

## Supporting information

### Highly efficient and selective electrochemical synthesis of substituted benzothiophenes and benzofurans in micro-continuous flow

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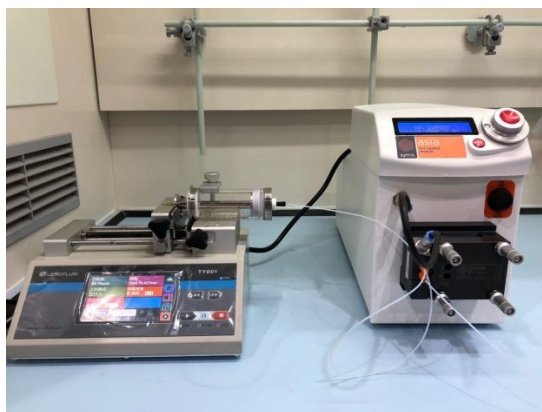
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## 1. General Information

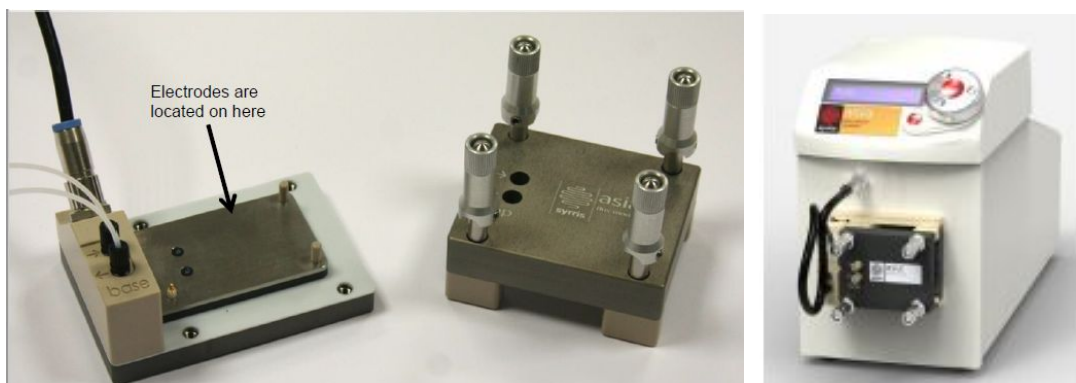
All reagents and solvents were commercially available and used without any further purification unless specified. Proton ( $^1\text{H}$  NMR) and carbon ( $^{13}\text{C}$  NMR) nuclear magnetic resonance spectra were recorded at 400 MHz and 100 MHz respectively. The chemical shifts are given in parts per million (ppm) on the delta ( $\delta$ ) scale.  $^1\text{H}$  NMR chemical shifts were determined relative to internal TMS at  $\delta$  0.0 ppm.  $^{13}\text{C}$  NMR chemical shifts were determined relative to  $\text{CDCl}_3$  at  $\delta$  77.00 ppm. The following abbreviations were used to explain multiplicities: s =singlet, d =doublet, dd = doublet of doublet, t = triplet, td = triplet of doublet, q = quartet, m = multiplet, and br = broad. Analytical TLC was performed on precoated silica gel plates. High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

## 2. Flow Electrochemistry Module

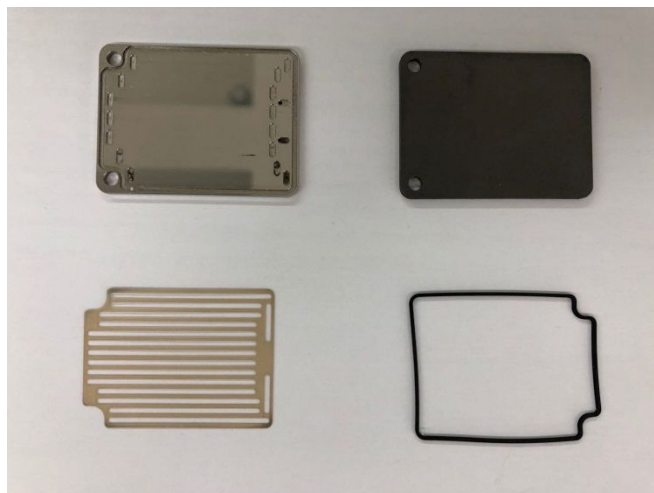
Reactions are performed in a novel flow electrochemistry system (the Asia Flux module). This system includes pumps, flow cell, working prototype cell holder and control module. The flow cell consists of pairs of electrodes separated by a gasket. Electrode materials include stainless steel, carbon, magnesium, and stainless steel with a platinum coating (also discussing copper, tin, and titanium) and the cell can be divided by a membrane to isolate the chemistry at the anode from the chemistry at the cathode. The working prototype cell holder holds the electrodes in place, enables quick fluidic and electrical connections and locates in the Syrris range of temperature controllers (e.g. The Asia Chip Climate Controller). The control module controls the current/voltage applied to the electrodes, displays the temperature, and locates the holder on the front of the module for room temperature applications.



**Figure S1.** Flow Electrochemistry Device



**Figure S2.** Flow cell holder and control module

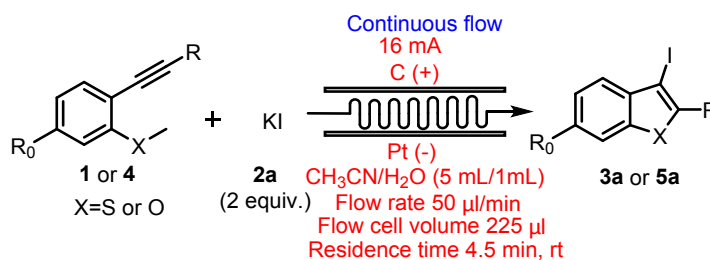


**Figure S3.** Flow cell materials and gasket

Description: Asia FLUX Flat Electrode-Carbon Filled PPS (Part Number: 2200959); Asia FLUX Flat Electrode-SS 316L Platinum Coated (Part Number: 2200740).

### 3. Experimental section

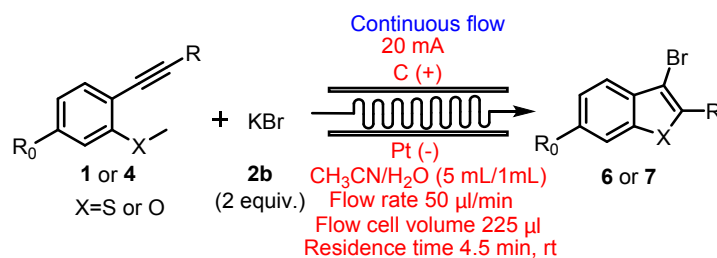
#### (1) General procedures for the synthesis of 3-iodine-substituted benzothiophenes and benzofurans.



**Figure S4.** Synthesis of 3a or 5a

First, assembled and installed the flow electrochemistry device, the anode was carbon plate, cathode was platinum plate and the cell volume were 225  $\mu\text{L}$ . Second, in a 50 mL beaker the corresponding substrates **1** or **4** (0.2 mmol, 1.0 equiv.) and **2a** KI (0.4mmol, 2.0 equiv.) were dissolved in 5 mL  $\text{CH}_3\text{CN}$  and 1 mL  $\text{H}_2\text{O}$  under the air. Then adjustment the current into 16 mA (substrates **4** was reacted under 30 mA) at the control module and the reaction mixture was pumped into the flow cell via a syringe. The flow rate was 50 $\mu\text{L}/\text{min}$  and residence time 4.5 minute. The outflow of the reaction mixture was collected then mixture was washed by 5 mL  $\text{H}_2\text{O}$  and extracted with ethyl acetate (10 mL  $\times$  3). The organic layer was dried over anhydrous sodium sulfate, and solvent was removed under vacuum. The resulting residue was purified by flash column chromatography using *n*-hexane as the eluent to afford the product in good yield.

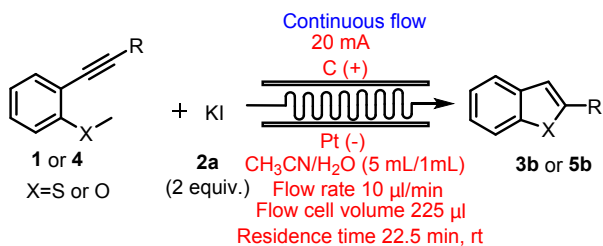
**(2) General procedures for the synthesis of 3- bromine-substituted benzothiophenes and benzofurans.**



**Figure S5.** Synthesis of **6** or **7**

First, assembled and installed the flow electrochemistry device, the anode was carbon plate, cathode was platinum plate and the cell volume were 225  $\mu\text{L}$ . Second, in a 50 mL beaker the corresponding substrates **1** or **4** (0.2 mmol, 1.0 equiv.) and **2b** KBr (0.4mmol, 2.0 equiv.) were dissolved in 5 mL  $\text{CH}_3\text{CN}$  and 1 mL  $\text{H}_2\text{O}$  under the air. Then adjustment the current into 20 mA (substrates **4** was reacted under 40 mA) at the control module and the reaction mixture was pumped into the flow cell via a syringe. The flow rate was 50 $\mu\text{L}/\text{min}$  and residence time 4.5 minute. The outflow of the reaction mixture was collected then mixture was washed by 5 mL  $\text{H}_2\text{O}$  and extracted with ethyl acetate (10 mL  $\times$  3). The organic layer was dried over anhydrous sodium sulfate, and solvent was removed under vacuum. The resulting residue was purified by flash column chromatography using *n*-hexane as the eluent to afford the product in good yield.

**(3) General procedures for the synthesis of dehalogenation benzothiophenes and benzofurans.**



**Figure S6.** Synthesis of **3b** or **5b**

First, assembled and installed the flow electrochemistry device, the anode was carbon plate, cathode was platinum plate and the cell volume were 225 μL. Second, in a 50 mL beaker the corresponding substrates **1** or **4** (0.2 mmol, 1.0 equiv.) and **2a** KI (0.4 mmol, 2.0 equiv.) were dissolved in 5 mL CH<sub>3</sub>CN and 1 mL H<sub>2</sub>O under the air. Then adjustment the current into 20 mA (substrates **4** was reacted under 40 mA) at the control module and the reaction mixture was pumped into the flow cell via a syringe. The flow rate was 10 μL/min and residence time 22.5 minute. The outflow of the reaction mixture was collected then mixture was washed by 5 mL H<sub>2</sub>O and extracted with ethyl acetate (10 mL × 3). The organic layer was dried over anhydrous sodium sulfate, and solvent was removed under vacuum. The resulting residue was purified by flash column chromatography using *n*-hexane as the eluent to afford the product in good yield.

#### 4. Cyclic voltammetry experiment

Cyclic voltammograms of **1a**, KI, KBr, KCl and **1a** + KI were performed in a three-electrode cell connected to a schlenk line under nitrogen at room temperature. The working electrode was a steady glassy carbon disk electrode (CHI101, Φ 3 mm, *L* 60 mm) while the counter electrode was a platinum wire (CHI115, Φ 0.5 mm, *L* 35 mm). The reference was an Ag/AgCl electrode (CHI111, Φ 4 mm Glass Tubing, Φ 0.5 mm Ag/AgCl Wire) submerged in saturated aqueous KCl solution. (1) **1a** (0.4 mmol) and a mixed solvent (CH<sub>3</sub>CN/H<sub>2</sub>O = 5/1, 12 mL) containing *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.8 mmol) were poured into the electrochemical cell in cyclic voltammetry experiments. The scan rate was 0.10 V/s, ranging from 0 V to 2.5 V. (2) KI (0.4 mmol) and a mixed solvent (CH<sub>3</sub>CN/H<sub>2</sub>O = 5/1, 12 mL) containing *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.8 mmol) were poured into the electrochemical cell in cyclic voltammetry experiments. The scan rate was 0.10 V/s, ranging from 0 V to 2.5 V. (3) KBr (0.4 mmol) and a mixed solvent (CH<sub>3</sub>CN/H<sub>2</sub>O = 5/1, 12 mL) containing *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.8 mmol) were poured into the electrochemical cell in cyclic voltammetry experiments. The scan rate was 0.10 V/s, ranging from 0 V to 2.5 V. (4) KCl (0.4 mmol) and a mixed solvent (CH<sub>3</sub>CN/H<sub>2</sub>O = 5/1, 12 mL) containing *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.8 mmol) were

poured into the electrochemical cell in cyclic voltammetry experiments. The scan rate was 0.10 V/s, ranging from 0 V to 2.5 V. (5) **1a** (0.4 mmol) + KI (0.8 mmol) and a mixed solvent (CH<sub>3</sub>CN/H<sub>2</sub>O = 5/1, 12 mL) containing *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.8 mmol) were poured into the electrochemical cell in cyclic voltammetry experiments. The scan rate was 0.10 V/s, ranging from 0 V to 2.5 V.

## 5. Electrospray Ionization-Time-of-Flight-Mass Spectrometry (ESI-TOF-MS) of compound **8**

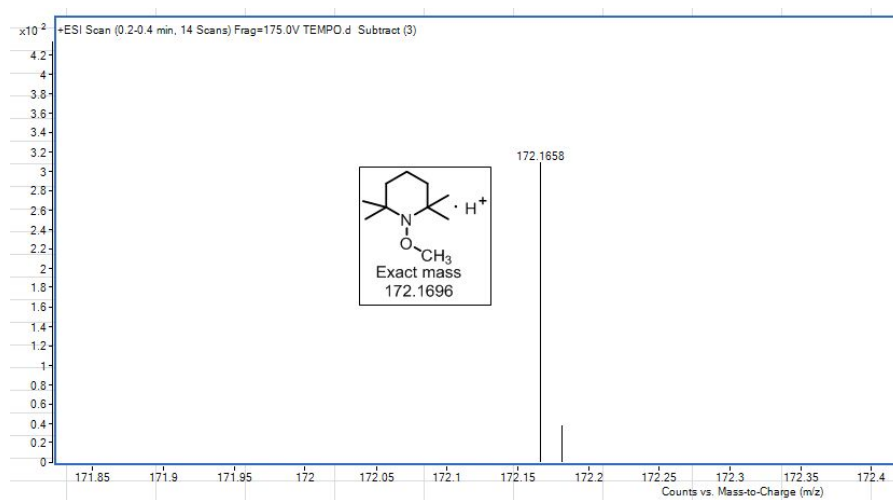
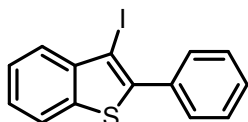


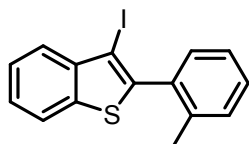
Figure S7. Mass spectrometry of **8**

## 6. Detail descriptions for products



3-Iodo-2-phenylbenzo[*b*] thiophene (**3aa**)

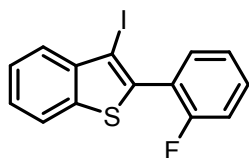
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.69 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.52 – 7.42 (m, 4H), 7.39 (t, *J* = 8.2 Hz, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 142.23, 141.95, 138.99, 134.68, 130.09, 128.94, 128.54, 126.35, 125.54, 125.50, 122.15, 79.48. HRMS (ESI-TOF) *m/z* Calcd for C<sub>14</sub>H<sub>9</sub>IS [M+H]<sup>+</sup>: 336.9542, found: 336.9547.



3-Iodo-2-(*o*-tolyl) benzo [*b*] thiophene (**3ab**)

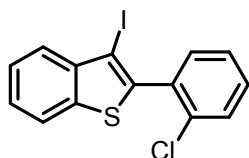
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.79 (d, *J* = 8.5 Hz, 2H), 7.50 – 7.44 (m, 1H), 7.43 – 7.35 (m, 2H), 7.33 – 7.26 (m, 3H), 2.24 (s, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 142.72, 141.13, 139.50, 137.72,

134.47, 130.89, 130.26, 129.37, 125.84, 125.71, 125.44, 125.39, 122.19, 82.49, 20.26. HRMS (ESI-TOF)  $m/z$  Calcd for  $C_{15}H_{11}IS$   $[M+H]^+$ :350.9699, found: 350.9696.



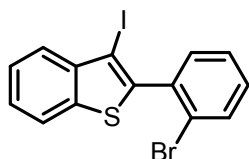
2-(2-Fluorophenyl)-3-iodobenzo [*b*] thiophene (**3ac**)

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.81 (t,  $J$  = 8.2 Hz, 2H), 7.53 – 7.37 (m, 4H), 7.26 (dd,  $J$  = 7.6, 1.1 Hz, 1H), 7.24 – 7.17 (m, 1H).  $^{19}F$  NMR (376 MHz,  $CDCl_3$ )  $\delta$  -110.72 (s, 1F).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  159.69 (d,  $J$  = 250.5 Hz), 141.26, 139.49, 136.49, 132.71, 131.14, 126.22, 125.72, 125.47, 124.10 (d,  $J$  = 3.7 Hz), 122.75 (d,  $J$  = 15.1 Hz), 122.14, 116.23 (d,  $J$  = 21.5 Hz), 83.14. HRMS (ESI-TOF)  $m/z$  Calcd for  $C_{14}H_8FIS$   $[M+H]^+$ :354.9448, found: 354.9445.



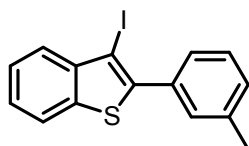
2-(2-Chlorophenyl)-3-iodobenzo [*b*] thiophene (**3ad**)

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.81 (d,  $J$  = 9.1 Hz, 2H), 7.56 – 7.51 (m, 1H), 7.51 – 7.45 (m, 1H), 7.45 – 7.33 (m, 4H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  140.92, 139.95, 139.49, 134.53, 133.94, 132.66, 130.59, 129.92, 126.68, 126.09, 125.74, 125.46, 122.22, 83.55. HRMS (ESI-TOF)  $m/z$  Calcd for  $C_{14}H_8ClIS$   $[M+H]^+$ :370.9153, found: 370.9157.



2-(2-Bromophenyl)-3-iodobenzo [*b*] thiophene (**3ae**)

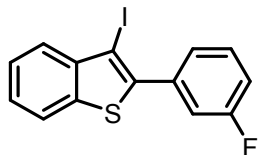
$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.81 (d,  $J$  = 9.0 Hz, 2H), 7.71 (d,  $J$  = 7.9 Hz, 1H), 7.51 – 7.45 (m, 1H), 7.45 – 7.38 (m, 3H), 7.33 (m, 1H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  141.66, 140.84, 139.42, 135.99, 133.06, 132.59, 130.75, 127.30, 126.11, 125.79, 125.50, 124.61, 122.27, 83.62. HRMS (ESI-TOF)  $m/z$  Calcd for  $C_{14}H_8BrIS$   $[M+H]^+$ :414.8648, found: 414.8644.





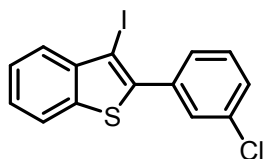
3-Iodo-2-(*m*-tolyl) benzo [*b*] thiophene (**3af**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82 (d,  $J$  = 8.1 Hz, 1H), 7.77 (d,  $J$  = 7.9 Hz, 1H), 7.53 – 7.42 (m, 3H), 7.40 – 7.32 (m, 2H), 7.24 (d,  $J$  = 7.4 Hz, 1H), 2.43 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.41, 141.94, 138.93, 138.27, 134.54, 130.68, 129.71, 128.42, 127.18, 126.29, 125.45, 122.12, 79.28, 21.48. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IS}$   $[\text{M}+\text{H}]^+$ : 350.9699, found: 350.9694.



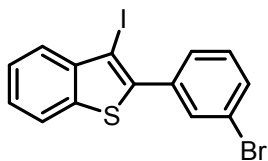
2-(3-Fluorophenyl)-3-iodobenzo [*b*] thiophene (**3ag**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (d,  $J$  = 8.1 Hz, 1H), 7.80 (d,  $J$  = 7.9 Hz, 1H), 7.51 – 7.38 (m, 5H), 7.18 – 7.09 (m, 1H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -112.28 (s, 1F).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.53 (d,  $J$  = 247.0 Hz), 141.82, 140.59 (d,  $J$  = 2.3 Hz), 138.87, 136.65 (d,  $J$  = 8.3 Hz), 130.12 (d,  $J$  = 8.6 Hz), 126.48, 125.86 (d,  $J$  = 3.0 Hz), 125.82, 125.63, 122.15, 117.09 (d,  $J$  = 22.8 Hz), 115.83 (d,  $J$  = 21.1 Hz), 80.02. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{FIS}$   $[\text{M}+\text{H}]^+$ : 354.9448, found: 354.9447.



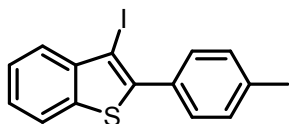
2-(3-Chlorophenyl)-3-iodobenzo [*b*] thiophene (**3ah**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J$  = 7.6 Hz, 1H), 7.73 (d,  $J$  = 7.9 Hz, 1H), 7.61 (d,  $J$  = 1.0 Hz, 1H), 7.49-7.51 (m, 1H), 7.45 – 7.39 (m, 1H), 7.37 – 7.30 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.77, 140.42, 138.91, 136.38, 134.41, 130.03, 129.78, 128.96, 128.28, 126.48, 125.84, 125.64, 122.17, 80.20. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{ClIS}$   $[\text{M}+\text{H}]^+$ : 370.9153, found: 370.9155.



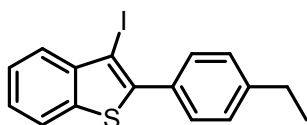
2-(3-Bromophenyl)-3-iodobenzo [*b*] thiophene (**3ai**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.86 – 7.81 (m, 2H), 7.78 (d,  $J$  = 8.0 Hz, 1H), 7.64 – 7.28 (m, 5H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  141.77, 140.28, 138.92, 136.65, 132.88, 131.87, 130.01, 128.74, 126.50, 125.86, 125.66, 122.49, 122.18, 80.28. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{BrIS}$   $[\text{M}+\text{H}]^+$ : 414.8648, found: 414.8646.



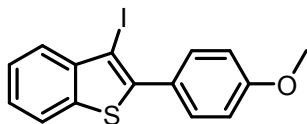
3-Iodo-2-(*p*-tolyl) benzo [*b*] thiophene (**3aj**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 8.1$  Hz, 1H), 7.77 (d,  $J = 7.9$  Hz, 1H), 7.58 (d,  $J = 8.1$  Hz, 2H), 7.50 – 7.42 (m, 1H), 7.37 (t,  $J = 7.0$  Hz, 1H), 7.28 (d,  $J = 7.9$  Hz, 2H), 2.42 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.37, 141.96, 138.99, 138.90, 131.72, 129.90, 129.25, 126.22, 125.41, 125.39, 122.09, 79.07, 21.41. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IS}$   $[\text{M}+\text{H}]^+$ : 350.9699, found: 350.9691.



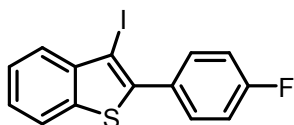
2-(4-Ethylphenyl)-3-iodobenzo [*b*] thiophene (**3ak**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 7.9$  Hz, 1H), 7.74 (d,  $J = 7.9$  Hz, 1H), 7.60 (d,  $J = 8.2$  Hz, 2H), 7.47 – 7.40 (m, 1H), 7.34 (t,  $J = 7.0$  Hz, 1H), 7.28 (d,  $J = 8.2$  Hz, 2H), 2.70 (q,  $J = 7.6$  Hz, 2H), 1.28 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  145.09, 142.30, 141.91, 138.80, 131.81, 129.88, 127.96, 126.15, 125.32 (d,  $J = 2.8$  Hz), 122.01, 78.95, 28.67, 15.29. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{16}\text{H}_{13}\text{IS}$   $[\text{M}+\text{H}]^+$ : 364.9855, found: 364.9857.



3-Iodo-2-(4-methoxyphenyl) benzo [*b*] thiophene (**3al**)

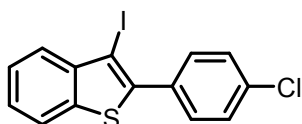
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78 (d,  $J = 8.4$  Hz, 1H), 7.72 (d,  $J = 8.0$  Hz, 1H), 7.60 (d,  $J = 8.8$  Hz, 2H), 7.42 (t,  $J = 7.6$  Hz, 1H), 7.33 (t,  $J = 7.6$  Hz, 1H), 6.96 (d,  $J = 8.8$  Hz, 2H), 3.82 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.17, 142.19, 142.02, 138.84, 131.37, 126.93, 126.19, 125.46, 125.37, 122.11, 114.02, 78.98, 55.43. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IOS}$   $[\text{M}+\text{H}]^+$ : 366.9648, found: 366.9644.



2-(4-Fluorophenyl)-3-iodobenzo [*b*] thiophene (**3am**)

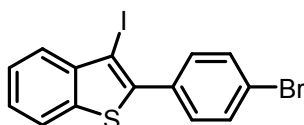
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 7.7$  Hz, 1H), 7.75 (d,  $J = 7.9$  Hz, 1H), 7.62 (dd,  $J = 8.8$ ,

5.3 Hz, 2H), 7.45 (t,  $J = 7.6$  Hz, 1H), 7.37 (t,  $J = 7.6$  Hz, 1H), 7.14 (t,  $J = 8.7$  Hz, 2H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -111.90 (s, 1F).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.99 (d,  $J = 249.6$  Hz), 141.73, 140.99, 138.80, 131.89, 131.80, 130.59 (d,  $J = 3.2$  Hz), 126.27, 125.55 (d,  $J = 7.0$  Hz), 122.06, 115.57 (d,  $J = 21.8$  Hz), 79.83. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{FIS}$   $[\text{M}+\text{H}]^+$ : 354.9448, found: 354.9441.



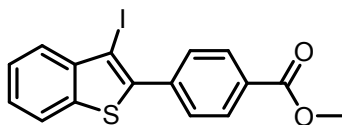
2-(4-Chlorophenyl)-3-iodobenzo [*b*] thiophene (**3an**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82 (d,  $J = 8.1$  Hz, 1H), 7.78 (d,  $J = 7.9$  Hz, 1H), 7.61 (d,  $J = 8.5$  Hz, 2H), 7.51 – 7.35 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.80, 140.76, 138.85, 133.05, 131.28, 128.78, 126.37, 125.72, 125.59, 122.12, 79.92. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{ClIS}$   $[\text{M}+\text{H}]^+$ : 370.9153, found: 370.9159.



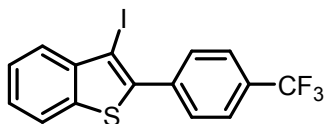
2-(4-Bromophenyl)-3-iodobenzo [*b*] thiophene (**3ao**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 8.1$  Hz, 1H), 7.77 (d,  $J = 7.9$  Hz, 1H), 7.62 – 7.56 (m, 2H), 7.56 – 7.51 (m, 2H), 7.49 – 7.43 (m, 1H), 7.42 – 7.35 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.87, 140.80, 138.90, 133.57, 131.78, 131.58, 126.43, 125.78, 125.65, 123.37, 122.17, 79.95. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{BrIS}$   $[\text{M}+\text{H}]^+$ : 414.8648, found: 414.8645.



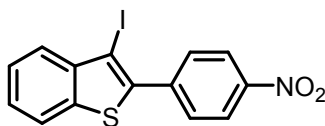
Methyl 4-(3-iodobenzo [*b*] thiophen-2-yl) benzoate (**3ap**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.14 (d,  $J = 8.4$  Hz, 2H), 7.88 – 7.75 (m, 4H), 7.49 (t,  $J = 8.1$  Hz, 1H), 7.42 (t,  $J = 8.1$  Hz, 1H), 3.96 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  166.65, 141.90, 140.80, 139.13, 139.00, 130.27, 130.04, 129.75, 126.55, 125.92, 125.68, 122.19, 80.32, 52.34. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{16}\text{H}_{11}\text{IO}_2\text{S}$   $[\text{M}+\text{H}]^+$ : 394.9597, found: 394.9593.



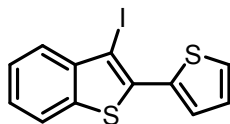
3-Iodo-2-(4-(trifluoromethyl) phenyl) benzo [*b*] thiophene (**3aq**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 (dd,  $J = 15.6, 7.4$  Hz, 4H), 7.74 (d,  $J = 8.2$  Hz, 2H), 7.54 – 7.47 (m, 1H), 7.42 (td,  $J = 7.6, 7.2, 1.2$  Hz, 1H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.66 (s, 3F).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.82, 140.29, 138.99, 138.27, 130.76 (q,  $J = 7.6$  Hz), 130.43, 126.58, 126.01, 125.75, 125.52 (q,  $J = 3.8$  Hz), 125.38 (t,  $J = 272$  Hz), 122.20, 80.48. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_8\text{F}_3\text{IS}$   $[\text{M}+\text{H}]^+$ : 404.9416, found: 404.9420.



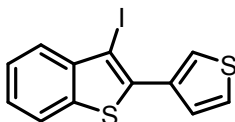
3-Iodo-2-(4-nitrophenyl) benzo [*b*] thiophene (**3ar**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.34 (d,  $J = 8.9$  Hz, 2H), 7.94 – 7.79 (m, 4H), 7.56 – 7.49 (m, 1H), 7.49 – 7.41 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  147.75, 141.83, 141.20, 139.22, 139.08, 130.95, 126.79, 126.37, 125.95, 123.79, 122.26, 81.36. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{INO}_2\text{S}$   $[\text{M}+\text{H}]^+$ : 381.9393, found: 381.9397.



3-Iodo-2-(thiophen-2-yl) benzo [*b*] thiophene (**3as**)

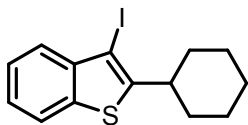
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (d,  $J = 8.1$  Hz, 1H), 7.71 (d,  $J = 7.9$  Hz, 1H), 7.57 (d,  $J = 3.7$  Hz, 1H), 7.42 (t,  $J = 5.9$  Hz, 2H), 7.34 (t,  $J = 7.5$  Hz, 1H), 7.16 – 7.09 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.32, 137.97, 135.91, 135.80, 128.66, 127.38, 127.28, 126.30, 125.80, 125.64, 121.90, 79.32. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{12}\text{H}_7\text{IS}_2$   $[\text{M}+\text{H}]^+$ : 342.9107, found: 342.9102.



3-Iodo-2-(thiophen-3-yl) benzo [*b*] thiophene (**3at**)

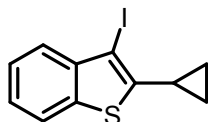
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.84 (dd,  $J = 3.0, 1.3$  Hz, 1H), 7.80 (d,  $J = 8.0$  Hz, 1H), 7.75 (d,  $J = 7.9$  Hz, 1H), 7.55 (dd,  $J = 5.0, 1.3$  Hz, 1H), 7.48 – 7.40 (m, 2H), 7.39 – 7.32 (m, 1H).  $^{13}\text{C}$  NMR (100

MHz, CDCl<sub>3</sub>)  $\delta$  142.08, 138.13, 137.19, 134.66, 128.41, 126.16, 125.89, 125.55, 125.51, 125.37, 122.03, 78.64. HRMS (ESI-TOF)  $m/z$  Calcd for C<sub>12</sub>H<sub>7</sub>IS<sub>2</sub> [M+H]<sup>+</sup>:342.9107, found: 342.9104.



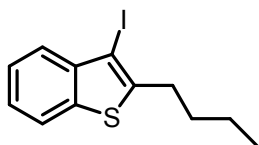
2-Cyclohexyl-3-iodobenzo [b] thiophene (**3au**)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.75 – 7.69 (m, 2H), 7.43 – 7.36 (m, 1H), 7.33 – 7.27 (m, 1H), 3.15 (m, 1H), 2.06 (d,  $J$  = 8.4 Hz, 2H), 1.87 (d,  $J$  = 6.6 Hz, 2H), 1.79 (d,  $J$  = 14.1 Hz, 1H), 1.49 (dd,  $J$  = 27.8, 14.7 Hz, 4H), 1.25 (m, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  150.54, 140.91, 137.31, 125.05, 124.89, 124.66, 122.38, 78.23, 42.98, 34.19, 26.51, 25.82. HRMS (ESI-TOF)  $m/z$  Calcd for C<sub>14</sub>H<sub>15</sub>IS [M+H]<sup>+</sup>:343.0012, found: 343.0015.



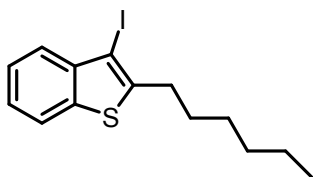
2-Cyclopropyl-3-iodobenzo [b] thiophene (**3av**)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.67 (d,  $J$  = 8.8 Hz, 2H), 7.43 – 7.36 (m, 1H), 7.32 – 7.26 (m, 1H), 2.32 (m, 1H), 1.21 – 1.13 (m, 2H), 0.89 (m, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  147.24, 141.50, 136.32, 125.13, 124.69, 124.41, 122.21, 80.22, 14.99, 10.33. HRMS (ESI-TOF)  $m/z$  Calcd for C<sub>11</sub>H<sub>9</sub>IS [M+H]<sup>+</sup>:300.9542, found: 300.9546.



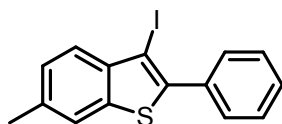
2-Butyl-3-iodobenzo [b] thiophene (**3aw**)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.72 (d,  $J$  = 7.9 Hz, 1H), 7.69 (d,  $J$  = 8.0 Hz, 1H), 7.40 (t,  $J$  = 8.1 Hz, 1H), 7.31 (t,  $J$  = 7.0 Hz, 1H), 3.02 – 2.91 (m, 2H), 1.82 – 1.66 (m, 2H), 1.52 – 1.38 (m, 2H), 1.03 – 0.86 (m, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  144.81, 141.18, 138.07, 125.06, 125.03, 124.79, 122.18, 80.04, 32.71, 32.69, 22.27, 13.88. HRMS (ESI-TOF)  $m/z$  Calcd for C<sub>12</sub>H<sub>13</sub>IS [M+H]<sup>+</sup>:316.9855, found: 316.9857.



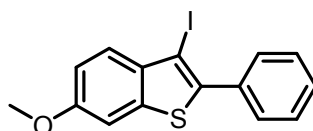
2-Hexyl-3-iodobenzo [*b*] thiophene (**3ax**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (dd,  $J = 11.7, 8.0$  Hz, 2H), 7.40 (t,  $J = 7.6$  Hz, 1H), 7.31 (t,  $J = 7.5$  Hz, 1H), 3.01 – 2.89 (m, 2H), 1.74 (p,  $J = 7.5$  Hz, 2H), 1.48 – 1.26 (m, 6H), 0.90 (t,  $J = 6.9$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  144.85, 141.19, 138.08, 125.06, 125.03, 124.80, 122.22, 80.04, 33.02, 31.58, 30.55, 28.81, 22.58, 14.10. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_{17}\text{IS}$  [ $\text{M}+\text{H}$ ] $^+$ : 345.0168, found: 345.0163.



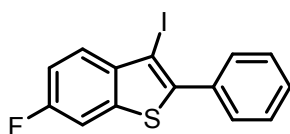
3-Iodo-6-methyl-2-phenylbenzo [*b*] thiophene (**3ay**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (dd,  $J = 8.0, 6.3$  Hz, 3H), 7.58 (s, 1H), 7.50 – 7.38 (m, 3H), 7.27 (d,  $J = 8.2$  Hz, 1H), 2.50 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  140.88, 139.82, 139.04, 135.62, 134.73, 129.99, 128.72, 128.43, 127.11, 125.84, 121.86, 78.96, 21.44. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IS}$  [ $\text{M}+\text{H}$ ] $^+$ : 350.9699, found: 350.9693.



3-Iodo-6-methoxy-2-phenylbenzo [*b*] thiophene (**3az**)

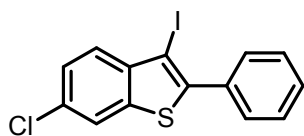
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 – 7.63 (m, 3H), 7.51 – 7.38 (m, 3H), 7.27 (d,  $J = 2.2$  Hz, 1H), 7.07 (dd,  $J = 8.9, 2.3$  Hz, 1H), 3.89 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.33, 139.96, 139.39, 136.02, 134.72, 129.95, 128.62, 128.45, 126.90, 115.30, 104.51, 78.47, 55.75. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IOS}$  [ $\text{M}+\text{H}$ ] $^+$ : 366.9648, found: 366.9641.



6-Fluoro-3-iodo-2-phenylbenzo [*b*] thiophene (**3aza**)

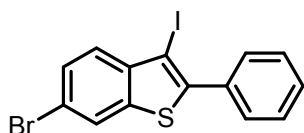
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78 (dd,  $J = 8.9, 5.1$  Hz, 1H), 7.66 (d,  $J = 8.1$  Hz, 2H), 7.53 – 7.39

(m, 4H), 7.20 (t,  $J = 7.7$  Hz, 1H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -116.12 (s, 1F).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  161.18 (d,  $J = 246.4$  Hz), 141.89 (d,  $J = 3.7$  Hz), 139.41 (d,  $J = 10.4$  Hz), 138.46 (d,  $J = 1.1$  Hz), 134.36, 129.94, 128.98, 128.55, 127.47 (d,  $J = 9.2$  Hz), 114.34 (d,  $J = 24.3$  Hz), 108.13 (d,  $J = 25.6$  Hz), 78.43. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{FIS}$   $[\text{M}+\text{H}]^+$ : 354.9488, found: 354.9479.



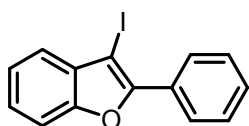
6-Chloro-3-iodo-2-phenylbenzo [*b*] thiophene (**3azb**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.83 – 7.60 (m, 4H), 7.44 (dd,  $J = 22.5, 7.9$  Hz, 4H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.68, 140.50, 139.63, 134.17, 131.66, 129.92, 129.09, 128.56, 127.09, 126.20, 121.55, 78.65. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{ClIS}$   $[\text{M}+\text{H}]^+$ : 370.9153, found: 370.9145.



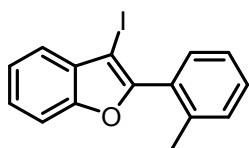
6-Bromo-3-iodo-2-phenylbenzo [*b*] thiophene (**3azc**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 1.7$  Hz, 1H), 7.67 (td,  $J = 5.7, 5.1, 2.9$  Hz, 3H), 7.55 (dd,  $J = 8.6, 1.7$  Hz, 1H), 7.51 – 7.42 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.73, 140.85, 140.11, 134.14, 129.93, 129.12, 128.85, 128.58, 127.41, 124.50, 119.44, 78.78. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{BrIS}$   $[\text{M}+\text{H}]^+$ : 414.8648, found: 414.8639.



3-Iodo-2-phenylbenzofuran (**5aa**)

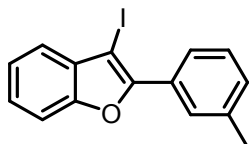
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 – 8.14 (m, 2H), 7.53 – 7.39 (m, 5H), 7.39 – 7.27 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.96, 153.11, 132.52, 130.04, 129.26, 128.54, 127.53, 125.70, 123.54, 121.88, 111.20, 61.15. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_9\text{IO}$   $[\text{M}+\text{H}]^+$ : 320.9771, found: 320.9775.



3-Iodo-2-(*o*-tolyl) benzofuran (**5ab**)

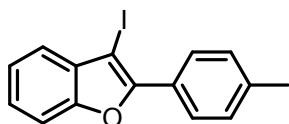
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.55 (d,  $J = 6.4$  Hz, 1H), 7.50 – 7.44 (m, 2H), 7.41 – 7.26 (m, 5H),

2.37 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.31, 154.49, 138.39, 131.47, 131.26, 130.68, 129.98, 129.47, 125.59, 125.41, 123.48, 121.65, 111.36, 64.83, 20.47. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IO}$   $[\text{M}+\text{H}]^+$ :334.9927, found: 334.9923.



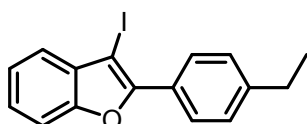
3-Iodo-2-(*m*-tolyl) benzofuran (**5ac**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 – 7.94 (m, 2H), 7.48 (d,  $J$  = 8.6 Hz, 1H), 7.46 – 7.21 (m, 5H), 2.45 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.93, 153.30, 138.26, 132.54, 130.09, 129.93, 128.42, 128.07, 125.61, 124.78, 123.49, 121.84, 111.16, 61.02, 21.57. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IO}$   $[\text{M}+\text{H}]^+$ :334.9927, found: 334.9929.



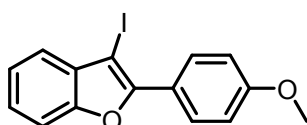
3-Iodo-2-(*p*-tolyl) benzofuran (**5ad**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J$  = 8.2 Hz, 2H), 7.50 – 7.41 (m, 2H), 7.38 – 7.26 (m, 4H), 2.41 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.88, 153.39, 139.43, 132.57, 129.25, 127.46, 127.23, 125.47, 123.46, 121.72, 111.12, 60.42, 21.50. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IO}$   $[\text{M}+\text{H}]^+$ :334.9927, found: 334.9924.



2-(4-Ethylphenyl)-3-iodobenzofuran (**5ae**)

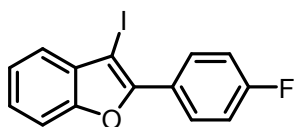
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.10 (d,  $J$  = 8.2 Hz, 2H), 7.46 (dd,  $J$  = 12.6, 8.4 Hz, 2H), 7.39 – 7.27 (m, 4H), 2.72 (q,  $J$  = 7.6 Hz, 2H), 1.29 (t,  $J$  = 7.6 Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.88, 153.40, 145.70, 132.58, 128.05, 127.54, 127.44, 125.46, 123.45, 121.71, 111.12, 60.39, 28.83, 15.36. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{16}\text{H}_{13}\text{IO}$   $[\text{M}+\text{H}]^+$ :349.0084, found: 349.0087.



3-Iodo-2-(4-methoxyphenyl) benzofuran (**5af**)

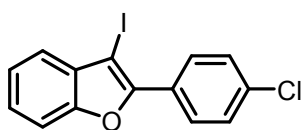


$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.11 (d,  $J = 8.8$  Hz, 2H), 7.49 – 7.38 (m, 2H), 7.36 – 7.25 (m, 2H), 7.00 (d,  $J = 8.8$  Hz, 2H), 3.86 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  160.38, 153.80, 153.28, 132.62, 129.07, 125.26, 123.44, 122.65, 121.56, 113.98, 111.03, 59.52, 55.40. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{IO}_2$   $[\text{M}+\text{H}]^+$ : 350.9876, found: 350.9879.



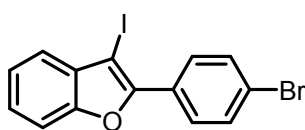
2-(4-Fluorophenyl)-3-iodobenzofuran (**5ag**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.16 (dd,  $J = 8.9, 5.3$  Hz, 2H), 7.46 (dd,  $J = 11.2, 7.0$  Hz, 2H), 7.40 – 7.29 (m, 2H), 7.19 (t,  $J = 8.7$  Hz, 2H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -110.83 (s, 1F).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  163.16 (d,  $J = 250.3$  Hz), 153.90, 152.33, 132.40, 129.53 (d,  $J = 8.2$  Hz), 126.25, 125.76, 123.62, 121.86, 115.67 (d,  $J = 21.9$  Hz), 111.17, 60.95. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{FIO}$   $[\text{M}+\text{H}]^+$ : 338.9677, found: 338.9671.



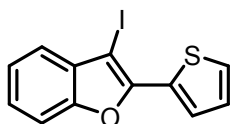
2-(4-Chlorophenyl)-3-iodobenzofuran (**5ah**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.16 – 8.09 (m, 2H), 7.51 – 7.42 (m, 4H), 7.41 – 7.29 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.92, 152.00, 135.17, 132.40, 128.81, 128.66, 128.50, 125.98, 123.69, 121.95, 111.22, 61.66. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{ClIO}$   $[\text{M}+\text{H}]^+$ : 354.9381, found: 354.9379.



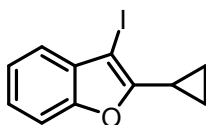
2-(4-Bromophenyl)-3-iodobenzofuran (**5ai**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 8.8$  Hz, 2H), 7.63 (d,  $J = 8.7$  Hz, 2H), 7.51 – 7.43 (m, 2H), 7.41 – 7.29 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  153.92, 152.01, 132.41, 131.76, 128.94, 128.85, 126.02, 123.70, 123.47, 121.96, 111.23, 61.75. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{BrIO}$   $[\text{M}+\text{H}]^+$ : 398.8876, found: 398.8872.



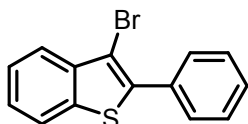
3-Iodo-2-(thiophen-2-yl) benzofuran (**5aj**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (dd,  $J = 3.7, 1.0$  Hz, 1H), 7.49 – 7.43 (m, 2H), 7.40 (dd,  $J = 7.5, 1.5$  Hz, 1H), 7.36 – 7.26 (m, 2H), 7.17 (dd,  $J = 5.0, 3.8$  Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.60, 150.31, 132.32, 131.95, 127.62, 127.18, 127.08, 125.69, 123.70, 121.46, 111.04, 60.79. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{12}\text{H}_7\text{IOS}$   $[\text{M}+\text{H}]^+$ : 326.9335, found: 326.9339.



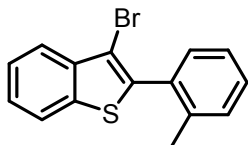
2-Cyclopropyl-3-iodobenzofuran (**5ak**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.32 – 7.26 (m, 2H), 7.24 – 7.19 (m, 2H), 2.18 (tt,  $J = 8.4, 5.1$  Hz, 1H), 1.17 – 1.10 (m, 2H), 1.08 – 1.00 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.64, 153.32, 131.44, 124.20, 123.18, 120.18, 110.75, 61.14, 9.72, 7.79. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{11}\text{H}_9\text{IO}$   $[\text{M}+\text{H}]^+$ : 284.9771, found: 284.9777.



3-Bromo-2-phenylbenzo [*b*] thiophene (**6a**)

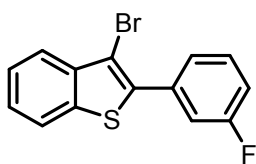
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 9.1$  Hz, 1H), 7.81 (d,  $J = 8.0$  Hz, 1H), 7.76 (dd,  $J = 8.2, 1.3$  Hz, 2H), 7.51 – 7.35 (m, 5H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  139.17, 138.26, 137.74, 133.10, 129.68, 128.82, 128.62, 125.49, 125.26, 123.70, 122.21, 104.98. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_9\text{BrS}$   $[\text{M}+\text{H}]^+$ : 288.9681, found: 288.9687.



3-Bromo-2-(*o*-tolyl) benzo [*b*] thiophene (**6b**)

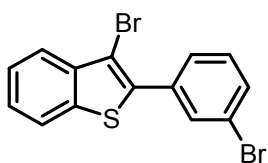
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (d,  $J = 7.5$  Hz, 1H), 7.81 (d,  $J = 7.8$  Hz, 1H), 7.51 – 7.45 (m, 1H), 7.44 – 7.37 (m, 1H), 7.37 – 7.26 (m, 4H), 2.28 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  138.47, 138.36, 138.26, 137.94, 132.48, 130.94, 130.28, 129.34, 125.69, 125.39, 125.19, 123.42, 122.28,

107.47, 20.16. HRMS (ESI-TOF)  $m/z$  Calcd for  $C_{15}H_{11}BrS$   $[M+H]^+$ :302.9838, found: 302.9832.



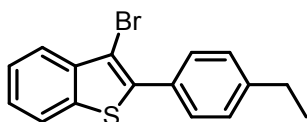
3-Bromo-2-(3-fluorophenyl) benzo *[b]* thiophene (**6c**)

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.88 (d,  $J$  = 9.2 Hz, 1H), 7.82 (d,  $J$  = 8.0 Hz, 1H), 7.57 – 7.38 (m, 5H), 7.13 (td,  $J$  = 8.4, 1.6 Hz, 1H).  $^{19}F$  NMR (376 MHz,  $CDCl_3$ )  $\delta$  -112.28 (s, 1F).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  162.63 (d,  $J$  = 246.6 Hz), 139.06, 137.68, 136.69, 135.08 (d,  $J$  = 8.5 Hz), 130.18 (d,  $J$  = 8.3 Hz), 125.82, 125.45, 125.41, 123.86, 122.23, 116.62 (d,  $J$  = 23.1 Hz), 115.73 (d,  $J$  = 21.1 Hz), 105.66. HRMS (ESI-TOF)  $m/z$  Calcd for  $C_{14}H_8BrFS$   $[M+H]^+$ :306.9587, found: 306.9583.



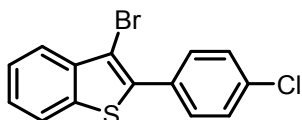
3-Bromo-2-(3-bromophenyl) benzo *[b]* thiophene (**6d**)

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.94 – 7.85 (m, 2H), 7.82 (d,  $J$  = 7.9 Hz, 1H), 7.69 (d,  $J$  = 7.8 Hz, 1H), 7.56 (d,  $J$  = 7.3 Hz, 1H), 7.53 – 7.46 (m, 1H), 7.43 (t,  $J$  = 8.1 Hz, 1H), 7.35 (t,  $J$  = 7.9 Hz, 1H).  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  138.98, 137.73, 136.37, 135.08, 132.45, 131.76, 130.09, 128.31, 125.85, 125.43, 123.87, 122.59, 122.24, 105.82. HRMS (ESI-TOF)  $m/z$  Calcd for  $C_{14}H_8Br_2S$   $[M+H]^+$ :366.8786, found: 366.8782.



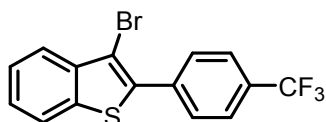
3-Bromo-2-(4-ethylphenyl) benzo *[b]* thiophene (**6e**)

$^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.85 (d,  $J$  = 8.1 Hz, 1H), 7.78 (d,  $J$  = 7.9 Hz, 1H), 7.68 (d,  $J$  = 8.2 Hz, 2H), 7.45 (t,  $J$  = 7.6 Hz, 1H), 7.37 (t,  $J$  = 7.6 Hz, 1H), 7.30 (d,  $J$  = 8.0 Hz, 2H), 2.71 (q,  $J$  = 7.6 Hz, 2H), 1.28 (t,  $J$  = 7.6 Hz, 3H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  145.16, 139.27, 138.48, 137.65, 130.41, 129.60, 128.17, 125.36, 125.21, 123.60, 122.18, 104.58, 28.76, 15.39. HRMS (ESI-TOF)  $m/z$  Calcd for  $C_{16}H_{13}BrS$   $[M+H]^+$ :316.9994, found: 316.9997.



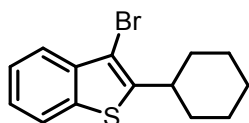
3-Bromo-2-(4-chlorophenyl) benzo [*b*] thiophene (**6f**)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 7.9 Hz, 1H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.52 – 7.38 (m, 4H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 139.06, 137.65, 136.87, 134.94, 131.54, 130.90, 128.89, 125.73, 125.40, 123.78, 122.22, 105.45. HRMS (ESI-TOF) *m/z* Calcd for C<sub>14</sub>H<sub>8</sub>BrClS [M+H]<sup>+</sup>:322.9291, found: 322.9297.



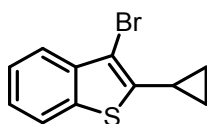
3-Bromo-2-(4-(trifluoromethyl) phenyl) benzo [*b*] thiophene (**6g**)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.90 (m, 3H), 7.83 (d, *J* = 8.6 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 2H), 7.55 – 7.47 (m, 1H), 7.47 – 7.39 (m, 1H). <sup>19</sup>F NMR (376 MHz, CDCl<sub>3</sub>) δ -62.70 (s, 3F). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 140.62, 138.98, 137.81, 136.68 (d, *J* = 1.3 Hz), 136.34, 129.96, 126.00, 125.62, 125.60 – 125.32 (m), 124.08 (q, *J* = 226 Hz), 123.95, 122.26, 106.17. HRMS (ESI-TOF) *m/z* Calcd for C<sub>15</sub>H<sub>8</sub>BrF<sub>3</sub>S [M+H]<sup>+</sup>:356.9555, found: 356.9557.



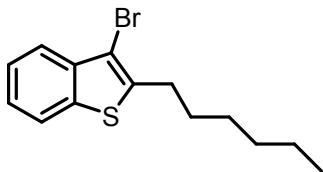
3-Bromo-2-cyclohexylbenzo [*b*] thiophene (**6h**)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.75 (d, *J* = 9.0 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.31 (t, *J* = 8.1 Hz, 1H), 3.28 – 3.01 (m, 1H), 2.05 (d, *J* = 8.5 Hz, 2H), 1.93 – 1.71 (m, 3H), 1.52 – 1.38 (m, 4H), 1.32 – 1.20 (m, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 146.86, 138.29, 136.60, 124.80, 122.46, 122.39, 103.87, 39.83, 33.95, 26.46, 25.80. HRMS (ESI-TOF) *m/z* Calcd for C<sub>14</sub>H<sub>15</sub>BrS [M+H]<sup>+</sup>:295.0151, found: 295.0155.



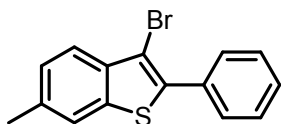
3-Bromo-2-cyclopropylbenzo [*b*] thiophene (**6i**)

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.69 (dd, *J* = 9.8, 8.7 Hz, 2H), 7.42 – 7.36 (m, 1H), 7.29 (td, *J* = 7.7, 7.2, 1.2 Hz, 1H), 2.35 (tt, *J* = 8.4, 5.1 Hz, 1H), 1.20 – 1.10 (m, 2H), 0.87 (dt, *J* = 6.7, 4.9 Hz, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 143.58, 138.82, 135.63, 124.97, 124.63, 122.31, 122.11, 106.23, 11.97, 10.11. HRMS (ESI-TOF) *m/z* Calcd for C<sub>11</sub>H<sub>9</sub>BrS [M+H]<sup>+</sup>:252.9681, found: 252.9685.



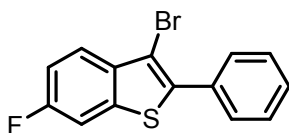
3-Bromo-2-hexylbenzo [*b*] thiophene (**6j**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.73 (d,  $J = 9.0$  Hz, 2H), 7.44 – 7.37 (m, 1H), 7.35 – 7.28 (m, 1H), 3.00 – 2.89 (m, 2H), 1.73 (p,  $J = 7.5$  Hz, 2H), 1.48 – 1.22 (m, 6H), 0.89 (t,  $J = 7.0$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  141.01, 138.42, 137.13, 124.85, 124.69, 122.62, 122.27, 105.69, 31.55, 30.33, 29.95, 28.80, 22.58, 14.10. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_{17}\text{BrS}$   $[\text{M}+\text{H}]^+$ : 297.0307, found: 297.0301.



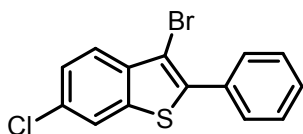
3-Bromo-6-methyl-2-phenylbenzo [*b*] thiophene (**6k**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (m, 3H), 7.60 (s, 1H), 7.51 – 7.38 (m, 3H), 7.28 (d,  $J = 8.2$  Hz, 1H), 2.51 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  137.88, 137.05, 136.92, 135.65, 133.22, 129.58, 128.61, 128.53, 126.94, 123.27, 121.97, 104.67, 21.53. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{BrS}$   $[\text{M}+\text{H}]^+$ : 302.9838, found: 302.9830.



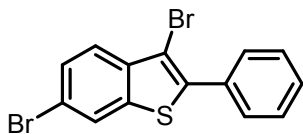
3-Bromo-6-fluoro-2-phenylbenzo [*b*] thiophene (**6l**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 – 7.68 (m, 3H), 7.62 – 7.36 (m, 4H), 7.25 – 7.15 (m, 1H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -115.75 (s, 1F).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  168.67 (d,  $J = 123.4$  Hz), 161.13 (d,  $J = 246.5$  Hz), 138.46 (d,  $J = 10.4$  Hz), 136.80 (d,  $J = 221.2$  Hz), 132.81, 129.53, 128.87, 128.64, 124.93 (d,  $J = 9.1$  Hz), 114.24 (d,  $J = 24.5$  Hz), 108.35 (d,  $J = 25.7$  Hz), 104.33. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{BrFS}$   $[\text{M}+\text{H}]^+$ : 306.9587, found: 306.9581.



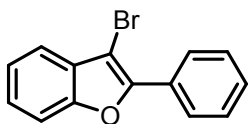
3-Bromo-6-chloro-2-phenylbenzo [*b*] thiophene (**6m**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.80 (d,  $J = 1.6$  Hz, 1H), 7.77 (d,  $J = 8.6$  Hz, 1H), 7.74 (d,  $J = 6.8$  Hz, 2H), 7.52 – 7.41 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  138.76, 138.55, 137.72, 132.65, 131.66, 129.55, 129.01, 128.67, 126.09, 124.55, 121.72, 104.54. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{BrClS}$   $[\text{M}+\text{H}]^+$ : 322.9291, found: 322.9283.



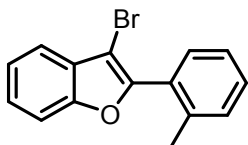
3,6-Dibromo-2-phenylbenzo *[b]* thiophene (**6n**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.95 (d,  $J = 1.3$  Hz, 1H), 7.76 – 7.67 (m, 3H), 7.56 (dd,  $J = 8.6$ , 1.6 Hz, 1H), 7.51 – 7.40 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  138.97, 138.79, 138.05, 132.59, 129.54, 129.03, 128.70, 128.67, 124.81, 124.64, 119.41, 104.64. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_8\text{Br}_2\text{S}$   $[\text{M}+\text{H}]^+$ : 366.8786, found: 366.8773.



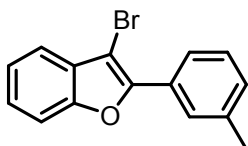
3-Bromo-2-phenylbenzofuran (**7a**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.18 (dd,  $J = 8.5$ , 1.3 Hz, 2H), 7.60 – 7.54 (m, 1H), 7.50 (t,  $J = 8.0$  Hz, 3H), 7.43 (d,  $J = 7.4$  Hz, 1H), 7.38 – 7.28 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.18, 150.33, 129.62, 129.56, 129.08, 128.62, 126.78, 125.62, 123.49, 119.92, 111.31, 93.84. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_9\text{BrO}$   $[\text{M}+\text{H}]^+$ : 272.9910, found: 272.9914.



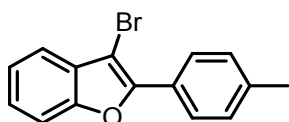
3-Bromo-2-(*o*-tolyl) benzofuran (**7b**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (dd,  $J = 7.5$ , 2.2 Hz, 2H), 7.50 (dd,  $J = 6.6$ , 2.2 Hz, 1H), 7.39 – 7.29 (m, 5H), 2.41 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.75, 152.89, 138.28, 130.80, 130.77, 129.90, 128.66, 128.56, 125.61, 125.31, 123.42, 119.87, 111.46, 95.99, 20.45. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{BrO}$   $[\text{M}+\text{H}]^+$ : 287.0066, found: 287.0061.



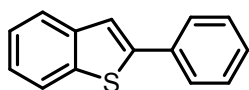
3-Bromo-2-(*m*-tolyl) benzofuran (**7c**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 (d,  $J = 9.0$  Hz, 2H), 7.58 – 7.54 (m, 1H), 7.53 – 7.48 (m, 1H), 7.42 – 7.29 (m, 3H), 7.23 (d,  $J = 7.6$  Hz, 1H), 2.45 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.14, 150.52, 138.32, 129.91, 129.64, 129.45, 128.52, 127.32, 125.53, 124.01, 123.45, 119.88, 111.27, 93.70, 21.59. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{BrO}$   $[\text{M}+\text{H}]^+$ : 287.0066, found: 287.0069.



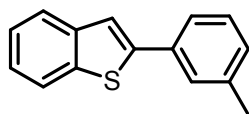
3-Bromo-2-(*p*-tolyl) benzofuran (**7d**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J = 8.3$  Hz, 2H), 7.54 (dd,  $J = 6.5, 1.9$  Hz, 1H), 7.49 (dd,  $J = 7.3, 1.8$  Hz, 1H), 7.36 – 7.27 (m, 4H), 2.41 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  153.08, 150.61, 139.24, 129.69, 129.33, 126.76, 126.72, 125.37, 123.42, 119.76, 111.23, 93.13, 21.50. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{11}\text{BrO}$   $[\text{M}+\text{H}]^+$ : 287.0066, found: 287.0061.



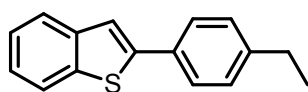
2-Phenylbenzo [*b*] thiophene (**3ba**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 7.7$  Hz, 1H), 7.75 (d,  $J = 7.1$  Hz, 1H), 7.73 – 7.67 (m, 2H), 7.52 (s, 1H), 7.40 (t,  $J = 7.5$  Hz, 2H), 7.32 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.30, 140.75, 139.56, 134.35, 129.00, 128.31, 126.55, 124.56, 124.37, 123.62, 122.32, 119.51. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_{10}\text{S}$   $[\text{M}+\text{H}]^+$ : 211.0576, found: 211.0572.



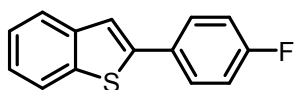
2-(*m*-tolyl) benzo [*b*] thiophene (**3bb**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 8.2$  Hz, 1H), 7.75 (d,  $J = 7.1$  Hz, 1H), 7.51 (d,  $J = 7.5$  Hz, 3H), 7.37 – 7.26 (m, 3H), 7.15 (d,  $J = 7.8$  Hz, 1H), 2.41 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.47, 140.75, 139.51, 138.65, 134.25, 129.12, 128.88, 127.24, 124.50, 124.27, 123.69, 123.54, 122.29, 119.37, 21.49. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{12}\text{S}$   $[\text{M}+\text{H}]^+$ : 225.0732, found: 225.0737.



