

## Electronic Supplementary Information

# Environmentally Benign Indole-Catalyzed Position-Selective Halogenation of Thioarenes and Other Aromatics

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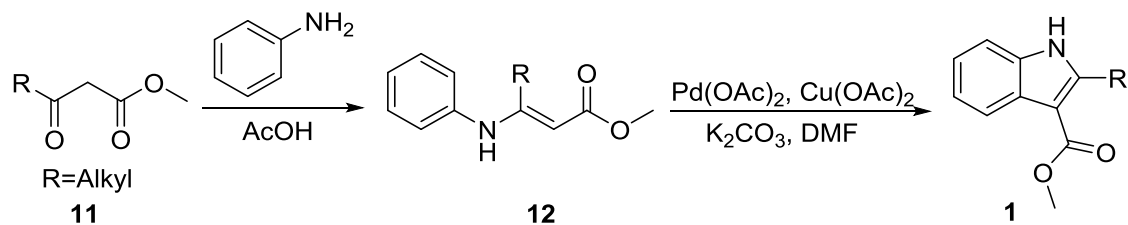
## **(A) General information**

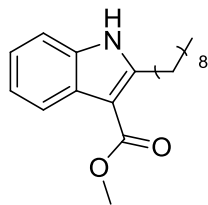
All reactions were carried out by standard procedures under air condition at room temperature unless stated otherwise. Commercially available reagents from Sigma Aldrich and J&K were used as received unless stated otherwise. The solvents were dried over a solvent purification system from Innovative Technology. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AMX400 (400 MHz) spectrometer or a Bruker Avance III 400MHz Spectrometer. Chemical shifts ( $\delta$ ) are reported in parts per million (ppm) relative to TMS ( $\delta$  0.00) for the  $^1\text{H}$  NMR and referenced to residual signals in NMR solvents ( $\text{CDCl}_3$  at  $\delta$  77.16) for the  $^{13}\text{C}$  NMR measurements. Coupling constant ( $J$ ) are quoted in Hz. High resolution mass spectra were obtained on a Finnigan MAT 95XL Mass Spectrometer. Analytical thin layer chromatography (TLC) was performed with Merck pre-coated TLC plates, silica gel 60F-254, layer thickness 0.25 mm. Flash chromatography separations were performed on Merck 60 (0.040-0.063 mm) mesh silica gel.

## (B) General procedure for the indole catalyst synthesis

The  $\beta$ -ketone ester **11** (1 mmol), aniline (1.5 mmol) and acetic acid (0.1 mmol) were charged to a 5 mL eggplant-shaped flask, which was placed in an ultrasound bath and the reaction was monitored by TLC. Upon completion of the reaction, the solution was diluted with EtOH (5 mL), dried over anhydrous  $\text{MgSO}_4$ , filtered, and concentrated under reduced pressure. The residue was briefly purified through a thin plug of silica gel eluted with  $\text{CH}_2\text{Cl}_2$  to give the enamine **12** which was used directly in the next step without further purification.

The enamine **12** was charged to a solution of DMF with  $\text{Pd}(\text{OAc})_2$  (0.1 mmol),  $\text{Cu}(\text{OAc})_2$  (3 mmol) and  $\text{K}_2\text{CO}_3$  (3 mmol) in a re-sealable tube. The tube was evacuated and backfilled with nitrogen three times. The screw cap was then closed and the re-sealable tube was placed in a preheated oil bath at 140 °C for 1 h. Upon completion of the reaction, the solution was cooled to room temperature and filtered through a thin plug of celite. The residue was washed with EtOAc and the filtrate was diluted with saturated aqueous  $\text{NH}_4\text{Cl}$  (5 mL). The aqueous layer was extracted with EtOAc ( $3 \times 10$  mL). The combined organic layer was washed with brine (5 mL), dried over anhydrous  $\text{MgSO}_4$ , filtered, and concentrated under reduced pressure. The residue was purified by flash column chromatography to yield indole catalyst **1**.





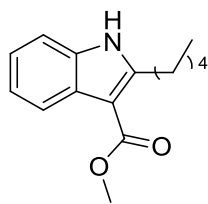
### Methyl 2-decyl-indole-3-carboxylate (1b)

Yield: 85%; Orange oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 9.18 (s, 1H), 8.16 (d, *J* = 7.7 Hz, 1H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.17-7.24 (m, 2H), 3.95 (s, 3H), 3.14 (t, *J* = 7.6 Hz, 2H), 1.67-1.74 (m, 2H), 1.22-1.33 (m, 12H), 0.89 (t, *J* = 6.8 Hz, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 166.8, 149.3, 134.7, 127.2, 122.3, 121.6, 121.3, 110.9, 103.4, 50.9, 31.9, 29.59, 29.56, 29.5, 29.4, 29.3, 28.1, 22.7, 14.2;

**HRMS** (EI) calcd for C<sub>19</sub>H<sub>27</sub>NO<sub>2</sub> [M]<sup>+</sup>: 301.2036; found: 301.2033.



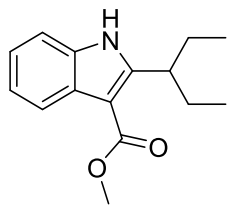
### Methyl 2-pentyl-indole-3-carboxylate (1c)

Yield: 87%; Yellow oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 8.97 (s, 1H), 8.15 (d, *J* = 7.5 Hz, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 7.18-7.24 (m, 2H), 3.95 (s, 3H), 3.14 (t, *J* = 7.8 Hz, 2H), 1.68-1.73 (m, 2H), 1.29-1.34 (m, 4H), 0.86 (s, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 166.7, 149.1, 134.7, 127.2, 122.3, 121.7, 121.3, 110.8, 103.5, 50.8, 31.6, 29.0, 28.0, 22.4, 14.0;

**HRMS** (EI) calcd for C<sub>15</sub>H<sub>19</sub>NO<sub>2</sub> [M]<sup>+</sup>: 245.1410; found: 245.1414.



**Methyl 2-ethylpropyl-indole-3-carboxylate (1d)**

Yield: 85%; Pale yellow oil.

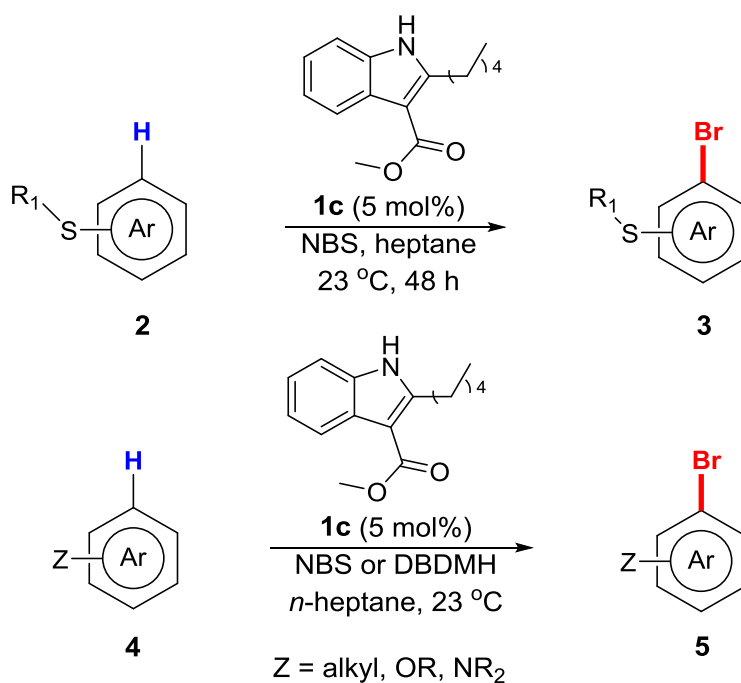
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 9.31 (s, 1H), 8.24 (d, *J* = 5.3 Hz, 1H), 7.41 (s, 1H), 7.28 (s, 2H), 4.01 (s, 4H), 1.76-1.87 (m, 4H), 0.93 (t, 6H);

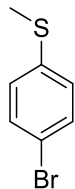
**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 167.2, 151.8, 135.1, 127.1, 122.4, 121.6, 121.5, 110.9, 105.0, 50.8, 40.0, 29.7, 27.8, 11.9;

**HRMS** (EI) calcd for C<sub>15</sub>H<sub>19</sub>NO<sub>2</sub> [M]<sup>+</sup>: 245.1410; found: 245.1412.

### (C) General Procedure for the Indole-Catalyzed Bromination

To a mixture of arene **2** or **4** (1.0 mmol, 1.0 equiv) and indole catalyst **1c** (12.3 mg, 0.05 mmol, 0.05 equiv) in *n*-heptane (2.0 mL) at 23 °C was added *N*-bromosuccinimide or 1,3-dibromo-5,5-dimethylhydantoin (1.05 mmol, 1.05 equiv) in the absence of light. The resultant mixture was stirred at 23 °C and monitored by TLC. Upon completion, the reaction mixture was filtered through a thin plug of silica gel. The filtrate was concentrated under reduced pressure to give the corresponding product **3** or **5**.





#### 4-Bromothioanisole (3a)

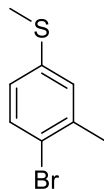
Yield: 92%; Colorless oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.39 (d,  $J = 8.6$  Hz, 2H), 7.11 (d,  $J = 8.6$  Hz, 2H), 2.46 (s, 3H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 137.8, 131.9, 128.2, 118.7, 16.0;

**HRMS** (EI) calcd for  $\text{C}_7\text{H}_7\text{BrS}$   $[\text{M}]^+$ : 201.9446; found: 201.9446.

**Reference:** *Synth. Commun.* **2013**, 43, 2057-2061.



#### 4-Bromo-3-methylthioanisole (3b)

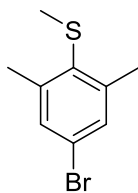
Yield: 97%; Colorless oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.41 (d,  $J = 8.3$  Hz, 1H), 7.11-7.12 (m, 1H), 6.92-6.95 (m, 1H), 2.46 (s, 3H), 2.37 (s, 3H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 138.3, 137.7, 132.6, 128.9, 125.5, 121.3, 22.9, 16.0;

**HRMS** (EI) calcd for  $\text{C}_8\text{H}_9\text{BrS}$   $[\text{M}]^+$ : 215.9603; found: 215.9601.

**Reference:** *J. Am. Chem. Soc.* **2009**, 131, 3291-3306.



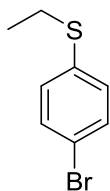
**4-Bromo-2,6-dimethylthioanisole (3c)**

Yield: 93%; Colorless oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.14 (s, 2H), 2.56 (s, 6H), 2.24 (s, 3H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 142.8, 135.3, 128.2, 128.1, 21.8, 18.4;

**HRMS** (EI) calcd for  $\text{C}_9\text{H}_{11}\text{BrS}$   $[\text{M}]^+$ : 229.9759; found: 229.9757.



**1-Bromo-4-(ethylthio)benzene (3d)**

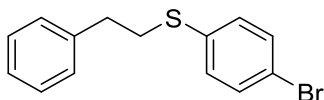
Yield: 94%; Colorless oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.39 (d,  $J = 8.5$  Hz, 2H), 7.18 (d,  $J = 8.4$  Hz, 2H), 2.92 (q,  $J = 7.3$  Hz, 2H), 1.30 (t,  $J = 7.3$  Hz, 3H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 136.0, 131.9, 130.6, 119.6, 27.8, 14.4;

**HRMS** (EI) calcd for  $\text{C}_8\text{H}_9\text{BrS}$   $[\text{M}]^+$ : 215.9603; found: 215.9607.

**Reference:** *J. Org. Chem.* **2001**, 66, 2104-2117.



**1-Bromo-4-[(2-phenylethyl)thio]benzene (3e)**

Yield: 92%; Colorless oil.

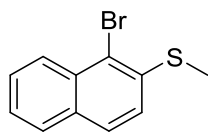


**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.41 (d, *J* = 8.3 Hz, 2H), 7.29-7.33 (m, 2H), 7.18-7.26 (m, 5H), 3.13-3.17 (m, 2H), 2.90-2.94 (m, 2H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 140.0, 135.7, 132.1, 130.8, 128.7, 128.6, 119.9, 35.6, 35.3;

**HRMS** (EI) calcd for C<sub>14</sub>H<sub>13</sub>BrS [M]<sup>+</sup>: 293.9895; found: 293.9894.

**Reference:** *Eur. J. Org. Chem.* **2011**, 4327-4334.



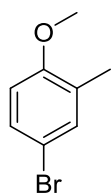
### 1-Bromo-2-(methylthio)naphthalene (3f)

Yield: 99%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 8.24 (d, *J* = 8.6 Hz, 1H), 7.78 (d, *J* = 8.9 Hz, 2H), 7.57-7.62 (m, 1H), 7.45-7.49 (m, 1H), 7.31 (d, *J* = 8.7 Hz, 1H), 2.6 (s, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 137.7, 132.6, 131.9, 128.3, 128.1, 128.0, 126.3, 125.7, 122.8, 120.4, 16.3;

**HRMS** (EI) calcd for C<sub>11</sub>H<sub>9</sub>BrS [M]<sup>+</sup>: 253.9582; found: 253.9582.



### 4-Bromo-2-methylanisole (5a)

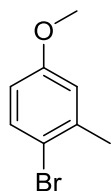
Yield: 95%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.24-7.27 (m, 2H), 6.67-6.69 (m, 1H), 3.80 (s, 1H), 2.19 (s, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 156.9, 133.3, 129.5, 129.1, 112.4, 111.6, 55.6, 16.2;

**HRMS** (EI) calcd for C<sub>8</sub>H<sub>9</sub>BrO [M]<sup>+</sup>: 199.9831; found: 199.9835.

**Reference:** *Org. Lett.* **2006**, 8, 3987-3990.



#### 4-Bromo-3-methylanisole (5b)

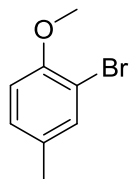
Yield: 99%; Colorless oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.40 (d,  $J = 8.6$  Hz, 1H), 6.79 (s, 1H), 6.62 (d,  $J = 8.6$  Hz, 1H), 3.77 (s, 3H), 2.37 (s, 3H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 158.9, 138.9, 132.9, 116.6, 115.5, 113.0, 55.5, 23.2;

**HRMS** (EI) calcd for  $\text{C}_8\text{H}_9\text{BrO}$   $[\text{M}]^+$ : 199.9831; found: 199.9836.

**Reference:** *J. Med. Chem.* **2013**, 56, 10132-10141.



#### 2-Bromo-4-methylanisole (5c)

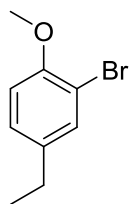
Yield: 97%; Colorless oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.36 (s, 1H), 7.06 (d,  $J = 8.3$  Hz, 1H), 6.80 (d,  $J = 8.3$  Hz, 1H), 3.86 (s, 3H), 2.27 (s, 3H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 153.8, 133.8, 131.5, 128.9, 111.9, 111.4, 56.4, 20.2;

**HRMS** (EI) calcd for  $\text{C}_8\text{H}_9\text{BrO}$   $[\text{M}]^+$ : 199.9831; found: 199.9831.

**Reference:** *Org. Lett.* **2001**, 3, 3795-3798.



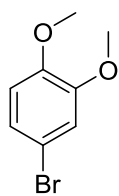
### 2-Bromo-4-ethylanisole (5d)

Yield: 92%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.38 (s, 1H), 7.07 (d, *J* = 8.4 Hz, 1H), 6.81 (d, *J* = 8.3 Hz, 1H), 3.86 (s, 3H), 2.57 (m, 2H); 1.21 (t, *J* = 7.6 Hz, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 153.8, 138.0, 132.7, 127.7, 112.0, 111.3, 56.2, 27.7, 15.8;

**HRMS** (EI) calcd for C<sub>9</sub>H<sub>11</sub>BrO [M]<sup>+</sup>: 213.9988; found: 213.9986.



### 4-Bromoveratrole (5e)

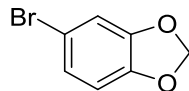
Yield: 90%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.00 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.95 (d, *J* = 2.2 Hz, 1H), 6.70 (d, *J* = 8.5 Hz, 1H), 3.84 (s, 3H), 3.83 (s, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 149.7, 148.8, 123.3, 114.7, 112.7, 112.4, 56.1, 56.0;

**HRMS** (EI) calcd for C<sub>8</sub>H<sub>9</sub>BrO<sub>2</sub> [M]<sup>+</sup>: 215.9780; found: 215.9784.

**Reference:** *J. Am. Chem. Soc.* **2009**, 131, 17500-17521.



### 1-Bromo-3,4-(methylenedioxy)benzene (5f)

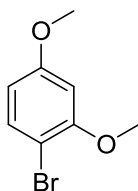
Yield: 92%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 6.94 (d, *J* = 7.6 Hz, 2H), 6.67 (d, *J* = 8.0 Hz, 1H), 5.95 (s, 2H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 148.6, 147.0, 124.3, 113.1, 112.3, 109.6, 101.7;

**HRMS** (EI) calcd for C<sub>7</sub>H<sub>5</sub>BrO<sub>2</sub> [M]<sup>+</sup>: 199.9467; found: 199.9466.

**Reference:** Imazaki, Y.; Shirakawa, E.; Ueno, R.; Hayashi, T. *J. Am. Chem. Soc.* **2012**, *134*, 14760-14763.



#### 1-Bromo-2,4-dimethoxybenzene (5g)

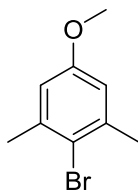
Yield: 97%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.40 (d, *J* = 8.6 Hz, 1H), 6.48 (d, *J* = 2.5 Hz, 1H), 6.39 (dd, *J* = 8.7, 2.6 Hz, 1H), 3.86 (s, 3H), 3.79 (s, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 160.3, 156.5, 133.2, 105.9, 102.5, 100.0, 56.2, 55.6;

**HRMS** (EI) calcd for C<sub>8</sub>H<sub>9</sub>BrO<sub>2</sub> [M]<sup>+</sup>: 215.9780; found: 215.9781.

**Reference:** *Synth. Commun.* **2001**, *31*, 2955-2963.



#### 4-Bromo-3,5-dimethylanisole (5h)

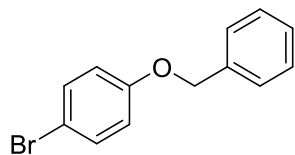
Yield: 89%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 6.66 (s, 2H), 3.77 (s, 3H), 2.40 (s, 6H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 158.1, 139.2, 118.3, 113.9, 55.4, 24.2;

**HRMS** (EI) calcd for C<sub>9</sub>H<sub>11</sub>BrO [M]<sup>+</sup>: 213.9988; found: 213.9984.

**Reference:** *J. Am. Chem. Soc.* **2007**, *129*, 3267-3286.



#### 4-Benzyloxybromobenzene (5i)

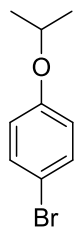
Yield: 93%; Colorless solid. M.p. 62–63 °C.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.32-7.43 (m, 7H), 6.84-6.88 (m, 2H), 5.04 (s, 2H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 157.9, 136.6, 132.4, 128.7, 128.2, 127.5, 116.8, 113.2, 70.3;

**HRMS** (EI) calcd for  $\text{C}_{13}\text{H}_{11}\text{BrO}$   $[\text{M}]^+$ : 261.9988; found: 261.9985.

**Reference:** *J. Med. Chem.* **2014**, *57*, 9578-9597.



#### 1-Bromo-4-(propan-2-yloxy)benzene (5j)

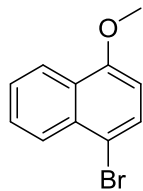
Yield: 90%; Colorless oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.35 (d,  $J = 9.0$  Hz, 2H), 6.76 (d,  $J = 8.9$  Hz, 2H), 4.46-4.52 (m, 1H), 1.32 (d,  $J = 6.1$  Hz, 6H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 157.1, 132.3, 117.7, 112.6, 70.3, 22.0;

**HRMS** (EI) calcd for  $\text{C}_9\text{H}_{11}\text{BrO}$   $[\text{M}]^+$ : 213.9988; found: 213.9984.

**Reference:** *J. Med. Chem.* **2012**, *55*, 4189-4204.



### 1-Bromo-4-methoxynaphthalene (5k)

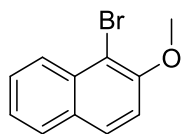
Yield: 90%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 8.33 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 7.62-7.68 (m, 2H), 7.56 (t, *J* = 7.3 Hz, 1H), 6.63 (d, *J* = 8.2 Hz, 1H), 3.96 (s, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 155.2, 132.4, 129.5, 127.8, 126.8, 125.9, 122.5, 113.2, 104.5, 55.6;

**HRMS** (EI) calcd for C<sub>11</sub>H<sub>9</sub>BrO [M]<sup>+</sup>: 235.9831; found: 235.9830.

**Reference:** *Synthesis*. **2009**, 12, 2040-2060.



### 1-Bromo-2-methoxynaphthalene (5l)

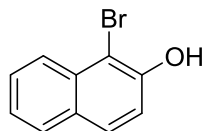
Yield: 98%; Colorless crystal. M.p. 82–83 °C.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 8.21 (d, *J* = 8.6 Hz, 1H), 7.80 (t, *J* = 7.9 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.42 (m, 1H), 7.28 (d, *J* = 9.0 Hz, 1H), 4.04 (s, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 153.7, 133.0, 129.8, 129.0, 128.1, 127.6, 126.1, 124.3, 113.5, 108.6, 57.0;

**HRMS** (EI) calcd for C<sub>11</sub>H<sub>9</sub>BrO [M]<sup>+</sup>: 235.9831; found: 235.9833.

**Reference:** *Macromolecular Research*. **2014**, 22, 1152-1155.



### 1-Bromo-2-naphthol (5m)

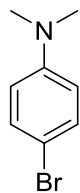
Yield: 93%; White solid. M.p. 80–81 °C.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 8.04 (d,  $J = 8.4$  Hz, 1H), 7.77 (q,  $J = 8.0$  Hz, 2H), 7.58 (t,  $J = 7.1$  Hz, 1H), 7.40 (t,  $J = 7.2$  Hz, 1H), 7.28 (d,  $J = 8.8$  Hz, 1H), 5.97 (s, 1H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 150.6, 132.3, 129.7, 129.4, 128.3, 127.9, 125.4, 124.2, 117.2, 106.2;

**HRMS** (EI) calcd for  $\text{C}_{10}\text{H}_7\text{BrO}$   $[\text{M}]^+$ : 221.9675; found: 221.9675.

**Reference:** *Org. Lett.* **2010**, 12, 3498-3501.



### 4-Bromo-*N,N*-dimethylaniline (5n)

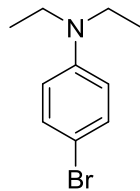
Yield: 90%; Pale yellow oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 7.30 (d,  $J = 7.9$  Hz, 2H), 6.59 (d,  $J = 7.9$  Hz, 2H), 2.92 (s, 6H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 149.8, 132.1, 114.6, 109.1, 41.0;

**HRMS** (EI) calcd for  $\text{C}_8\text{H}_{10}\text{BrN}$   $[\text{M}]^+$ : 198.9991; found: 198.9992.

**Reference:** *J. Org. Chem.* **2006**, 26, 9851-9853.



**4-Bromo-*N,N*-diethylaniline (5o)**

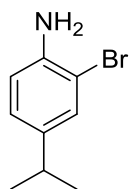
Yield: 90%; Pale yellow oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.24 (d, *J* = 8.5 Hz, 2H), 6.52 (d, *J* = 8.0 Hz, 2H), 3.30 (q, *J* = 6.9 Hz, 4H), 1.12 (t, *J* = 8.5 Hz, 6H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 146.0, 131.9, 113.5, 107.0, 44.5, 12.5;

**HRMS** (EI) calcd for C<sub>10</sub>H<sub>14</sub>BrN [M]<sup>+</sup>: 227.0304; found: 227.0302.

**Reference:** *J. Org. Chem.* **2006**, 26, 9851-9853.



**4-Amino-2-Bromocumene (5p)**

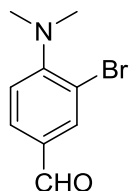
Yield: 90%; Pale yellow oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.29 (s, 1H), 6.98 (d, *J* = 8.1 Hz, 1H), 6.71 (d, *J* = 8.1 Hz, 1H), 3.96 (s, 2H), 2.76-2.83 (m, 1H), 1.21 (d, *J* = 6.9 Hz, 6H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 141.9, 140.5, 130.3, 126.5, 115.9, 109.4, 33.1, 24.2;

**HRMS** (EI) calcd for C<sub>9</sub>H<sub>12</sub>BrN [M]<sup>+</sup>: 213.0148; found: 213.0146.

**Reference:** *J. Med. Chem.* **2012**, 55, 7360-7377.



**3-Bromo-4-*N,N*-dimethylaminobenzaldehyde (5q)**

Yield: 95%; Colorless oil.

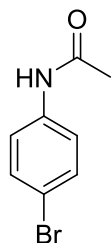


**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 9.77(s, 1H), 7.99 (d, *J* = 1.9 Hz, 1H), 7.70 (dd, *J* = 8.3, 0.9 Hz, 1H), 7.03 (d, *J* = 8.3 Hz, 1H), 2.91 (s, 6H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 189.7, 156.9, 135.9, 131.0, 129.9, 119.4, 116.5, 43.5;

**HRMS** (EI) calcd for C<sub>9</sub>H<sub>10</sub>BrNO [M]<sup>+</sup>: 226.9940; found: 226.9941.

**Reference:** *Journal of Molecular Catalysis A: Chemical*. **2007**, 267, 30-33.



**N-(4-bromophenyl)acetamide (5r)**

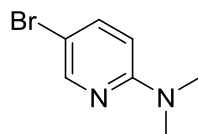
Yield: 87%; White crystal. M.p. 168–169 °C.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.38-7.43 (m, 4H), 7.30 (br s, 1H), 2.17 (s, 3H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 168.5, 137.1, 132.1, 121.5, 117.0, 24.7;

**HRMS** (ESI) calcd for C<sub>8</sub>H<sub>8</sub>BrNO [M+H]<sup>+</sup>: 213.9862; found: 213.9864.

**Reference:** Kumar, L.; Mahajan, T.; Sharma, V.; Agarwal, D. D. *Ind. Eng. Chem. Res.* **2011**, 50, 705-712.



**5-Bromo-2-dimethylaminopyridine (5s)**

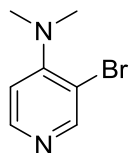
Yield: 91%; Colorless oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 8.15 (d, *J* = 2.3 Hz, 1H), 7.47 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.38 (d, *J* = 9.0 Hz, 1H), 3.04 (s, 6H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 157.8, 148.3, 139.3, 107.3, 106.0, 38.2;

**HRMS** (EI) calcd for C<sub>7</sub>H<sub>9</sub>BrN<sub>2</sub> [M]<sup>+</sup>: 199.9944; found: 199.9944.

**Reference:** *ACS. Comb. Sci.* **2005**, 7, 879-886.



### 3-Bromo-4-dimethylaminopyridine (5t)

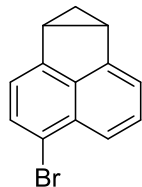
Yield: 90%; White solid. M.p. 84–85 °C.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 8.48 (s, 1H), 8.24 (d, *J* = 5.6 Hz, 1H), 6.77 (d, *J* = 5.6 Hz, 1H), 2.95 (s, 6H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 157.1, 153.2, 148.5, 113.8, 112.3, 42.6;

**HRMS** (ESI) calcd for C<sub>7</sub>H<sub>9</sub>BrN<sub>2</sub> [M + Na]<sup>+</sup>: 222.98413; found: 222.98415.

**Reference:** *Synth. Commun.* **2009**, 39, 215-219.



### 3-Bromo-7,7a-dihydro-6bH-cyclopropa[a]acenaphthylene (5u)

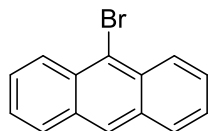
Yield: 96%; Yellow oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.74 (d, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.48 (dd, *J* = 8.4, 6.8 Hz, 1H), 7.40 (d, *J* = 7.2 Hz, 1H), 7.21 (d, *J* = 7.2 Hz, 1H), 3.06-3.01 (m, 1H), 2.99-2.95 (m, 1H), 1.53 (td, *J* = 8.0, 4.0 Hz, 1H), 0.82-0.79 (m, 1H);

**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 146.6, 146.4, 137.6, 131.4, 130.4, 128.6, 122.2, 120.4, 120.3, 117.3, 28.0, 24.4, 23.7;

**HRMS** (APCI) calcd for C<sub>13</sub>H<sub>9</sub>Br [M+H]<sup>+</sup>: 244.99574; found: 244.99604.

**Reference:** *PCT Int. Appl.*, **2015**, WO 2015179448, 26 Nov 2015.



**9-Bromoanthracene (5v)**

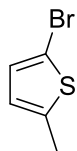
Yield: 81%; Yellow solid. M.p. 100–101 °C.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 8.50 (d,  $J = 8.7$  Hz, 2H), 8.4 (s, 1H), 7.96 (d,  $J = 8.3$  Hz, 2H), 7.60 (t,  $J = 7.7$  Hz, 2H), 7.51 (t,  $J = 7.7$  Hz, 2H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 134.0, 132.3, 130.6, 128.7, 127.7, 127.3, 127.1, 125.6;

**HRMS** (EI) calcd for  $\text{C}_{14}\text{H}_9\text{Br}$   $[\text{M}]^+$ : 255.9882; found: 255.9880.

**Reference:** *Green Chemistry Letters and Reviews*. **2012**, 5, 639-642.



**5-Bromo-2-methylthiophene (5w)**

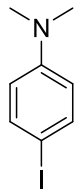
Yield: 92%; Colorless oil.

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 6.82 (s, 1H), 6.51 (s, 1H), 2.42 (s, 3H);

$^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ): ( $\delta$ , ppm) 141.4, 129.6, 125.5, 108.5, 15.5;

**HRMS** (EI) calcd for  $\text{C}_5\text{H}_5\text{BrS}$   $[\text{M}]^+$ : 175.9290; found: 175.9292.

**Reference:** *Synthesis*. **2002**, 9, 1133-1135.



**4-Iodo-*N,N*-dimethylaniline (6)**

Yield: 91%; Pale yellow oil.

**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.46-7.49 (m, 2H), 6.49-6.52 (m, 2H), 2.93 (d, *J* = 3.1 Hz, 6H);

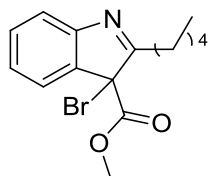
**<sup>13</sup>C NMR** (100 MHz, CDCl<sub>3</sub>): (δ, ppm) 150.1, 137.6, 114.8, 77.5, 40.5;

**HRMS** (EI) calcd for C<sub>8</sub>H<sub>10</sub>IN [M]<sup>+</sup>: 246.9858; found: 246.9858.

**Reference:** *Tetrahedron*. **2002**, 58, 2405-2413.

## (D) Procedure for the preparation compound **1c-Br**

To a solution of indole catalyst **1c** (0.3 mmol, 60.9 mg, 1.0 equiv) in dichloromethane (3 mL) at 23 °C was added *N*-bromosuccinimide (56 mg, 0.315 mmol, 1.05 equiv). After 15 minutes, the solution was concentrated under reduced pressure. The residue was dissolved in *n*-hexane (5 mL) and the resultant suspension was filtered through sintered glass funnel. The filtrate was concentrated under reduced pressure and compound **1c-Br** was obtained (99% yield) as a yellow oil.



### Methyl 3-Bromo-2-pentyl-3*H*-indole-3-carboxylate (**1c-Br**)

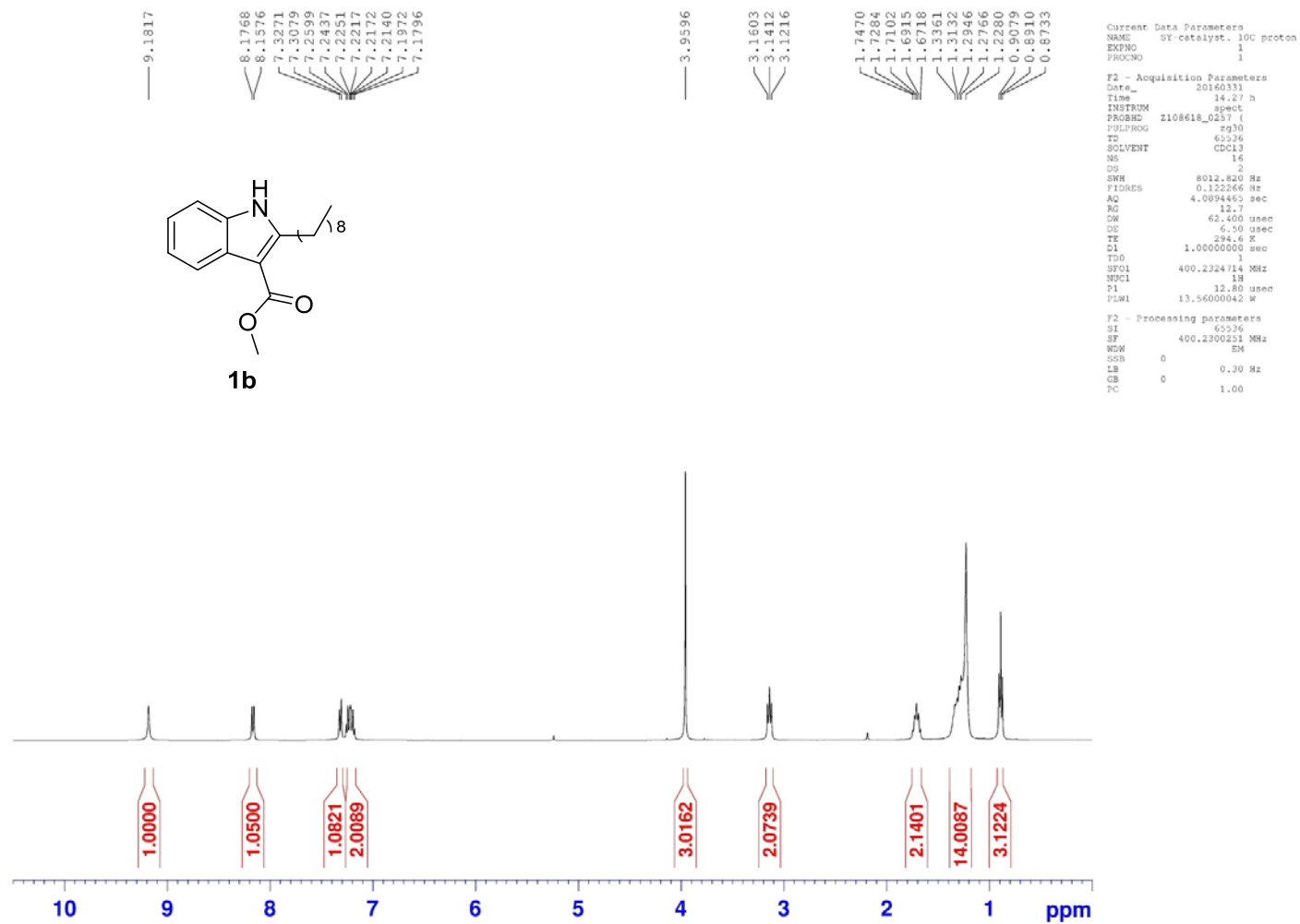
Yield: 99%; Yellow oil.

