# Regioselective ethoxycarbonylation of Indoles and Indazoles using DEAD and Tetraethylammonium cyanide

Appaswami Lalitha,*[a] Samikannu Ramesh [a,b] and Pirama Nayagam Arunachalam [b]
[a]*Department of Chemistry, Periyar University, Salem- 636011, India.
[b]Syngene International Ltd, Bangalore, India- 560 099, India

Fax: +91-427-2345124
E-mail: lalitha2531@yahoo.co.in

**Contents:**



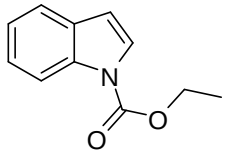
## 1. General Experimental Details

General procedure: Under nitrogen atmosphere, a reaction flask charged with indole or indazole (0.2 mmol),[a] tetraethyl ammonium cyanide (0.4 mmol),[a] and aectonitrile (2 mL) was cooled to 0 °C and DEAD (0.4mmol)[a] was added slowly (dropwise) at this temperature. After the addition, reaction mass was slowly warmed to RT and at RT the reaction mass was stirred for 12hduring while the reaction was monitored by TLC. After the completion of the reaction , 10 mL of ethylacetate was added and the mixture was washed with water (3×5 mL). Then the organic layer was concentrated in vacuum and the residue was purified by flash column chromatography on a silica gel to give the desired product. Thin layer chromatography was performed on silica gel plates. Silica gel (Merck, 230-400 mesh) was used for flash column chromatography. $^{1}$H and $^{13}$C NMR spectra were recorded on a Bruker (400 MHz) spectrometer and the COSY spectra were recorded on a Varian (500MHz) spectrometer. Chemical shift values (δ) are given in ppm and are referenced to residual solvent peaks ($^{1}$H and $^{13}$C NMR). Coupling constants (*J*) were reported in hertz (Hz). Mass spectra and high resolution mass spectra (LC-MS) were also reported. X-ray crystal structure was obtained by Bruker CCD area detector diffractometer.

[a](For nitro subsituted indole or indazole, the reaction mixture composition was as follows : indole/indazole (0.2 mmol), tetraethyl ammonium cyanide (0.6 mmol), DEAD (0.6 mmol))

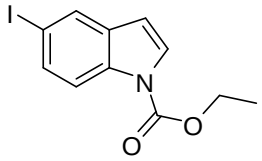
## 2. Characterization data for compounds

**01**



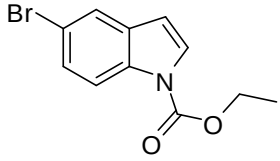
**Ethyl 1*H*- indole-1-carboxylate (2a)** (Reported[1]): Yellow viscous oil, $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.37–1.41 (t, $J$ = 4,4 Hz,3H), 4.39–4.44 (q, $J$ = 4 Hz, 2H), 6.51–6.52 (d, $J$ = 4 Hz, 1H), 7.14–7.18 (m, 1H, ArH), 7.23–7.27 (m 1H, ArH), 7.48–7.50 (dd, 1H),7.50–7.54 (d, $J$ = 16 Hz, 1H ArH) 8.10–8.12 (b, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.39, 63.14, 107.90, 115.14, 120.95, 122.88, 124.39, 125.53, 130.50, 135.23, 151.07 ppm. MS: m/z = 189.22 $(M)^+$.

**02**



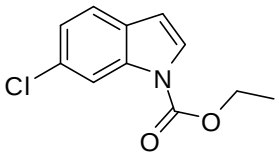
**Ethyl 5-iodo-1*H*-indole-1-carboxylate (2b)** (Reported[2]): Viscous oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.37–1.40 (t, 3H), 4.38–4.43 (q, 2H), 6.45–6.45 (d, $J$ = 4 Hz, 1H), 7.04–7.07 (dd, 1H, ArH), 7.51–7.52 (d, 1H, ArH), 7.69 (s, 1H ArH),7.97–7.99 (b, $J$ = 7.2 Hz, 1H) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.42, 28.40, 63.13, 108.00, 110.85, 115.30, 116.41, 126.41, 131.09, 133.75,153.11 ppm. MS: m/z = 315.11 $(M)^+$.

**03**



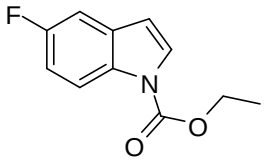
**Ethyl 5-bromo-1*H*-indole-1-carboxylate (2c)** (Reported[3]) : Yellow viscous oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.47–1.50 (t, 3H), 4.48–4.54 (q, 2H), 6.57–6.58 (d, $J$ = 4 Hz, 1H), 7.21–7.24 (dd, ArH), 7.46–7.48 (dd, 1H, ArH), 7.61–7.62 (d, 1H, ArH), 8.22 (b, 1H) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.40, 63.51, 107.64, 115.47, 121.64, 123.53, 126.14, 128.97, 130.42 ppm. MS: m/z = 268.11 $(M)^+$.

**04**



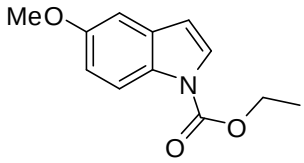

**Ethyl 6-chloro-1*H*-indole-1-carboxylate (2d)** (Reported[4]**):** Colorless viscous oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.46–1.49 (t, 3H), 4.47–4.53 (q, 2H), 6.55–6.56 (d, $J$ = 4 Hz, 1H), 7.20–7.23 (q, 1H, ArH), 7.45–7.47 (d, 1H, ArH), 7.60–7.61 (d, 1H, ArH), 8.21(b, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.40,63.51, 107.63, 115.47, 121.64, 123.53, 126.14, 128.97, 130.42, 150.73 ppm. MS: m/z = 223.66 $(M)^+$.

**05**



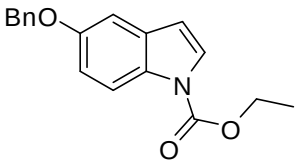

**Ethyl 5-fluoro-1*H*-indole-1-carboxylate (2e)** (Reported[5]): Light yellow viscous oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.38–1.41 (t, 3H), 4.39–4.45 (q, 2H), 6.47–6.48 (dd, $J$ = 4Hz, 1H), 6.95–7.00 (dt 1H, ArH), 7.13–7.16 (dd, 1H, ArH), 7.58–7.59 (d, 1H, ArH), 8.04–8.05 (b, 1H ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.39, 63.32, 106.31, 106.54, 107.60, 107.64, 112.06, 112.31, 116.01, 116.10, 127.09, 131.30, 131.40, 131.62, 150.82, 158.19, 160.56 ppm. MS: m/z = 207.22 $(M)^+$.

**06**



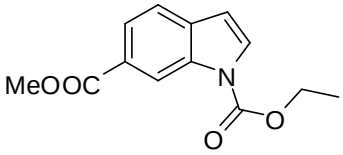

**Ethyl 5-methoxy-1*H*-indole-1-carboxylate (2f)** (Reported[1d]): Colorless Viscous oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.44–1.48 (t, 3H),3.85 (s, 3H), 4.45–4.50 (q, 2H), 6.51–6.52 (dd, $J$ = 4 Hz, 1H), 6.92–6.95 (dd, 1H, ArH), 7.03–7.03 (d, 1H, ArH), 7.58–7.59 (d, $J$ = 4 Hz,1H, ArH), 8.04–8.06 (b, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.41,55.68, 63.07, 103.63, 107.76, 113.14, 115.83, 126.18, 129.96, 131.36, 151.00, 156.06 ppm. MS: m/z = 219.24 $(M)^+$.

07



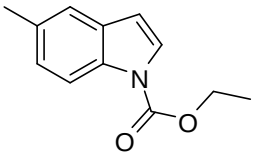

**Ethyl 5-(benzyloxy)-1*H*-indole-1-carboxylate (2g)** (Reported[6]): Yellow pasty mass. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.35–1.39 (t, 3H), 4.36–4.41 (q, 2H), 5.028 (s, 3H),6.42–6.43 (d, $J$ = 4 Hz, 1H), 6.92–6.95 (dd, 1H, ArH), 7.02–7.03 (d, $J$ = 4 Hz, 1H, ArH), 7.22–7.24 (t, 1H, ArH),7.25–7.30 (dt 2H, ArH), 7.37–7.39 (d, $J$ = 8 Hz, 2H ArH) 7.50–7.51 (d, $J$ = 4 Hz, 1H, ArH), 7.97–7.99(b, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.40, 63.07, 70.60, 105.05, 107.78, 113.92, 115.85, 126.20, 127.45, 127.87, 128.53, 130.13, 131.31, 137.29, 150.98, 155.21 ppm. MS: m/z = 309.37 $(M)^+$.

08



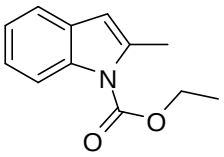

**4- Ethyl 6-methyl-1*H*-indole-1,6-carboxylate (2h)** (Not Reported): Off white soild. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.48–1.51 (t, 3H), 3.94 (s, 3H), 4.50–4.56 (q, 2H), 6.63–6.64 (d, $J$ = 4 Hz, 1H), 7.58–7.60 (dd $J$ = 4 Hz, 1H, ArH), 7.76–7.77 (d, $J$ = 4 Hz,1H, ArH), 7.93–7.96 (dd, 1H, ArH), 8.88 (b, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.35, 52.06, 63.59, 107.75, 117.02, 120.65, 124.15, 126.26, 128.50, 134.23, 134.67, 150.71,167.6 ppm. MS: m/z = 247.25 $(M)^+$.

09



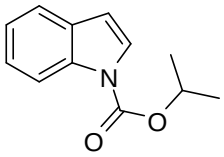

**Ethyl 5-methyl-1*H*-indole-1-carboxylate (2i)** (Reported[7]): Yellow pasty mass. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.45–1.49 (t, 3H), 2.45 (s, 3H) 4.46–4.52 (q, 2H), 6.52–6.53 (d, $J$ = 4 Hz, 1H), 7.14–7.16 (d, $J$ = 8 Hz, 1H, ArH), 7.36 (s, 1H, ArH), 7.58–7.59 (d, $J$ = 4 Hz, 1H, ArH), 8.04–8.06 (b, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.44, 21.30, 63.06, 107.68, 114.76, 120.90, 125.60, 125.76, 130.75, 132.37 ppm. MS: m/z = 203.24 $(M)^+$.

10



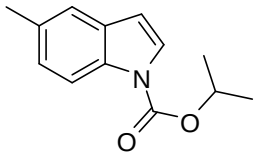
**Ethyl 2-methyl-1*H*-indole-1-carboxylate (2j)** (Reported[1d, 8]) : Yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.39–1.42 (t, 3H), 2.62 (s, 3H), 4.48–4.53 (q, 2H), 6.34 (s, 1H), 7.18–7.26 (m, 2H, ArH), 7.43–7.45 (d, 1H, ArH), 8.10–8.12 (b,1H ArH,) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.37, 16.85, 62.92, 108.41, 115.55, 119.58, 122.85, 123.29, 129.60, 137.88, 152.33 ppm. MS: m/z = 203.24 $(M)^+$.

11



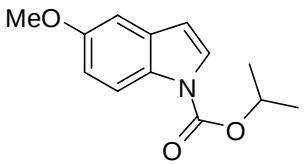

**Isopropyl-1*H*-indole-1-carboxylate (2k)** (Reported[1d]) : Viscous oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.36–1.38 (d, $J$ = 8 Hz,6H), 5.16–5.22 (m, 1H), 6.49–6.50 (d, $J$ = 4 Hz, 1H), 7.13–7.17 (m, 1H, ArH), 7.22–7.26 (m, 1H, ArH), 7.47–7.49 (d, $J$ = 8 Hz,1H, ArH),7.53–7.54 (d, $J$ = 4 Hz, 1H, ArH) 8.09–8.11 (b, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 21.98, 71.33, 107.69, 115.16, 120.93, 122.79, 124.31, 125.59, 130.53, 135.23, 150.65 ppm. MS: m/z = 203.24 $(M)^+$.

12




**Isopropyl 5-methyl-1*H*-indole-1-carboxylate (2l)** (Not Reported) : Yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.37–1.38 (d, $J$ = 4.4 Hz,6H), 2.36(s, 3H), 5.15–5.22 (m, 1H), 6.43–6.44 (d, $J$ = 4 Hz, 1H), 7.05–7.07 (dd, $J$ = 4 Hz, 1H, ArH), 7. 27 (s, 1H, ArH), 7.49–7.50 (d, 1H, ArH), 7.95–7.97 (b, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 21.27,22.01, 71.20, 107.45, 114.78, 120.85, 125.68, 130.77, 132.26, 133.43, 150.68, ppm. MS: m/z = 217.27 $(M)^+$.

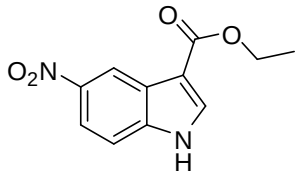
13




**Isopropyl 5-methoxy-1*H*-indole-1-carboxylate (2m)** (Not Reported): Yellow oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.44–1.46 (d, $J$ = 8 Hz,6H), 3.85 (s, 3H), 5.22–5.29 (m, 1H), 6.51–6.52 (dd, $J$ = 4 Hz, 1H), 6.92–6.95 (dd, $J$ = 4 Hz, 1H ArH), 7.03 (d, 1H, ArH),

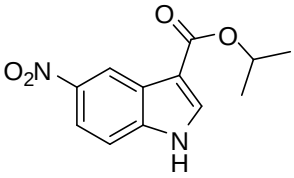
7.59 (d, 1H, ArH), 8.03–8.06 (b,1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 22.01, 55.69, 71.25, 103.60, 107.56, 113.09, 115.86, 126.25, 127.66, 131.38, 150.59, 156.01 ppm. MS: m/z = 233.27 $(M)^+$.

14



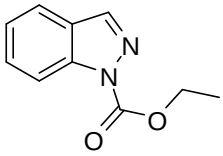
**Ethyl 5-nitro-1*H*-indole-3-carboxylate (2n)** (Reported[11]): Off white solid. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.53–1.57 (t, 3H), 4.61–4.66 (q, 2H), 8.36–8.46 (m, 3H, ArH), 8.70–8.71 (d, $J$ = 4 Hz, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.34, 64.97, 115.12, 118.00, 124.10, 140.68 ppm. MS: m/z = 234.21 $(M)^+$.

**15**



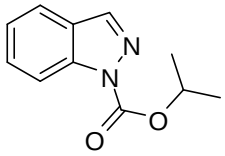
**Isopropyl 5-nitro-1*H*-indole-3-carboxylate (2o)** (Not Reported): Off white solid. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.53–1.55 (d, $J$ = 4.4 Hz,6H), 5.37–5.43 (m, 1H), 8.35–8.45 (dd, 3H, ArH), 8.70–8.71 (dd, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 21.87, 73.67, 115.15, 117.98, 123.99, 125.51, 140.54, 142.18, 144.53, 149.66 ppm. MS: m/z = 248.24 $(M)^+$.

**16**



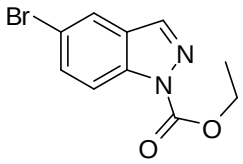
**Ethyl 1*H*-indazole-1-carboxylate (2p)** (Reported[9 a,b]) **:** Yellow color oil. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.52–1.57 (t, 3H), 4.58–4.63 (q, 2H), 7.33–7.37 (t, 1H, ArH), 7.55–7.59 (t, 1H, ArH), 7.75–7.77 (d, $J$ = 8 Hz,1H, ArH), 8.20 (s, 1H, ArH),8.25–8.27 (d, $J$ = 8 Hz, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.43, 64.05, 114.52, 121.15, 124.00, 125.88, 129.21, 139.88, 140.13, 150.74 ppm. MS: m/z = 190.20 $(M)^+$.

**17**



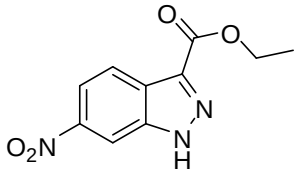
**Isopropyl 1*H*-indazole-1-carboxylate (2q)** (Not Reported): Yellow color viscous oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.52–1.53 (d, $J$ = 4.4 Hz,6H), 5.35–5.42 (m, 1H), 7.32–7.36 (t, 1H, ArH), 7.54–7.58 (t, 1H, ArH), 7.74–7.76 (d, $J$ = 8 Hz,1H, ArH), 8.20 (s, 1H, ArH),8.23–8.26 (d, $J$ = 12 Hz, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 21.95, 72.43, 114.58, 115.21, 121.13, 123.89, 125.89, 129.12, 139.87, 139.98, 150.33 ppm. MS: m/z = 204.23 $(M)^+$.