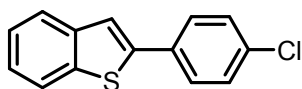
2-(4-Ethylphenyl) benzo [*b*] thiophene (**3bc**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 7.8$  Hz, 1H), 7.74 (d,  $J = 7.4$  Hz, 1H), 7.63 (d,  $J = 8.1$  Hz, 2H), 7.49 (s, 1H), 7.37 – 7.25 (m, 3H), 2.68 (q,  $J = 7.6$  Hz, 2H), 1.26 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.67, 144.46, 140.82, 139.40, 131.78, 128.48, 126.51, 124.47, 124.14, 123.44, 122.26, 118.90, 28.66, 15.51. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{16}\text{H}_{14}\text{S}$   $[\text{M}+\text{H}]^+$ : 239.0889, found: 239.0891.



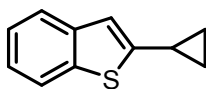
2-(4-Fluorophenyl) benzo [b] thiophene (**3bd**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 7.8$  Hz, 1H), 7.75 (d,  $J = 7.2$  Hz, 1H), 7.66 (dd,  $J = 8.8$ , 5.2 Hz, 2H), 7.45 (s, 1H), 7.37 – 7.27 (m, 2H), 7.10 (t,  $J = 8.7$  Hz, 2H).  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -113.33 (s, 1F).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.74 (d,  $J = 248.4$  Hz), 143.03, 140.64, 139.41, 130.54 (d,  $J = 3.2$  Hz), 128.15 (d,  $J = 8.1$  Hz), 124.58, 124.35, 123.52, 122.22, 119.41, 115.92 (d,  $J = 21.9$  Hz). HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_9\text{FS}$   $[\text{M}+\text{H}]^+$ : 229.0482, found: 229.0487.



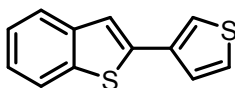
2-(4-Chlorophenyl) benzo [b] thiophene (**3be**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.82 (d,  $J = 8.0$  Hz, 1H), 7.78 – 7.74 (m, 1H), 7.63 (d,  $J = 8.6$  Hz, 2H), 7.51 (s, 1H), 7.42 – 7.36 (m, 2H), 7.36 – 7.28 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.85, 140.60, 139.52, 134.11, 132.86, 129.14, 127.67, 124.69, 124.60, 123.68, 122.30, 119.90. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_9\text{ClS}$   $[\text{M}+\text{H}]^+$ : 245.0186, found: 245.0187.



2-Cyclopropylbenzo [b] thiophene (**3bf**)

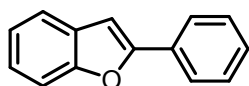
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.74 – 7.68 (m, 1H), 7.61 (d,  $J = 7.7$  Hz, 1H), 7.31 – 7.16 (m, 2H), 6.96 (s, 1H), 2.20 – 2.07 (m, 1H), 1.09 – 0.99 (m, 2H), 0.86 – 0.76 (m, 2H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  149.42, 140.26, 138.48, 124.16, 123.35, 122.52, 122.10, 118.81, 11.95, 10.00. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{11}\text{H}_{10}\text{S}$   $[\text{M}+\text{H}]^+$ : 175.0576, found: 175.0579.



2-(Thiophen-3-yl) benzo [b] thiophene (**3bg**)

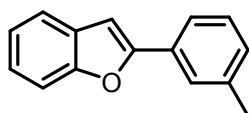


$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.78 (d,  $J$  = 8.2 Hz, 1H), 7.72 (d,  $J$  = 7.3 Hz, 1H), 7.49 (dd,  $J$  = 2.9, 1.4 Hz, 1H), 7.42 – 7.38 (m, 2H), 7.36 (dd,  $J$  = 5.0, 2.9 Hz, 1H), 7.34 – 7.25 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  140.53, 139.06, 138.97, 135.74, 126.60, 126.14, 124.57, 124.30, 123.47, 122.24, 121.32, 119.43. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{12}\text{H}_8\text{S}_2$   $[\text{M}+\text{H}]^+$ : 217.0140, found: 217.0137.



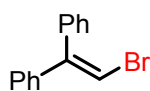
2-Phenylbenzofuran (**5ba**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (dd,  $J$  = 8.4, 1.2 Hz, 2H), 7.58 (d,  $J$  = 7.4 Hz, 1H), 7.52 (d,  $J$  = 8.2 Hz, 1H), 7.44 (t,  $J$  = 7.6 Hz, 2H), 7.35 (d,  $J$  = 8.0 Hz, 1H), 7.29 (d,  $J$  = 7.1 Hz, 1H), 7.21 (d,  $J$  = 7.9 Hz, 1H), 7.02 (d,  $J$  = 0.8 Hz, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  155.95, 154.92, 130.52, 129.25, 128.81, 128.57, 124.96, 124.28, 122.95, 120.92, 111.20, 101.32. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_{11}\text{O}$   $[\text{M}+\text{H}]^+$ : 195.0804, found: 195.0808.



2-(*m*-tolyl) benzofuran (**5bb**)

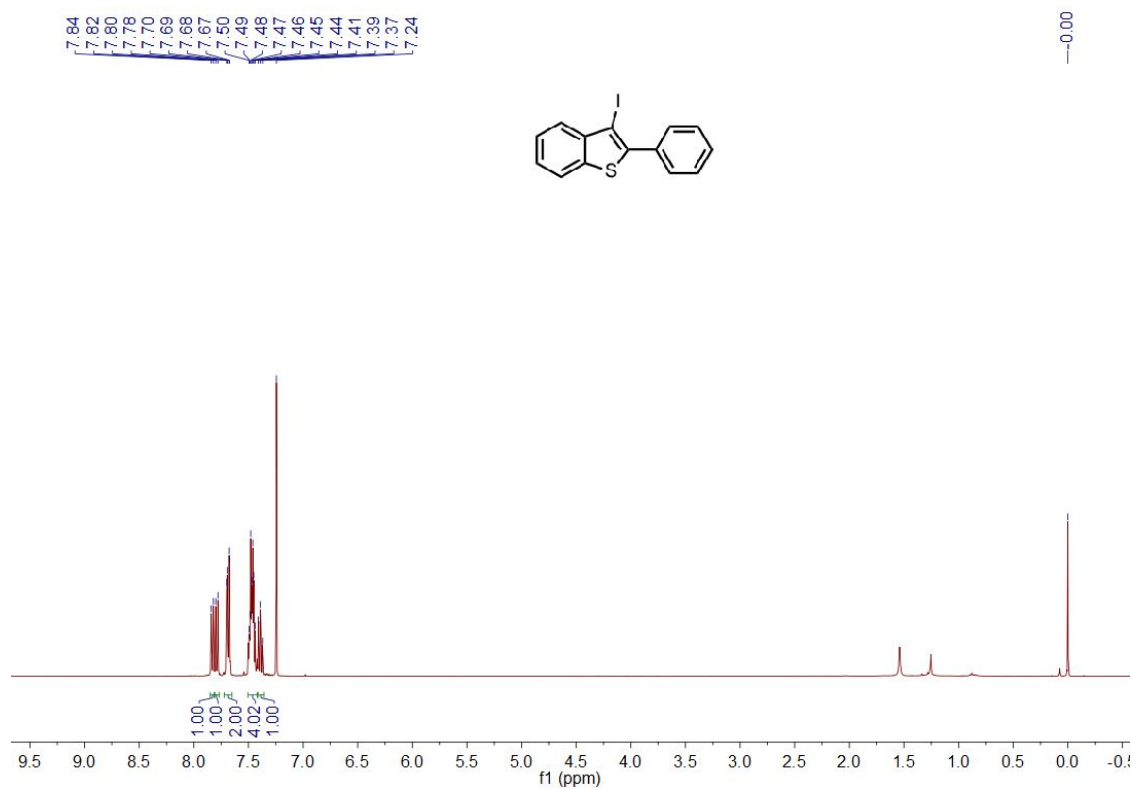
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64 – 7.57 (m, 2H), 7.50 (d,  $J$  = 7.4 Hz, 1H), 7.44 (d,  $J$  = 8.0 Hz, 1H), 7.29 – 7.19 (m, 2H), 7.19 – 7.12 (m, 1H), 7.09 (d,  $J$  = 7.5 Hz, 1H), 2.35 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  156.14, 154.88, 138.47, 130.42, 129.41, 129.29, 128.72, 125.56, 124.19, 122.91, 122.17, 120.87, 111.16, 101.21, 21.52. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{15}\text{H}_{12}\text{O}$   $[\text{M}+\text{H}]^+$ : 209.0961, found: 209.0967.



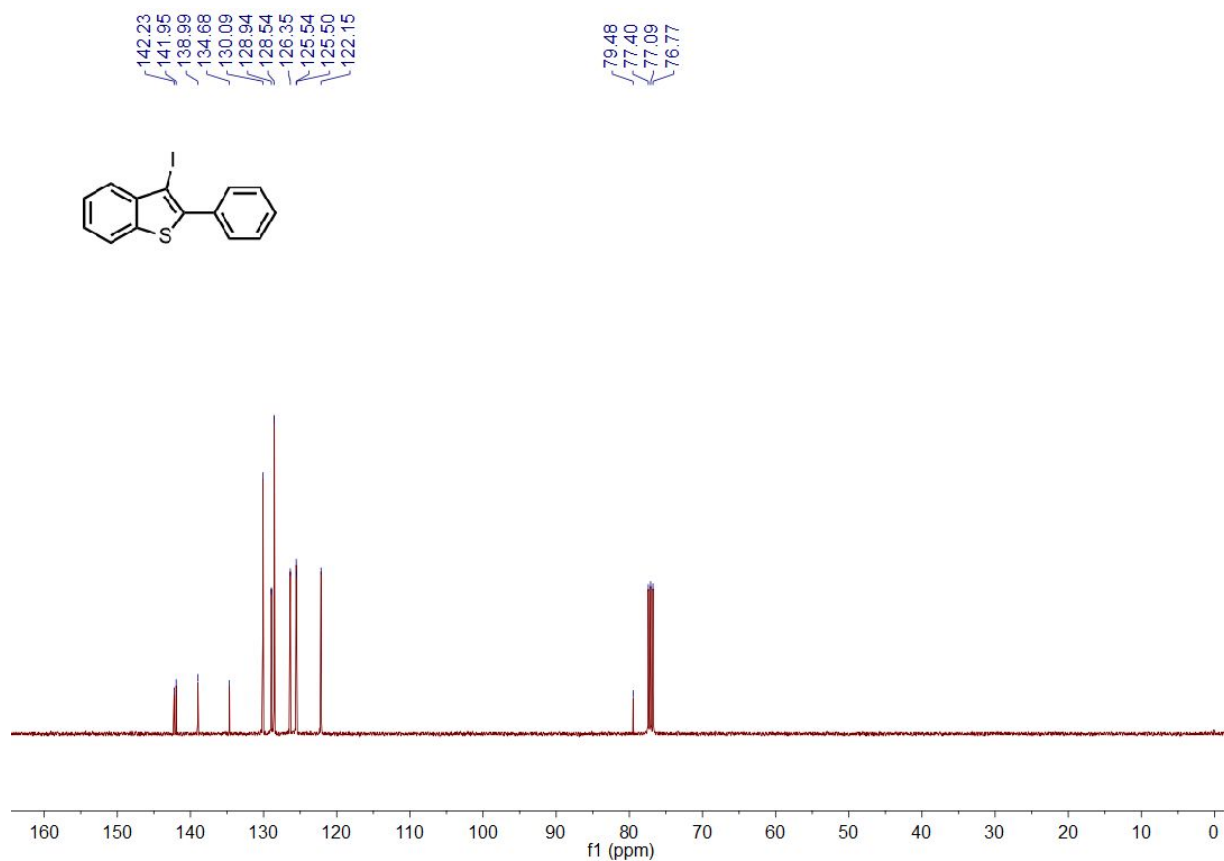
(2-Bromoethene-1,1-diyl) dibenzene (**9**)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44 – 7.33 (m, 3H), 7.33 – 7.27 (m, 5H), 7.22 (d,  $J$  = 2.3 Hz, 2H), 6.78 (s, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  146.83, 140.70, 139.07, 129.65, 128.42, 128.22, 128.11, 127.97, 127.61, 105.17. HRMS (ESI-TOF)  $m/z$  Calcd for  $\text{C}_{14}\text{H}_{11}\text{Br}$   $[\text{M}+\text{Na}]^+$ : 280.9936, found: 280.9924.

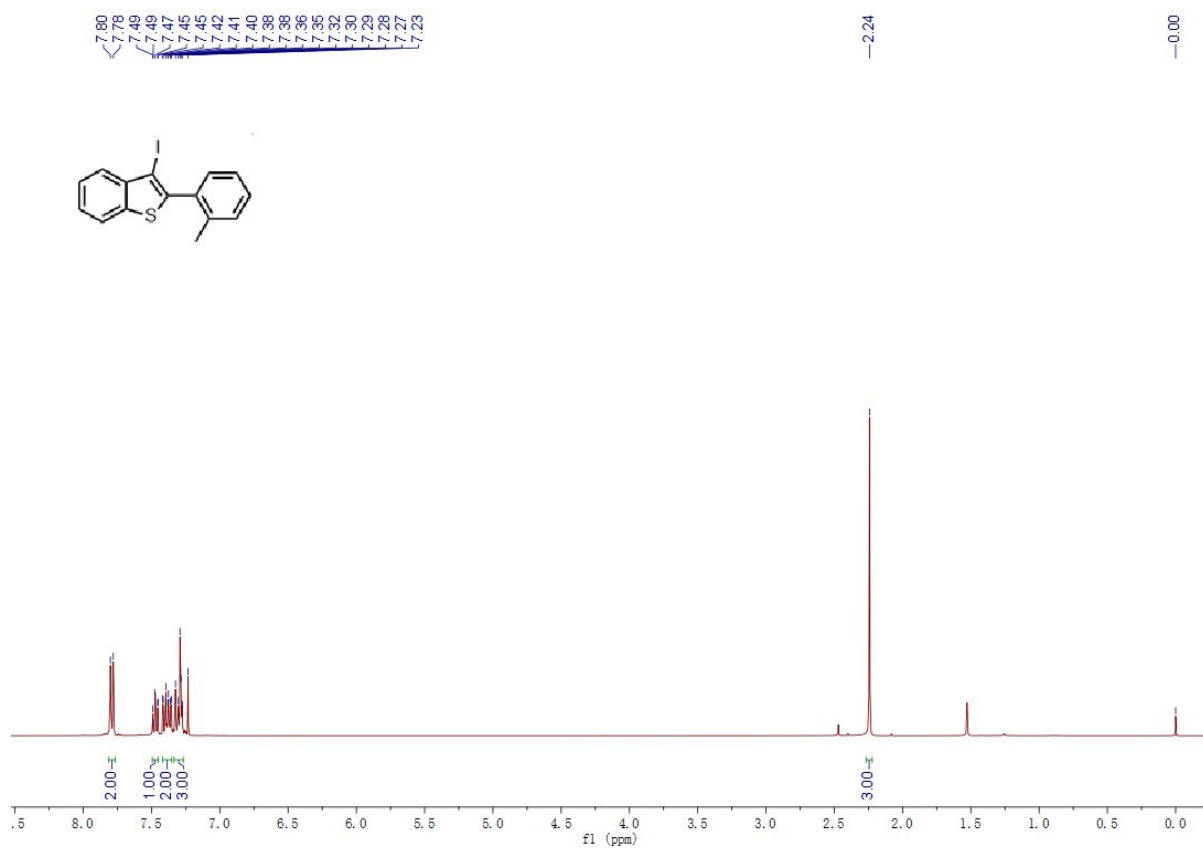
## 7. $^1\text{H}$ NMR, $^{19}\text{F}$ NMR and $^{13}\text{C}$ NMR spectra



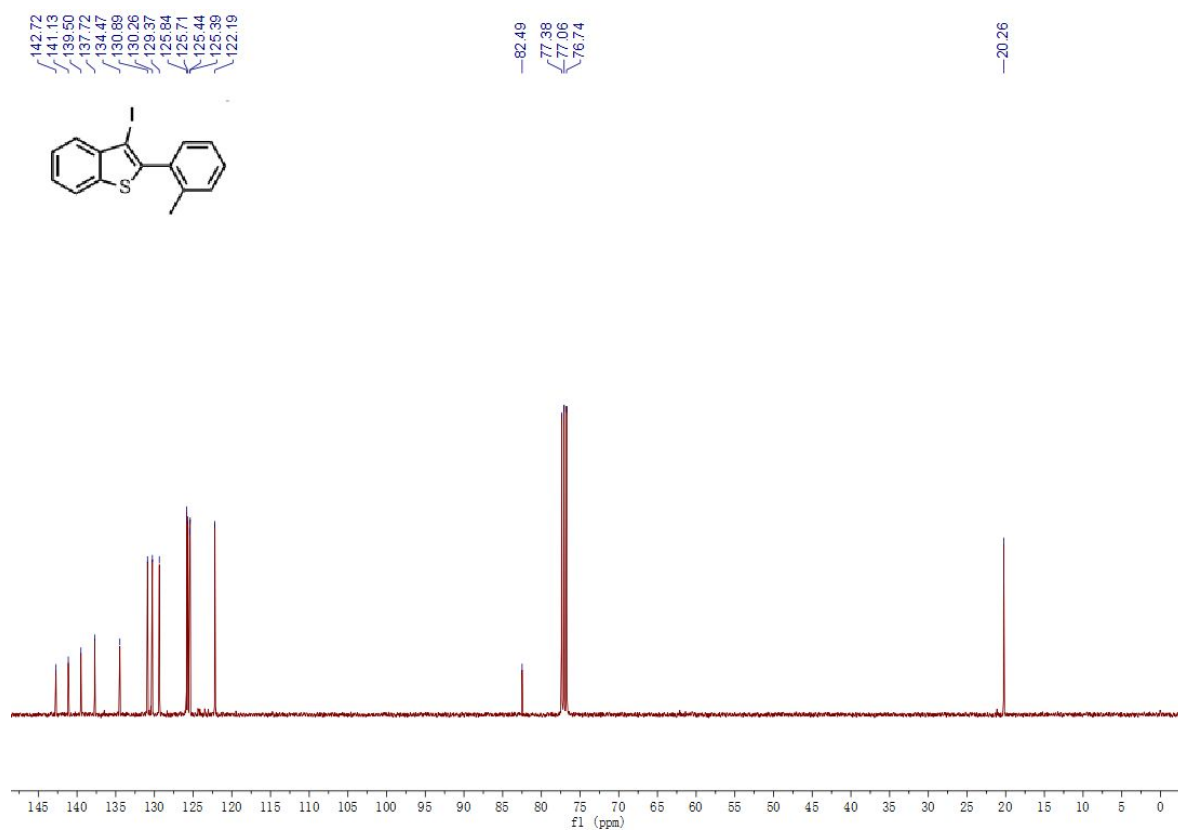
**Figure S8.** Copies of  $^1\text{H}$  NMR Spectrum for Compound **3aa** (400 Hz,  $\text{CDCl}_3$ )



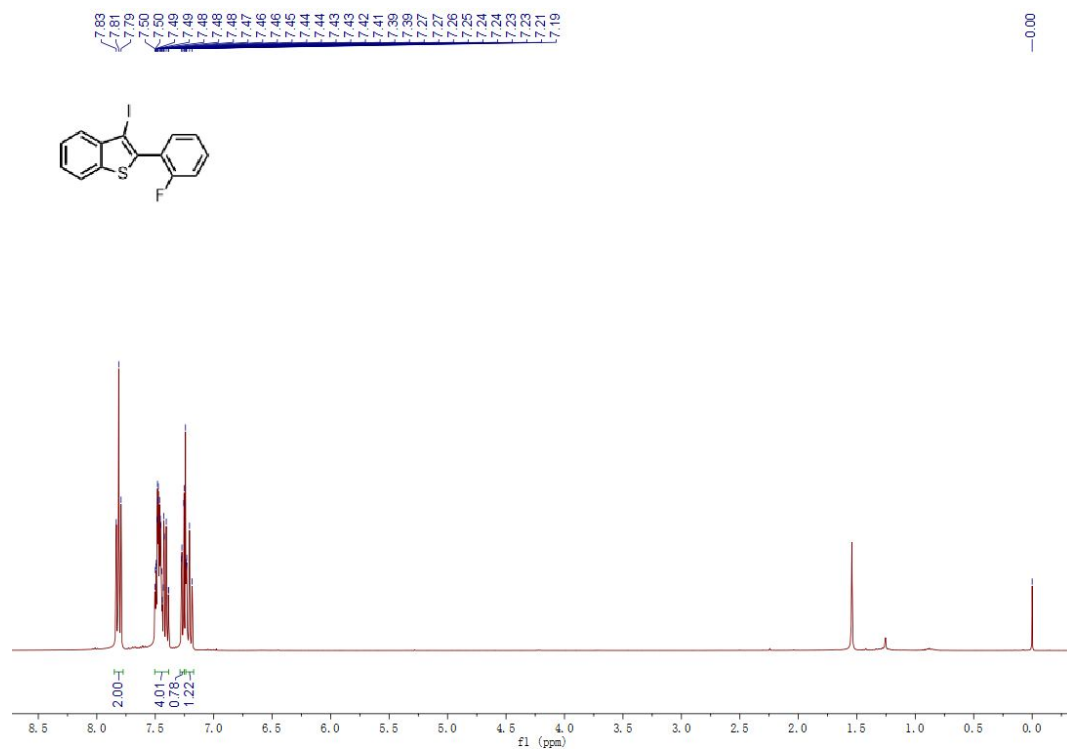
**Figure S9.** Copies of  $^{13}\text{C}$  NMR Spectrum for Compound **3aa** (100 Hz,  $\text{CDCl}_3$ )



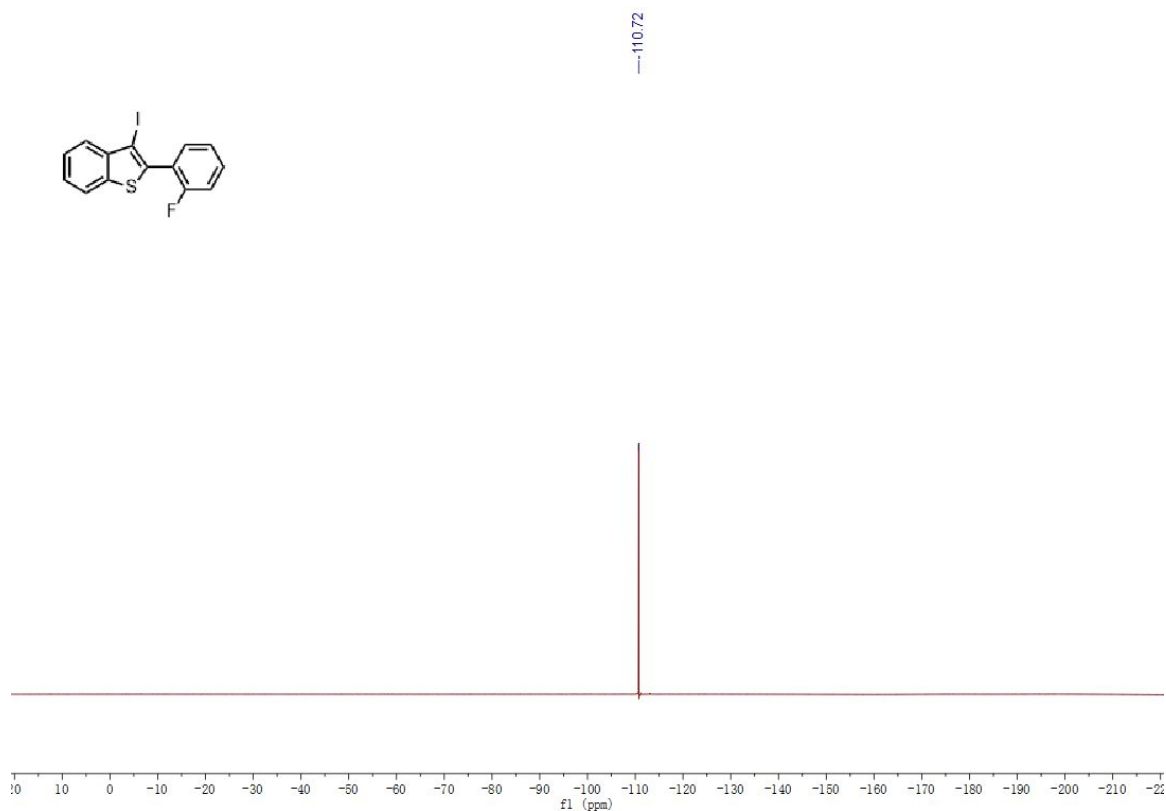
**Figure S10.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ab** (400 Hz, CDCl<sub>3</sub>)



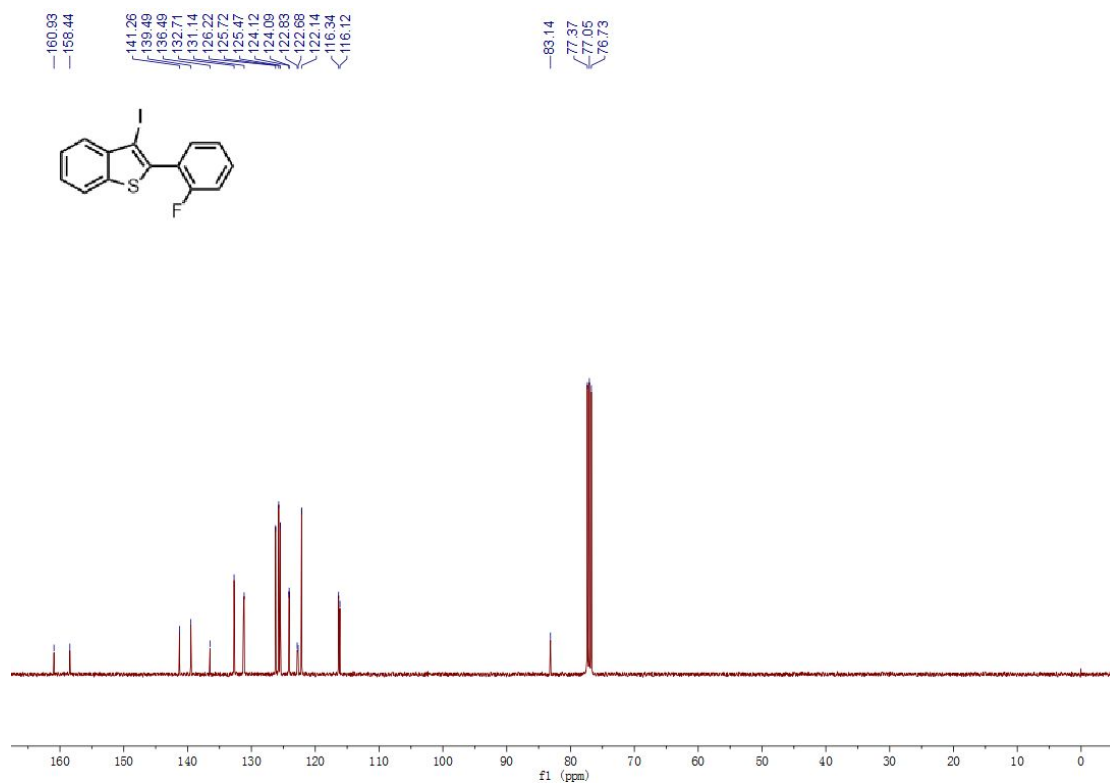
**Figure S11.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ab** (100 Hz, CDCl<sub>3</sub>)



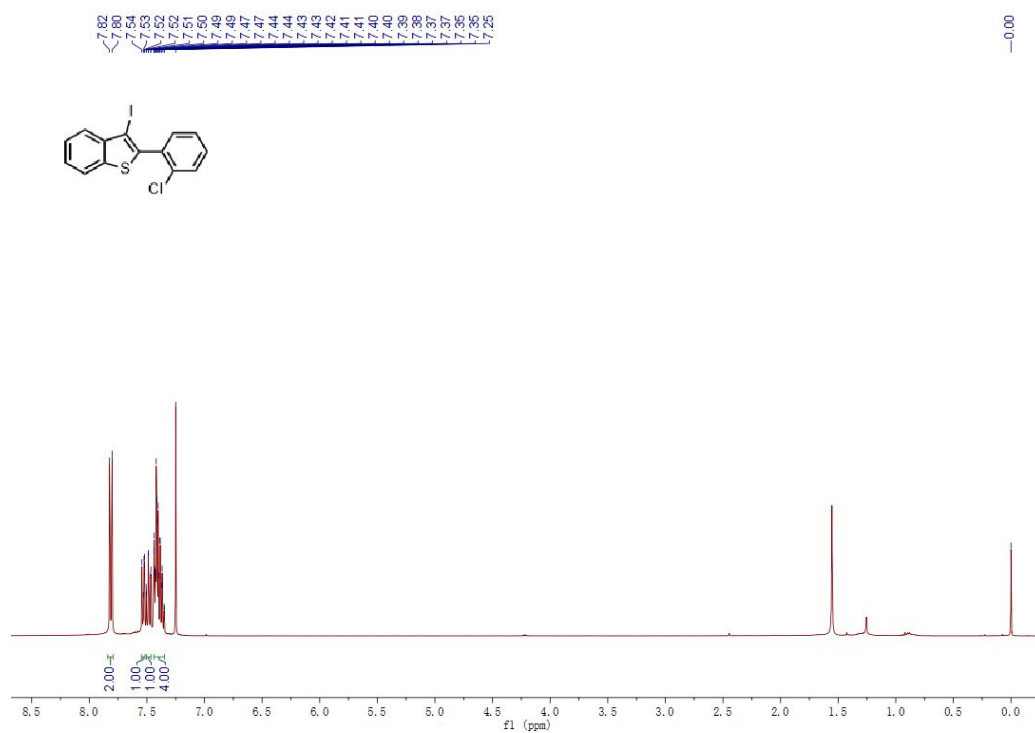
**Figure S12.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ac** (400 Hz, CDCl<sub>3</sub>)



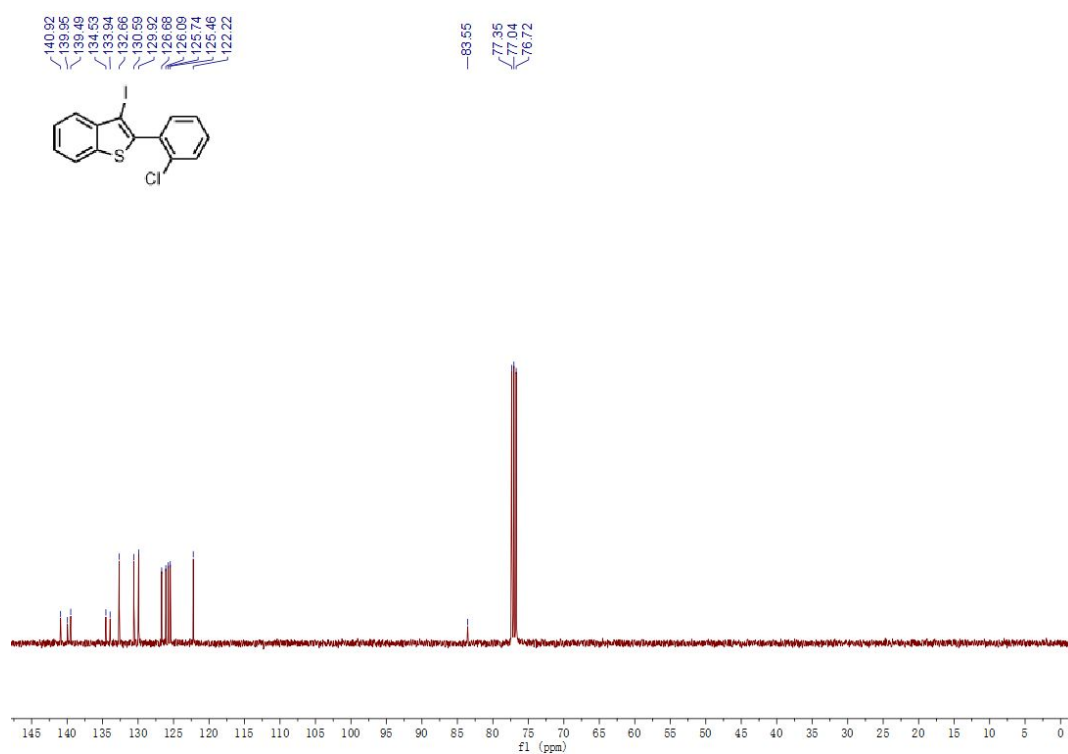
**Figure S13.** Copies of <sup>19</sup>F NMR Spectrum for Compound **3ac** (376 Hz, CDCl<sub>3</sub>)



**Figure S14.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ac** (100 Hz, CDCl<sub>3</sub>)

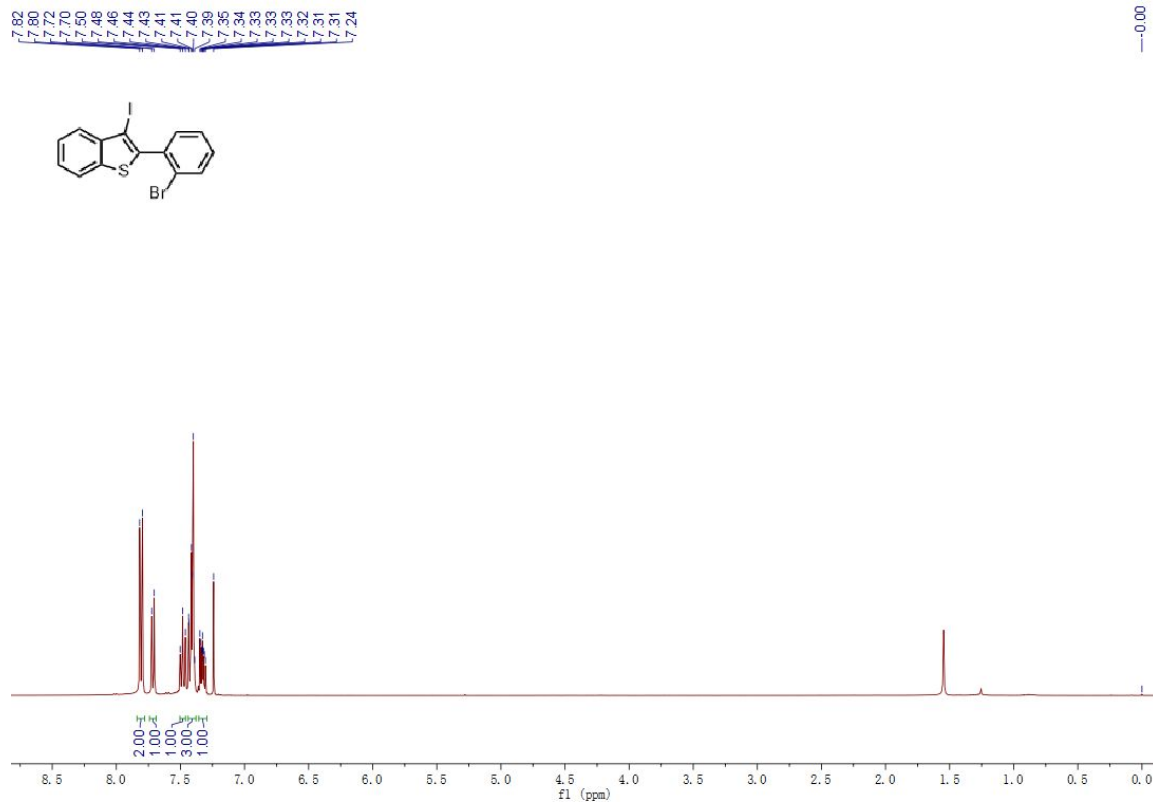


**Figure S15.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ad** (400 Hz, CDCl<sub>3</sub>)

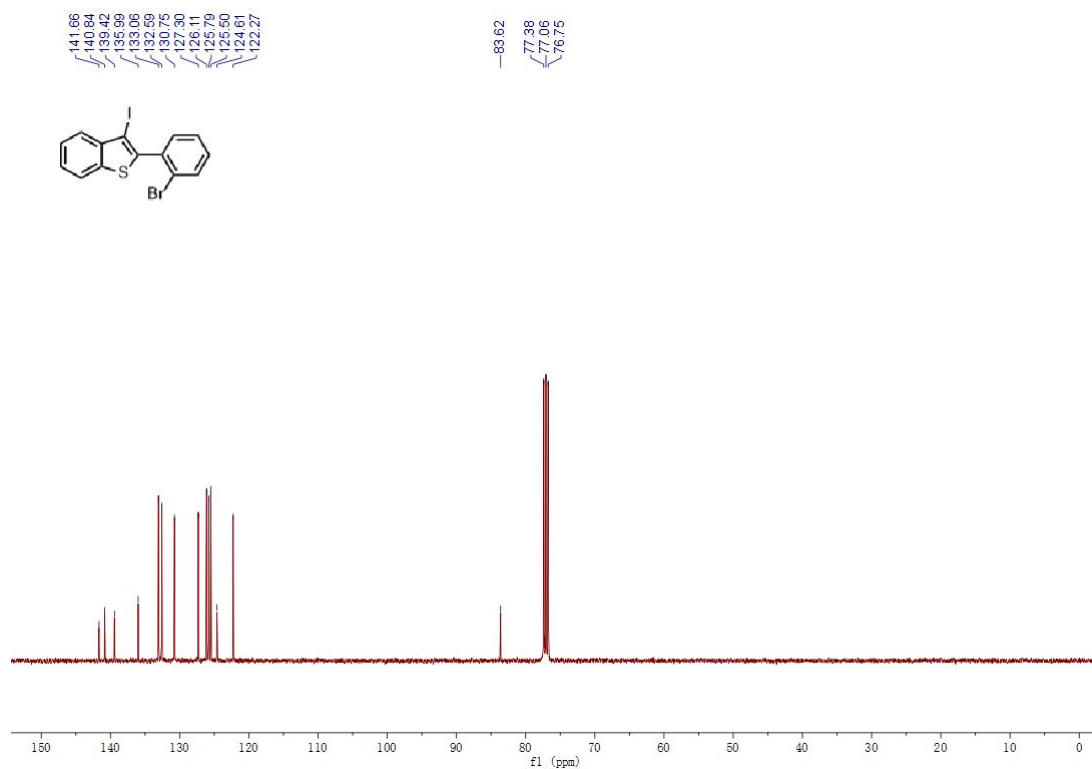


**Figure S16.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ad** (100 Hz, CDCl<sub>3</sub>)

2-(2-Bromophenyl)-3-iodobenzo [*b*] thiophene (**3ae**)

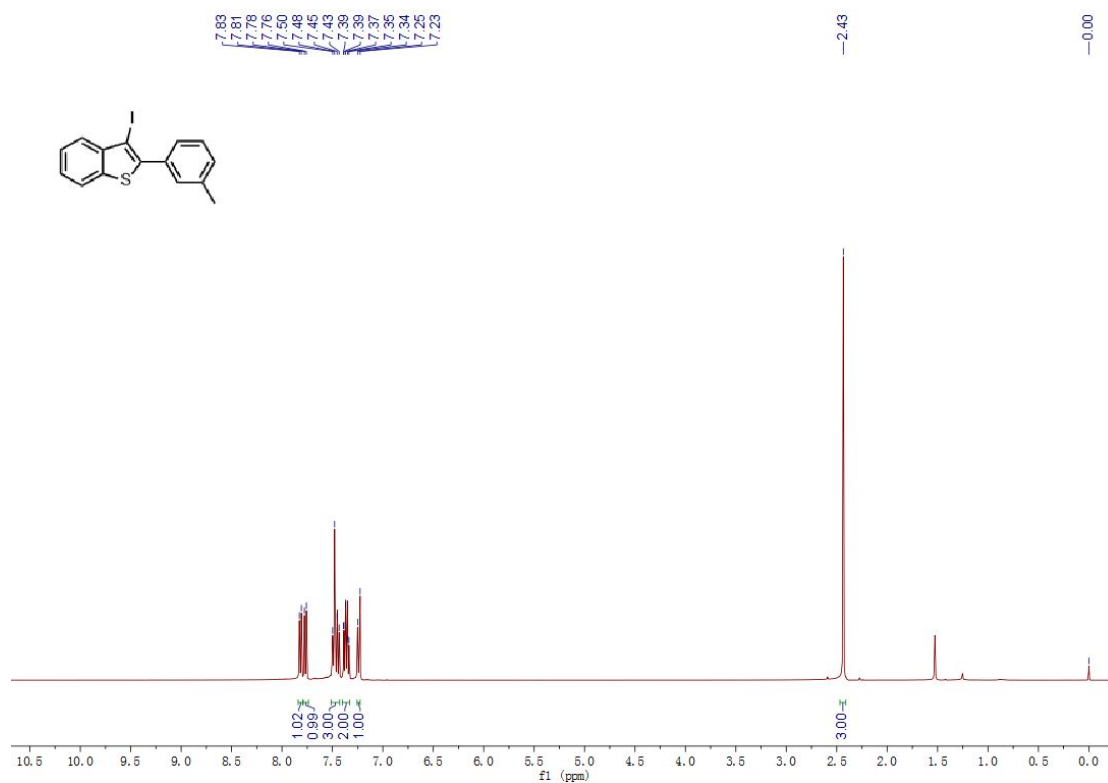


**Figure S17.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ae** (400 Hz, CDCl<sub>3</sub>)

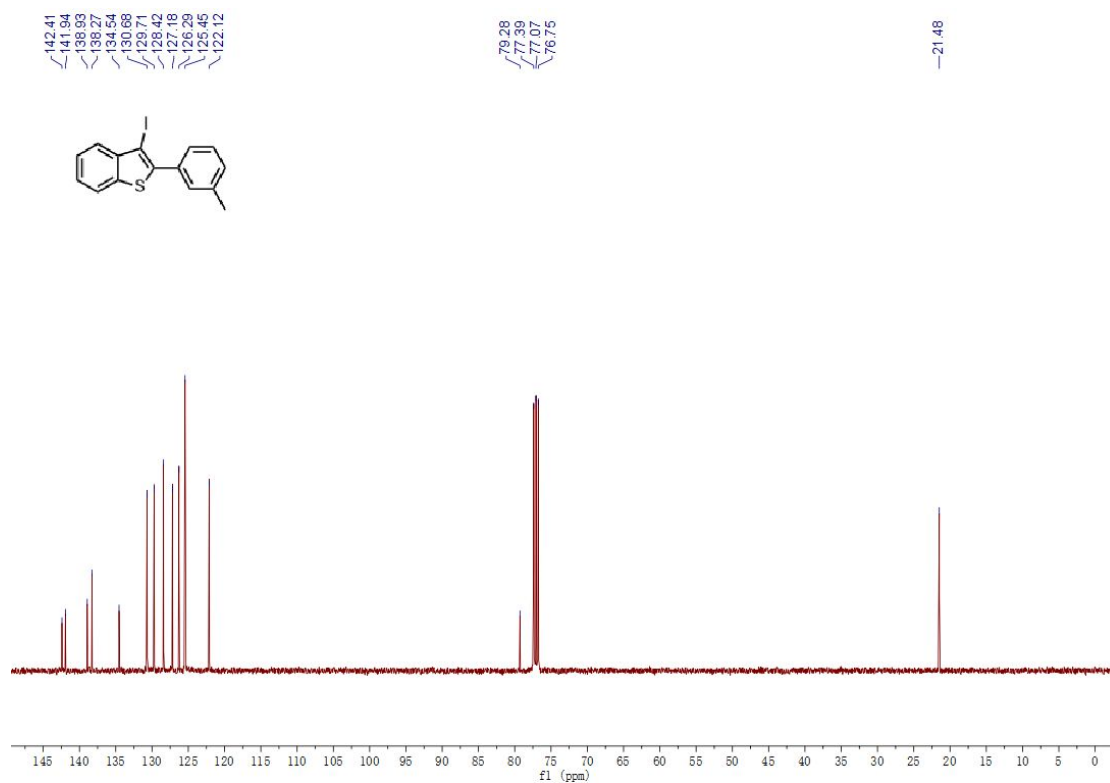


**Figure S18.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ae** (100 Hz, CDCl<sub>3</sub>)

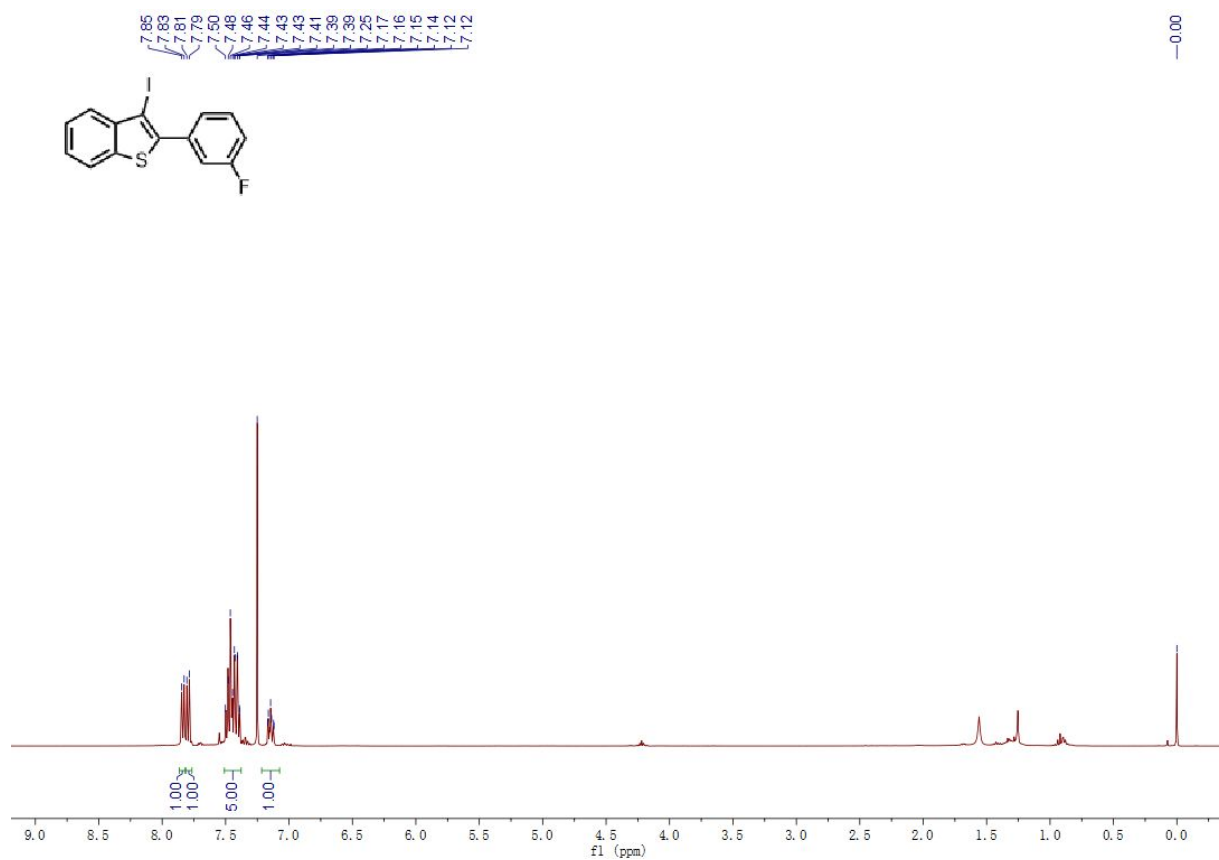
3-Iodo-2-(*m*-tolyl) benzo [*b*] thiophene (**3af**)



**Figure S19.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3af** (400 Hz, CDCl<sub>3</sub>)

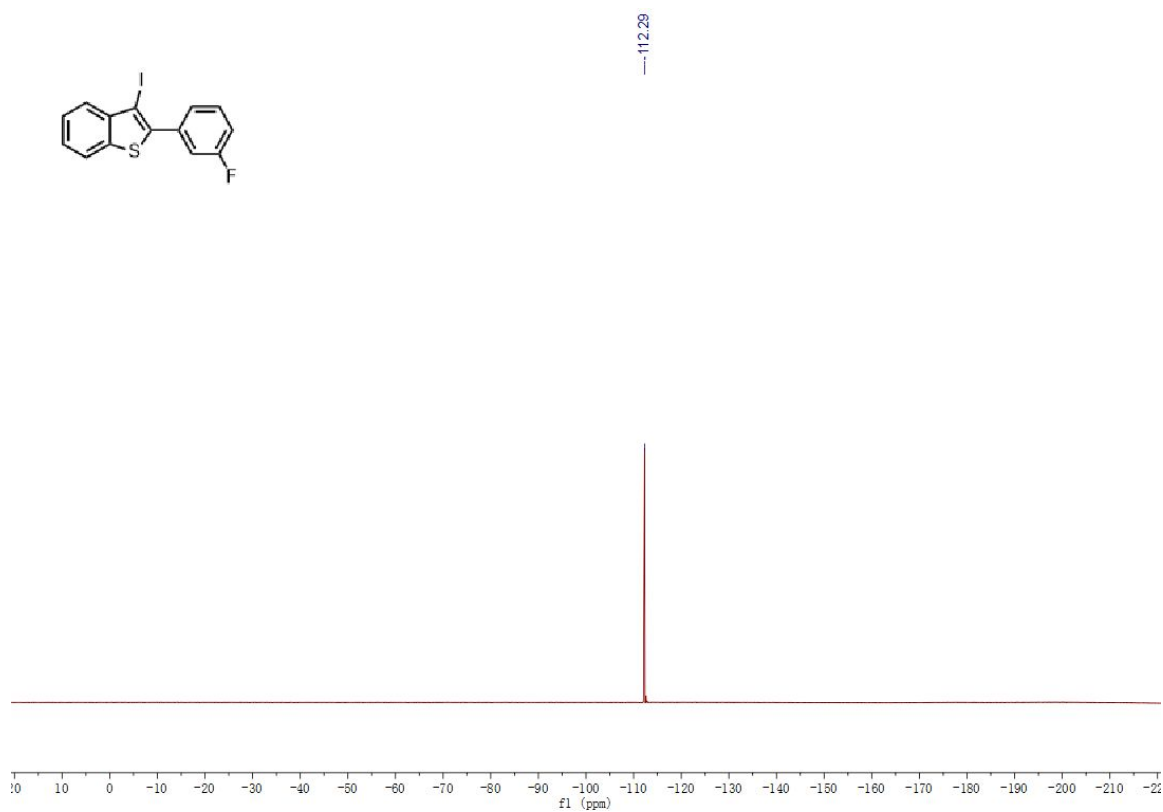


**Figure S20.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3af** (100 Hz, CDCl<sub>3</sub>)

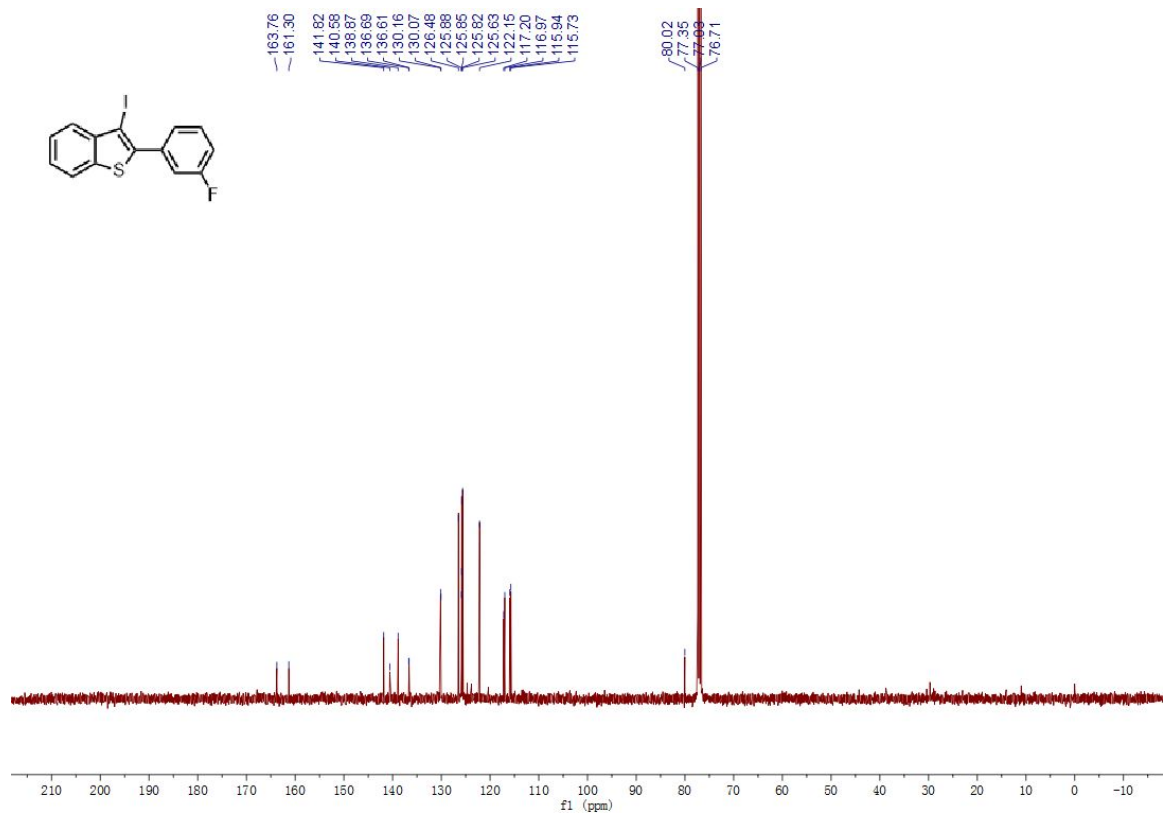


**Figure S21.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ag** (400 Hz, CDCl<sub>3</sub>)

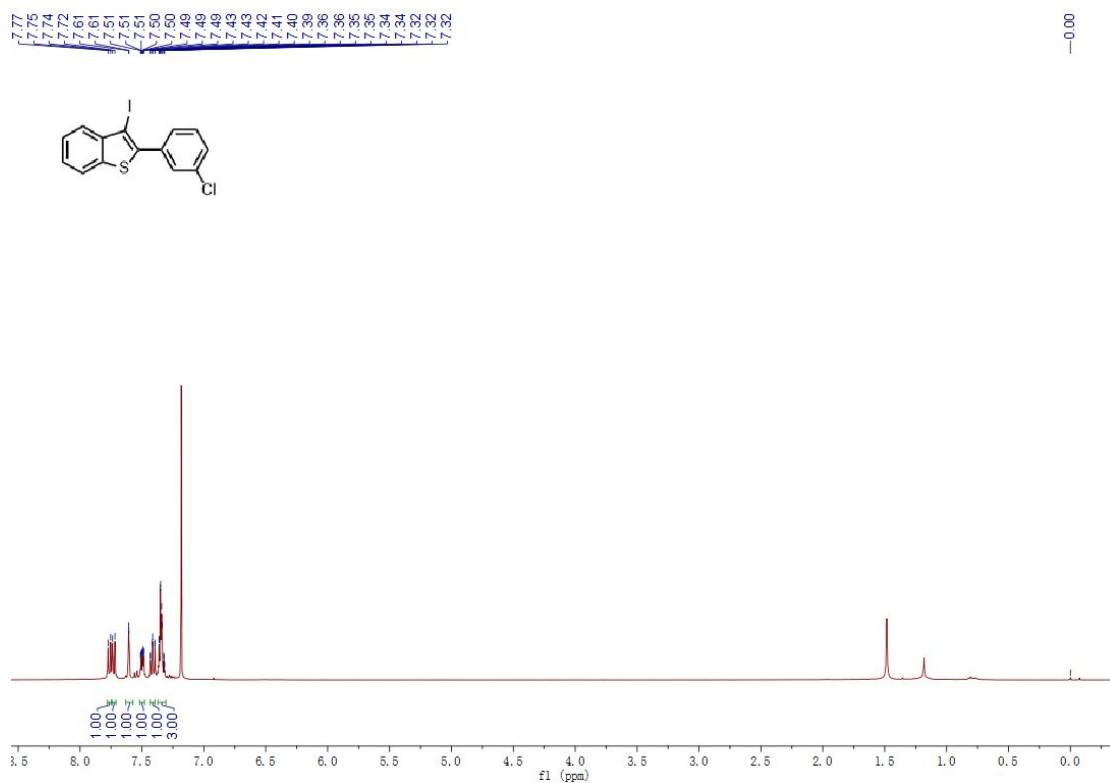




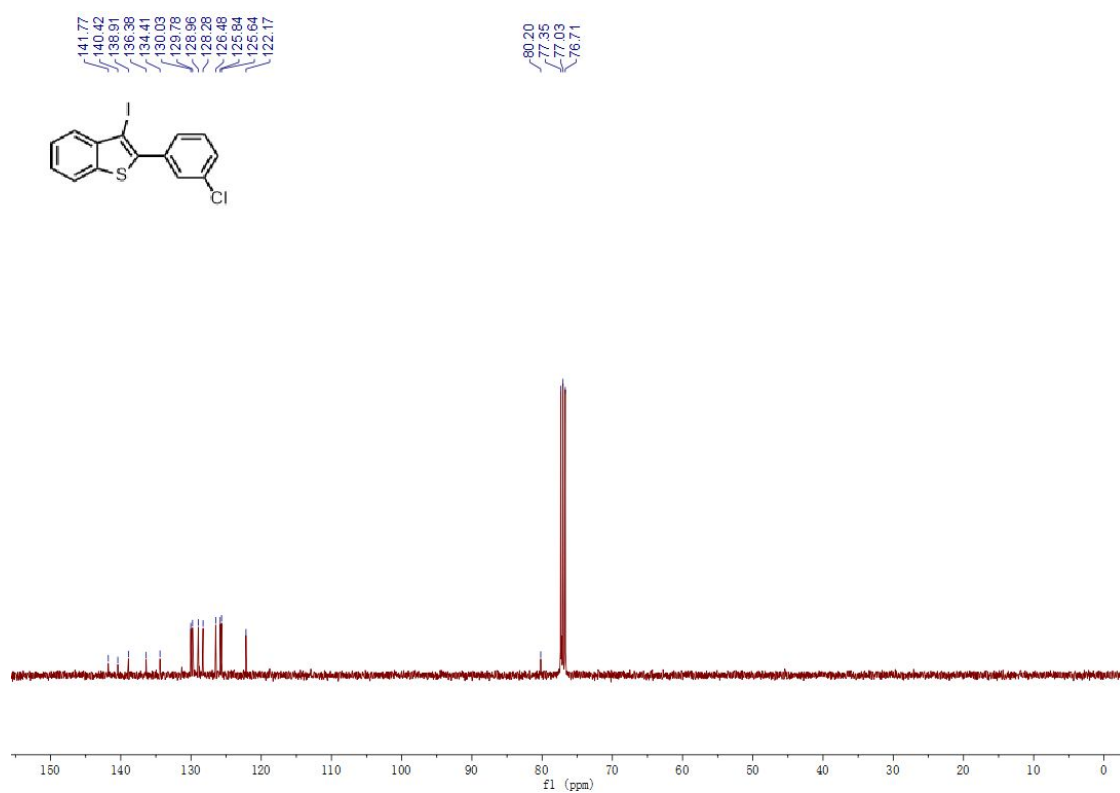
**Figure S22.** Copies of <sup>19</sup>F NMR Spectrum for Compound **3ag** (376 Hz, CDCl<sub>3</sub>)



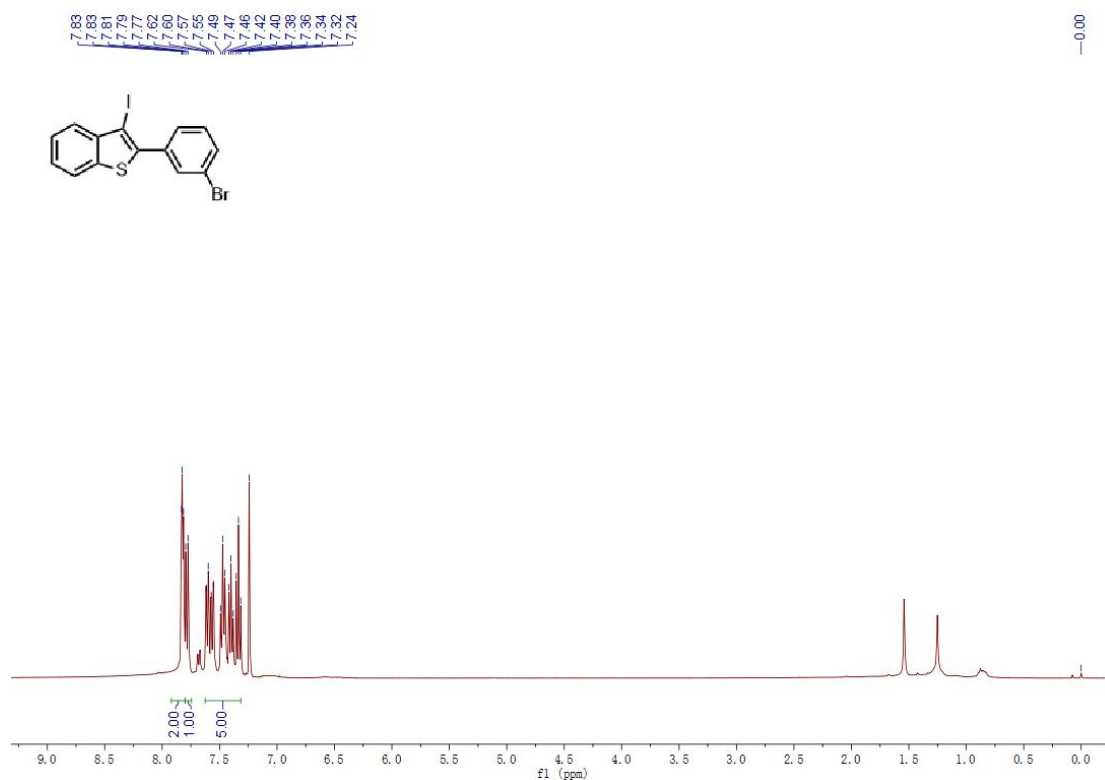
**Figure S23.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ag** (100 Hz, CDCl<sub>3</sub>)



