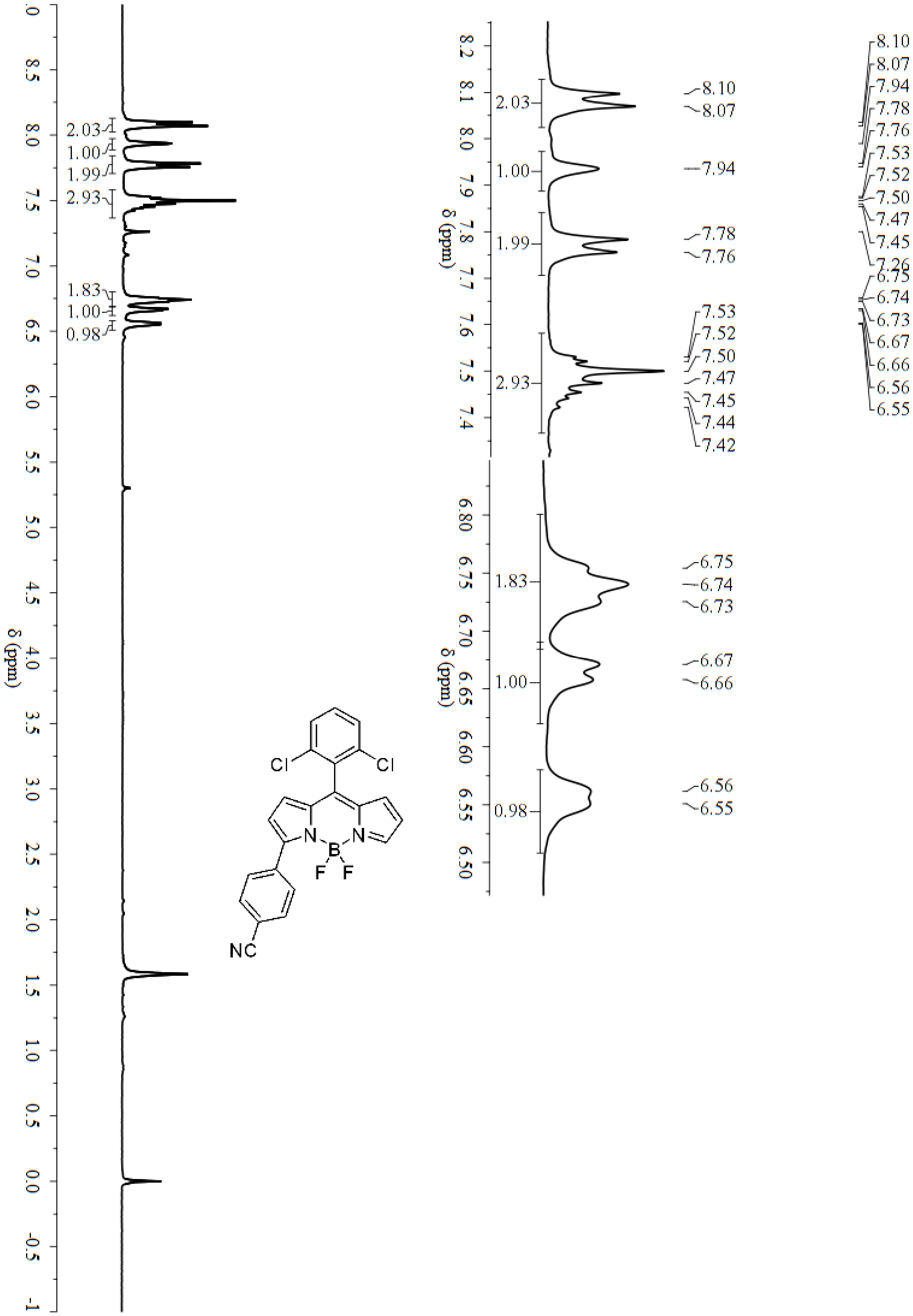
^{13}C NMR spectrum of **3a** in $CDCl_3$



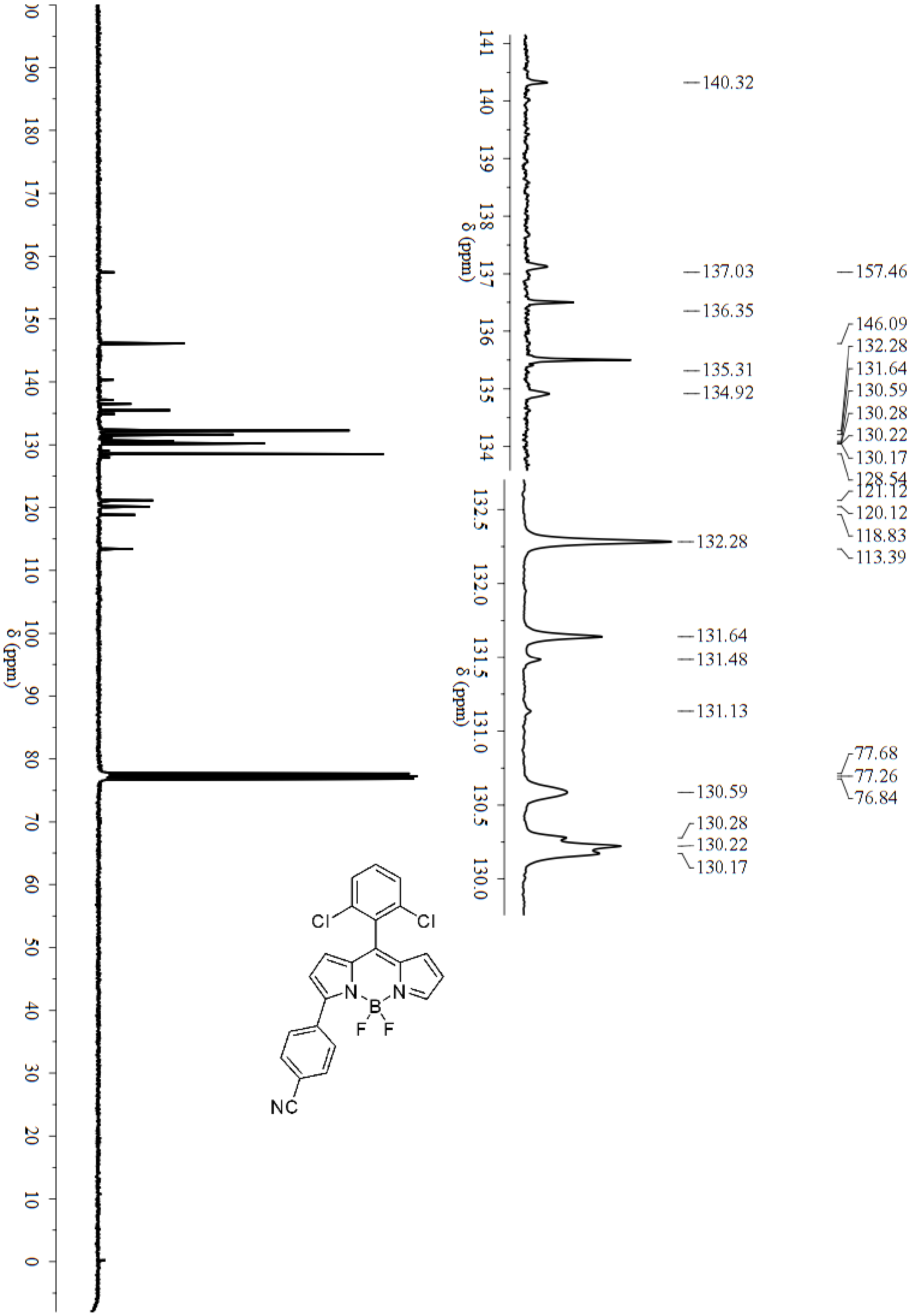
[1]H NMR spectrum of **3b** in $CDCl_3$



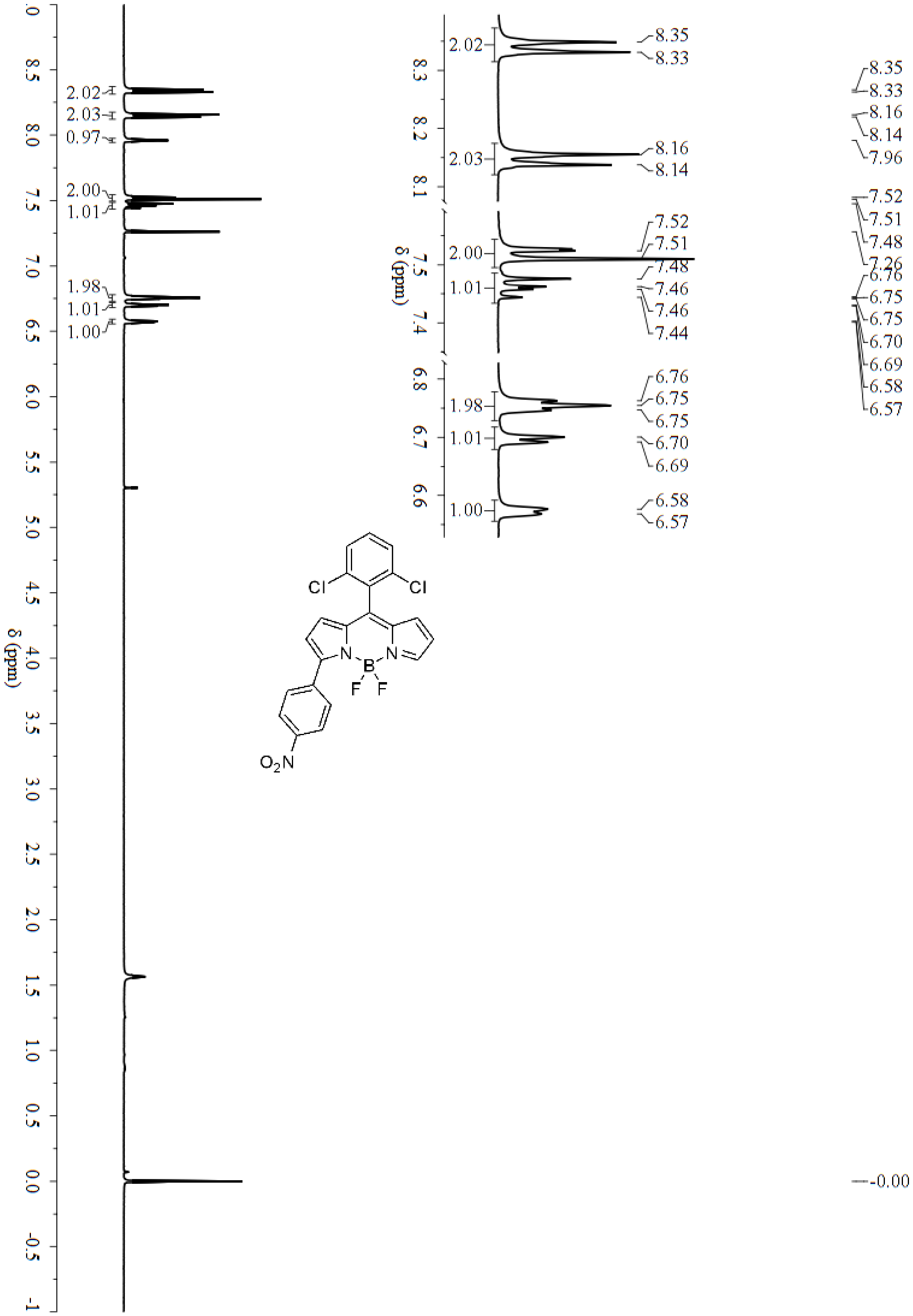
^{13}C NMR spectrum of **3b** in $CDCl_3$



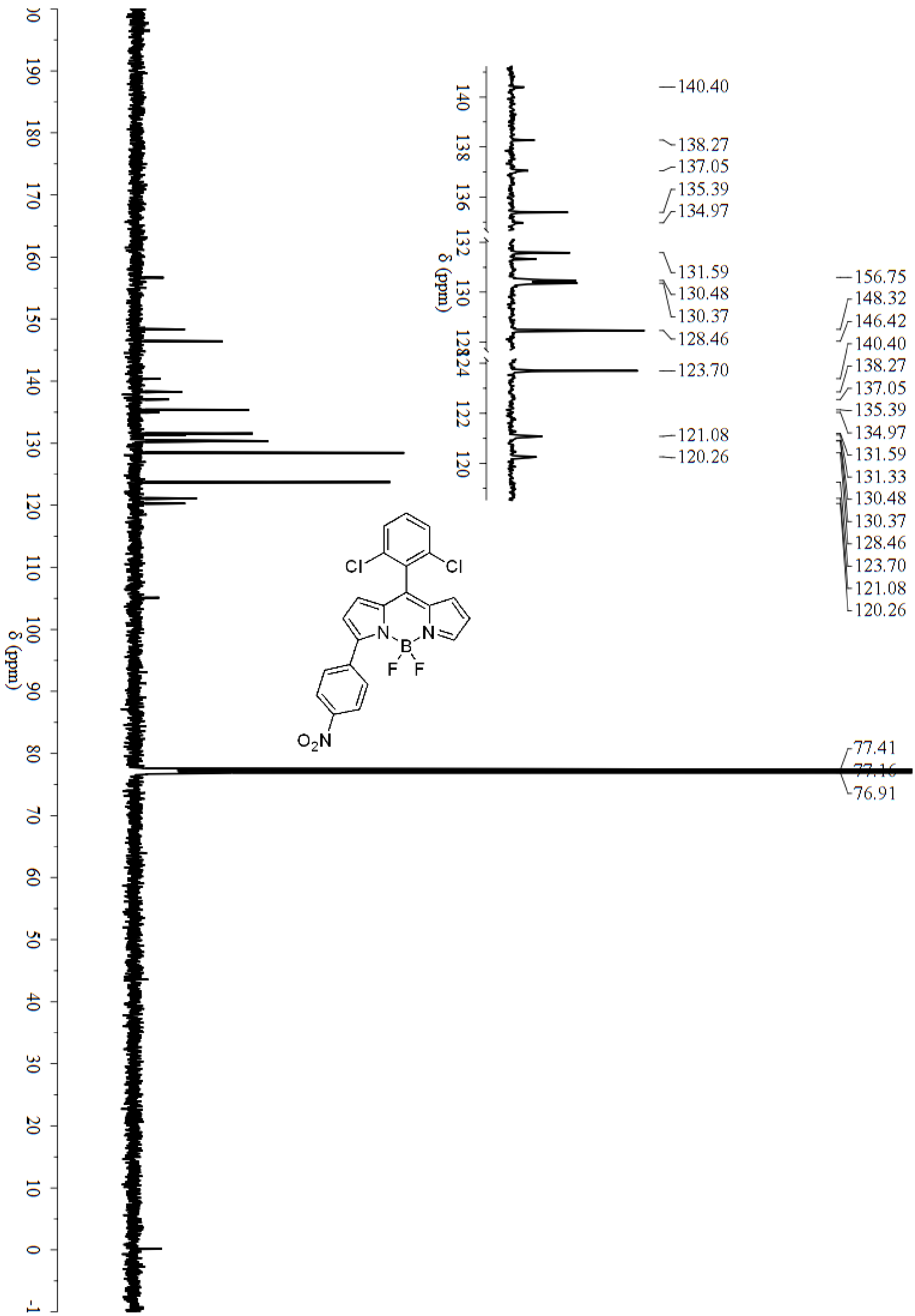
[1]H NMR spectrum of **3c** in $CDCl_3$



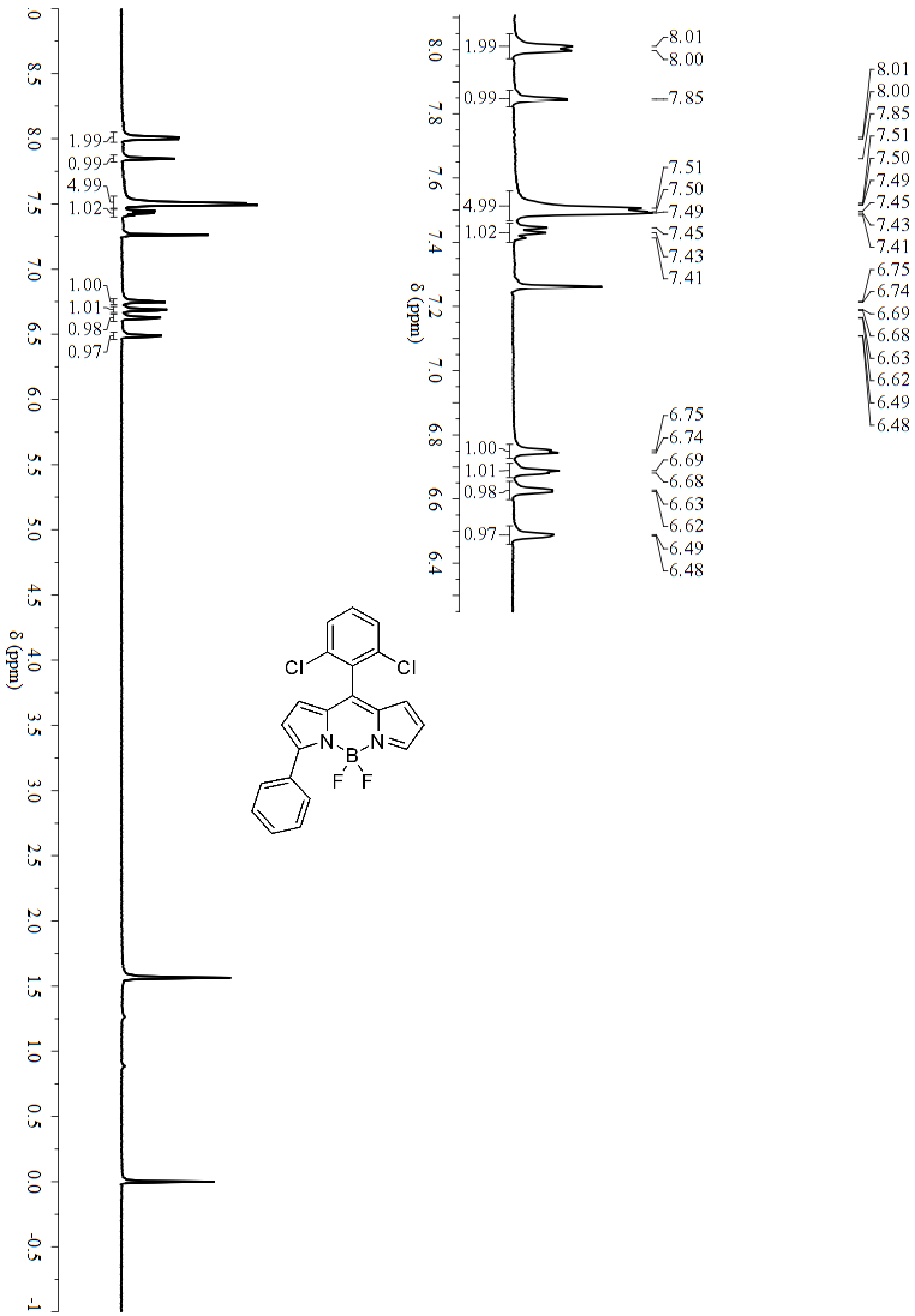
^{13}C NMR spectrum of **3c** in $CDCl_3$



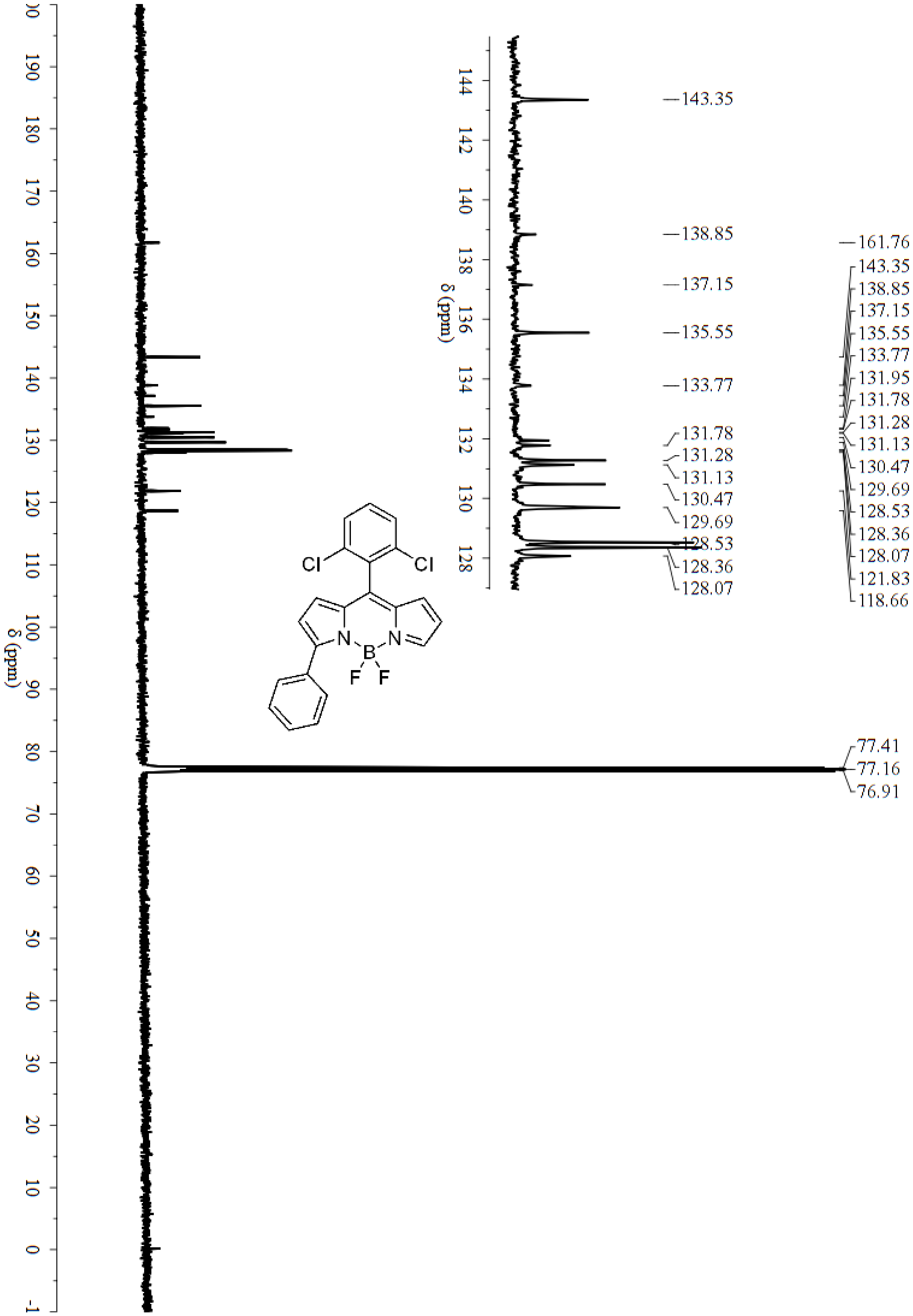
^{1}H NMR spectrum of **3d** in $CDCl_3$



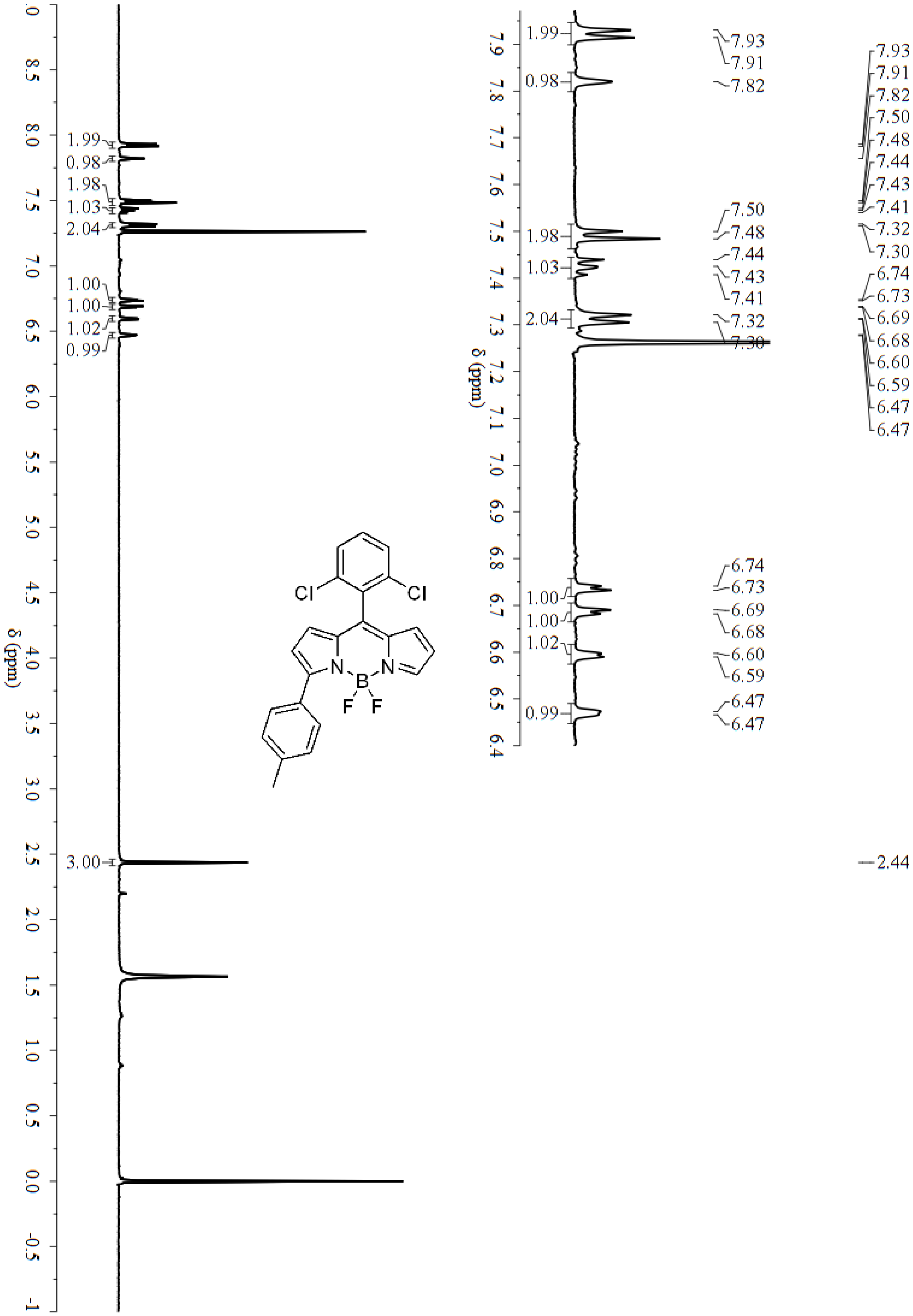
[13]C NMR spectrum of **3d** in $CDCl_3$



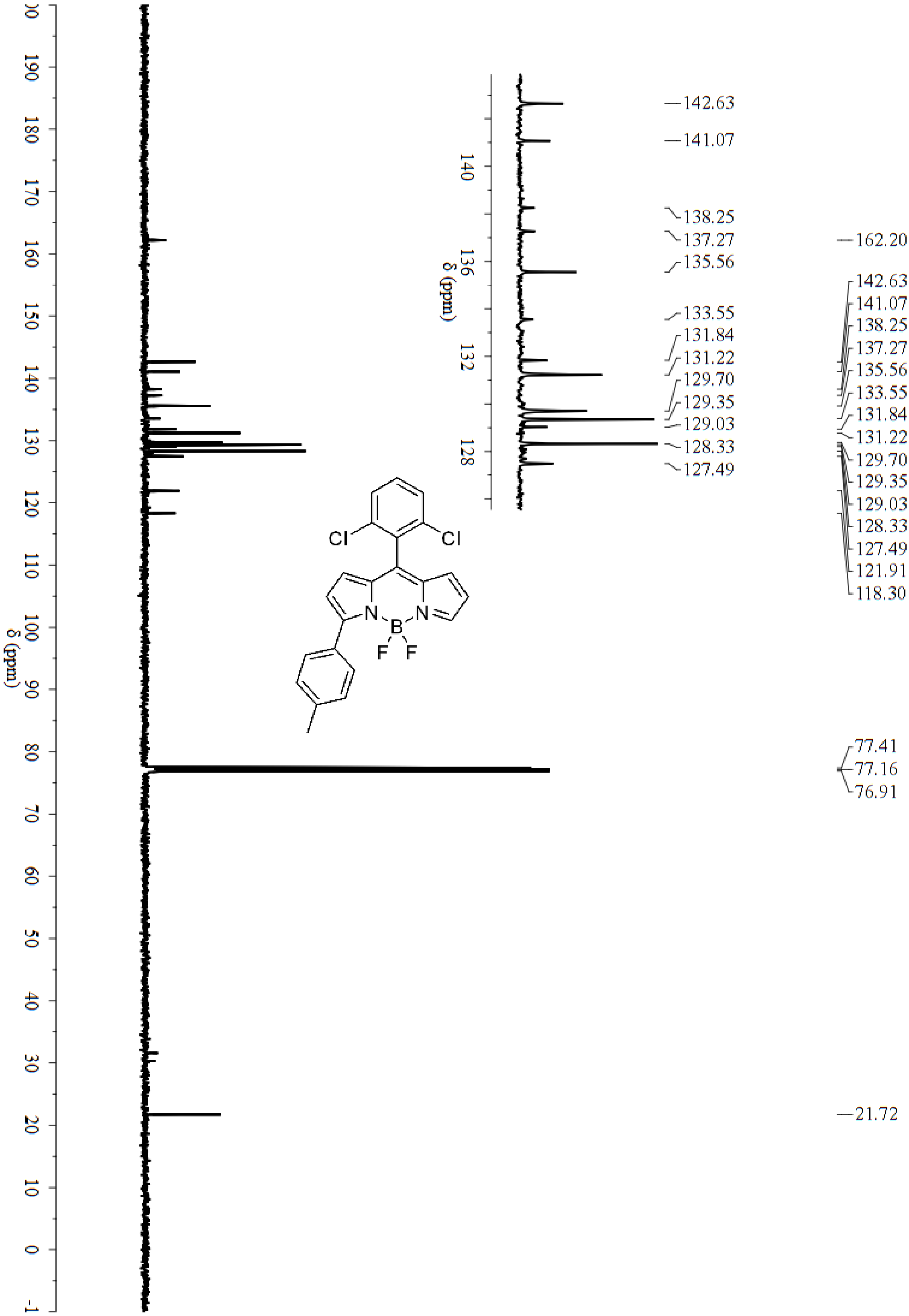
[1]H NMR spectrum of **3e** in $CDCl_3$



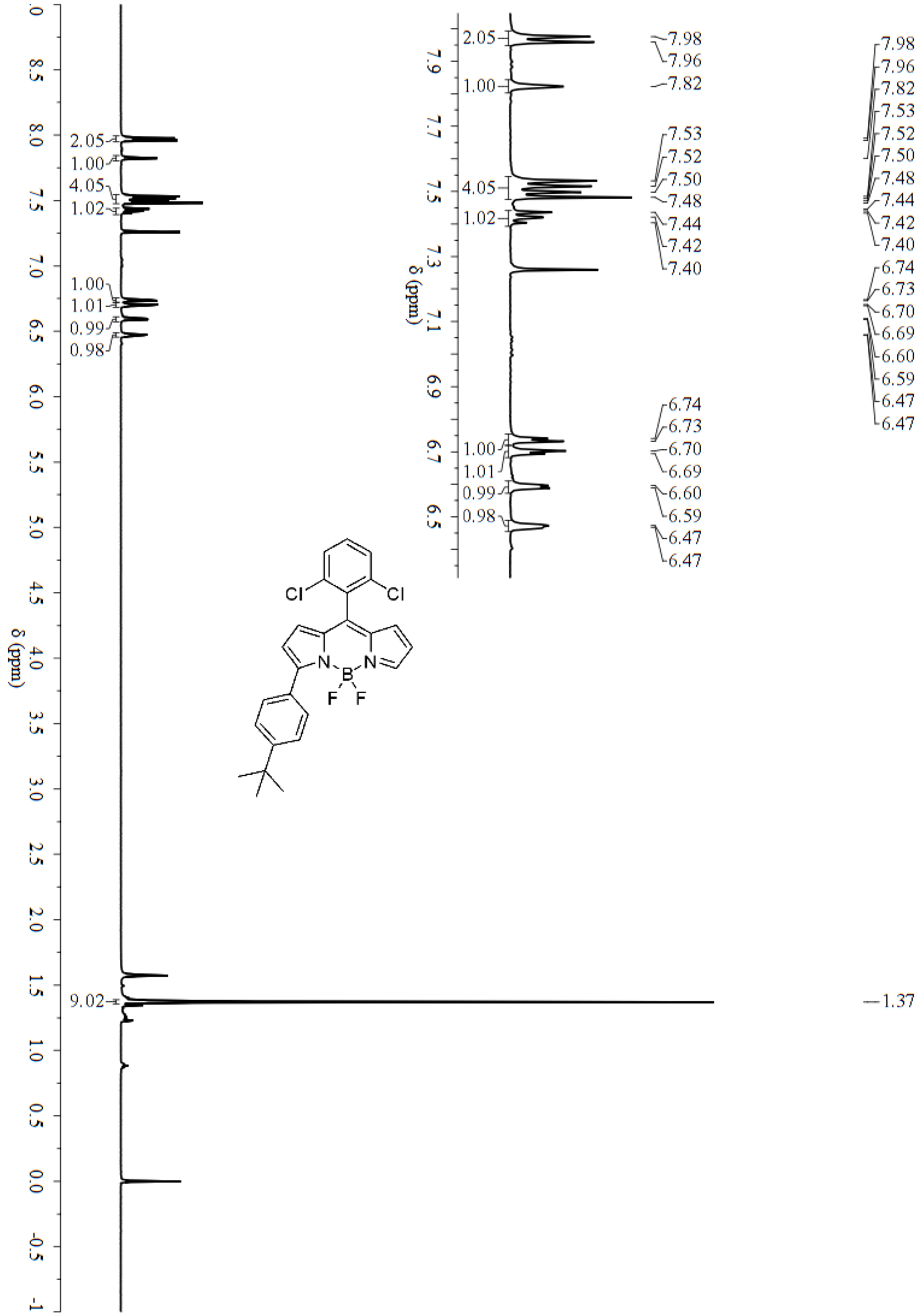
[13]C NMR spectrum of **3e** in $CDCl_3$