**18**



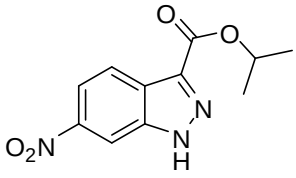
**Ethyl 5-bromo-1*H*-Indazole-1-carboxylate (2r)** (Not Reported): Yellow color oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.50–1.54 (t, 3H), 4.56–4.62 (q, 2H), 7.62–7.65 (dd, 1H, ArH), 7.88–7.89 (d, $J$ = 4 Hz, 1H, ArH), 8.12–8.14 (d, $J$ = 8 Hz, 2H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.38, 64.38, 115.92, 117.23, 123.71, 127.42, 132.28, 138.69, 138.97, 150.41 ppm. MS: m/z = 269.10 $(M)^+$.

**19**



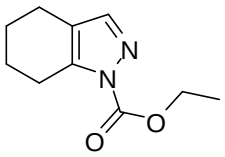
**Ethyl 5-nitro-1*H*-indazole-3-carboxylate (2s)** (Reported [12]): Off white solid. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.53–1.57 (t, 3H), 4.61–4.66 (q, 2H,), 8.36–8.46 (m, 3H, ArH), 8.70–8.71 (d, $J$ = 4 Hz, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.34, 64.97, 115.12, 118.00, 124.10, 140.68 ppm. MS: m/z = 235.20 $(M)^+$.

**20**



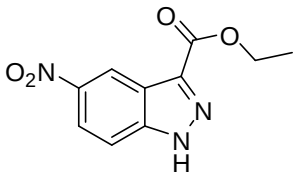
**Isopropyl 5-nitro-1*H*-indazole-3-carboxylate (2t)** (Not Reported) : Off white solid. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.53–1.55 (d, $J$ = 8 Hz, 6H), 5.37–5.43 (m, 1H), 8.35–8.45 (dd, 3H, ArH), 8.70–8.71 (d, $J$ = 4 Hz, 1H, ArH) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 21.87, 73.67, 115.15, 117.98, 123.99, 125.51, 140.54, 142.18, 144.53, 149.66 ppm. MS: m/z = 249.23 $(M)^+$.

**21**




**Ethyl 3a,4,5,6,7,7a- hexahydro-1*H*- indazole-1-carboxylate (2u)** (Reported[10]): Yellow color viscous oil. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$= 1.41–1.46 (t, 3H), 1.66–1.84 (m, 6H), 2.47–2.57 (q, 2H), 2.71–2.93 (q, 2H), 4.45–4.50 (q, 2H), 7.81 (s, 1H) ppm. $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ = 14.35, 20.50, 20.59, 22.33, 22.64, 22.97, 23.75, 24.17, 63.83, 64.12, 120.12, 120.26,127.14, 142.87, 149.75,155.47 ppm. MS: m/z = 194.24 $(M)^+$.

**22**




**Ethyl 5-nitro-1*H*-indazole-3-carboxylate (2v)** (Reported[13]): Off white solid. $^{1}$H NMR (300 MHz, DMSO–d6): $\delta$= 1.45–1.411 (t, 3H), 4.58–4.51 (q, 2H), 8.31–8.34 (dd, 1H, ArH), 8.49–8.46 (dd, 1H, ArH), 8.69–8.691 (d, 1H, ArH), 8.90–8.91 (dd, 1H, ArH) ppm. MS: m/z = 235.20 $(M)^+$.

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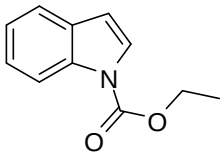
# $^{1}$H NMR – 2a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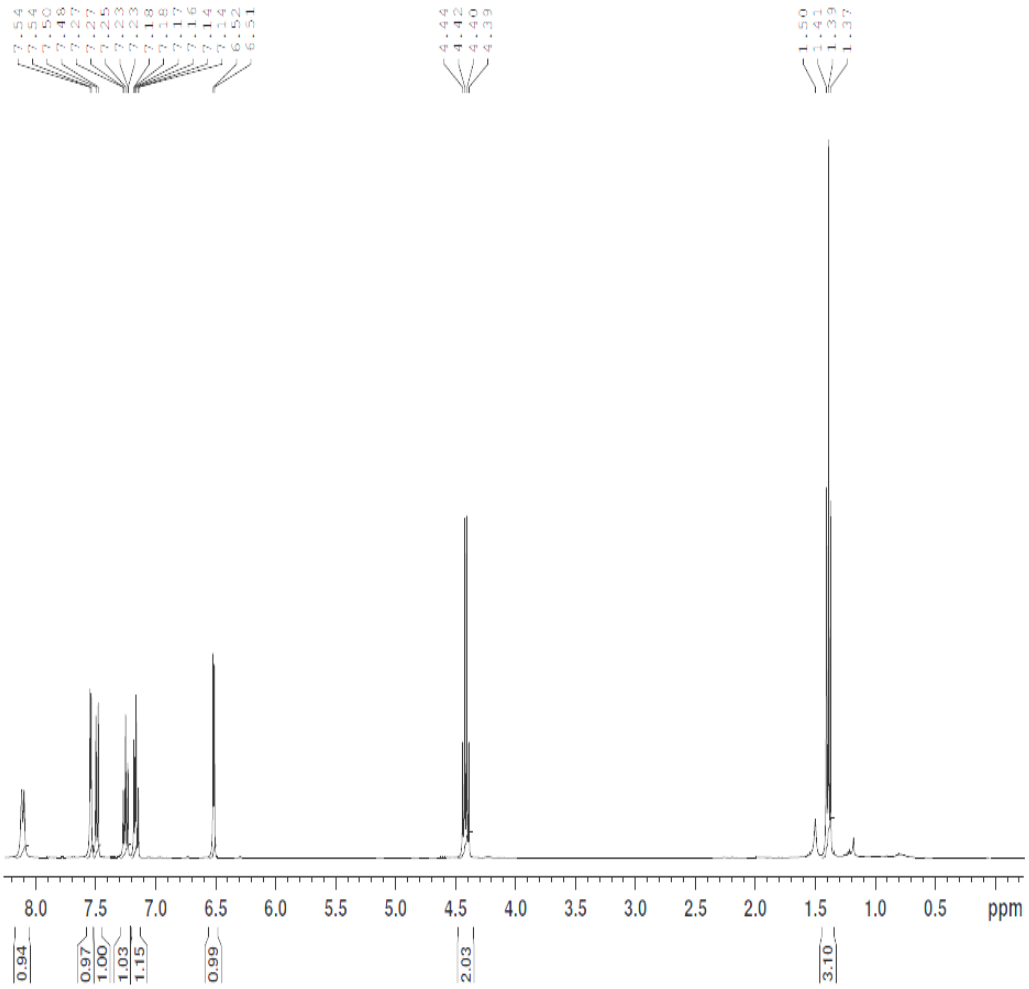
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4.39
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1.41
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2.03
3.10

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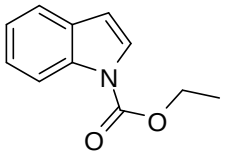


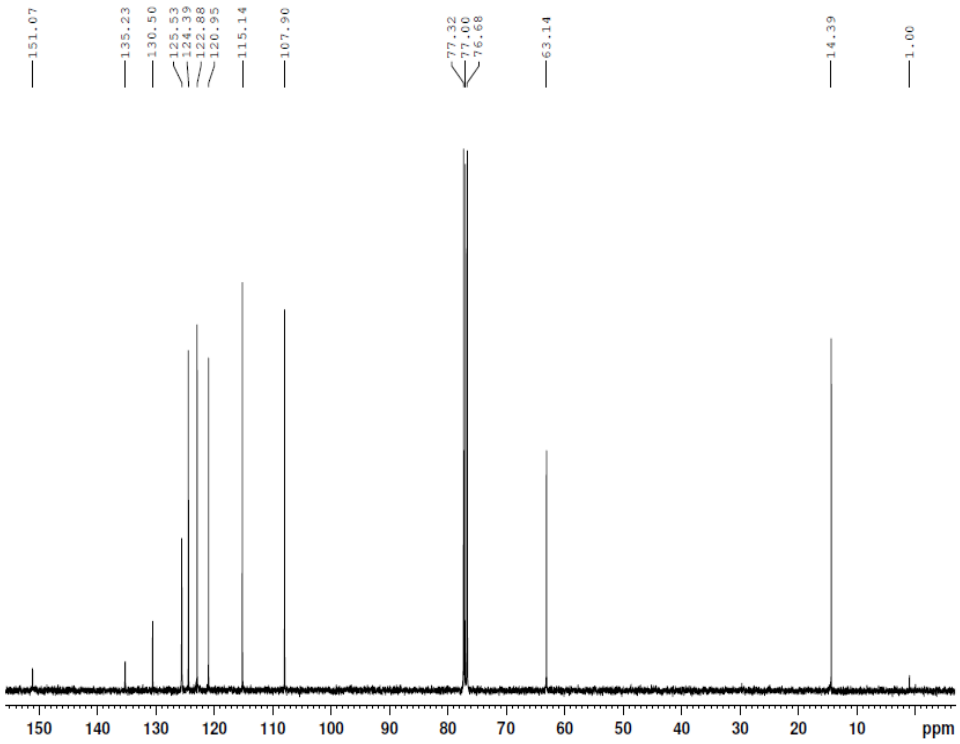

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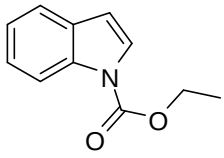


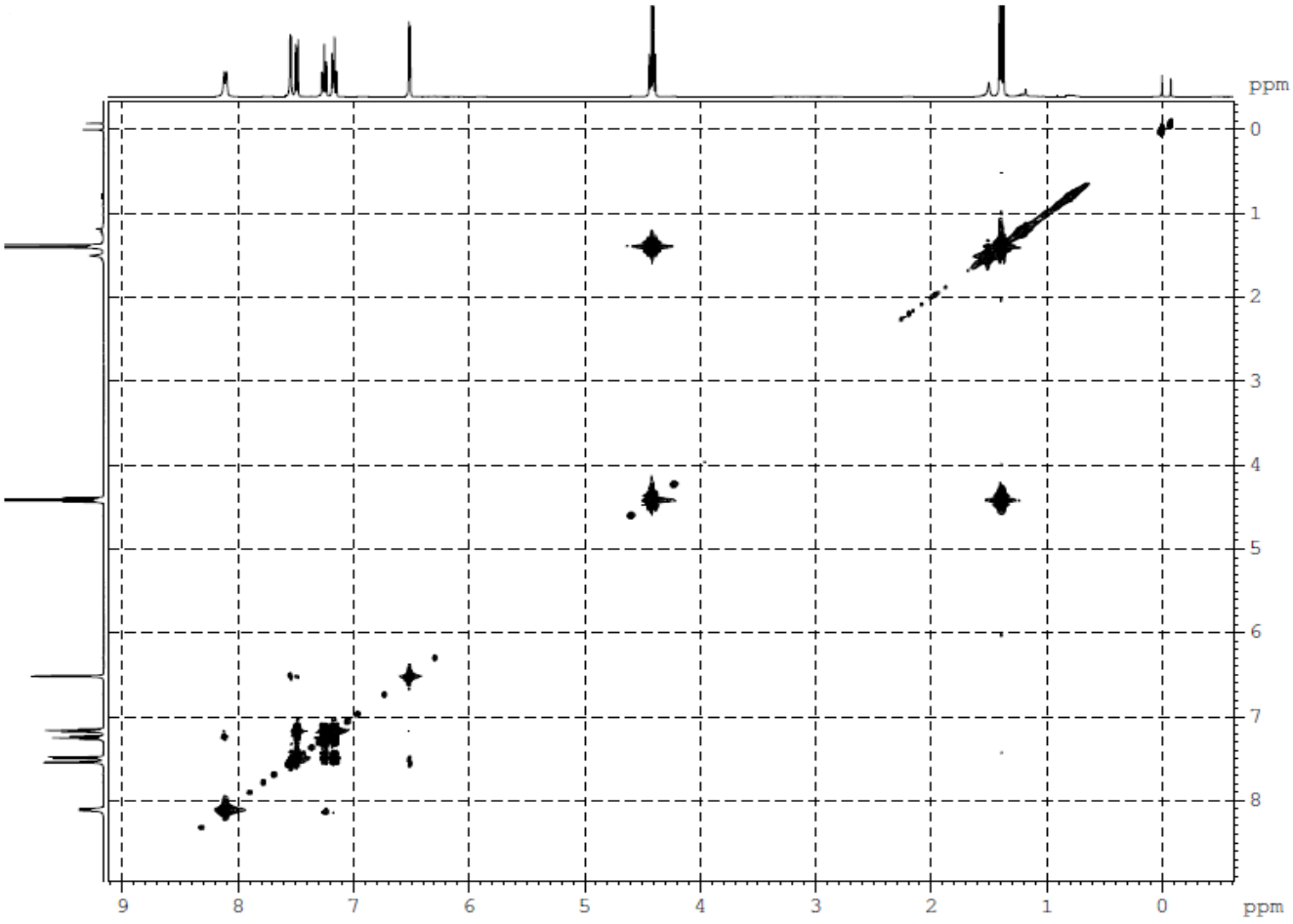

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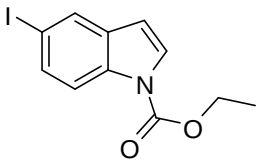


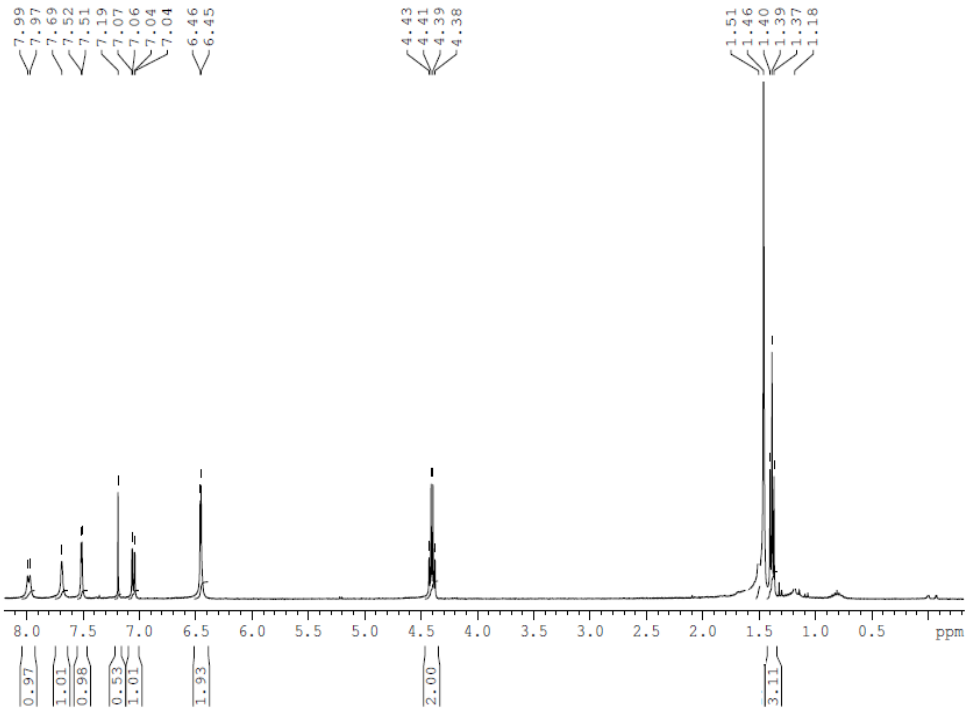

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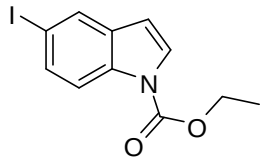