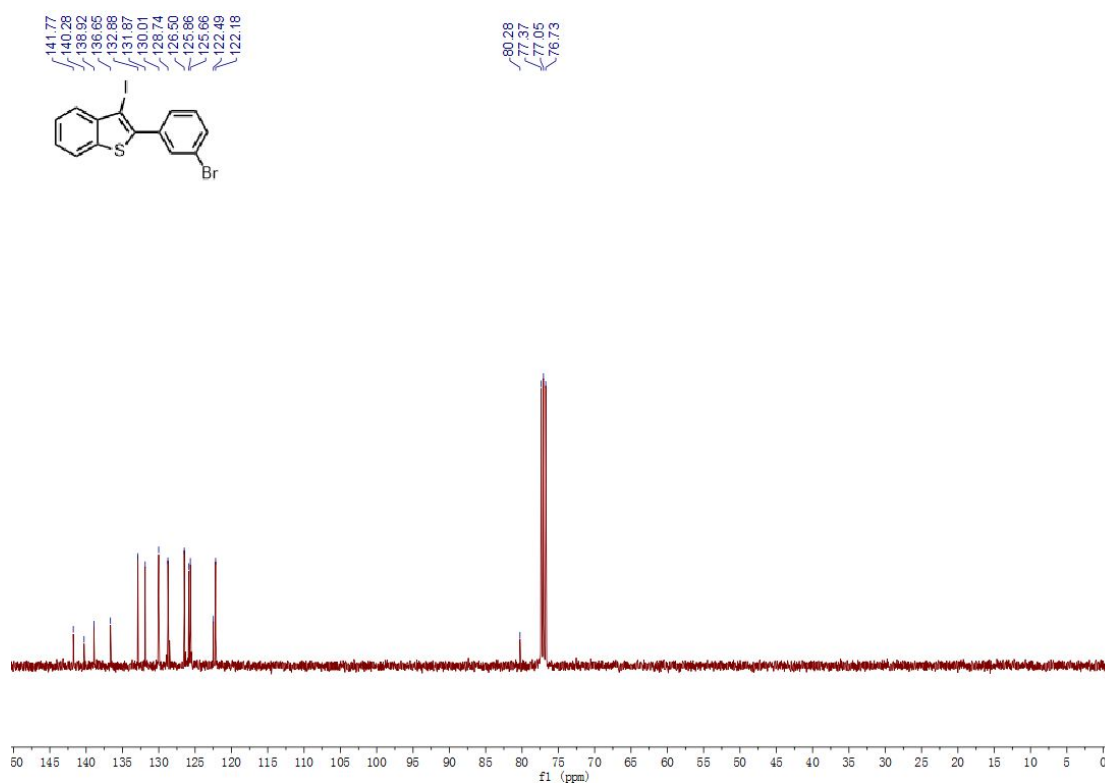
**Figure S24.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ah** (400 Hz, CDCl<sub>3</sub>)



**Figure S25.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ah** (100 Hz, CDCl<sub>3</sub>)



**Figure S26.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ai** (400 Hz, CDCl<sub>3</sub>)



**Figure S27.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ai** (100 Hz, CDCl<sub>3</sub>)

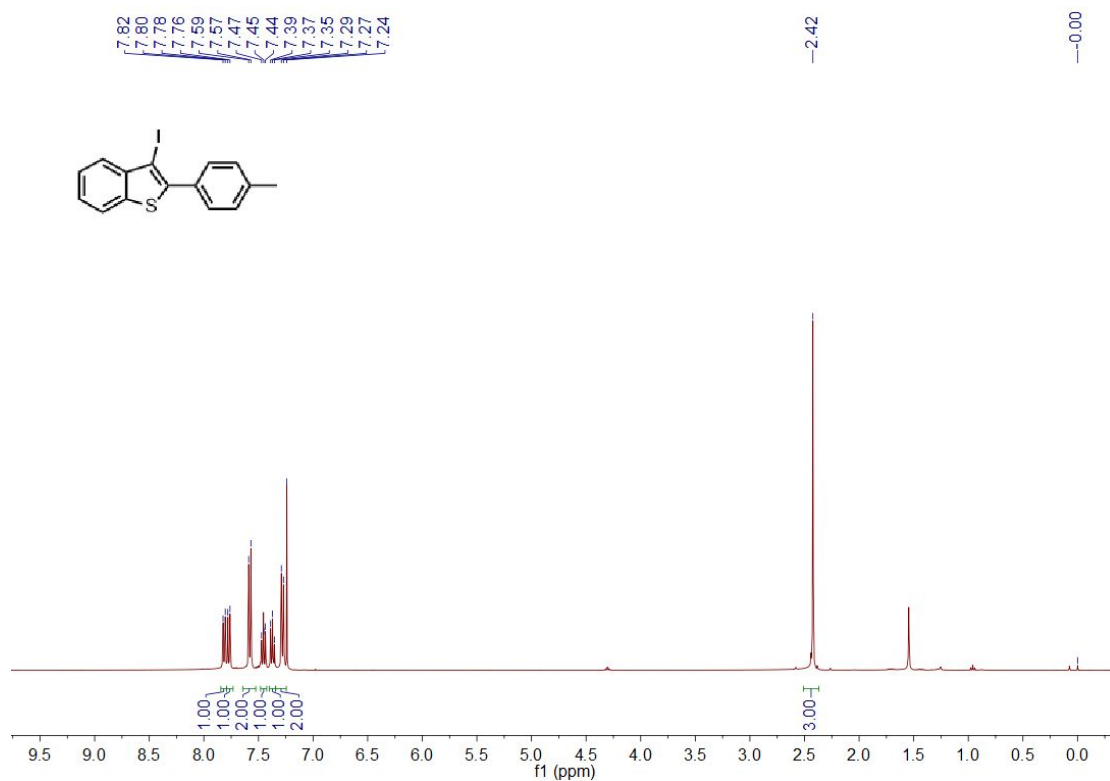


Figure S28. Copies of <sup>1</sup>H NMR Spectrum for Compound **3aj** (400 Hz, CDCl<sub>3</sub>)

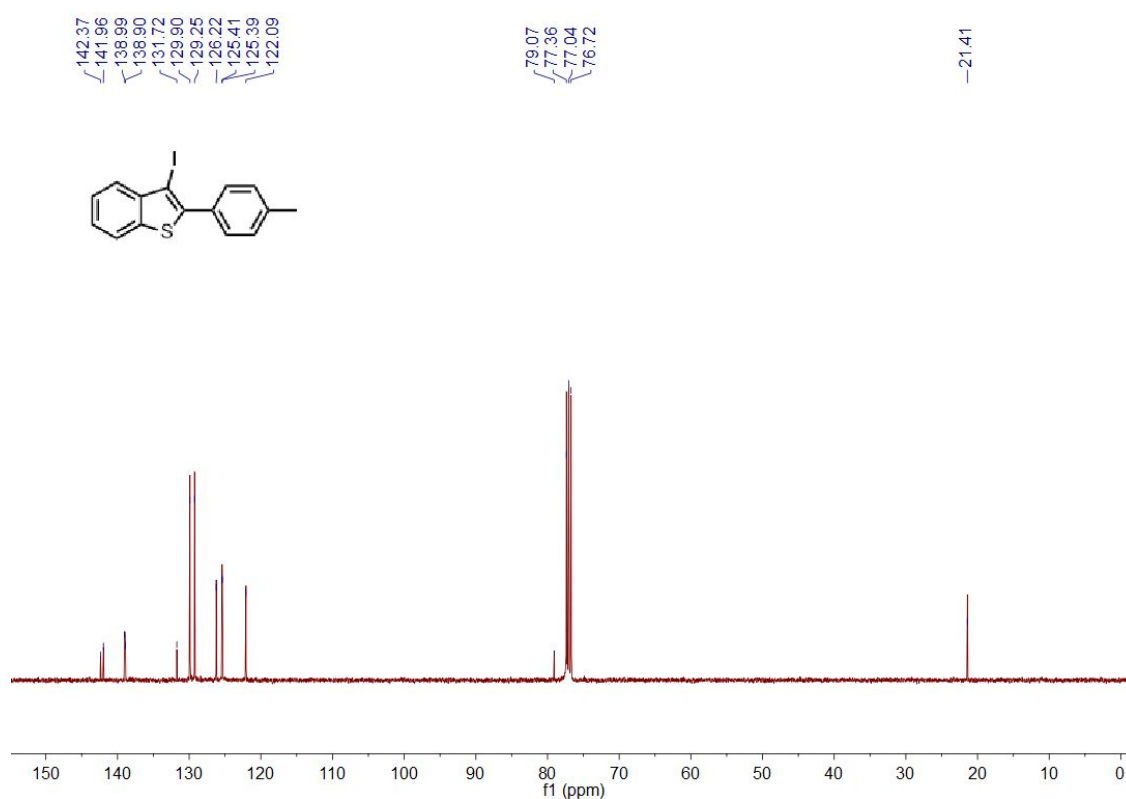
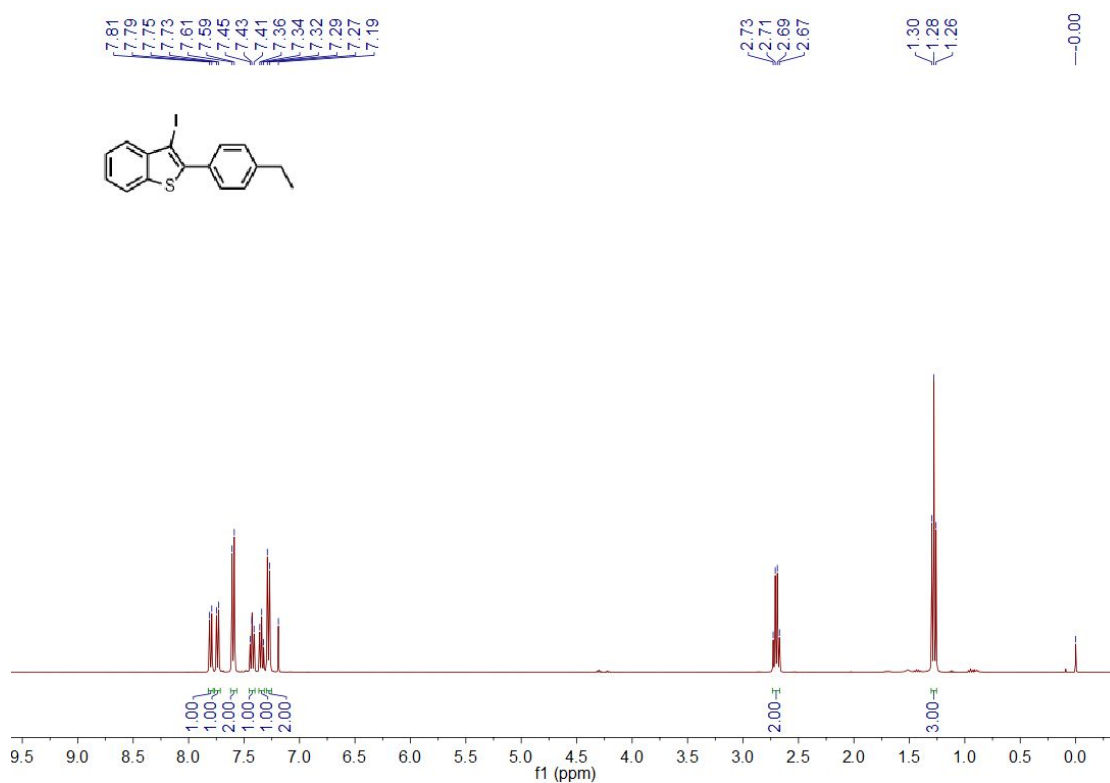
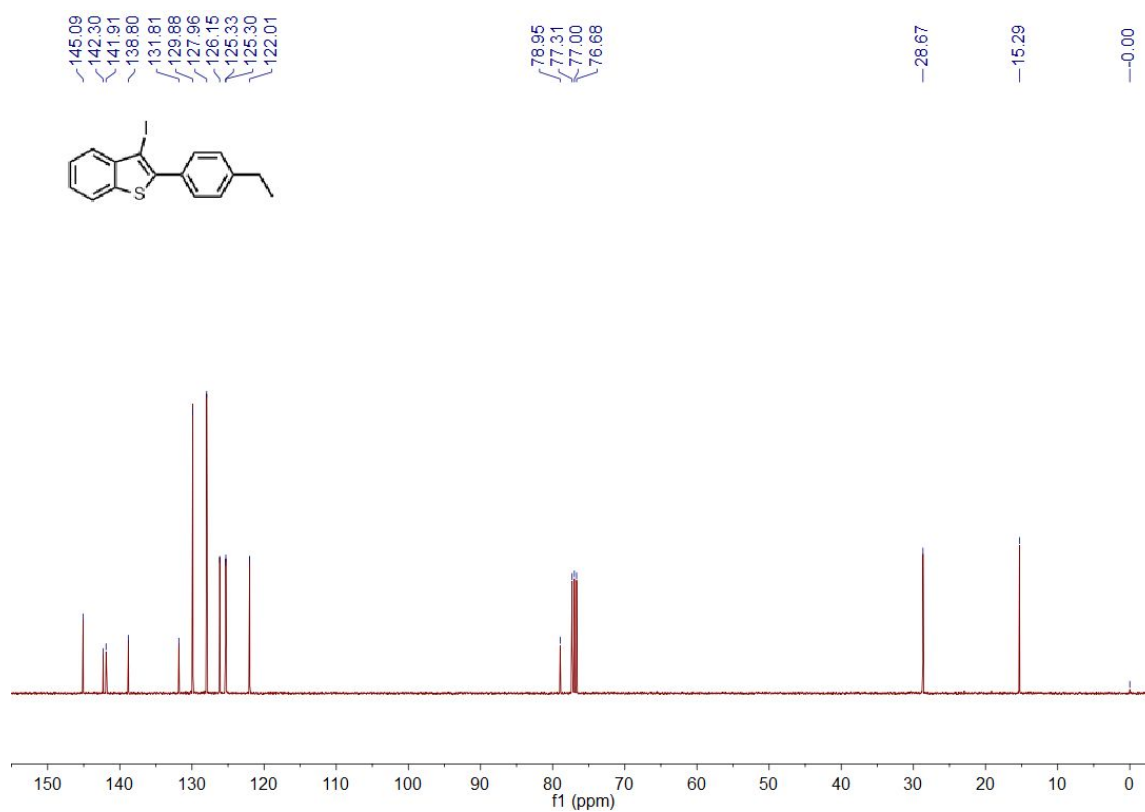


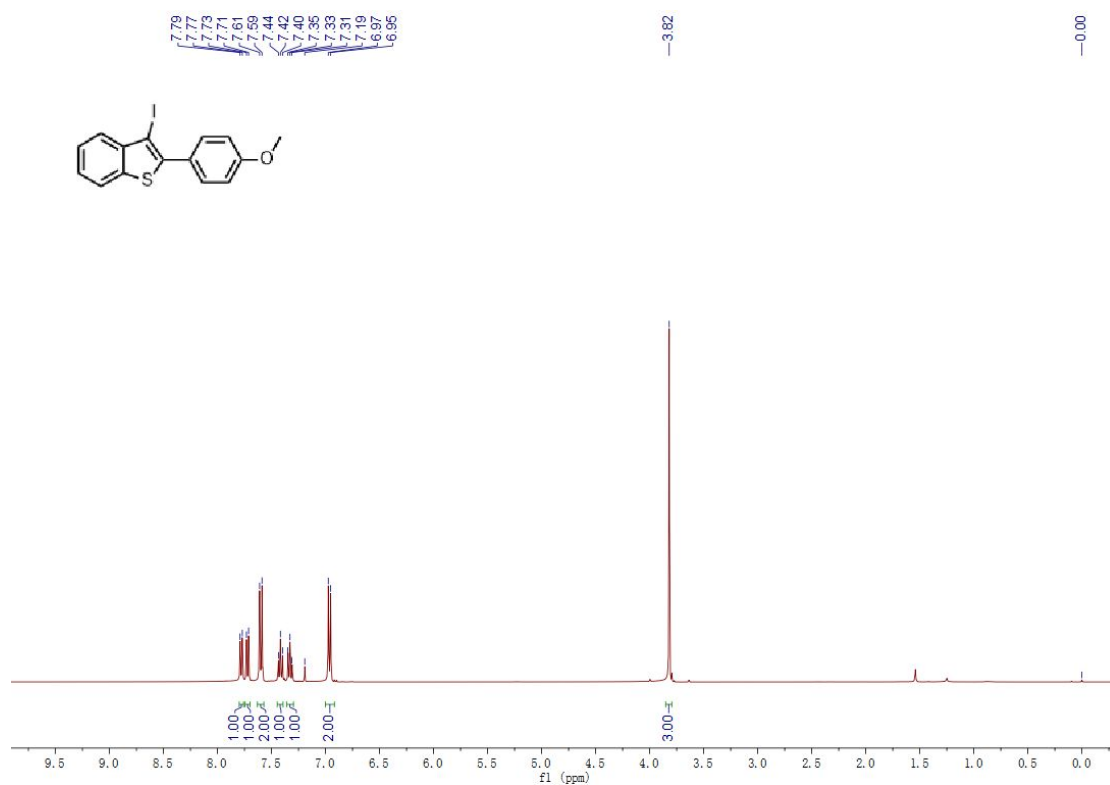
Figure S29. Copies of <sup>13</sup>C NMR Spectrum for Compound **3aj** (100 Hz, CDCl<sub>3</sub>)



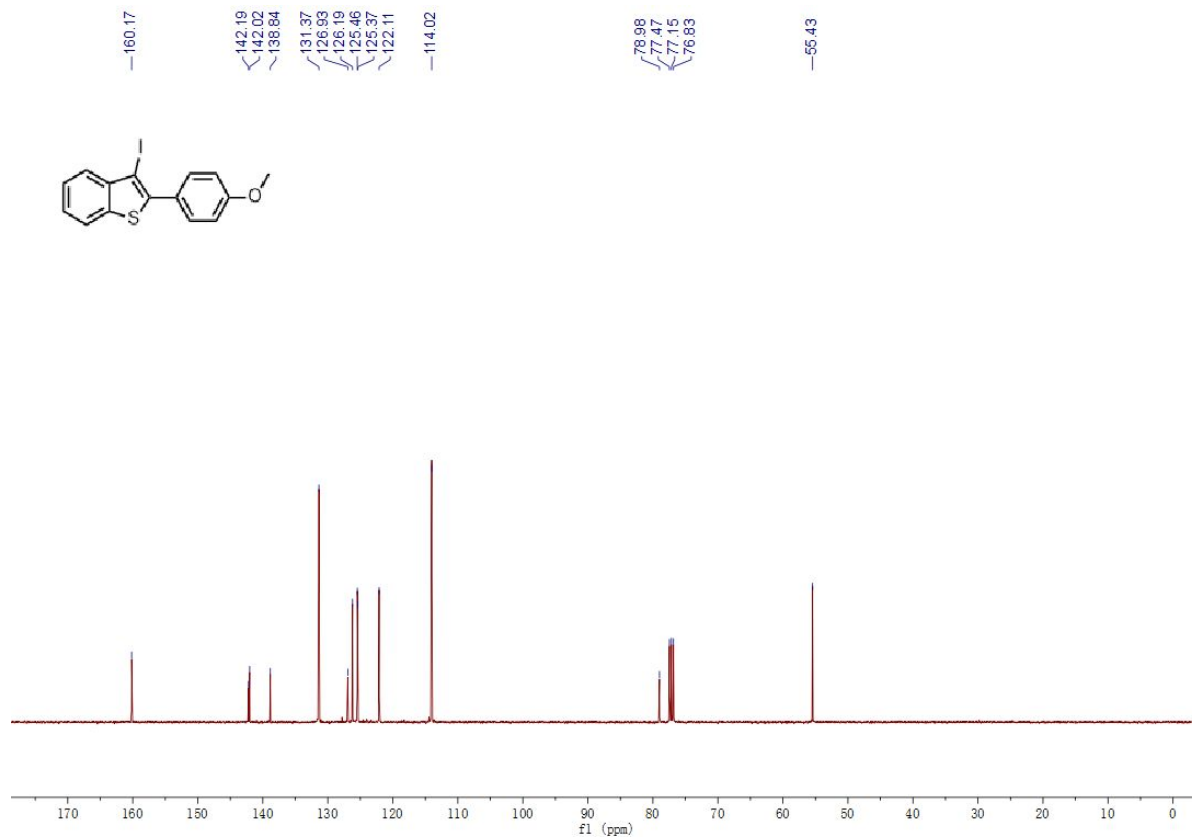
**Figure S30.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ak** (400 Hz, CDCl<sub>3</sub>)



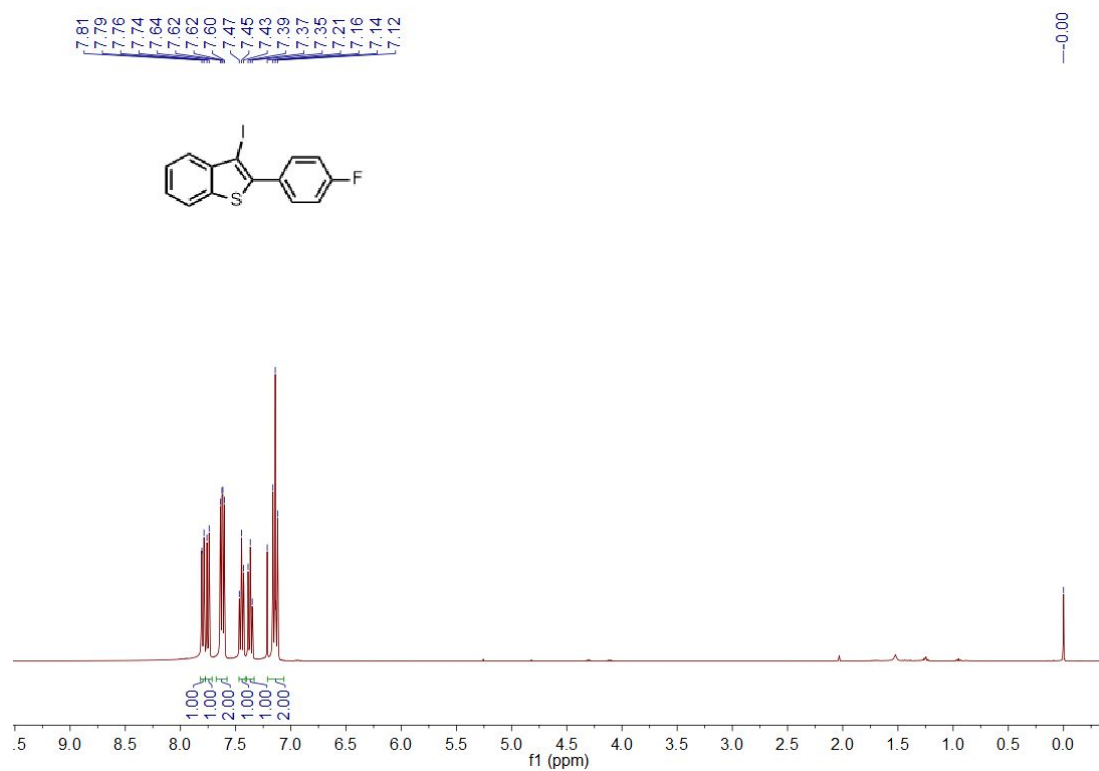
**Figure S31.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ak** (100 Hz, CDCl<sub>3</sub>)



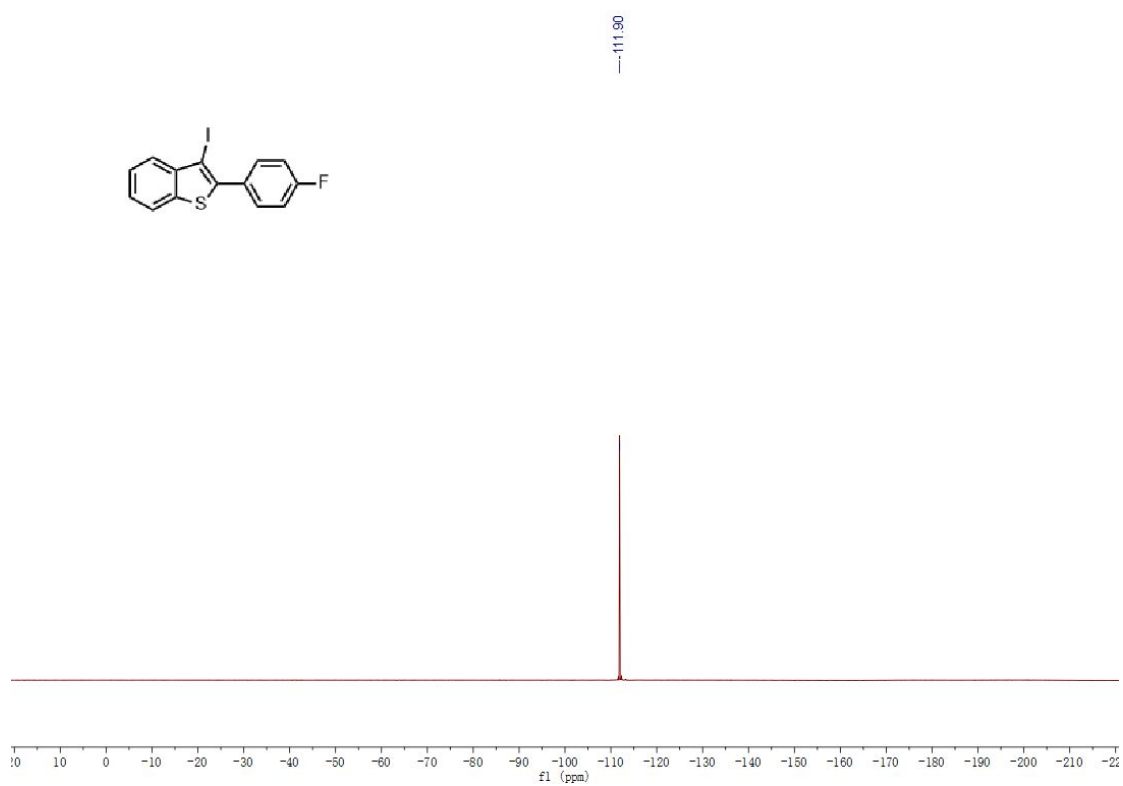
**Figure S32.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3al** (400 Hz, CDCl<sub>3</sub>)



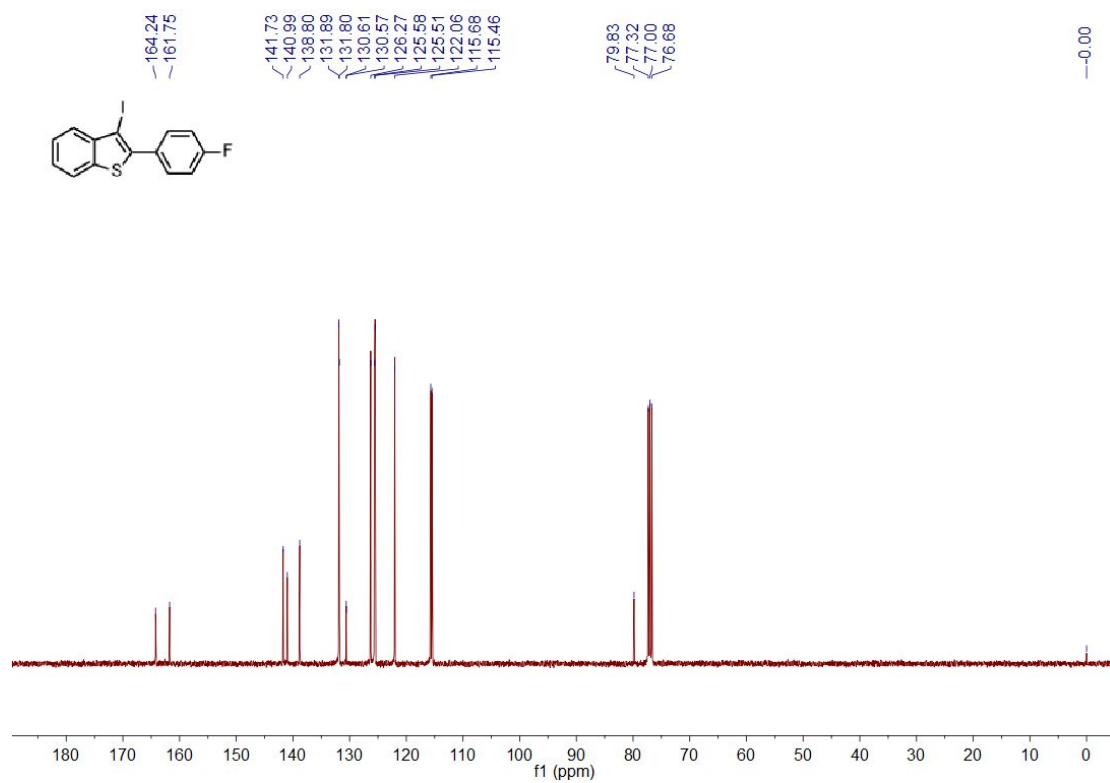
**Figure S33.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3al** (100 Hz, CDCl<sub>3</sub>)



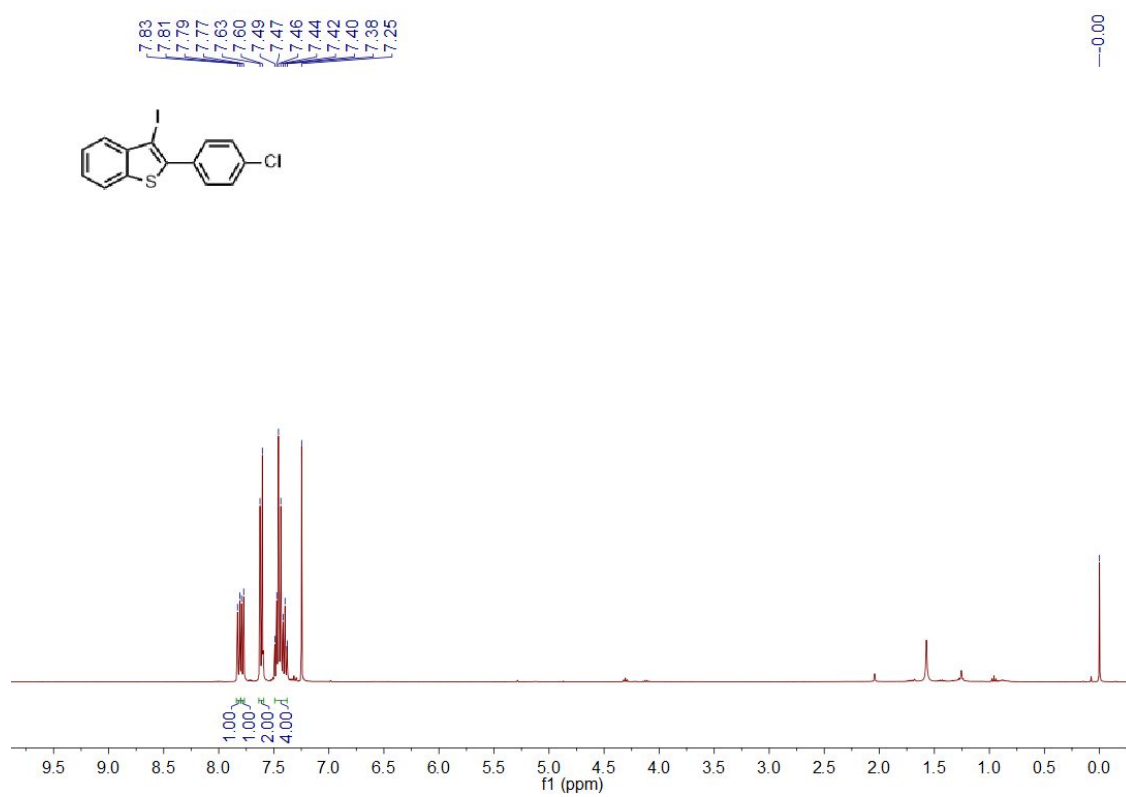
**Figure S34.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3am** (400 Hz, CDCl<sub>3</sub>)



**Figure S35.** Copies of <sup>19</sup>F NMR Spectrum for Compound **3am** (400 Hz, CDCl<sub>3</sub>)

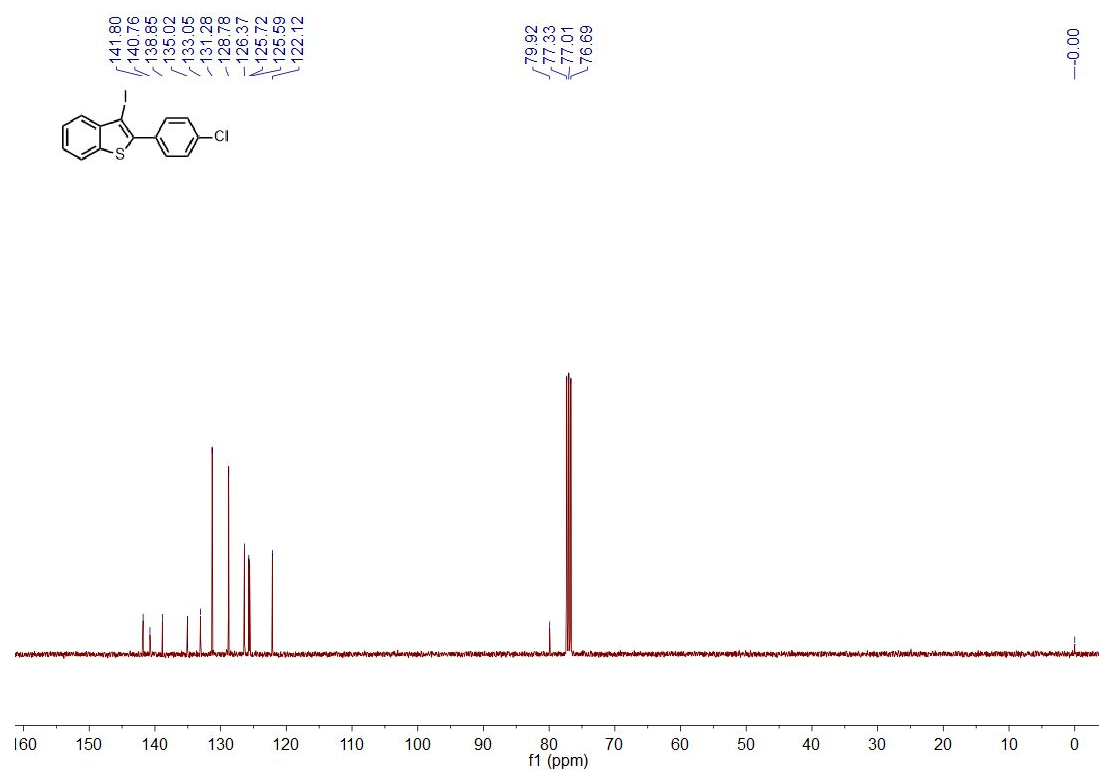


**Figure S36.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3am** (100 Hz, CDCl<sub>3</sub>)

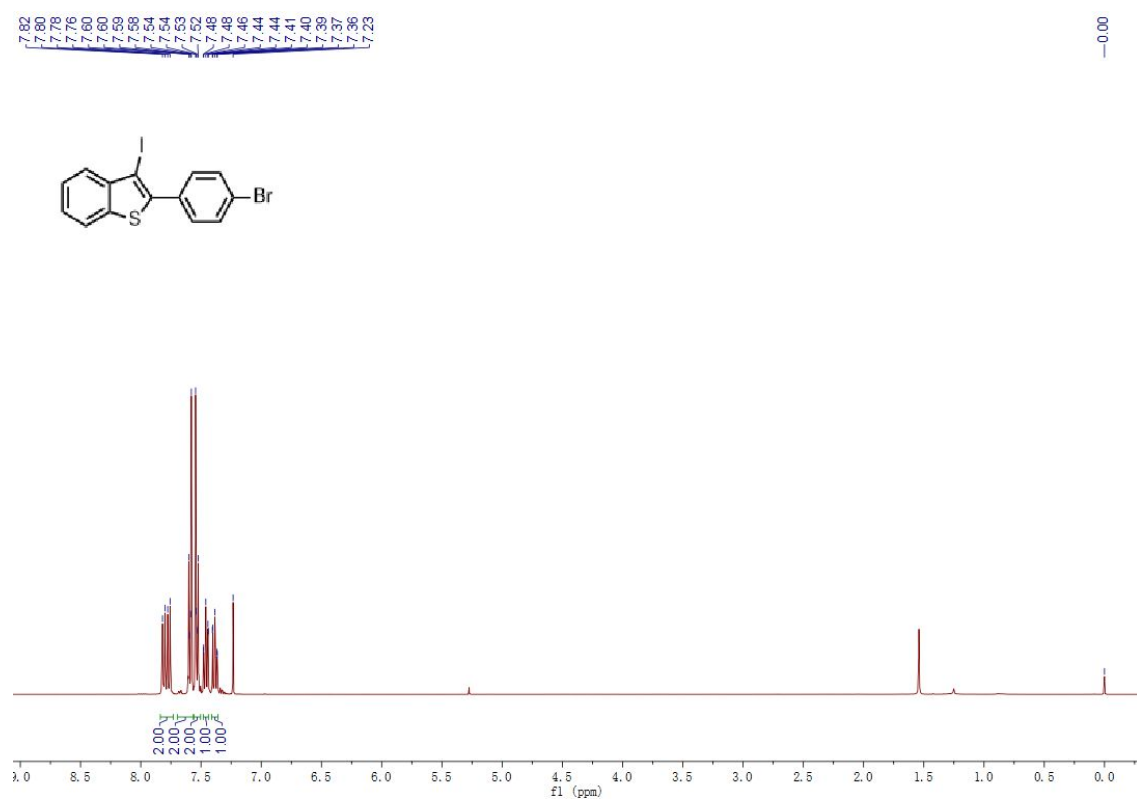


**Figure S37.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3an** (400 Hz, CDCl<sub>3</sub>)

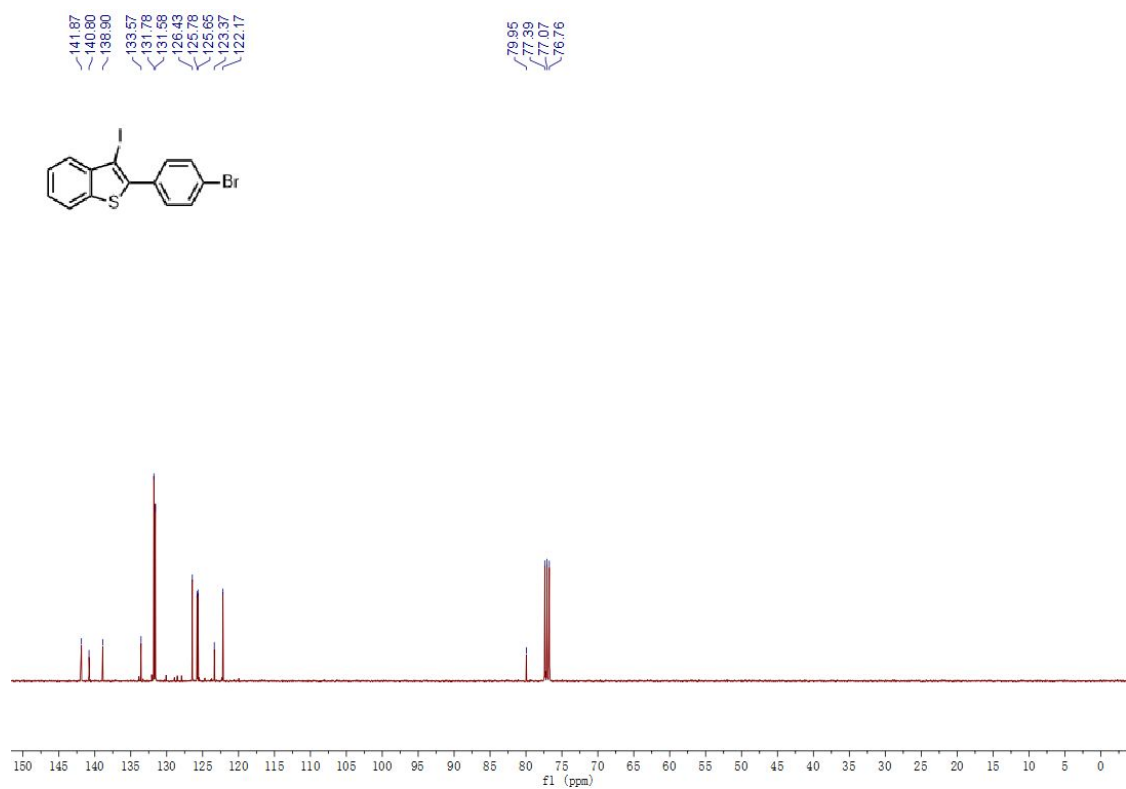




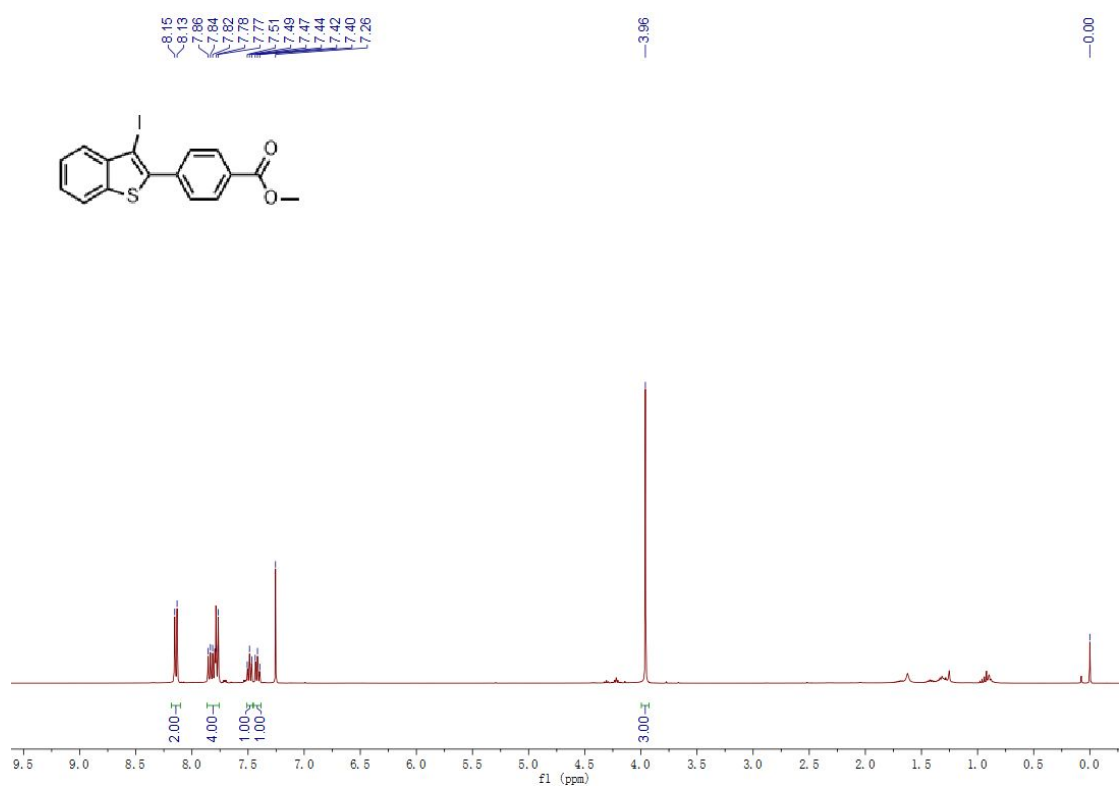
**Figure S38.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3an** (100 Hz, CDCl<sub>3</sub>)



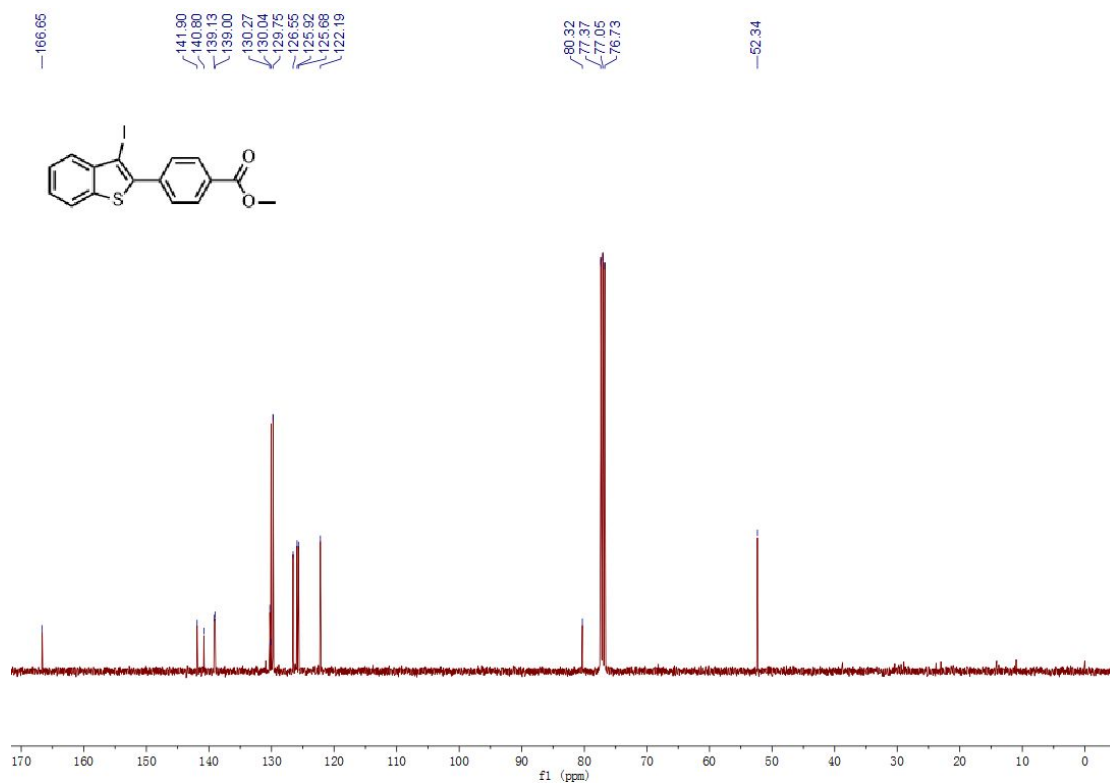
**Figure S39.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ao** (400 Hz, CDCl<sub>3</sub>)



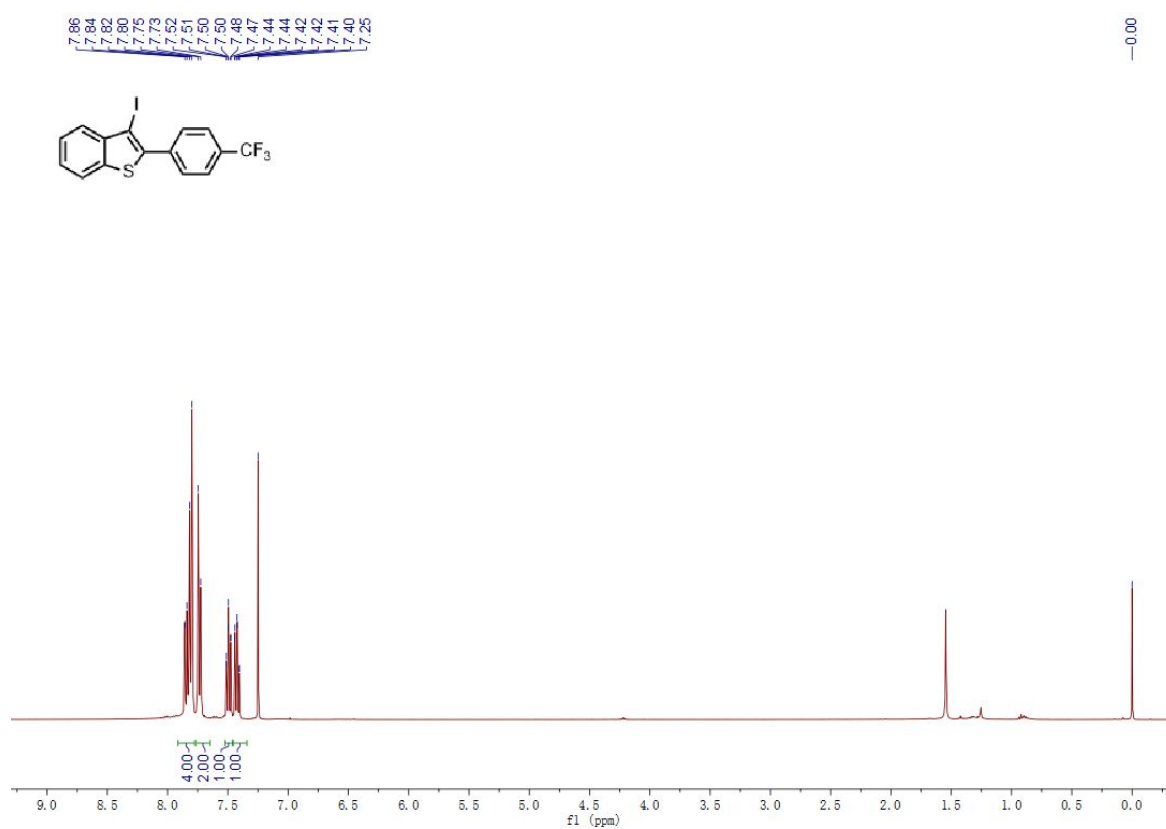
**Figure S40.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ao** (100 Hz, CDCl<sub>3</sub>)



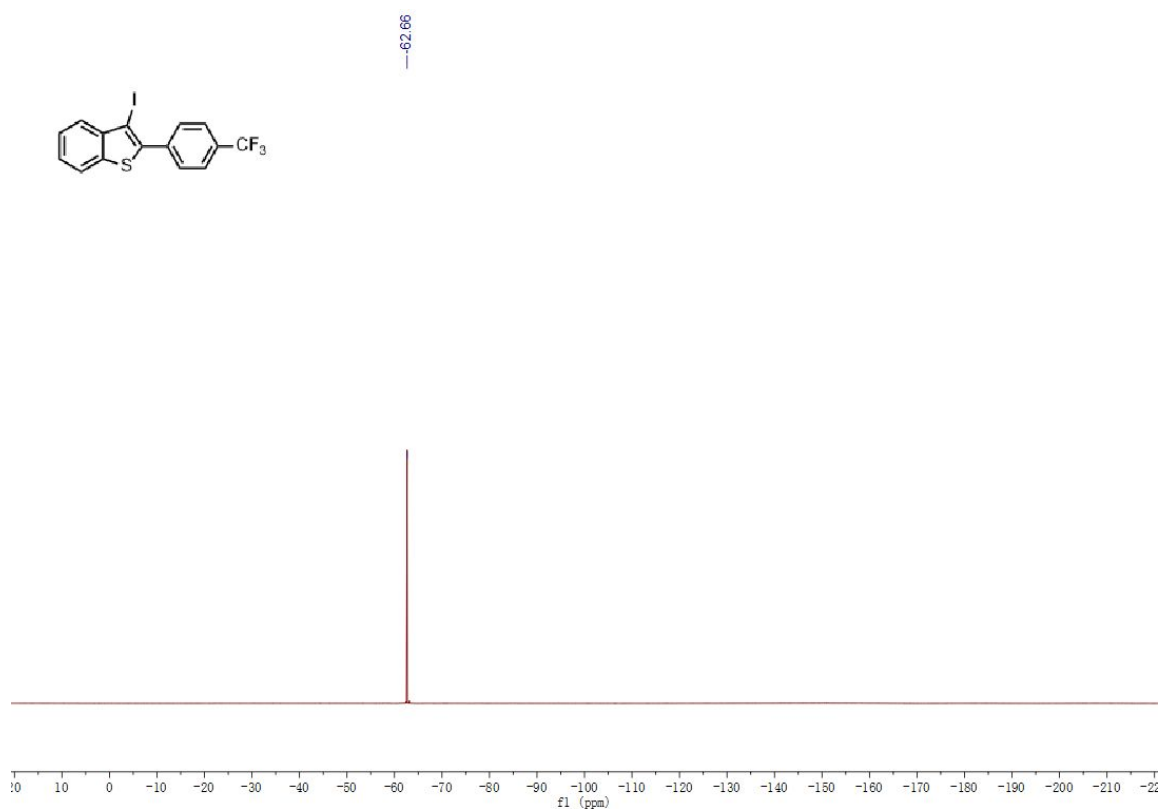
**Figure S41.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ap** (400 Hz, CDCl<sub>3</sub>)



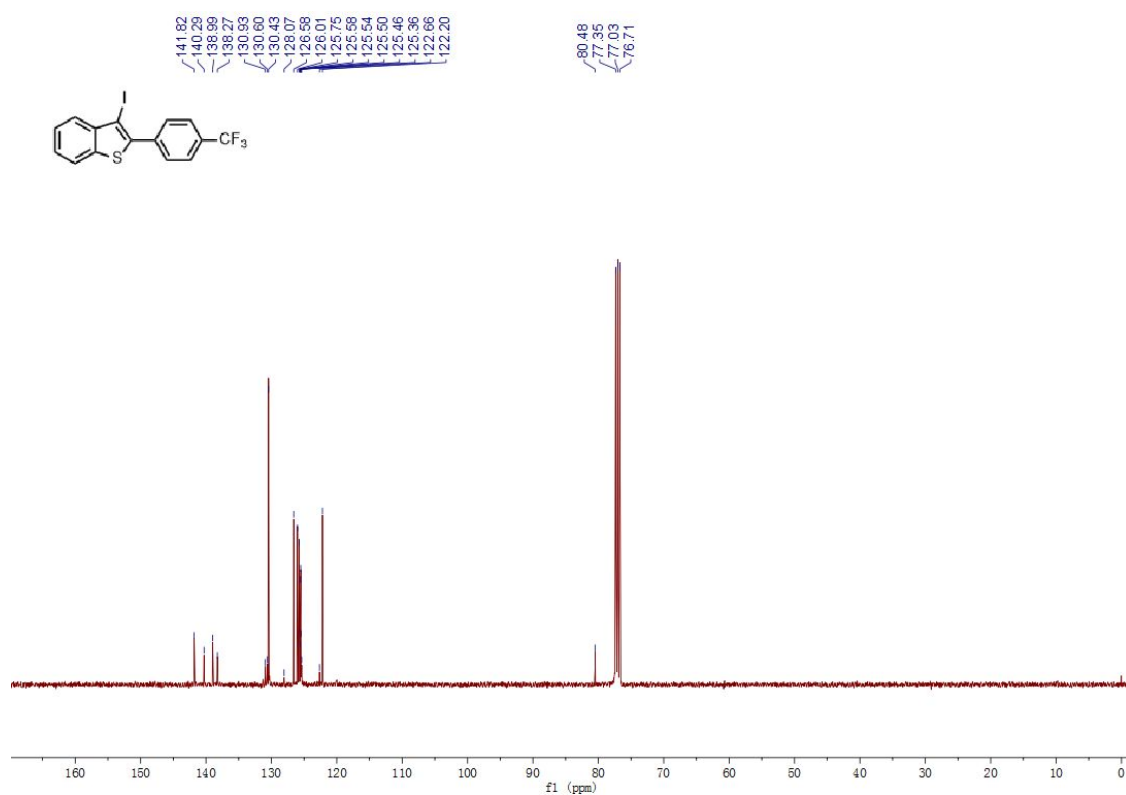
**Figure S42.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ap** (100 Hz, CDCl<sub>3</sub>)



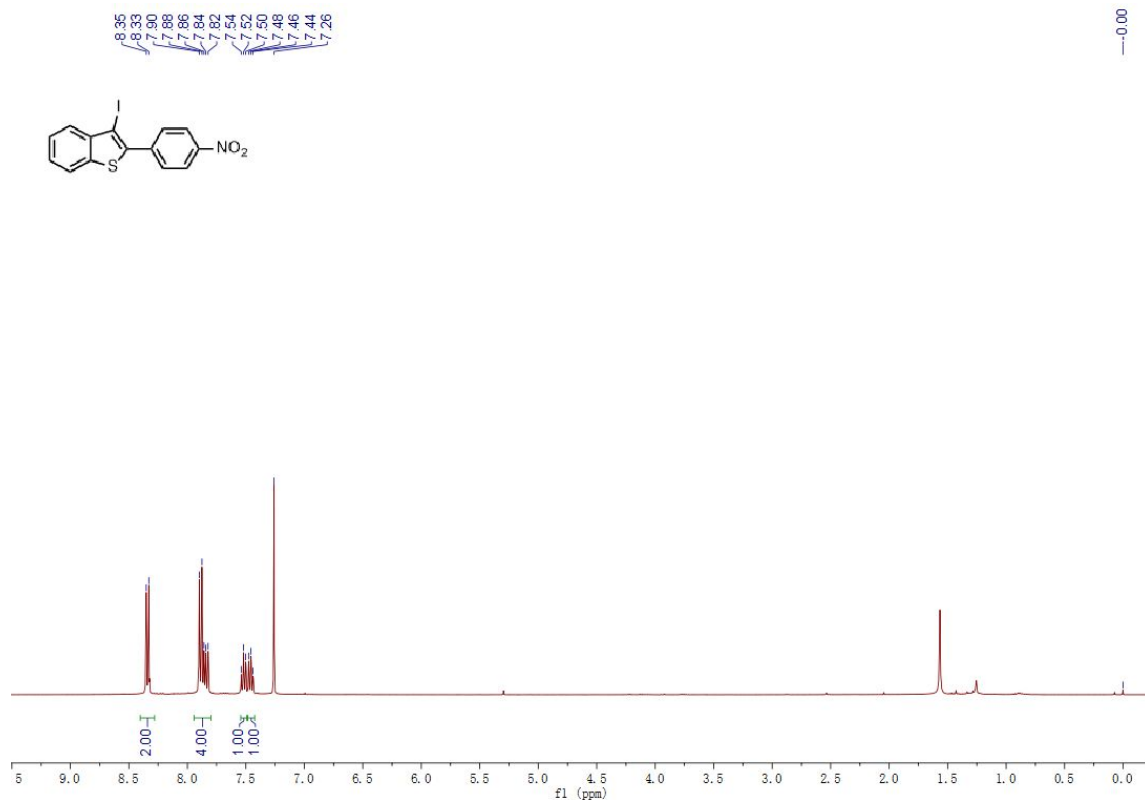
**Figure S43.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3aq** (400 Hz, CDCl<sub>3</sub>)



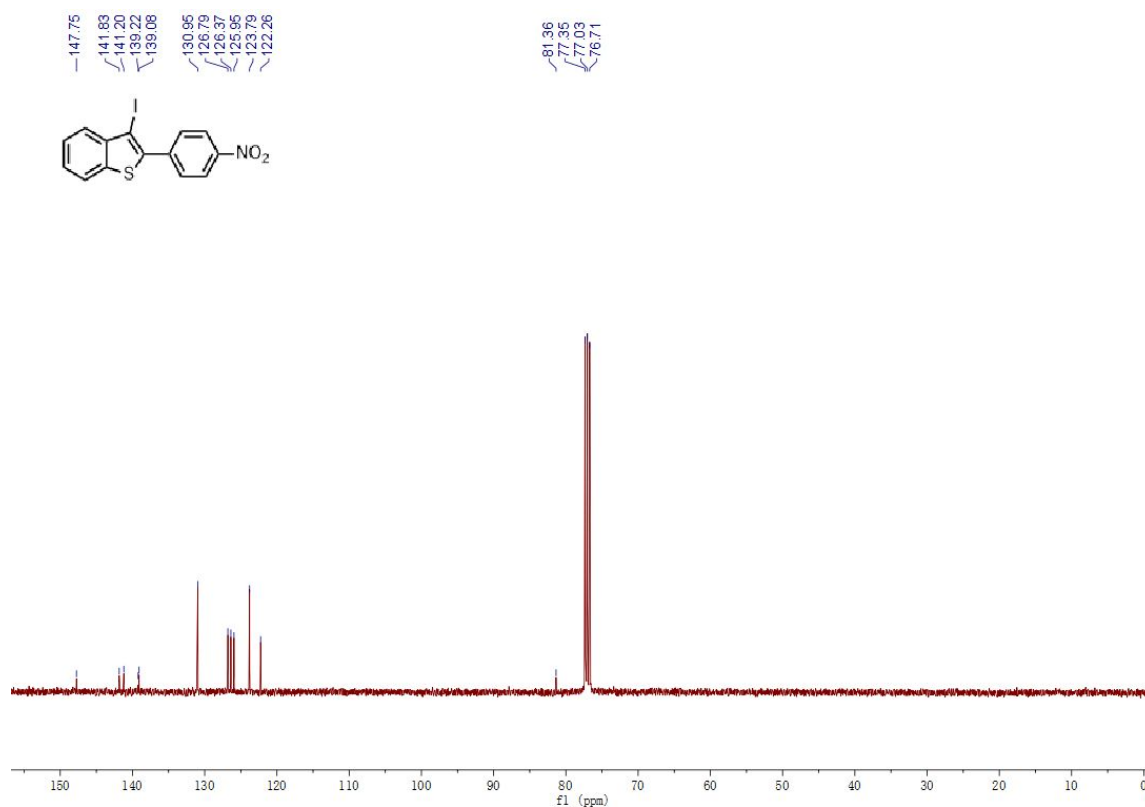
**Figure S44.** Copies of <sup>19</sup>F NMR Spectrum for Compound **3aq** (376 Hz, CDCl<sub>3</sub>)



