Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

for

Dithienoazaborine Derivatives with Selective π-Conjugated Extension via Late-Stage Functionalization

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Contents

1. Materials and instrumentation

General. All reactions were performed using standard Schlenk and glovebox (Vigor) techniques at argon atmosphere. Diethyl ether, tetrahydrofuran, hexanes, toluene and 1,2-dichlorobenzene were distilled from sodium/benzophenone prior to use. Aniline (99.5%), 4-hexylaniline (98%), N-bromosuccinimide (NBS) (98%), bis(pinacolato)diboron (B_2Pin_2) (98%), bromobenzene (99.5%), tributylphenyltin (97%), 2-bromothiophene (98%), 2-(tributylstannyl)thiophene (97%), sodium tert-butoxide ($NaOBu^t$) (98%), tri-tert-butylphosphine tetrafluoroborate ($[HP^tBu_3]BF_4$) (98%), 4,4′-di-tert-butyl-2,2′-dipyridyl (dtbpy) (98%), (1,5-Cyclooctadiene)(methoxy)iridium(I) Dimer ($[Ir(OMe)(Cod)]_2$) (96%), tri-o-tolylphosphine (P-(o-Tolyl)$_3$) (98%), methyl trioctyl ammonium chloride (aliquat-336) (98%), tris(dibenzylideneacetone) dipalladium ($Pd_2(dba)_3$) (98%), tetrakis(triphenylphosphine) palladium ($Pd(PPh_3)_4$) (99%), and potassium carbonate (99%) were purchased from Energy Chemical Inc. Phenylborondichloride ($PhBCl_2$) was obtained from Sigma-Aldrich. 3-bromo-2,2'-bithiophene (**1**) was prepared according to literature procedures,[1] (3-hexylthiophene-2,5-diyl)bis(tributylstannane) (**8a**) was prepared according to literature procedures,[2] and 2,5-dibromo-3-hexylthiophene (**8b**) was prepared according to literature procedures.[3] Unless otherwise indicated, all other reagents and solvents were used as commercially available without further purification. Column chromatographic purification of products was accomplished using 200-300 mesh silica gel.

NMR spectra were measured on a Bruker Avance-400 as well as JOEL 400 (^{11}B NMR spectra of **7b** and **7c**) spectrometer in the solvents indicated; chemical shifts are reported in units (ppm) by assigning TMS resonance in the ^{1}H spectrum as 7.26 ppm, $CDCl_3$ resonance in the ^{13}C spectrum as 77.0 ppm. Coupling constants are reported in Hz with multiplicities denoted as s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). UV-Vis measurements were performed using DH-2000-BAL Scan spectrophotometer. Fluorescence measurements were conducted on an FLS920 system. The photoluminescence quantum efficiency, time-resolved fluorescence were obtained using Edinburgh FLSP980 fluorescence spectrophotometer equipped with a xenon lamp (Xe900), a picosecond pulsed laser (EPL-375), a microsecond flash-lamp (μF900) and an integrating sphere, respectively. Single crystal X-ray diffraction analysis was carried out on a Bruker Apex Duo instrument. The molecular weight of the oligomers was determined by gel permeation chromatography (GPC) on a PL-GPC 220-type at the temperature of 150 °C. 1,2,4-Trichlorobenzene (TCB) was used as the eluent at a flow rate of 1.0 mL min^{-1} and monodisperse polystyrene was used as the standard. High-resolution mass spectra (HRMS) were collected on a Bruker maXisUHR-TOF mass spectrometer in an ESI positive mode for all small molecules. The mass spectrometry data of oligomers were collected on a Bruker maxis MALDI-TOF mass spectrometer in electron spray ionization-positive mode.

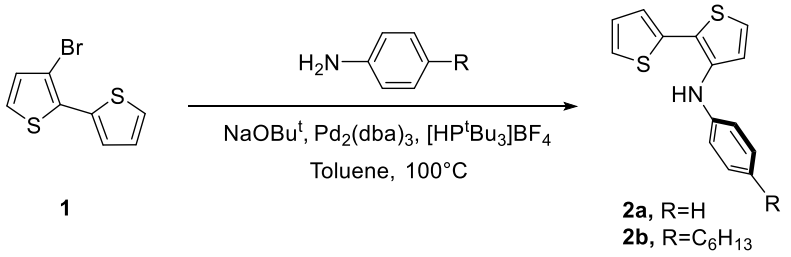
Cyclic voltammograms were recorded with a CHI660E/B15721b electrochemical analyzer using degassed and dried DCM under an argon atmosphere. The CV cell consisted of a gold electrode, a Pt wire counter electrode, and an Ag/AgCl reference electrode. All measurements were performed using DCM solutions of samples with a concentration of 1 mM and 0.1 M $Bu_4N^+PF_6^-$ as a supporting electrolyte with a scan rate of 100 mVs^{-1}. Potentials are determined against a ferrocene/ferrocenyl ion couple

(Fc/Fc$^+$). Thermogravimetric analysis (TGA) measurements were carried out in the temperature range of 30−700 °C by using a STA7300 thermal analysis system in nitrogen, at a heating rate of 10 K min^{-1}. A solution of n-tetrabutylammonium fluoride (TBAF) was prepared as the mother liquid which was used to carry out fluorescence titration experiments, and the concentration of this mother liquid was 1mM. In the exploration of the reversibility of optical behaviors, the concentration of added F^- was only 0.5 equivalent of BN compound in the solution.

All the computational calculations reported in this work were performed using the Gaussian 09 code. The geometries for the ground state of dimers for **7a** and **7b** was optimized at the B3LYP level with the B3LYP/6-31G(d) basis set. The geometries for the ground state of **3a**, **3b**, **5a**, **5b**, **6a** and **6b** were optimized at the B3LYP level with the 6-31G(d) and 6-31+G** basis set. The geometries for the ground state of **3a-F**, **3b-F**, **5a-F**, **5b-F**, **6a-F** and **6b-F** were optimized at the B3LYP level with the 6-31+G** basis set.[4-6] The simulated UV–Vis spectra for optimized molecules were performed at the time dependent density functional theory (TD-DFT)[7-8] at the ground-state equilibrium geometries were determined using the PBE0, in association with the 6-311+G** basis set. It should be pointed out that the structures of all stationary points were fully optimized, and frequency calculations were performed at the same level. The frequency calculations confirmed the nature of all revealed equilibrium geometries: there were no imaginary frequencies.

2. Experimental procedures and data

2.1 General procedure for the synthesis of N-phenyl-[2,2'-bithiophen]-3-amine (2a) and N-(4-hexylphenyl)-[2,2'-bithiophen]-3-amine (2b):



A solution of 3-bromo-2,2'-bithiophene (2.45 g, 10 mmol), aniline (11 mmol), $NaOBu^t$ (1.16 g, 12.10 mmol), $Pd_2(dba)_3$ (293 mg, 0.32 mmol) and $[HP^tBu_3]BF_4$ (153.75 mg, 0.53 mmol) in 20 mL of toluene was heated for 20 h at 100 °C. And then the reaction mixture was cooled to room temperature, after filtration, the filtrate was concentrated under reduced pressure and the residue was purified by column chromatography over silica gel (petroleum ether : dichlorome = 10 : 1) to afford compound **2a** and compound **2b** as light yellow crystals. (1.85 g, 72%).

Compound **2a**. Yield: 1.85g (72%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.26-7.16 (m, 5H, Ar*H*), 7.09-7.02 (m, 2H, Ar*H*), 6.87 (dd, *J* = 5.5 Hz, 3.5 Hz, 3H, Ar*H*), 5.55 (s, 1H, N*H*).

^{13}C NMR (100 MHz, $CDCl_3$): δ 144.96, 136.57, 135.04, 129.39, 127.42, 124.91, 124.71, 124.64, 122.97, 122.60, 119.85, 115.36 (Ar-C).

HRMS (ESI$^+$) *m*/*z*: $[M + H]^+$ calcd for $C_{14}H_{12}NS_2$, 258.04057, found, 258.04001.

Mp (°C): 86.3-87.8.

Compound **2b**. Yield: 2.39 g (70%).

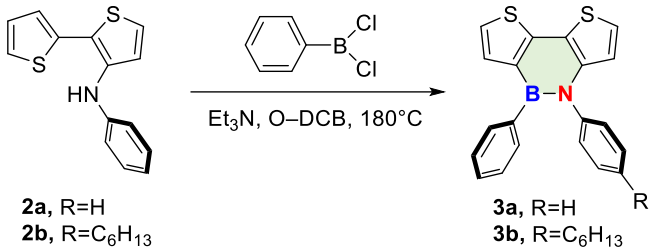
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24 (d, *J* = 5.1 Hz, 1H, Ar*H*), 7.17 (dd, *J* = 10.3 Hz, 4.5 Hz, 2H, Ar*H*), 7.07-7.02 (m, 4H, Ar*H*), 6.82 (d, *J* = 8.3 Hz, 2H, Ar*H*), 5.54 (s, 1H, N*H*), 2.56-2.51 (m, 2H, -CH_2), 1.63-1.55 (m, 2H, -CH_2), 1.37-1.27 (m, 6H, -CH_2), 0.89 (t, *J* = 6.6 Hz, 3H, -CH_3).

^{13}C NMR (100 MHz, $CDCl_3$): δ 142.47, 137.41, 135.24, 134.75, 129.22, 127.43, 124.69, 124.50, 124.15, 122.95, 115.89 (Ar-C), 35.19, 31.79, 31.73, 29.04, 22.66, 14.14 (hexyl-C).

HRMS (ESI$^+$) *m*/*z*: [M + H]$^+$ calcd for $C_{20}H_{24}NS_2$, 342.13447, found, 342.13396.

Mp (°C): 50.7-51.9.

2.2 General procedure for the synthesis of 4,5-diphenyl-4,5-dihydrodithieno[3,2-c: 2',3'-e][1,2]azaborinine (3a) and 4-(4-hexylphenyl)-5-phenyl-4,5-dihydrodithieno[3, 2-c:2',3'-e][1,2] azaborinine (3b):



2a, R=H
2b, R=C_6H_{13}

3a, R=H
3b, R=C_6H_{13}

To a solution of **2a** or **2b** (5 mmol) and triethylamine (1.14 g, 11.25 mmol) in o-dichlorobenzene (20 mL) was added dropwise a solution of $PhBCl_2$ (1.19 g, 7.5 mmol) in o-dichlorobenzene (5 mL) via syringe. The reaction mixture was heated at 180 °C for 15h. After removal of the solvent under reduced pressure, the residue was purified by column chromatography over silica gel (petroleum ether : dichlorome = 10 : 1) to afford compound **3a** and compound **3b** as white solids.

Compound **3a**. Yield: 1.15g (67%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (d, *J* = 5.0 Hz, 1H, Ar*H*), 7.36-7.26 (m, 6H), 7.22-7.15 (m, 6H, Ar*H*), 6.61 (d, *J* = 5.5 Hz, 1H, Ar*H*).

^{13}C NMR (100 MHz, $CDCl_3$): δ 147.21, 145.01, 143.39, 133.74, 132.68, 128.99, 128.67, 127.29, 127.09, 127.08, 122.65, 122.09, 120.11, 118.82 (Ar-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 34.50 (br).

HRMS (ESI$^+$) *m*/*z*: [M + H]$^+$ calcd for $C_{20}H_{15}BNS_2$, 344.0734, found, 344.0730.

Mp (°C): 183.2–185.1.

Compound **3b**. Yield: 1.52g (71%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 (d, *J* = 5.0 Hz, 1H, Ar*H*), 7.33-7.29 (m, 2H, Ar*H*), 7.26-7.15 (m, 5H, Ar*H*), 7.09 (dd, *J* = 21.6 Hz, 8.2 Hz, 4H, Ar*H*), 6.64 (d, *J* = 5.5 Hz, 1H, Ar*H*), 2.60 (t, *J* = 7.6 Hz, 2H, -CH_2), 1.64-1.57 (m, 2H, -CH_2), 1.30 (s, 6H, -CH_2), 0.90 (t, *J* = 6.6 Hz, 3H, -CH_3).

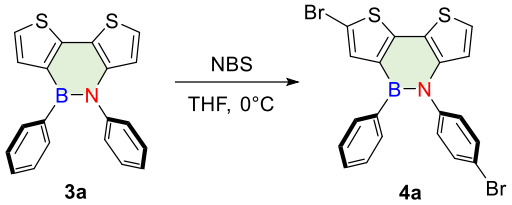
^{13}C NMR (100 MHz, $CDCl_3$): δ 147.16, 143.65, 142.54, 141.70, 133.84, 132.69, 128.88, 128.30, 127.21, 127.03, 122.52, 121.98, 120.26, 118.68 (Ar-C), 35.44, 31.73, 31.28, 28.76, 22.65, 14.14 (hexyl-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 34.27 (bs).

HRMS (ESI$^+$) *m*/*z*: [M + H]$^+$ calcd for $C_{26}H_{27}BNS_2$, 428.1673, found, 428.1672.

Mp (°C): 84.4–85.9.

2.3 Synthesis of 7-bromo-4-(4-bromophenyl)-5-phenyl-4,5-dihydrodithieno[3,2-c:2', 3'-e][1,2]azaborinine (4a):



To a solution of compound **3a** (1.03 g, 3 mmol) in THF (15 mL) at 0 °C was added dropwise a solution of NBS (1.19 g, 7.5 mmol) in THF (5 mL) via syringe. Then the mixture was slowly warmed to room temperature and stirred overnight. The solvent was removed under reduced pressure, the product was purified via column chromatography over silica gel (petroleum ether : dichlorome = 5 : 1) to afford compound **4a** as a white solid (0.96 g, 63%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46 (d, *J* = 8.4 Hz, 2H, Ar*H*), 7.36 (s, 1H, Ar*H*), 7.24 (s, 6H, Ar*H*), 7.06 (d, *J* = 8.4 Hz, 2H, Ar*H*), 6.60 (d, *J* = 5.5 Hz, 1H, Ar*H*).

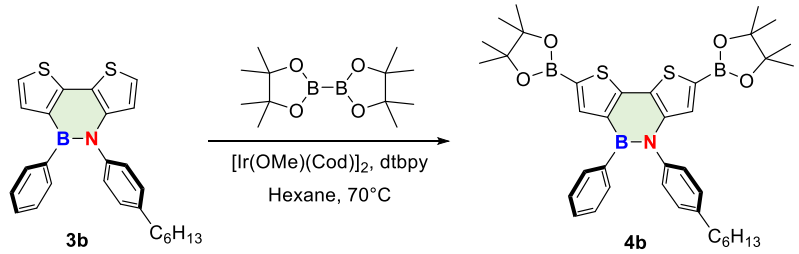
^{13}C NMR (100 MHz, $CDCl_3$): δ 148.54, 143.77, 142.93, 134.95, 133.47, 132.27, 130.21, 127.69, 127.43, 123.43, 120.94, 119.73, 118.19, 109.78 (Ar-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 34.14 (bs).

HRMS (ESI$^+$) *m*/*z*: [M + H]$^+$ calcd for $C_{20}H_{13}BBr_2NS_2$, 499.8944, found, 499.8909.

Mp (°C): 223.8–225.5.

2.4 Synthesis of 4-(4-hexylphenyl)-5-phenyl-2,7-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-4,5-dihydrodithieno[3,2-c:2',3'-e][1,2]azaborinine (4b):



A solution of compound **3b** (427 mg, 1 mmol), B_2Pin_2 (533.27 mg, 2.1 mmol), dtbpy (21.47 mg, 0.08 mmol) and $[Ir(OMe)(Cod)]_2$ (26.52 mg, 0.04 mmol) in 8 mL of hexane was heated for 15 h at 70 °C. Then the reaction mixture was cooled to room temperature, and the precipitate was isolated via vacuum filtration and washed with hexane. The remaining solid was purified by column chromatography over silica gel (petroleum ether : dichlorome = 1 : 1) to afford compound **4b** as a light brown solid (489 mg, 72%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (s, 1H, Ar*H*), 7.27 (dd, *J* = 4.8, 2.0 Hz, 2H, Ar*H*), 7.18-7.15 (m, 4H, Ar*H*), 7.10 (d, *J* = 8.3 Hz, 2H, Ar*H*), 7.04 (d, *J* = 8.3 Hz, 2H, Ar*H*), 2.63-2.58 (m, 2H, -CH_2), 1.65-1.59 (m, 2H, -CH_2), 1.36 (s, 12H, -CH_3), 1.33 (s, 12H, -CH_3), 1.31 (s, 6H, -CH_2), 0.90 (t, *J* = 6.7 Hz, 3H, -CH_3).

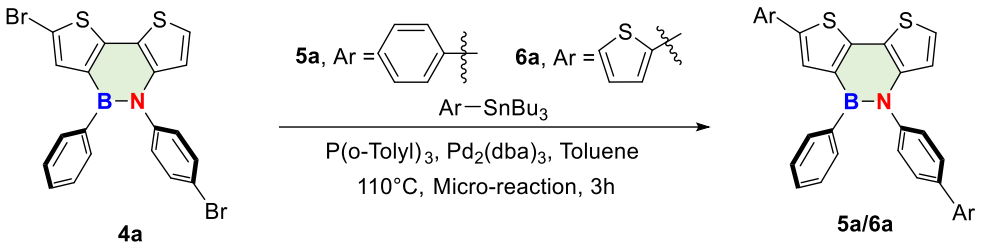
^{13}C NMR (100 MHz, $CDCl_3$): δ 151.79, 145.14, 143.95, 142.26, 141.61, 133.67, 128.94, 128.68, 128.36, 127.16, 127.01, 124.54, 84.49, 84.26 (Ar-C), 35.43, 31.73, 31.15, 28.78 (hexyl-C), 24.79, 24.73 (CH_3-C), 22.65, 14.15 (hexyl-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 29.84 (bs).

HRMS (ESI^+) *m*/*z*: $[M + H]^+$ calcd for $C_{38}H_{49}B_3NO_4S_2$, 680.3377, found, 680.3383.

Mp (°C): 227.5–228.4.

2.5 General procedure for the synthesis of 4-([1,1'-biphenyl]-4-yl)-5,7-diphenyl-4,5-dihydrodithieno[3,2-c:2',3'-e][1,2]azaborinine (5a) and 5-phenyl-7-(thiophen-2-yl)-4-(4-(thiophen-2-yl)phenyl)-4,5-dihydr-odithieno[3,2-c:2',3'-e][1,2]azaborinine (6a):



Compound **4a** (0.154 g, 0.3 mmol), Ar-$SnBu_3$ (0.66 mmol), $Pd_2(dba)_3$ (8.24 mg, 0.009 mmol) and P-(*o*-Tolyl)$_3$ (13.70 mg, 0.045 mmol) were dissolved in 10 mL of toluene in a vial suitable for microwave reactions, the reaction mixture was stirred at 110 °C for 3 h in a microwave reactor. After the mixture was filtered and evaporated, the residue was purified by column chromatography over silica gel (petroleum ether : dichlorome = 5 : 1) to afford compound **5a** and compound **6a** as light brown solids.

Compound **5a**. Yield: 71.3 mg (48%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71-7.65 (m, 3H, Ar*H*), 7.60 (dd, *J* = 14.1Hz, 7.8 Hz, 4H, Ar*H*), 7.45 (t, *J* = 7.5 Hz, 2H, Ar*H*), 7.41-7.34 (m, 5H, Ar*H*), 7.31-7.27 (m, 2H, Ar*H*), 7.26-7.21 (m, 5H, Ar*H*), 6.71 (d, *J* = 5.5 Hz, 1H, Ar*H*).

^{13}C NMR (100 MHz, $CDCl_3$): δ 146.75, 144.16, 143.49, 141.12, 140.16, 139.80, 134.39, 133.75, 128.93, 128.86, 128.29, 127.57, 127.53, 127.03, 126.24, 122.94, 120.19 (Ar-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 35.53 (bs).

HRMS (ESI^+) *m*/*z*: $[M + H]^+$ calcd for $C_{32}H_{23}BNS_2$, 496.1359, found, 496.1349.

Mp (°C): 233.3–234.9.

Compound **6a**. Yield: 65.5 mg (43%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61-7.57 (m, 2H, Ar*H*), 7.49 (s, 1H, Ar*H*), 7.37-7.29 (m, 4H, Ar*H*), 7.25-7.22 (m, 6H, Ar*H*), 7.21-7.18 (m, 2H, Ar*H*), 7.09 (dd, *J* = 5.1Hz, 3.6 Hz, 1H, Ar*H*), 7.04 (dd, *J* = 5.1Hz, 3.6 Hz, 1H, Ar*H*), 6.68 (d, *J* = 5.5 Hz, 1H, Ar*H*).

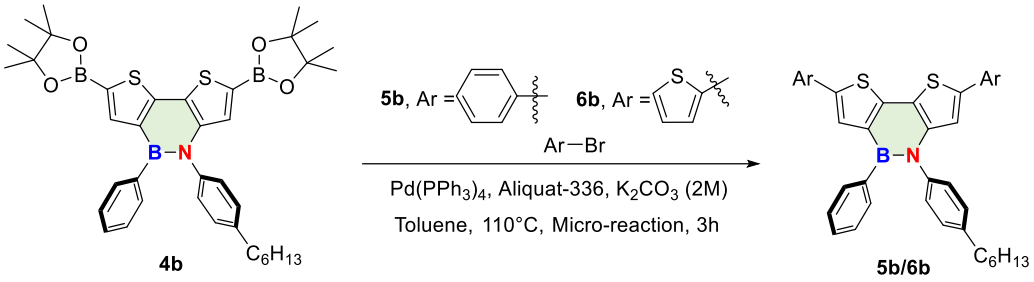
^{13}C NMR (100 MHz, $CDCl_3$): δ 144.07, 143.53, 143.44, 134.18, 133.70, 133.20, 129.04, 128.71, 128.16, 127.86, 127.49, 127.35, 126.33, 125.15, 124.63, 124.25, 123.42, 123.08, 120.08 (Ar-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 33.68 (bs).

HRMS (ESI^+) *m*/*z*: $[M + H]^+$ calcd for $C_{28}H_{19}BNS_4$, 508.0488, found, 508.0480.

Mp (°C): 227.7–229.5.

2.6 General procedure for the synthesis of 4-(4-hexylphenyl)-2,5,7-triphenyl-4,5-dihydrodithieno[3,2-c:2',3'-e][1,2]azaborinine (5b) and 4-(4-hexylphenyl)-5-phenyl-2,7-di(thiophen-2-yl)-4,5-dihydrodi-thieno[3,2-c:2',3'-e][1,2]azaborinine (6b):



Compound **4b** (0.17 g, 0.25 mmol), Ar-Br (0.54 mmol), Aliquat-336 (10.1 mg, 0.025 mmol), $Pd(PPh_3)_4$ (14.5 mg, 0.0125 mmol) and Ar_2-sparged aqueous potassium carbonate (2.0 M, 3.6 mL, 2.0 mmol) were dissolved in 10 mL of toluene in a vial suitable for microwave reactions, the reaction mixture was stirred at 110 °C for 3 h in a microwave reactor. The resulting mixture was poured into 30 mL of $CHCl_3$ while stirring, filtered through a pad of Celite, and the solvent removed under reduced pressure. The remaining solid was dissolved in 30 mL of toluene and washed three times with 30 mL portions of water. The organic layer was dried over $MgSO_4$ and the solvent was evaporated. The product was purified by column chromatography over silica gel (petroleum ether : dichlorome = 5 : 1) to afford compound **5b** and compound **6b** as light brown and light yellow solids.

Compound **5b**. Yield: 74.6 mg (51%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (dd, *J* = 9.6Hz, 2.4 Hz, 3H, Ar*H*), 7.58-7.55 (m, 2H, Ar*H*), 7.41-7.28 (m, 8H, Ar*H*), 7.24-7.19 (m, 3H, Ar*H*), 7.13 (q, *J* = 8.4 Hz, 4H, Ar*H*), 6.85 (s, 1H, Ar*H*), 2.67-2.61 (m, 2H, -CH_2), 1.67-1.61 (m, 2H, -CH_2), 1.32 (s, 6H, -CH_2), 0.91 (t, *J* = 6.7 Hz, 3H, -CH_3).

^{13}C NMR (100 MHz, $CDCl_3$): δ 146.38, 144.29, 142.32, 141.80, 141.09, 140.90, 134.43, 134.01, 133.77, 128.97, 128.94, 128.91, 128.40, 128.30, 128.11, 127.47, 127.29, 127.12, 126.22, 125.83, 118.24, 115.85 (Ar-C), 35.46, 31.73, 31.20, 28.74, 22.66, 14.14 (hexyl-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 33.59 (bs).

HRMS (ESI^+) *m/z*: $[M + H]^+$ calcd for $C_{38}H_{35}BNS_2$, 580.2299, found, 580.2276.

Mp (°C): 120.6–122.3.

Compound **6b**. Yield: 67.1 mg (45%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49 (s, 1H, Ar*H*), 7.30 (d, *J* = 7.3 Hz, 2H, Ar*H*), 7.22 (t, *J* = 6.5 Hz, 7H, Ar*H*), 7.11 (dd, *J* = 23.5Hz, 8.0 Hz, 4H, Ar*H*), 7.02 (dt, *J* = 8.3Hz, 4.3 Hz, 2H, Ar*H*), 6.67 (s, 1H, Ar*H*), 2.63 (t, *J* = 7.5 Hz, 2H, -CH_2), 1.67-1.59 (m, 2H, -CH_2), 1.31 (s, 6H, -CH_2), 0.90 (t, *J* = 6.3 Hz, 3H, -CH_3).

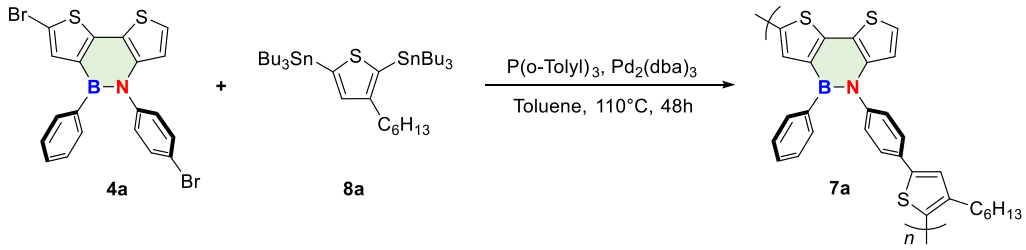
^{13}C NMR (100 MHz, $CDCl_3$): δ 145.75, 144.11, 142.14, 141.88, 137.49, 137.19, 134.19, 133.73, 128.99, 128.86, 128.22, 128.02, 127.87, 127.34, 127.14, 125.31, 124.61, 124.51, 124.23, 117.40, 116.17 (Ar-C), 35.44, 31.72, 31.19, 28.72, 22.66, 14.15 (hexyl-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 33.26 (bs).

HRMS (ESI$^+$) *m/z*: $[M + H]^+$ calcd for $C_{34}H_{31}BNS_4$, 592.1426, found, 592.1372.

Mp (°C): 144.4–146.1.

2.7 Synthesis of 7a:



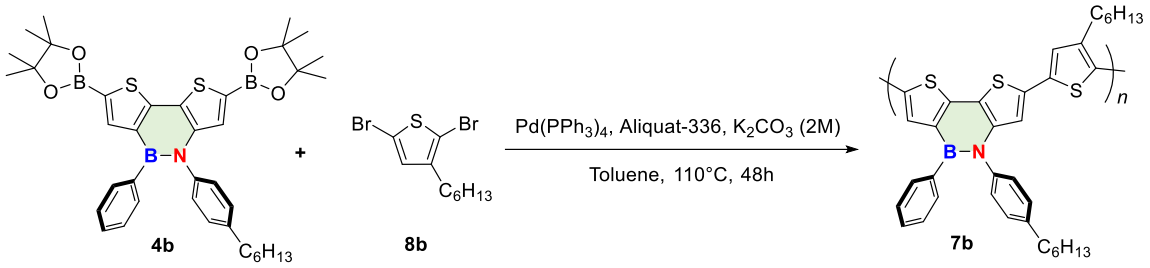
Monomer **4a** (0.216 g, 0.43 mmol), monomer **8a** (0.322 g, 0.43 mmol), $Pd_2(dba)_3$ (6.0 mg, 0.0065 mmol) and P(*o*-Tolyl)$_3$ (10.0 mg, 0.033 mmol) were dissolved in 10 mL of toluene in a Schlenk flask. The reaction mixture was stirred for 48 h at 110 °C. The reaction mixture was then cooled to room temperature, the solvent was removed in vacuo, and the residue was dissolved in 1 mL $CHCl_3$, then reprecipitated in MeOH (200 mL), the precipitate was purified by Soxhlet extraction using acetone to remove the residual monomer and then extracted with chloroform to get a dark purple solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 (s, 3H, Ar*H*), 7.23-6.85 (m, 8H, Ar*H*), 6.63 (s, 1H, Ar*H*), 2.62 (s, 4H, -CH_2), 1.62 (s, 4H, -CH_2), 1.31 (s, 12H, -CH_2), 0.90 (s, 6H, -CH_3).

^{11}B NMR (128 MHz, $CDCl_3$): δ 18.77 (bs).

Mn = 2.83 kg/mol, Mw = 5.08 kg/mol, PDI = 1.80 by GPC.

2.8 Synthesis of 7b:



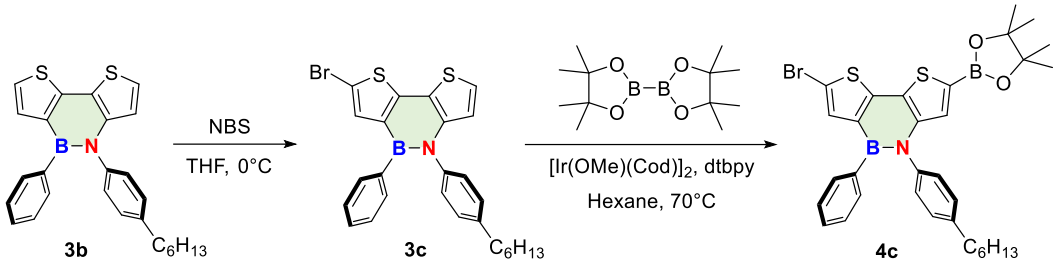
Monomer **4b** (0.272 g, 0.4 mmol), monomer **8b** (0.13 g, 0.4 mmol), $Pd(PPh_3)_4$ (24 mg, 0.02 mmol), Aliquant336 (16 mg, 0.04 mmol) and Ar_2-sparged aqueous potassium carbonate (2.0 M, 3.6 mL, 2.0 mmol) were dissolved in 10 mL of toluene in a Schlenk flask. The reaction mixture was stirred for 48 h at 110 °C. The reaction mixture was then cooled to room temperature, the solvent was removed in vacuo, and the residue was dissolved in 1 mL $CHCl_3$, then reprecipitated in MeOH (200 mL), the precipitate was purified by Soxhlet extraction using acetone to remove the residual monomer and then extracted with chloroform to get a dark purple solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.3 Hz, 1H, Ar*H*), 7.51-7.42 (m, 2H, Ar*H*), 7.33 (d, *J* = 24.3 Hz, 3H, Ar*H*), 7.25-7.16 (m, 5H, Ar*H*), 7.09 (dd, *J* = 14.7Hz, 7.1 Hz, 2H, Ar*H*), 6.64 (dd, *J* = 30.7Hz, 5.3 Hz, 1H, Ar*H*), 2.54 (s, 2H, -CH_2), 1.59 (s, 2H, -CH_2), 1.27 (s, 6H, -CH_2), 0.86 (d, *J* = 4.7 Hz, 3H, -CH_3).

^{11}B NMR (128 MHz, $CDCl_3$): δ 18.82 (bs).

Mn = 1.77 kg/mol, Mw = 3.70 kg/mol, PDI = 2.09 by GPC.

2.9 Synthesis of 7c:



Compound **3c** was prepared as a yellow solid (0.99 g, 65%) by following the procedure of **4a** using compound **3b** (1.28 g, 3 mmol) instead of **3a** (1.03 g, 3 mmol) and using NBS (0.5 g, 3.15 mmol) instead of NBS (1.19 g, 7.5 mmol). Compound **4c** was prepared as light brown solid by following the procedure of **4b** using compound **3c (**506.33 mg, 1 mmol**)** instead of **3b** (427 mg, 1 mmol). Yield: 474 mg (75%).