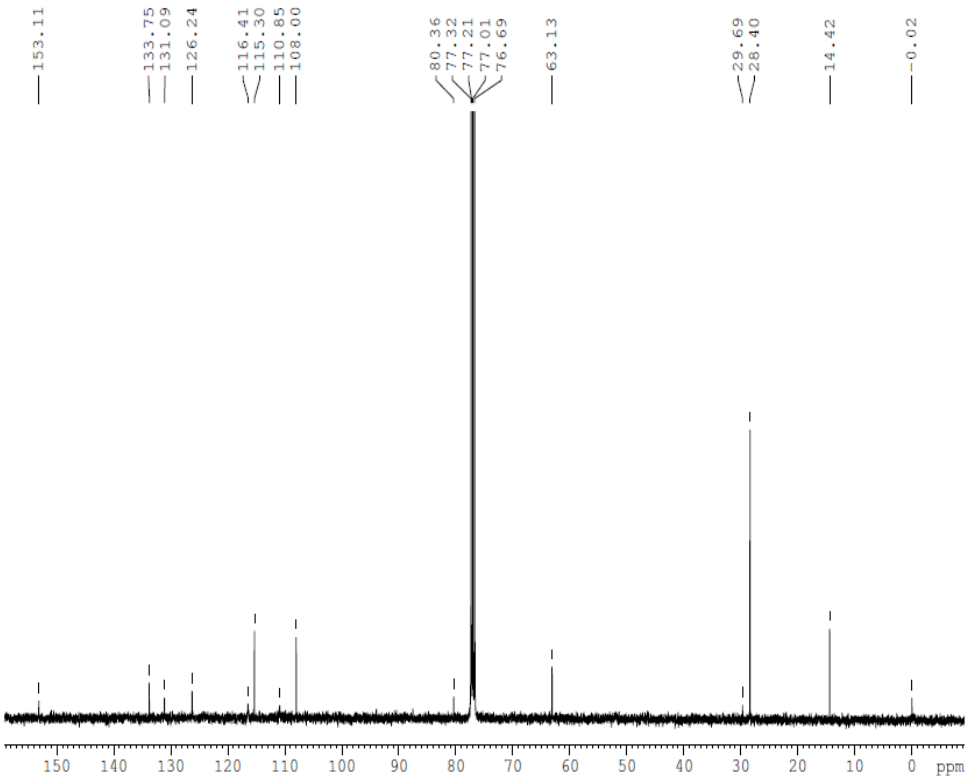

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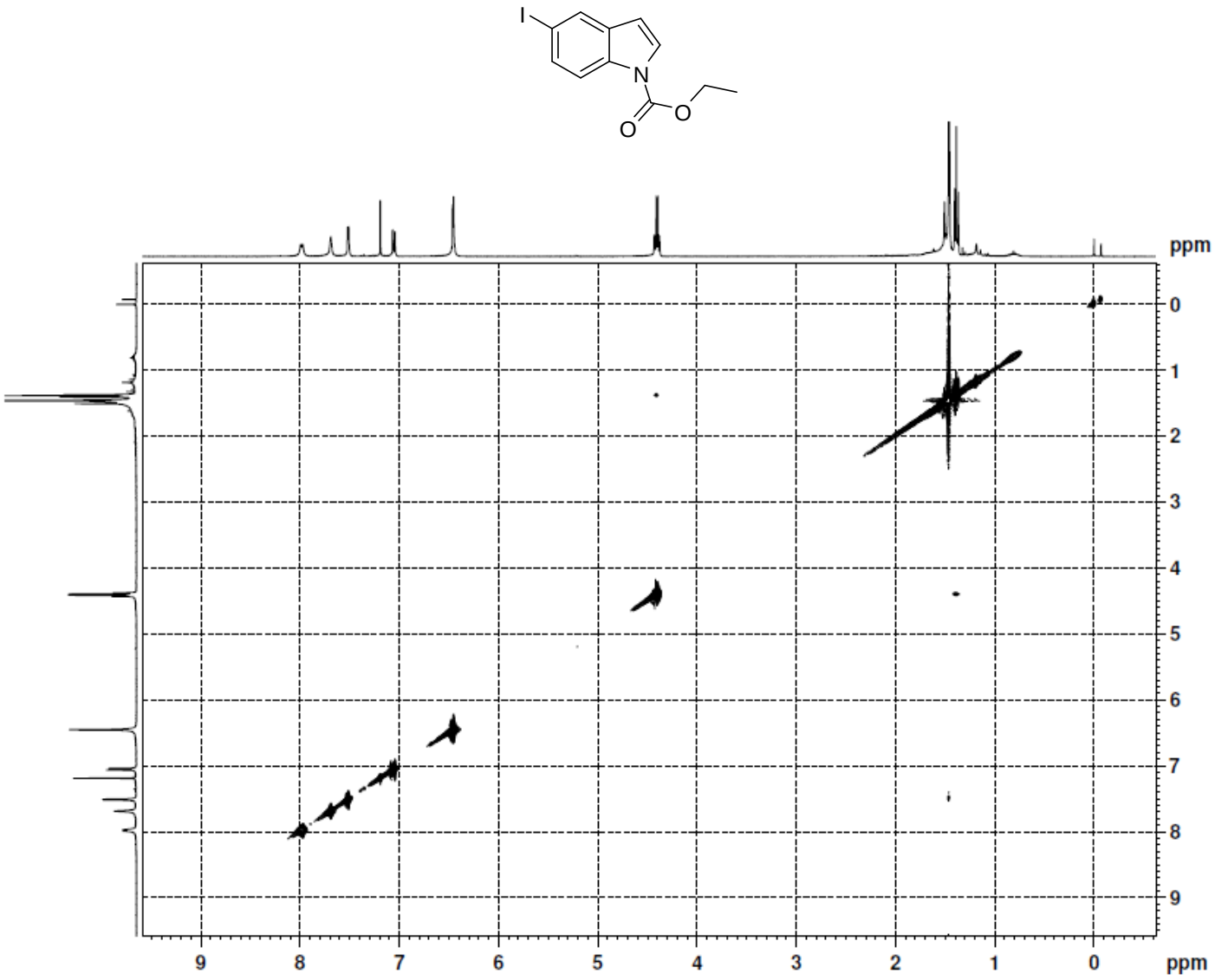

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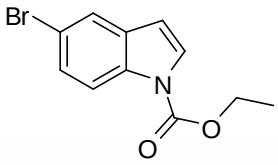


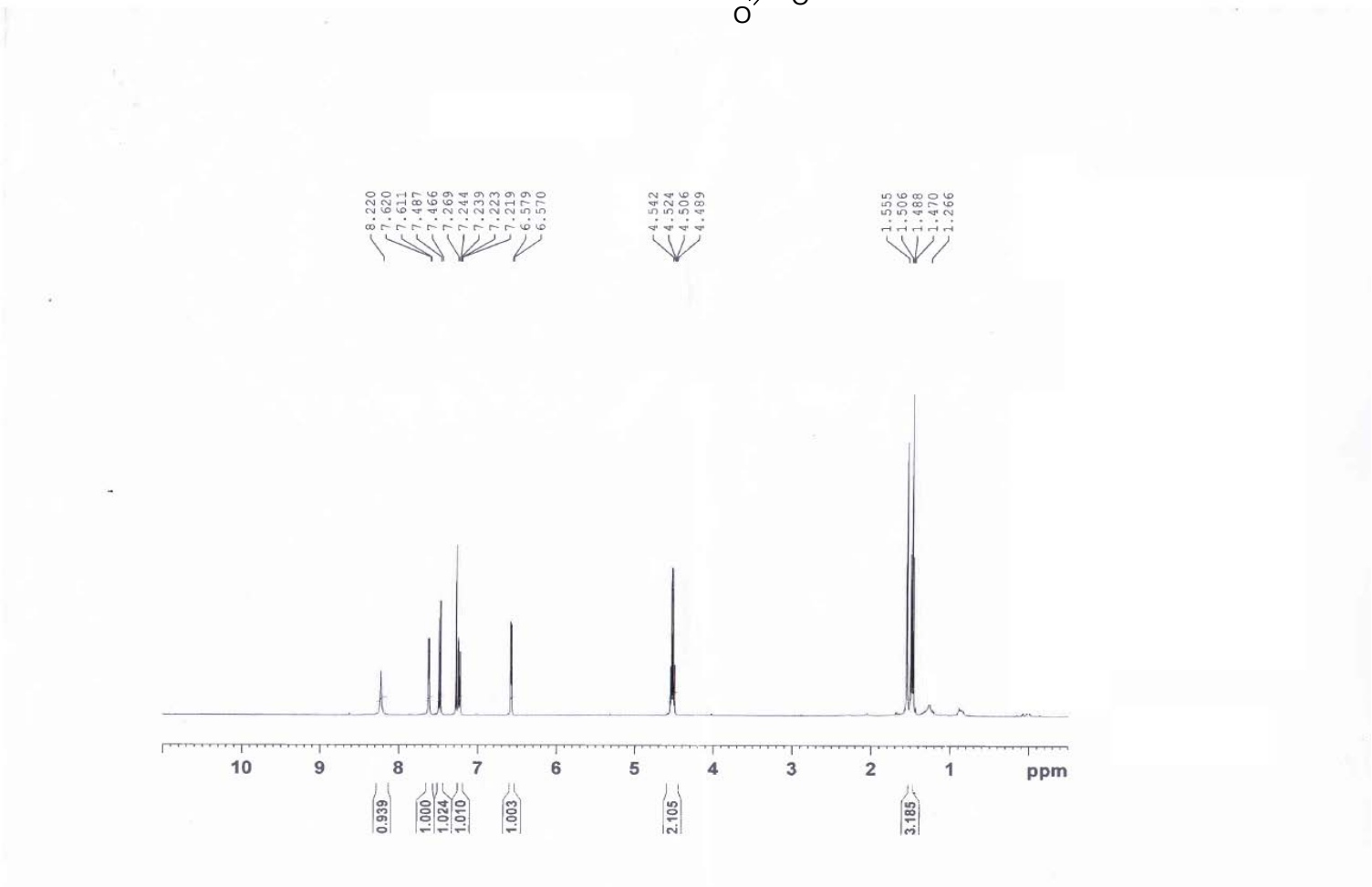

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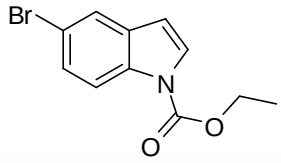


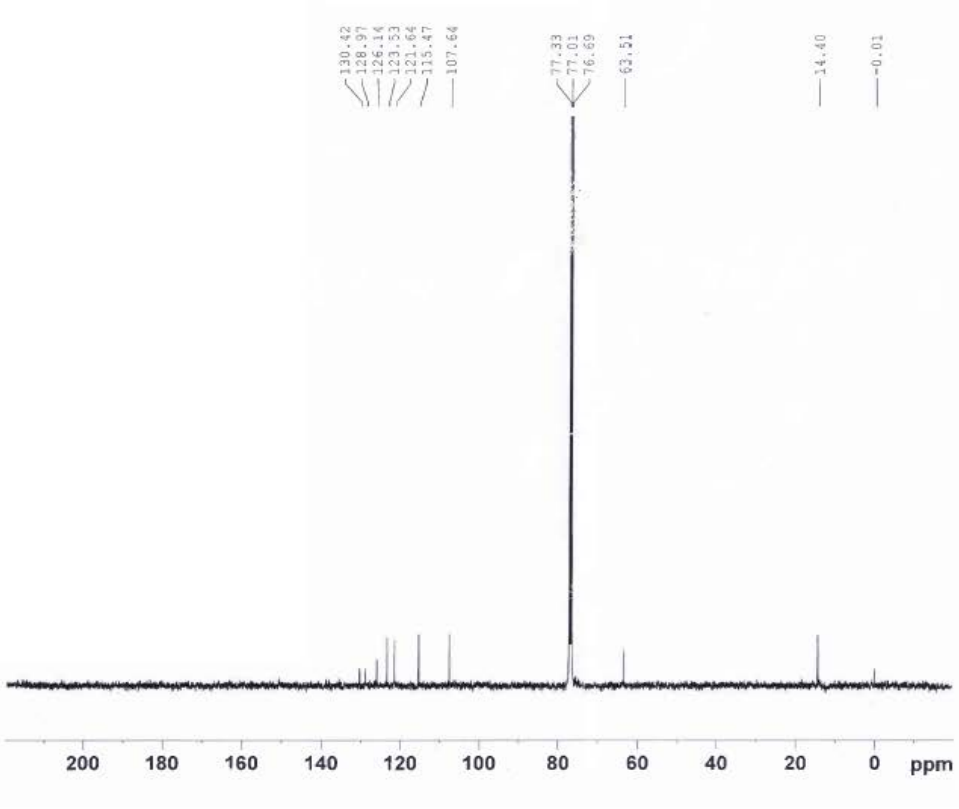

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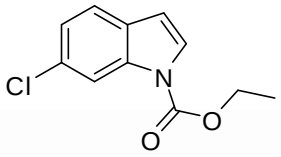


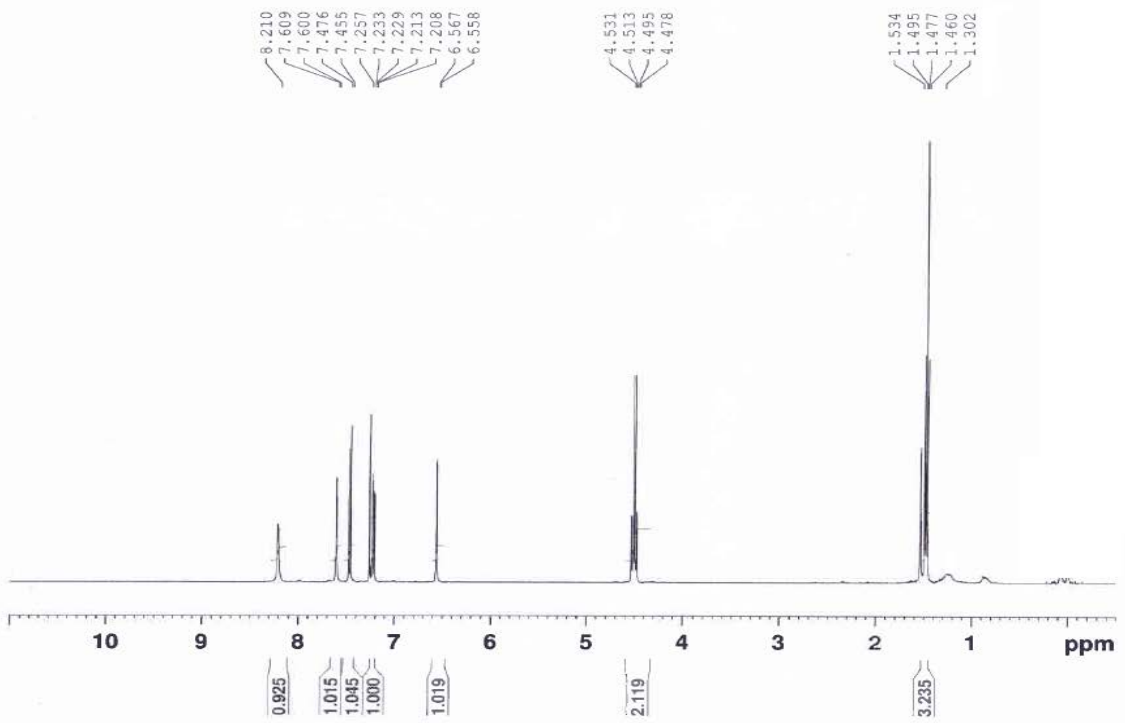

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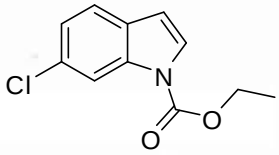