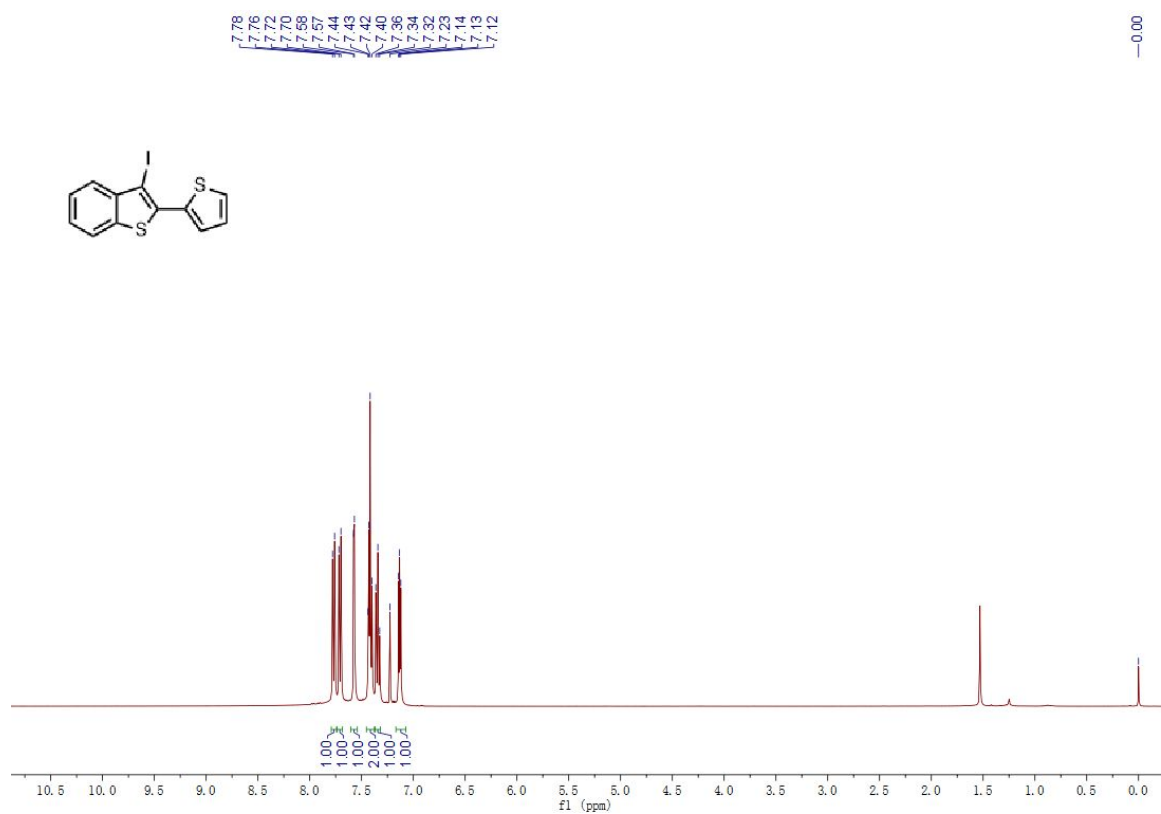
**Figure S45.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3aq** (100 Hz, CDCl<sub>3</sub>)



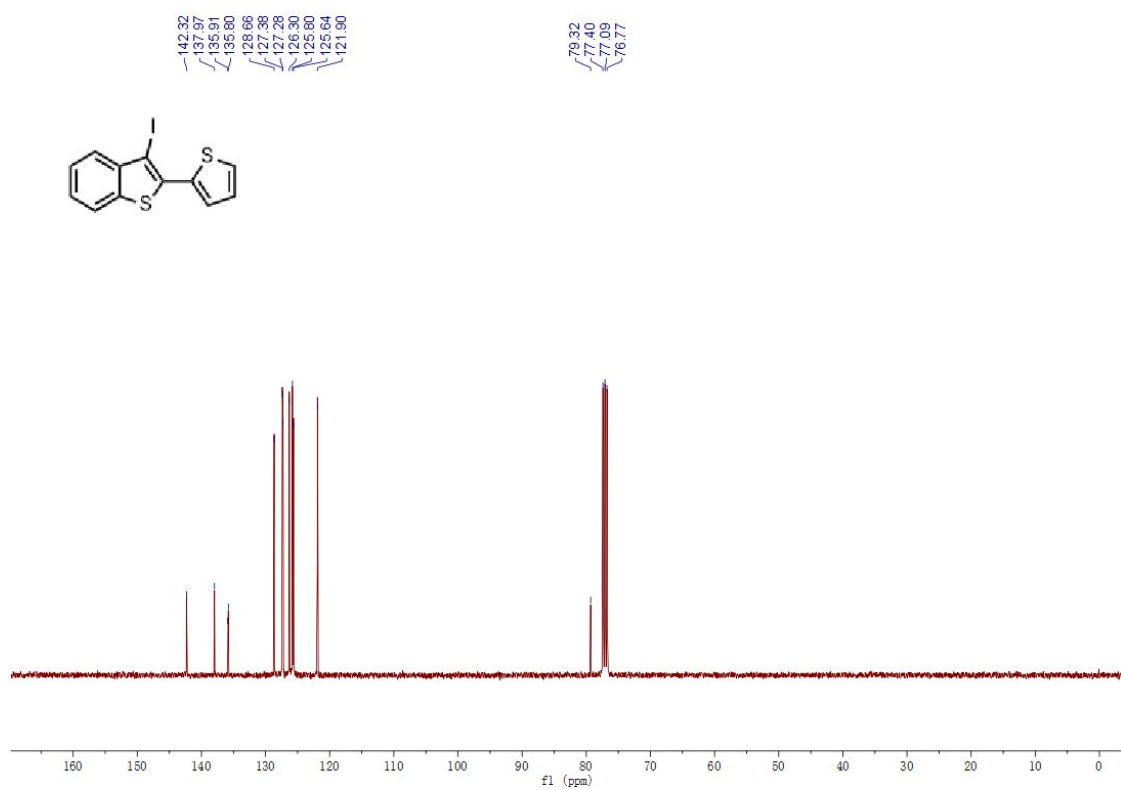
**Figure S46.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ar** (400 Hz, CDCl<sub>3</sub>)



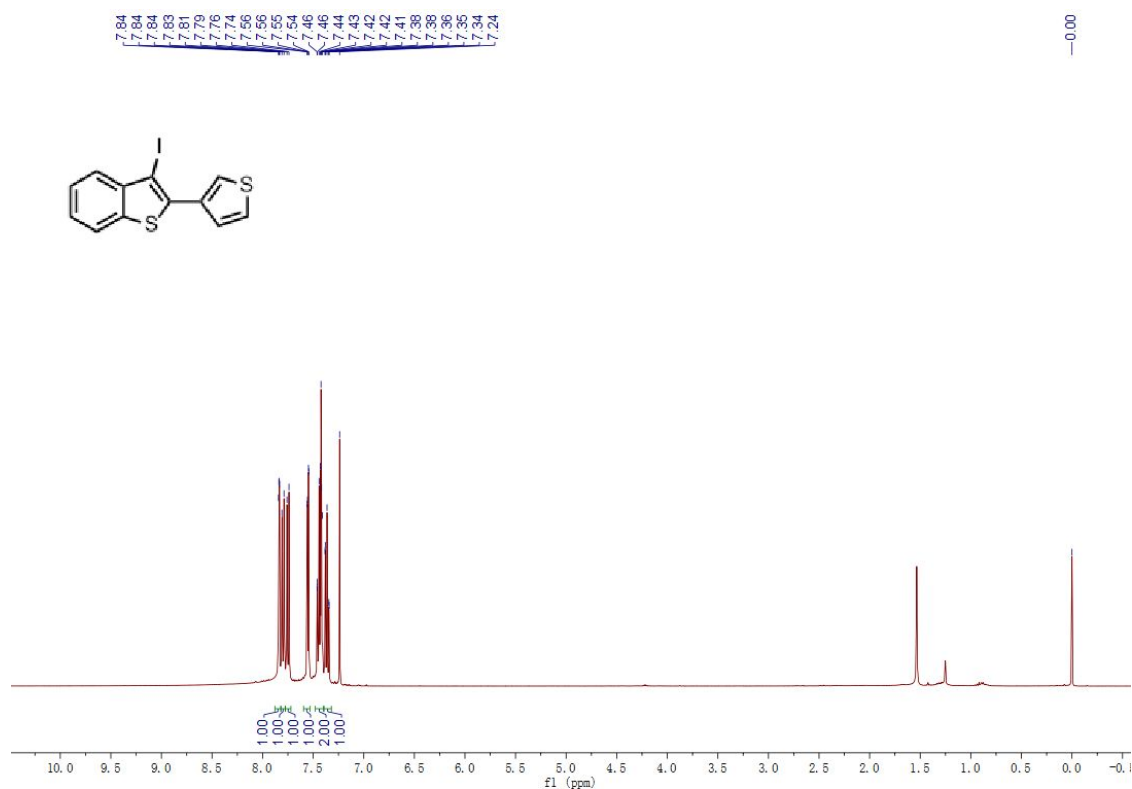
**Figure S47.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ar** (100 Hz, CDCl<sub>3</sub>)



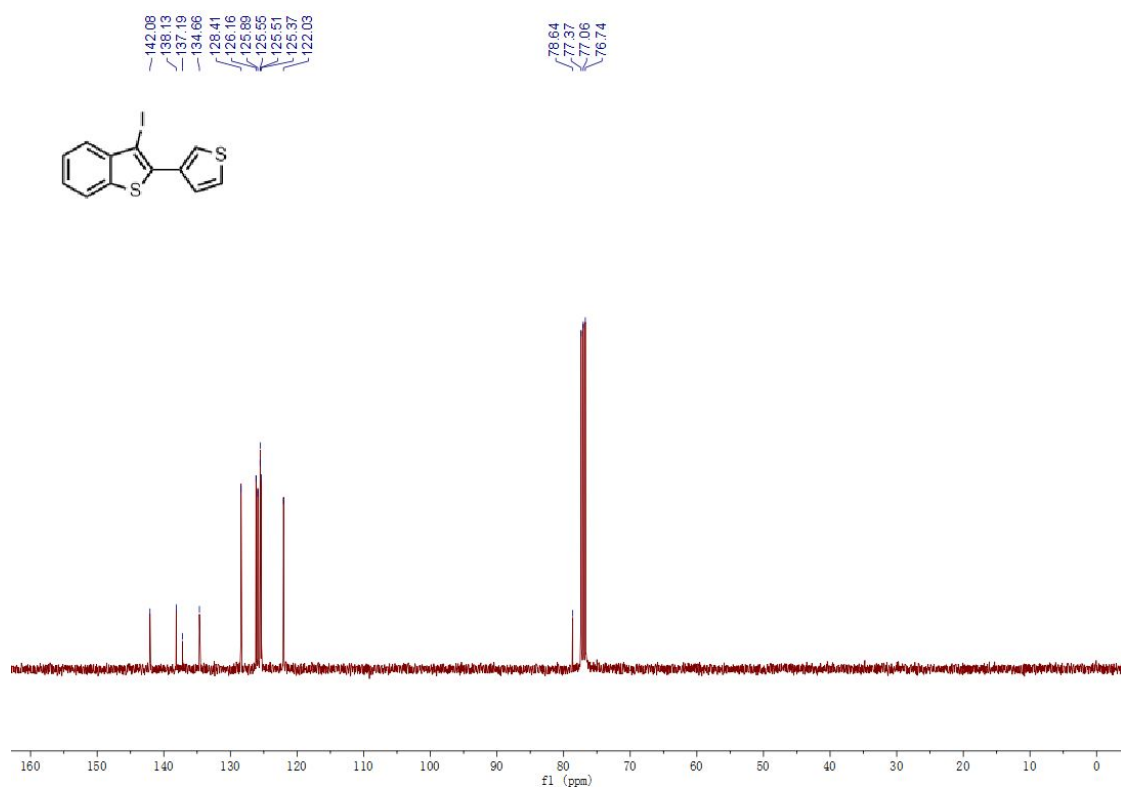
**Figure S48.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3as** (400 Hz, CDCl<sub>3</sub>)



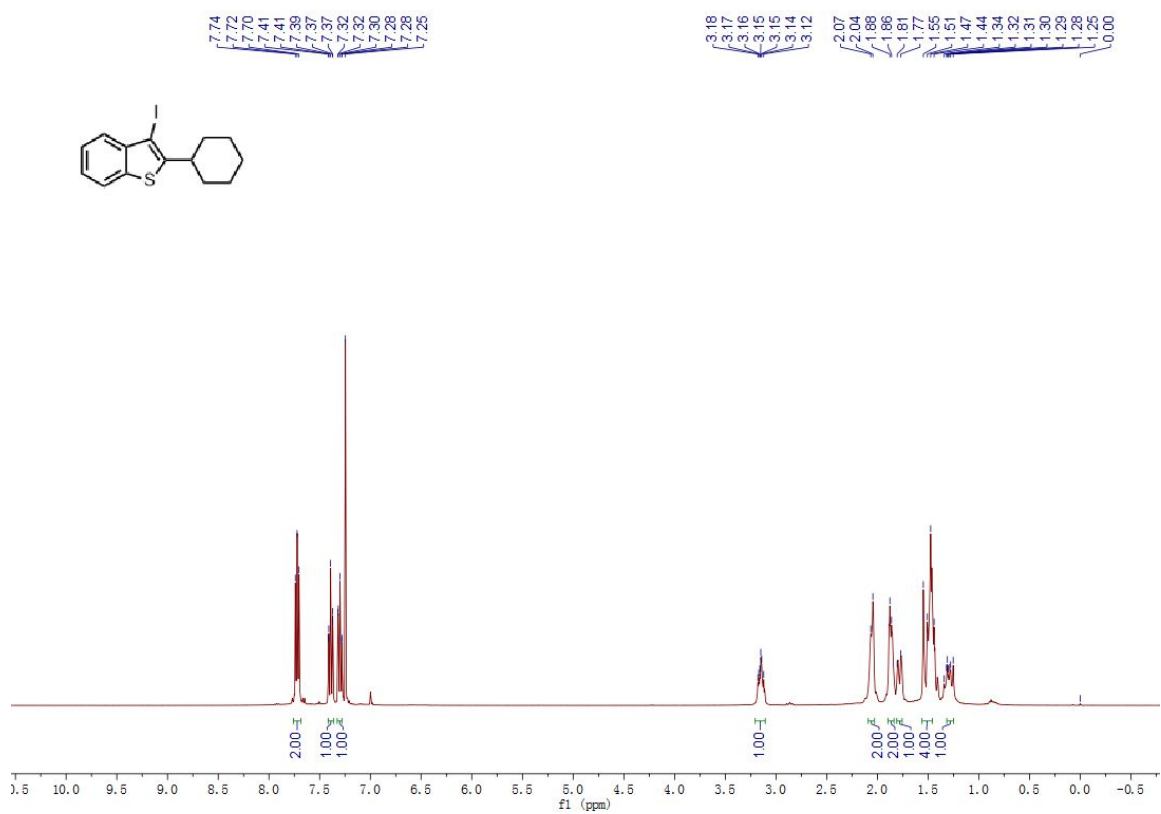
**Figure S49.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3as** (100 Hz, CDCl<sub>3</sub>)



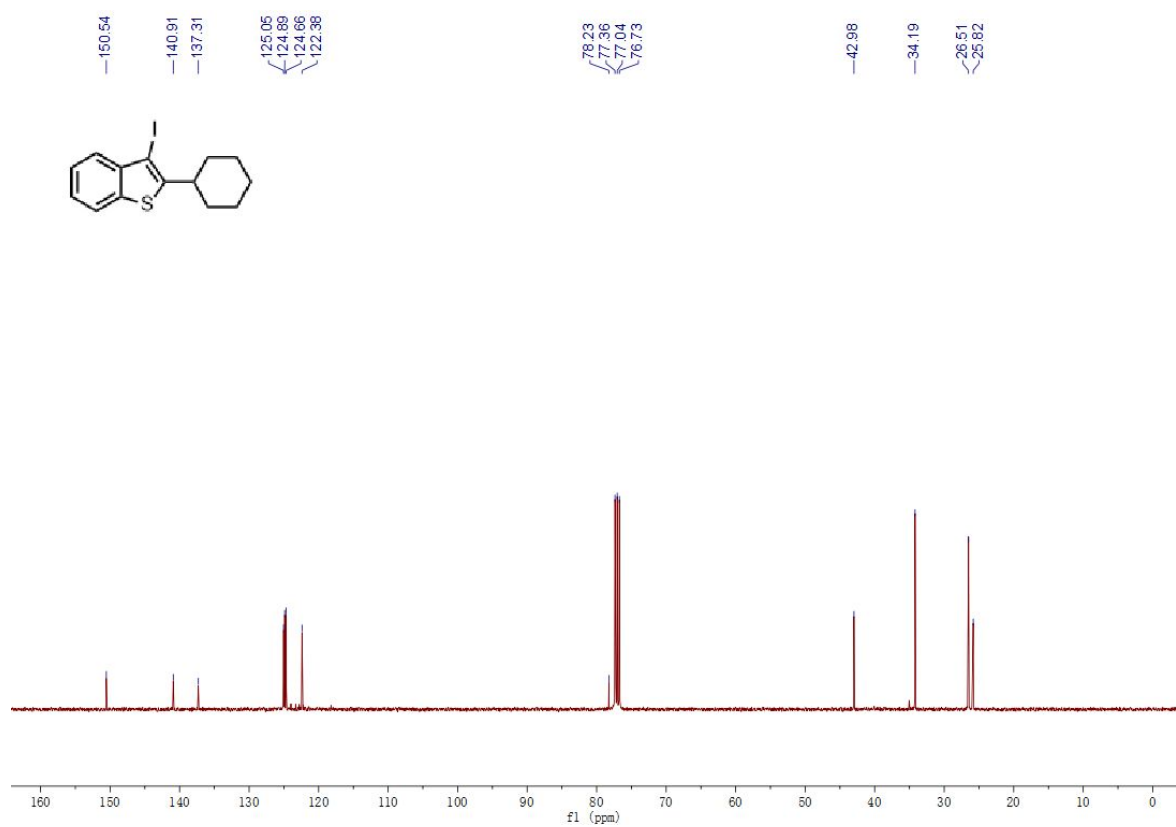
**Figure S50.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3at** (400 Hz, CDCl<sub>3</sub>)



**Figure S51.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3at** (100 Hz, CDCl<sub>3</sub>)

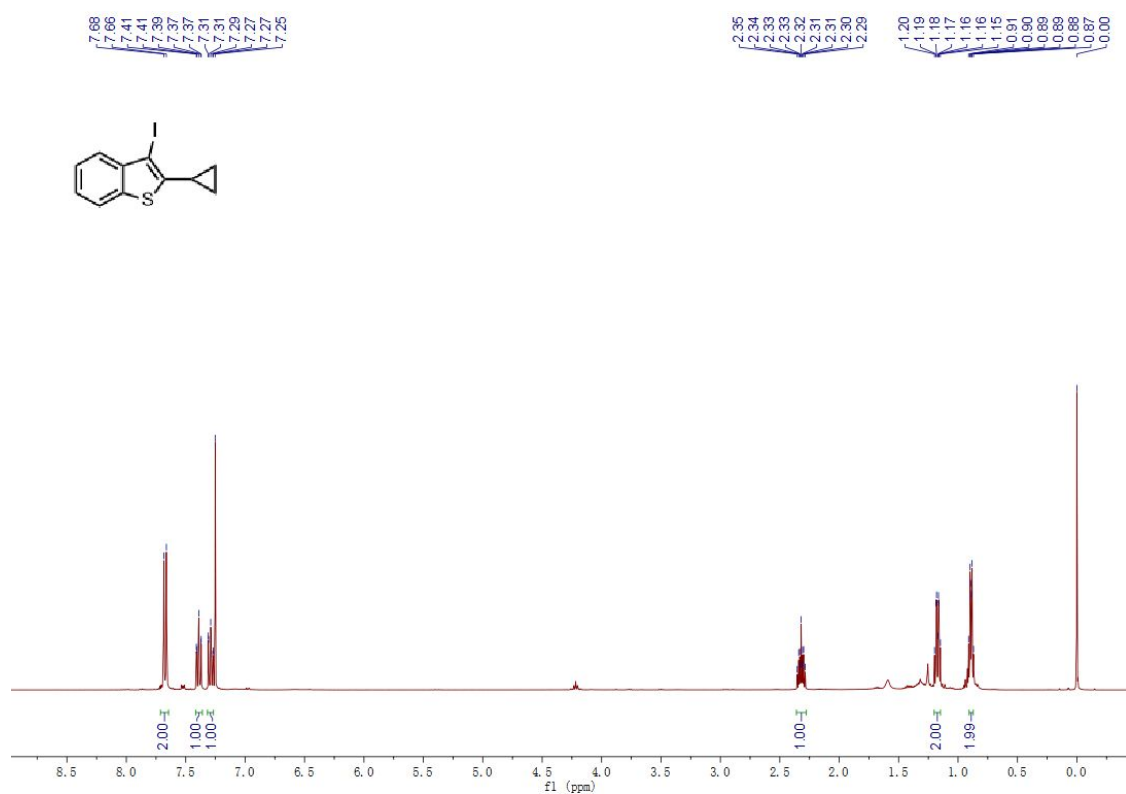


**Figure S52.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3au** (400 Hz, CDCl<sub>3</sub>)

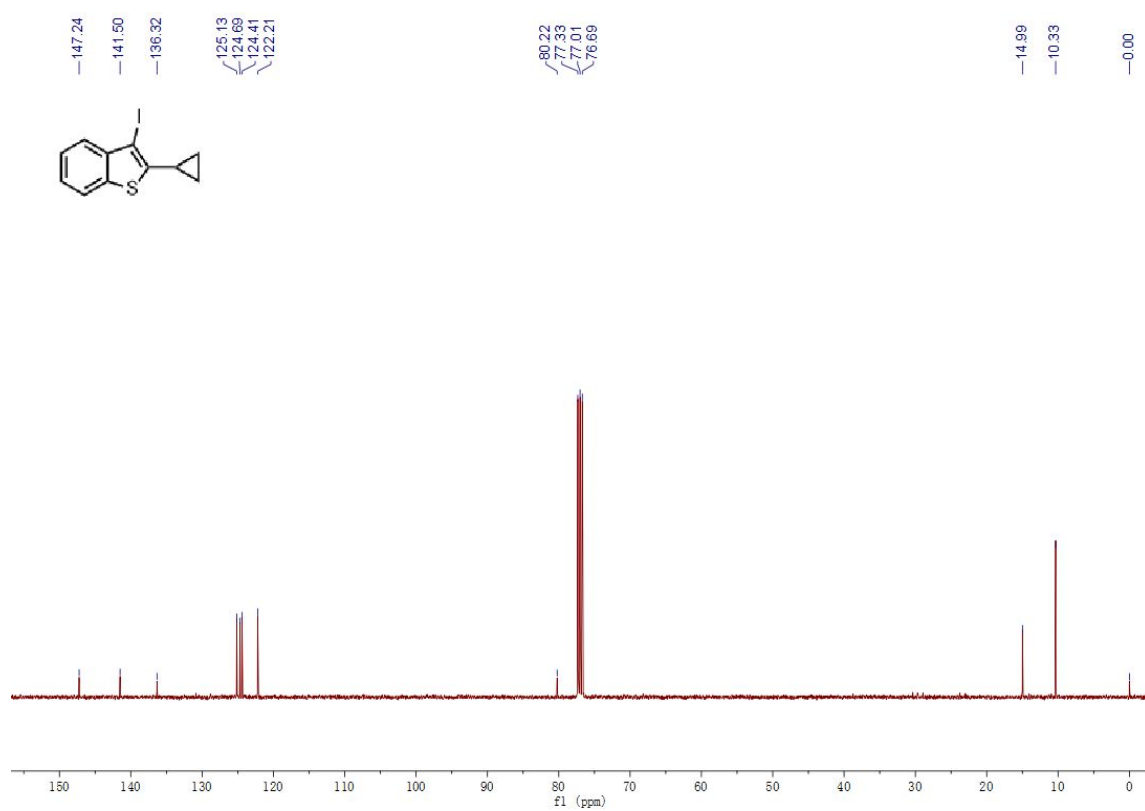


**Figure S53.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3au** (100 Hz, CDCl<sub>3</sub>)

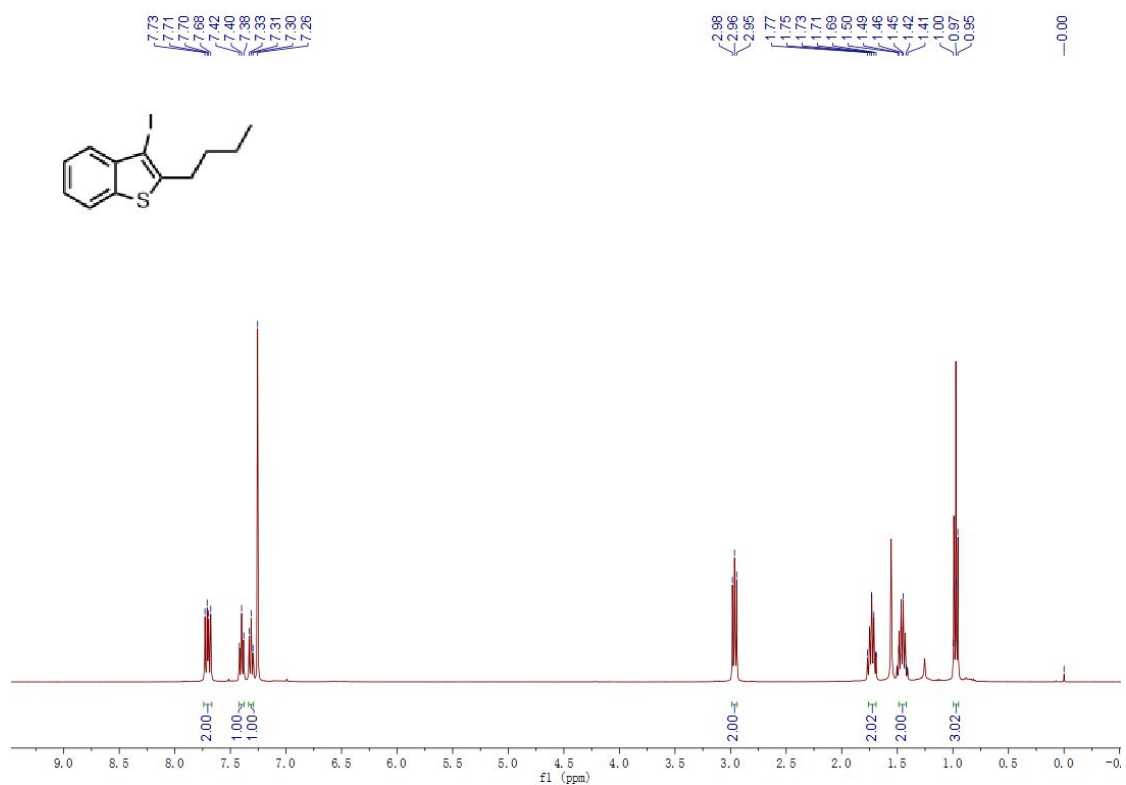




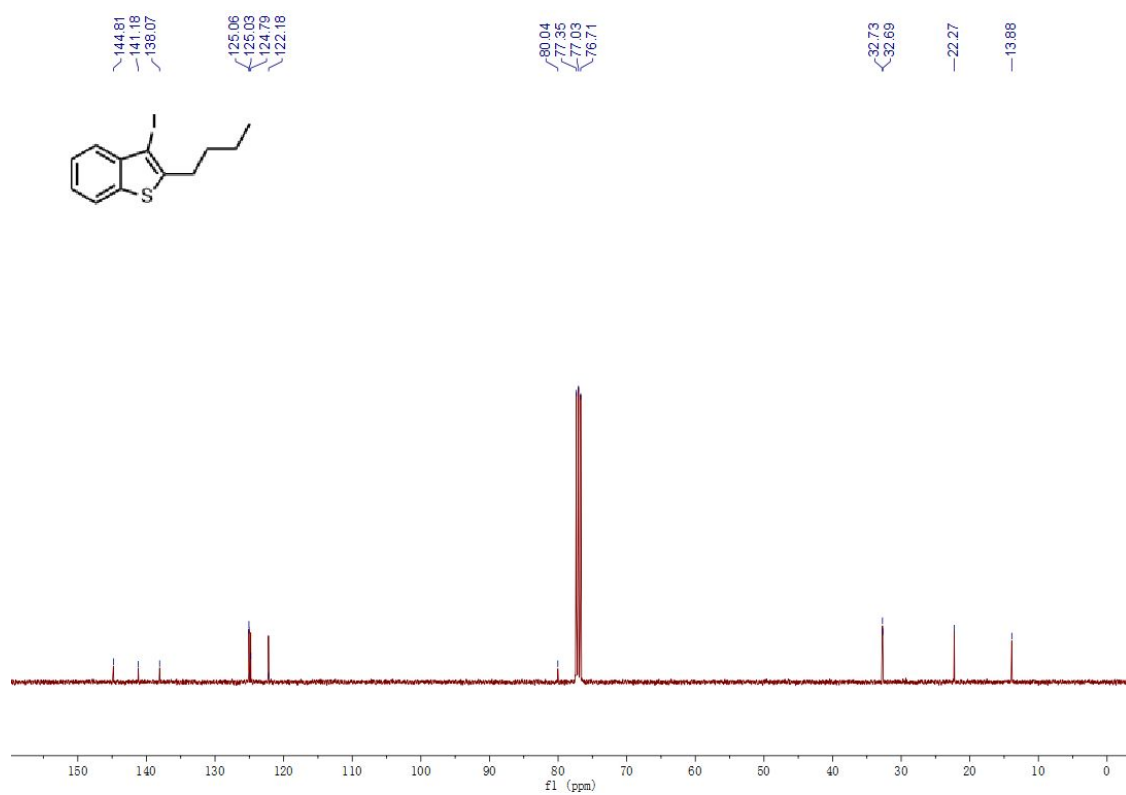
**Figure S54.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3av** (400 Hz, CDCl<sub>3</sub>)



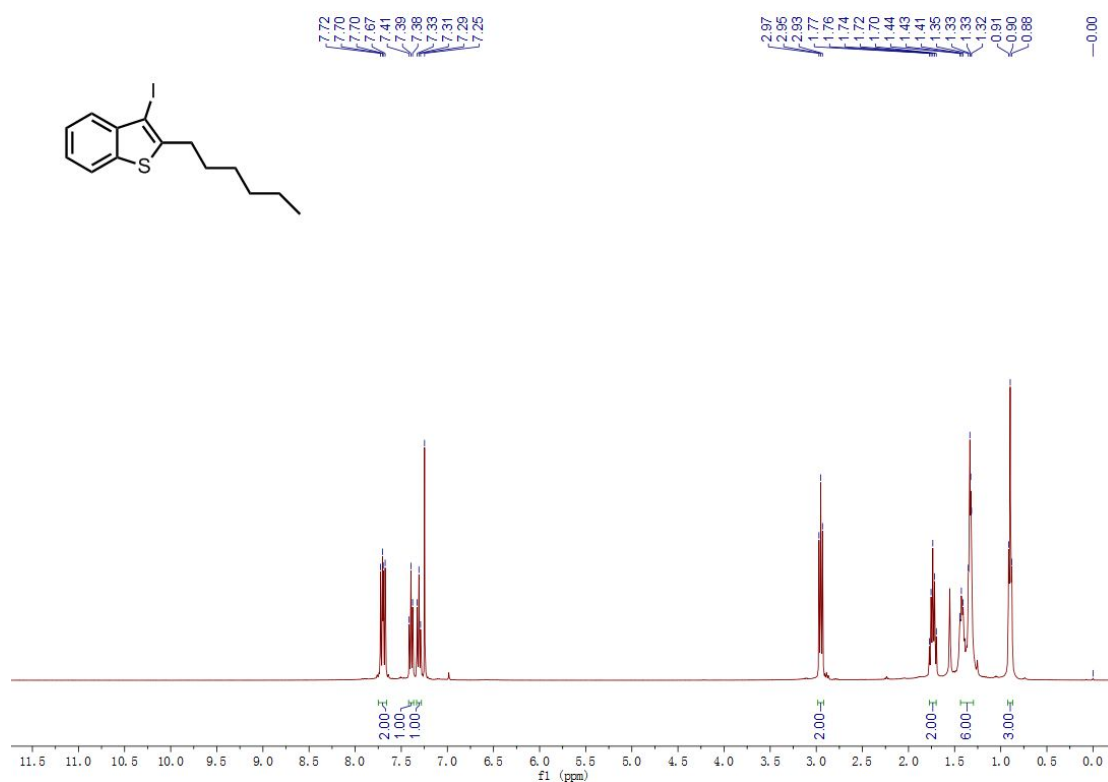
**Figure S55.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3av** (100 Hz, CDCl<sub>3</sub>)



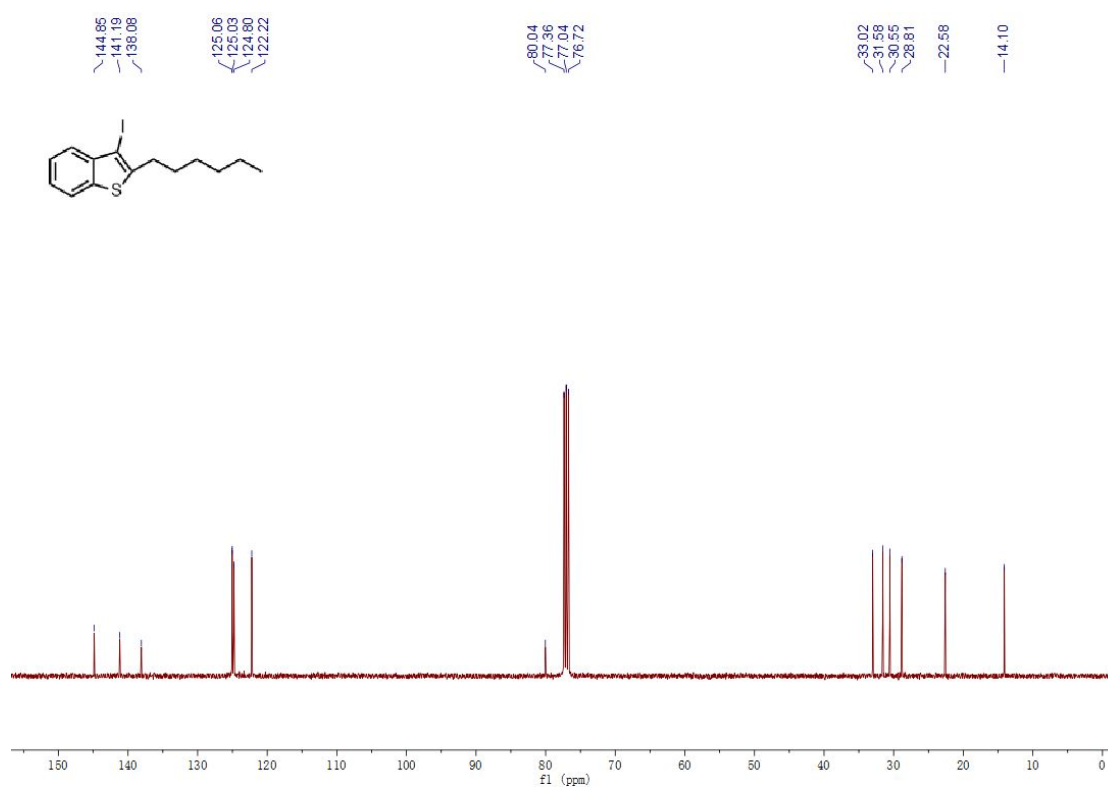
**Figure S56.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3aw** (400 Hz, CDCl<sub>3</sub>)



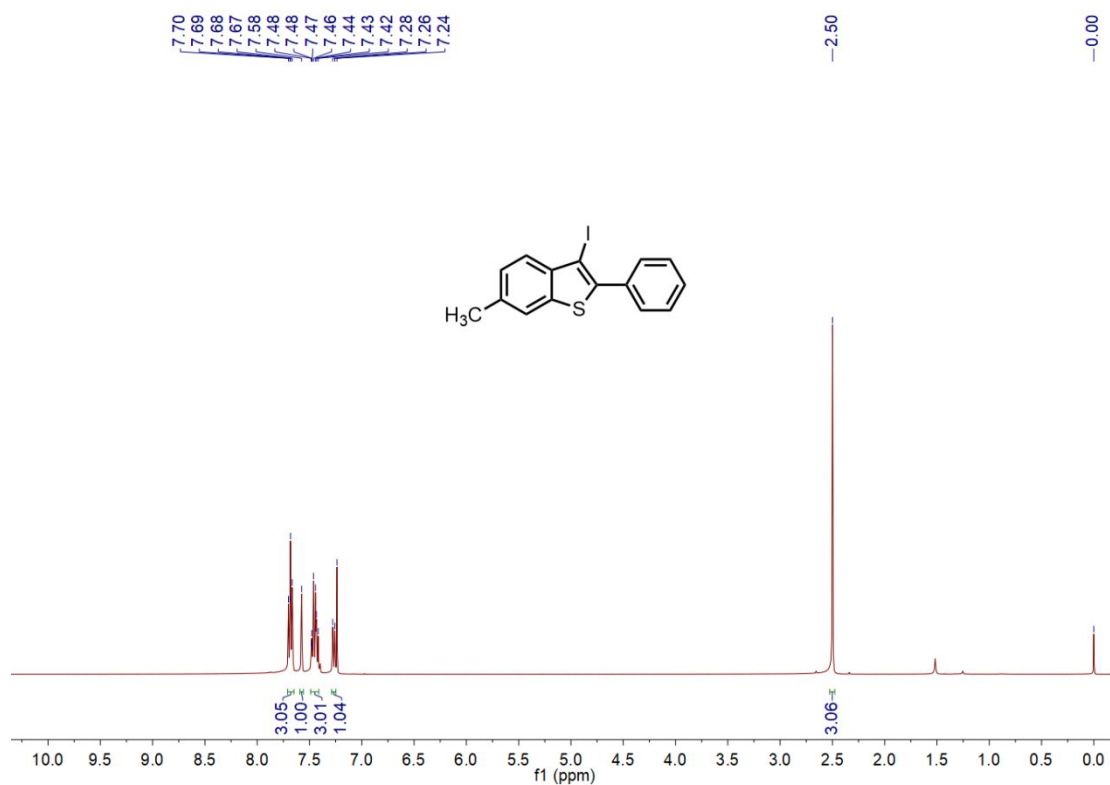
**Figure S57.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3aw** (100 Hz, CDCl<sub>3</sub>)



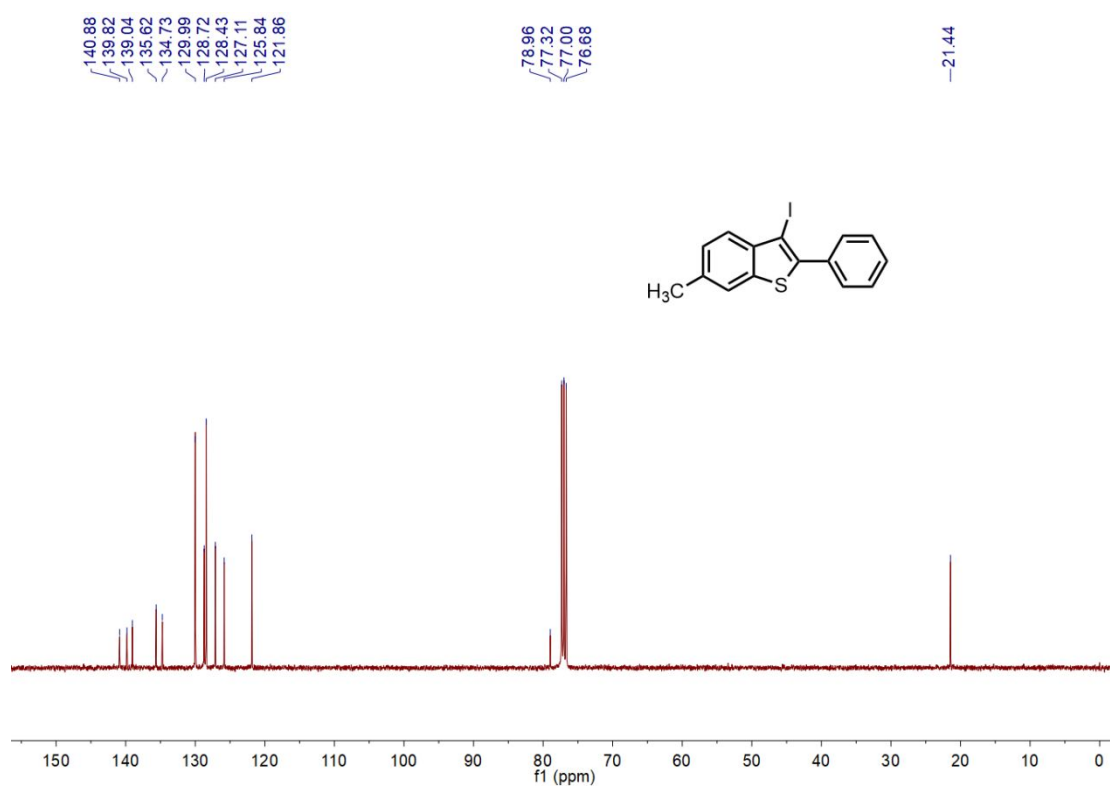
**Figure S58.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ax** (400 Hz, CDCl<sub>3</sub>)



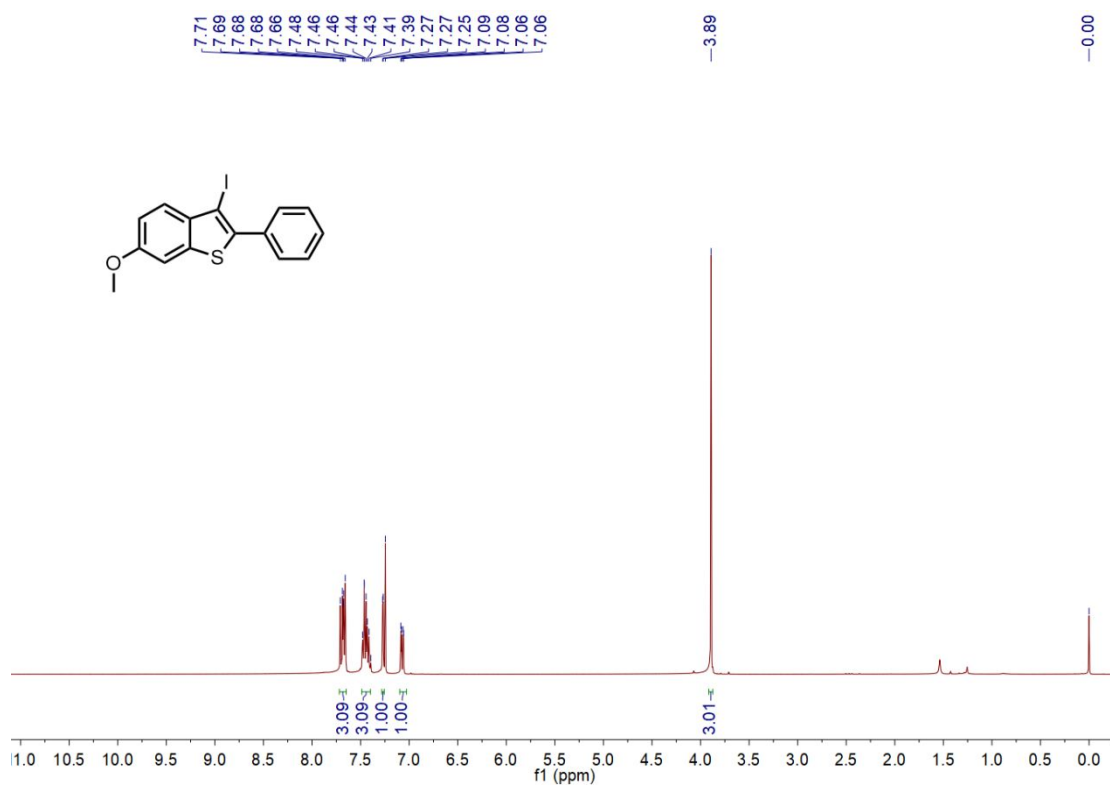
**Figure S59.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ax** (100 Hz, CDCl<sub>3</sub>)



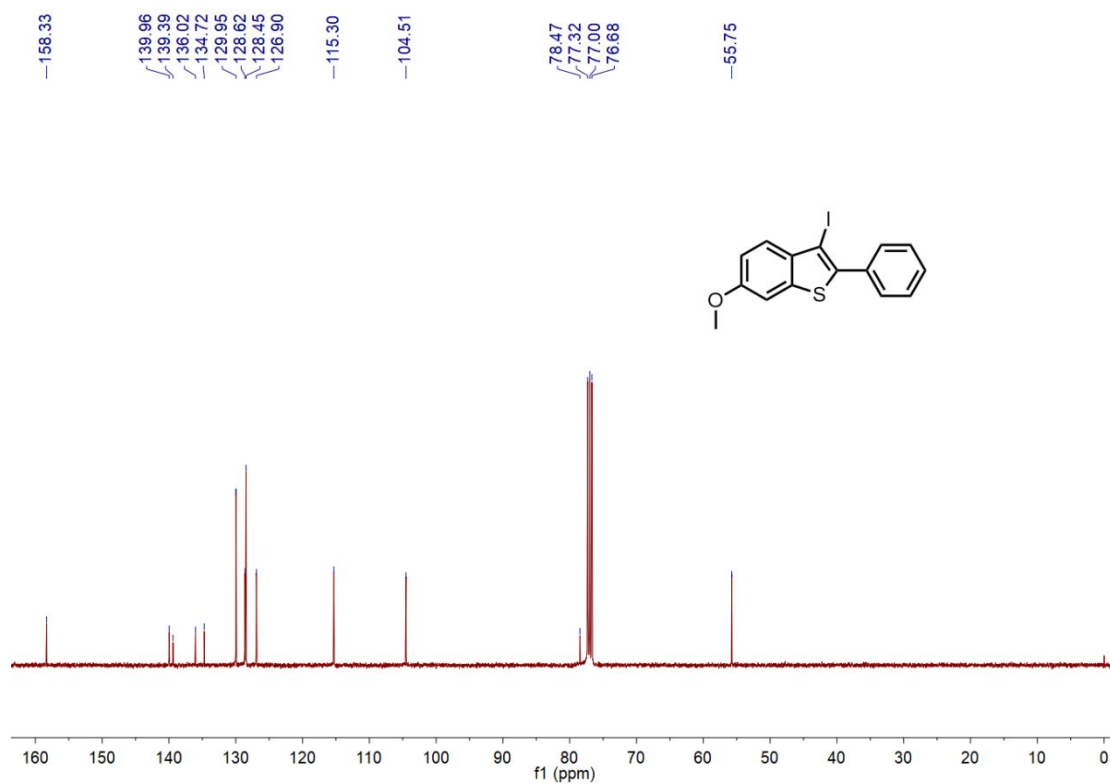
**Figure S60.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ay** (400 Hz, CDCl<sub>3</sub>)



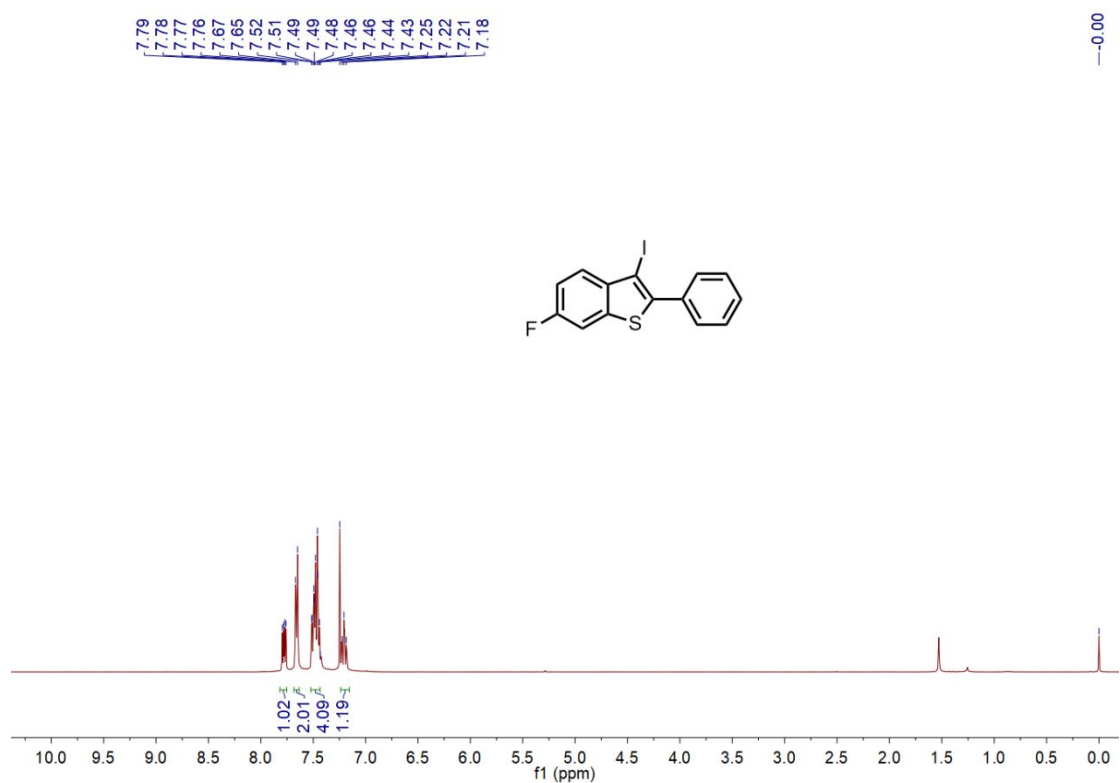
**Figure S61.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ay** (100 Hz, CDCl<sub>3</sub>)



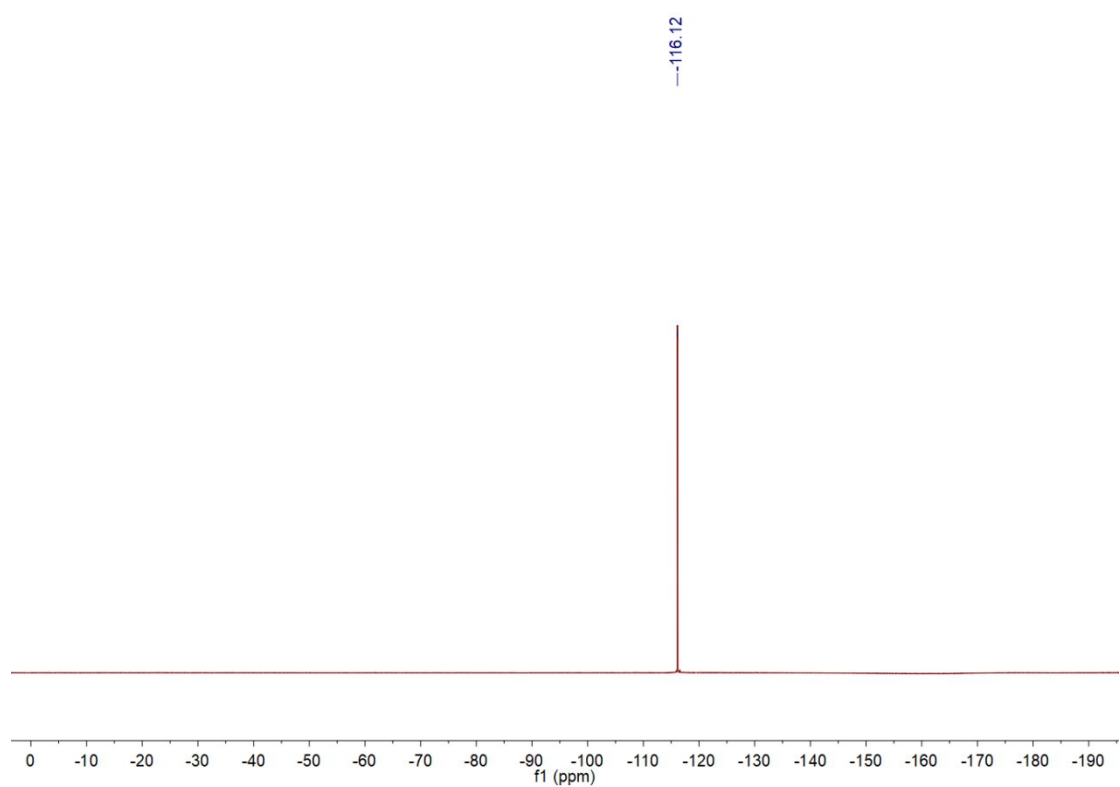
**Figure S62.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3az** (400 Hz, CDCl<sub>3</sub>)



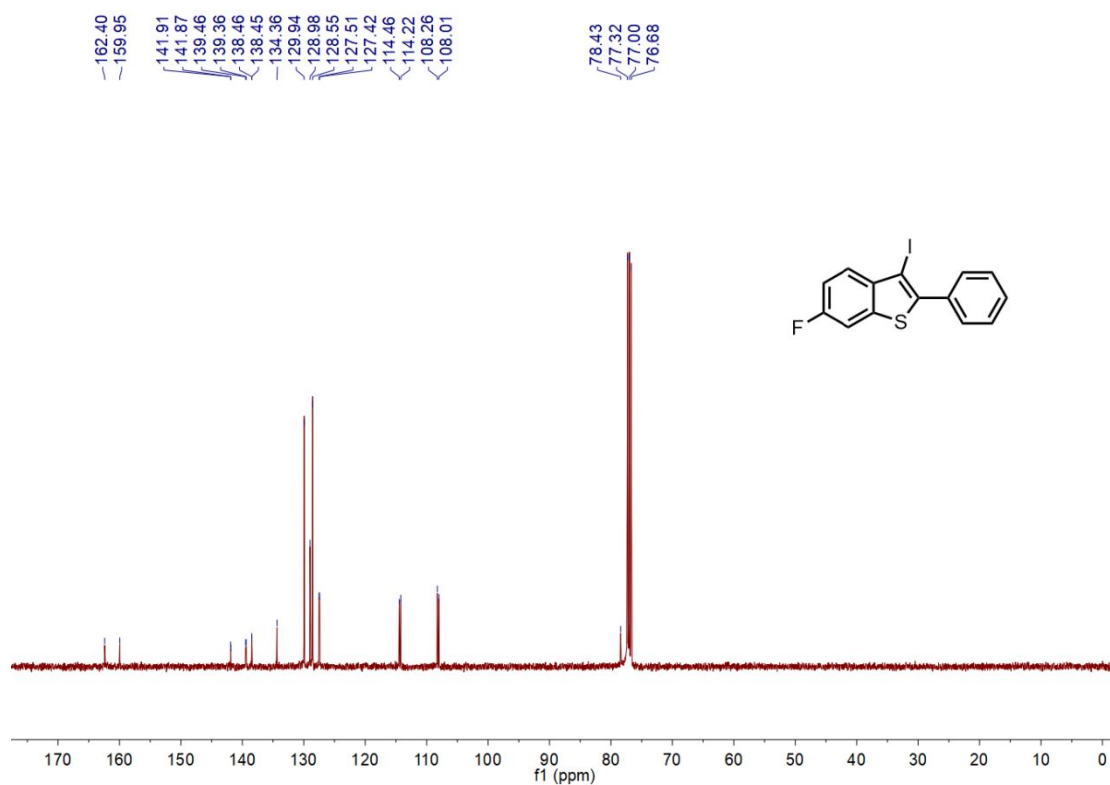
**Figure S63.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3az** (100 Hz, CDCl<sub>3</sub>)



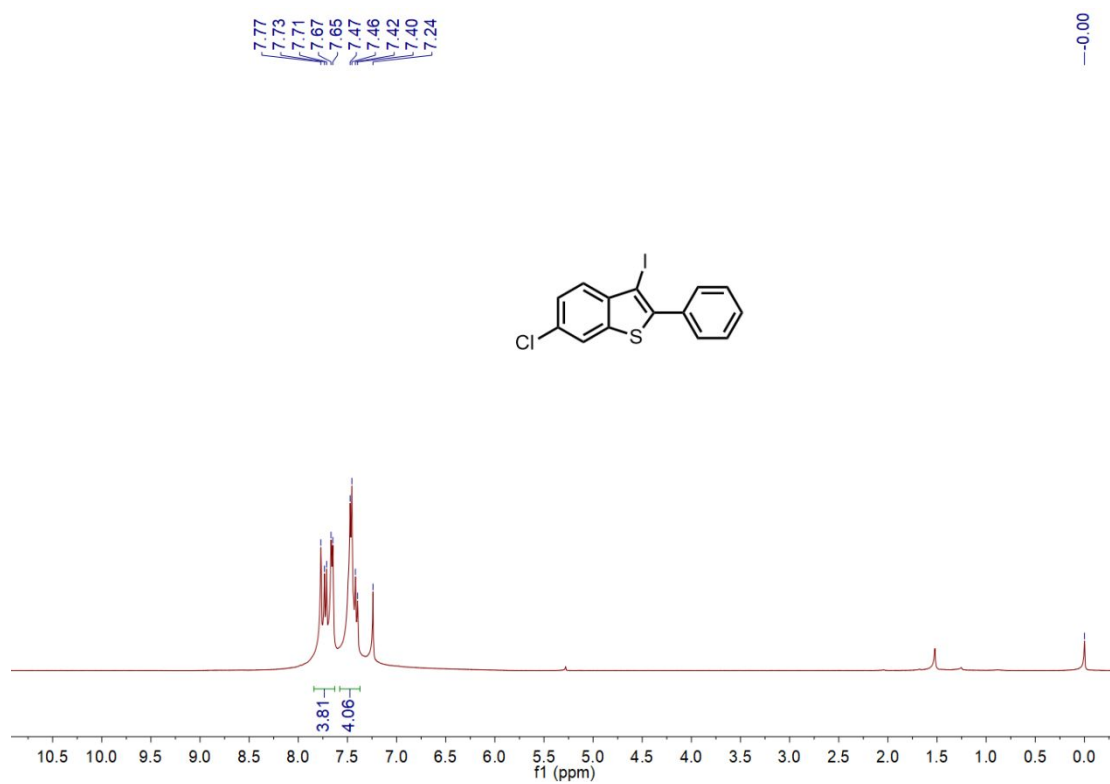
**Figure S64.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3aza** (400 Hz, CDCl<sub>3</sub>)



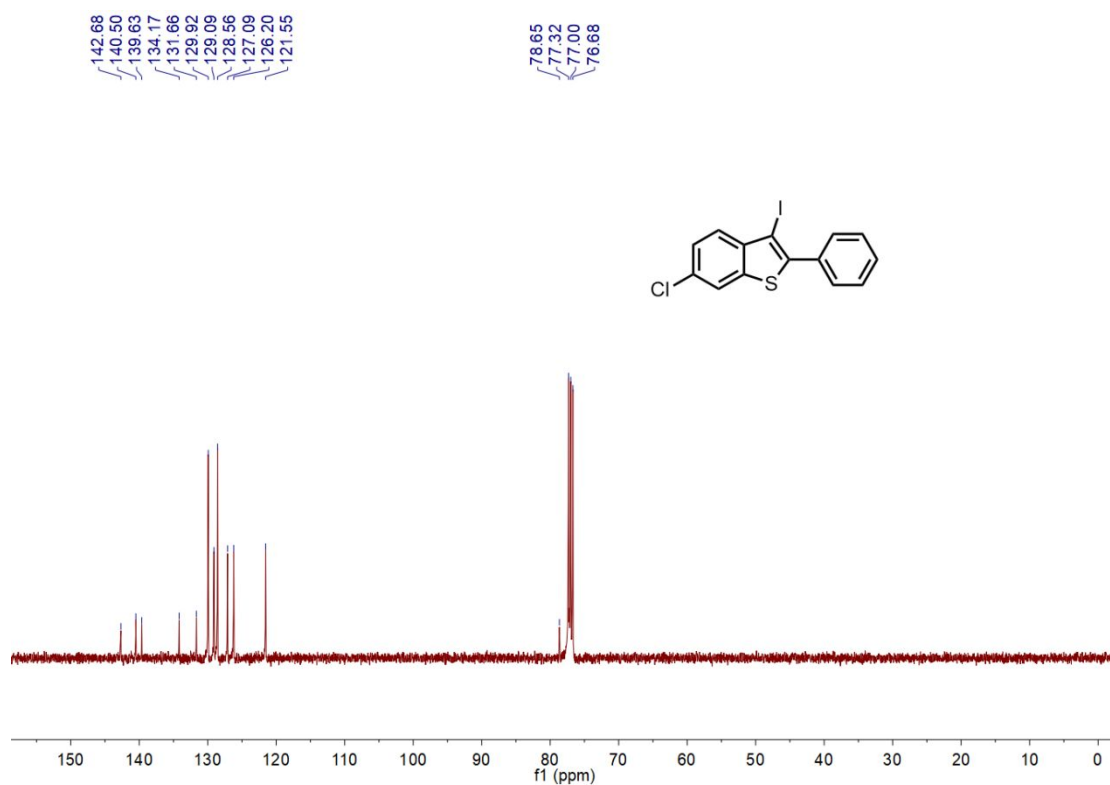
**Figure S65.** Copies of <sup>19</sup>F NMR Spectrum for Compound **3aza** (376 Hz, CDCl<sub>3</sub>)