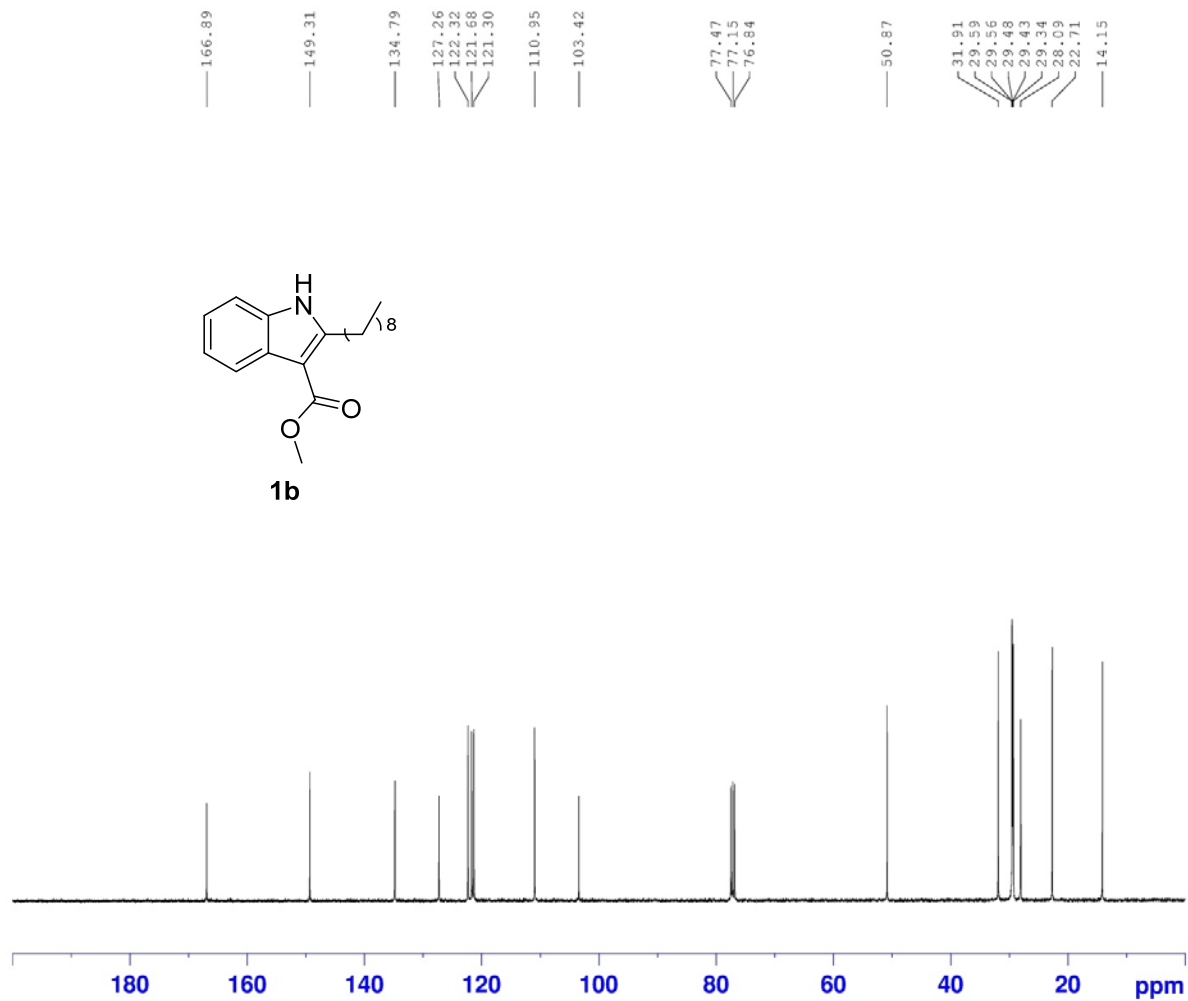
**<sup>1</sup>H NMR** (400 MHz, CDCl<sub>3</sub>): (δ, ppm) 7.52-7.57 (m, 2H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 3.73 (s, 3H), 2.72 (s, 2H), 1.80-1.91 (m, 2H), 1.33-1.45 (m, 2H), 0.91 (t, *J* = 7.0 Hz, 3H);

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>): (δ, ppm) 180.4, 166.4, 153.4, 136.2, 130.8, 126.7, 124.4, 120.9, 60.0, 54.0, 31.6, 30.0, 29.5, 26.2, 22.4, 14.0;

**HRMS** (EI) calcd for C<sub>15</sub>H<sub>18</sub>BrNO<sub>2</sub> [M]<sup>+</sup>: 323.0515; found: 323.0519.

**(E) <sup>1</sup>H and <sup>13</sup>C NMR Spectra**

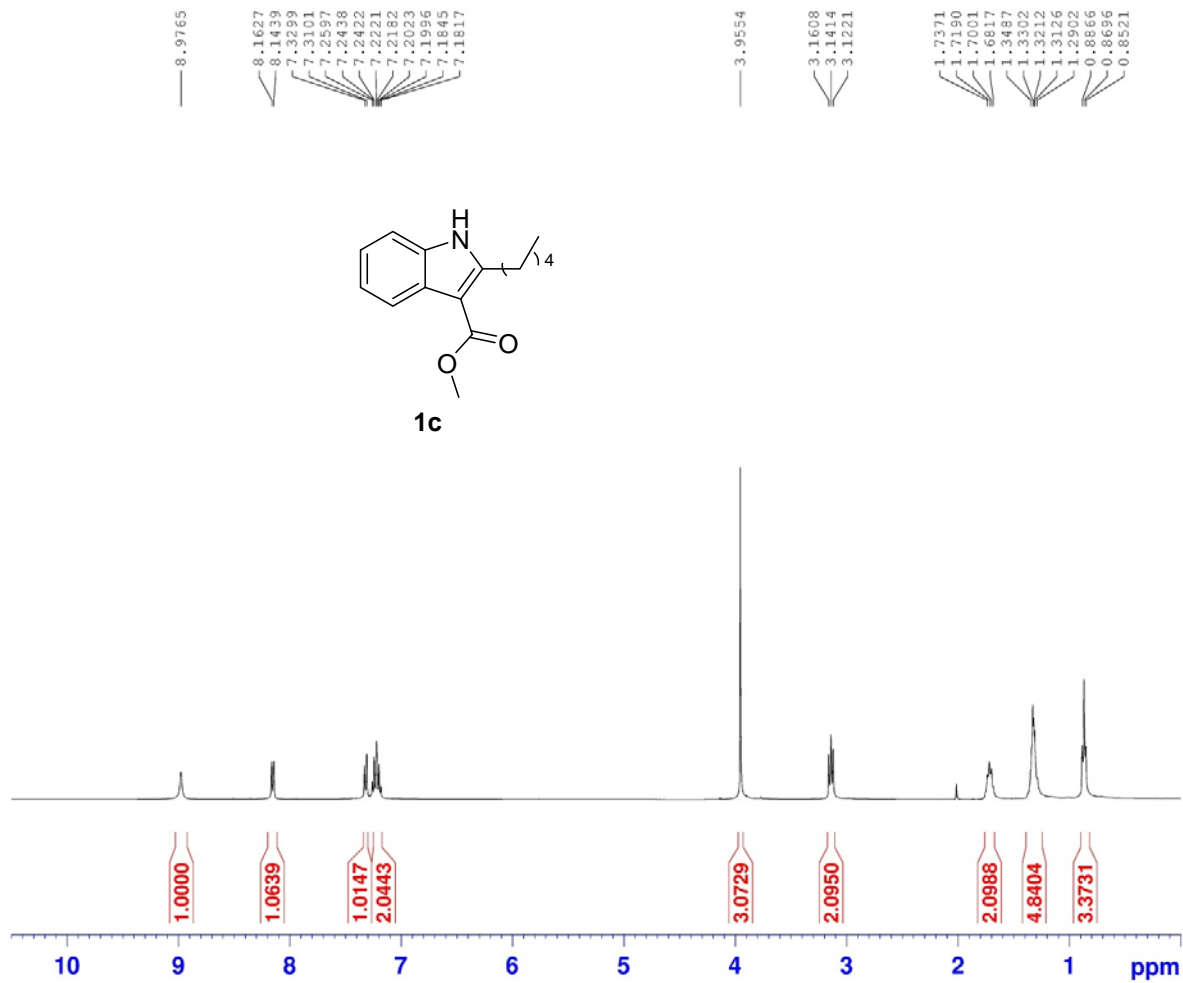




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 P1 9.50 usec  
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 SFO2 400.2316009 MHz  
 NUC2 1H  
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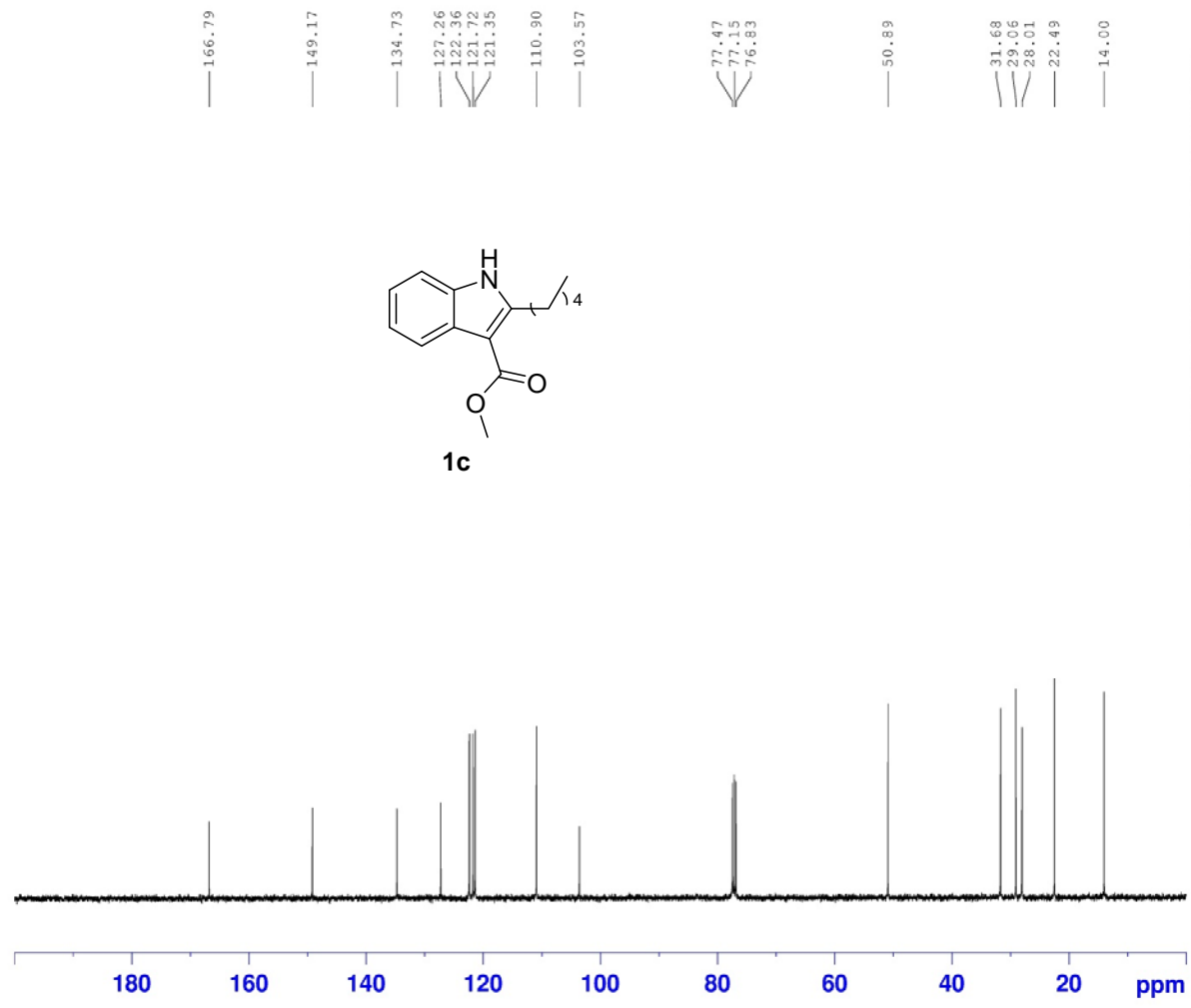


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 FIDRES 0.122266 Hz  
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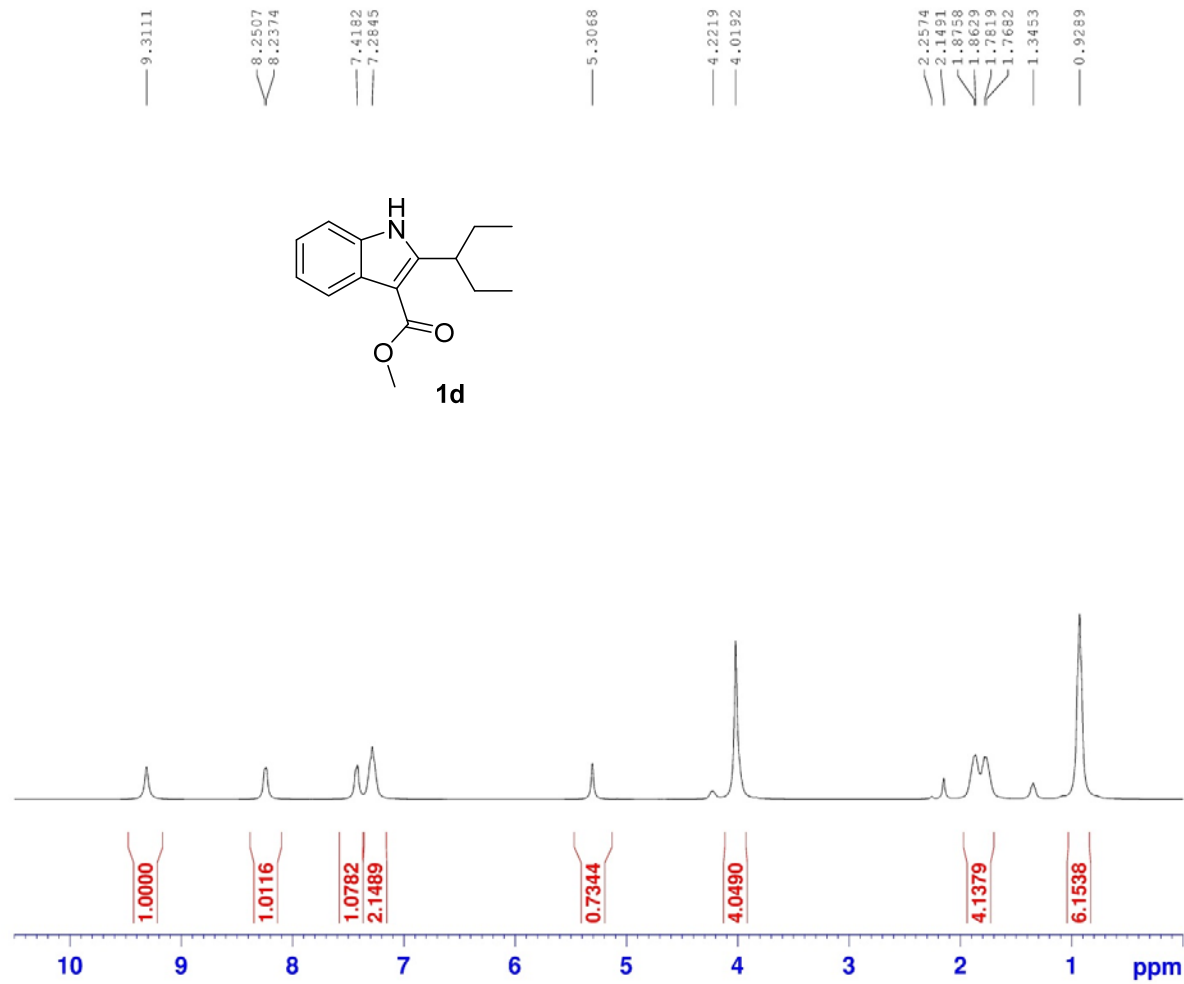
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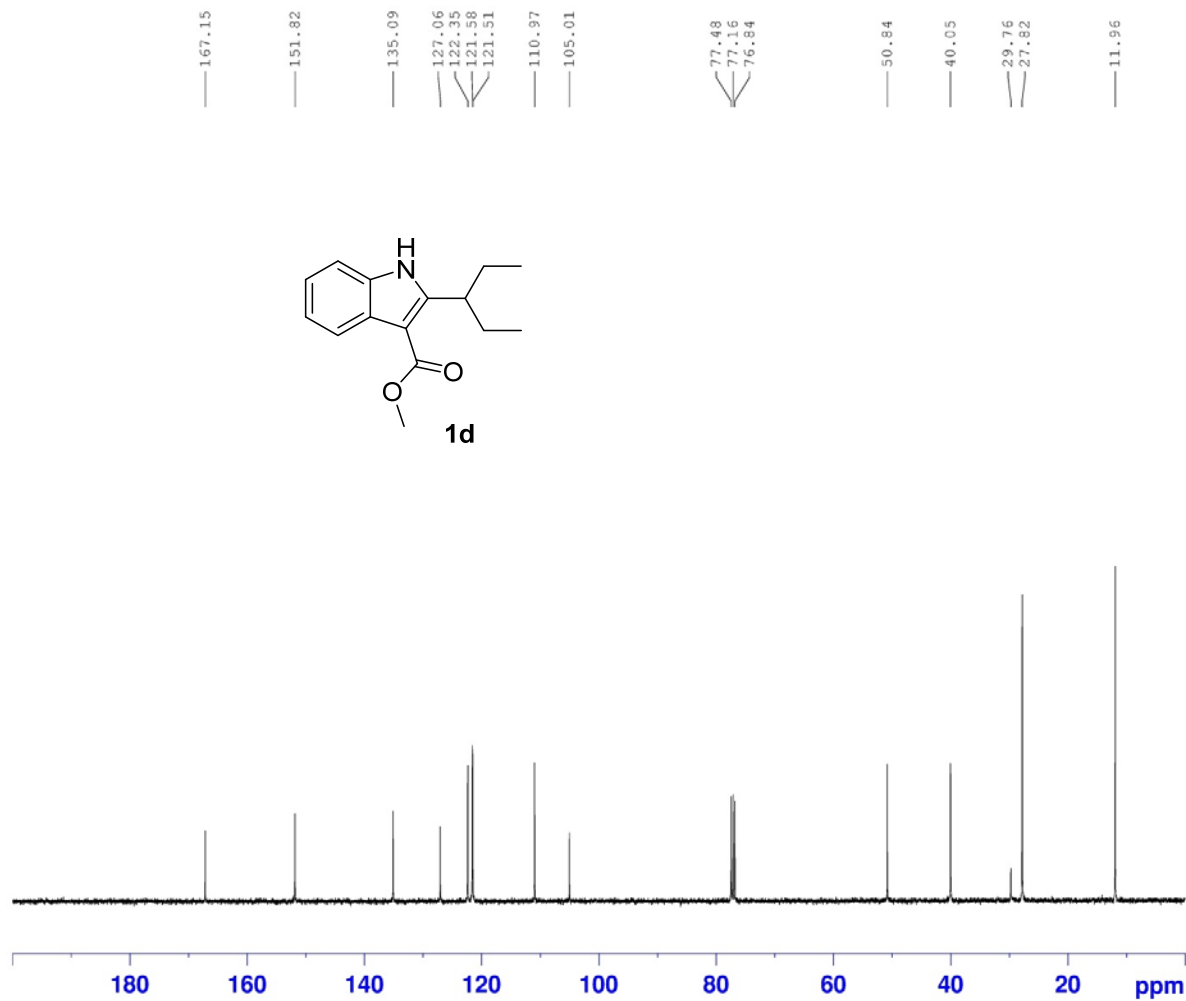
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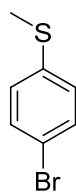
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 FIDRES 0.366798 Hz  
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 DE 6.50 usec  
 TE 294.9 K  
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 SFO2 400.2316009 MHz  
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 PLW2 13.56000042 W  
 PLW12 0.27428001 W  
 PLW13 0.13796000 W

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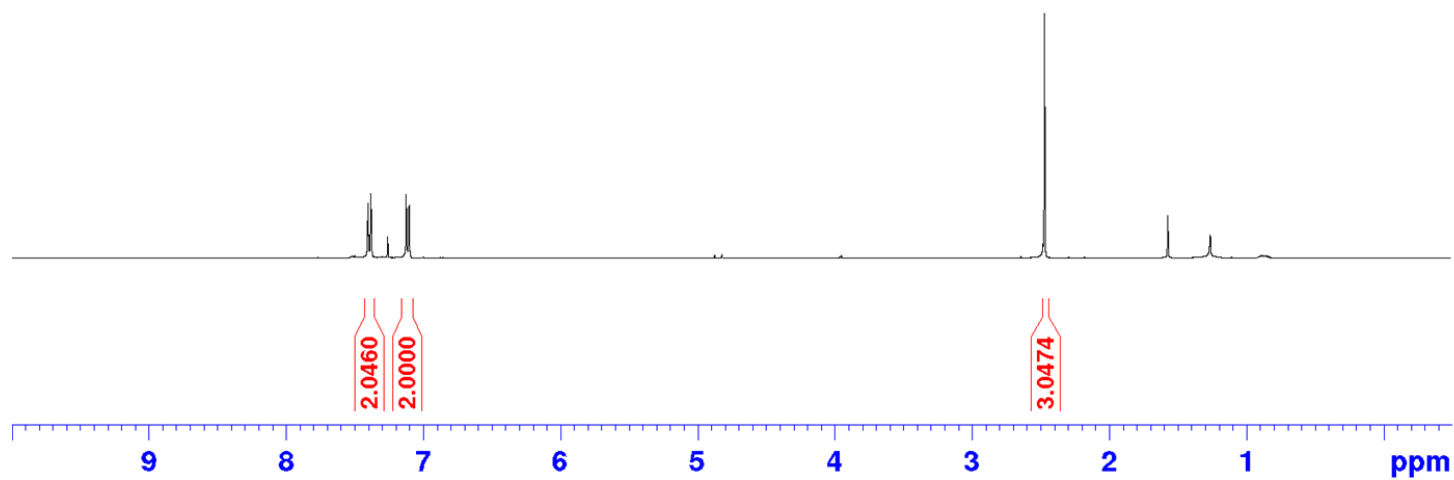


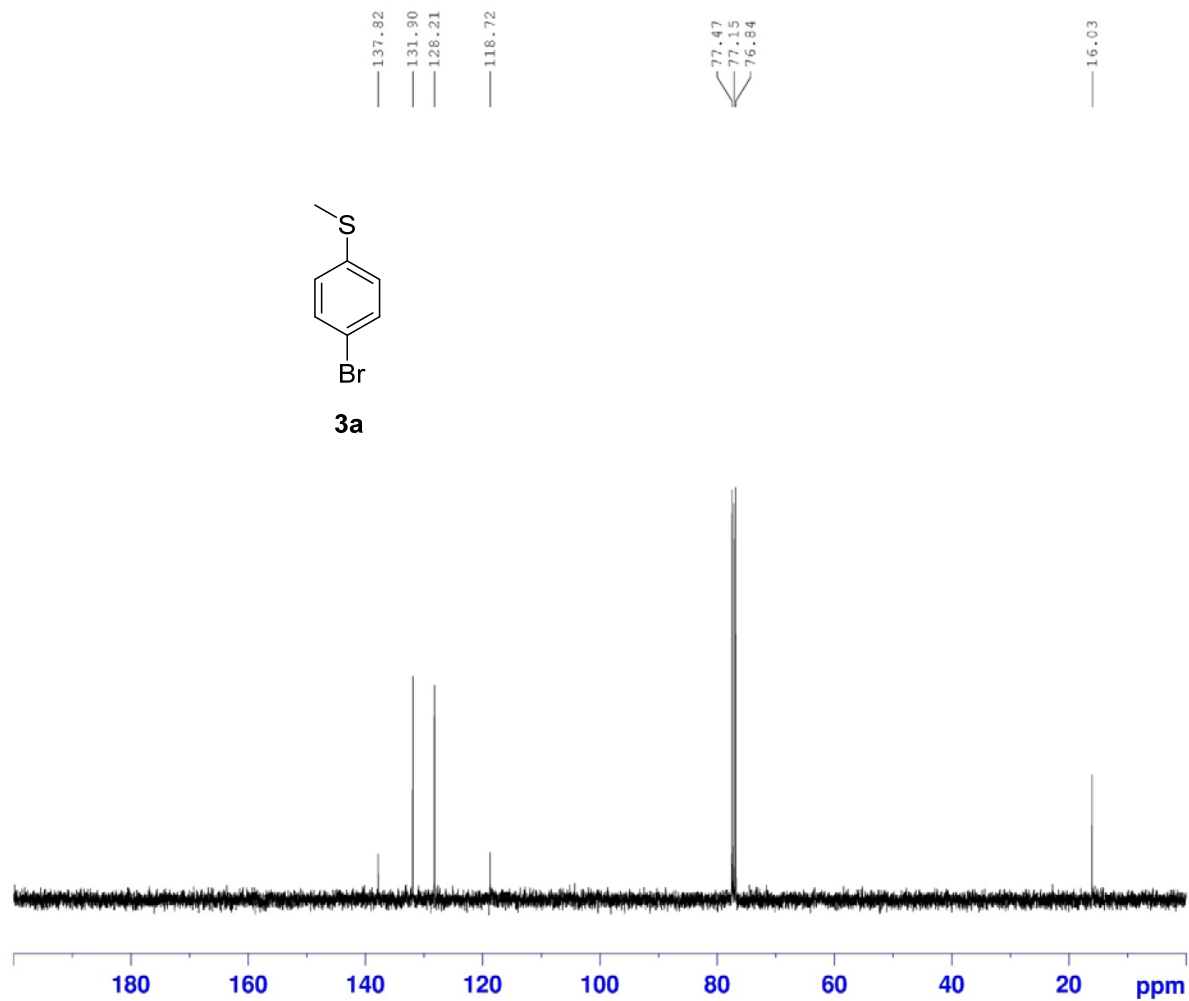
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PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160606  
Time 13.26 h  
INSTRUM spect  
PROBHD Z108618\_0257 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 4  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 114  
DW 62.400 usec  
DE 6.50 usec  
TE 295.0 K  
D1 1.00000000 sec  
TD0 1  
SF01 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters  
SI 65536  
SF 400.2300106 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





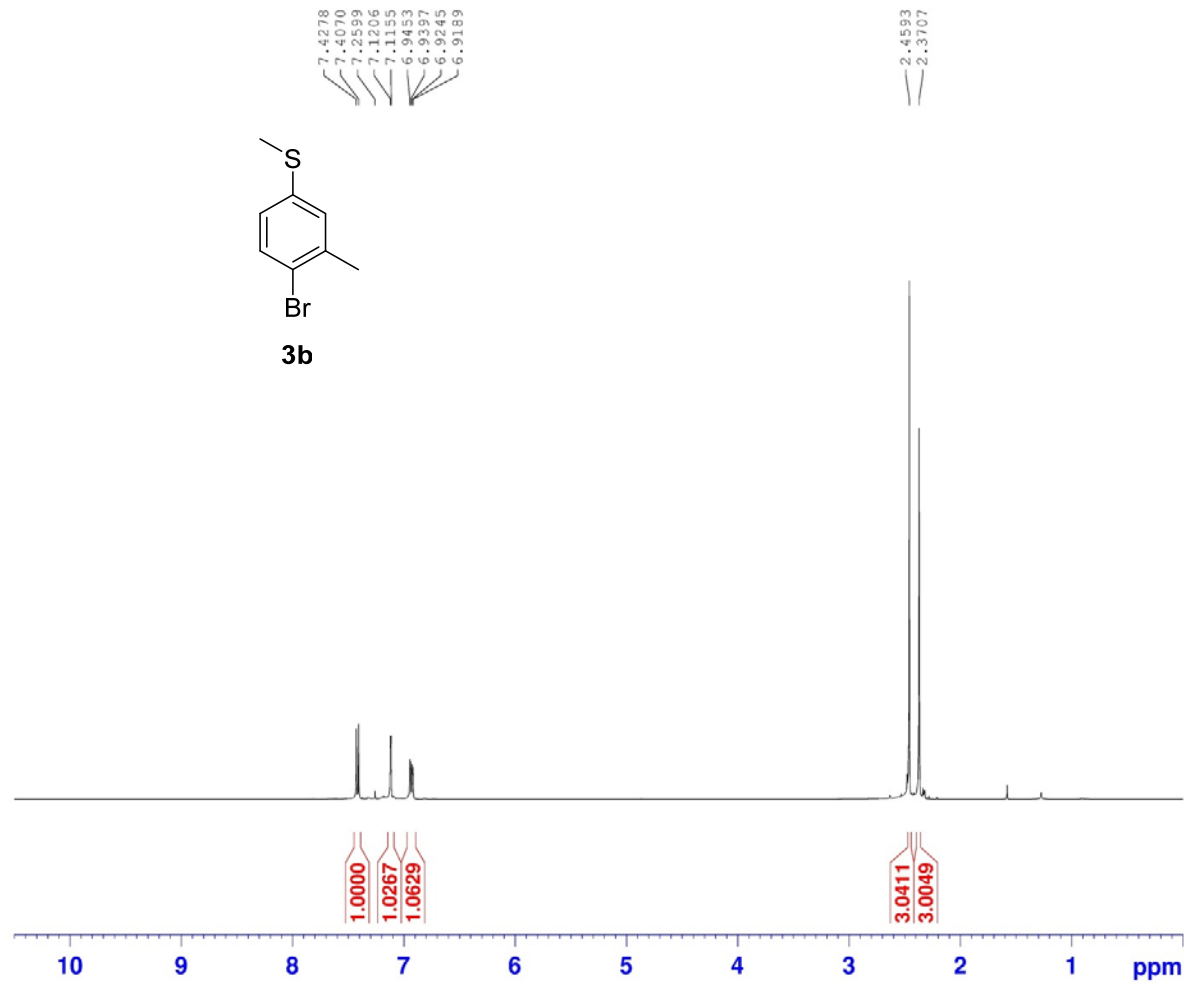
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Current Data Parameters
NAME      SY-13901 carbon
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160427
Time     16.58 h
INSTRUM  spect
PROBHD   Z824601_0021
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       35
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       200
DW       20.800 usec
DE       6.50 usec
TE       294.9 K
D1       2.0000000 sec
d11      0.0300000 sec
TD0      1
SFO1     100.6228298 MHz
NUC1     13C
P1       9.50 usec
PLM1     41.2500000 W
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLM2     8.31000042 W
PLW12    0.23083000 W
PLW13    0.11611000 W

F2 - Processing parameters
SI       32768
SF       100.6127579 MHz
WDW      EM
SSB      0
LR       1.00 Hz
GB       0
FC       1.40

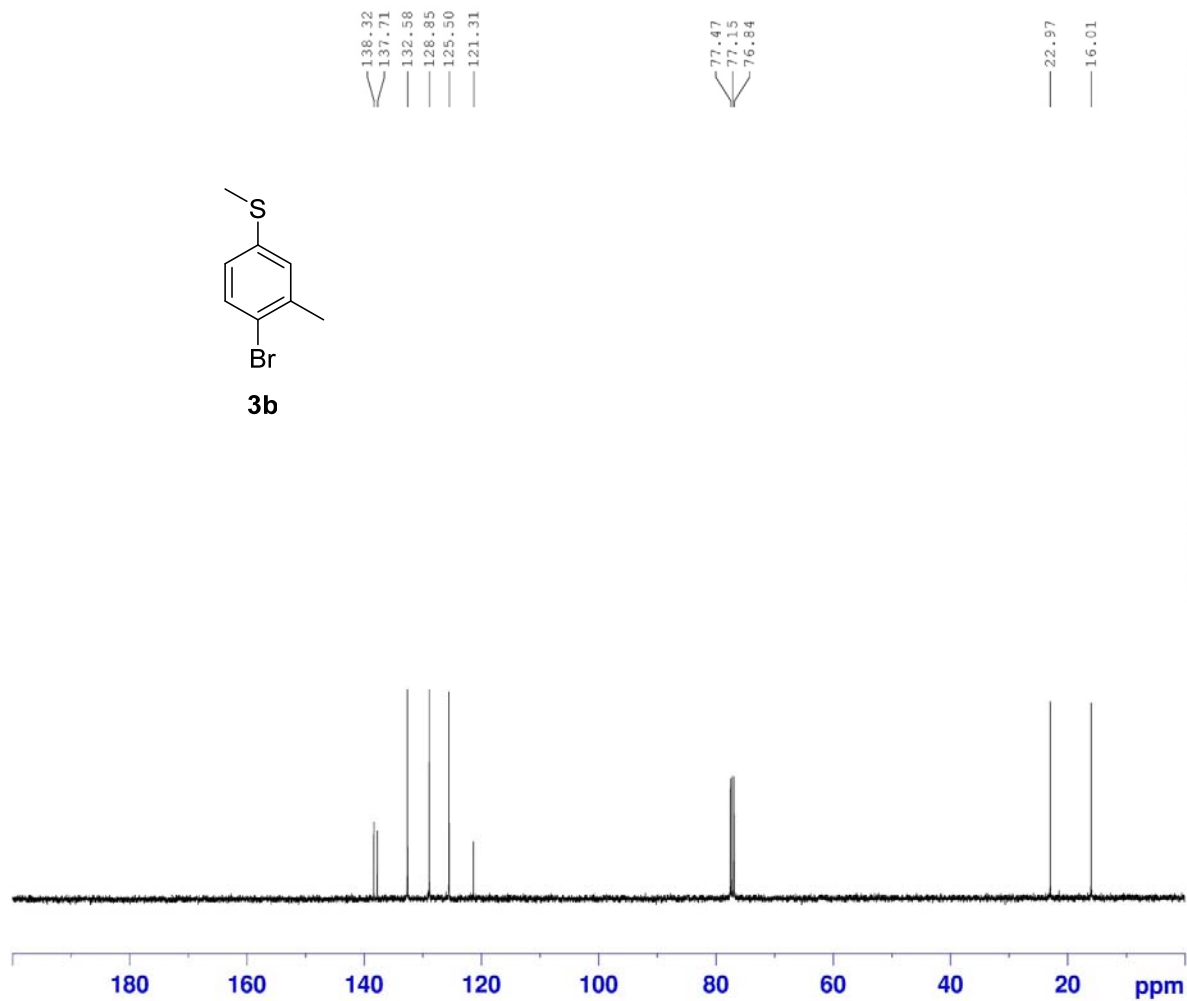
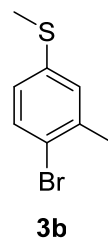
```



Current Data Parameters  
 NAME SY-12603  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160926  
 Time 13.32 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 7  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.2 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300101 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



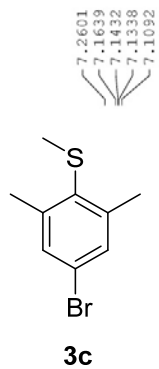
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Current Data Parameters
NAME      SY-12603-Carbon
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160926
Time     13.35 h
INSTRUM  spect
PROBHD   Z108618_0257
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       20
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       120
DW       20.800 usec
DE       6.50 usec
TE       295.4 K
D1       2.00000000 sec
d11      0.03000000 sec
TD0      1
SFO1     100.6479773 MHz
NUC1     13C
P1       9.50 usec
PLM1     55.34000015 W
SFO2     400.2316009 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLM2     13.56000042 W
PLW12    0.27428001 W
PLW13    0.13796000 W

F2 - Processing parameters
SI       32768
SF       100.6379101 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
FC       1.40

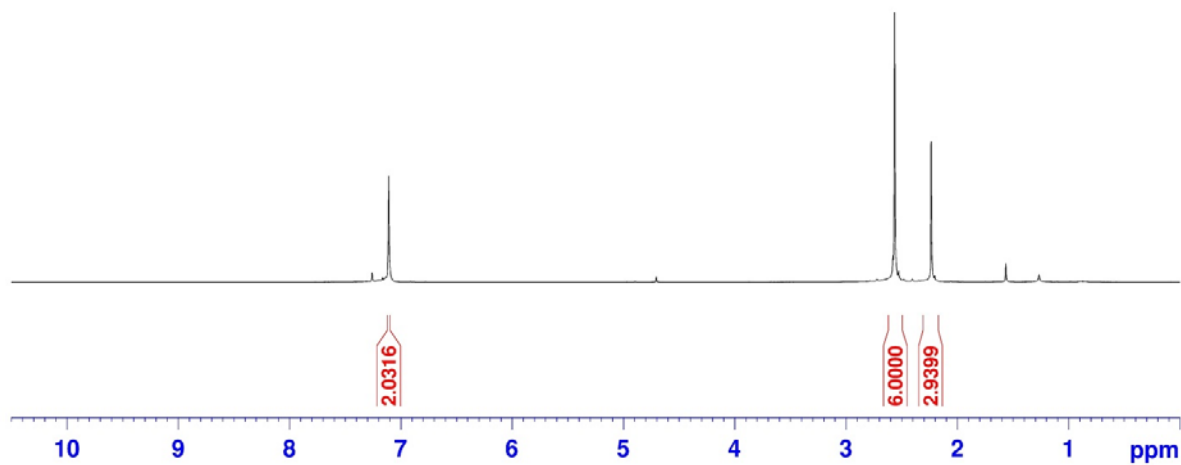
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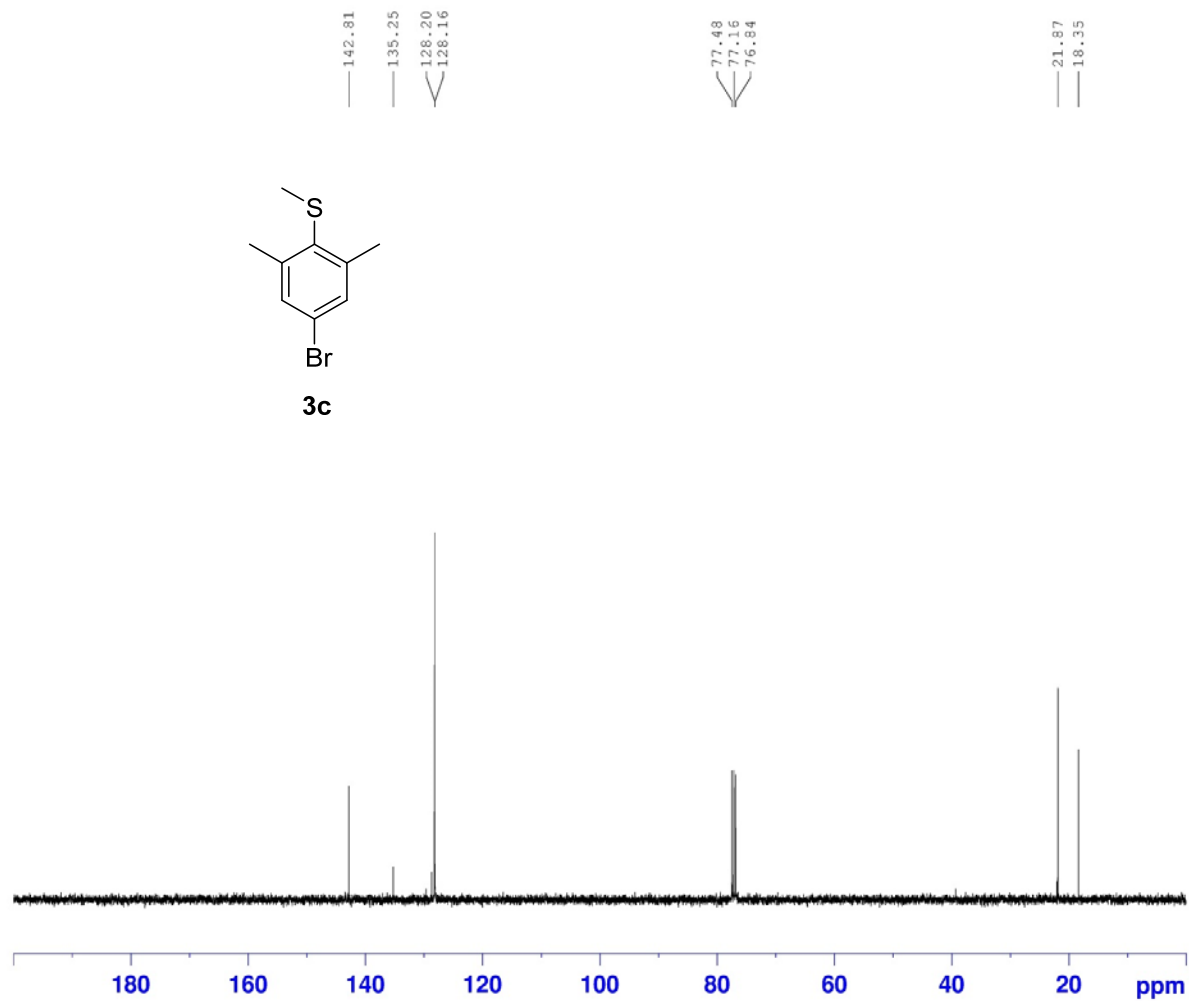
7.2601  
 7.1639  
 7.1432  
 7.1338  
 7.1092

2.5636  
 2.2355

Current Data Parameters  
 NAME SY-12608  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20170116  
 Time 17.43 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 7  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.3 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W  
 F2 - Processing parameters  
 SI 65536  
 SF 400.1300098 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00