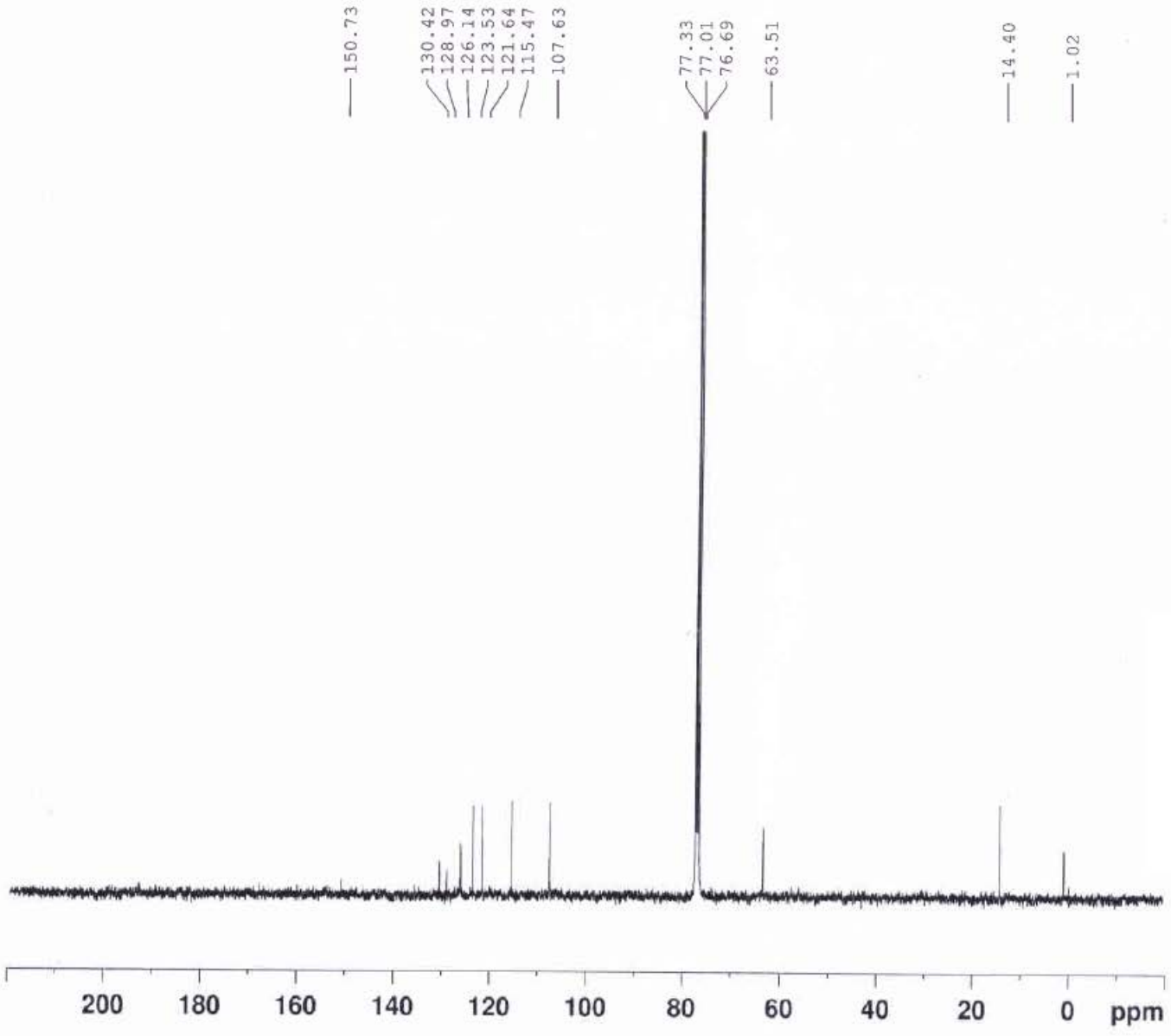

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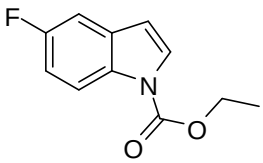


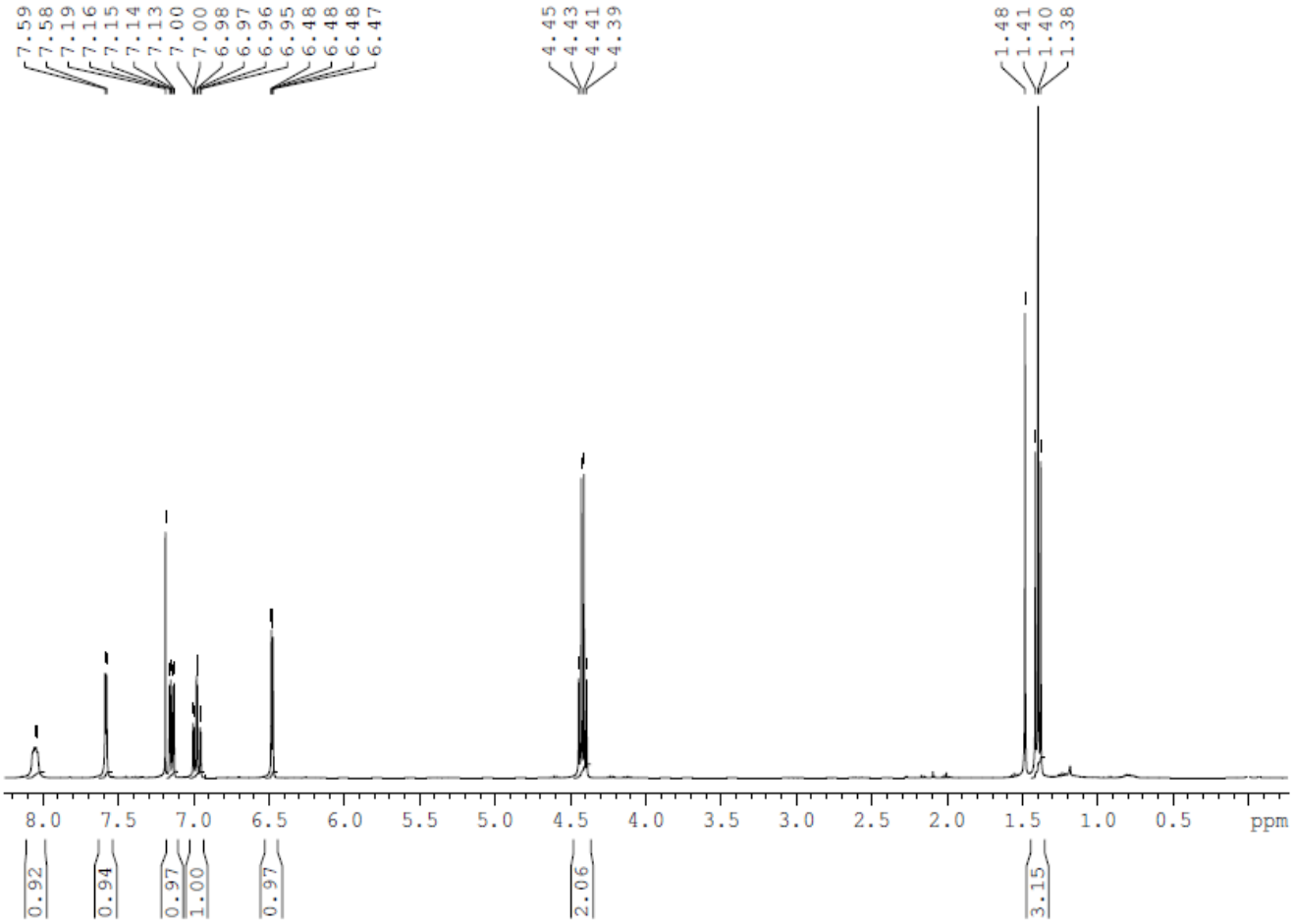

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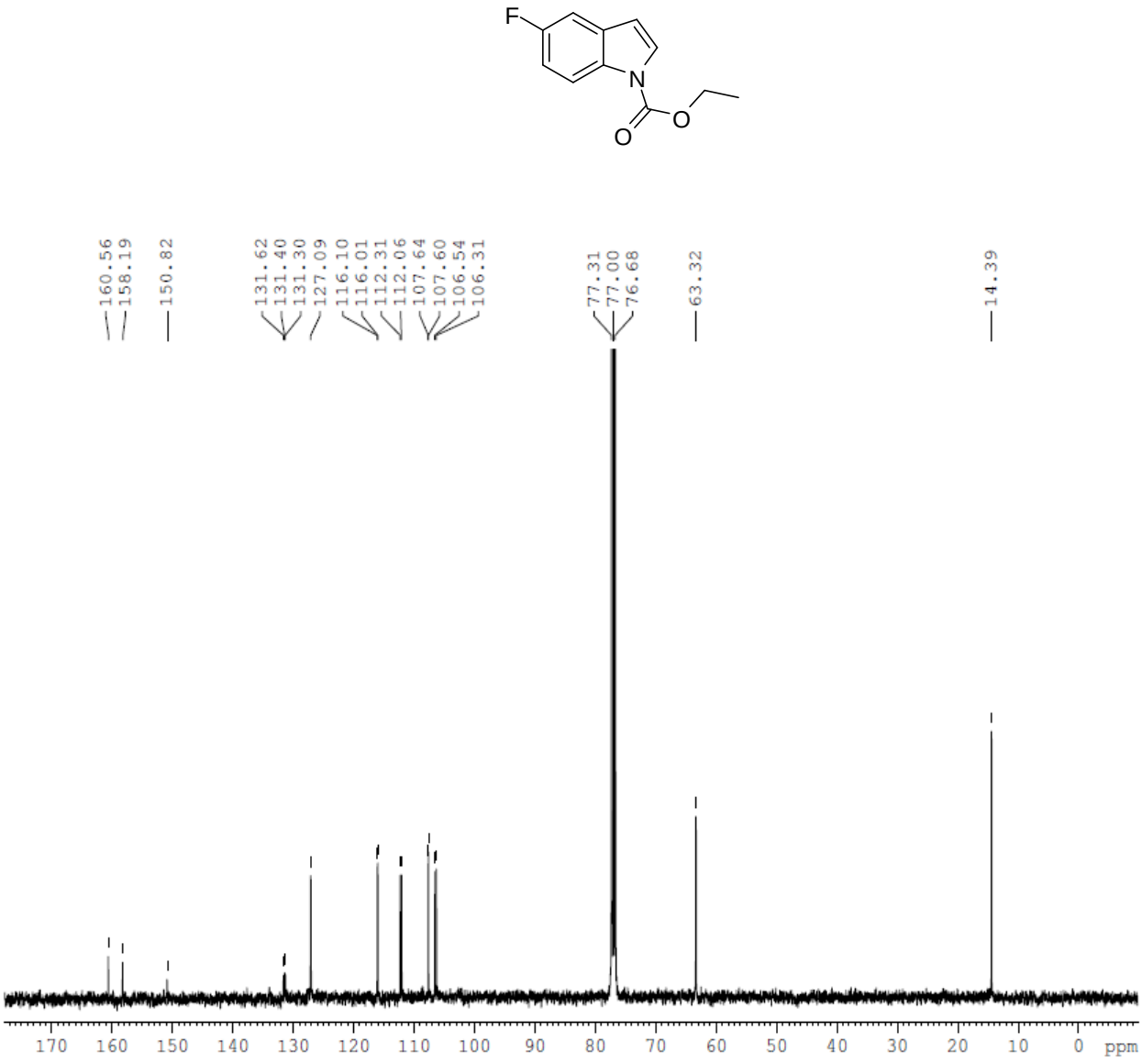

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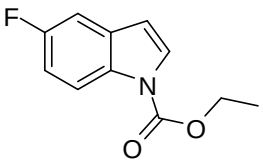


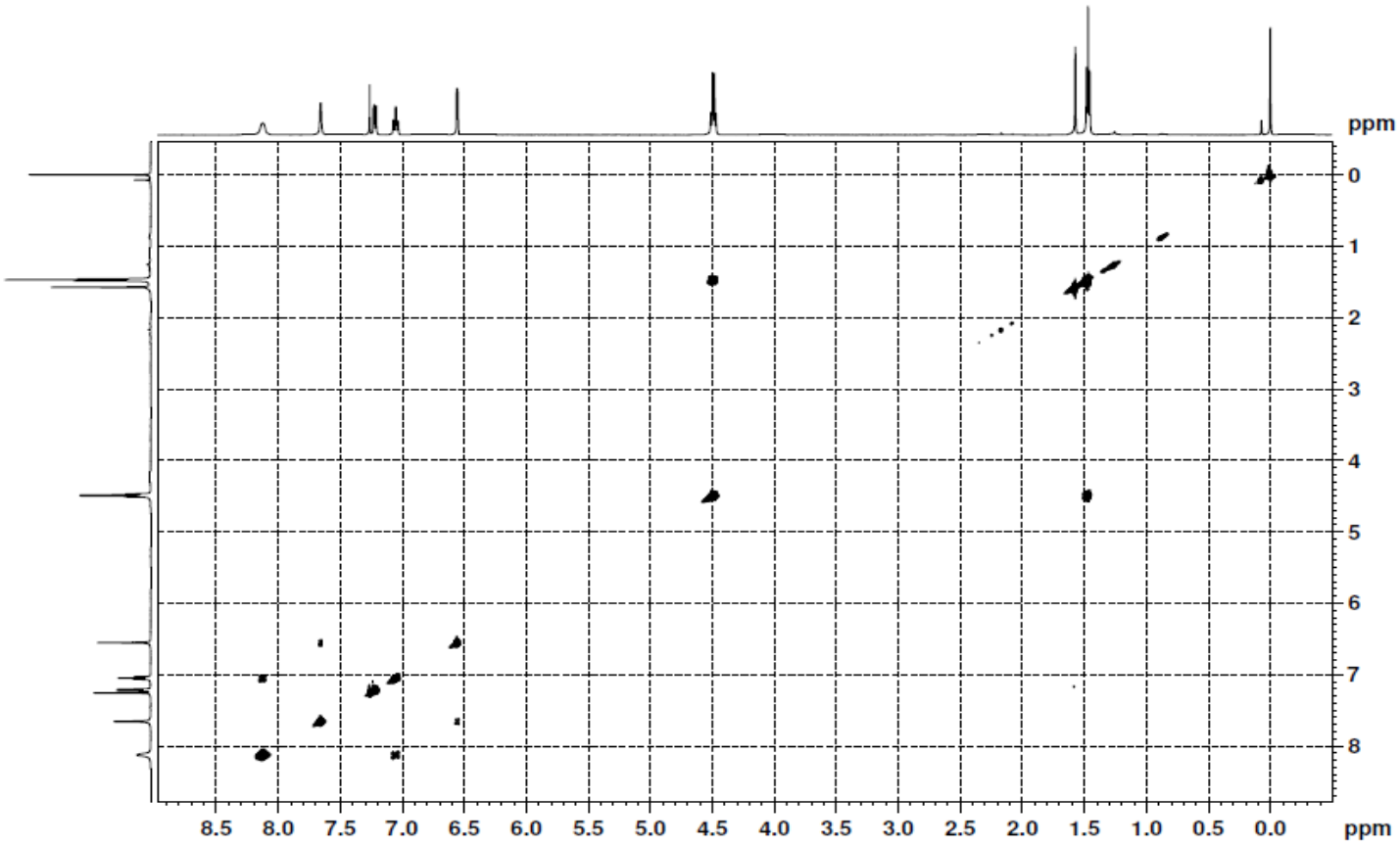

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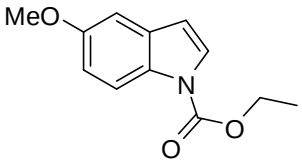


