

## Supporting information

For

**An efficient and green method for regio- and chemo-selective Friedel–Crafts acylations using a deep eutectic solvent ([CholineCl][ZnCl<sub>2</sub>]<sub>3</sub>)**

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## Section 1. Spectral data

### [CholineCl][ZnCl<sub>2</sub>]<sub>3</sub><sup>1</sup>

IR  $\nu_{\max}$  3543, 1619, 1475 cm<sup>-1</sup>.

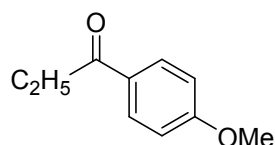
<sup>1</sup>H-NMR (300 MHz, DMSO-*d*6):  $\delta$  5.23 (s, 1H), 3.81-3.78 (m, 2H), 3.34-3.32 (m, 2H), 3.04 (s, 9H).

<sup>13</sup>C-NMR (75 MHz, DMSO-*d*6):  $\delta$  67.8, 55.9, 54.2, 54.1, 54.0.

HRMS (ESI): [Choline + H]<sup>+</sup> 105.0504

[ZnCl<sub>3</sub>]<sup>-</sup> 170.8356, [Zn<sub>2</sub>Cl<sub>5</sub>]<sup>-</sup> 306.6968, [Zn<sub>3</sub>Cl<sub>7</sub>]<sup>-</sup> 444.5604

### 4-Methoxypropiophenone<sup>2</sup>



<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.87 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 3.79 (s, 3H), 2.88 (q, *J* = 7.3 Hz, 2H), 1.14 (t, *J* = 7.3 Hz, 3H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  199.4, 163.3, 130.2, 130.1, 113.7, 55.4, 31.4, 8.4.

GC-MS (EI, 70 eV): *m/z* 164 (M<sup>+</sup>).

### 3-Propionylindole<sup>3</sup>

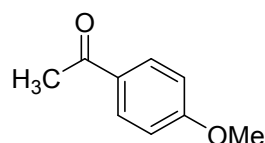


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.70 (br s, 1H), 8.41–8.40 (m, 1H), 7.88 (s, 1H), 7.43–7.41 (m, 1H), 7.30–7.28 (m, 2H), 2.93 (q, *J* = 7.4 Hz, 2H), 1.28 (t, *J* = 7.4 Hz, 3H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  197.1, 136.3, 130.9, 125.6, 123.7, 122.6, 122.5, 117.9, 111.4, 33.1, 9.0.

GC-MS (EI, 70 eV) *m/z* = 173 [M<sup>+</sup>].

### 4-Methoxyacetophenone<sup>4</sup>

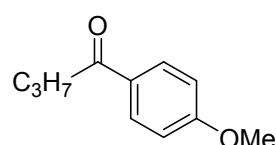


**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>):  $\delta$  7.93 (d,  $J$  = 9.0 Hz, 2H), 6.93 (d,  $J$  = 9.0 Hz, 2H), 3.86 (s, 3H), 2.55 (s, 3H).

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>)  $\delta$  196.7, 163.5, 130.6, 130.3, 113.7, 55.4, 26.3.

**GC-MS** (EI, 70 eV):  $m/z$  150 (M<sup>+</sup>).

#### 4-Methoxybutyrophenone<sup>2</sup>

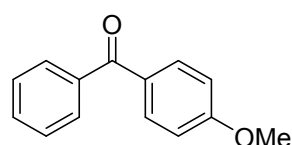


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.92 (d,  $J$  = 8.9 Hz, 2H), 6.91 (d,  $J$  = 8.9 Hz, 2H), 3.84 (s, 3H), 2.87 (t,  $J$  = 7.3 Hz, 2H), 1.74 (dd,  $J$  = 14.7, 7.4 Hz, 2H), 0.98 (t,  $J$  = 7.4 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>)  $\delta$  199.1, 163.3, 131.0, 130.3, 113.7, 55.4, 40.2, 18.0, 13.9.

**GC-MS** (EI, 70 eV):  $m/z$  178 (M<sup>+</sup>).

#### 4-Methoxybenzophenone<sup>5</sup>

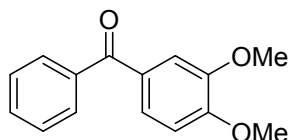


**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>):  $\delta$  7.86-7.81 (m, 2H), 7.75 (dd,  $J$  = 8.3, 1.4 Hz, 2H), 7.55 (d,  $J$  = 7.5 Hz, 1H), 7.49-7.44 (m, 2H), 6.96 (d,  $J$  = 9.0 Hz, 2H), 3.88 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>)  $\delta$  195.6, 163.2, 138.3, 132.6, 131.9, 130.2, 129.8, 128.2, 113.6, 55.5.

**GC-MS** (EI, 70 eV):  $m/z$  212 (M<sup>+</sup>).

#### 3,4-Dimethoxybenzophenone<sup>5</sup>

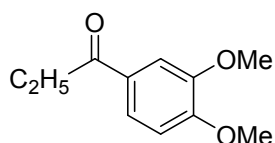


**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>): δ 7.77 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.49 (s, 1H), 7.46-7.36 (m, 3H), 6.90 (m, 2H), 3.96 (s, 3H), 3.95 (s, 3H).

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 195.6, 153.0, 149.0, 138.3, 131.9, 130.2, 129.7, 128.2, 125.5, 112.1, 109.7, 56.1, 56.0.

**GC-MS** (EI, 70 eV): *m/z* 242 (M<sup>+</sup>).

### 3,4-Dimethoxypropiophenone<sup>2</sup>

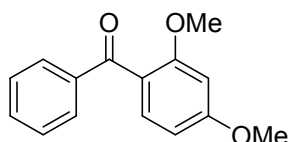


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>): δ 7.58 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.53 (d, *J* = 2.0 Hz, 1H), 6.87 (d, *J* = 8.4 Hz, 1H), 3.93 (s, 3H), 3.92 (s, 3H), 2.95 (q, *J* = 7.3 Hz, 2H), 1.21 (t, *J* = 7.3 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>): δ 199.5, 153.1, 149.0, 130.2, 122.5, 110.2, 110.0, 56.0, 56.0, 31.3, 8.6.

**GC-MS** (EI, 70 eV): *m/z* 194 (M<sup>+</sup>).

### 2,4-Dimethoxybenzophenone<sup>6</sup>

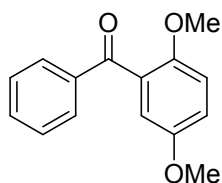


**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>): δ 7.77 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.49 (s, 1H), 7.42 (dt, *J* = 1.8, 0.6 Hz, 1H), 7.39 (s, 2H), 6.53 (dd, *J* = 9.6, 5.3 Hz, 2H), 3.86 (s, 3H), 3.69 (s, 3H).

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 195.6, 163.4, 159.6, 138.8, 132.3, 132.2, 129.7, 128.0, 121.5, 104.6, 98.8, 55.6, 55.5.

**GC-MS** (EI, 70 eV): *m/z* 242 (M<sup>+</sup>).

### 2,5-Dimethoxybenzophenone<sup>6</sup>

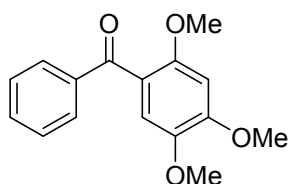


**<sup>1</sup>H NMR** (300 MHz, CDCl<sub>3</sub>): δ 7.84-7.80 (m, 2H), 7.57-7.52 (m, 1H), 7.47-7.38 (m, 2H), 7.01 (dd, *J* = 9.0, 3.0 Hz, 1H), 6.92 (dd, *J* = 6.0, 3.0 Hz, 2H), 3.78 (s, 3H), 3.66 (s, 3H).

**<sup>13</sup>C NMR** (75 MHz, CDCl<sub>3</sub>) δ 196.2, 153.5, 151.5, 137.6, 133.0, 129.8, 128.2, 117.3, 114.4, 113.1, 56.3, 55.8.

**GC-MS** (EI, 70 eV): *m/z* 242 (M<sup>+</sup>).

### 2, 4, 5-Trimethoxybenzophenone<sup>2</sup>

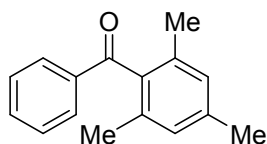


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>): δ 7.76 (d, *J* = 8.2 Hz, 2H), 7.51 (t, *J* = 6.8 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.02 (s, 1H), 6.55 (s, 1H), 3.94 (s, 3H), 3.83 (s, 3H), 3.64 (s, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>): δ 195.5, 153.4, 152.6, 143.3, 139.0, 132.3, 130.1, 129.5, 128.4, 128.0, 120.1, 113.6, 97.8, 56.6, 56.5, 56.2.

**GC-MS** (EI, 70 eV): *m/z* 272 (M<sup>+</sup>).

### 2, 4, 6-Trimethylbenzophenone<sup>6</sup>

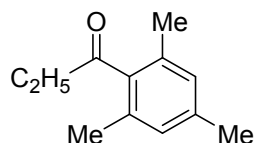


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>): δ 7.80 (d, *J* = 7.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 6.90 (s, 2H), 2.33 (s, 3H), 2.08 (s, 6H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 200.8, 138.5, 137.4, 136.9, 134.2, 133.5, 129.4, 128.8, 128.4, 21.2, 19.4.

**GC-MS** (EI, 70 eV): *m/z* 223 (M+H).

## 2, 4, 6-Trimethylpropiophenone<sup>2</sup>

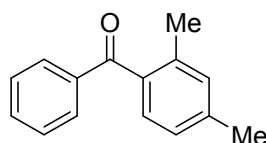


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  6.83 (s, 2H), 2.70 (q,  $J = 7.3$  Hz, 2H), 2.28 (s, 3H), 2.18 (s, 6H), 1.19 (t,  $J = 7.3$  Hz, 3H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  211.4, 139.9, 138.1, 132.4, 128.4, 37.9, 21.0, 19.0, 7.6.

GC-MS (EI, 70 eV):  $m/z$  176 (M<sup>+</sup>).

## 2, 4-Dimethylbenzophenone<sup>7</sup>

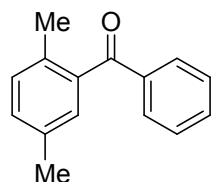


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.77 (dd,  $J = 8.3, 1.2$  Hz, 2H), 7.54 (t,  $J = 7.4$  Hz, 1H), 7.42 (m, 2H), 7.21 (d,  $J = 7.7$  Hz, 1H), 7.09 (s, 1H), 7.02 (d,  $J = 7.7$  Hz, 1H), 2.36 (s, 3H), 2.31 (s, 3H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  198.5, 140.6, 138.3, 137.3, 135.7, 132.8, 131.9, 130.1, 129.2, 128.4, 127.5, 125.8, 21.4, 20.1.

GC-MS (EI, 70 eV):  $m/z$  210 (M<sup>+</sup>).

## 2, 5-Dimethylbenzophenone<sup>7</sup>

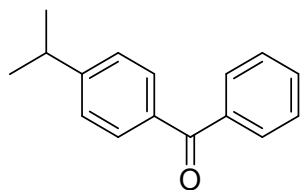


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.82 – 7.80 (m, 2H), 7.80 – 7.56 (m, 1H), 7.47 – 7.44 (m, 2H), 7.21 – 7.17 (m, 2H), 7.13 (s, 1H), 2.34 (s, 3H), 2.28 (s, 3H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  198.9, 138.6, 137.8, 134.8, 133.4, 133.0, 130.9, 130.8, 130.1, 128.9, 128.4, 121.3, 20.8, 19.5.

GC-MS (EI, 70 eV):  $m/z$  210 (M<sup>+</sup>).

#### 4-Isopropylbenzophenone<sup>6</sup>

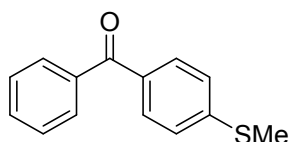


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.85 – 7.78 (m, 2H), 7.76 (d,  $J$  = 8.2 Hz, 2H), 7.58 (t,  $J$  = 7.4 Hz, 1H), 7.48 (t,  $J$  = 7.7 Hz, 2H), 7.34 (d,  $J$  = 8.2 Hz, 2H), 3.00 (s, 1H), 1.30 (t,  $J$  = 6.4 Hz, 6H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  196.2, 154.0, 138.0, 135.3, 132.1, 130.4, 130.0, 128.2, 126.4, 121.7, 34.3, 24.1, 23.7.

GC-MS (EI, 70 eV)  $m/z$ : 224 ([M]<sup>+</sup>).

#### 4-Methylthiobenzophenone<sup>6</sup>

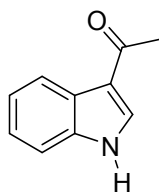


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.75 (m, 4H), 7.57 (t,  $J$  = 7.4 Hz, 1H), 7.47 (t,  $J$  = 7.6 Hz, 2H), 7.31 – 7.27 (m, 2H), 2.53 (s, 3H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  195.8, 145.3, 137.9, 133.7, 132.2, 130.6, 129.8, 128.3, 124.9, 14.9.

GC-MS (EI, 70 eV):  $m/z$  228 (M<sup>+</sup>).

#### 3-Acetylidole<sup>8,9</sup>

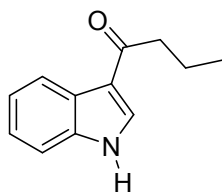


<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.76 (br s, 1H), 8.40–8.39 (m, 1H), 7.87 (s, 1H), 7.43–7.41 (m, 1H), 7.30–7.29 (m, 2H), 2.56 (s, 3H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  193.6, 136.4, 131.4, 125.4, 123.7, 122.7, 122.4, 118.7, 111.3, 27.6.

**GC-MS** (EI, 70 eV):  $m/z$  (%) = 159 (50, [M<sup>+</sup>]).

### 3-Butyrylindole<sup>9-11</sup>

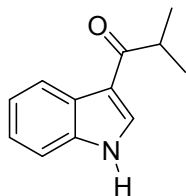


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>):  $\delta$  8.85 (br s, 1H), 8.43–8.41 (m, 1H), 7.88 (d,  $J$  = 2.6 Hz, 1H), 7.43–7.41 (m, 1H), 7.30–7.28 (m, 2H), 2.86 (t,  $J$  = 7.4, 2H), 1.83 (hept,  $J$  = 7.4 Hz, 2H), 1.03 (t,  $J$  = 7.4 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>):  $\delta$  196.7, 136.4, 131.1, 125.5, 123.7, 122.6, 122.5, 118.3, 111.4, 41.9, 18.6, 14.1.

**GC-MS** (EI, 70 eV)  $m/z$  = 187 [M<sup>+</sup>].

### 3-Isobutyrylindole<sup>8,9</sup>

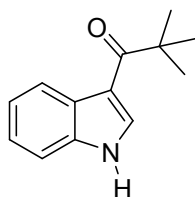


**<sup>1</sup>H NMR** (300 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  11.90 (br s, 1H), 8.34 (s, 1H), 8.24–8.19 (m, 1H), 7.48–7.45 (m, 1H), 7.23–7.14 (m, 2H), 3.45 (hept,  $J$  = 6.8 Hz, 1H), 1.12 (d,  $J$  = 6.8 Hz, 6H).

**<sup>13</sup>C NMR** (75 MHz, DMSO-*d*<sub>6</sub>):  $\delta$  199.4, 136.7, 133.4, 125.7, 122.7, 121.6, 121.5, 114.9, 112.0, 35.8, 19.8.

**GC-MS** (EI, 70 eV)  $m/z$  = 187 [M<sup>+</sup>].

### 3-Pivaloylindole<sup>8,9,11</sup>



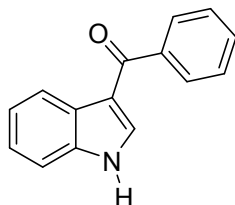


**<sup>1</sup>H NMR** (300 MHz, DMSO-*d*<sub>6</sub>): δ 11.84 (br s, 1H), 8.34 (s, 1H), 8.29–8.26 (m, 1H), 7.46–7.43 (m, 1H), 7.21–7.11 (m, 2H), 1.34 (s, 9H).

**<sup>13</sup>C NMR** (75 MHz, DMSO-*d*<sub>6</sub>): δ 201.1, 135.6, 132.4, 127.2, 122.5, 122.0, 121.4, 112.2, 111.7, 43.4, 28.6.

**GC-MS** (EI, 70 eV) *m/z* = 201 [M<sup>+</sup>].

### 3-Benzoylindole<sup>8,11</sup>

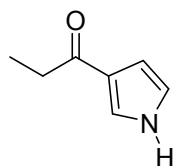


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 8.65 (br s, 1H), 8.43 (dd, *J* = 6.2, 2.9 Hz, 1H), 7.84 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.69 (d, *J* = 2.7 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.50–7.44 (m, 3H), 7.35–7.33 (m, 2H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 207.8, 140.7, 136.3, 133.5, 131.3, 128.8, 128.3, 126.40, 124.0, 122.8, 122.6, 111.3.

**GC-MS** (EI, 70 eV) *m/z* = 221 [M<sup>+</sup>].

### 3-Propionylpyrrole<sup>12</sup>

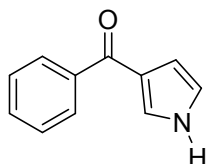


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 9.62 (s, 1H), 7.04 – 7.02 (m, 1H), 6.93 – 6.91 (m, 1H), 6.29 – 6.26 (m, 1H), 2.84 – 2.79 (q, 2H), 1.24 – 1.20 (t, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 191.6, 131.7, 124.3, 115.8, 110.5, 31.1, 9.0.

**GC-MS** (EI, 70 eV) *m/z* = 123 [M<sup>+</sup>].

### 3-Benzoylpyrrole<sup>13</sup>

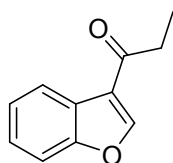


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 9.58 (s, 1H), 7.85 – 7.83 (m, 2H), 7.52 – 7.49 (m, 1H), 7.44 – 7.41 (m, 2H), 7.09 – 7.08 (m, 1H), 6.84 – 6.83 (m, 1H), 6.30 – 6.28 (m, 1H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 184.7, 138.3, 131.8, 128.9, 128.3, 125.0, 119.3, 117.4, 111.0.

**GC-MS** (EI, 70 eV) *m/z* = 171 [M<sup>+</sup>].

### 3-Propionylbenzofurane<sup>14</sup>

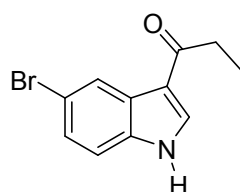


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 8.25 (s, 2H), 7.54 – 7.51 (m, 1H), 7.38 – 7.36 (m, 2H), 2.94 – 2.88 (q, 2H), 1.28 – 1.25 (t, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 196.36, 155.63, 150.53, 125.55, 124.49, 124.36, 122.90, 121.99, 111.46, 33.71, 8.23.

**GC-MS** (EI, 70 eV) *m/z* = 174 [M<sup>+</sup>].

### 3-Propionyl-5-bromoindole<sup>15</sup>

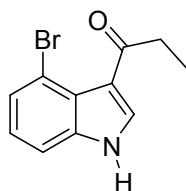


**<sup>1</sup>H NMR** (300 MHz, DMSO-*d*<sub>6</sub>): δ 12.06 (br s, 1H), 8.35 (s, 1H), 8.31 (d, *J* = 2.0 Hz, 1H), 7.42 (d, *J* = 8.6 Hz, 1H), 7.31 (dd, *J* = 8.6, 2.0 Hz, 1H), 2.85 (q, *J* = 7.4 Hz, 2H), 1.09 (t, *J* = 7.4 Hz, 3H).

**<sup>13</sup>C NMR** (75 MHz, DMSO-*d*<sub>6</sub>): δ 196.4, 135.8, 135.2, 127.6, 125.7, 123.9, 115.9, 114.8, 114.6, 32.3, 9.4.

**GC-MS** (EI, 70 eV) *m/z* = 253 [M<sup>+</sup>].

### 3-Propionyl-4-bromoindole



Reddish brown solid, mp. 112–113 °C.

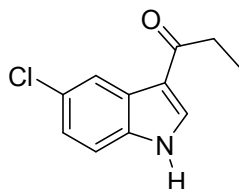
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 9.59 (br s, 1H), 7.40 (dt, *J* = 8.3, 0.8 Hz, 1H), 7.33 (dd, *J* = 7.5, 0.7 Hz, 1H), 7.24 (dd, *J* = 2.3, 0.9 Hz, 1H), 7.19 (dd, *J* = 8.2, 7.6 Hz, 1H), 3.04 (q, *J* = 7.4 Hz, 2H), 1.30 (t, *J* = 7.4 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 194.1, 137.4, 135.0, 128.5, 126.8, 123.8, 116.8, 111.5, 108.9, 31.6, 8.6.

**GC-MS** (EI, 70 eV) *m/z* = 251 [M<sup>+</sup>].

**HR-ESI-MS**: *m/z* calcd for ([M+Na]<sup>+</sup>) 273.9838, found 273.9814..

### 3-Propionyl-5-chloroindole<sup>16</sup>

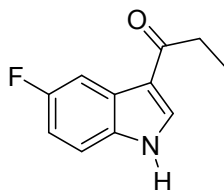


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 8.57 (br s, 1H), 8.41 (d, *J* = 1.9 Hz, 1H), 7.88 (d, *J* = 2.4 Hz, 1H), 7.33 (d, *J* = 8.6 Hz, 1H), 7.24 (dd, *J* = 8.7, 2.4 Hz, 1H), 2.90 (q, *J* = 7.4 Hz, 2H), 1.26 (t, *J* = 7.4 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 196.5, 138.7, 137.3, 134.6, 131.3, 124.1, 122.2, 117.7, 112.2, 33.0, 29.7, 8.8.

**GC-MS** (EI, 70 eV) *m/z* = 207 [M<sup>+</sup>].

### 3-Propionyl-5-fluoroindole<sup>17</sup>

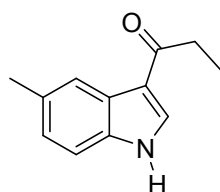


**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 8.64 (s, 1H), 8.08 (dd, *J* = 9.7, 2.5 Hz, 1H), 7.90 (d, *J* = 2.5 Hz, 1H), 7.33 (dd, *J* = 8.8, 4.3 Hz, 1H), 7.03 (td, *J* = 8.9, 2.5 Hz, 1H), 2.90 (q, *J* = 7.4 Hz, 2H), 1.26 (t, *J* = 7.4 Hz, 3H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>-*d*<sub>1</sub>): δ 196.6, 159.6 (d, *J* = 239.4 Hz), 132.3 (d, *J* = 20.8), 126.3 (d, *J* = 11.1 Hz), 118.1, 112.2 (d, *J* = 25.0 Hz), 107.9 (d, *J* = 25.0 Hz), 32.9, 8.8.

**GC-MS** (EI, 70 eV) *m/z* = 191 [M<sup>+</sup>].

### 3-Propionyl-5-methylindole



Pale yellow solid, mp. 208–209 °C

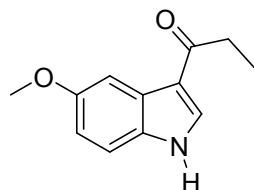
**<sup>1</sup>H NMR** (300 MHz, DMSO-*d*<sub>6</sub>): δ 11.75 (br s, 1H), 8.23 (s, 1H), 8.04–7.93 (m, 1H), 7.33 (d, *J* = 8.3 Hz, 1H), 7.02 (dd, *J* = 8.3, 1.5 Hz, 1H), 2.84 (q, *J* = 7.4 Hz, 2H), 2.39 (s, 3H), 1.10 (t, *J* = 7.4 Hz, 3H).

**<sup>13</sup>C NMR** (75 MHz, DMSO-*d*<sub>6</sub>): δ 195.7, 134.9, 133.4, 130.3, 125.7, 124.1, 121.0, 115.6, 111.6, 31.8, 21.3, 9.2.

**GC-MS** (EI, 70 eV) *m/z*: 187 [M<sup>+</sup>].

**HR-ESI-MS**: *m/z* calcd for ([M+Na]<sup>+</sup>) 210.0889, found 210.0917.

### 3-Propionyl-5-methoxyindole



White solid, mp. 182–183 °C

**<sup>1</sup>H NMR** (300 MHz, DMSO-*d*<sub>6</sub>): δ 11.74 (br s, 1H), 8.21 (s, 1H), 7.69 (d, *J* = 2.5 Hz, 1H), 7.33 (d, *J* = 8.8 Hz, 1H), 6.81 (dd, *J* = 8.8, 2.6 Hz, 1H), 3.75 (s, 3H), 2.82 (q, *J* = 7.4 Hz, 2H), 1.09 (t, *J* = 7.4 Hz, 3H).