```

Current Data Parameters
NAME      SY-12604-carbon
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20161006
Time     10.52 h
INSTRUM  spect
PROBHD   Z824601_0021
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       14
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       200
DW       20.800 usec
DE       6.50 usec
TE       295.2 K
D1       2.0000000 sec
d11      0.0300000 sec
TD0      1
SFO1     100.6228298 MHz
NUC1     13C
P1       9.50 usec
PLM1     41.2500000 W
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLM2     8.31000042 W
PLW12    0.23083000 W
PLW13    0.11611000 W

F2 - Processing parameters
SI       32768
SF       100.6127631 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
FC       1.40

```

7.4042  
7.3830  
7.2597  
7.1901  
7.1690

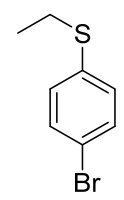
2.9471  
2.9288  
2.9105  
2.8922

1.3217  
1.3034  
1.2850

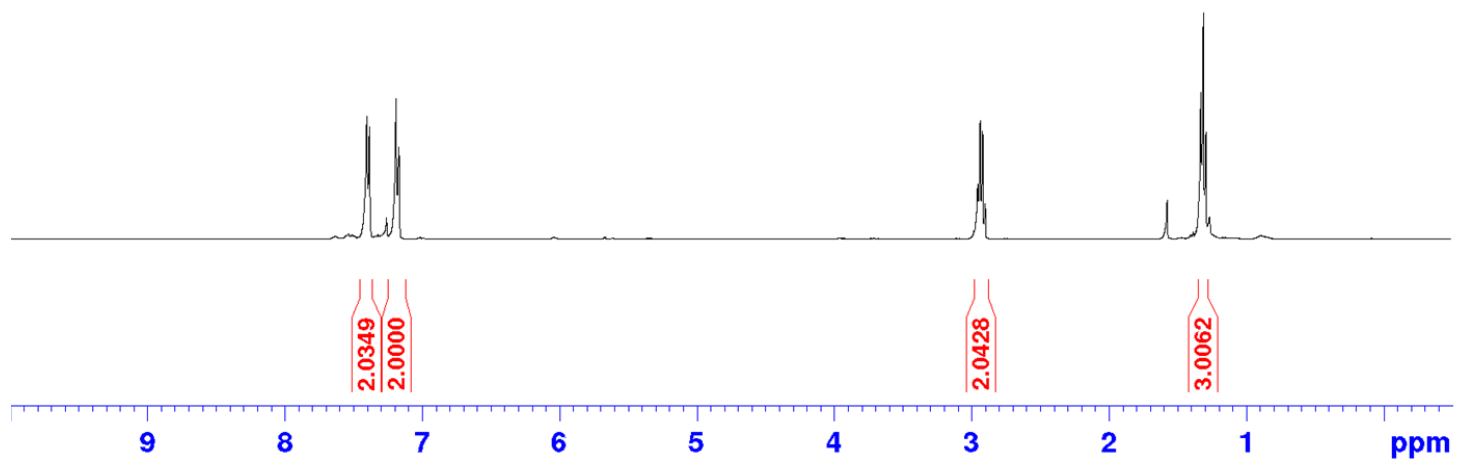
Current Data Parameters  
NAME SY-18506  
EXPNO 1  
PROCNO 1

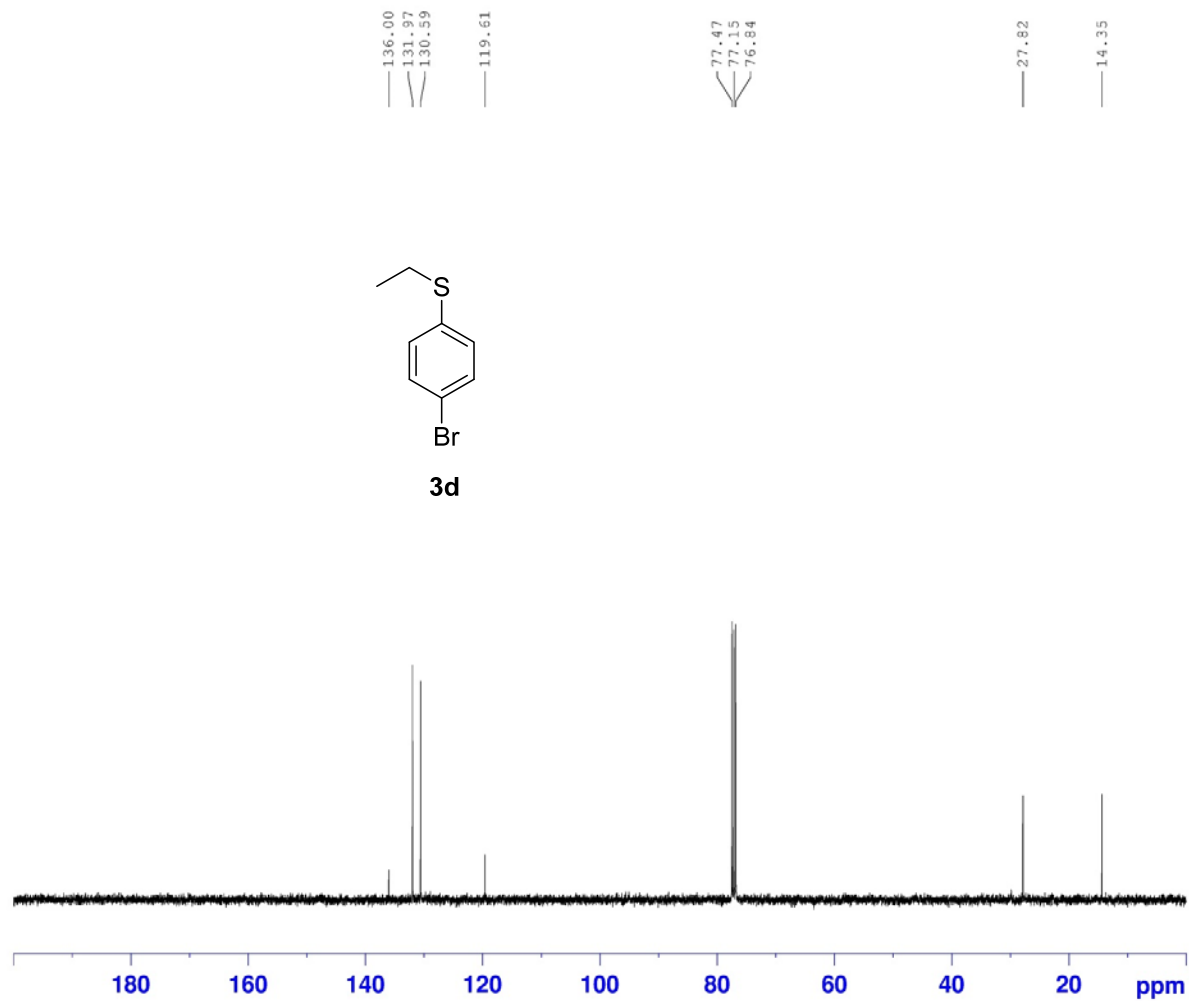
F2 - Acquisition Parameters  
Date\_ 20160630  
Time 13.46 h  
INSTRUM spect  
PROBHD Z824601\_0021 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 12  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 128  
DW 62.400 usec  
DE 6.50 usec  
TE 295.3 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P1 15.00 usec  
PLW1 8.31000042 W

F2 - Processing parameters  
SI 65536  
SF 400.1300091 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



3d





```

Current Data Parameters
NAME          sv-18506-c13
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20150630
Time          13.49 h
INSTRUM       spect
PROBHD        Z824601_0021
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            80
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            295.4 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SFO1          100.6228298 MHz
NUC1          13C
P1            9.50 usec
PLM1          41.25000000 W
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          8.31000042 W
PLW12         0.23083000 W
PLW13         0.11611000 W

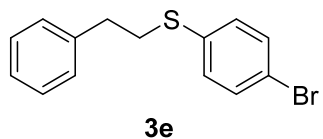
F2 - Processing parameters
SI            32768
SF            100.6127586 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

```

7.4257  
7.4050  
7.3340  
7.3152  
7.2969  
7.2596  
7.2396  
7.2227  
7.2048  
7.1878

3.1761  
3.1578  
3.1370  
2.9428  
2.9221  
2.9038

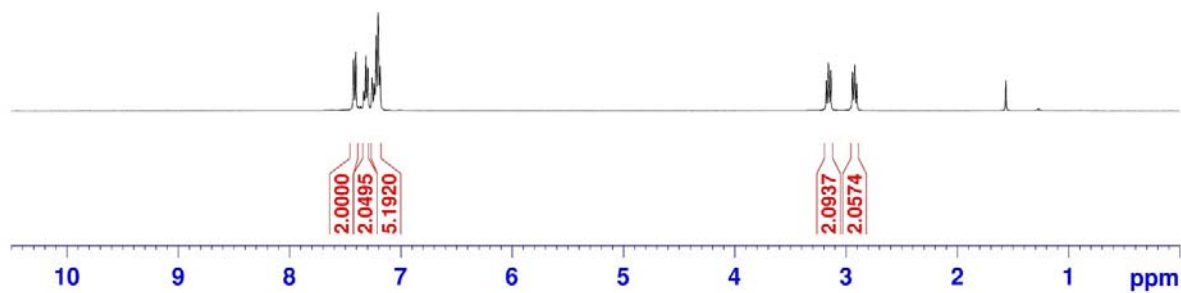
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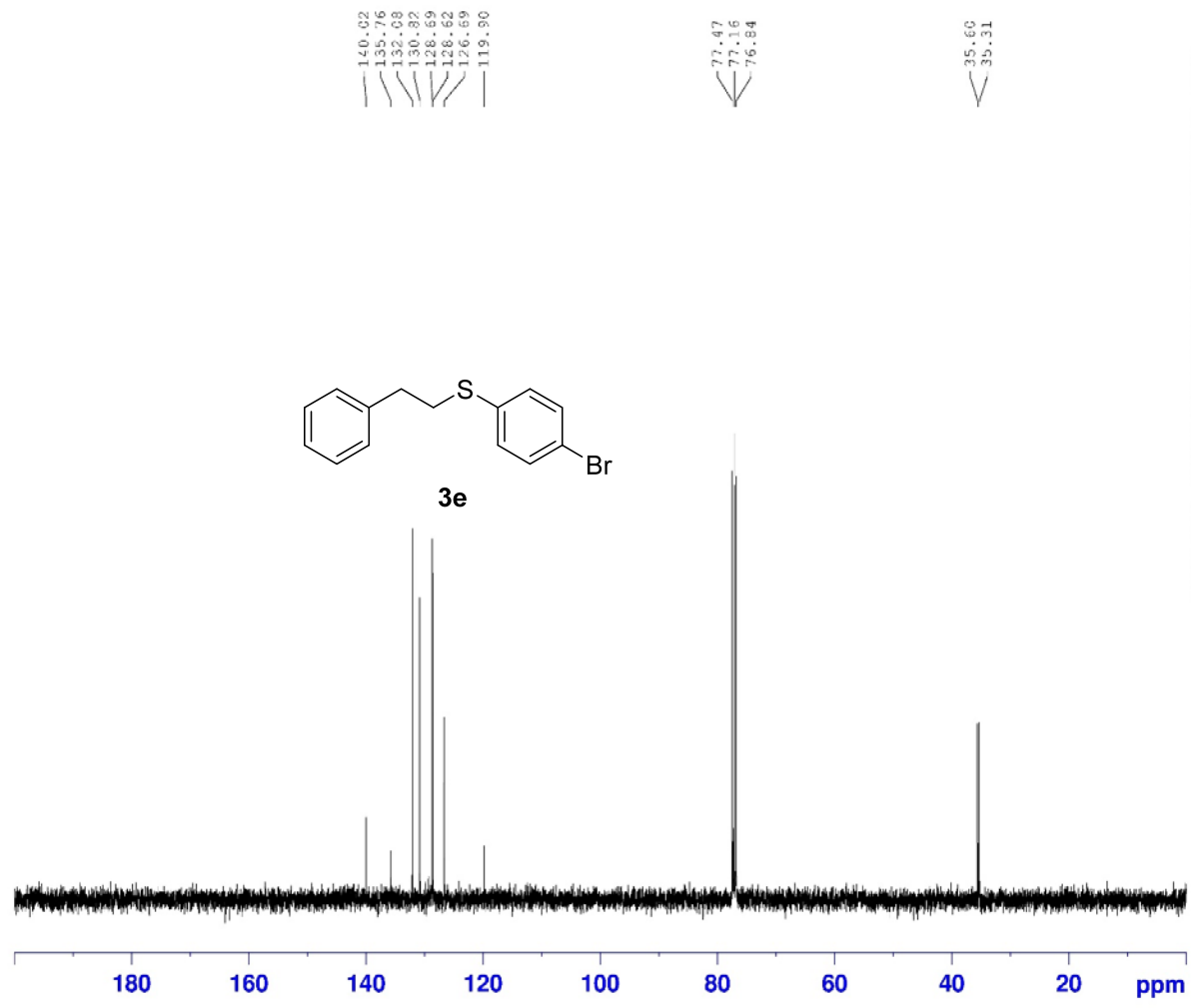


Current Data Parameters  
NAME SY-8607  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170109  
Time 18.00 h  
INSTRUM spect  
PROBHD Z824601\_0021 (1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 10  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 128  
DW 62.400 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.00000000 sec  
TDO 1  
SFO1 400.1324708 MHz  
NUC1 1H  
P1 15.00 usec  
PLW1 8.31000042 W

F2 - Processing parameters  
SI 65536  
SF 400.1300093 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



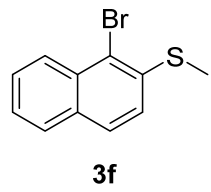
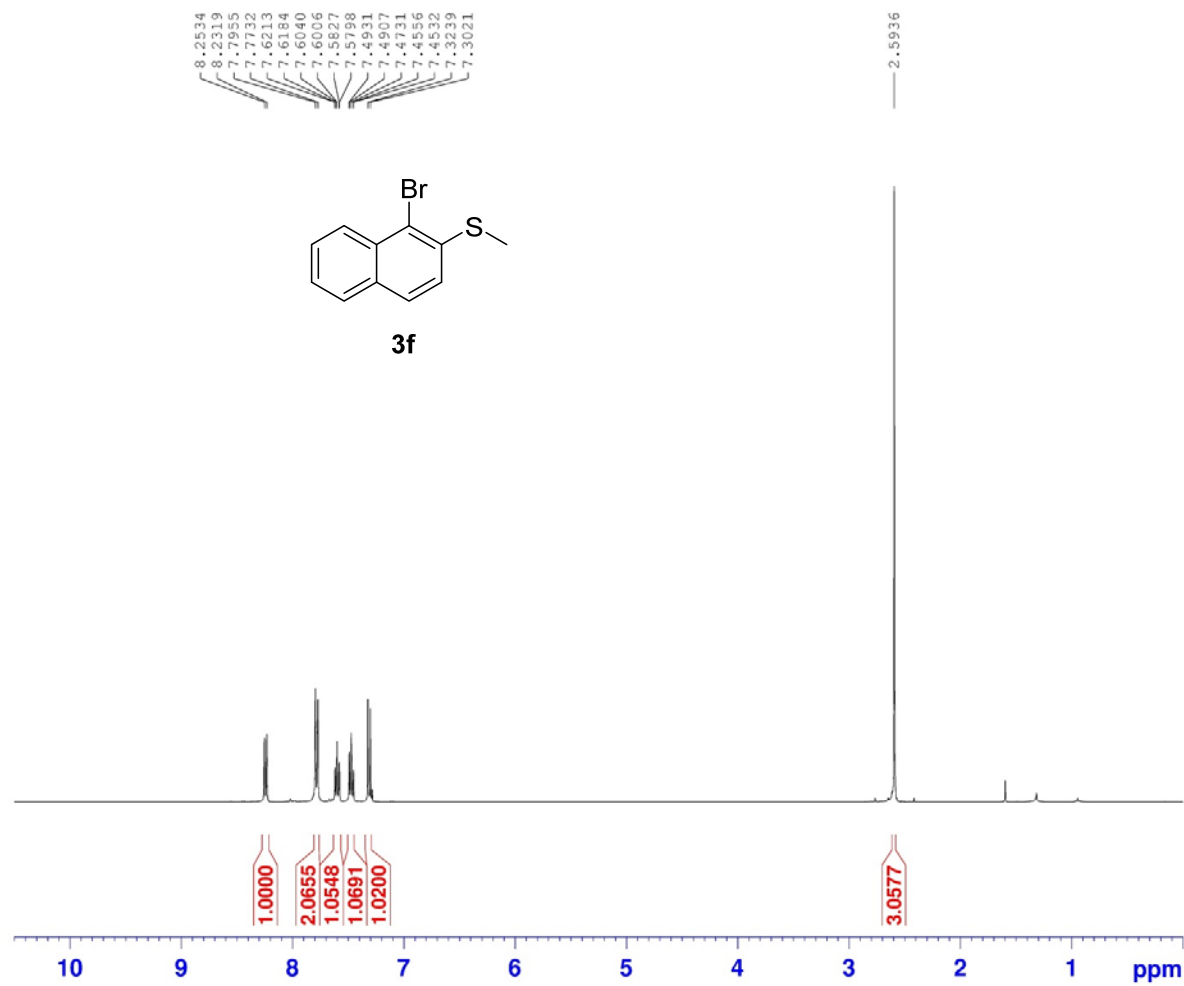


```

Current Data Parameters
NAME      SY-8607 carbon
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20110109
Time     18.03 h
INSTRUM  spect
PROBHD   5824601 0021
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        41
DS        4
SWH       24036.481 Hz
FIDRES   0.366798 Hz
AQ        1.3631488 sec
RG        202
AW        20.300 usec
DE        6.56 usec
TE        296.3 K
D1        2.0000000 sec
d11       0.0300000 sec
TE0       1
SFO1     100.6228298 MHz
NUC1      13C
P1        3.56 usec
PLW1     41.2500000 W
SFO2     400.1316005 MHz
NUC2      1H
CPDPRG2  waltz16
NUC3      13C
PLW2     30.00 usec
PLW3     8.3100000 W
PLW12    0.2398300 W
PLW13    0.1161000 W

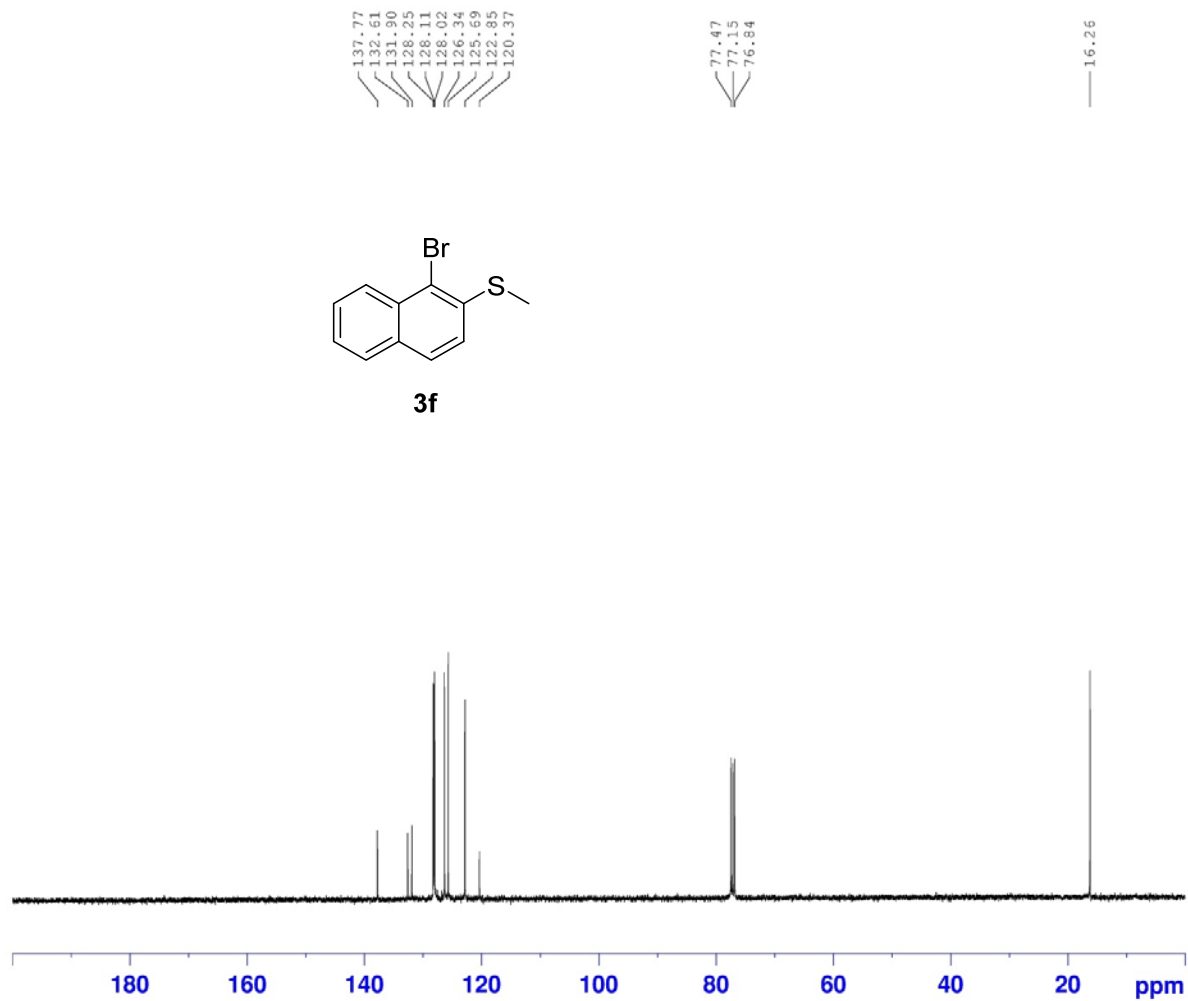
F2 - Processing parameters
SI        32768
SF        100.6127580 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



Current Data Parameters  
 NAME SY-12606  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161006  
 Time 11.26 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 3  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 71.8  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.8 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



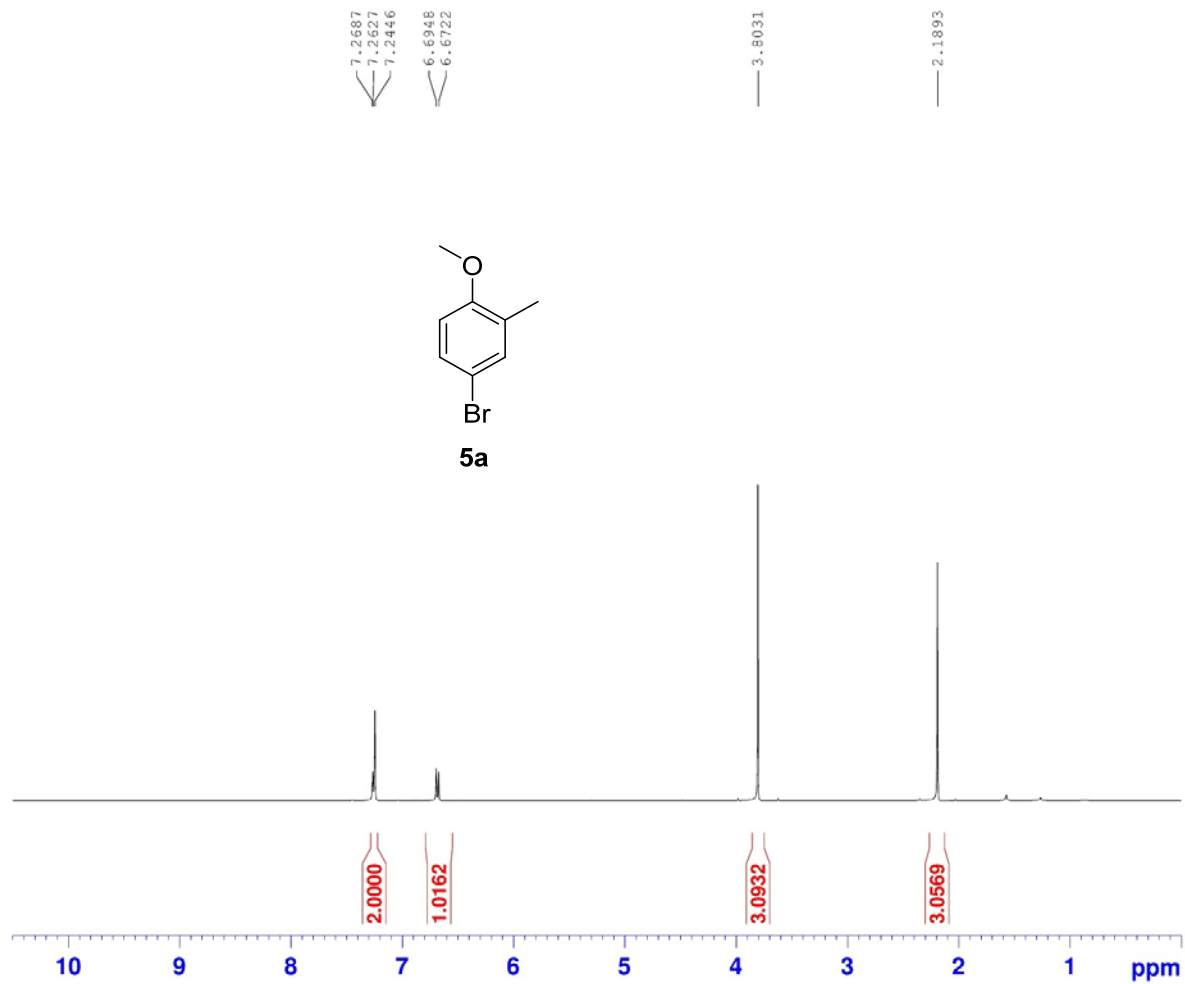
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Current Data Parameters
NAME          SY-12606-cl3
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20161011
Time          12.32 h
INSTRUM       spect
PROBHD        E108618_0257 (
PULPROG       zgpg30
ID            65536
SOLVENT       CDCl3
NS            102
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            144
DW            20.800 usec
DE            6.50 usec
TE            296.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SFO1          100.6479773 MHz
NUC1          13C
P1            9.50 usec
PLW1          55.3400015 W
SFO2          400.2316009 MHz
NUC2          1H
CPDPRG12     waltz16
PCPD2        90.00 usec
PLW2         13.56000042 W
PLW12        0.27428001 W
PLW13        0.13796000 W

F2 - Processing parameters
SI            32768
SF            100.6379123 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40

```

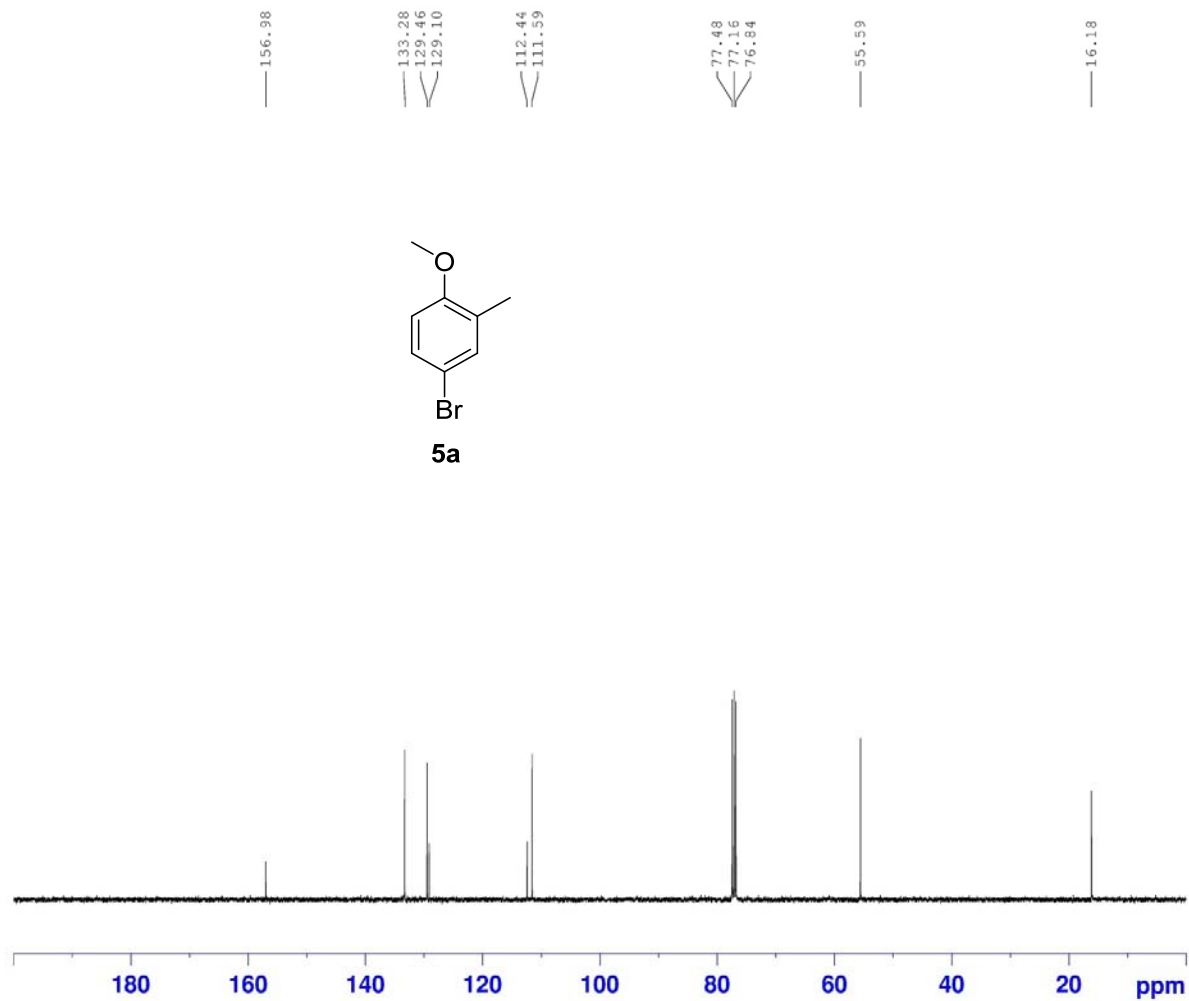


Current Data Parameters  
 NAME sy-15519-H  
 EXRNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20151028  
 Time 14.07 h  
 INSTRUM spect  
 PROBHD E108618\_0257 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 64  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.3 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 F1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300101 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





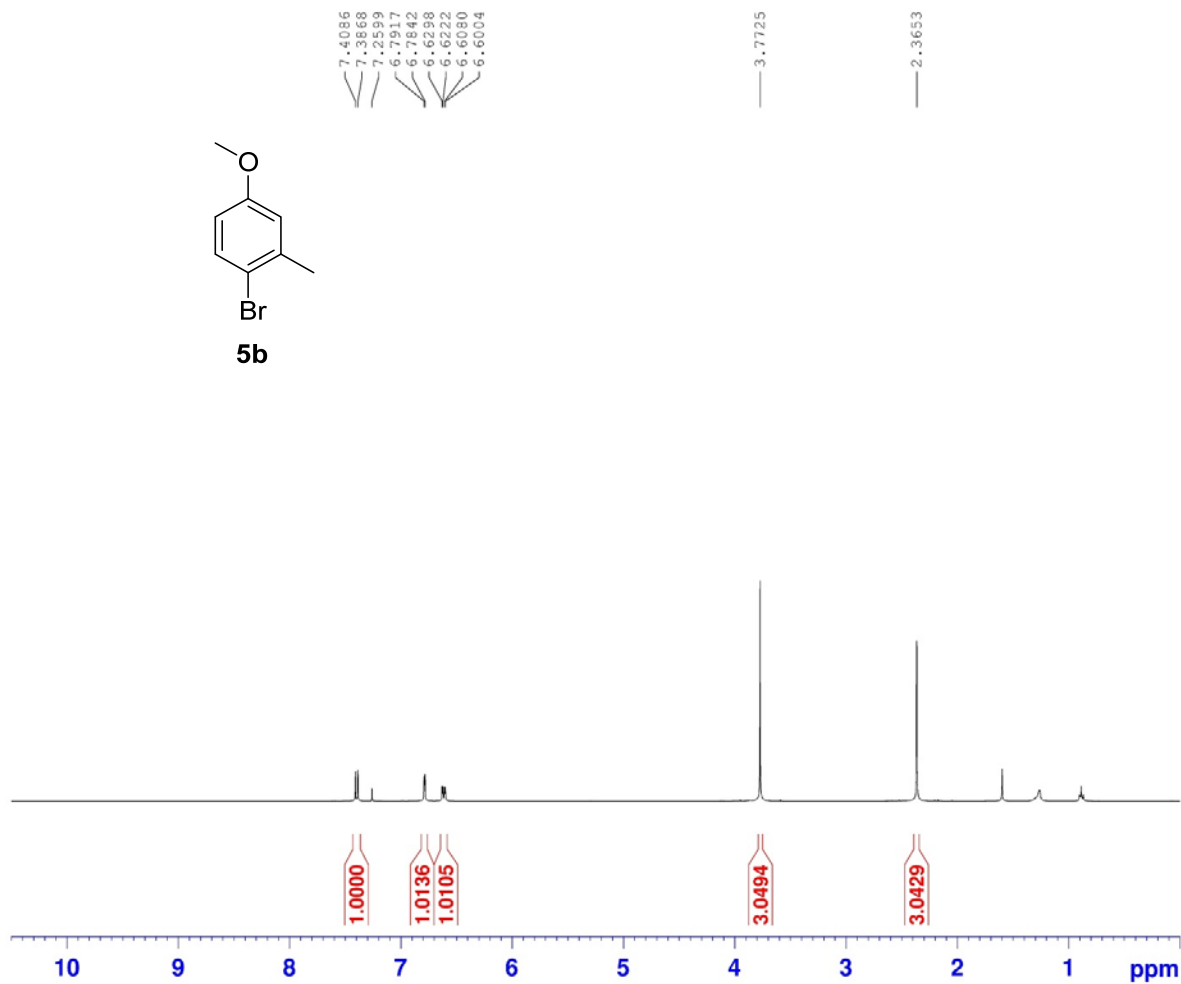
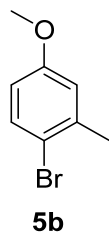
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Current Data Parameters
NAME          sy-15519-c
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20151028
Time          13.42 h
INSTRUM       spect
PROBHD        Z824601_0021
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            104
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            200
DW            20.800 usec
DE            6.50 usec
TE            294.6 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SFO1          100.6228298 MHz
NUC1          13C
P1            9.50 usec
PLM1          41.25000000 W
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          8.31000042 W
PLW12         0.23083000 W
PLW13         0.11611000 W

F2 - Processing parameters
SI            32768
SF            100.6127574 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

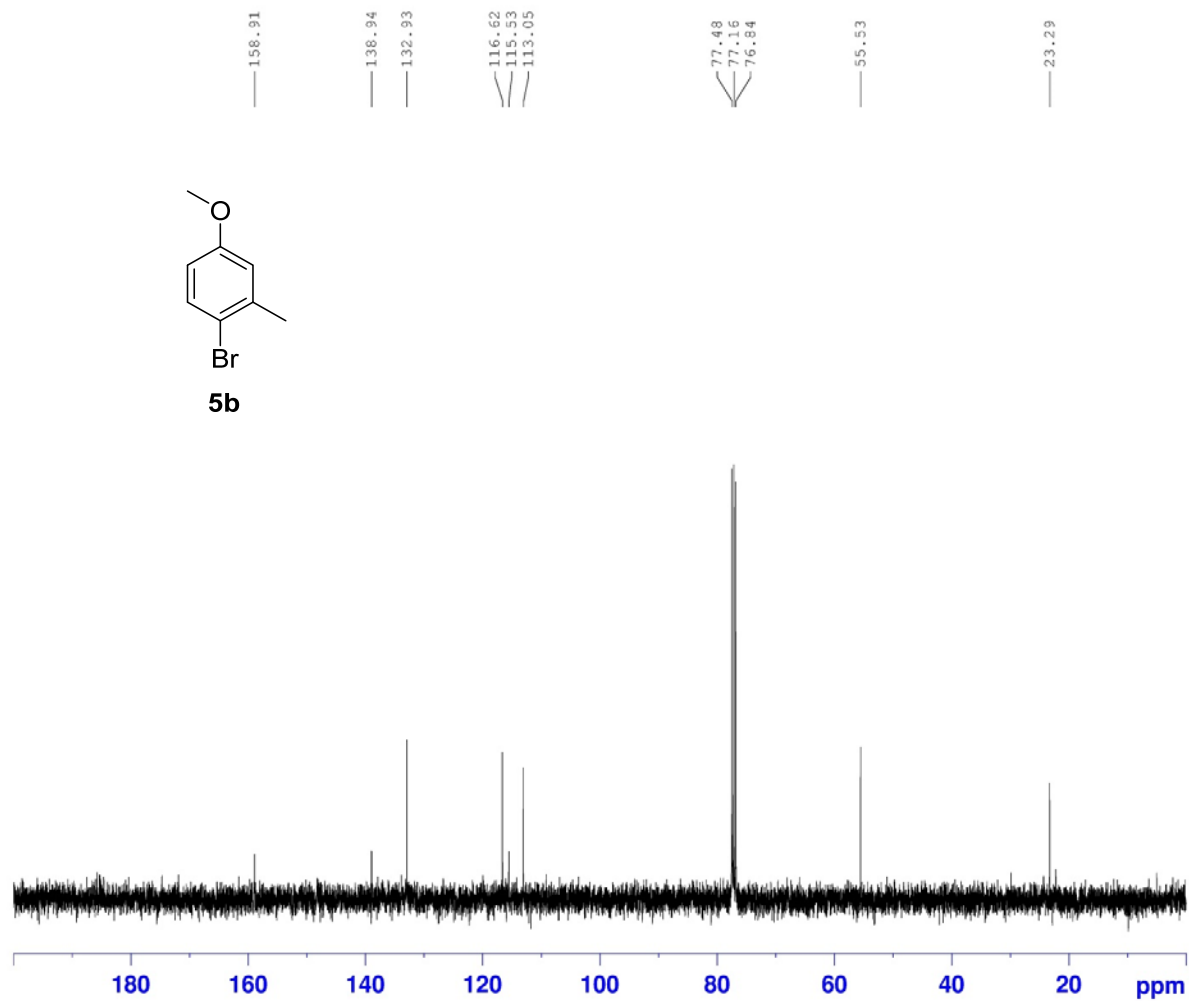
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Current Data Parameters  
 NAME SY-13102 proton  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160427  
 Time 16.46 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 12  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.6 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300089 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



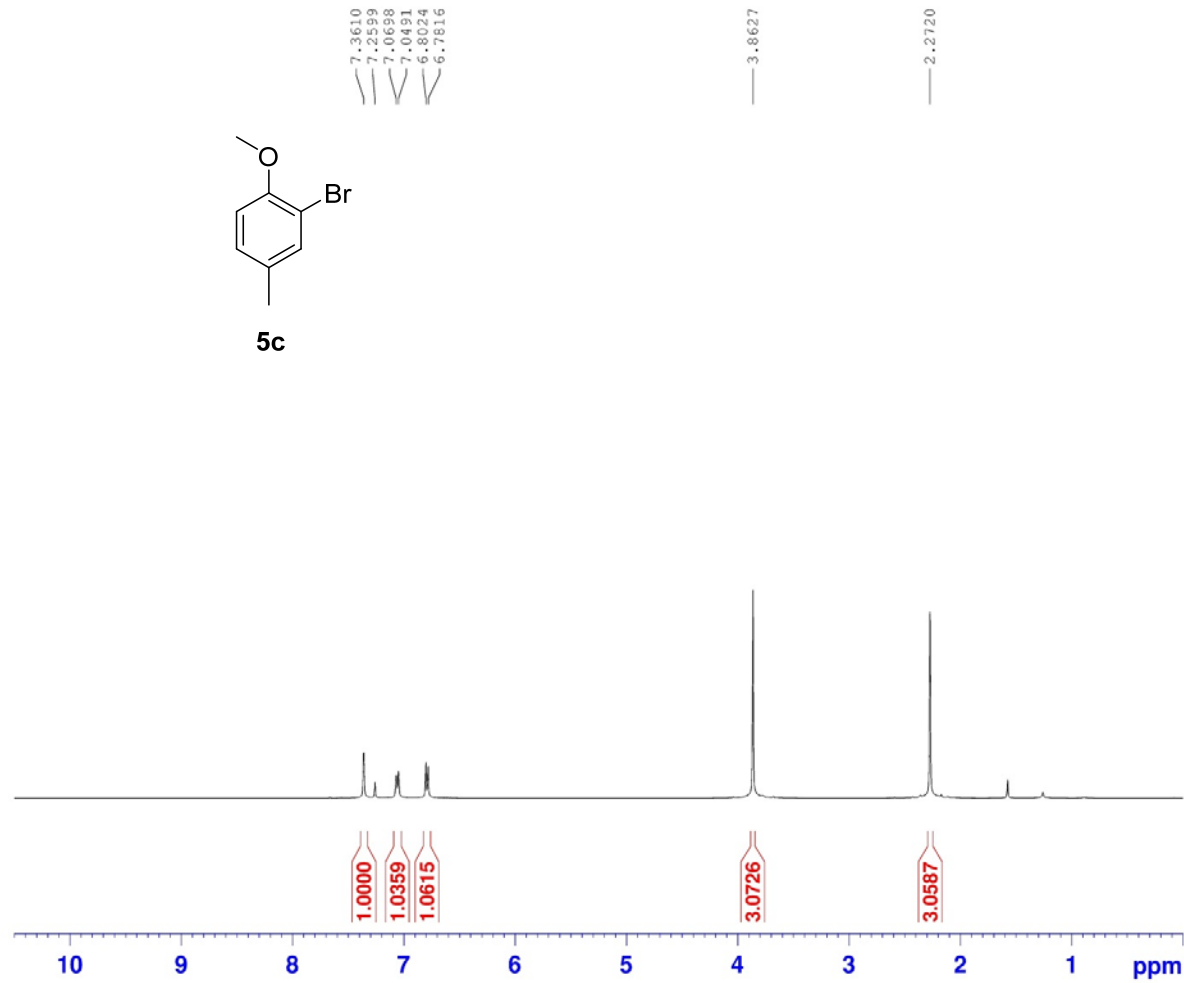
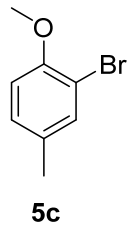
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Current Data Parameters
NAME      SY-13102 carbon13
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150428
Time     11.13 h
INSTRUM  spect
PROBHD   Z824601_0021
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       29
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       203
DW       20.800 usec
DE       6.50 usec
TE       296.4 K
D1       2.0000000 sec
d11      0.0300000 sec
TD0      1
SFO1     100.6228298 MHz
NUC1     13C
P1       9.50 usec
PLM1     41.2500000 W
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLM2     8.31000042 W
PLW12    0.23083000 W
PLW13    0.11611000 W

F2 - Processing parameters
SI       32768
SF       100.6127564 MHz
WDW      EM
SSB      0
LR       1.00 Hz
GB       0
FC       1.40

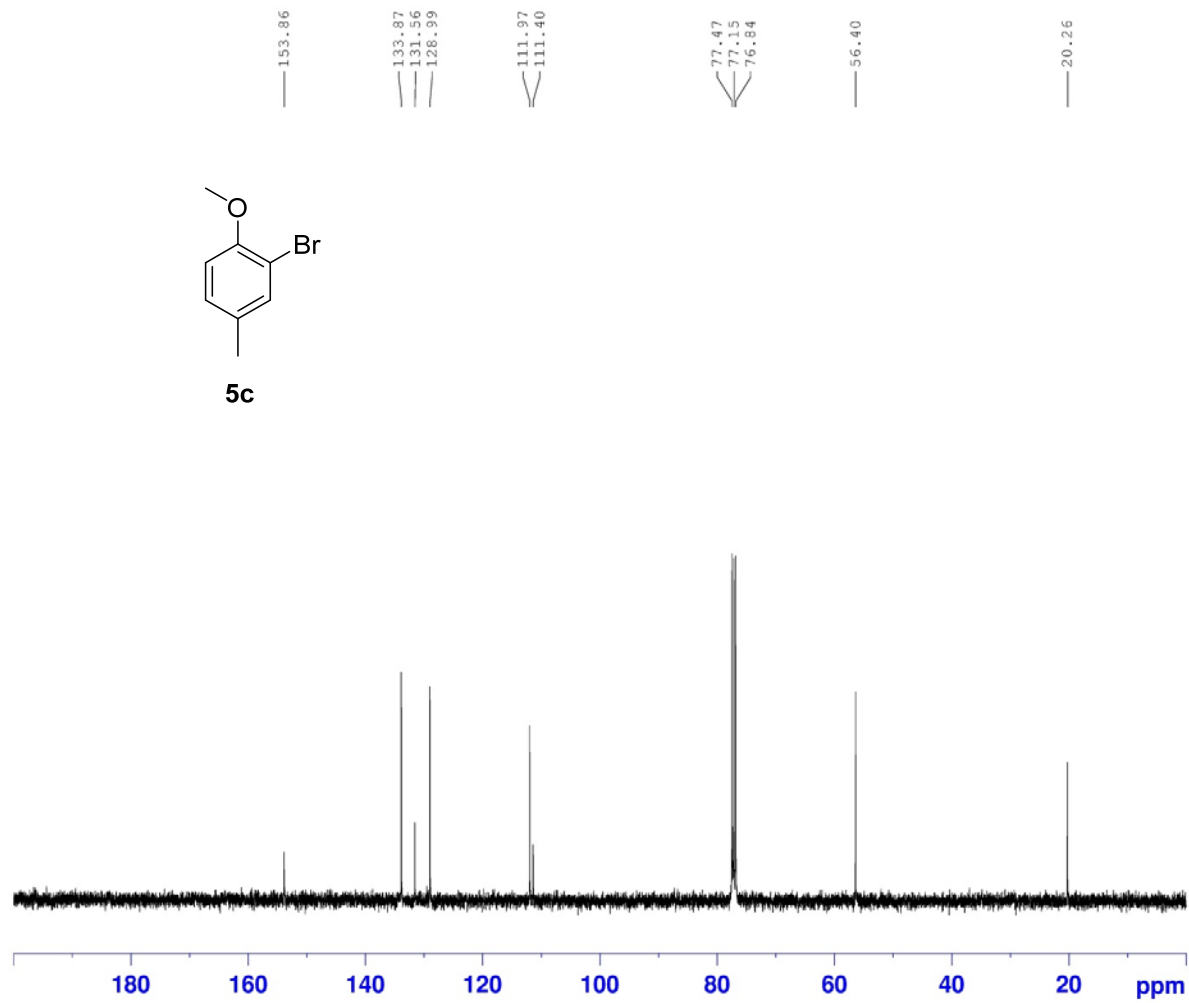
```