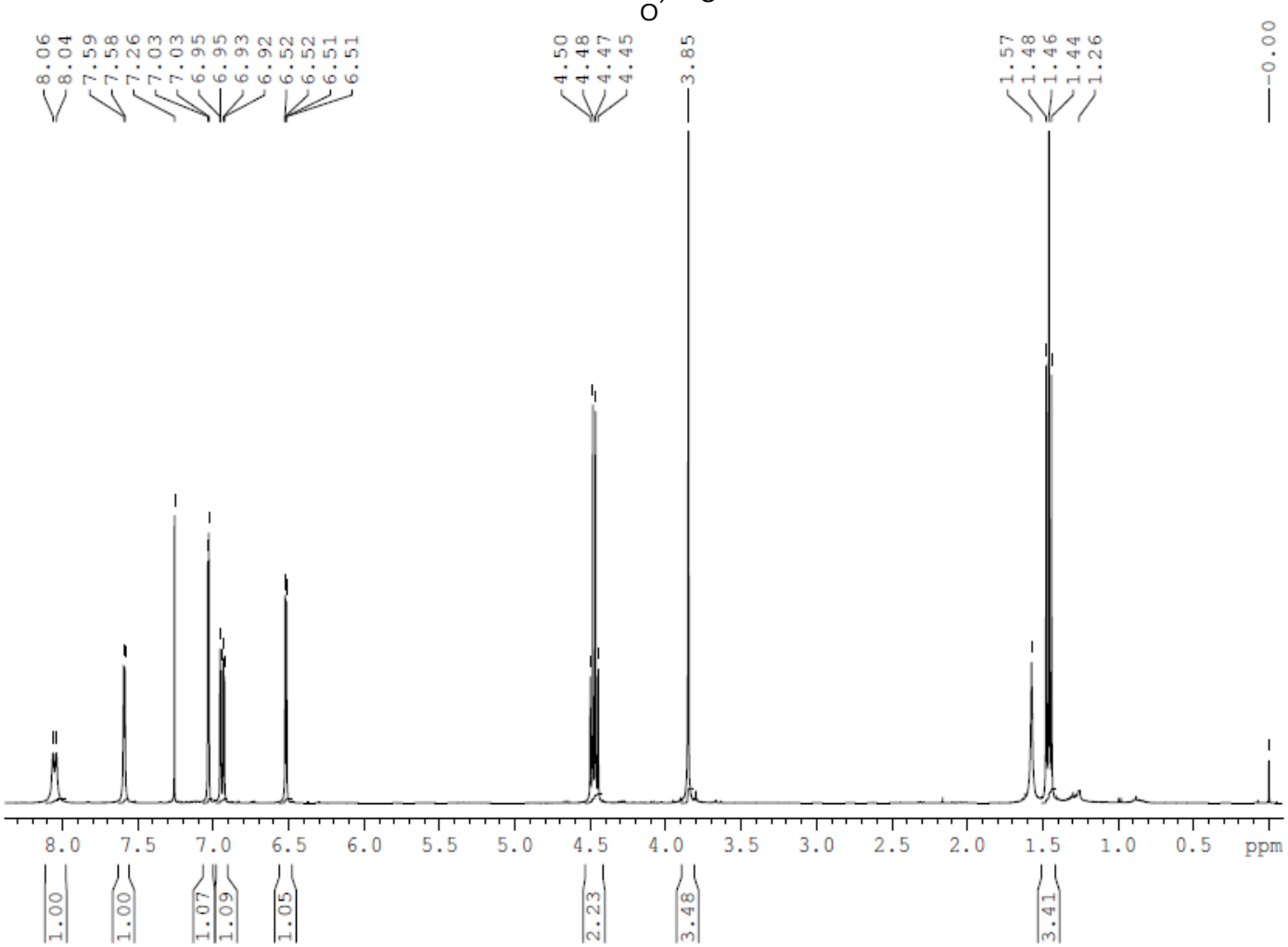

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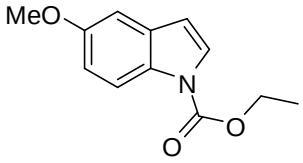


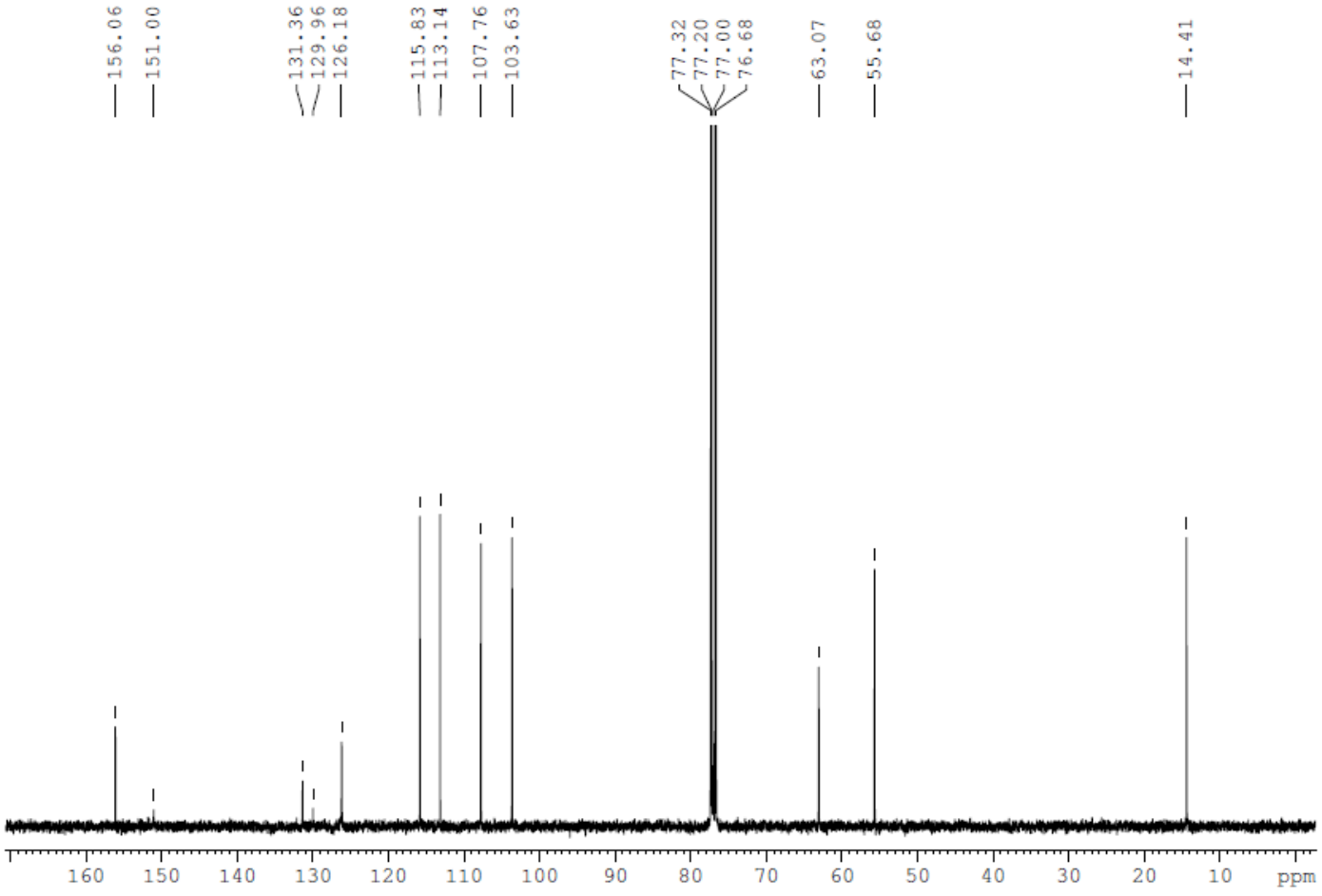

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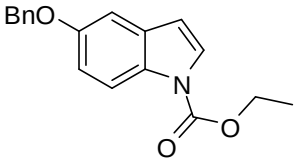


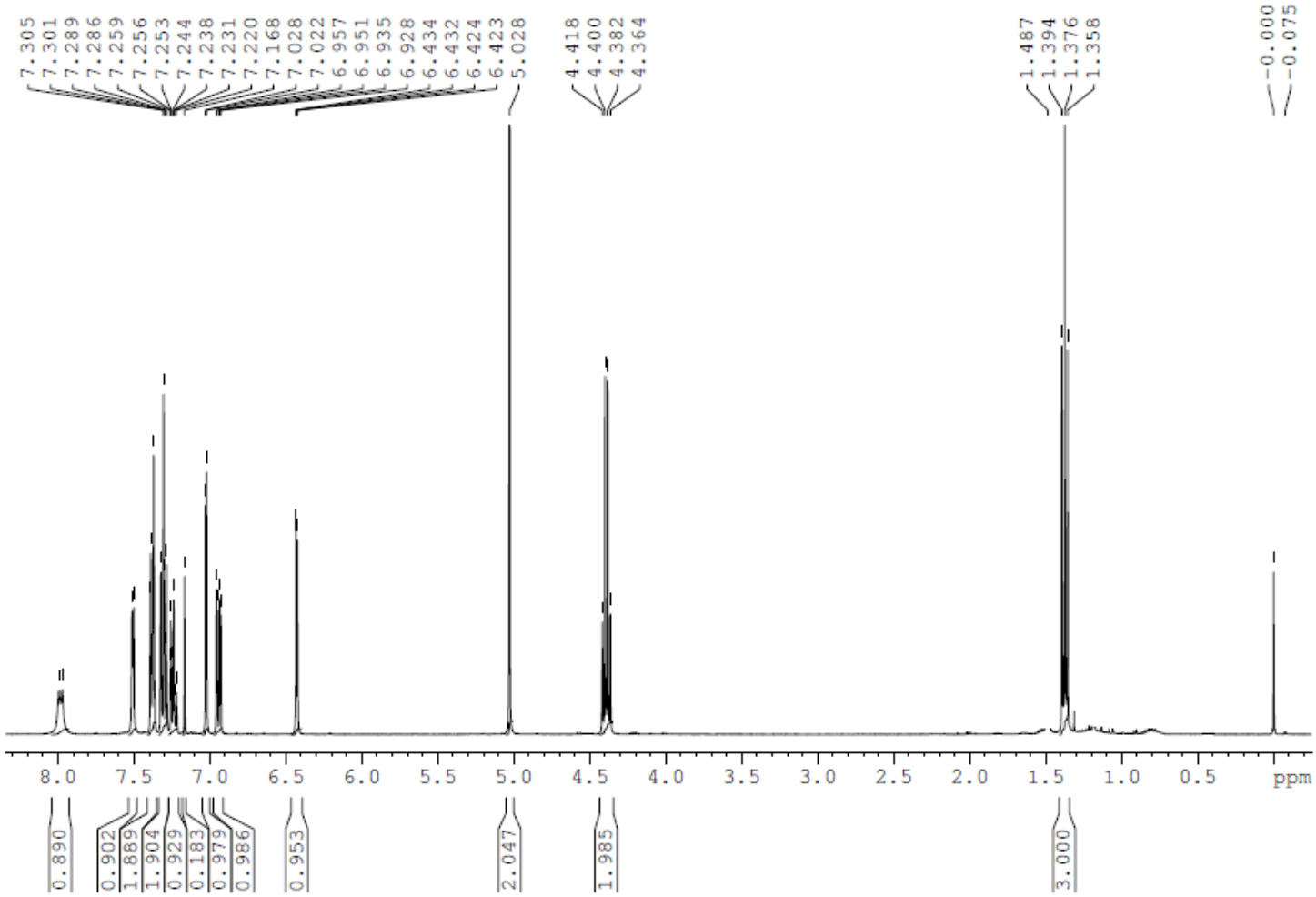

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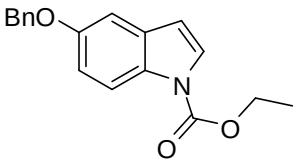


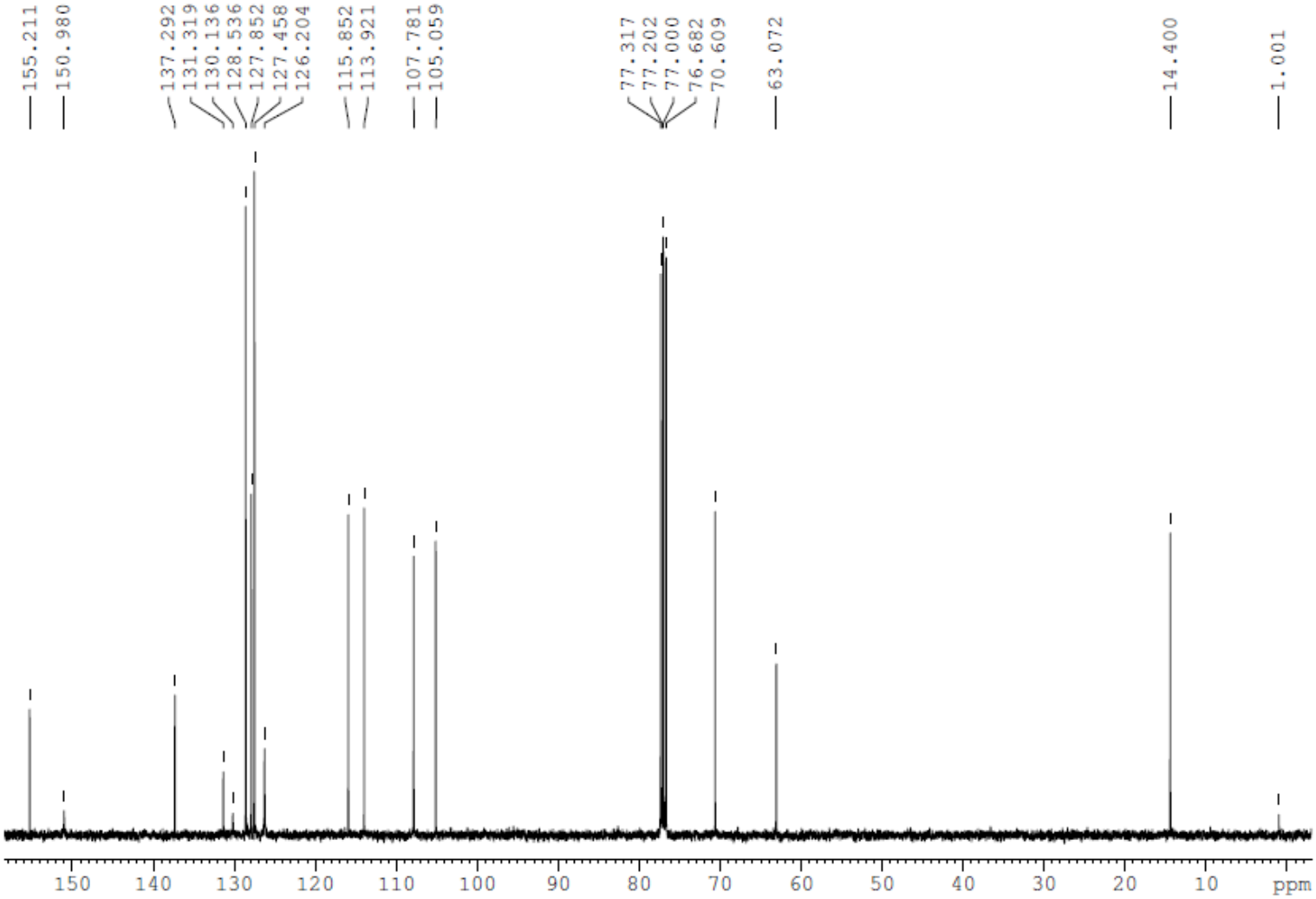

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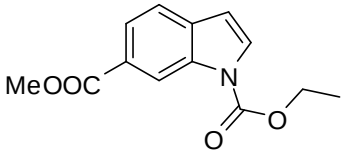