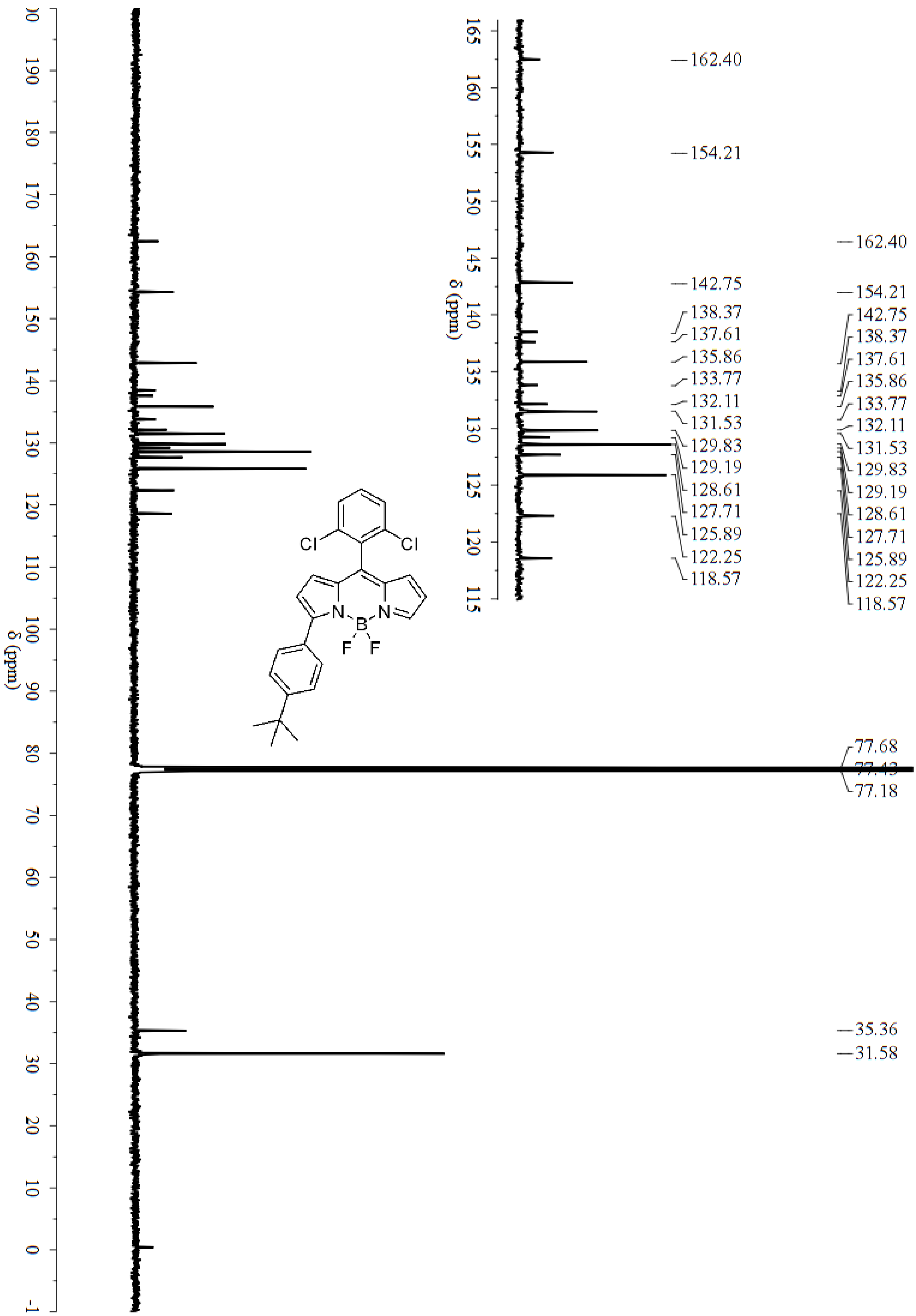
[1]H NMR spectrum of **3f** in $CDCl_3$



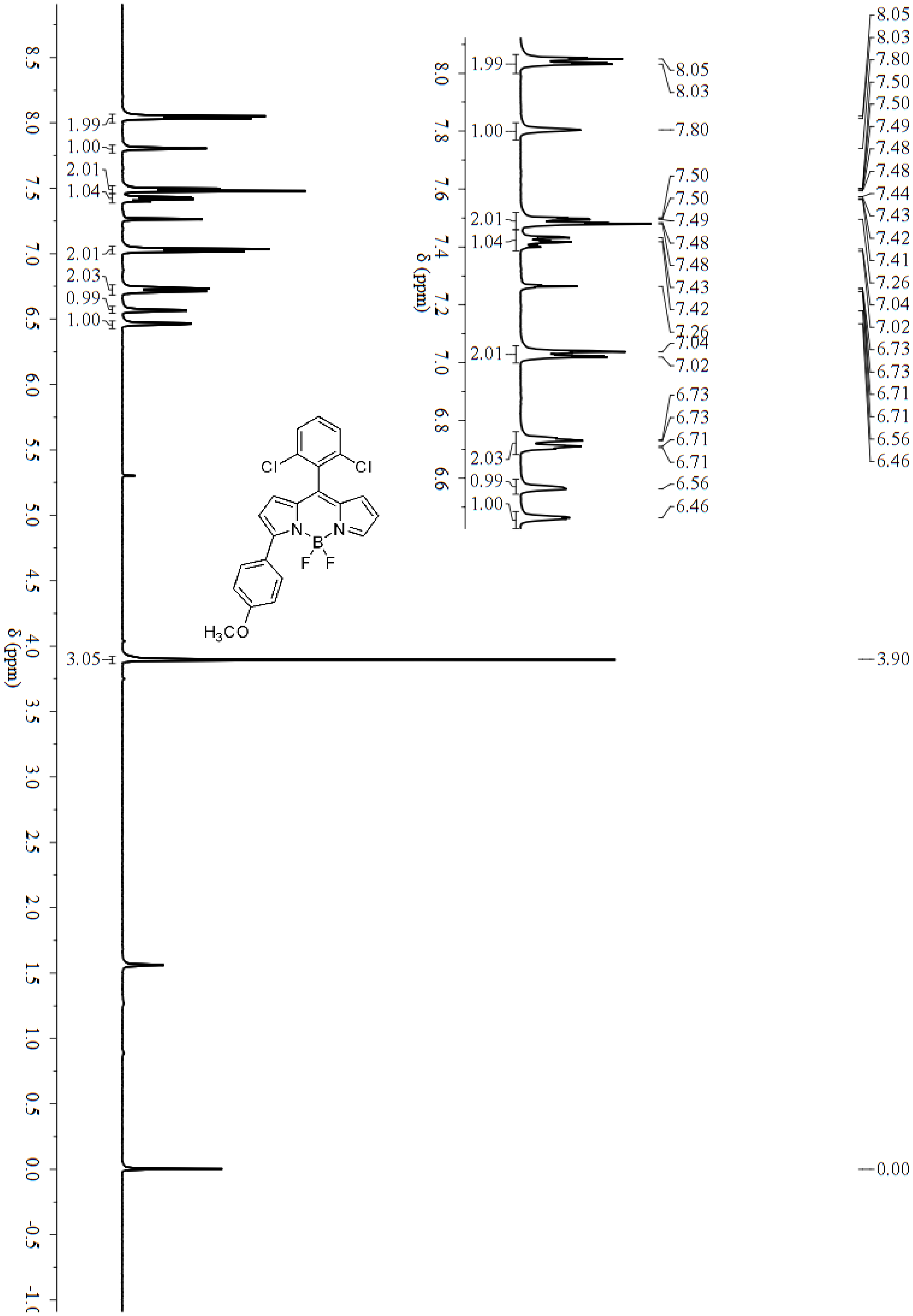
^{13}C NMR spectrum of **3f** in $CDCl_3$



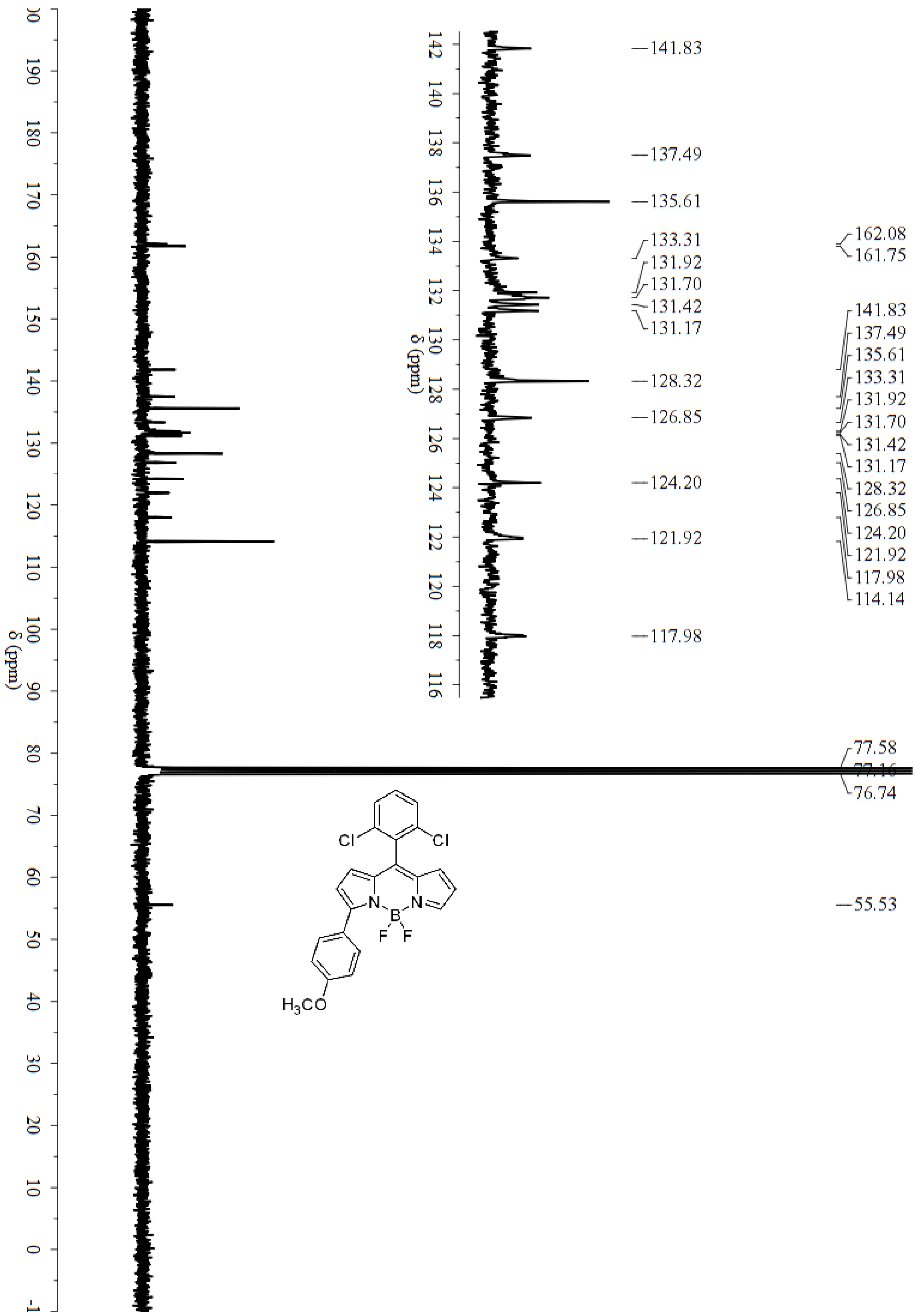
[1]H NMR spectrum of **3g** in $CDCl_3$



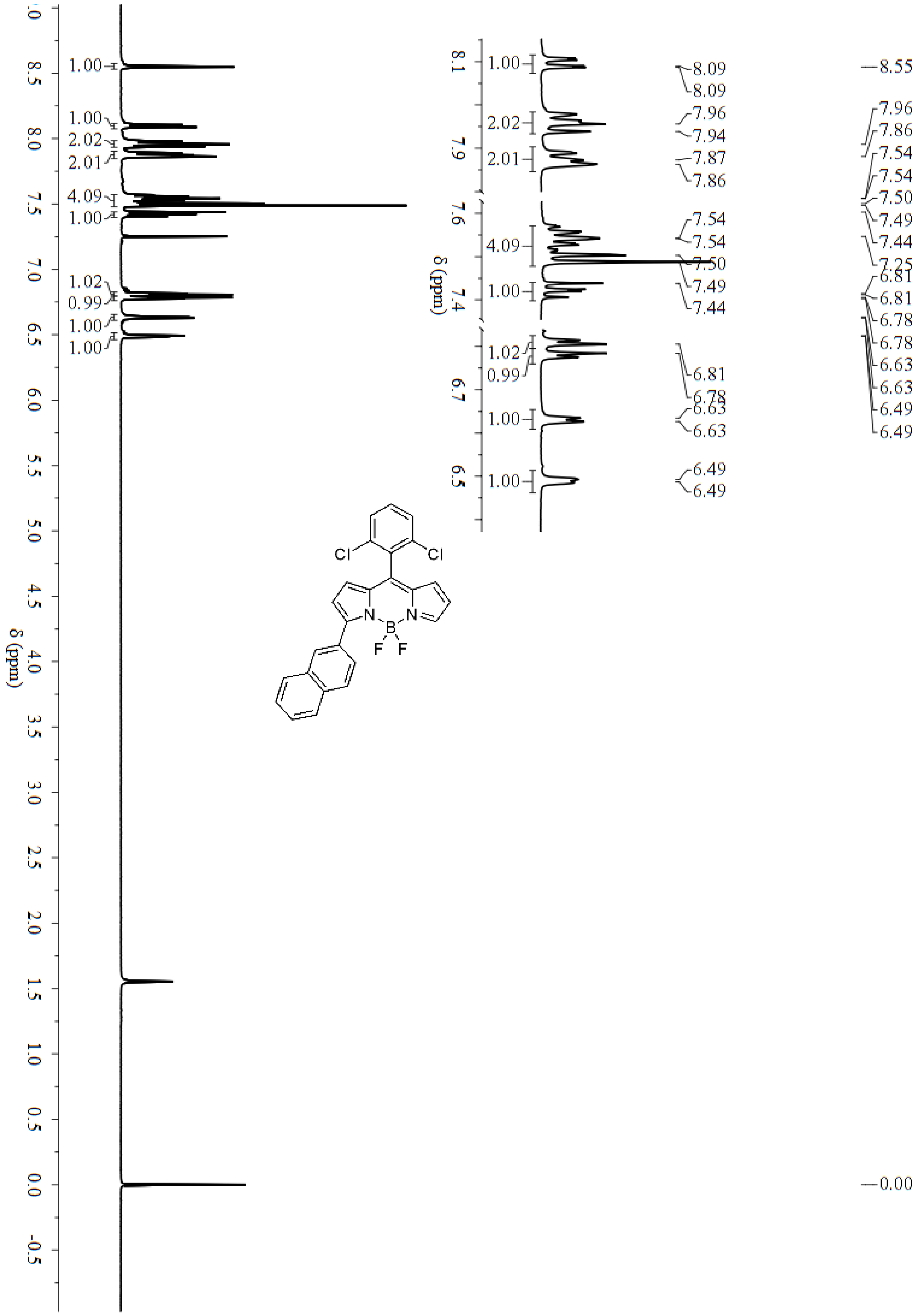
^{13}C NMR spectrum of **3g** in $CDCl_3$



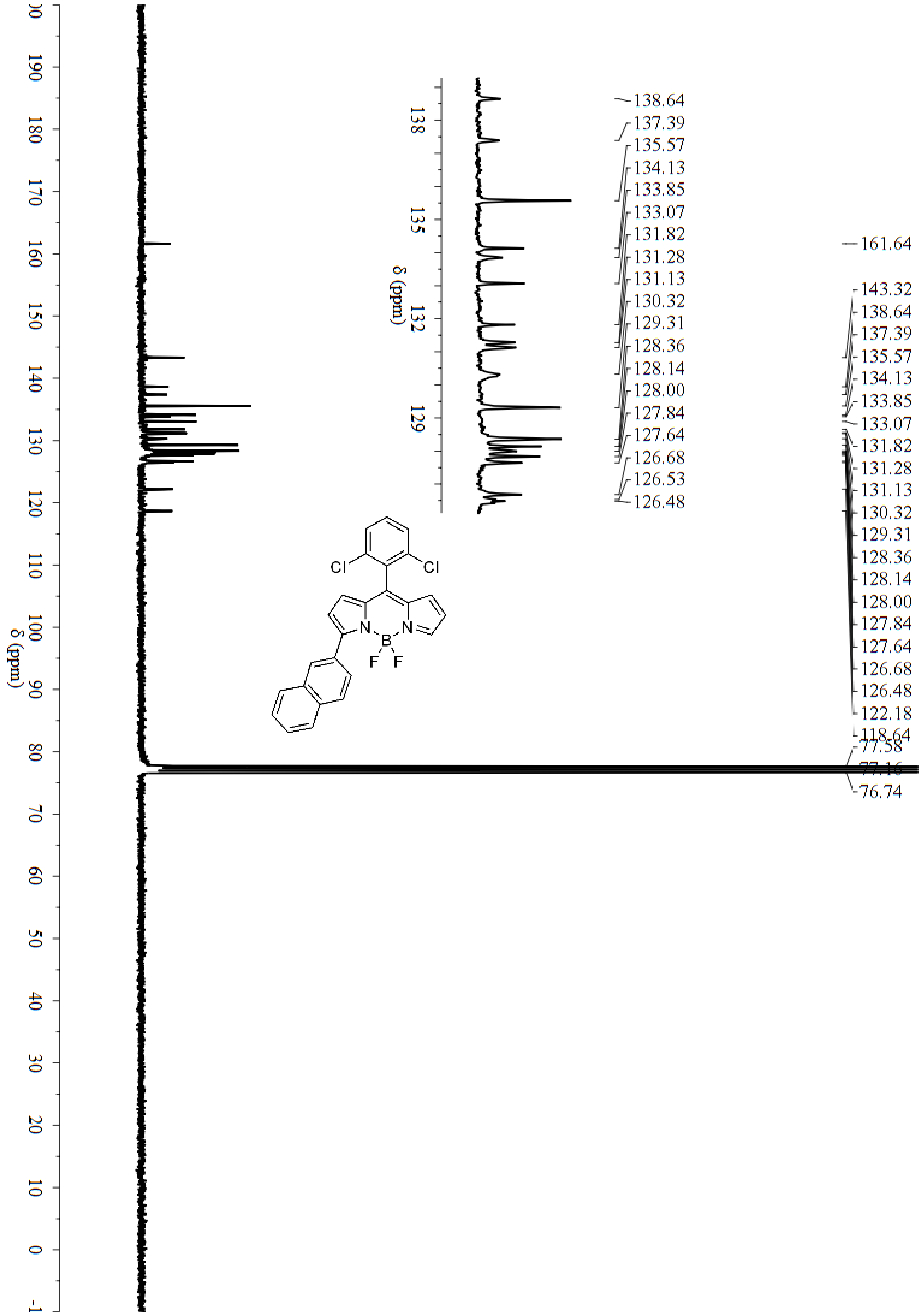
[1]H NMR spectrum of **3h** in $CDCl_3$



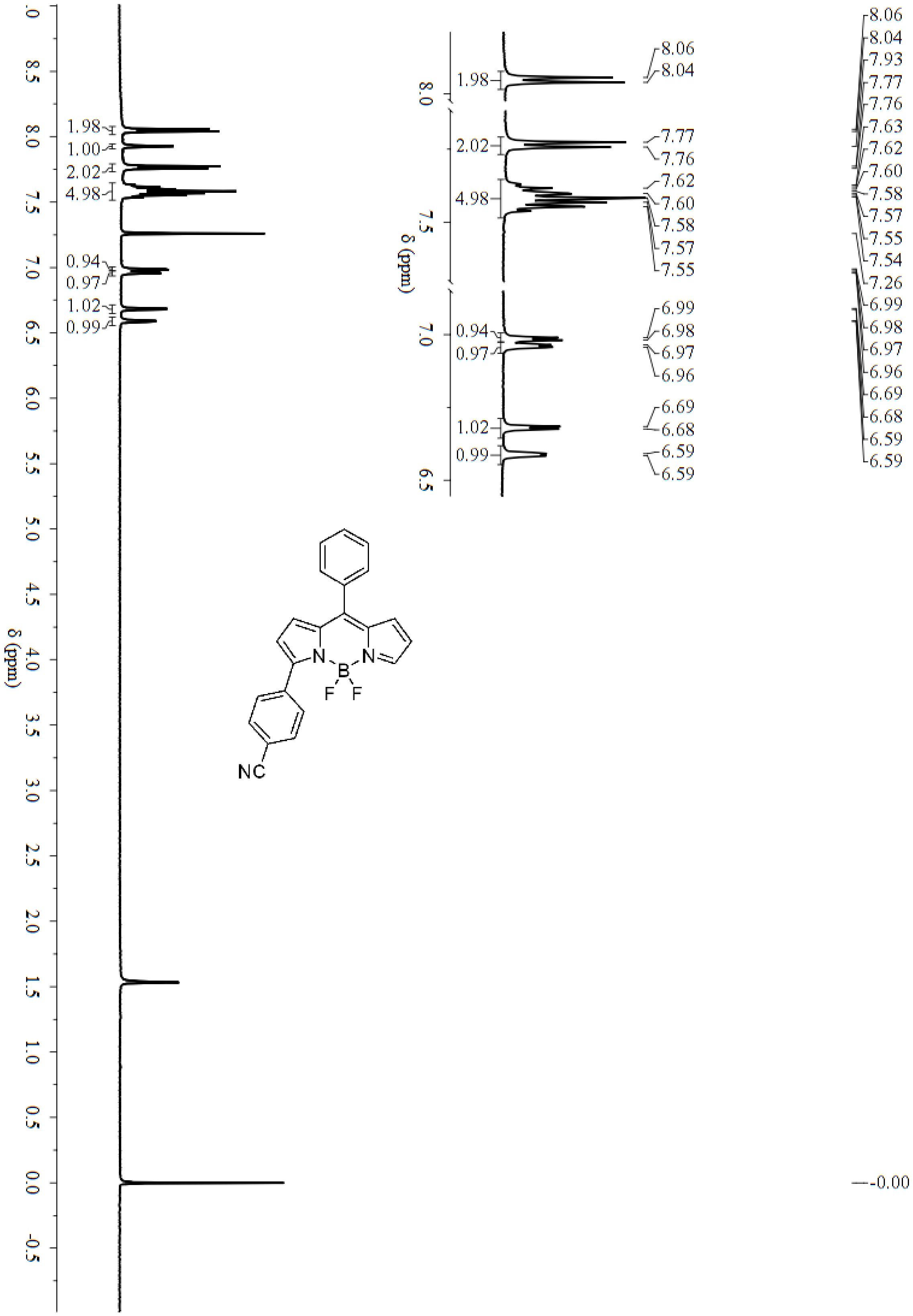
^{13}C NMR spectrum of **3h** in $CDCl_3$



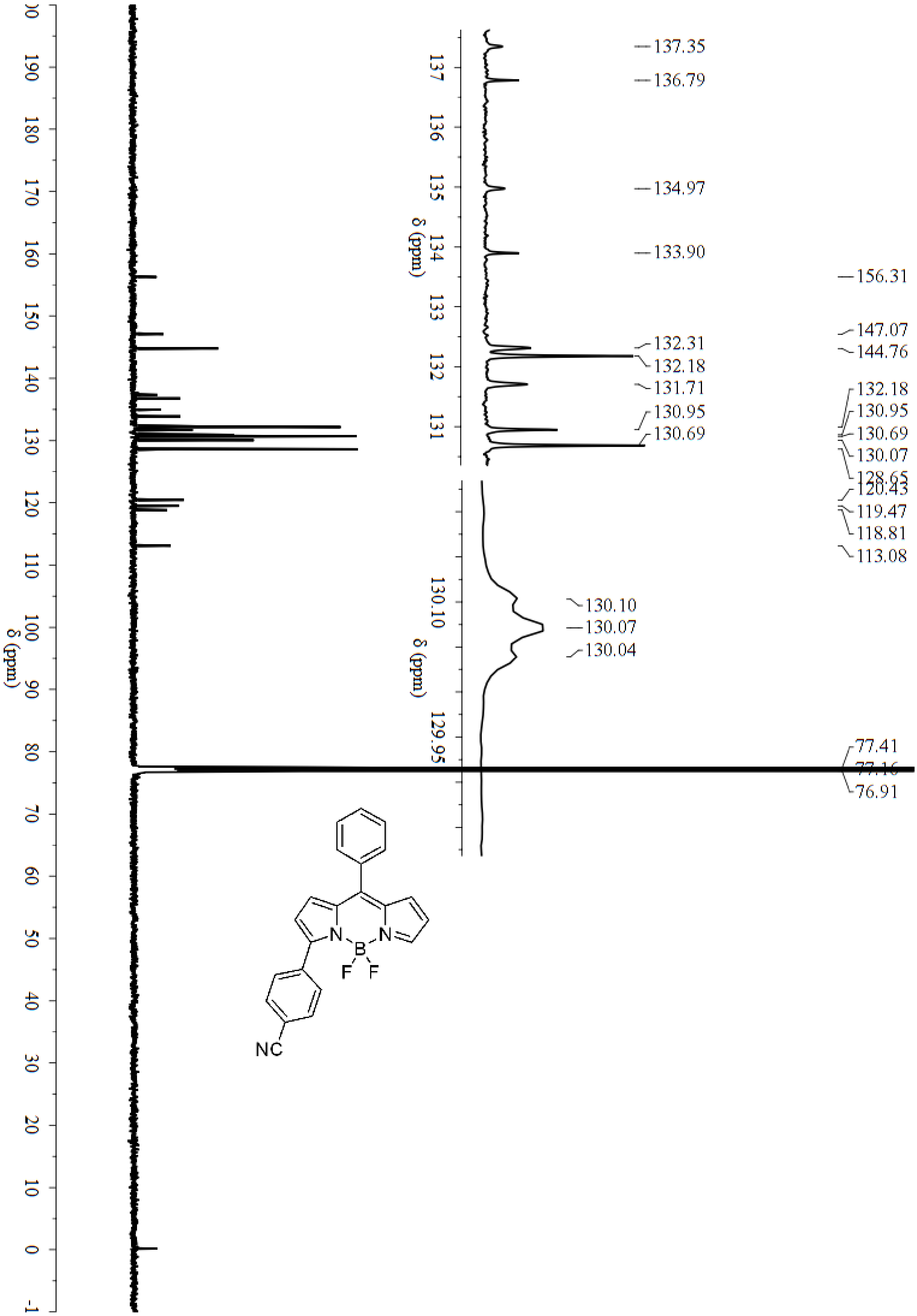
[1]H NMR spectrum of **3i** in $CDCl_3$



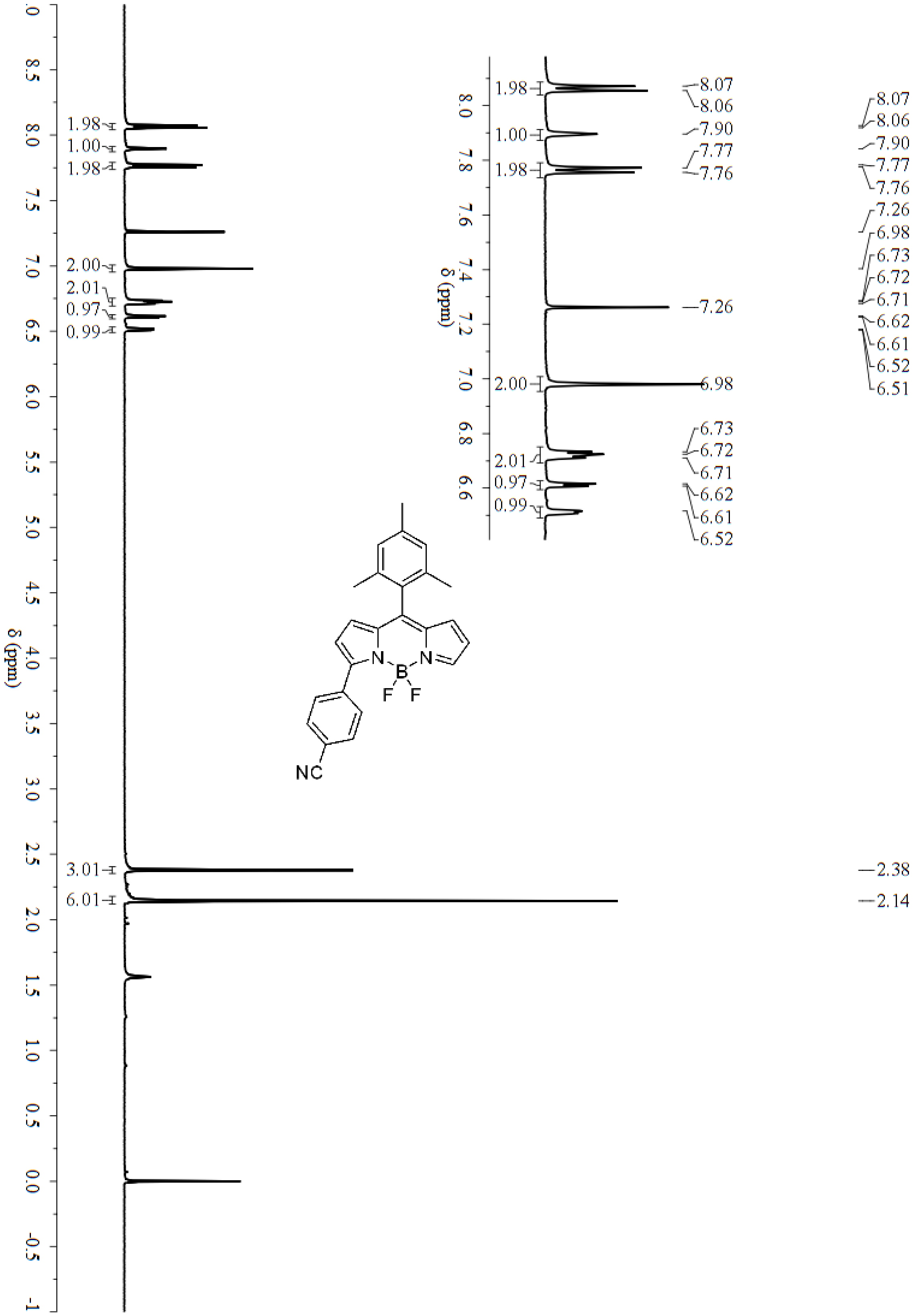
^{13}C NMR spectrum of **3i** in $CDCl_3$.



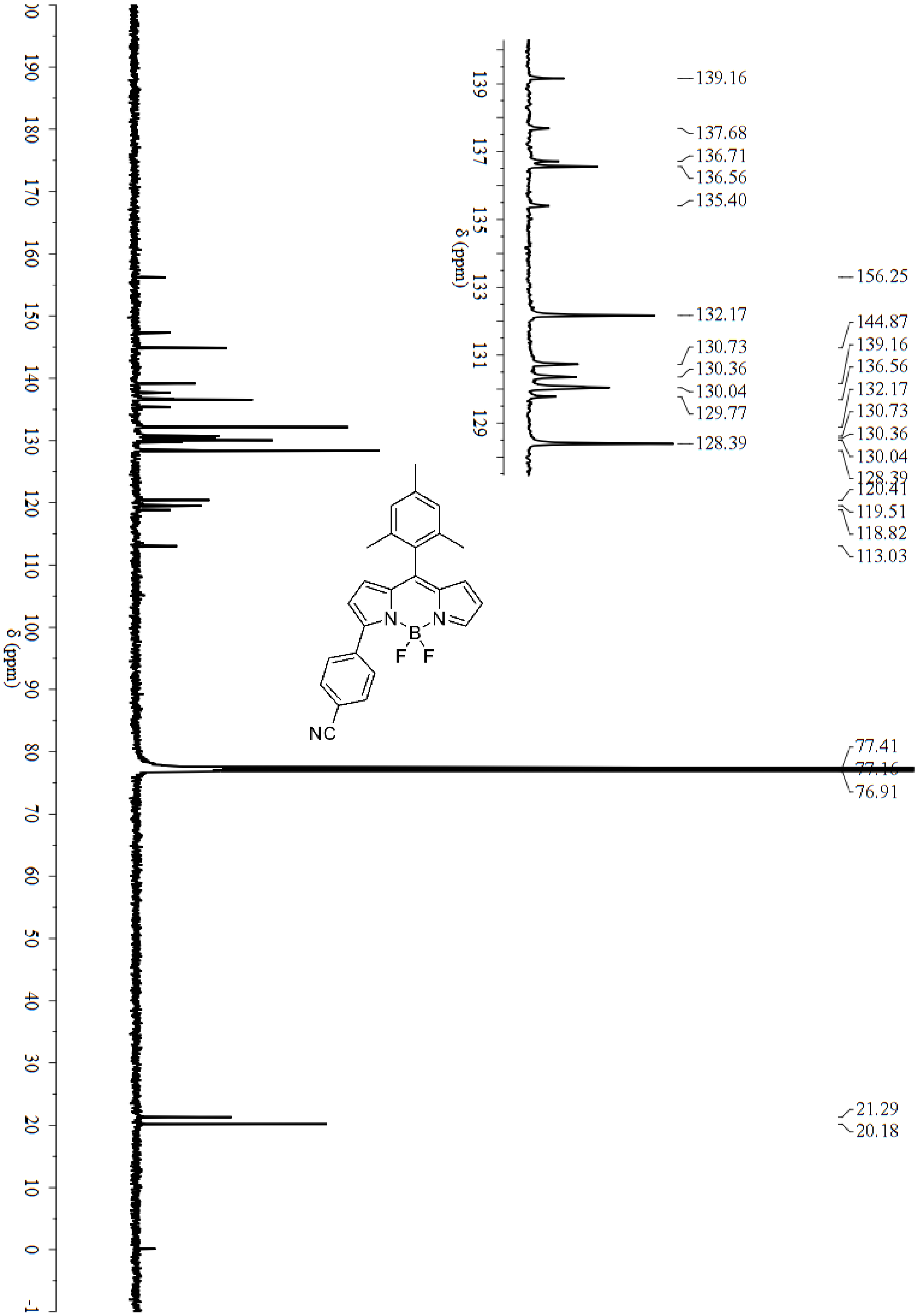
^{1}H NMR spectrum of **3j** in $CDCl_3$



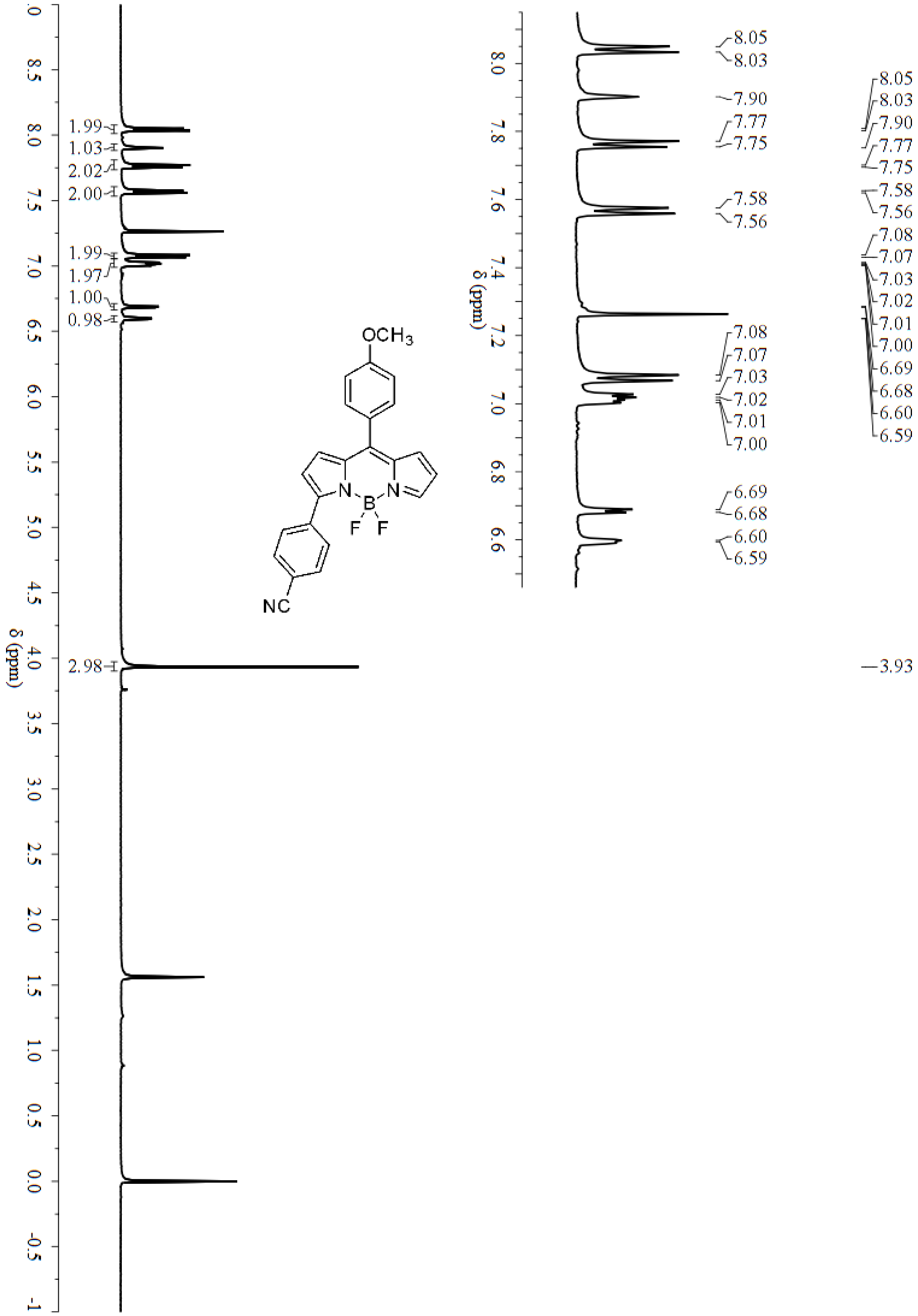
^{13}C NMR spectrum of **3j** in $CDCl_3$



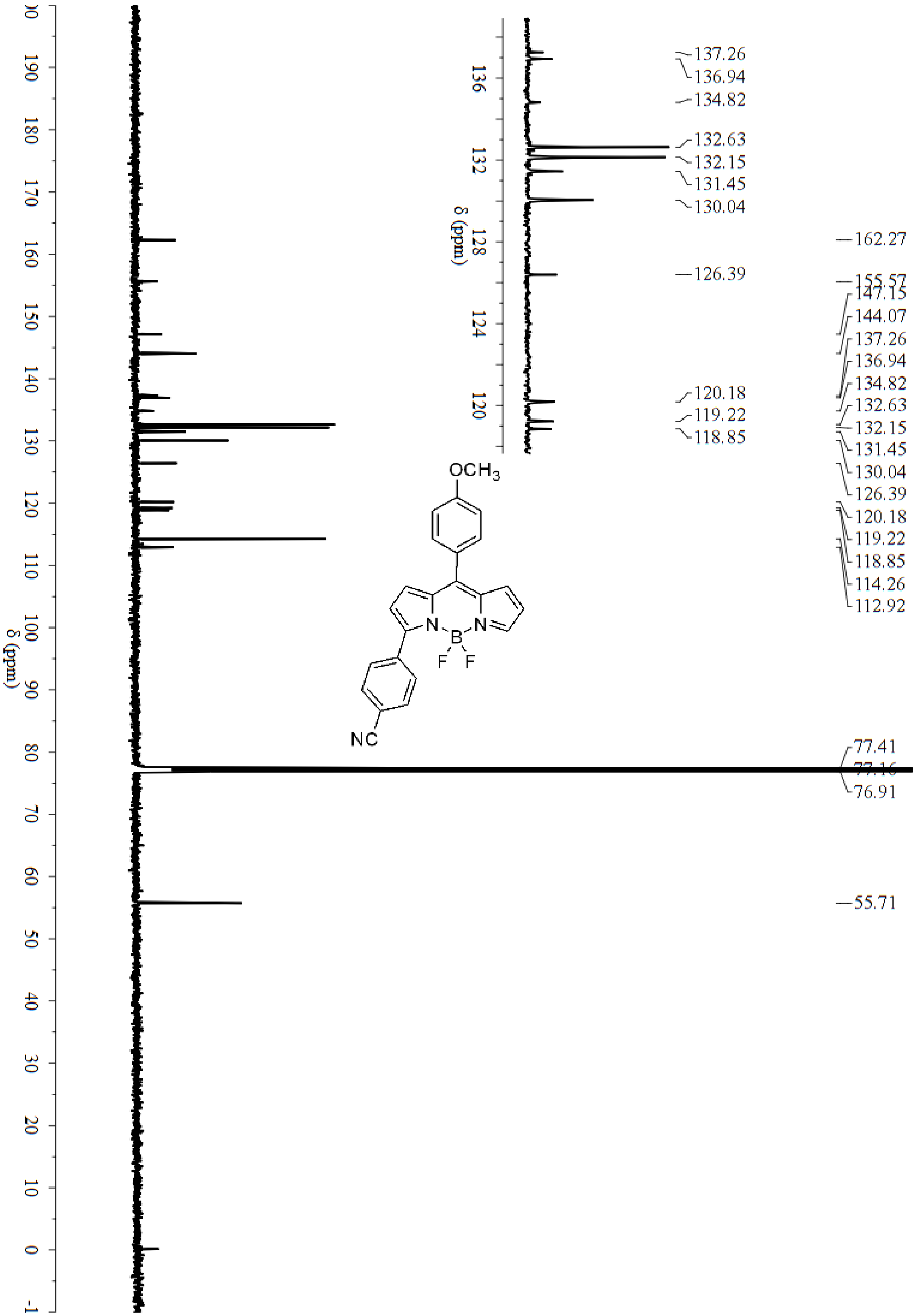
^{1}H NMR spectrum of **3k** in $CDCl_3$