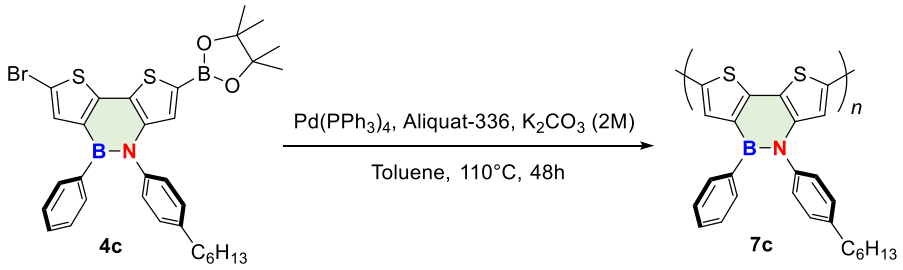
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (s, 1H, Ar*H*), 7.24 – 7.21 (m, 2H, Ar*H*), 7.18 (t, *J* = 6.4 Hz, 3H, Ar*H*), 7.14 – 7.09 (m, 3H, Ar*H*), 7.03 (d, *J* = 8.1 Hz, 2H, Ar*H*), 2.61 (t, *J* = 7.6 Hz, 2H, -CH_2), 1.64 – 1.59 (m, 2H, -CH_2), 1.33 (s, 12H, -CH_3), 1.31 (s, 4H, -CH_2), 1.25 (s, 2H, -CH_2), 0.89 (d, *J* = 7.0 Hz, 3H, -CH_3).

^{13}C NMR (101 MHz, $CDCl_3$): δ 148.11, 144.55, 142.01, 141.82, 135.13, 133.61, 129.00, 128.53, 128.25, 127.41, 127.11, 123.52, 110.69, 84.54 (Ar-C), 35.43, 31.73, 31.15, 28.78 (hexyl-C), 24.73 (CH_3-C), 22.65, 14.14 (hexyl-C).

^{11}B NMR (128 MHz, $CDCl_3$): δ 28.53 (bs).

HRMS (ESI$^+$) *m/z*: $[M + H]^+$ calcd for $C_{32}H_{37}B_2BrNO_2S_2$, 632.1663, found, 632.1682.

Mp (°C): 224.5–226.1.



Oligomer **7c** was prepared by following the procedure of **7b** using compound **4c** (0.25 g, 0.4 mmol) instead of monomer **4b** (0.272 g, 0.4 mmol) and monomer **8b** (0.13 g, 0.4 mmol). Oligomer was isolated as a dark purple solid after filtration.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 81.5Hz, 27.1 Hz, 4H, Ar*H*), 7.26 – 6.37 (m, 7H, Ar*H*), 2.80 – 2.46 (m, 2H, -CH_2), 1.67 – 1.52 (m, 2H, -CH_2), 1.45 – 1.23 (m, 6H, -CH_2), 1.00 – 0.81 (m, 3H, -CH_2).

^{11}B NMR (128 MHz, $CDCl_3$): δ 18.70 (bs).

Mn = 1.27 kg/mol, Mw = 1.81 kg/mol, PDI = 1.41 by GPC.

3. Single-crystal X-ray structure determination

X-ray Crystallography. Crystals of appropriate quality for X-ray diffraction studies were removed from a vial (in a glove box) and immediately covered with a thin layer of hydrocarbon oil (Paratone-N). A suitable crystal was then selected, attached to a glass fiber, and quickly placed in a glass vial. All data were collected using a Bruker APEX II CCD detector/D8 diffractometer using Mo/Cu Kα radiation. The data were corrected for absorption through Gaussian integration from indexing of the crystal faces. Structures were solved using the direct methods programs SHELXS-97, and refinements were completed using the program SHELXL-97.[9]

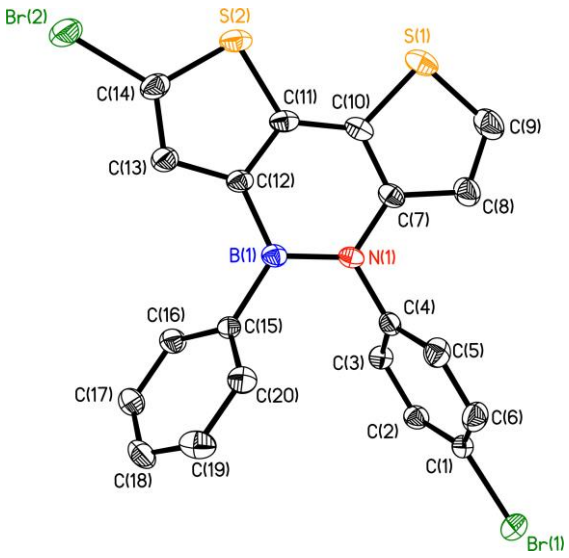


Figure S1. Molecular Structure of **4a** with thermal ellipsoids presented at a 50% probability level. All hydrogen atoms have been omitted for clarity. Selected bond lengths (Å): Br(1)-C(1), 1.901(4); Br(2)-C(14), 1.870(4); N(1)-C(7), 1.395(5); N(1)-B(1), 1.444(5); N(1)-C(4), 1.451(5); C(15)-B(1), 1.579(5); C(12)-B(1), 1.523(6); Bond angles (deg): C(7)-N(1)-B(1), 122.3(3); C(7)-N(1)-C(4), 115.8(3); B(1)-N(1)-C(4), 121.9(3); C(20)-C(15)-B(1), 122.7(3); C(16)-C(15)-B(1), 119.9(3); C(3)-C(4)-N(1), 118.5(3); C(5)-C(4)-N(1), 121.2(3); C(11)-C(12)-B(1), 119.0(4); C(13)-C(12)-B(1), 129.9(4); C(10)-C(7)-N(1), 120.8(3); N(1)-C(7)-C(8), 126.5(4); C(6)-C(1)-Br(1), 120.2(3); C(2)-C(1)-Br(1), 118.3(3); C(13)-C(14)-Br(2), 127.4(4); S(2)-C(14)-Br(2), 119.2(2); N(1)-B(1)-C(12), 115.6(3); N(1)-B(1)-C(15), 121.4(3); C(12)-B(1)-C(15), 123.0(3).

Table S1. Crystal data and structure refinement for compound **4a** (CCDC 1980884).

Empirical formula	$C_{20}H_{12}BBr_2NS_2$
Formula weight	501.06
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C 2/c

Unit cell dimensions	a = 11.7998(4) Å α = 90 deg.
	b = 17.9358(7) Å β = 98.223(2) deg.
	c = 18.6892(9) Å γ = 90 deg.
Volume	3914.7(3) Å ^3
Z, Calculated density	8, 1.700 Mg/m^3
Absorption coefficient	4.358 mm^-1
F(000)	1968
Crystal size	0.21 x 0.15 x 0.12 mm
Theta range for data collection	2.081 to 26.431 deg.
Limiting indices	-13<=h<=14, -22<=k<=22, -23<=l<=22
Reflections collected / unique	14954 / 4012 [R(int) = 0.0247]
Completeness to theta = 25.242	99.80%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4012 / 0 / 235
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R1 = 0.0436, wR2 = 0.1162
R indices (all data)	R1 = 0.0627, wR2 = 0.1261
Extinction coefficient	n/a
Largest diff. peak and hole	0.918 and -0.971 e. Å ^-3

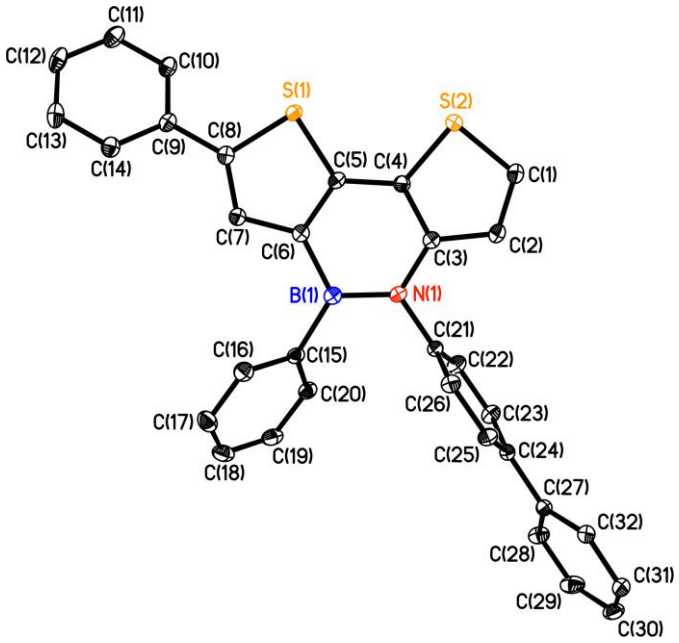


Figure S2. Molecular Structure of **5a** with thermal ellipsoids presented at a 50% probability level. All hydrogen atoms have been omitted for clarity. Selected bond lengths (Å): N(1)-C(3), 1.3992(19); N(1)-C(21), 1.4559(18); N(1)-B(1), 1.440(2); C(6)-B(1), 1.543(2); C(15)-B(1), 1.581(2). Bond angles (deg):

C(3)-N(1)-C(21), 114.47(12); C(3)-N(1)-B(1), 122.38(12); B(1)-N(1)-C(21), 123.00(12); N(1)-C(3)-C(2), 127.02(13); C(4)-C(3)-N(1), 120.76(13); C(5)-C(6)-B(1), 118.80(13); C(7)-C(6)-B(1), 130.98(13); C(16)-C(15)-B(1), 120.58(14); C(20)-C(15)-B(1), 122.40(14); C(22)-C(21)-N(1), 120.68(13); C(26)-C(21)-N(1), 119.17(13); N(1)-B(1)-C(6), 115.50(13); N(1)-B(1)-C(15), 122.54(13); C(6)-B(1)-C(15), 121.88(13).

Table S2. Crystallographic experimental details for compound **5a** (CCDC 1980885).

Empirical formula	$C_{32}H_{22}BNS_2$
Formula weight	495.44
Temperature	296.15 K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 1 21/n 1
Unit cell dimensions	a = 13.881(3) Å α = 90 deg.
	b = 10.825(2) Å β = 96.789(3) deg.
	c = 16.729(3) Å γ = 90 deg.
Volume	2496.1(9) Å^3
Z, Calculated density	32, 1.318 Mg/m^3
Absorption coefficient	0.236 mm^-1
F(000)	1032
Crystal size	0.21 x 0.16 x 0.11 mm
Theta range for data collection	1.805 to 26.549 deg.
Limiting indices	-17<=h<=17, -13<=k<=13, -21<=l<=20
Reflections collected / unique	26172 / 5185 [R(int) = 0.0282]
Completeness to theta = 25.242	100.00%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5185 / 0 / 325
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0321, wR2 = 0.0785
R indices (all data)	R1 = 0.0416, wR2 = 0.0840
Extinction coefficient	n/a
Largest diff. peak and hole	0.305 and -0.234 e. Å^-3

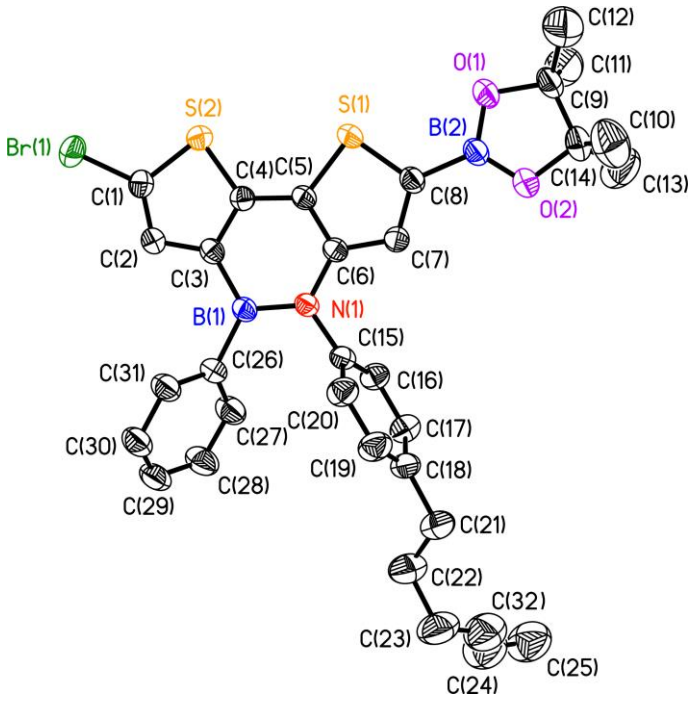


Figure S3. Molecular Structure of **4c** with thermal ellipsoids presented at a 50% probability level. All hydrogen atoms have been omitted for clarity. Selected bond lengths (Å): Br(1)-C(1), 1.879(4); O(1)-B(2), 1.343(6); O(2)-B(2), 1.322(6); N(1)-C(6), 1.400(5); N(1)-C(15), 1.447(5); N(1)-B(1), 1.442(5); C(3)-B(1), 1.528(6); C(8)-B(2), 1.552(6); C(26)-B(1), 1.570(6) Bond angles (deg): B(2)-O(1)-C(9), 108.3(4); B(2)-O(2)-C(10), 110.6(4); C(6)-N(1)-C(15), 117.3(3); C(6)-N(1)-B(1), 122.0(3); B(1)-N(1)-C(15), 120.7(3); C(2)-C(3)-B(1), 129.8(3); C(4)-C(3)-B(1), 119.2(4); N(1)-C(6)-C(7), 127.2(3); C(5)-C(6)-N(1), 120.6(3); C(7)-C(8)-B(2), 128.2(4); B(2)-C(8)-S(1), 121.2(3); C(16)-C(15)-N(1), 120.7(4); C(20)-C(15)-N(1), 120.4(4); C(27)-C(26)-B(1), 123.2(4); C(31)-C(26)-B(1), 121.1(4); N(1)-B(1)-C(3), 115.9(3); N(1)-B(1)-C(26), 121.4(4); C(3)-B(1)-C(26), 122.6(4); O(1)-B(2)-C(8), 122.3(4); O(2)-B(2)-O(1), 113.7(4); O(2)-B(2)-C(8), 124.0(4).

Table S3. Crystal data and structure refinement for compound **4c** (CCDC 1989882).

Empirical formula	$C_{32}H_{36}B_2BrNO_2S_2$	
Formula weight	632.29	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P -1	
Unit cell dimensions	a = 10.337(6) Å	α = 80.485(10) deg.
	b = 12.780(8) Å	β = 69.729(9) deg.
	c = 13.153(7) Å	γ = 81.294(9) deg.
Volume	1599.2(16) A^3	
Z, Calculated density	12, 1.303 Mg/m^3	

Absorption coefficient	1.444 mm^-1
F(000)	646
Crystal size	0.280 x 0.21 x 0.16 mm
Theta range for data collection	1.624 to 25.799 deg.
Limiting indices	-12<=h<=12, -15<=k<=15, -15<=l<=15
Reflections collected / unique	16144 / 6046 [R(int) = 0.0230]
Completeness to theta = 25.242	99.80%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6046 / 602 / 366
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0626, wR2 = 0.1844
R indices (all data)	R1 = 0.0861, wR2 = 0.2068
Extinction coefficient	n/a
Largest diff. peak and hole	0.869 and -0.561 e. Å ^-3

4. GPC data for 7a, 7b and 7c

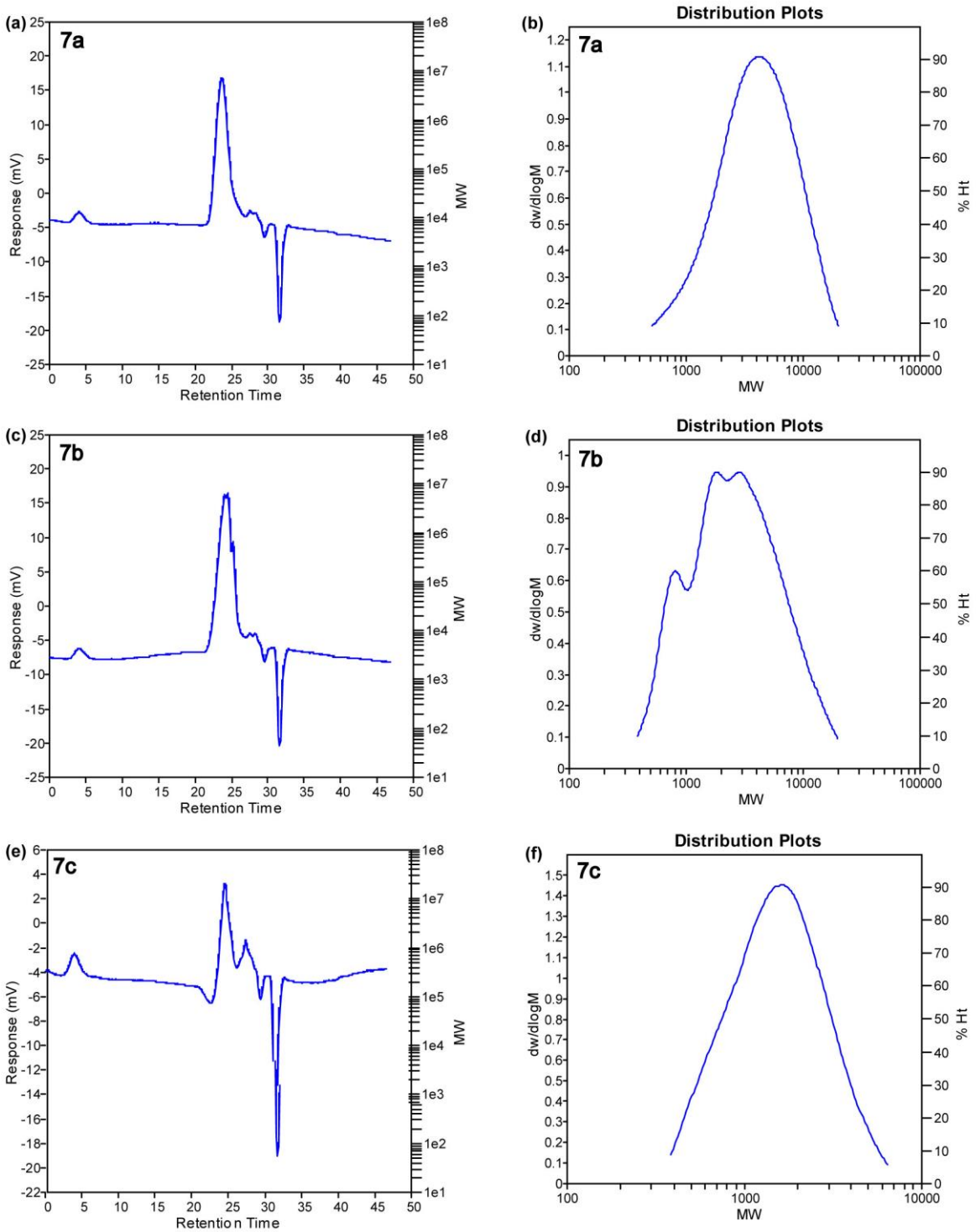


Figure S4. GPC data of **7a**, **7b** and **7c** with 1,2,4Trichlorobenzene (TCB) as an eluent at 1 mL/min at the temperature of 150 °C.

5. MALDI mass spectra of 7a, 7b and 7c

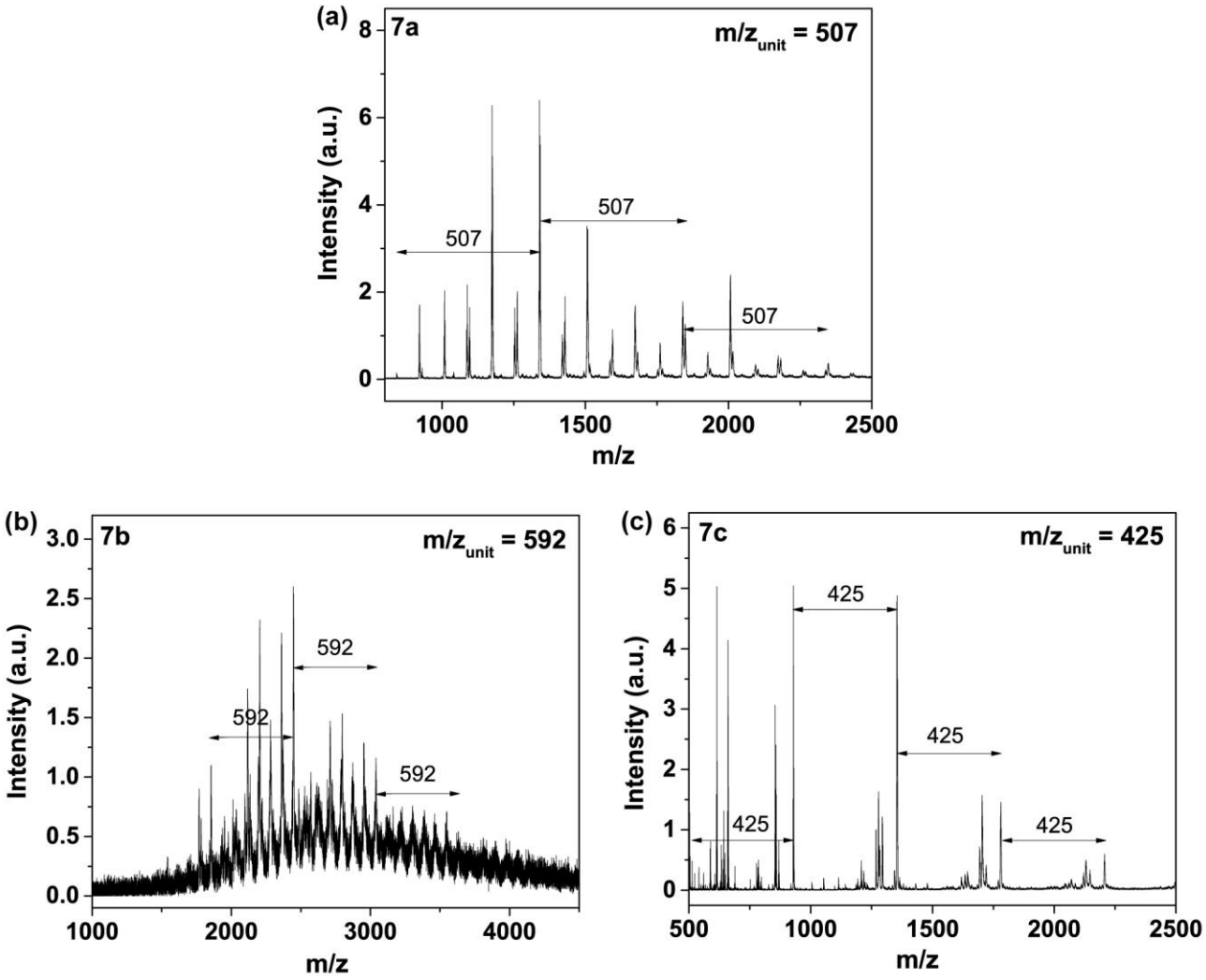


Figure S5. MALDI mass spectra of **7a**, **7b** and **7c**.

6. TGA data of BNDT derivatives

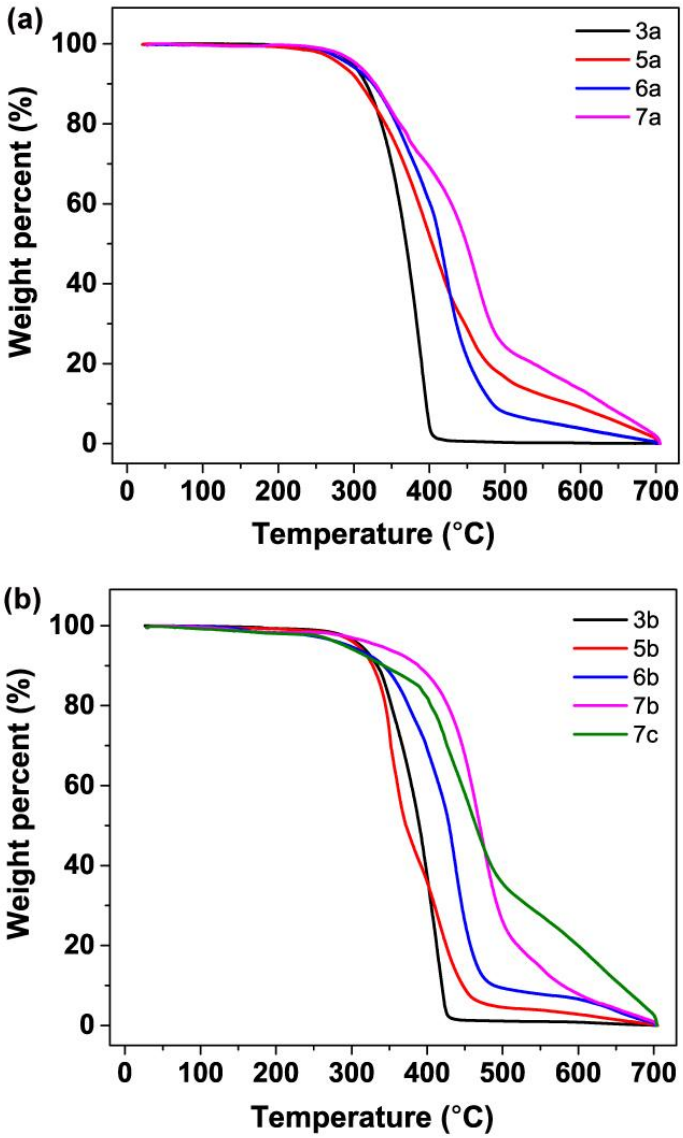
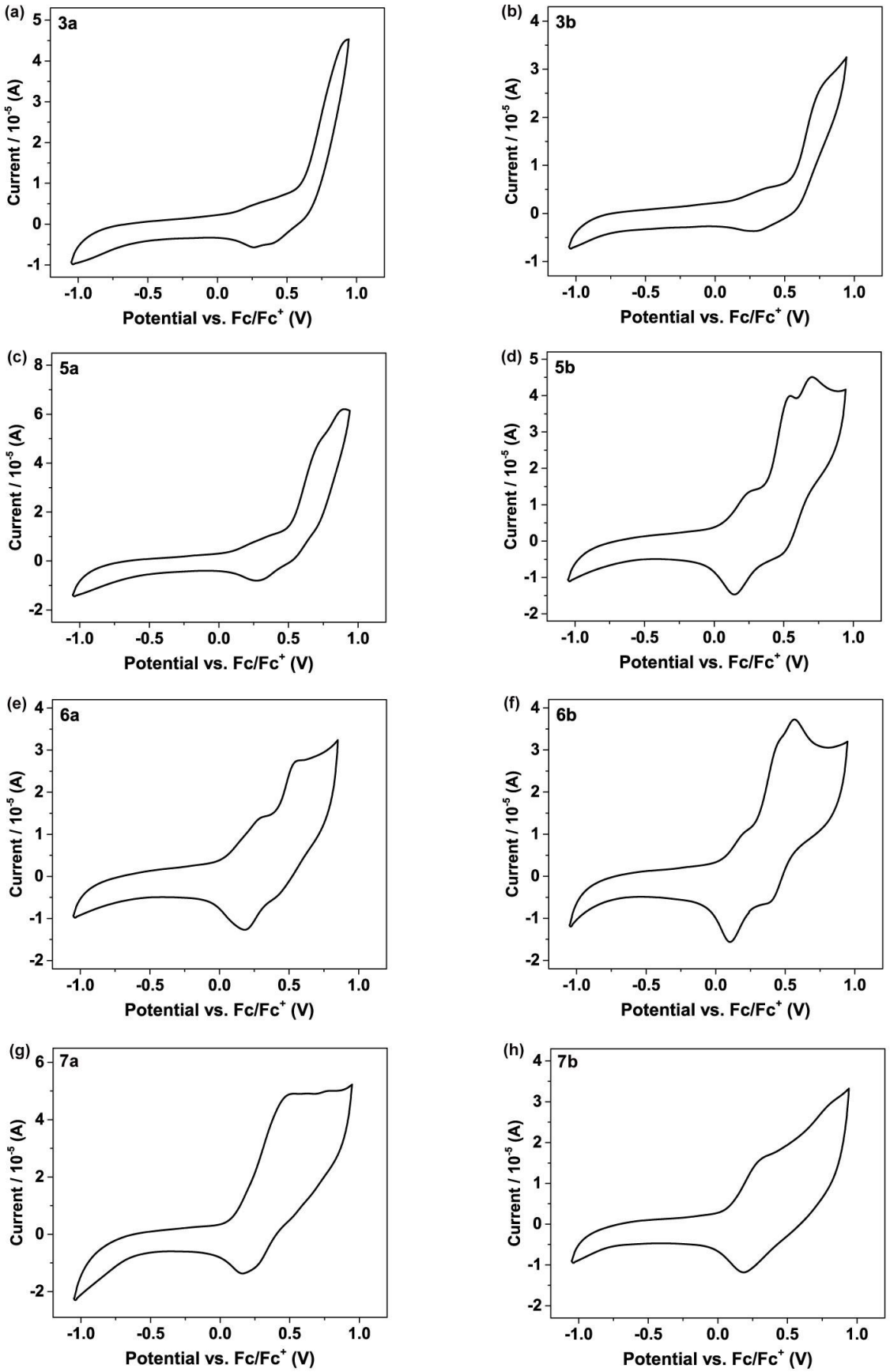


Figure S6. TGA of **BNDT** derivatives.

7. The cyclic voltammograms



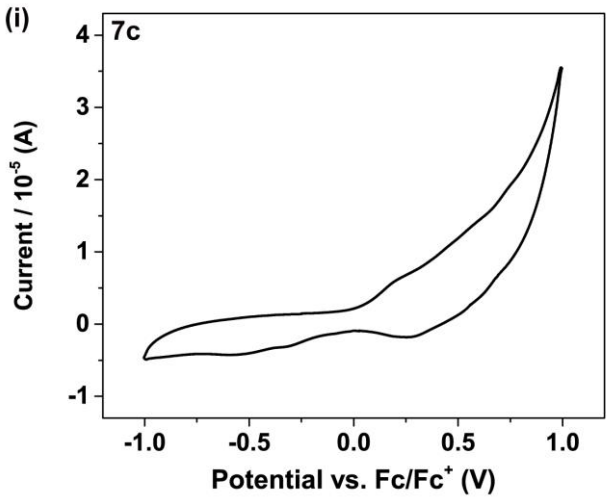


Figure S7. Cyclic voltammograms of **3a** (a), **3b** (b), **5a** (c), **5b** (d), **6a** (e), **6b** (f), **7a** (g)，**7b** (h) and **7c** (i) in DCM (c = 10^{-3} M) with $Bu_4N^+PF_6^-$ (0.1 M) as a supporting electrolyte, vs. Fc/Fc^+. (Fc = ferrocene).

Table S4. Electronic properties of **BNDT** derivatives

Entry	E_g [a](eV)	$E_{ox,onset}$ [b](V)	HOMO(eV) (Exp)[c]	LUMO(eV) (Exp)[d]	HOMO(eV) (Cal)[e]	LUMO(eV) (Cal)[e]	E_g (eV) (Cal)[e]
3a	3.50	0.35	-5.15	-1.65	-5.35	-1.14	4.21
5a	3.18	0.28	-5.08	-1.90	-5.14	-1.36	3.78
6a	3.04	0.24	-5.04	-2.00	-5.07	-1.50	3.57
7a	2.71	-0.04	-4.76	-2.05	--	--	--
3b	3.51	0.34	-5.14	-1.63	-5.32	-1.10	4.21
5b	2.88	0.23	-5.03	-2.15	-5.01	-1.58	3.43
6b	2.67	0.16	-4.96	-2.29	-4.89	-1.79	3.10
7b	2.05	-0.07	-4.73	-2.68	--	--	--
7c	2.03	-0.06	-4.74	-2.71	--	--	--

[a] *Eg* estimated from the UV-Vis absorption spectra.

[b] Oxidation onset potentials measured by cyclic voltammetry.

[c] HOMO = -($E_{ox,\ onset}$ + 4.8) eV.

[d] LUMO = HOMO + *Eg*.

Theoretical calculations have been carried out by using the GAUSSIAN09 suite of programs in gas-phase at the B3LYP/6-31G(d) level[e], respectively.

