

## Magnetically separable triazine-based Cu(II)-vitamin B<sub>5</sub> complex in nitromethane toward efficient heterogeneous cyanation reaction of aryl halides

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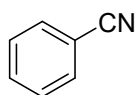
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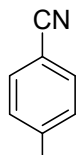
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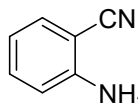
### Characterization of aryl nitrile derivatives:



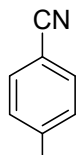
Benzonitrile (2a). Colorless oil; <sup>1</sup>H NMR (499 MHz, DMSO-*d*<sub>6</sub>) δ 7.80 (d, *J* = 7.6 Hz, 2H), 7.71 – 7.68 (m, 1H), 7.55 (t, *J* = 7.6 Hz, 2H); <sup>13</sup>C NMR (126 MHz, DMSO-*d*<sub>6</sub>) δ 132.64, 131.17, 128.80, 118.60, 112.66. HRMS (ESI): Calcd for C<sub>7</sub>H<sub>5</sub>N (M + H)<sup>+</sup> 103.04, found 103.10.



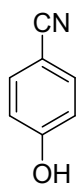
4-Aminobenzonitrile (2d). White solid, mp 83-85 ° C; <sup>1</sup>H NMR (499 MHz, DMSO-*d*<sub>6</sub>) δ 7.36 (d, *J* = 8.1 Hz, 2H), 6.59 (d, *J* = 8.2 Hz, 2H), 6.11 (s, 2H); <sup>13</sup>C NMR (126 MHz, DMSO-*d*<sub>6</sub>) δ 150.98, 133.14, 118.42, 114.65, 98.61. HRMS (ESI): Calcd for C<sub>7</sub>H<sub>6</sub>N<sub>2</sub> (M + H)<sup>+</sup> 118.05, found 118.10.



2-Aminobenzonitrile (2f). Beige-brown solid, mp 49-50 ° C;  $^1\text{H}$  NMR (499 MHz, DMSO- $d_6$ )  $\delta$  7.35 (d,  $J$  = 7.9 Hz, 1H), 7.28 (t,  $J$  = 7.5 Hz, 1H), 6.76 (d,  $J$  = 8.5 Hz, 1H), 6.57 (t,  $J$  = 7.5 Hz, 1H), 5.98 (s, 2H);  $^{13}\text{C}$  NMR (126 MHz, DMSO- $d_6$ )  $\delta$  151.11, 133.59, 13.94, 118.02, 116.74, 94.30, 115.05. HRMS (ESI): Calcd for  $\text{C}_7\text{H}_6\text{N}_2$  (M +H) $^+$  118.05, found 118.10.



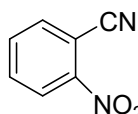
4-Nitrobenzonitrile (2h). Yellow solid, mp 147-149 ° C;  $^1\text{H}$  NMR (499 MHz, DMSO- $d_6$ )  $\delta$  8.37 (d,  $J$  = 8.3 Hz, 2H), 8.16 (d,  $J$  = 8.3 Hz, 2H);  $^{13}\text{C}$  NMR (126 MHz, DMSO- $d_6$ )  $\delta$  15.01, 133.80, 123.92, 117.93, 117.07. HRMS (ESI): Calcd for  $\text{C}_7\text{H}_4\text{N}_2\text{O}_2$  (M +H) $^+$  148.03, found 148.10.



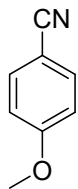
4-Hydroxybenzonitrile (2i). White solid, mp 110-112 ° C;  $^1\text{H}$  NMR (499 MHz, DMSO- $d_6$ )  $\delta$  10.59 (s, 1H), 7.59 (d,  $J$  = 8.2 Hz, 2H), 6.88 (d,  $J$  = 8.3 Hz, 2H);  $^{13}\text{C}$  NMR (126 MHz, DMSO- $d_6$ )  $\delta$  161.81, 134.20, 118.55, 116.26, 102.34. HRMS (ESI): Calcd for  $\text{C}_7\text{H}_5\text{NO}$  (M +H) $^+$  119.04, found 119.20.



Picolinonitrile (2j). White solid, mp 28-30 ° C;  $^1\text{H}$  NMR (499 MHz, DMSO- $d_6$ )  $\delta$  8.75 (d,  $J$  = 4.8 Hz, 1H), 8.07 – 8.01 (m, 2H), 7.73 (t,  $J$  = 6.1 Hz, 1H);  $^{13}\text{C}$  NMR (126 MHz, DMSO- $d_6$ )  $\delta$  151.37, 138.00, 133.98, 128.20, 127.66, 117.32. HRMS (ESI): Calcd for  $\text{C}_6\text{H}_4\text{N}_2$  (M +H) $^+$  104.04, found 104.10.

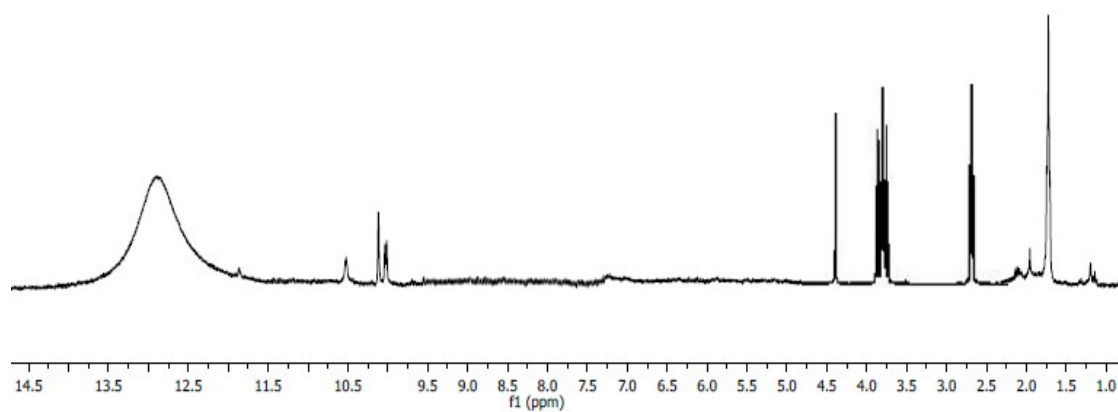


2-Nitrobenzonitrile (2k). Yellow solid, mp 109-110 ° C;  $^1\text{H}$  NMR (499 MHz, DMSO- $d_6$ )  $\delta$  8.42 – 8.35 (m, 1H), 8.17 (dd,  $J$  = 5.7, 3.4 Hz, 1H), 7.98 (dd,  $J$  = 6.0, 3.4 Hz, 2H);  $^{13}\text{C}$  NMR (126 MHz, DMSO- $d_6$ )  $\delta$  149.39, 135.51, 134.36, 133.83, 124.14, 115.13, 107.96. HRMS (ESI): Calcd for  $\text{C}_7\text{H}_4\text{N}_2\text{O}_2$  (M +H) $^+$  148.03, found 148.10.