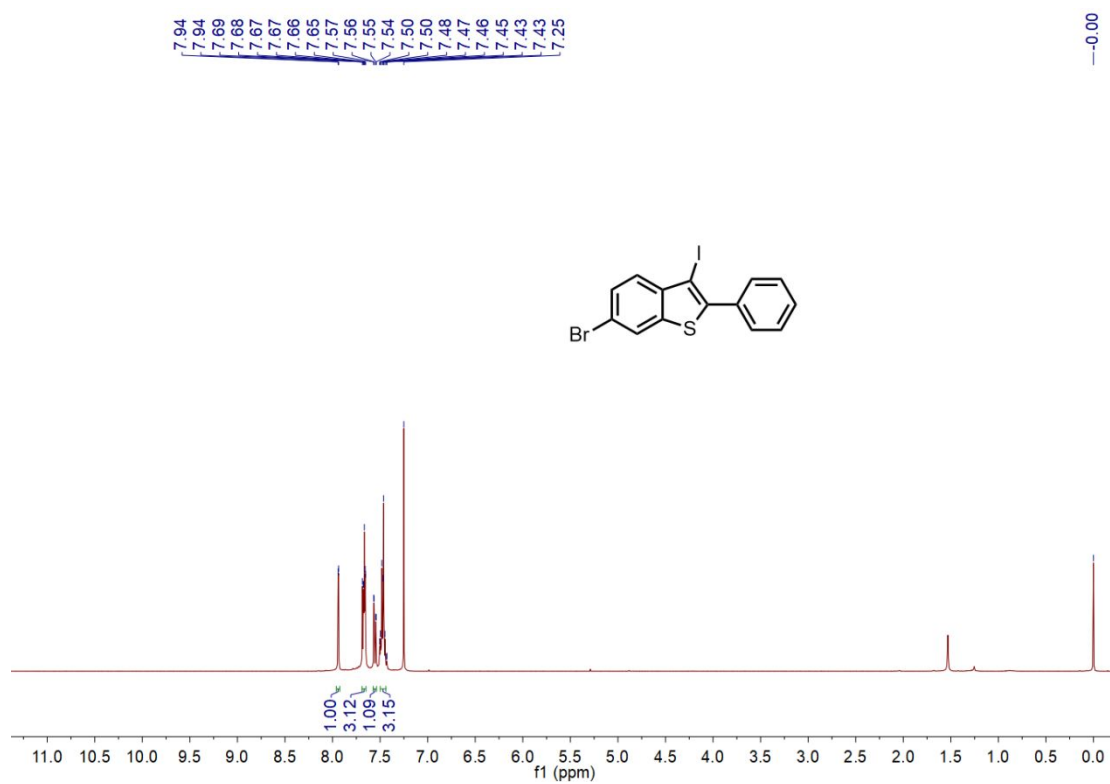
**Figure S66.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3aza** (100 Hz, CDCl<sub>3</sub>)



**Figure S67.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3azb** (400 Hz, CDCl<sub>3</sub>)

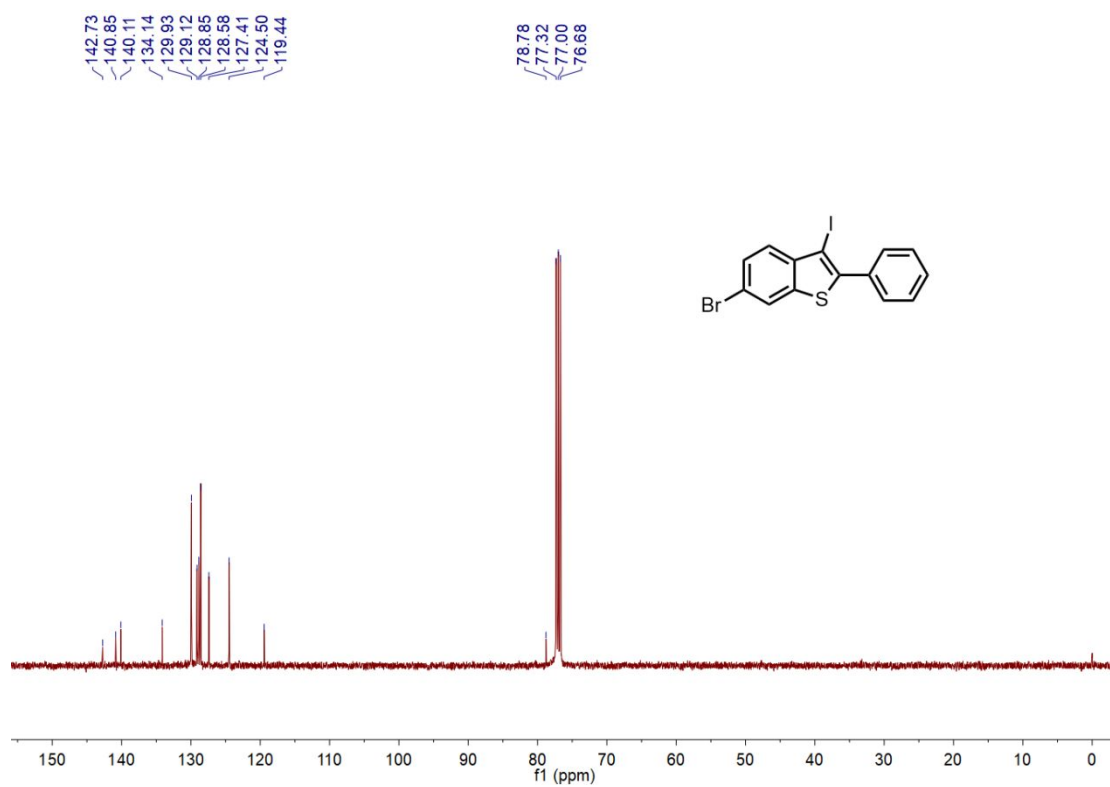


**Figure S68.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3azb** (100 Hz, CDCl<sub>3</sub>)

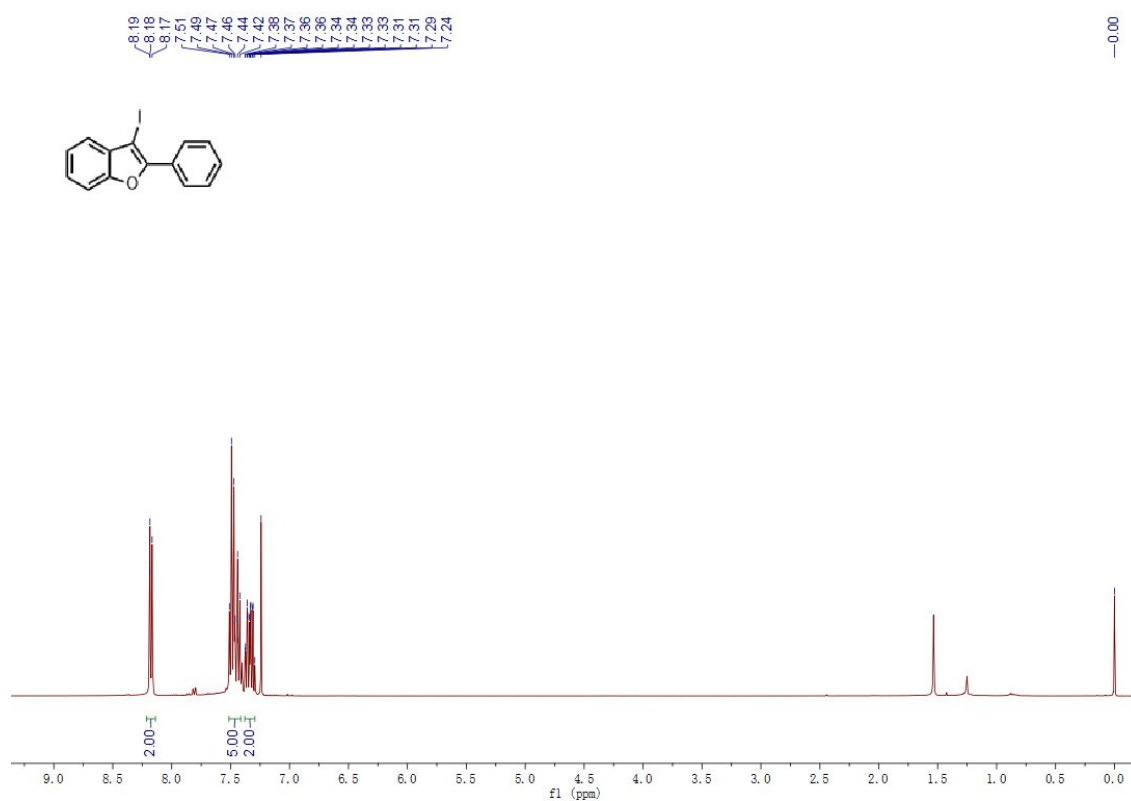


**Figure S69.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3azc** (400 Hz, CDCl<sub>3</sub>)

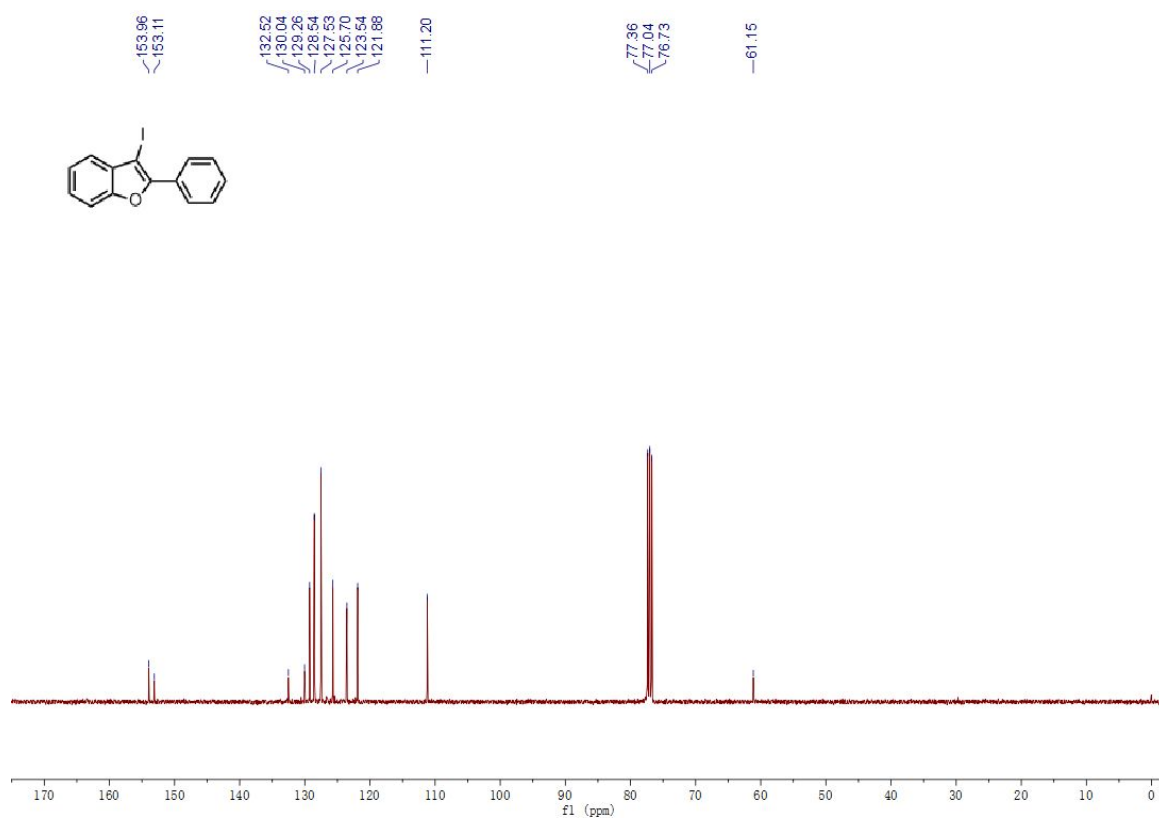




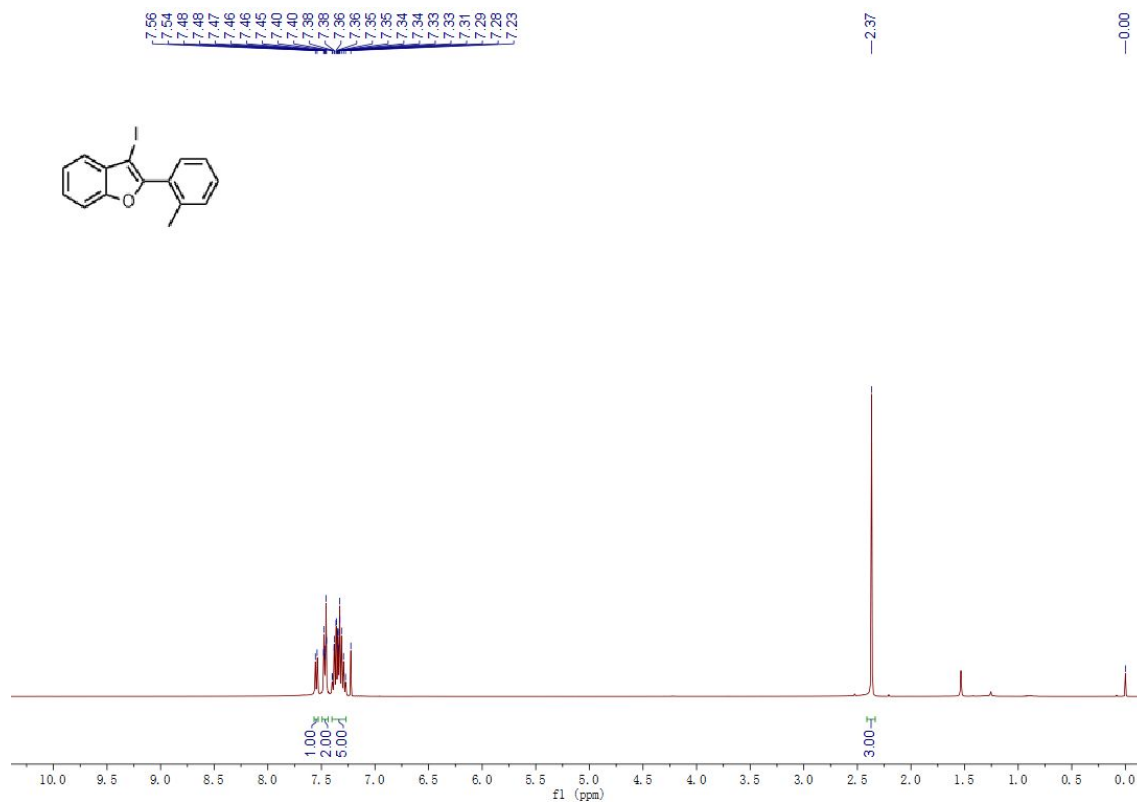
**Figure S70.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3azc** (100 Hz, CDCl<sub>3</sub>)



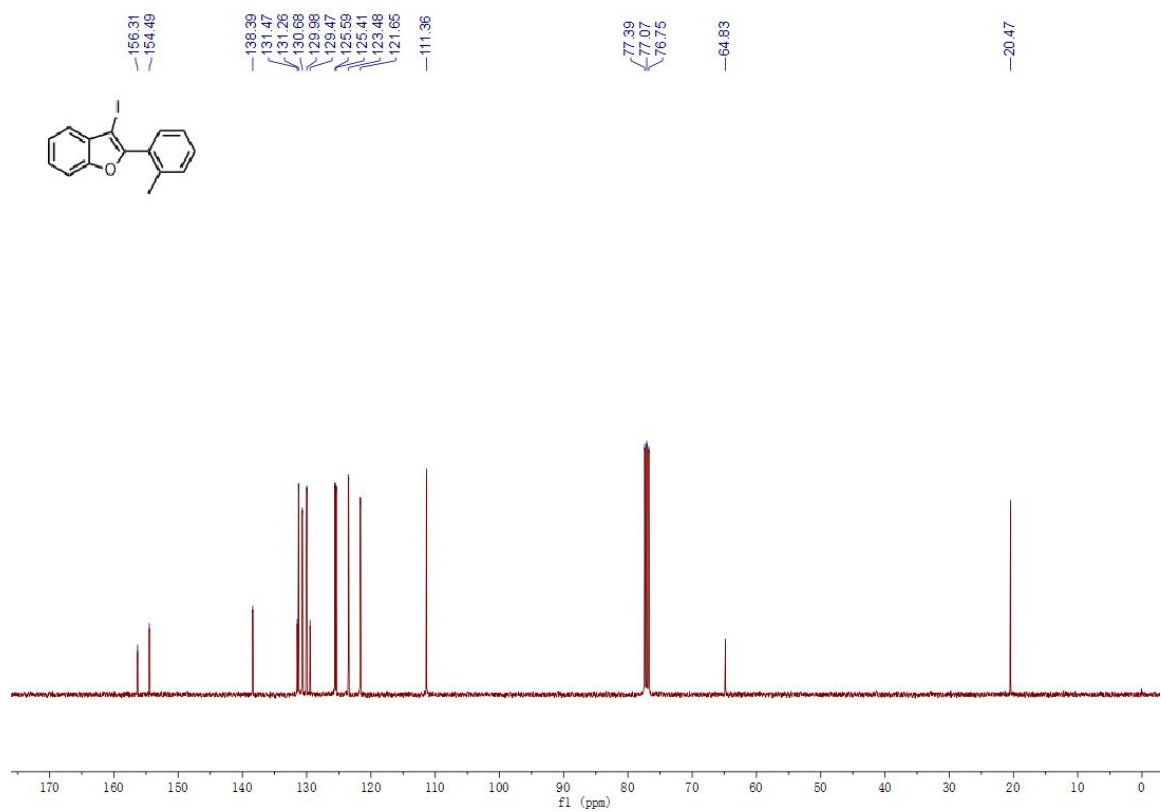
**Figure S71.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5aa** (400 Hz, CDCl<sub>3</sub>)



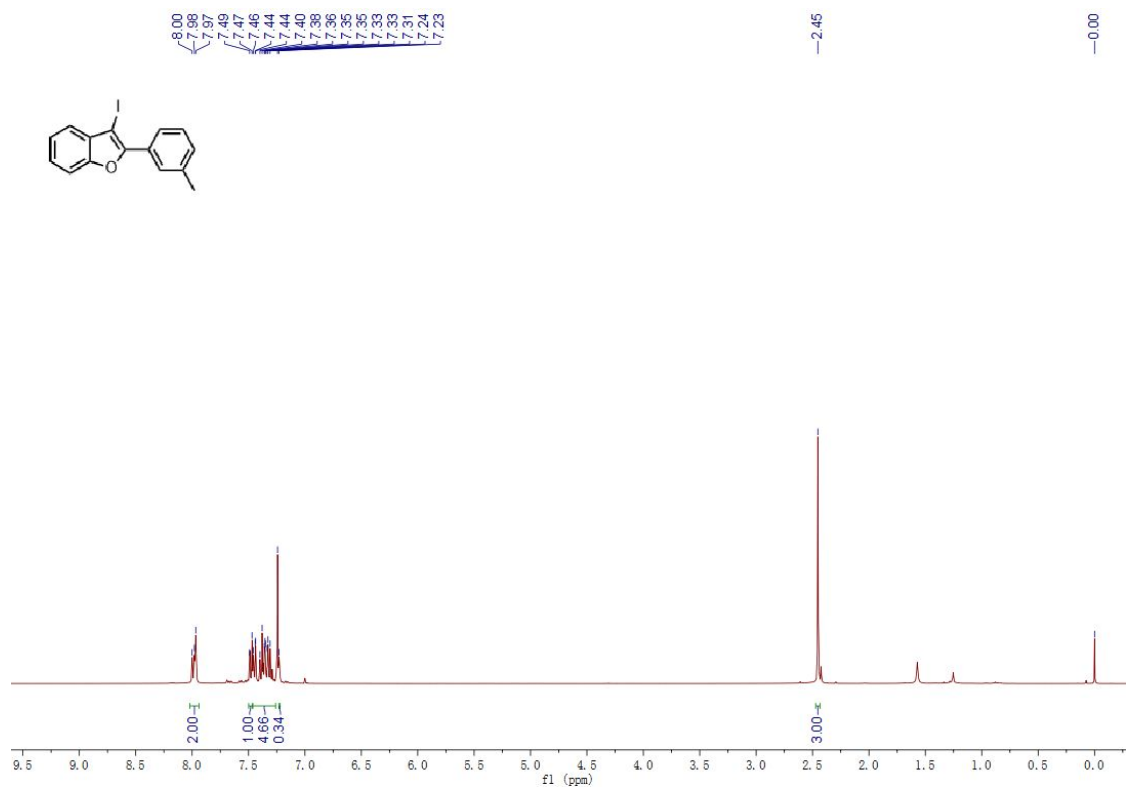
**Figure S72.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5aa** (100 Hz, CDCl<sub>3</sub>)



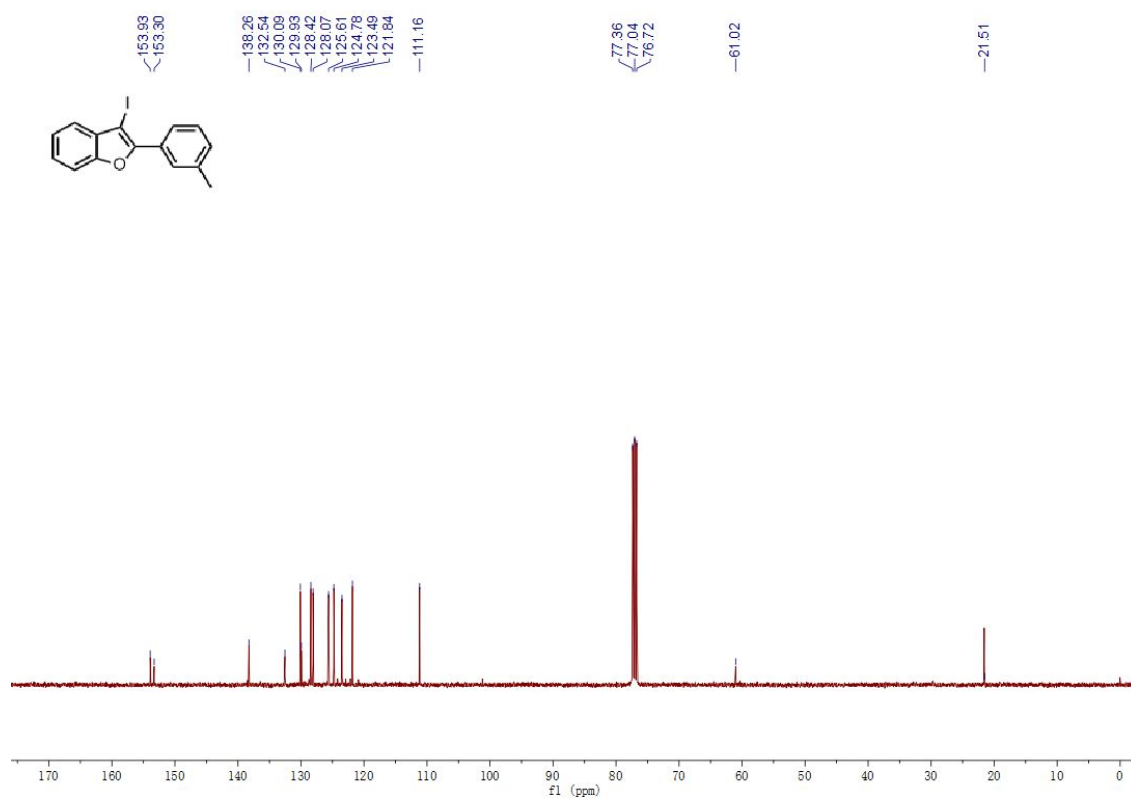
**Figure S73.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ab** (400 Hz, CDCl<sub>3</sub>)



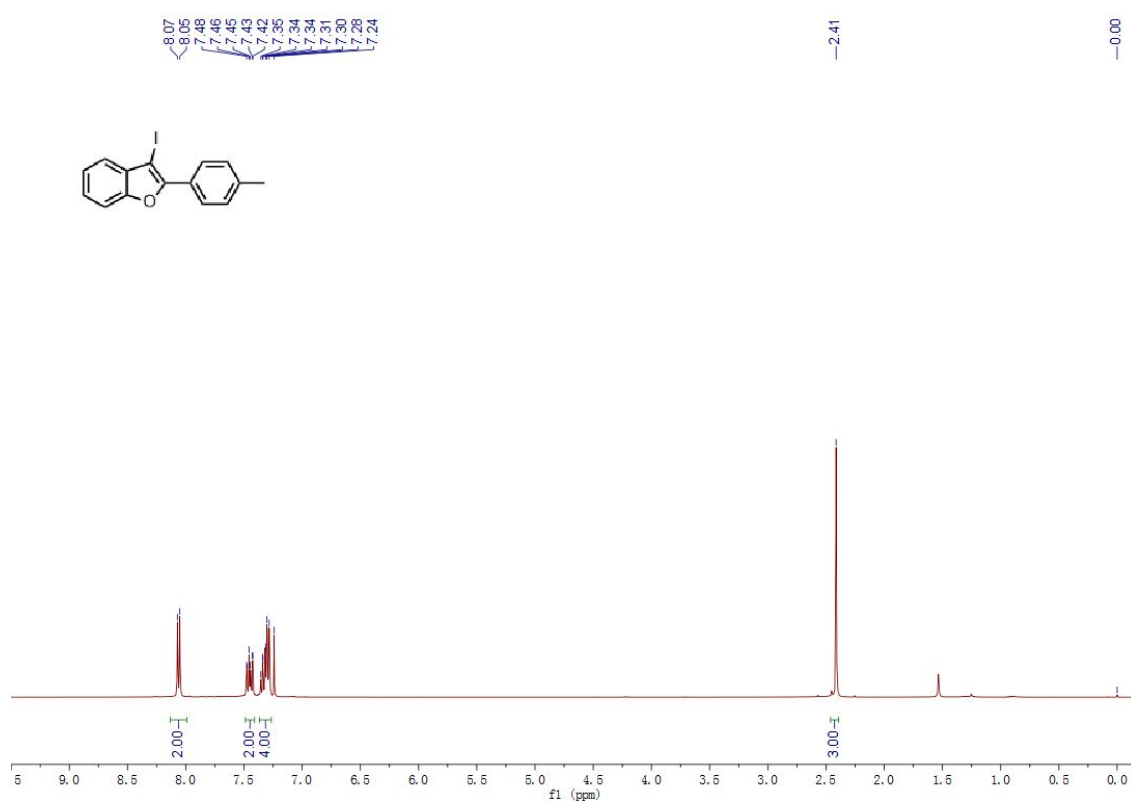
**Figure S74.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5ab** (100 Hz, CDCl<sub>3</sub>)



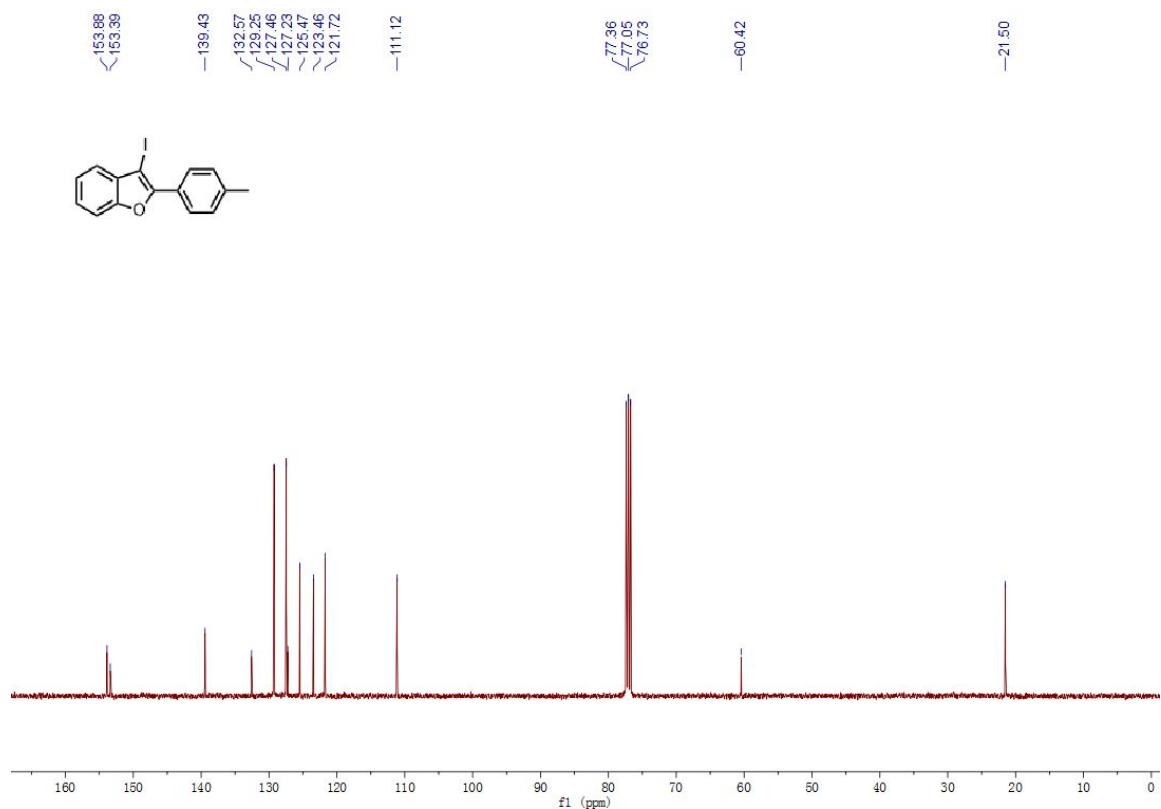
**Figure S75.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ac** (400 Hz, CDCl<sub>3</sub>)



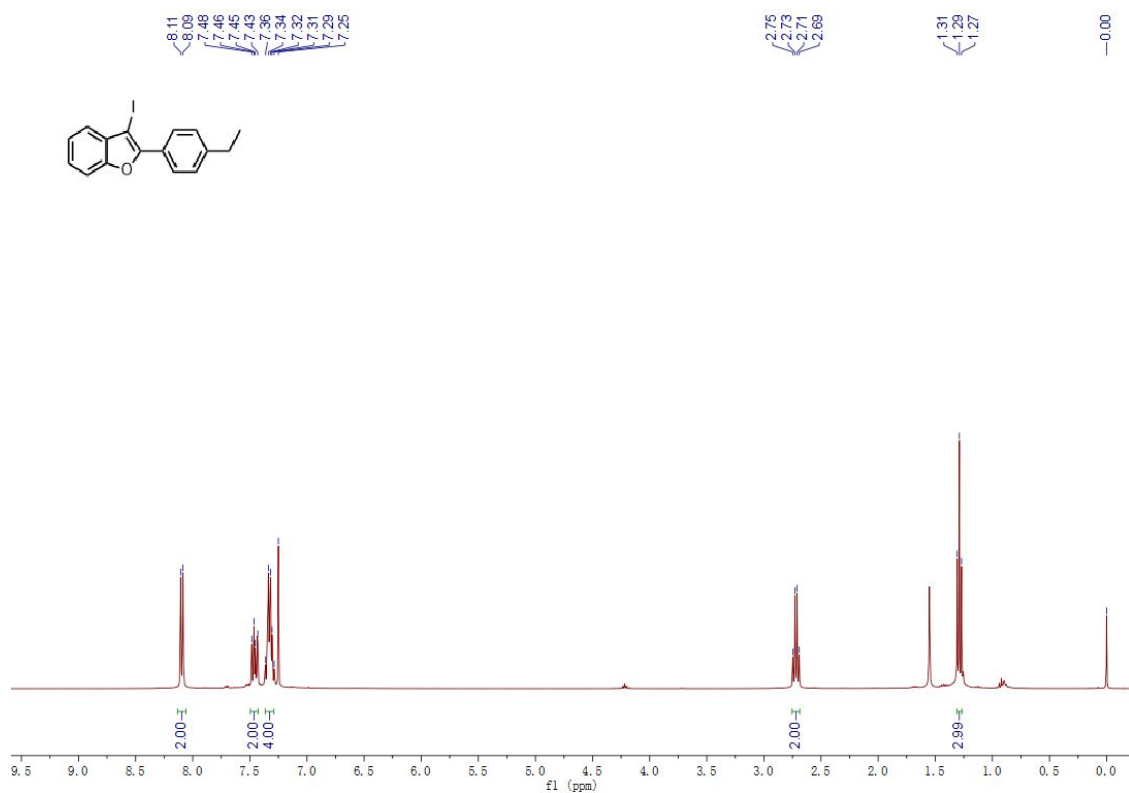
**Figure S76.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5ac** (100 Hz, CDCl<sub>3</sub>)



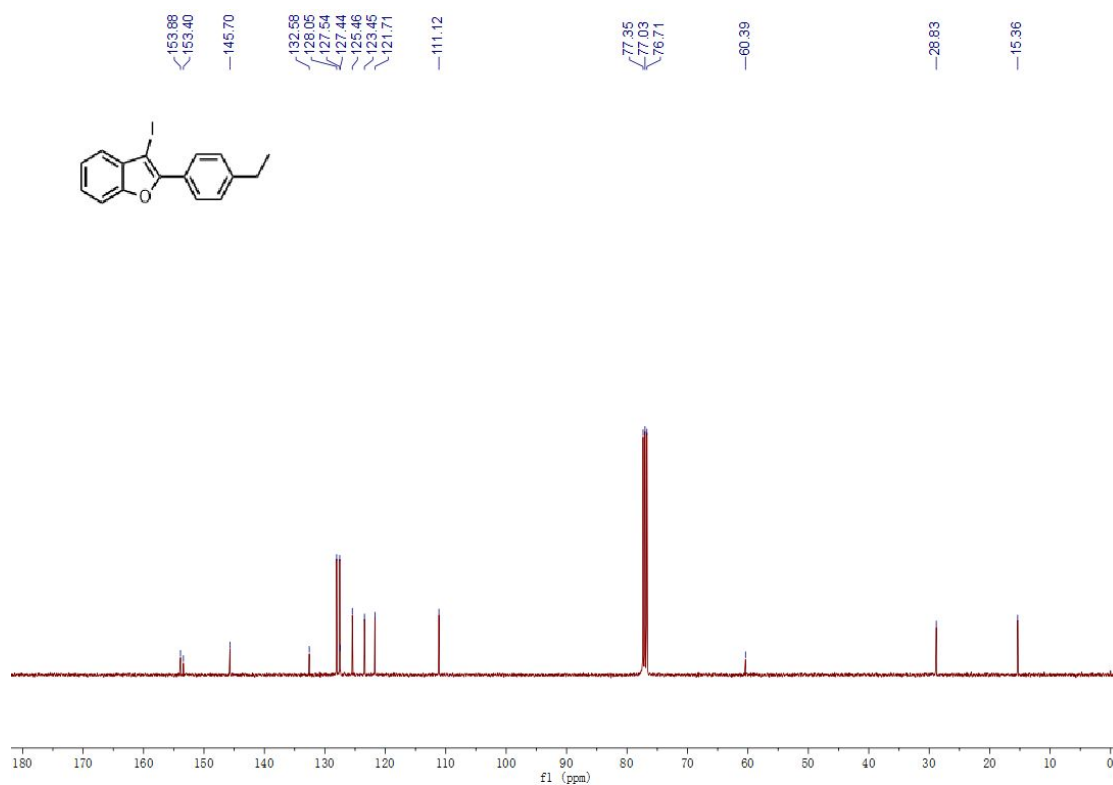
**Figure S77.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ad** (400 Hz, CDCl<sub>3</sub>)



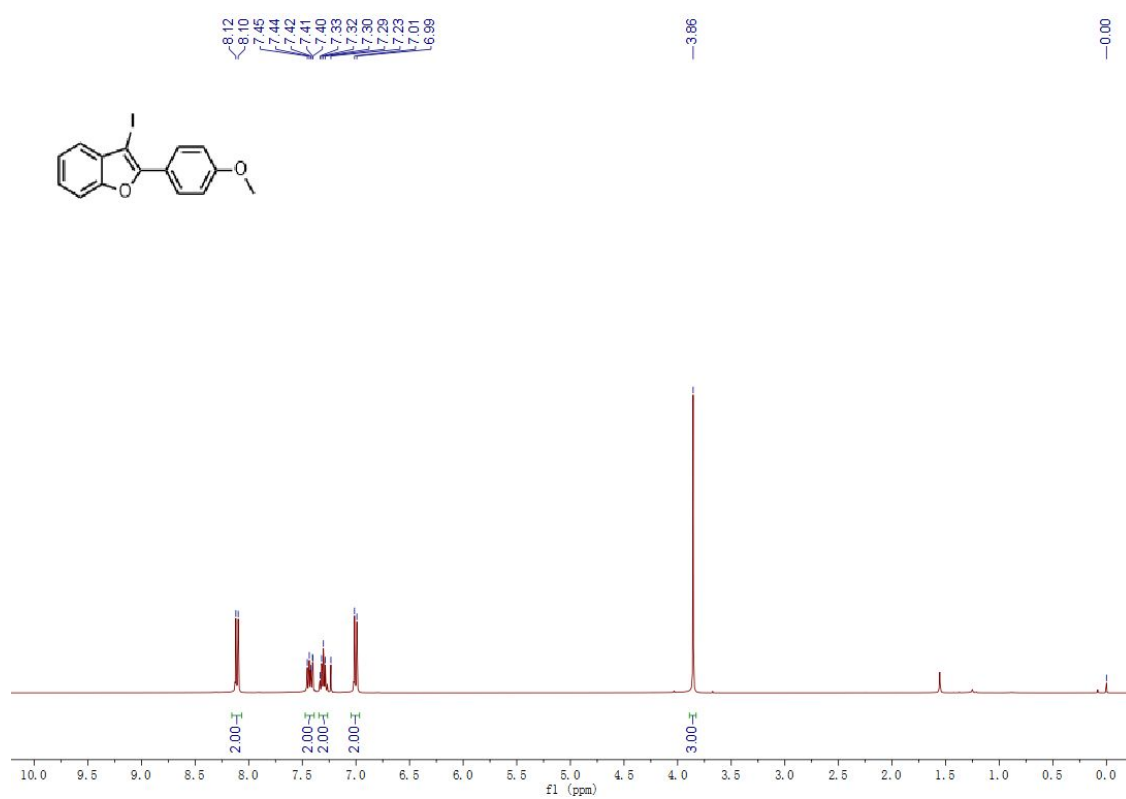
**Figure S78.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5ad** (100 Hz, CDCl<sub>3</sub>)



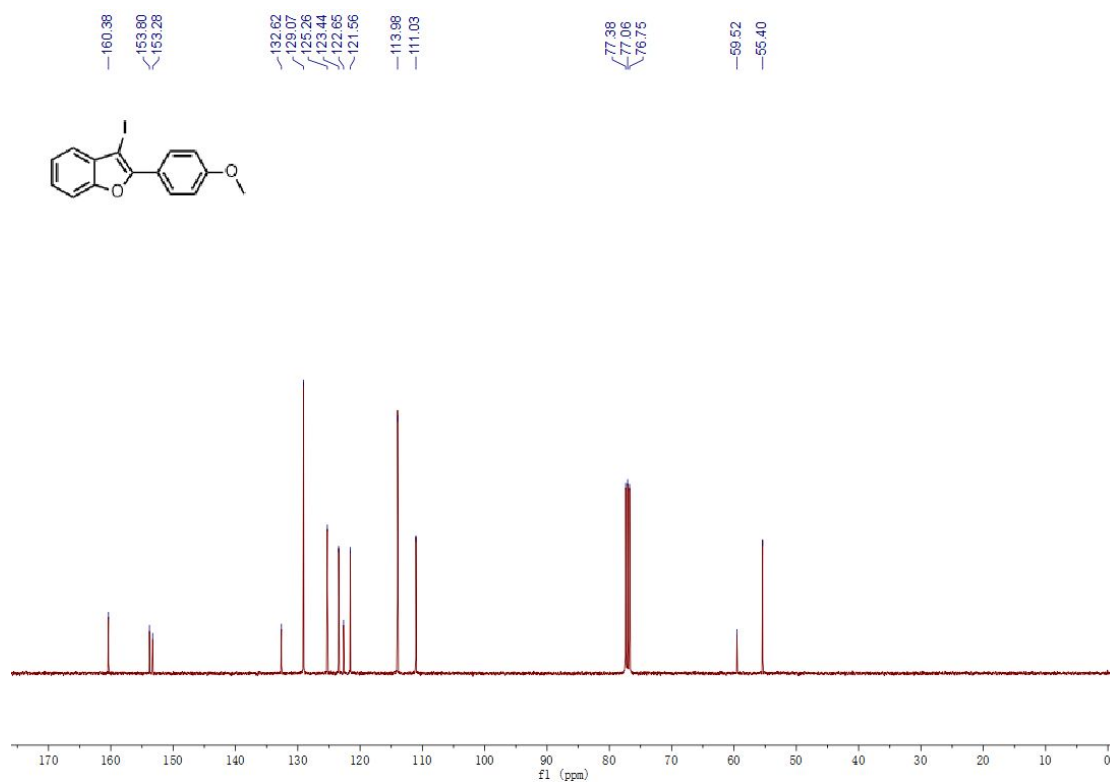
**Figure S79.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ae** (400 Hz, CDCl<sub>3</sub>)



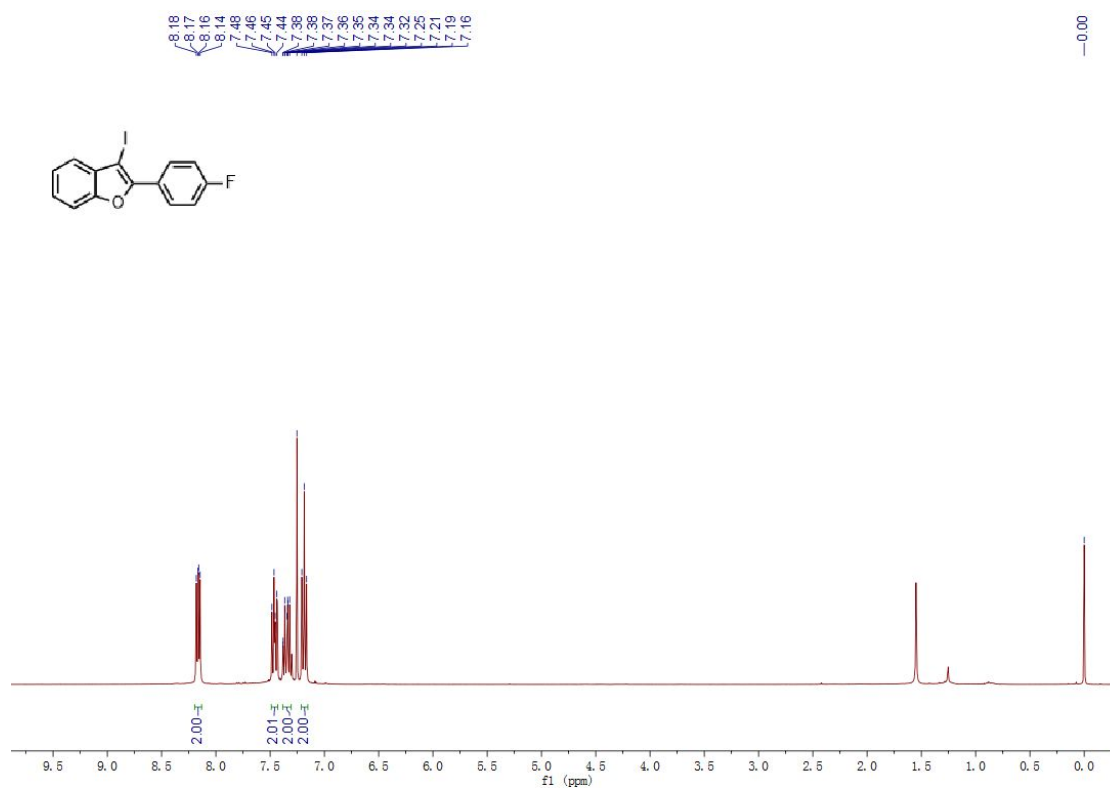
**Figure S80.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5ae** (100 Hz, CDCl<sub>3</sub>)



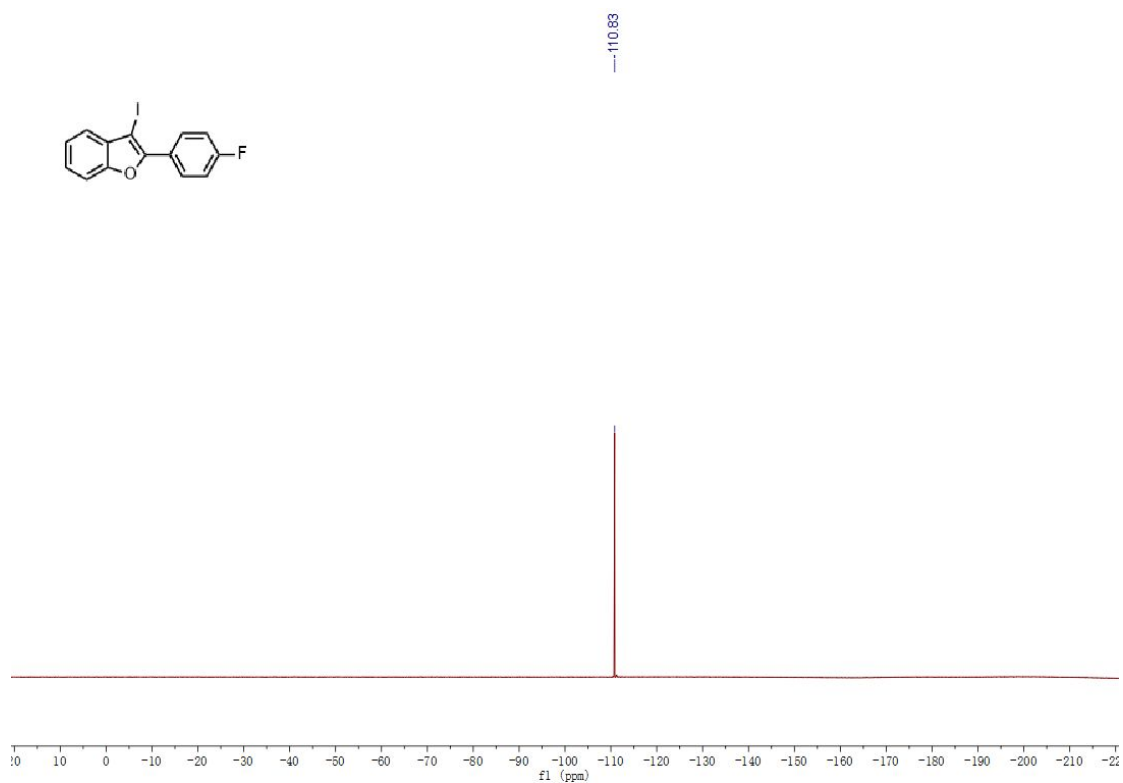
**Figure S81.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5af** (400 Hz, CDCl<sub>3</sub>)



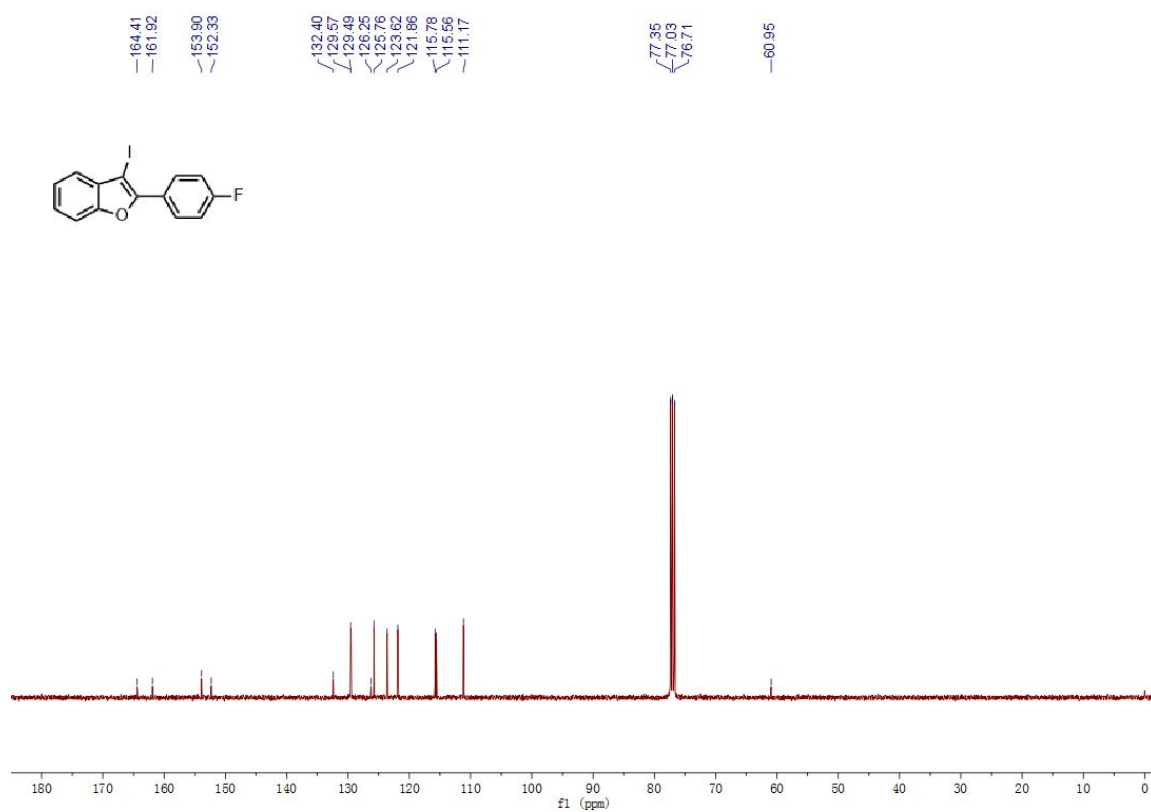
**Figure S82.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5af** (100 Hz, CDCl<sub>3</sub>)



**Figure S83.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ag** (400 Hz, CDCl<sub>3</sub>)

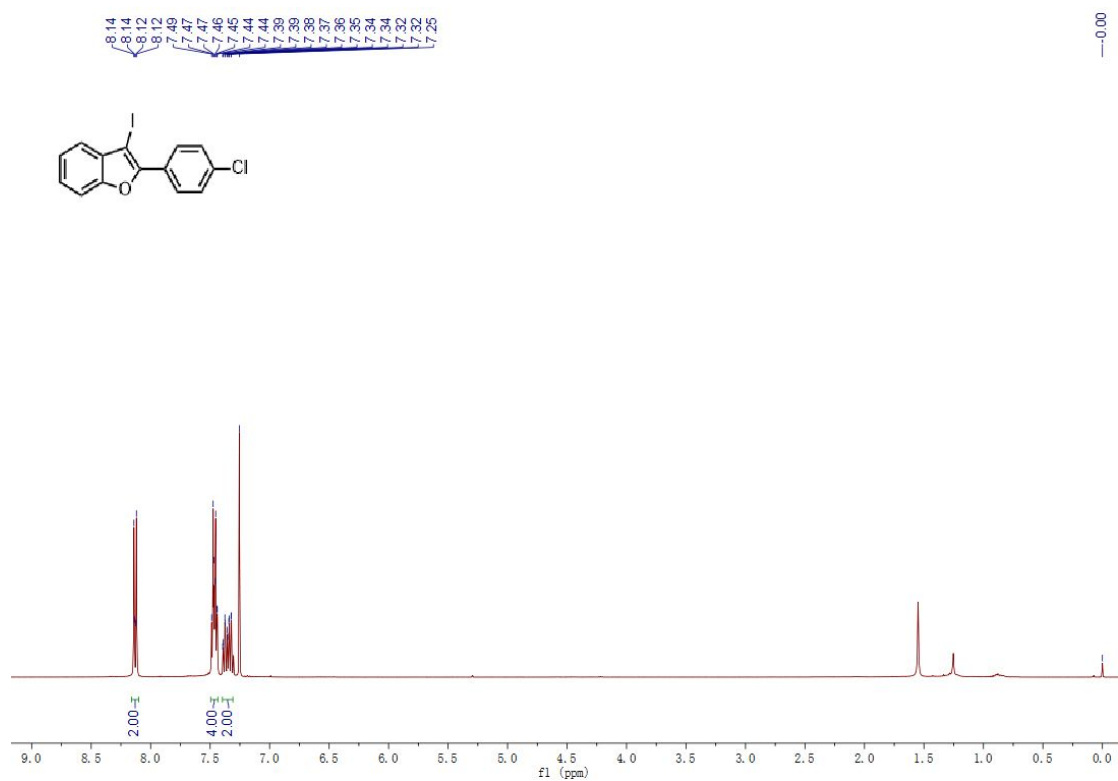


**Figure S84.** Copies of  $^{19}\text{F}$  NMR Spectrum for Compound **5ag** (376 Hz,  $\text{CDCl}_3$ )

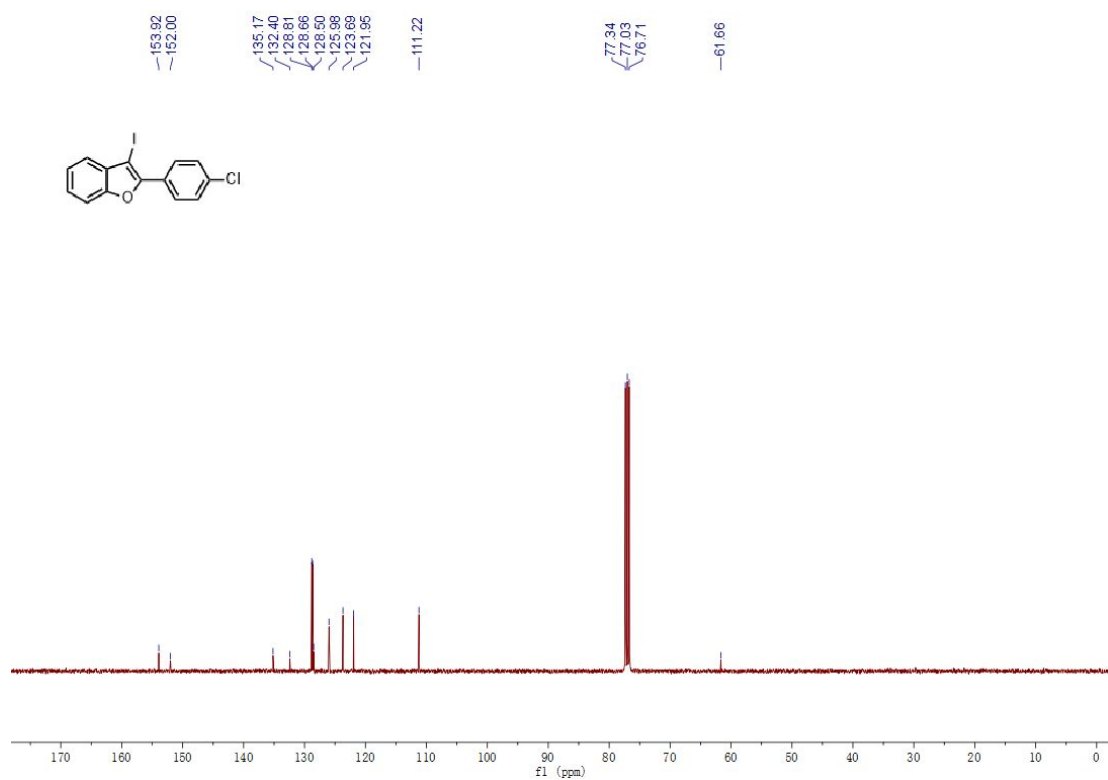


**Figure S85.** Copies of  $^{13}\text{C}$  NMR Spectrum for Compound **5ag** (100 Hz,  $\text{CDCl}_3$ )

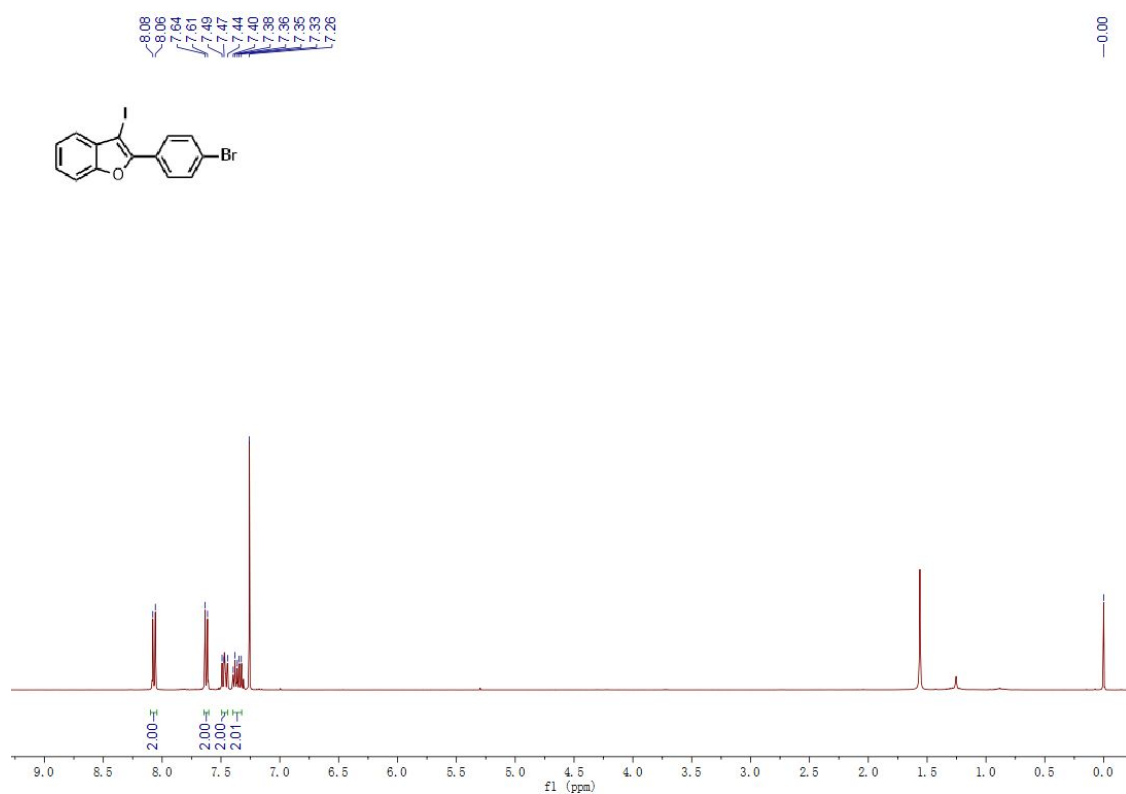




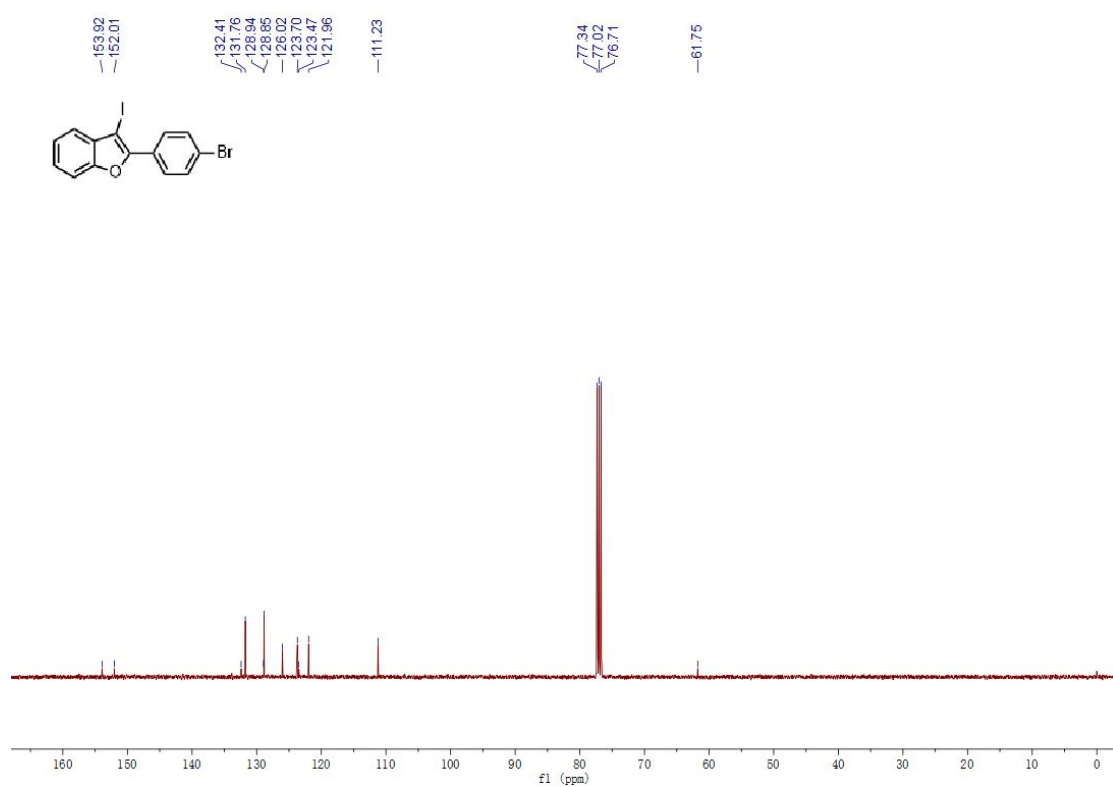
**Figure S86.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ah** (400 Hz, CDCl<sub>3</sub>)



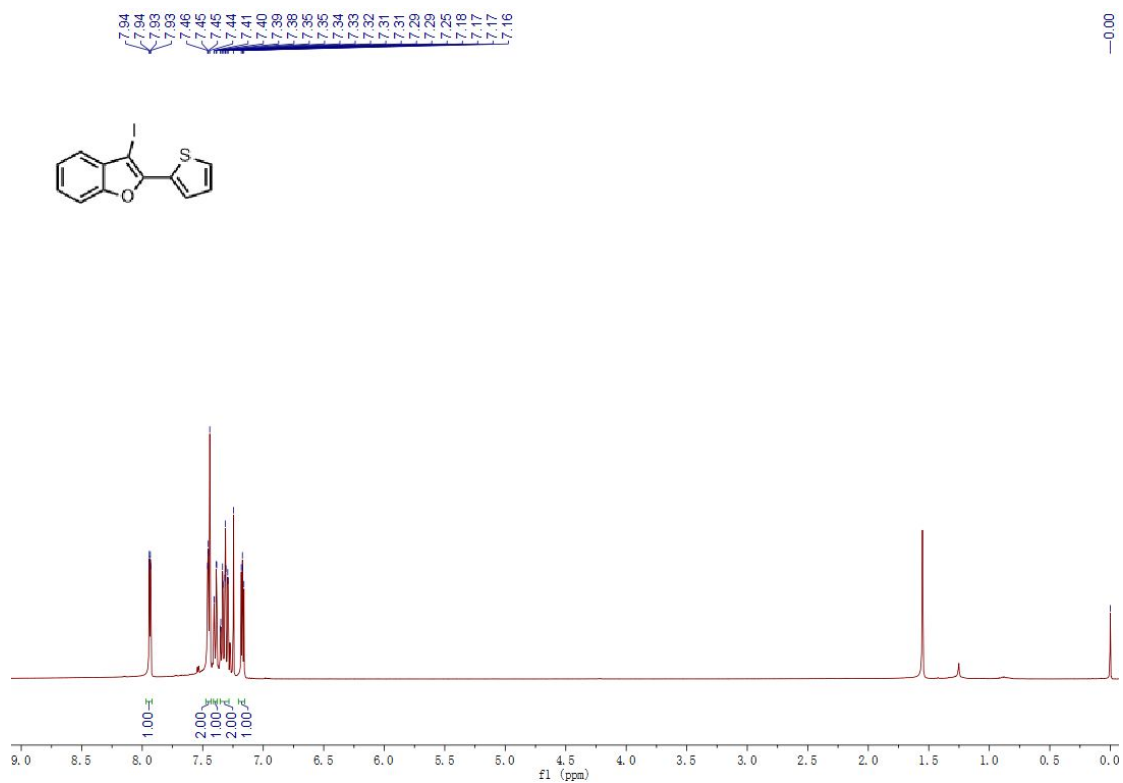
**Figure S87.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5ah** (100 Hz, CDCl<sub>3</sub>)