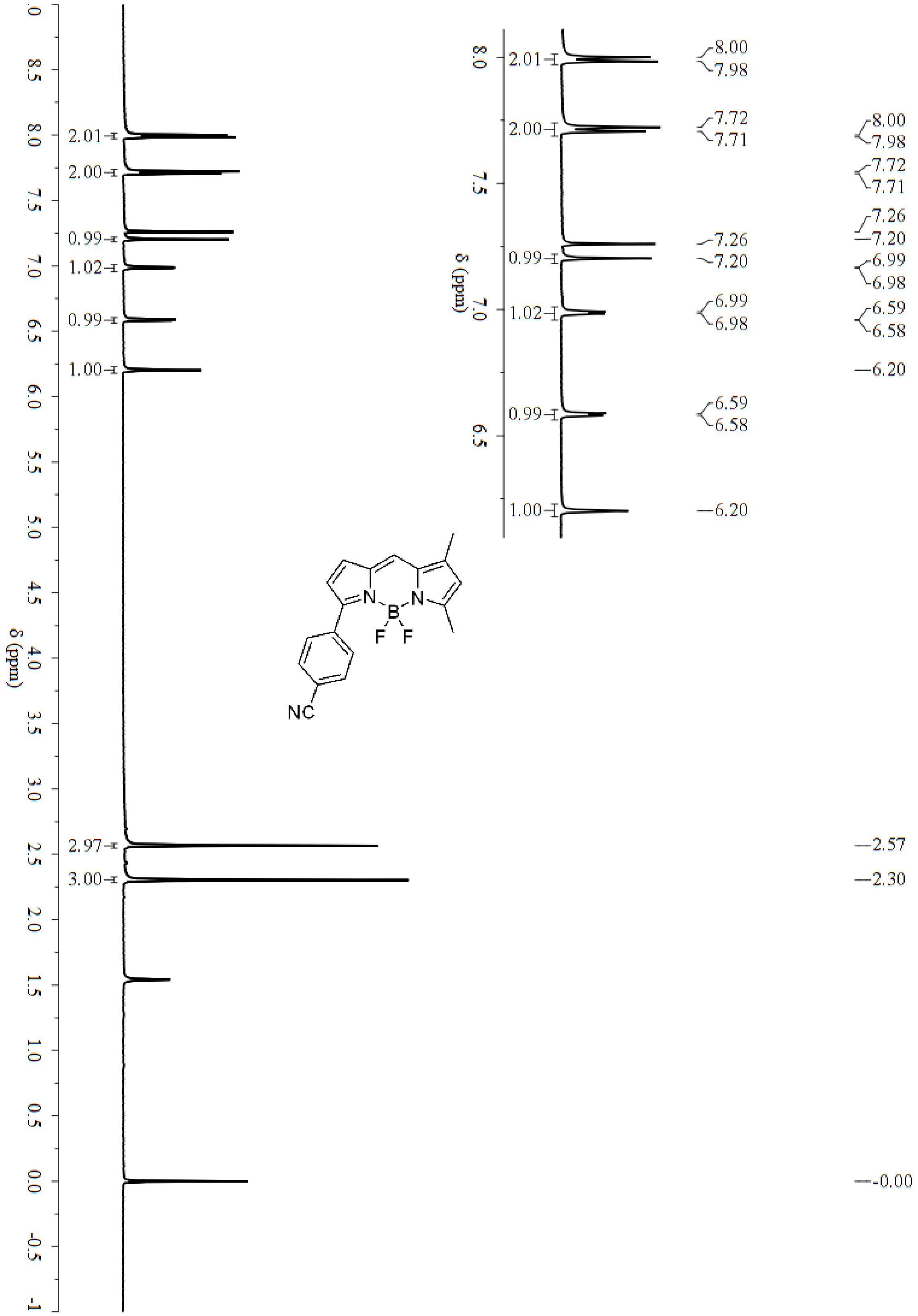
[13]C NMR spectrum of **3k** in $CDCl_3$



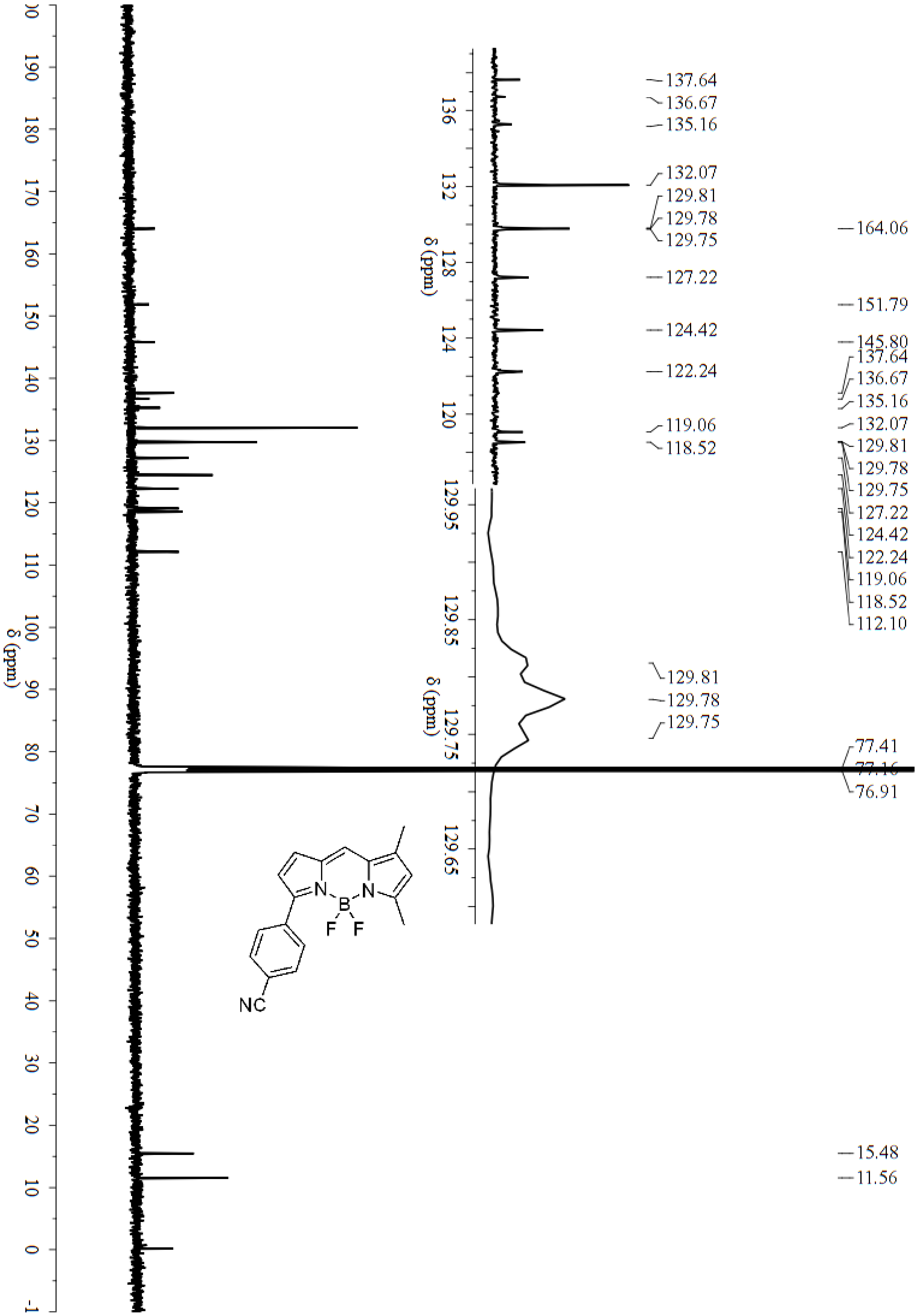
[1]H NMR spectrum of **3l** in $CDCl_3$



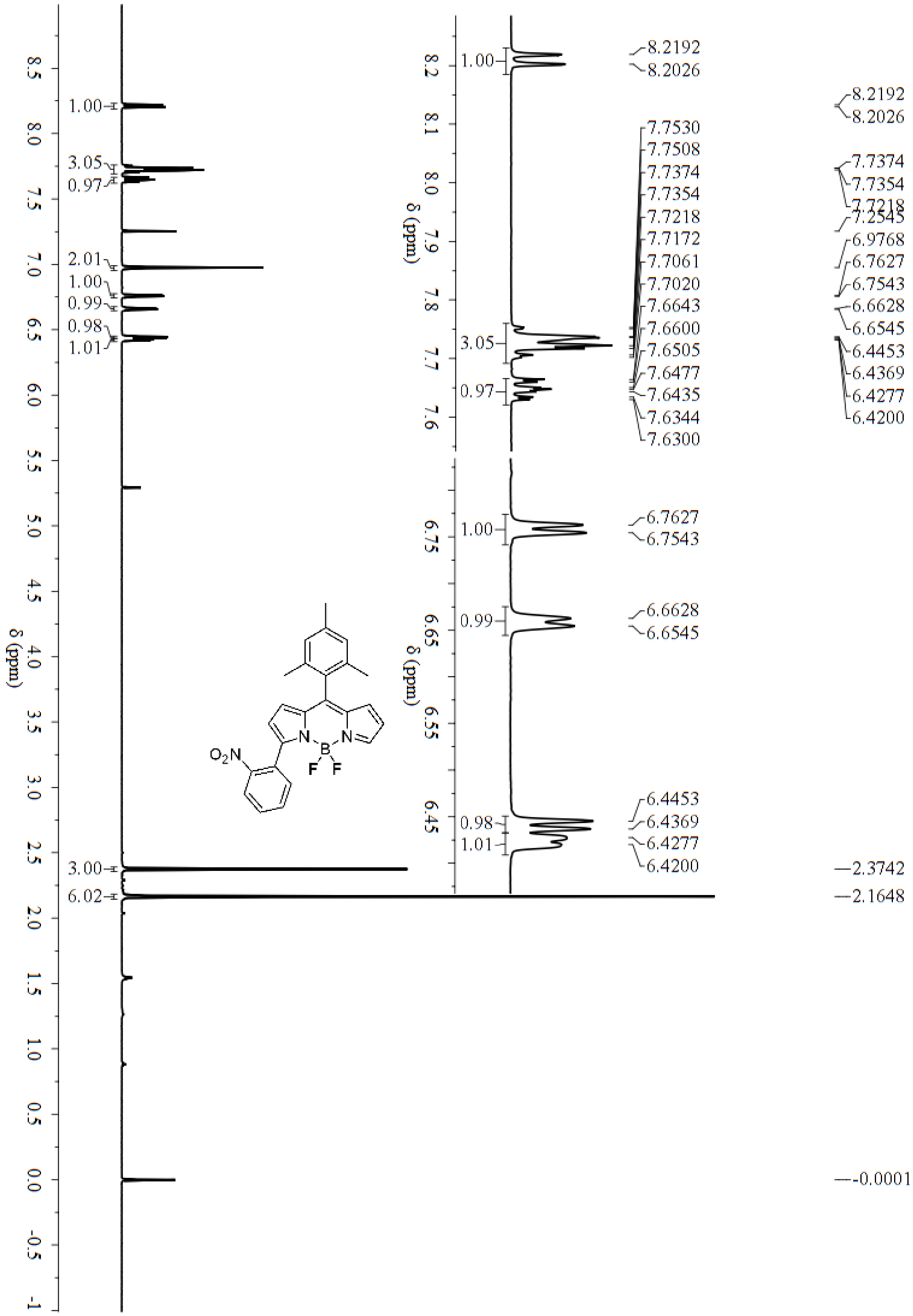
^{13}C NMR spectrum of **3l** in $CDCl_3$



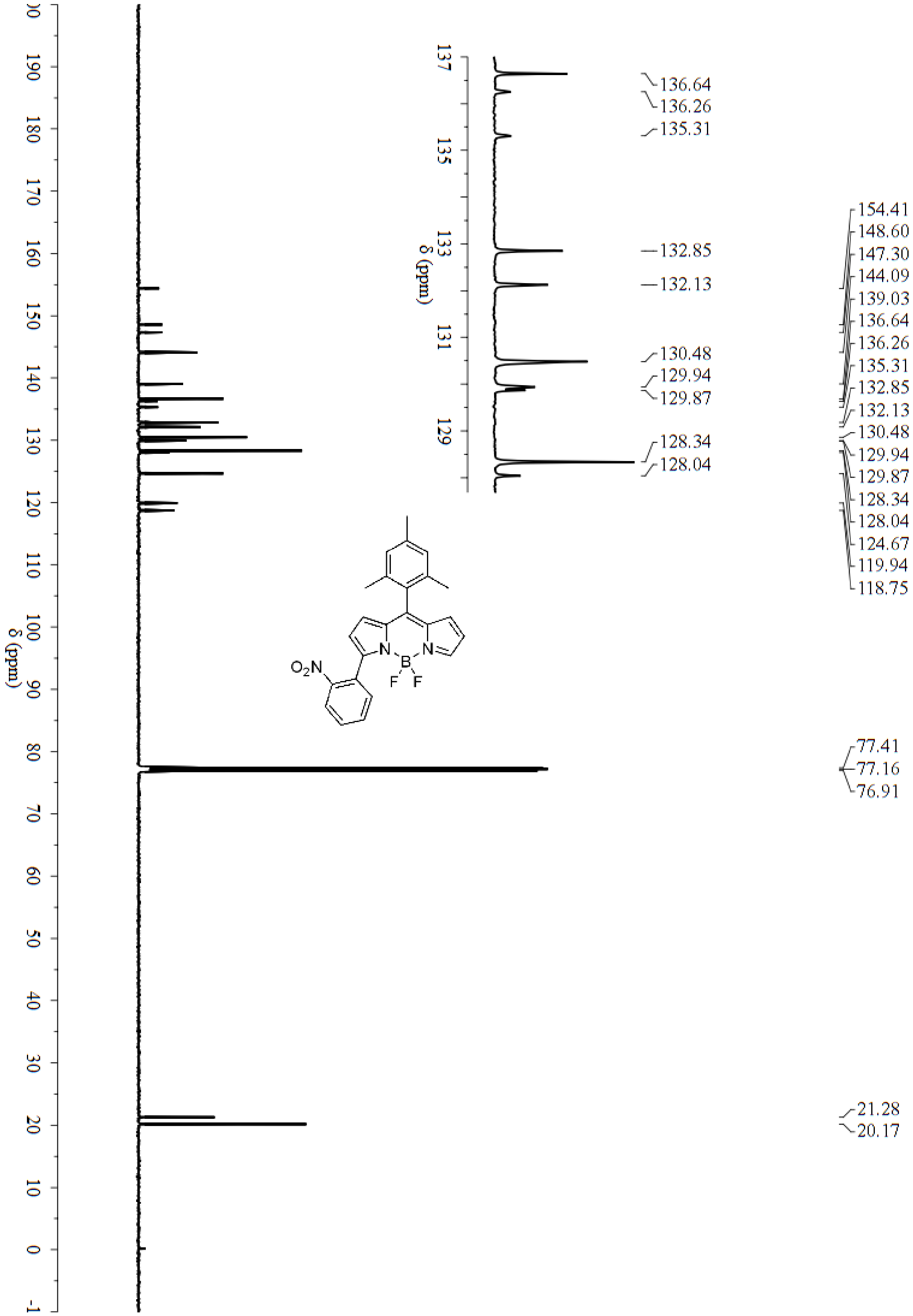
^{1}H NMR spectrum of **3m** in $CDCl_3$



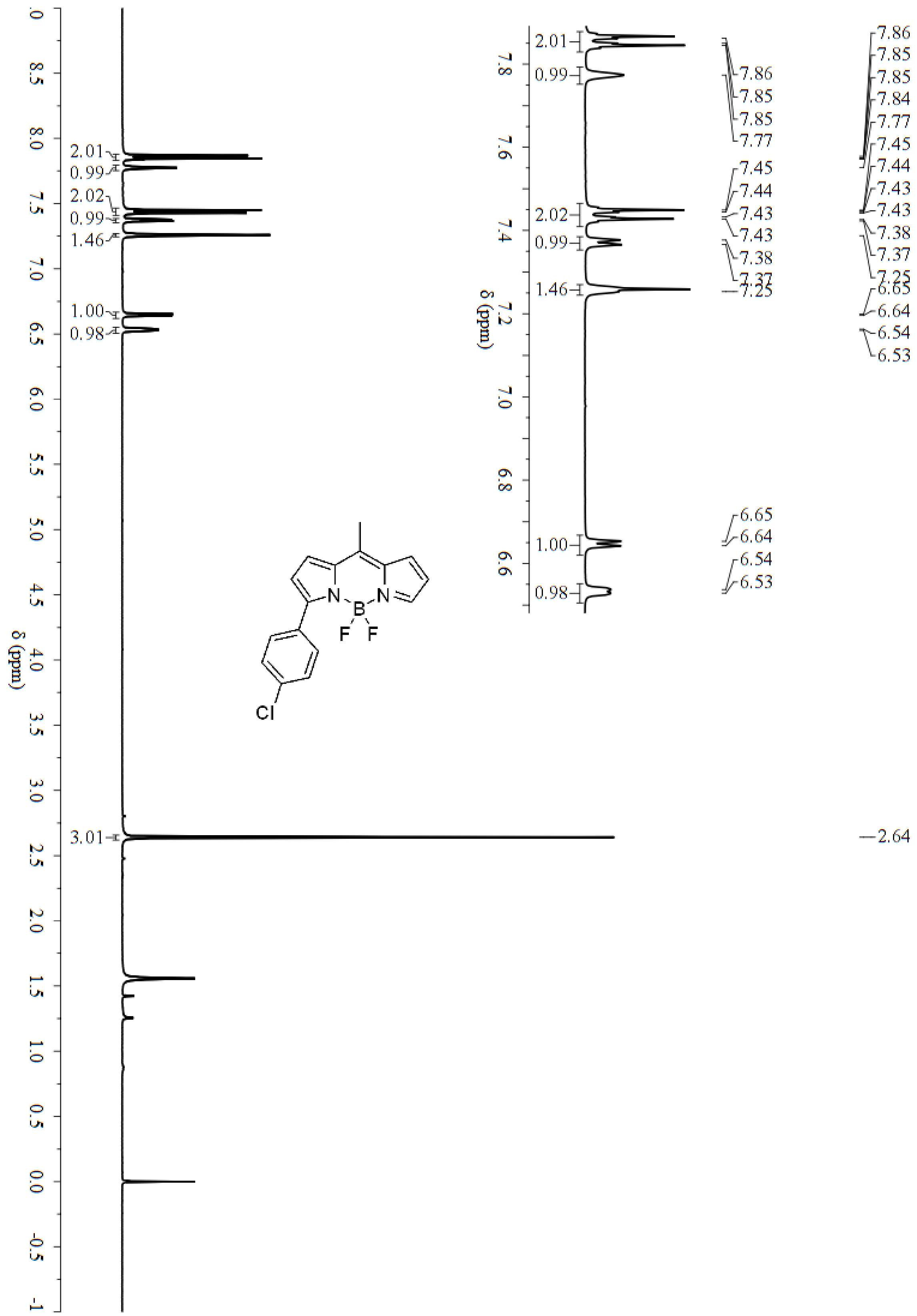
^{13}C NMR spectrum of **3m** in $CDCl_3$



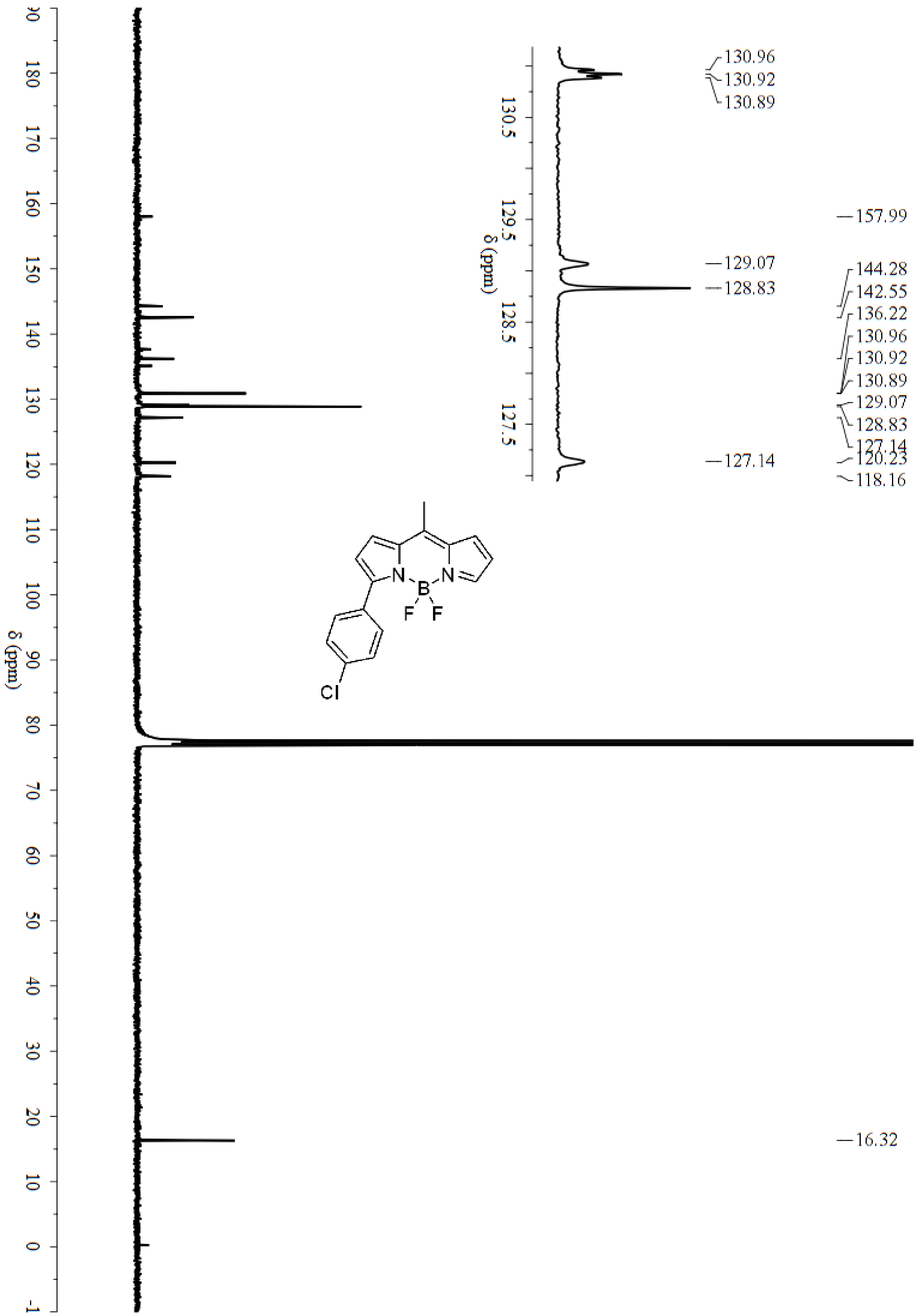
[1]H NMR spectrum of **3n** in $CDCl_3$



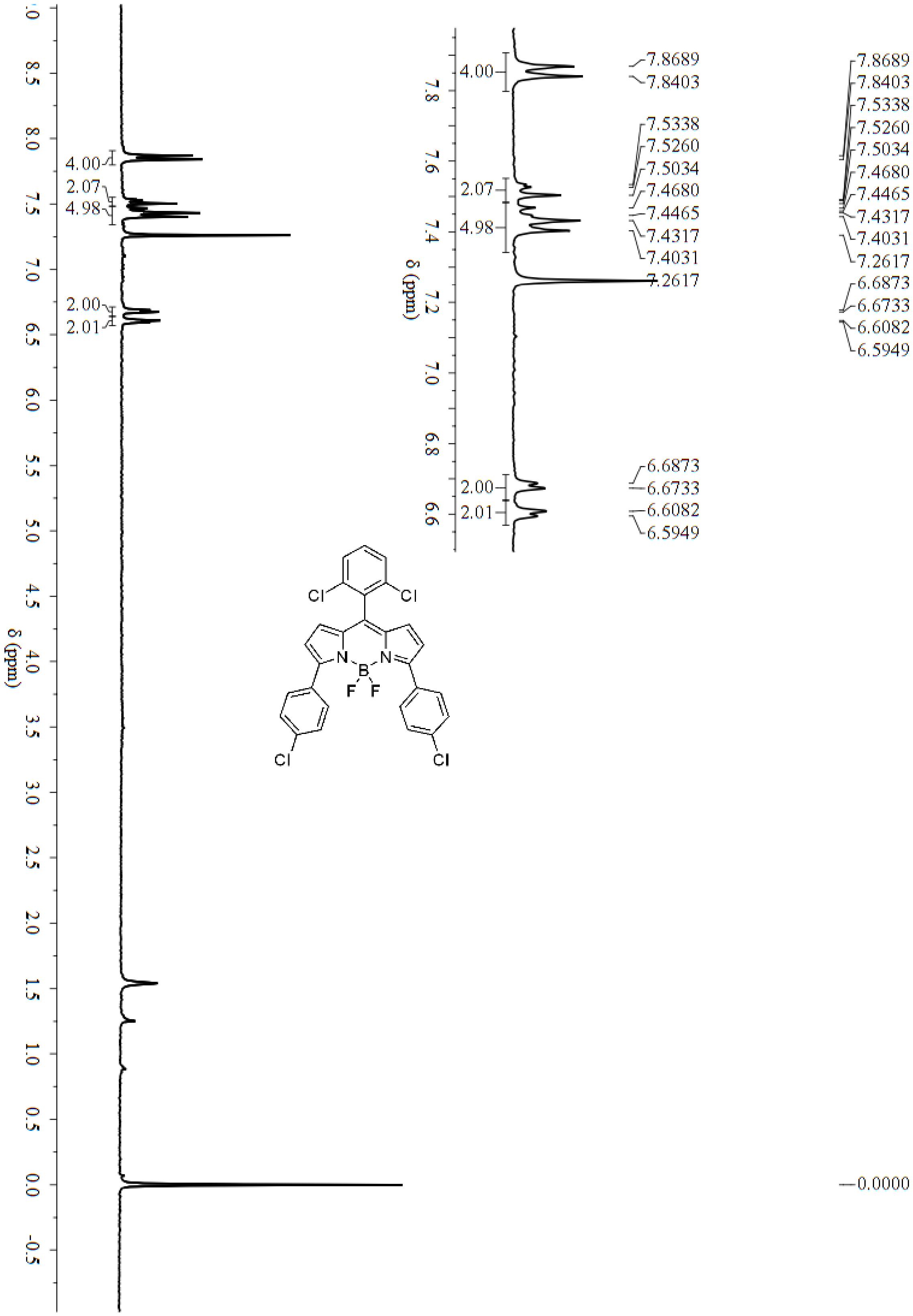
^{13}C NMR spectrum of **3n** in $CDCl_3$



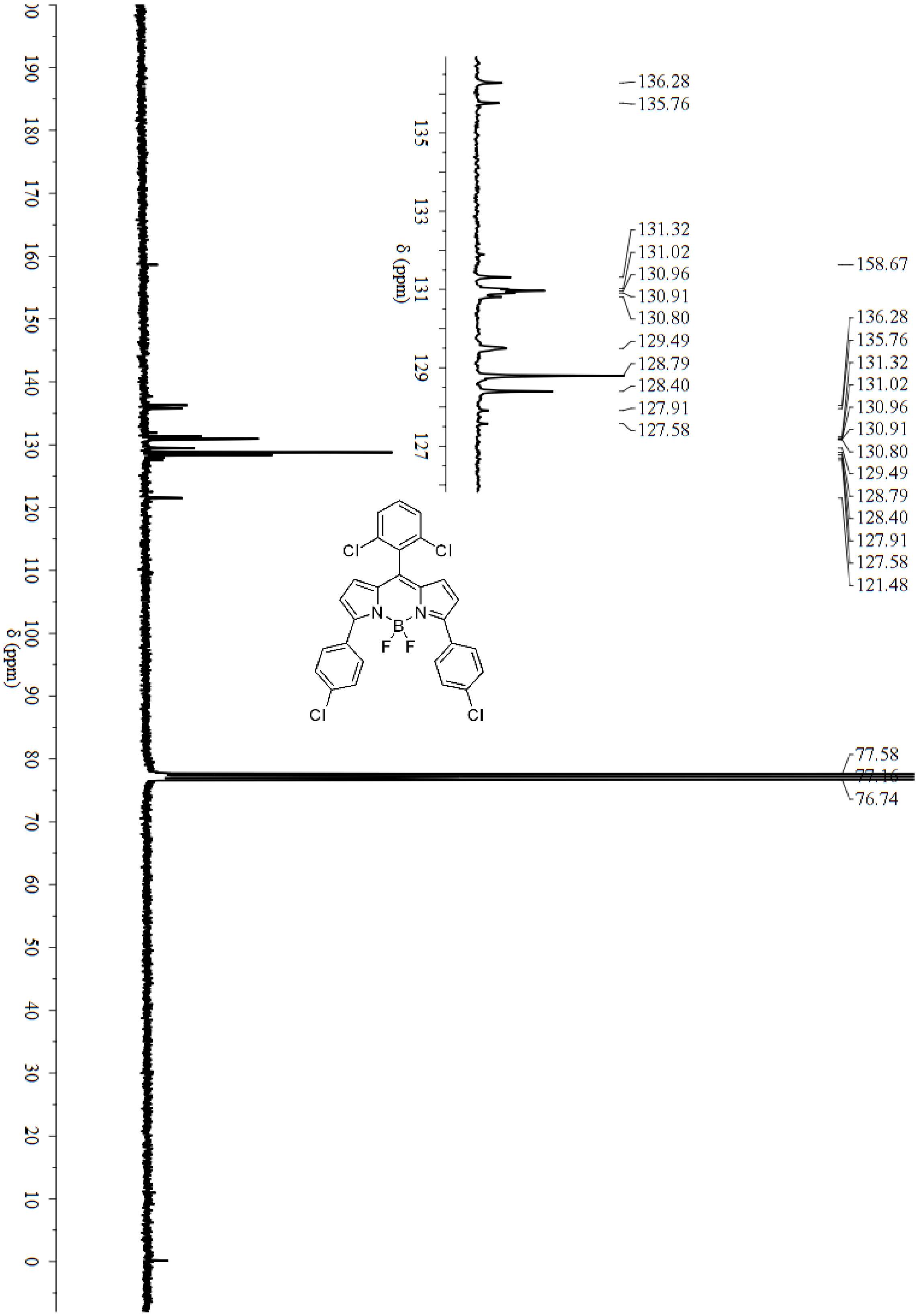
[1]H NMR spectrum of **3o** in $CDCl_3$



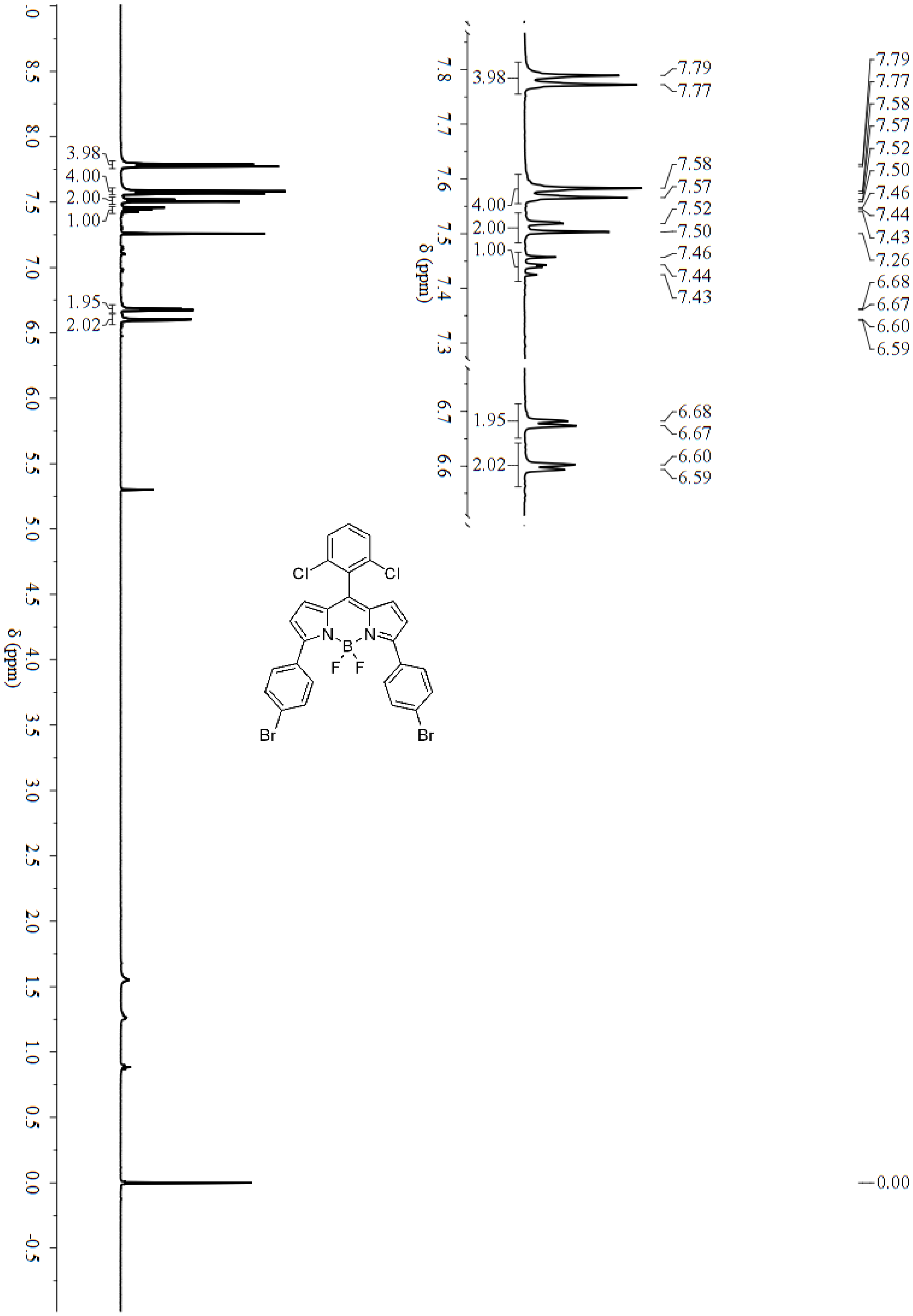
[13]C NMR spectrum of **3o** in $CDCl_3$