8. The excitation and emission spectra

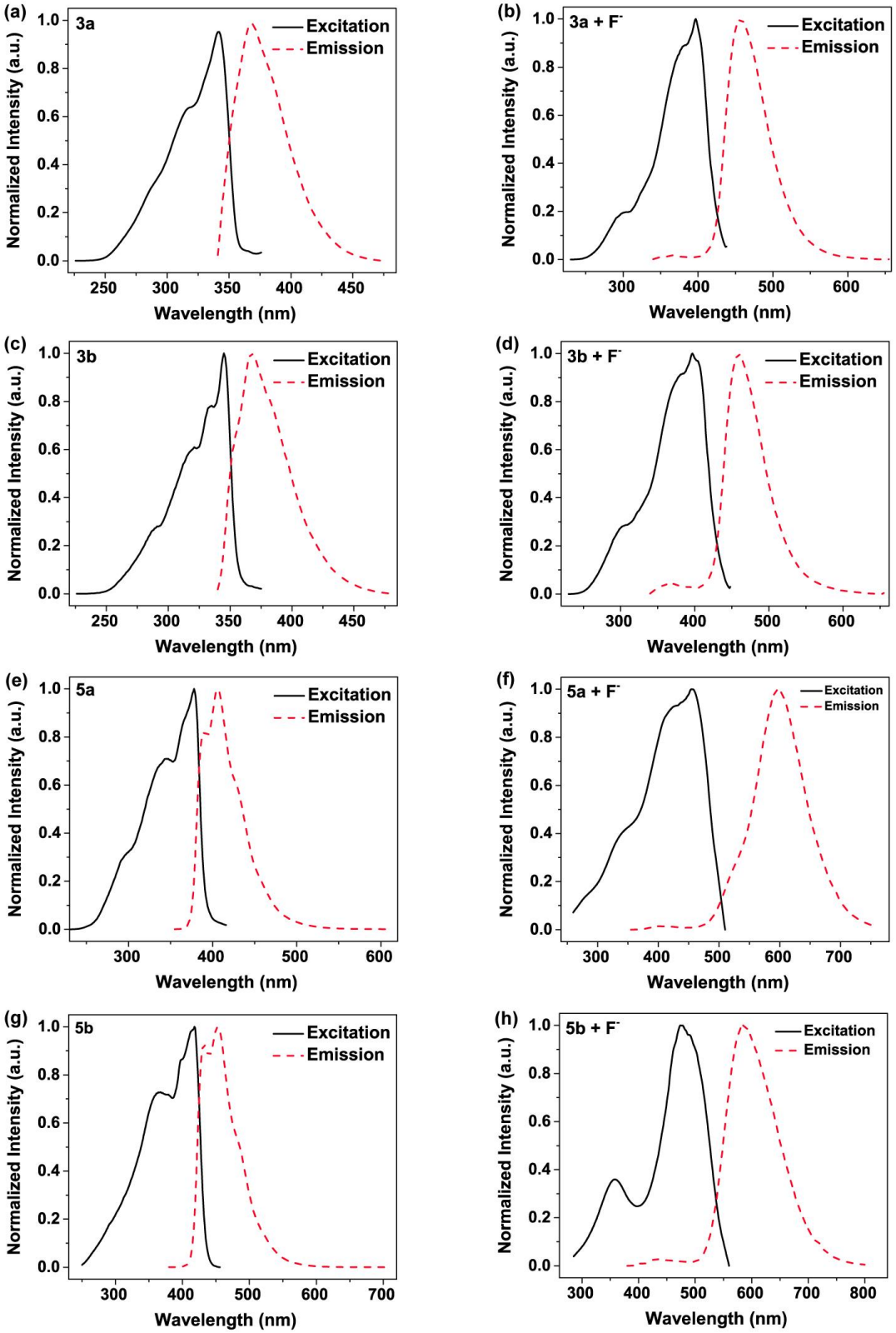


Figure S8. Excitation and emission spectra of **BNDT** derivatives without TABF (left) and after the addition of TBAF (right). (a and b) **3a**, [**3a**] = 10 μM; (c and d) **3b**, [**3b**] = 10 μM; (e and f) **5a**, [**5a**] = 10 μM; (g and h) **5b**, [**5b**] = 10 μM.

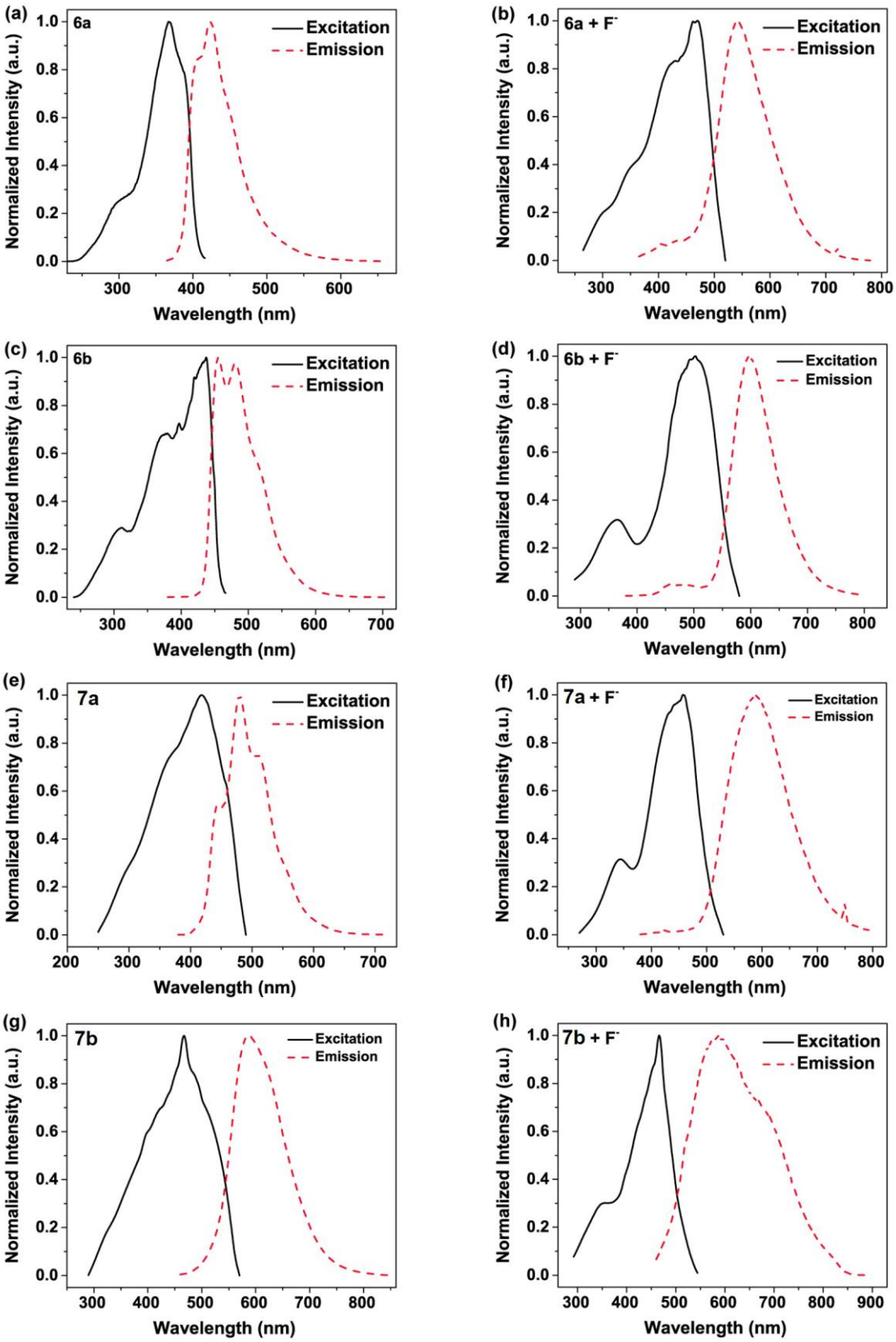


Figure S9. Excitation and emission spectra of **BNDT** derivatives without TABF (left) and after the addition of TBAF (right). (a and b) **6a**, [**6a**] = 10 μM; (c and d) **6b**, [**6b**] = 10 μM; (e and f) **7a**, [**7a**] = 10 μM; (g and h) **7b**, [**7b**] = 10 μM.

9. Fluoride titration experiments of BNDT derivatives

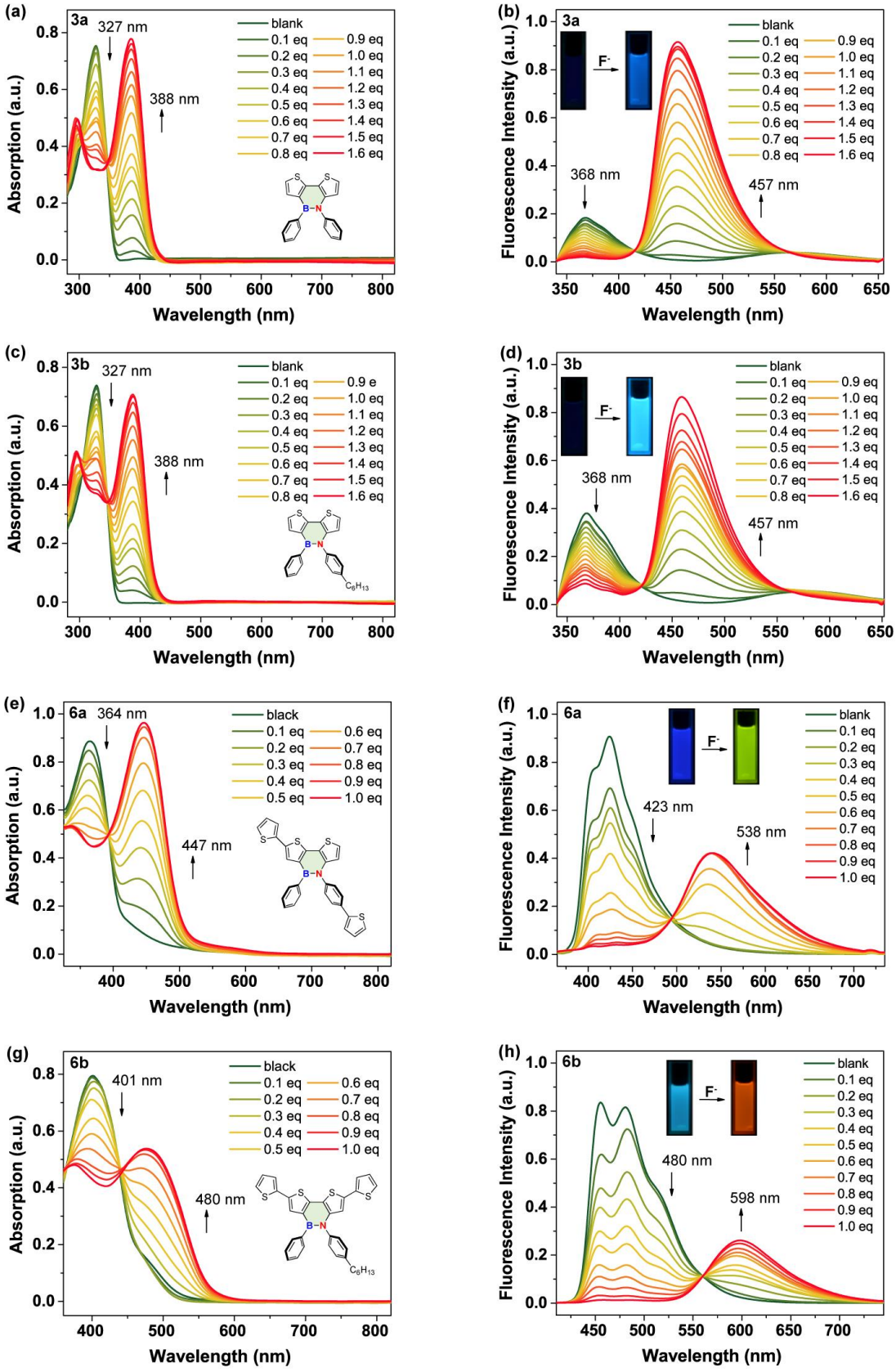


Figure S10. Spectral changes in the UV-Vis absorption (left) and fluorescence (right) of **3a**, **3b**, **6a** and **6b** after the addition of F^-. [F^-] = 1μM.

10. Plots of changed emission intensity

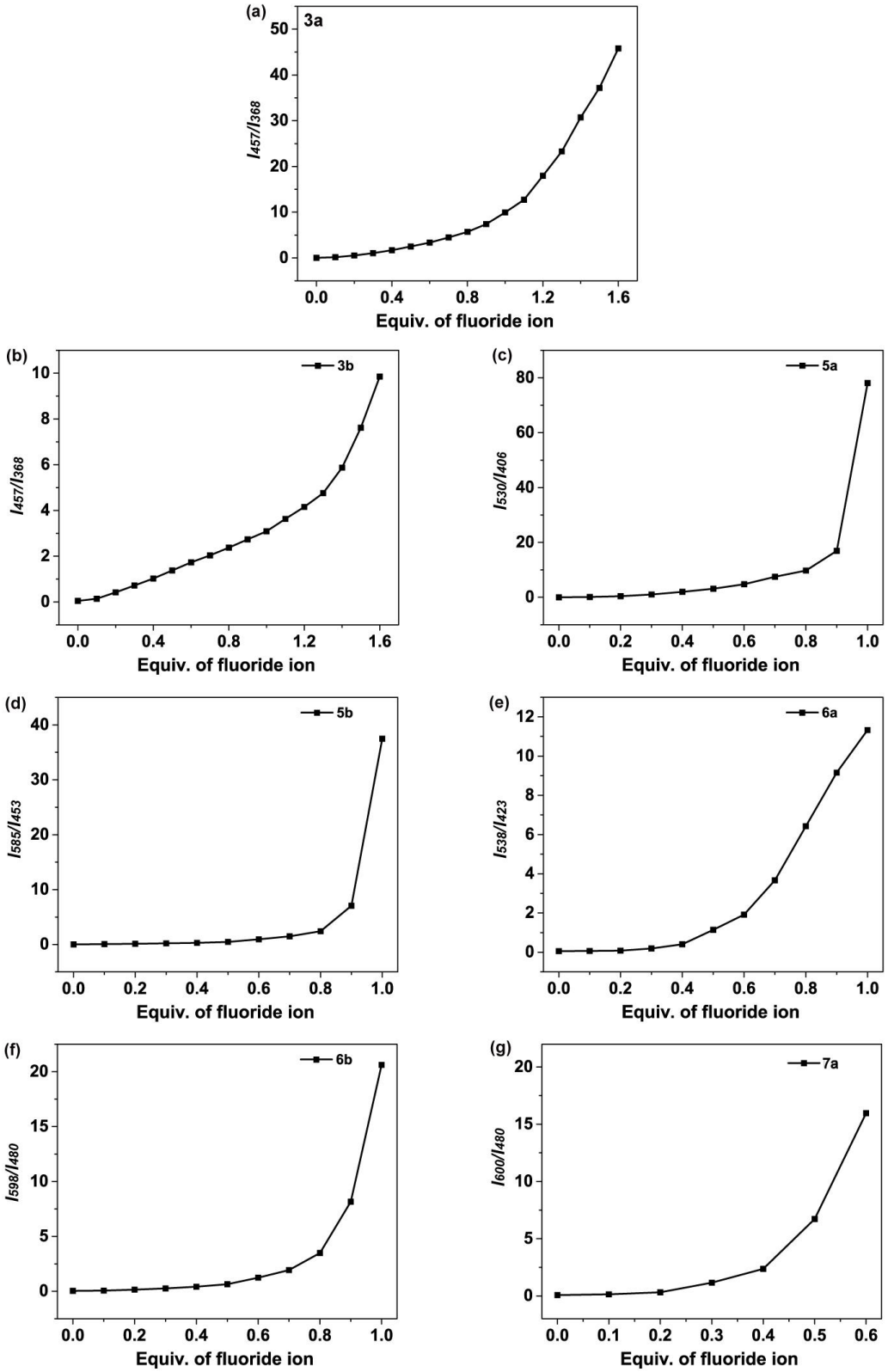


Figure S11. The plots of emission intensity ratio of **BNDT** derivatives at different equivalents of F^-. (a) **3a**, $\lambda_{em} = I_{457}/I_{368}$; (b) **3b**, $\lambda_{em} = I_{457}/I_{368}$; (c) **5a**, $\lambda_{em} = I_{530}/I_{406}$; (d) **5b**, $\lambda_{em} = I_{585}/I_{453}$; (e) **6a**, $\lambda_{em} = I_{538}/I_{423}$; (f) **6b**, $\lambda_{em} = I_{598}/I_{480}$; (g) **7a**, $\lambda_{em} = I_{600}/I_{480}$.

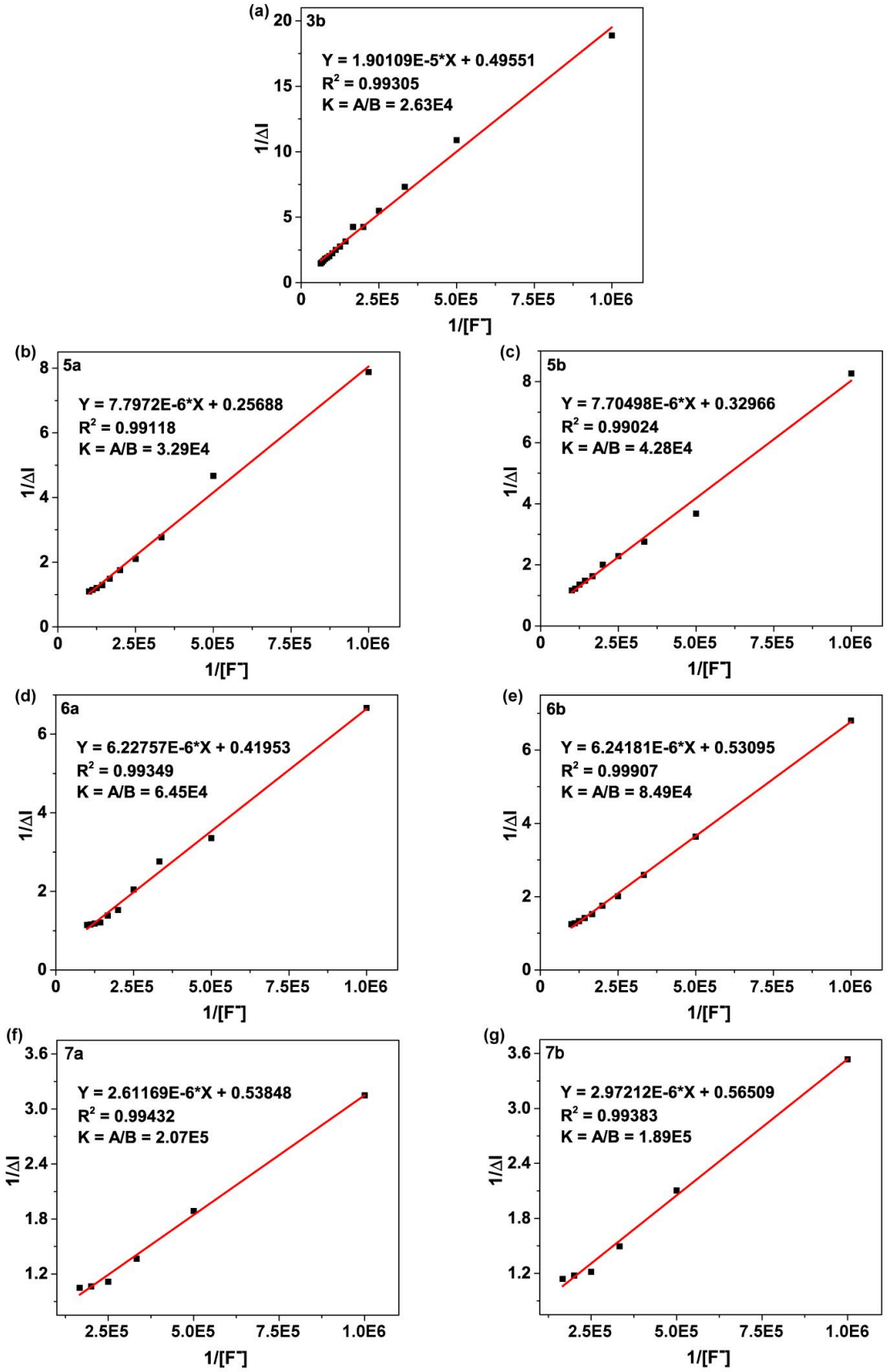


Figure S12. Benesi-Hilderbrand plots of **BNDT** derivatives at different [F^-]. $1/\Delta I = A + B/[F^-]$, $K = A/B$.[10-11]

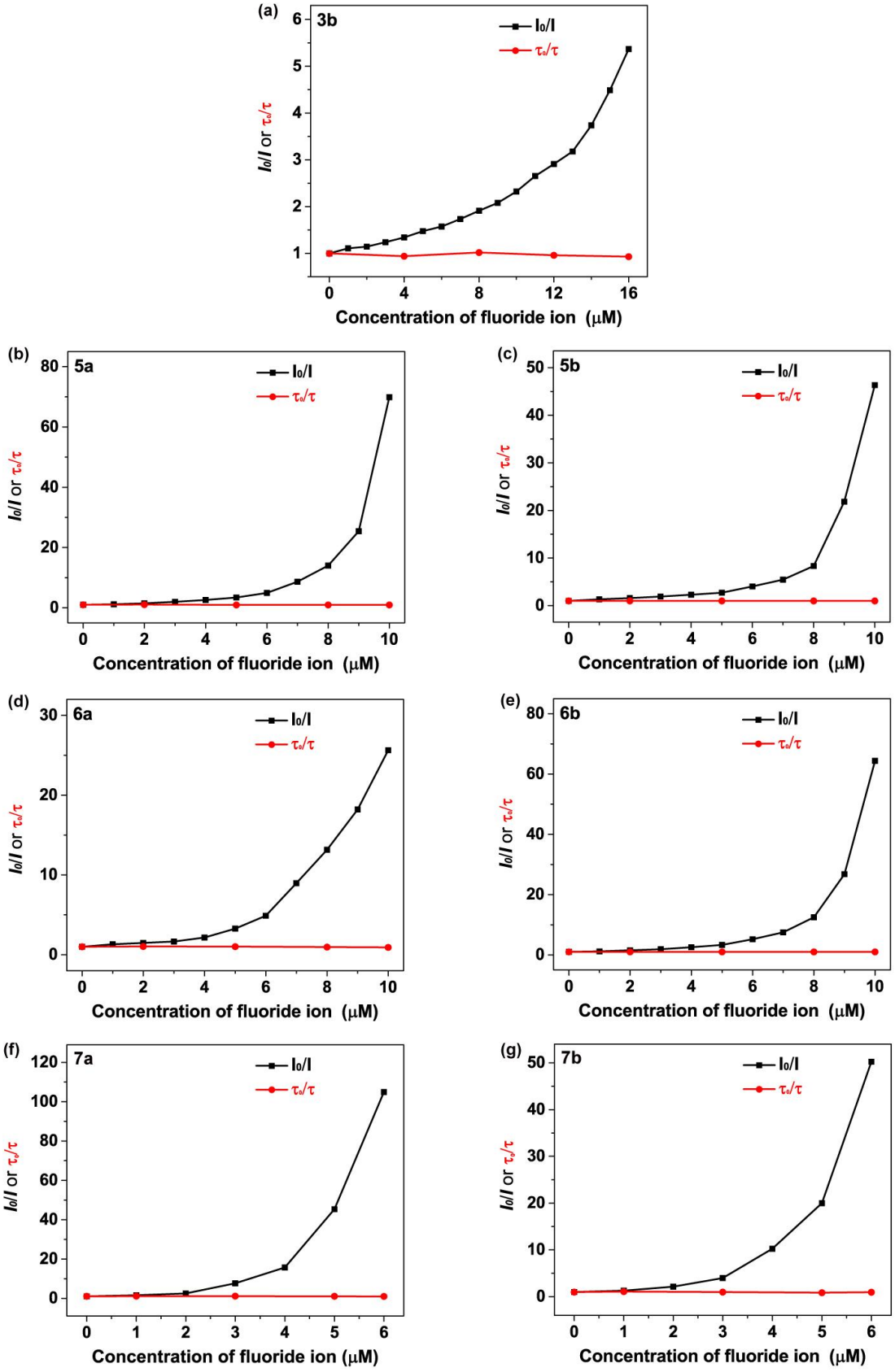


Figure S13. Plots of the ratios of fluorescence intensity (I_0/I) and lifetime change (τ_0/τ) as a function of [F^-] of **BNDT** derivatives in THF upon addition of F^-.

11. Quenching efficiencies of BNDT derivatives

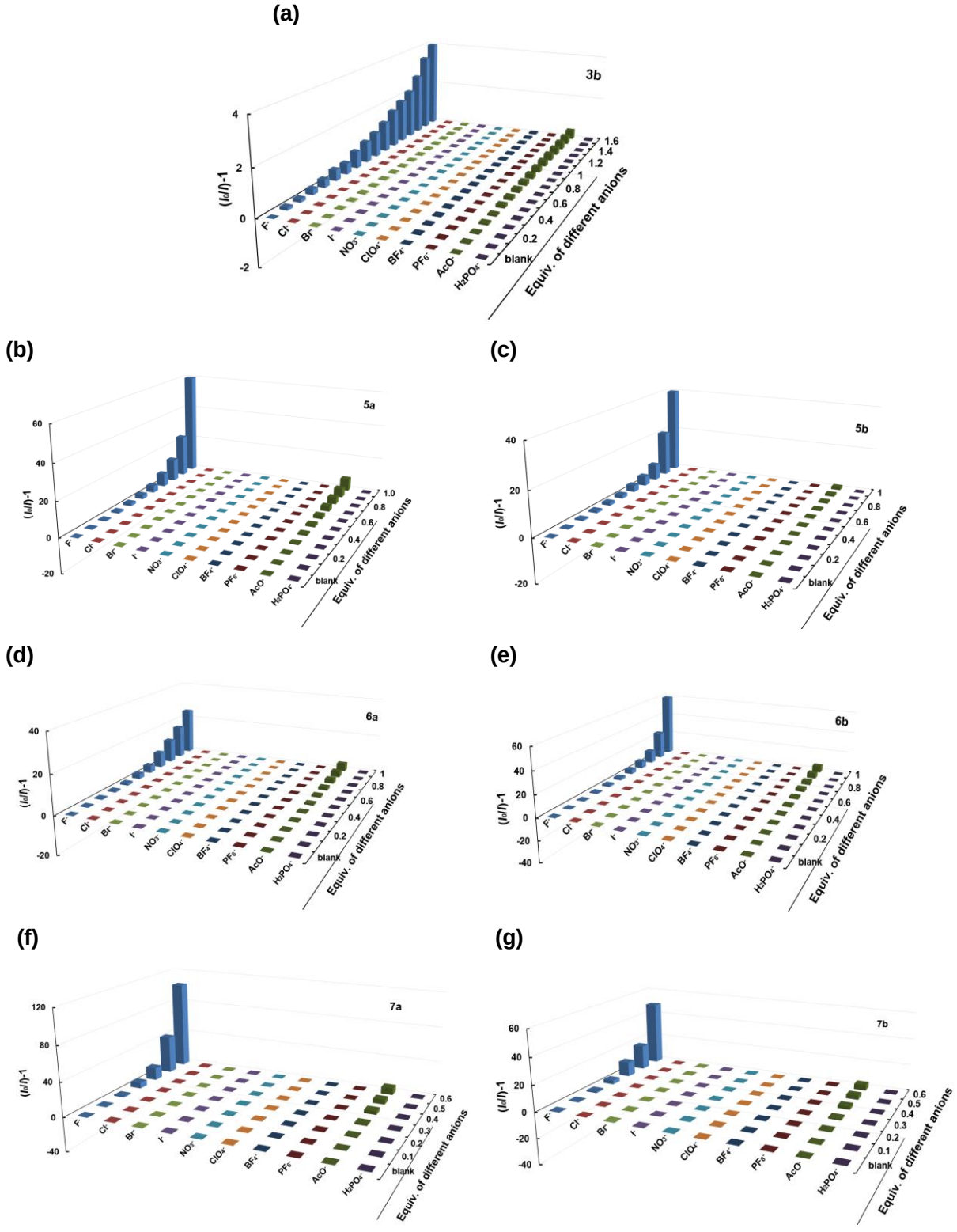


Figure S14. (I_0/I)-1 of F^- and other anions for the emission of **BNDT** derivatives in THF (10 μM) at different equivalents of anions.

12. Reversibility of BNDT derivatives

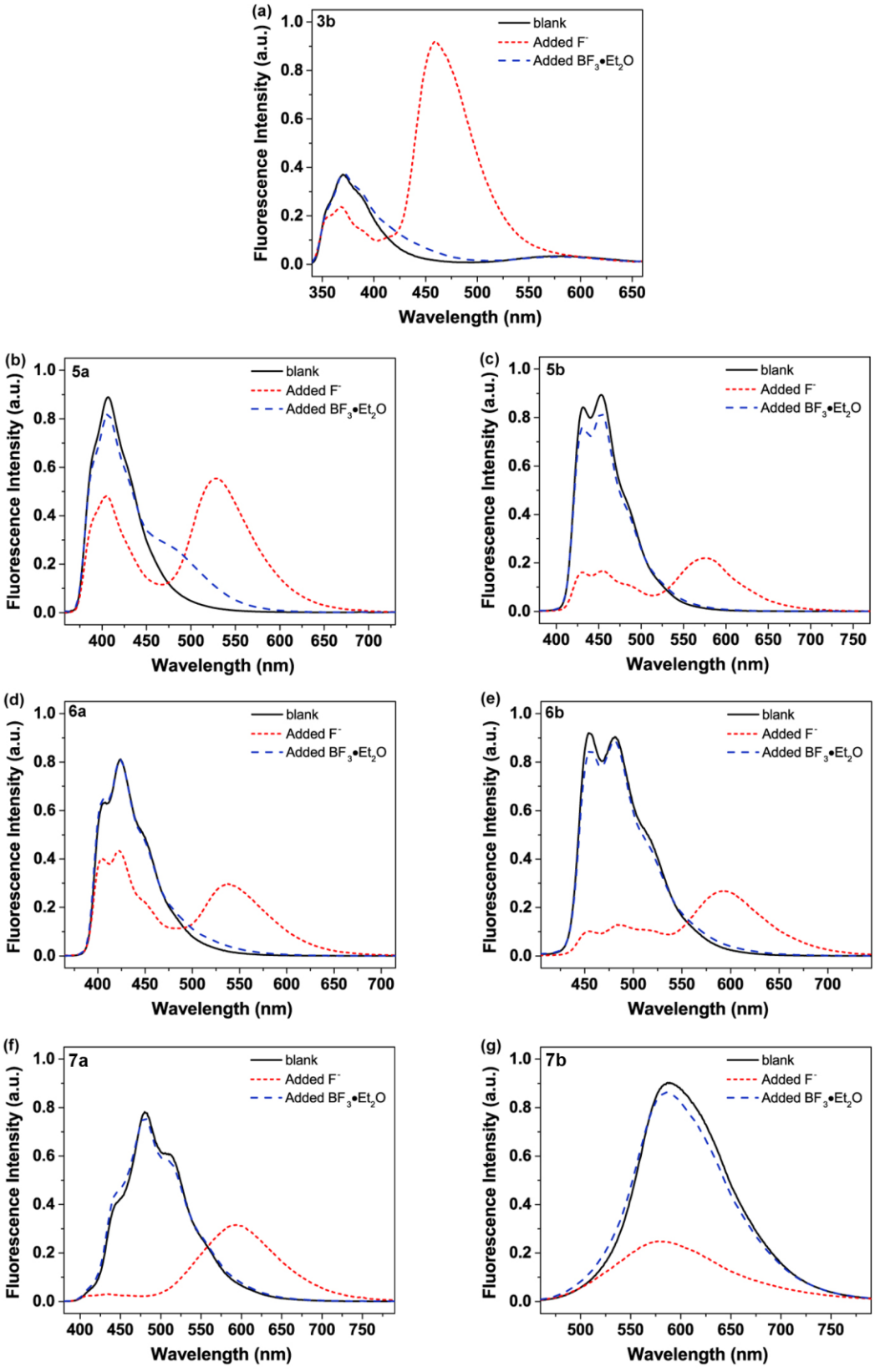
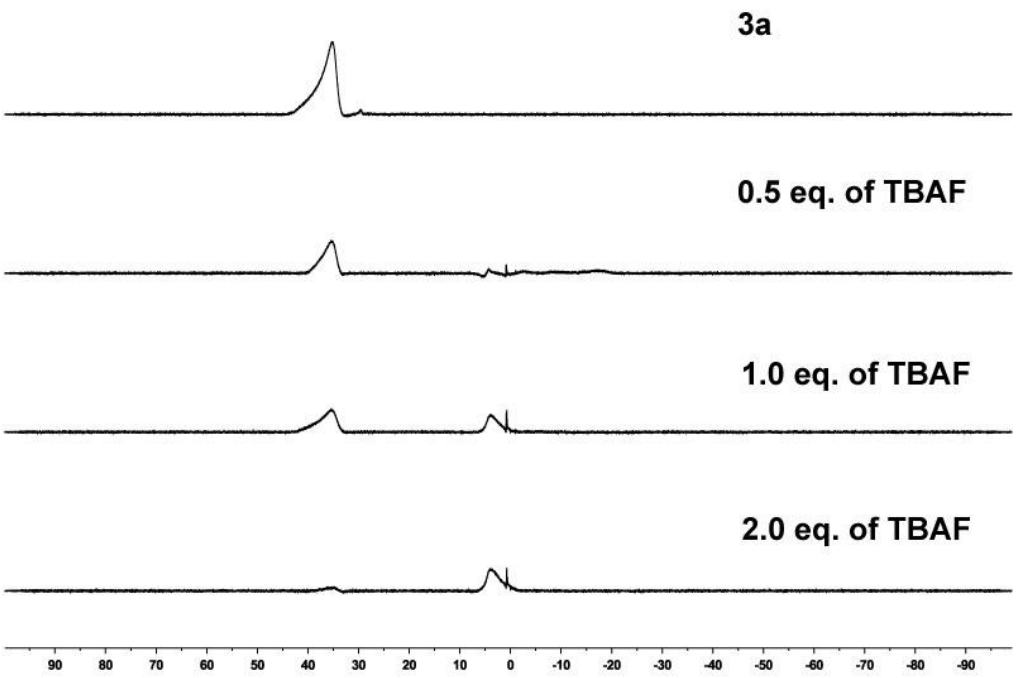


Fig S15. Spectral changes in the fluorescence of **BNDT** derivatives after the addition of F^- (short dashed line) and BF_3•Et_2O (dashed line). [F^-] = 5μM. [BF_3•Et_2O] >>5μM.