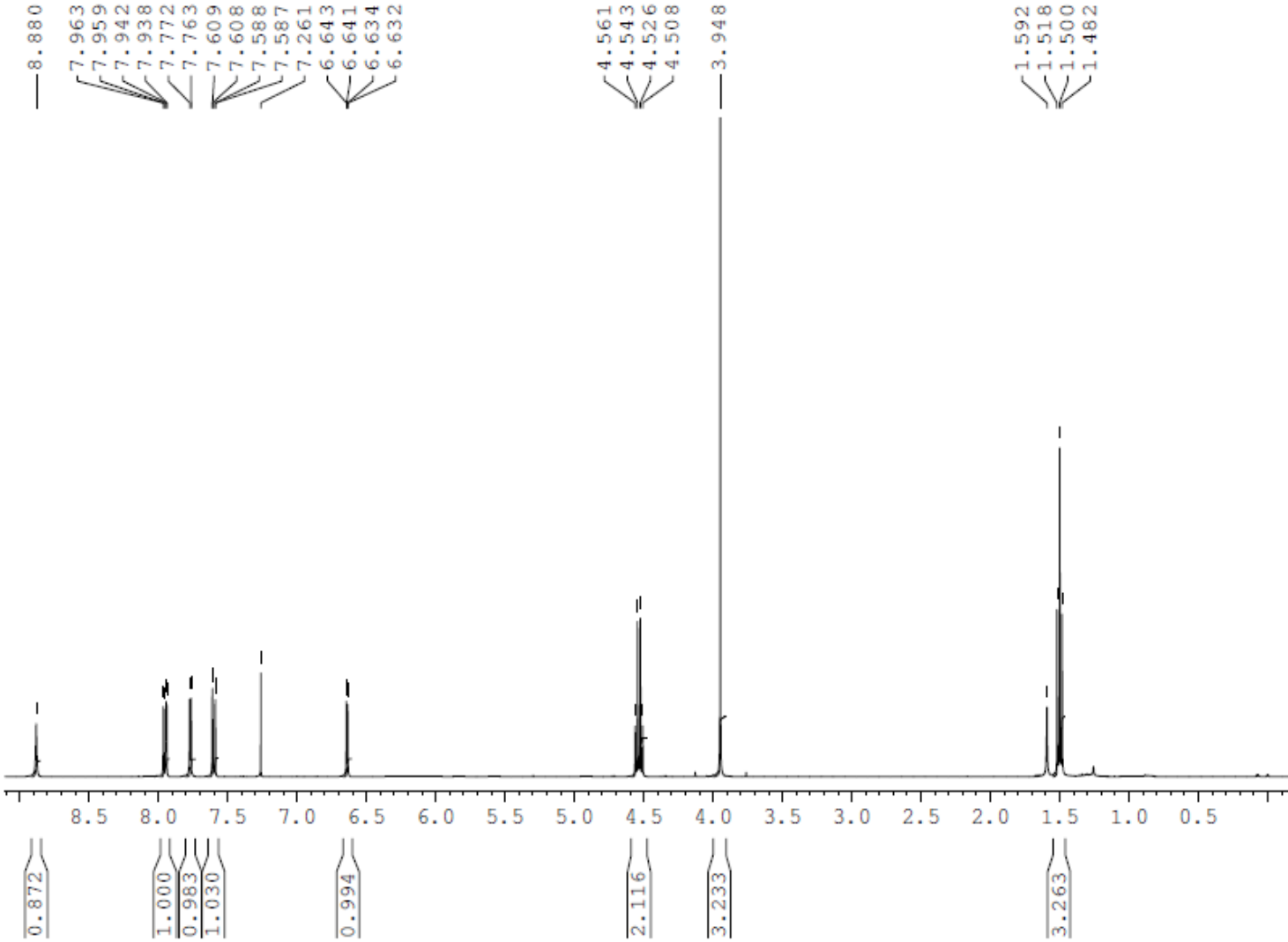

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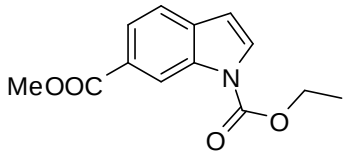


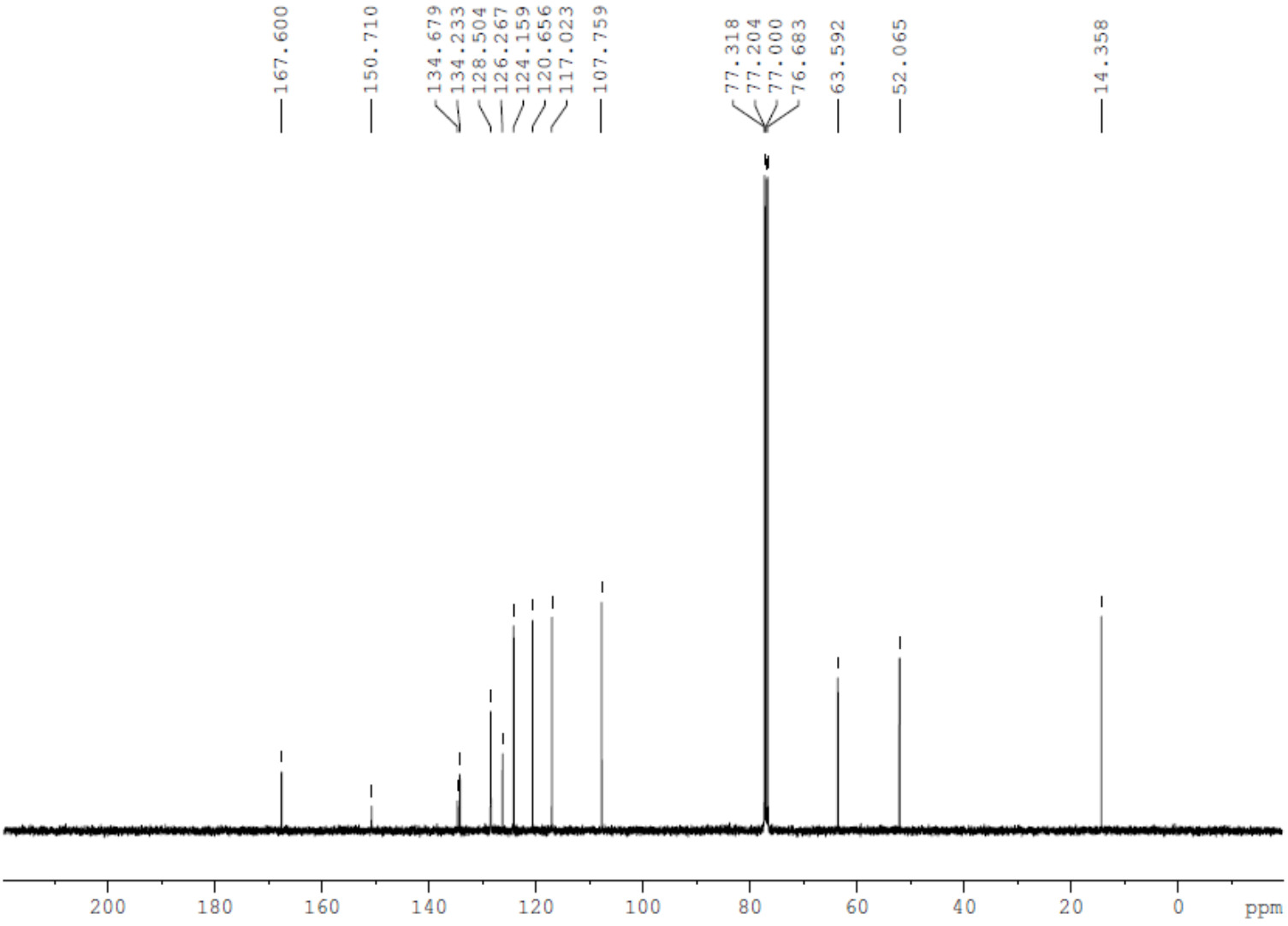

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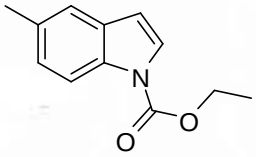
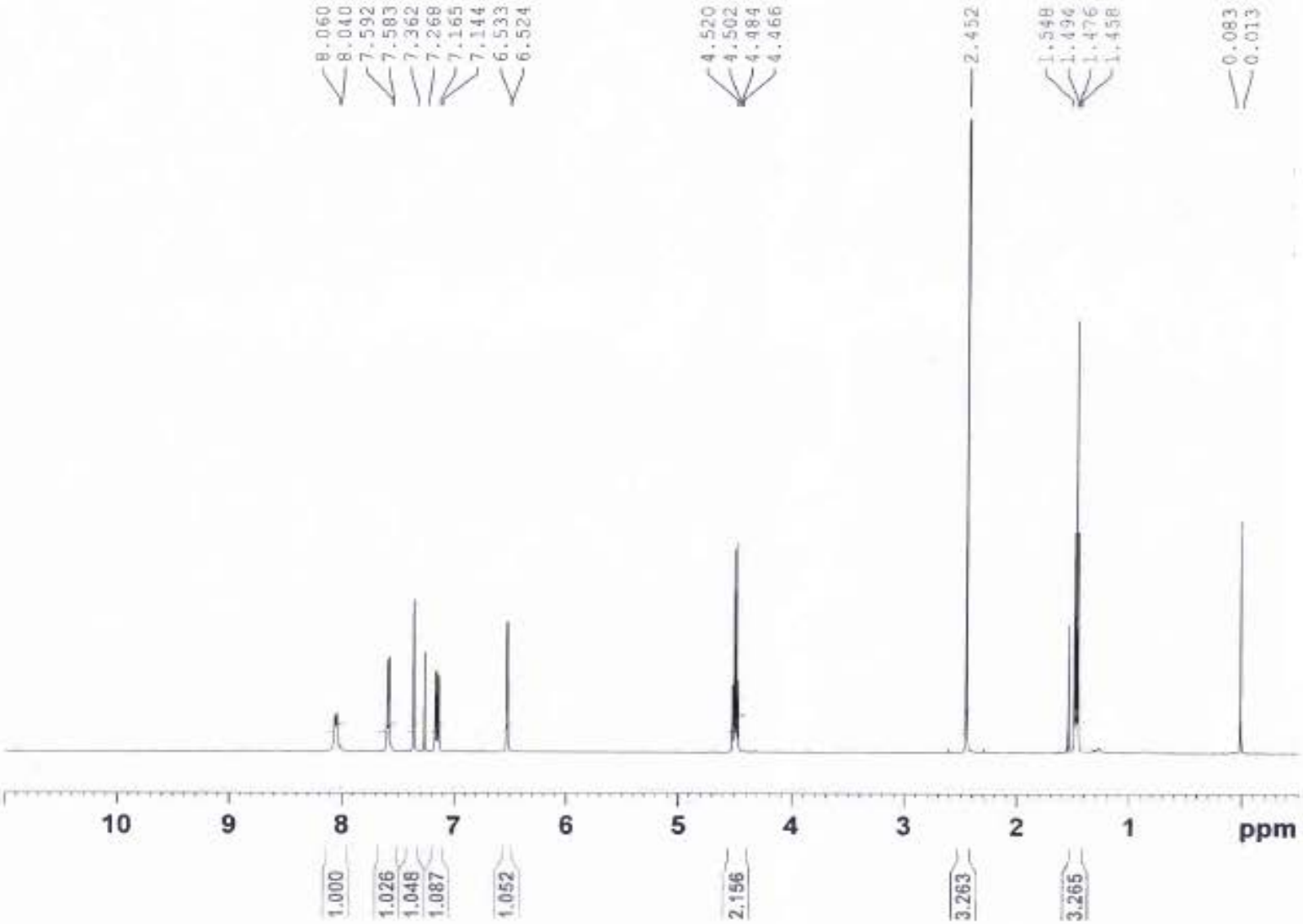
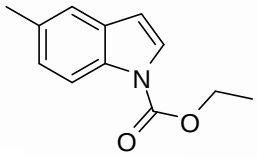
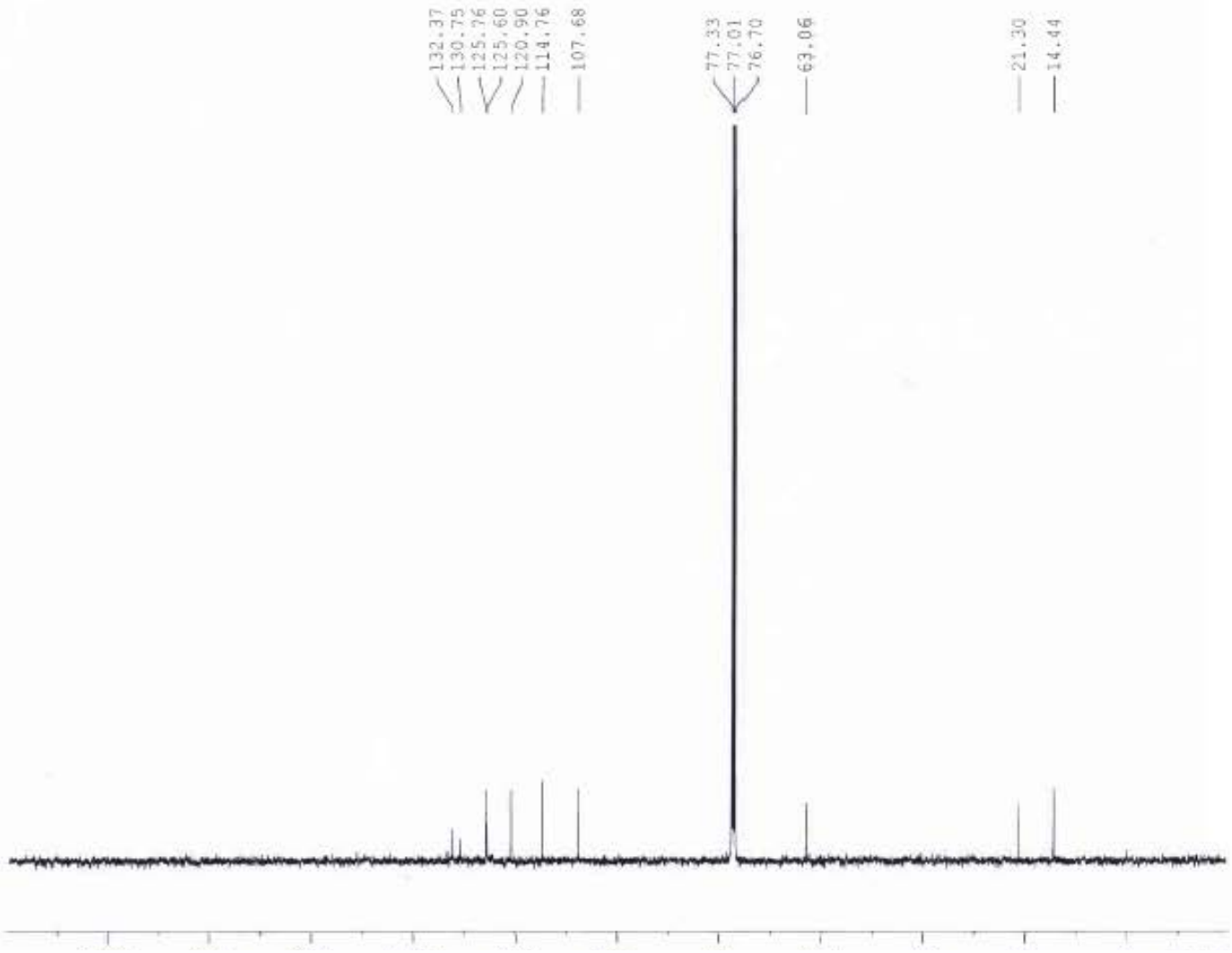