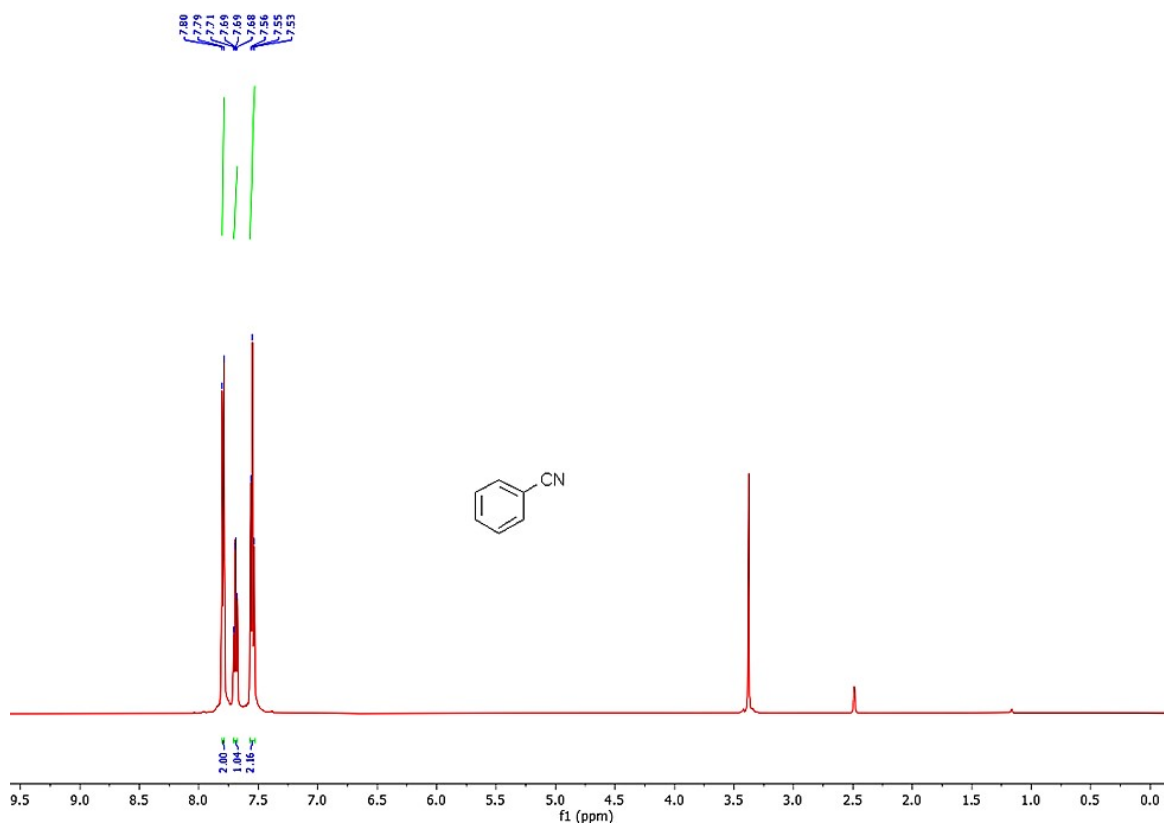


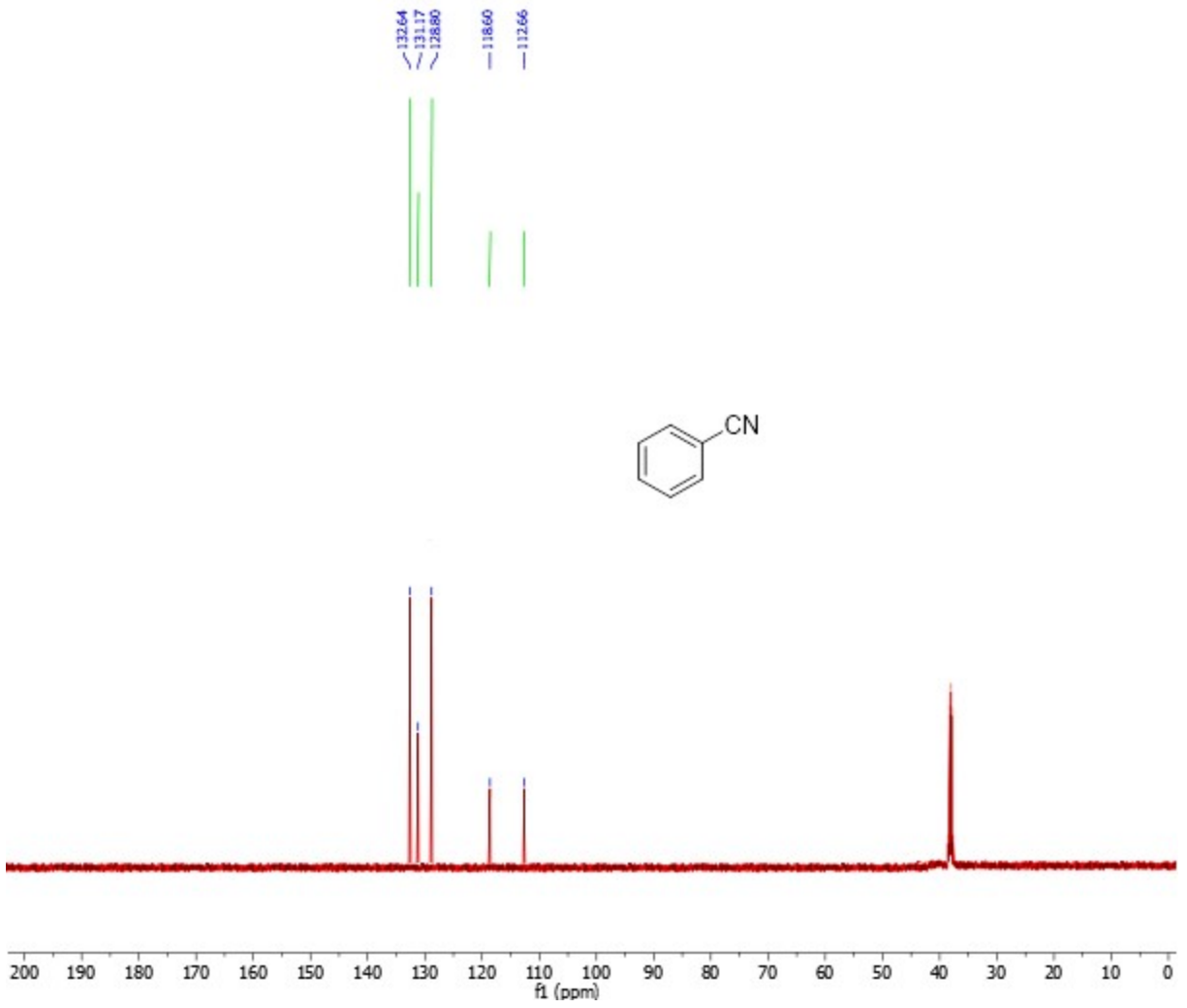
4-Methoxybenzotrile (2m). White solid, mp 60-61 ° C; <sup>1</sup>H NMR (499 MHz, DMSO-*d*<sub>6</sub>) δ 7.76 (d, *J* = 8.6 Hz, 2H), 7.09 (d, *J* = 8.6 Hz, 2H), 3.83 (s, 3H); <sup>13</sup>C NMR (126 MHz, DMSO-*d*<sub>6</sub>) δ 163.10, 133.88, 118.55, 114.22, 104.08, 55.32.. HRMS (ESI): Calcd for C<sub>13</sub>H<sub>13</sub>N<sub>2</sub>O (M +H)<sup>+</sup> 133.05, found 133.10.