13. ^{11}B and ^{19}F NMR spectra of fluoride titration experiments

(a)



(b)

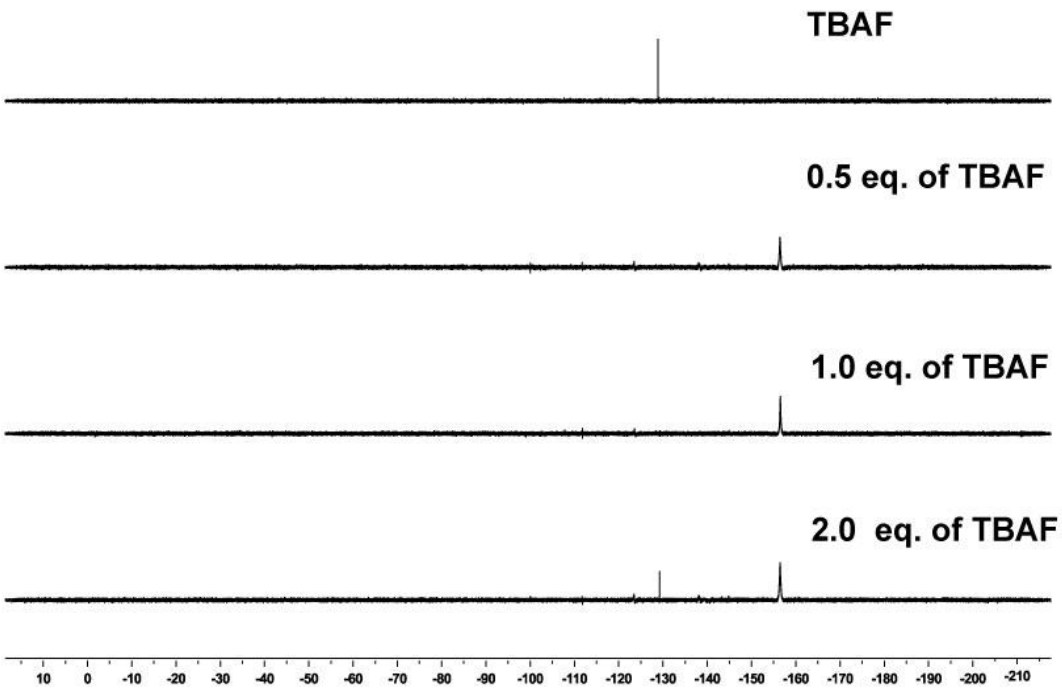


Fig S16. (a) ^{11}B NMR spectra of **3a** and a mixture of **3a** after addition of 0.5, 1.0 and 2.0 equivs. of TBAF. **(b)** ^{19}F NMR spectra of TBAF and a mixture of **3a** after addition of 0.5, 1.0 and 2.0 equivs. of TBAF.

14. The Calculated UV-Vis spectra

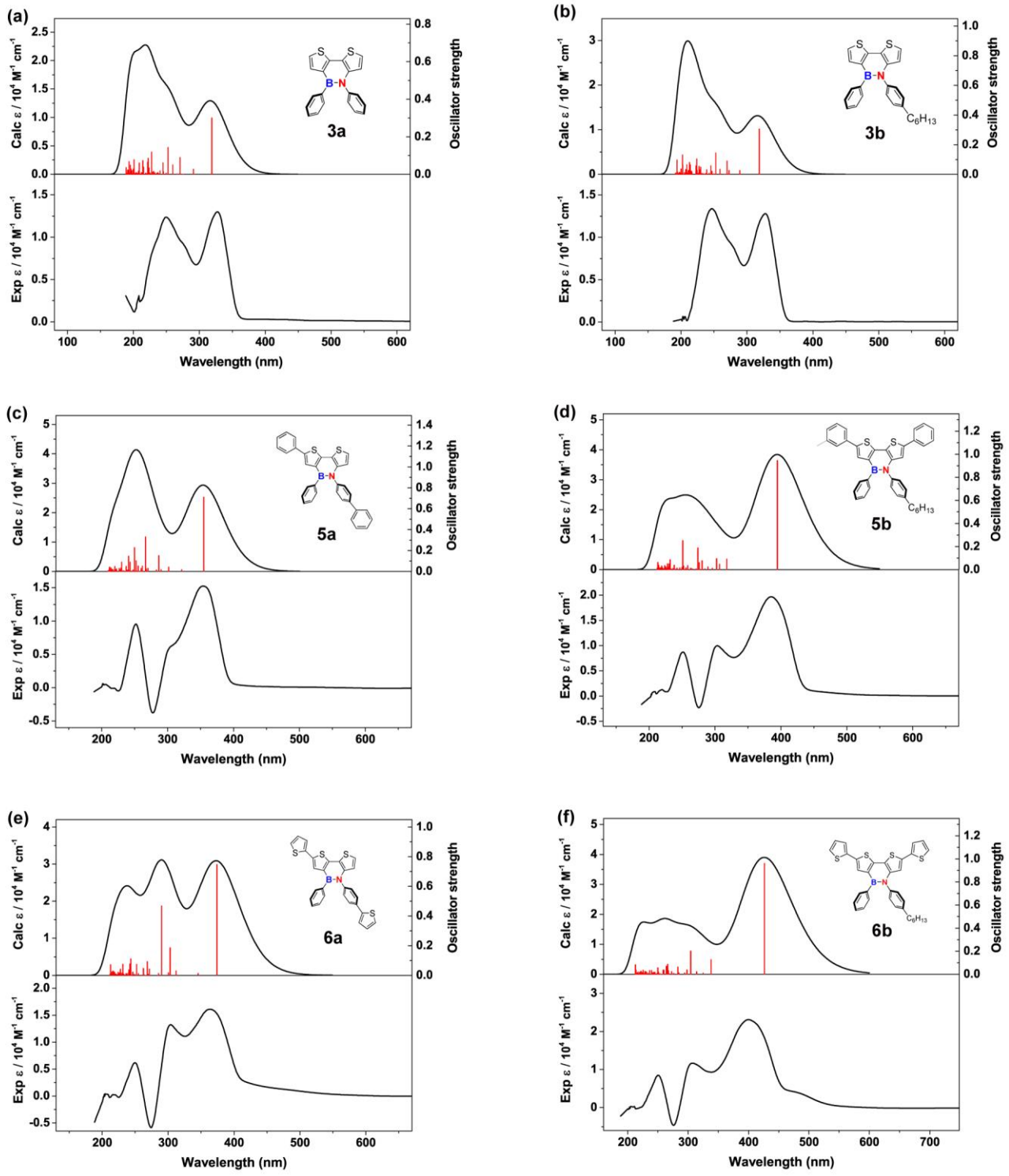


Figure S17. Calculated UV-Vis absorbance spectra at the TD-PBE0/6-311+G**//B3LYP/6-31+G** level of theory in gas-phase, and experimental UV-Vis spectra of **BNDT** derivatives.

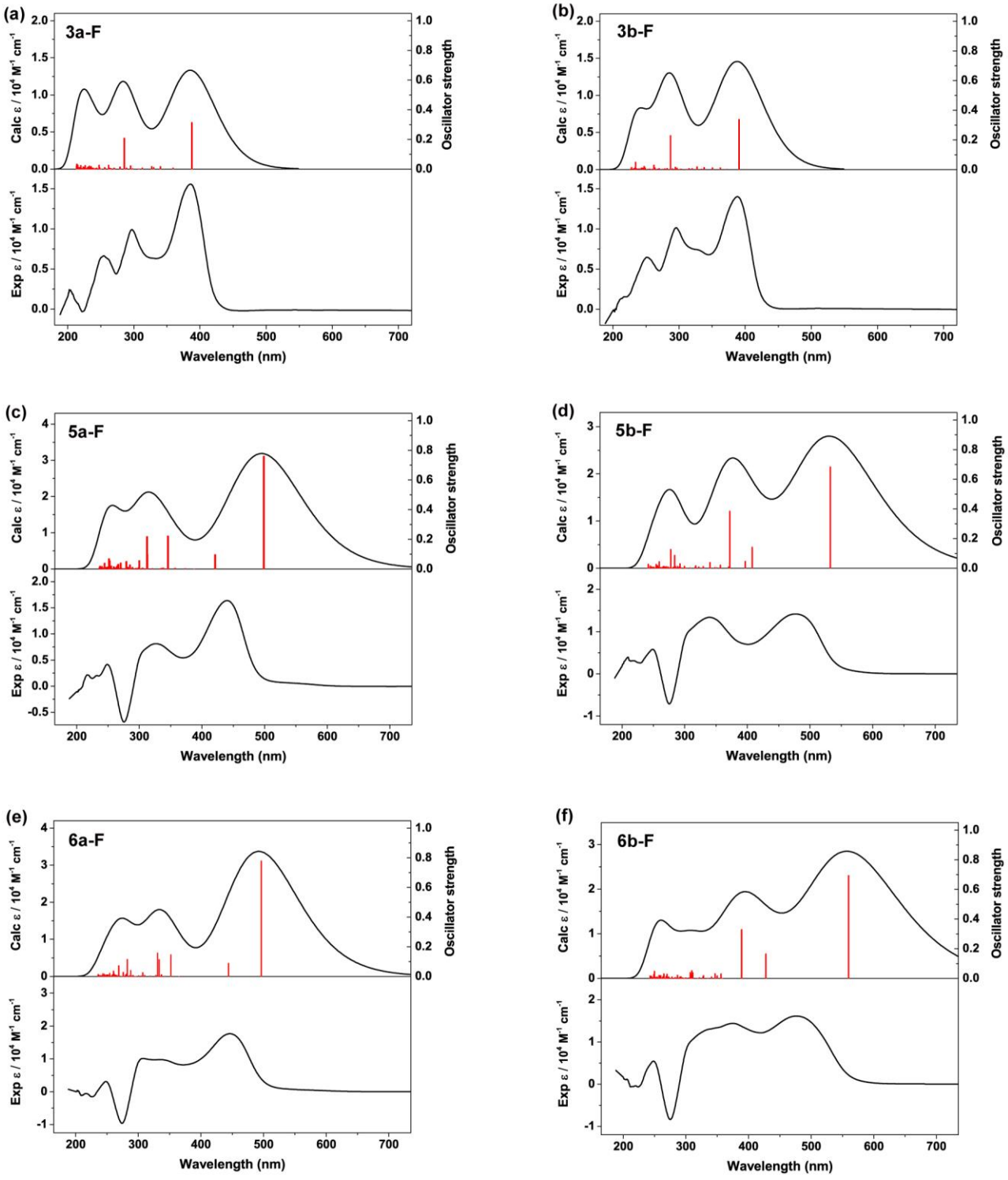


Figure S18. Calculated UV-Vis absorbance spectra at the TD-PBE0/6-311+G**//B3LYP/6-31+G** level of theory in gas-phase, and experimental UV-Vis spectra of **BNDT** derivatives after addition of TBAF.

Table S5. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **3a**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
318.86	0.3011	HOMO -> LUMO	95.22%
252.40	0.1432	HOMO-2 -> LUMO	72.01%
		HOMO -> LUMO+3	10.58%
227.44	0.1181	HOMO-6 -> LUMO	25.92%
		HOMO-5 -> LUMO+1	5.78%
		HOMO-2 -> LUMO+1	9.68%
		HOMO-1 -> LUMO+3	8.82%
		HOMO -> LUMO+9	9.68%

Table S6. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **3b**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
318.76	0.3066	HOMO -> LUMO	95.22%
252.72	0.1459	HOMO-2 -> LUMO	62.50%
		HOMO -> LUMO+3	14.15%
223.90	0.1052	HOMO-6 -> LUMO	25.63%
		HOMO -> LUMO+7	10.31%
		HOMO -> LUMO+9	7.22%
		HOMO -> LUMO+10	29.33%
202.36	0.1308	HOMO-6 -> LUMO+1	10.22%
		HOMO-1 -> LUMO+7	6.70%
		HOMO -> LUMO+14	13.21%
		HOMO -> LUMO+16	14.36%
		HOMO -> LUMO+17	9.25%

Table S7. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **5a**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
354.55	0.7112	HOMO -> LUMO	97.72%
286.34	0.1514	HOMO-1 -> LUMO	60.72%
		HOMO -> LUMO+2	5.31%
		HOMO -> LUMO+3	14.36%
266.15	0.3303	HOMO-1 -> LUMO+1	86.86%
252.01	0.1023	HOMO-7 -> LUMO	8.40%

		HOMO-5 -> LUMO	55.97%
		HOMO-4 -> LUMO	9.50%
249.43	0.2277	HOMO-2 -> LUMO+1	6.25%
		HOMO-1 -> LUMO+2	12.10%
		HOMO-1 -> LUMO+3	5.51%
240.67	0.1464	HOMO-7 -> LUMO	33.78%
		HOMO-5 -> LUMO	9.42%
		HOMO-1 -> LUMO+2	12.40%
		HOMO-1 -> LUMO+3	17.88%

Table S8. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **5b**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
394.29	0.9452	HOMO -> LUMO	98.56%
317.65	0.0909	HOMO-1 -> LUMO	14.58%
		HOMO -> LUMO+1	69.86%
		HOMO -> LUMO+2	10.76%
302.62	0.0952	HOMO-1 -> LUMO	76.38%
		HOMO -> LUMO+1	8.99%
		HOMO -> LUMO+2	6.41%
273.66	0.1888	HOMO-3 -> LUMO	86.86%
250.77	0.2514	HOMO-1 -> LUMO+1	57.89%
		HOMO-1 -> LUMO+2	22.04%

Table S9. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **6a**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
374.09	0.7465	HOMO -> LUMO	98.22%
303.00	0.1863	HOMO-1 -> LUMO	69.38%
		HOMO-1 -> LUMO+2	17.29%
290.14	0.4682	HOMO-1 -> LUMO+1	90.86%
268.47	0.0927	HOMO-9 -> LUMO+1	5.51%
		HOMO-3 -> LUMO	18.73%
		HOMO-2 -> LUMO+1	11.42%
		HOMO-1 -> LUMO+2	26.65%
		HOMO-1 -> LUMO+3	15.79%
		HOMO -> LUMO+4	7.61%
243.24	0.1118	HOMO-8 -> LUMO	12.80%
		HOMO-2 -> LUMO+2	41.95%
		HOMO-2 -> LUMO+3	17.76%

Table S10. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **6b**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
426.47	0.9599	HOMO -> LUMO	99.12%
338.10	0.1280	HOMO -> LUMO+1	91.13%
304.34	0.2019	HOMO-2 -> LUMO	75.40%
		HOMO-1 -> LUMO	10.13%
266.22	0.0868	HOMO-7 -> LUMO	13.21%
		HOMO-6 -> LUMO	8.57%
		HOMO-1 -> LUMO+1	28.43%
		HOMO -> LUMO+7	30.11%

Table S11. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **3a-F**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
397.92	0.3139	HOMO -> LUMO	97.72%
285.78	0.2092	HOMO-1 -> LUMO	92.75%

Table S12. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **3b-F**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
390.69	0.3378	HOMO -> LUMO+1	95.77%
287.10	0.2302	HOMO-1 -> LUMO+1	89.51%

Table S13. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **5a-F**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
498.51	0.7597	HOMO -> LUMO	98.56%
420.89	0.0963	HOMO -> LUMO+1	97.16%
345.59	0.2218	HOMO-1 -> LUMO	96.05%
312.54	0.0980	HOMO-1 -> LUMO+1	19.85%
		HOMO -> LUMO+9	8.41%

		HOMO -> LUMO+13	6.05%
312.34	0.2179	HOMO-1 -> LUMO+1	76.14%
		HOMO -> LUMO+13	14.69%

Table S14. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **5b-F**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
532.86	0.6833	HOMO -> LUMO	99.12%
408.08	0.1421	HOMO -> LUMO+1	91.13%
372.23	0.3853	HOMO-1 -> LUMO	96.61%
278.00	0.1273	HOMO-6 -> LUMO	60.94%
		HOMO-5 -> LUMO	10.31%
		HOMO-4 -> LUMO	6.06%
		HOMO -> LUMO+20	8.41%

Table S15. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **6a-F**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
496.23	0.7787	HOMO -> LUMO	98.28%
443.95	0.0887	HOMO -> LUMO+1	97.72%
352.04	0.1467	HOMO-1 -> LUMO	94.67%
333.23	0.1140	HOMO-1 -> LUMO+1	25.49%
		HOMO -> LUMO+2	9.86%
		HOMO -> LUMO+4	7.14%
		HOMO -> LUMO+5	38.37%
		HOMO -> LUMO+6	9.77%
330.66	0.1577	HOMO-1 -> LUMO+1	65.21%
		HOMO -> LUMO+4	15.79%
		HOMO -> LUMO+5	12.10%

Table S16. Calculated ($\lambda_{TD\text{-}DFT}$) wavelengths of **6b-F**. Molecular orbitals (MOs) involved in the main electronic transition，f corresponds to the oscillator strength. (TD-PBE0/6-311+G**//B3LYP/6-31+G**)

$\lambda_{TD\text{-}DFT}$	Oscillator Strength, f	MOs	
559.77	0.6933	HOMO -> LUMO	99.12%
427.78	0.1656	HOMO -> LUMO+1	96.33%
388.99	0.3291	HOMO-1 -> LUMO	97.16%

15. DFT calculations and comparison of HOMO/LUMO plots

Comparison of HOMO/LUMO plots for **3a**, **3b**, **5a**, **5b**, **6a**, **6b**, **3a-F, 3b-F, 5a-F, 5b-F, 6a-F** and **6b-F** at the B3LYP level with the 6-31+G** basis set.

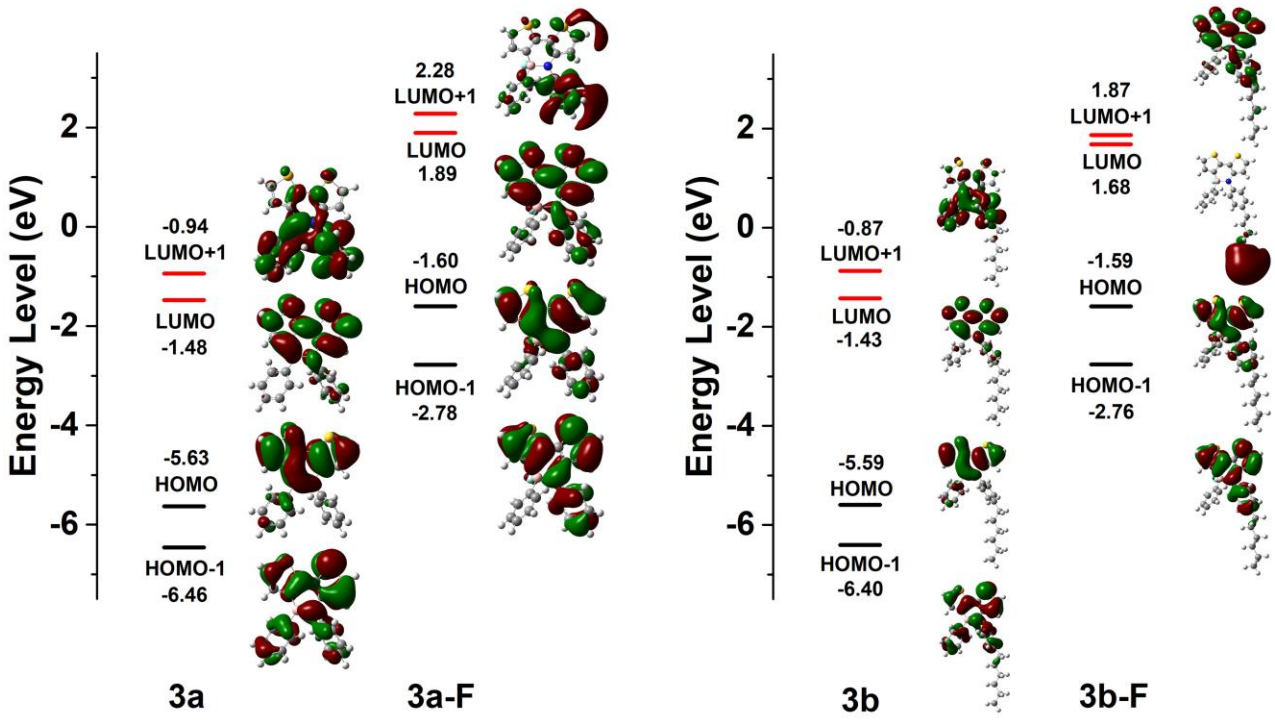


Figure S19. HOMO-1, HOMO, LUMO and LUMO+1 energy levels of **3a**, **3b**, **3a-F** and **3b-F** in the gas-phase at the B3LYP/6-31+G** level.

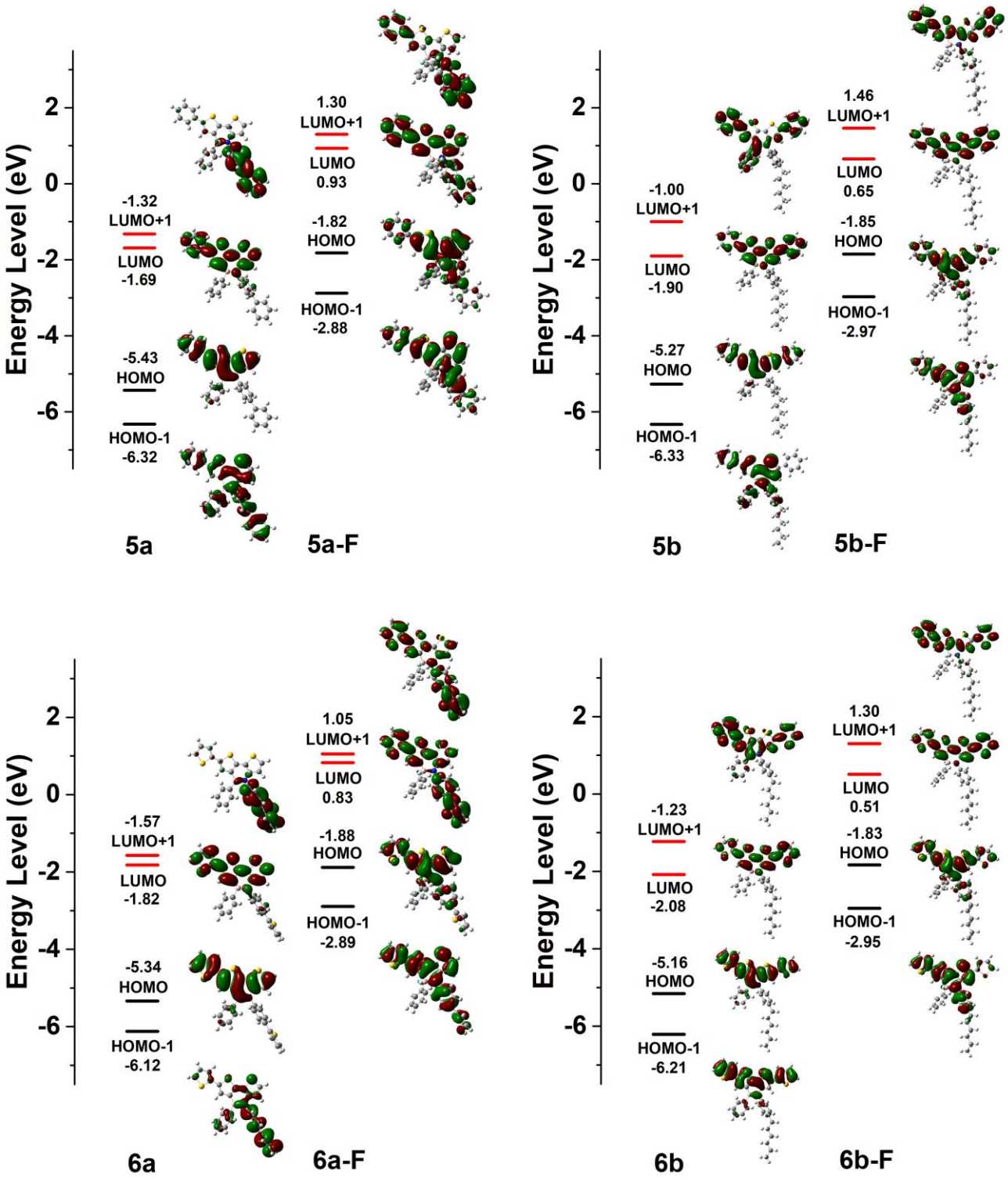


Figure S20. HOMO-1, HOMO, LUMO and LUMO+1 energy levels of **5a**, **5b**, **6a**, **6b**, **5a-F, 5b-F, 6a-F** and **6b-F** in the gas-phase at the B3LYP/6-31+G** level.