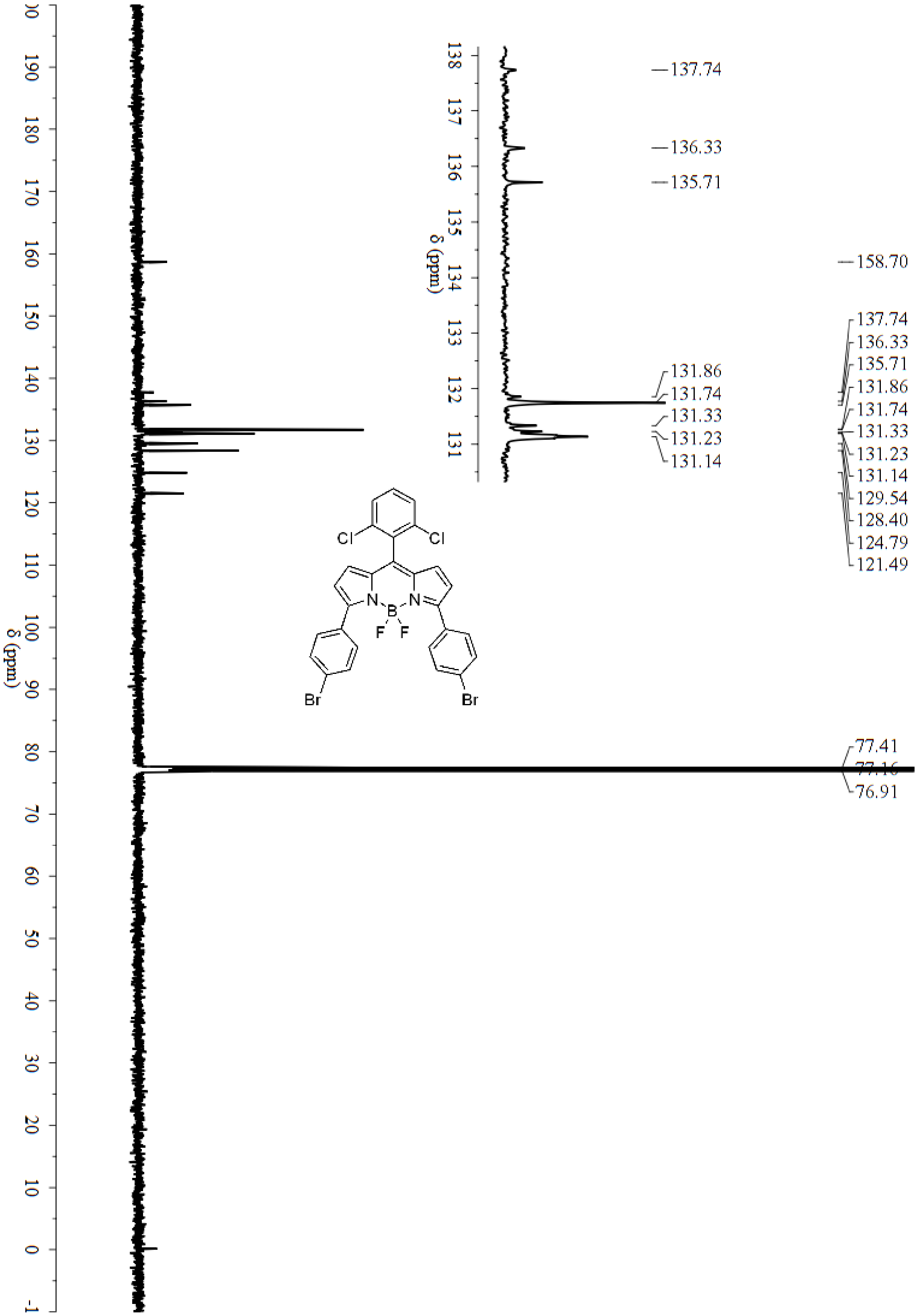
¹H NMR spectrum of **4a** in $CDCl_3$



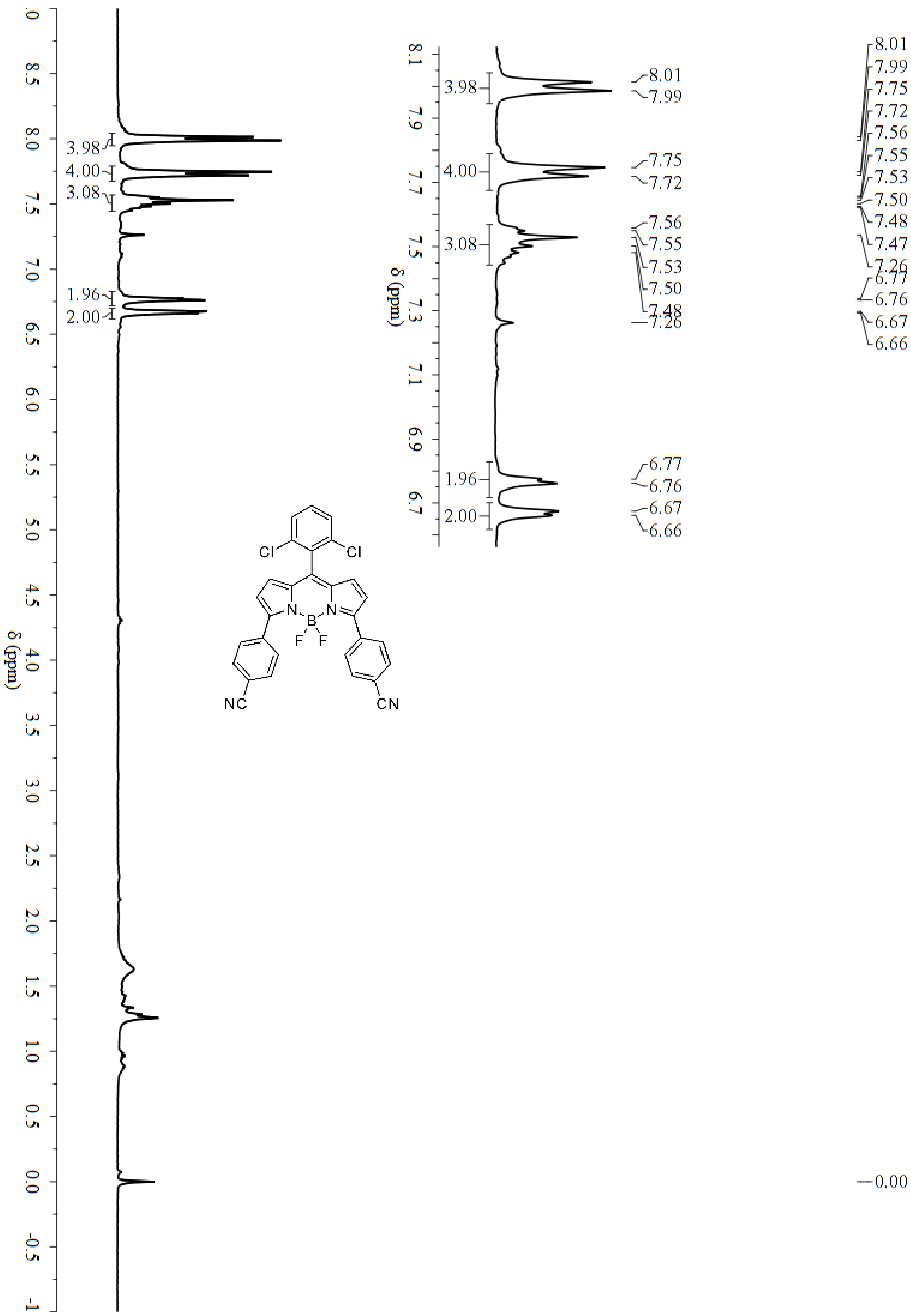
^{13}C NMR spectrum of **4a** in $CDCl_3$



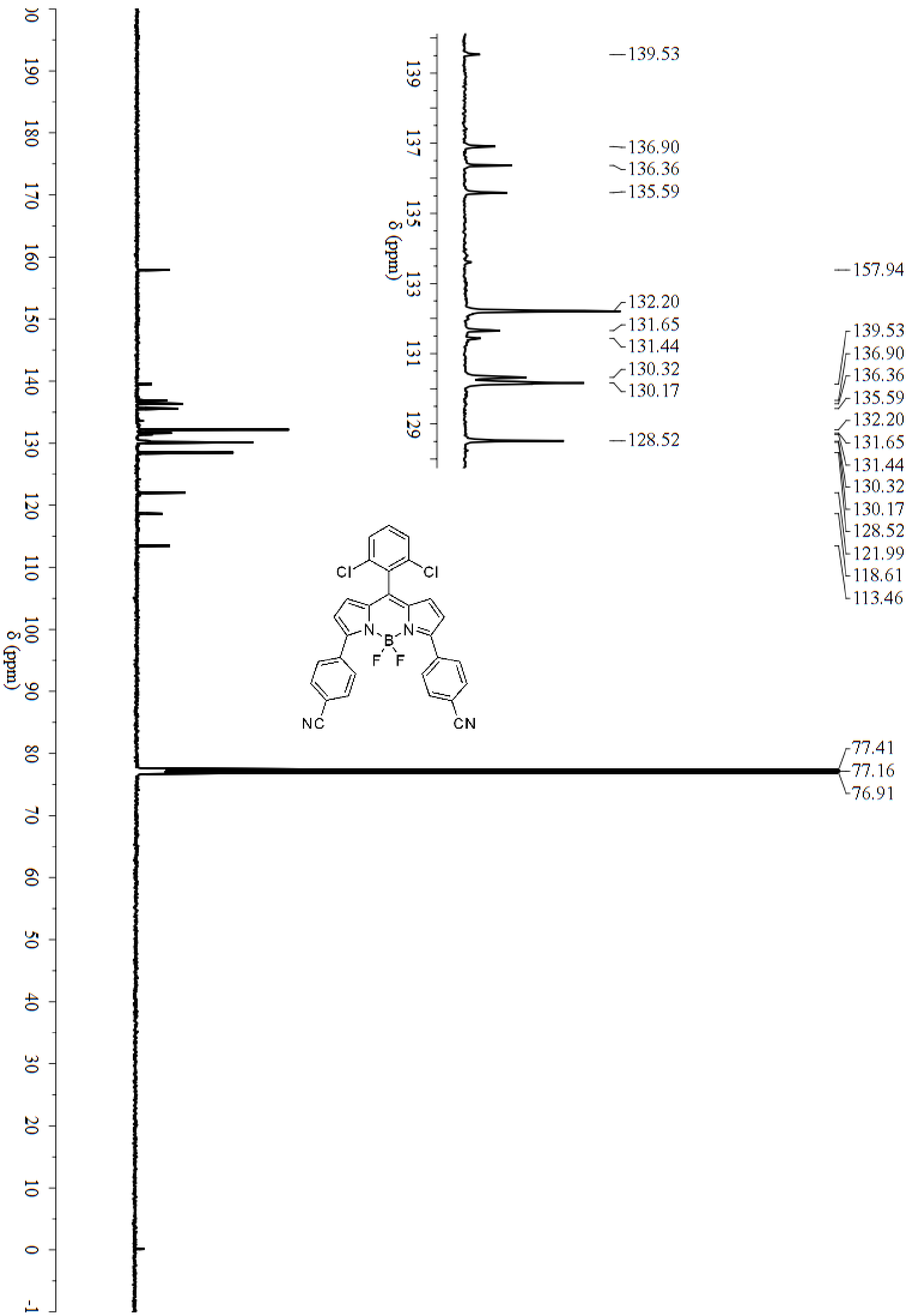
[1]H NMR spectrum of **4b** in $CDCl_3$



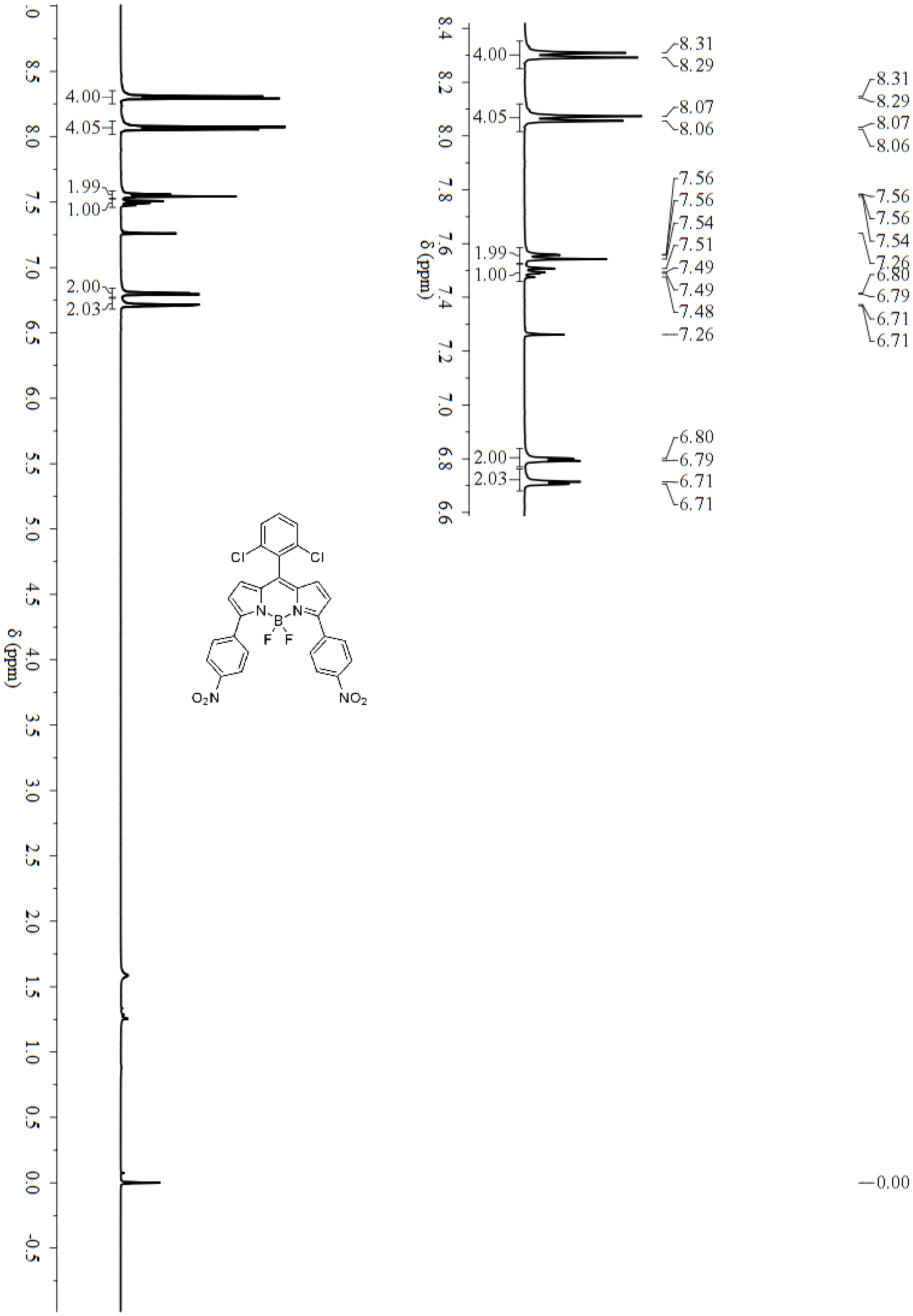
^{13}C NMR spectrum of **4b** in $CDCl_3$



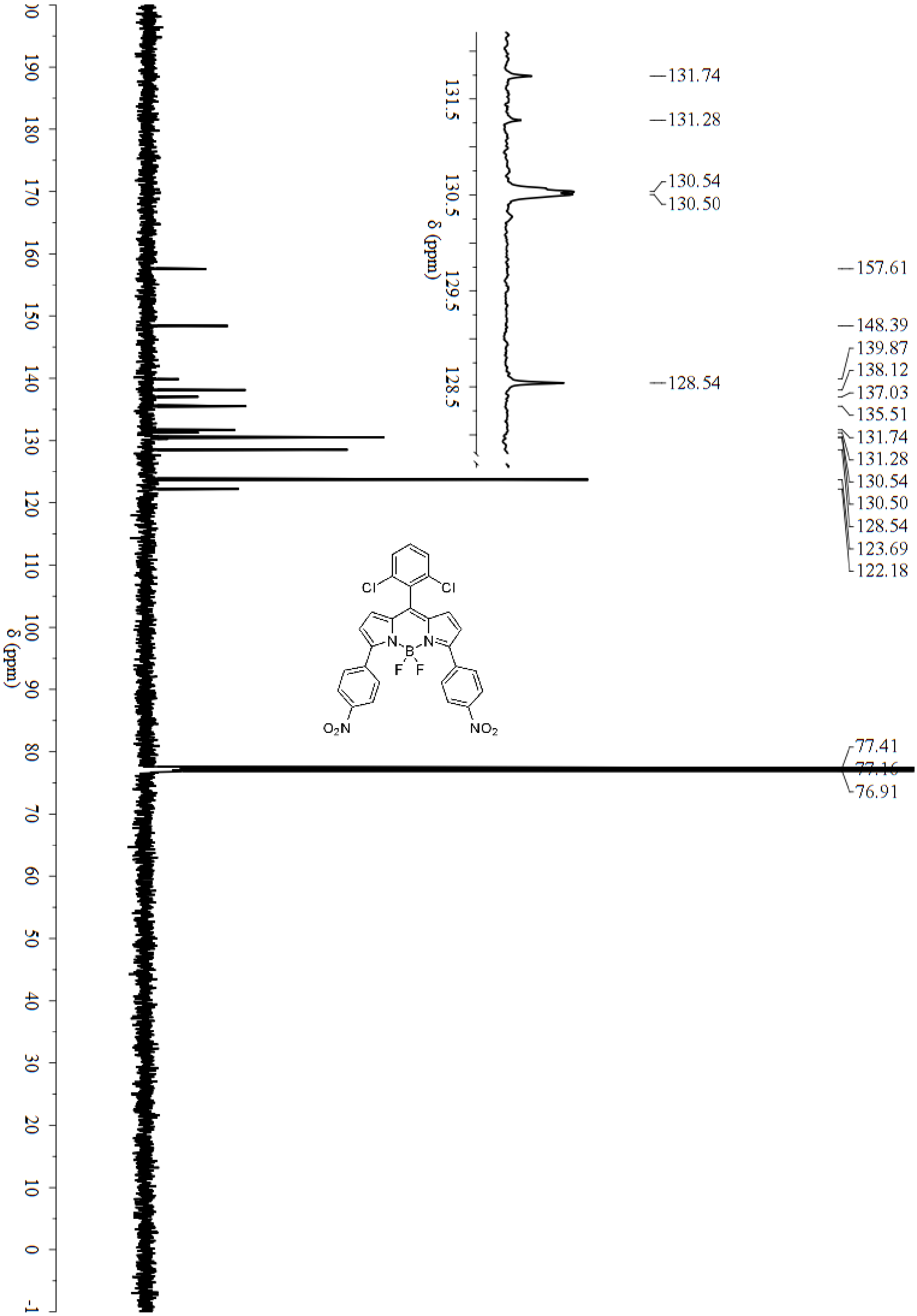
[1]H NMR spectrum of **4c** in $CDCl_3$



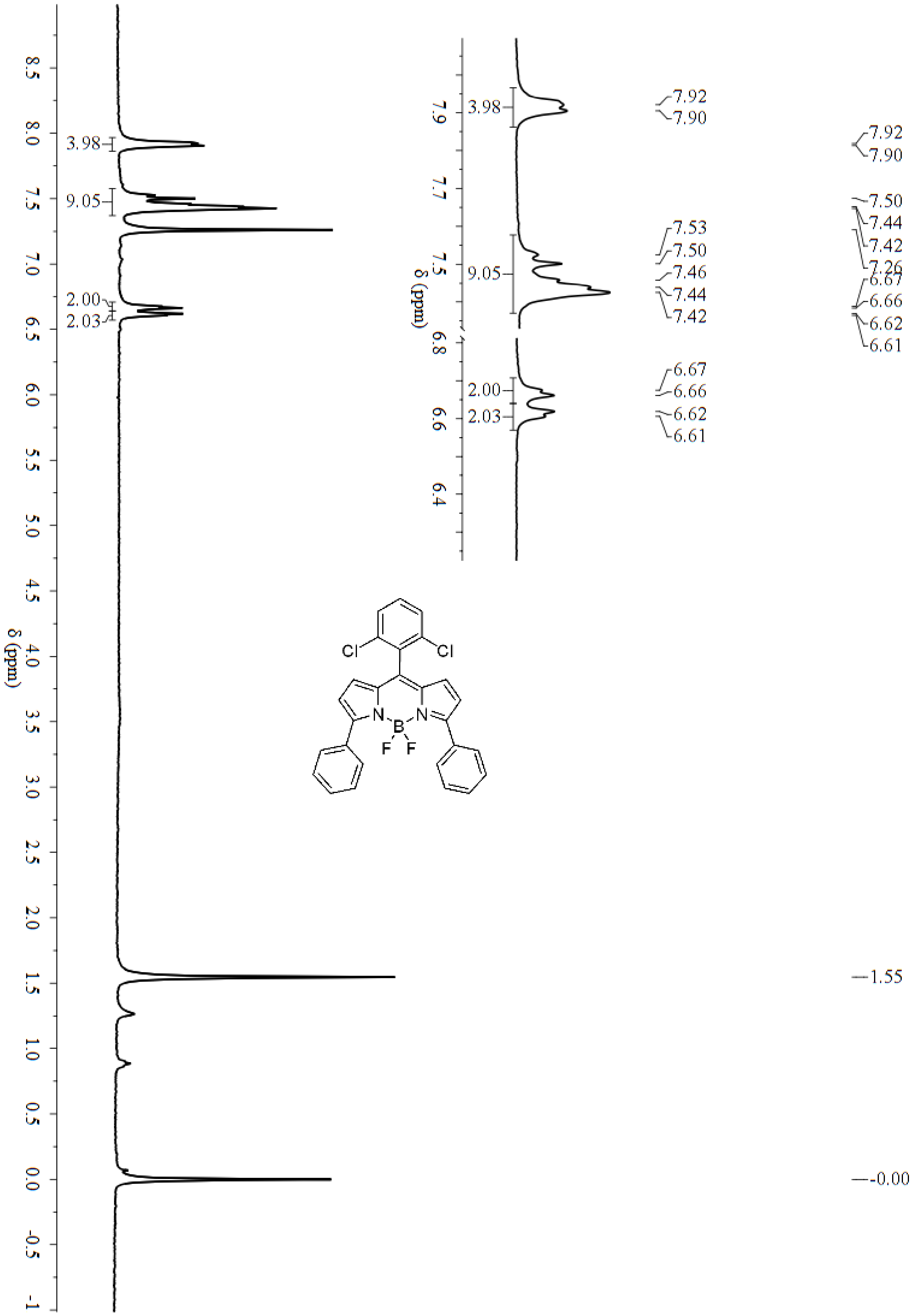
^{13}C NMR spectrum of **4c** in $CDCl_3$



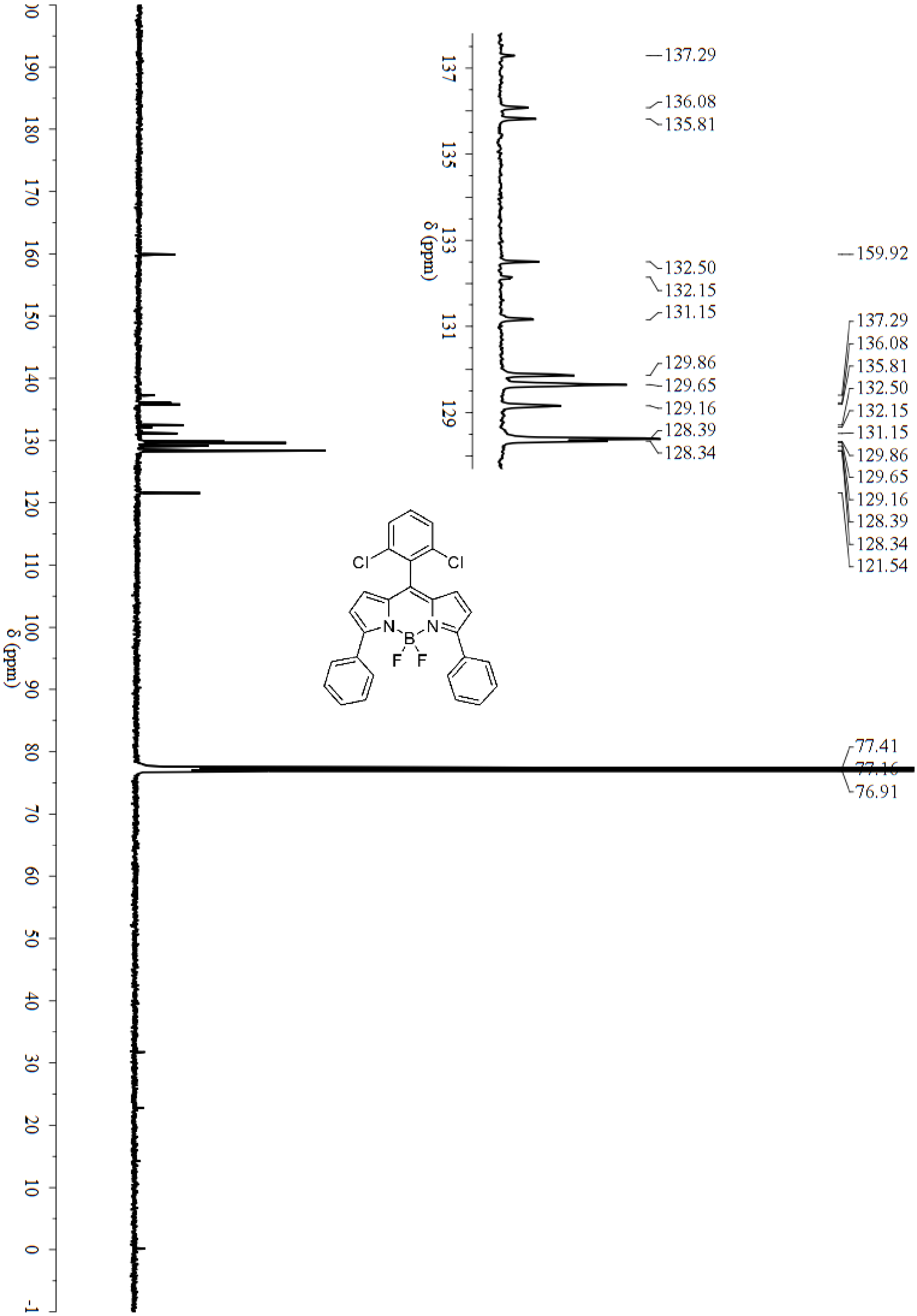
[1]H NMR spectrum of **4d** in $CDCl_3$



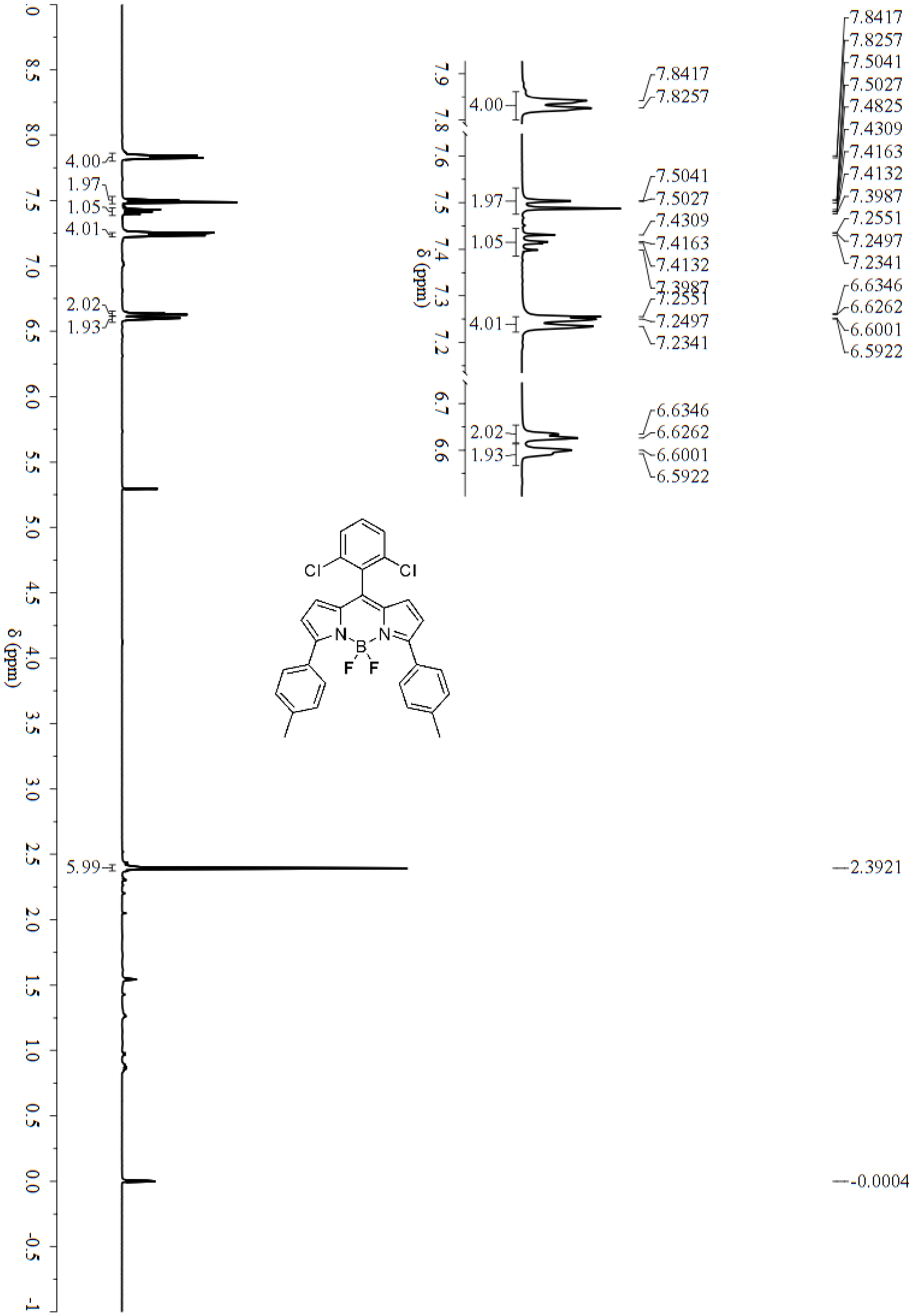
^{13}C NMR spectrum of **4d** in $CDCl_3$



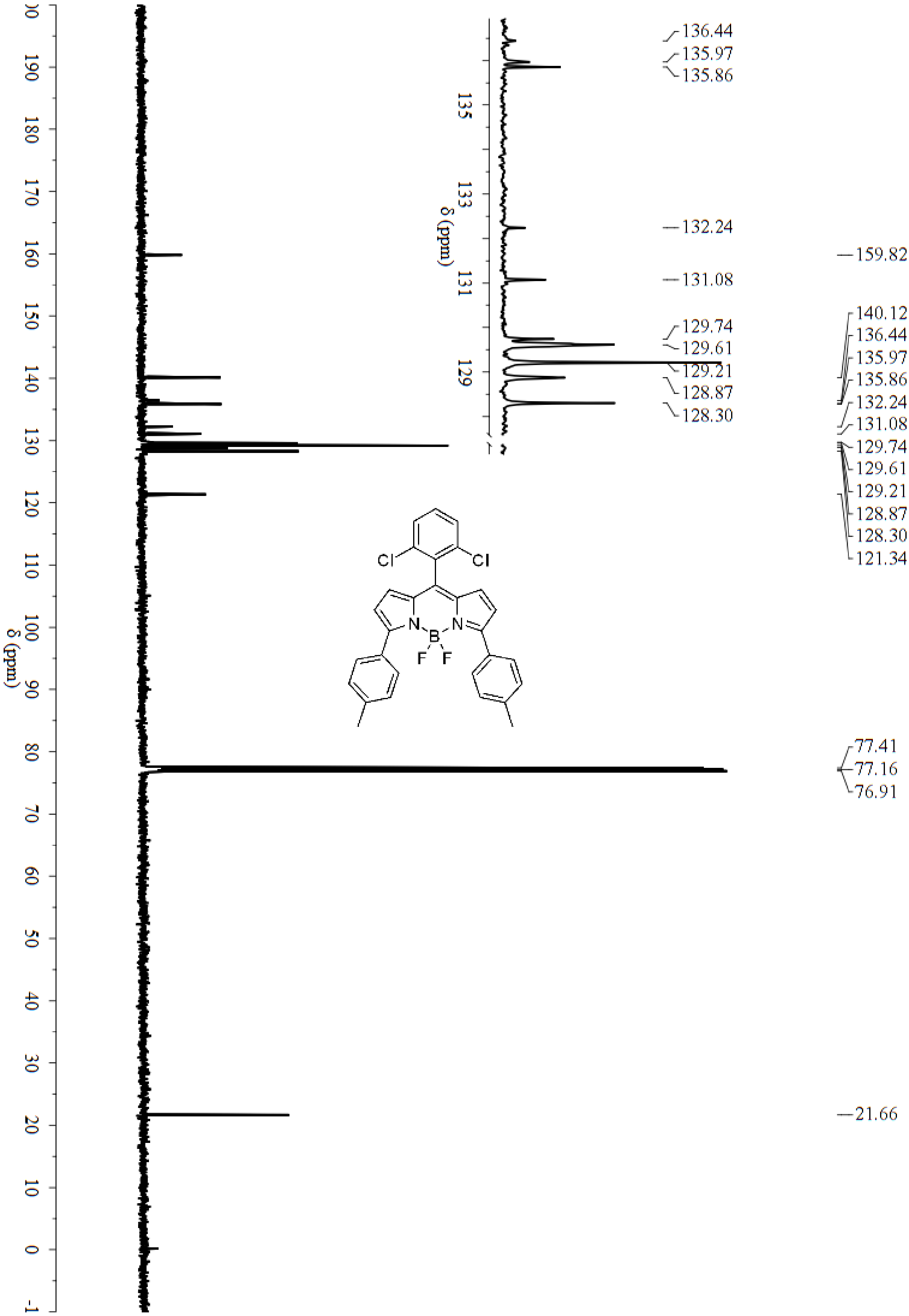
^{1}H NMR spectrum of **4e** in $CDCl_3$



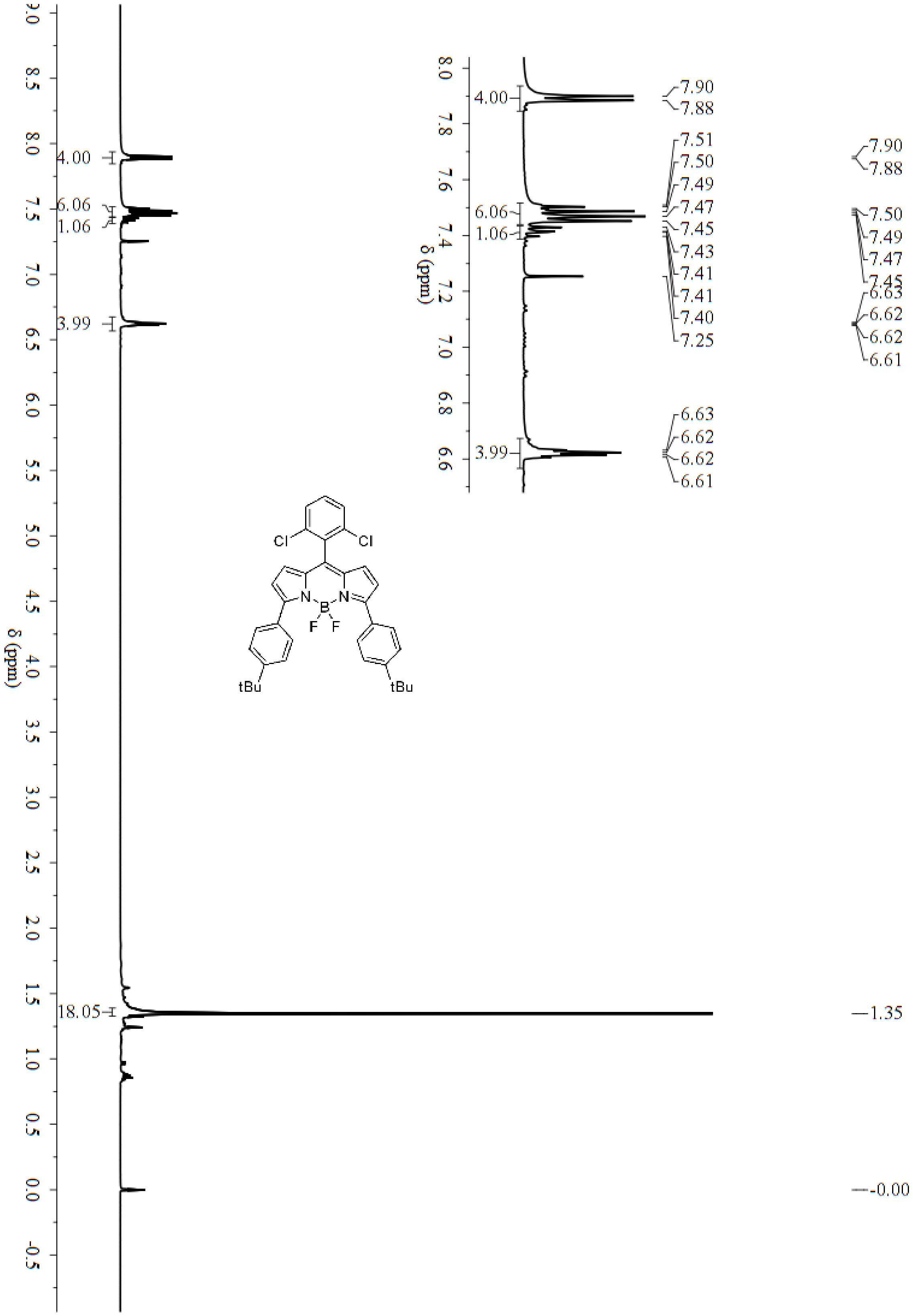
^{13}C NMR spectrum of **4e** in $CDCl_3$