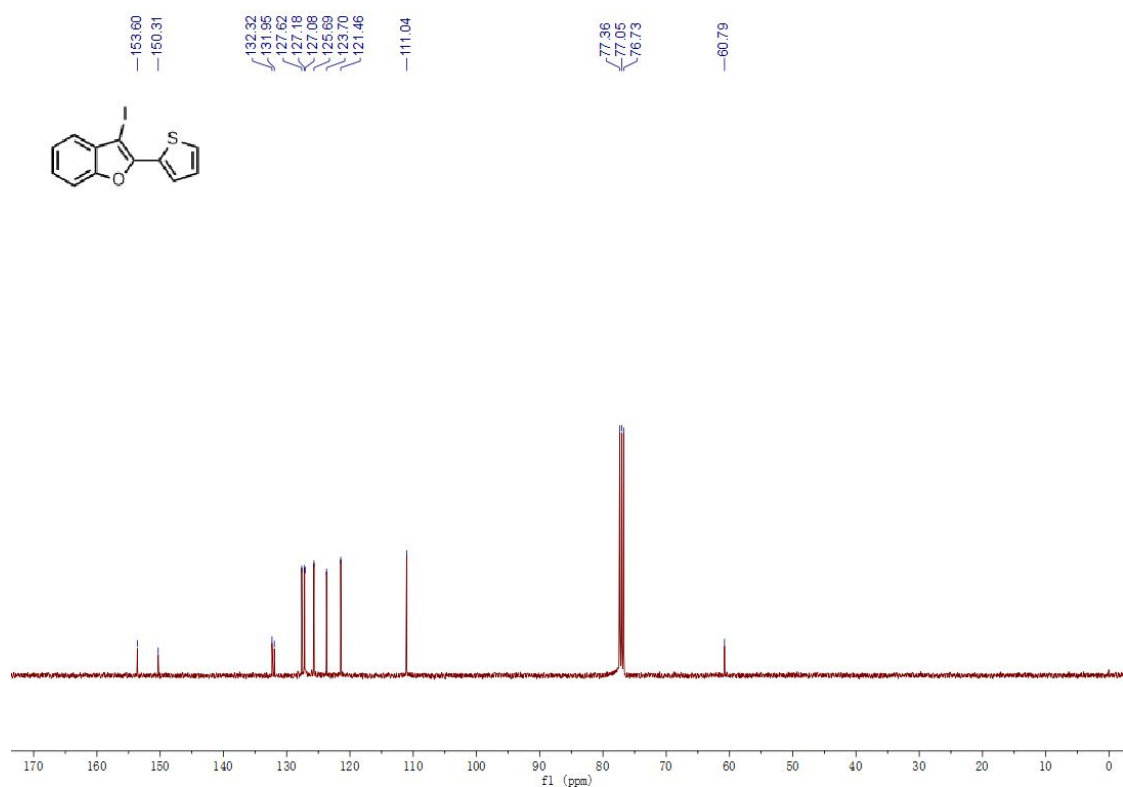
**Figure S88.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ai** (400 Hz, CDCl<sub>3</sub>)



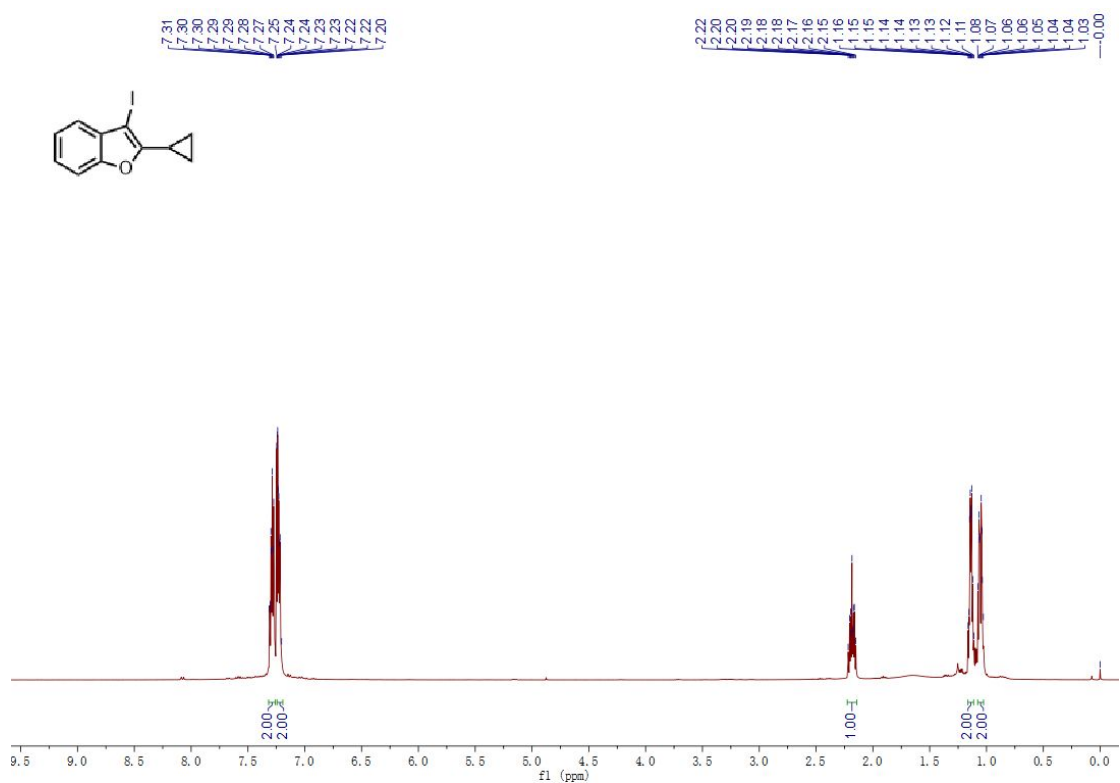
**Figure S89.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5ai** (100 Hz, CDCl<sub>3</sub>)



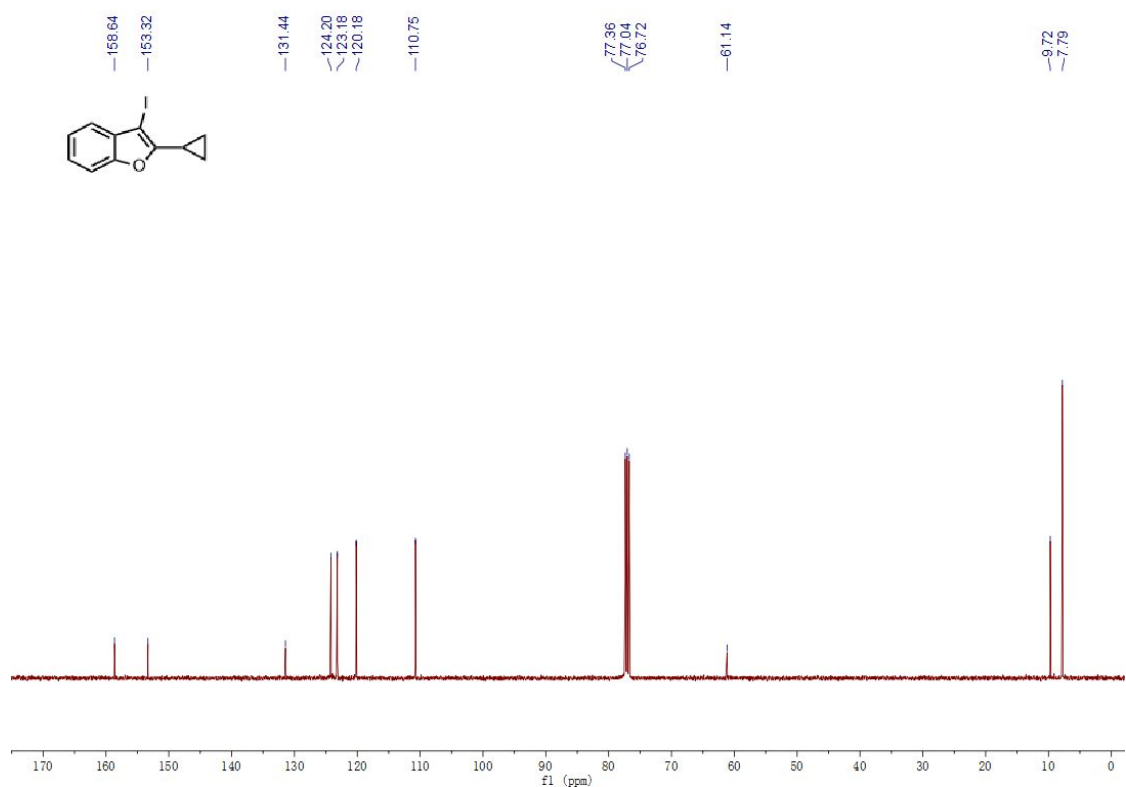
**Figure S90.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5aj** (400 Hz, CDCl<sub>3</sub>)



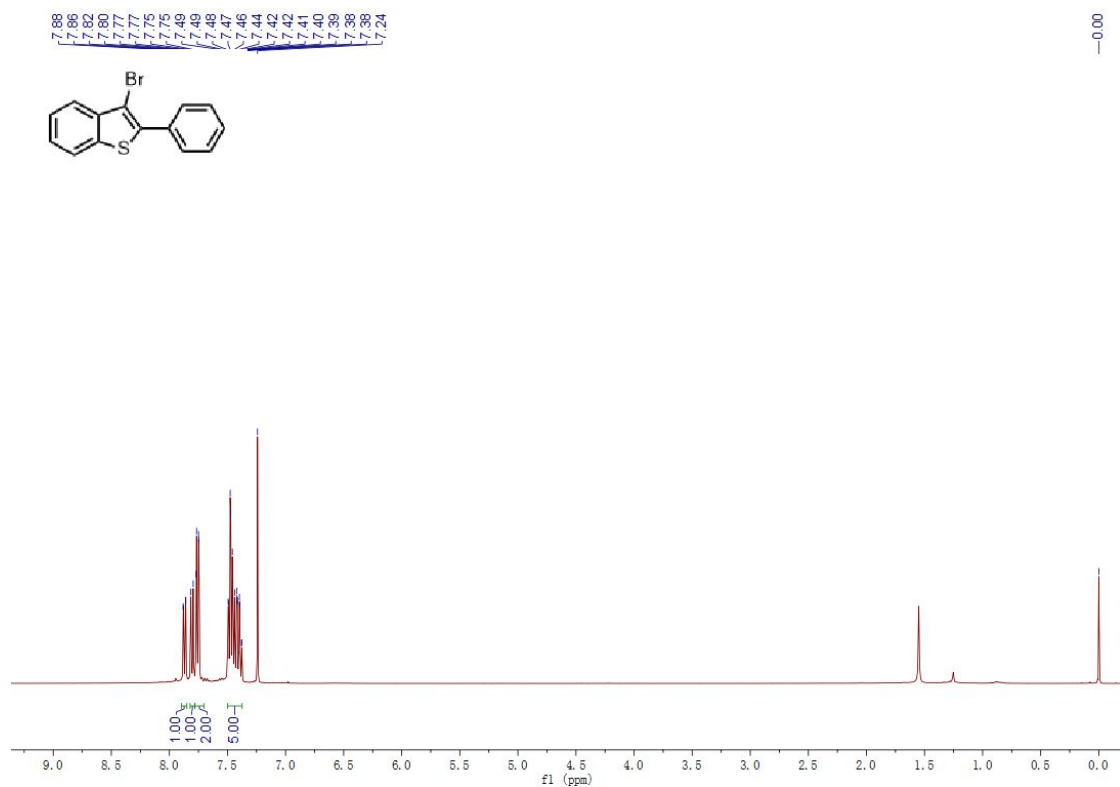
**Figure S91.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5aj** (100 Hz, CDCl<sub>3</sub>)



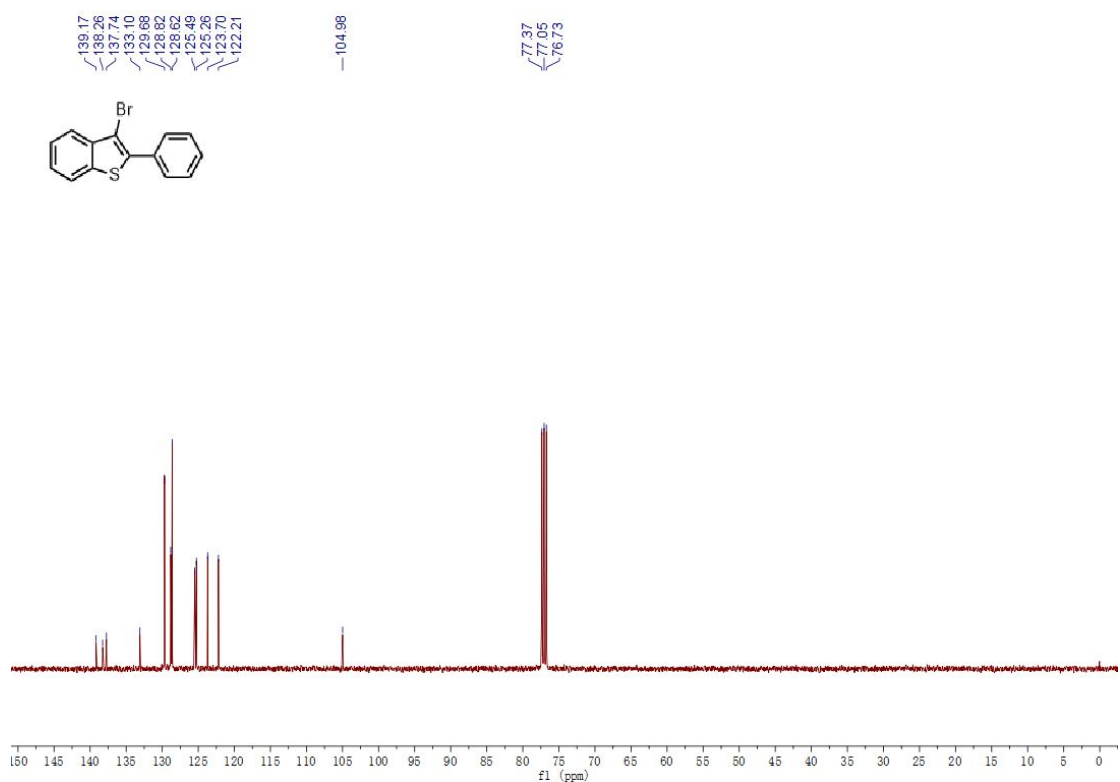
**Figure S92.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ak** (400 Hz, CDCl<sub>3</sub>)



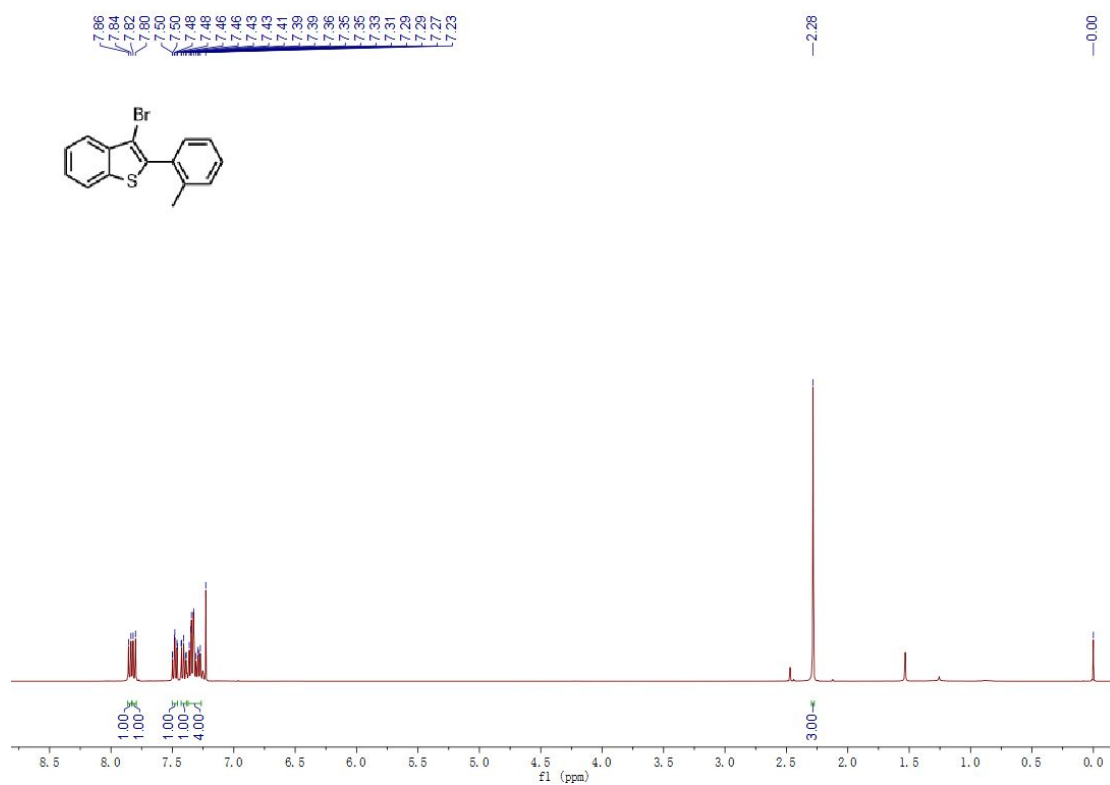
**Figure S93.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5ak** (100 Hz, CDCl<sub>3</sub>)



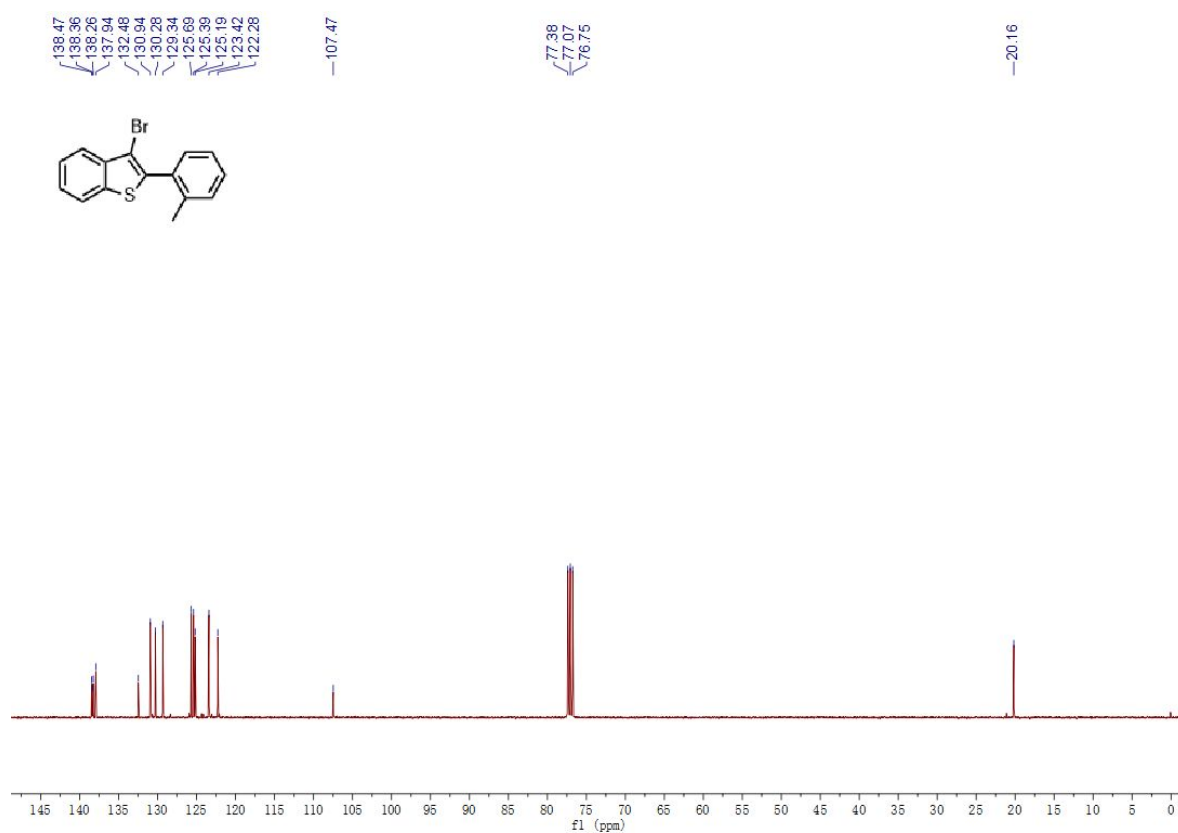
**Figure S94.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6a** (400 Hz, CDCl<sub>3</sub>)



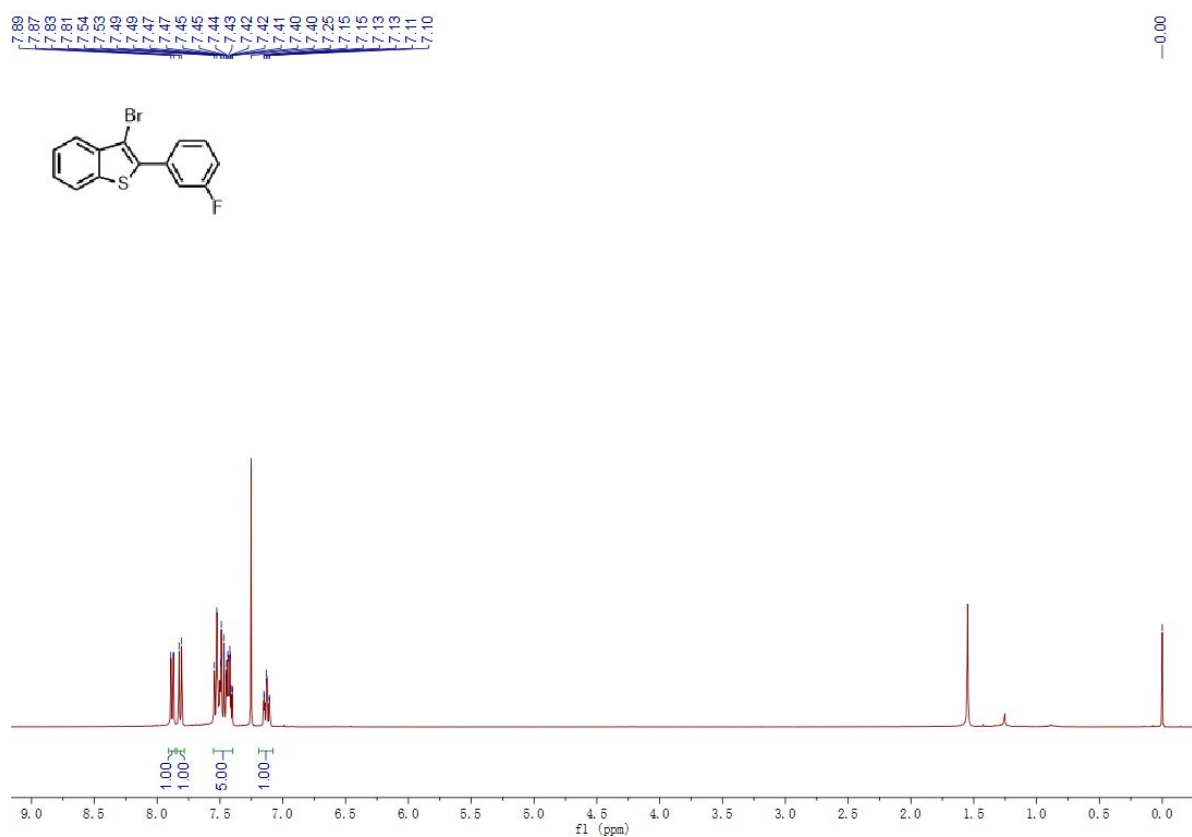
**Figure S95.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6a** (100 Hz, CDCl<sub>3</sub>)



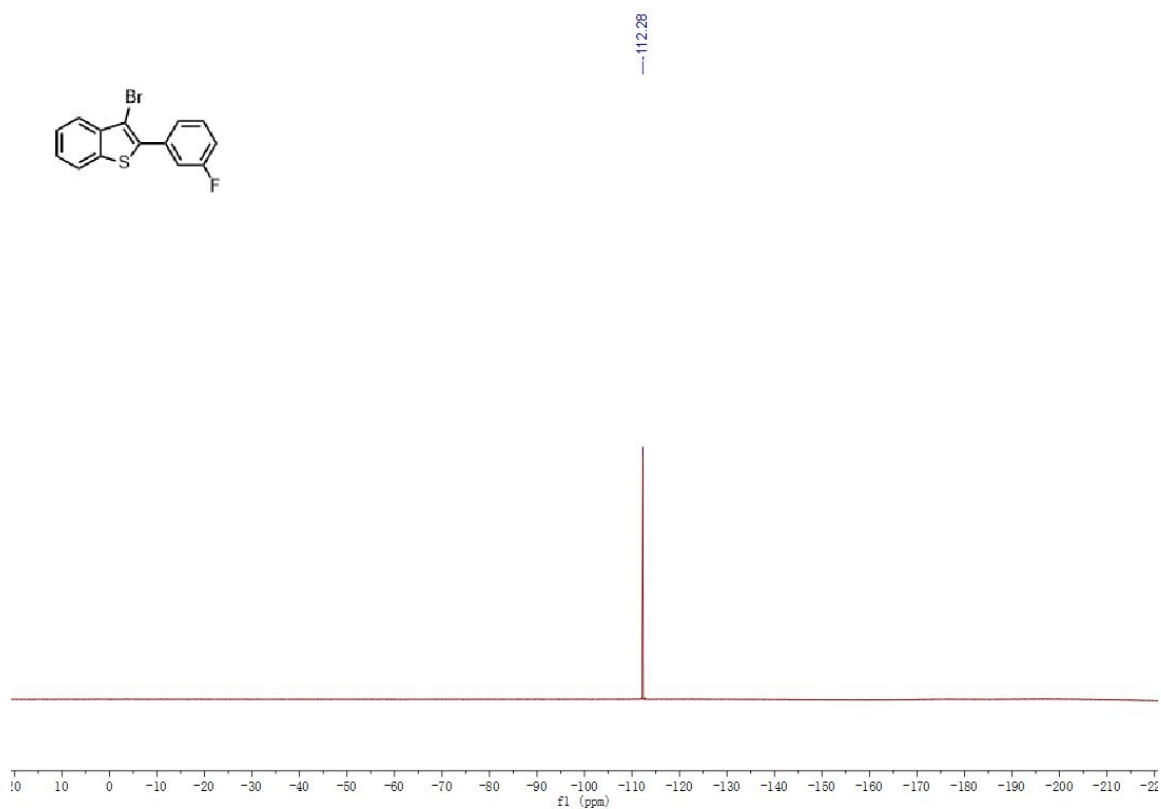
**Figure S96.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6b** (400 Hz, CDCl<sub>3</sub>)



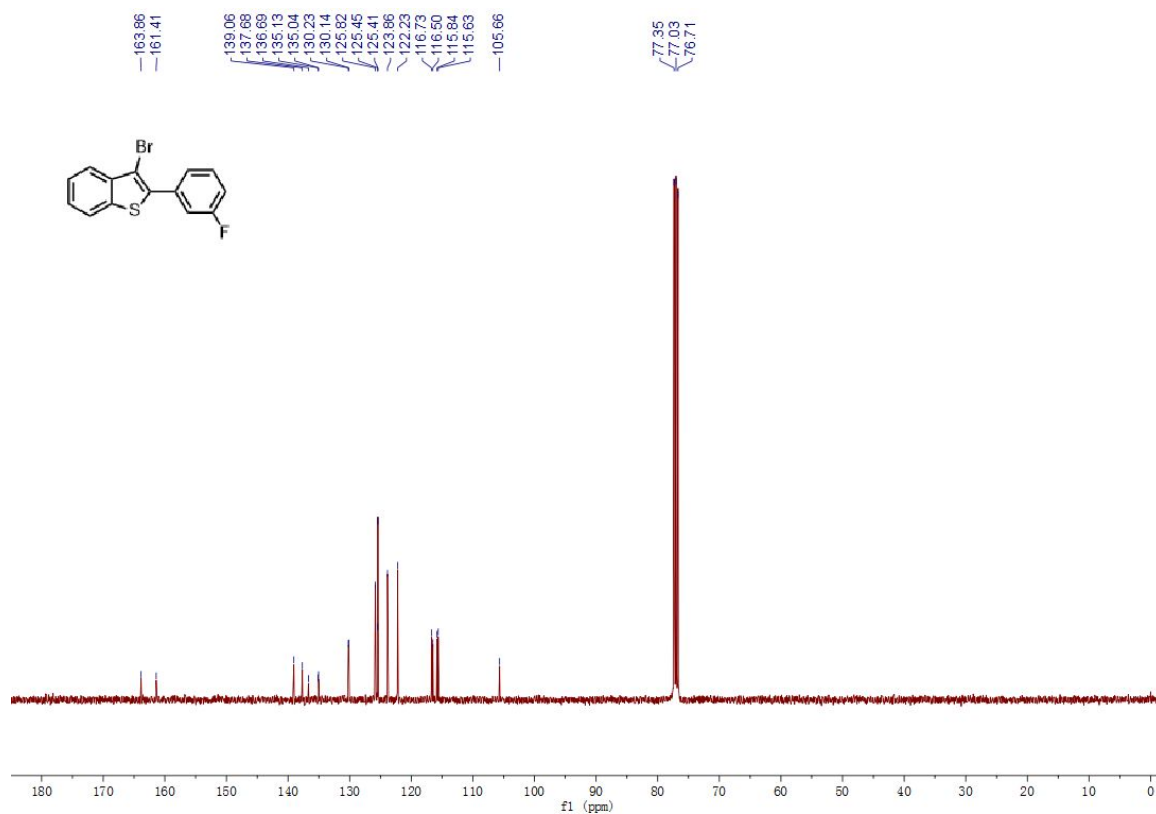
**Figure S97.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6b** (100 Hz, CDCl<sub>3</sub>)



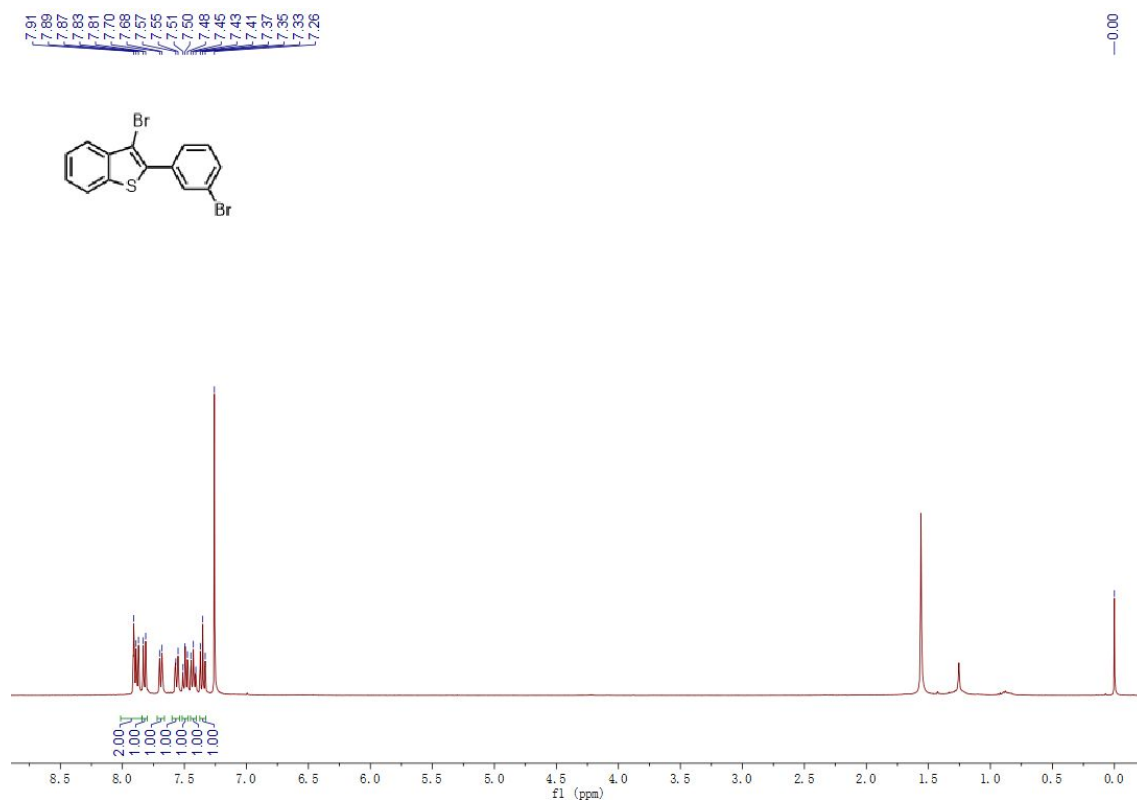
**Figure S98.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6c** (400 Hz, CDCl<sub>3</sub>)



**Figure S99.** Copies of <sup>19</sup>F NMR Spectrum for Compound **6c** (376 Hz, CDCl<sub>3</sub>)

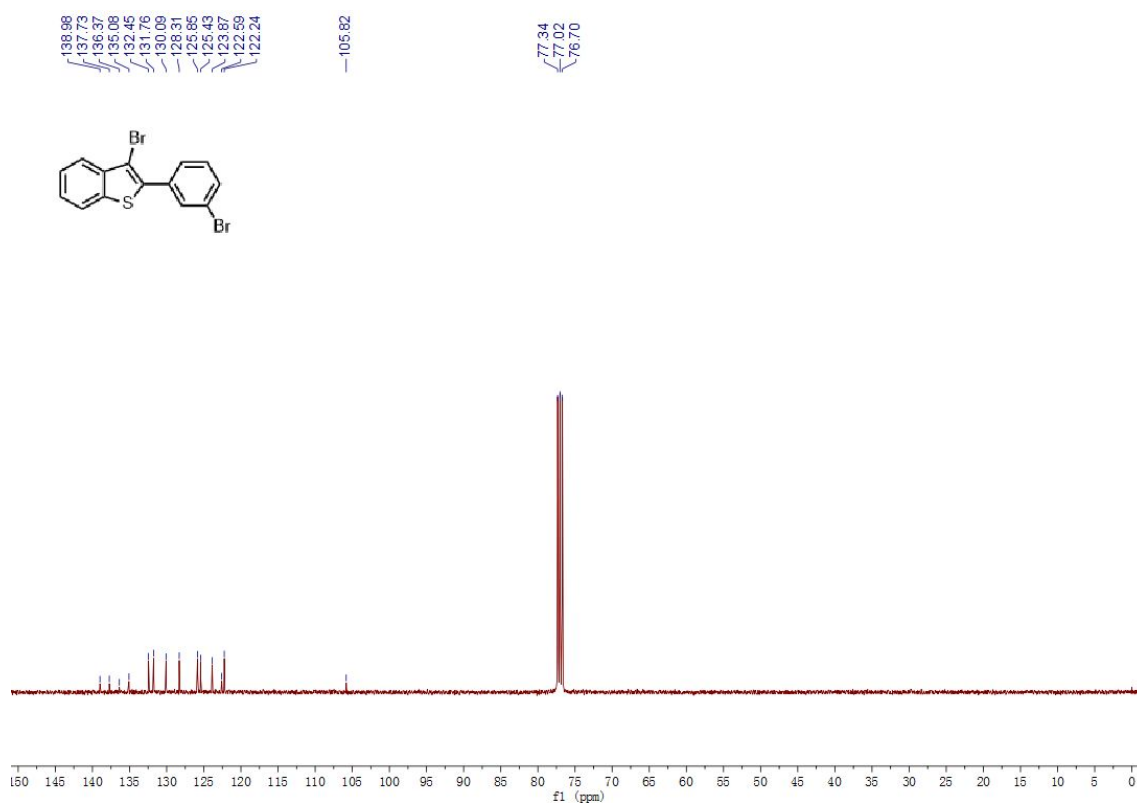


**Figure S100.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6c** (100 Hz, CDCl<sub>3</sub>)

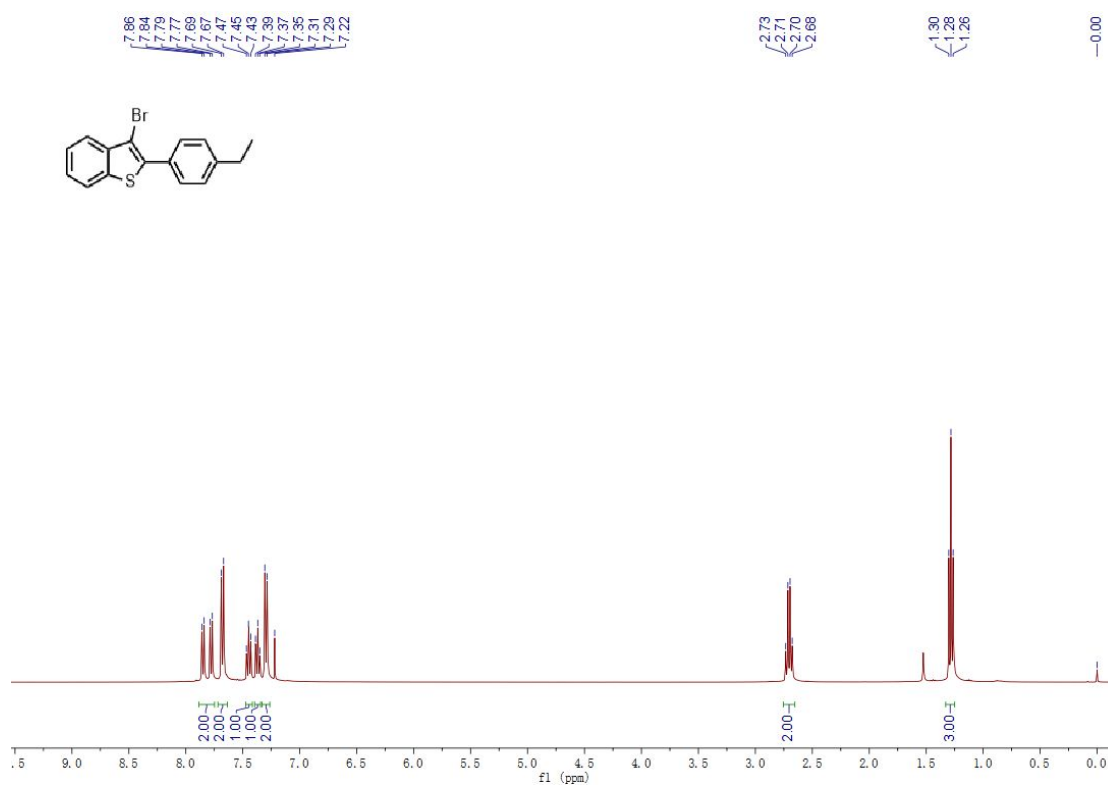


**Figure S101.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6d** (400 Hz, CDCl<sub>3</sub>)

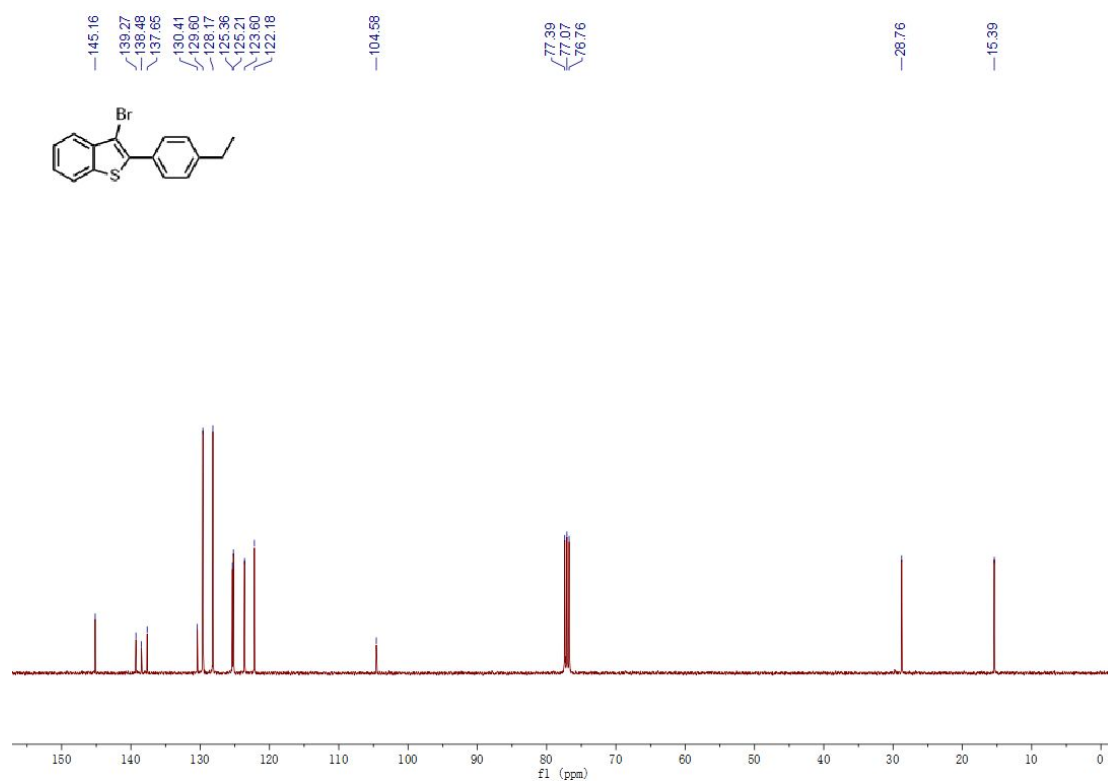




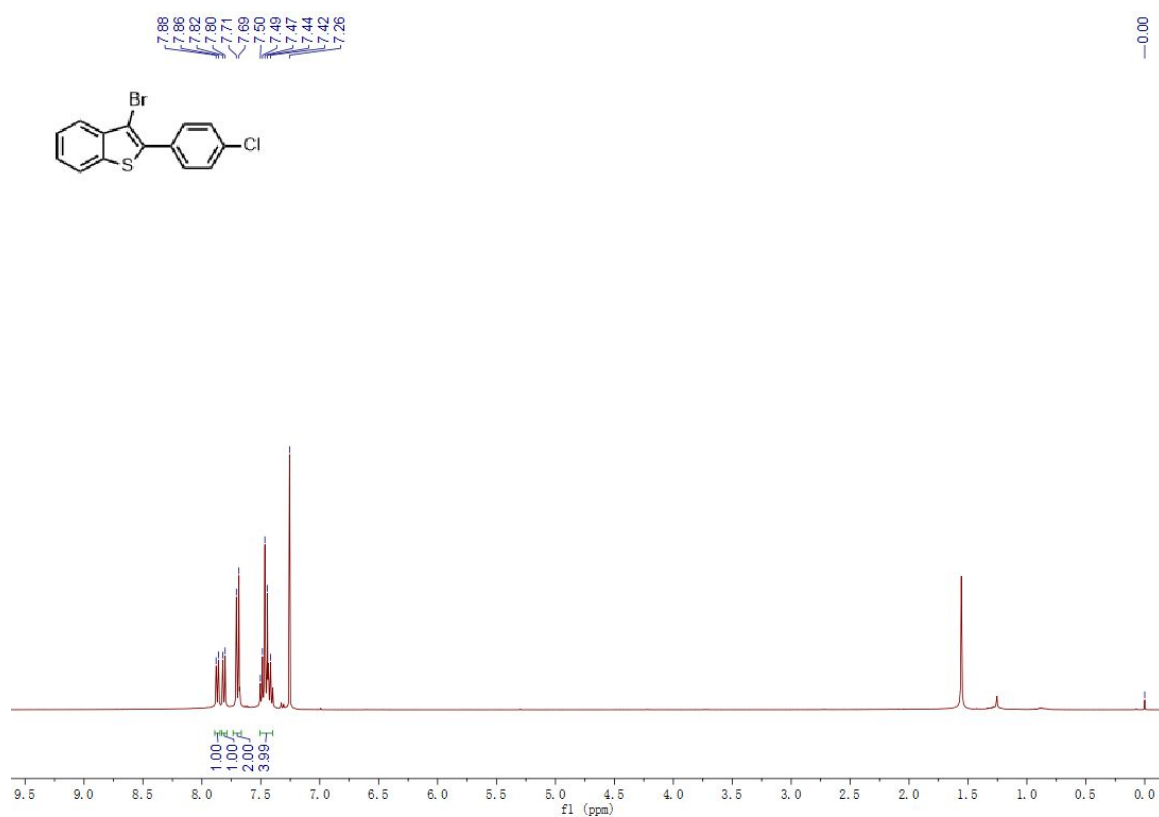
**Figure S102.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6d** (100 Hz, CDCl<sub>3</sub>)



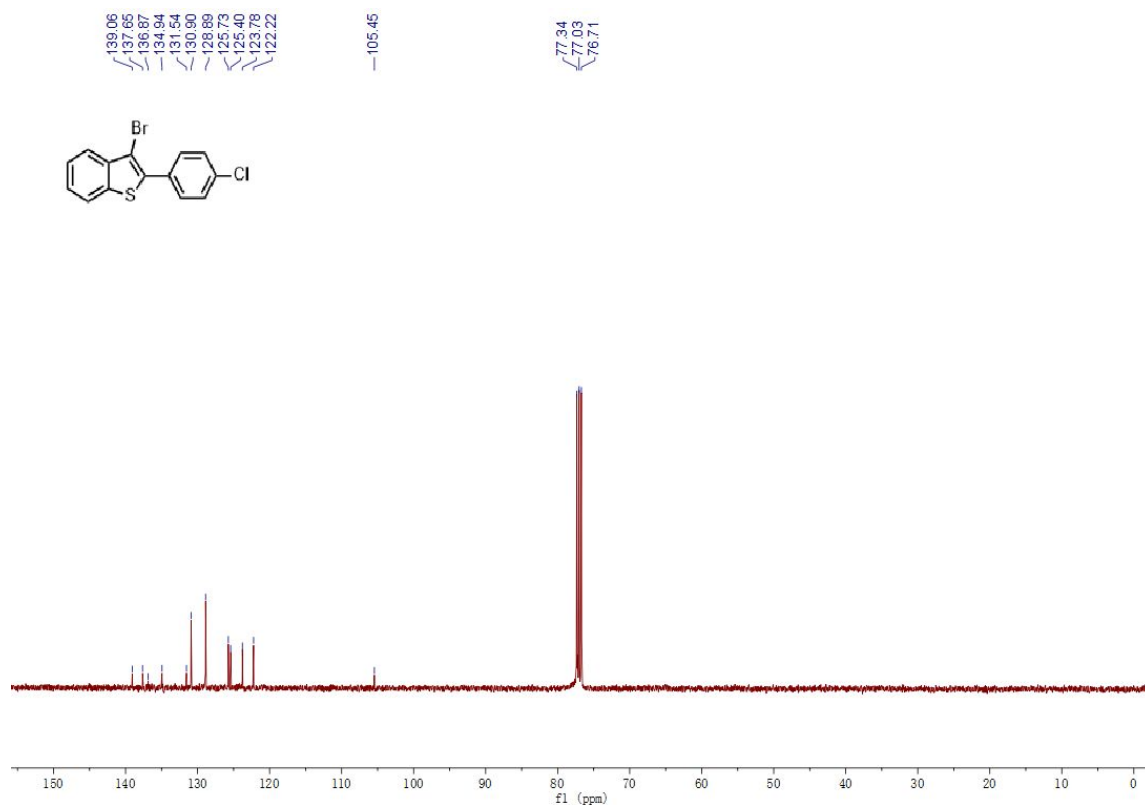
**Figure S103.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6e** (400 Hz, CDCl<sub>3</sub>)



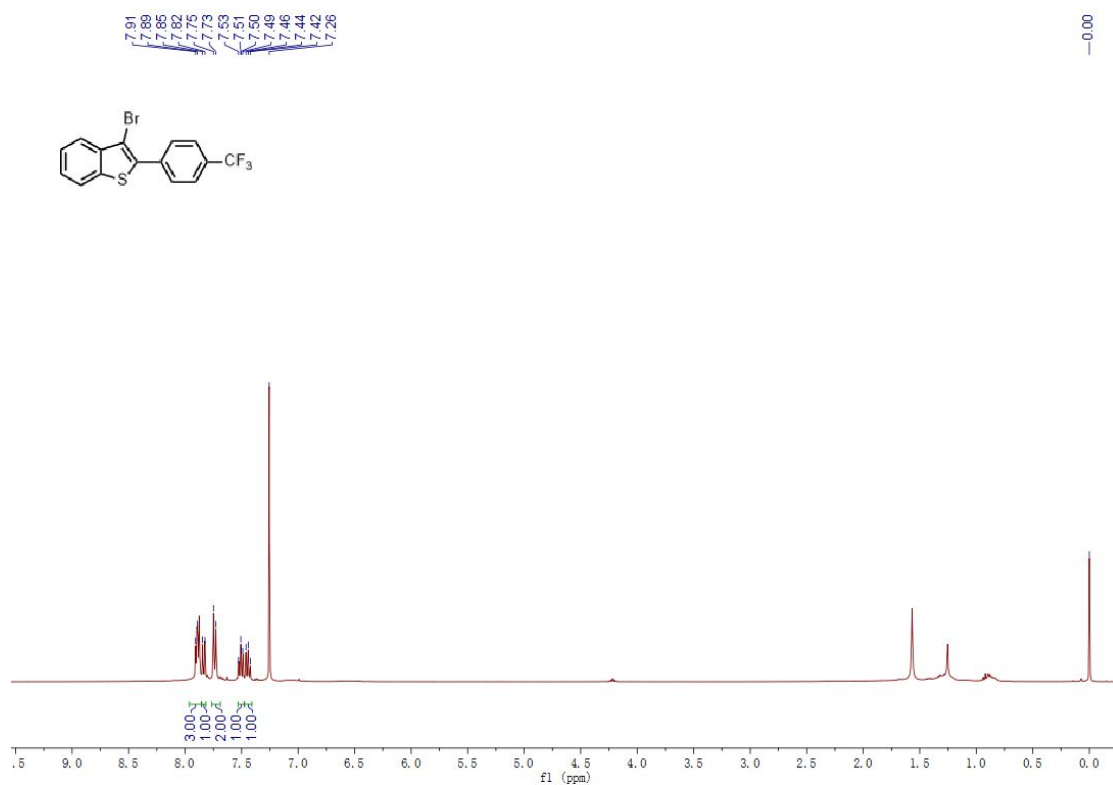
**Figure S104.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6e** (100 Hz, CDCl<sub>3</sub>)



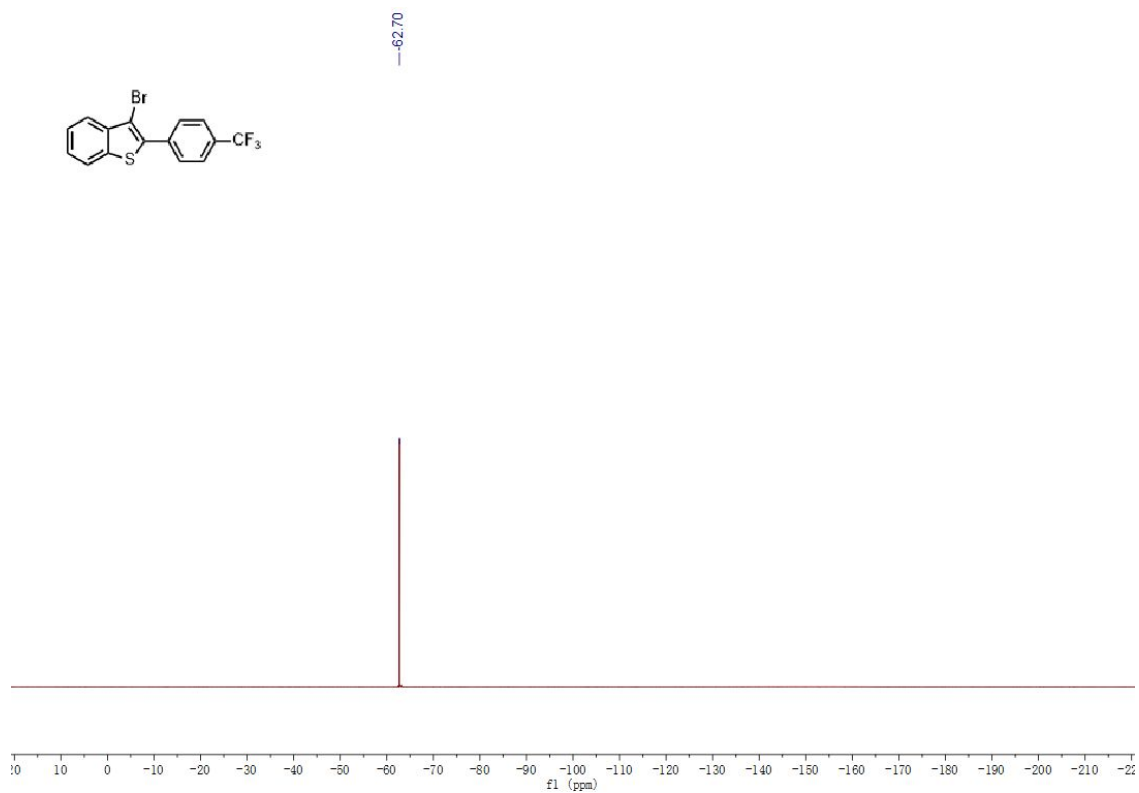
**Figure S105.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6f** (400 Hz, CDCl<sub>3</sub>)



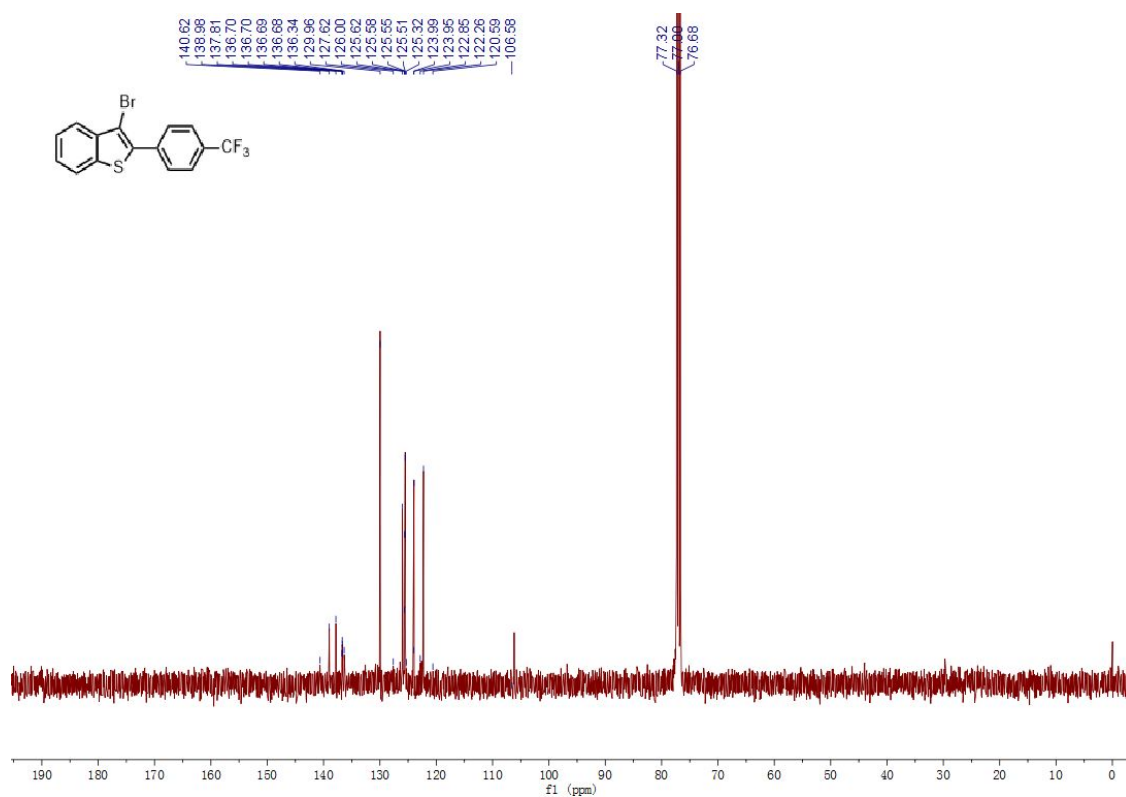
**Figure S106.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6f** (100 Hz, CDCl<sub>3</sub>)



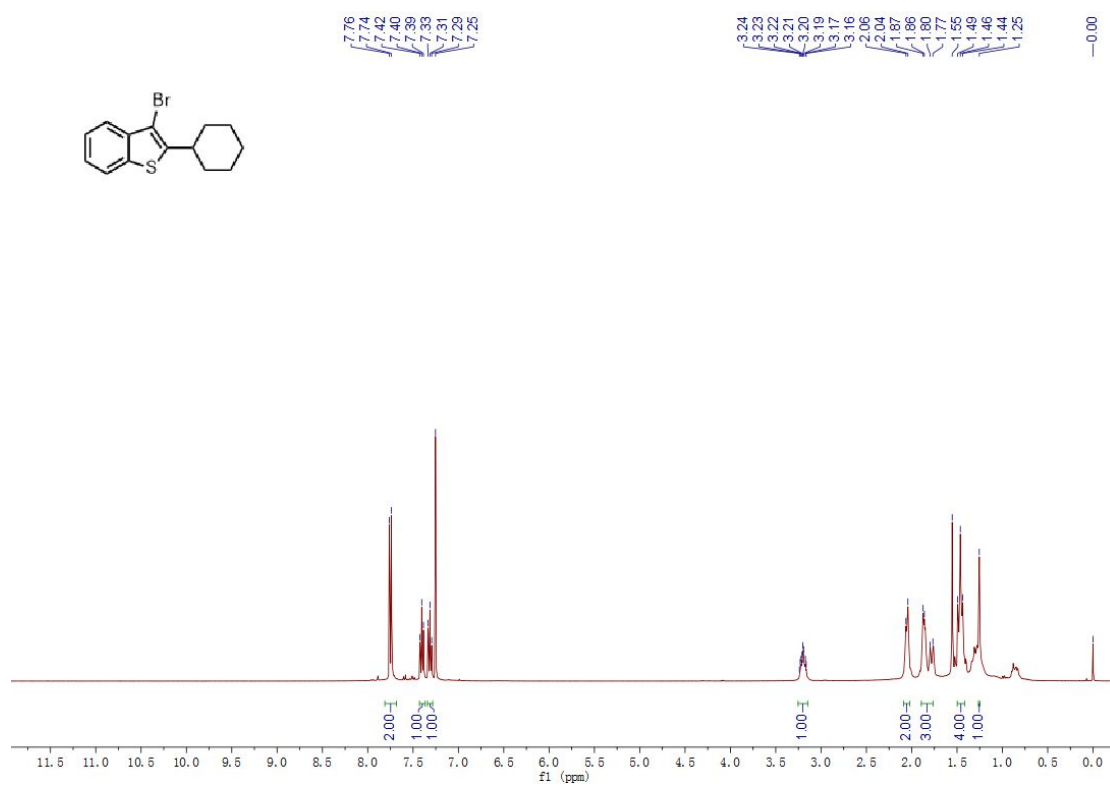
**Figure S107.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6g** (400 Hz, CDCl<sub>3</sub>)



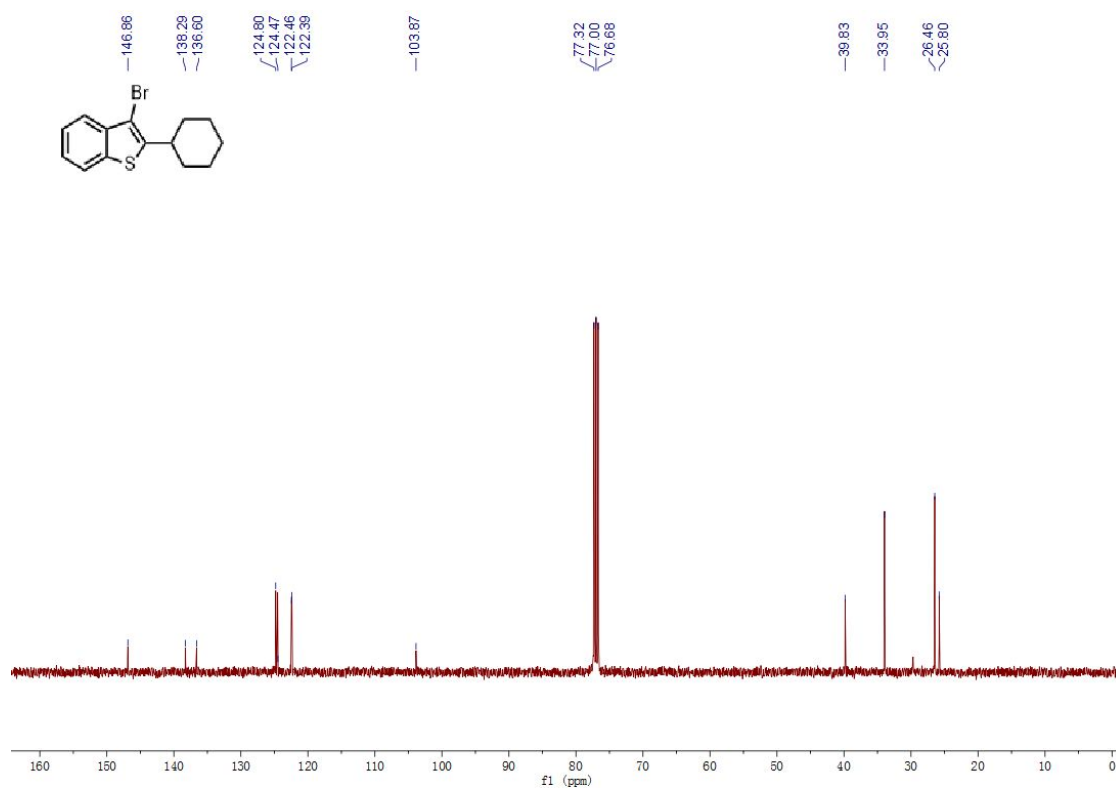
**Figure S108.** Copies of <sup>19</sup>F NMR Spectrum for Compound **6g** (376 Hz, CDCl<sub>3</sub>)