16. ^{1}H NMR and ^{13}C NMR spectra

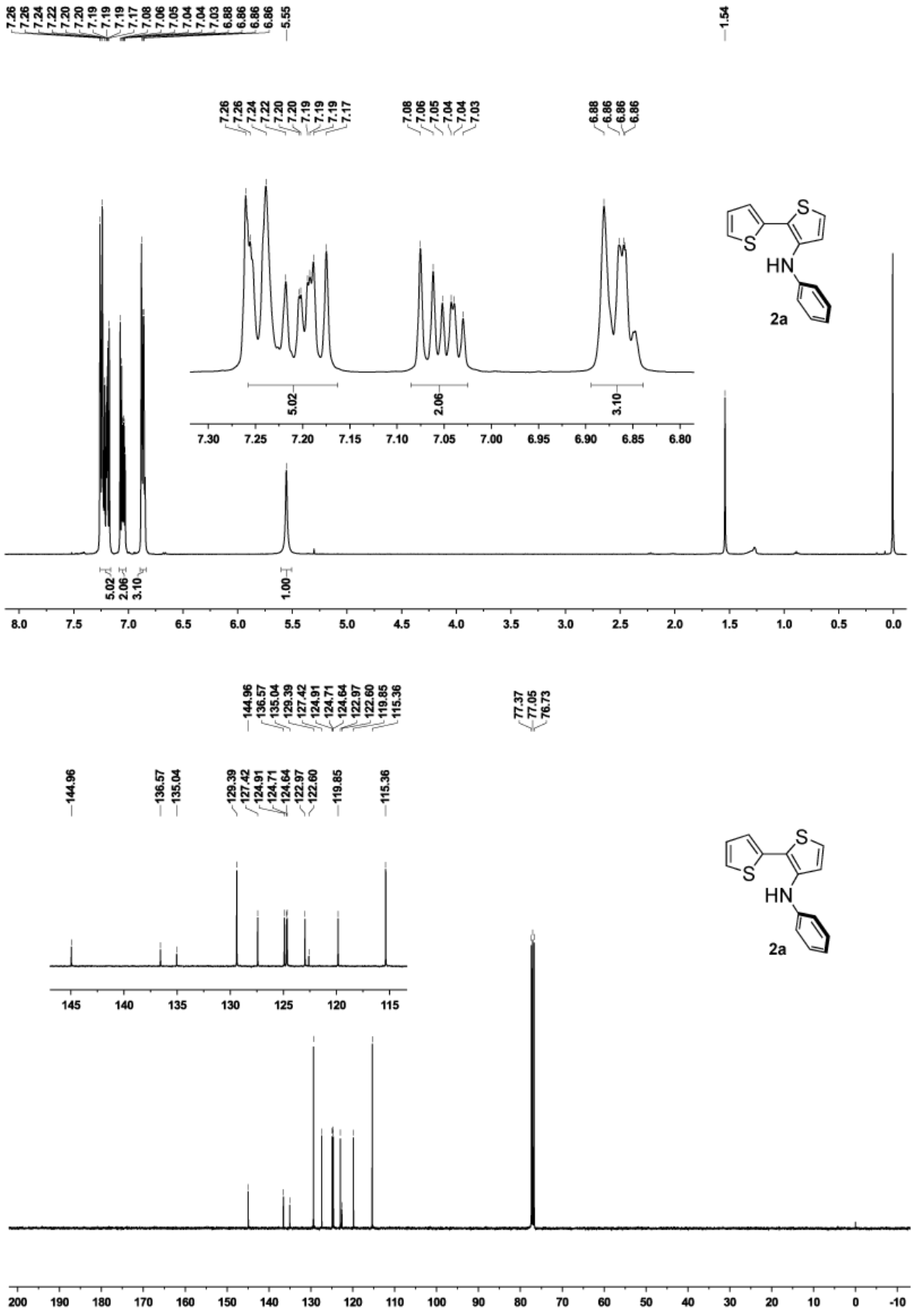


Figure S21. ^{1}H NMR and ^{13}C NMR spectra of **2a** in $CDCl_3$

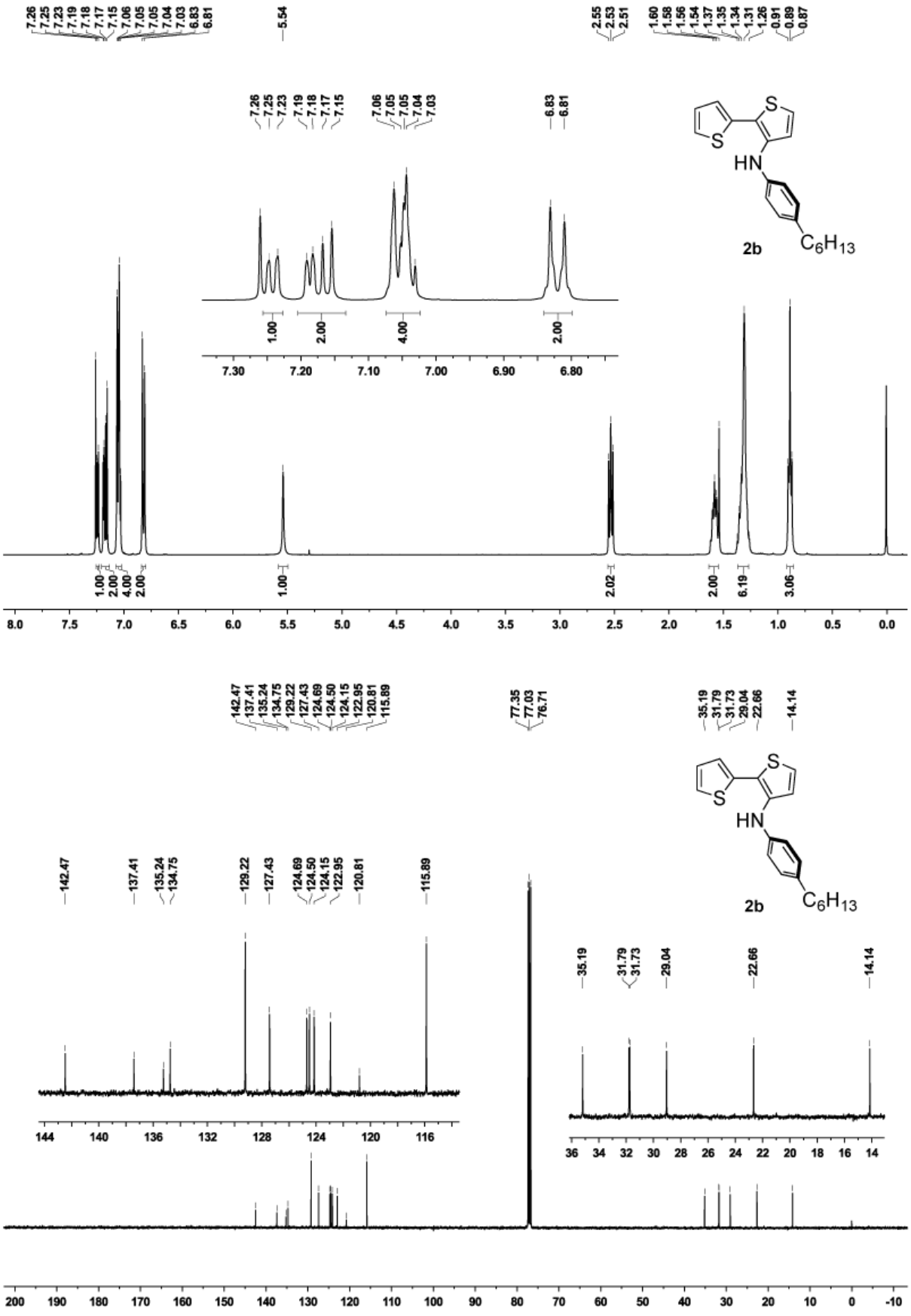


Figure S22. ^{1}H NMR and ^{13}C NMR spectra of **2b** in $CDCl_3$

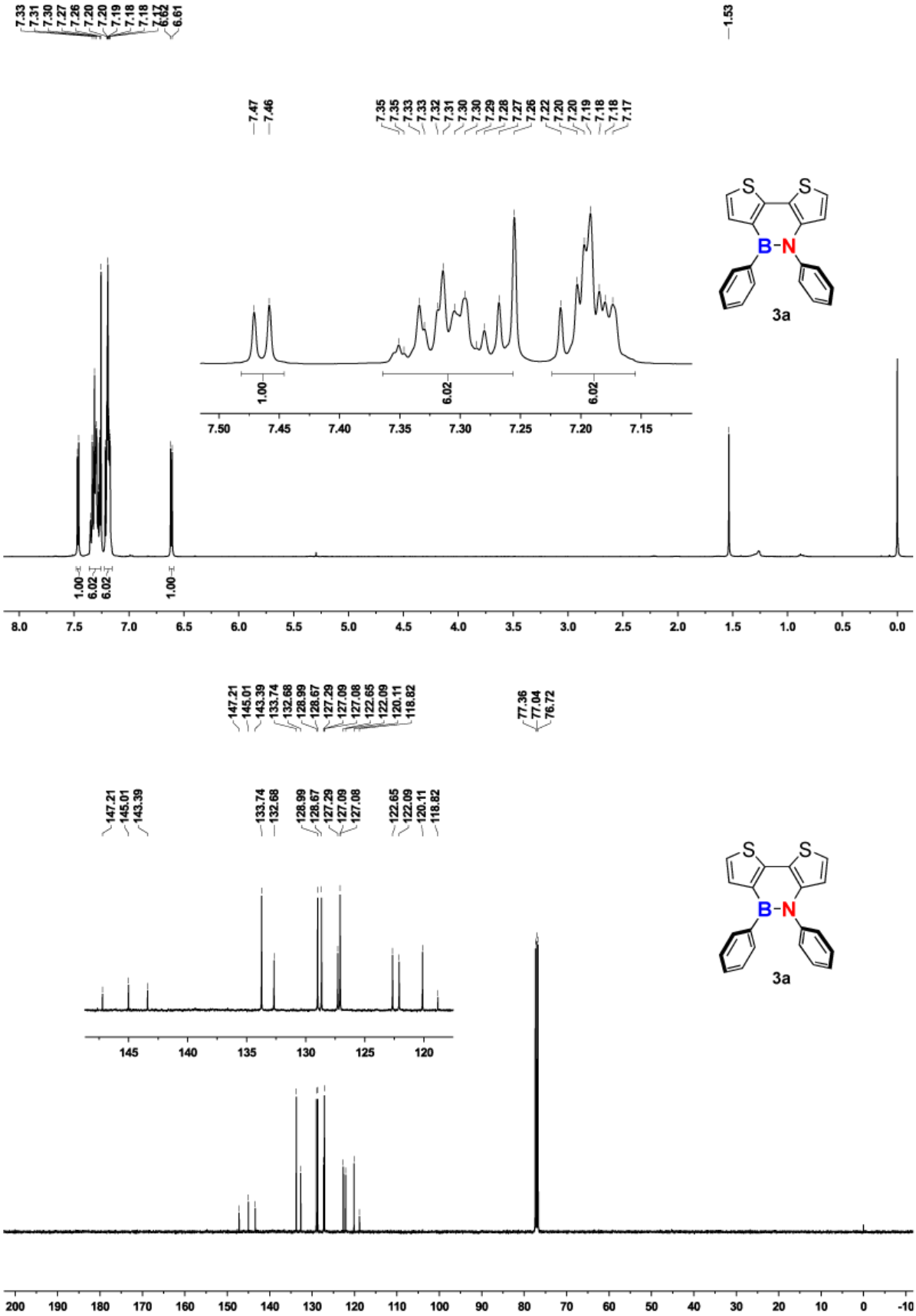


Figure S23. ^{1}H NMR and ^{13}C NMR spectra of **3a** in $CDCl_3$

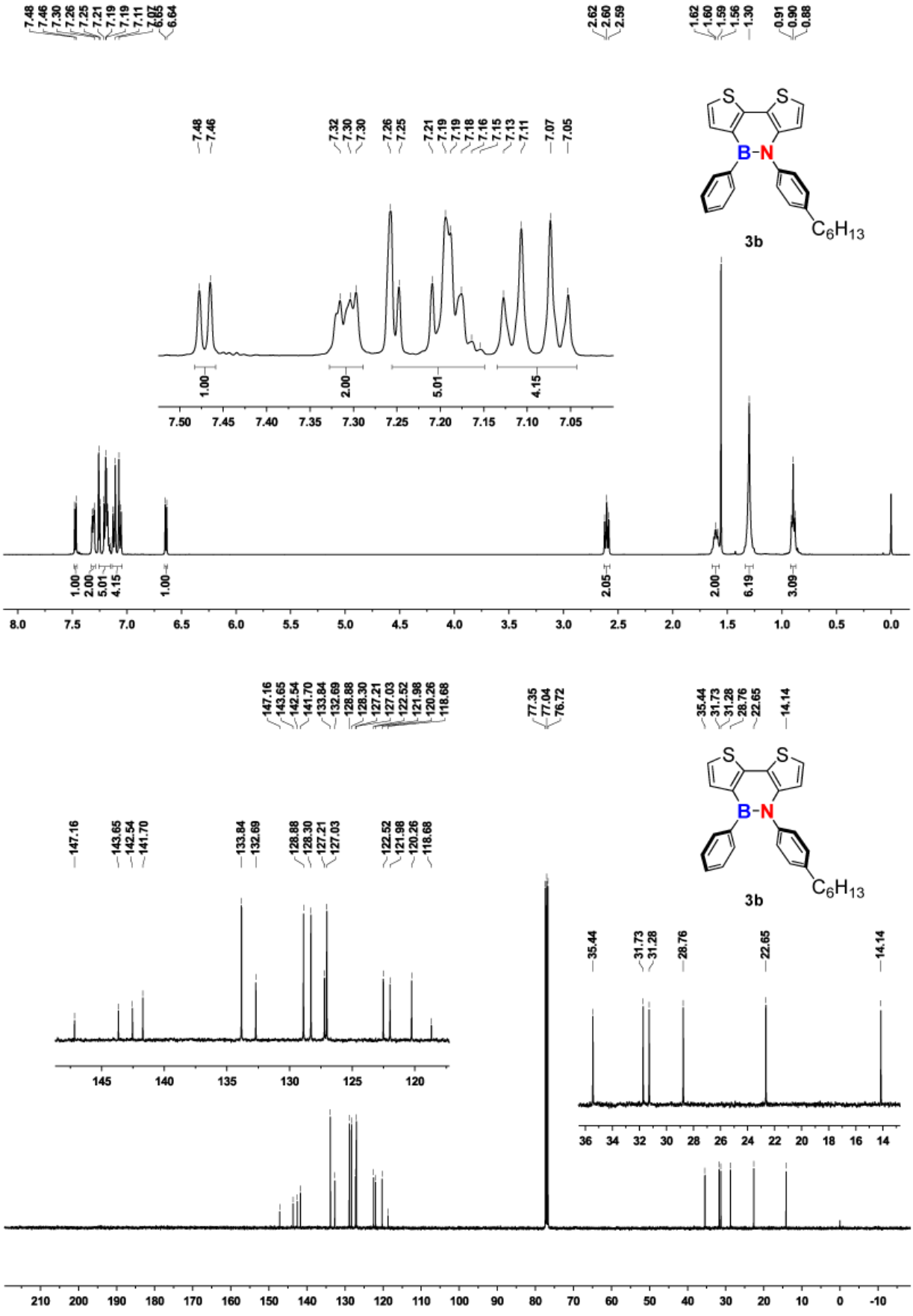


Figure S24. ^{1}H NMR and ^{13}C NMR spectra of **3b** in $CDCl_3$

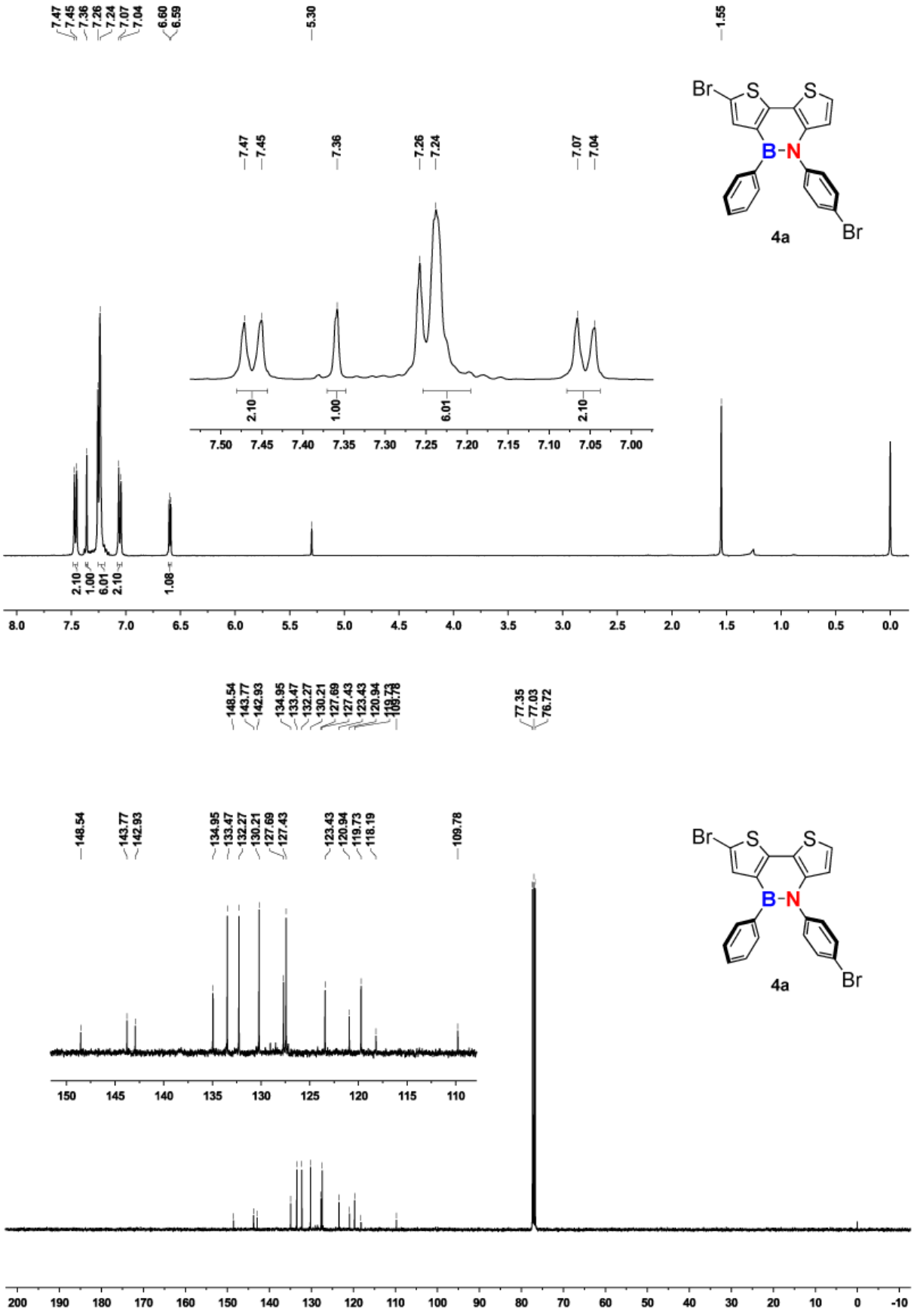


Figure S25. ^{1}H NMR and ^{13}C NMR spectra of **4a** in $CDCl_3$

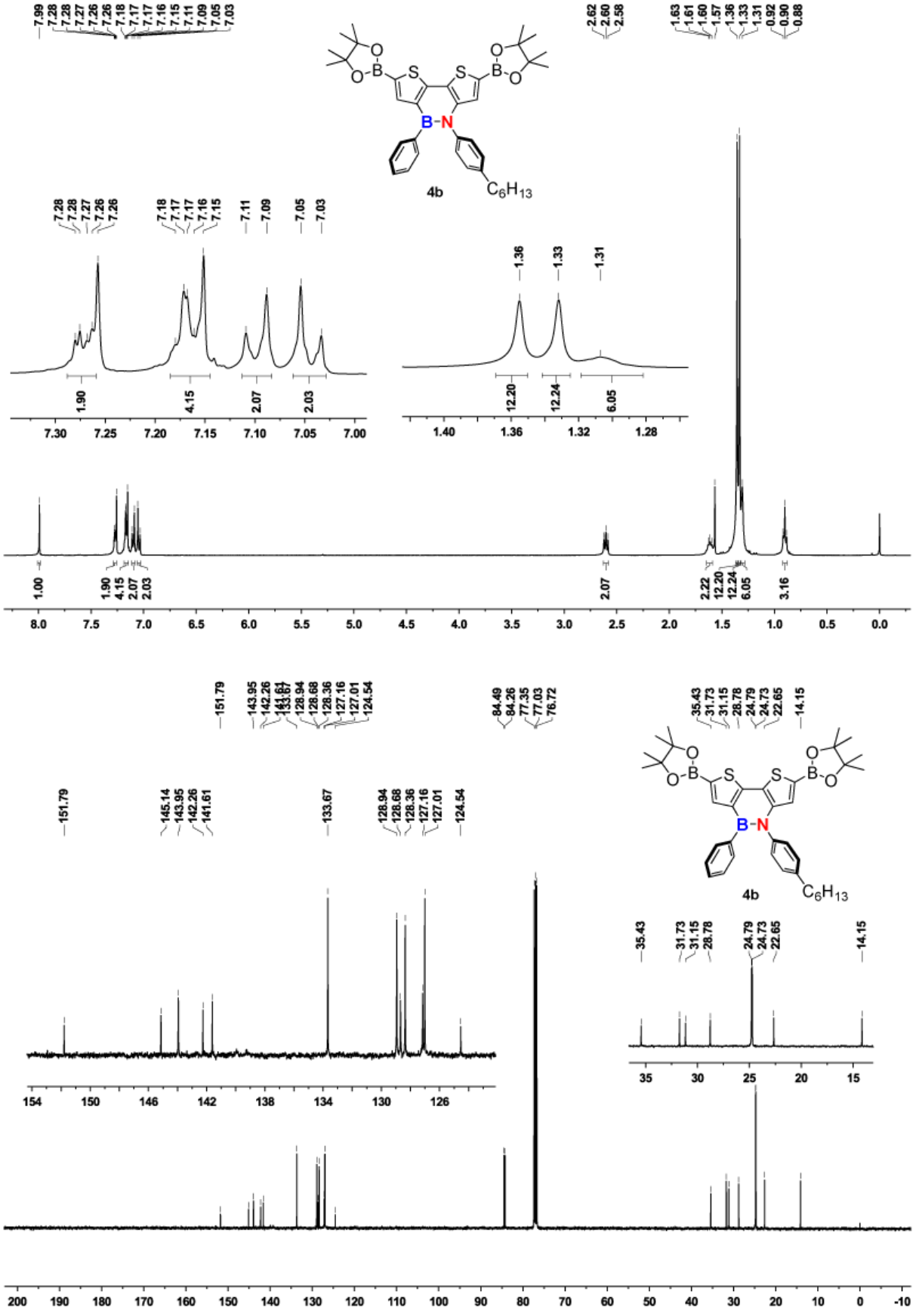


Figure S26. ^{1}H NMR and ^{13}C NMR spectra of **4b** in $CDCl_3$

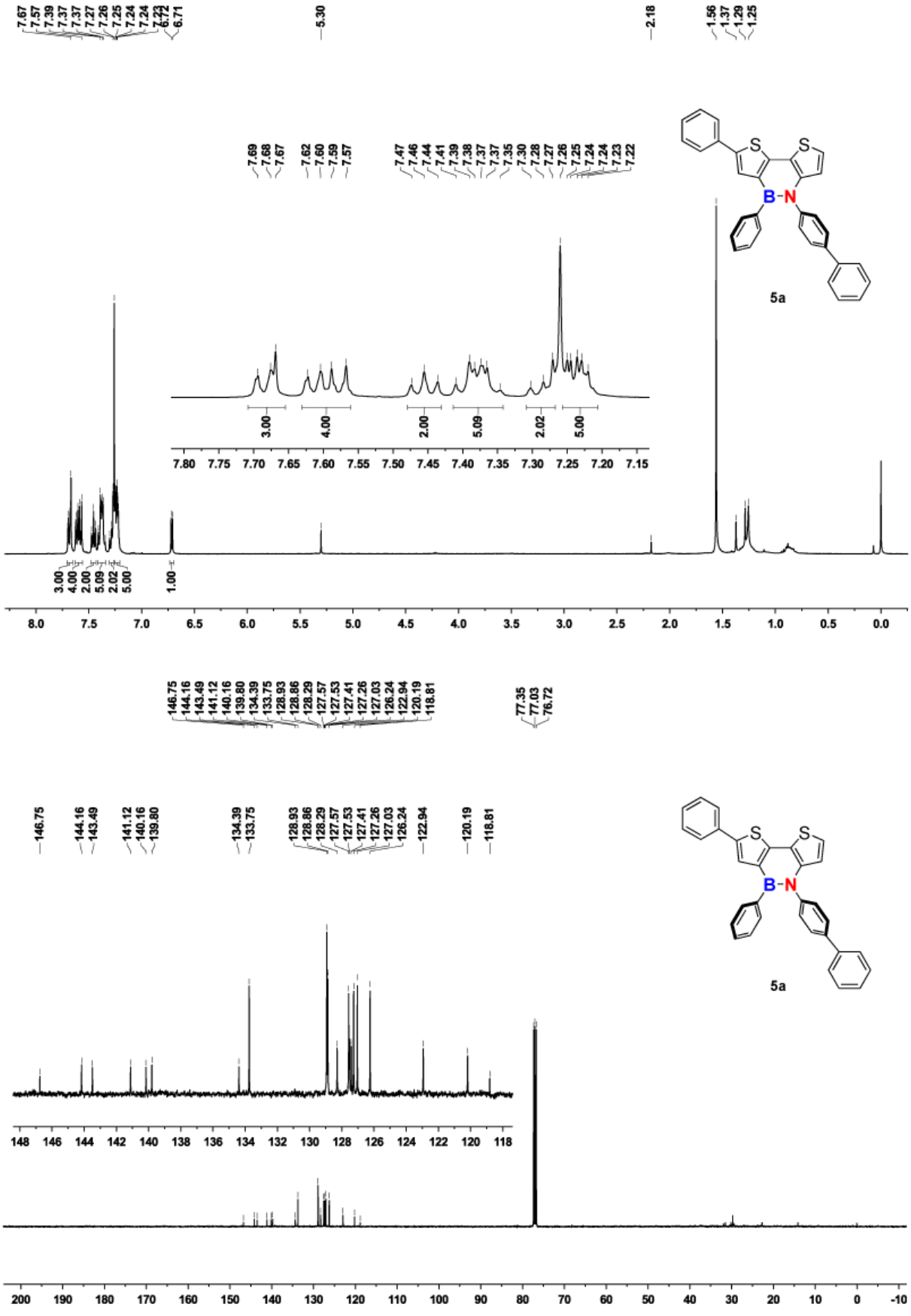


Figure S27. ^{1}H NMR and ^{13}C NMR spectra of **5a** in $CDCl_3$

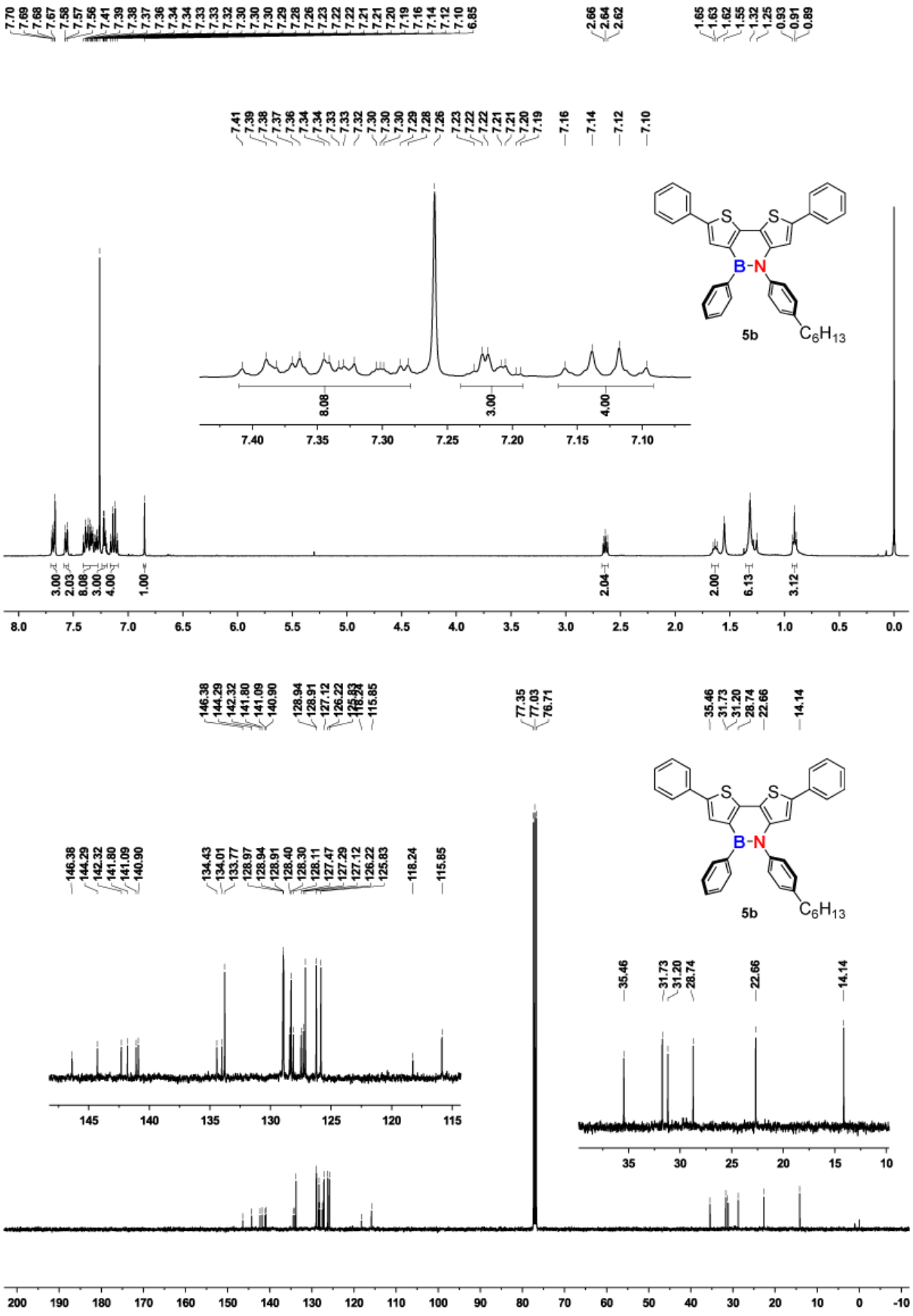


Figure S28. ^{1}H NMR and ^{13}C NMR spectra of **5b** in $CDCl_3$

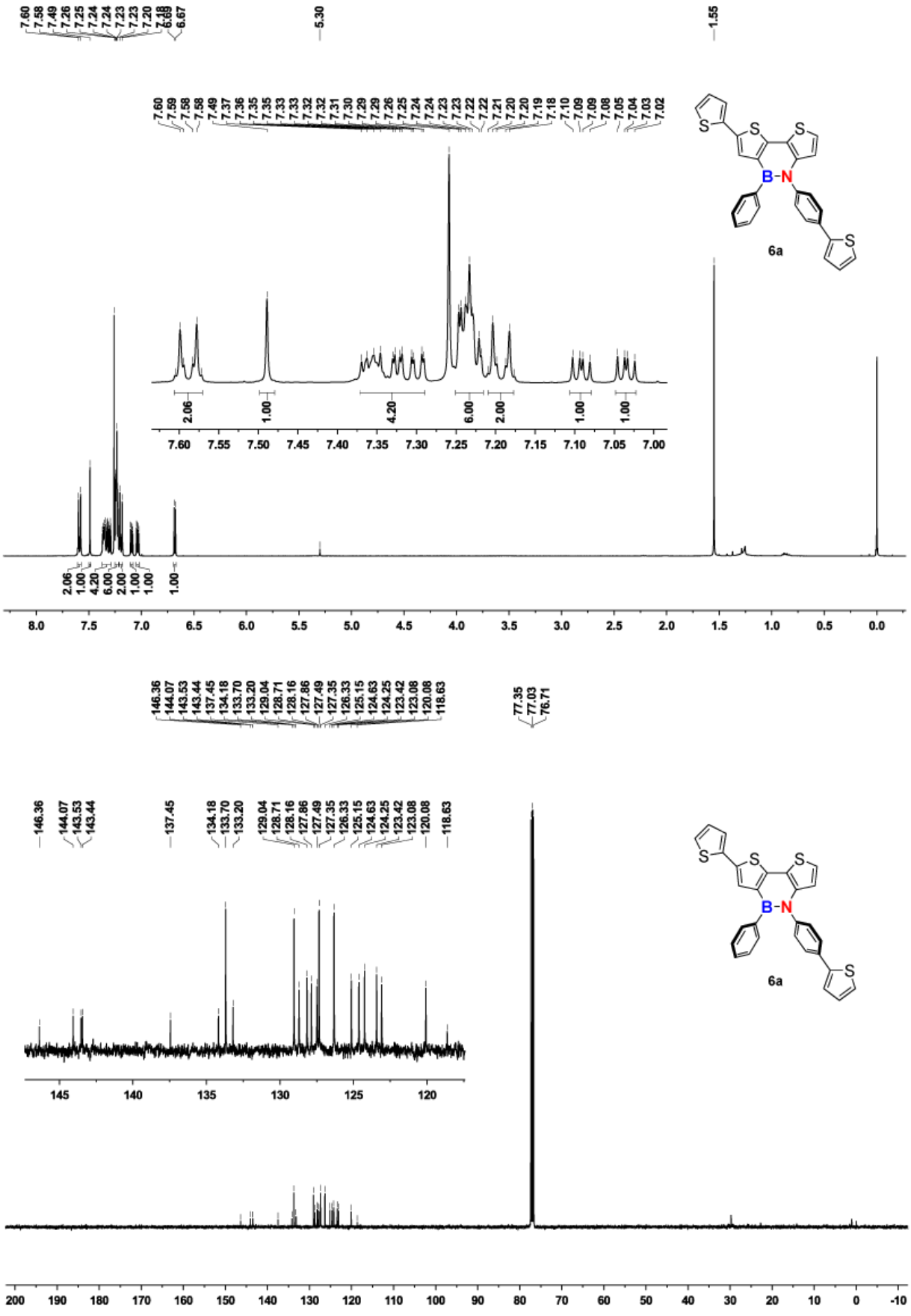


Figure S29. ^{1}H NMR and ^{13}C NMR spectra of **6a** in $CDCl_3$

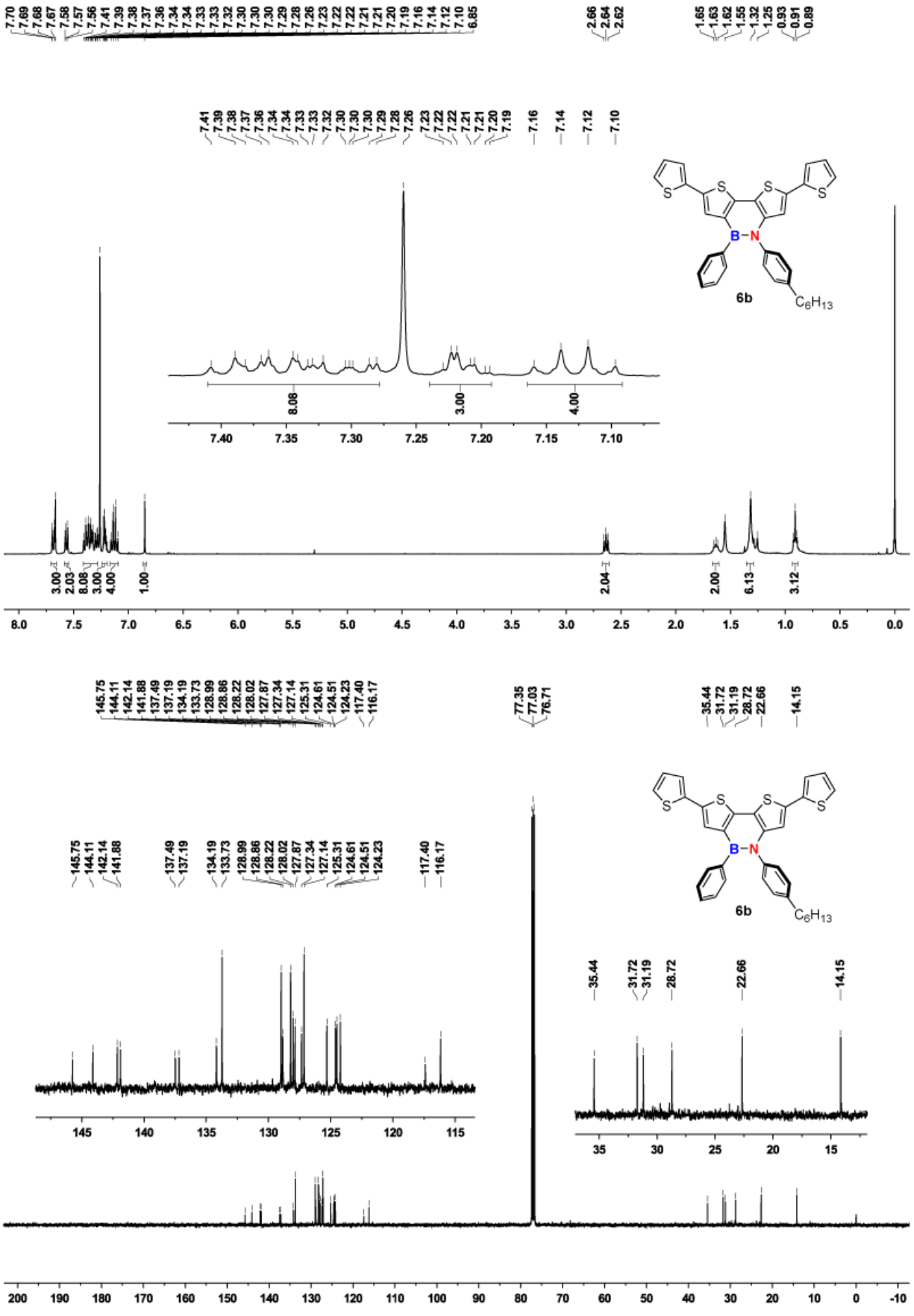


Figure S30. ^{1}H NMR and ^{13}C NMR spectra of **6b** in $CDCl_3$

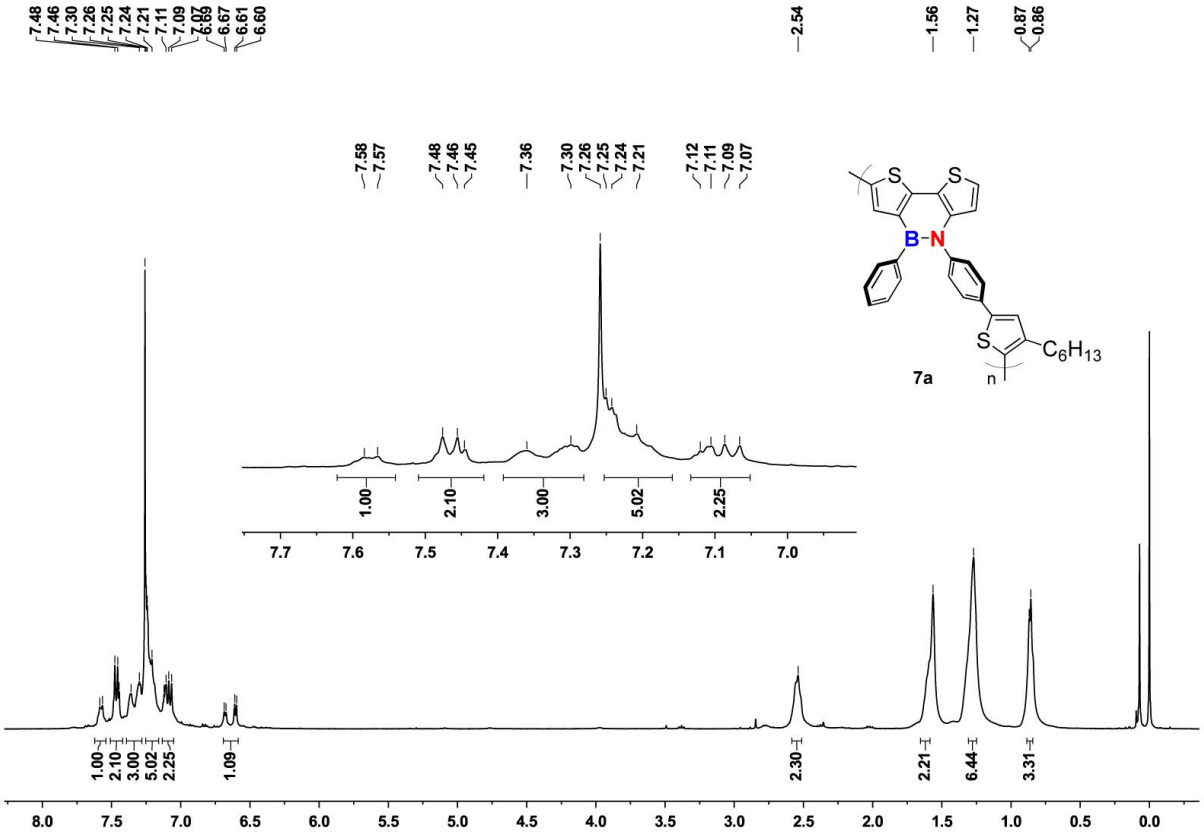


Figure S31. ^{1}H NMR spectra of **7a** in $CDCl_3$

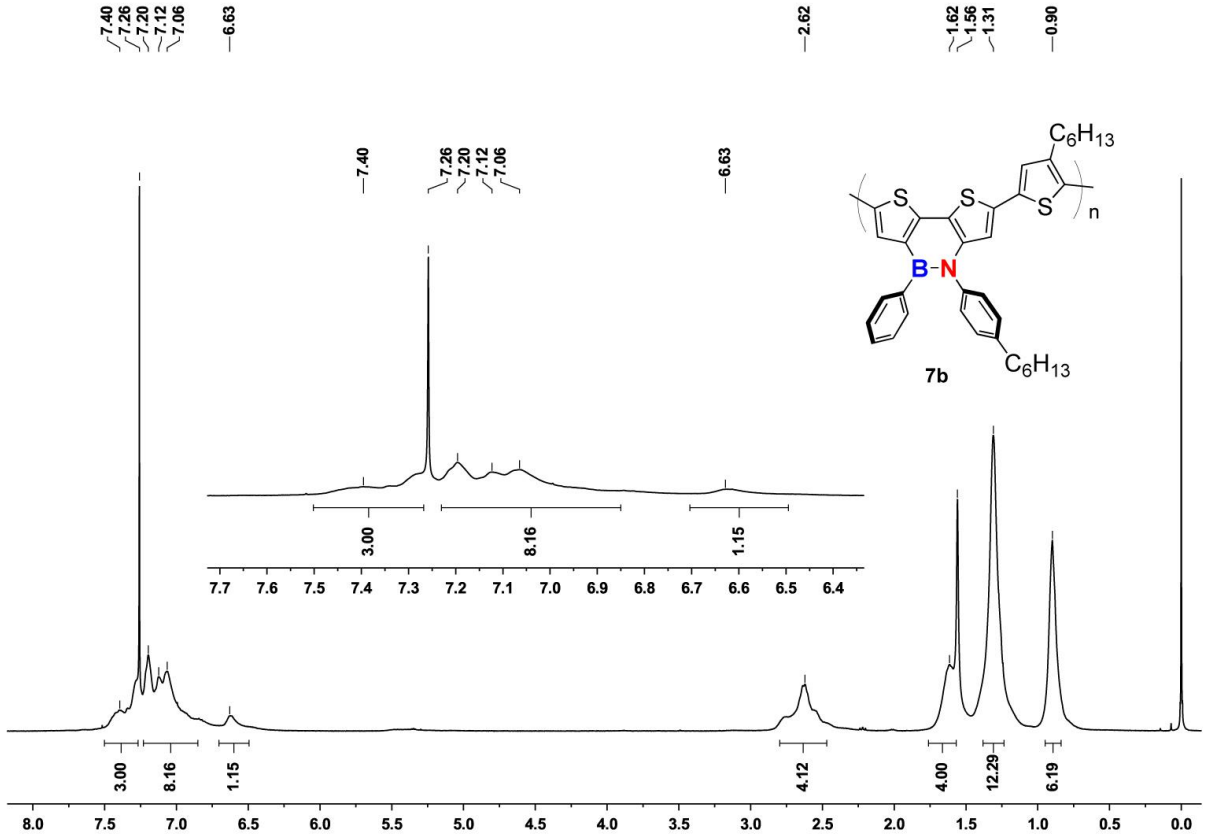


Figure S32. ^{1}H NMR spectra of **7b** in $CDCl_3$

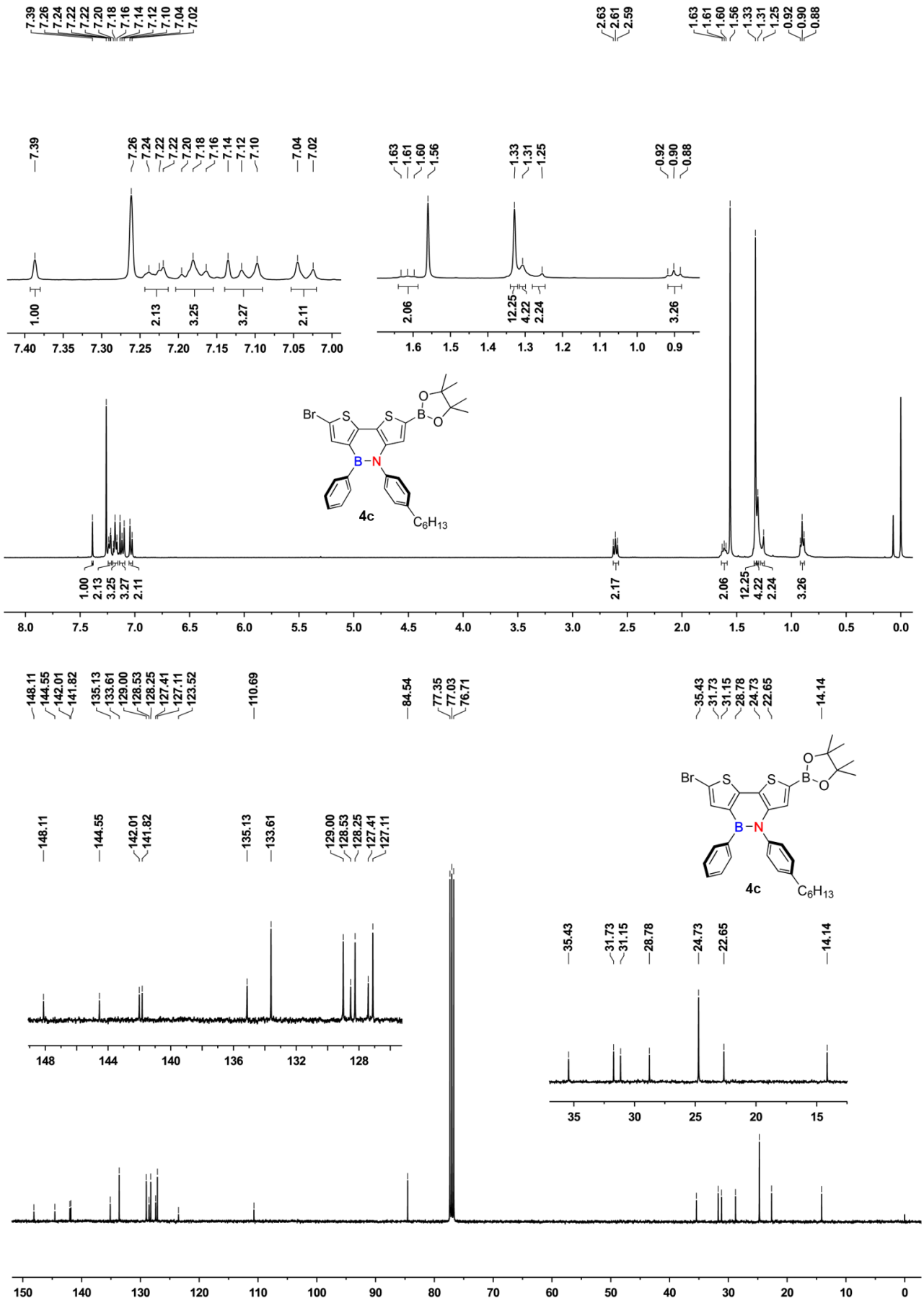


Figure S33. ^{1}H NMR and ^{13}C NMR spectra of **4c** in $CDCl_3$

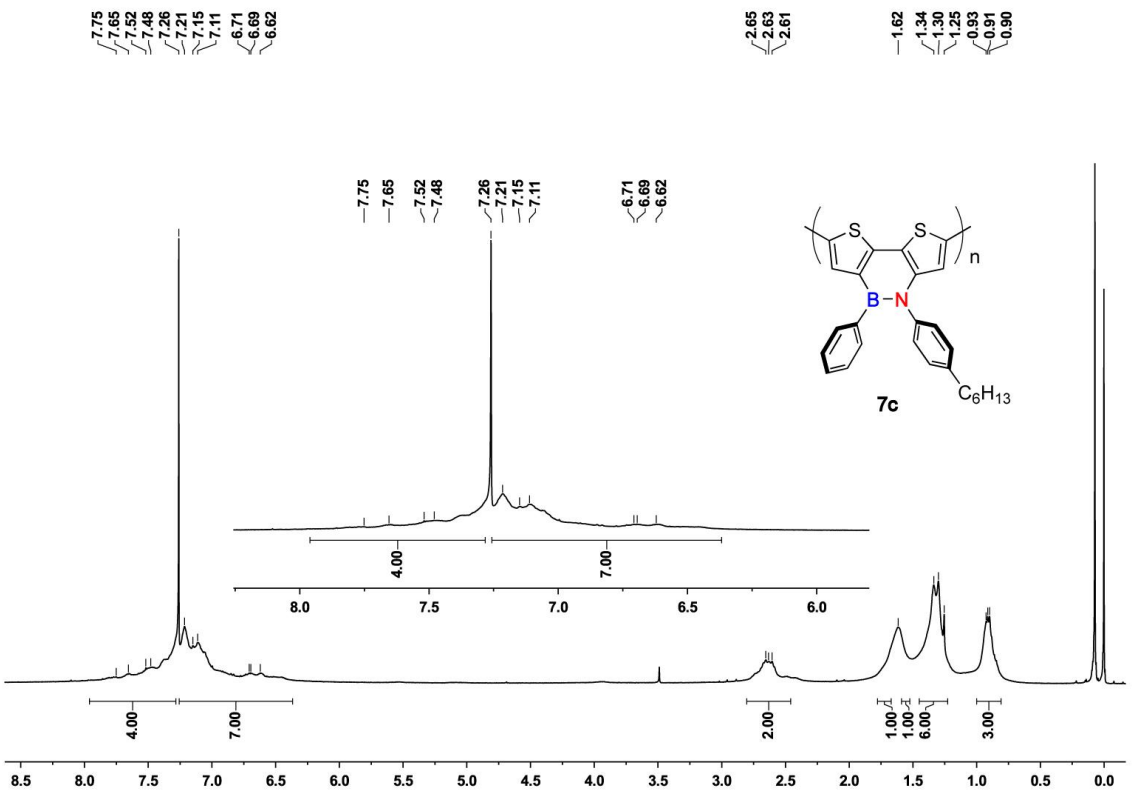


Figure S34. ^{1}H NMR spectra of **7c** in $CDCl_3$

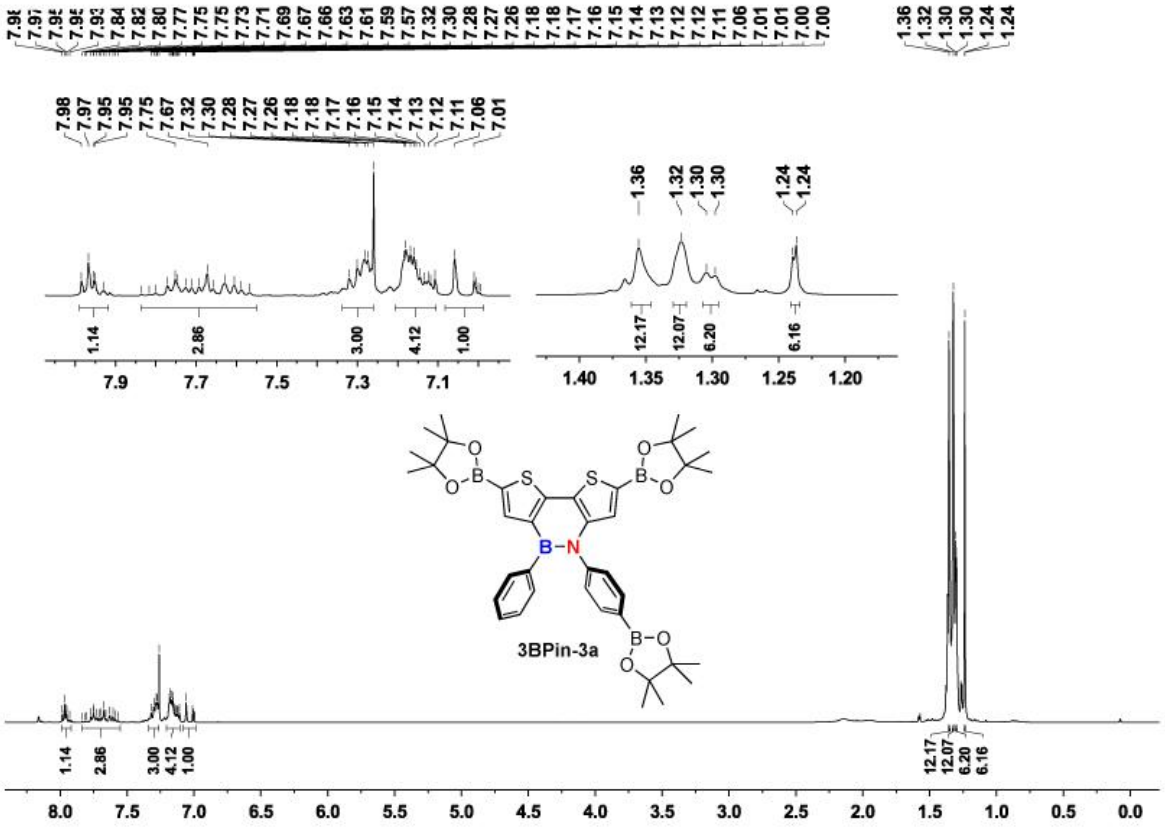


Figure S35. ^{1}H NMR spectra of **3BPin-3a** in $CDCl_3$

17. ^{11}B NMR spectra

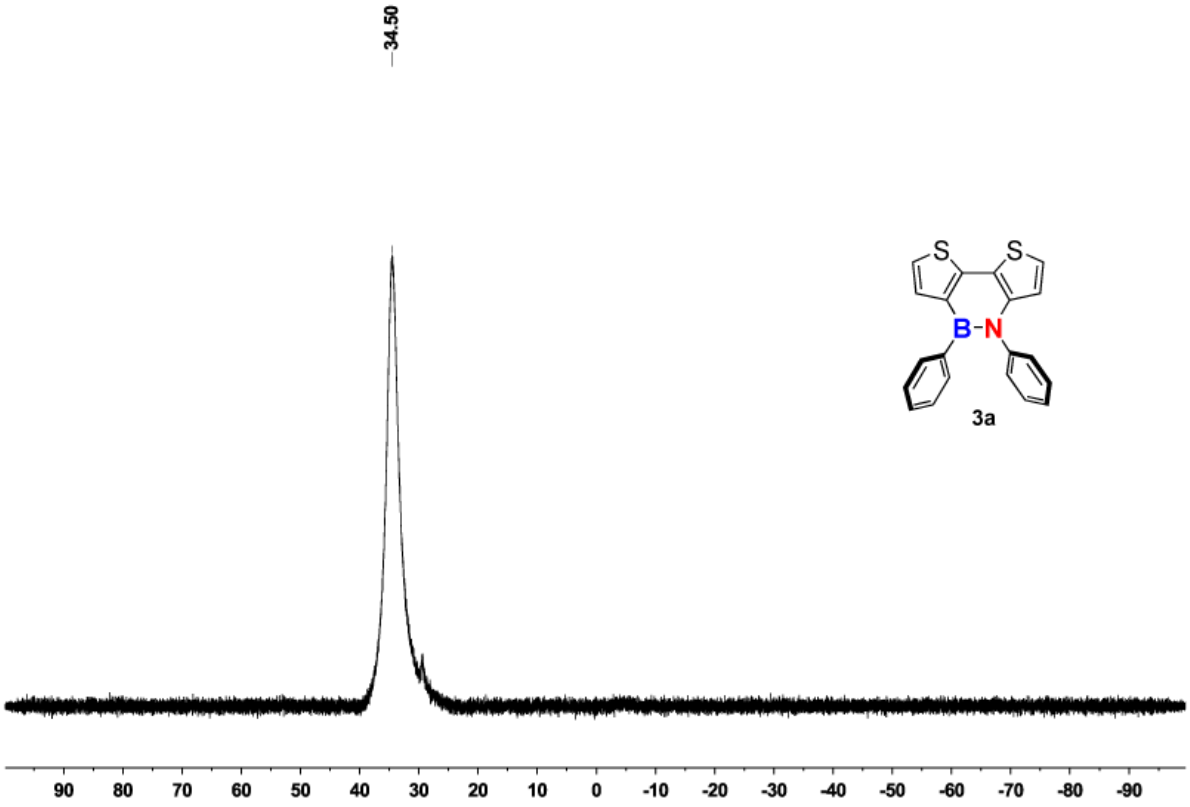


Figure S36. ^{11}B NMR spectra of **3a** in $CDCl_3$

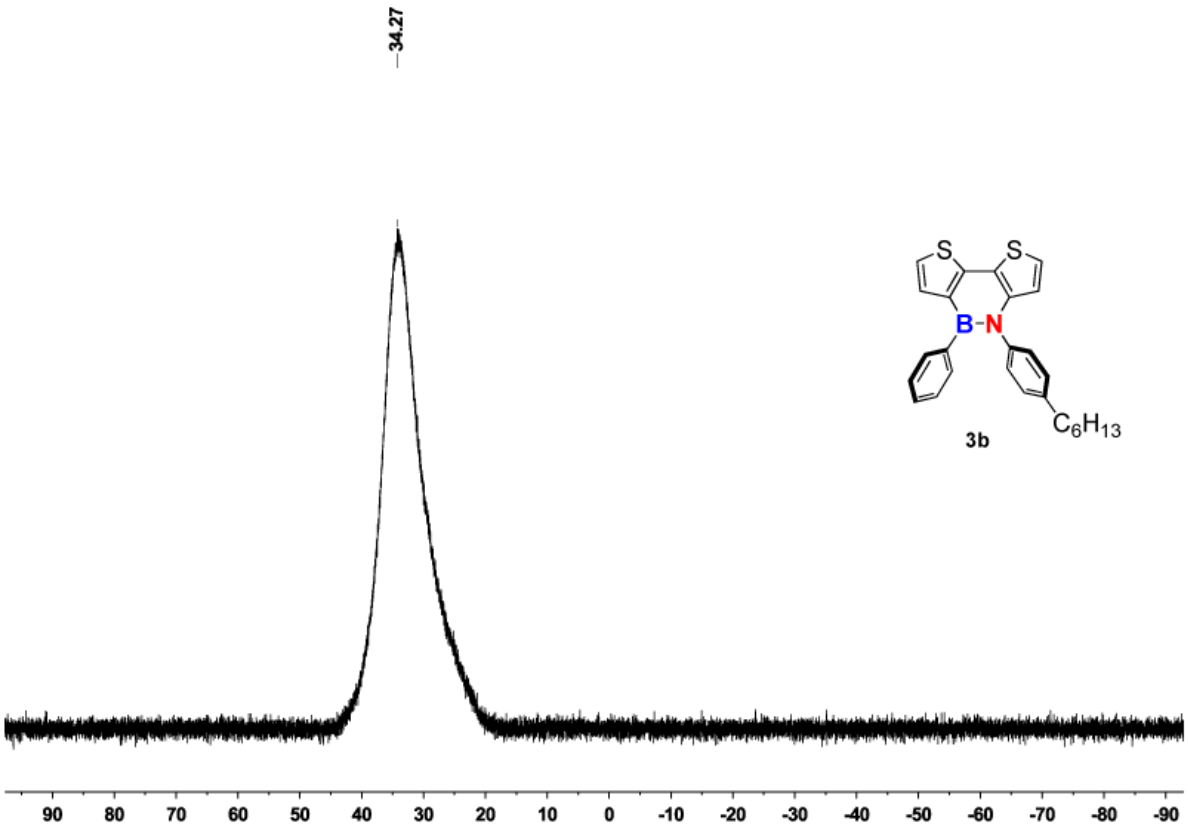


Figure S37. ^{11}B NMR spectra of **3b** in $CDCl_3$

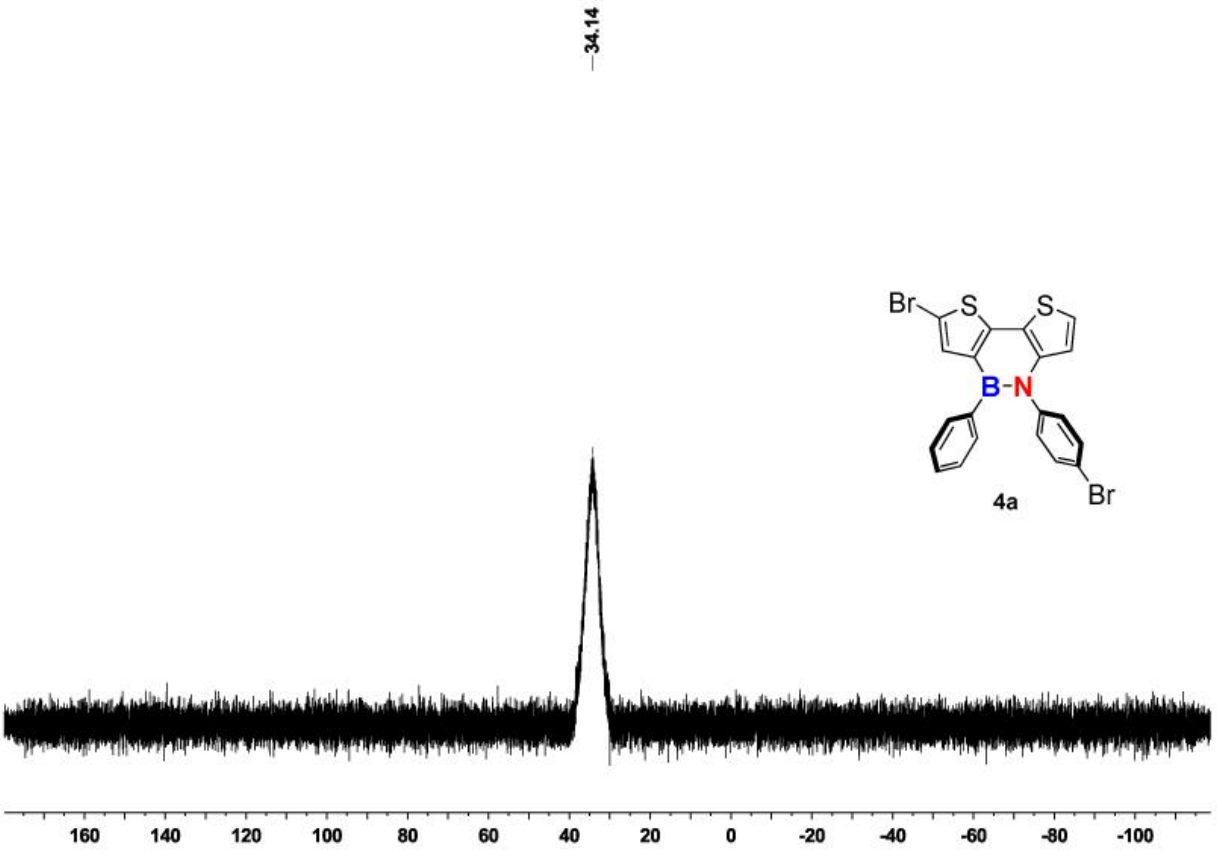


Figure S38. ^{11}B NMR spectra of **4a** in $CDCl_3$

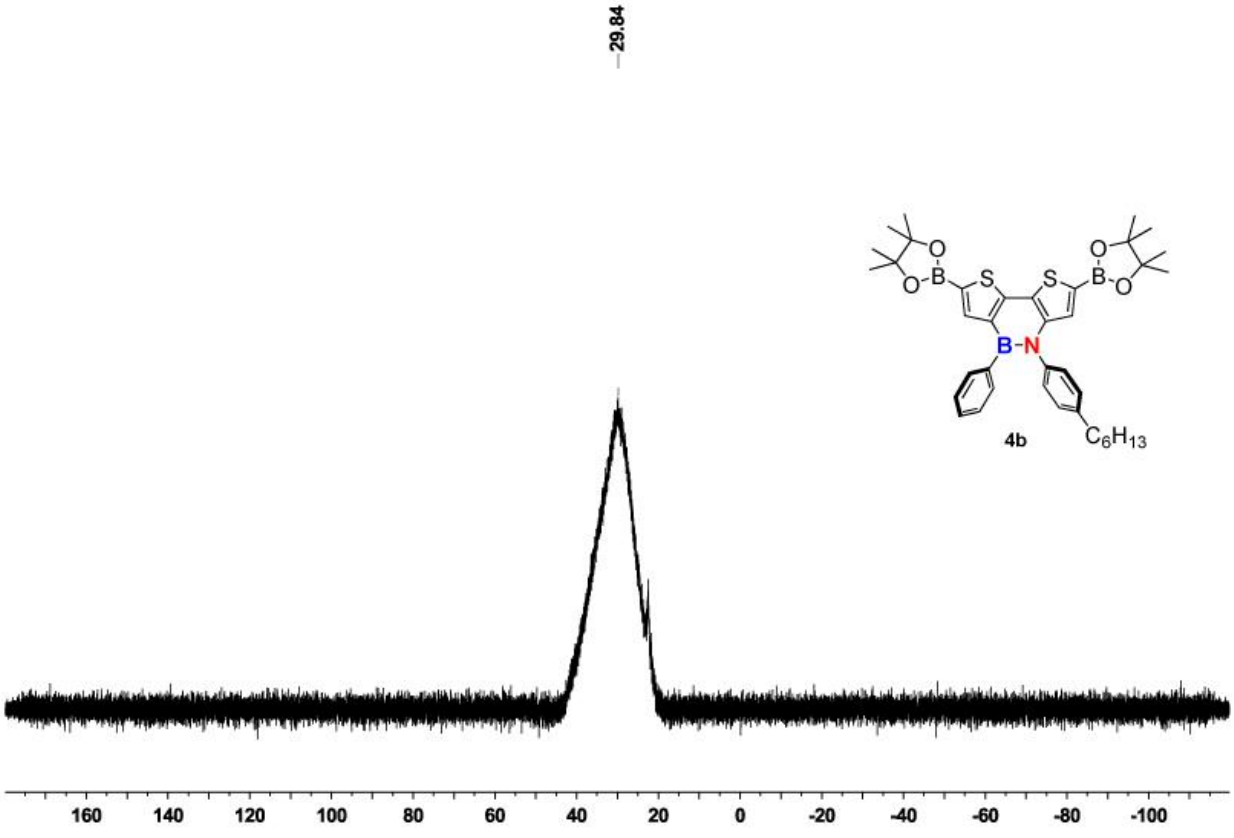


Figure S39. ^{11}B NMR spectra of **4b** in $CDCl_3$

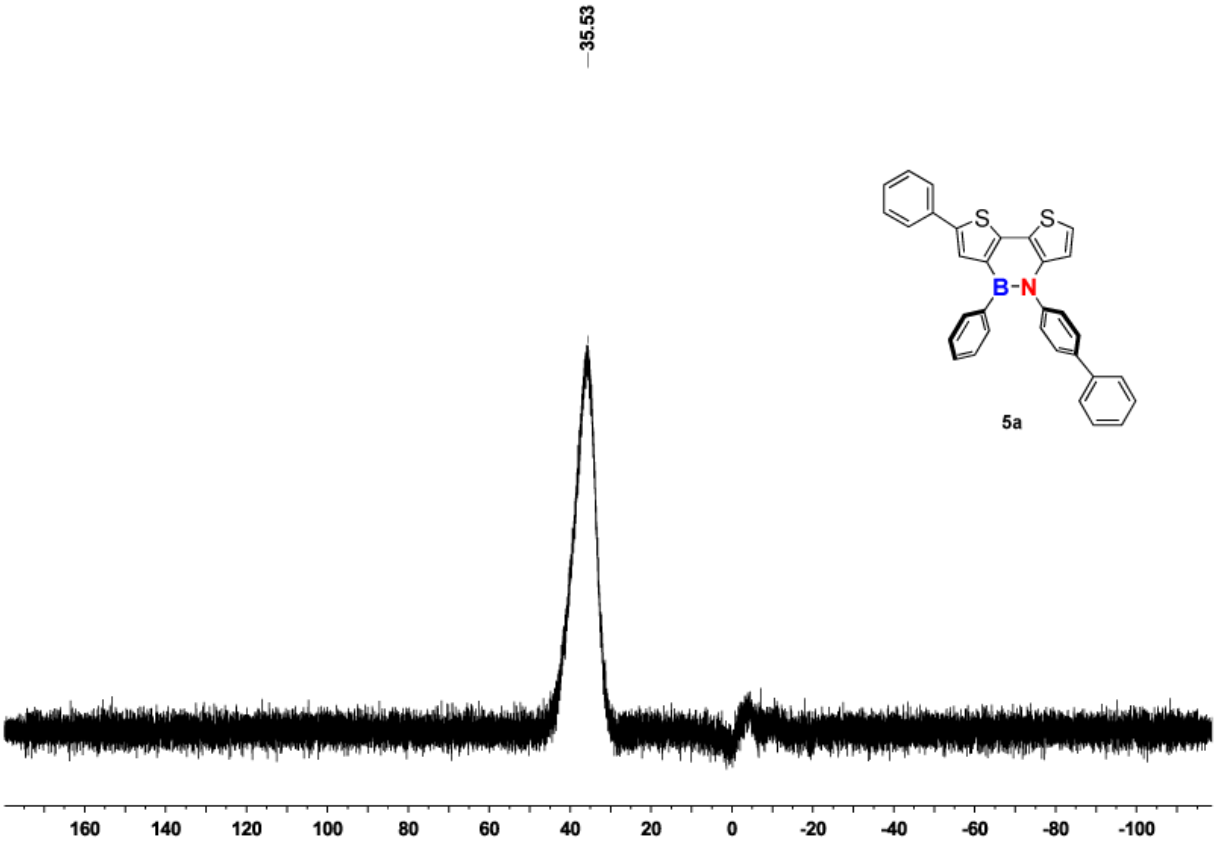


Figure S40. ^{11}B NMR spectra of **5a** in $CDCl_3$

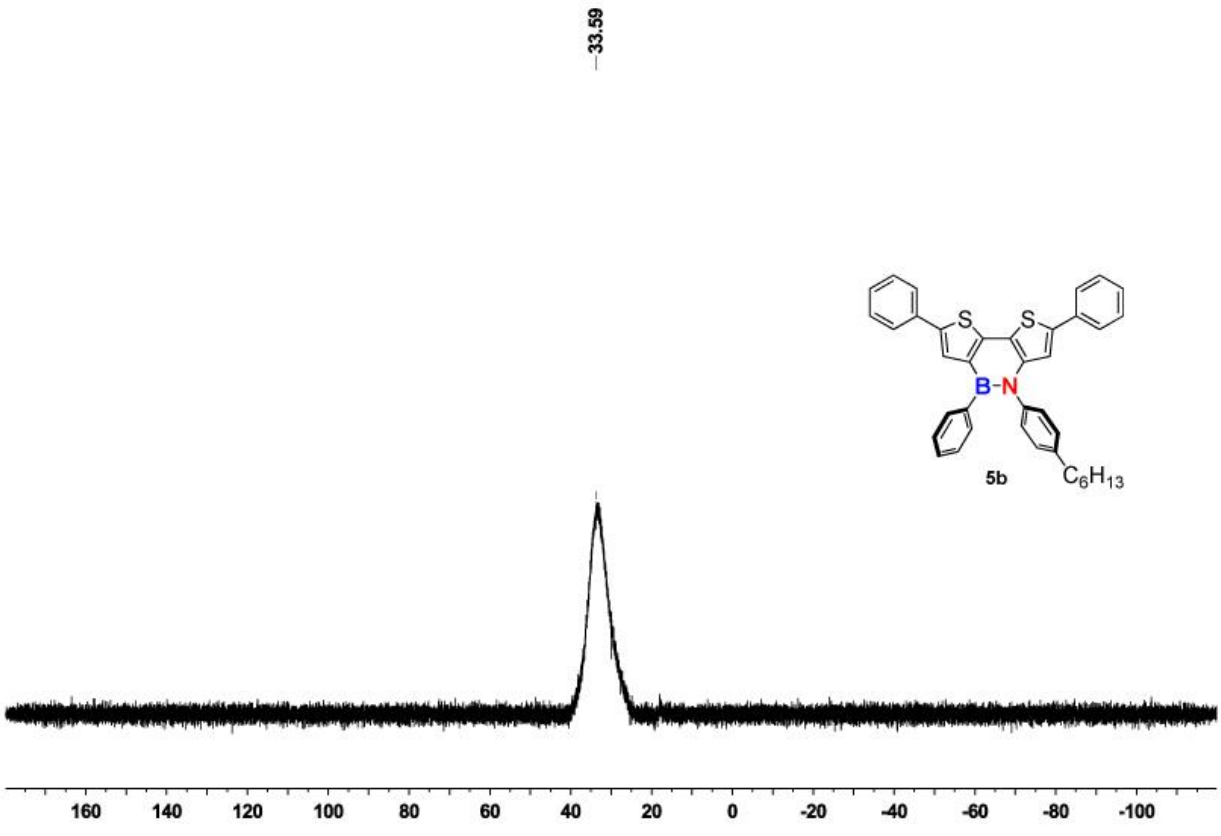


Figure S41. ^{11}B NMR spectra of **5b** in $CDCl_3$

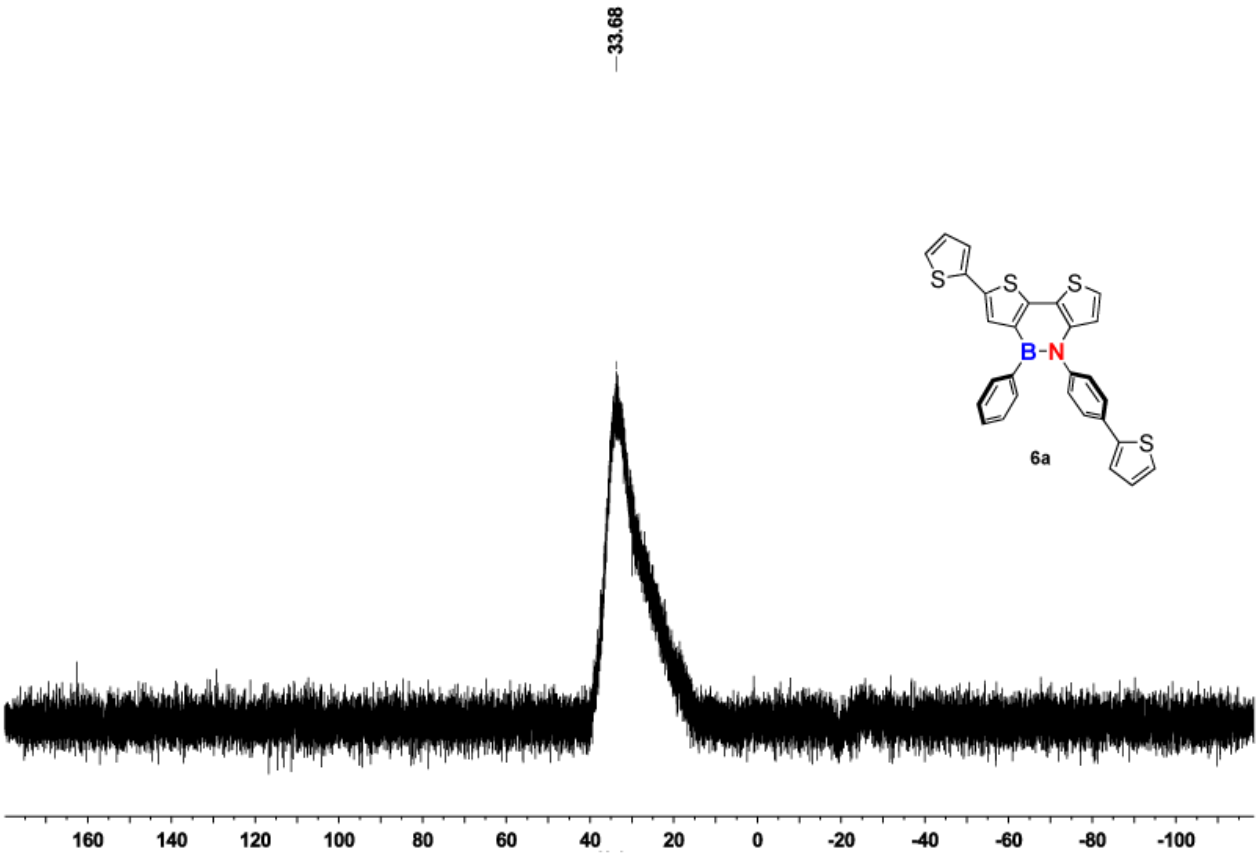


Figure S42. ^{11}B NMR spectra of **6a** in $CDCl_3$

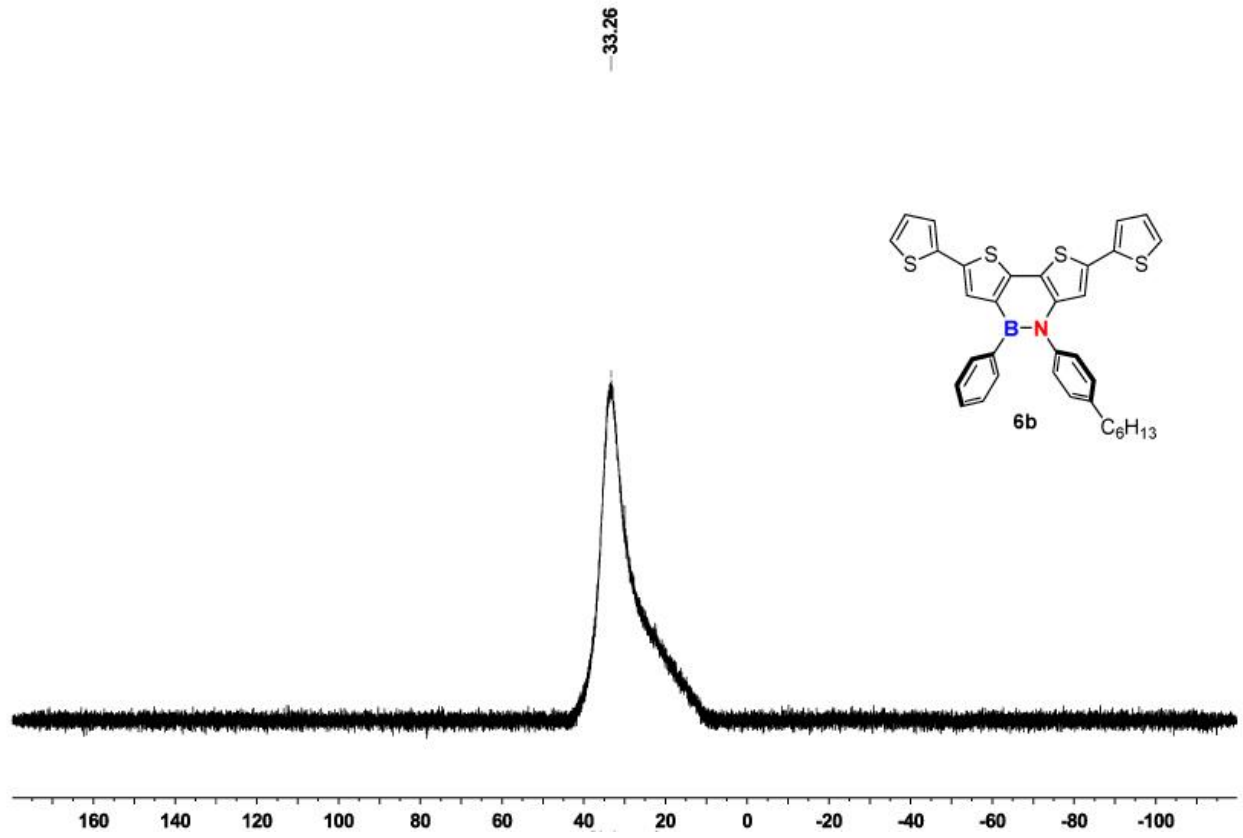


Figure S43. ^{11}B NMR spectra of **6b** in $CDCl_3$

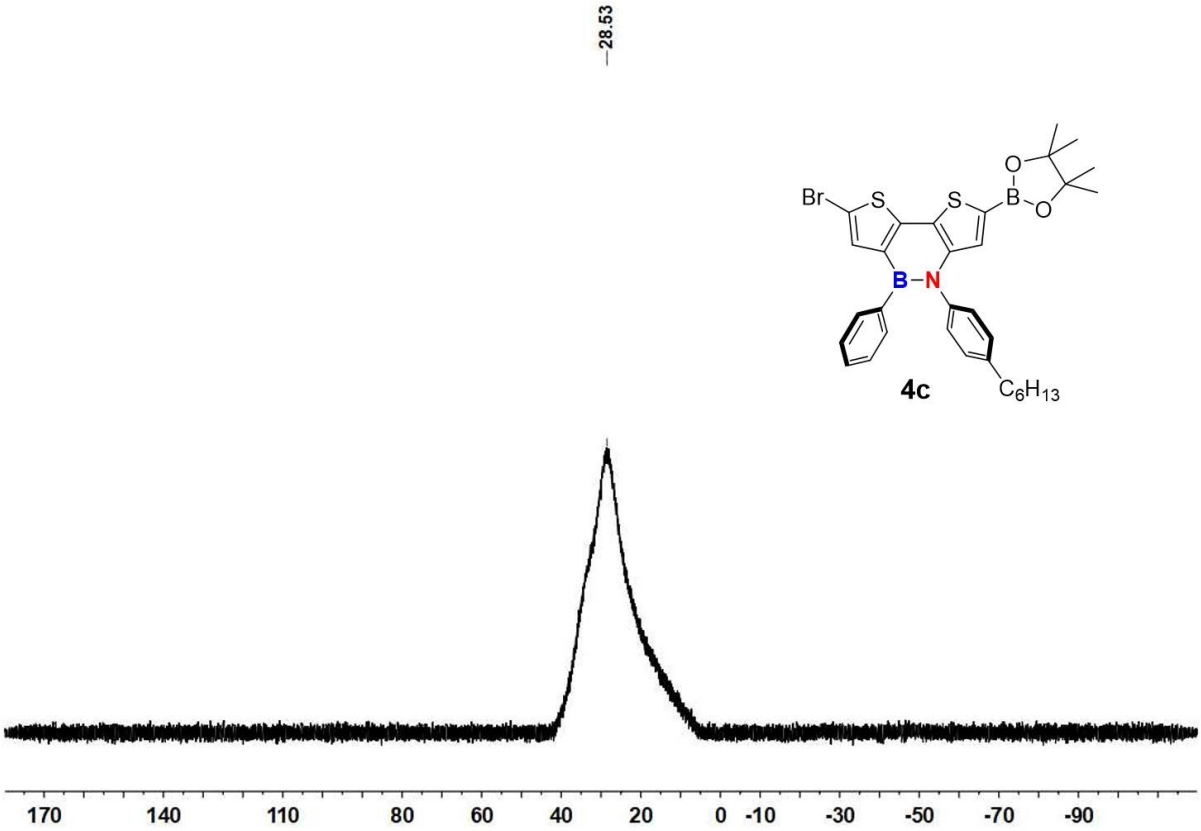


Figure S44. ^{11}B NMR spectra of **4c** in $CDCl_3$

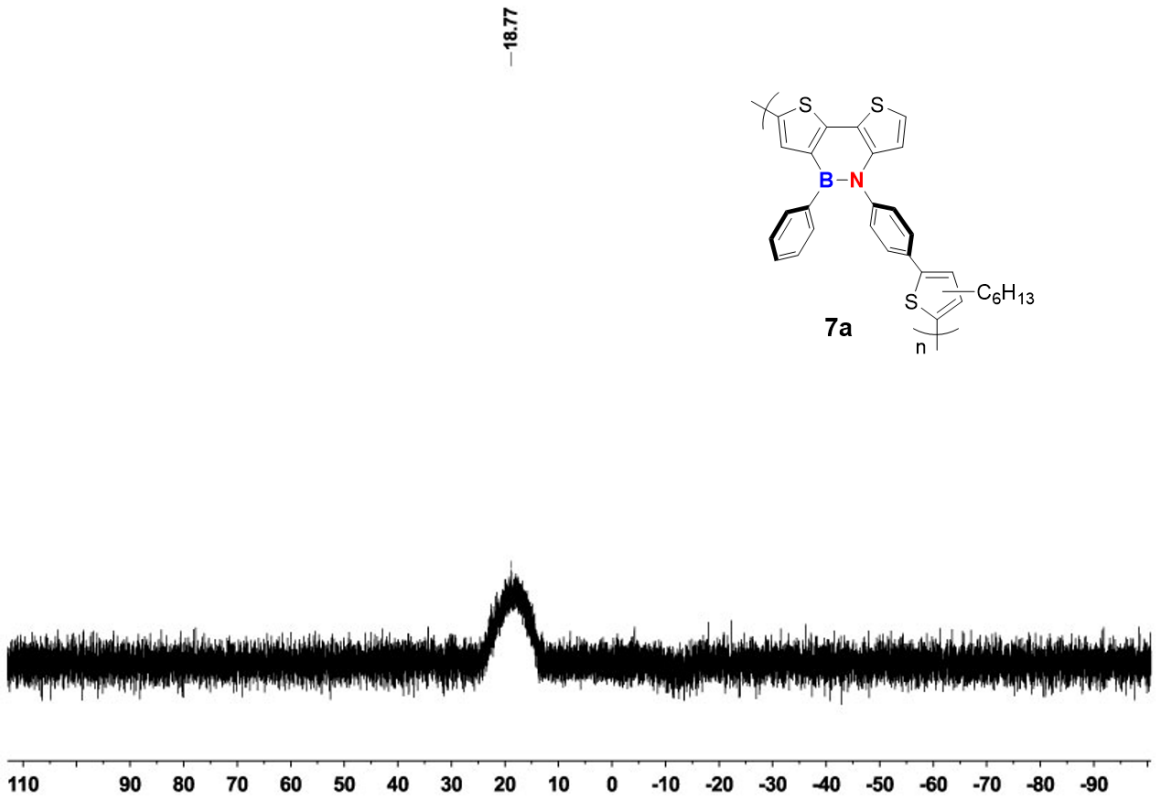


Figure S45. ^{11}B NMR spectra of **7a** in $CDCl_3$