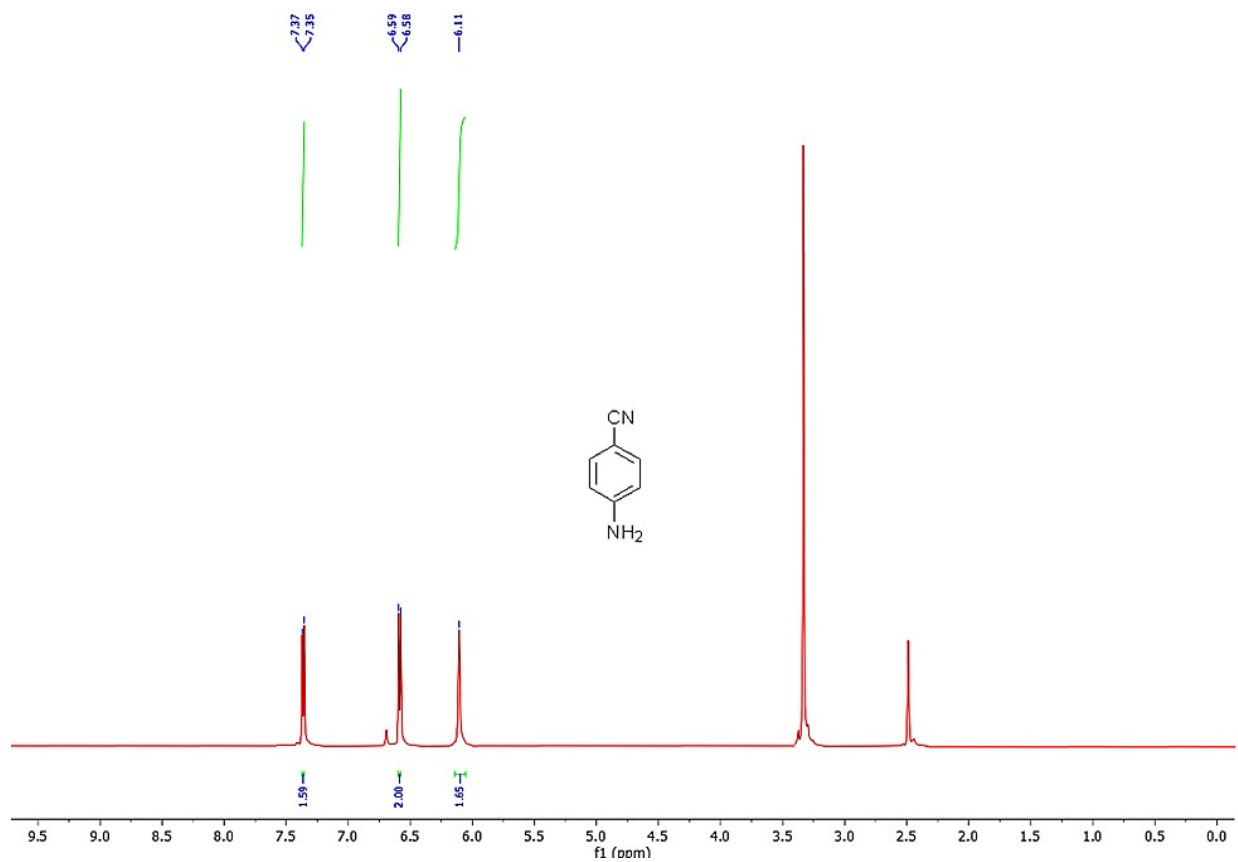
### <sup>1</sup>H NMR of TCT/B<sub>5</sub>

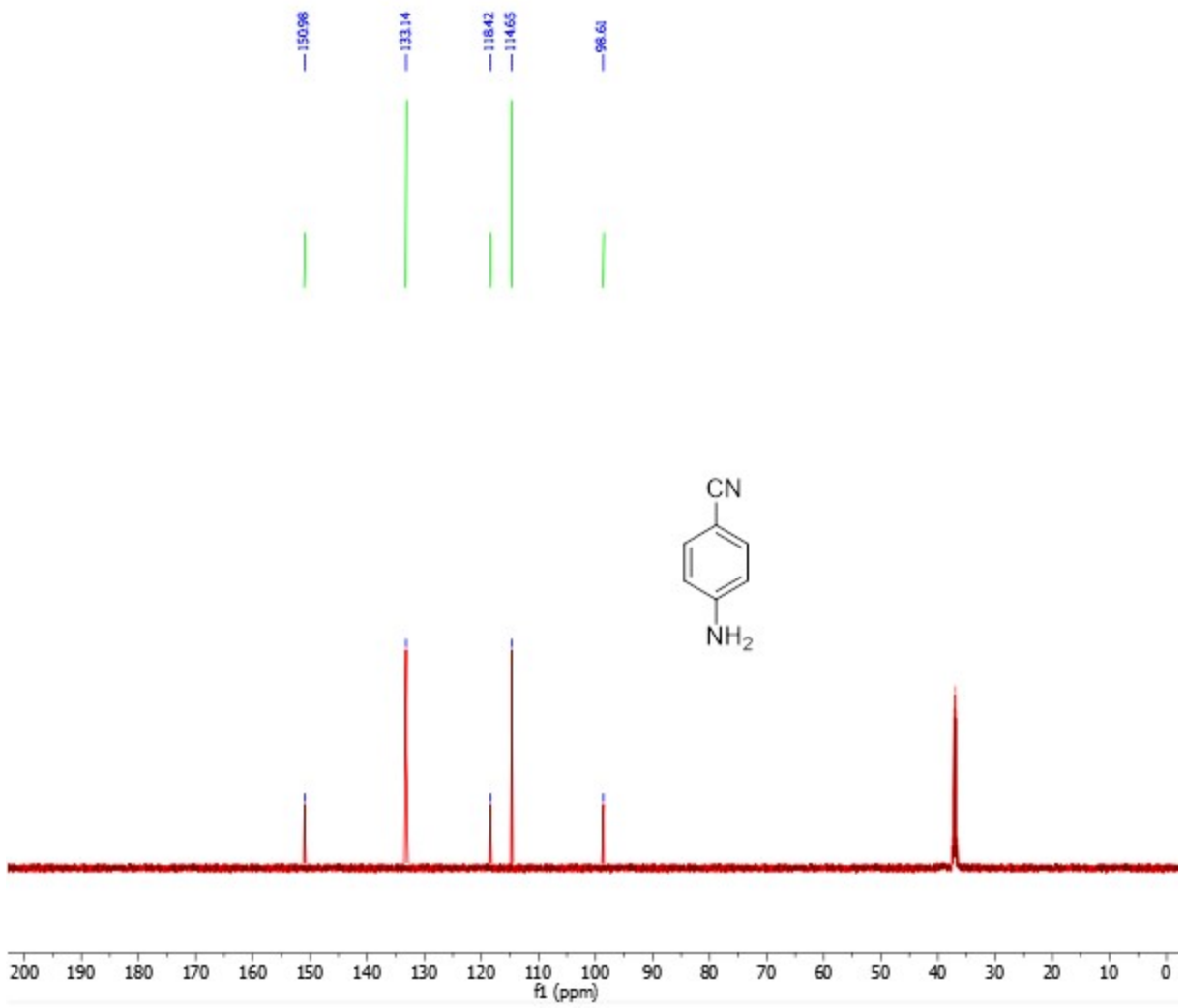


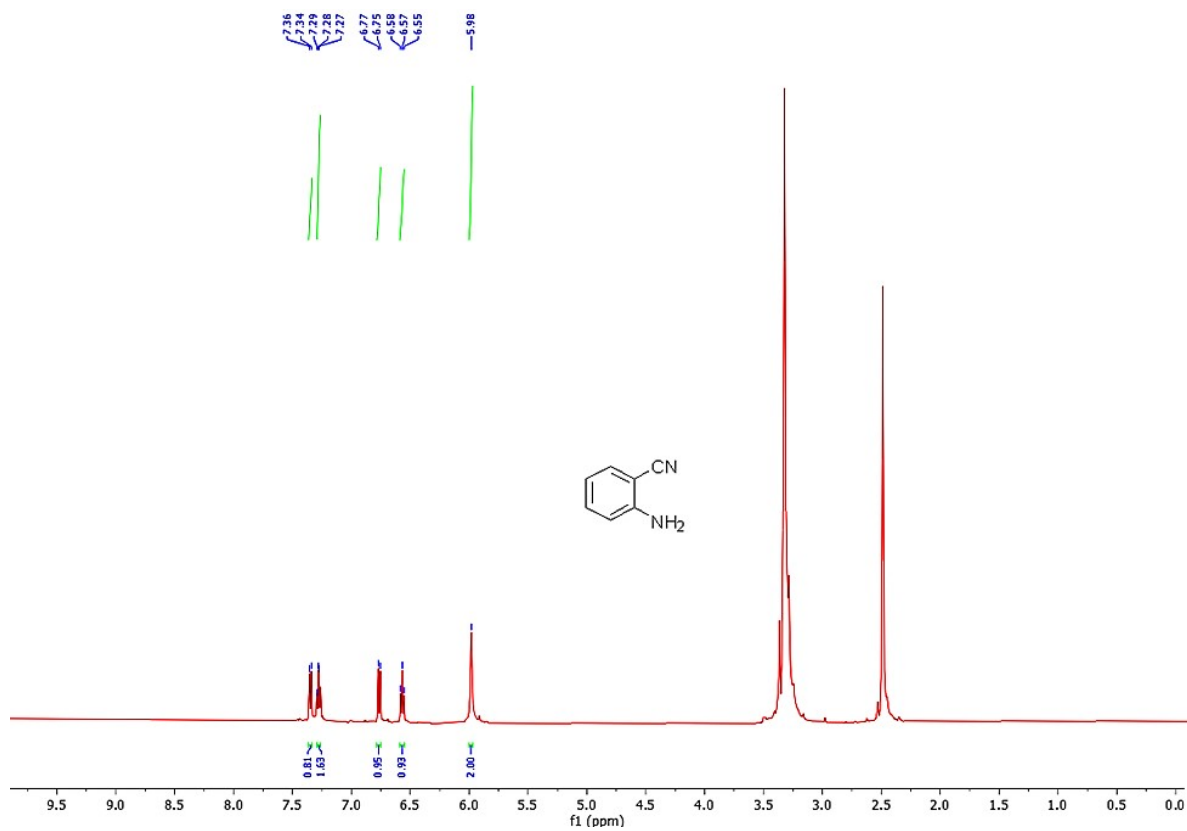
**$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of aryl nitrile derivatives:**