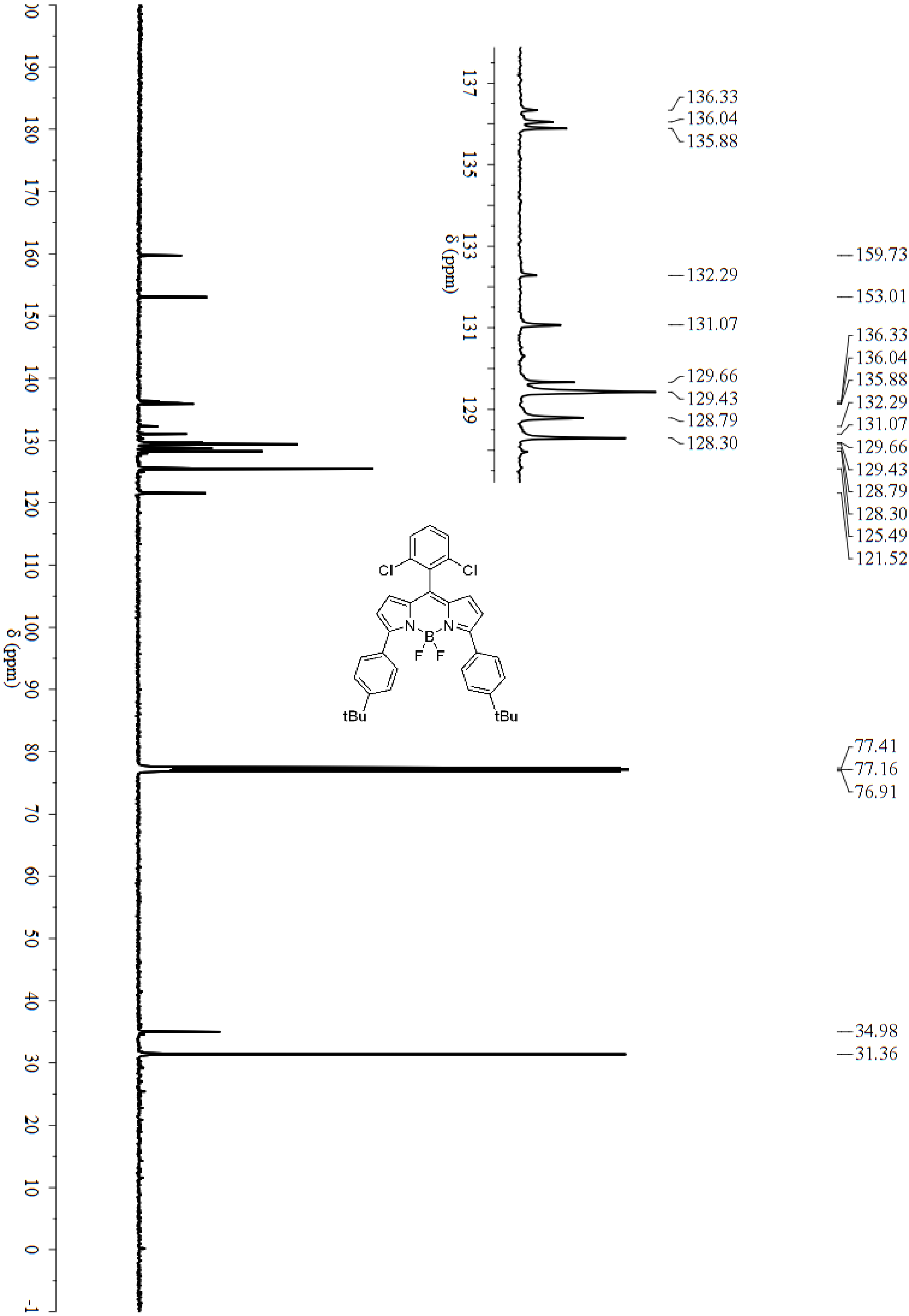
[1]H NMR spectrum of **4f** in $CDCl_3$



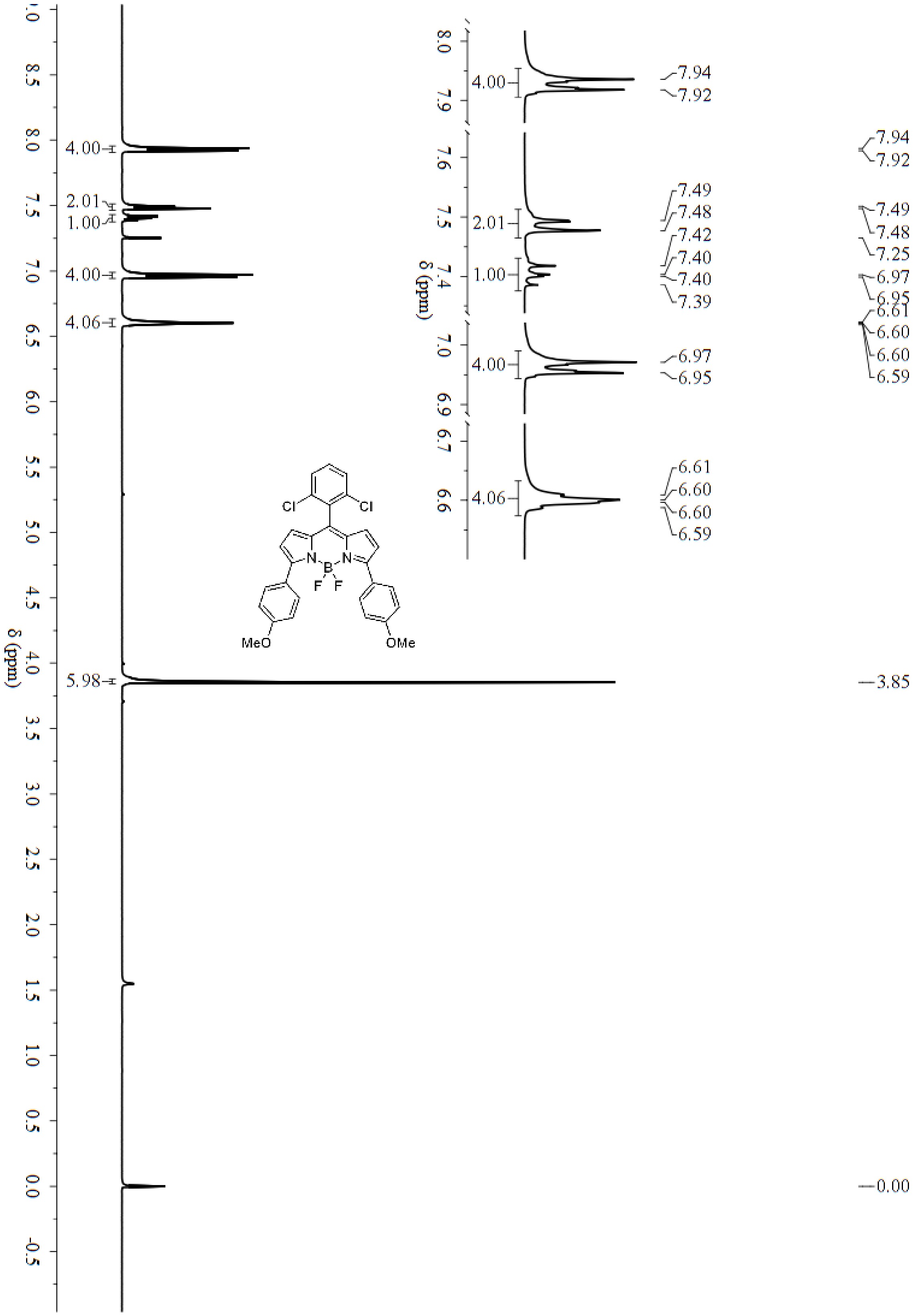
^{13}C NMR spectrum of **4f** in $CDCl_3$



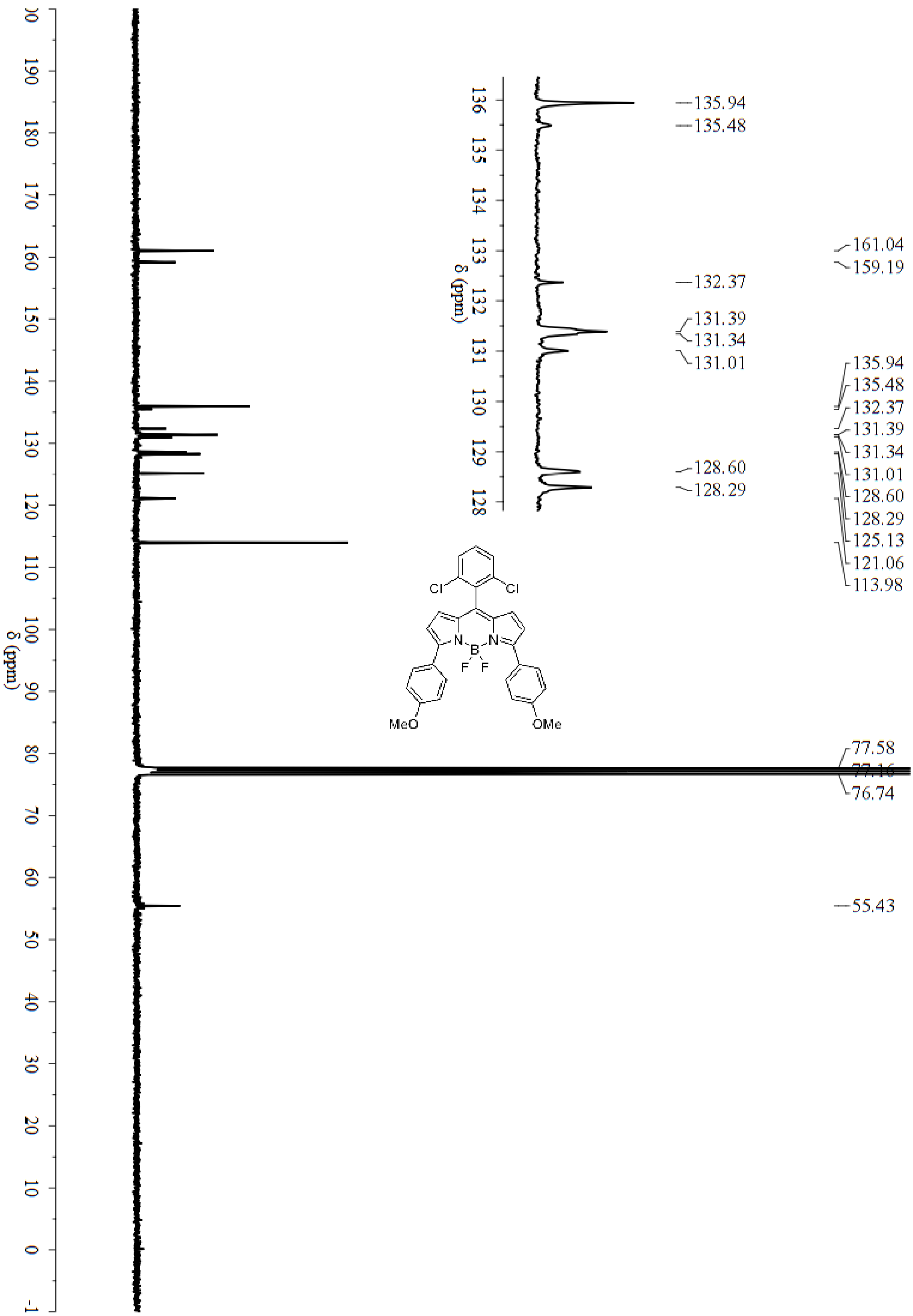
[1]H NMR spectrum of **4g** in $CDCl_3$



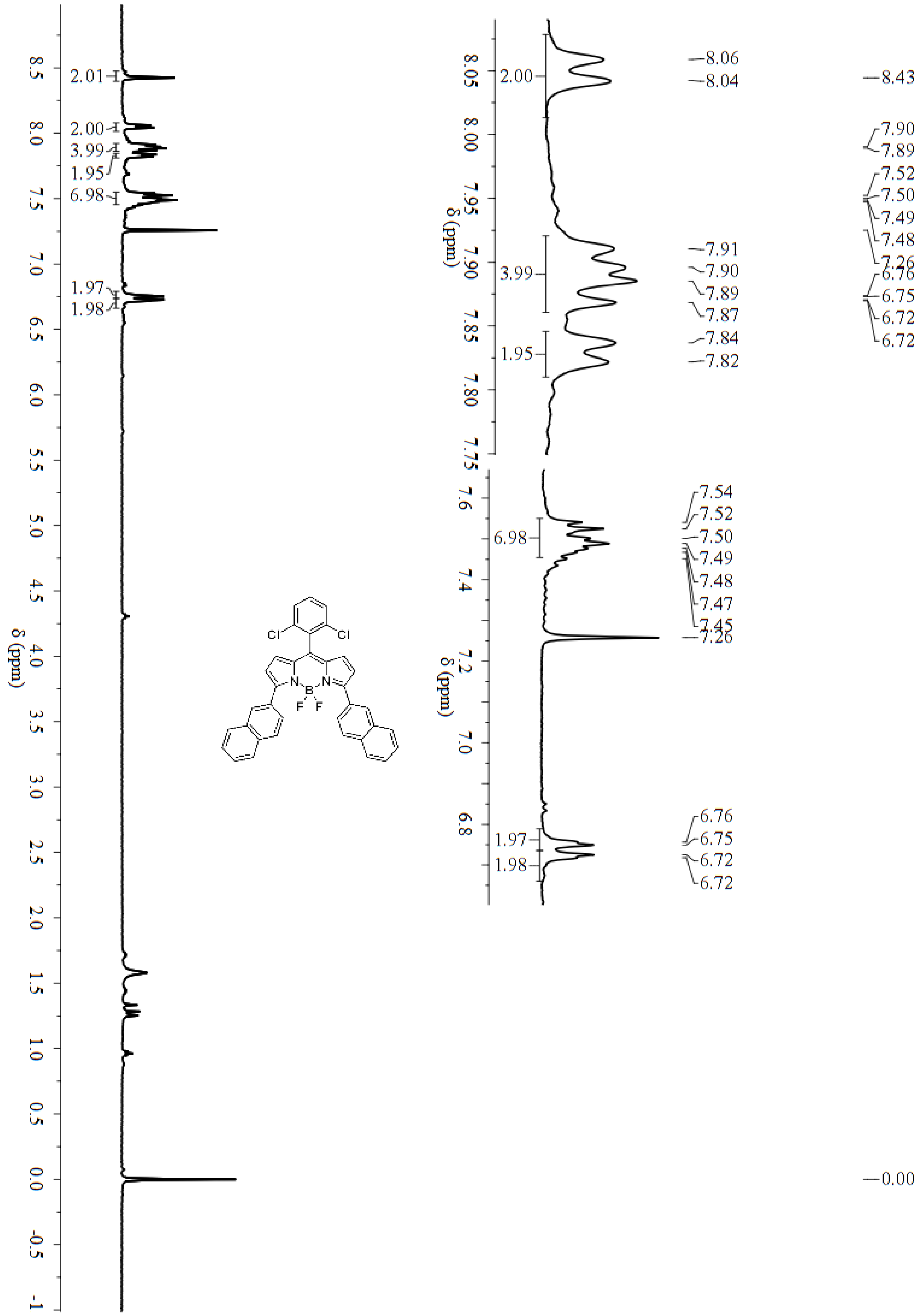
^{13}C NMR spectrum of **4g** in $CDCl_3$



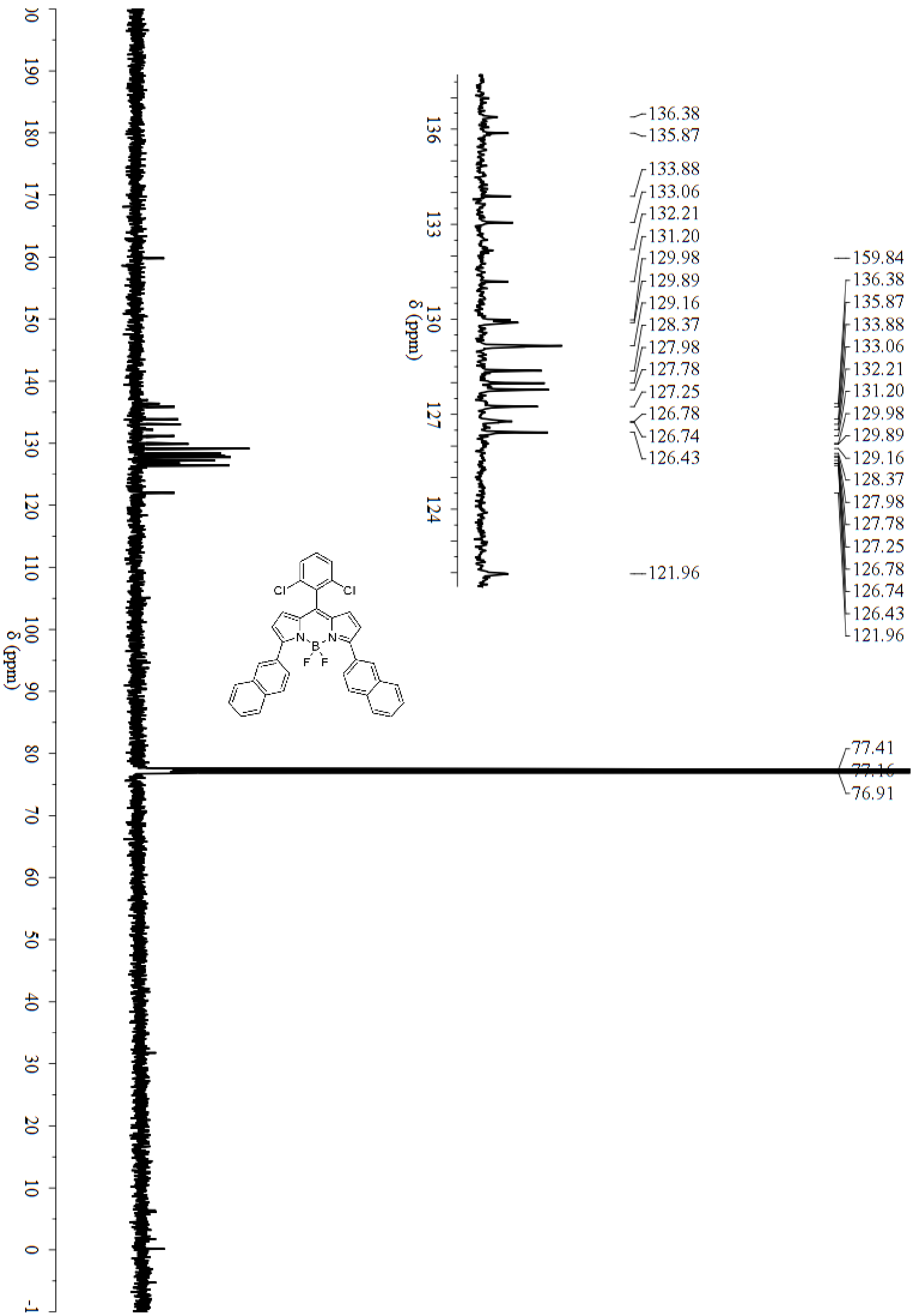
^{1}H NMR spectrum of **4h** in $CDCl_3$



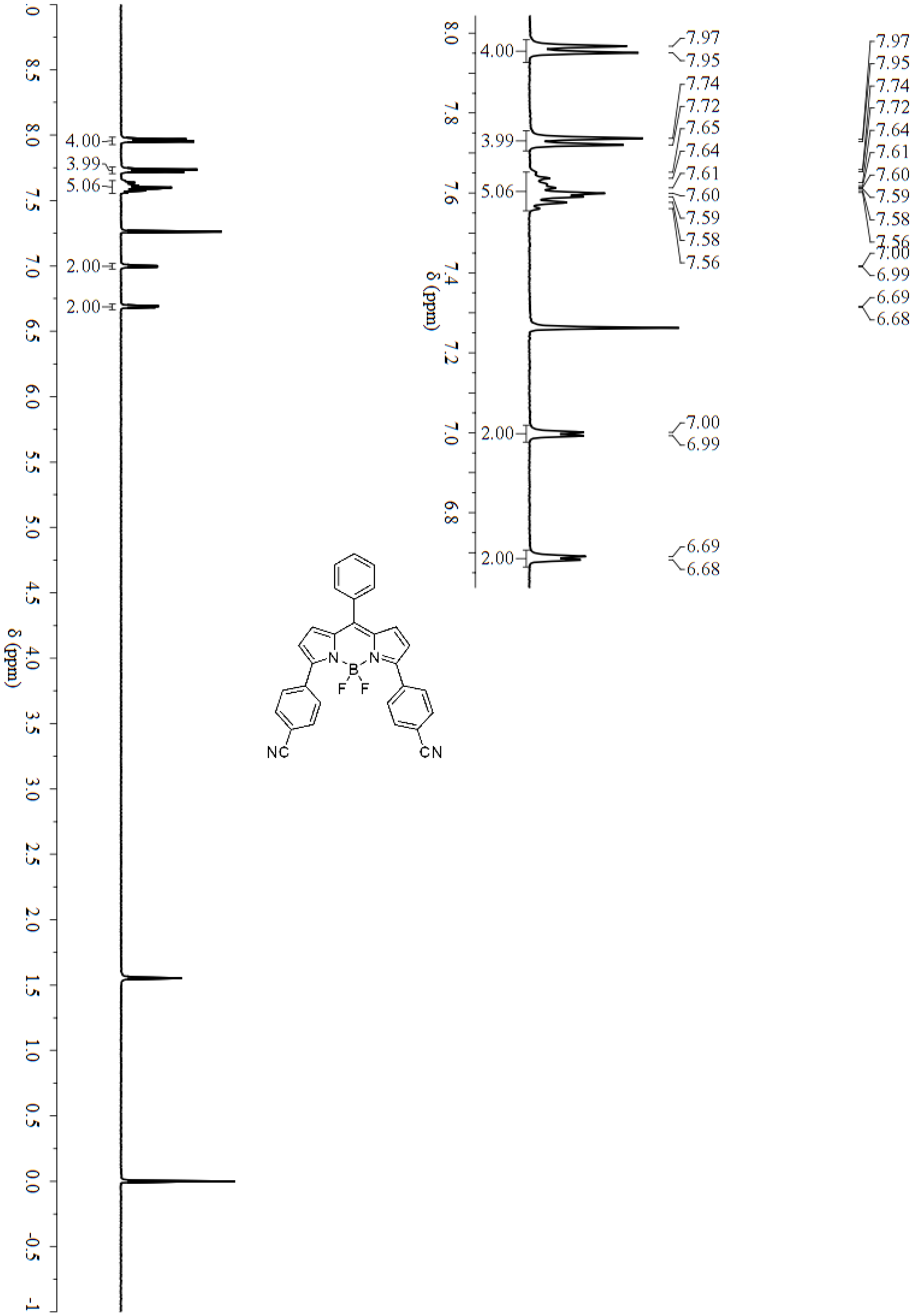
^{13}C NMR spectrum of **4h** in $CDCl_3$



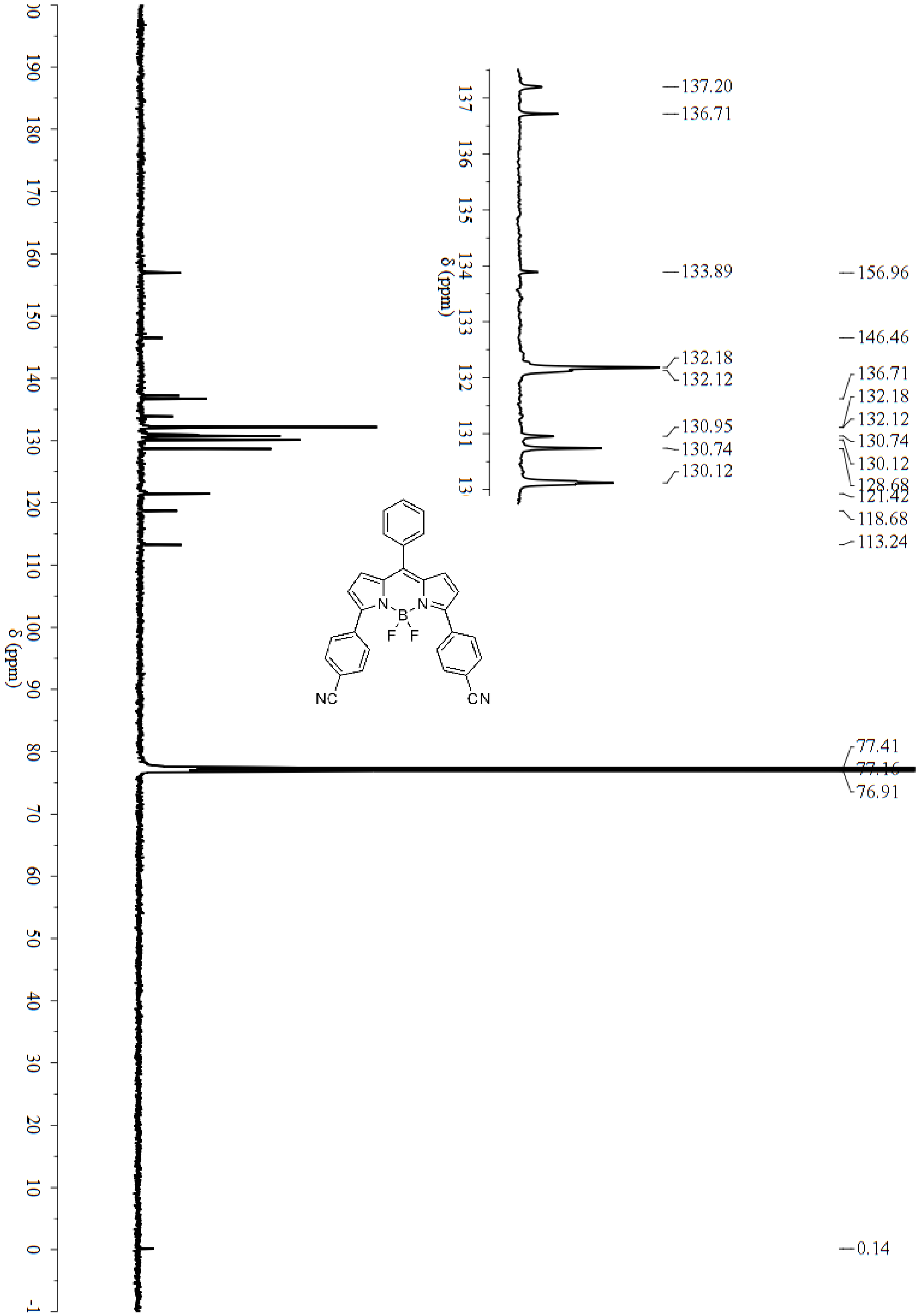
[1]H NMR spectrum of **4i** in $CDCl_3$



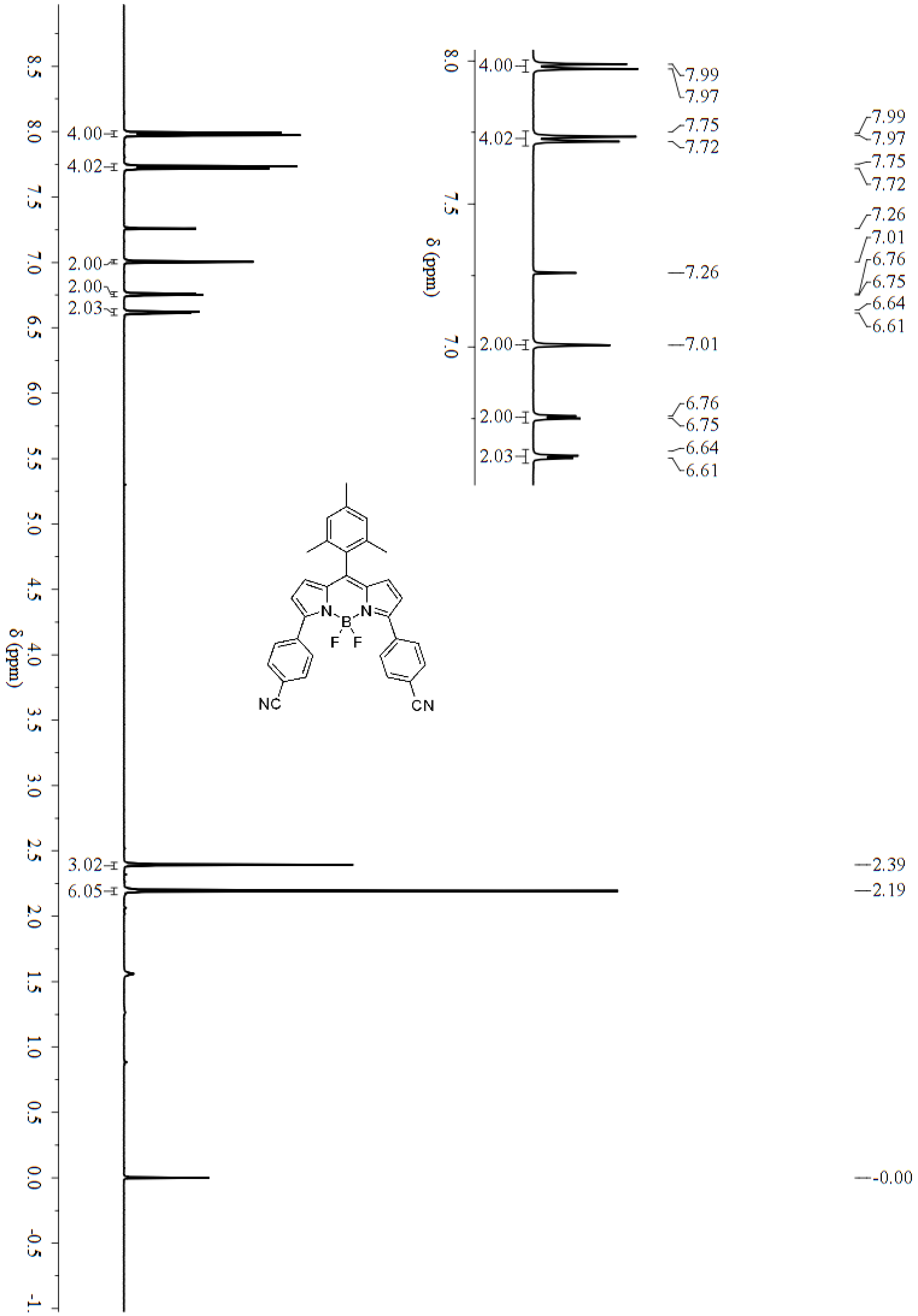
^{13}C NMR spectrum of **4i** in $CDCl_3$



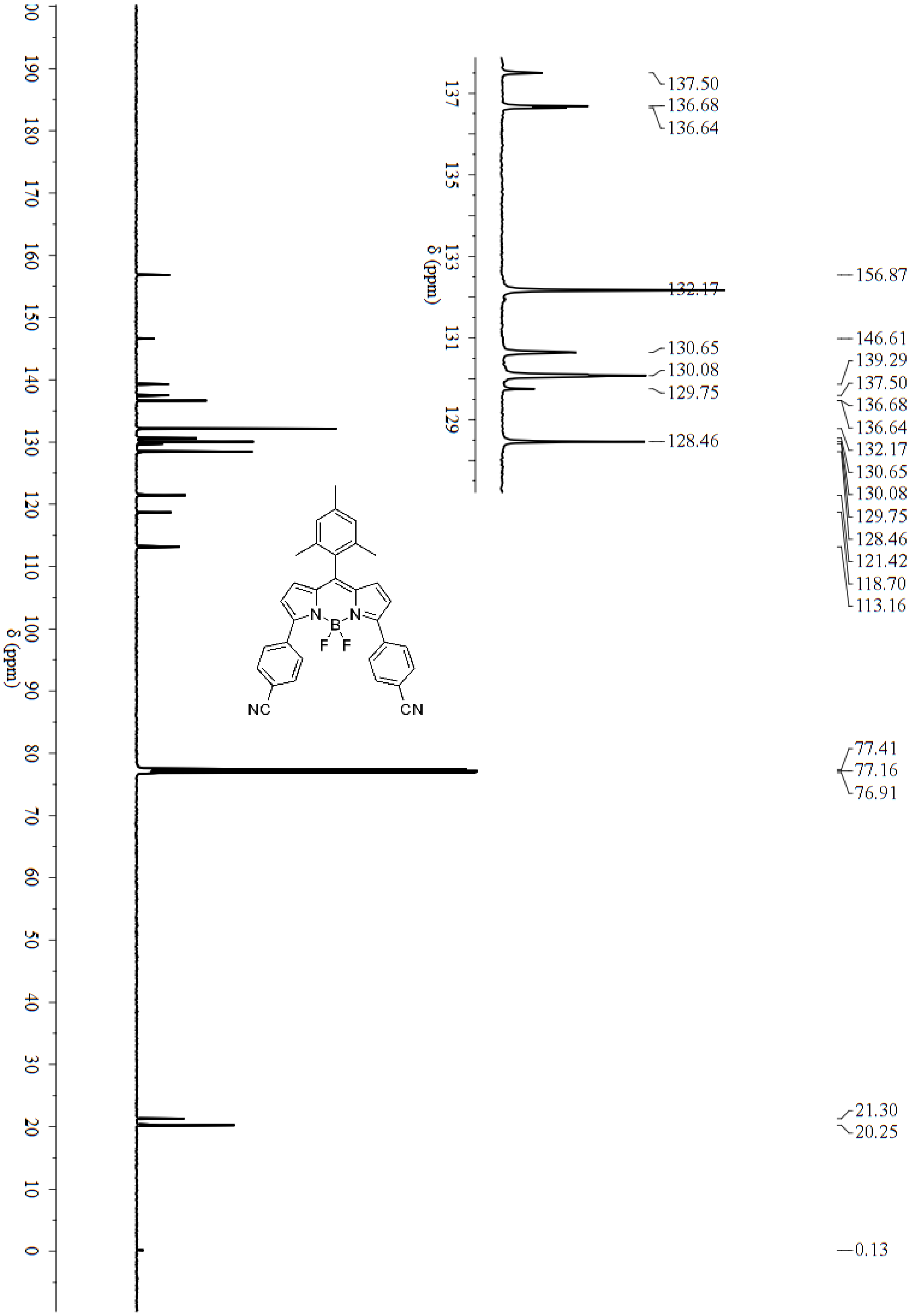
^{1}H NMR spectrum of **4j** in $CDCl_3$



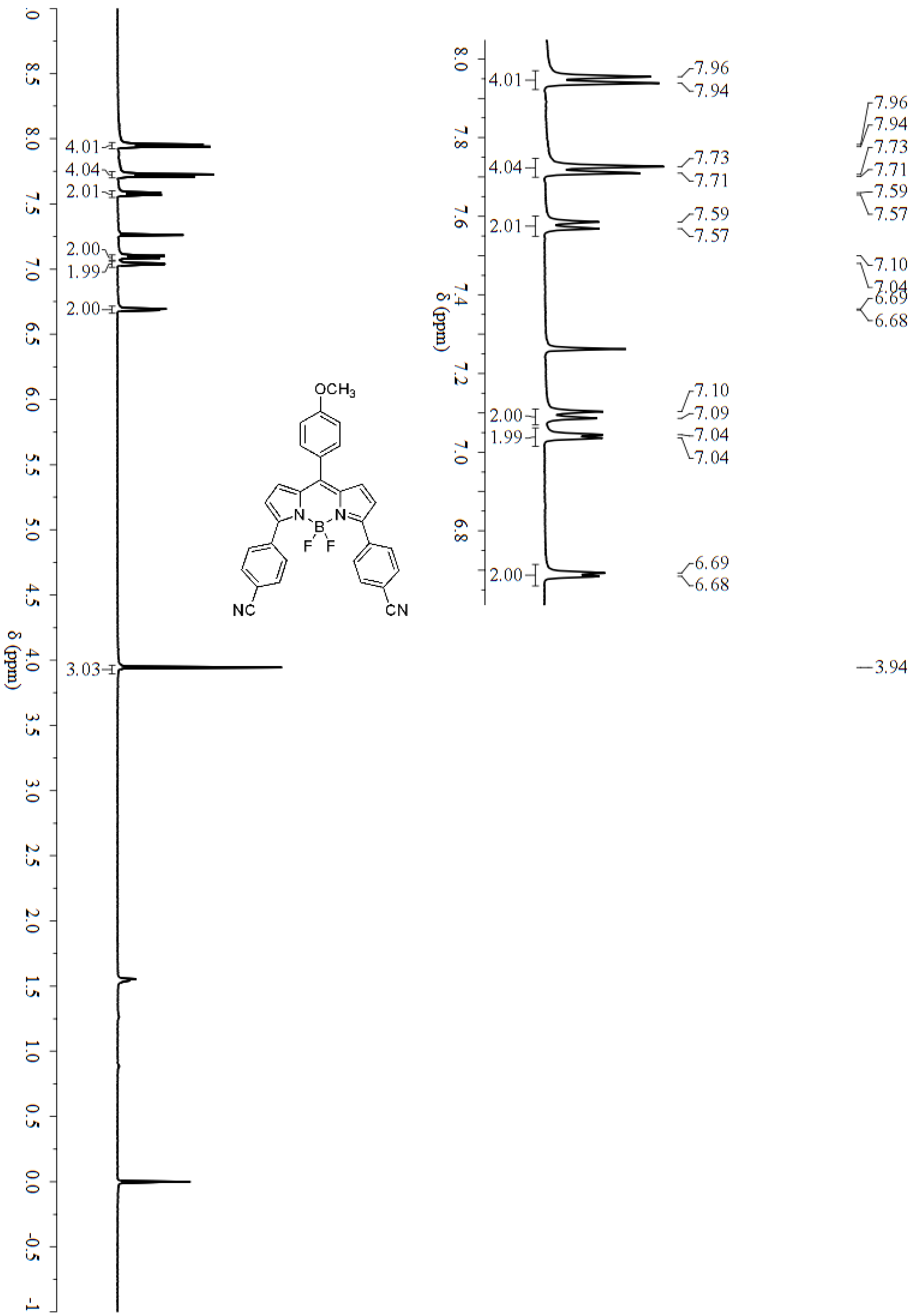
^{13}C NMR spectrum of **4j** in $CDCl_3$