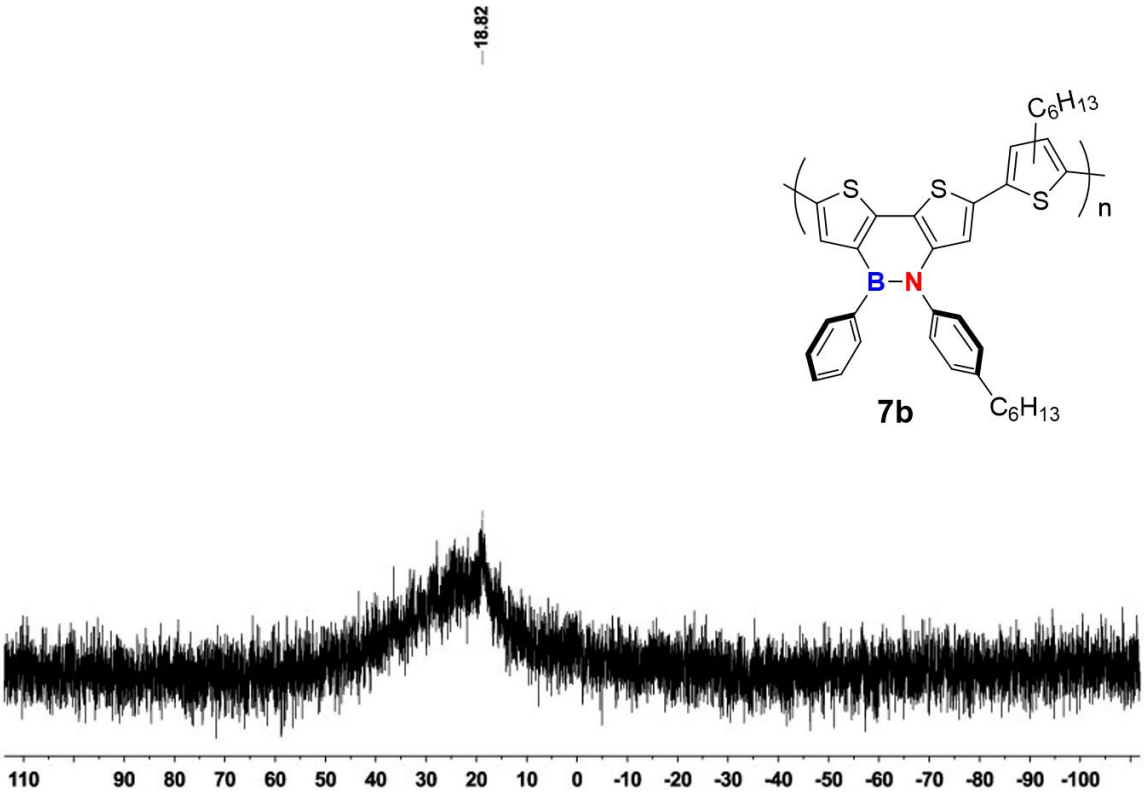


Figure S46. ^{11}B NMR spectra of **7b** in $CDCl_3$

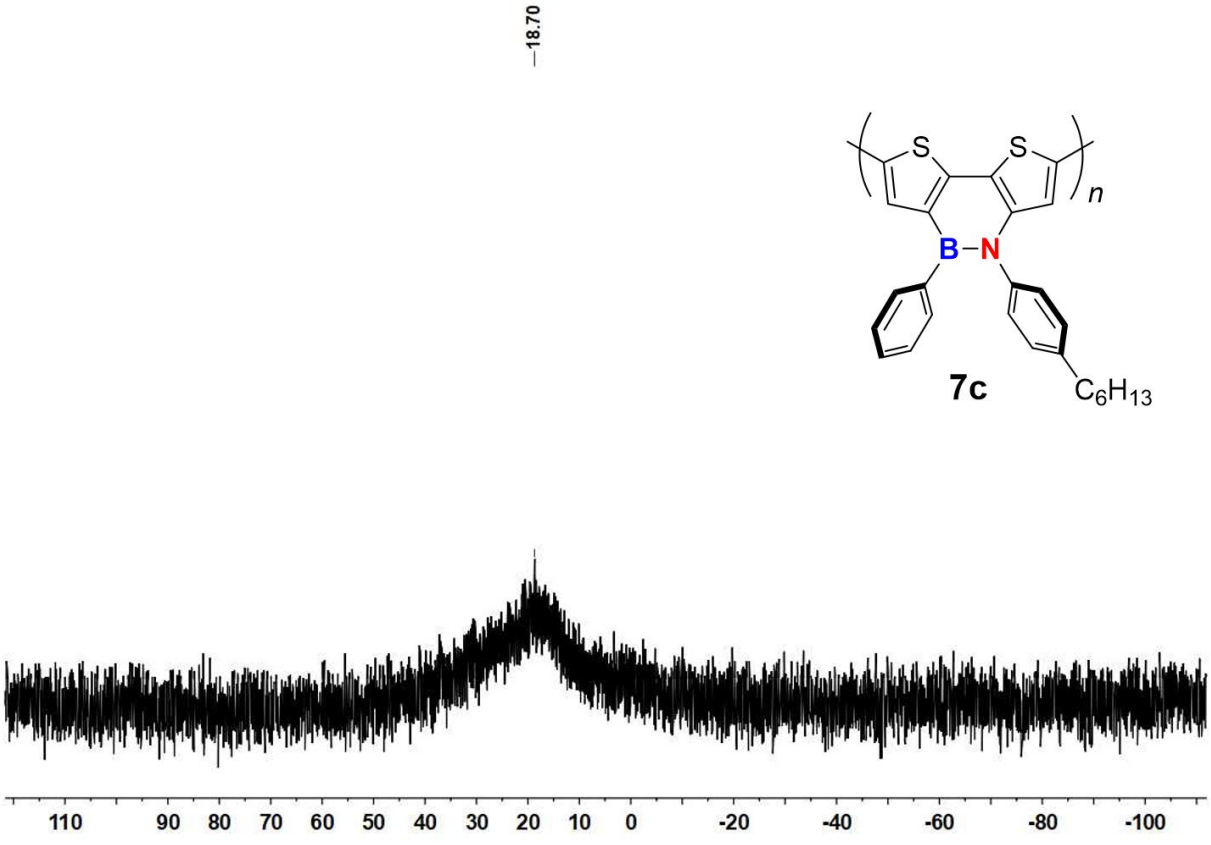


Figure S47. ^{11}B NMR spectra of **7c** in $CDCl_3$

18. Coordinates of molecular structures

Table S17. Cartesian coordinates of optimized geometry of **3a** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.73342	3.24797	-0.18545
2	6	0	-1.40847	2.9274	-0.15813
3	6	0	-1.15257	1.51301	-0.07373
4	6	0	-2.35459	0.79085	-0.04858
5	16	0	-3.75687	1.83134	-0.1157
6	5	0	0.18098	0.75607	-0.0436
7	7	0	0.08249	-0.69003	1.71E-4
8	6	0	-1.15176	-1.34369	0.0438
9	6	0	-2.35124	-0.62622	0.01668
10	6	0	-1.36406	-2.75977	0.14053
11	6	0	-2.68934	-3.08767	0.1745
12	16	0	-3.73126	-1.69829	0.0972
13	6	0	2.55892	1.28409	-1.03383
14	6	0	3.76149	1.99508	-1.03197
15	6	0	4.01915	2.93663	-0.03157
16	6	0	3.05993	3.16754	0.95778
17	6	0	1.85202	2.46455	0.93798
18	6	0	1.57346	1.49827	-0.05027
19	6	0	1.25497	-1.53499	0.03415
20	6	0	1.99593	-1.65326	1.21253
21	6	0	3.132	-2.46616	1.24176
22	6	0	3.52456	-3.16848	0.09936
23	6	0	2.77695	-3.05392	-1.07651
24	6	0	1.64381	-2.23793	-1.11087
25	1	0	-3.18804	4.22756	-0.24646
26	1	0	-0.62241	3.67254	-0.20204
27	1	0	-0.56861	-3.49152	0.18426
28	1	0	-3.12227	-4.07612	0.24292
29	1	0	2.38535	0.55292	-1.81855
30	1	0	4.49862	1.81134	-1.80912
31	1	0	4.95655	3.48601	-0.02489
32	1	0	3.24875	3.89755	1.74051
33	1	0	1.11419	2.66547	1.71148
34	1	0	1.68484	-1.10263	2.09444
35	1	0	3.70932	-2.54865	2.15788

36	1	0	4.40808	-3.7994	0.12396
37	1	0	3.07742	-3.59451	-1.96937
38	1	0	1.05945	-2.13928	-2.02102

Table S18. Cartesian coordinates of optimized geometry of **3b** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.57467	2.23835	-0.29323
2	6	0	4.22253	2.39404	-0.21204
3	6	0	3.49811	1.15415	-0.1086
4	6	0	4.37709	0.06138	-0.12658
5	16	0	6.04869	0.5551	-0.25522
6	5	0	1.98756	0.9031	-0.02269
7	7	0	1.58207	-0.48764	0.02633
8	6	0	2.51544	-1.52675	0.02391
9	6	0	3.88714	-1.26786	-0.05406
10	6	0	2.2285	-2.92985	0.11709
11	6	0	3.35868	-3.69616	0.09909
12	16	0	4.81328	-2.75185	-0.02513
13	6	0	1.03876	3.07415	1.01094
14	6	0	0.14982	4.15143	1.06626
15	6	0	-0.85825	4.27581	0.10675
16	6	0	-0.97093	3.31264	-0.89991
17	6	0	-0.08904	2.2298	-0.93729
18	6	0	0.93764	2.08068	0.01574
19	6	0	0.19149	-0.8737	0.11275
20	6	0	-0.46939	-1.38359	-1.00832
21	6	0	-1.81309	-1.75161	-0.9201
22	6	0	-2.52639	-1.61778	0.28071
23	6	0	-1.84407	-1.11138	1.39624
24	6	0	-0.49911	-0.74506	1.31945
25	6	0	-9.75241	0.87695	-0.44492
26	6	0	-8.83278	-0.30369	-0.11232
27	6	0	-7.34101	0.04311	-0.20888
28	6	0	-6.41298	-1.13344	0.12151
29	6	0	-4.92306	-0.78041	0.02961
30	6	0	-3.99644	-1.9691	0.36005