<sup>13</sup>C NMR (75 MHz, DMSO-*d*<sub>6</sub>): δ 195.7, 155.3, 133.6, 131.4, 126.1, 115.8, 112.7, 112.103.0, 55.2, 31.7, 9.1.

GC-MS (EI, 70 eV) *m/z*: 203 [M<sup>+</sup>].

HR-ESI-MS *m/z* calcd for ([M+Na]<sup>+</sup>) 226.0839, found 226.0856.

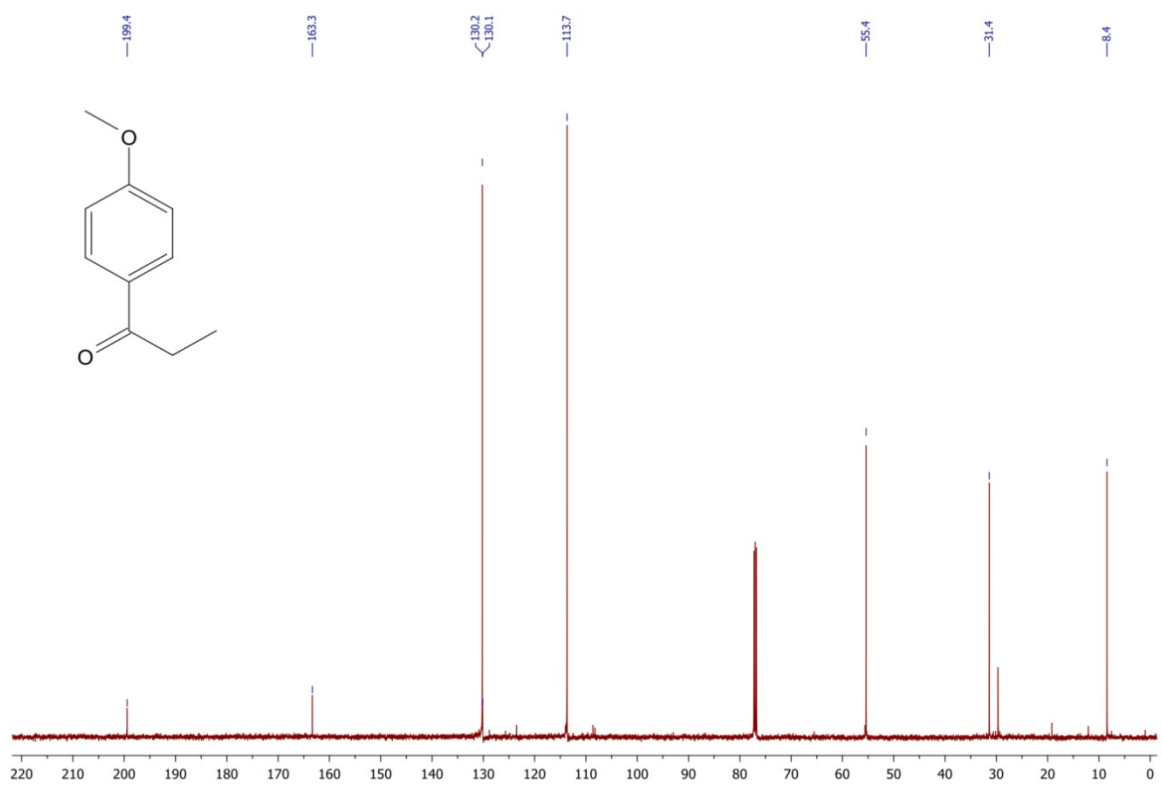
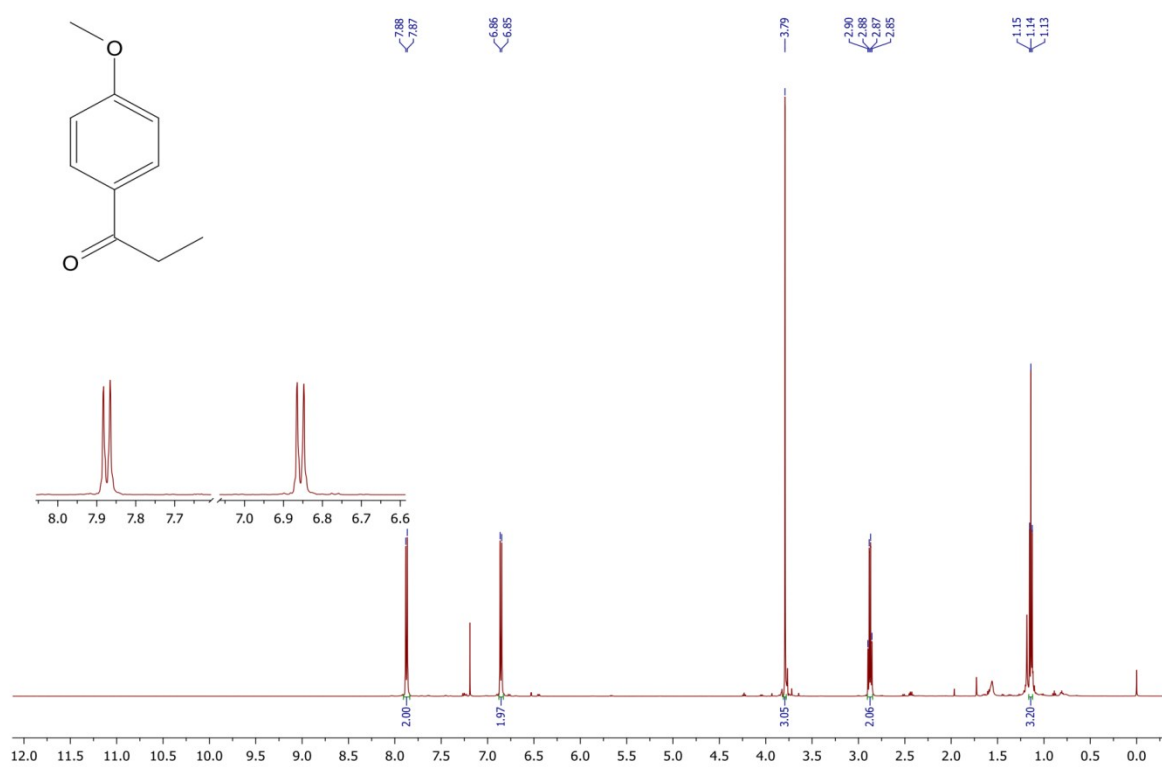
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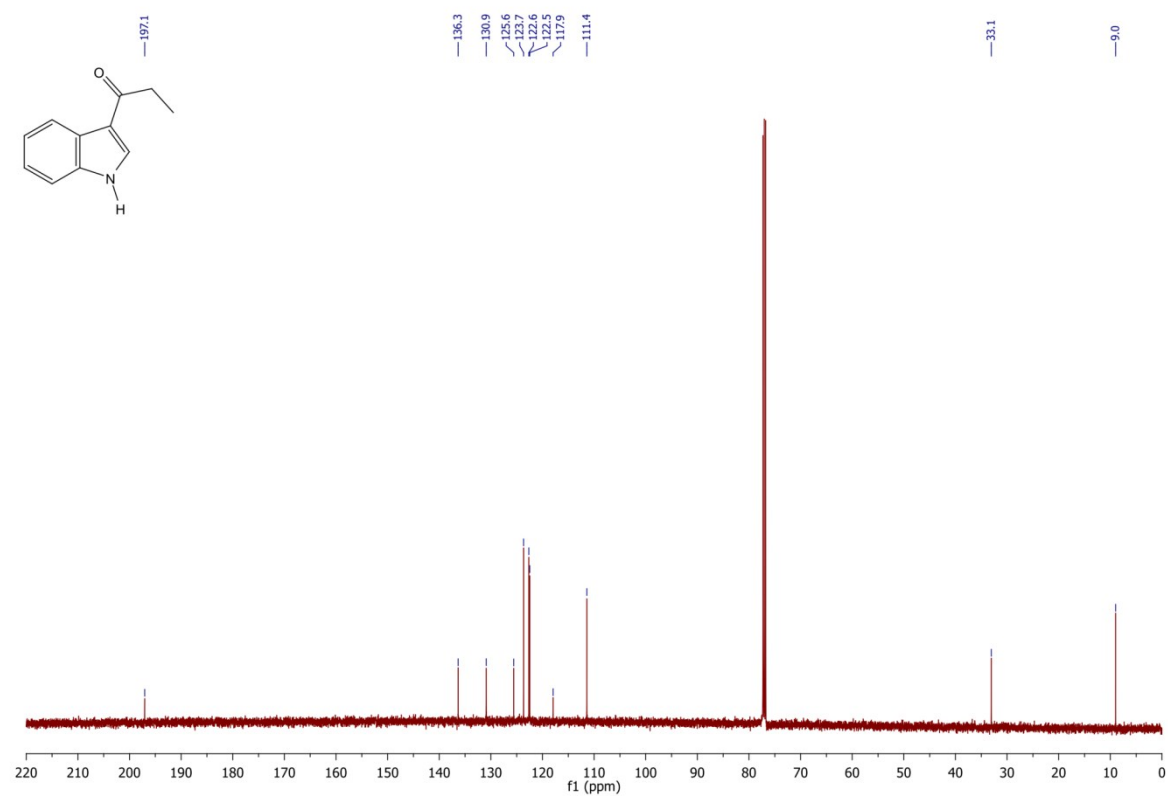
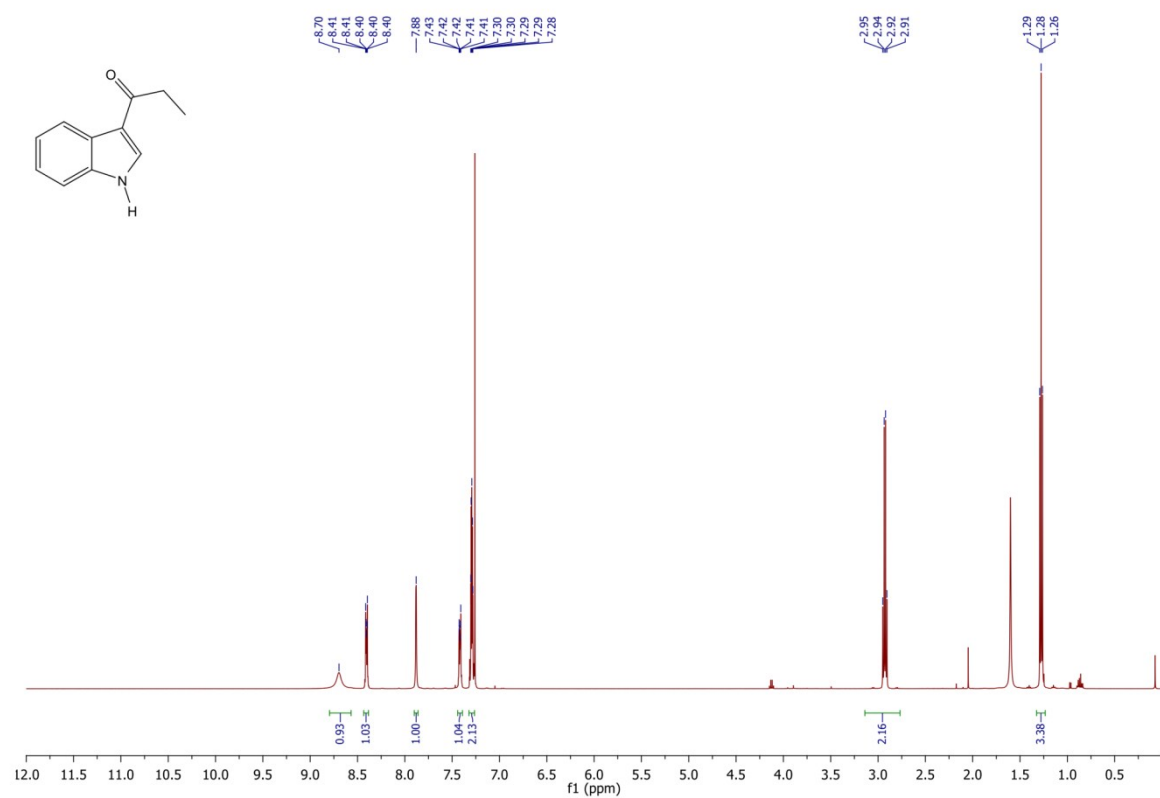
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## Section 6. NMR spectra

### $^1\text{H}$ and $^{13}\text{C}$ NMR of 4-methoxypropiophenone



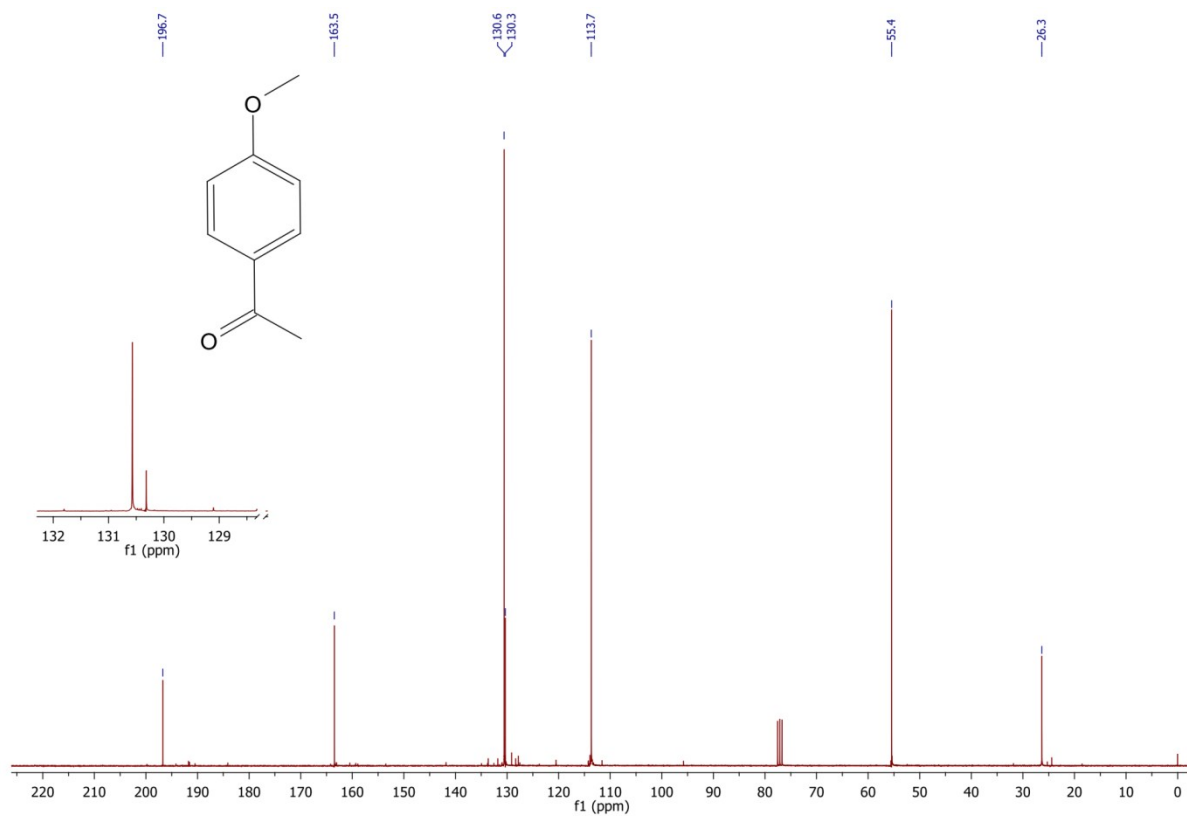
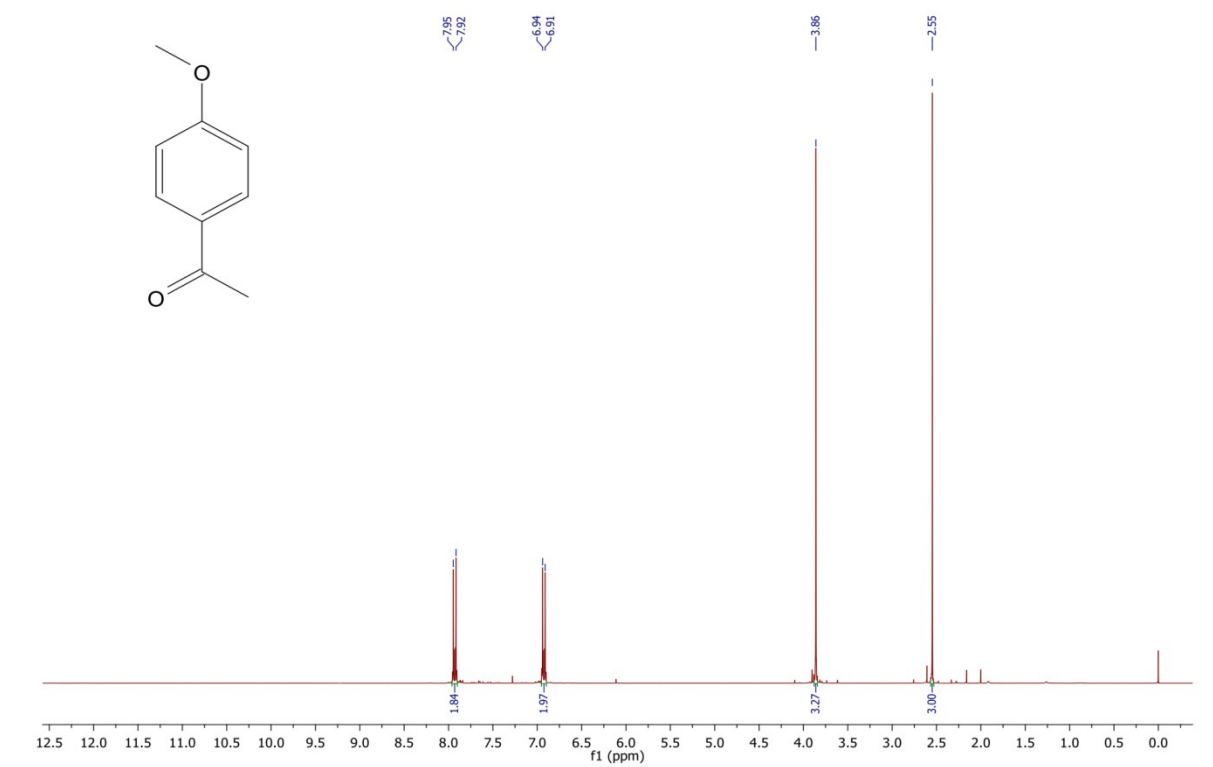
# $^1\text{H}$ and $^{13}\text{C}$ NMR of propionylindole



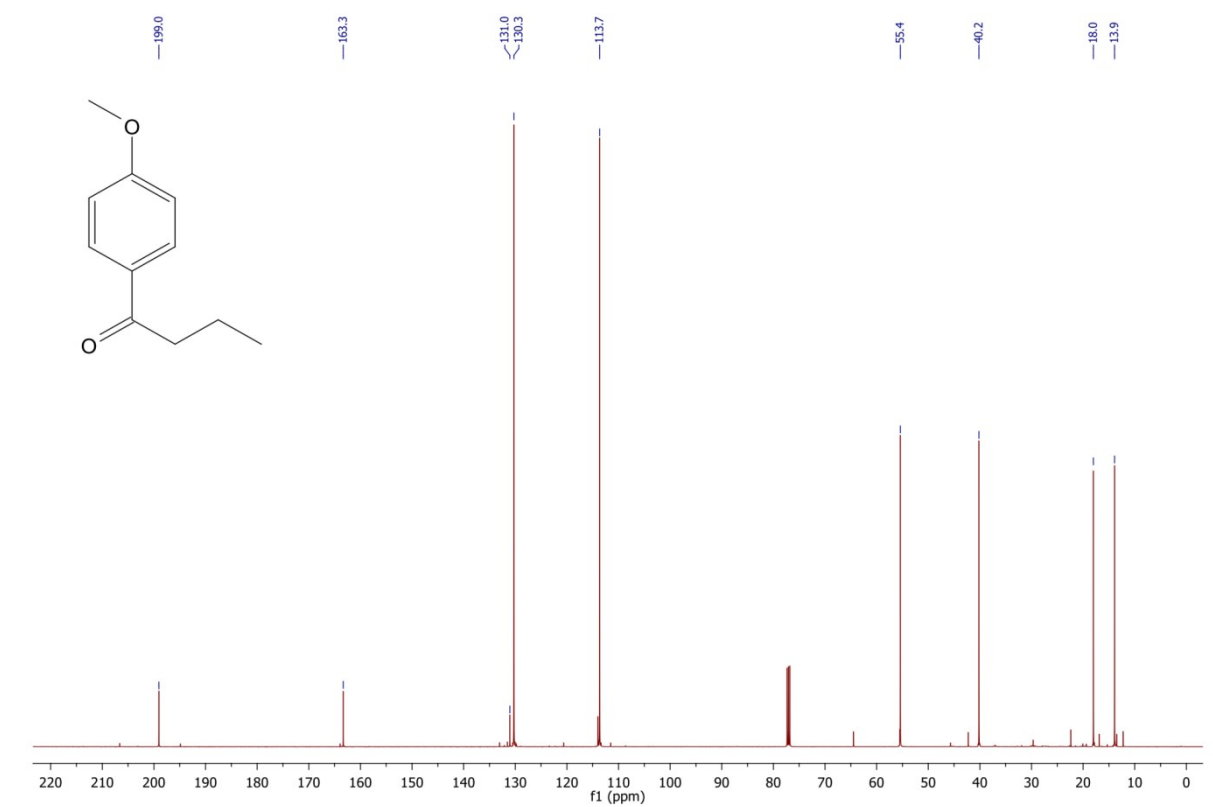
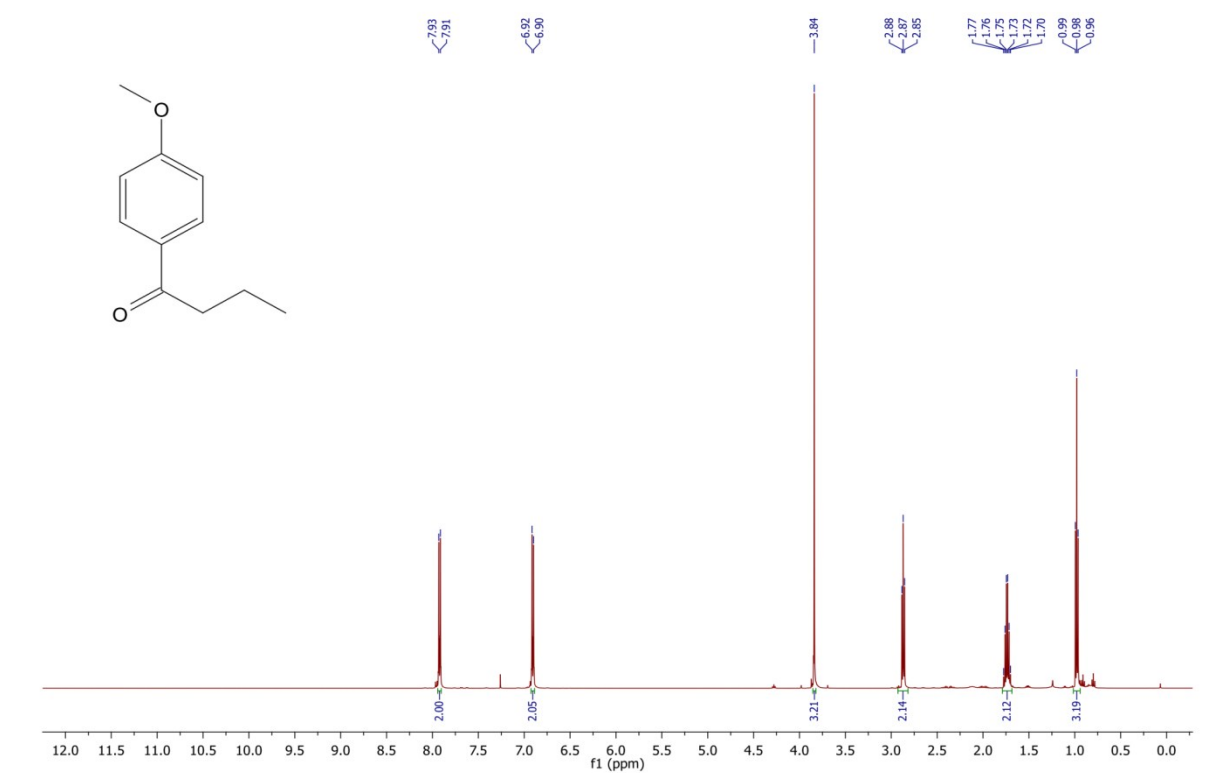