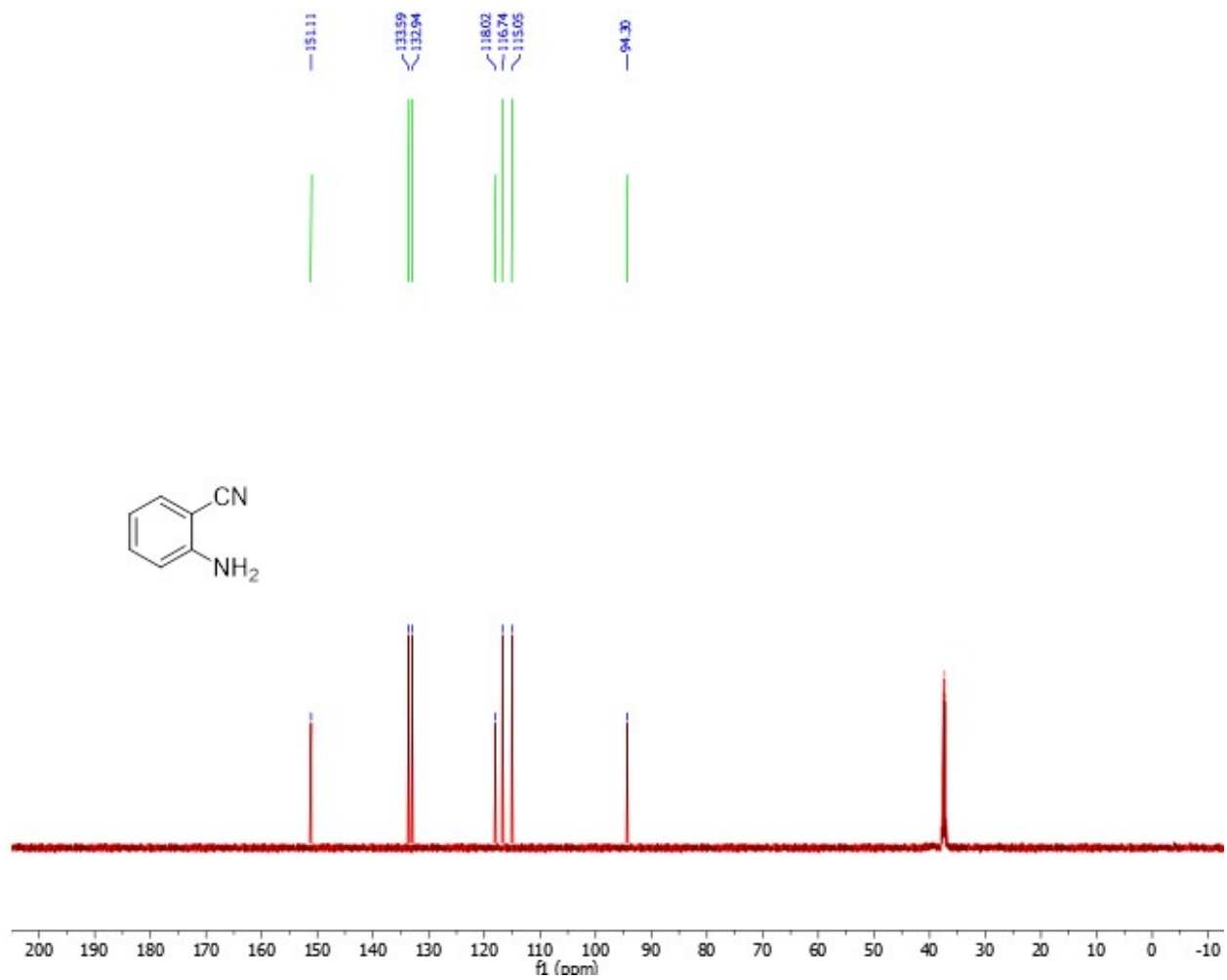


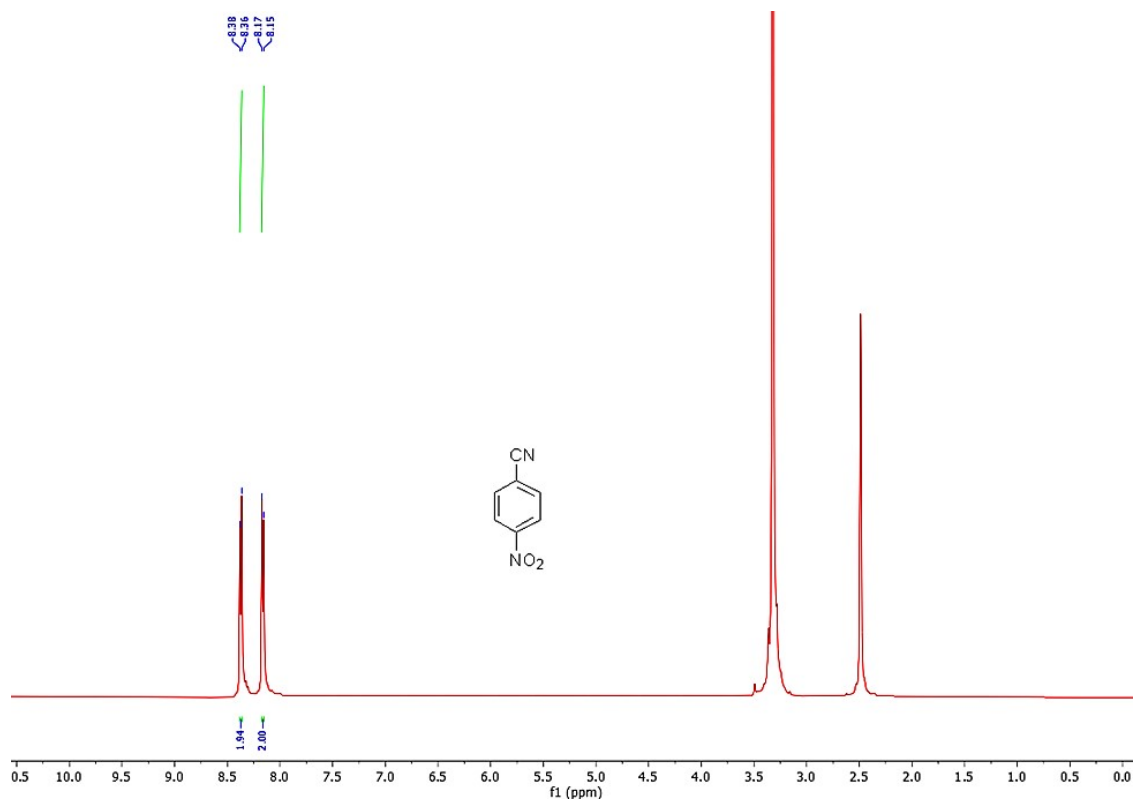


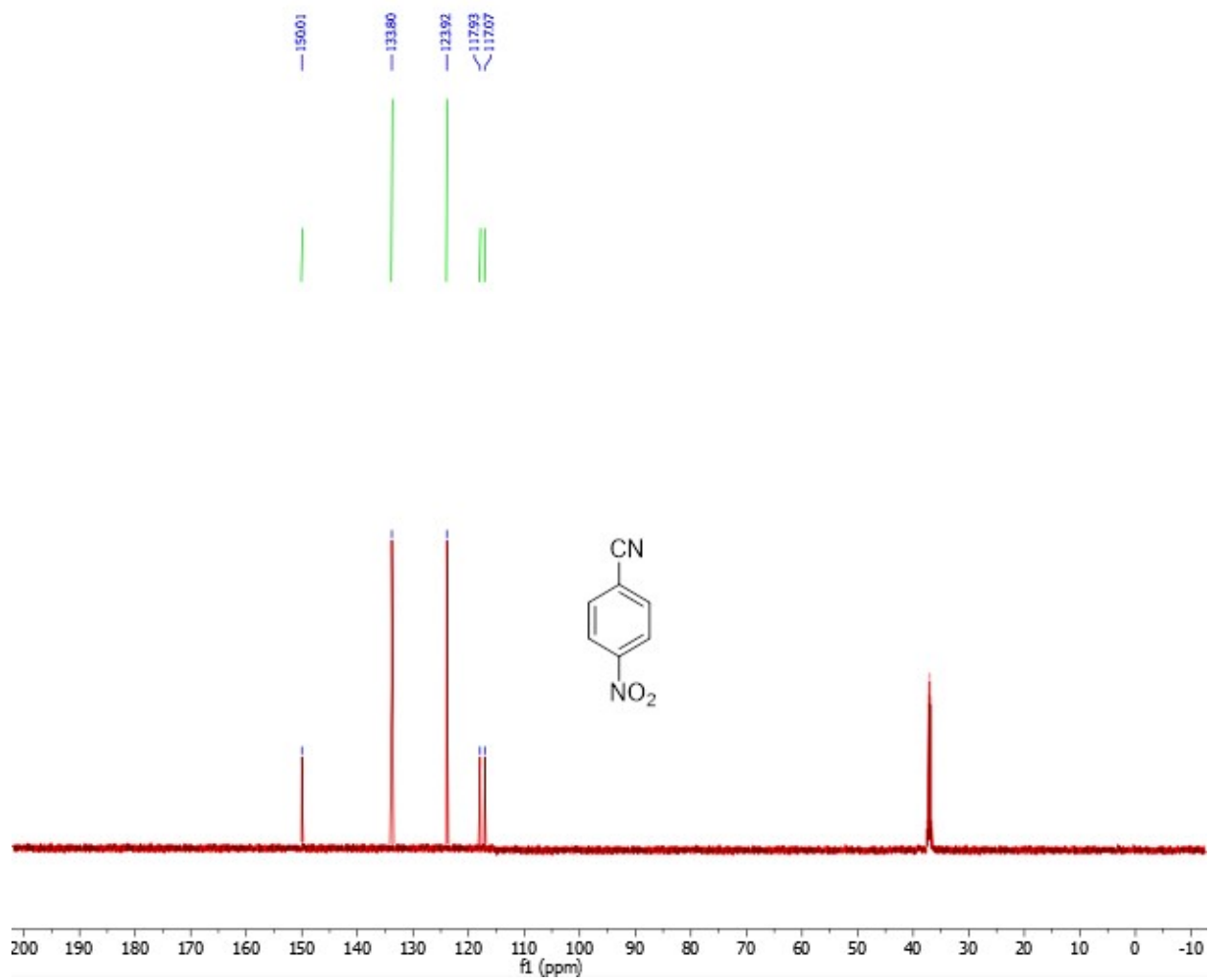