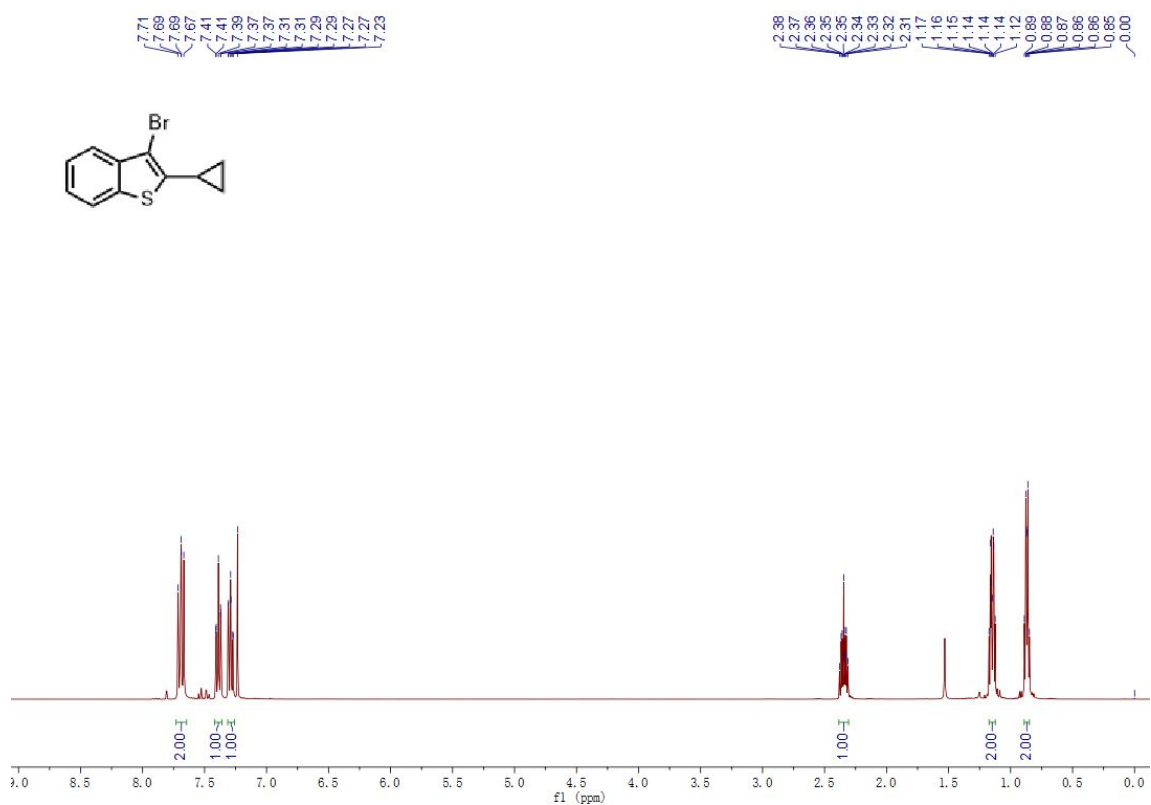
**Figure S109.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6g** (100 Hz, CDCl<sub>3</sub>)



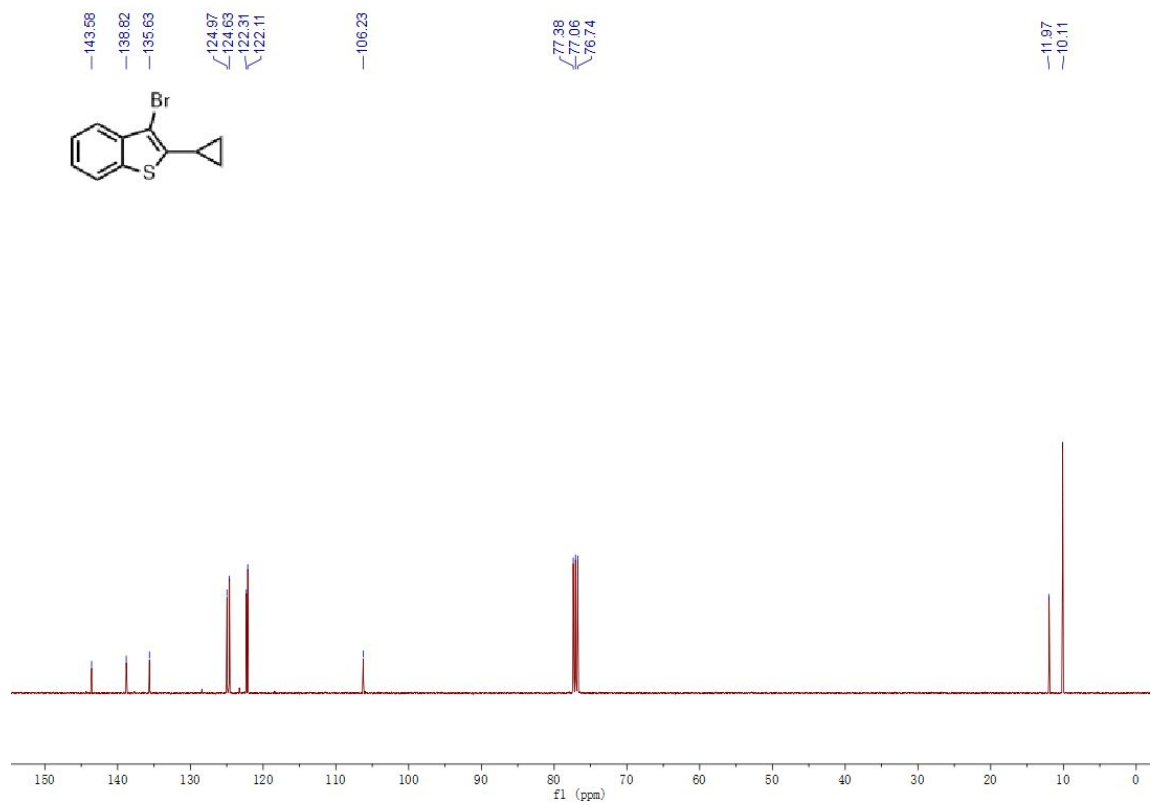
**Figure S110.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6h** (400 Hz, CDCl<sub>3</sub>)



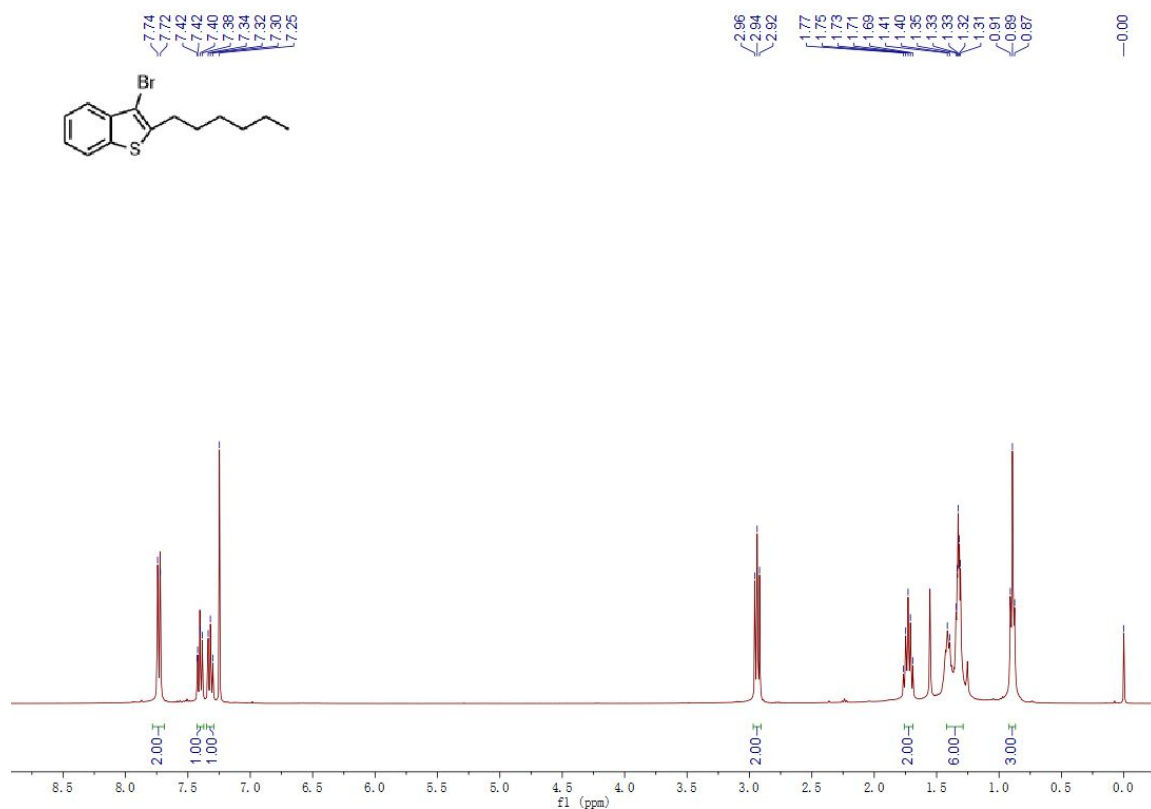
**Figure S111.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6h** (100 Hz, CDCl<sub>3</sub>)



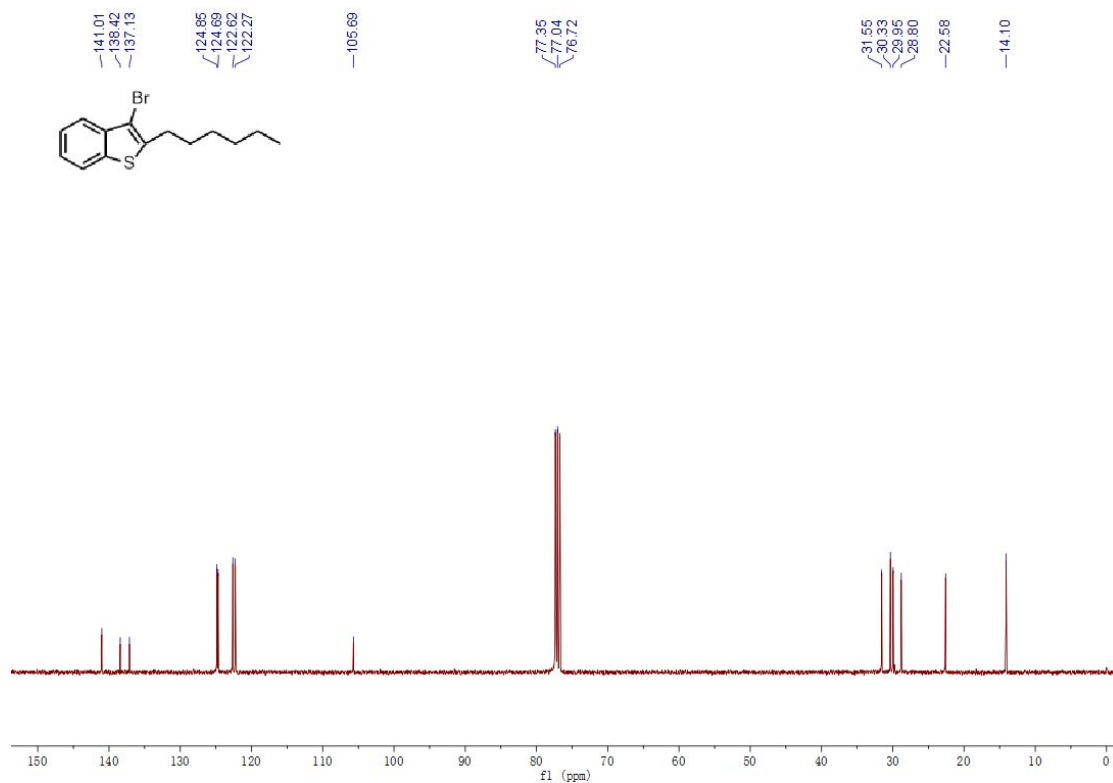
**Figure S112.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6i** (400 Hz, CDCl<sub>3</sub>)



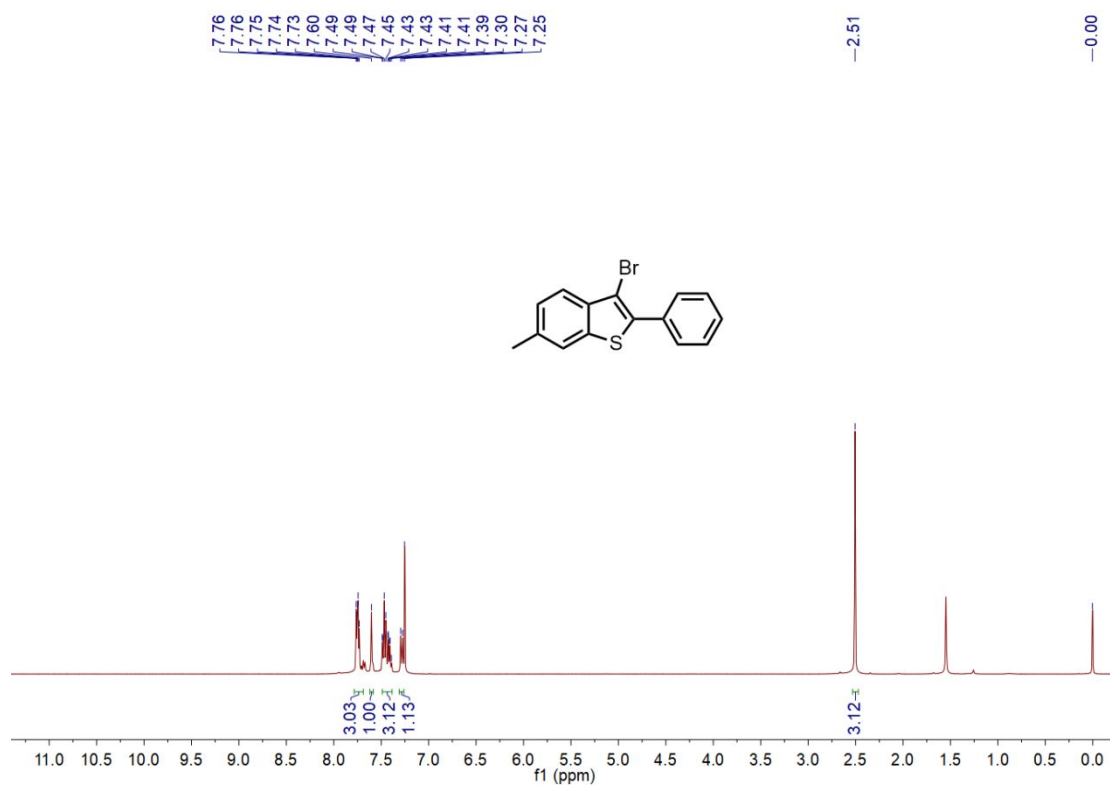
**Figure S113.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6i** (100 Hz, CDCl<sub>3</sub>)



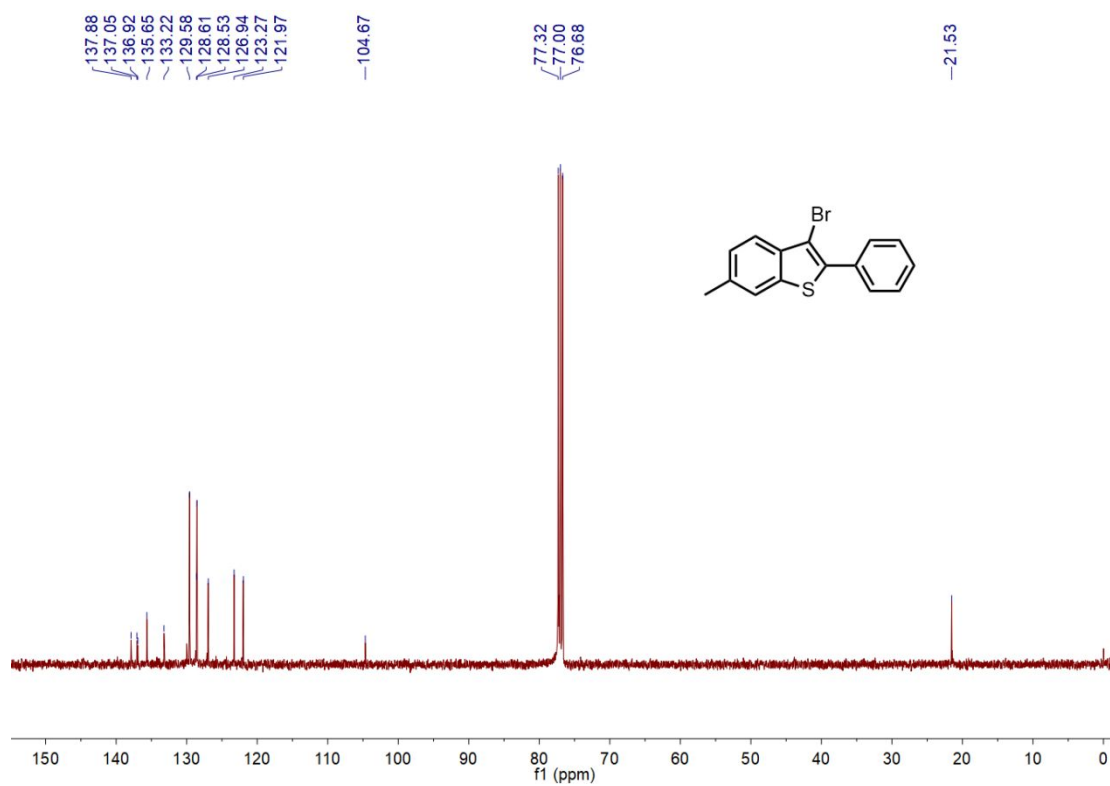
**Figure S114.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6j** (400 Hz, CDCl<sub>3</sub>)



**Figure S115.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6j** (100 Hz, CDCl<sub>3</sub>)

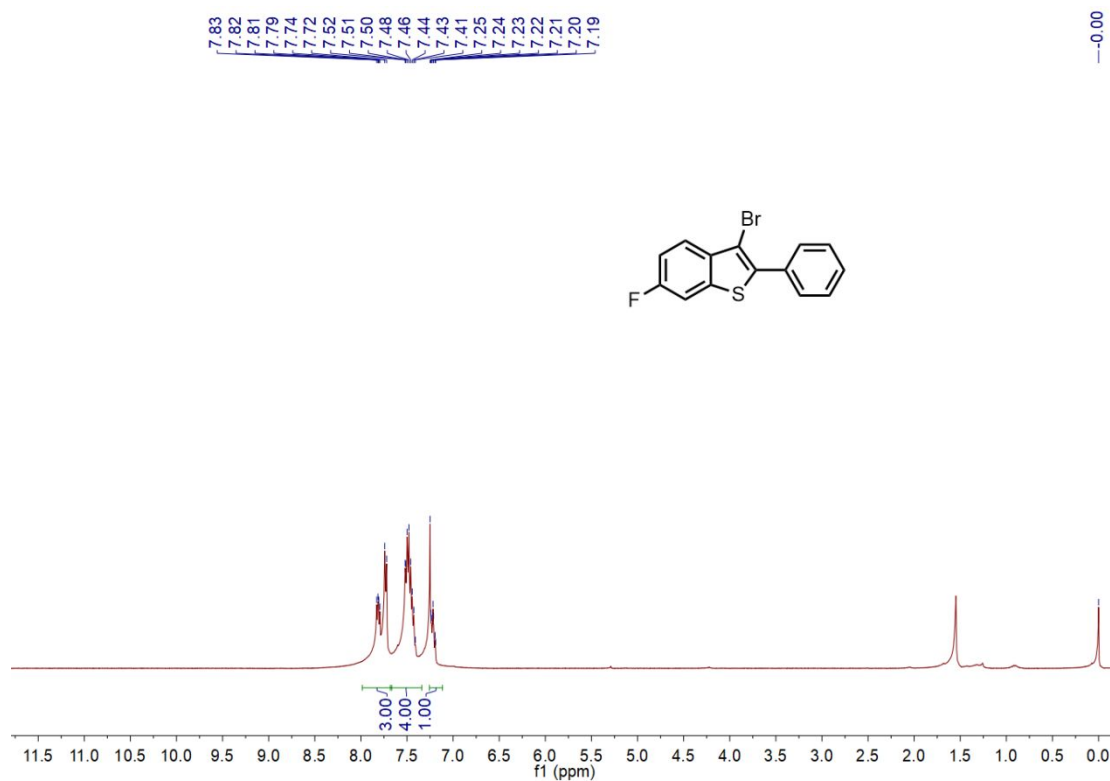


**Figure S116.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6k** (400 Hz, CDCl<sub>3</sub>)

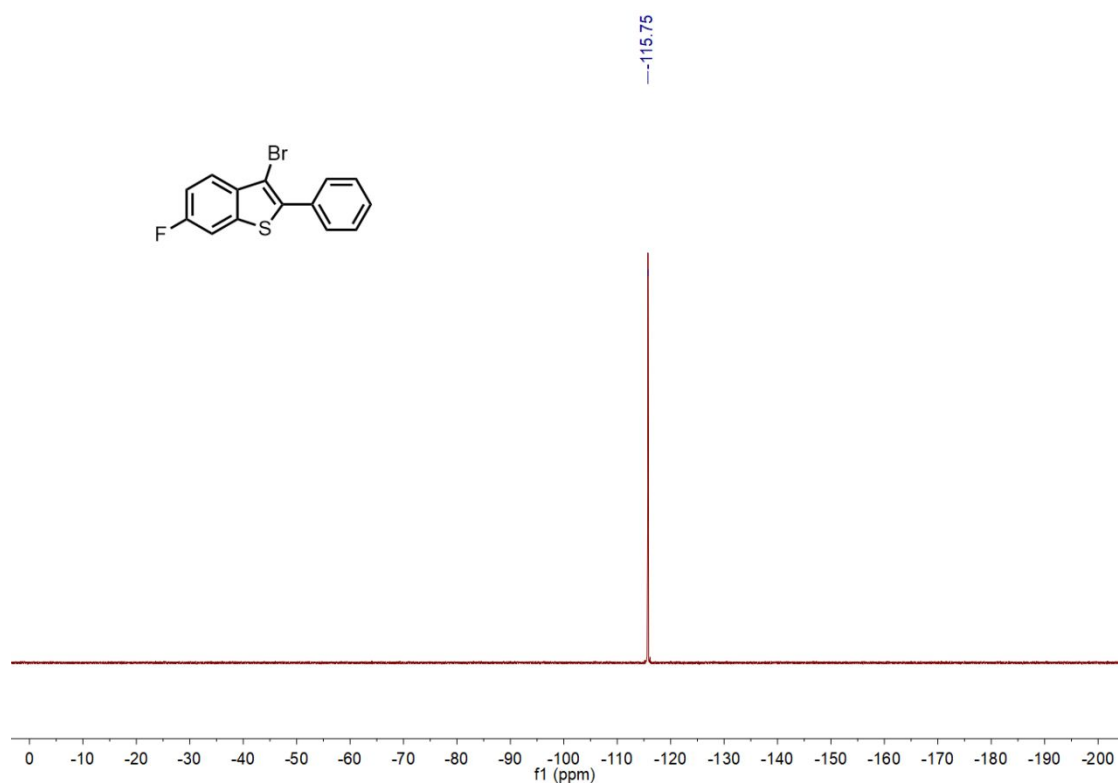


**Figure S117.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6k** (100 Hz, CDCl<sub>3</sub>)

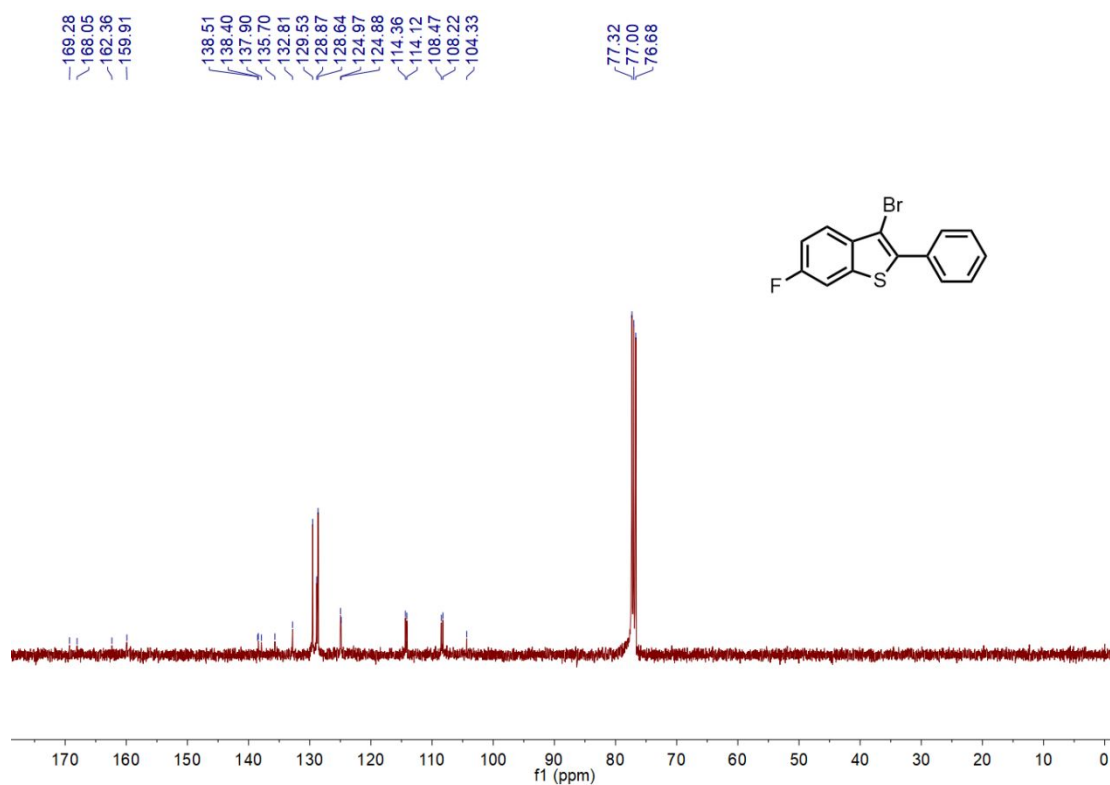




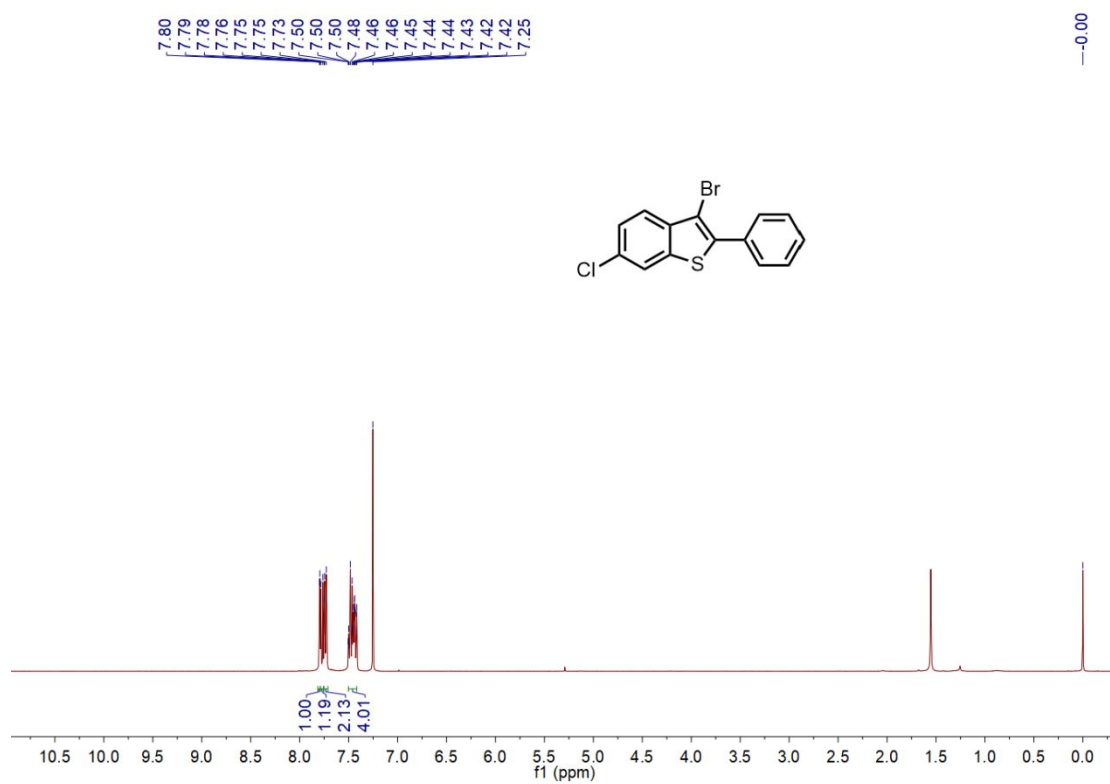
**Figure S118.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6I** (400 Hz, CDCl<sub>3</sub>)



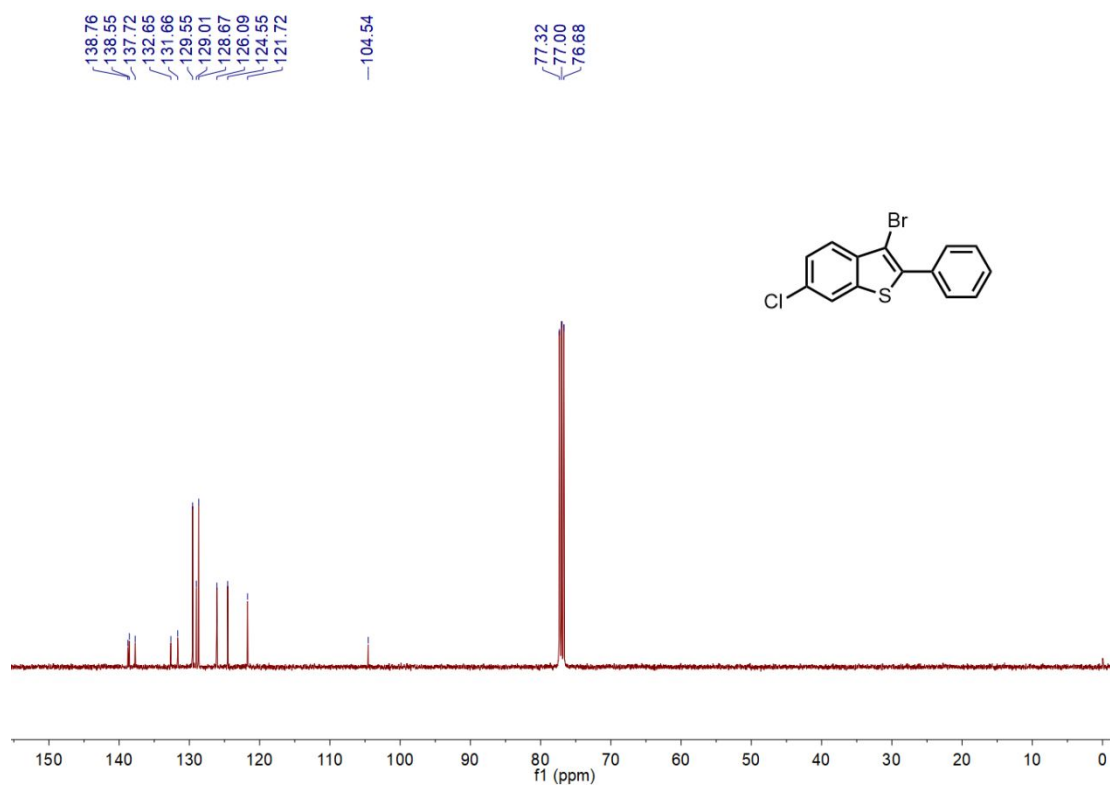
**Figure S119.** Copies of <sup>19</sup>F NMR Spectrum for Compound **6I** (376 Hz, CDCl<sub>3</sub>)



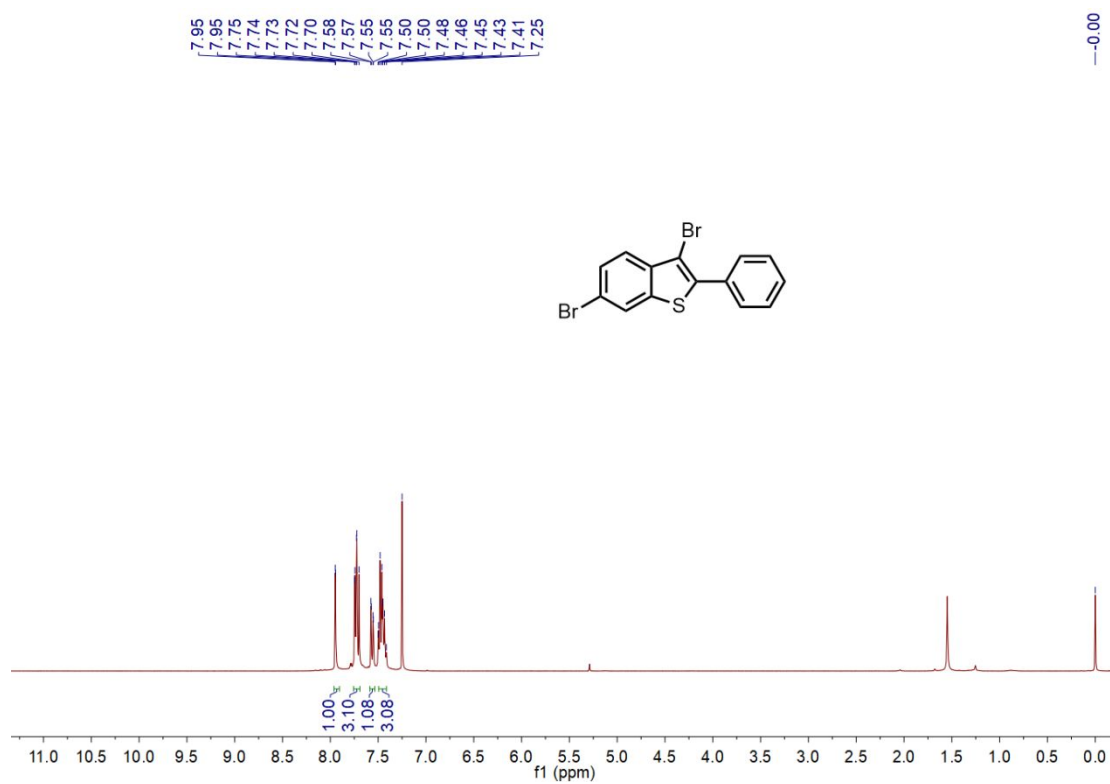
**Figure S120.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6l** (100 Hz, CDCl<sub>3</sub>)



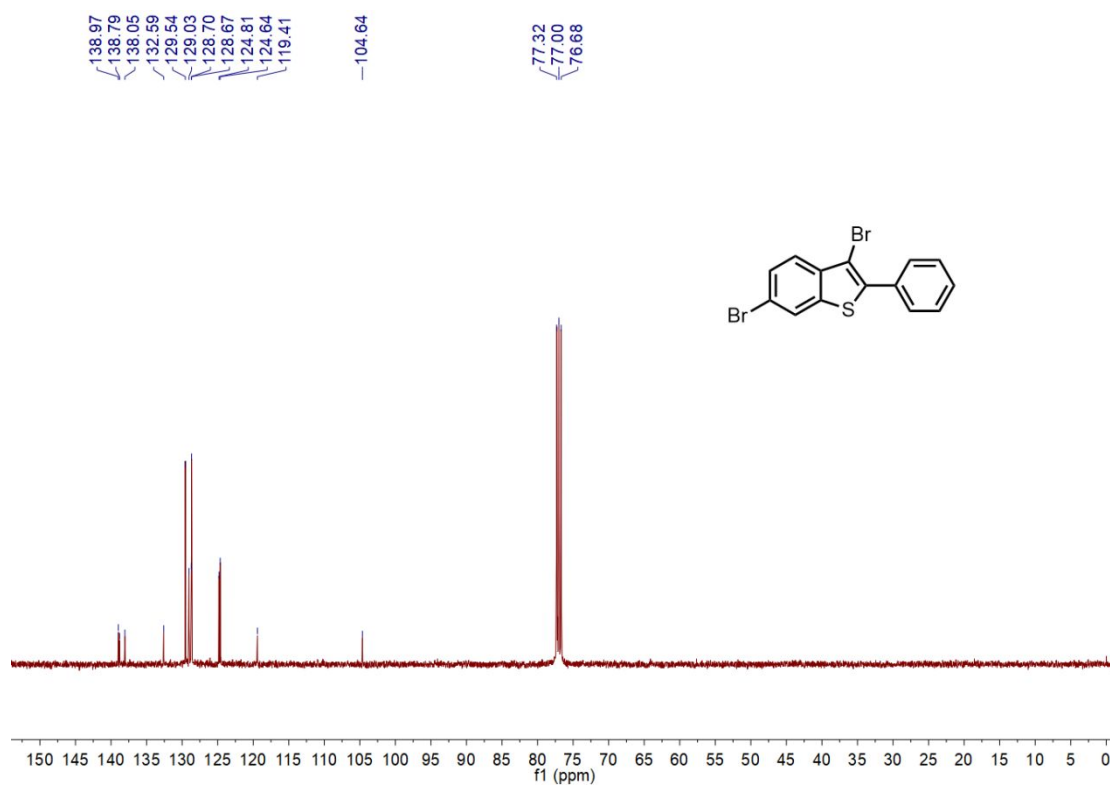
**Figure S121.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6m** (400 Hz, CDCl<sub>3</sub>)



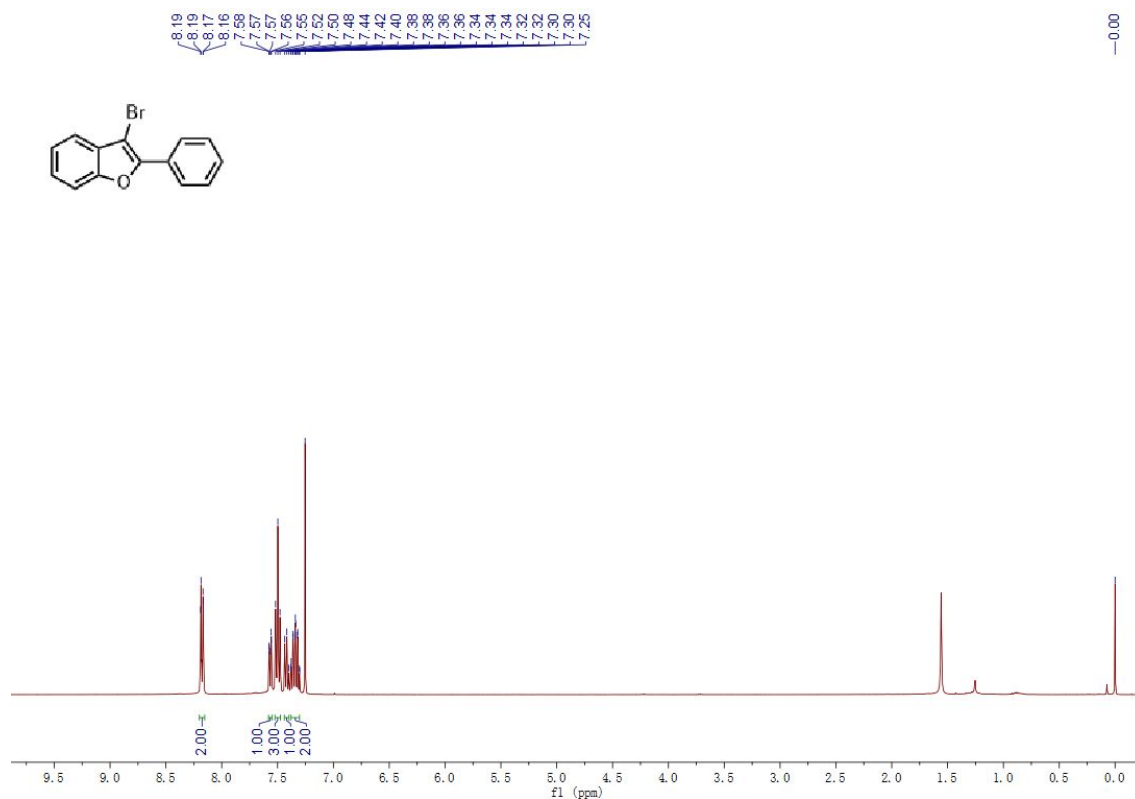
**Figure S122.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6m** (100 Hz, CDCl<sub>3</sub>)



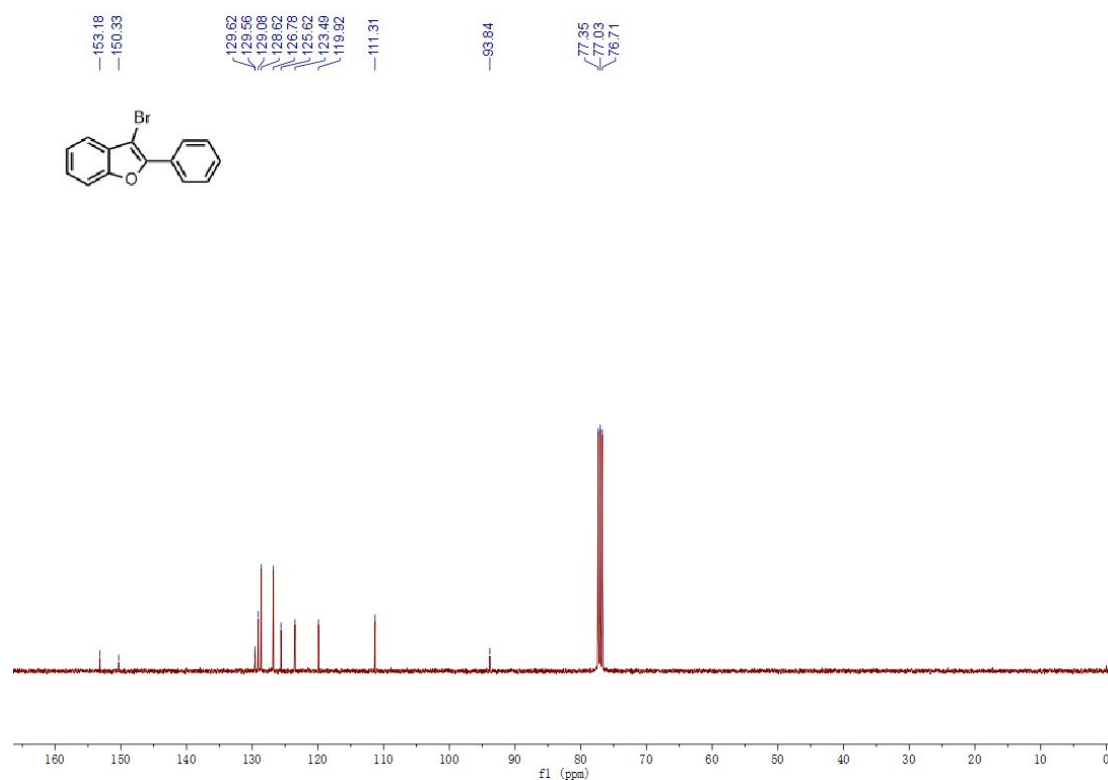
**Figure S123.** Copies of <sup>1</sup>H NMR Spectrum for Compound **6n** (400 Hz, CDCl<sub>3</sub>)



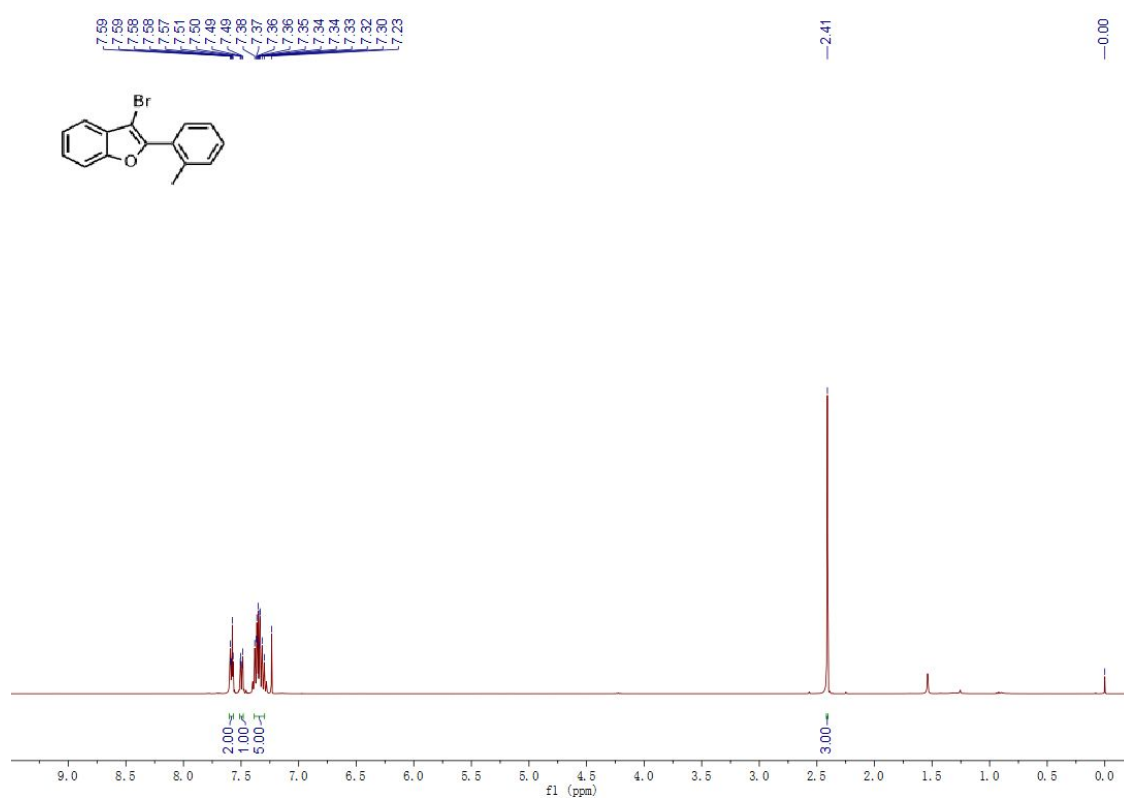
**Figure S124.** Copies of <sup>13</sup>C NMR Spectrum for Compound **6n** (100 Hz, CDCl<sub>3</sub>)



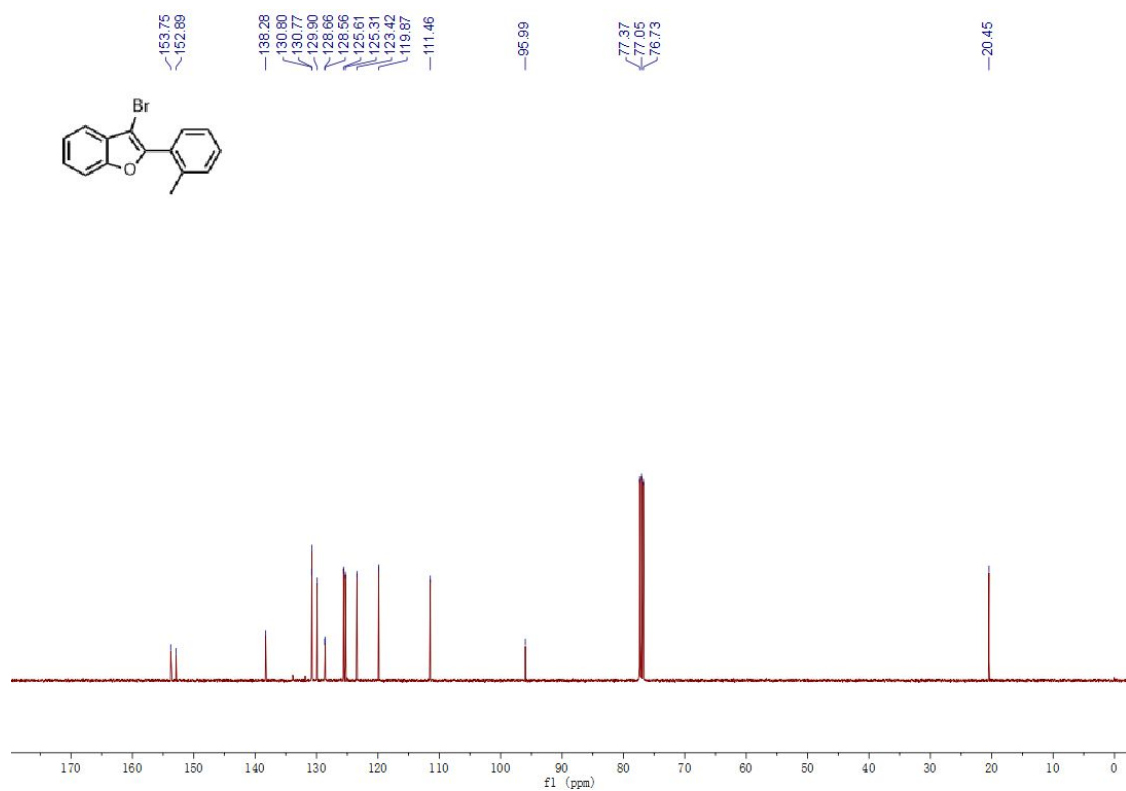
**Figure S125.** Copies of <sup>1</sup>H NMR Spectrum for Compound **7a** (400 Hz, CDCl<sub>3</sub>)



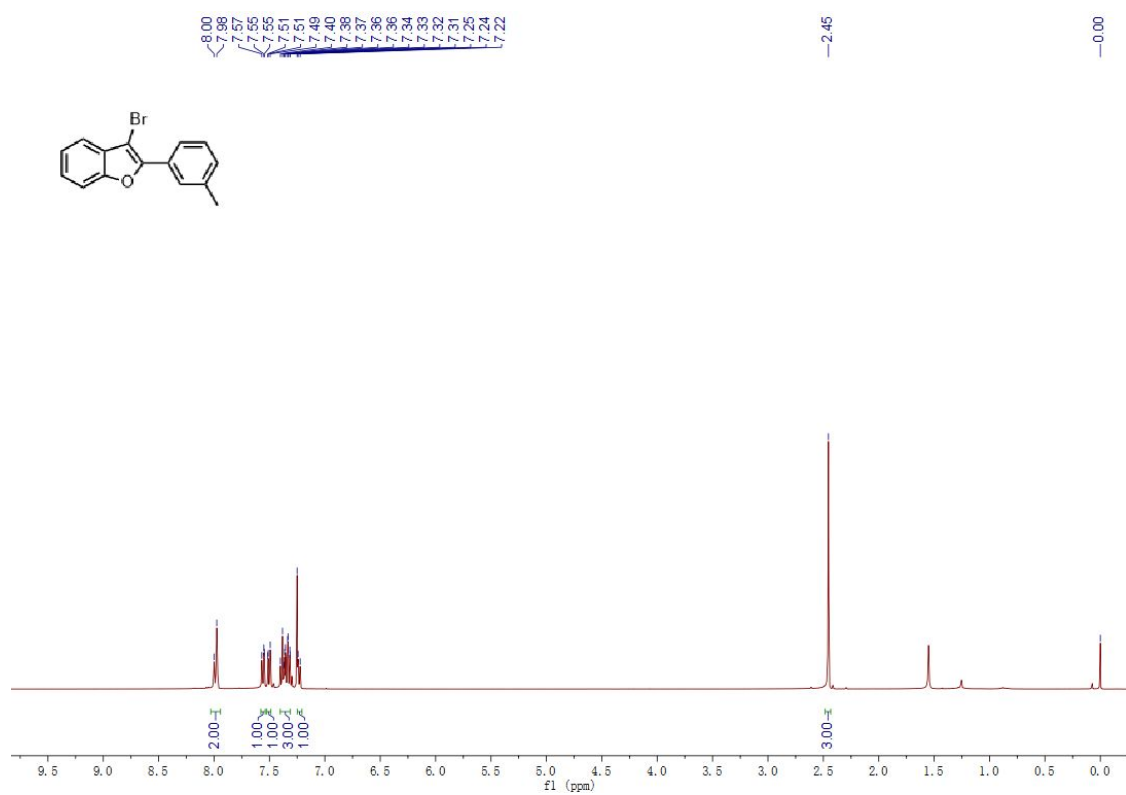
**Figure S126.** Copies of <sup>13</sup>C NMR Spectrum for Compound **7a** (100 Hz, CDCl<sub>3</sub>)



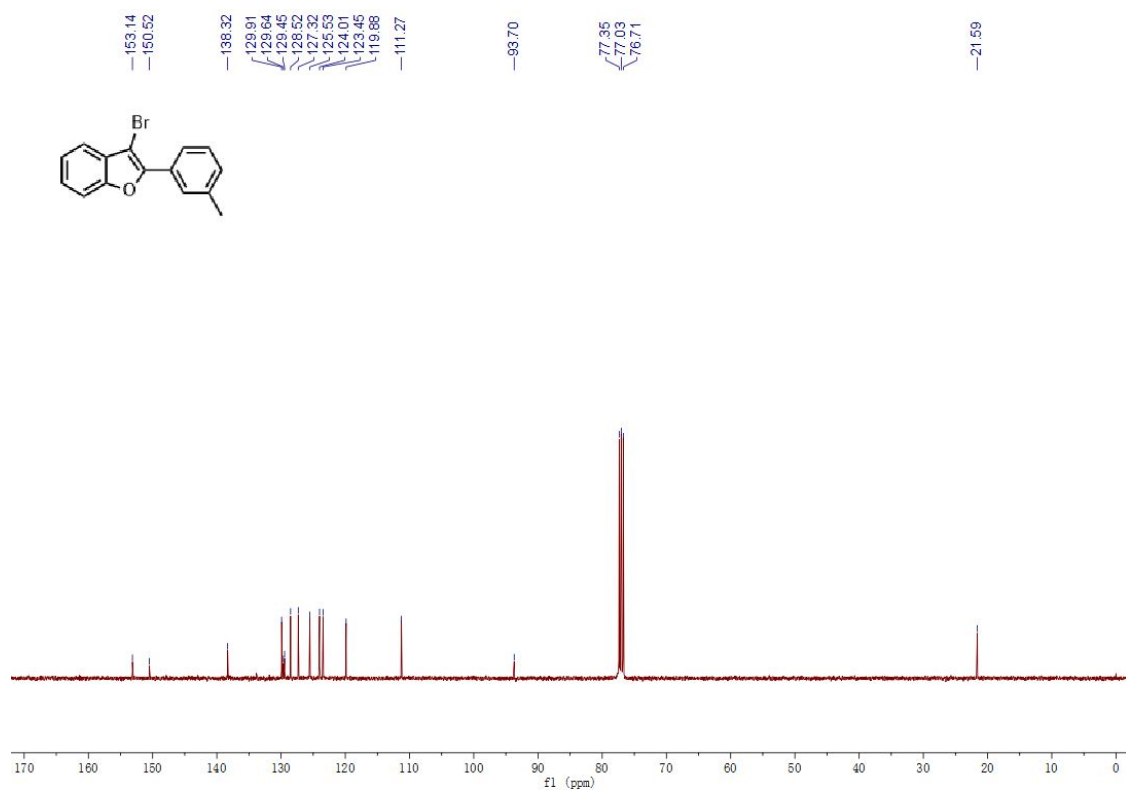
**Figure S127.** Copies of <sup>1</sup>H NMR Spectrum for Compound **7b** (400 Hz, CDCl<sub>3</sub>)



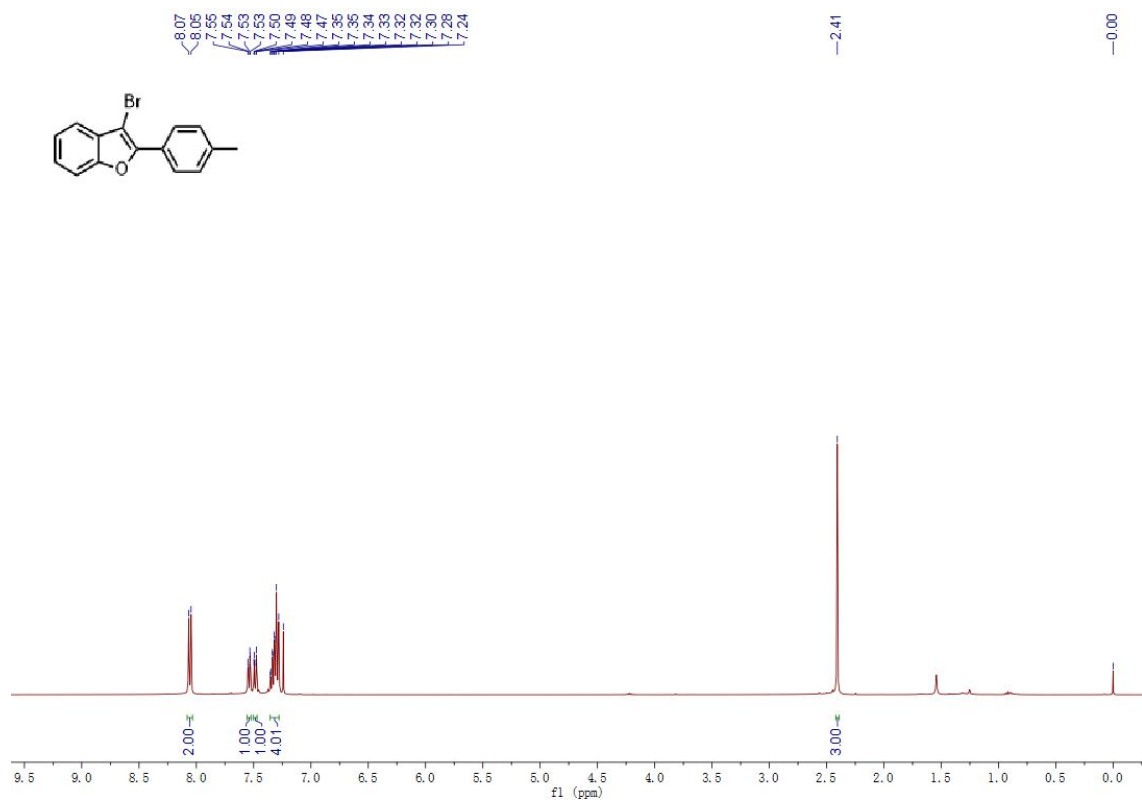
**Figure S128.** Copies of <sup>13</sup>C NMR Spectrum for Compound **7b** (100 Hz, CDCl<sub>3</sub>)



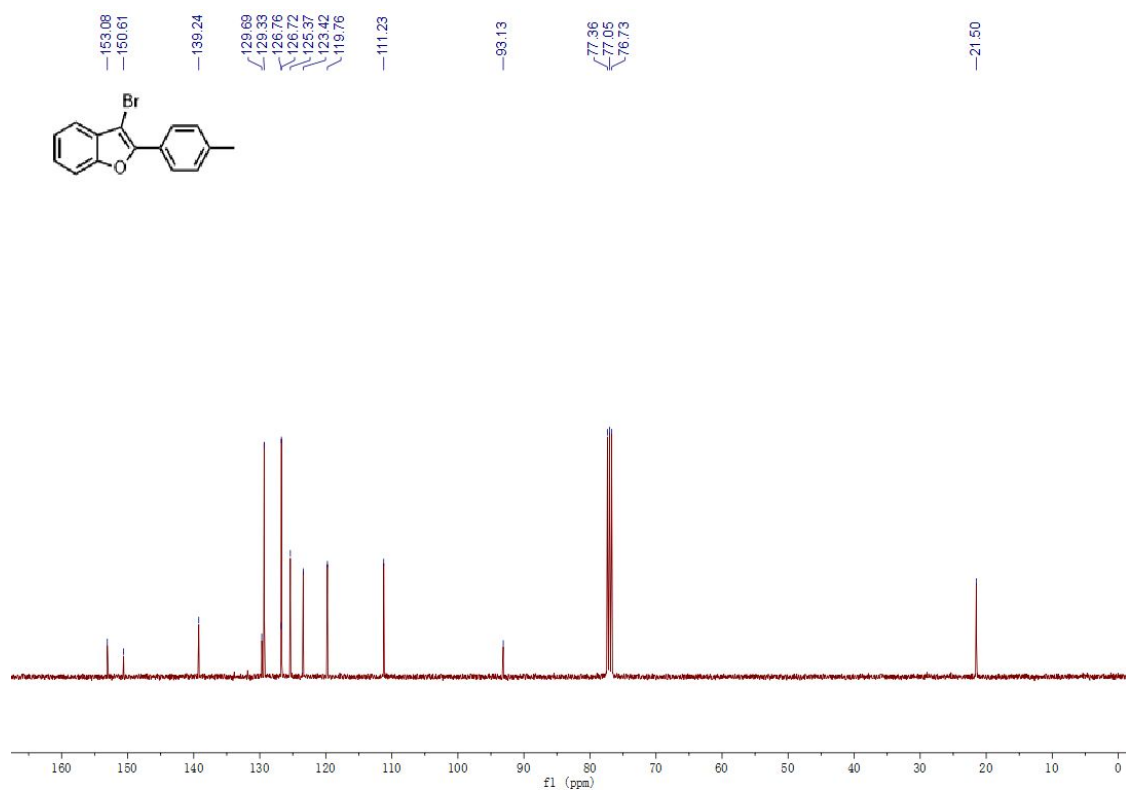
**Figure S129.** Copies of <sup>1</sup>H NMR Spectrum for Compound **7c** (400 Hz, CDCl<sub>3</sub>)