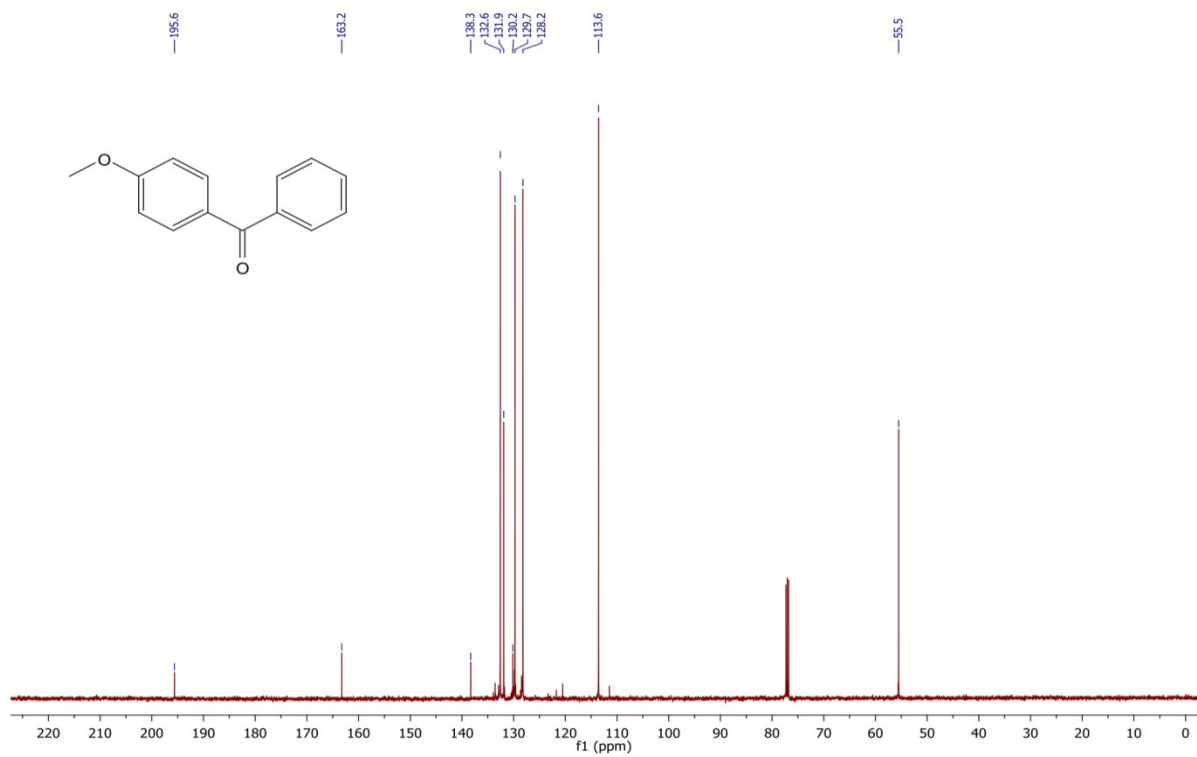
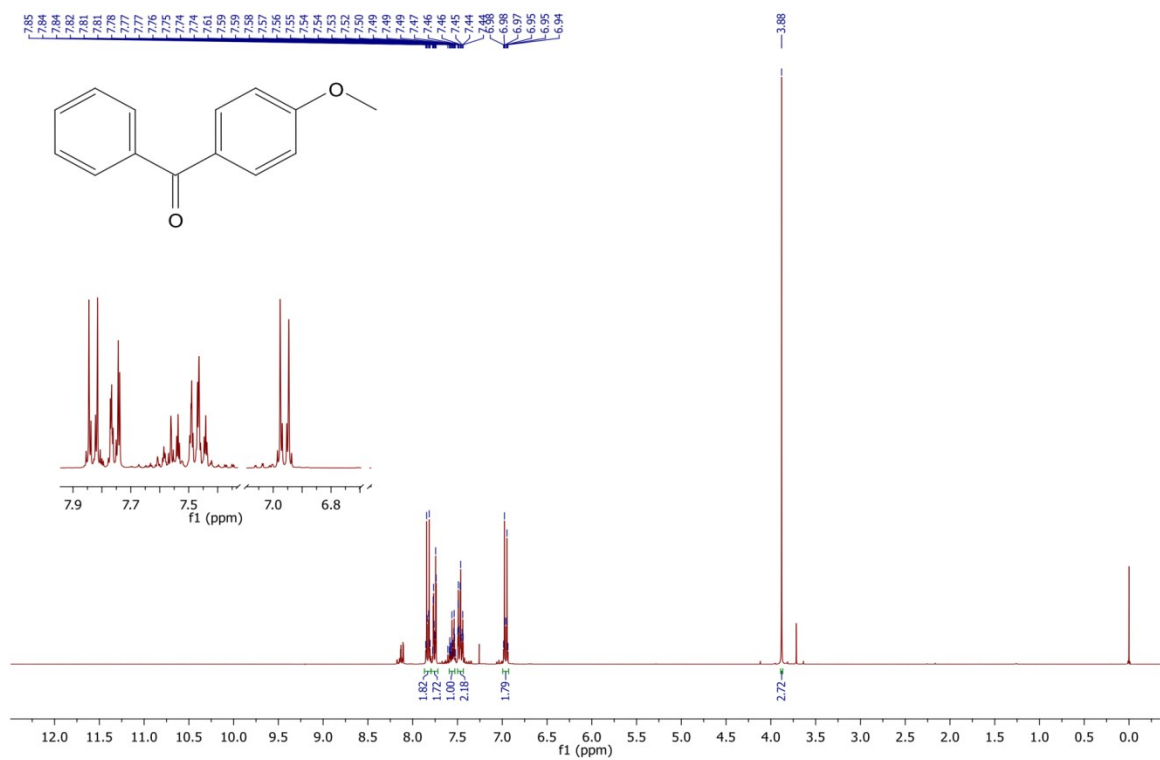
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 4-methoxyacetophenone



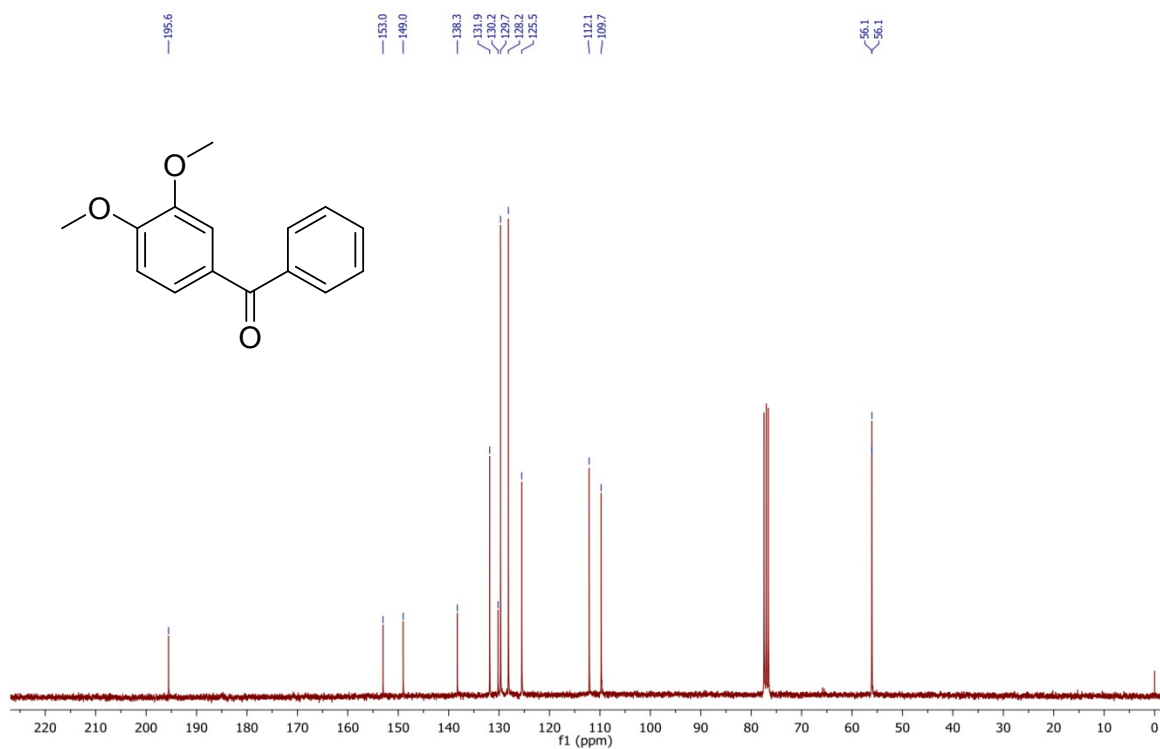
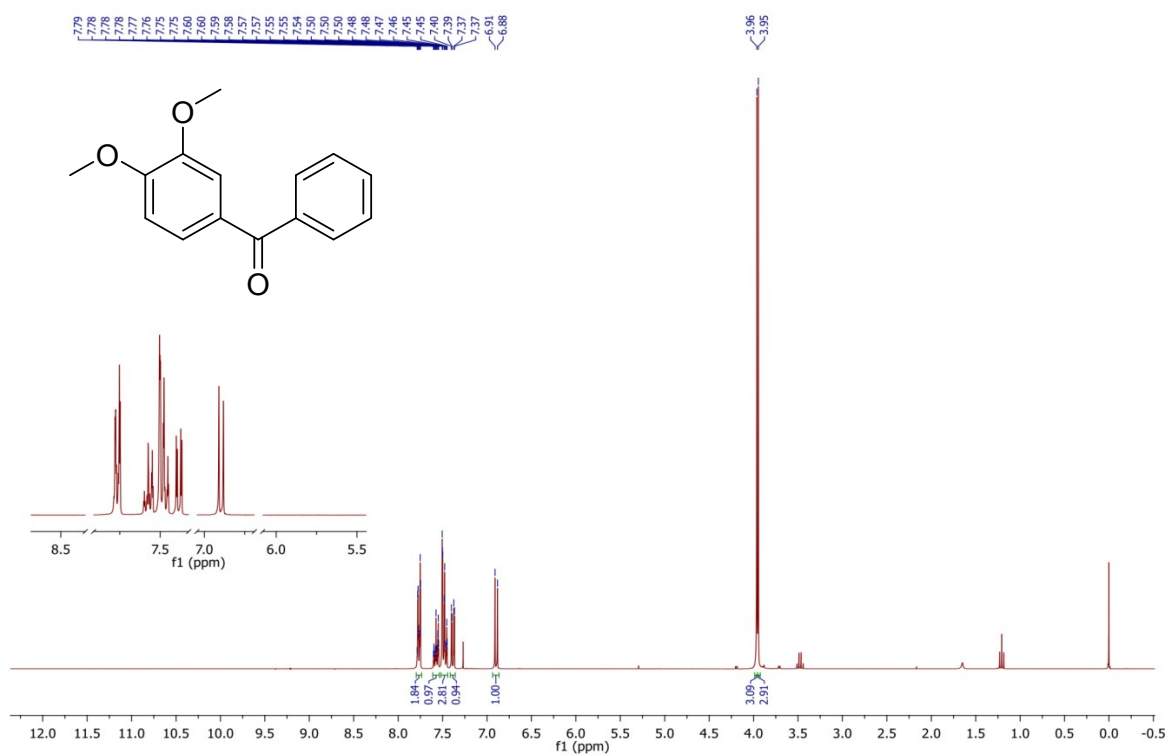
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 4-methoxybutyrophenone



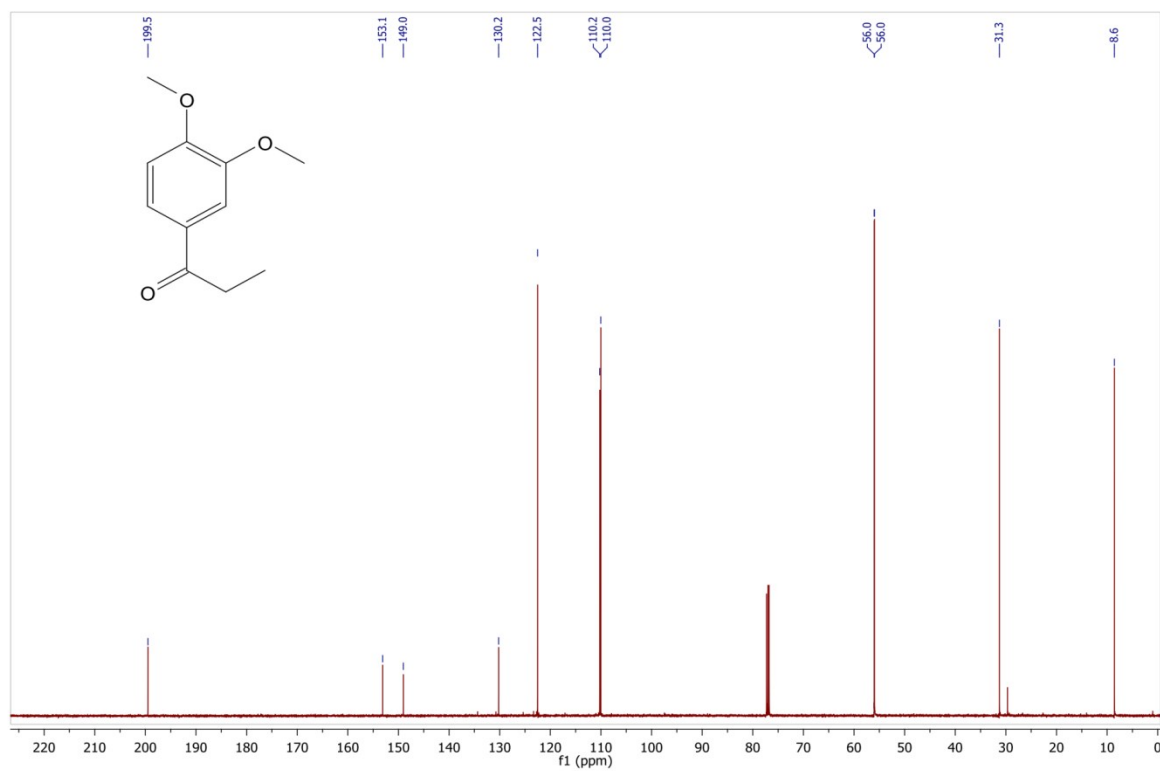
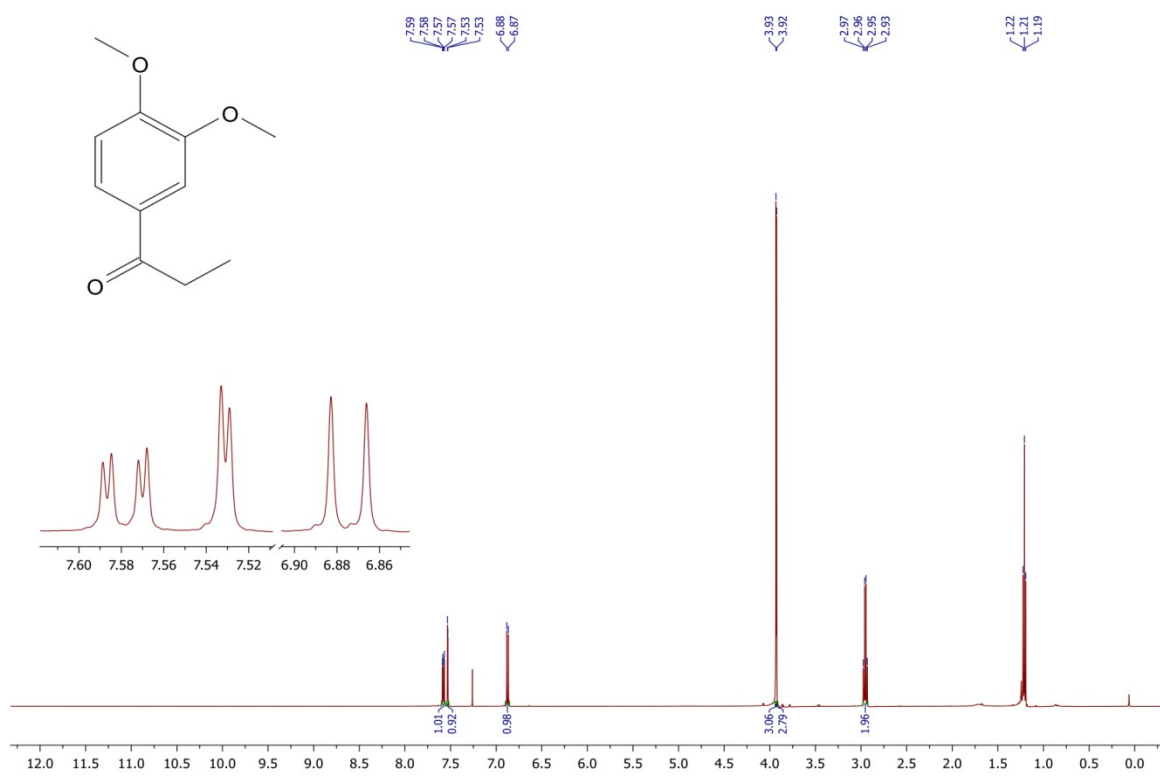
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 4-methoxybenzophenone



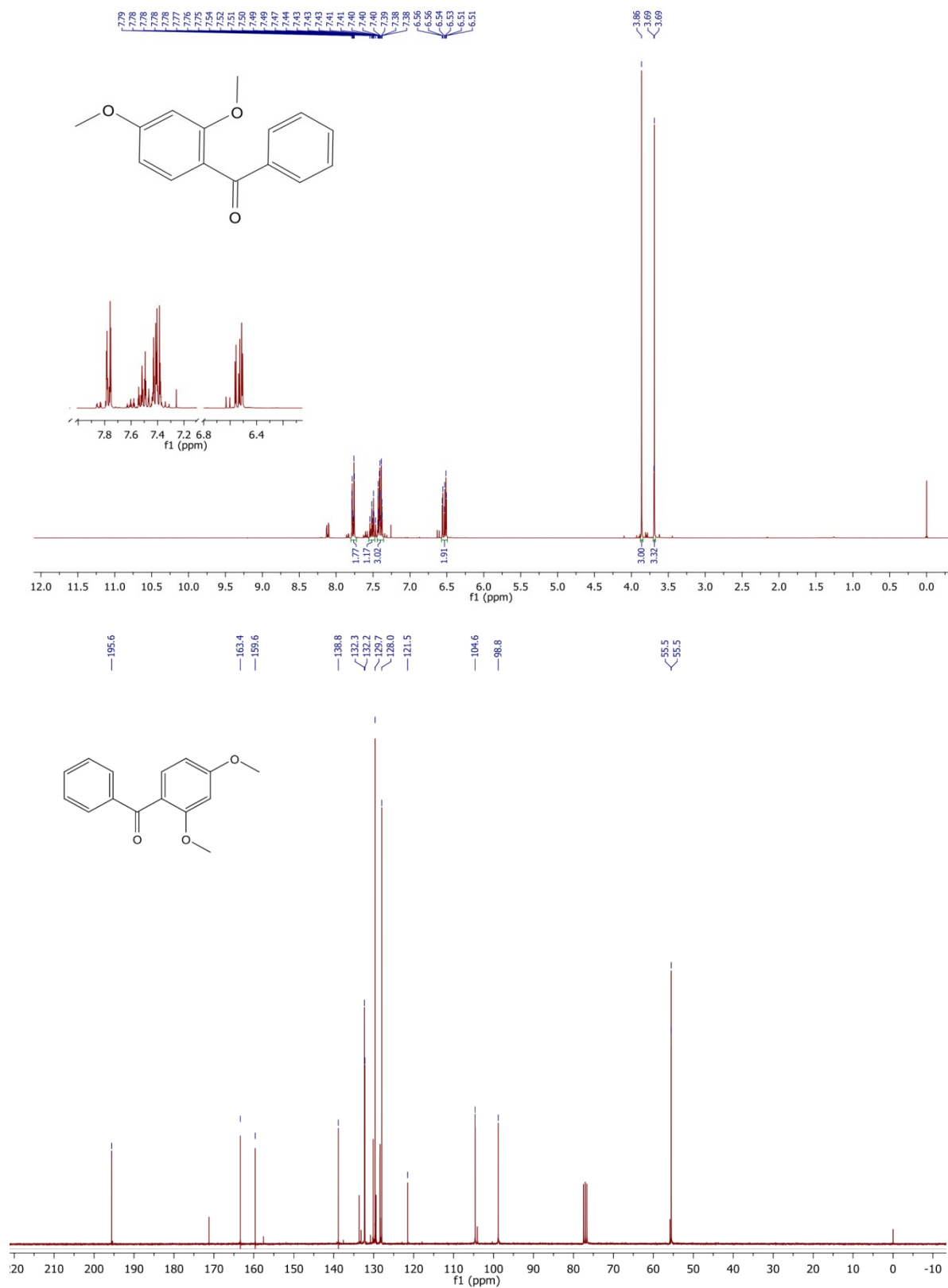
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3,4-dimethoxybenzophenone