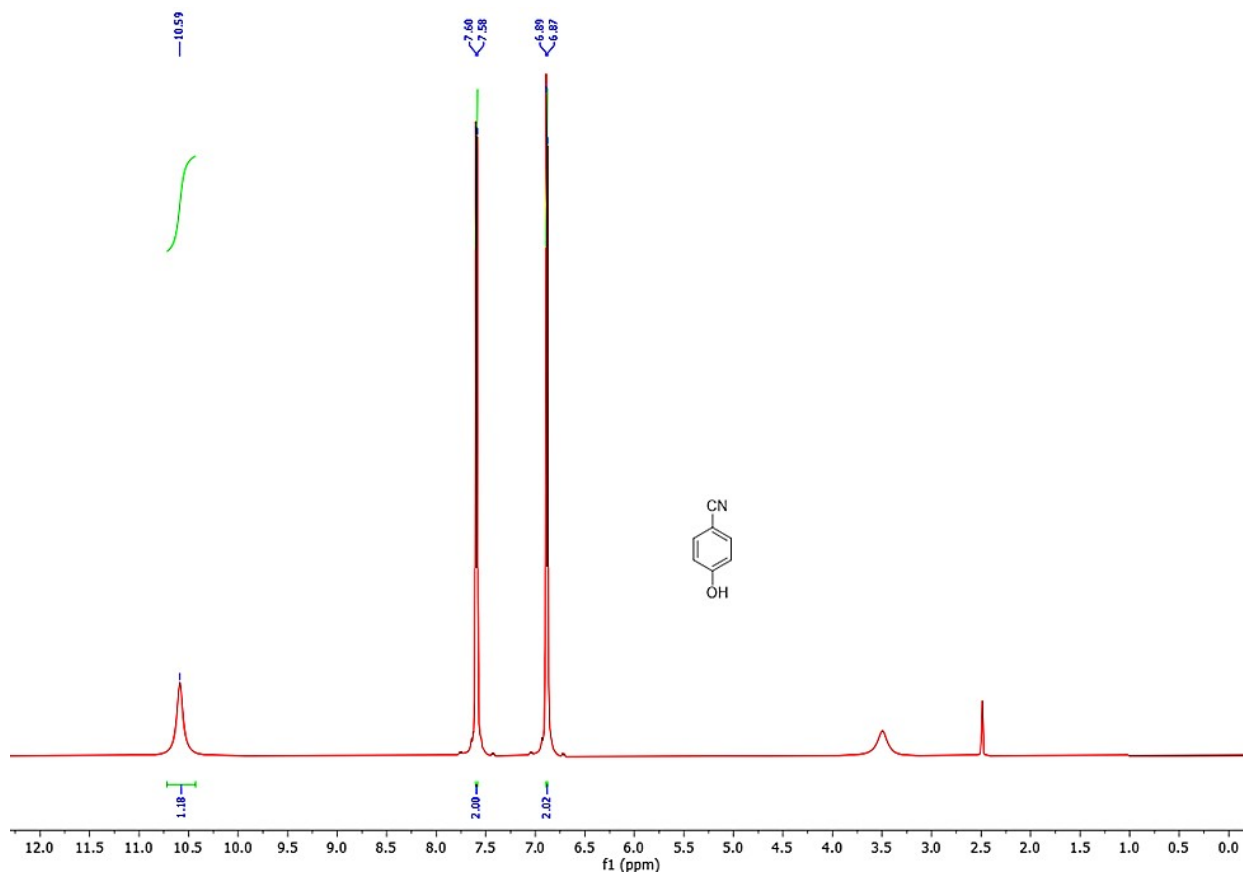


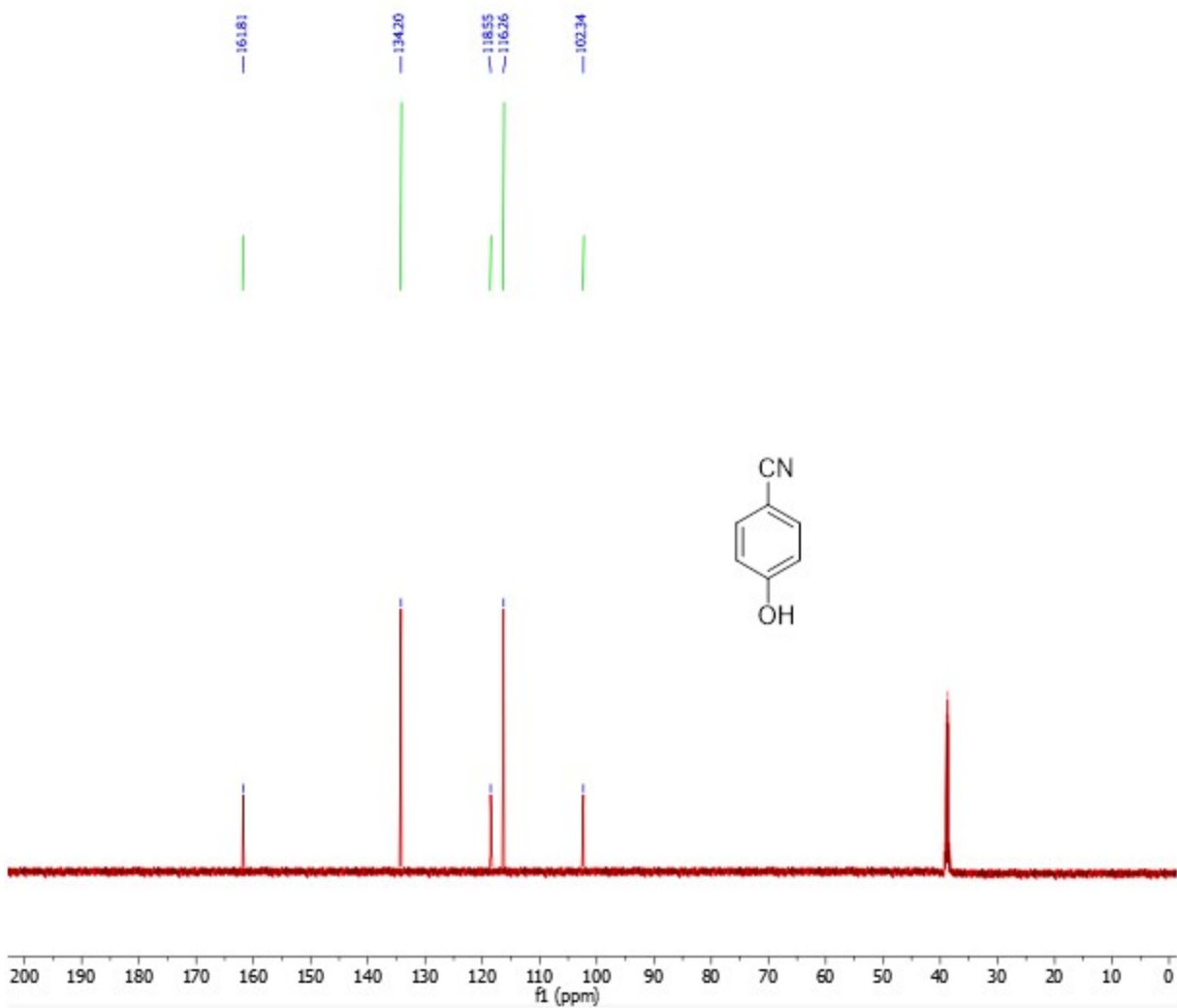