Current Data Parameters  
 NAME SY-1-123-02-03 pure  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160408  
 Time 9.23 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300099 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

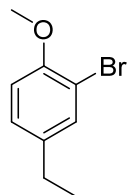


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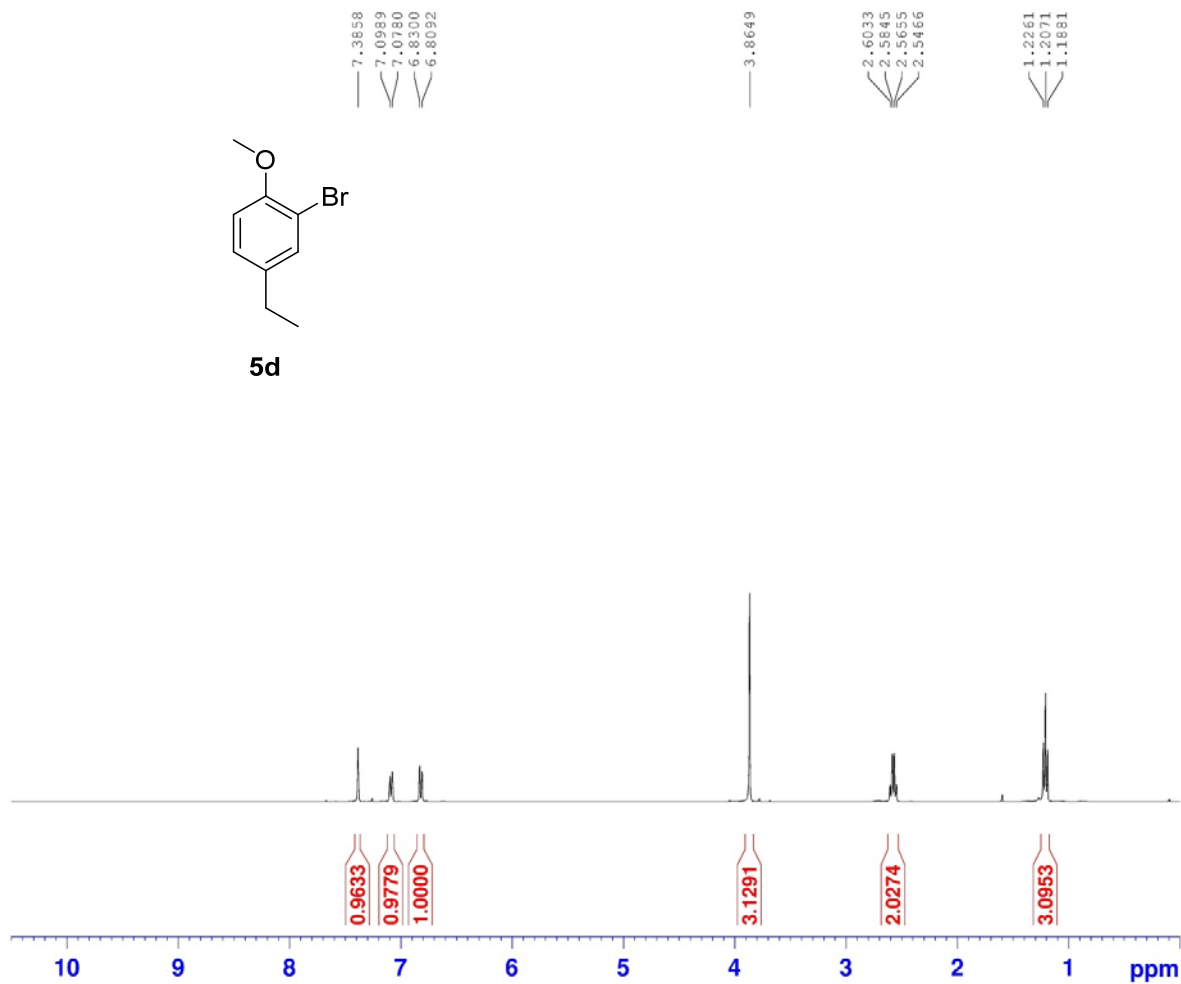
Current Data Parameters
NAME      ST-1-13-02-03 pure C13
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160408
Time     9.27 h
INSTRUM  spect
PROBHD   zgpg30
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       104
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       203
DM       20.800 usec
DE       6.30 usec
IE       297.3 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
SFO1     100.6228298 MHz
NUC1     13C
P1       9.30 usec
PLM1     41.2500000 W
SFO2     400.1316005 MHz
NUC2     1H
CPCPRG12  waltz16
PCPD2    90.00 usec
PLM2     8.3100004 W
PLM12    0.23083000 W
PLM13    0.11611000 W

F2 - Processing parameters
SI       32768
SF       100.6127579 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```



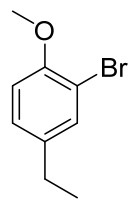
**5d**



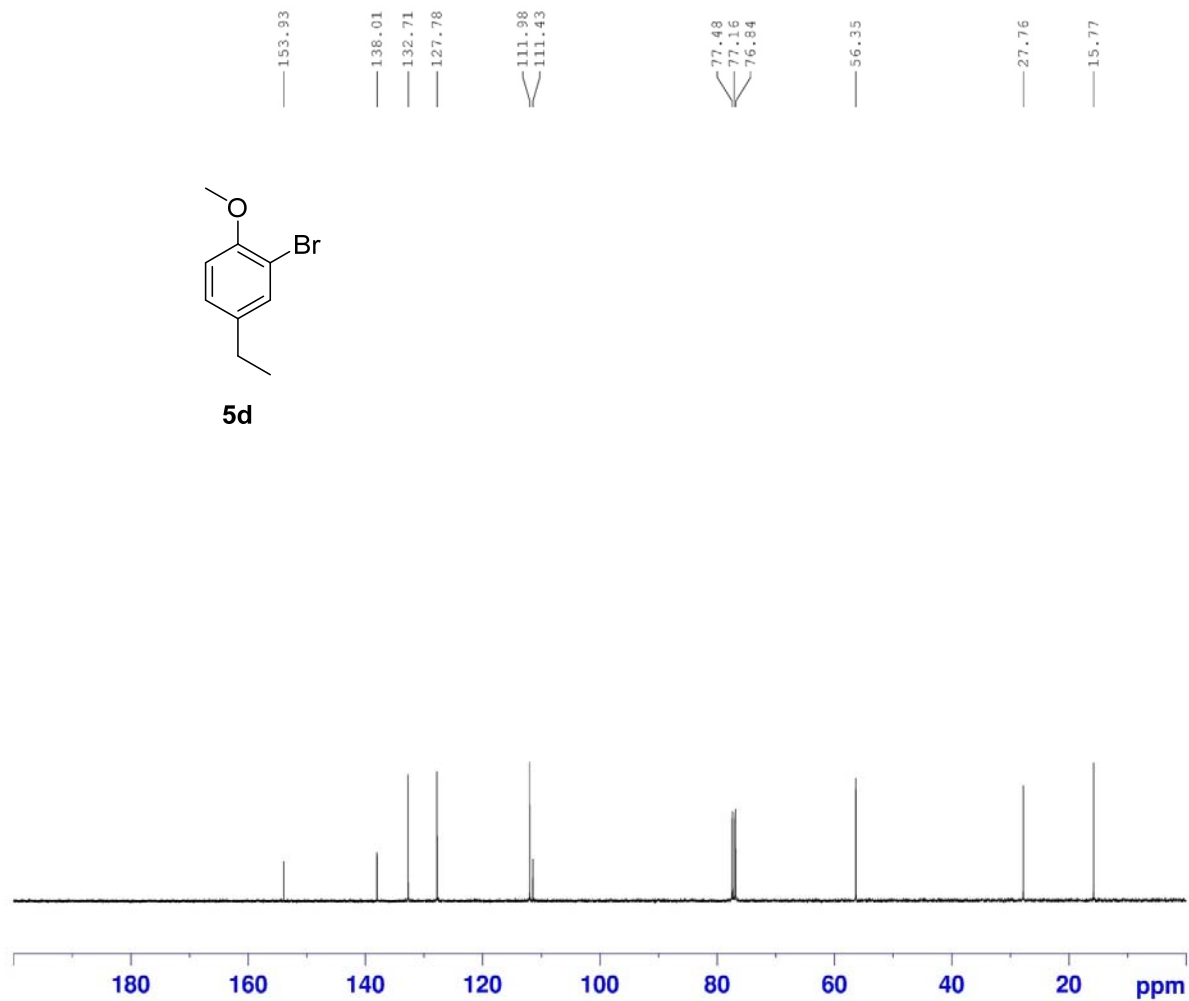
Current Data Parameters  
 NAME 15523-H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20151029  
 Time 23.46 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.8 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300102 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



5d



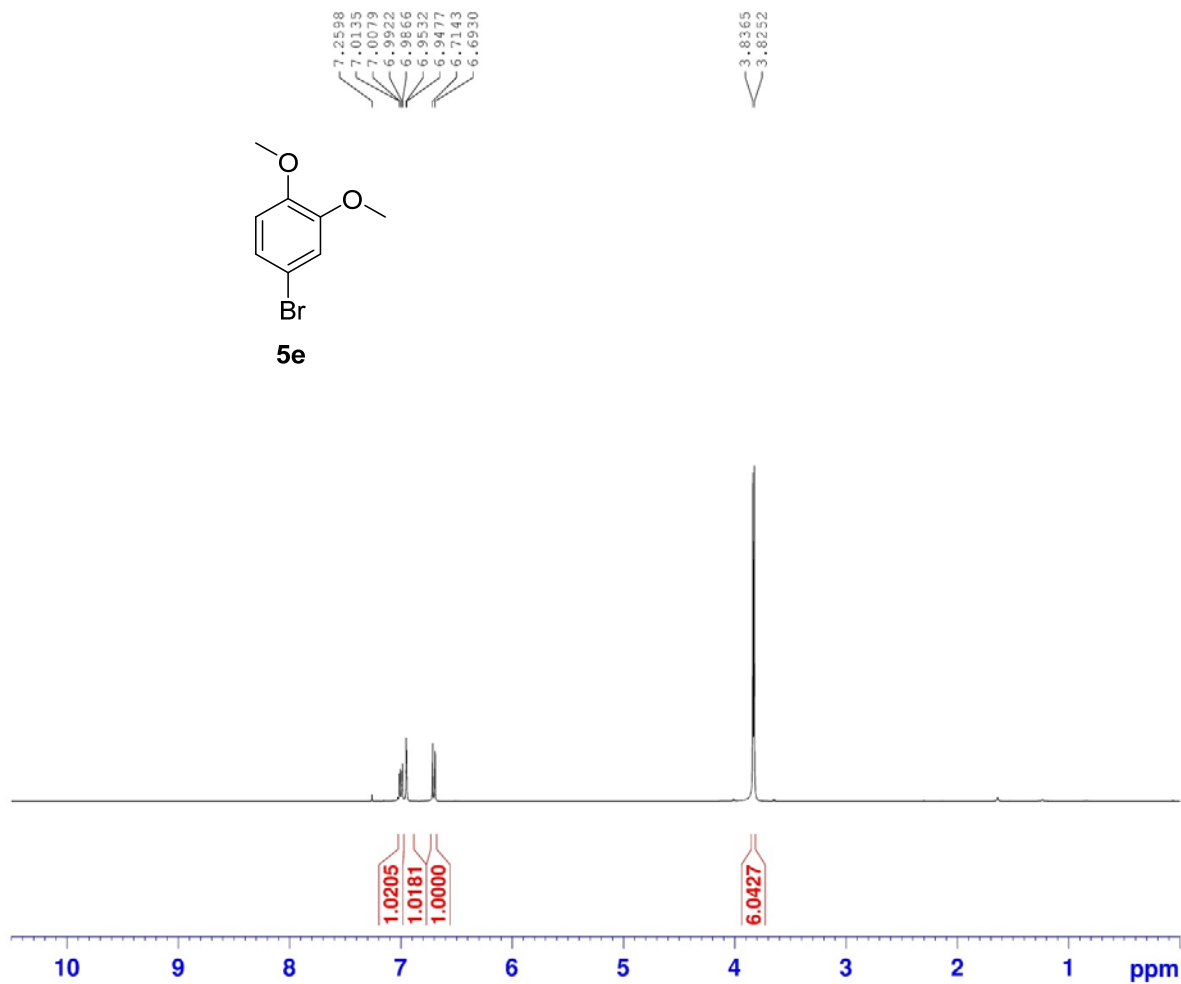
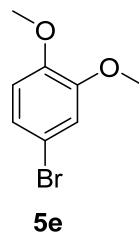
```

Current Data Parameters
NAME          15523-c
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20151029
Time          23.55 h
INSTRUM       spect
PROBHD        Z108618_0257 f
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            11
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            1
DW            20.800 usec
DE            6.50 usec
TE            295.1 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SF01          100.6479773 MHz
NUC1          13C
P1            9.50 usec
PLM1          55.34000015 W
SF02          400.2316009 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI            32768
SF            100.6379081 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

```

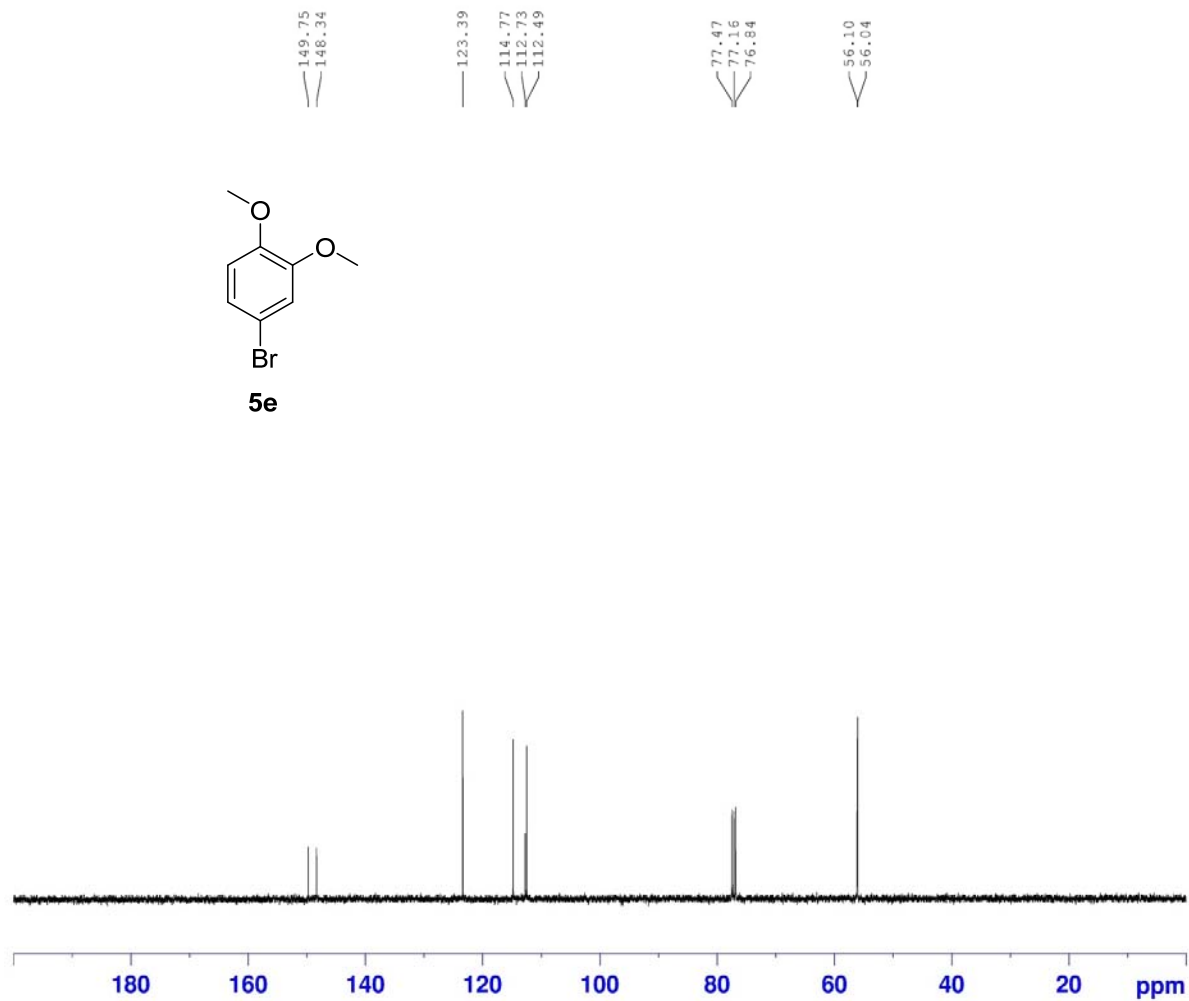
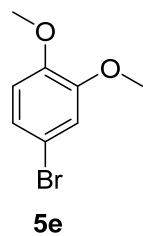


Current Data Parameters  
 NAME SY-15516-H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160120  
 Time 18.52 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300102 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



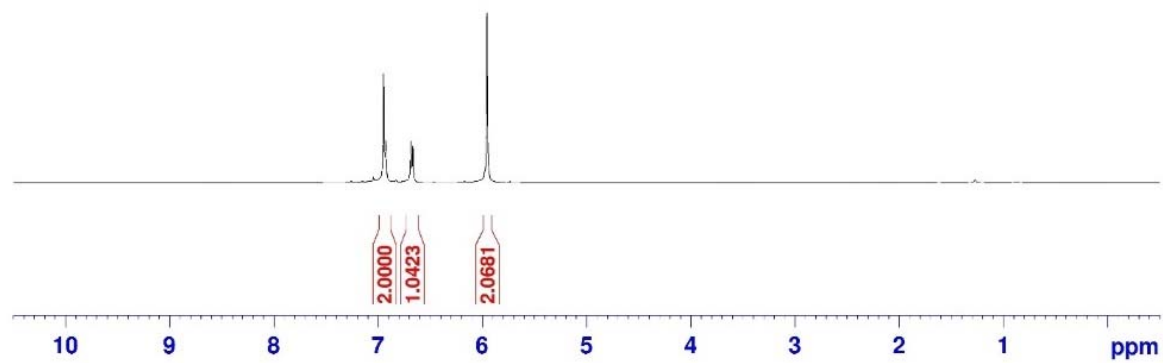
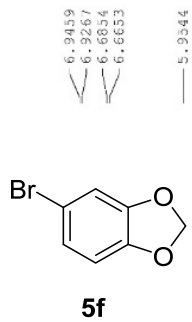


```

Current Data Parameters
NAME          sy-15516-c
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20160120
Time          18.55 h
INSTRUM       spect
PROBHD        Z108618_0257
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            204
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            1
DW            20.800 usec
DE            6.50 usec
TE            296.3 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SFO1          100.6479773 MHz
NUC1          13C
P1            9.50 usec
PLM1          55.34000015 W
SFO2          400.2316009 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI            32768
SF            100.6379105 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40
  
```

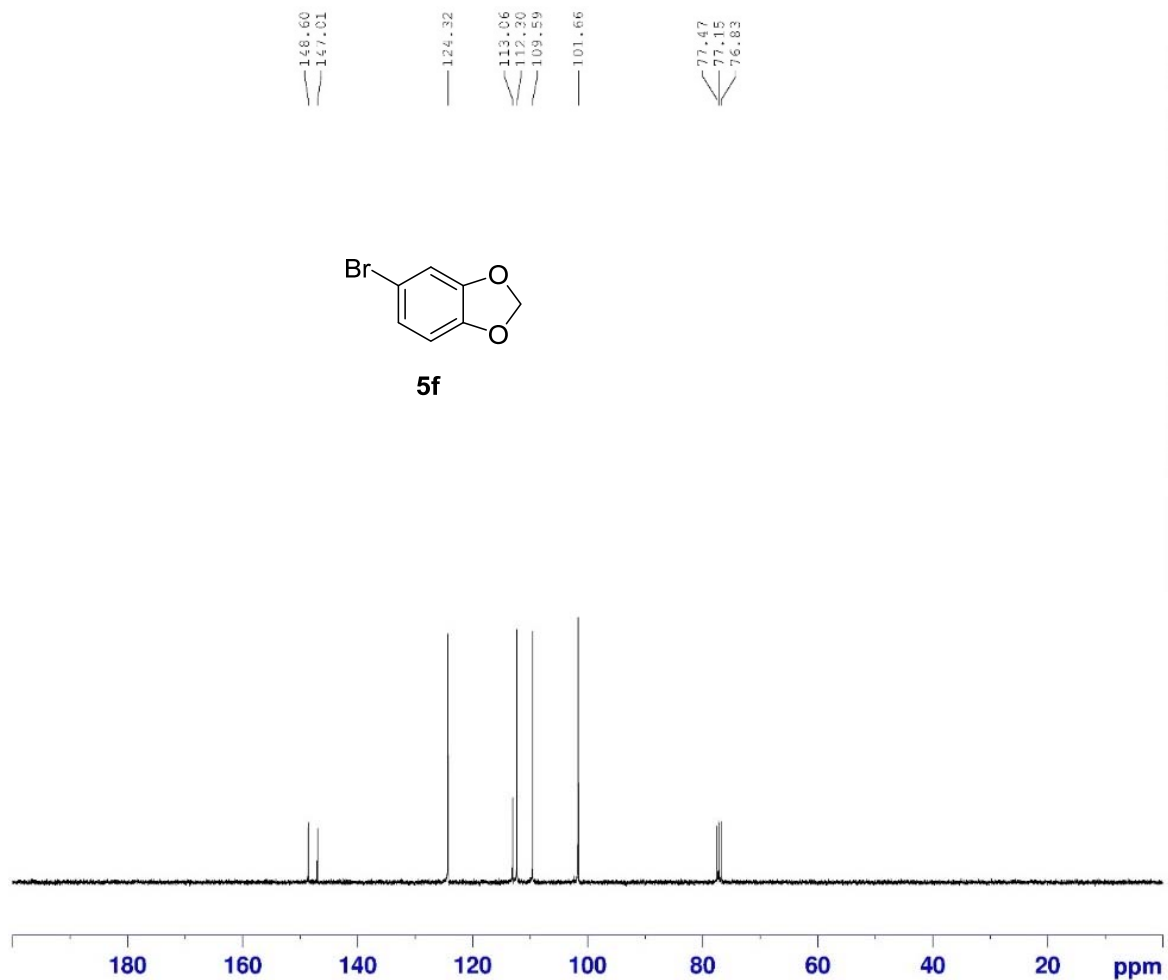


```

Current Data Parameters
NAME      15526-C (2)
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160125
Time     18.01 h
INSTRUM  spect
PROBHD   zgpg30_0021
PULPROG  zgpg30
TD       65536
F2       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894463 sec
RG       57
OR       62.100 usec
DE       6.50 usec
TE       291.5 K
D1       1.0000000 sec
TD0      -
SFOL     403.1324708 MHz
NUC1     1H
PC1      -5.00 usec
PL1      8.31000342 W

F2 - Processing parameters
SI       65536
SF       403.1300100 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```



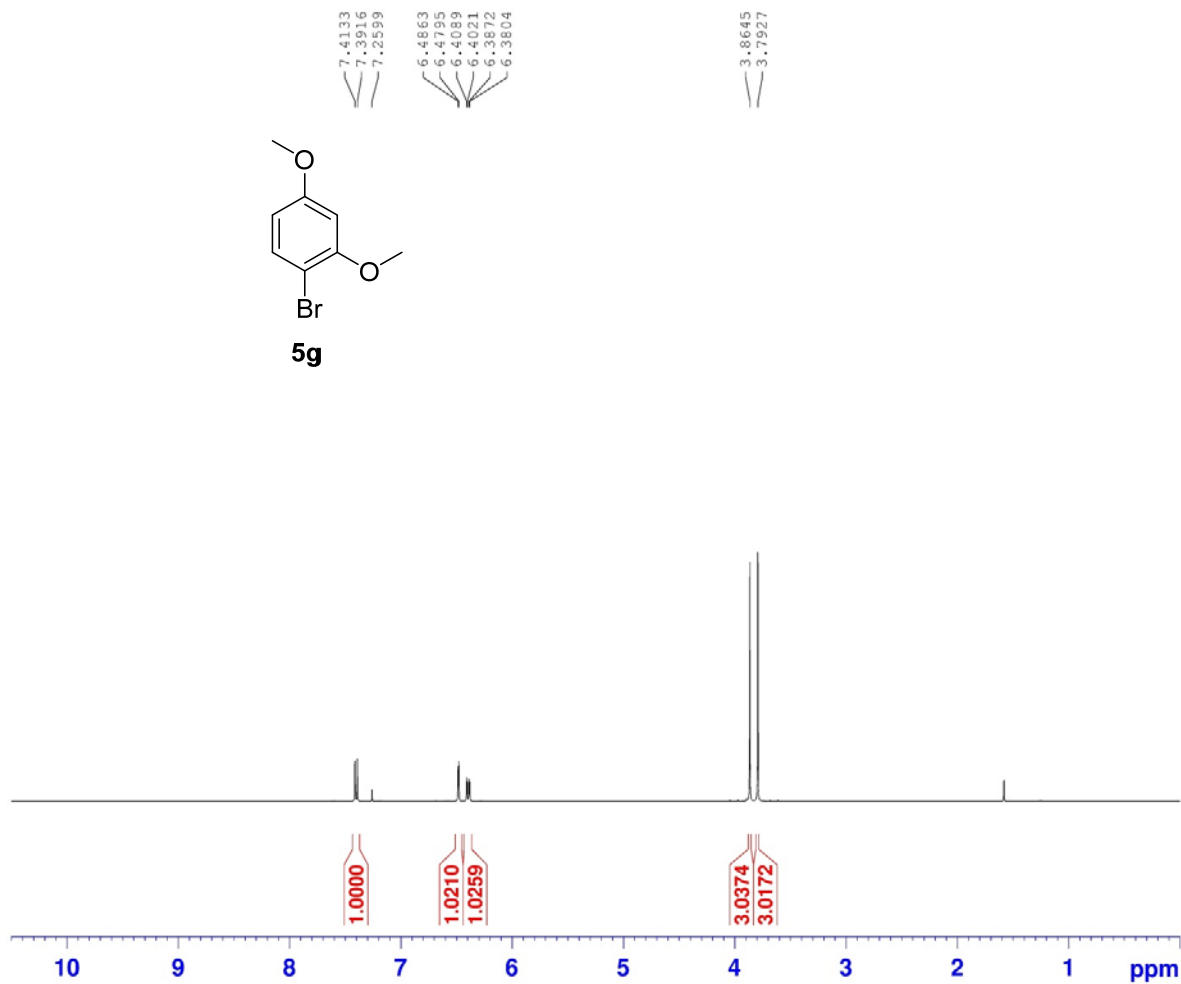
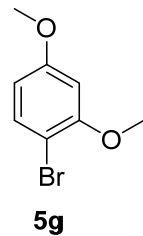
```

Current Date Parameters
NAME      15326-C
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20160125
Time      18.00 h
INSTRUM   spect
PROBHD    zgpg30
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         56
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3651488 sec
RG         200
DK         30.800 usec
DE         6.50 usec
TE         295.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1      100.6228730 MHz
NUC1       13C
P1         9.50 usec
PLW1      41.2500000 w
SFO2      400.1316005 MHz
P2         14
CPDPRG2   waltz16
ICPDUC    30.00 usec
PLW2      8.3100042 w
PLW12     0.2306300 w
PLW13     0.11611800 w

F2 - Processing parameters
SI         32768
SF         100.6127692 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