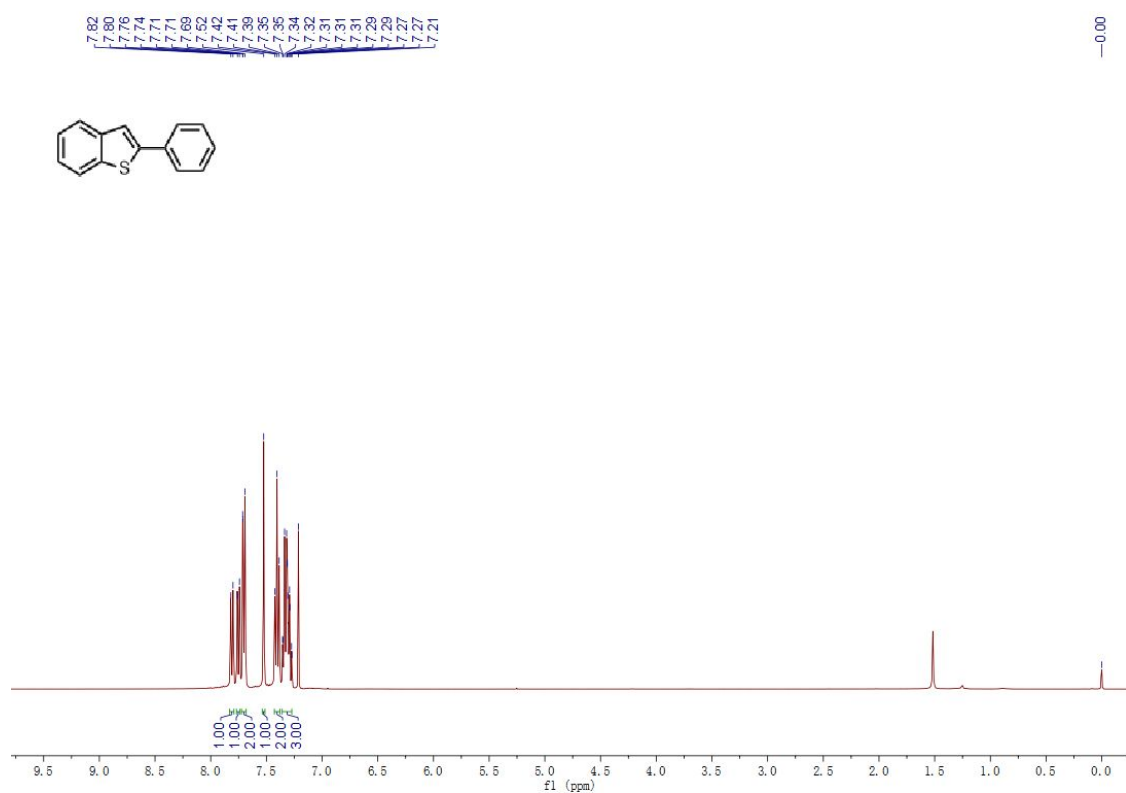
**Figure S130.** Copies of <sup>13</sup>C NMR Spectrum for Compound 7c (100 Hz, CDCl<sub>3</sub>)



**Figure S131.** Copies of <sup>1</sup>H NMR Spectrum for Compound 7d (400 Hz, CDCl<sub>3</sub>)

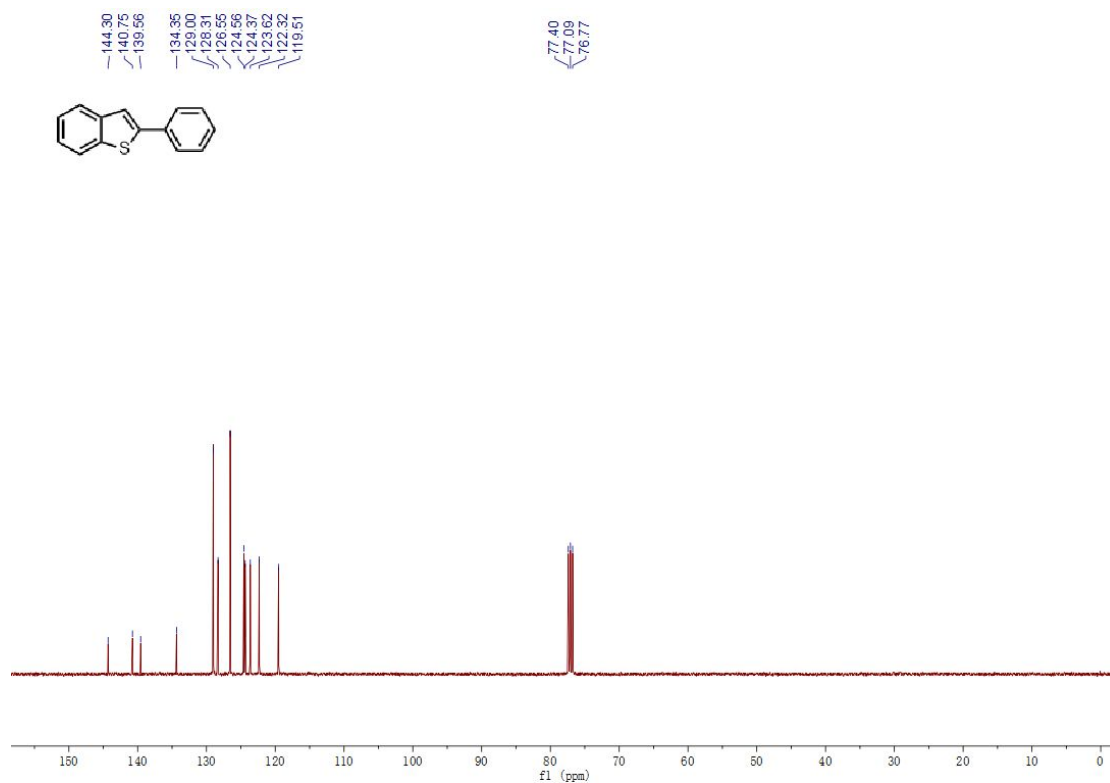


**Figure S132.** Copies of <sup>13</sup>C NMR Spectrum for Compound **7d** (100 Hz, CDCl<sub>3</sub>)

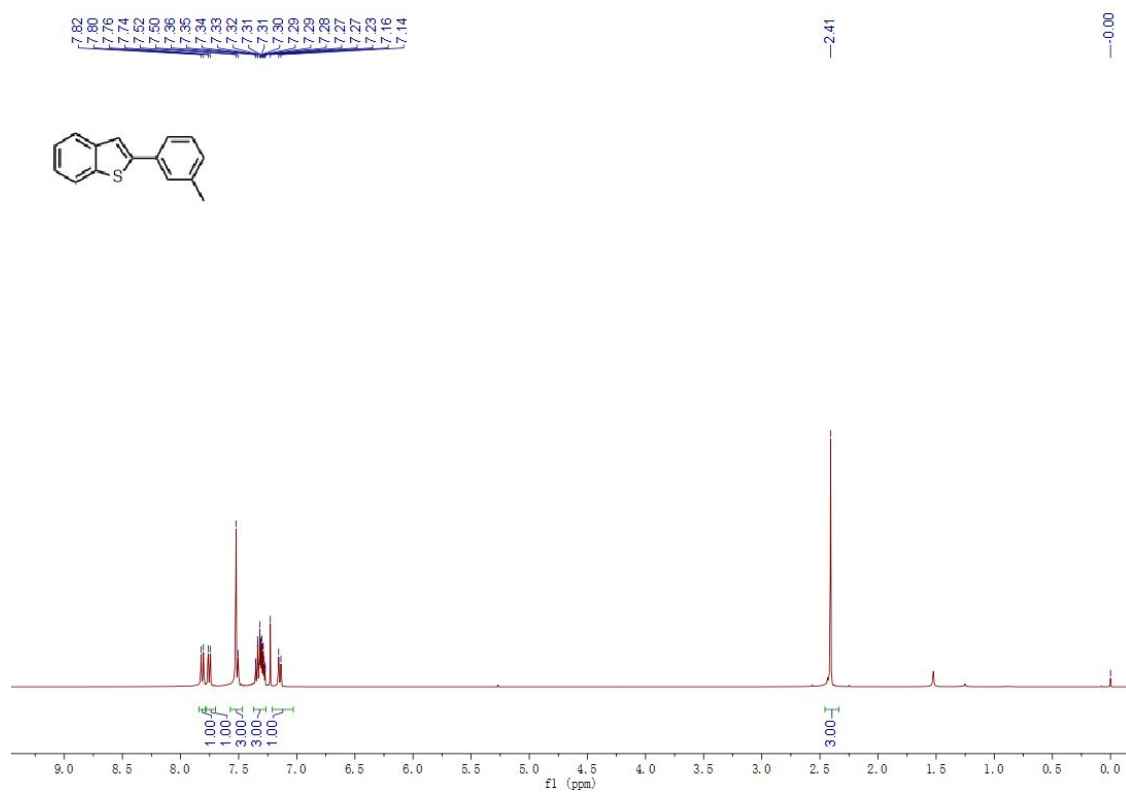


**Figure S133.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3ba** (400 Hz, CDCl<sub>3</sub>)

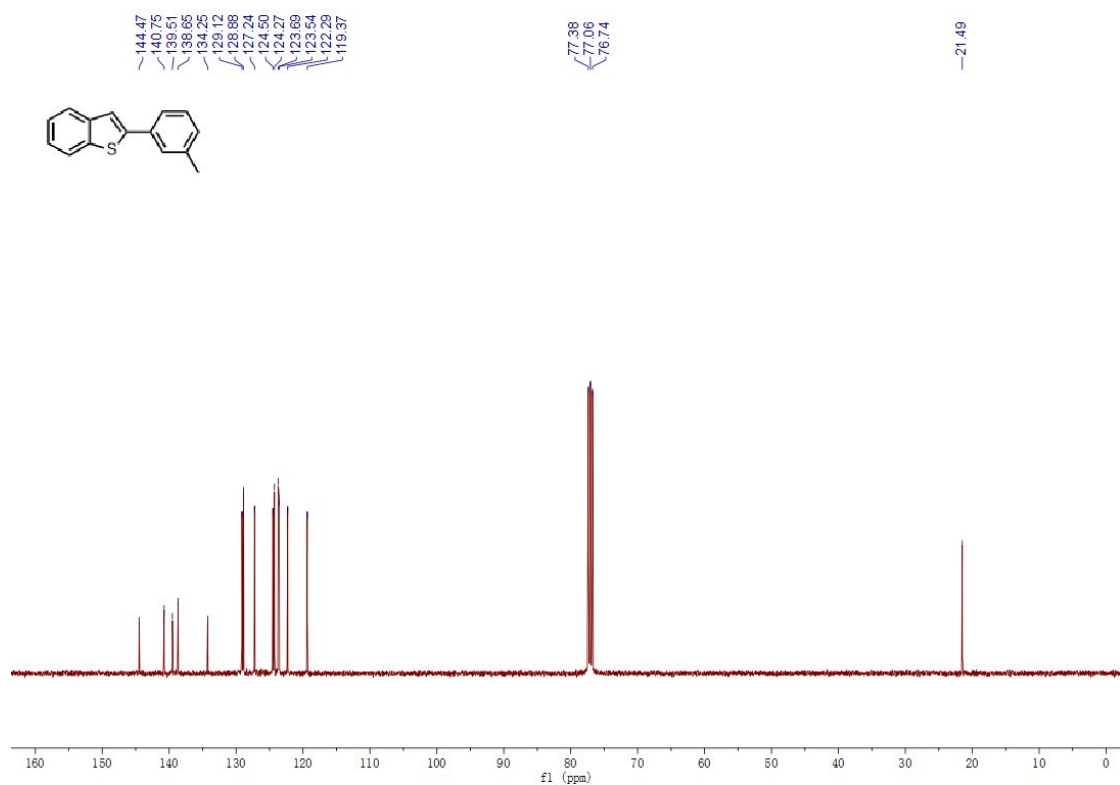




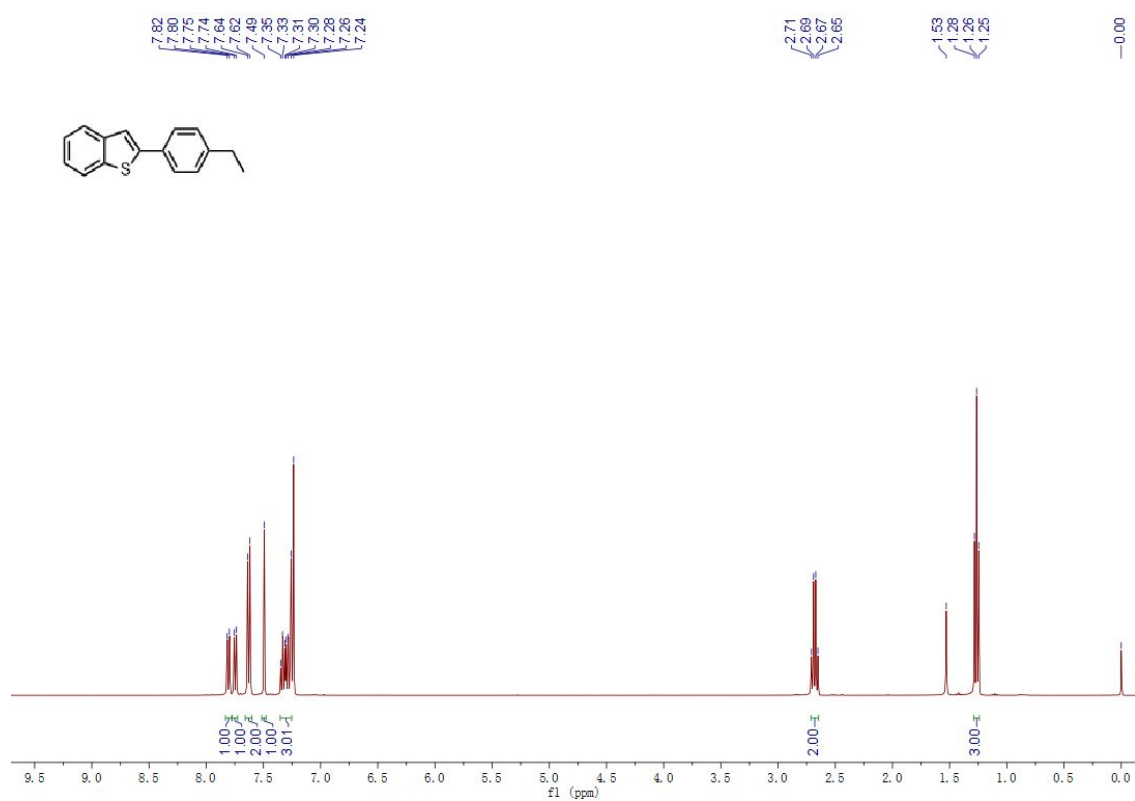
**Figure S134.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3ba** (100 Hz, CDCl<sub>3</sub>)



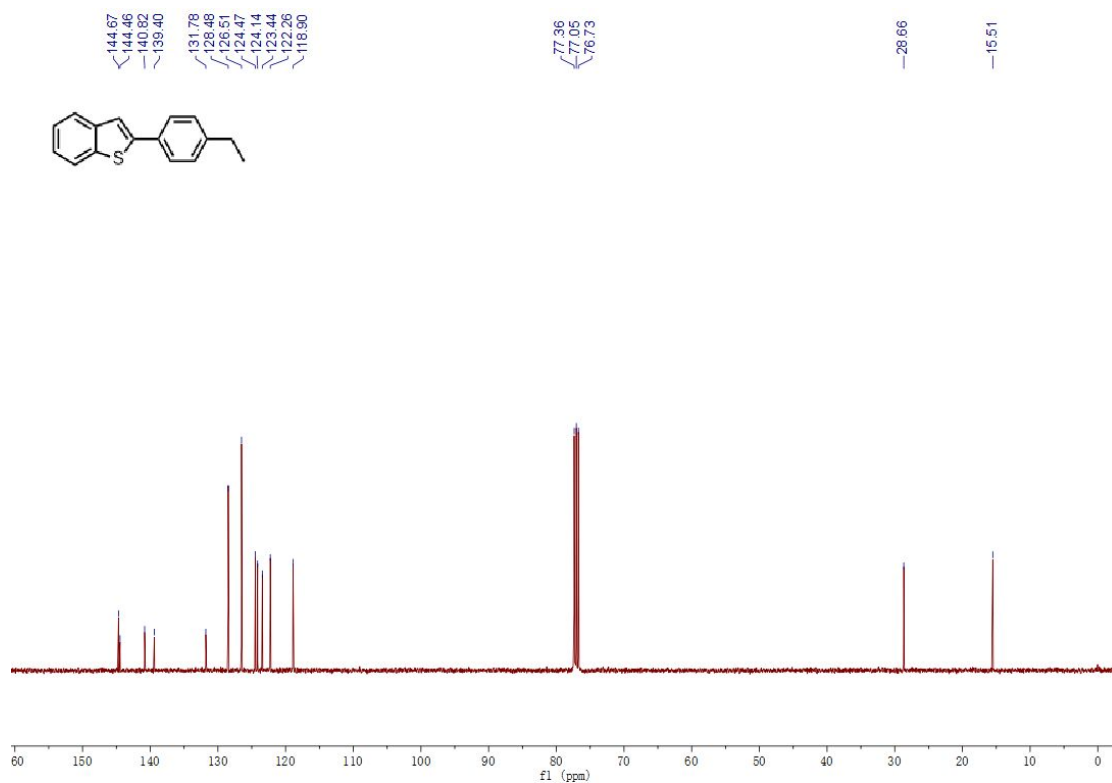
**Figure S135.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3bb** (400 Hz, CDCl<sub>3</sub>)



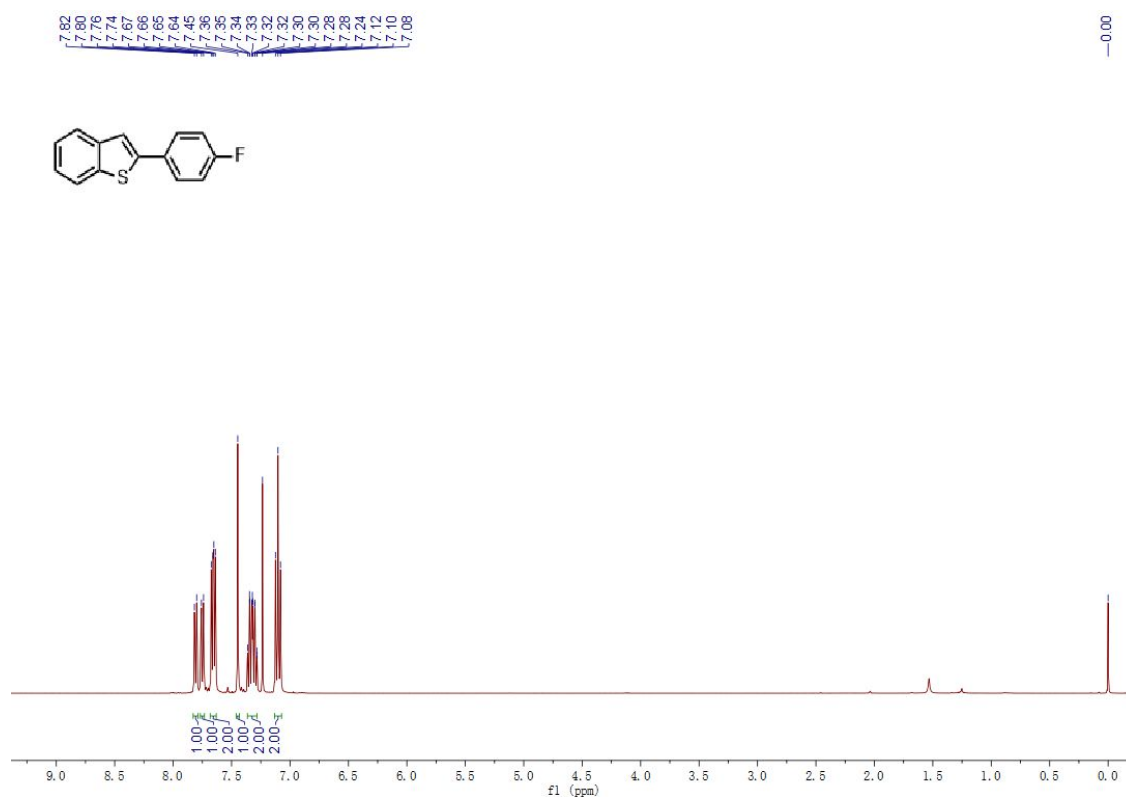
**Figure S136.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3bb** (100 Hz, CDCl<sub>3</sub>)



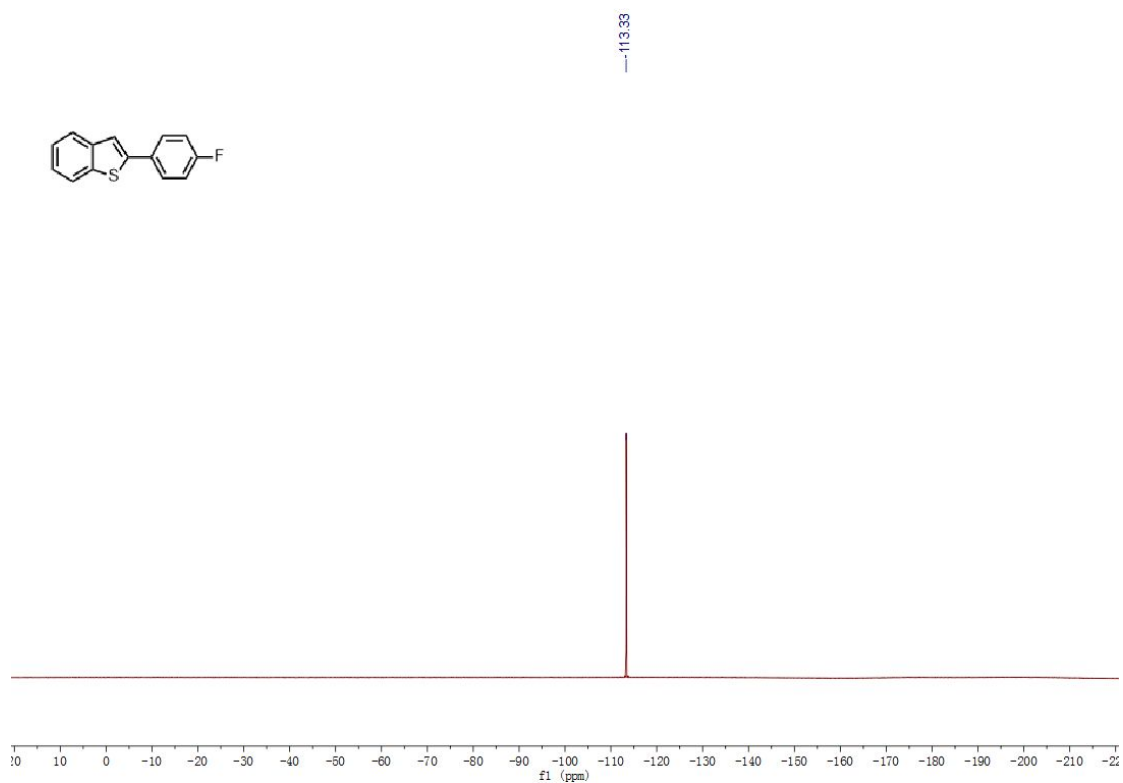
**Figure S137.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3bc** (400 Hz, CDCl<sub>3</sub>)



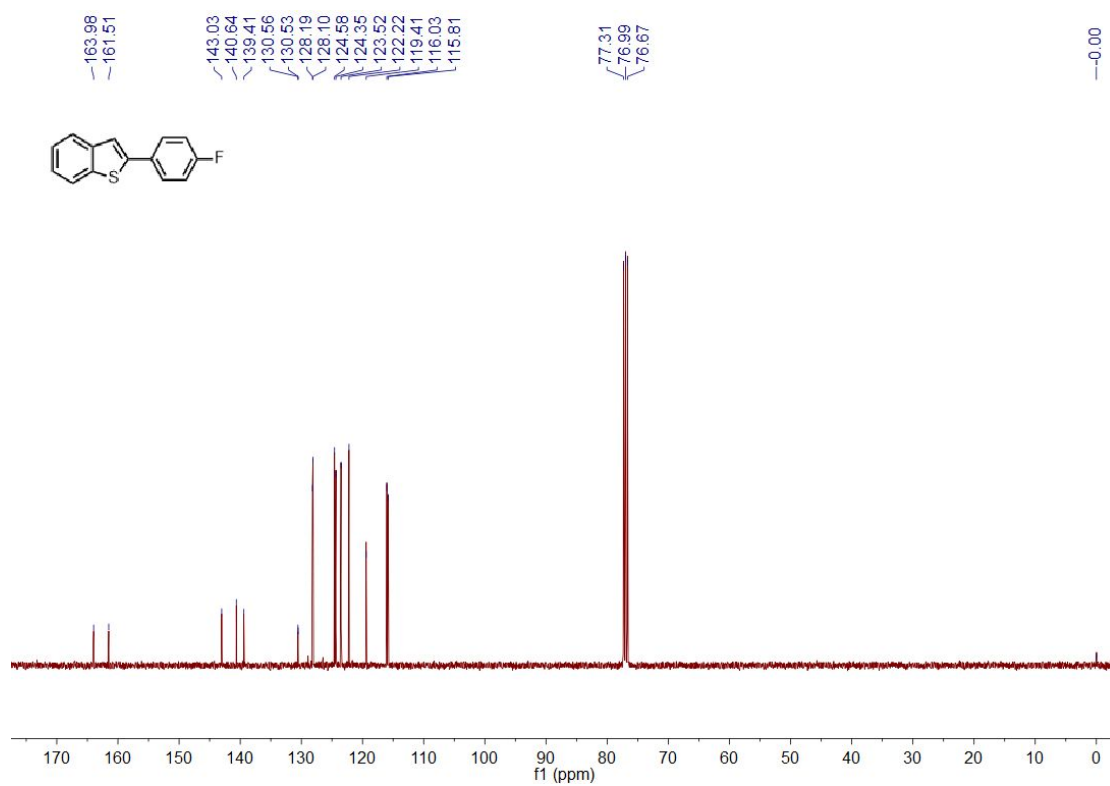
**Figure S138.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3bc** (100 Hz, CDCl<sub>3</sub>)



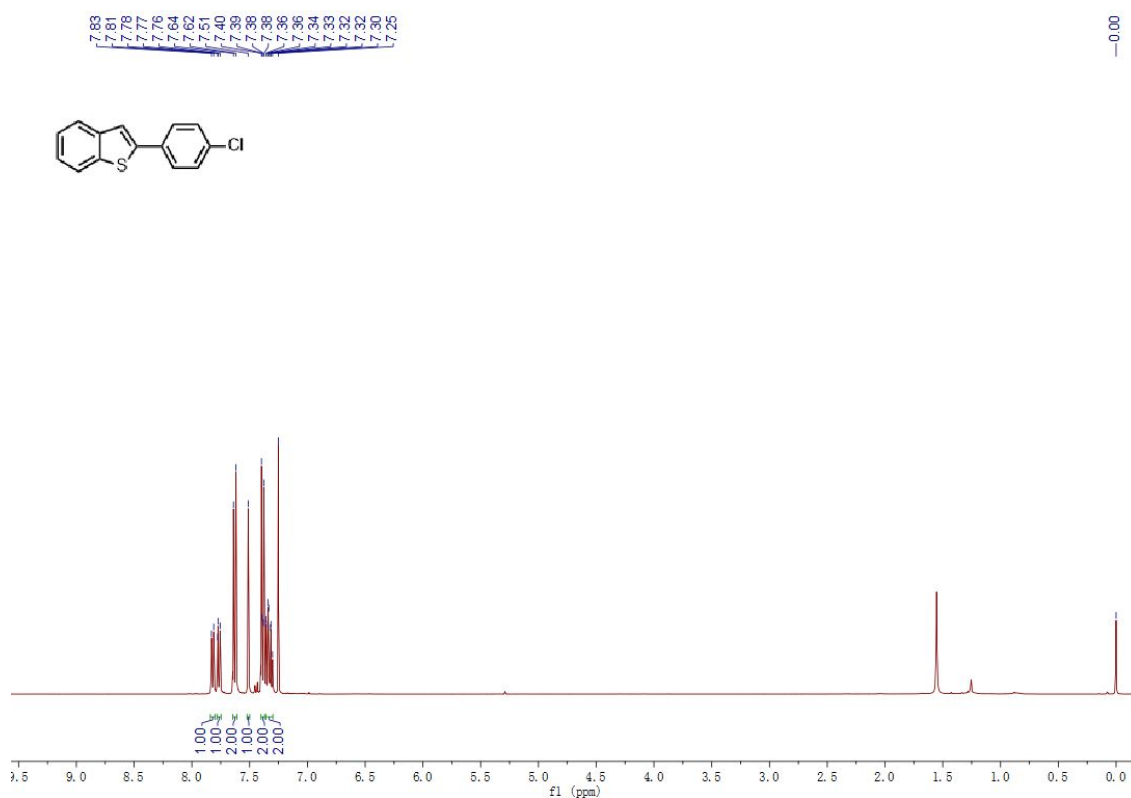
**Figure S139.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3bd** (400 Hz, CDCl<sub>3</sub>)



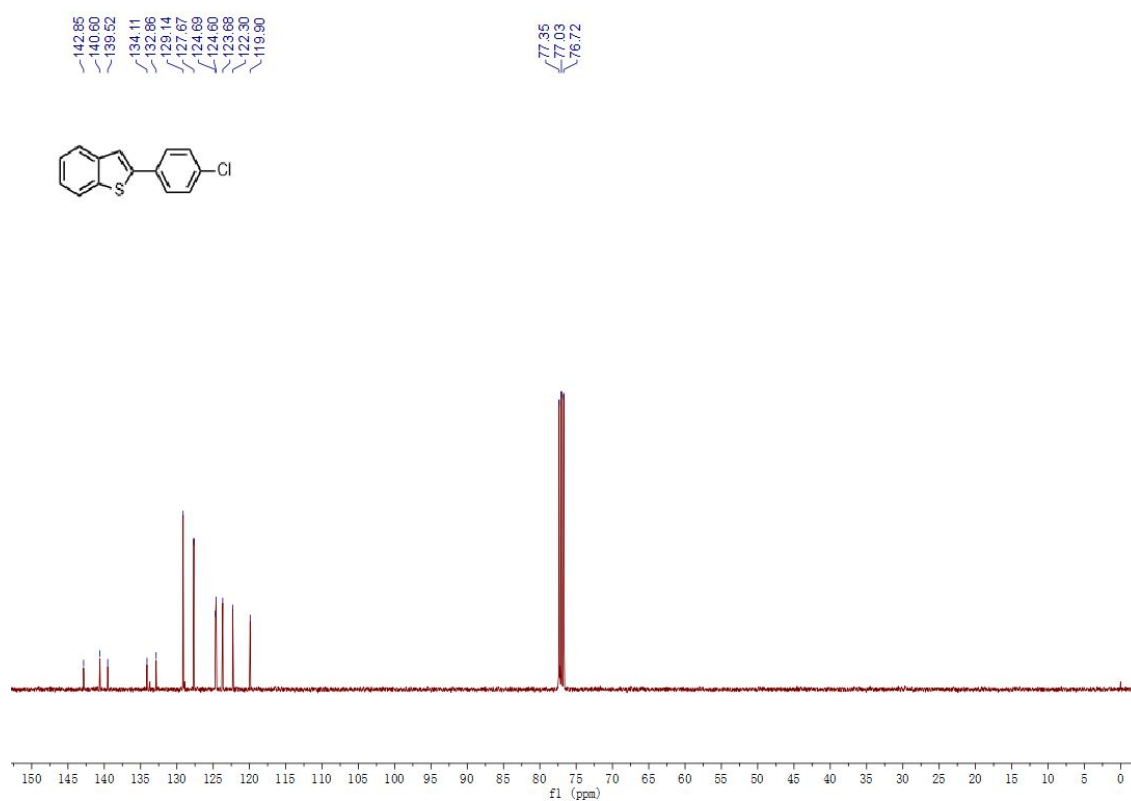
**Figure S140.** Copies of  $^{19}\text{F}$  NMR Spectrum for Compound **3bd** (376 Hz,  $\text{CDCl}_3$ )



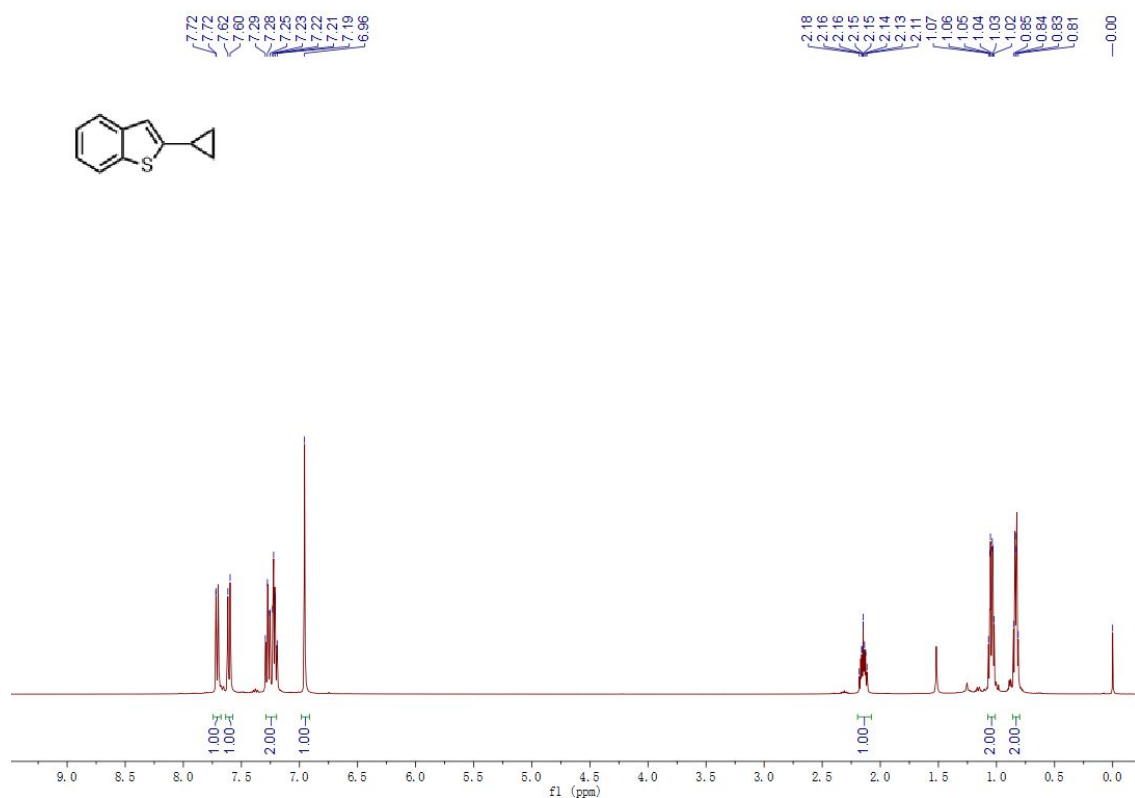
**Figure S141.** Copies of  $^{13}\text{C}$  NMR Spectrum for Compound **3bd** (100 Hz,  $\text{CDCl}_3$ )



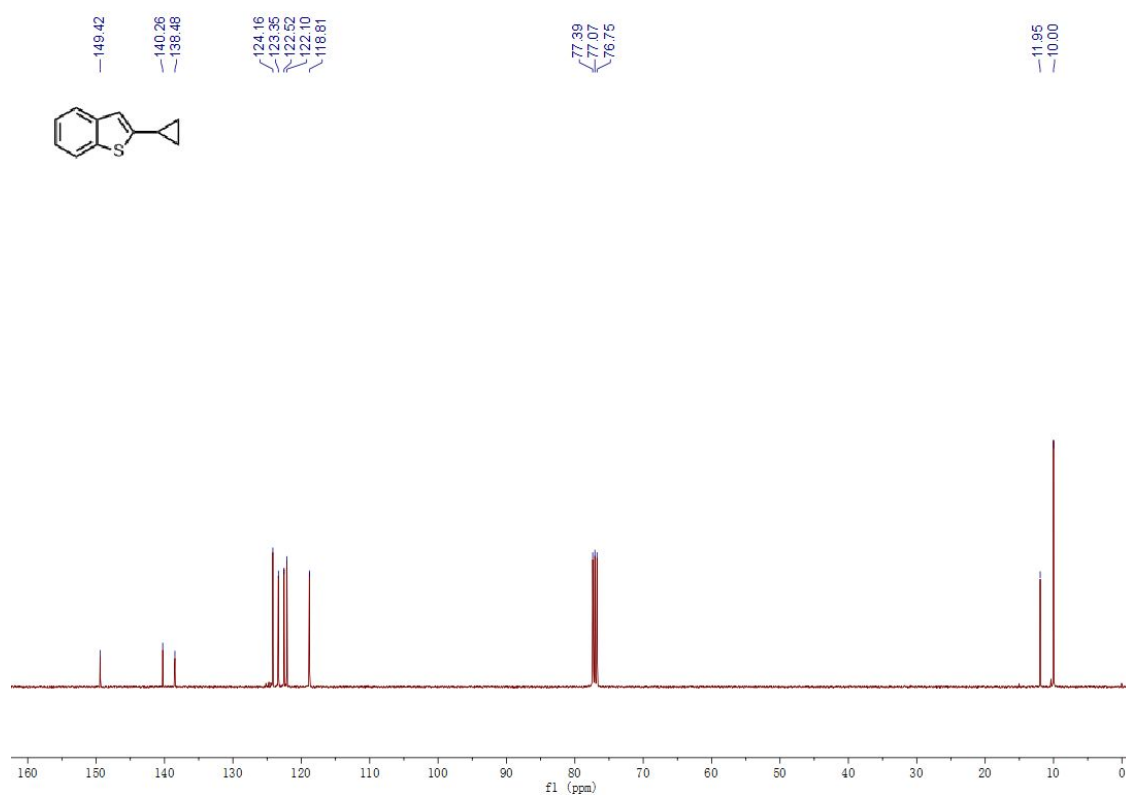
**Figure S142.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3be** (400 Hz, CDCl<sub>3</sub>)



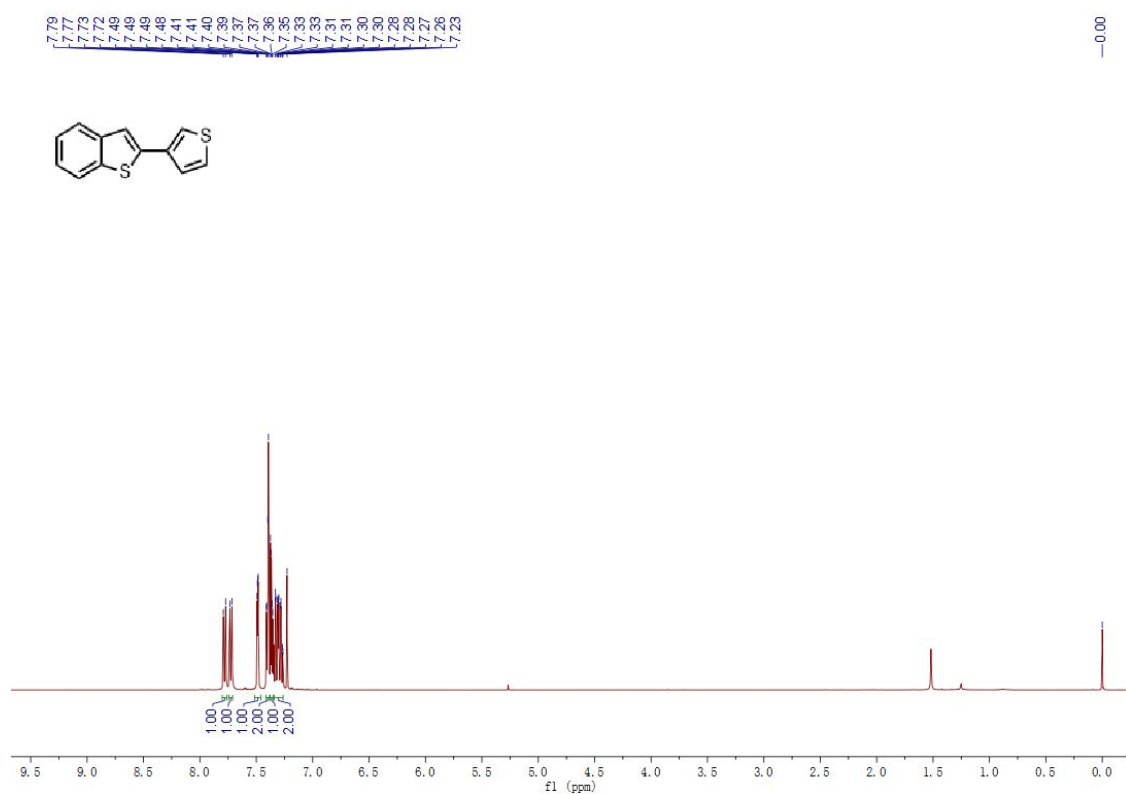
**Figure S143.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3be** (100 Hz, CDCl<sub>3</sub>)



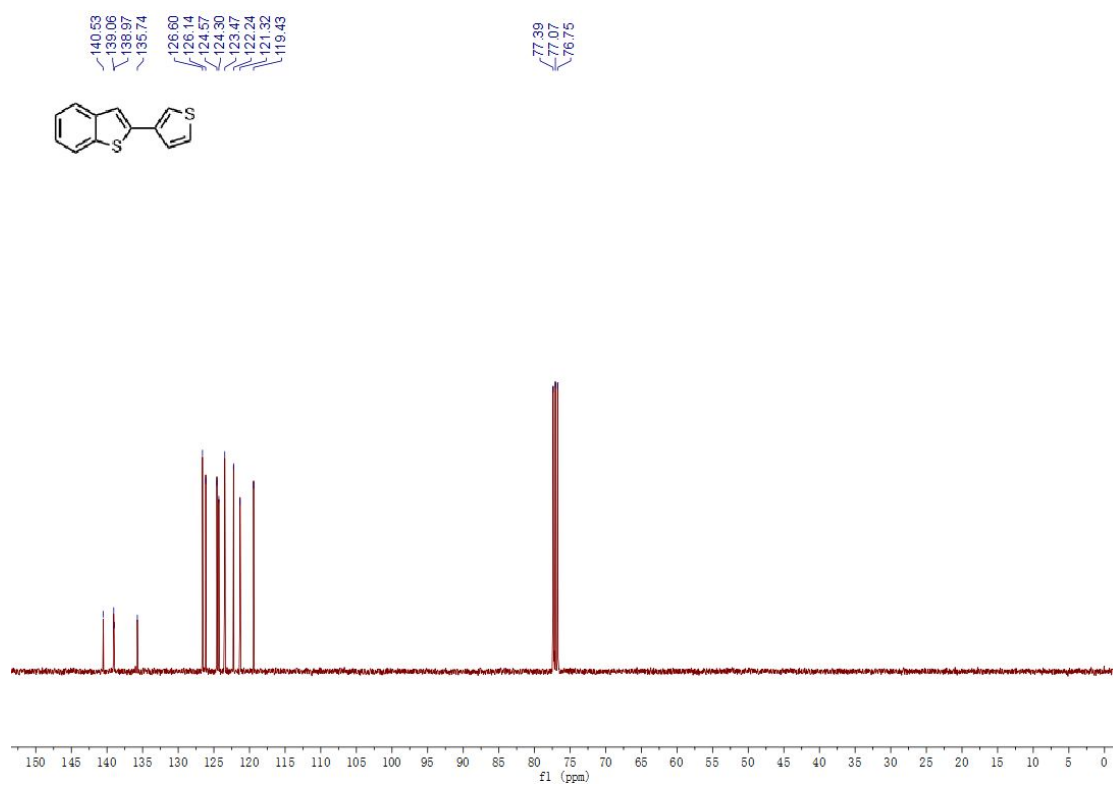
**Figure S144.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3bf** (400 Hz, CDCl<sub>3</sub>)



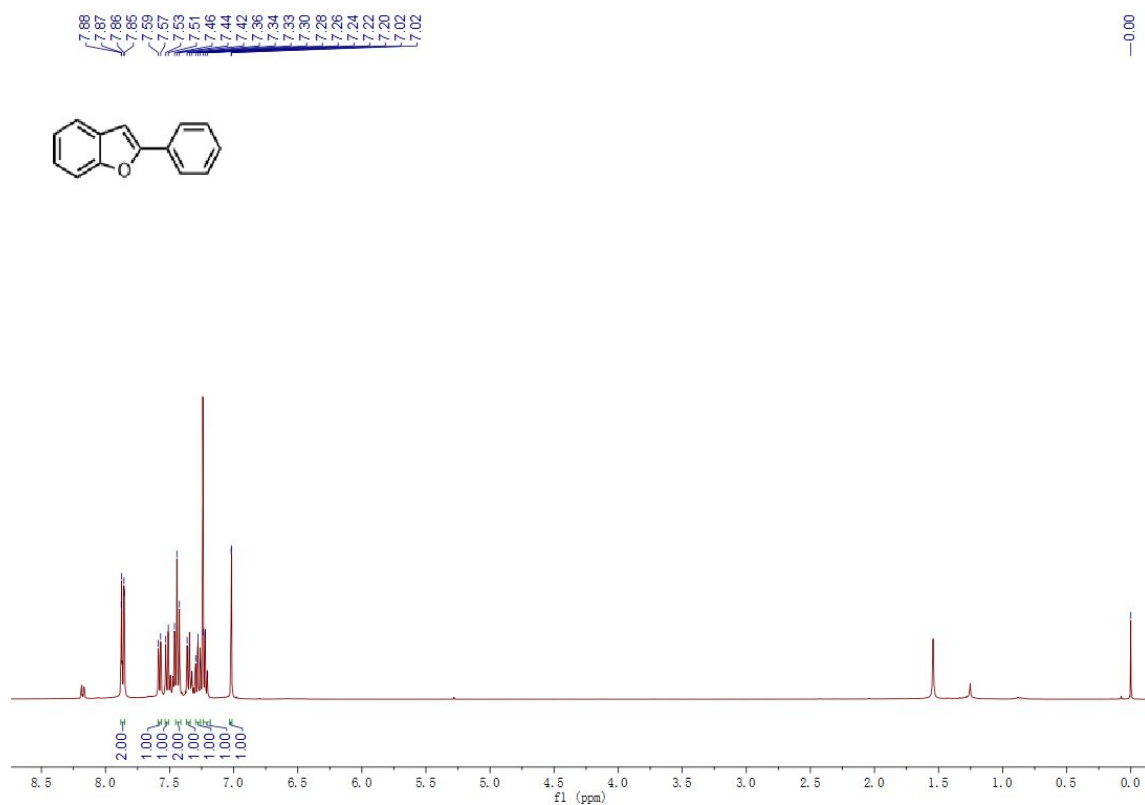
**Figure S145.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3bf** (100 Hz, CDCl<sub>3</sub>)



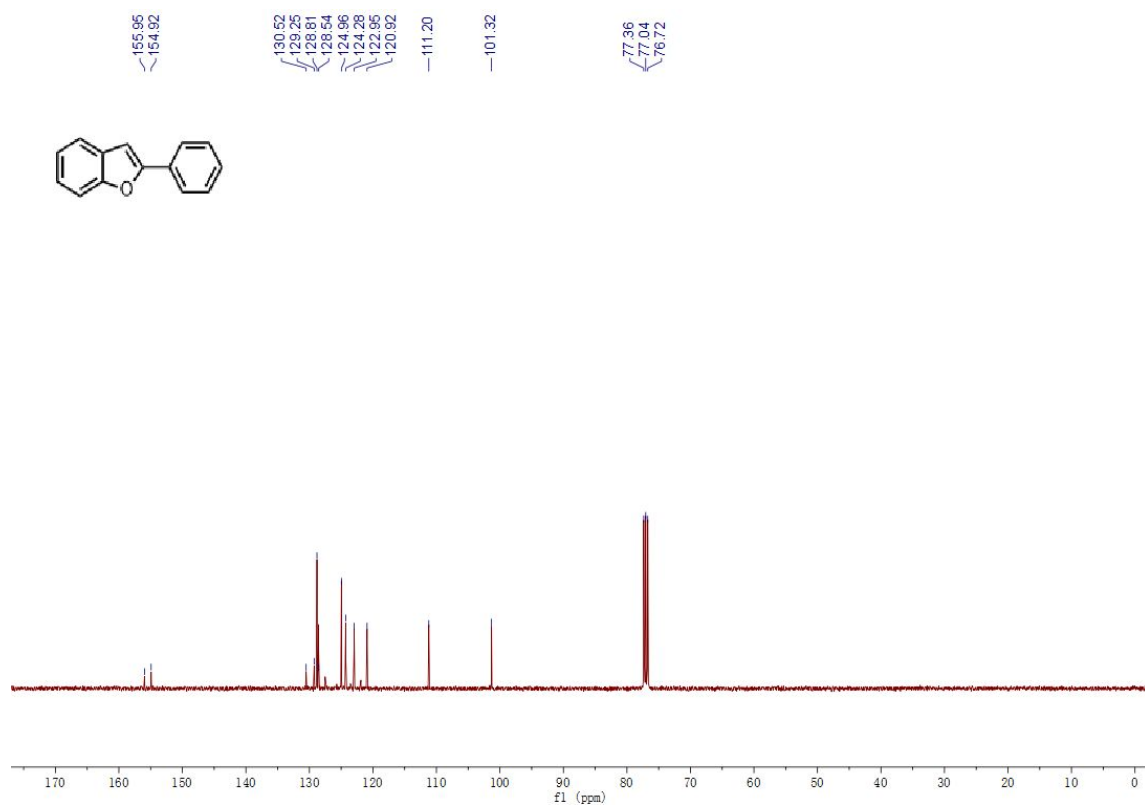
**Figure S146.** Copies of <sup>1</sup>H NMR Spectrum for Compound **3bg** (400 Hz, CDCl<sub>3</sub>)



**Figure S147.** Copies of <sup>13</sup>C NMR Spectrum for Compound **3bg** (100 Hz, CDCl<sub>3</sub>)

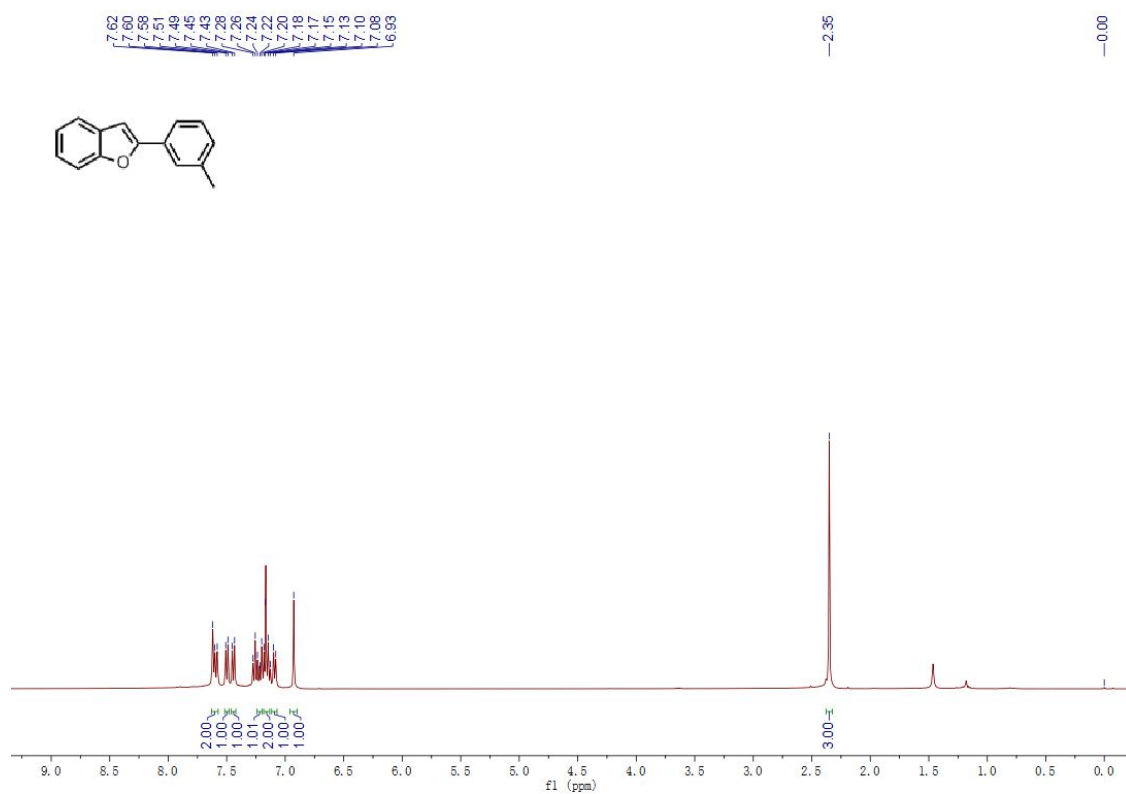


**Figure S148.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5ba** (400 Hz, CDCl<sub>3</sub>)

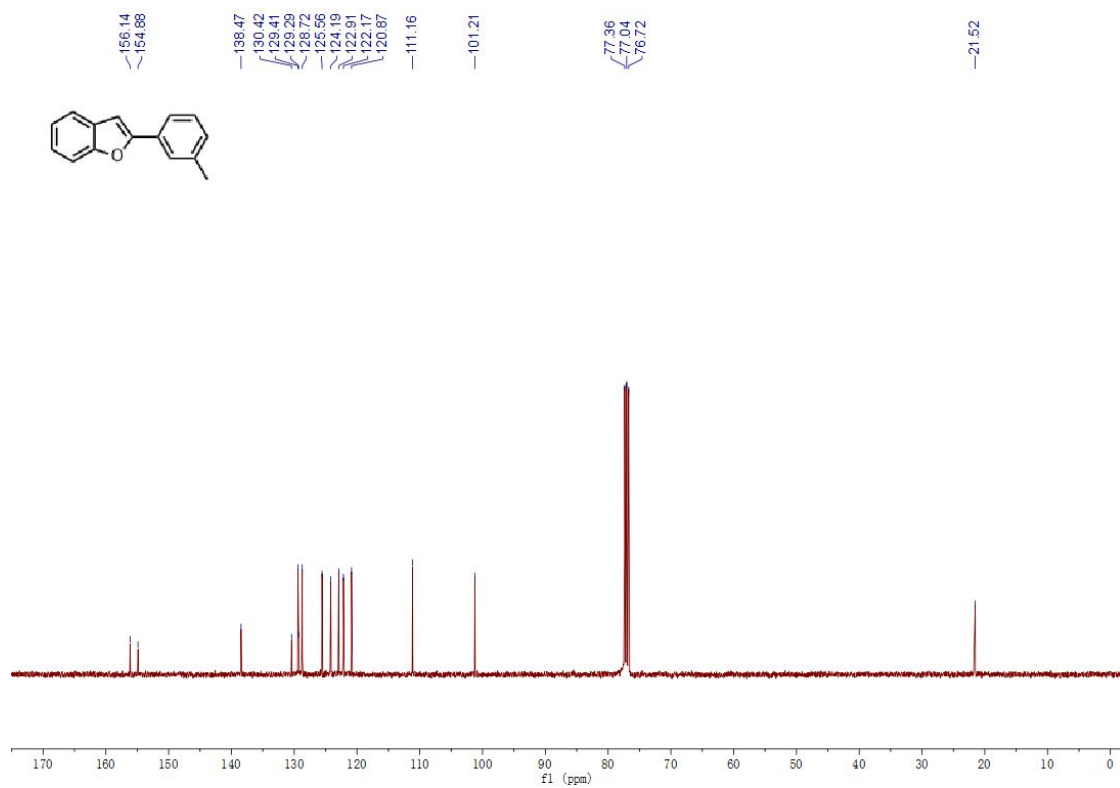


**Figure S149.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5ba** (100 Hz, CDCl<sub>3</sub>)

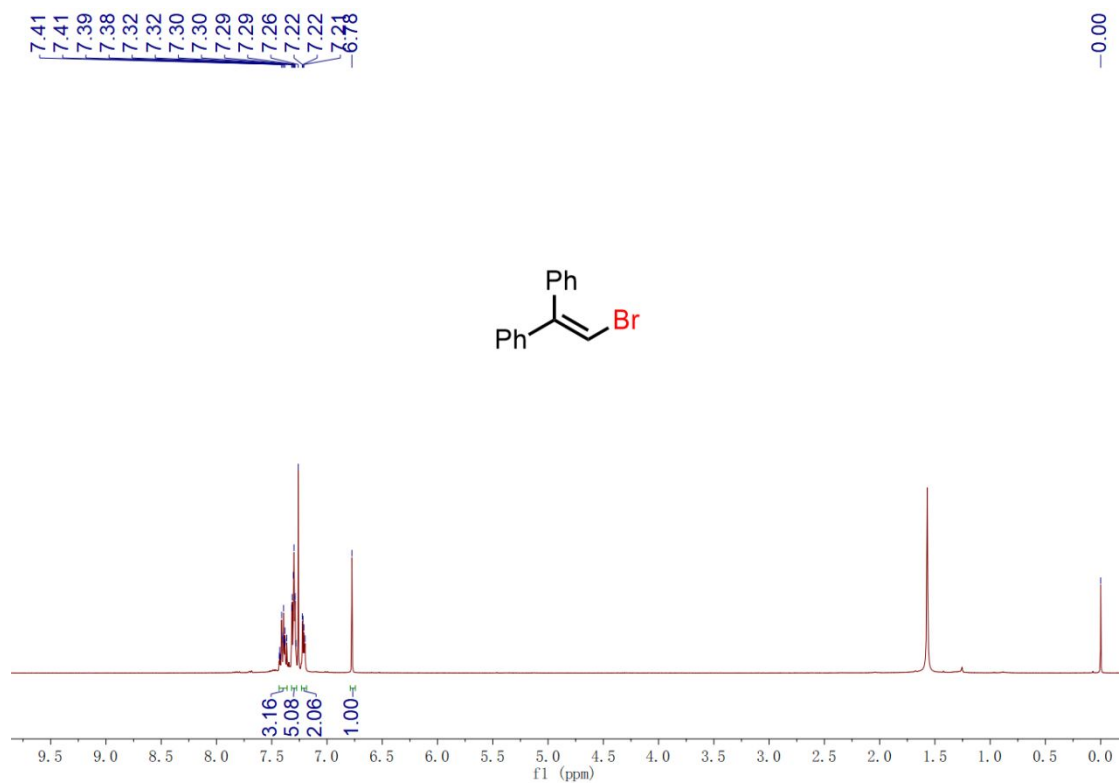




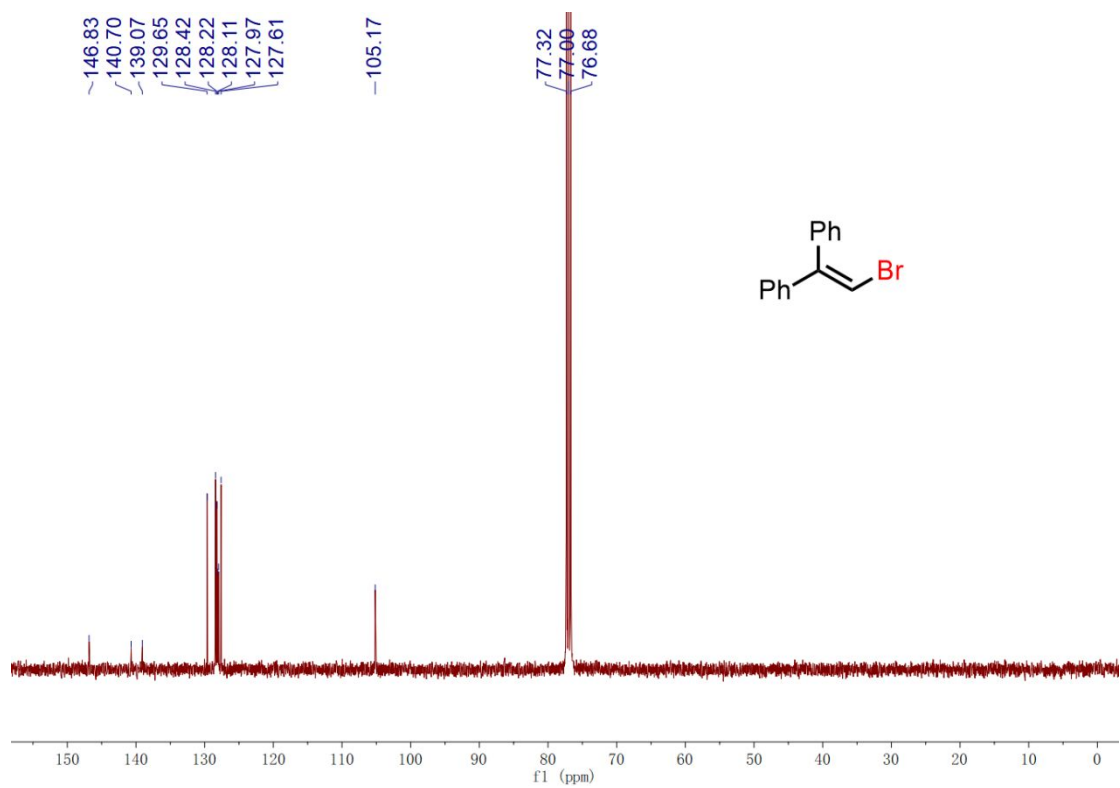
**Figure S150.** Copies of <sup>1</sup>H NMR Spectrum for Compound **5bb** (400 Hz, CDCl<sub>3</sub>)



**Figure S151.** Copies of <sup>13</sup>C NMR Spectrum for Compound **5bb** (100 Hz, CDCl<sub>3</sub>)



**Figure S152.** Copies of <sup>1</sup>H NMR Spectrum for Compound **9** (400 Hz, CDCl<sub>3</sub>)



**Figure S153.** Copies of <sup>13</sup>C NMR Spectrum for Compound **9** (100 Hz, CDCl<sub>3</sub>)