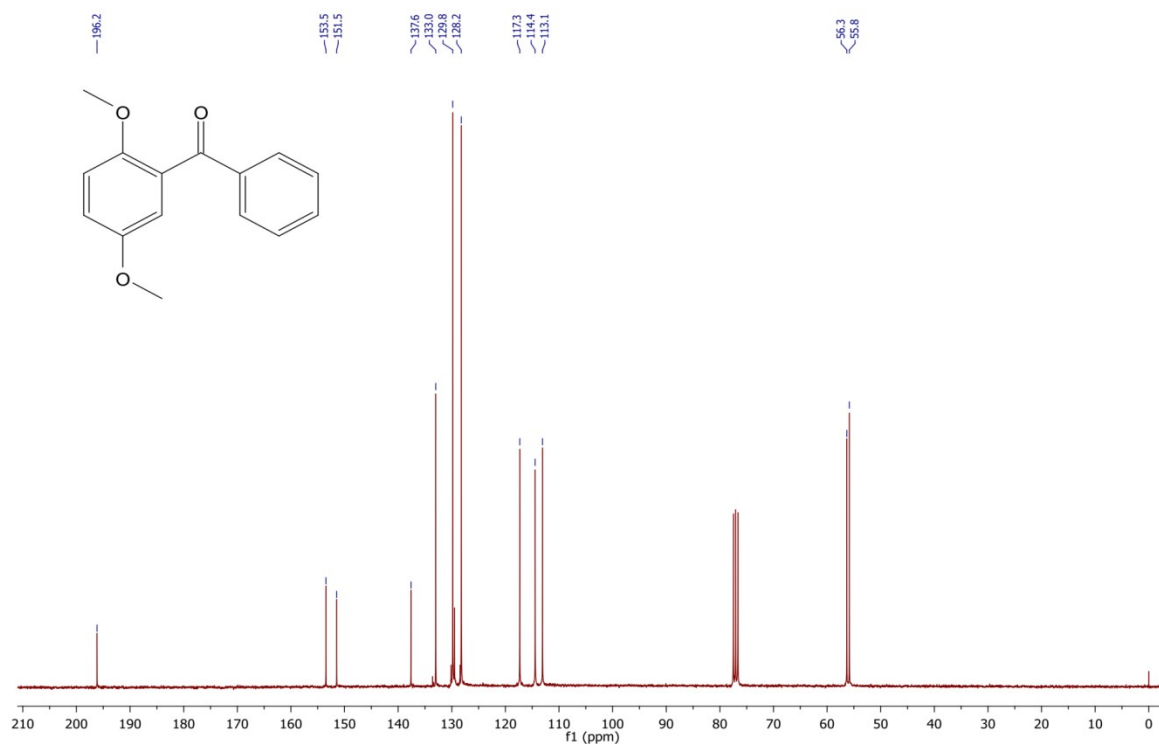
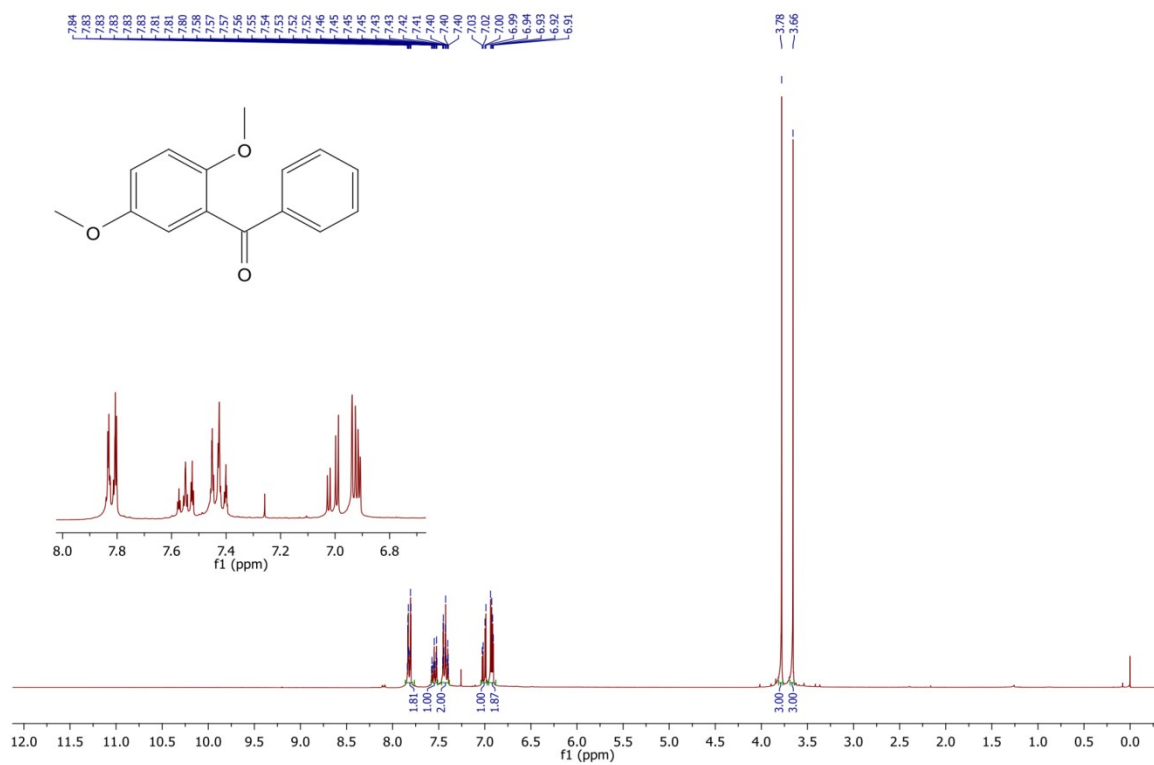
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3,4-dimethoxypropiophenone



# $^1\text{H}$ and $^{13}\text{C}$ NMR of 2,4-dimethoxybenzophenone

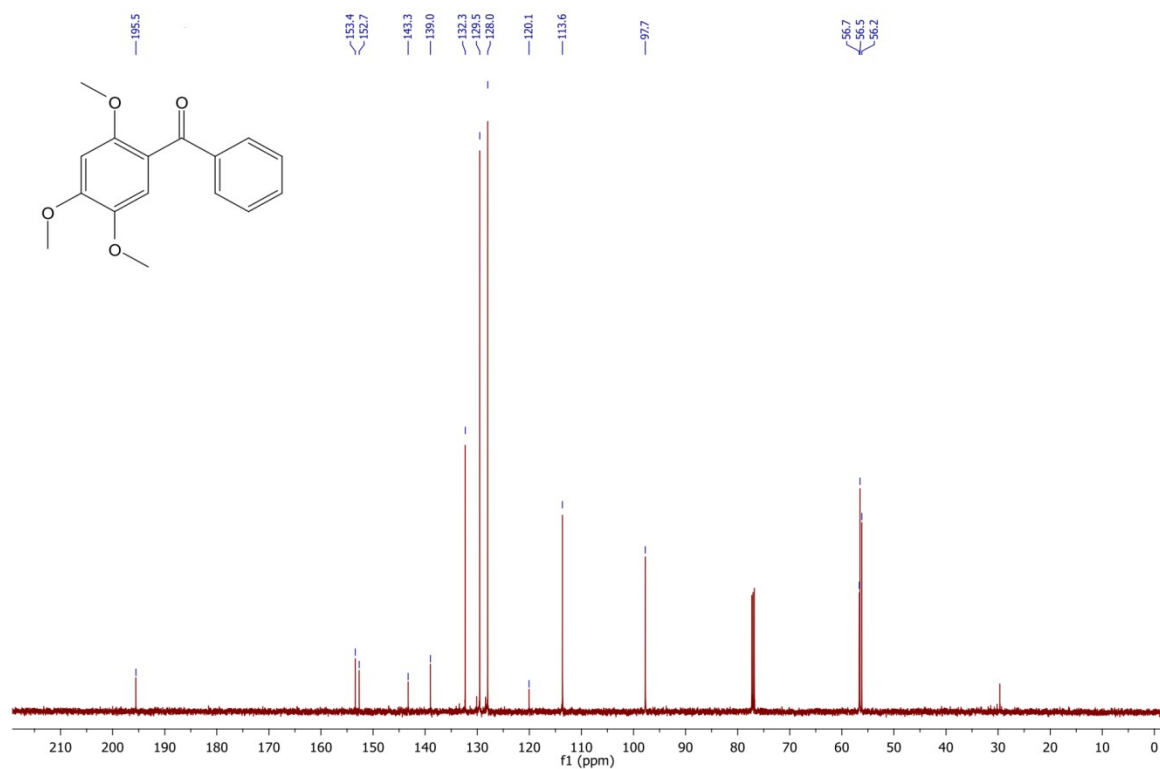
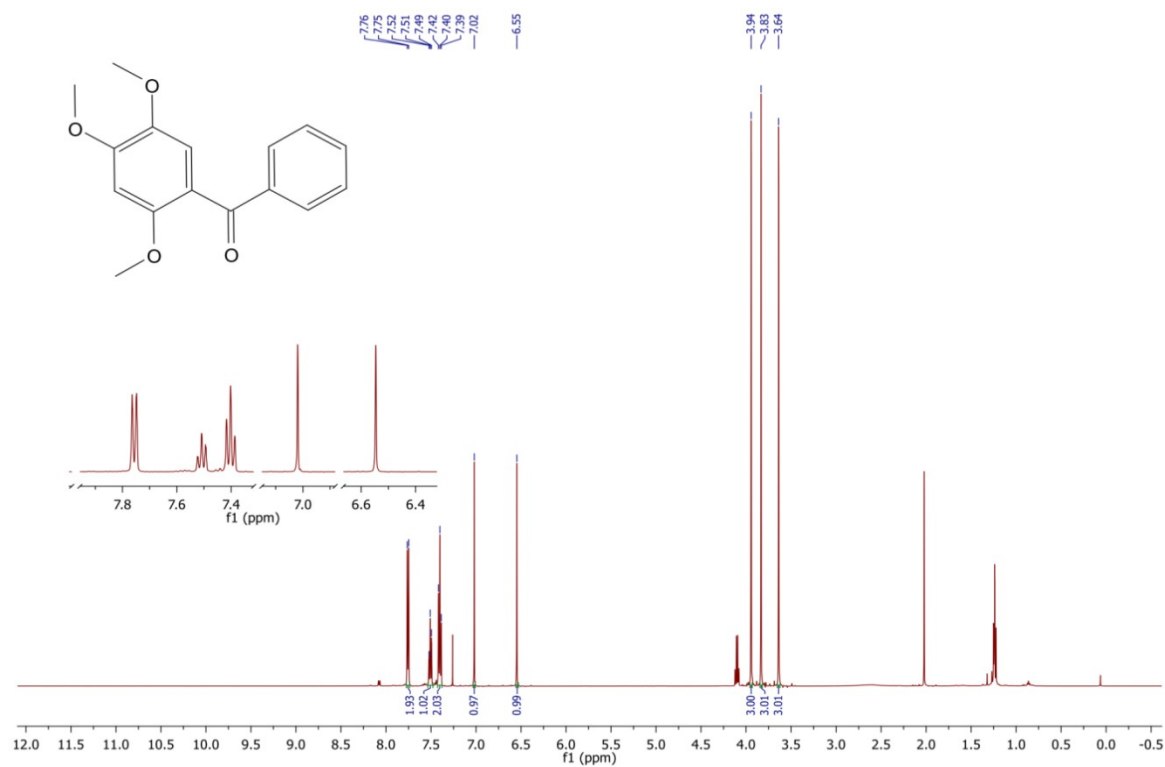


# $^1\text{H}$ and $^{13}\text{C}$ NMR of 2,5-dimethoxybenzophenone

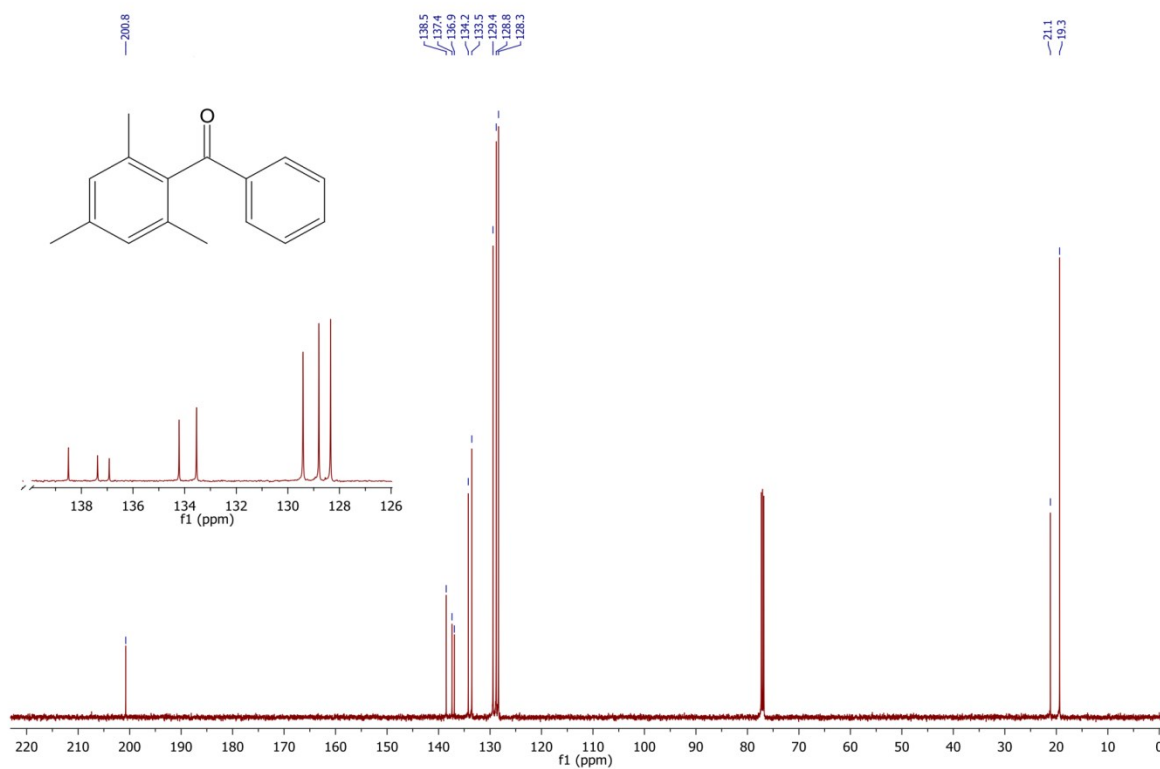
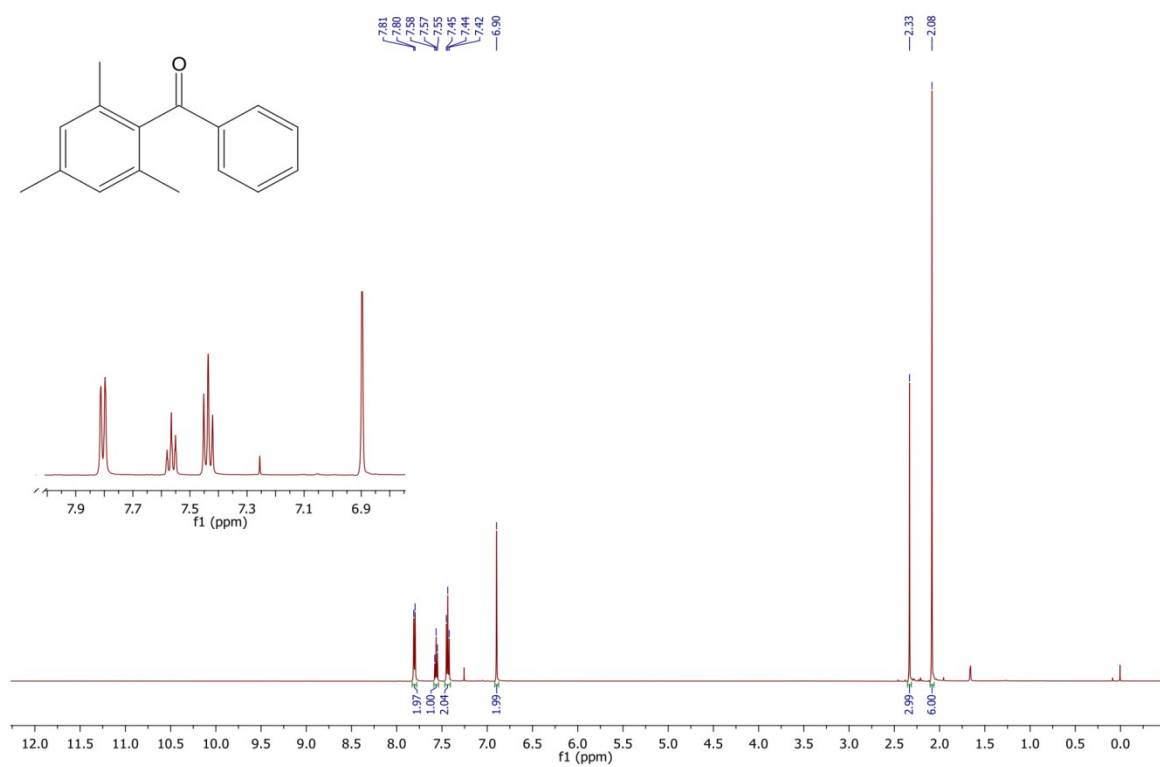




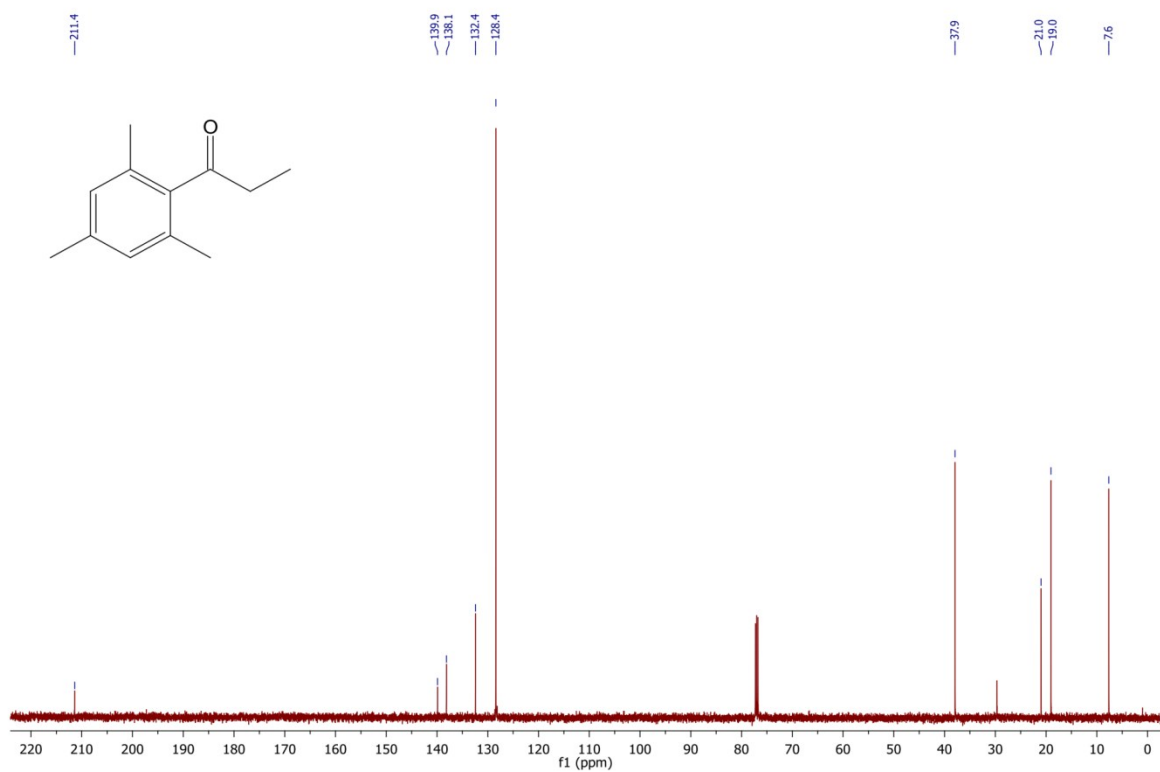
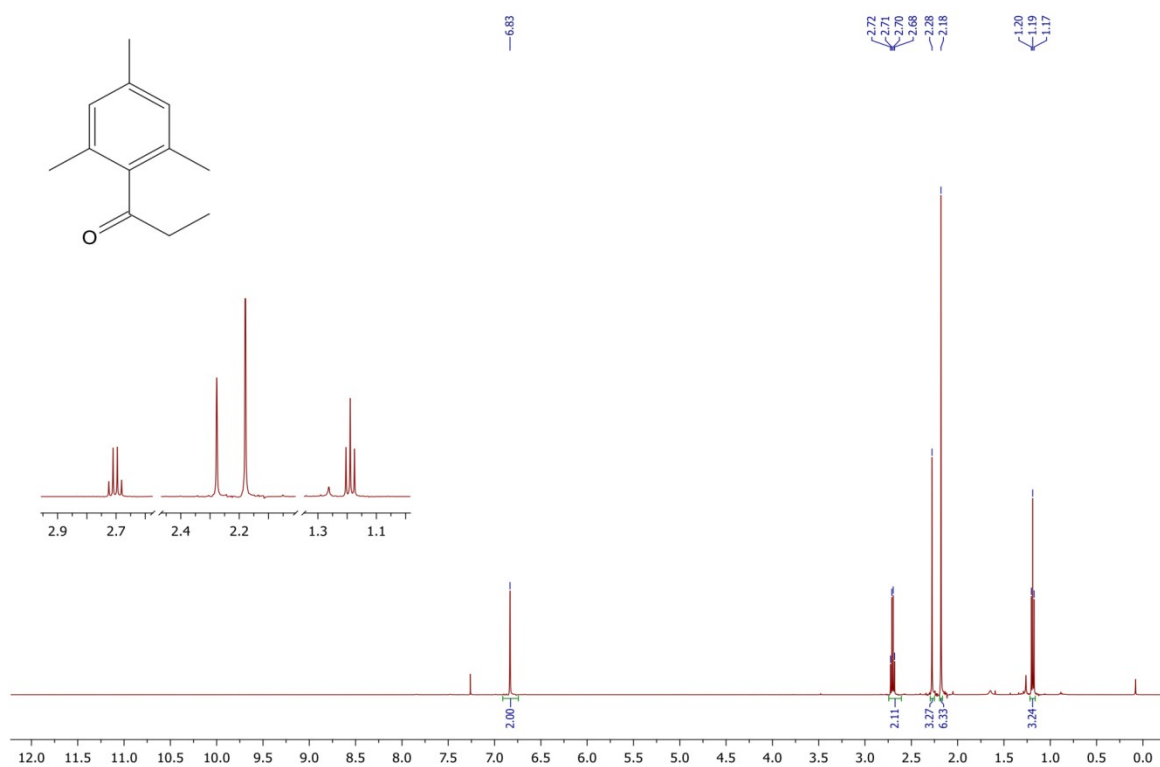
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 2,4,5-trimethoxybenzophenone



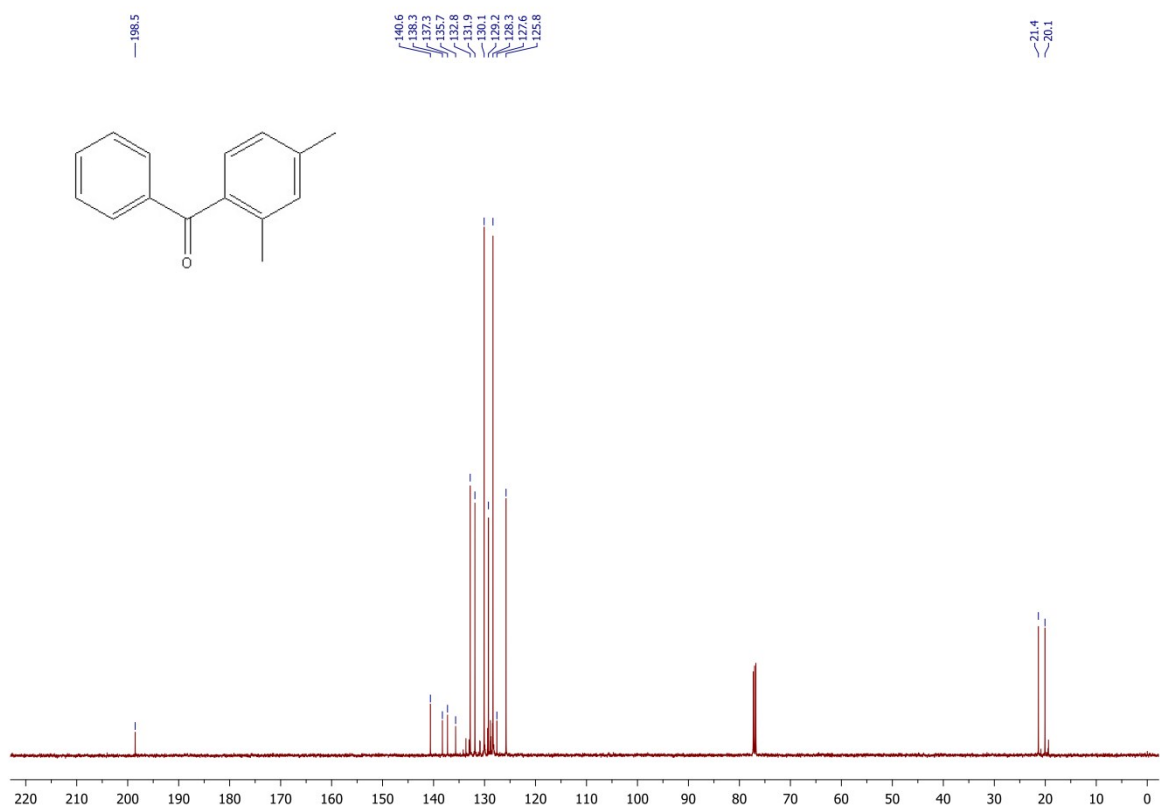
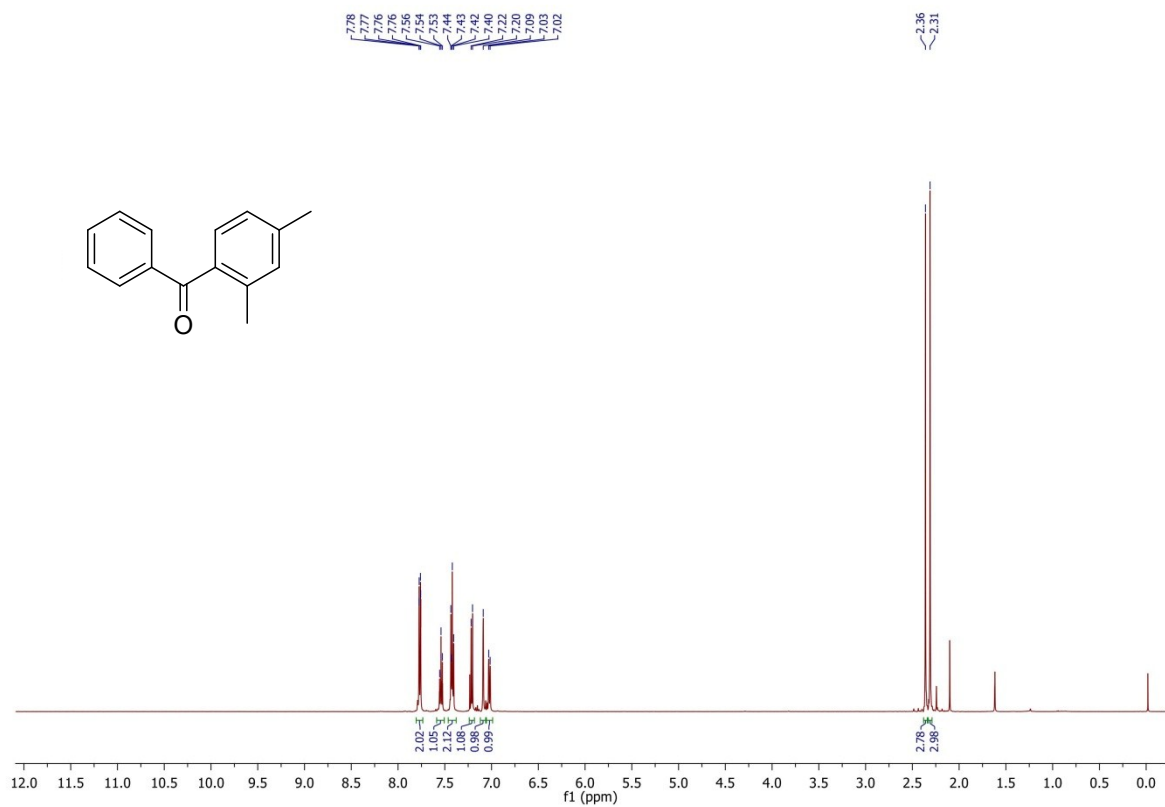
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 2,4,6-trimethylbenzophenone