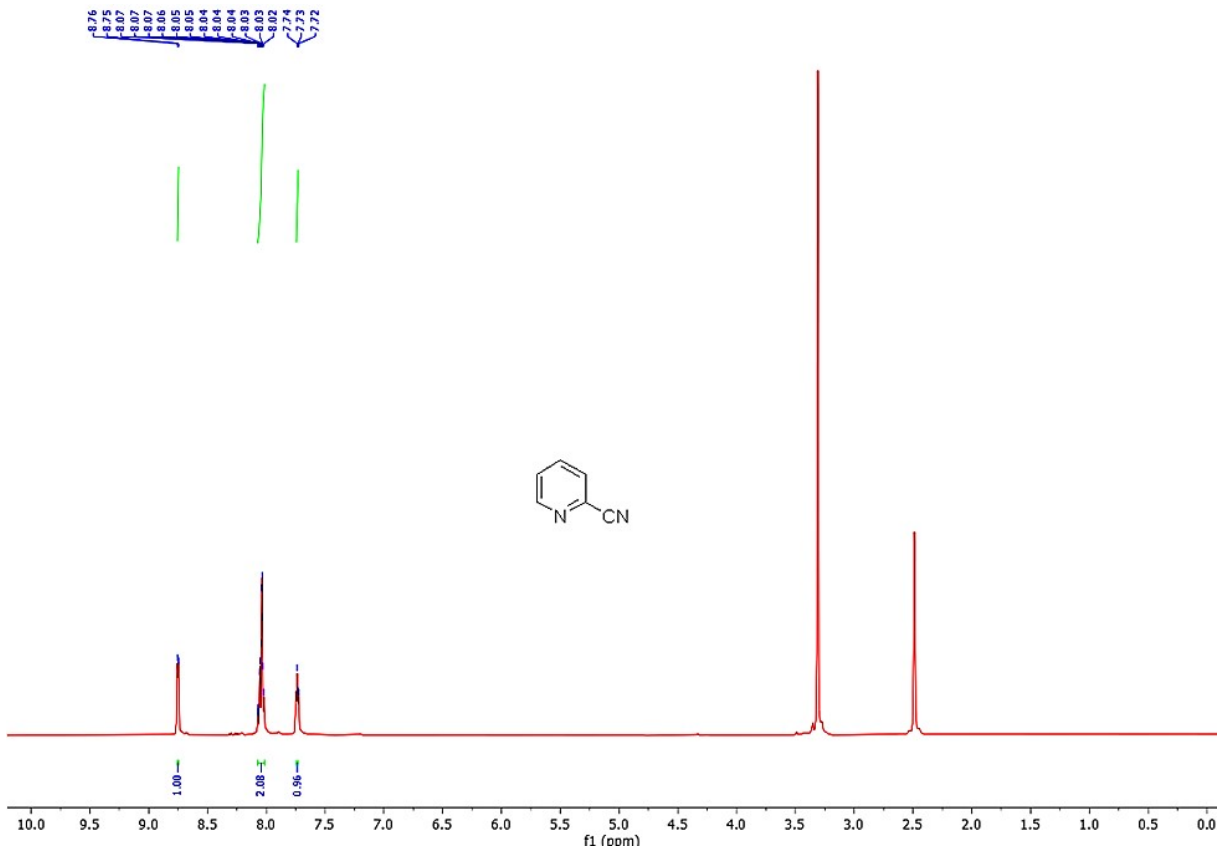


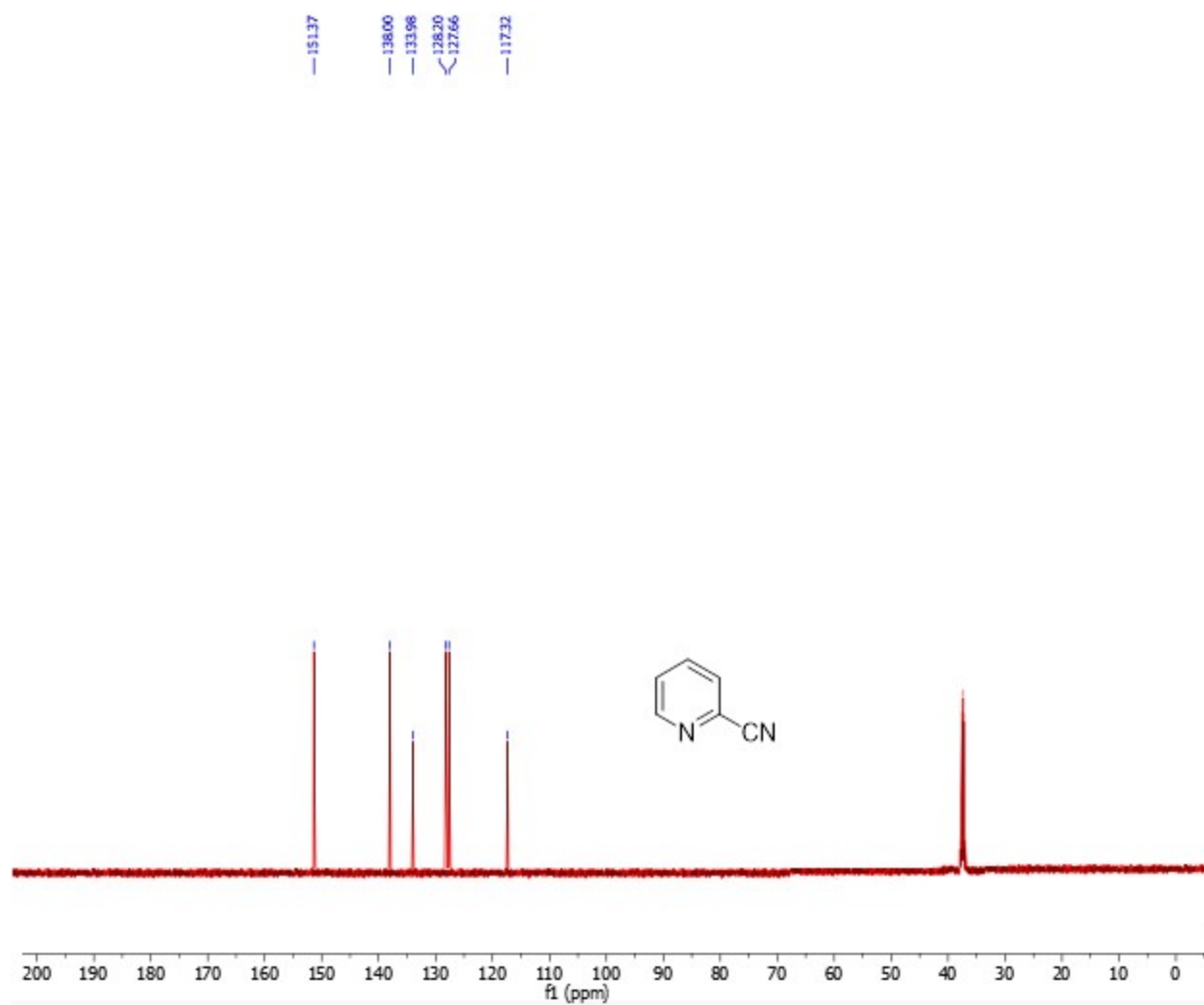


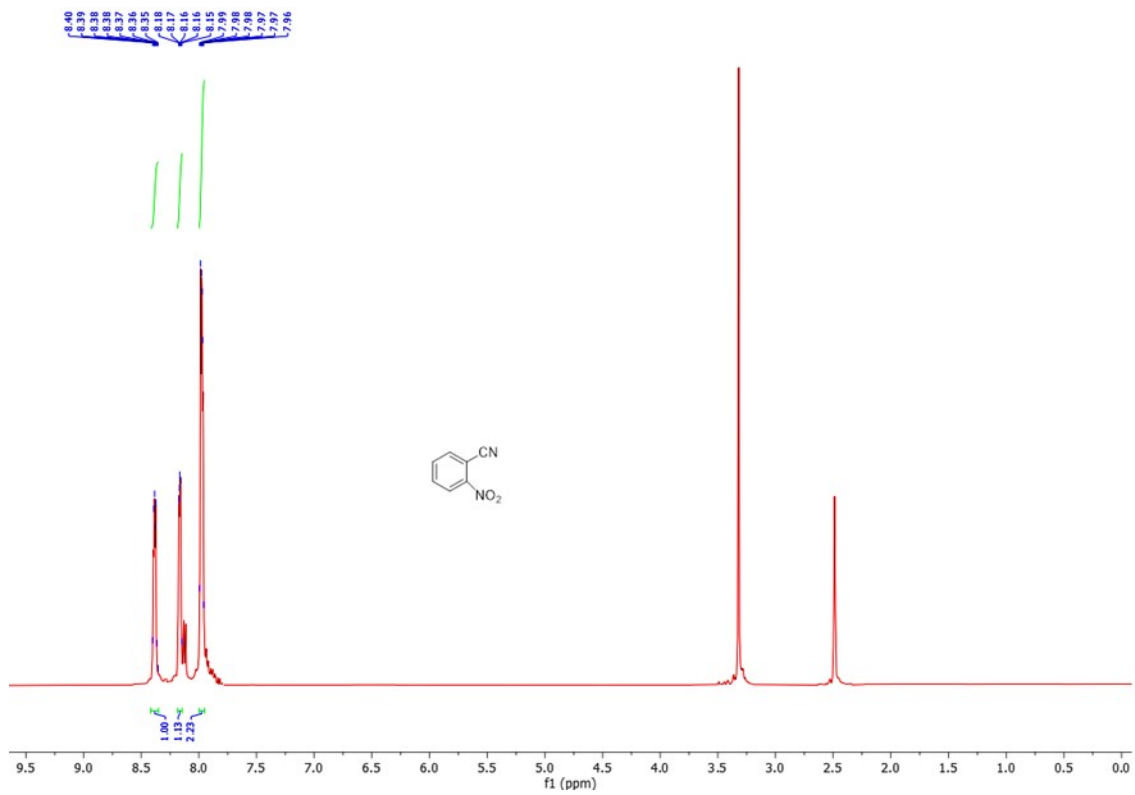