31	1	0	6.3365	3.00148	-0.37833

32	1	0	3.74022	3.36467	-0.23031
33	1	0	1.2308	-3.34053	0.19497
34	1	0	3.4255	-4.77399	0.15361
35	1	0	1.82228	3.00064	1.76183
36	1	0	0.24818	4.89475	1.8531
37	1	0	-1.54675	5.1157	0.14078
38	1	0	-1.74748	3.40289	-1.65489
39	1	0	-0.20165	1.49093	-1.72593
40	1	0	0.07026	-1.48988	-1.94506
41	1	0	-2.31489	-2.14703	-1.80009
42	1	0	-2.37049	-1.00295	2.34145
43	1	0	0.01692	-0.35449	2.19086
44	1	0	-10.80837	0.59681	-0.36466
45	1	0	-9.57864	1.71839	0.23639
46	1	0	-9.58055	1.23773	-1.46605
47	1	0	-9.05353	-1.141	-0.78892
48	1	0	-9.05454	-0.66493	0.90155
49	1	0	-7.12038	0.88066	0.46884
50	1	0	-7.11945	0.40628	-1.22311
51	1	0	-6.63129	-1.9696	-0.55884
52	1	0	-6.63748	-1.49846	1.13445
53	1	0	-4.69749	0.05018	0.71192
54	1	0	-4.69135	-0.416	-0.98047
55	1	0	-4.21467	-2.79451	-0.32972
56	1	0	-4.23097	-2.33434	1.36814

Table S19. Cartesian coordinates of optimized geometry of **5a** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.35595	-0.05207	0.05007
2	6	0	3.16593	-0.73593	0.04661
3	6	0	1.99314	0.08769	0.00087
4	6	0	2.33888	1.4469	-0.02189
5	16	0	4.06586	1.69289	0.00846
6	5	0	0.51205	-0.31248	-0.00224
7	7	0	-0.43539	0.78522	-0.0136
8	6	0	-0.01856	2.11812	-0.05338
9	6	0	1.34008	2.4515	-0.05448

10	6	0	-0.86468	3.27461	-0.12186
11	6	0	-0.15386	4.44022	-0.16337
12	16	0	1.56549	4.1852	-0.12711
13	6	0	0.51042	-2.6975	-0.99749
14	6	0	0.15167	-4.04832	-1.01439
15	6	0	-0.67056	-4.56578	-0.01014
16	6	0	-1.13257	-3.72065	1.00278
17	6	0	-0.78295	-2.36809	1.00238
18	6	0	0.04608	-1.81996	0.00378
19	6	0	-1.86235	0.56049	-0.01405
20	6	0	-2.60921	0.7728	1.14856
21	6	0	-3.98551	0.54939	1.14856
22	6	0	-4.65037	0.10898	-0.00985
23	6	0	-3.88359	-0.09404	-1.17013
24	6	0	-2.5071	0.13117	-1.17582
25	6	0	-8.36854	0.49061	0.68543
26	6	0	-8.90004	-0.60464	-8.99E-4
27	6	0	-8.04184	-1.46647	-0.68927
28	6	0	-6.66537	-1.23513	-0.69127
29	6	0	-6.11643	-0.13638	-0.00641
30	6	0	-6.99205	0.72214	0.68188
31	6	0	8.10321	-0.39938	-0.40933
32	6	0	6.81285	0.12989	-0.4413
33	6	0	5.72282	-0.58781	0.08714
34	6	0	5.97389	-1.85355	0.65378
35	6	0	7.26252	-2.38447	0.67489
36	6	0	8.33559	-1.66074	0.14496
37	1	0	3.11997	-1.81879	0.05431
38	1	0	-1.94553	3.23565	-0.1419
39	1	0	-0.54277	5.44775	-0.21561
40	1	0	1.15864	-2.31645	-1.78337
41	1	0	0.51817	-4.69567	-1.80673
42	1	0	-0.94643	-5.61671	-0.01486
43	1	0	-1.76825	-4.11363	1.79181
44	1	0	-1.15959	-1.73133	1.79806
45	1	0	-2.10659	1.09858	2.05465
46	1	0	-4.5457	0.68914	2.06819
47	1	0	-4.37189	-0.41035	-2.08682
48	1	0	-1.92874	-0.02476	-2.08085
49	1	0	-9.02668	1.17202	1.21713
50	1	0	-9.97105	-0.78471	0.00101
51	1	0	-8.44262	-2.32652	-1.21825
52	1	0	-6.00636	-1.92696	-1.2077