# $^1\text{H}$ and $^{13}\text{C}$ NMR of 2,4,6-trimethylpropiophenone

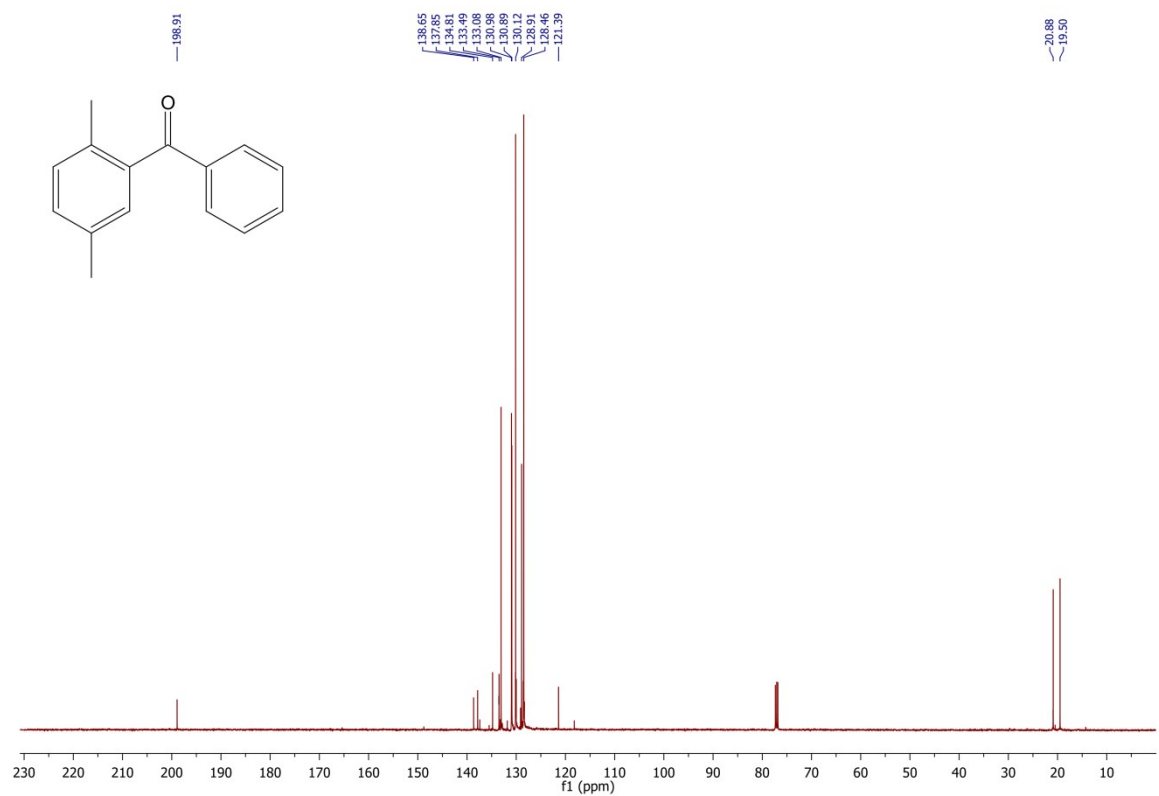
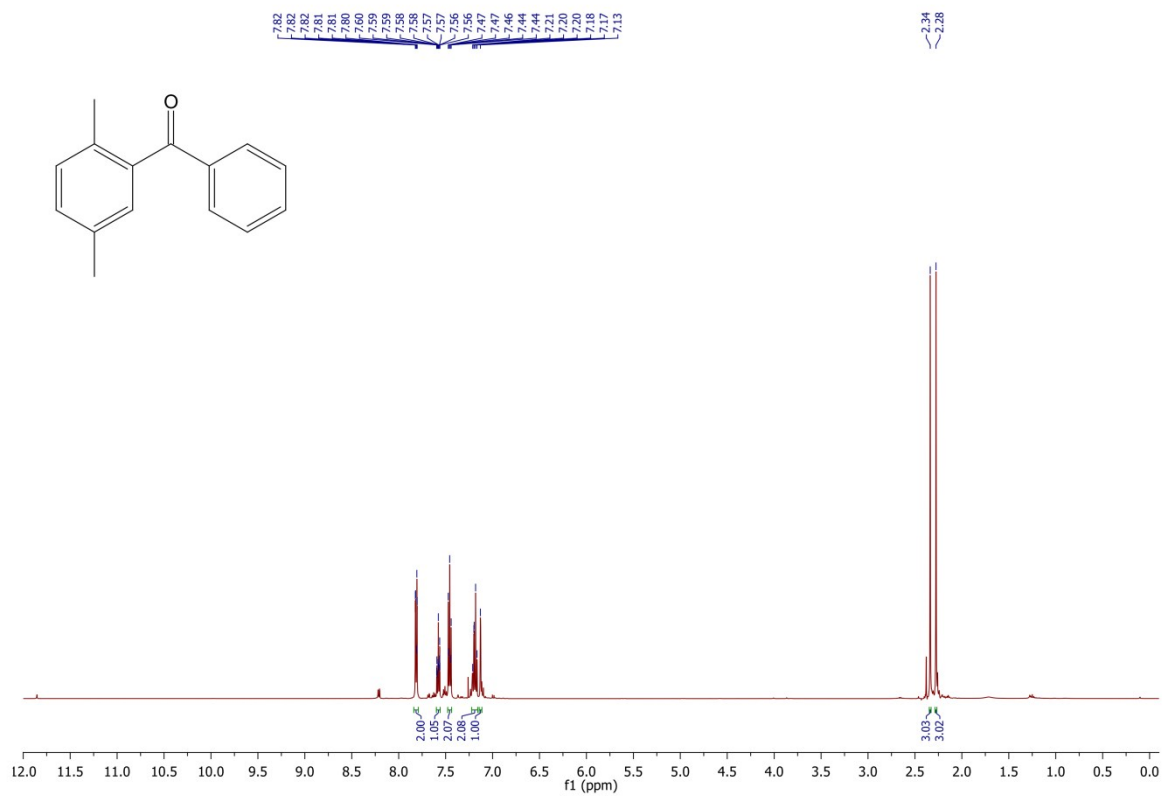


# $^1\text{H}$ and $^{13}\text{C}$ NMR of 2,4-dimethylbenzophenone

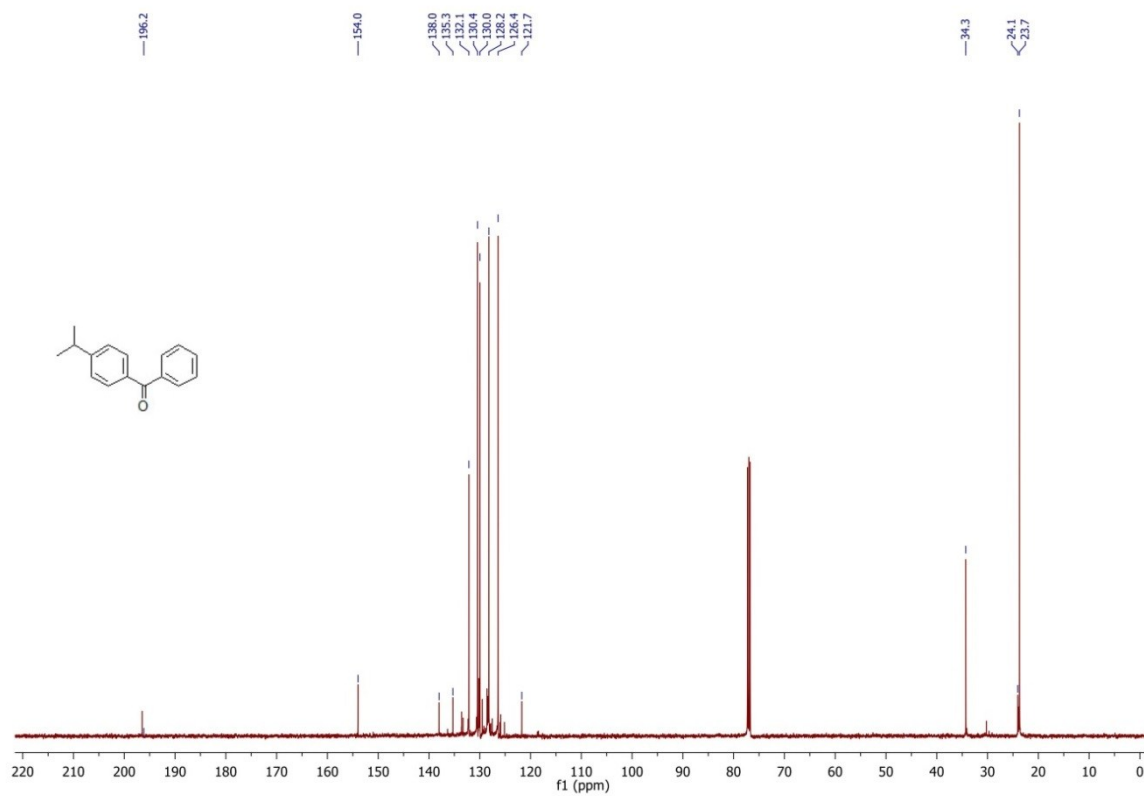
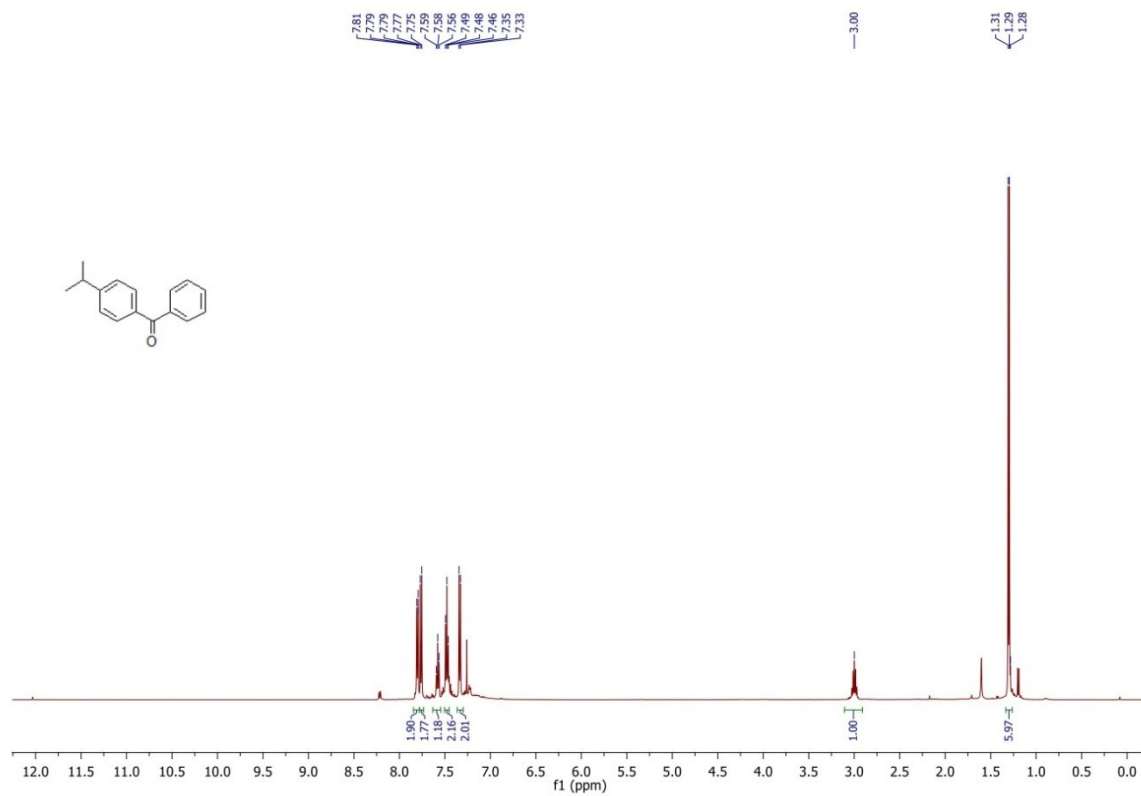


## **$^1\text{H}$ and $^{13}\text{C}$ NMR of 2, 5-dimethylpropiophenone**

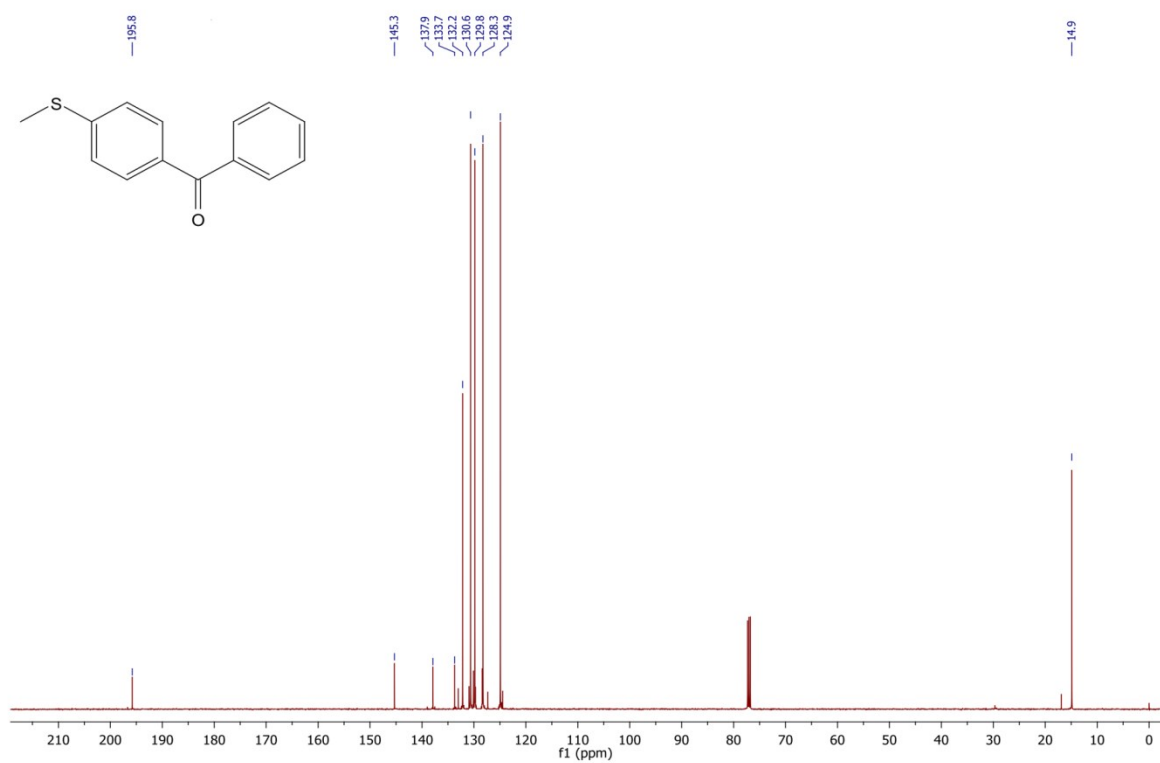
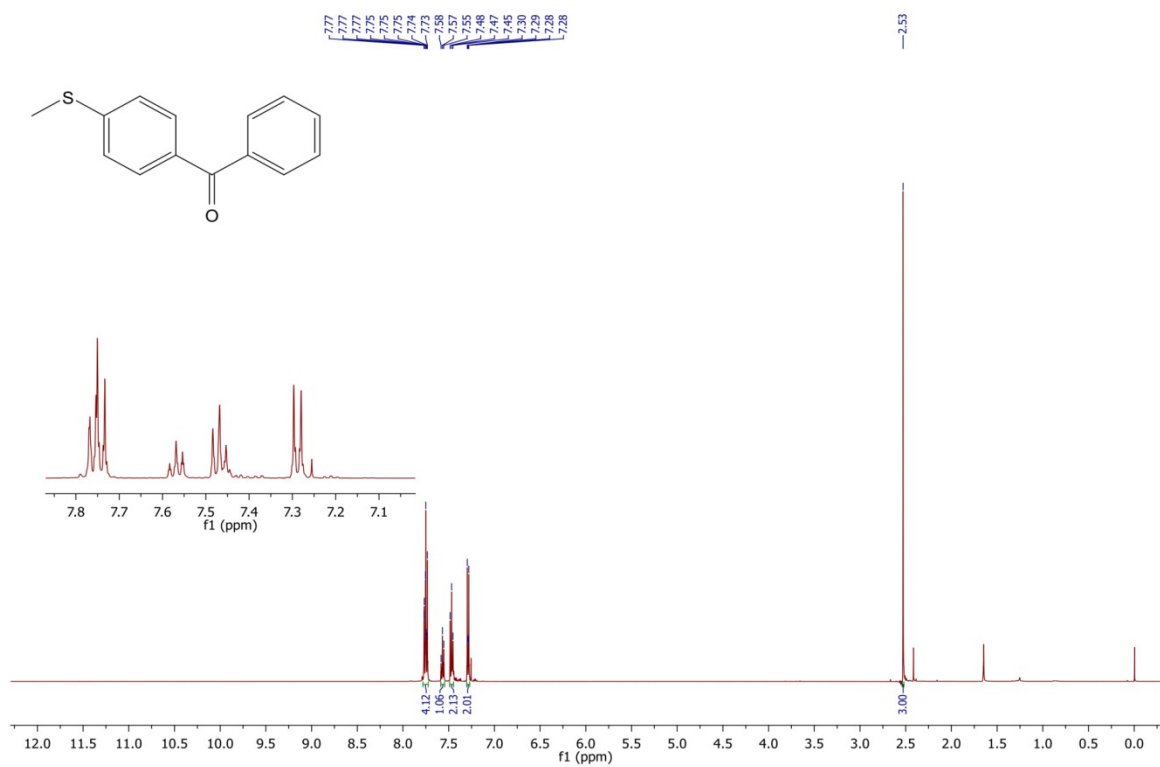
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 2,5-dimethylbenzophenone



# $^1\text{H}$ and $^{13}\text{C}$ NMR of 4-isopropylbenzophenone

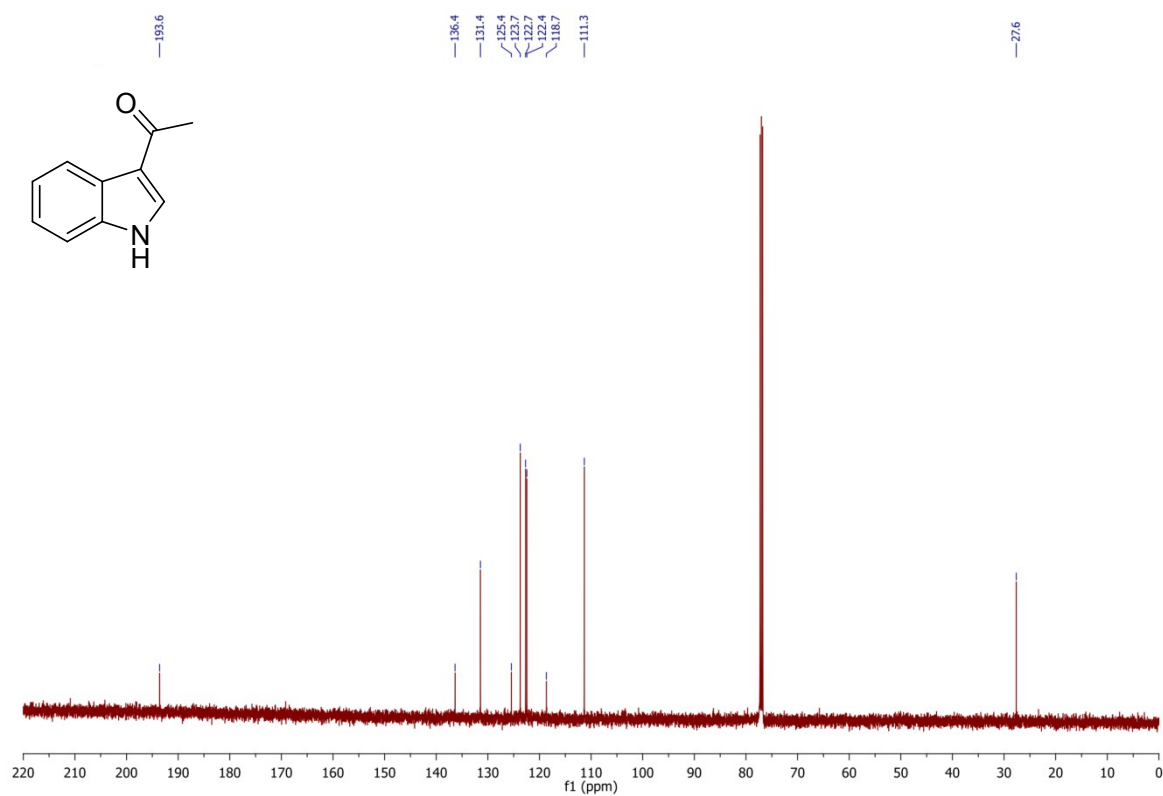
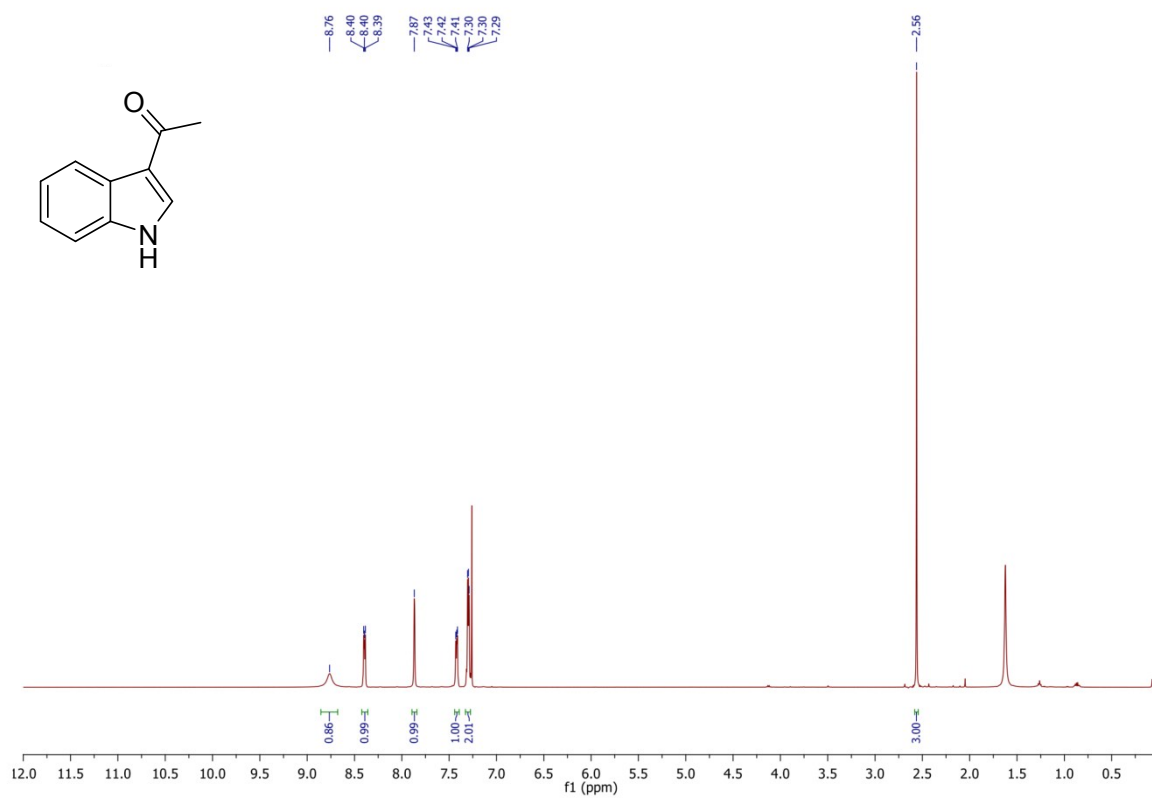