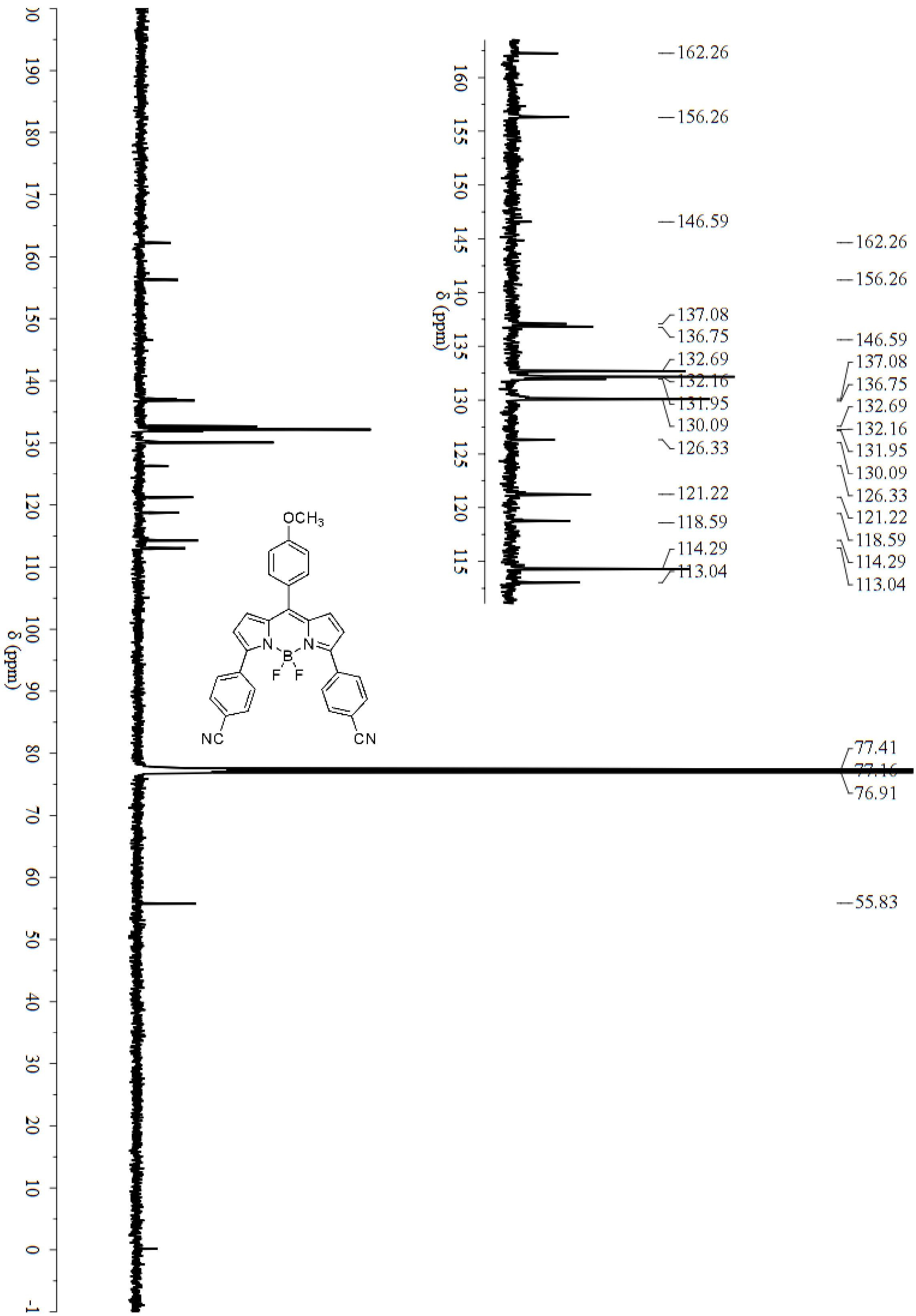
[1]H NMR spectrum of **4k** in $CDCl_3$



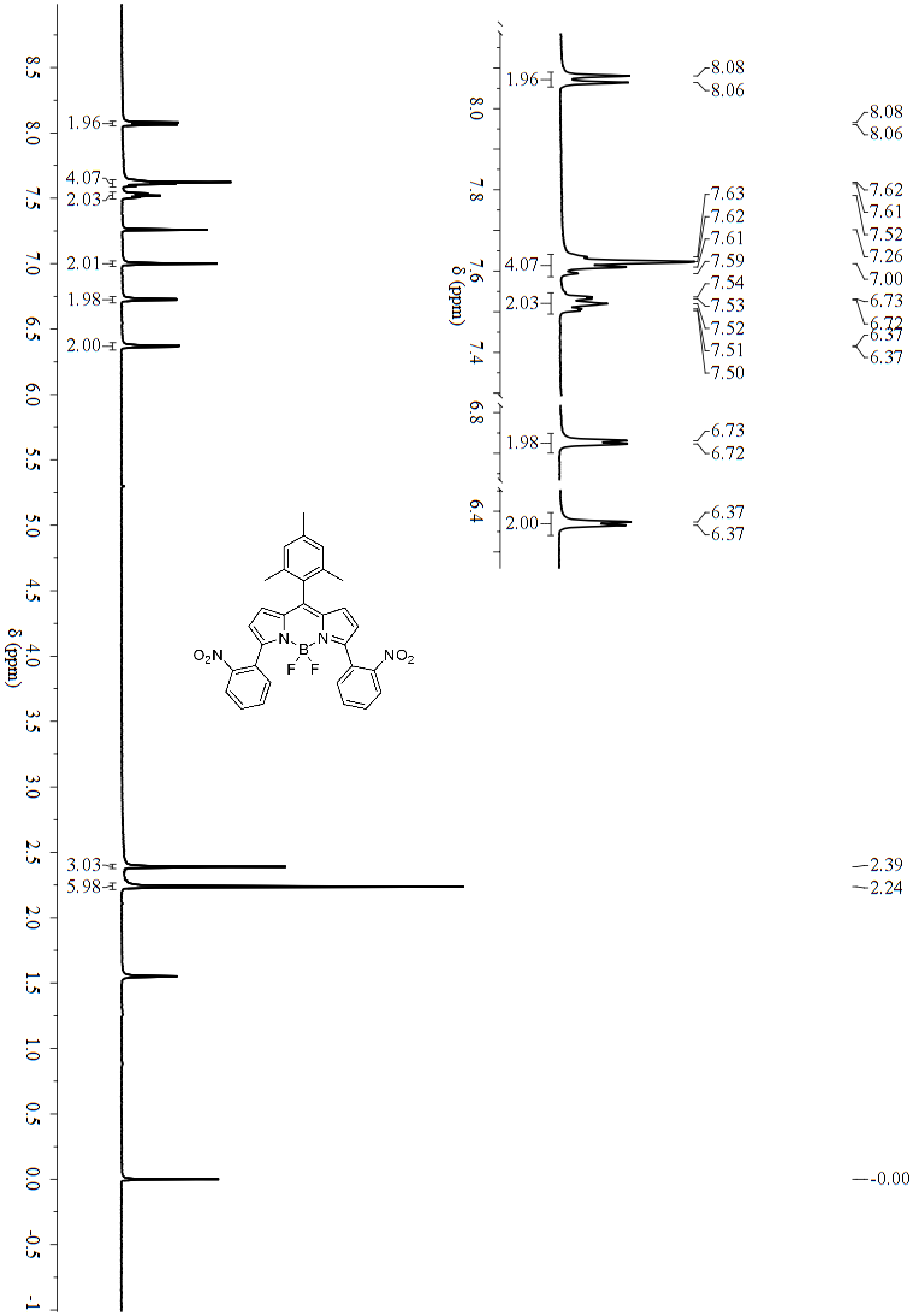
^{13}C NMR spectrum of **4k** in $CDCl_3$



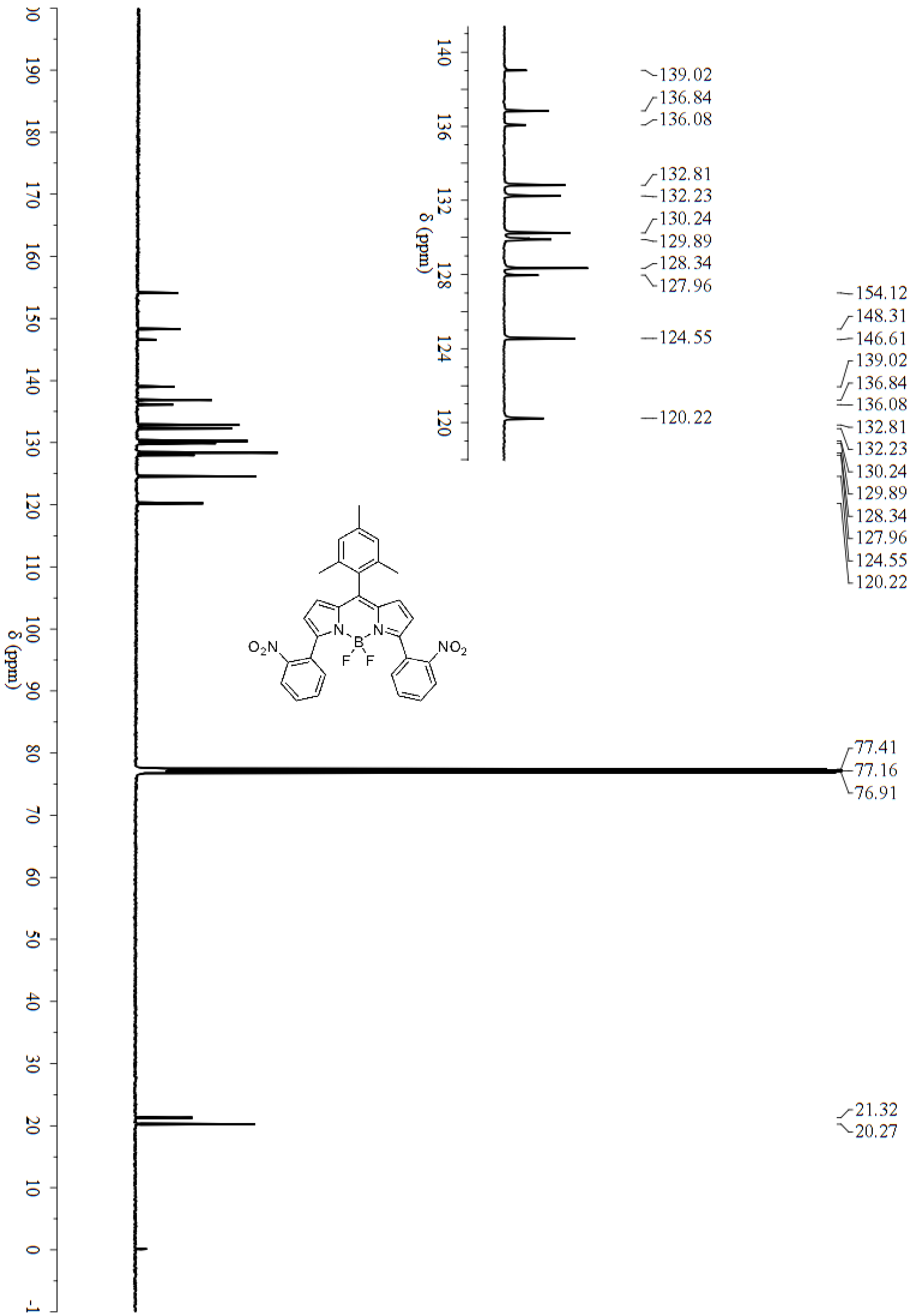
^{1}H NMR spectrum of **4l** in $CDCl_3$



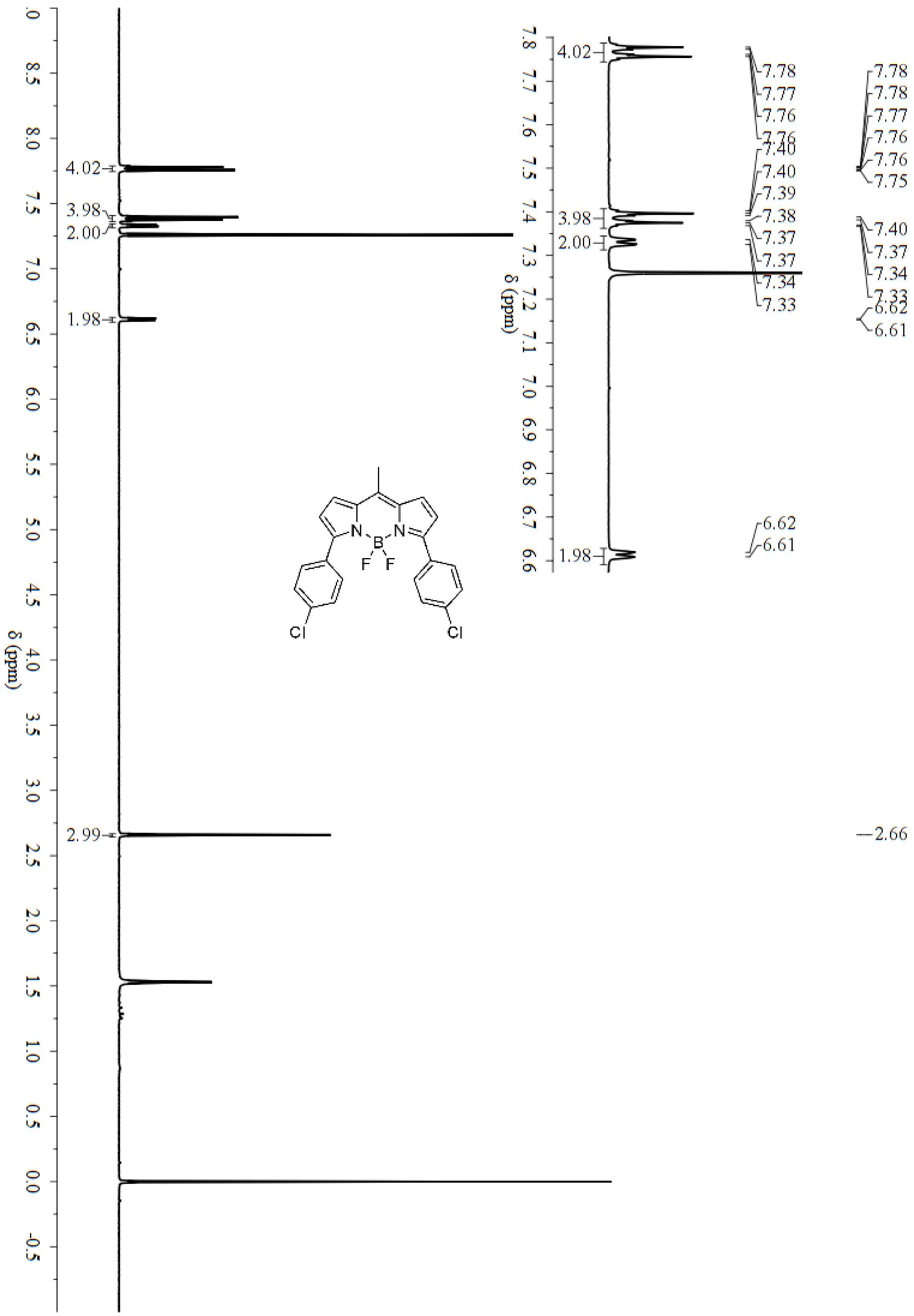
^{13}C NMR spectrum of **4l** in $CDCl_3$



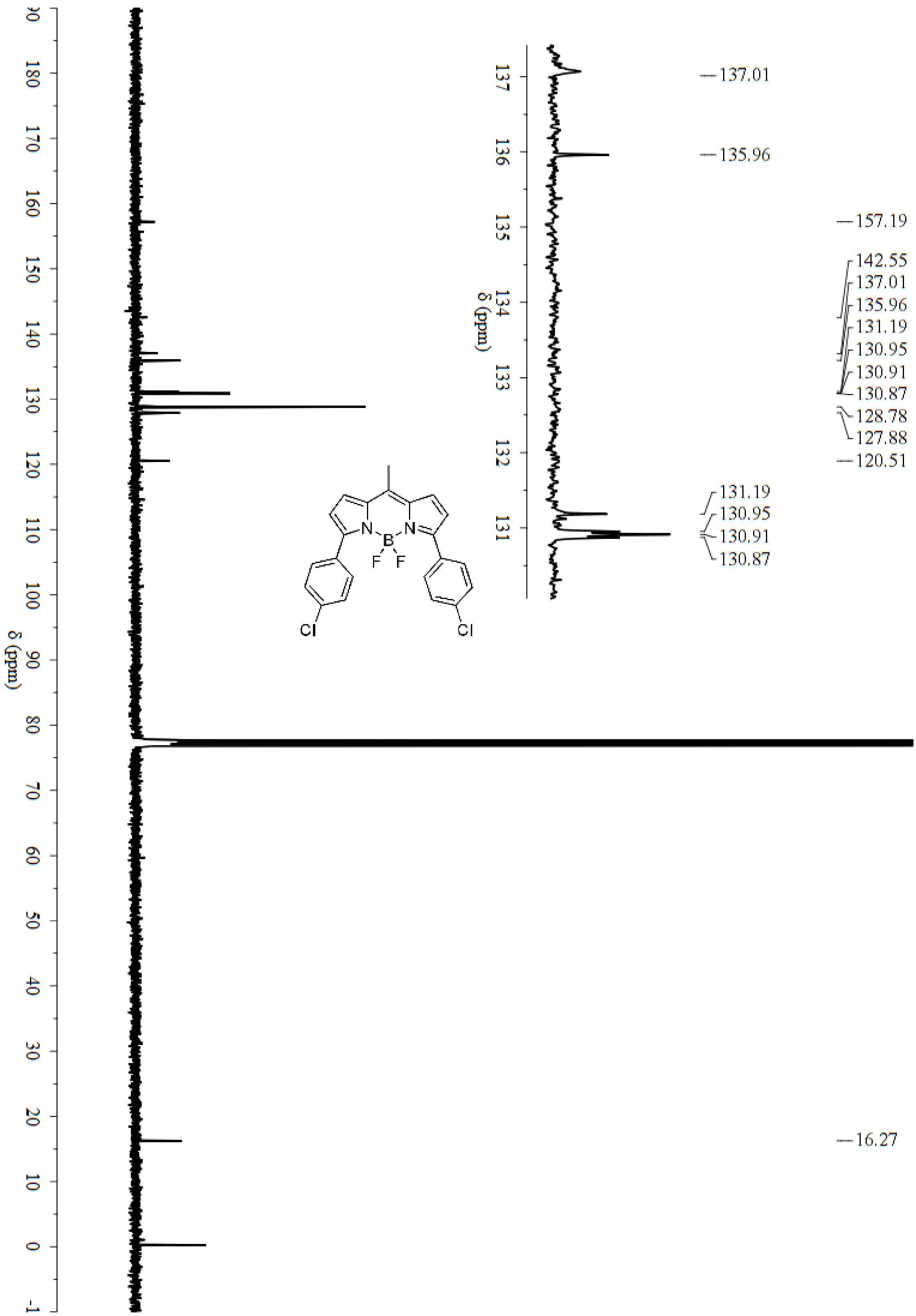
[1]H NMR spectrum of **4n** in $CDCl_3$



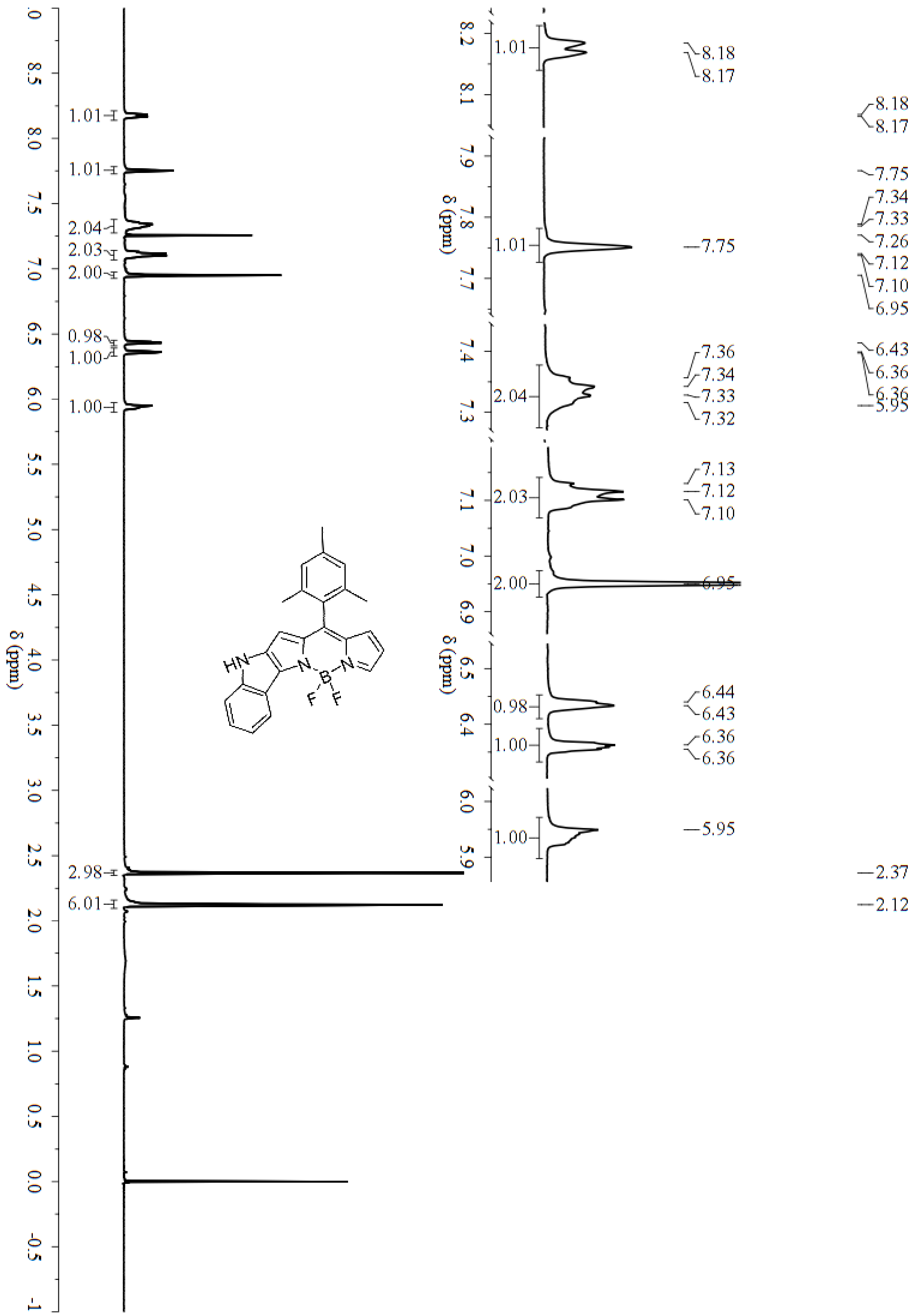
^{13}C NMR spectrum of **4n** in $CDCl_3$



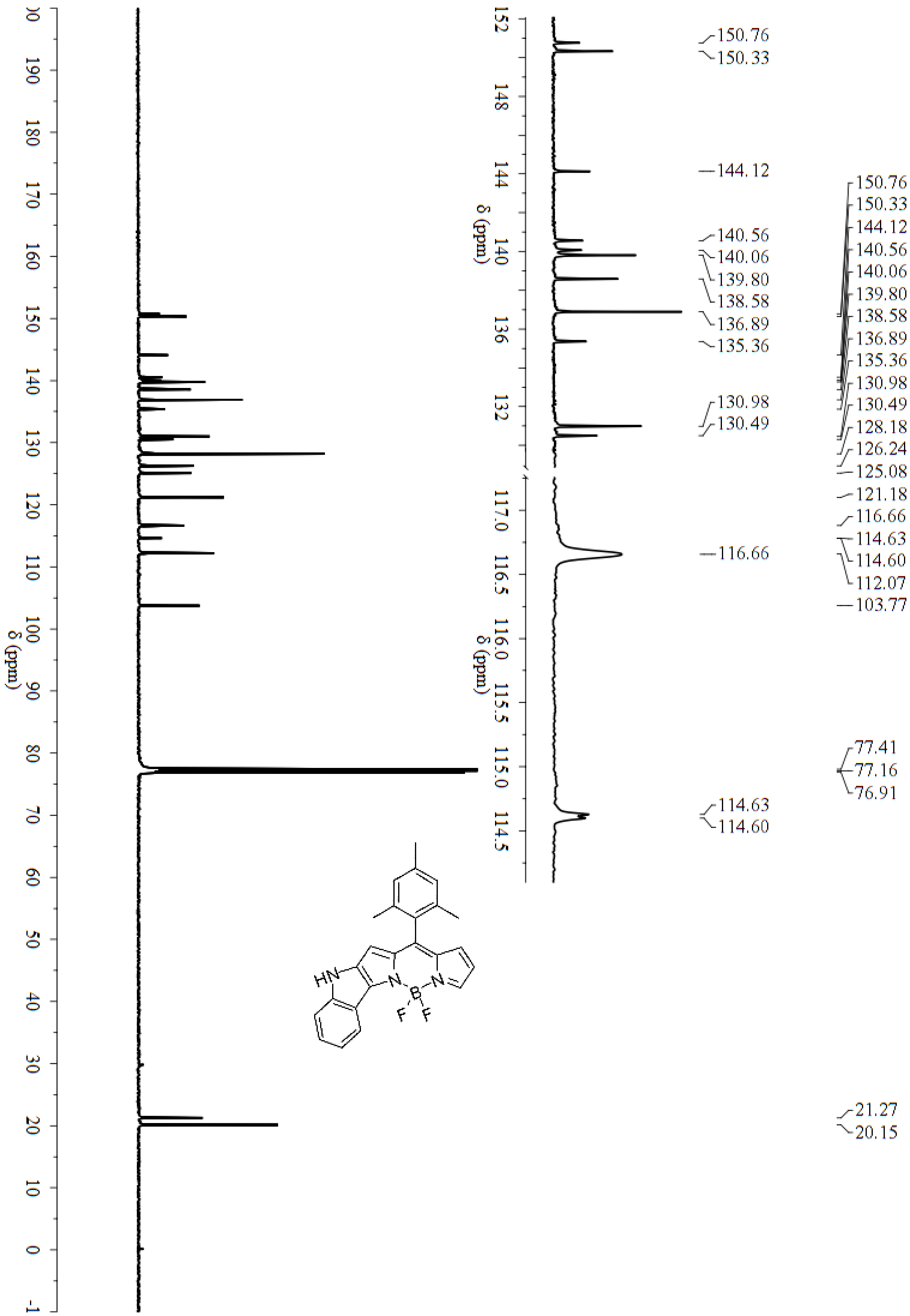
[1]H NMR spectrum of **4o** in $CDCl_3$



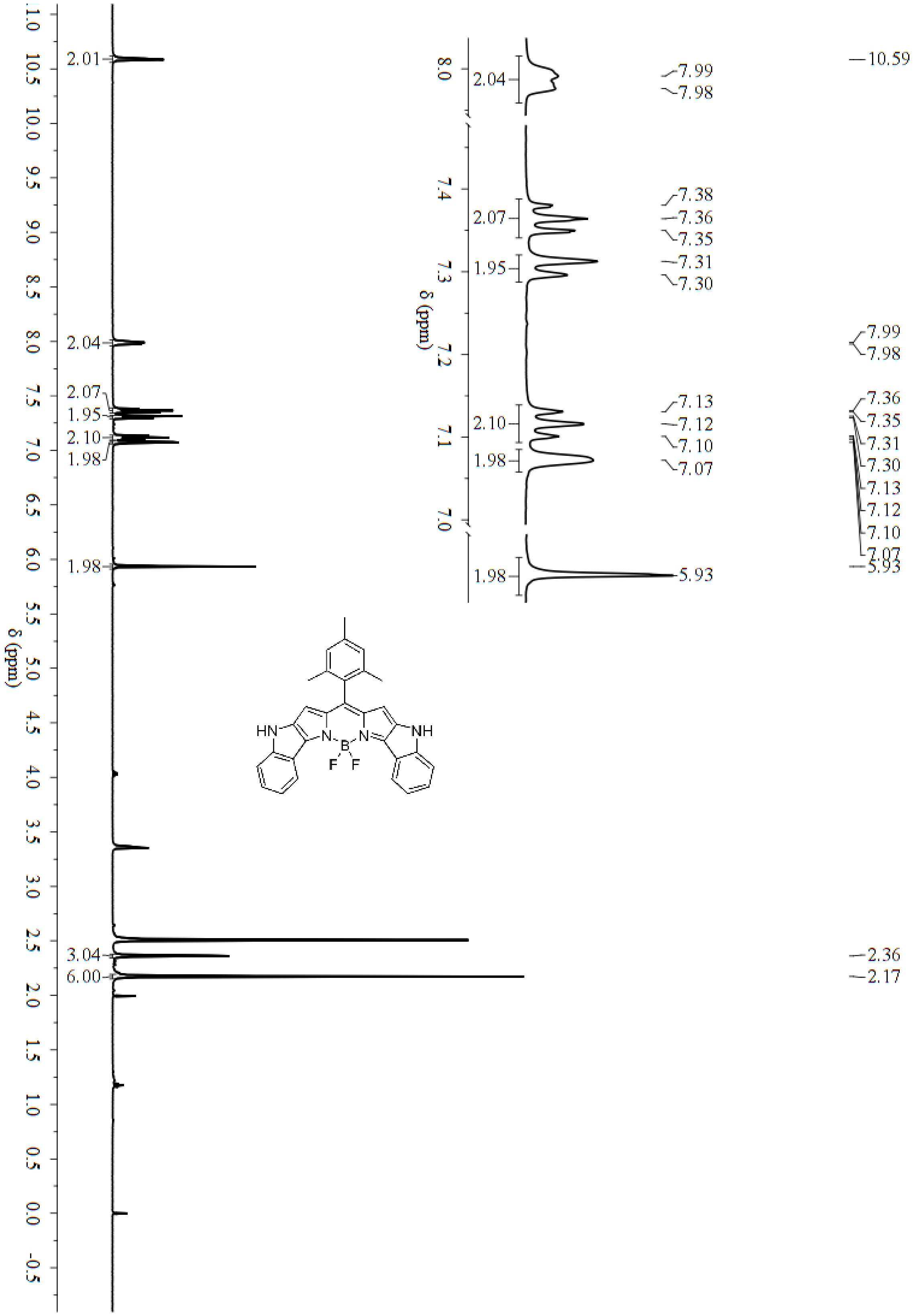
^{13}C NMR spectrum of **4o** in $CDCl_3$



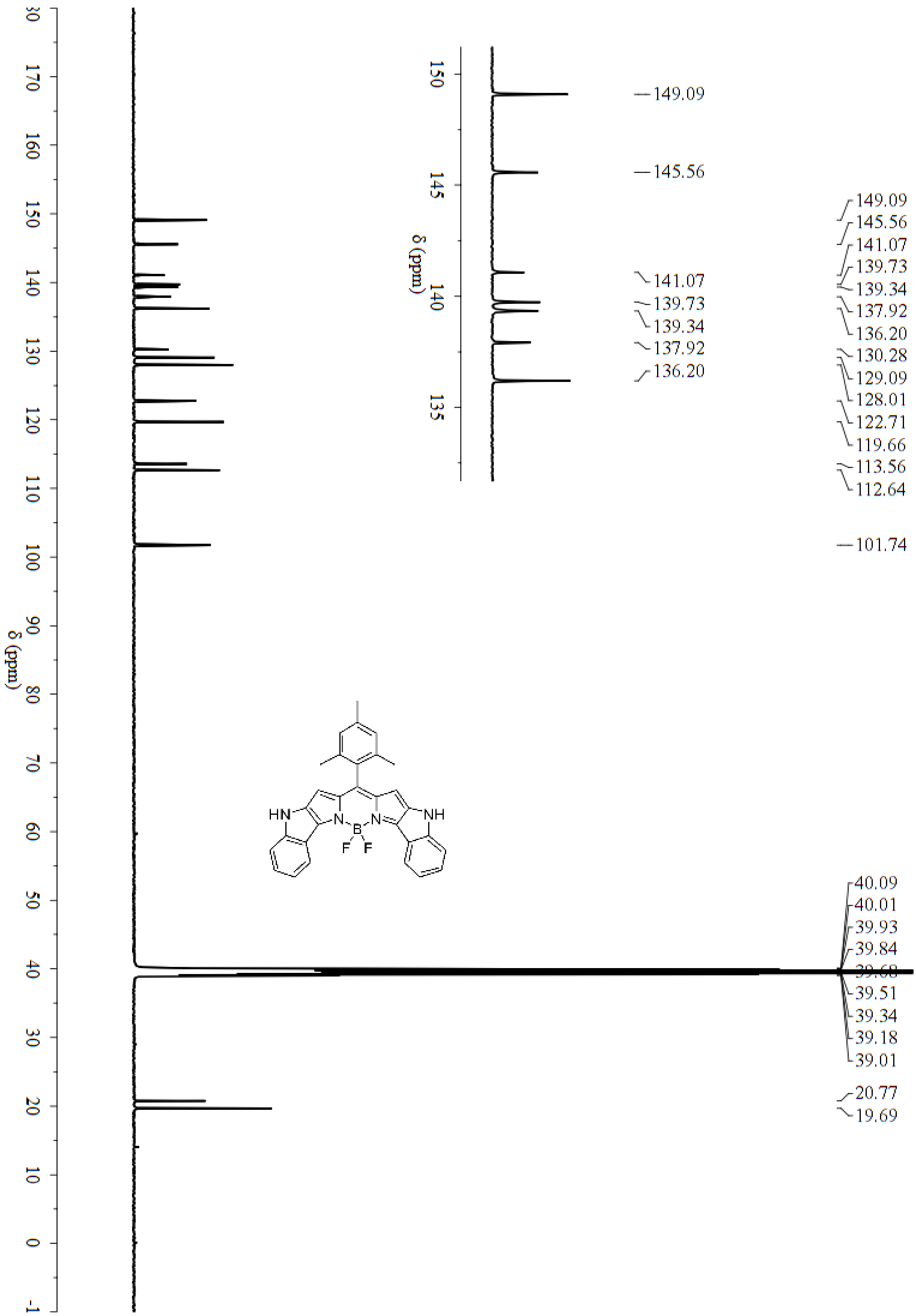
[1]H NMR spectrum of **5a** in $CDCl_3$



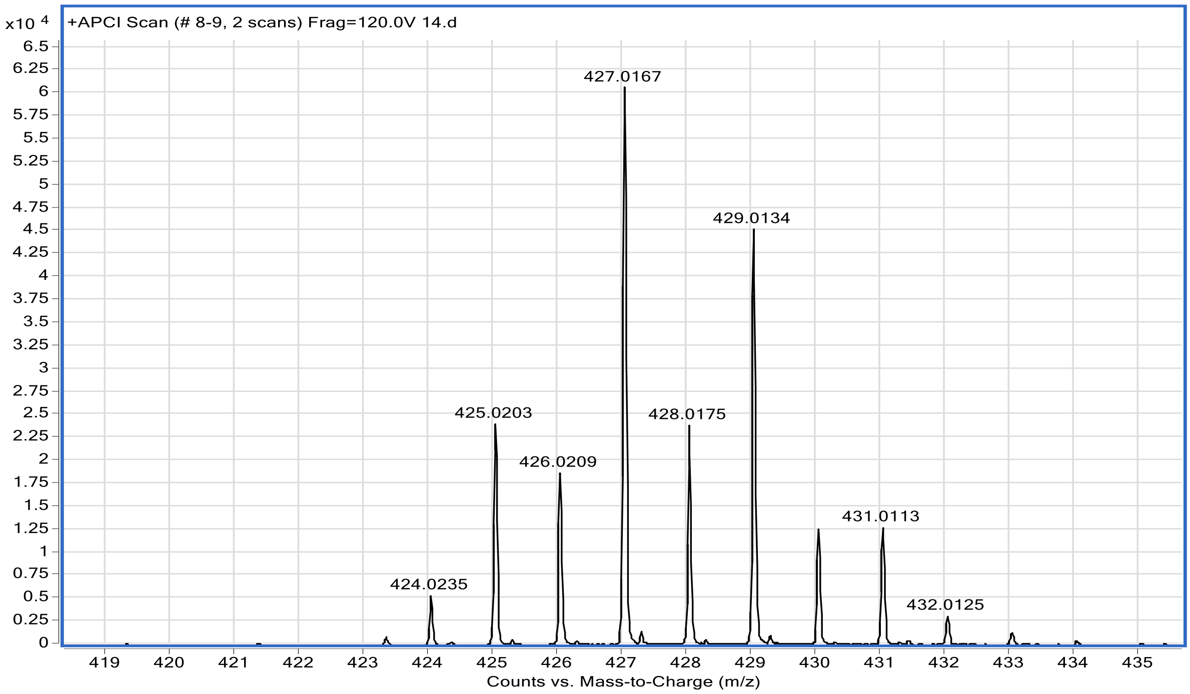
^{13}C NMR spectrum of **5a** in $CDCl_3$



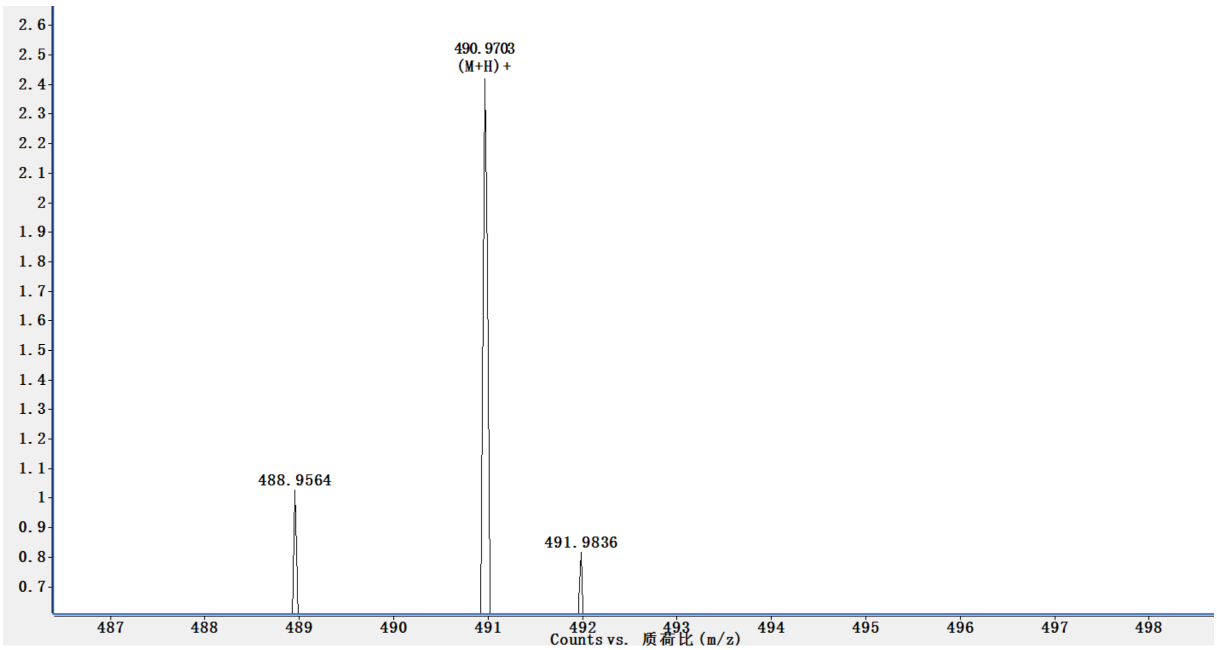
^{1}H NMR spectrum of **5b** in d_6-DMSO



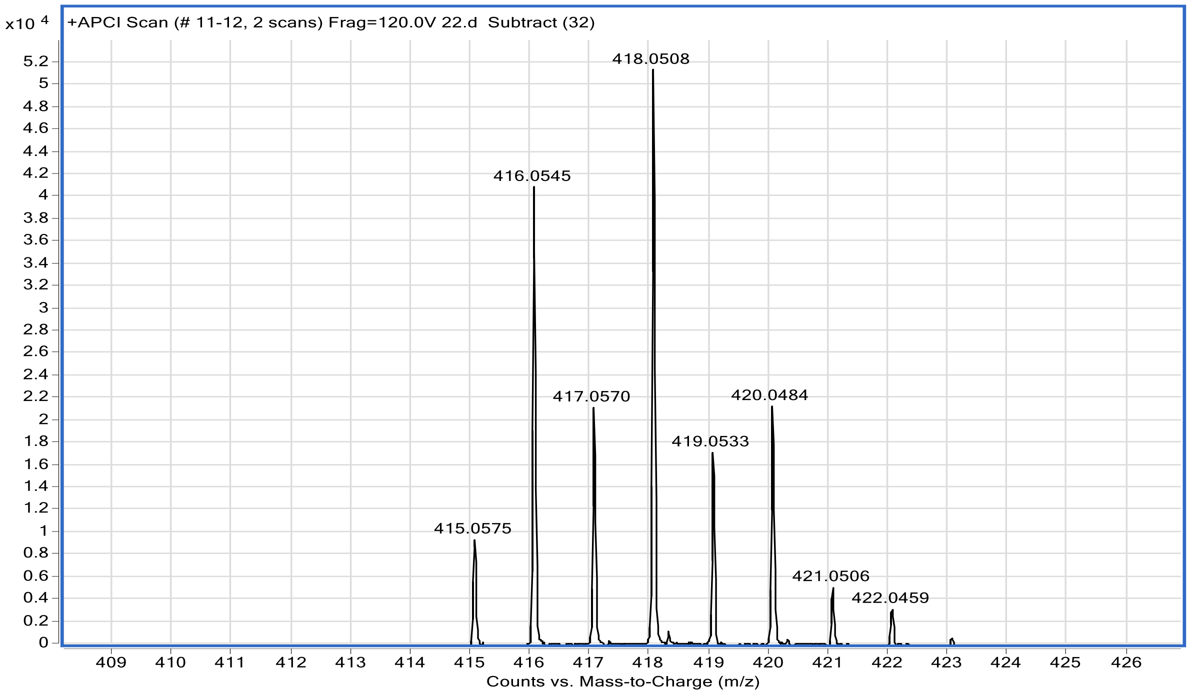
^{13}C NMR spectrum of **5b** in d_6-DMSO