53	1	0	-6.59406	1.59092	1.19832
54	1	0	8.92689	0.17323	-0.82606
55	1	0	6.64682	1.10153	-0.89767
56	1	0	5.15592	-2.4132	1.09628
57	1	0	7.43112	-3.36159	1.11871
58	1	0	9.33985	-2.07326	0.16809

Table S20. Cartesian coordinates of optimized geometry of **5b** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.54272	-1.76698	-0.06736
2	6	0	-3.22375	-2.14467	-0.01037
3	6	0	-2.28355	-1.06382	0.02979
4	6	0	-2.94454	0.17386	-0.01115
5	16	0	-4.67967	-0.00243	-0.07587
6	5	0	-0.75022	-1.09667	0.06791
7	7	0	-0.09308	0.19539	0.05372
8	6	0	-0.81746	1.38955	0.03442
9	6	0	-2.21631	1.38669	-0.00386
10	6	0	-0.27489	2.71099	0.05811
11	6	0	-1.23054	3.69954	0.03101
12	16	0	-2.85001	3.01574	-0.01239
13	6	0	-0.19096	-3.37461	1.1575
14	6	0	0.47715	-4.60054	1.22452
15	6	0	1.40849	-4.94357	0.24093
16	6	0	1.66889	-4.04863	-0.8006
17	6	0	1.00987	-2.81775	-0.84972
18	6	0	0.06263	-2.4482	0.12543
19	6	0	1.34654	0.32144	0.10216
20	6	0	2.06579	0.63617	-1.05413
21	6	0	3.45466	0.76351	-0.99982
22	6	0	4.15567	0.57961	0.20171
23	6	0	3.4159	0.2705	1.35226
24	6	0	2.02598	0.14463	1.30893
25	6	0	-1.0248	5.15311	0.04211
26	6	0	-5.73973	-2.61544	-0.11802
27	6	0	-1.96127	6.03341	-0.53287
28	6	0	-1.74739	7.41158	-0.52298

29	6	0	-0.59111	7.94266	0.05479
30	6	0	0.3472	7.07981	0.62993
31	6	0	0.13175	5.70264	0.63014
32	6	0	-6.95171	-2.15417	-0.66704
33	6	0	-8.07696	-2.97728	-0.7156
34	6	0	-8.01862	-4.28361	-0.22348
35	6	0	-6.8218	-4.7555	0.3252
36	6	0	-5.69933	-3.93154	0.38493
37	6	0	10.83073	-3.13524	-0.58184
38	6	0	10.13495	-1.80368	-0.27681
39	6	0	8.60361	-1.89765	-0.31197
40	6	0	7.89813	-0.56859	-0.01132
41	6	0	6.36784	-0.66746	-0.05106
42	6	0	5.66566	0.674	0.2454
43	1	0	-2.91712	-3.18413	-0.02911
44	1	0	0.78607	2.92036	0.06498
45	1	0	-0.91946	-3.12977	1.9272
46	1	0	0.26672	-5.28809	2.03957
47	1	0	1.92443	-5.89883	0.28409
48	1	0	2.38766	-4.30774	-1.57351
49	1	0	1.23483	-2.13641	-1.66552
50	1	0	1.53522	0.78243	-1.99066
51	1	0	4.00179	1.01012	-1.90666
52	1	0	3.93228	0.12853	2.29855
53	1	0	1.46519	-0.09284	2.20754
54	1	0	-2.85268	5.63473	-1.00856
55	1	0	-2.48269	8.07049	-0.97572
56	1	0	-0.42431	9.01565	0.06025
57	1	0	1.24471	7.48116	1.09188
58	1	0	0.85307	5.04685	1.10758
59	1	0	-7.00964	-1.14935	-1.0755
60	1	0	-8.99907	-2.59769	-1.14651
61	1	0	-8.89424	-4.92465	-0.26327
62	1	0	-6.7651	-5.76587	0.72038
63	1	0	-4.78679	-4.30237	0.84069
64	1	0	11.92098	-3.0339	-0.54996
65	1	0	10.5597	-3.50426	-1.57821
66	1	0	10.54681	-3.90618	0.14441
67	1	0	10.4666	-1.04428	-0.9986
68	1	0	10.45214	-1.44313	0.7116
69	1	0	8.2716	-2.65677	0.41123
70	1	0	8.28695	-2.2609	-1.30057
71	1	0	8.23171	0.19044	-0.7341

72	1	0	8.21331	-0.20606	0.97805
73	1	0	6.04748	-1.0292	-1.03754
74	1	0	6.02702	-1.4187	0.67408
75	1	0	5.98145	1.03149	1.23387
76	1	0	6.00679	1.42297	-0.48099

Table S21. Cartesian coordinates of optimized geometry of **6a** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.3779	0.05073	-0.02557
2	6	0	-3.20136	-0.65917	-0.01814
3	6	0	-2.01431	0.14311	-0.00895
4	6	0	-2.33346	1.50903	-0.00198
5	16	0	-4.05692	1.79123	-0.00427
6	5	0	-0.54084	-0.28544	0.01468
7	7	0	0.42639	0.79473	0.05554
8	6	0	0.0354	2.13585	0.04072
9	6	0	-1.31689	2.49472	0.0157
10	6	0	0.90355	3.27759	0.02471
11	6	0	0.21512	4.45705	-0.00162
12	16	0	-1.50888	4.23392	-0.01399
13	6	0	0.70304	-2.38524	0.9896
14	6	0	1.02949	-3.74317	0.96404
15	6	0	0.5672	-4.55712	-0.07387
16	6	0	-0.2322	-4.00321	-1.07699
17	6	0	-0.56799	-2.64713	-1.03449
18	6	0	-0.10266	-1.80053	-0.00739
19	6	0	1.8484	0.54384	0.08036
20	6	0	2.51164	0.13263	-1.07744
21	6	0	3.8823	-0.11956	-1.04894
22	6	0	4.62886	0.04856	0.13152
23	6	0	3.94729	0.48069	1.28582
24	6	0	2.57483	0.71731	1.2629
25	6	0	6.07321	-0.21919	0.17807
26	6	0	-5.74402	-0.43511	-0.03904
27	6	0	6.83409	-0.63153	1.25139
28	6	0	8.21577	-0.79961	0.94271
29	6	0	8.50452	-0.51374	-0.36582

30	16	0	7.0884	-0.02823	-1.23891
31	6	0	-6.90491	0.24575	-0.34904
32	6	0	-8.07712	-0.55976	-0.26366
33	6	0	-7.80905	-1.85013	0.11034
34	16	0	-6.11293	-2.10019	0.37806
35	1	0	-3.17828	-1.74324	-0.02935
36	1	0	1.98373	3.21983	0.02923
37	1	0	0.62355	5.45808	-0.01688
38	1	0	1.07924	-1.77306	1.80455
39	1	0	1.64736	-4.16496	1.7523
40	1	0	0.82536	-5.61219	-0.09888
41	1	0	-0.59873	-4.62617	-1.88855
42	1	0	-1.19825	-2.23748	-1.82056
43	1	0	1.94852	-0.00692	-1.99451
44	1	0	4.37296	-0.47045	-1.95179
45	1	0	4.50021	0.64746	2.20474
46	1	0	2.06243	1.0477	2.16176
47	1	0	6.41019	-0.83849	2.22748
48	1	0	8.95945	-1.1277	1.66
49	1	0	9.46123	-0.55554	-0.86819
50	1	0	-6.91384	1.28835	-0.64691
51	1	0	-9.07545	-0.19578	-0.47795
52	1	0	-8.50204	-2.66882	0.24729

Table S22. Cartesian coordinates of optimized geometry of **6b** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.60579	-1.63395	-0.12767
2	6	0	3.29509	-2.04338	-0.06012
3	6	0	2.33452	-0.98319	-0.00305
4	6	0	2.96878	0.26914	-0.04432
5	16	0	4.70913	0.13324	-0.12153
6	5	0	0.802	-1.04815	0.05257
7	7	0	0.11892	0.23103	0.04815
8	6	0	0.81755	1.43914	0.02105
9	6	0	2.21674	1.46488	-0.02871
10	6	0	0.24833	2.74716	0.06967
11	6	0	1.18633	3.75498	0.04418

12	16	0	2.81999	3.10727	-0.04918
13	6	0	-0.94807	-2.79567	-0.83574
14	6	0	-1.57944	-4.04064	-0.78107
15	6	0	-1.26966	-4.94079	0.24234
16	6	0	-0.31725	-4.58866	1.20212
17	6	0	0.3227	-3.34821	1.12955
18	6	0	0.01953	-2.41645	0.11558
19	6	0	-1.32289	0.32803	0.1086
20	6	0	-1.99004	0.11971	1.31706
21	6	0	-3.38184	0.2156	1.37069
22	6	0	-4.13547	0.52525	0.22927
23	6	0	-3.44658	0.74161	-0.97373
24	6	0	-2.05569	0.64451	-1.03862
25	6	0	5.81446	-2.43048	-0.19928
26	6	0	0.97191	5.18732	0.07931
27	6	0	1.87024	6.18987	0.38994
28	6	0	1.30655	7.49599	0.32927
29	6	0	-0.01731	7.48781	-0.02528
30	16	0	-0.59593	5.87704	-0.30585
31	6	0	7.09078	-2.04143	-0.5568
32	6	0	8.04006	-3.10318	-0.52277
33	6	0	7.48832	-4.29753	-0.1407
34	16	0	5.79351	-4.14108	0.19735
35	6	0	-10.71783	-3.36166	-0.48369
36	6	0	-10.05588	-2.01067	-0.18915
37	6	0	-8.52302	-2.06209	-0.24274
38	6	0	-7.85049	-0.71412	0.04868
39	6	0	-6.31856	-0.7733	-0.00659
40	6	0	-5.64683	0.58489	0.28401
41	1	0	3.01428	-3.09075	-0.07286
42	1	0	-0.81443	2.93596	0.14423
43	1	0	-1.21137	-2.11075	-1.63685
44	1	0	-2.31489	-4.30686	-1.53563
45	1	0	-1.76369	-5.90737	0.2896
46	1	0	-0.06791	-5.28041	2.00241
47	1	0	1.06807	-3.09672	1.88058
48	1	0	-1.41859	-0.11869	2.20863
49	1	0	-3.88878	0.04976	2.31815
50	1	0	-4.00469	0.98952	-1.87346
51	1	0	-1.53458	0.81466	-1.97643
52	1	0	2.89791	5.99166	0.67342
53	1	0	1.85969	8.40211	0.54809
54	1	0	-0.68775	8.32834	-0.14058

55	1	0	7.33561	-1.02726	-0.8523
56	1	0	9.0867	-2.98431	-0.77867
57	1	0	7.9716	-5.25917	-0.0361
58	1	0	-11.81001	-3.29077	-0.43846
59	1	0	-10.40343	-4.12298	0.24014
60	1	0	-10.44893	-3.72481	-1.48281
61	1	0	-10.37092	-1.65742	0.80258
62	1	0	-10.41742	-1.26207	-0.90788
63	1	0	-8.16136	-2.81099	0.47689
64	1	0	-8.20847	-2.41758	-1.23486
65	1	0	-8.16471	-0.35858	1.04089
66	1	0	-8.21169	0.03463	-0.67152
67	1	0	-5.95172	-1.51623	0.71442
68	1	0	-5.99914	-1.12642	-0.99652
69	1	0	-6.01069	1.32524	-0.44006
70	1	0	-5.96352	0.9354	1.2747

Table S23. Cartesian coordinates of optimized geometry of **3a-F** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.72267	-3.19472	-0.02034
2	6	0	1.44008	-2.85498	0.32197
3	6	0	1.17839	-1.44552	0.34346
4	6	0	2.31235	-0.73338	-0.00724
5	16	0	3.68872	-1.77723	-0.3555
6	5	0	-0.20207	-0.70001	0.7535
7	7	0	-0.10723	0.80822	0.27537
8	6	0	1.12131	1.42577	0.07427
9	6	0	2.30401	0.69656	-0.07711
10	6	0	1.37835	2.84499	0.05001
11	6	0	2.69549	3.16168	-0.13151
12	16	0	3.69808	1.74445	-0.25463
13	6	0	-1.7302	-1.46977	-1.29053
14	6	0	-2.79291	-2.17589	-1.86137
15	6	0	-3.66001	-2.91643	-1.04954
16	6	0	-3.44482	-2.9361	0.33154
17	6	0	-2.37767	-2.21942	0.88751
18	6	0	-1.49254	-1.46332	0.0975

19	6	0	-1.27905	1.58592	0.15868
20	6	0	-2.29063	1.49891	1.1362
21	6	0	-3.47301	2.22889	1.00685
22	6	0	-3.67842	3.07656	-0.08649
23	6	0	-2.68094	3.16991	-1.06365
24	6	0	-1.50343	2.43072	-0.94841
25	1	0	3.16642	-4.1786	-0.09814
26	1	0	0.68432	-3.59705	0.56078
27	1	0	0.60632	3.59365	0.17383
28	1	0	3.13991	4.14604	-0.18782
29	1	0	-1.06469	-0.90358	-1.93972
30	1	0	-2.94676	-2.14988	-2.93877
31	1	0	-4.489	-3.46852	-1.48768
32	1	0	-4.11035	-3.50765	0.97675
33	1	0	-2.22241	-2.23644	1.9635
34	1	0	-2.12675	0.85215	1.99036
35	1	0	-4.23834	2.1383	1.77448
36	1	0	-4.59908	3.64671	-0.18045
37	1	0	-2.82757	3.80744	-1.93305
38	1	0	-0.75099	2.48491	-1.72938
39	9	0	-0.34921	-0.72474	2.21016

Table S24. Cartesian coordinates of optimized geometry of **3b-F** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.40424	2.22836	-0.48779
2	6	0	-4.14773	2.33043	0.0492
3	6	0	-3.44451	1.08686	0.17114
4	6	0	-4.21676	0.04127	-0.30529
5	16	0	-5.79049	0.57292	-0.89374
6	5	0	-1.97295	0.83732	0.8054
7	7	0	-1.49782	-0.61515	0.38918
8	6	0	-2.41167	-1.60321	0.04511
9	6	0	-3.731	-1.30538	-0.30784
10	6	0	-2.18292	-3.02732	0.04914
11	6	0	-3.28064	-3.76105	-0.30444
12	16	0	-4.66144	-2.75469	-0.63475
13	6	0	-0.49229	2.06966	-1.03646

14	6	0	0.35445	3.08717	-1.48533
15	6	0	0.79988	4.07282	-0.59671
16	6	0	0.38586	4.02004	0.73747
17	6	0	-0.45893	2.99074	1.17157
18	6	0	-0.92003	1.98501	0.30253
19	6	0	-0.13216	-0.96147	0.47993
20	6	0	0.63604	-0.55527	1.58814
21	6	0	1.99761	-0.84982	1.66088
22	6	0	2.65382	-1.56891	0.65161
23	6	0	1.88468	-1.97925	-0.44771
24	6	0	0.52629	-1.67722	-0.53984
25	6	0	9.72296	0.85826	-1.15577
26	6	0	8.87371	-0.22591	-0.48127
27	6	0	7.36613	0.05308	-0.54533
28	6	0	6.50719	-1.0285	0.12346
29	6	0	5.00065	-0.7466	0.057
30	6	0	4.14128	-1.84355	0.71849
31	1	0	-6.12892	3.01052	-0.67224
32	1	0	-3.72272	3.27983	0.36049
33	1	0	-1.23623	-3.47886	0.31697
34	1	0	-3.36459	-4.83678	-0.37782
35	1	0	-0.83059	1.31503	-1.74431
36	1	0	0.66808	3.11356	-2.52752
37	1	0	1.45839	4.86808	-0.94009
38	1	0	0.72308	4.77959	1.44123
39	1	0	-0.77068	2.95504	2.21256
40	1	0	0.1438	-0.0103	2.38546
41	1	0	2.56109	-0.51935	2.53241
42	1	0	2.35972	-2.5316	-1.25767
43	1	0	-0.035	-1.98175	-1.41814
44	1	0	10.79312	0.62918	-1.093
45	1	0	9.46516	0.95902	-2.21703
46	1	0	9.56298	1.83562	-0.68467
47	1	0	9.17836	-0.32609	0.57012
48	1	0	9.08165	-1.19751	-0.95159
49	1	0	7.06255	0.15686	-1.59737
50	1	0	7.15801	1.02446	-0.07359
51	1	0	6.81173	-1.1324	1.17586
52	1	0	6.71649	-1.99977	-0.35007
53	1	0	4.69151	-0.63682	-0.99134
54	1	0	4.78186	0.21585	0.53848
55	1	0	4.44939	-1.94811	1.76834
56	1	0	4.36279	-2.80512	0.23386

57	9	0	-2.05854	0.90534	2.26599

Table S25. Cartesian coordinates of optimized geometry of **5a-F** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.12658	0.02083	-0.80614
2	6	0	-2.979	-0.73739	-0.65331
3	6	0	-1.85588	-0.05746	-0.10863
4	6	0	-2.16394	1.26811	0.15095
5	16	0	-3.81995	1.67372	-0.26583
6	5	0	-0.38892	-0.68218	0.20247
7	7	0	0.6261	0.54806	0.38146
8	6	0	0.16737	1.80397	0.75879
9	6	0	-1.18037	2.16933	0.66698
10	6	0	0.95118	2.85509	1.35975
11	6	0	0.22166	3.96159	1.69075
12	16	0	-1.46657	3.7745	1.31067
13	6	0	-0.49629	-1.14976	2.82859
14	6	0	-0.56441	-1.98533	3.94758
15	6	0	-0.55356	-3.37563	3.78762
16	6	0	-0.47265	-3.91095	2.49853
17	6	0	-0.40439	-3.06094	1.38808
18	6	0	-0.41323	-1.65917	1.51791
19	6	0	1.97847	0.38129	0.05228
20	6	0	2.71766	1.37617	-0.6273
21	6	0	4.05558	1.18906	-0.95844
22	6	0	4.73232	-0.00633	-0.65236
23	6	0	3.98604	-1.00661	0.00108
24	6	0	2.65264	-0.82455	0.34642
25	6	0	8.41435	0.67264	-1.33295
26	6	0	8.87902	-0.59169	-1.7085
27	6	0	7.98104	-1.66356	-1.73593
28	6	0	6.64062	-1.47282	-1.39808
29	6	0	6.15383	-0.20696	-1.0124
30	6	0	7.07541	0.8599	-0.98645
31	6	0	-7.83348	-0.01154	-1.61496
32	6	0	-6.59353	0.39427	-1.1225
33	6	0	-5.43258	-0.38738	-1.31587

34	6	0	-5.58284	-1.59815	-2.03158
35	6	0	-6.82458	-2.00525	-2.51338
36	6	0	-7.96382	-1.21651	-2.31238
37	1	0	-2.94401	-1.79139	-0.9089
38	1	0	2.01387	2.77207	1.54886
39	1	0	0.57288	4.87271	2.15553
40	1	0	-0.50321	-0.07179	2.9777
41	1	0	-0.62492	-1.55381	4.94503
42	1	0	-0.6062	-4.03044	4.65476
43	1	0	-0.46052	-4.99061	2.35848
44	1	0	-0.3301	-3.4879	0.3906
45	1	0	2.21886	2.29064	-0.93077
46	1	0	4.56972	1.97007	-1.51356
47	1	0	4.46994	-1.93919	0.28009
48	1	0	2.11996	-1.61424	0.86077
49	1	0	9.10011	1.51573	-1.29676
50	1	0	9.922	-0.73905	-1.97546
51	1	0	8.32223	-2.6516	-2.03515
52	1	0	5.95089	-2.30936	-1.45717
53	1	0	6.73914	1.84191	-0.66699
54	1	0	-8.70498	0.61616	-1.44509
55	1	0	-6.52242	1.32469	-0.56659
56	1	0	-4.71068	-2.2154	-2.22037
57	1	0	-6.90157	-2.94215	-3.05985
58	1	0	-8.9305	-1.53368	-2.69367
59	9	0	0.04328	-1.45288	-0.93626

Table S26. Cartesian coordinates of optimized geometry of **5b-F** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.4243	-1.82938	-0.07977
2	6	0	3.14561	-2.12287	0.3601
3	6	0	2.24793	-1.02396	0.4423
4	6	0	2.87282	0.14798	0.03273
5	16	0	4.54725	-0.10355	-0.43706
6	5	0	0.72115	-1.02905	0.98967
7	7	0	0.04171	0.33252	0.54697
8	6	0	0.79541	1.4566	0.26317

9	6	0	2.1743	1.38725	0.00397
10	6	0	0.33514	2.81342	0.23006
11	6	0	1.30482	3.74825	-0.06248
12	16	0	2.86349	2.96785	-0.29064
13	6	0	-0.42323	-2.47517	-0.93195
14	6	0	-1.06758	-3.61351	-1.42457
15	6	0	-1.40582	-4.65865	-0.55718
16	6	0	-1.09087	-4.54338	0.79983
17	6	0	-0.44901	-3.39396	1.27778
18	6	0	-0.09979	-2.32673	0.43041
19	6	0	-1.36903	0.45394	0.56815
20	6	0	-2.11163	-0.03813	1.65638
21	6	0	-3.50495	0.03647	1.65979
22	6	0	-4.21624	0.61002	0.59641
23	6	0	-3.47121	1.10445	-0.48468
24	6	0	-2.07917	1.02167	-0.50636
25	6	0	1.15519	5.19872	-0.17249
26	6	0	5.56169	-2.72777	-0.25558
27	6	0	2.26606	6.06844	-0.12228
28	6	0	2.10985	7.44991	-0.22594
29	6	0	0.83826	8.01311	-0.3737
30	6	0	-0.27481	7.16618	-0.42348
31	6	0	-0.12093	5.78439	-0.33164
32	6	0	6.877	-2.2464	-0.442
33	6	0	7.95342	-3.11736	-0.6074
34	6	0	7.75952	-4.50192	-0.58635
35	6	0	6.46306	-4.99805	-0.40262
36	6	0	5.38442	-4.13111	-0.24584
37	6	0	-10.73225	-3.01539	-1.28069
38	6	0	-10.09217	-1.76725	-0.66112
39	6	0	-8.55812	-1.80818	-0.65589
40	6	0	-7.90877	-0.56349	-0.03626
41	6	0	-6.37523	-0.60628	-0.0334
42	6	0	-5.72991	0.64781	0.59106
43	1	0	2.84946	-3.1264	0.64801
44	1	0	-0.68721	3.08685	0.45477
45	1	0	-0.16327	-1.67651	-1.62451
46	1	0	-1.30641	-3.68745	-2.48394
47	1	0	-1.90643	-5.54775	-0.93465
48	1	0	-1.34678	-5.34817	1.48703
49	1	0	-0.21266	-3.31208	2.33581
50	1	0	-1.57677	-0.47504	2.49194
51	1	0	-4.05061	-0.35342	2.51771

52	1	0	-3.98902	1.54774	-1.33409
53	1	0	-1.52958	1.38484	-1.36979
54	1	0	3.26099	5.65488	0.01469
55	1	0	2.98734	8.09015	-0.18196
56	1	0	0.71652	9.08997	-0.45007
57	1	0	-1.27113	7.58385	-0.54544
58	1	0	-0.99588	5.1458	-0.39773
59	1	0	7.05677	-1.17523	-0.44485
60	1	0	8.95162	-2.70937	-0.74709
61	1	0	8.59857	-5.18044	-0.71315
62	1	0	6.28814	-6.07116	-0.39065
63	1	0	4.38664	-4.54043	-0.12757
64	1	0	-11.82661	-2.95393	-1.27093
65	1	0	-10.44423	-3.92077	-0.73295
66	1	0	-10.41491	-3.14647	-2.32224
67	1	0	-10.45367	-1.64488	0.36971
68	1	0	-10.42785	-0.87513	-1.20867
69	1	0	-8.19655	-1.93037	-1.68735
70	1	0	-8.22233	-2.70177	-0.10988
71	1	0	-8.27081	-0.44287	0.99587
72	1	0	-8.24647	0.3302	-0.58256
73	1	0	-6.03029	-1.49397	0.51341
74	1	0	-6.0069	-0.72272	-1.06168
75	1	0	-6.07536	1.5343	0.04091
76	1	0	-6.09874	0.7589	1.62023
77	9	0	0.73962	-1.0867	2.44966

Table S27. Cartesian coordinates of optimized geometry of **6a-F** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.33601	0.00792	-0.03631
2	6	0	-3.1509	-0.62904	-0.35967
3	6	0	-1.99189	0.19438	-0.37255
4	6	0	-2.31609	1.50029	-0.03288
5	16	0	-4.0309	1.71608	0.29277
6	5	0	-0.47784	-0.23498	-0.76539
7	7	0	0.50088	0.93124	-0.29804
8	6	0	0.04023	2.2265	-0.1083

9	6	0	-1.32161	2.52012	0.03629
10	6	0	0.83438	3.43034	-0.09251
11	6	0	0.1	4.56932	0.08086
12	16	0	-1.60374	4.2424	0.20702
13	6	0	0.06581	-1.80284	1.31647
14	6	0	0.33743	-3.03587	1.91557
15	6	0	0.46174	-4.186	1.12783
16	6	0	0.31068	-4.07992	-0.2576
17	6	0	0.04262	-2.83616	-0.84252
18	6	0	-0.0832	-1.66303	-0.07664
19	6	0	1.87887	0.67687	-0.17391
20	6	0	2.54198	-0.13706	-1.11512
21	6	0	3.89444	-0.43214	-0.98148
22	6	0	4.6609	0.07483	0.08511
23	6	0	3.99717	0.88916	1.02425
24	6	0	2.6416	1.17332	0.90496
25	6	0	6.08709	-0.23014	0.23743
26	6	0	-5.67195	-0.53088	0.0535
27	6	0	6.8463	-0.27603	1.38971
28	6	0	8.21679	-0.60383	1.16812
29	6	0	8.50991	-0.8111	-0.15432
30	16	0	7.1034	-0.59289	-1.15135
31	6	0	-6.85459	0.10303	0.39849
32	6	0	-7.99366	-0.75276	0.37982
33	6	0	-7.6936	-2.04115	0.02279
34	16	0	-5.99254	-2.22757	-0.30034
35	1	0	-3.11307	-1.68964	-0.5909
36	1	0	1.90882	3.44035	-0.22187
37	1	0	0.45968	5.58817	0.1264
38	1	0	-0.03286	-0.92104	1.94726
39	1	0	0.45053	-3.10231	2.99603
40	1	0	0.6723	-5.14885	1.5882
41	1	0	0.4035	-4.96582	-0.88348
42	1	0	-0.06902	-2.76463	-1.92171
43	1	0	1.97316	-0.53235	-1.94821
44	1	0	4.36182	-1.08229	-1.71676
45	1	0	4.55255	1.30715	1.85947
46	1	0	2.15492	1.77984	1.66213
47	1	0	6.42126	-0.11129	2.3732
48	1	0	8.94979	-0.69636	1.96272
49	1	0	9.4568	-1.08208	-0.60094
50	1	0	-6.89701	1.1547	0.65855
51	1	0	-8.99748	-0.42092	0.62419

52	1	0	-8.35783	-2.88933	-0.06955
53	9	0	-0.37345	-0.36935	-2.21395

Table S28. Cartesian coordinates of optimized geometry of **6b-F** (B3LYP/6-31+G**)

Standard orientation: (Ground State)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.51712	-1.66626	-0.10708
2	6	0	3.24537	-2.0095	0.3198
3	6	0	2.31377	-0.941	0.40428
4	6	0	2.90443	0.25523	0.01084
5	16	0	4.59279	0.06501	-0.4485
6	5	0	0.78404	-0.99748	0.94215
7	7	0	0.06831	0.35135	0.51599
8	6	0	0.78805	1.49846	0.24617
9	6	0	2.17062	1.47139	-0.01014
10	6	0	0.28838	2.841	0.22384
11	6	0	1.23555	3.80295	-0.05798
12	16	0	2.81726	3.0738	-0.29662
13	6	0	-0.30976	-2.44602	-1.00482
14	6	0	-0.92562	-3.59197	-1.51569
15	6	0	-1.24815	-4.65394	-0.663
16	6	0	-0.94634	-4.54805	0.69767
17	6	0	-0.33312	-3.391	1.19412
18	6	0	-4.06E-4	-2.30705	0.36171
19	6	0	-1.34648	0.43469	0.54578
20	6	0	-2.06858	-0.07688	1.63833
21	6	0	-3.46328	-0.03698	1.65051
22	6	0	-4.19475	0.51968	0.59189
23	6	0	-3.46953	1.03306	-0.49356
24	6	0	-2.07608	0.98477	-0.52402
25	6	0	5.67993	-2.50135	-0.28454
26	6	0	1.0662	5.23483	-0.15045
27	6	0	2.02731	6.23082	-0.17761
28	6	0	1.48808	7.54567	-0.27318
29	6	0	0.11822	7.56353	-0.31711
30	16	0	-0.53808	5.95328	-0.25686
31	6	0	6.95614	-2.15518	-0.69897
32	6	0	7.86068	-3.25416	-0.75663

33	6	0	7.28748	-4.44339	-0.3892
34	16	0	5.61225	-4.23334	0.03666
35	6	0	-10.63656	-3.27817	-1.19741
36	6	0	-10.02175	-2.00938	-0.59439
37	6	0	-8.48719	-2.01209	-0.60446
38	6	0	-7.86299	-0.74661	-0.00132
39	6	0	-6.32888	-0.75217	-0.01218
40	6	0	-5.70887	0.5219	0.5973
41	1	0	2.98265	-3.03119	0.57858
42	1	0	-0.74303	3.08976	0.43983
43	1	0	-0.06166	-1.63384	-1.68596
44	1	0	-1.15388	-3.65897	-2.57782
45	1	0	-1.72586	-5.5494	-1.05476
46	1	0	-1.18956	-5.36647	1.37321
47	1	0	-0.10661	-3.31662	2.2548
48	1	0	-1.51744	-0.50091	2.46991
49	1	0	-3.99397	-0.44041	2.51152
50	1	0	-4.0034	1.46594	-1.3382
51	1	0	-1.54103	1.36362	-1.3898
52	1	0	3.0884	6.01837	-0.11148
53	1	0	2.09638	8.44361	-0.29805
54	1	0	-0.54424	8.41605	-0.37641
55	1	0	7.23005	-1.13717	-0.95211
56	1	0	8.89843	-3.16191	-1.0599
57	1	0	7.73851	-5.42498	-0.34202
58	1	0	-11.73197	-3.24413	-1.17668
59	1	0	-10.32018	-4.17156	-0.64565
60	1	0	-10.32673	-3.40966	-2.24117
61	1	0	-10.37588	-1.88754	0.43906
62	1	0	-10.38511	-1.13048	-1.14562
63	1	0	-8.1238	-2.8925	-0.05472
64	1	0	-8.1329	-2.13375	-1.6385
65	1	0	-8.21848	-0.62611	1.03308
66	1	0	-8.22742	0.13387	-0.55184
67	1	0	-5.95792	-1.62719	0.53804
68	1	0	-5.96689	-0.86754	-1.04282
69	1	0	-6.07866	1.39561	0.04274
70	1	0	-6.07269	0.6326	1.62829
71	9	0	0.80057	-1.07335	2.40066

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Author Contributions

Sikun Zhang and Gang He conceived the idea for the study. Sikun Zhang prepared the samples and conducted characterizations. Xiaodong Yang, Xu Liu and Letian Xu helped to prepare and characterize the samples. Sikun Zhang and Gang He contributed to the DFT calculations. Bin Rao and Ni Yan discussed the manuscript. Sikun Zhang and Gang He wrote the manuscript and all the authors revised and polished the manuscript.