# $^1\text{H}$ and $^{13}\text{C}$ NMR of 4-methylthiobenzophenone

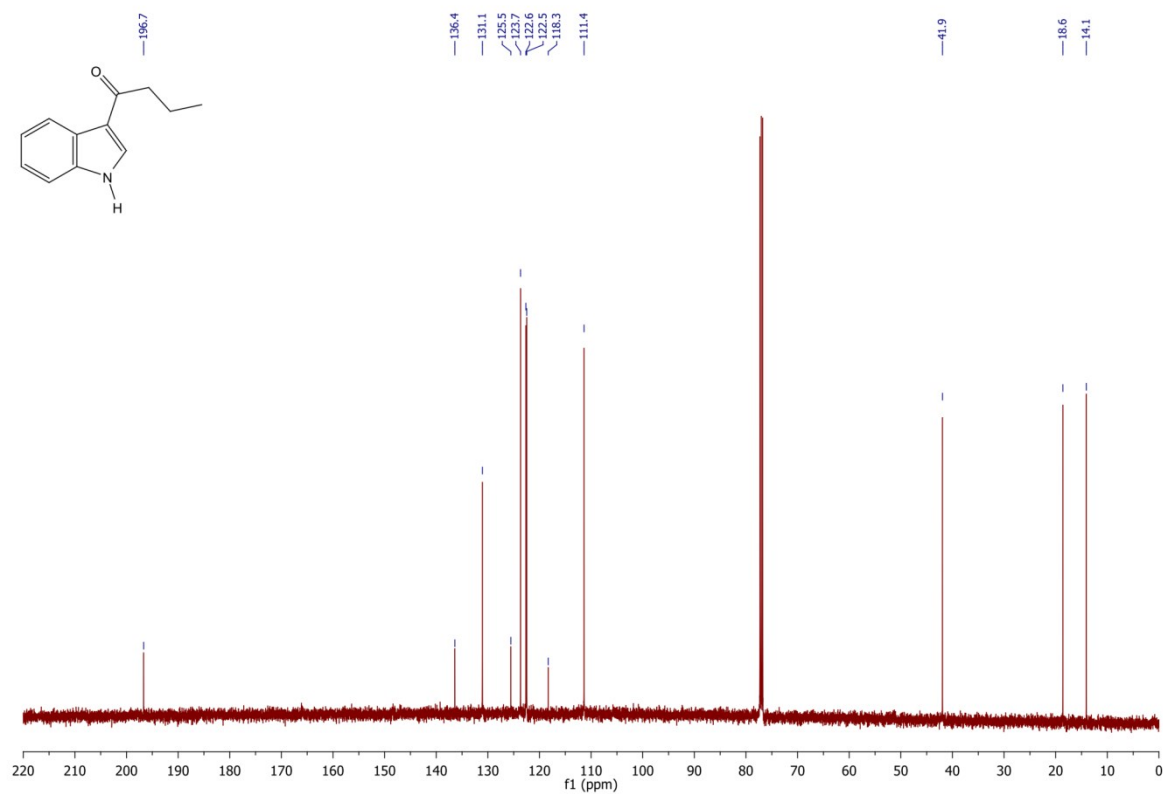
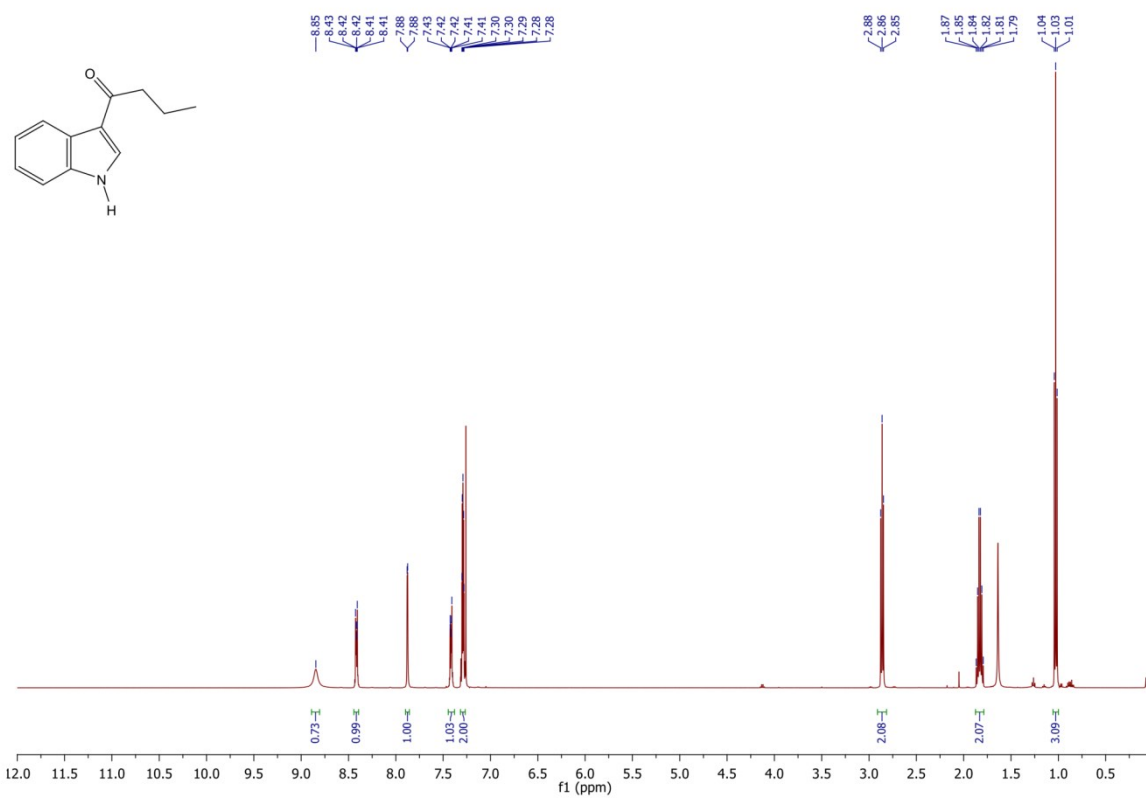




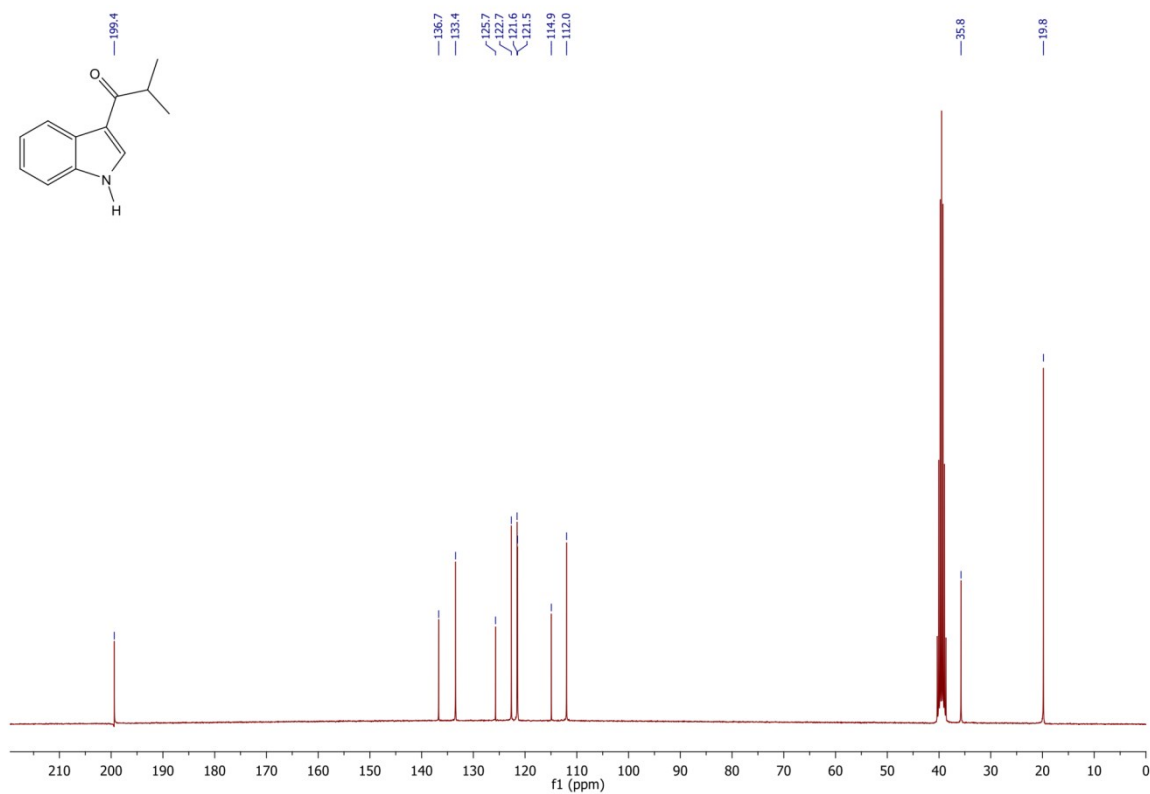
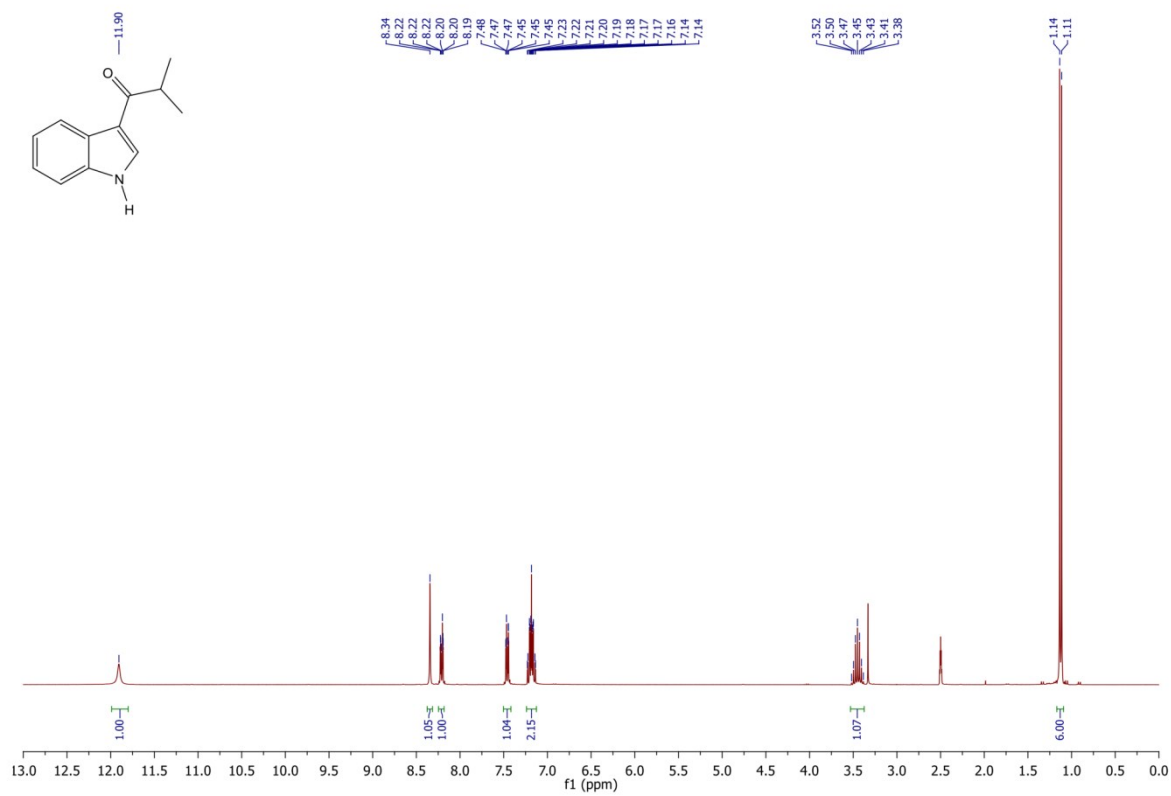
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-acetylindole



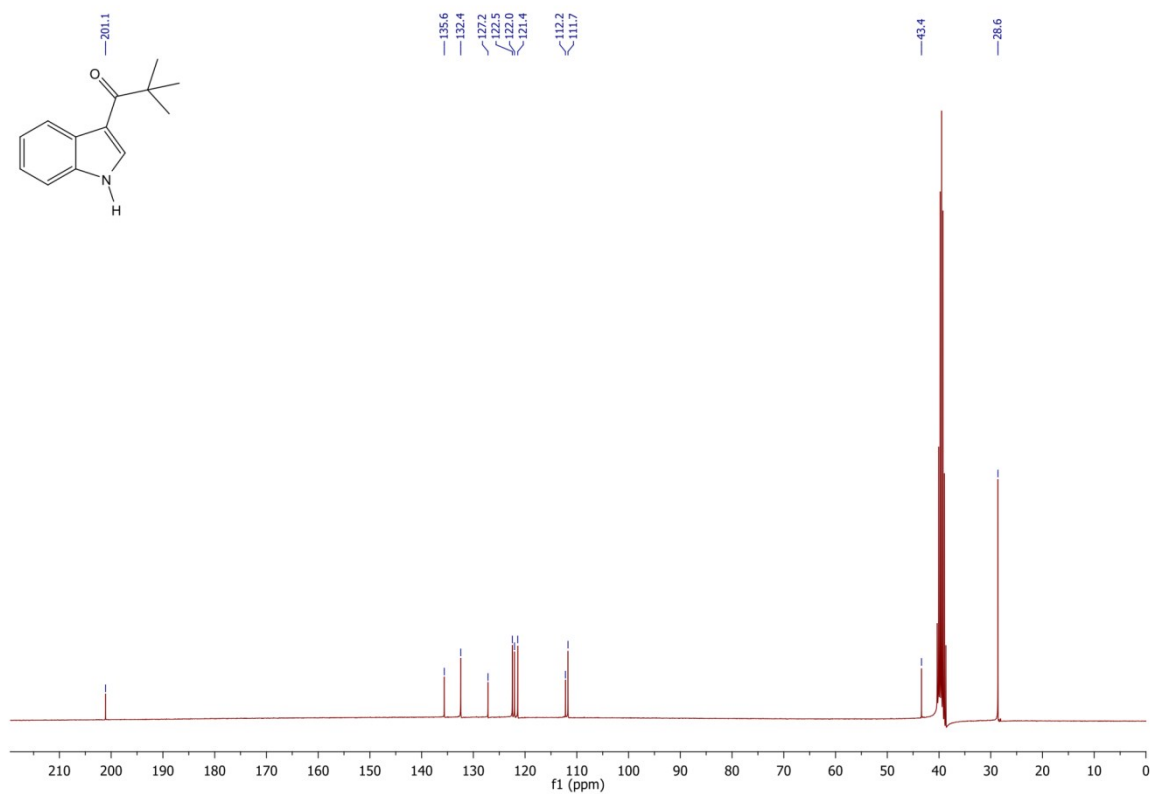
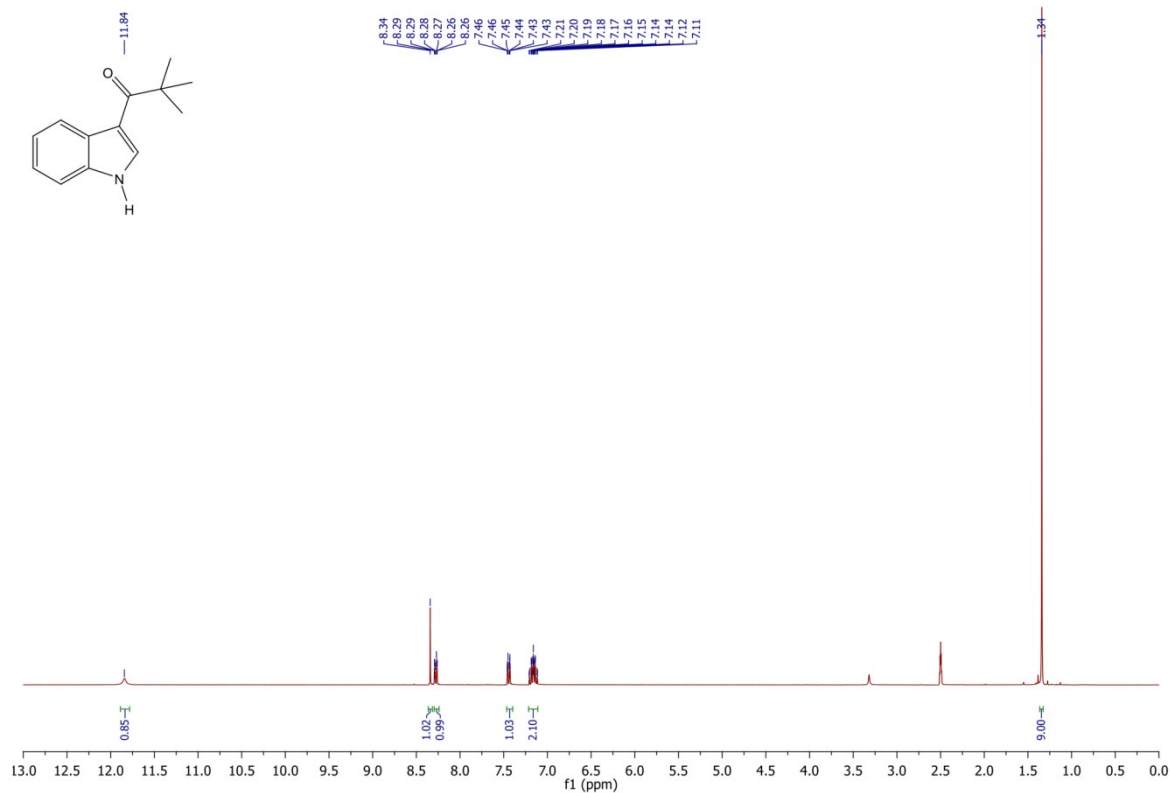
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-butyrylindole



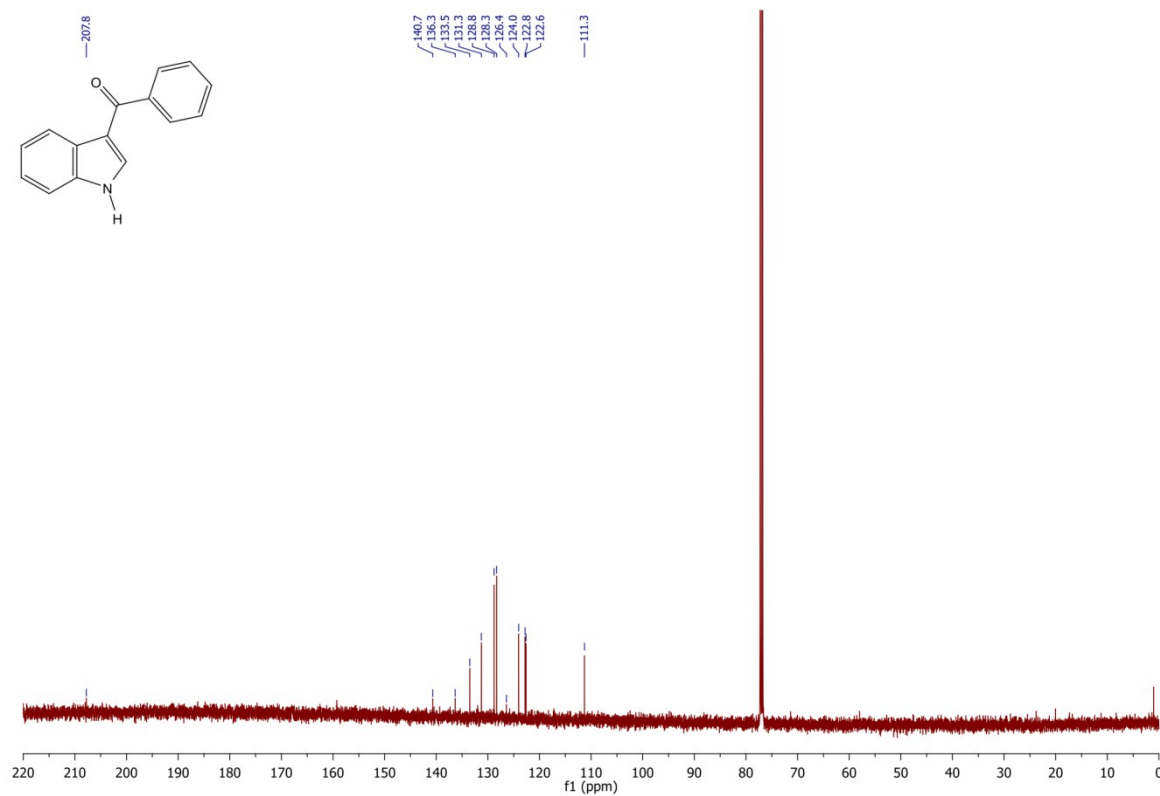
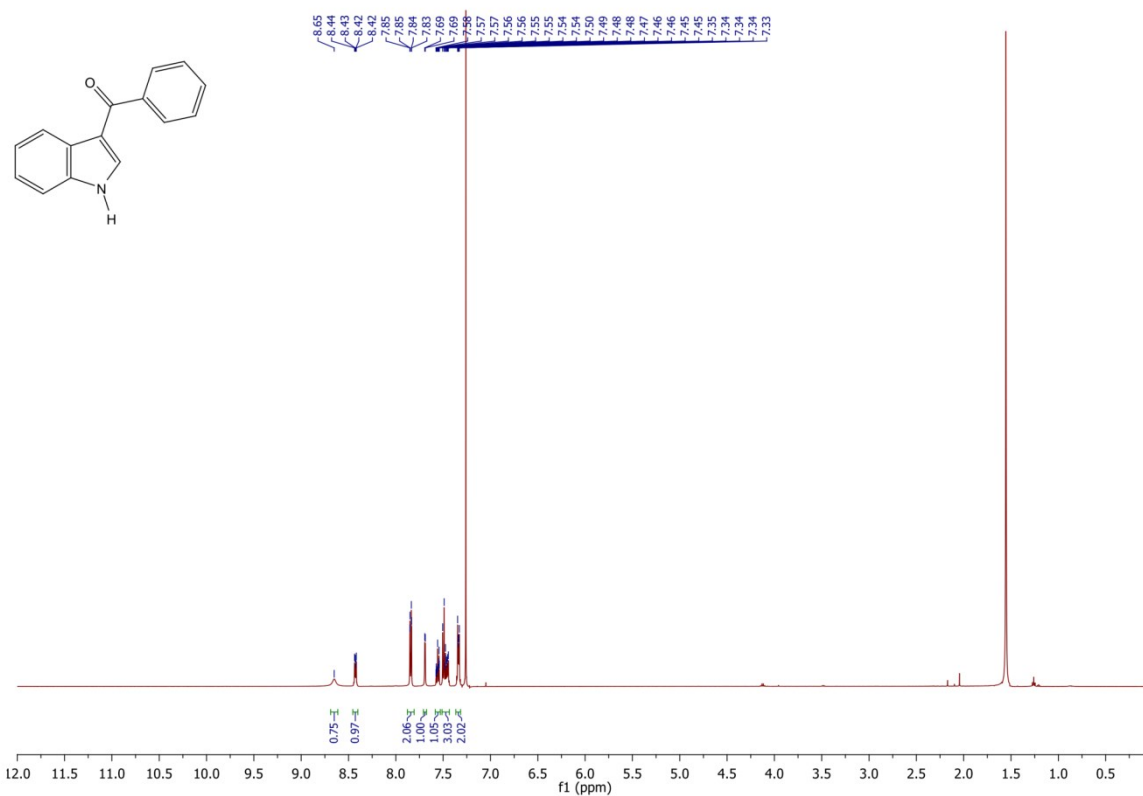
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-isobutyrylindole