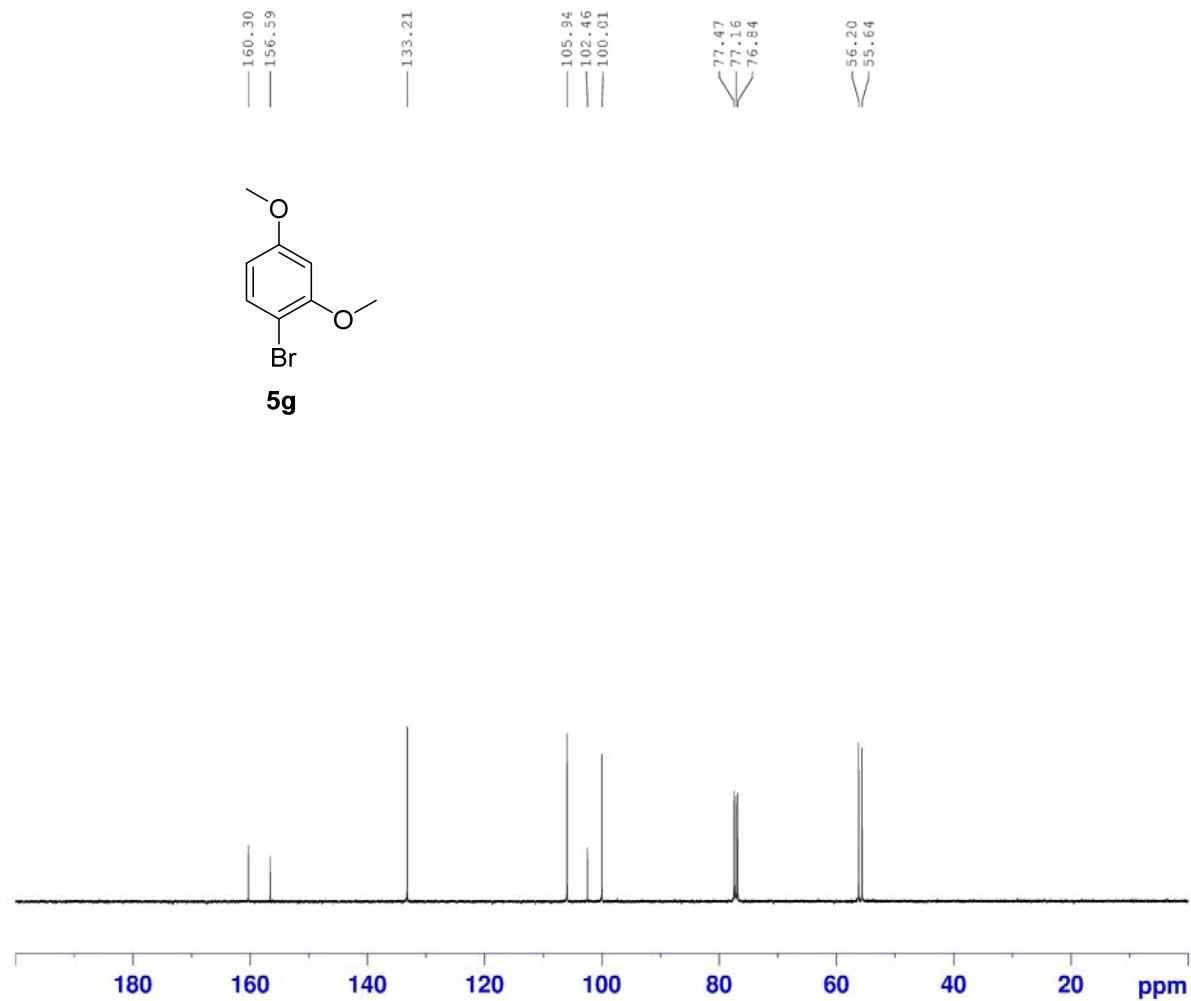
```



Current Data Parameters  
 NAME SY-15518-proton  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20161024  
 Time 13.33 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 4  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 80.6  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.5 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300101 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



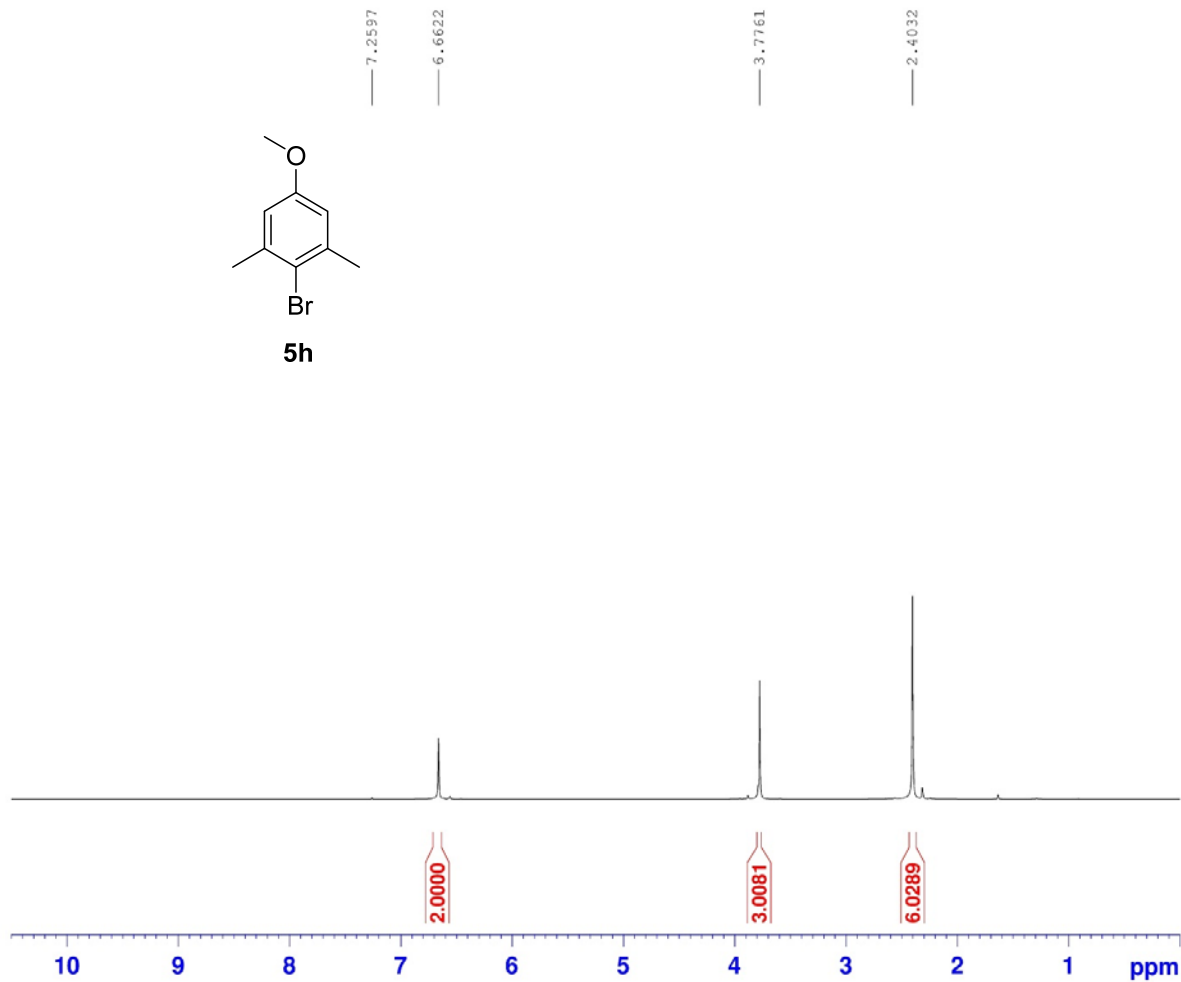
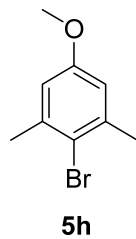
```

Current Data Parameters
NAME          SY-15518-c
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20151030
Time          9.39 h
INSTRUM       spect
PROBHD        Z108618_0257
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            100
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            144
DW            20.800 usec
DE            6.50 usec
TE            294.3 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SFO1          100.6479773 MHz
NUC1          13C
P1            9.50 usec
PLM1          55.34000015 W
SFO2          400.2316009 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI            32768
SF            100.6379075 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

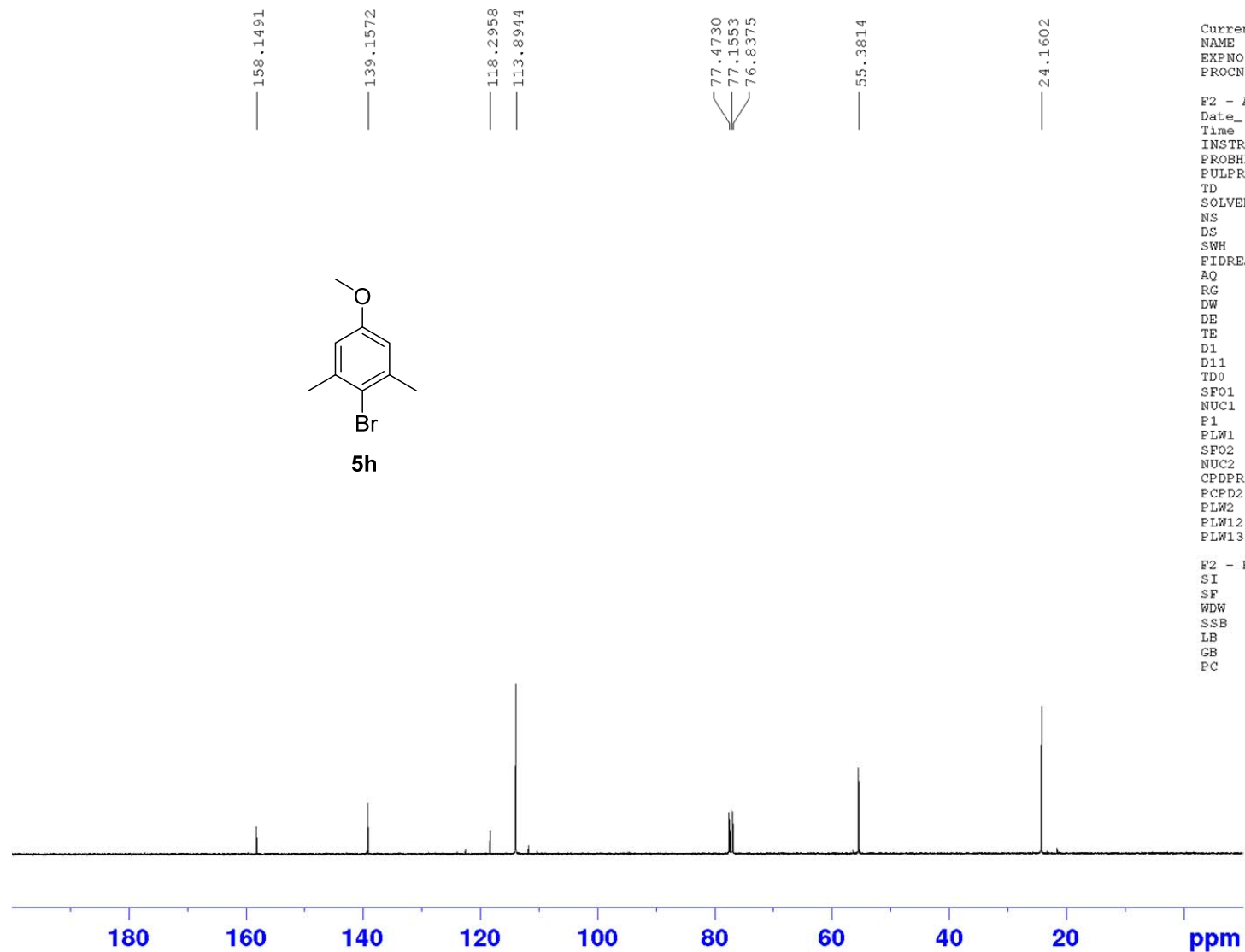
```



Current Data Parameters  
 NAME SY-103-05  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160411  
 Time 17.59 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 FULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300098 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



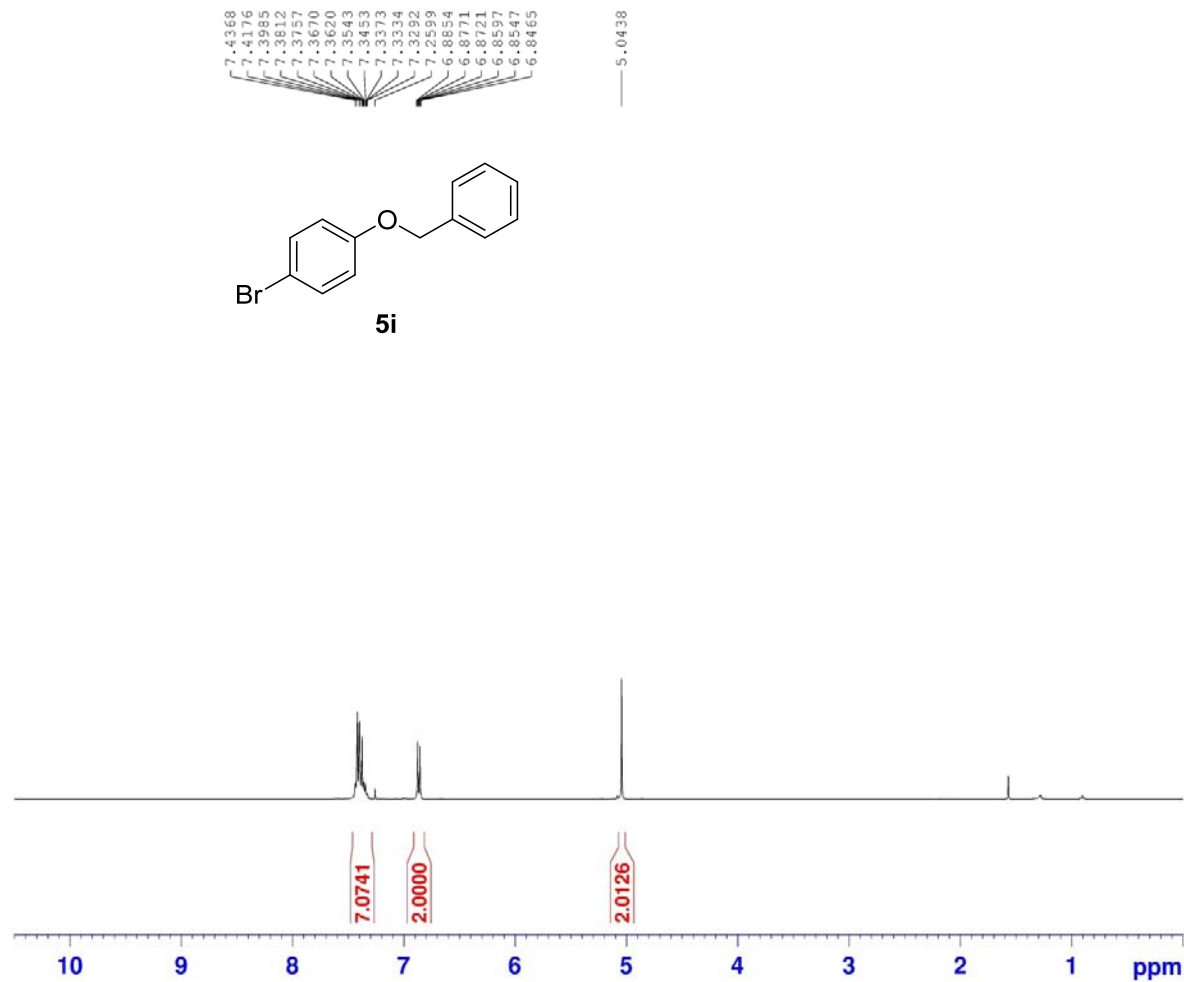
```

Current Data Parameters
NAME      SY-103-05 C13
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20160411
Time      18.02 h
INSTRUM   spect
PROBHD    Z108618_0257 (
PULPROG   zgpg30
TD         65536
SOLVENT   CDC13
NS         81
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         128
DW         20.800 usec
DE         6.50 usec
TE         294.6 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
SF01       100.6479773 MHz
NUC1       13C
P1         9.50 usec
PLW1       55.3400015 W
SFO2       400.2316009 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2      90.00 usec
PLW2       13.5600042 W
PLW12      0.27428001 W
PLW13      0.13796000 W

F2 - Processing parameters
SI         32768
SF         100.6379072 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

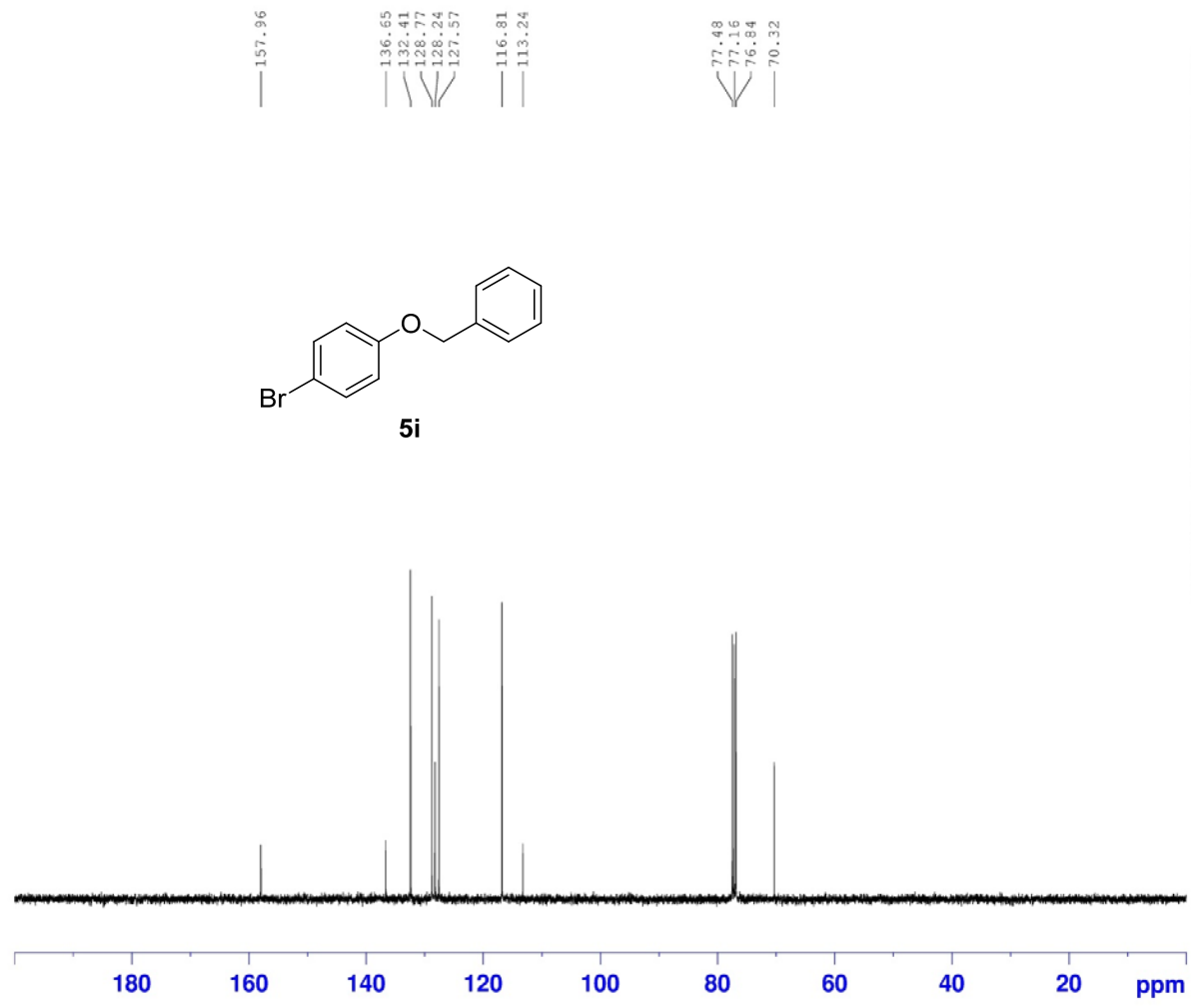


Current Data Parameters  
 NAME SY-10308  
 EXFNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160413  
 Time 10.12 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 f  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 114  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.5 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300097 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





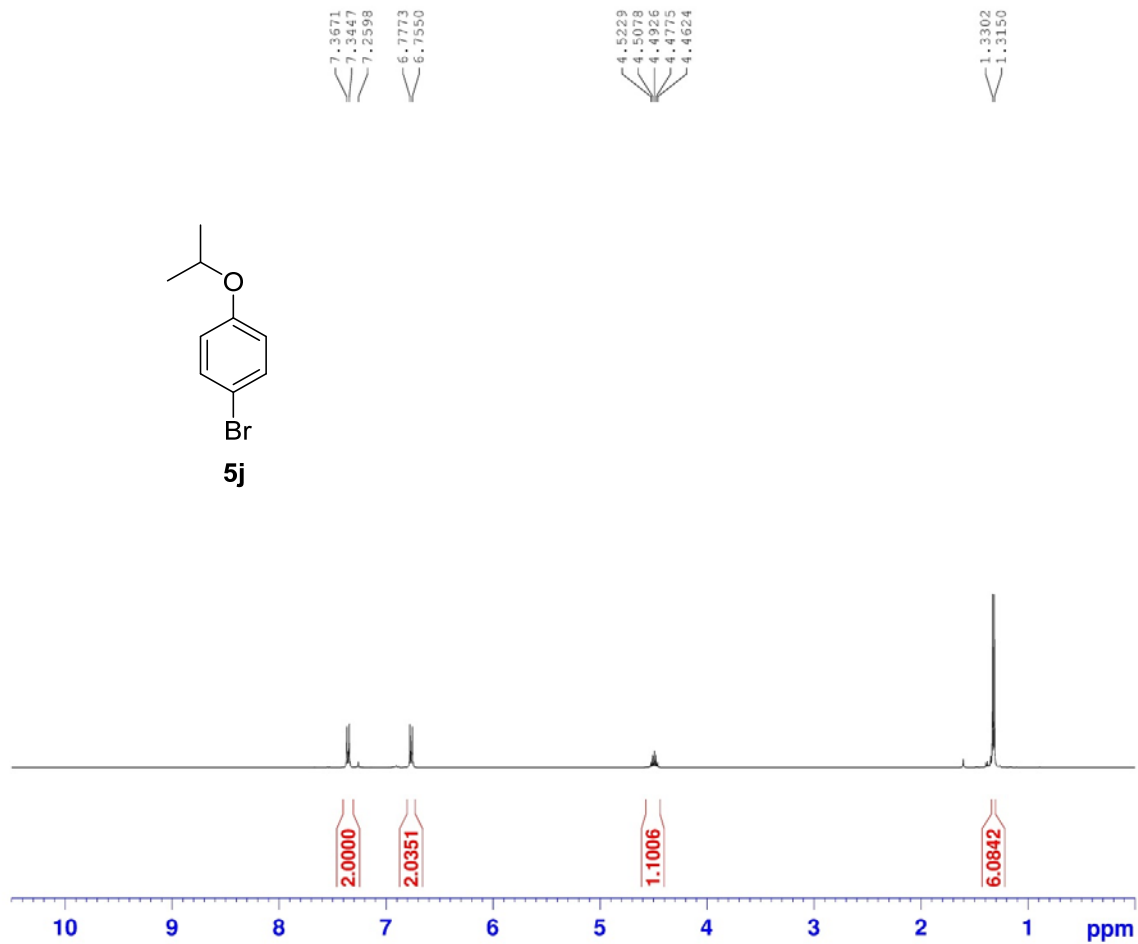
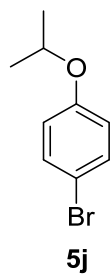
```

Current Data Parameters
NAME      SY-10308 Cl3
EXPNO    1
PROCNO   1

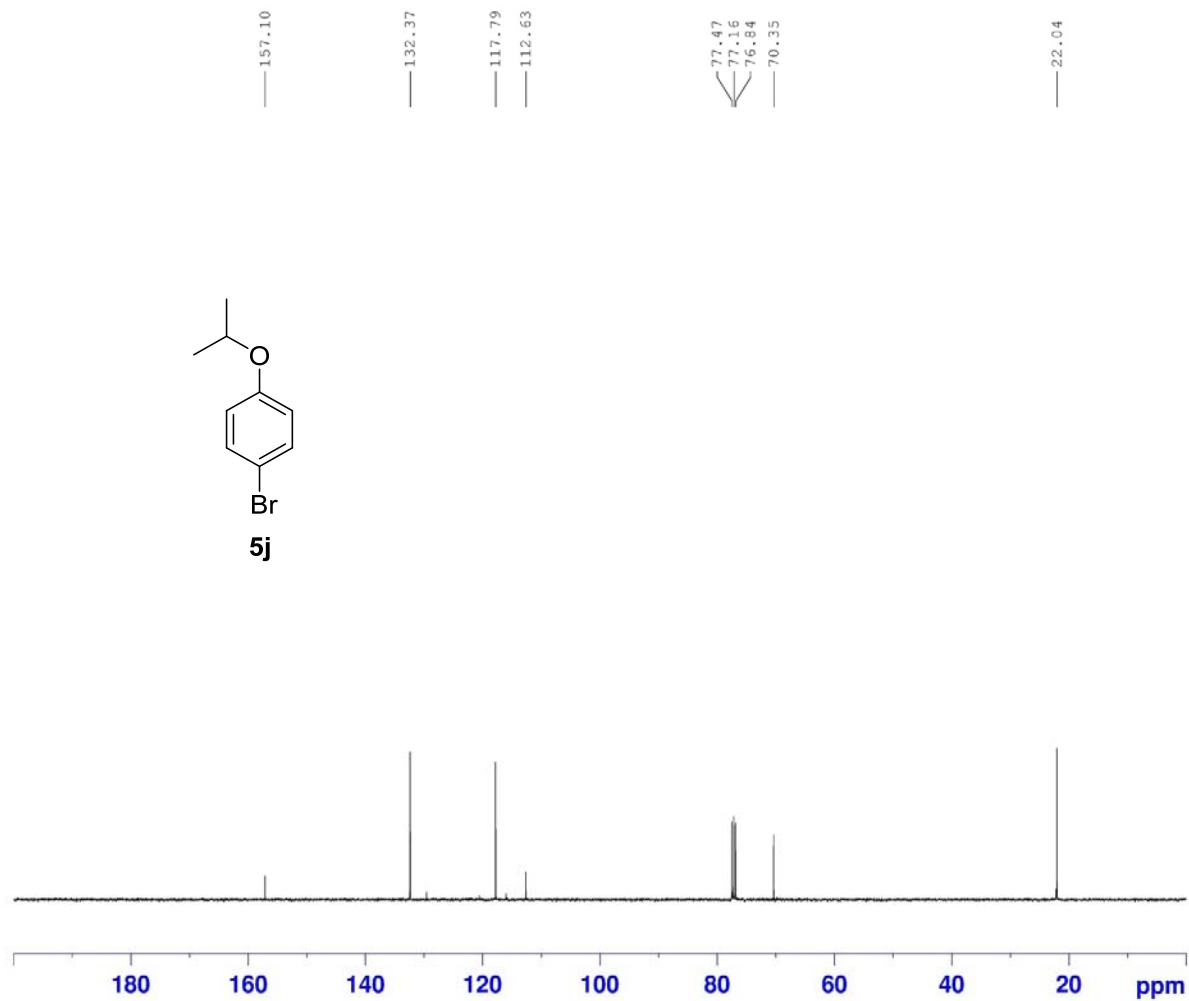
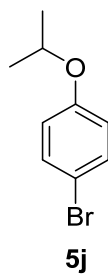
F2 - Acquisition Parameters
Date_    20160413
Time     10.16 h
INSTRUM  spect
PROBHD   Z824601_0021 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       70
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       203
DW       20.800 usec
DE       6.50 usec
TE       294.6 K
D1       2.0000000 sec
D11      0.0300000 sec
TD0      1
SFO1     100.6228298 MHz
NUC1     13C
P1       9.50 usec
PLW1     41.2500000 W
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG12 waltz16
PCPD2    90.00 usec
PLW2     8.31000042 W
PLW12    0.23083000 W
PLW13    0.11611000 W

F2 - Processing parameters
SI       32768
SF       100.6127594 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```



Current Data Parameters  
 NAME ST-10701  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20160413  
 Time 9.59 h  
 INSTRUM spect  
 PROBHD 2024601\_0021 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 80.6  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.2 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W  
 F2 - Processing parameters  
 SI 65536  
 SF 400.1300097 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 FC 1.00



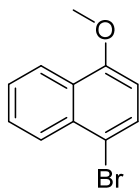
```

Current Data Parameters
NAME      sv-10701 c13
EXPNO     1
PROCNO    1

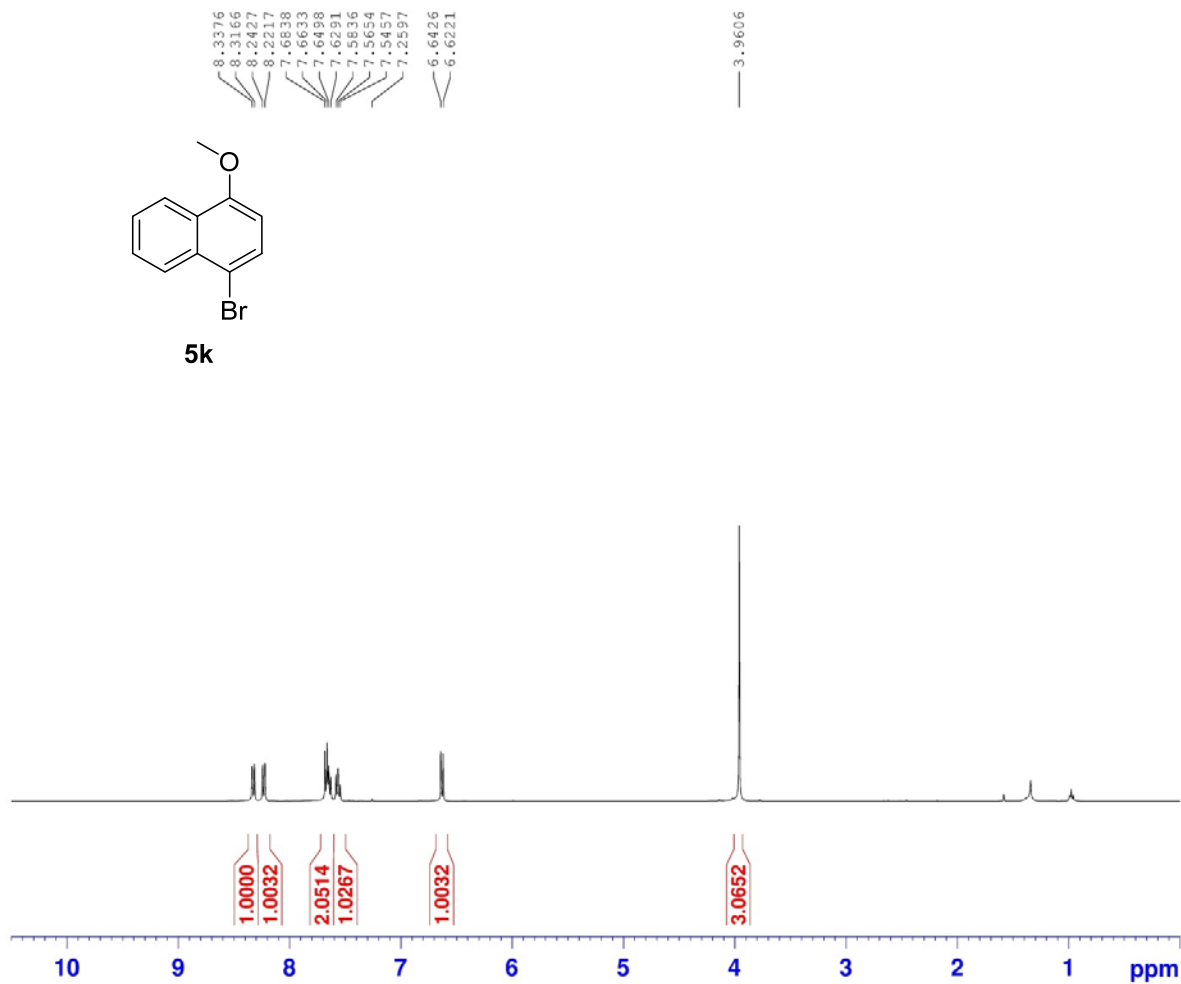
F2 - Acquisition Parameters
Date_     20160413
Time      10.02 h
INSTRUM   spect
PROBHD    Z824601_0021 f
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        102
DS        4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         200
DW         20.800 usec
DE         6.50 usec
TE         294.4 K
D1         2.00000000 sec
d11        0.03000000 sec
TD0        1
SFO1       100.6228298 MHz
NUC1       13C
P1         9.50 usec
PLM1       41.25000000 W
SFO2       400.1316005 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2     90.00 usec
PLM2       8.31000042 W
PLW12     0.23083000 W
PLW13     0.11611000 W

F2 - Processing parameters
SI         32768
SF         100.6127586 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
FC         1.40

```



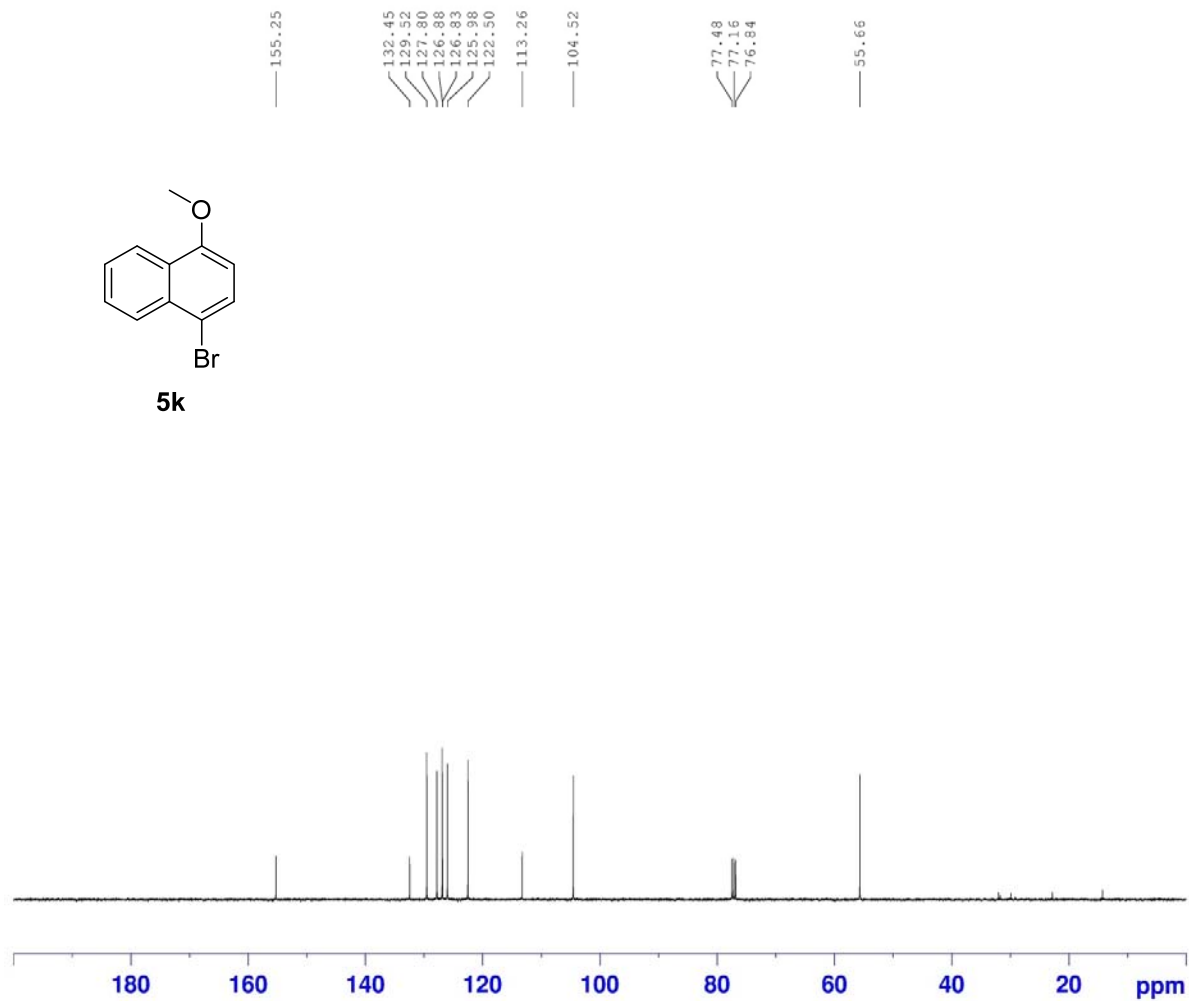
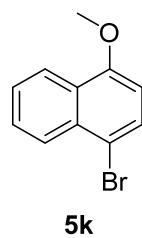
5k



Current Data Parameters  
 NAME SY-13303  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160425  
 Time 12.20 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.0 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1300098 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



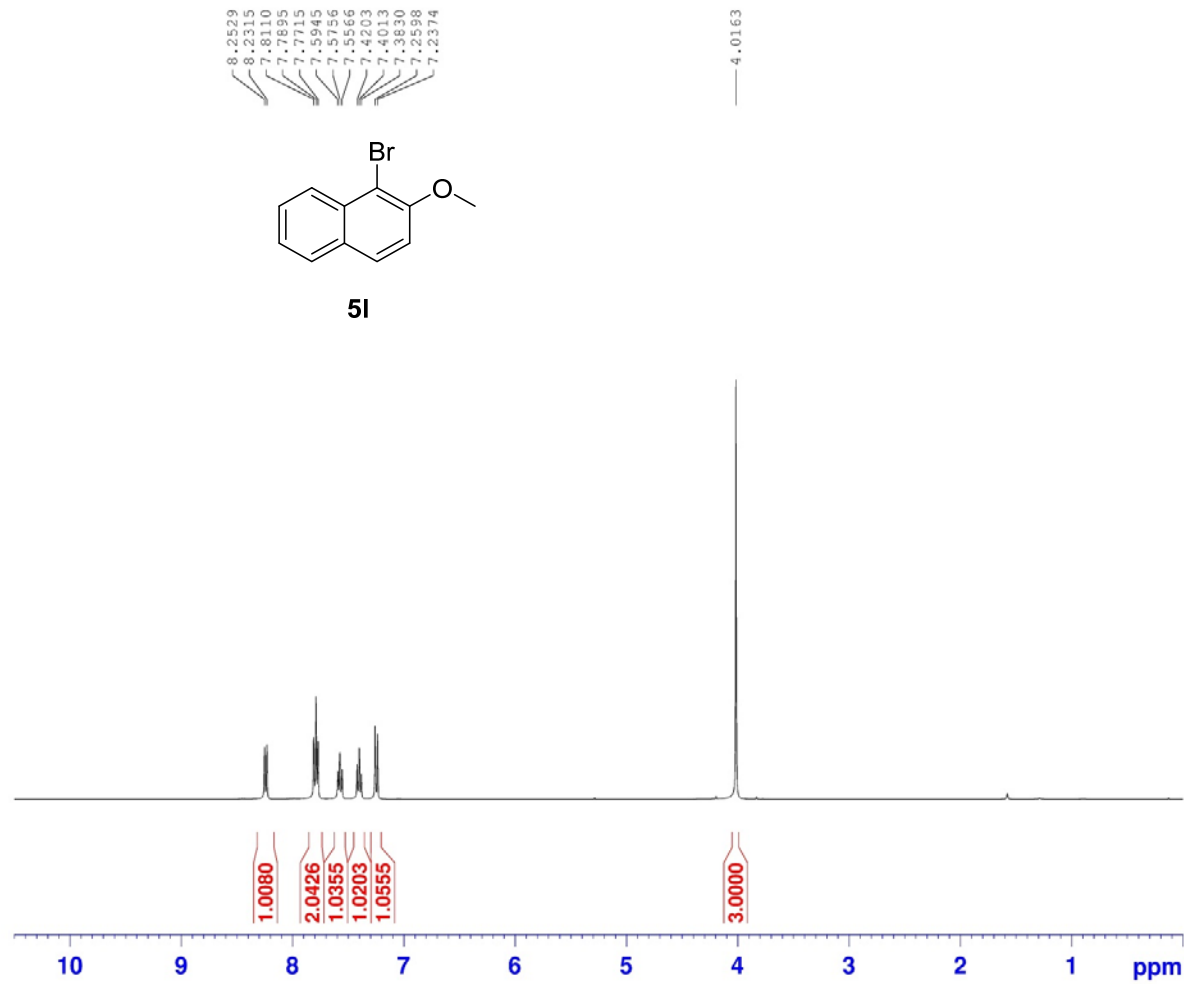
```