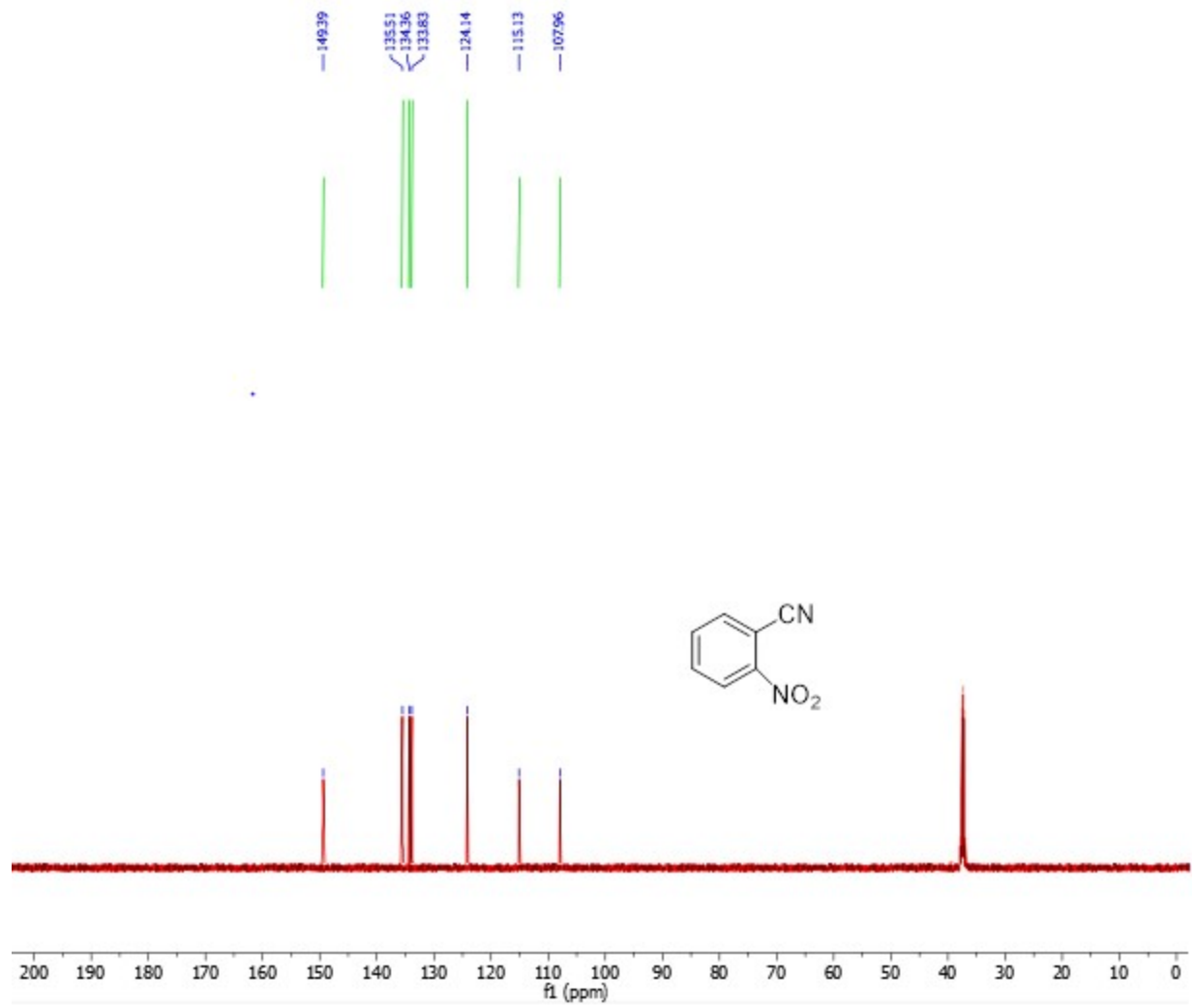


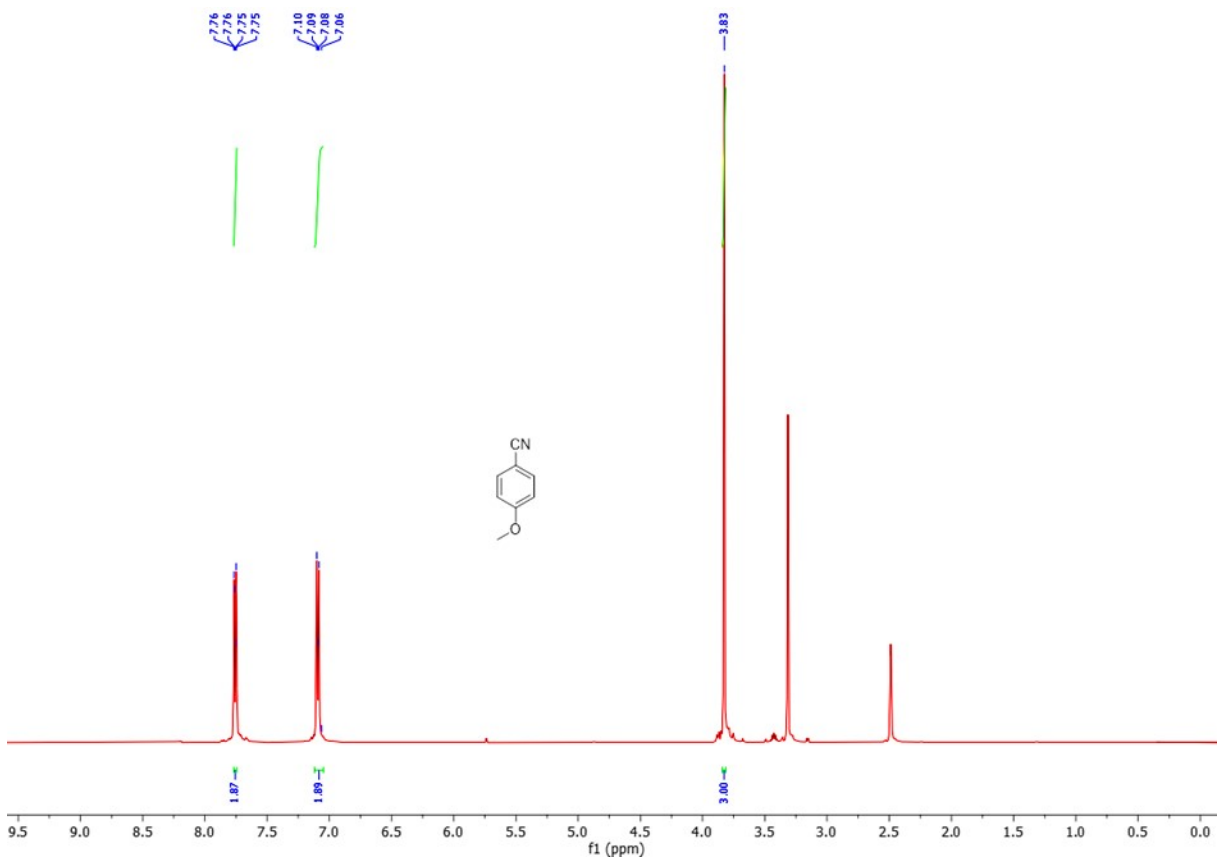