# $^{13}$C NMR – 2i



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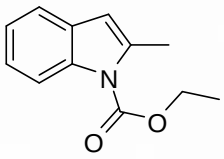
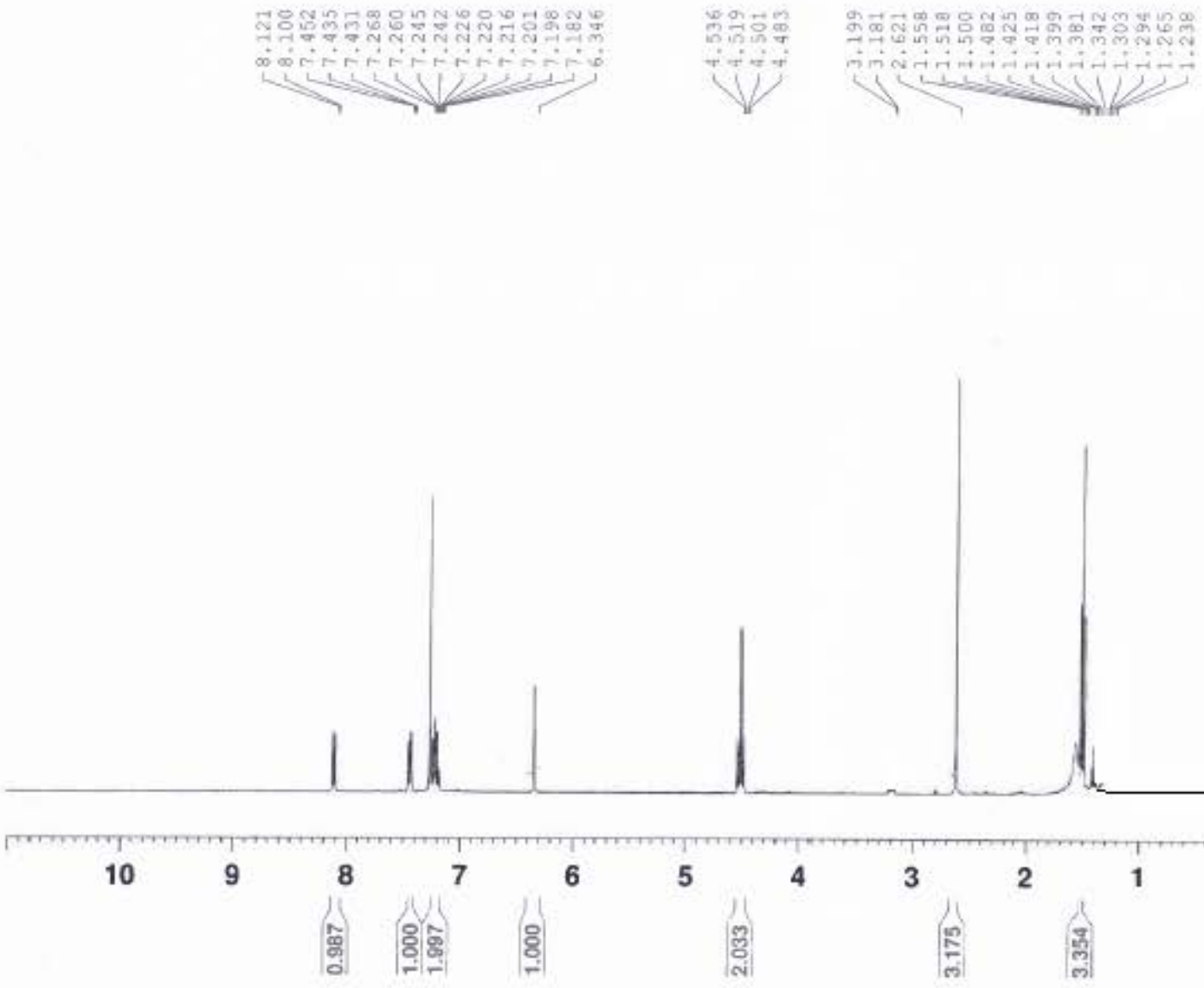
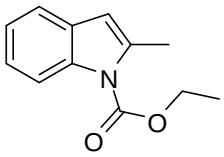
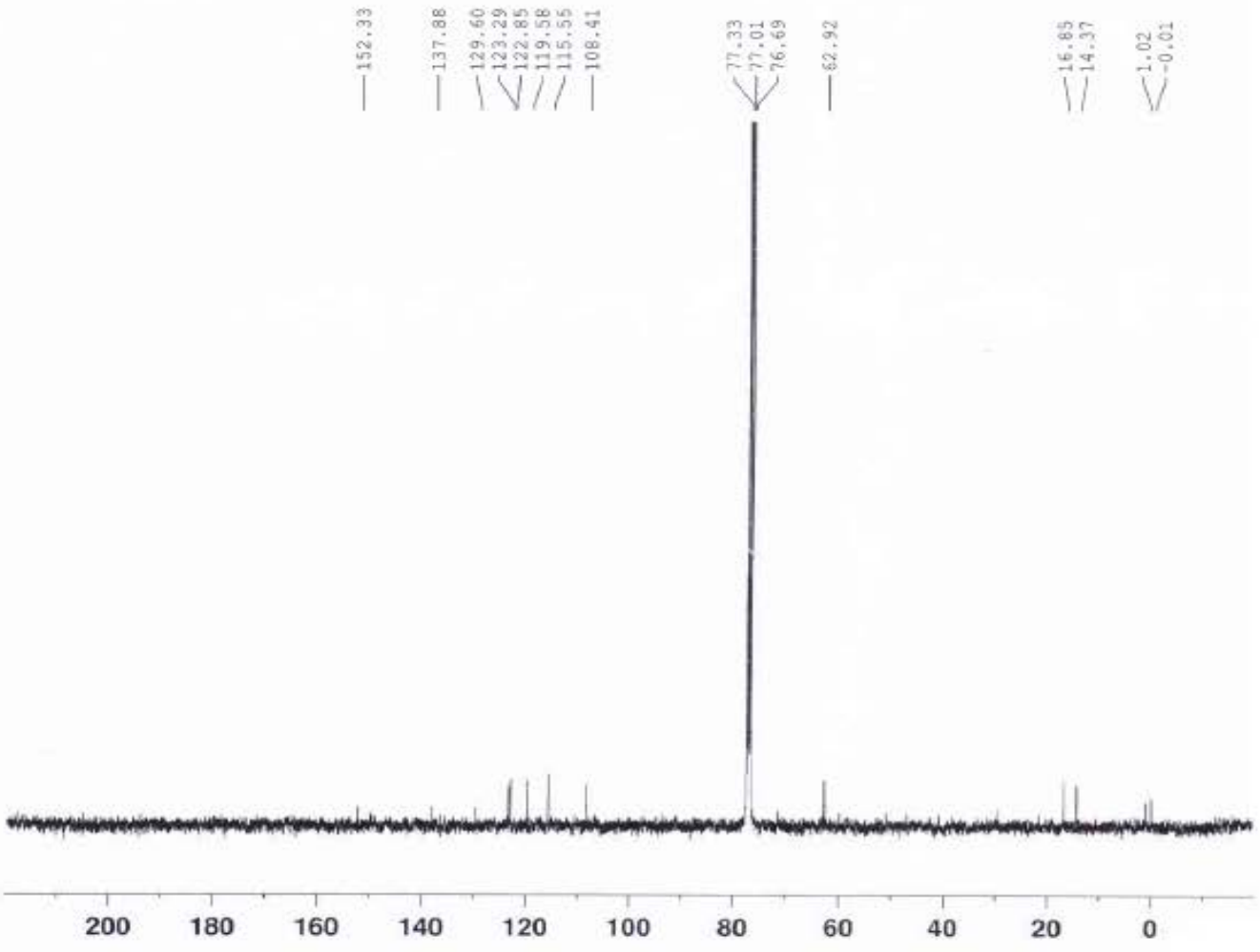