Current Data Parameters
NAME          SV-13303-C13
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20150425
Time          12.24 h
INSTRUM       spect
PROBHD        Z824601_0021
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            45
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            200
DW            20.800 usec
DE            6.50 usec
TE            296.2 K
D1            2.0000000 sec
d11           0.0300000 sec
TD0           1
SF01          100.6228298 MHz
NUC1          13C
P1            9.50 usec
PLM1          41.2500000 W
SF02          400.1316005 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          8.31000042 W
PLW12        0.23083000 W
PLW13        0.11611000 W

F2 - Processing parameters
SI            32768
SF            100.6127711 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

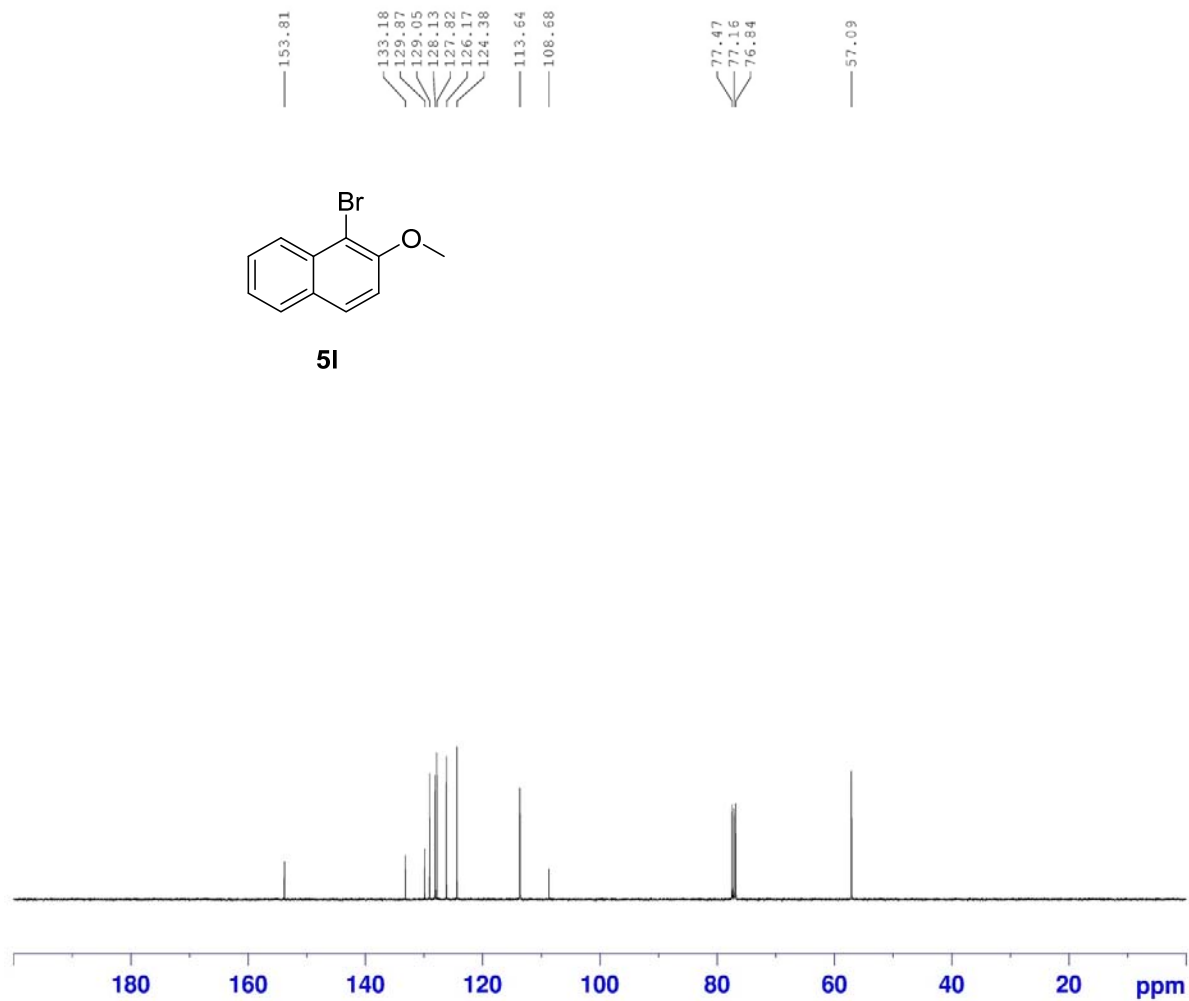
```



Current Data Parameters  
 NAME sy-15522-H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20151119  
 Time 15.17 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300117 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



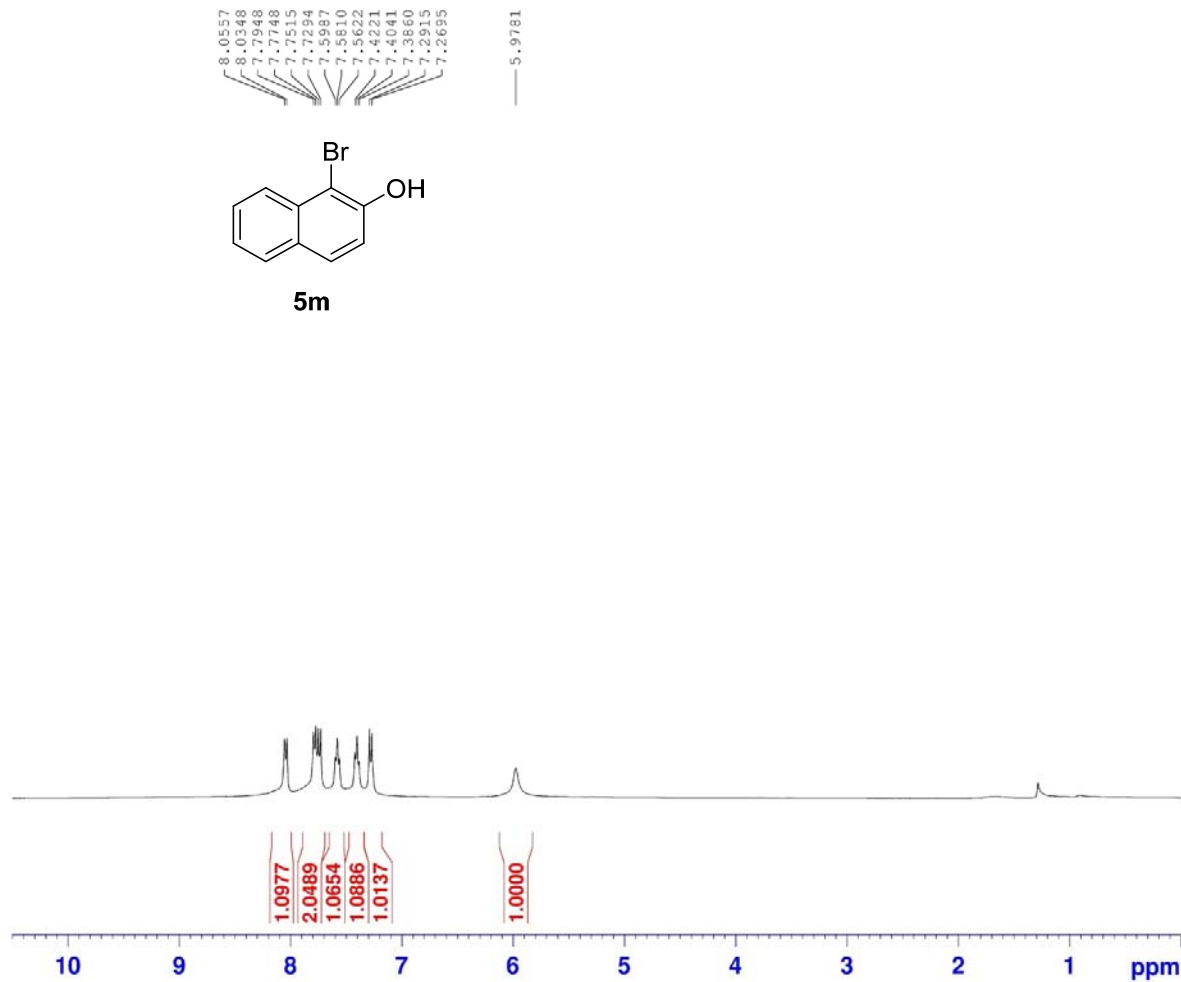
```

Current Data Parameters
NAME          sy-15522-c
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20160224
Time          20.06 h
INSTRUM       spect
PROBHD        Z824601_0021
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            152
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            200
DW            20.800 usec
DE            6.50 usec
TE            295.8 K
D1            2.0000000 sec
d11           0.0300000 sec
TD0           1
SF01          100.6228298 MHz
NUC1          13C
P1            9.50 usec
PLM1          41.2500000 W
SF02          400.1316005 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          8.31000042 W
PLW12         0.23083000 W
PLW13         0.11611000 W

F2 - Processing parameters
SI            32768
SF            100.6127656 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

```

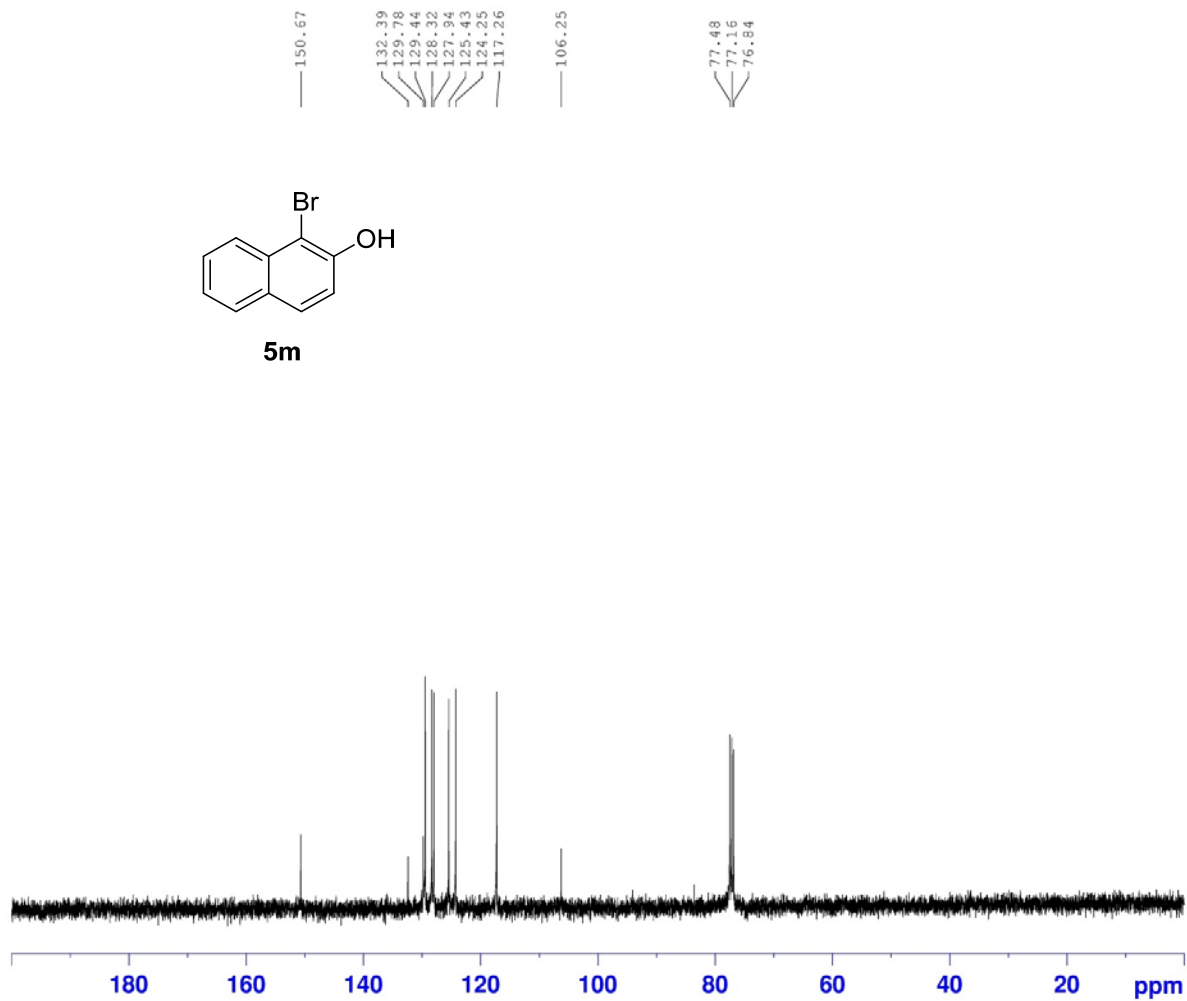
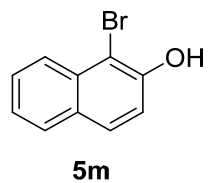


Current Data Parameters  
 NAME SY-10101 proton  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160412  
 Time 12.11 h  
 INSTRUM spect  
 PROBHD Z108618\_0257 (   
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 57  
 DN 62.400 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300099 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





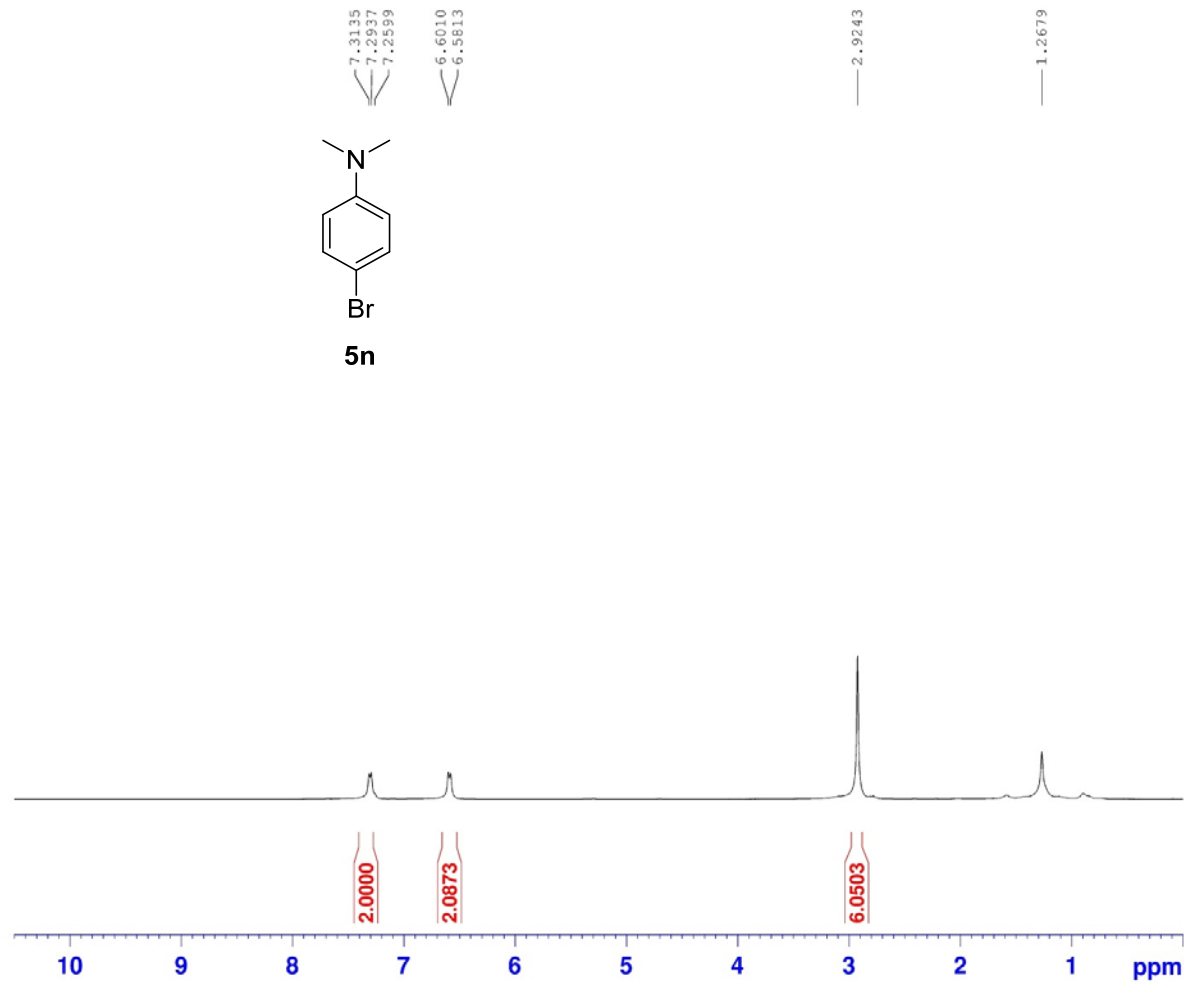
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Current Data Parameters
NAME          sv-10101 C13
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20150412
Time          12.15 h
INSTRUM       spect
PROBHD        Z108618_0257 f
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            52
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            144
DW            20.800 usec
DE            6.50 usec
TE            295.1 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SFO1          100.6479773 MHz
NUC1          13C
P1            9.50 usec
PLM1          55.34000015 W
SFO2          400.2316009 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI            32768
SF            100.6379079 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

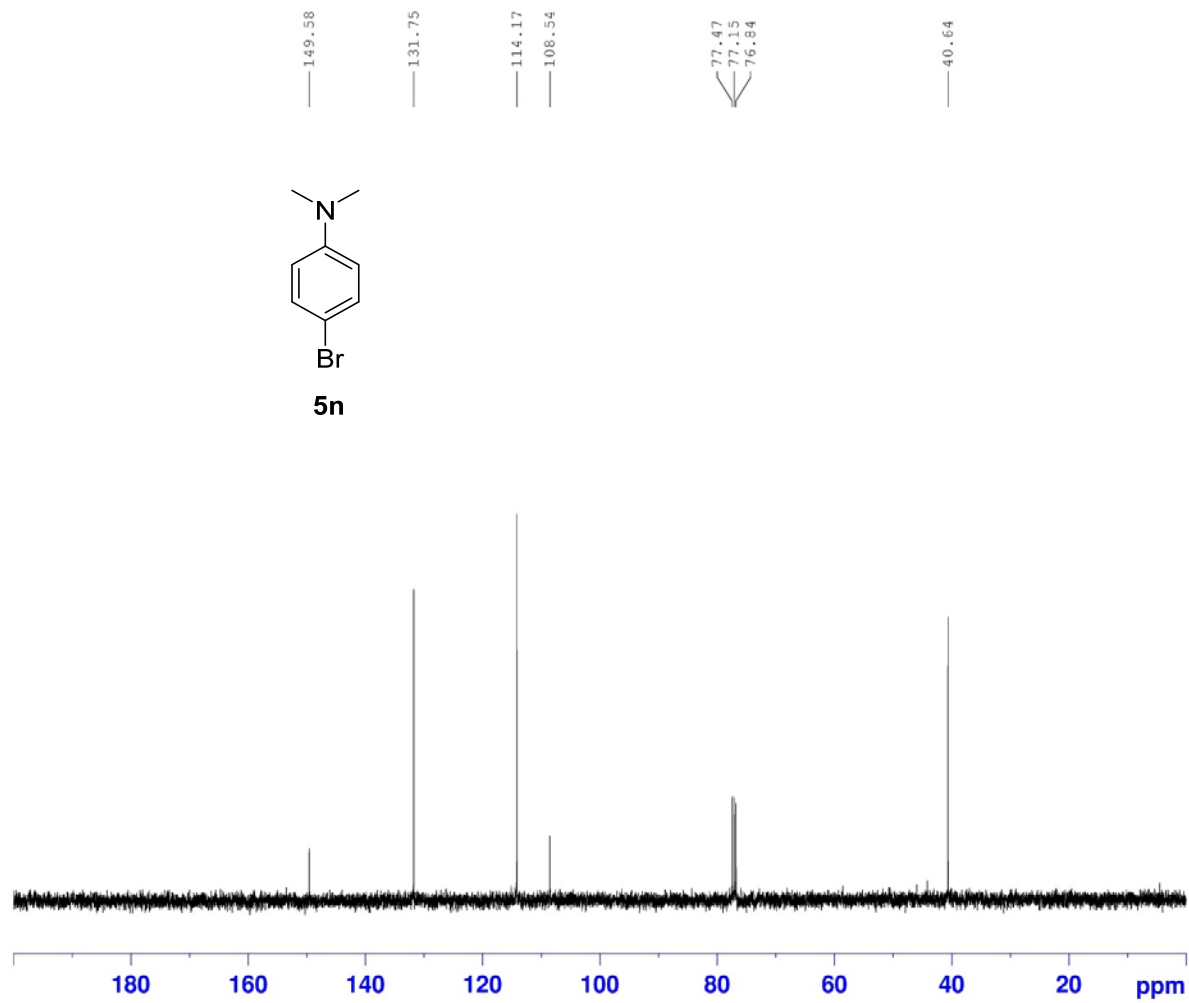
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Current Data Parameters  
 NAME SY-15520  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160601  
 Time 13.31 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 50.8  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.6 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300128 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



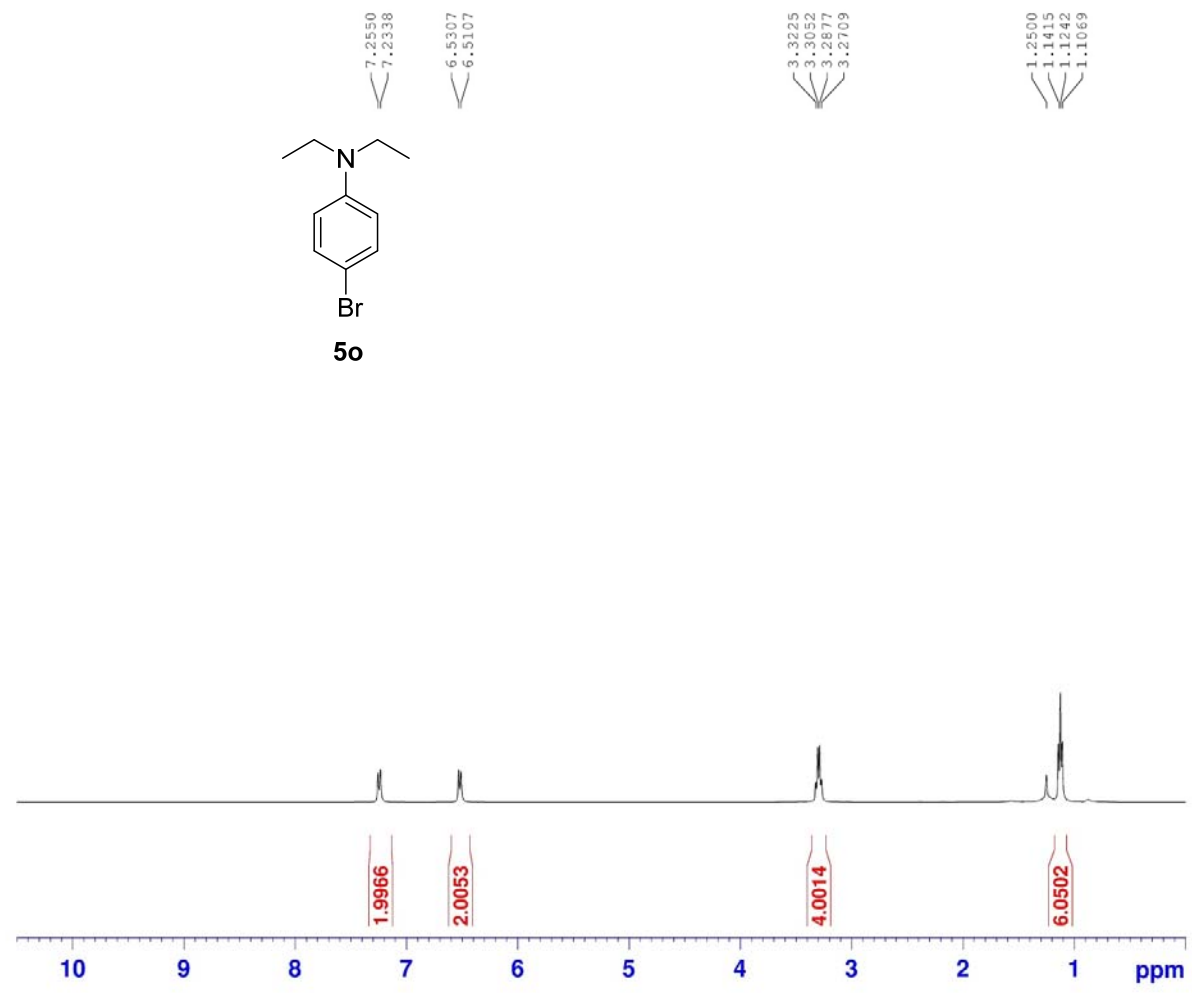
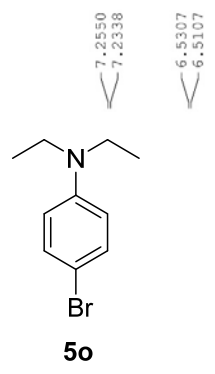
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Current Data Parameters
NAME          SY-15520-c
EXPNO         1
PROCNO        1

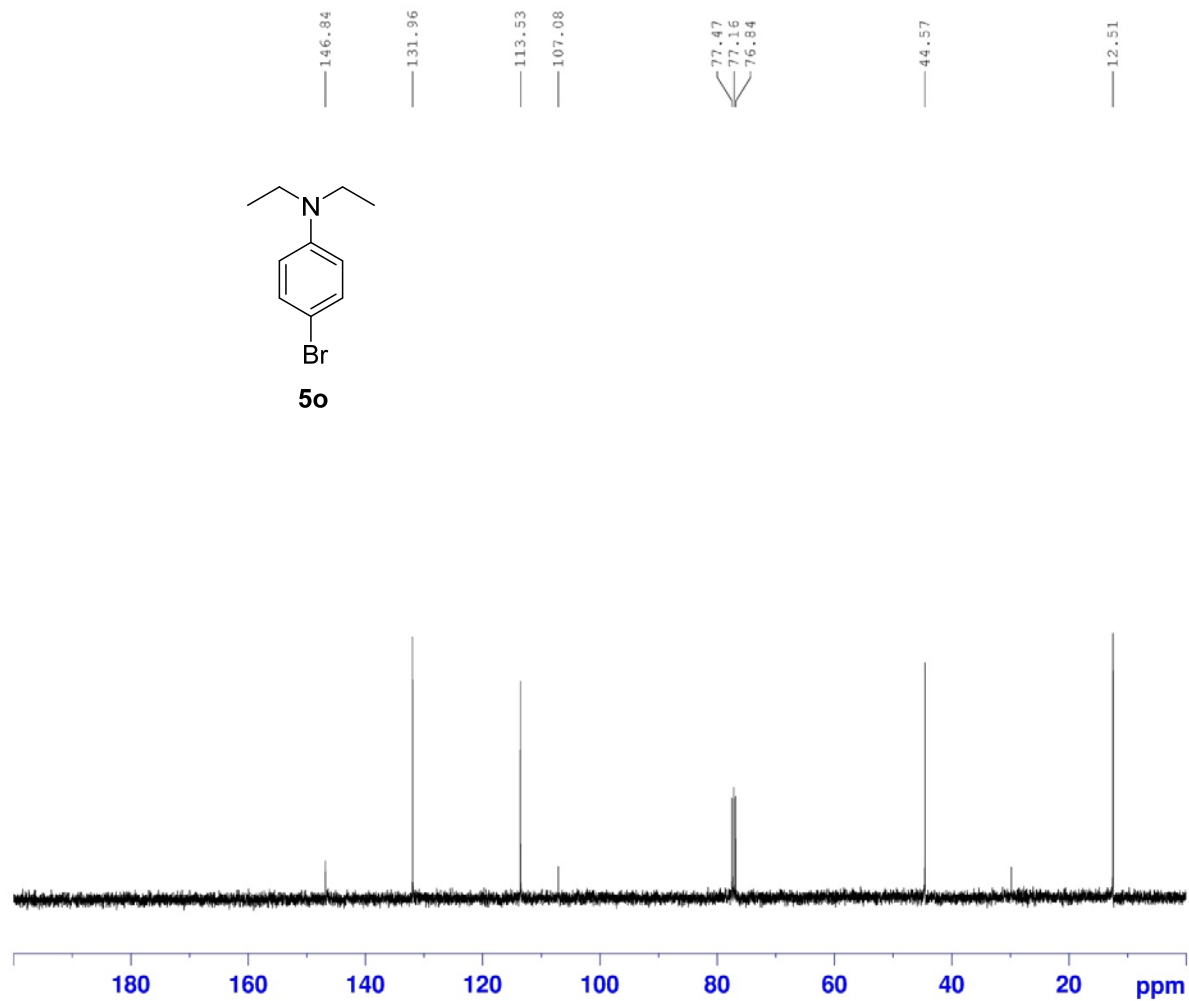
F2 - Acquisition Parameters
Date_         20161031
Time          13.46 h
INSTRUM       spect
PROBHD        Z108618_0257
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            100
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            1
DW            20.800 usec
DE            6.50 usec
TE            295.1 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SFO1          100.6479773 MHz
NUC1          13C
P1            9.50 usec
PLM1          55.34000015 W
SFO2          400.2316009 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI            32768
SF            100.6379087 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

```



Current Data Parameters  
 NAME SY-15521  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20160601  
 Time 13.47 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 FULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.7 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2300231 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



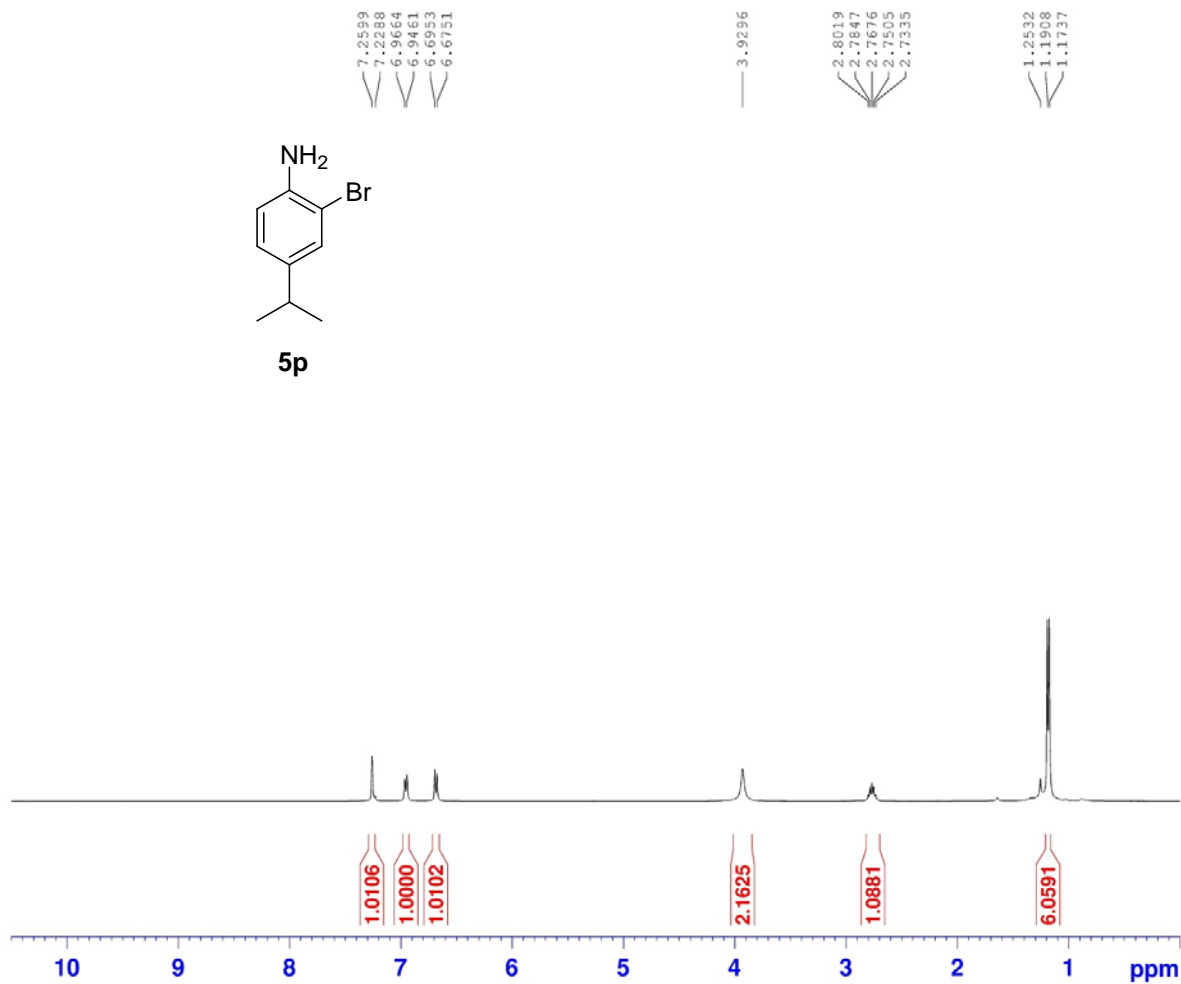
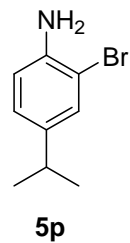
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Current Data Parameters
NAME      SV-15521-C13
EXPNO    1
PROCNO   1

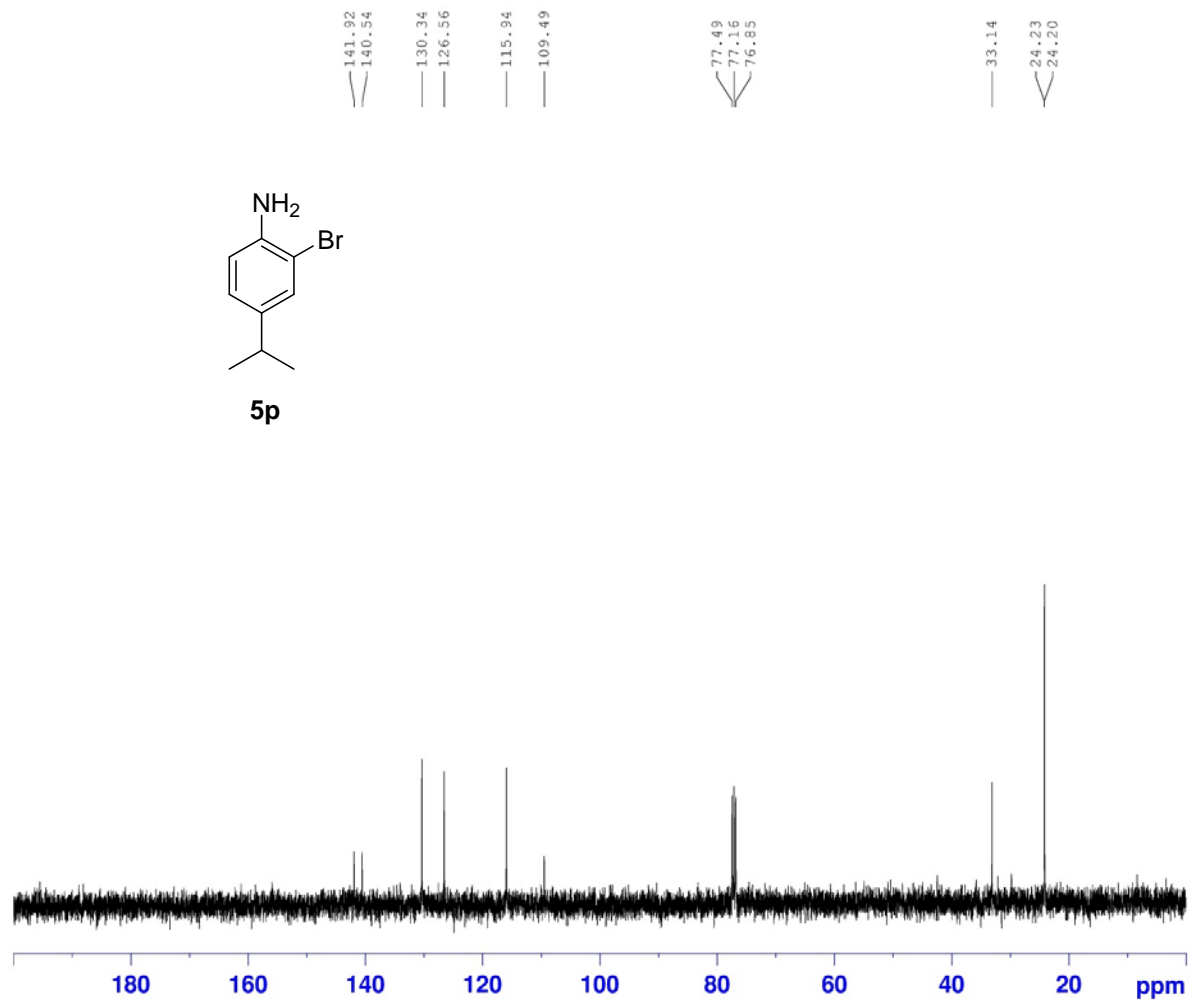
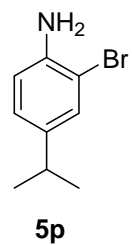
F2 - Acquisition Parameters
Date_    20150601
Time     13.53 h
INSTRUM  spect
PROBHD   Z108618_0257 f
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       250
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       1
DW       20.800 usec
DE       6.50 usec
TE       296.2 K
D1       2.0000000 sec
d11      0.0300000 sec
TD0      1
SFO1     100.6479773 MHz
NUC1     13C
P1       9.50 usec
PLM1     55.3400015 W
SFO2     400.2316009 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLM2     13.56000042 W
PLW12    0.27428001 W
PLW13    0.13796000 W