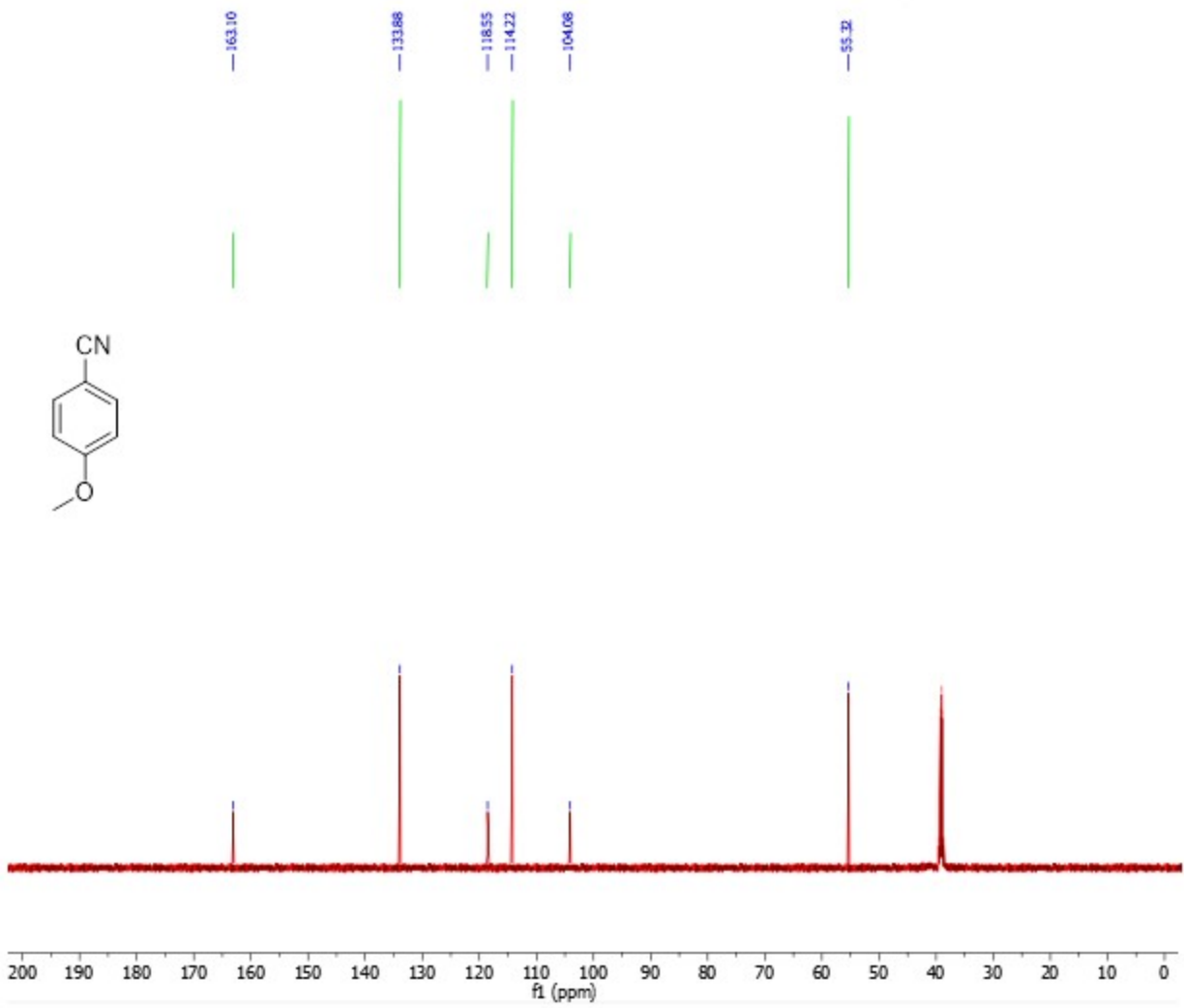












**References:**

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