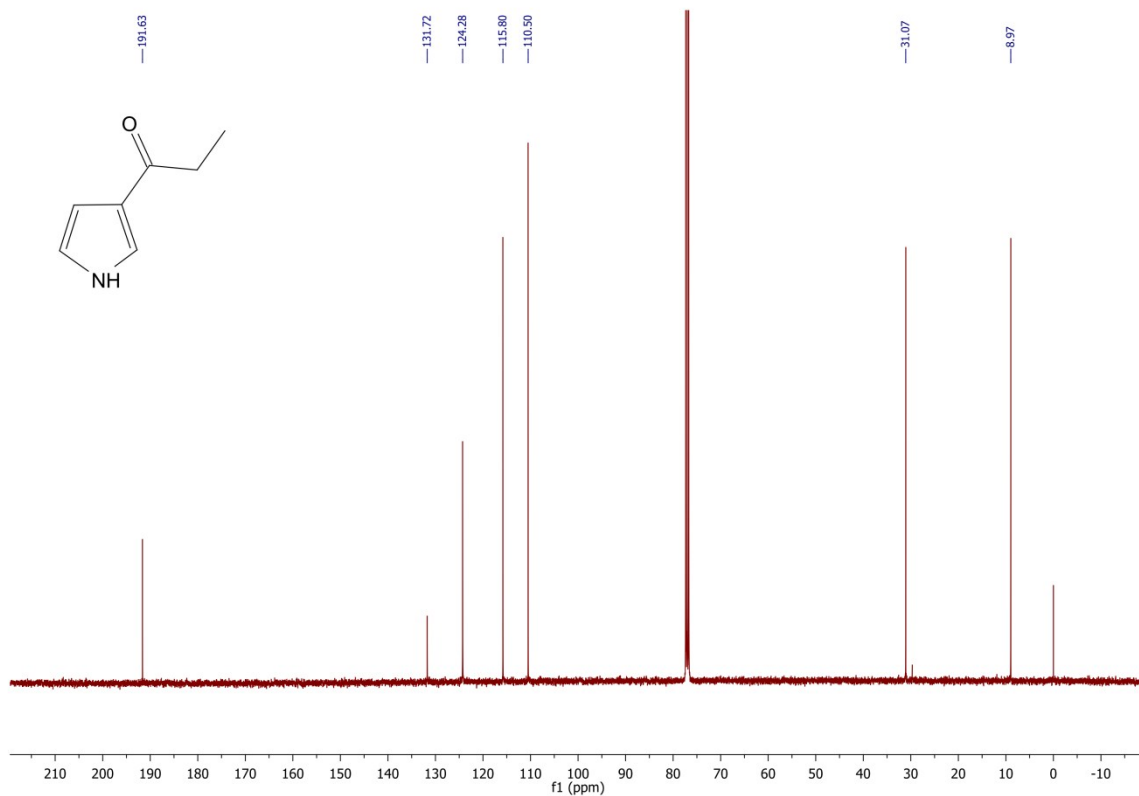
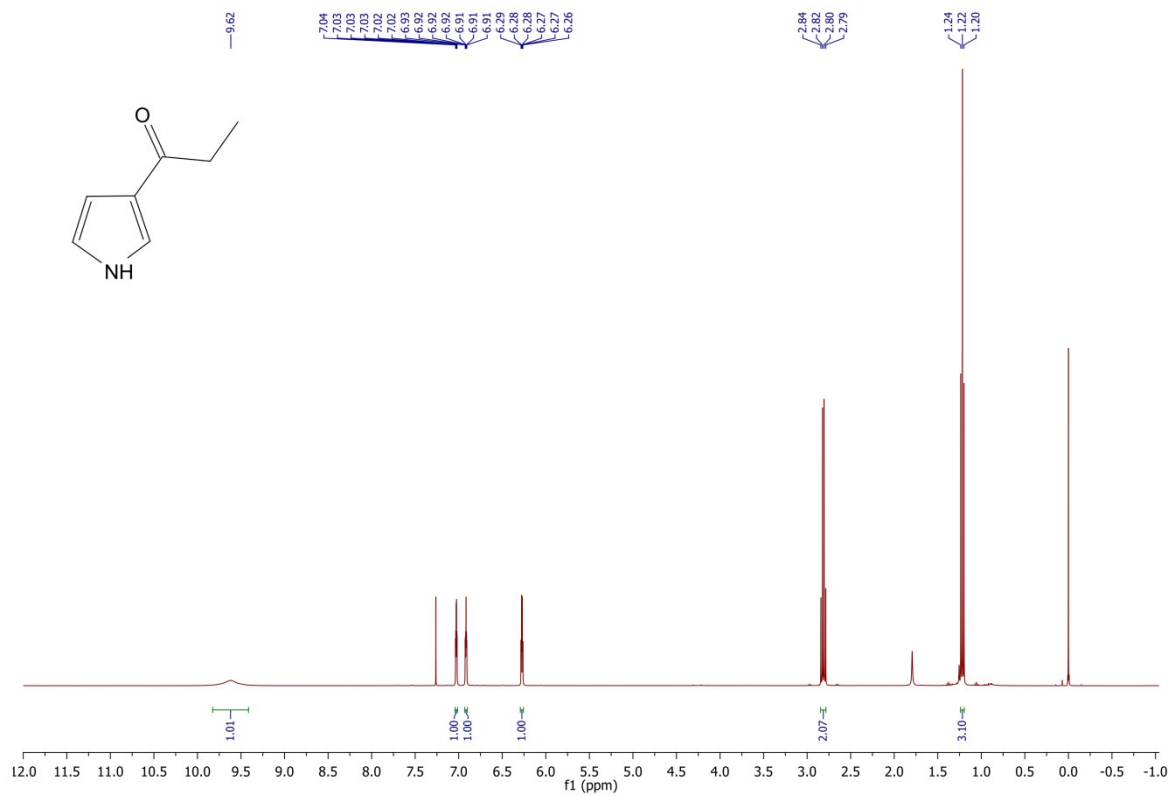
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-pivaloylindole



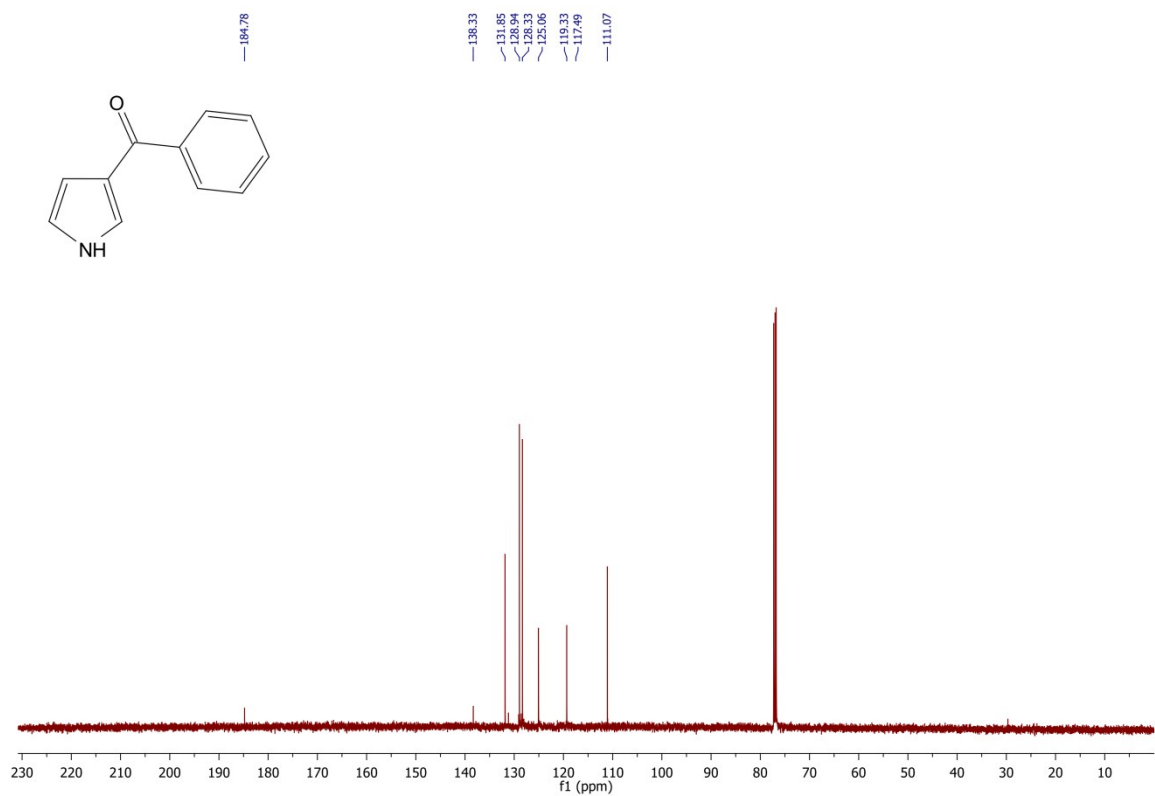
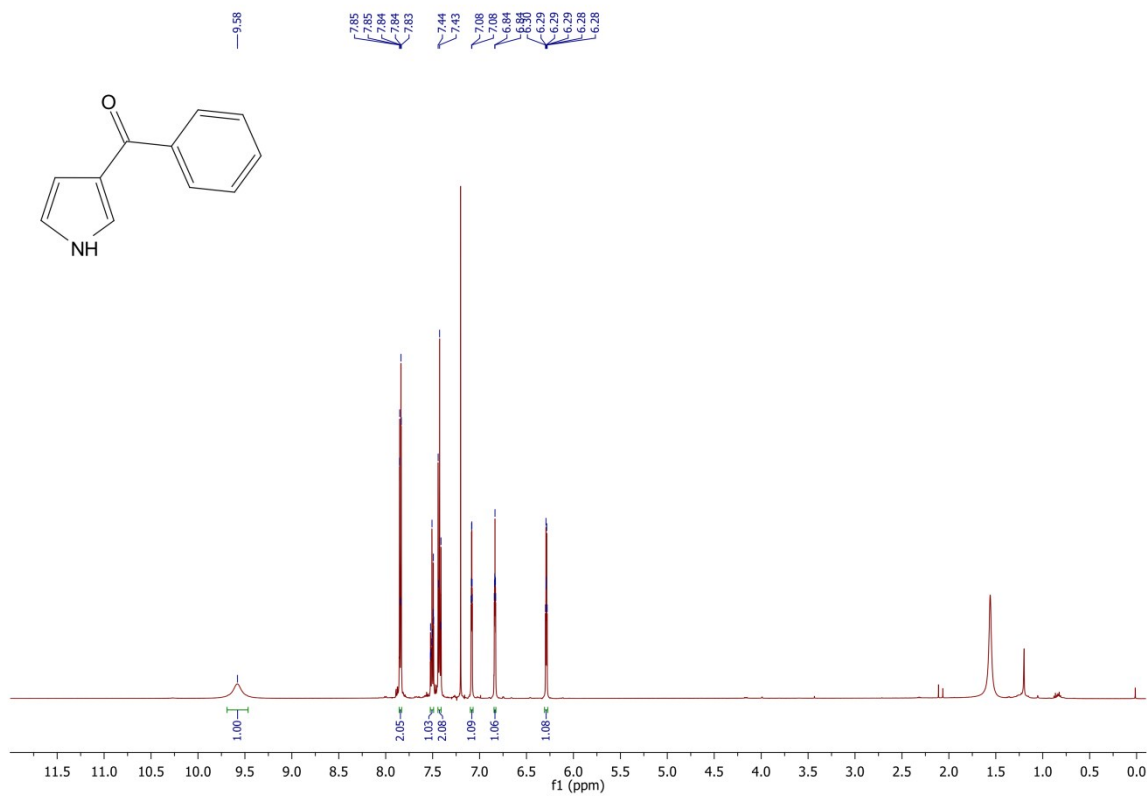
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-benzoylindole



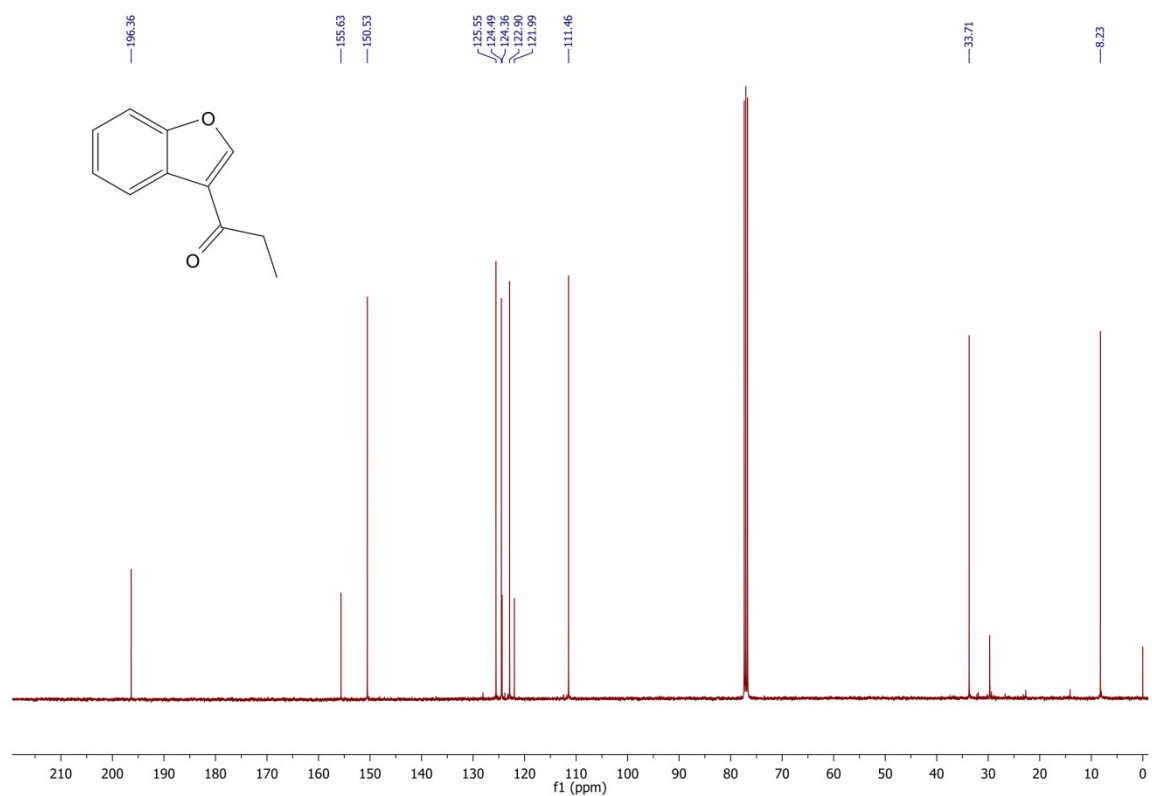
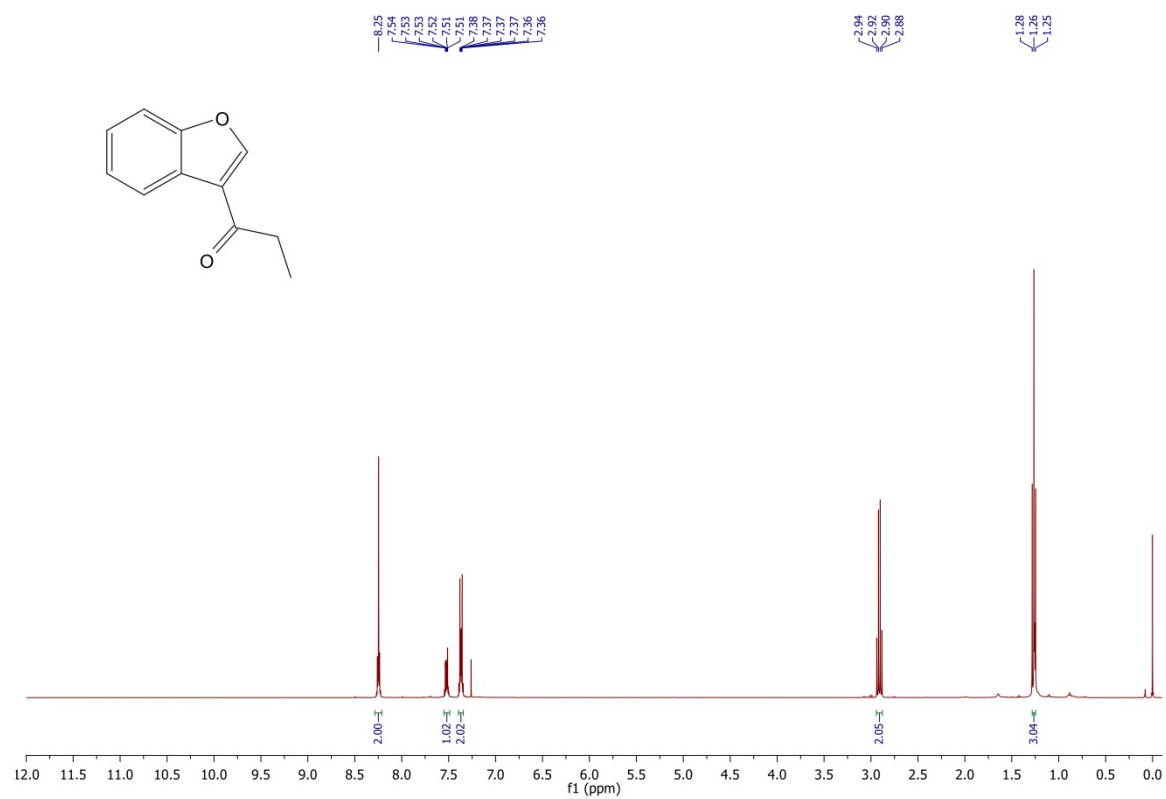
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-propionylpyrrole



# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-benzoylpyrrole

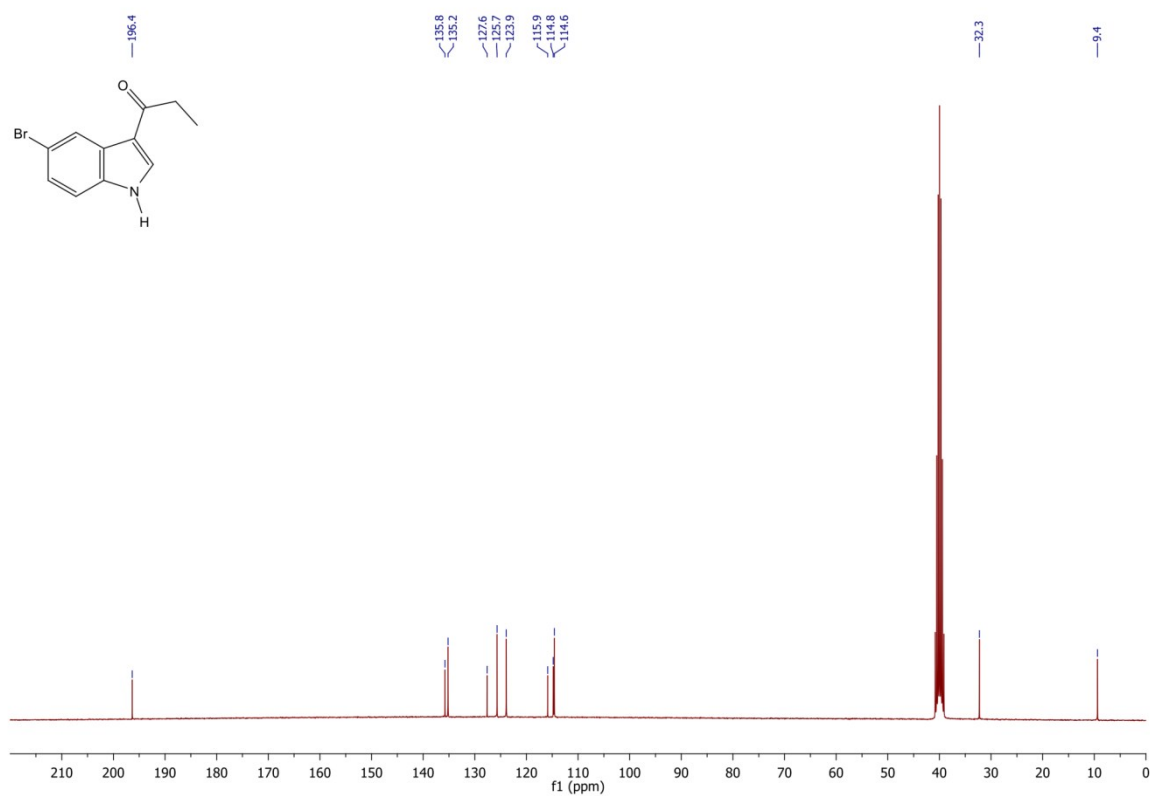
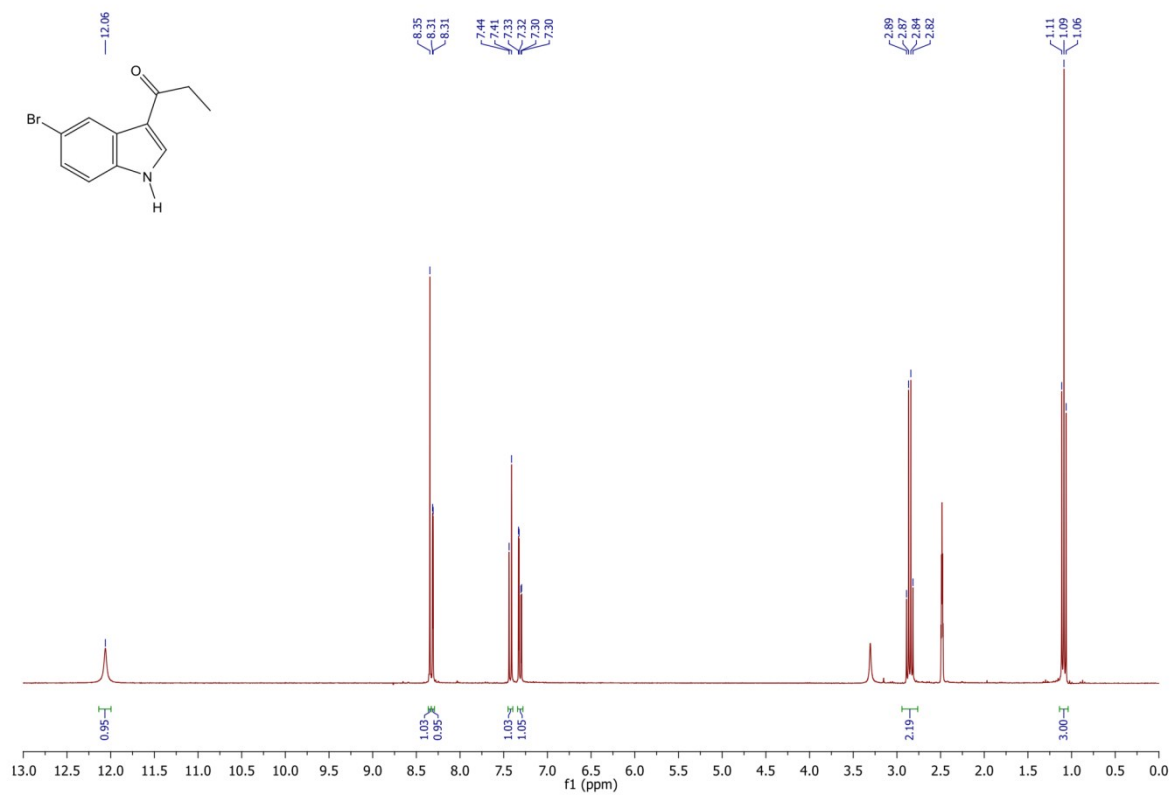


# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-propionylbenzofuran

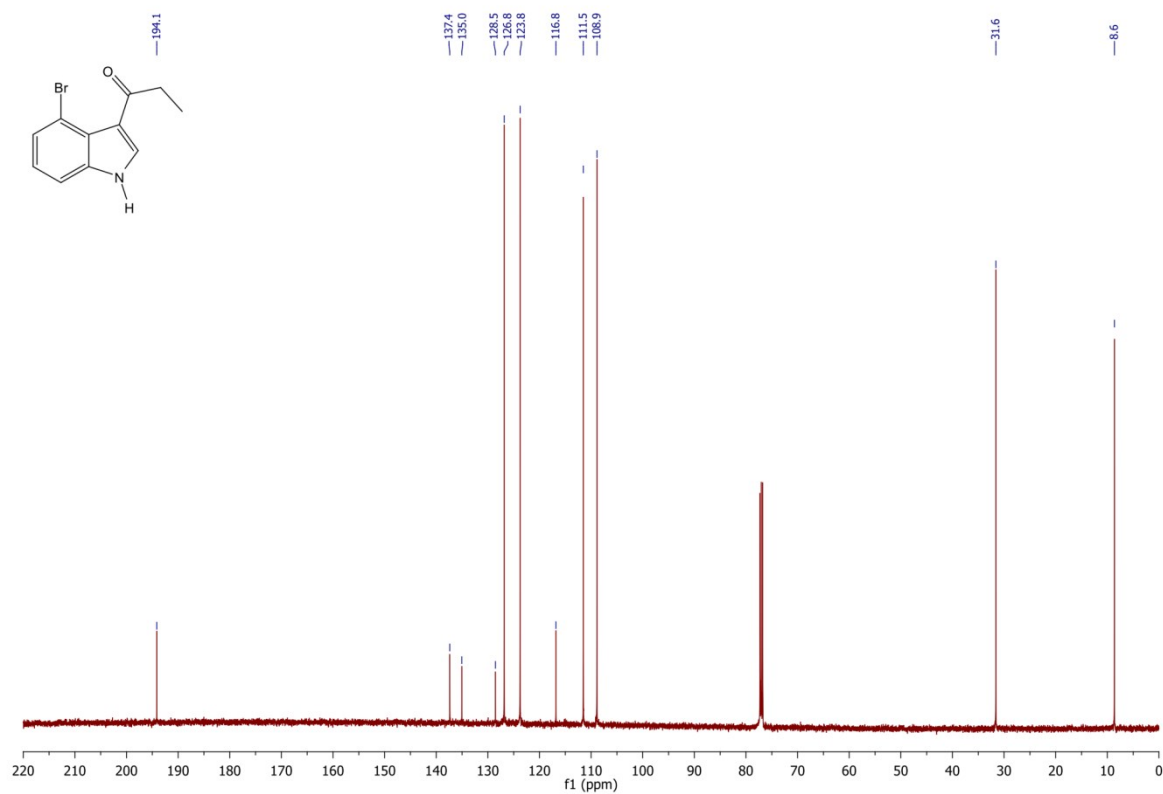
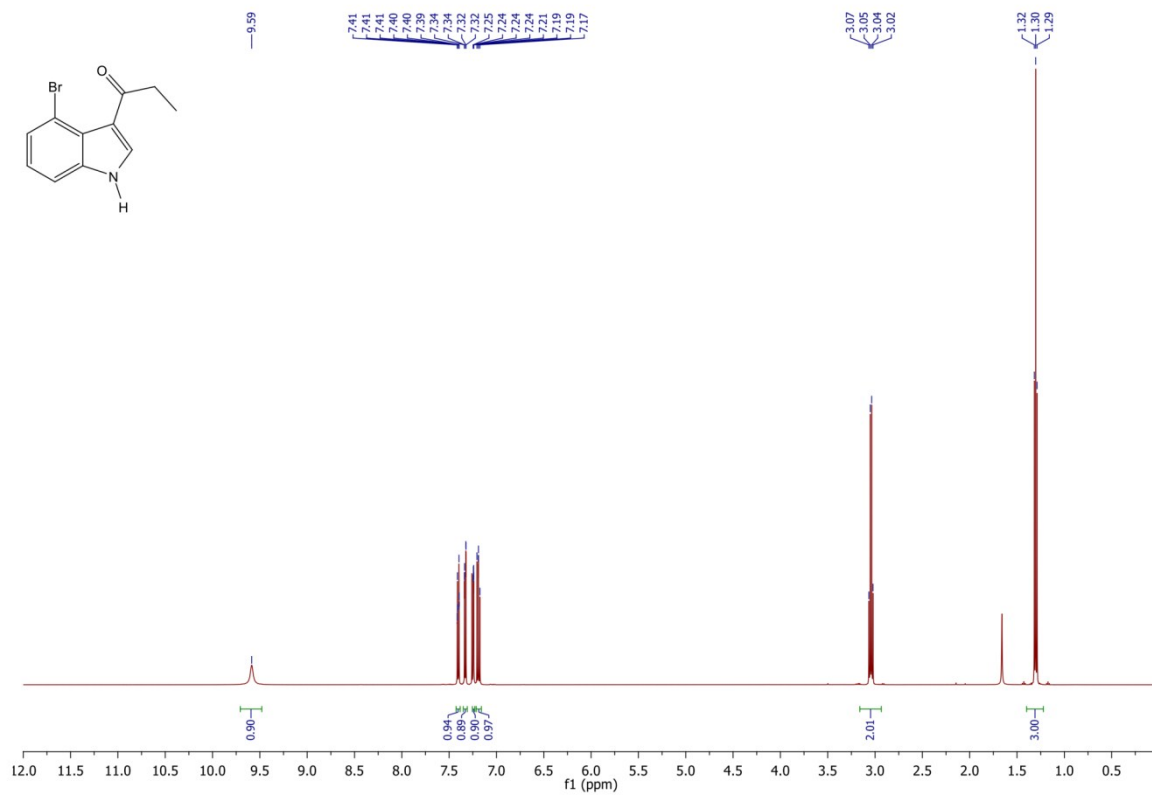




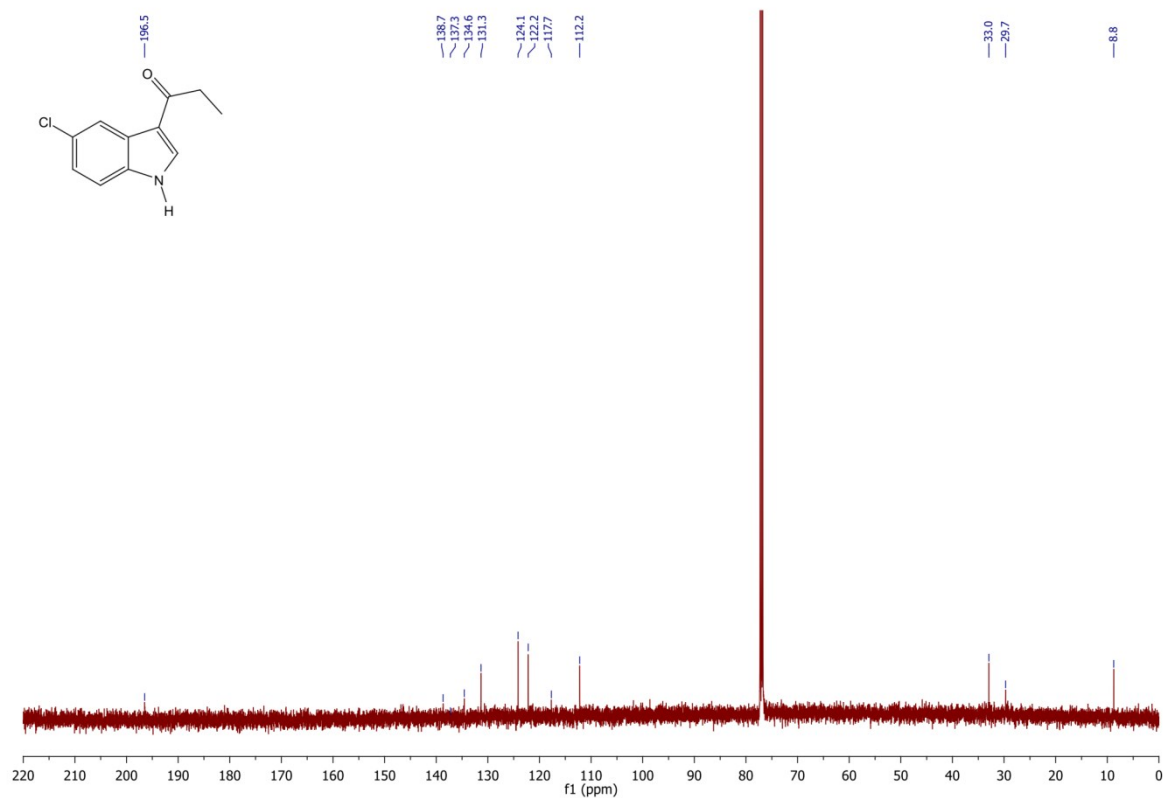
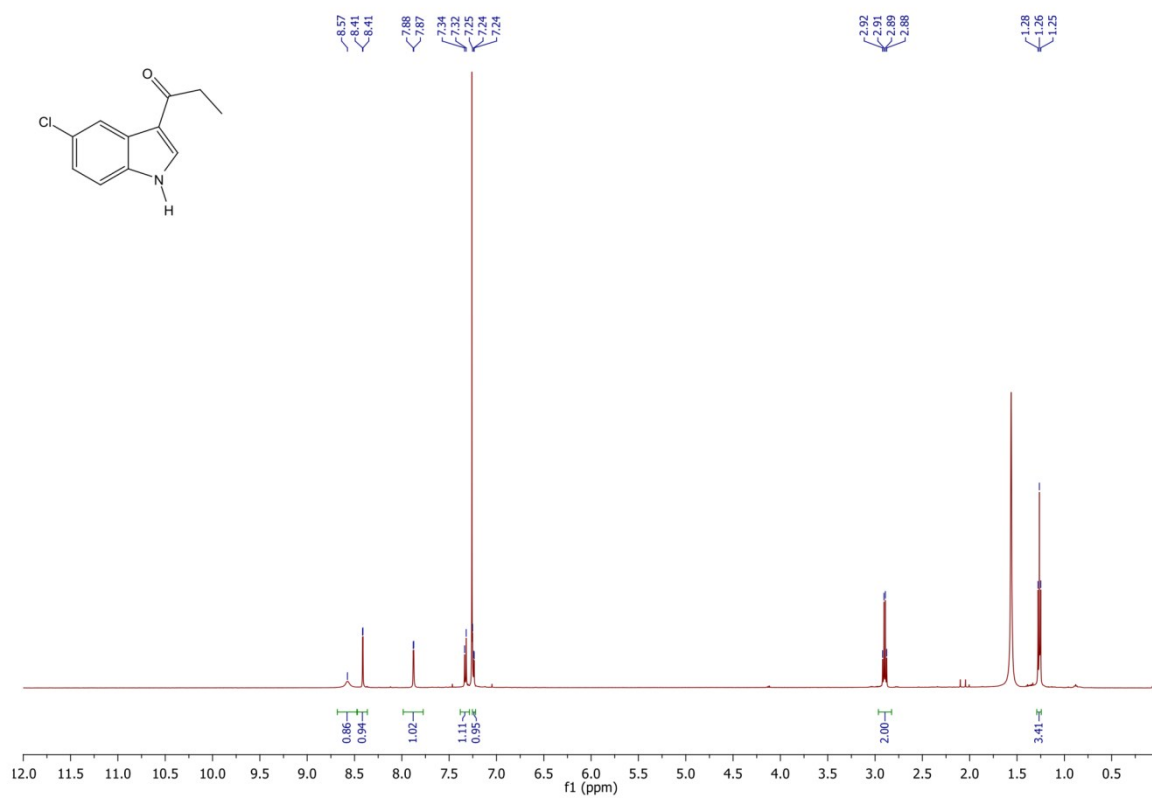
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-propionyl-5-bromoindole



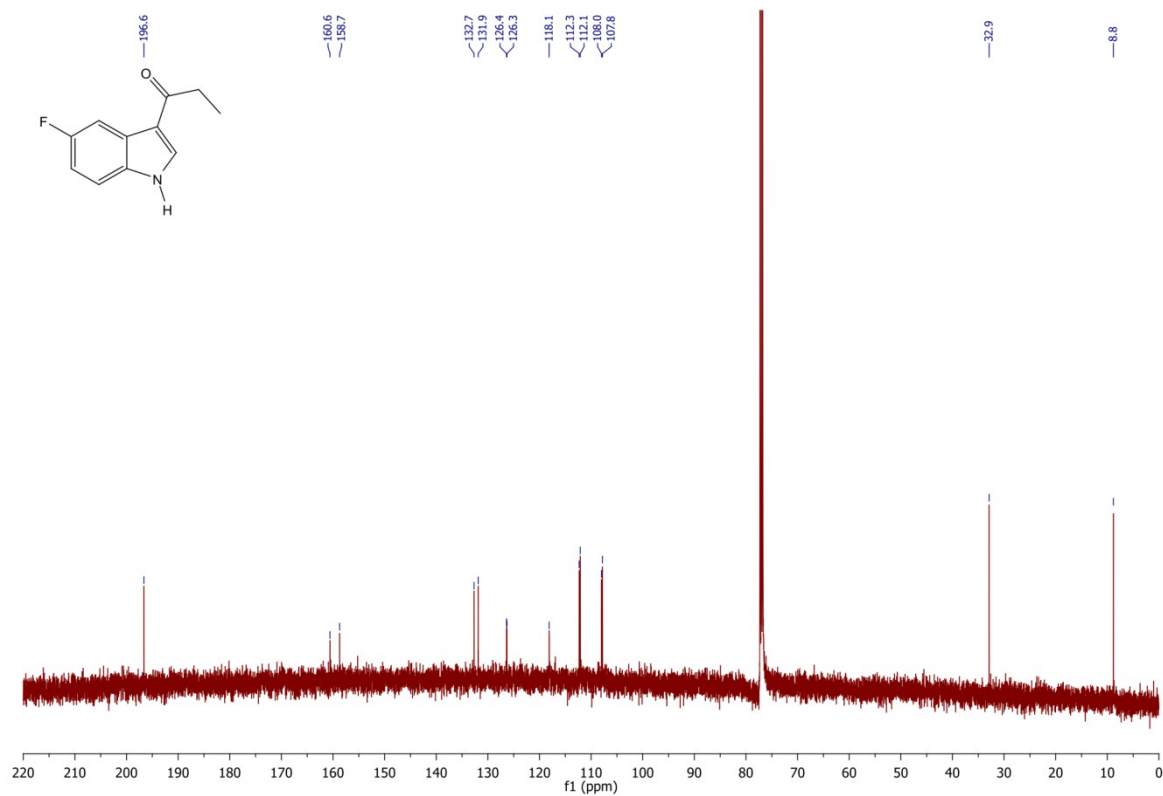
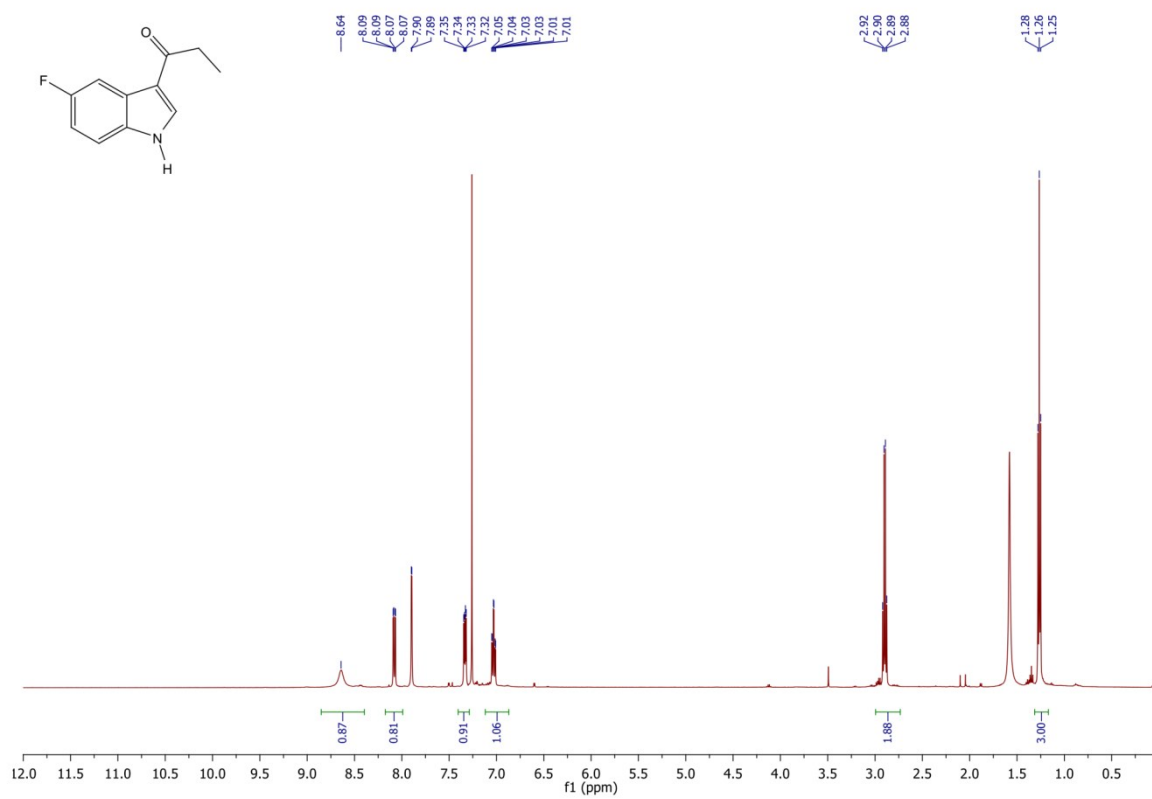
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-propionyl-4-bromoindole



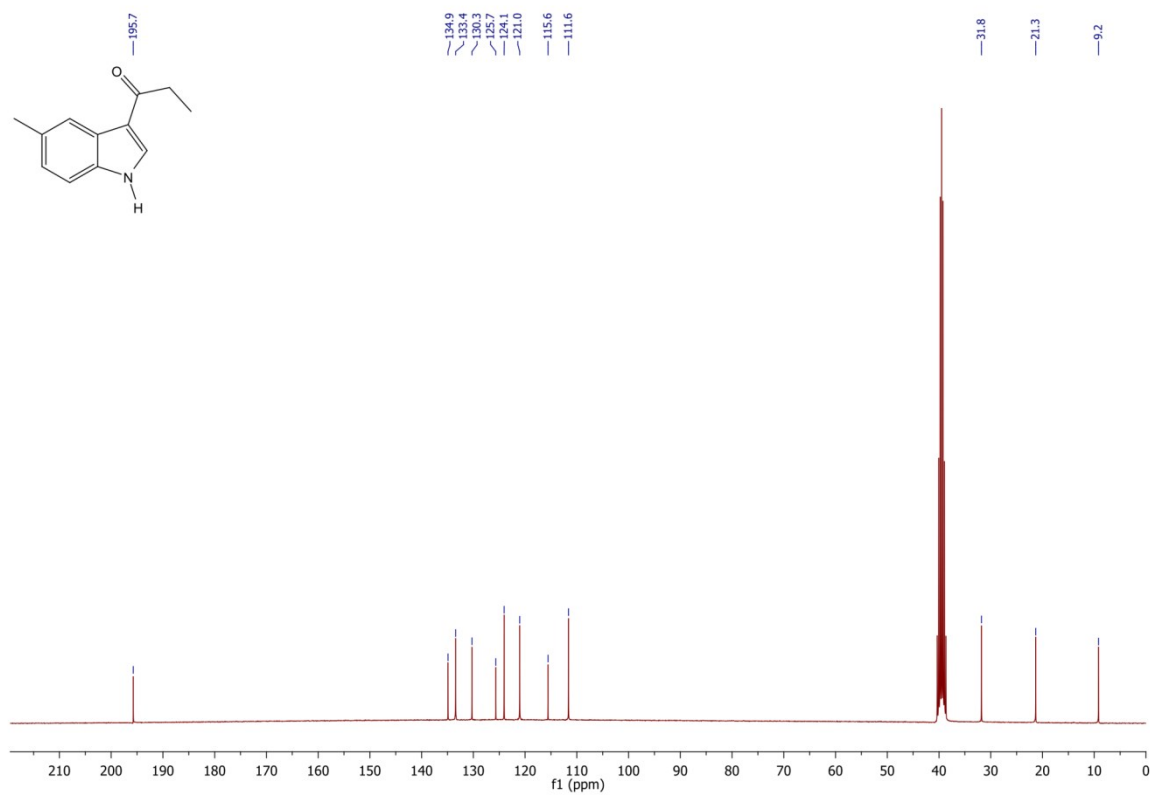
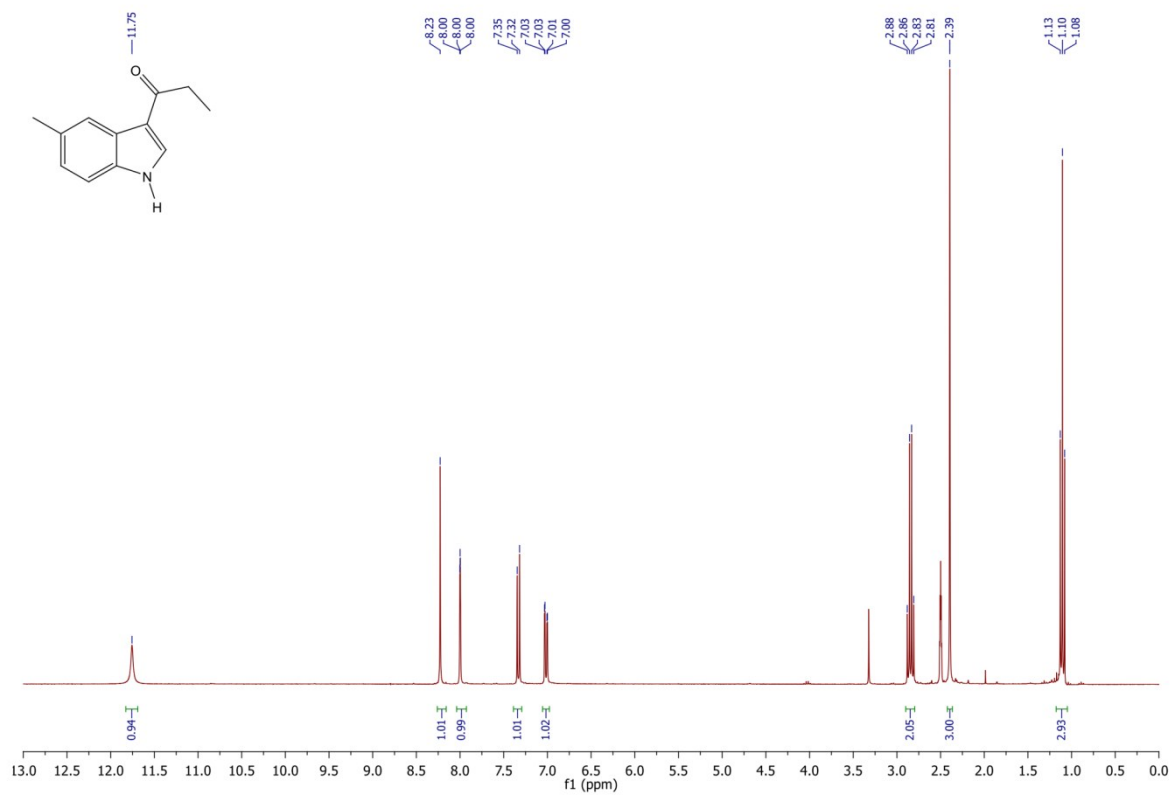
# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-propionyl-5-chloroindole



# $^1\text{H}$ and $^{13}\text{C}$ NMR of 3-propionyl-5-fluoroindole



# <sup>1</sup>H and <sup>13</sup>C NMR of 3-propionyl-5-methylindole



# <sup>1</sup>H and <sup>13</sup>C NMR of 3-propionyl-5-methoxyindole