F2 - Processing parameters
SI       32768
SF       100.6379057 MHz
WDW      EM
SSB      0
LR       1.00 Hz
GB       0
FC       1.40

```



Current Data Parameters  
 NAME SY-15524-2  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20160603  
 Time 11.25 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 4  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.5 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W  
 F2 - Processing parameters  
 SI 65536  
 SF 400.2300234 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

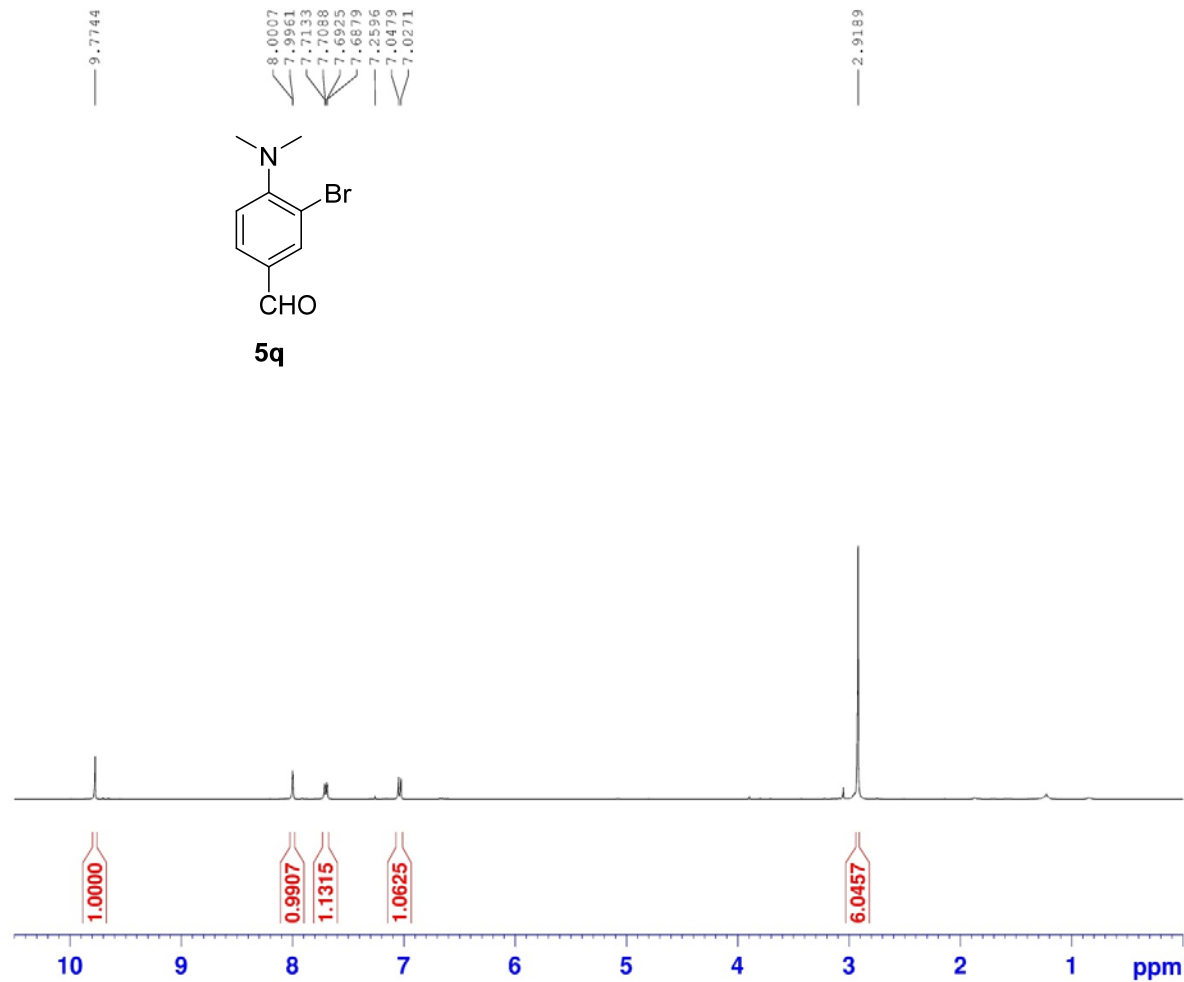


```

Current Data Parameters
NAME      SY-15524-2-C13
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150603
Time     12.50 h
INSTRUM  spect
PROBHD   Z108618_0257
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        250
DS        4
SWH       24038.461 Hz
FIDRES    0.366798 Hz
AQ         1.3631488 sec
RG         1
DW         20.800 usec
DE         6.50 usec
TE         295.3 K
D1         2.00000000 sec
d11       0.03000000 sec
TD0        1
SFO1      100.6479773 MHz
NUC1       13C
P1         9.50 usec
PLM1       55.34000015 W
SFO2      400.2316009 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     90.00 usec
PLM2       13.56000042 W
PLW12     0.27428001 W
PLW13     0.13796000 W

F2 - Processing parameters
SI         32768
SF         100.6379079 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
FC         1.40
  
```

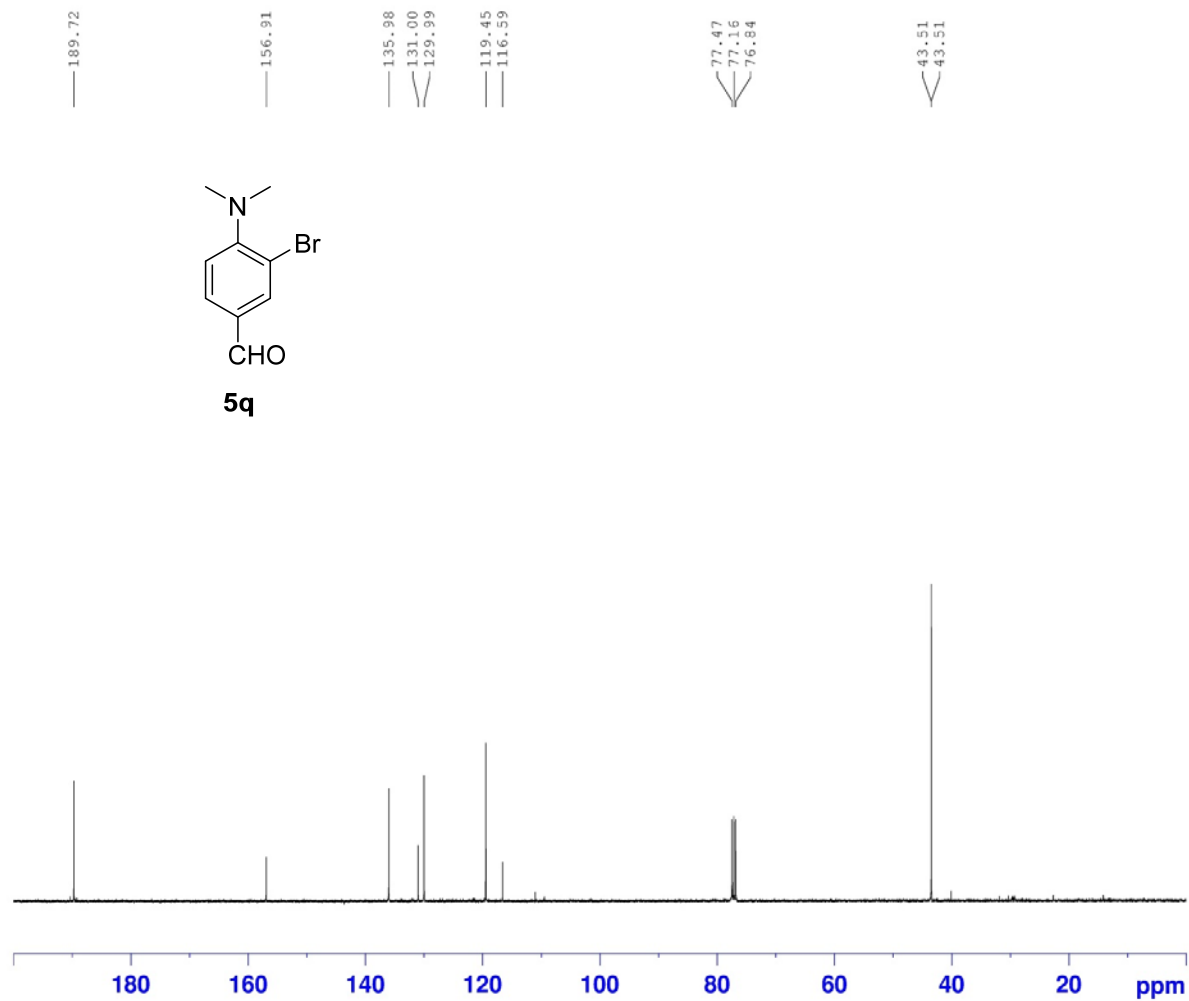


Current Data Parameters  
 NAME SY-105-03  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160411  
 Time 17.47 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.8 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300097 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





```

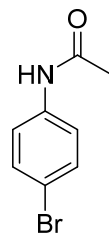
Current Data Parameters
NAME      SY-105-03 C13
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20150411
Time      17.50 h
INSTRUM   spect
PROBHD    Z108618_0257 f
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         86
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         101
DW         20.800 usec
DE         6.50 usec
TE         295.2 K
D1         2.00000000 sec
d11        0.03000000 sec
TD0        1
SFO1       100.6479773 MHz
NUC1        13C
P1          9.50 usec
PLM1        55.34000015 W
SFO2        400.2316009 MHz
NUC2         1H
CPDPRG2    waltz16
PCPD2      90.00 usec
PLM2        13.56000042 W
PLW12       0.27428001 W
PLW13       0.13796000 W

F2 - Processing parameters
SI          32768
SF          100.6379101 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
FC          1.40

```

7.4341  
7.4266  
7.4110  
7.4062  
7.3904  
7.3831  
7.3014  
7.2601



**5r**

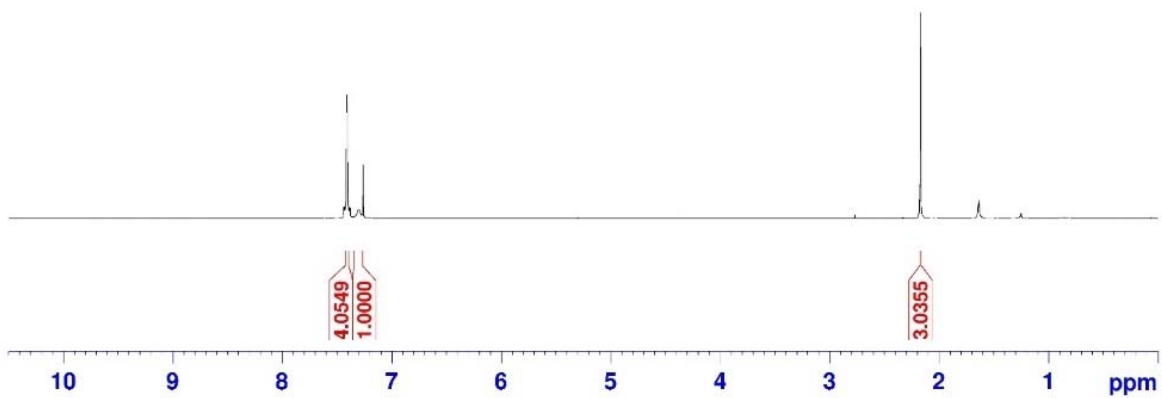
— 2.1889

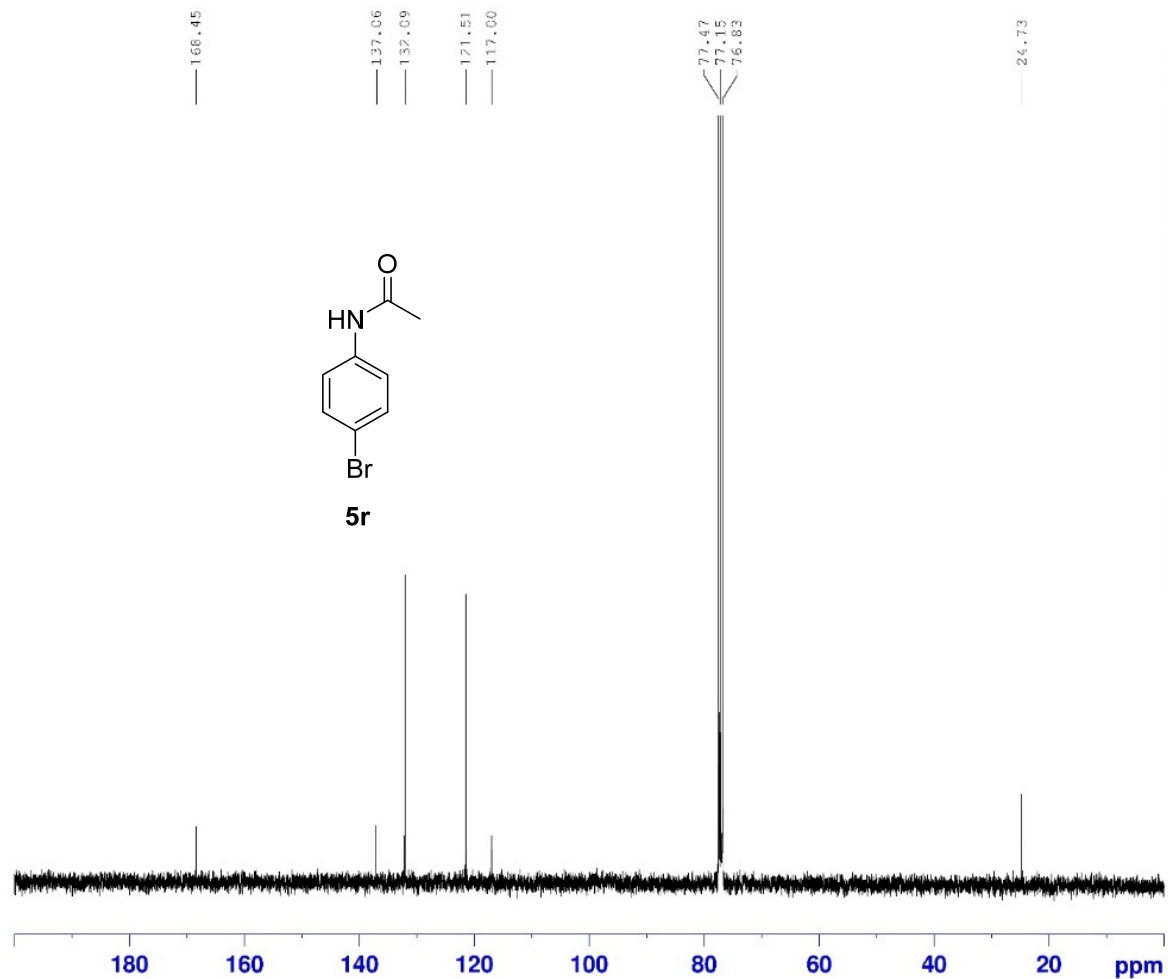
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Current Data Parameters
NAME      15527-H
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150329
Time     12.37 h
INSTRUM  spect
FACOMB   2108618_0257 1
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       21
DS       2
SWH      8012.820 Hz
FIDRES   0.122265 Hz
AQ       4.0894465 sec
RG       144
SR       62.100 usec
DE       6.50 usec
TE       291.3 K
D1       1.00000000 sec
TD0      1
SF01     400.232414 MHz
NUC1     1H
P1       -2.80 usec
PLW1     13.5600042 W

F2 - Processing parameters
SI       65536
SF       400.230098 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

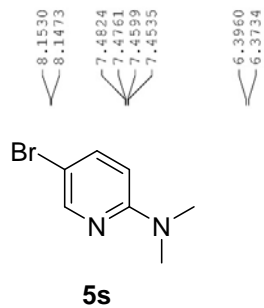




Current Data Parameters  
 NAME 15527-0  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160401  
 Time 13.30 h  
 INSTRUM spect  
 PROBHD 5324601.0021.1  
 PULPROG zgpg30  
 TD 85536  
 SOLVENT H2O  
 NS 421  
 DS 4  
 SFO 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631480 sec  
 RG 203  
 DW 30.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
 DI 2.00300000 sec  
 D11 0.03000000 sec  
 TCO 1  
 SFO1 100.6228798 MHz  
 SPC1 13C  
 P1 9.50 usec  
 PLW1 41.2500000 W  
 SFO2 400.1316005 MHz  
 SPC2 1H  
 CPDPRG2 waltz16  
 ICDPC 30.00 usec  
 PLW2 8.3100042 W  
 PLW3 0.23081000 W  
 PLW4 0.11611000 W

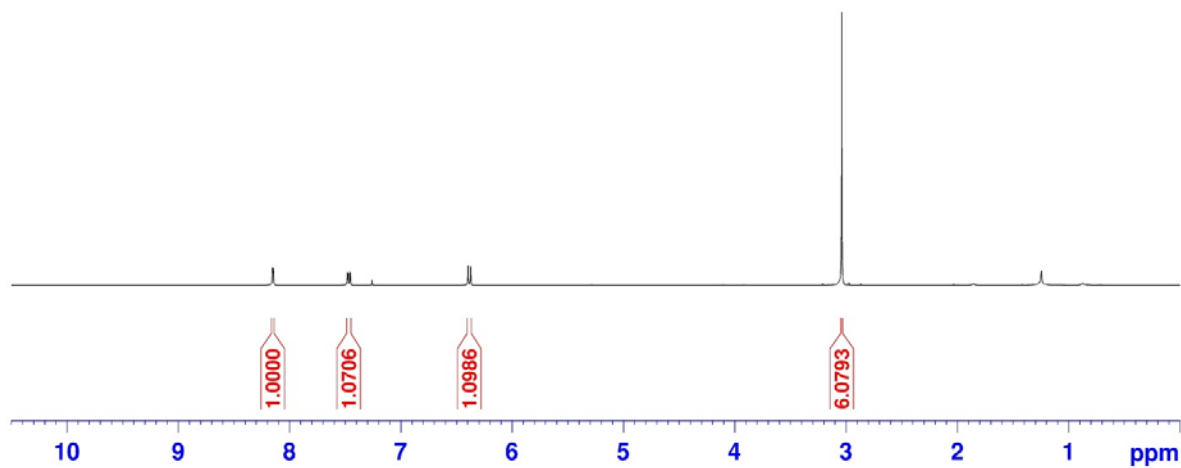
F2 - Processing parameters  
 SI 32768  
 SF 100.6127566 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 TC 1.40

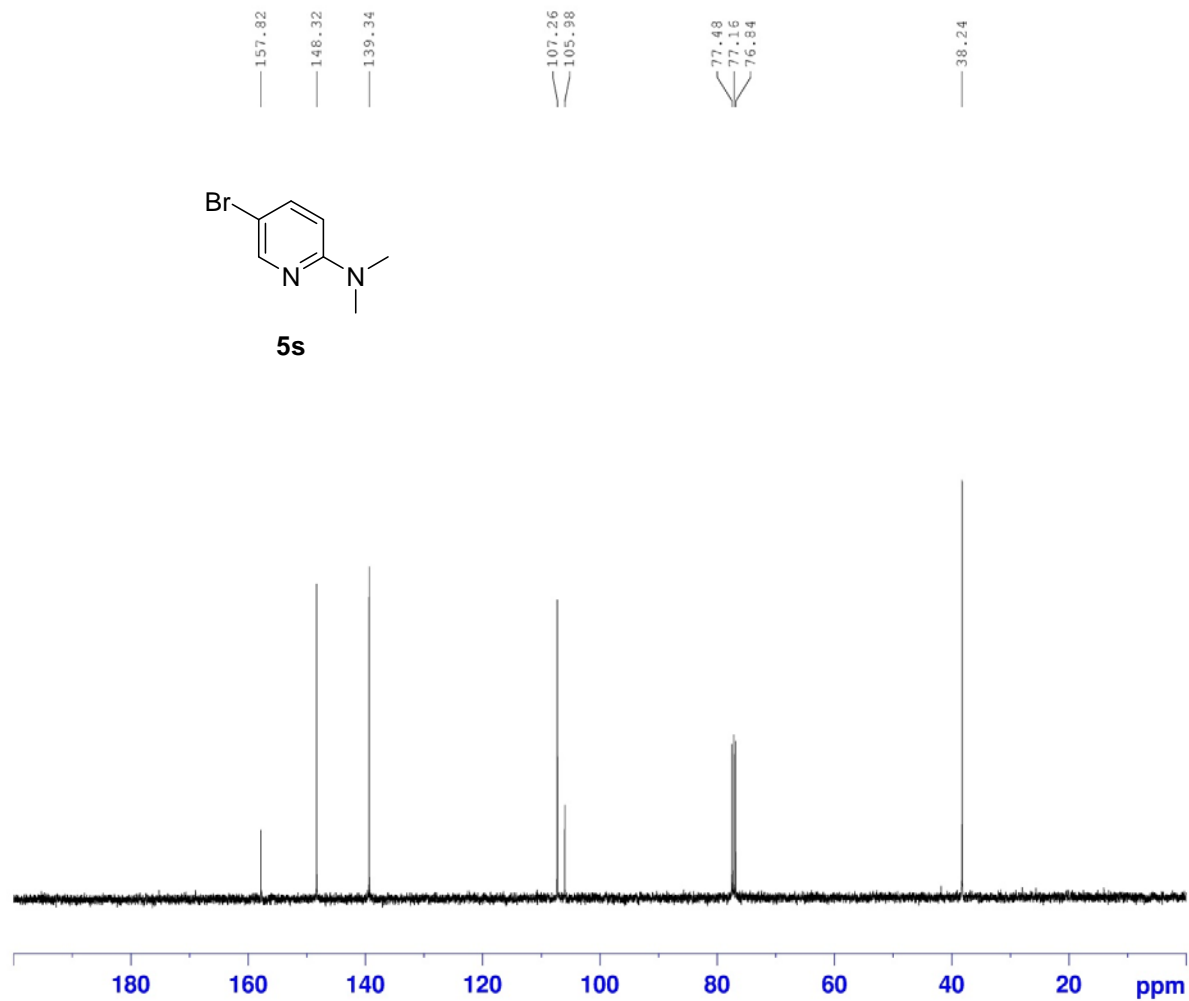


Current Data Parameters  
 NAME SY-1450212  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160525  
 Time 16.14 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 7  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 57  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.1 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300107 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





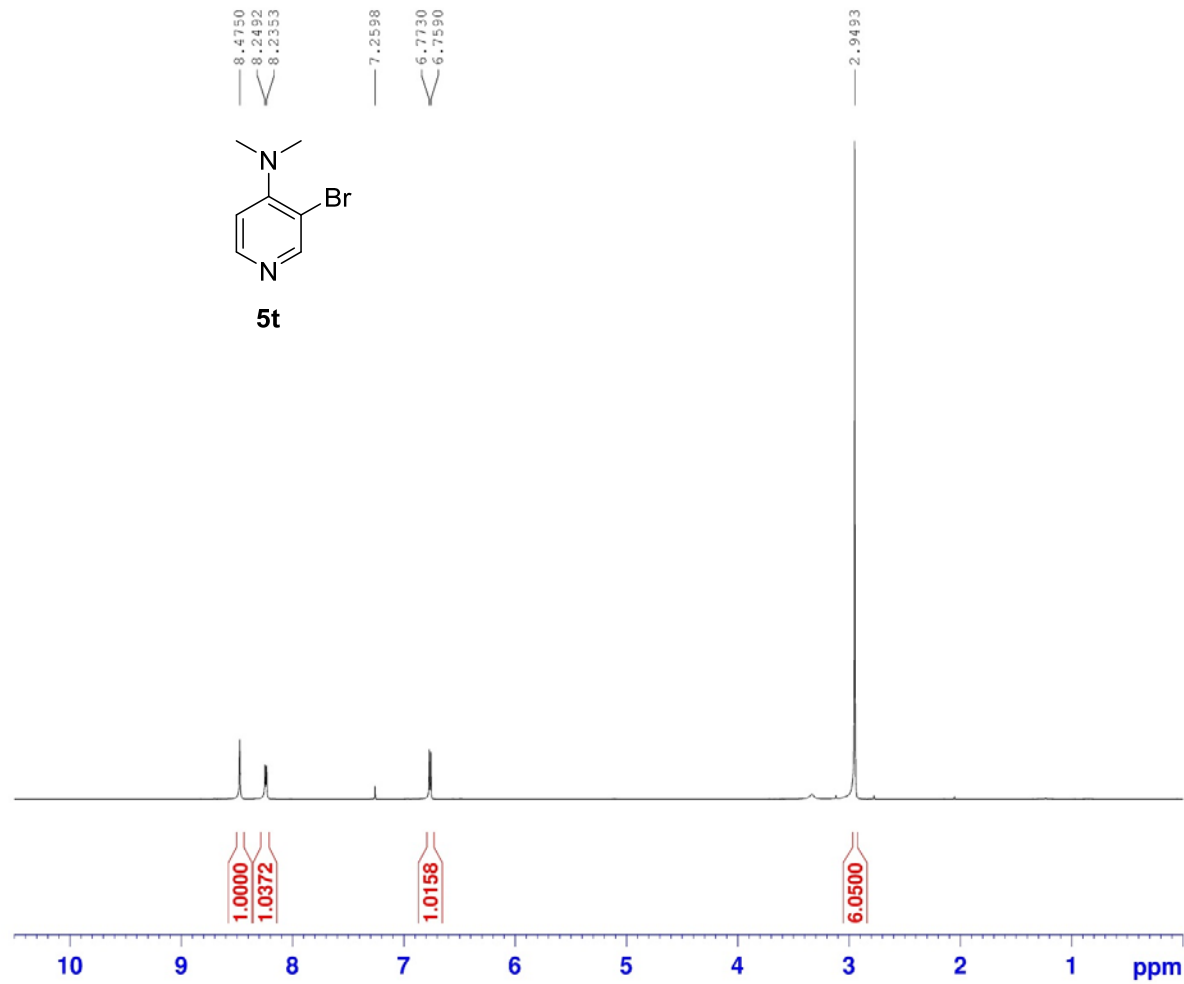
```

Current Data Parameters
NAME          SY-15501-c
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20161031
Time          13.36 h
INSTRUM       spect
PROBHD        Z108618_0257 f
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            23
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            161
DW            20.800 usec
DE            6.50 usec
TE            295.3 K
D1            2.0000000 sec
d11           0.0300000 sec
TD0           1
SF01          100.6479773 MHz
NUC1           13C
P1            9.50 usec
PLM1          55.34000015 W
SF02          400.2316009 MHz
NUC2           1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI            32768
SF            100.6379094 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

```



Current Data Parameters

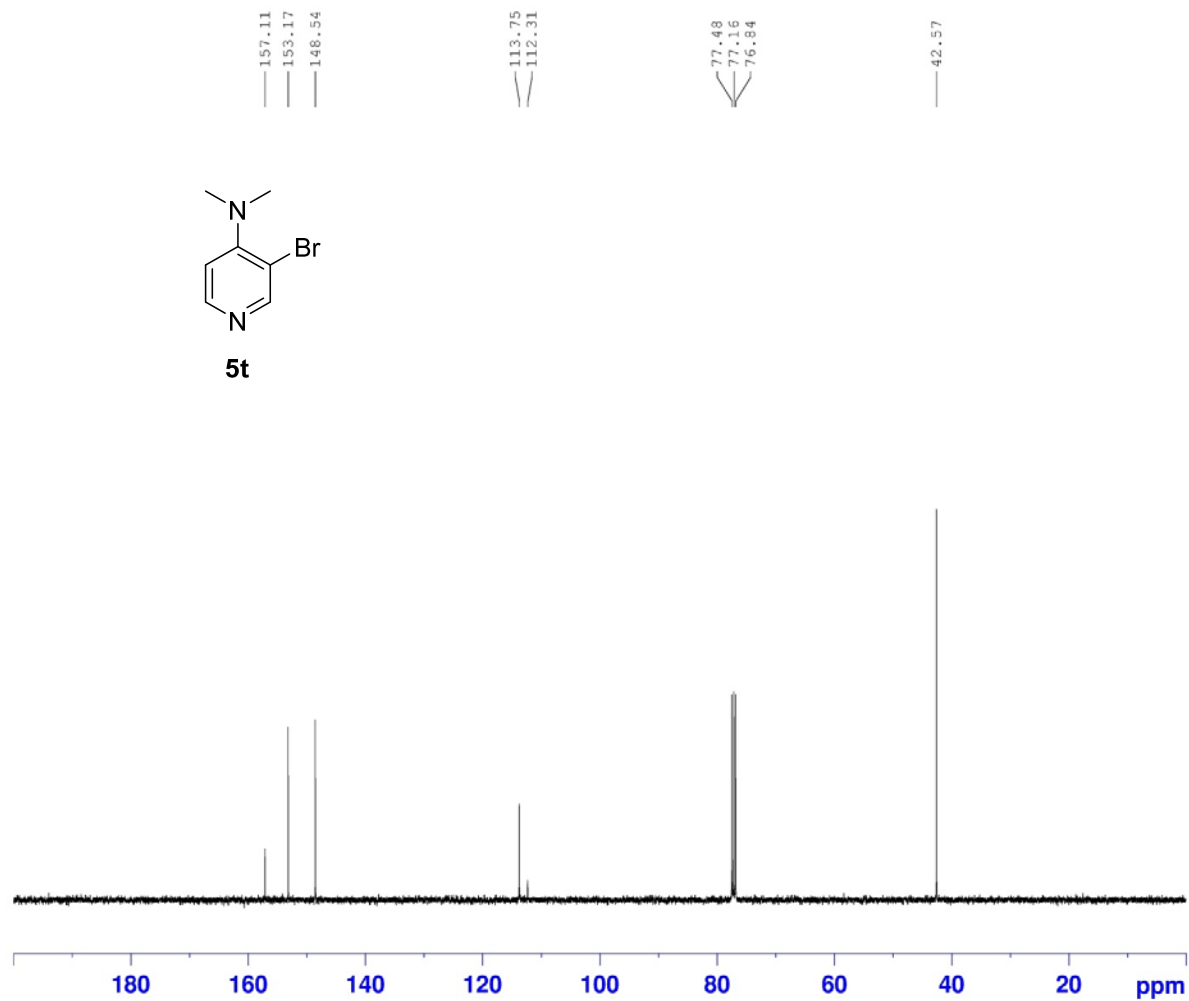
NAME	SY-15512-H
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20161102
Time	18.29 h
INSTRUM	spect
PROBHD	Z108618_0237 (
FULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	3
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894465 sec
RG	71.8
DW	62.400 usec
DE	6.50 usec
TE	295.9 K
D1	1.00000000 sec
TDO	1
SFO1	400.2324714 MHz
NUC1	1H
PI	12.80 usec
PLW1	13.56000042 W

F2 - Processing parameters

SI	65536
SF	400.2300098 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



```

Current Data Parameters
NAME          SV-15512-c
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20161104
Time          13.04 h
INSTRUM       spect
PROBHD        Z824601_0021
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            100
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            203
DW            20.800 usec
DE            6.50 usec
TE            294.5 K
D1            2.00000000 sec
d11           0.03000000 sec
TD0           1
SF01          100.6228298 MHz
NUC1          13C
P1            9.50 usec
PLM1          41.25000000 W
SF02          400.1316005 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          8.31000042 W
PLW12         0.23083000 W
PLW13         0.11611000 W

F2 - Processing parameters
SI            32768
SF            100.6127615 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

```

kzh-1,8-naphthyl-cp

7.753  
7.732  
7.610  
7.591  
7.501  
7.484  
7.480  
7.463  
7.413  
7.395  
7.260  
7.220  
7.202

3.056  
3.044  
3.034  
3.024  
3.014  
2.992  
2.982  
2.972  
2.962  
2.950

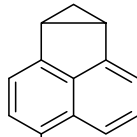
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1.524  
1.514  
1.504  
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0.812  
0.802  
0.792



Current Data Parameters  
NAME kzh20170829  
EXPNO 3  
PROCNO 1

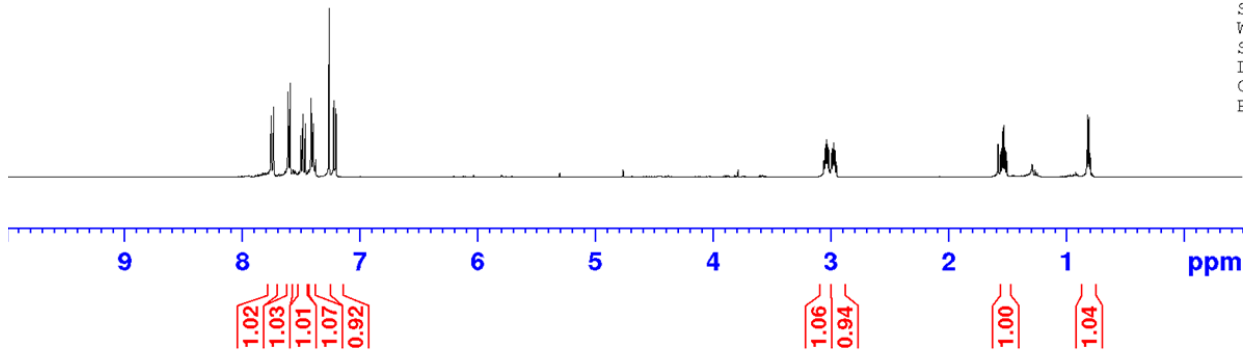
F2 - Acquisition Parameters  
Date\_ 20170830  
Time 17.42 h  
INSTRUM spect  
PROBHD Z108618\_0257 {  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 50.8  
DW 62.400 usec  
DE 6.50 usec  
TE 294.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters  
SI 65536  
SF 400.2300101 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



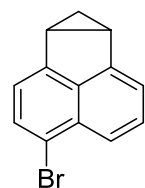
Br

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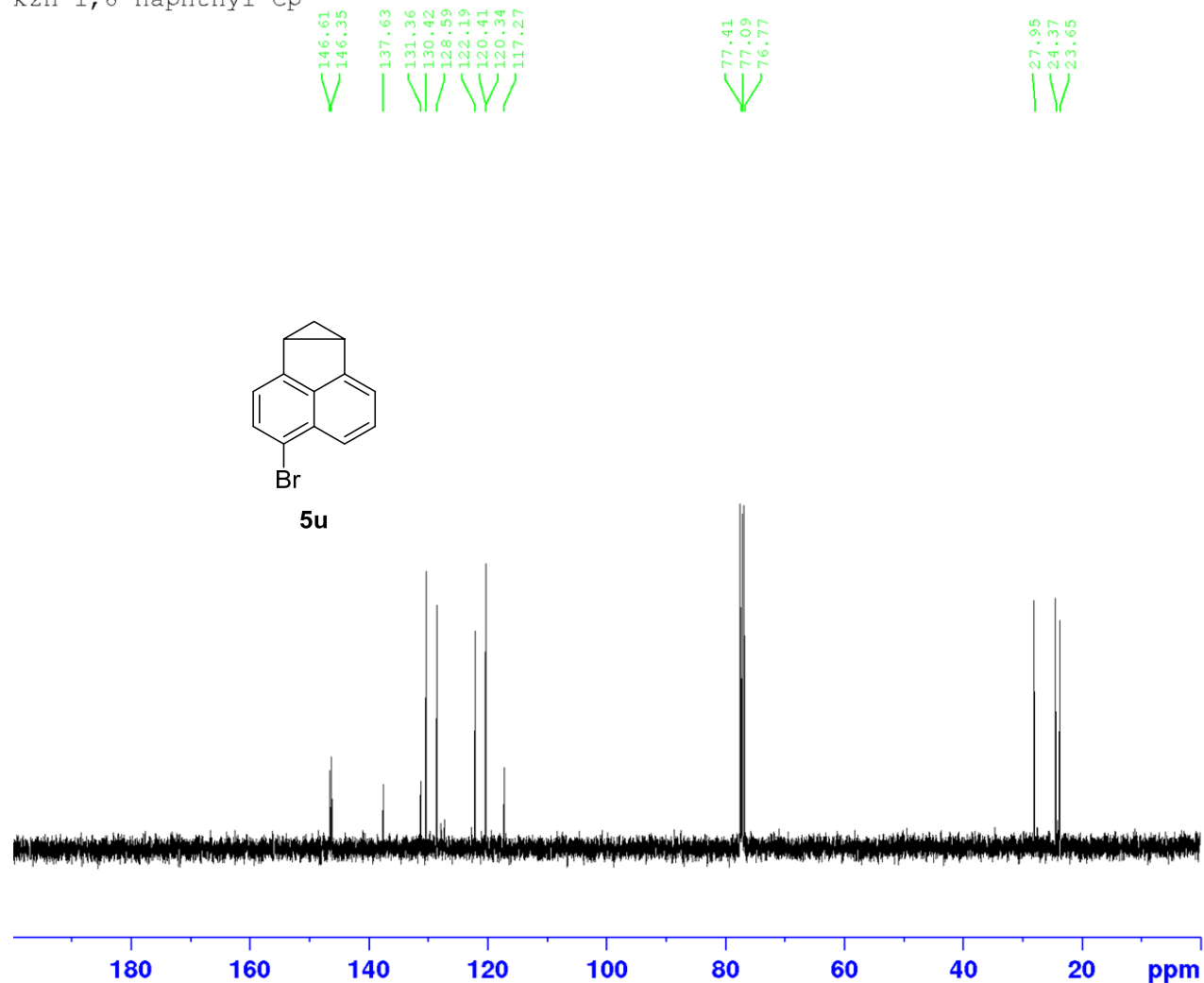




kzh-1,8-naphthyl-cp



5u

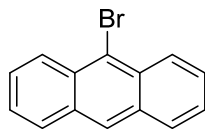


Current Data Parameters  
NAME kzh20170829  
EXPNO 5  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170830  
Time 17.53 h  
INSTRUM spect  
PROBHD Z108618\_0257 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 10  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 161  
DW 20.800 usec  
DE 6.50 usec  
TE 295.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 100.6479773 MHz  
NUC1 13C  
P1 9.50 usec  
PLW1 55.34000015 W  
SFO2 400.2316009 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 13.56000042 W  
PLW12 0.27428001 W  
PLW13 0.13796000 W

F2 - Processing parameters  
SI 32768  
SF 100.6379135 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

8.5387  
8.5166  
8.4000  
7.9835  
7.9625  
7.6213  
7.6041  
7.5830  
7.5182  
7.4992  
7.4809  
7.2559

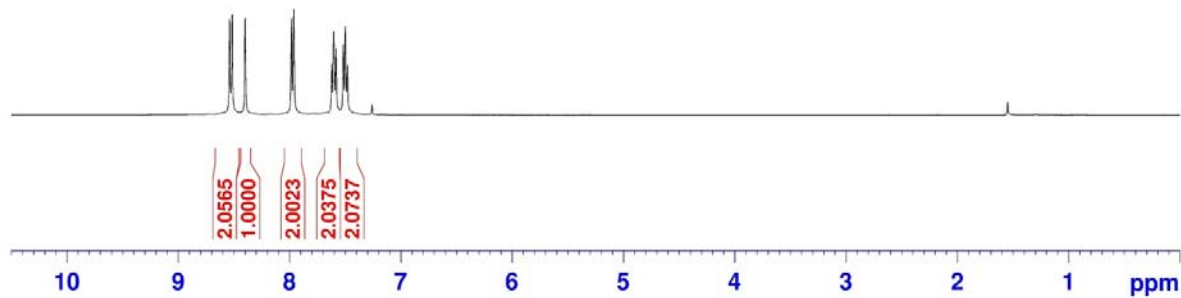


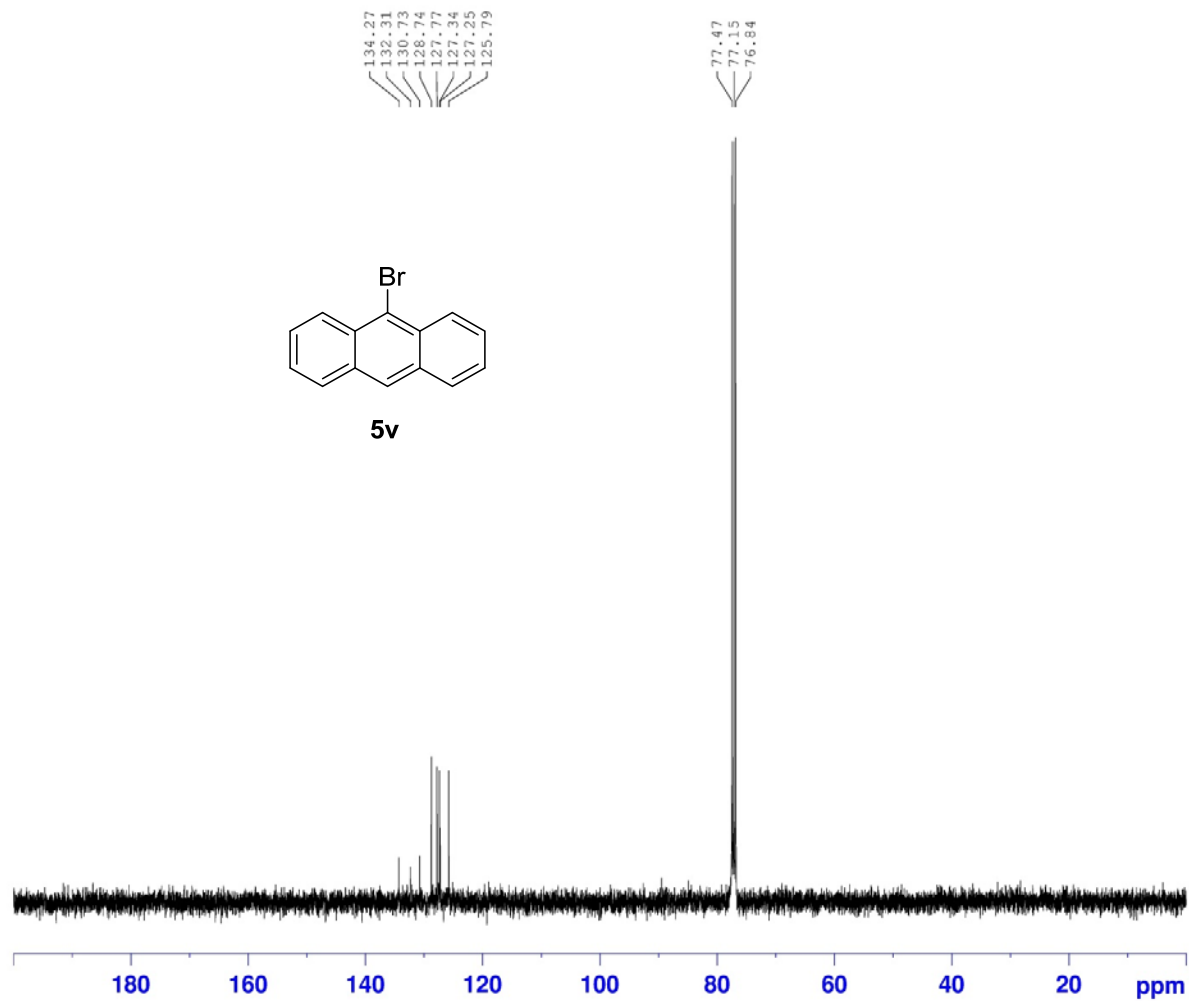
**5v**

Current Data Parameters  
NAME sy-15513  
EXFNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160521  
Time 13.45 h  
INSTRUM spect  
PROBHD Z108618\_0257 f  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 64  
DW 62.400 usec  
DE 6.50 usec  
TE 295.1 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.2324714 MHz  
NUC1 1H  
P1 12.80 usec  
PLW1 13.56000042 W

F2 - Processing parameters  
SI 65536  
SF 400.2300107 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





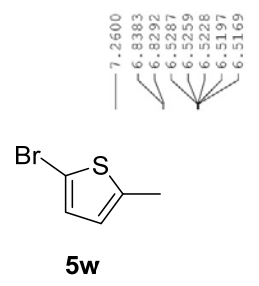
```