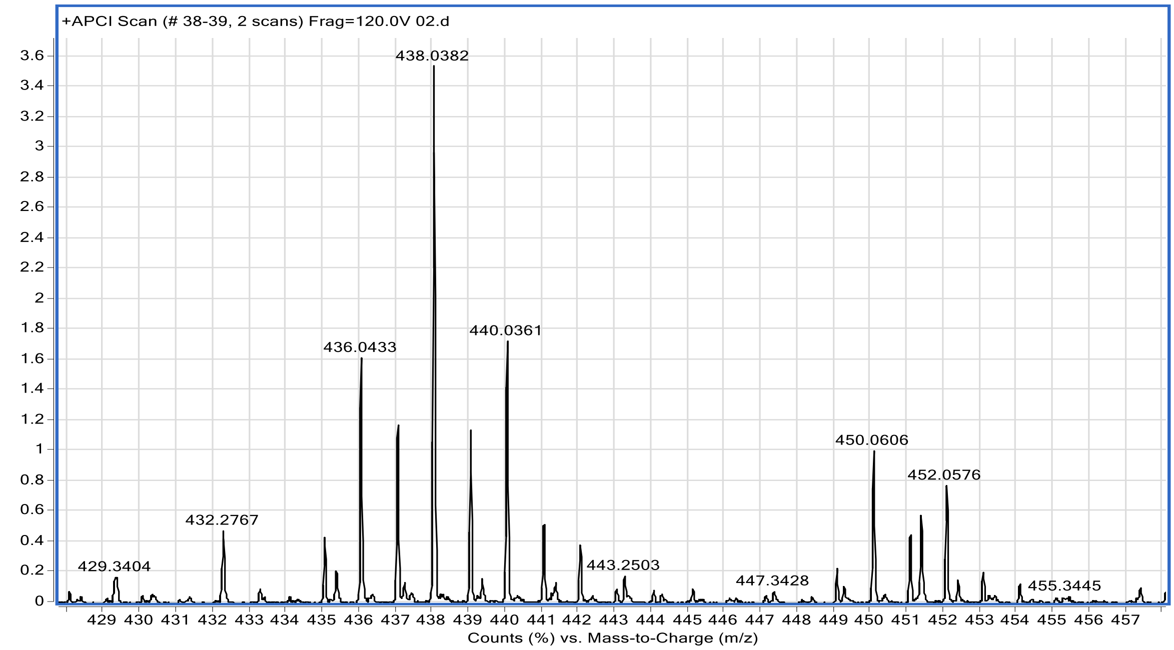
HRMS for **3a**



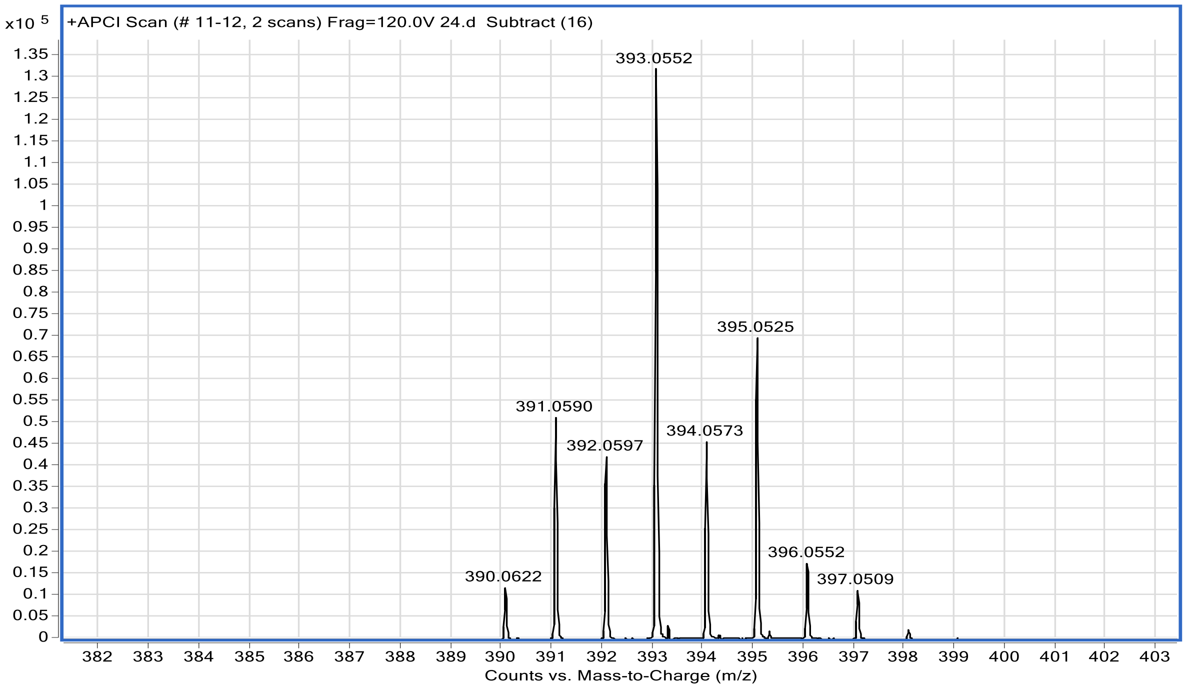
HRMS for **3b**



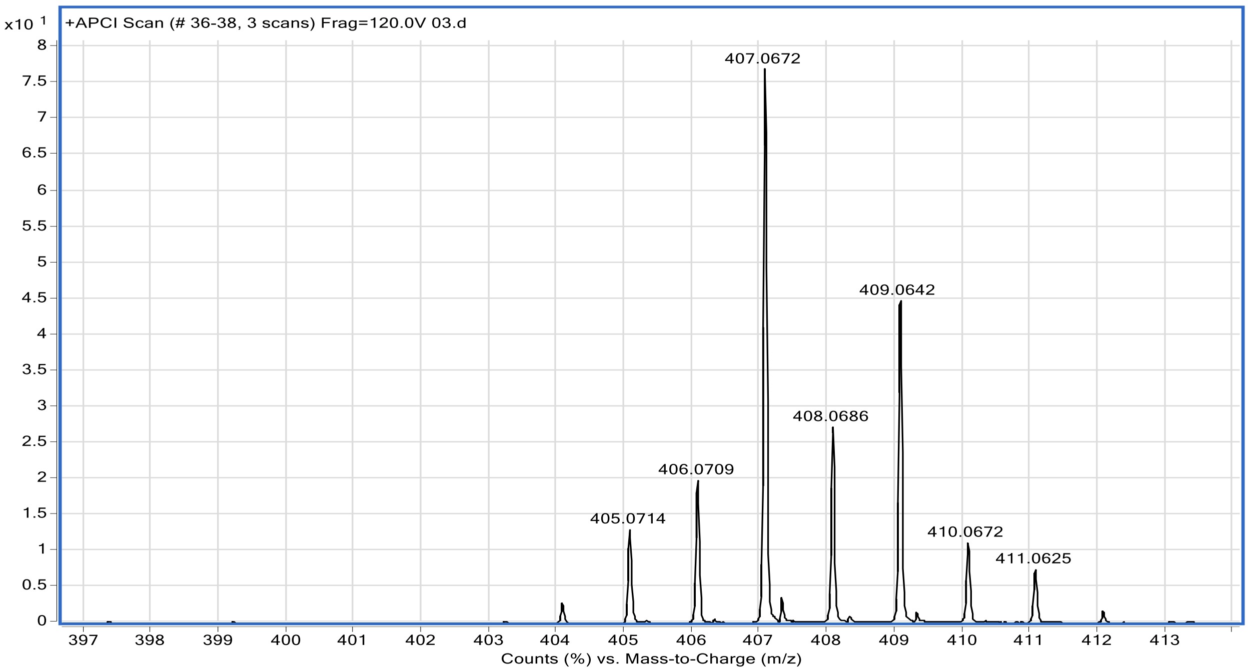
HRMS for **3c**



HRMS for **3d**



HRMS for **3e**



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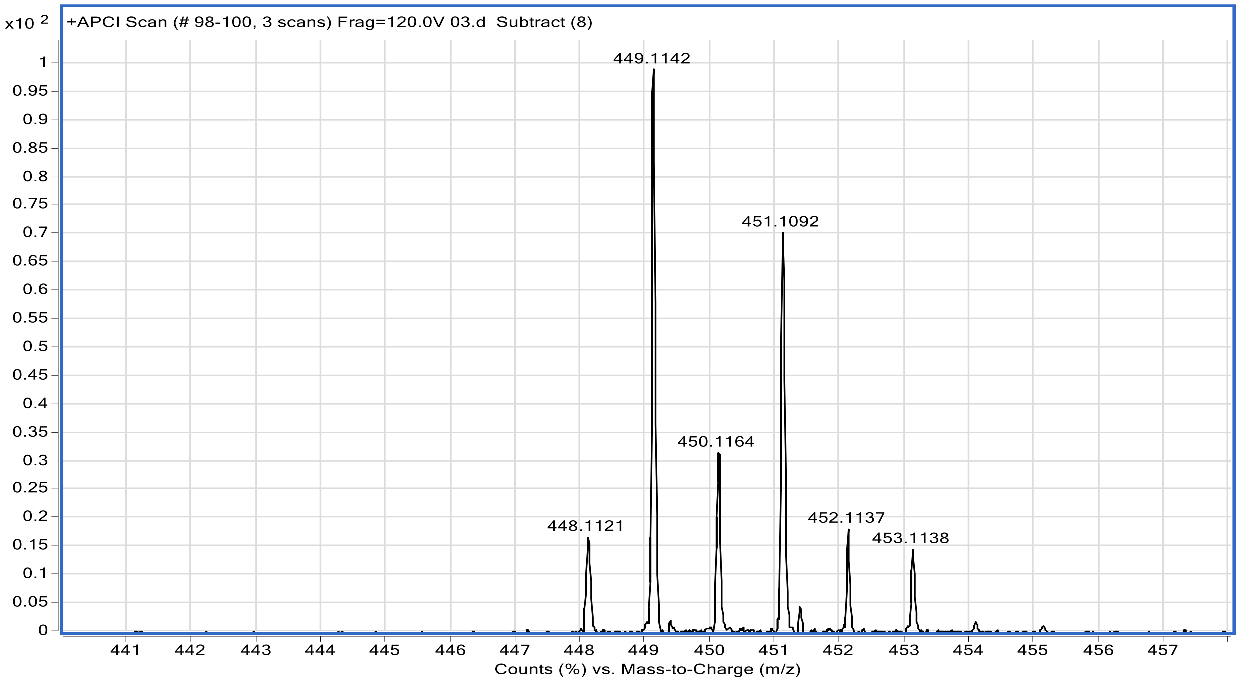

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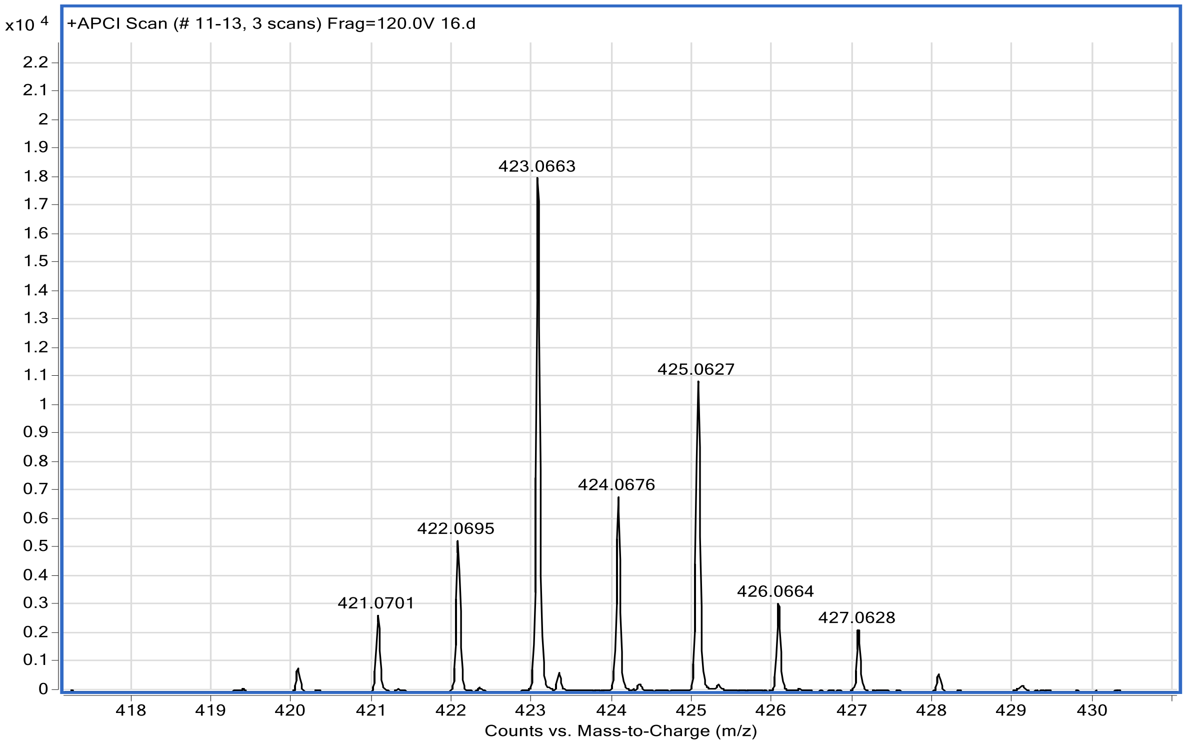

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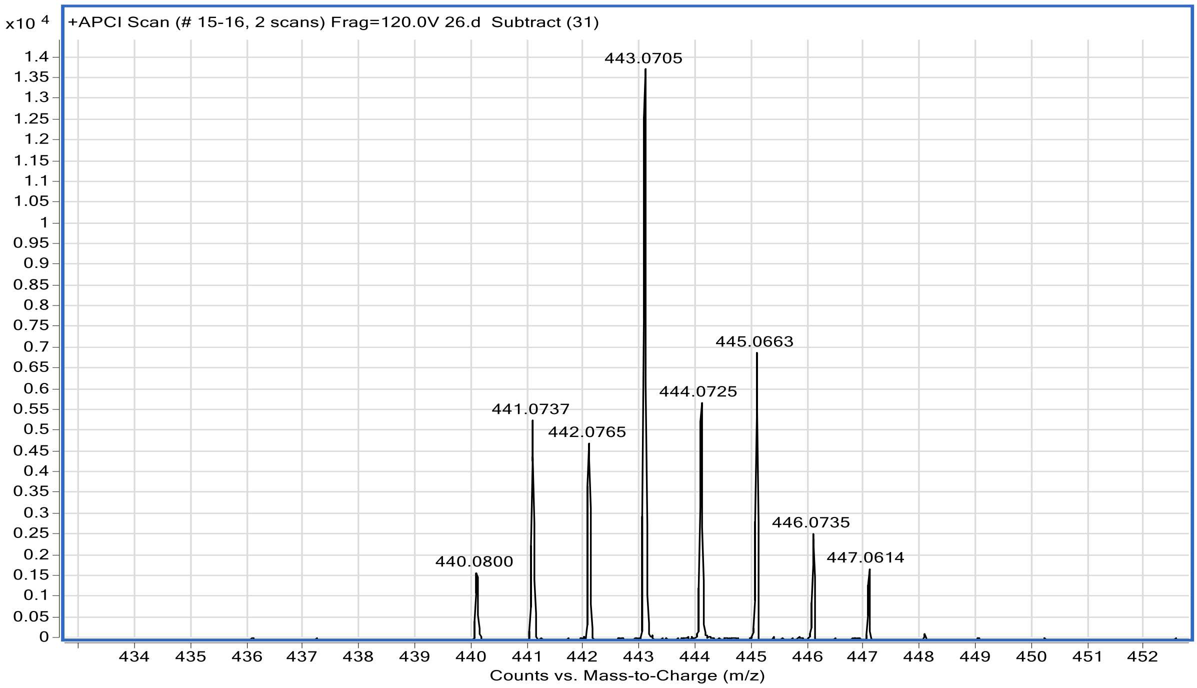
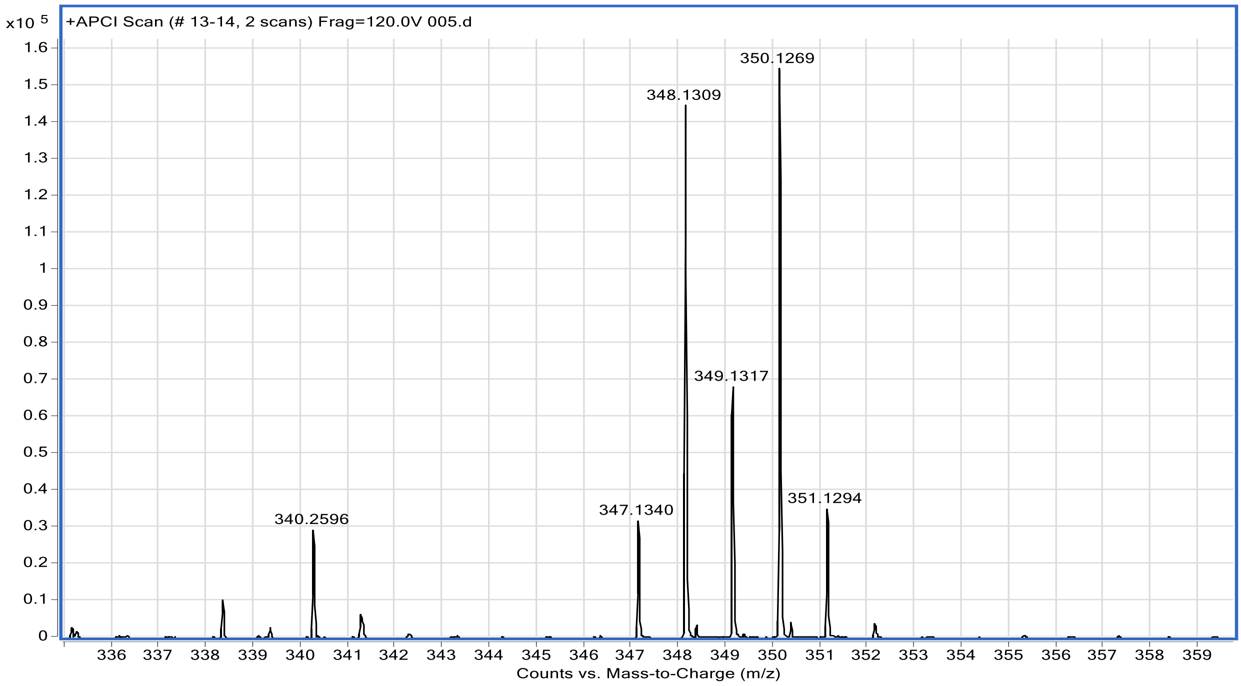
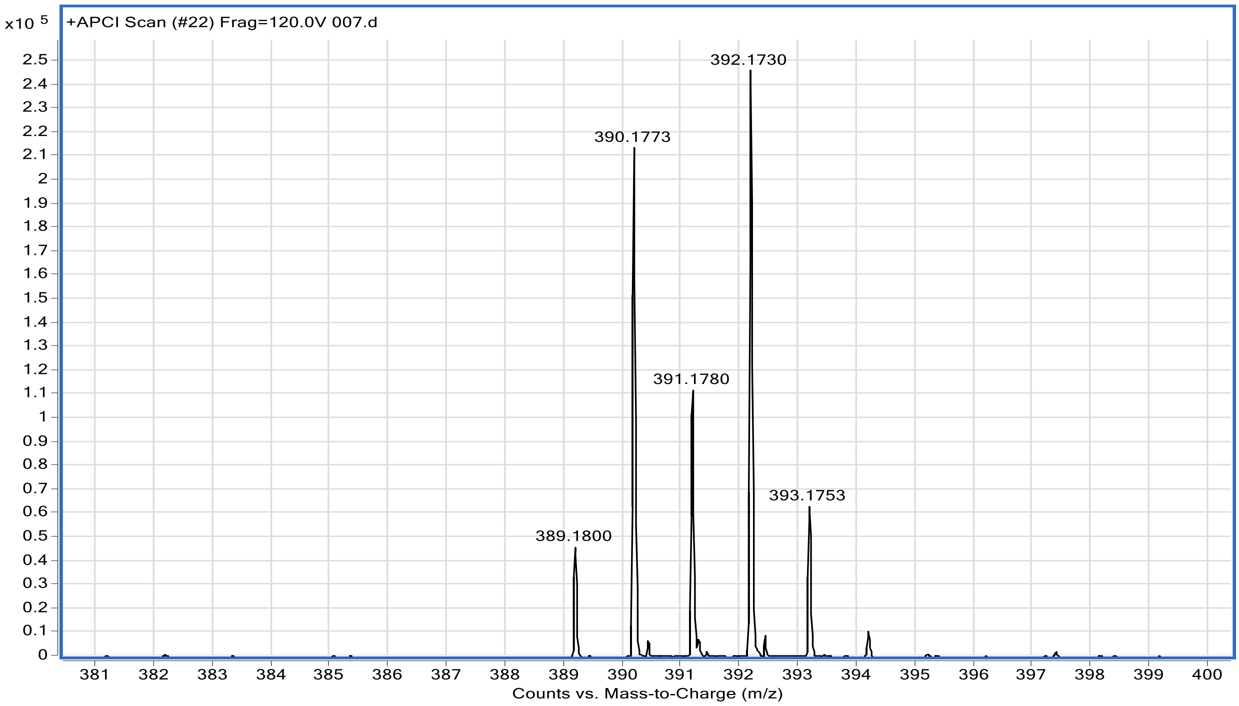


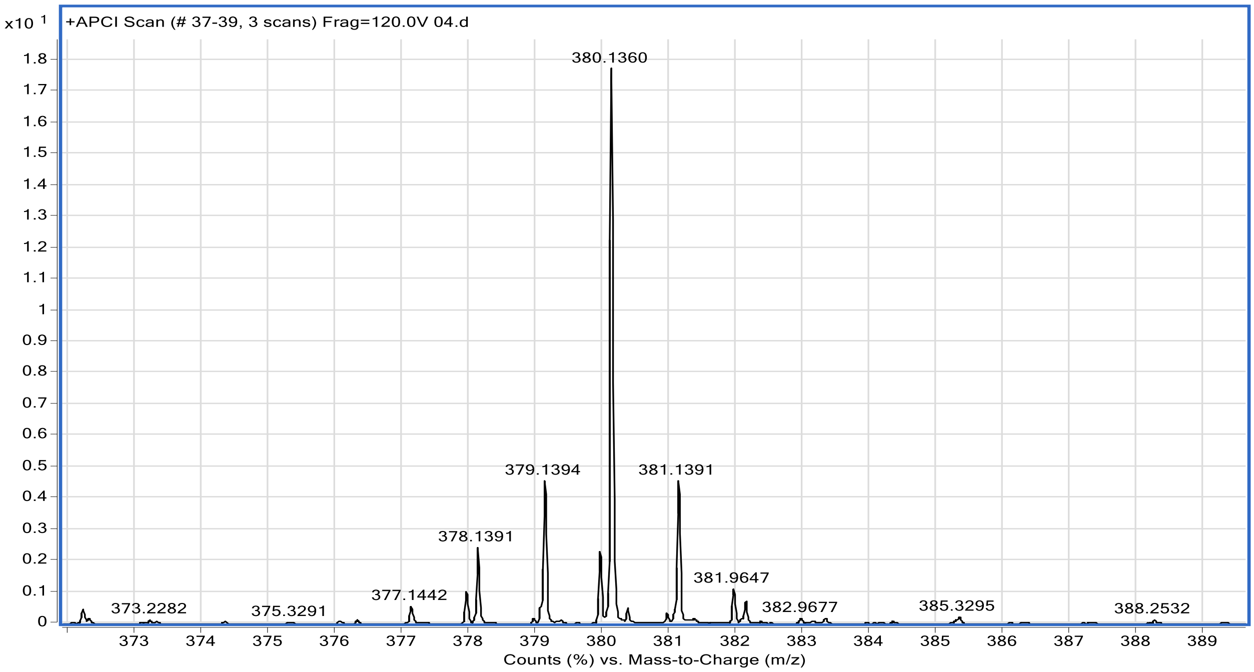
HRMS for **3i**



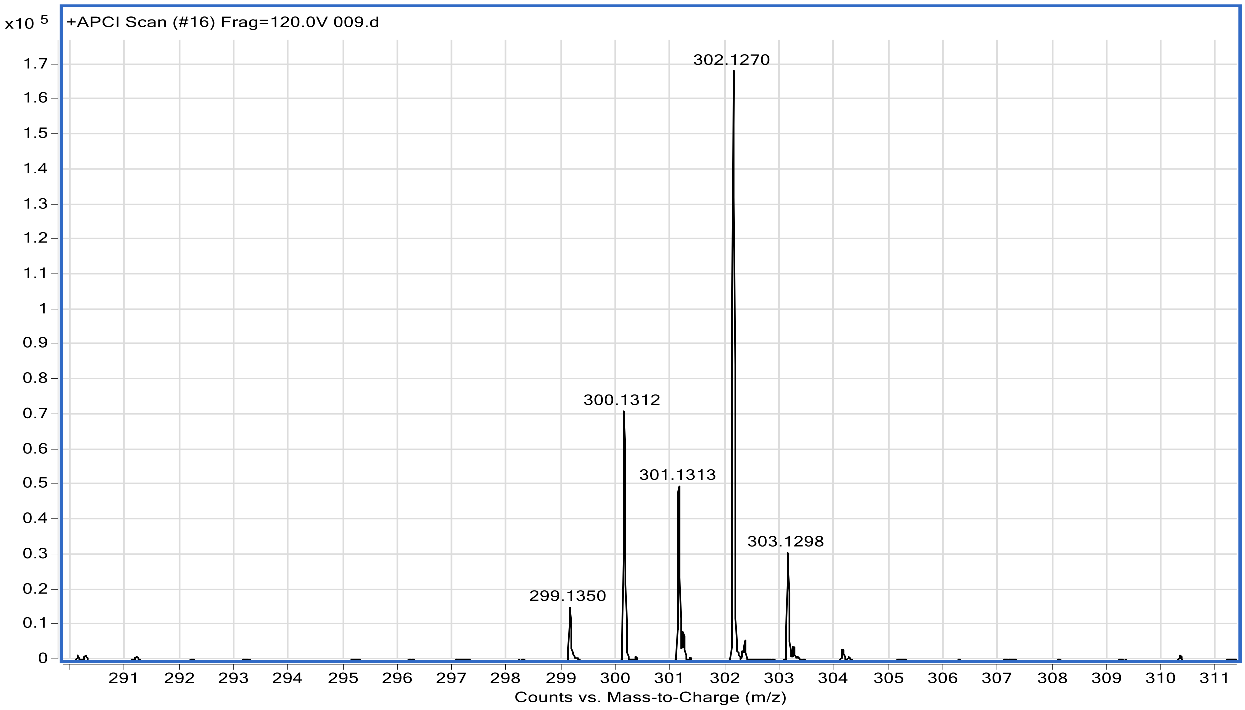
HRMS for **3j**



HRMS for **3k**



HRMS for **3l**



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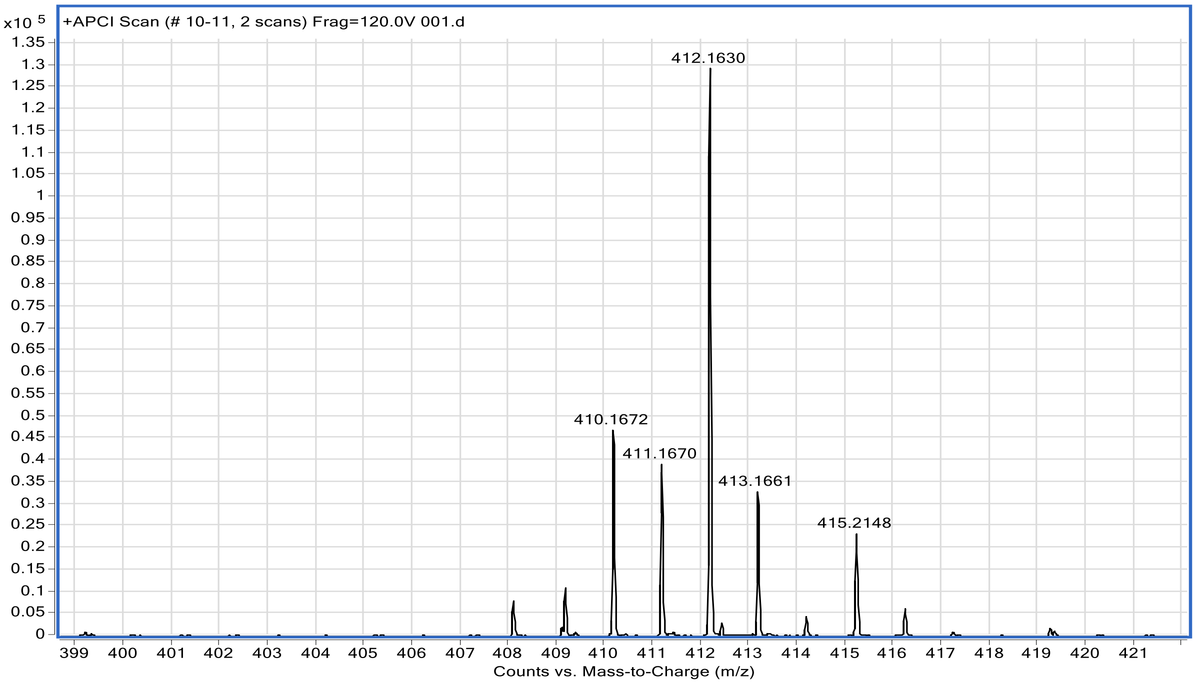

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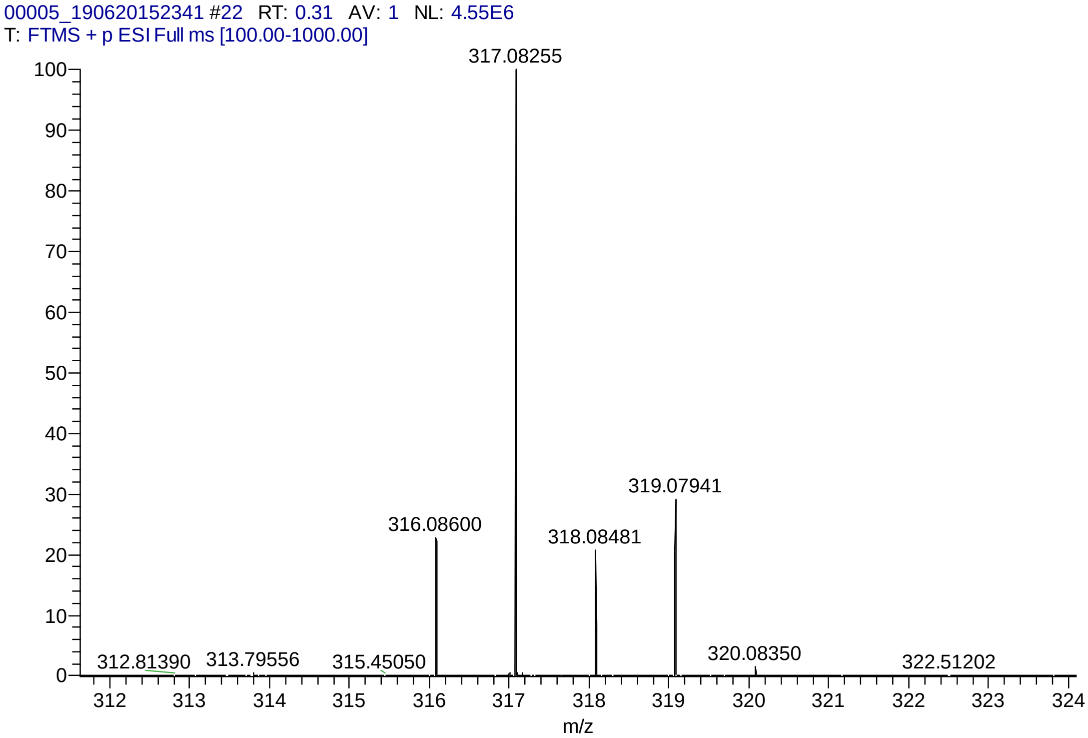
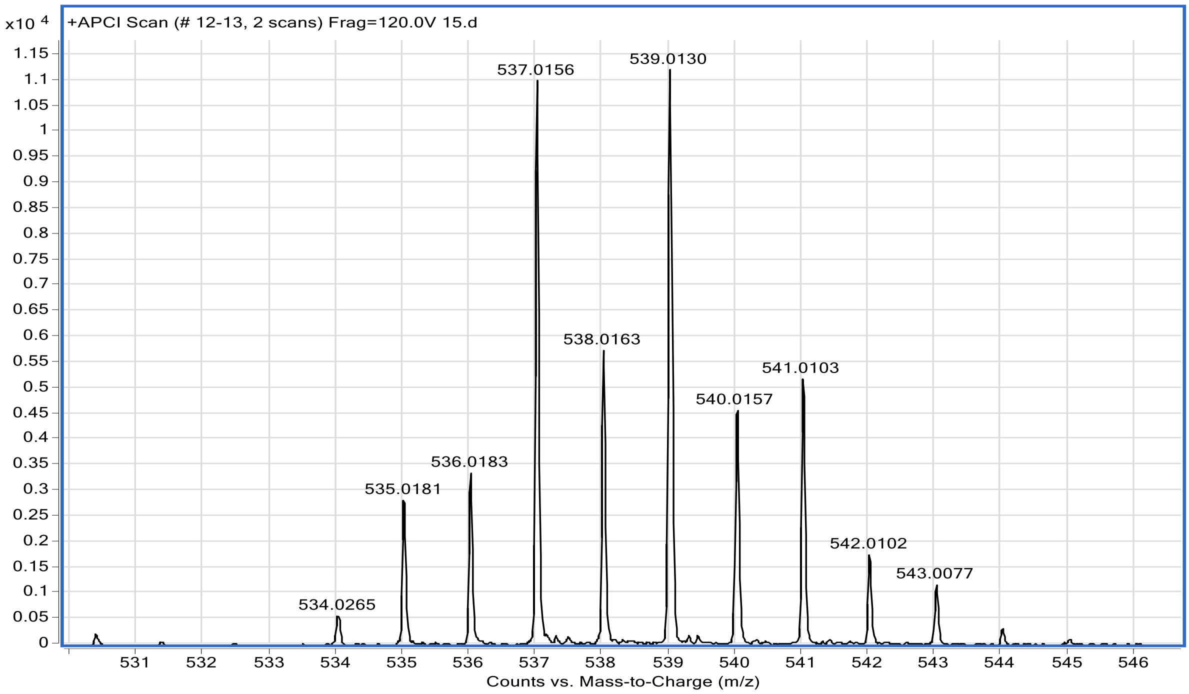
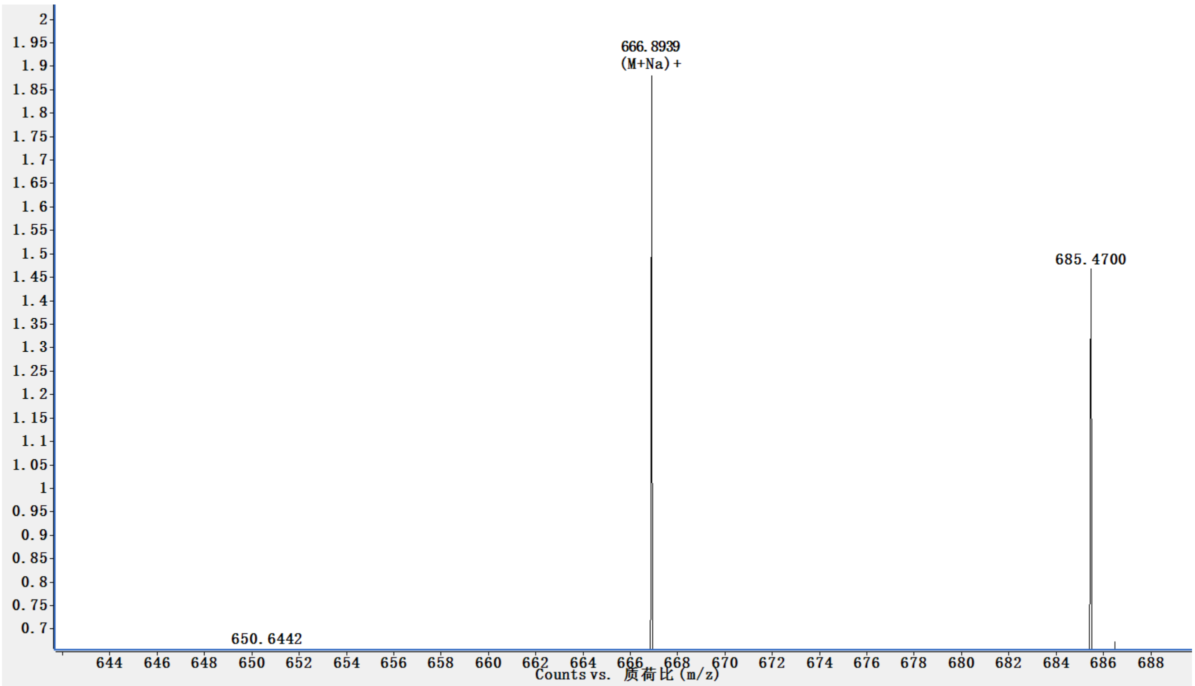


HRMS for **3o**



HRMS for **4a**



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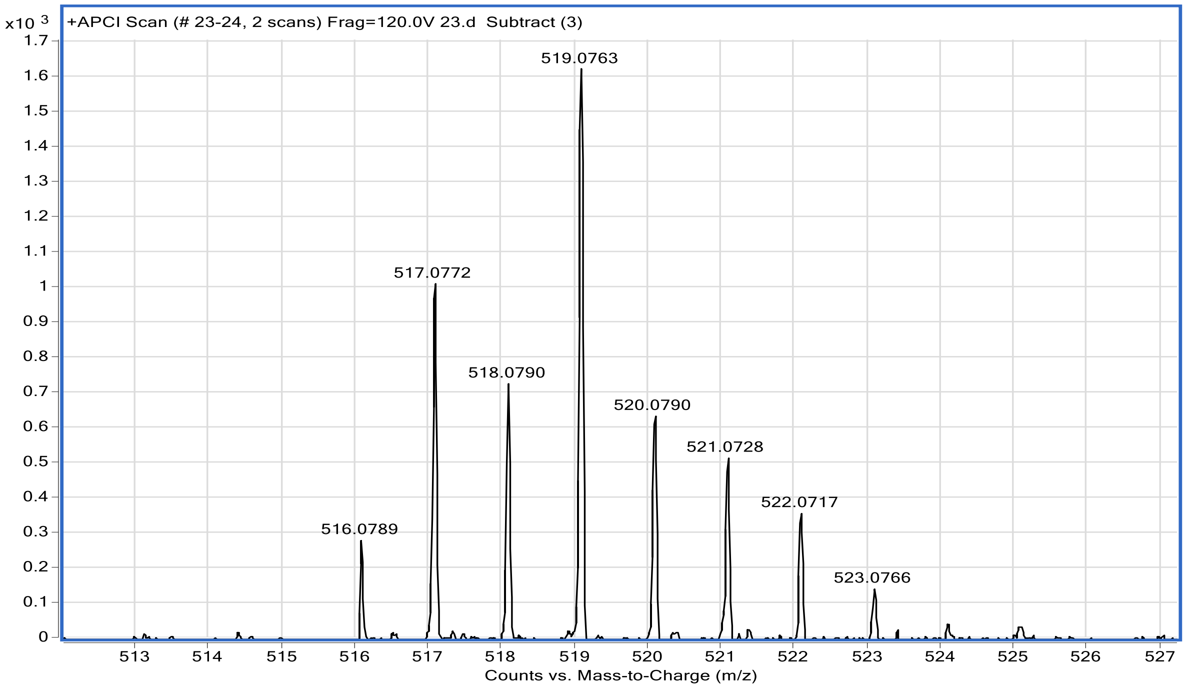

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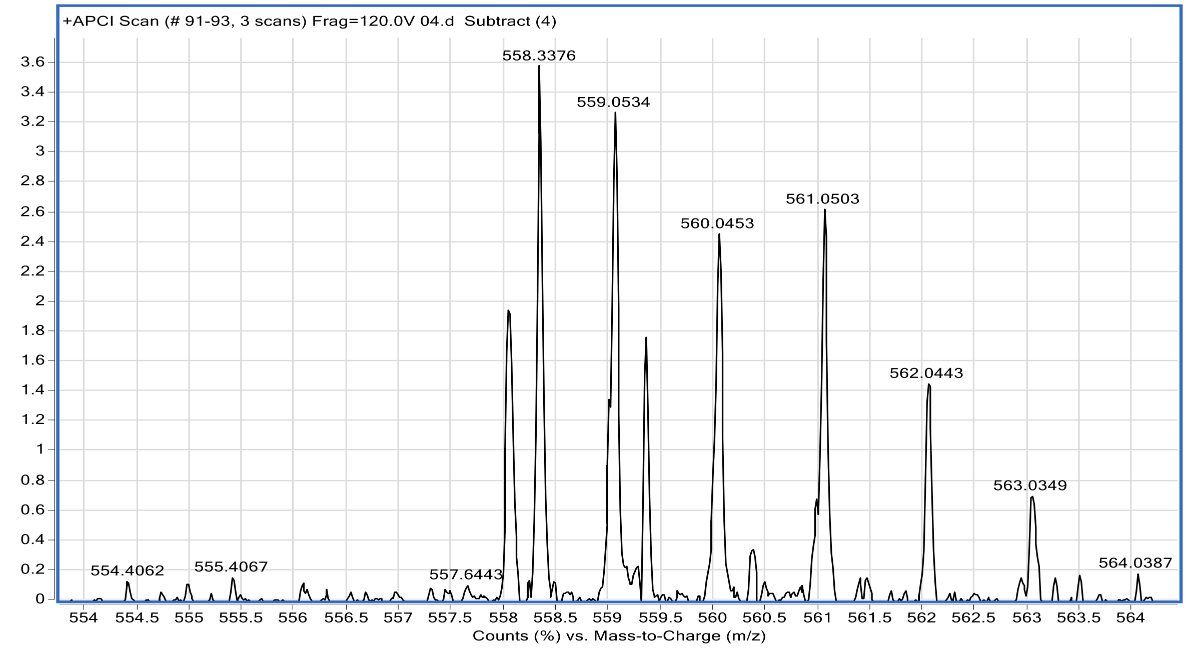

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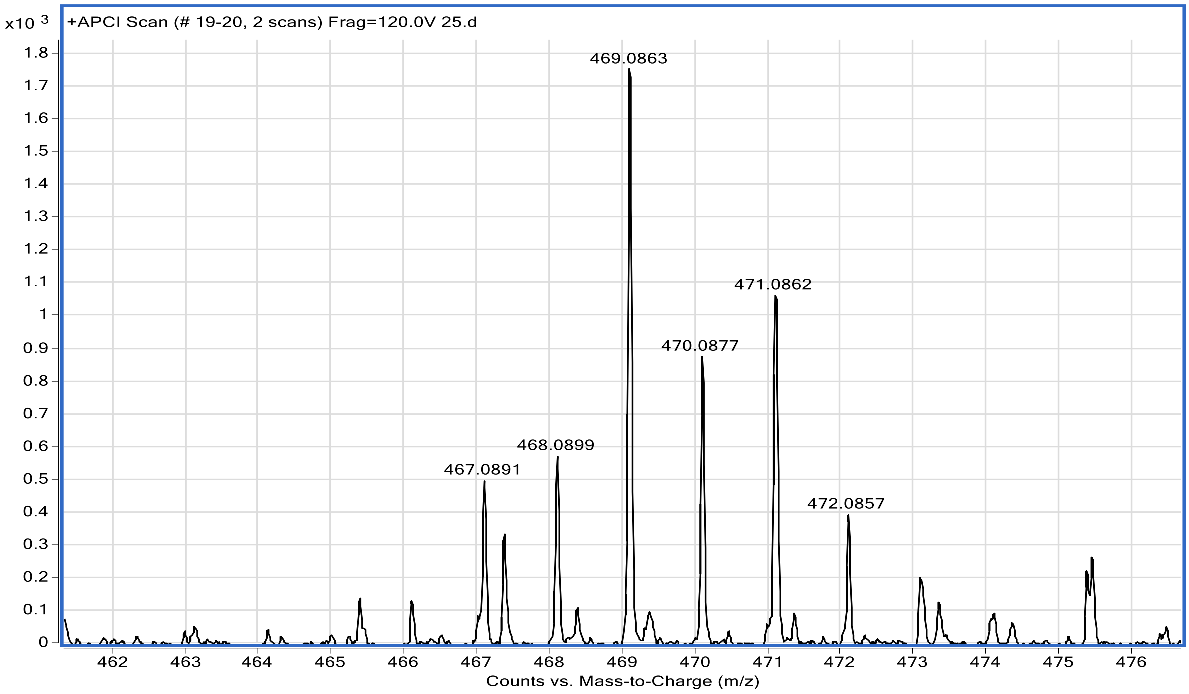

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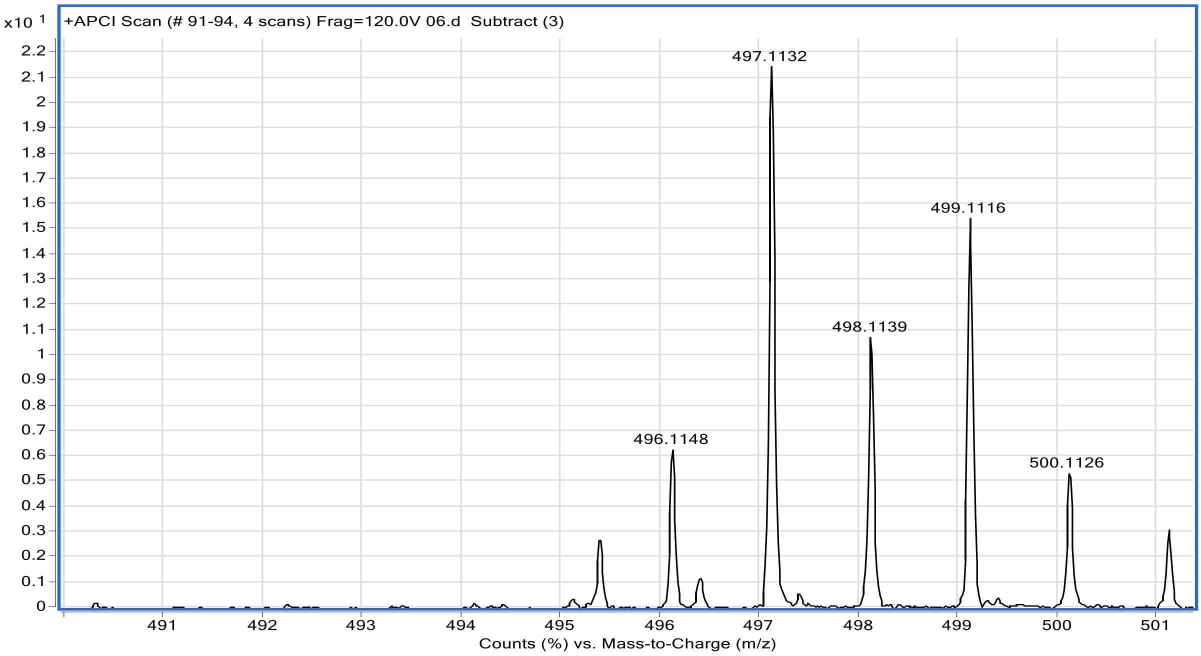

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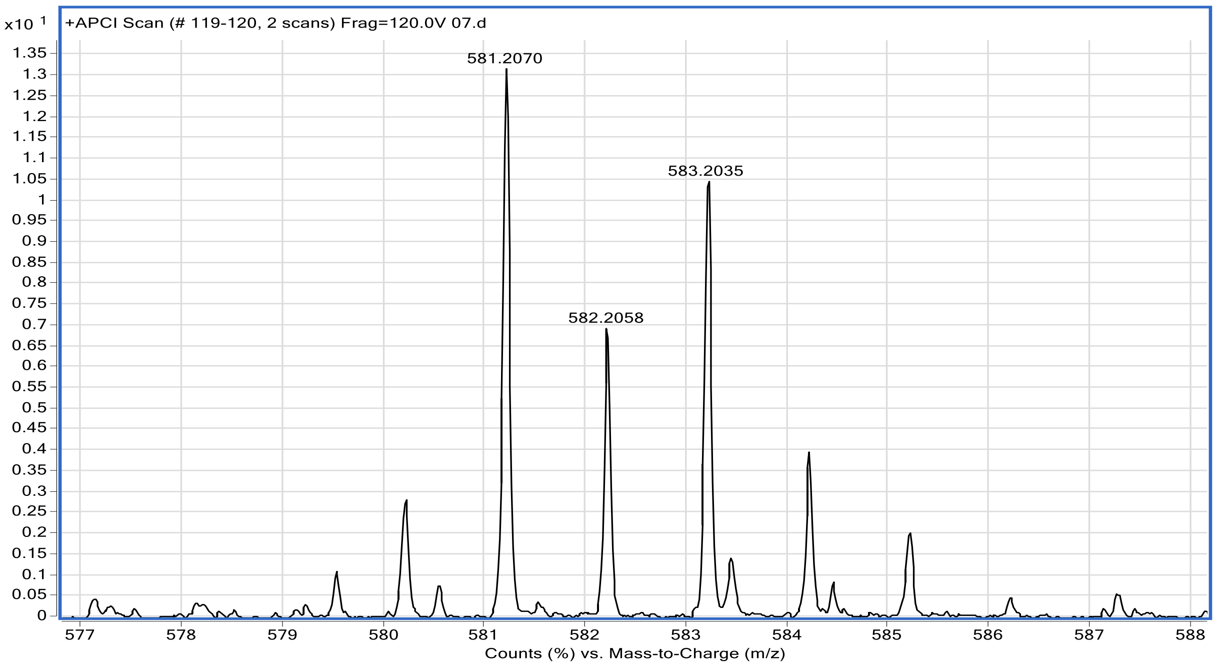

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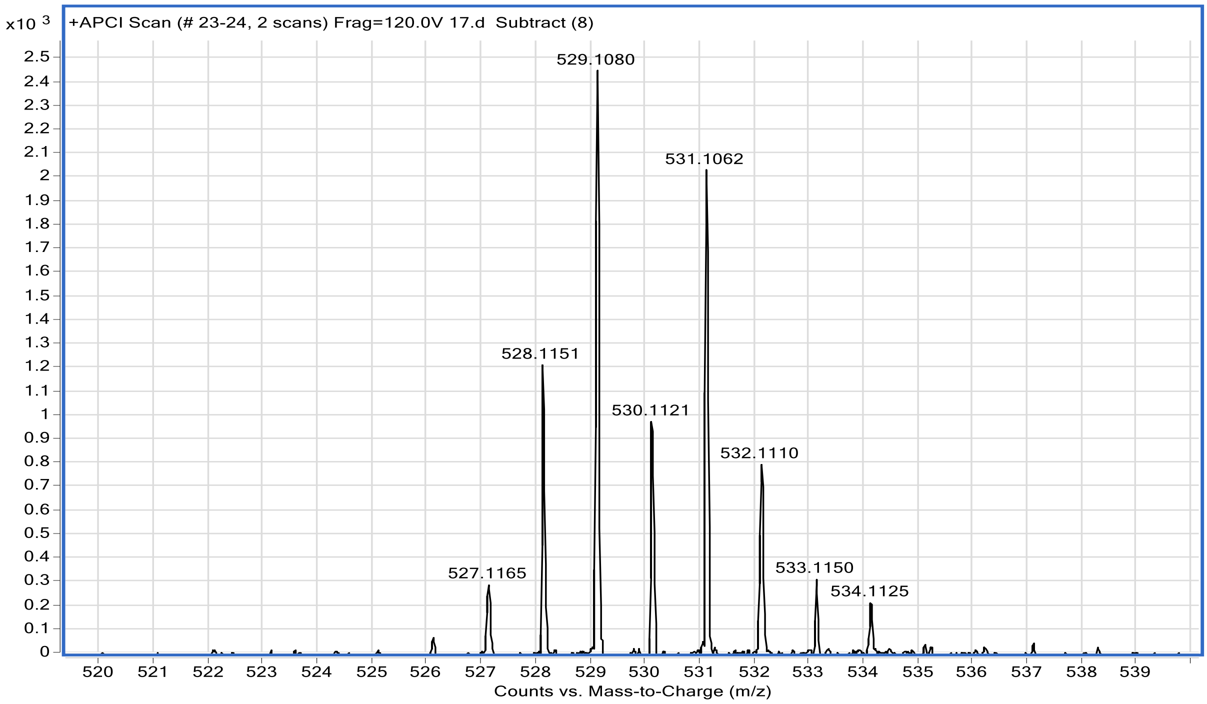

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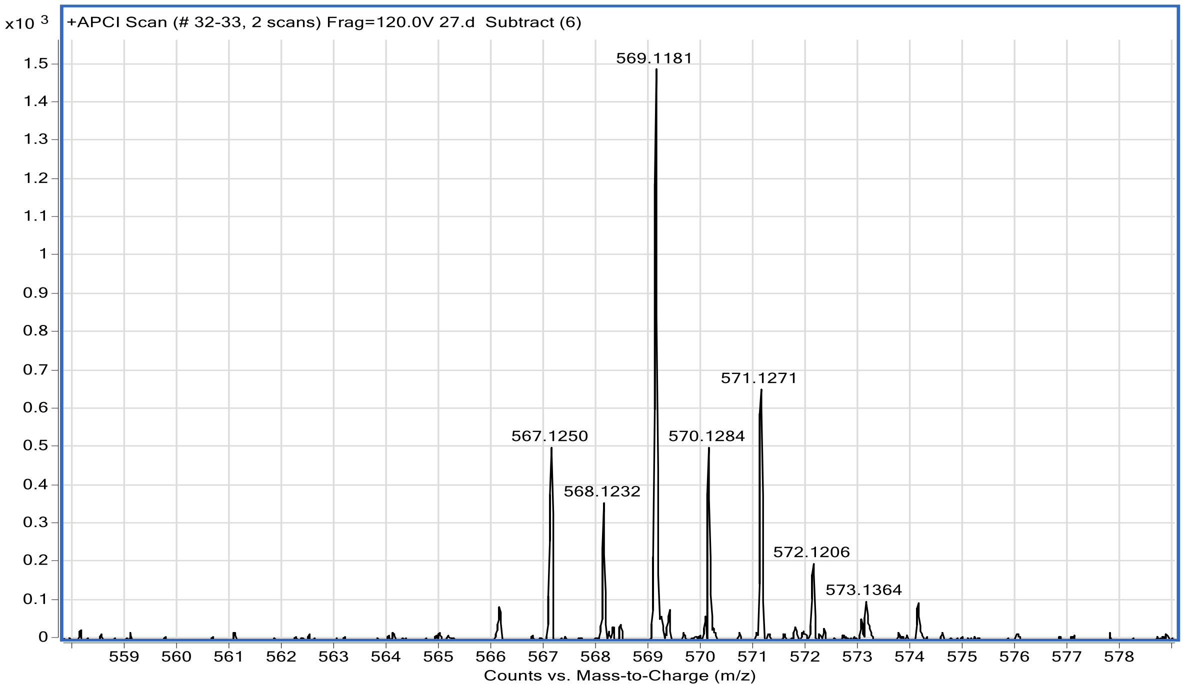

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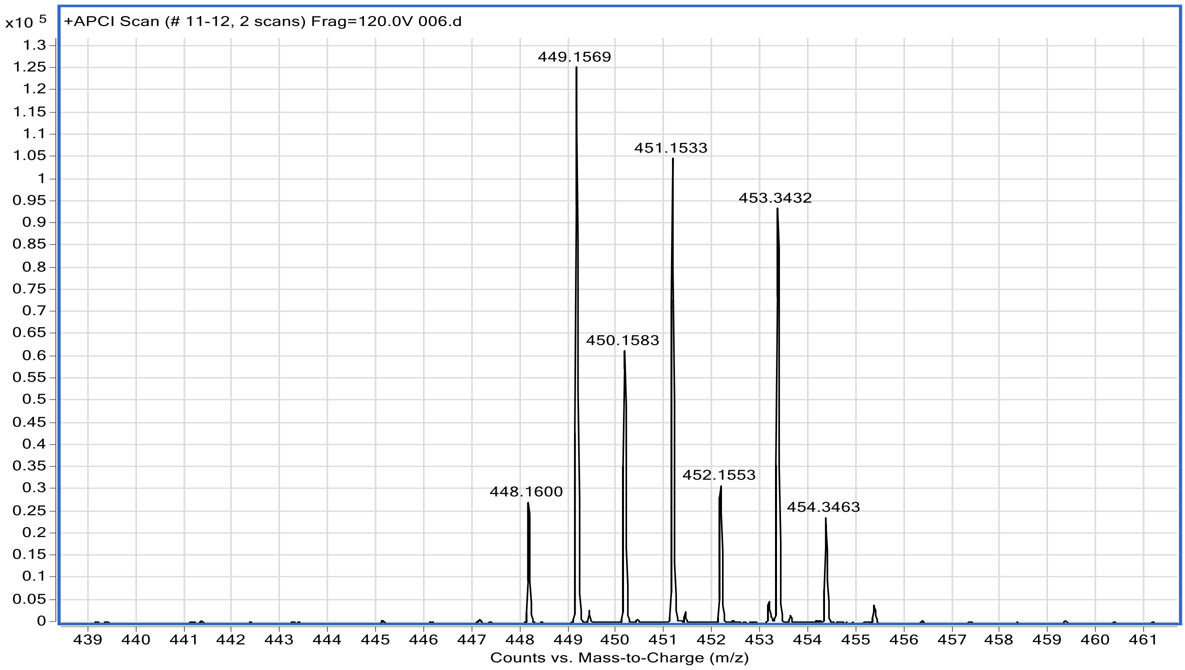

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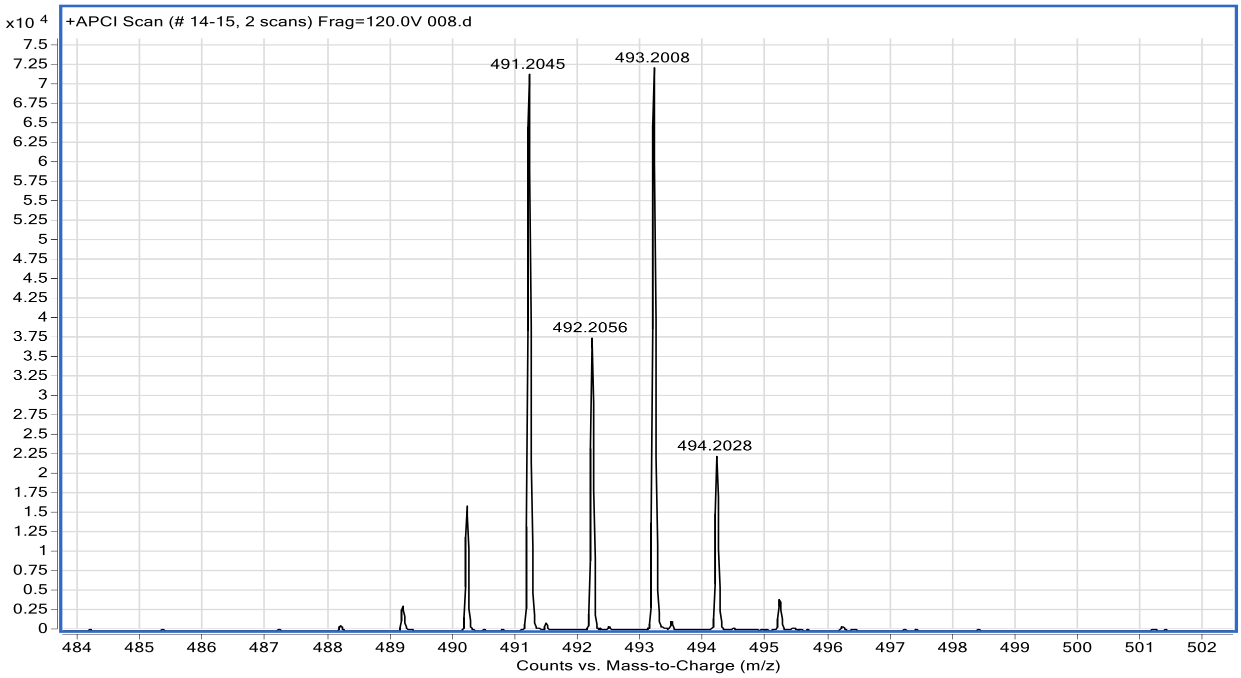
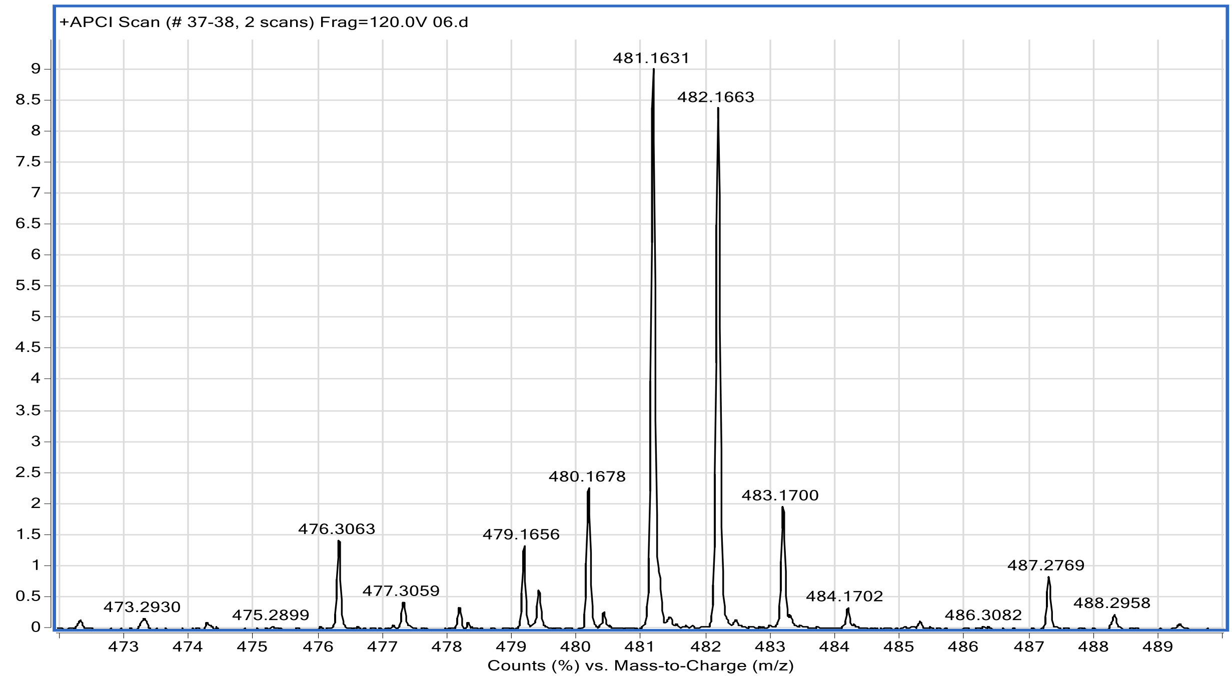
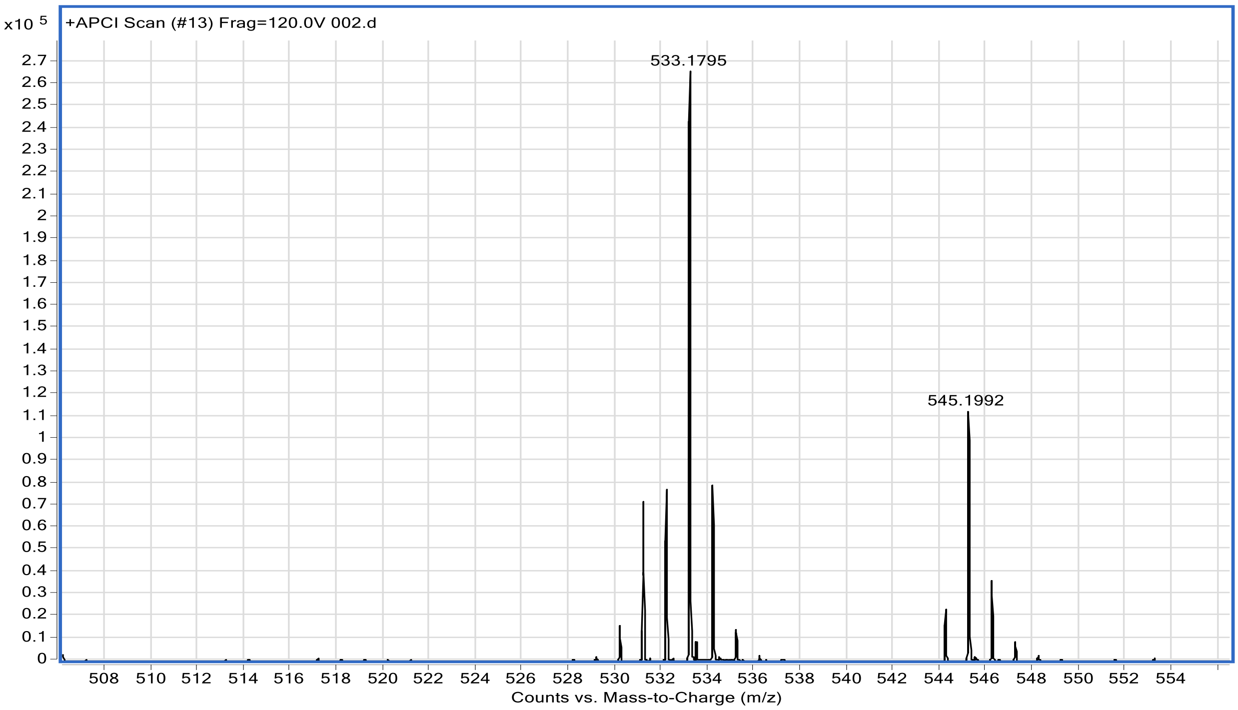


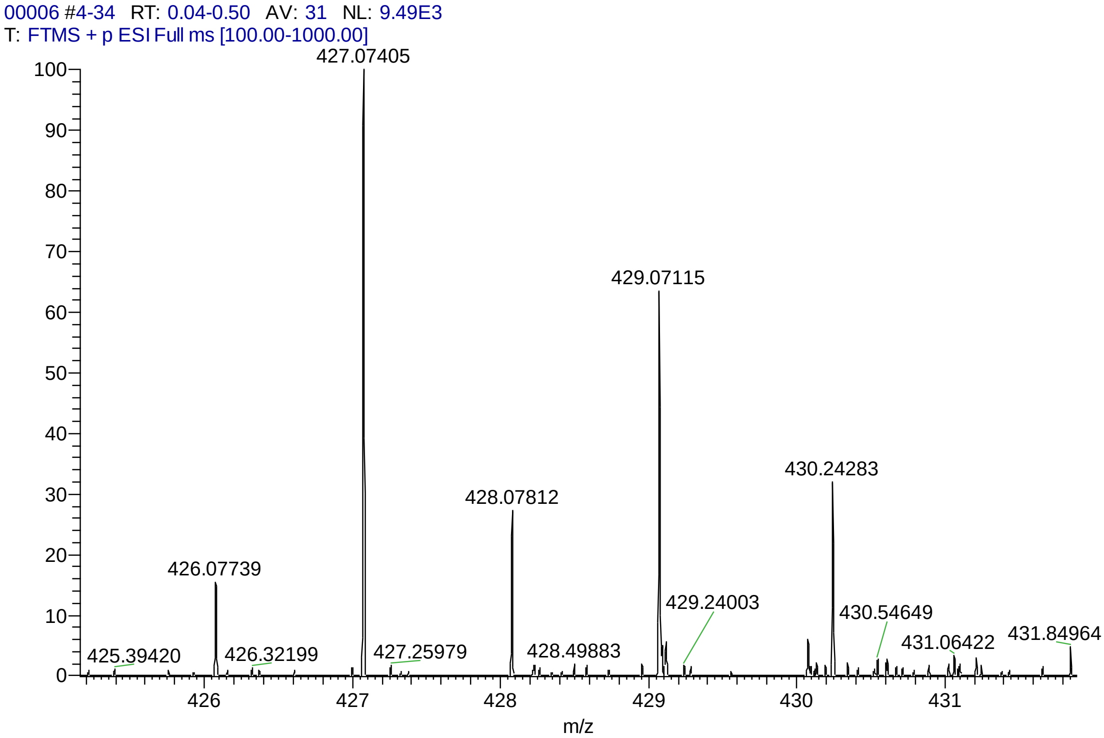
HRMS for **4k**



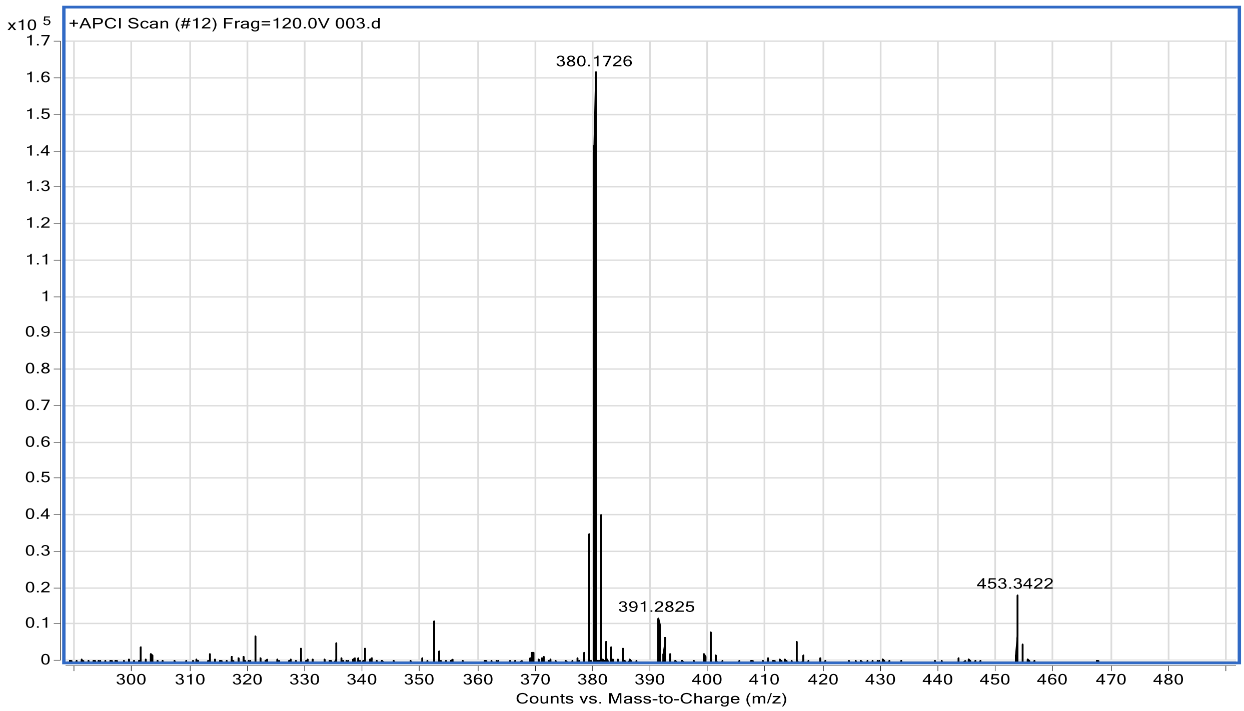
HRMS for **4l**



HRMS for **4n**



HRMS for **4o**



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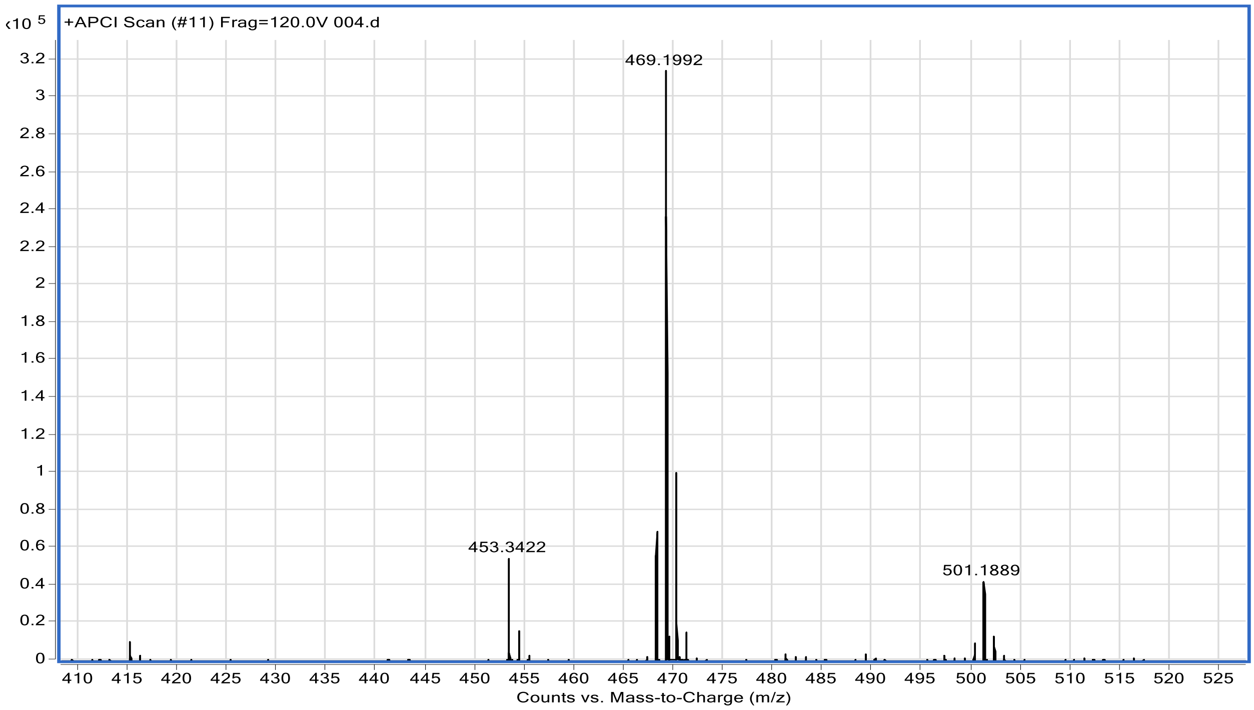
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469.1992
453.3422
501.1889
Counts vs. Mass-to-Charge (m/z)

HRMS for **5b**

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