Current Data Parameters
NAME          sy-15513-c
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20160309
Time          19.48 h
INSTRUM       spect
PROBHD        Z824601_0021 f
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            232
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            200
DW            20.800 usec
DE            6.50 usec
TE            296.2 K
D1            2.0000000 sec
d11           0.0300000 sec
TD0           1
SFO1          100.6228298 MHz
NUC1          13C
P1            9.50 usec
PLM1          41.2500000 W
SFO2          400.1316005 MHz
NUC2          1H
CPDPRG2       waltz16
PCPD2         90.00 usec
PLM2          8.31000042 W
PLW12         0.23083000 W
PLW13         0.11611000 W

F2 - Processing parameters
SI            32768
SF            100.6127557 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
FC            1.40

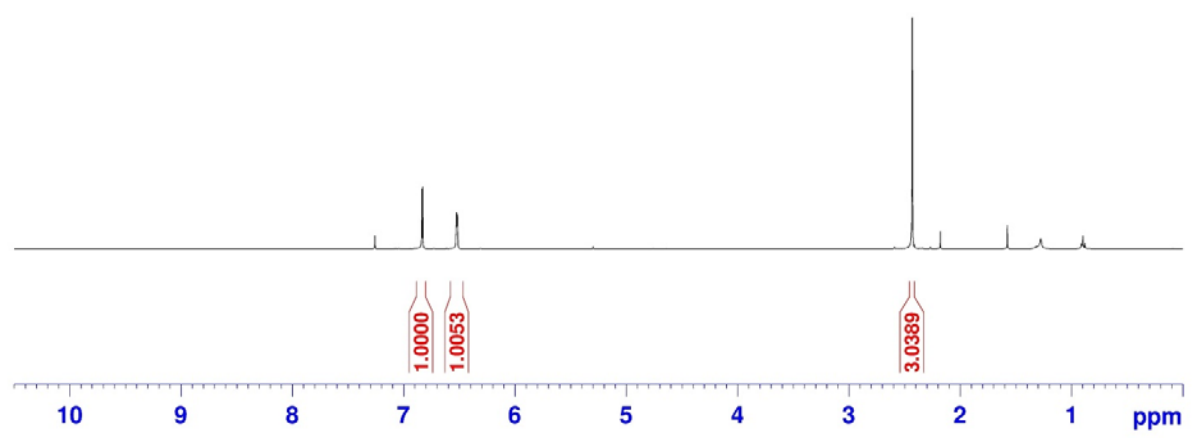
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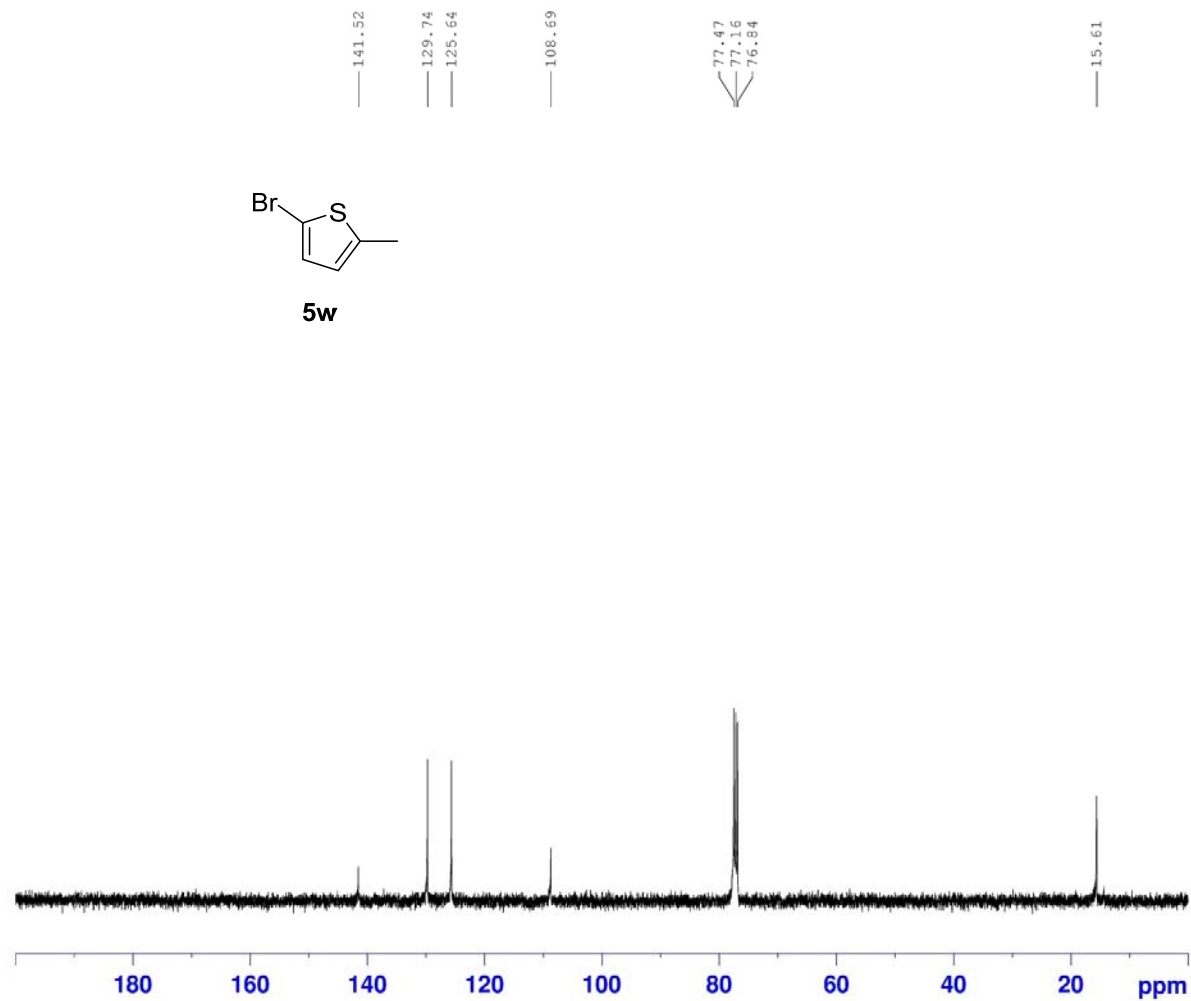


7.2600  
 6.8383  
 6.8292  
 6.8287  
 6.8259  
 6.8228  
 6.8197  
 6.8169

2.4326  
 2.4300

Current Data Parameters  
 NAME SY-15511-H  
 EXPNO 1  
 PROCNO 1  
  
 F2 - Acquisition Parameters  
 Date\_ 20161027  
 Time 10.42 h  
 INSTRUM spect  
 PROBHD Z824601\_0021 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 5  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 101  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.1324708 MHz  
 NUC1 1H  
 P1 15.00 usec  
 PLW1 8.31000042 W  
  
 F2 - Processing parameters  
 SI 65536  
 SF 400.1300098 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





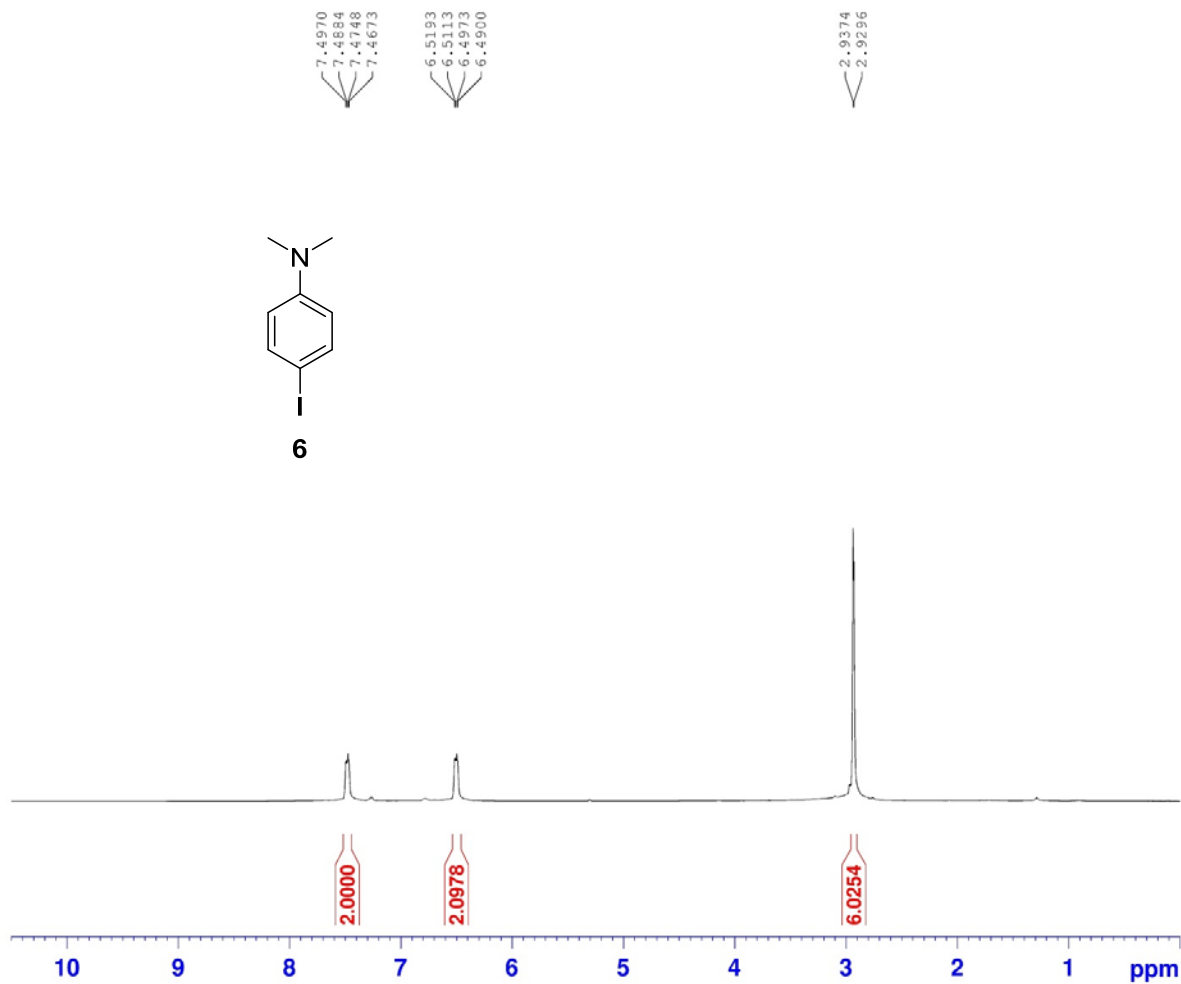
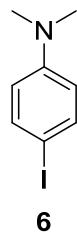
```

Current Data Parameters
NAME      SY-15511-Carbon
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160729
Time     18.01 h
INSTRUM  spect
PROBHD   Z824601_0021 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       228
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       203
DW       20.800 usec
DE       6.50 usec
TE       294.7 K
D1       2.0000000 sec
d11      0.0300000 sec
TD0      1
SFO1     100.6228298 MHz
NUC1     13C
P1       9.50 usec
PLM1     41.2500000 W
SFO2     400.1316005 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLM2     8.31000042 W
PLW12    0.23083000 W
PLW13    0.11611000 W

F2 - Processing parameters
SI       32768
SF       100.6127586 MHz
WDW      EM
SSB      0
LR       1.00 Hz
GB       0
FC       1.40

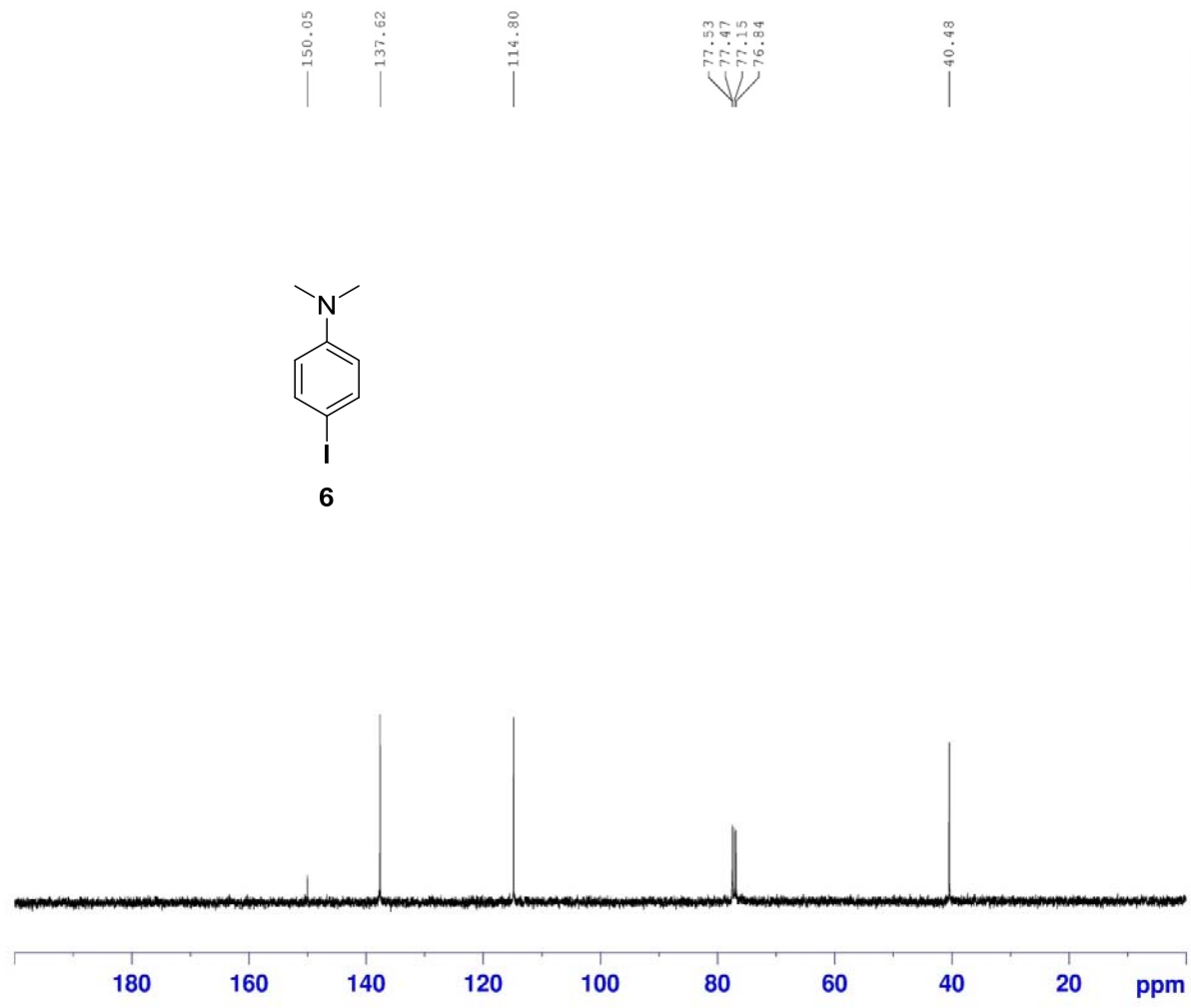
```



Current Data Parameters  
 NAME SY-123-0102pure  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160407  
 Time 11.59 h  
 INSTRUM spect  
 PROBHD Z108618\_0237 (1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 32  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.2 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PLW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300102 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



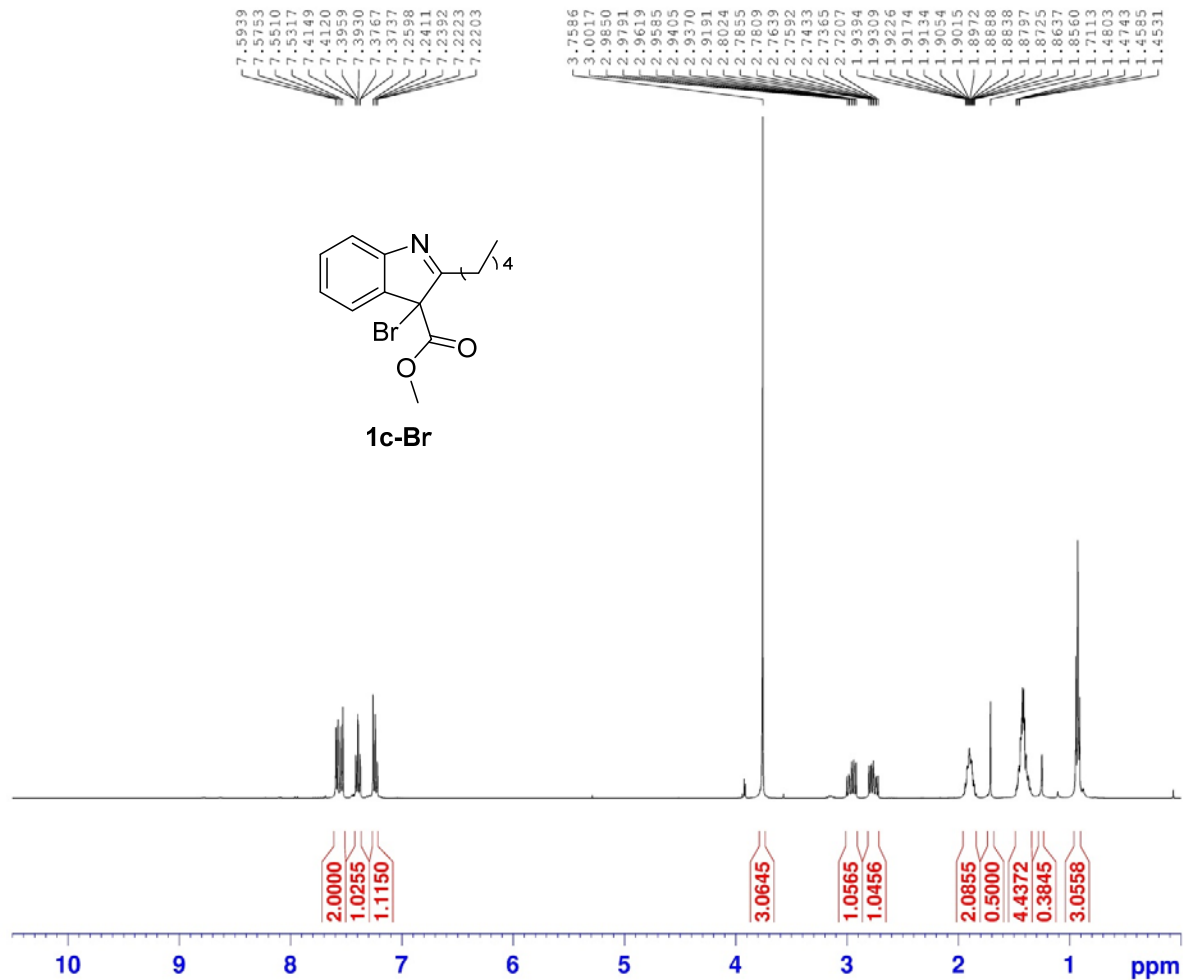
```

Current Data Parameters
NAME      SY-123-0102pure c13
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160407
Time     12.03 h
INSTRUM  spect
PROBHD   Z108618_0257 (
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       500
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       1
DM       20.800 usec
DE       6.50 usec
TE       294.4 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
SFO1     100.6479773 MHz
NUC1     13C
P1       9.50 usec
PLW1     55.3400015 W
SFO2     400.2316009 MHz
NUC2     1H
CPDPRG12 waltz16
PCPD2    90.00 usec
PLW2     13.56000042 W
PLW12    0.27428001 W
PLW13    0.13796000 W

F2 - Processing parameters
SI       32768
SF       100.6379101 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```

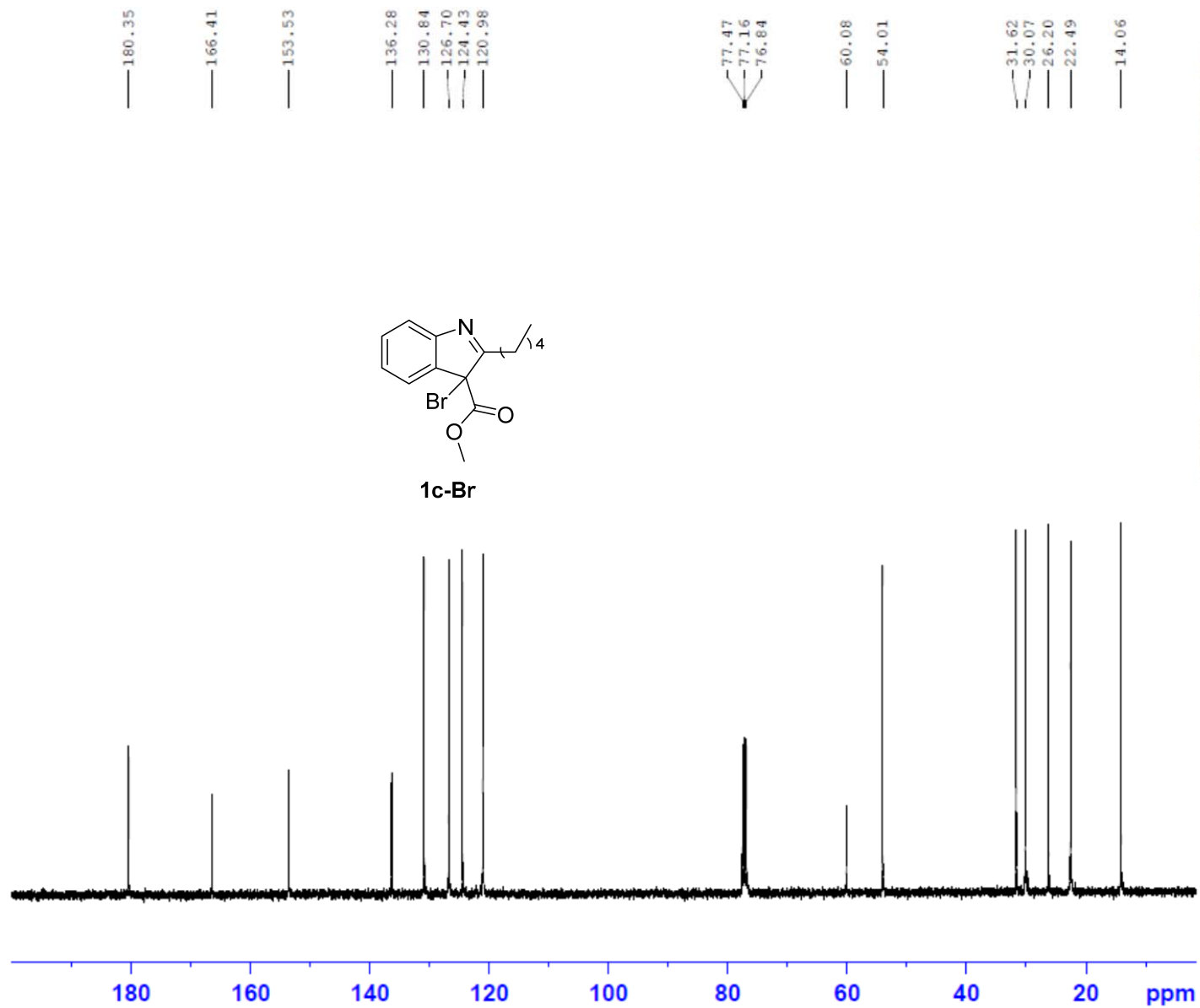


Current Data Parameters  
 NAME SY-C-Br  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160718  
 Time 14.08 h  
 INSTRUM spect  
 PROBHD z108618\_0237 (   
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 60  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RC 64  
 DN 62.400 usec  
 DE 6.50 usec  
 TE 295.9 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.2324714 MHz  
 NUC1 1H  
 P1 12.80 usec  
 PEW1 13.56000042 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300104 MHz  
 WDN EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00





```

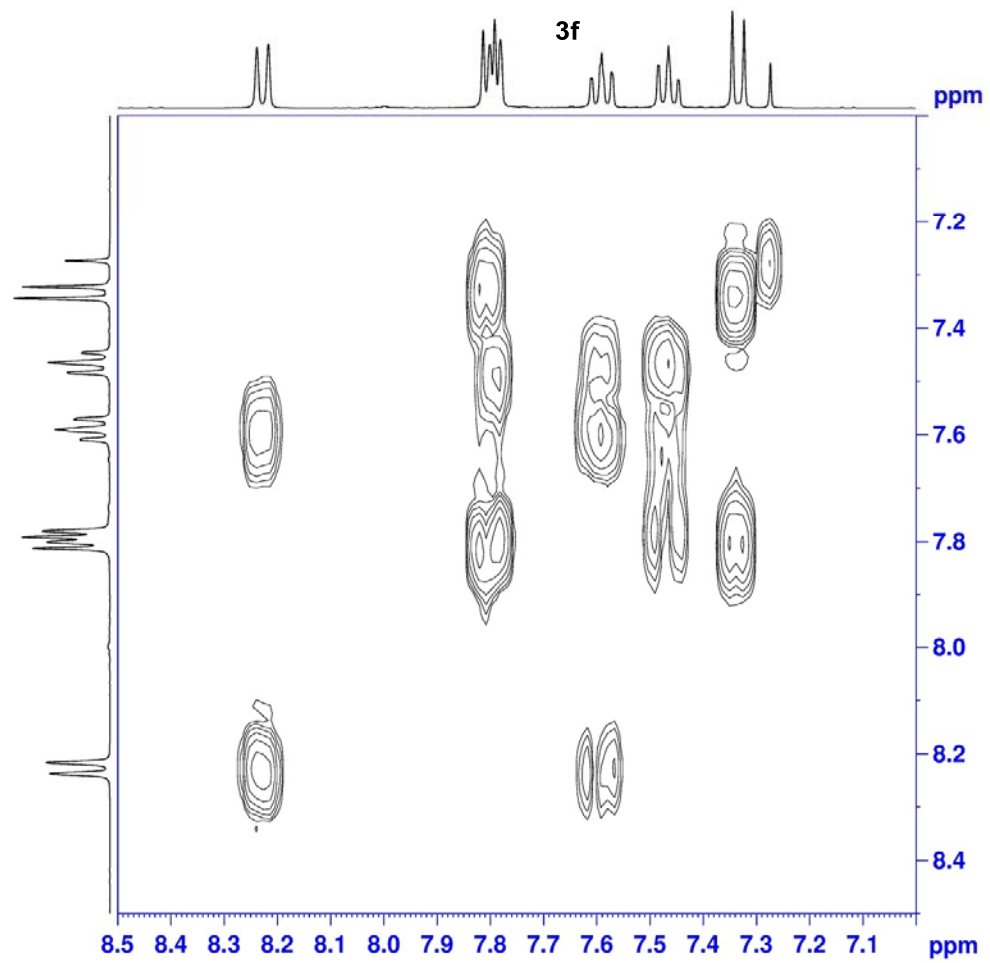
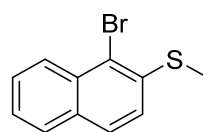
Current Data Parameters
NAME      C2 Cat intermediate carbon
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20170824
Time     19.27 h
INSTRUM  spect
PROBHD   Z108618_0257 |
PULPROG  zgpg30
TD       83536
SOLVENT  CDCl3
NS       101
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       114
DM       20.800 usec
DE       6.50 usec
TE       295.1 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
SFO1     100.6479773 MHz
NUC1     13C
P1       9.50 usec
PLW1     55.34000015 W
SFO2     400.2316009 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLW2     13.56000042 W
PLW12    0.27428001 W
PLW13    0.13798000 W

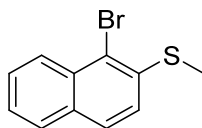
F2 - Processing parameters
SI       32768
SF       100.6379123 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

```

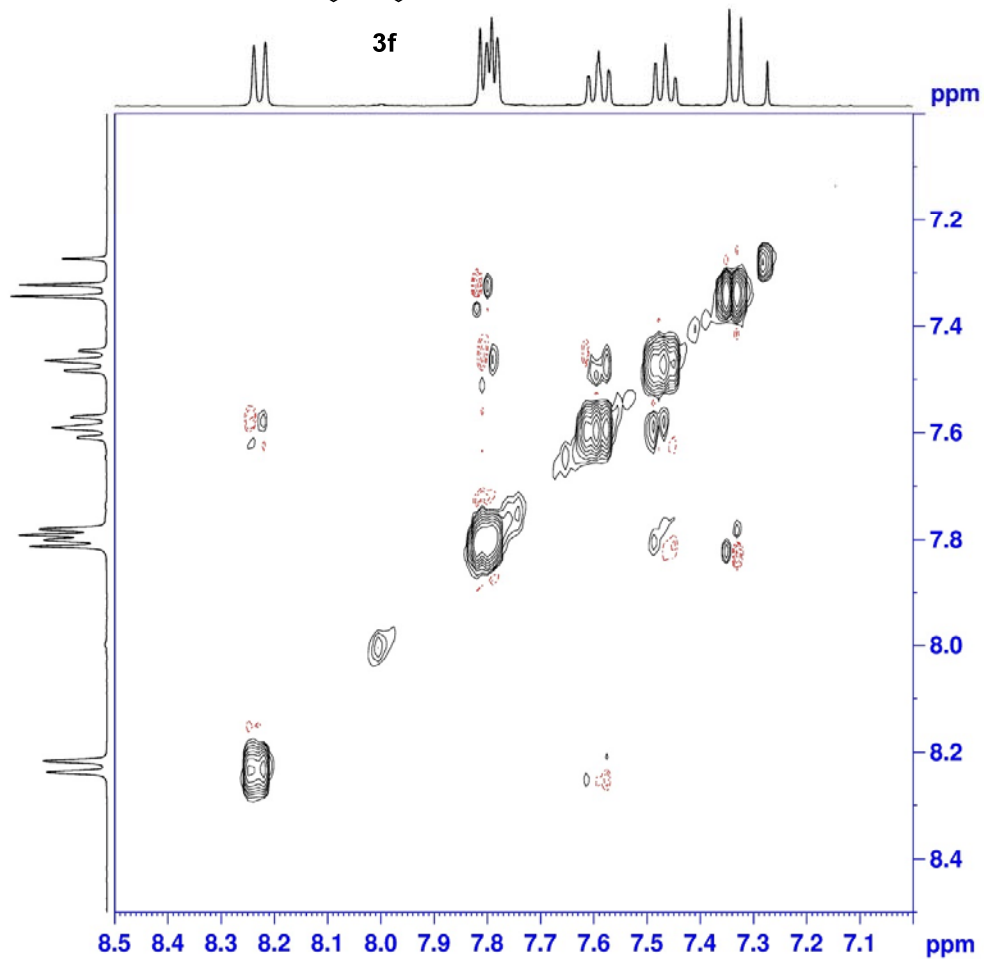
12606 1H NMR cdc13



12606 cdcl3



3f



Current Data Parameters  
NAME kzh-SY-12606-20170118  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20170118  
Time 19.58  
INSTRUM spect  
PROBHD 2824601\_0021 (r  
PULPROG roesyphpp.2  
TD 2048  
SOLVENT CDCl3  
NS 2  
DS 32  
SWH 4000.000 Hz  
FIDRES 1.953125 Hz  
AQ 0.2560000 sec  
RG 203  
DW 125.000 usec  
DE 6.50 usec  
TE 295.0 K  
d0 -0.00001355 sec  
D1 2.0000000 sec  
d11 0.0300000 sec  
d12 0.00002000 sec  
in0 0 sec  
l4 794  
P15 200000.00 usec  
ST1CNT 0  
d0orig -0.00001355 sec  
phlloop 0  
t1loop 0  
SFO1 400.1318806 MHz  
NUC1 1H  
P1 15.00 usec  
P17 2500.00 usec  
P25 126.00 usec  
PLW1 8.31000042 W  
PLW10 2.07750010 W  
PLW27 0.47108999 W

F1 - Acquisition parameters  
ID 256  
SFO1 400.1319 MHz  
FIDRES 15.625000 Hz  
SW 9.997 ppm  
FMODE States-TPPI

F2 - Processing parameters  
SI 1024  
SF 400.1300000 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 States-TPPI  
SF 400.1300000 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0