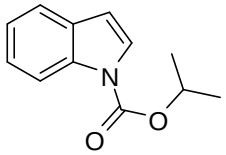



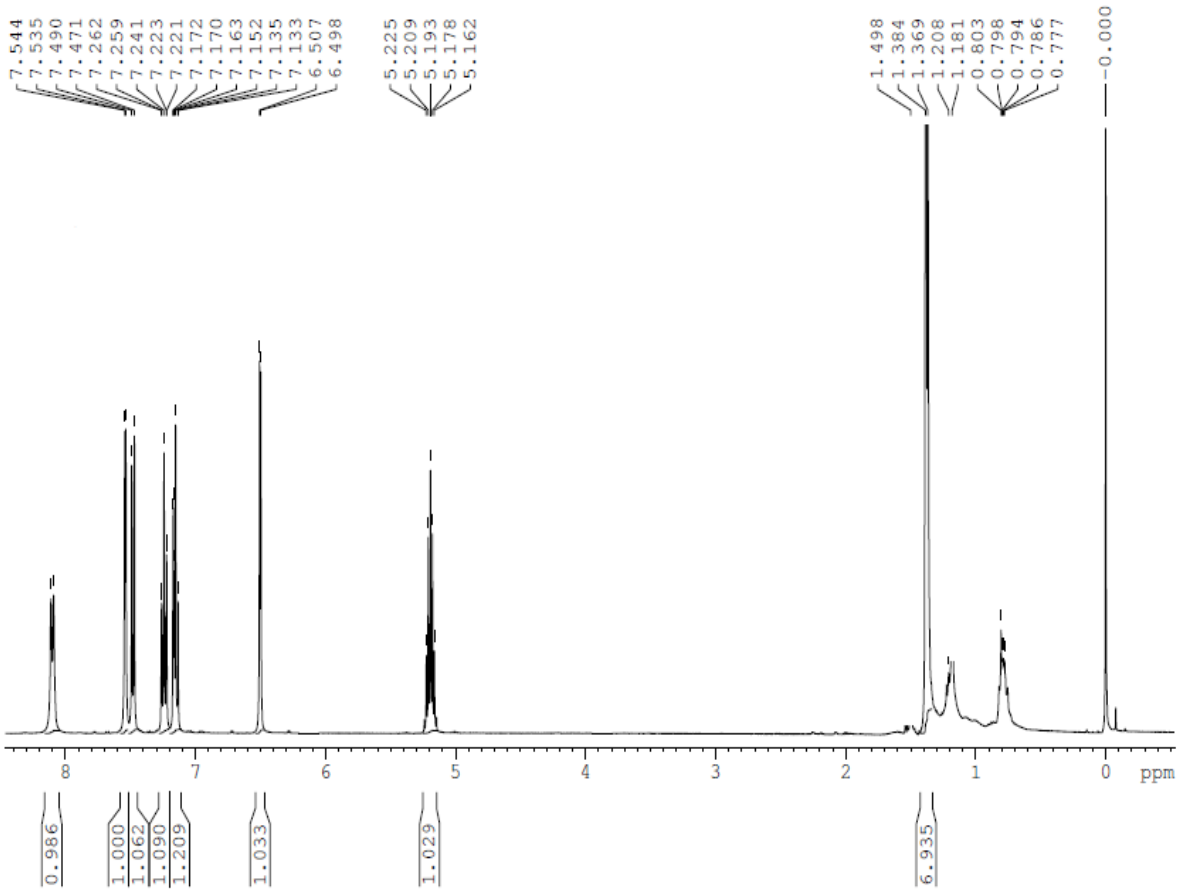
# $^{13}$C NMR – 2j



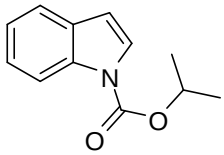



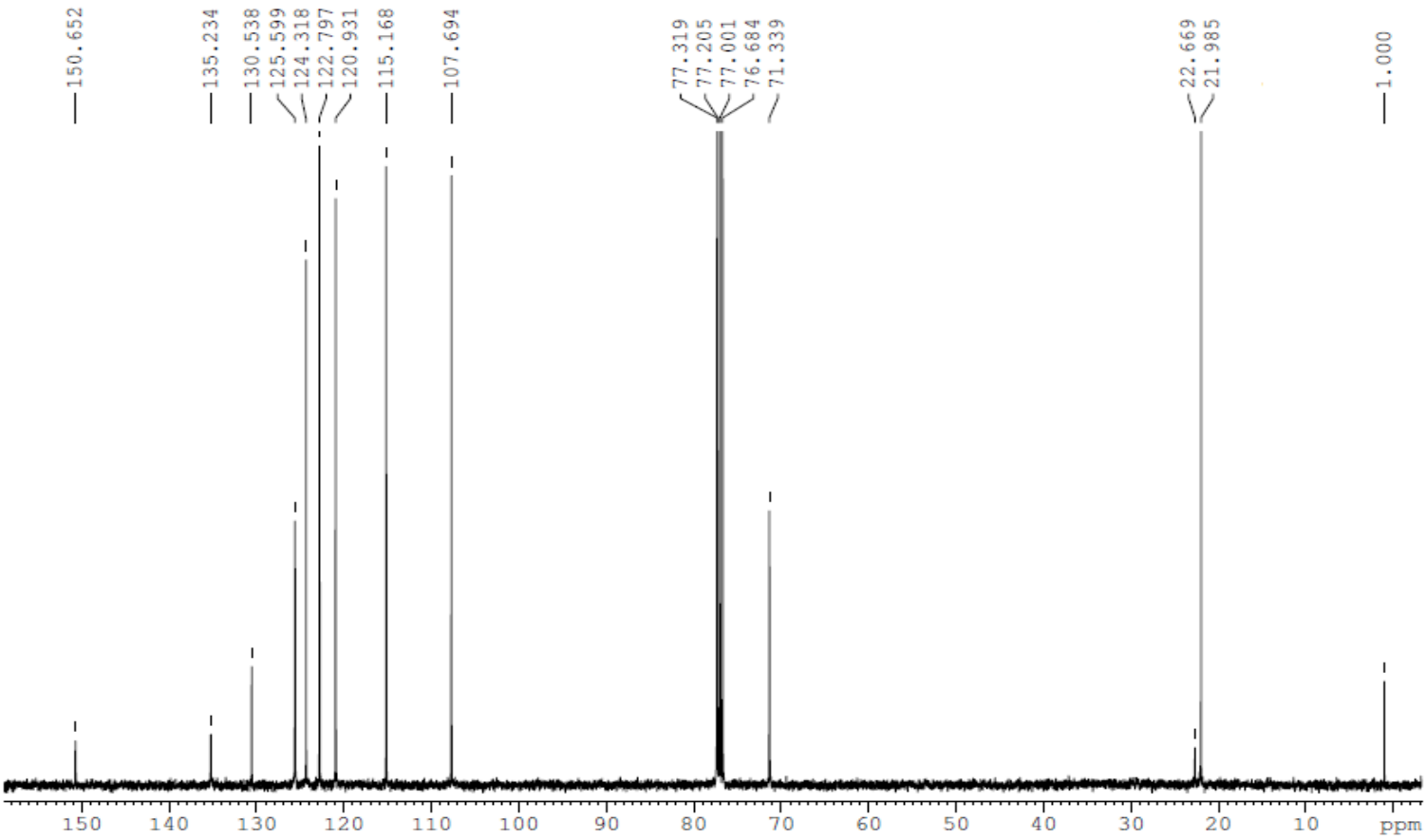
# $^{1}$H NMR – 2k



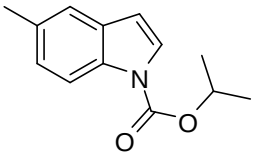



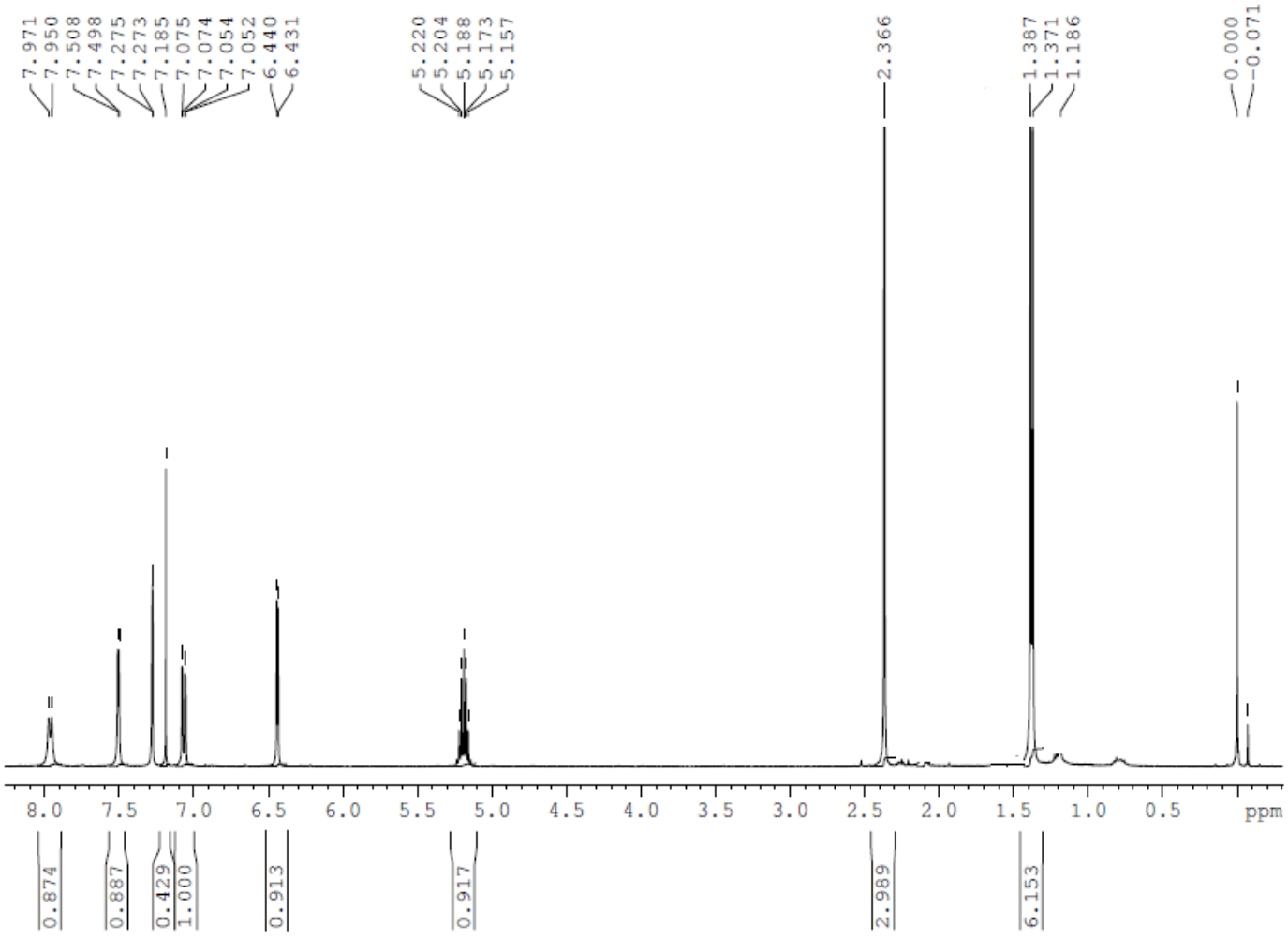
# $^{13}$C NMR – 2k



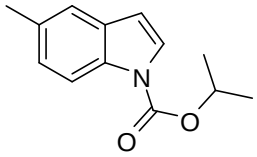



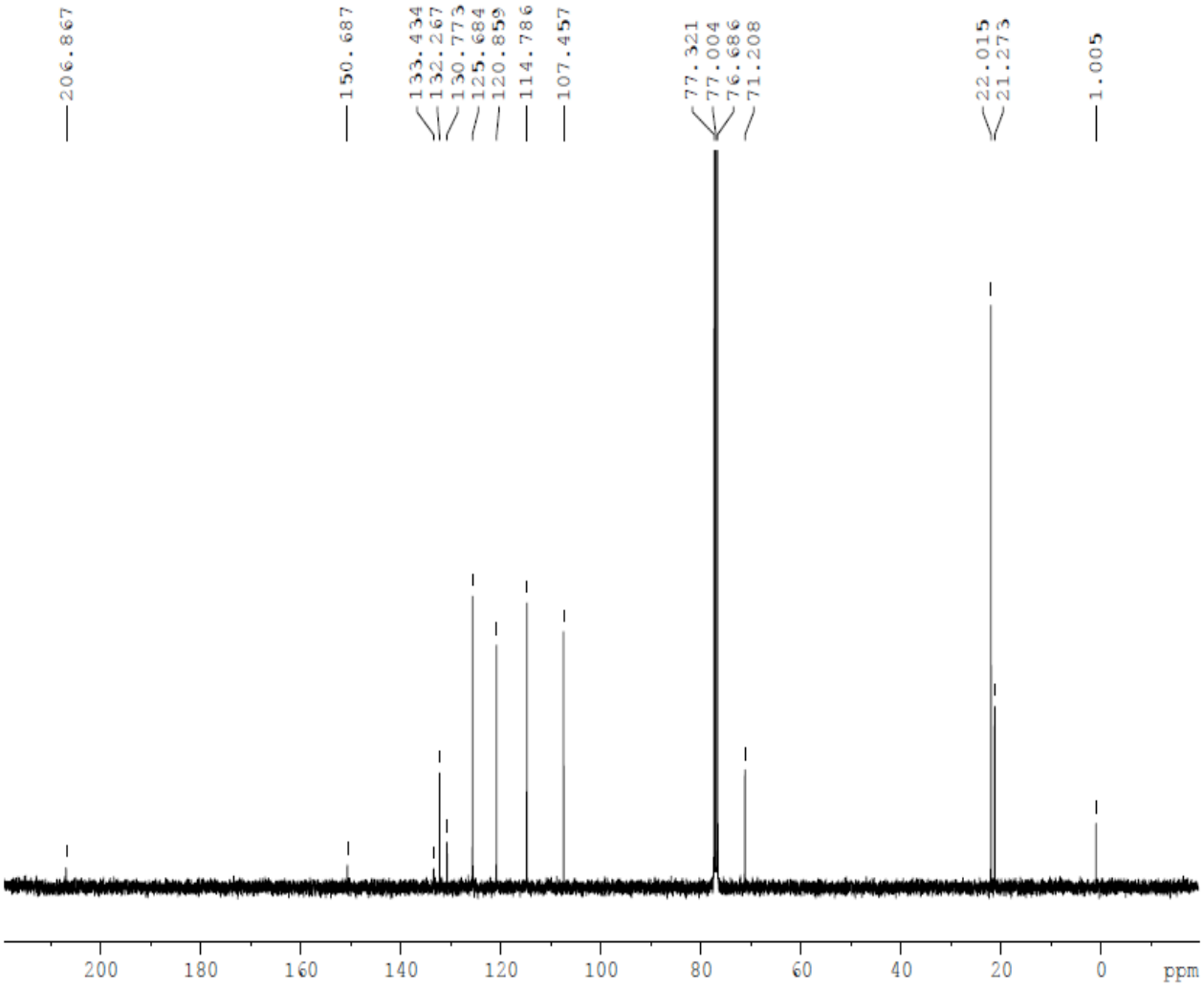
# $^{1}$H NMR – 2l



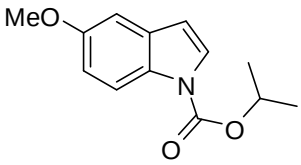



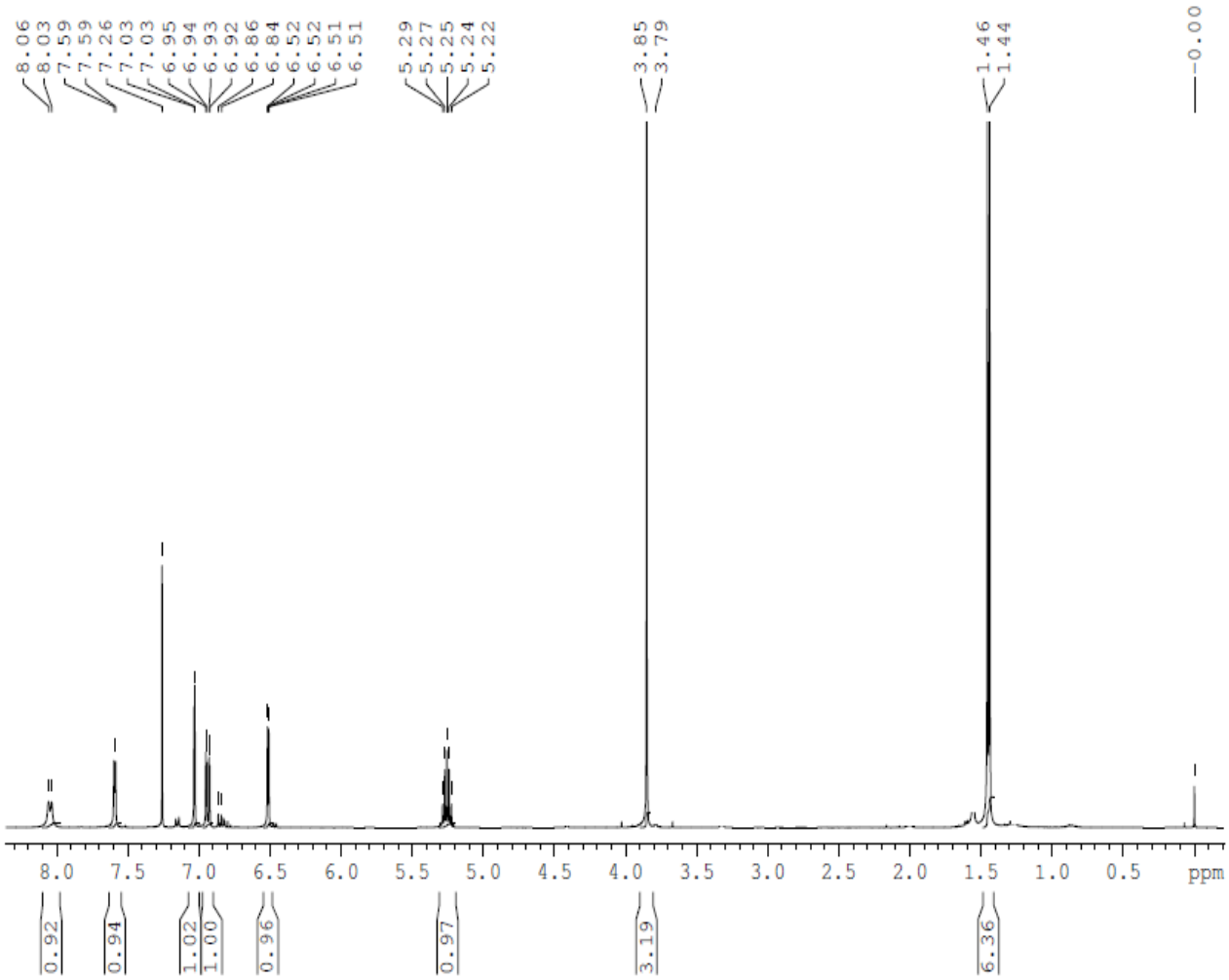
# $^{13}$C NMR – 2l



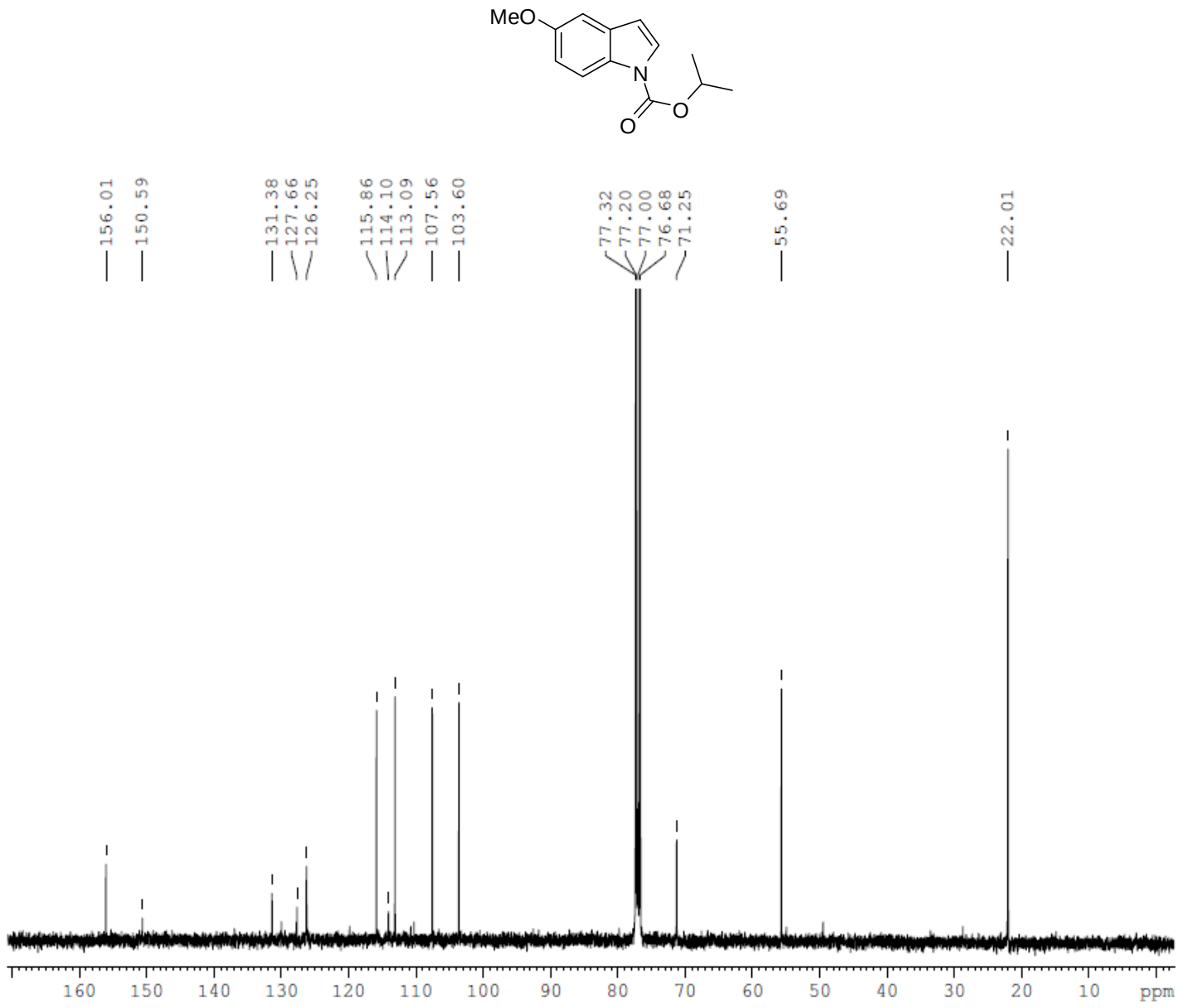



# $^{1}$H NMR – 2m

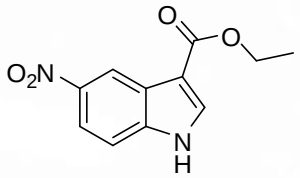


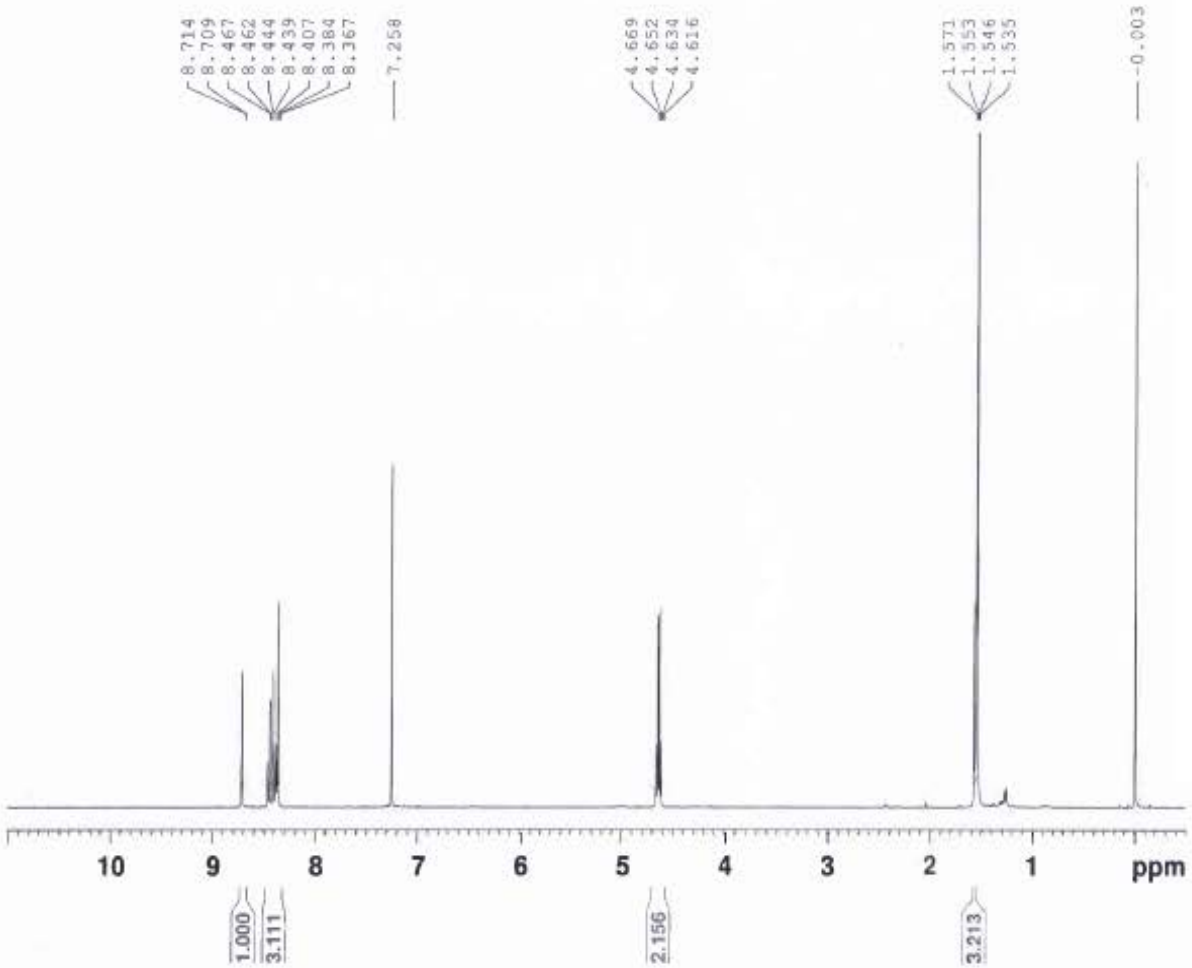



# $^{13}$C NMR – 2m

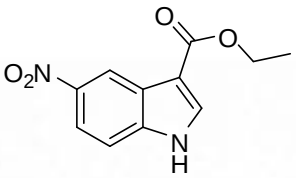


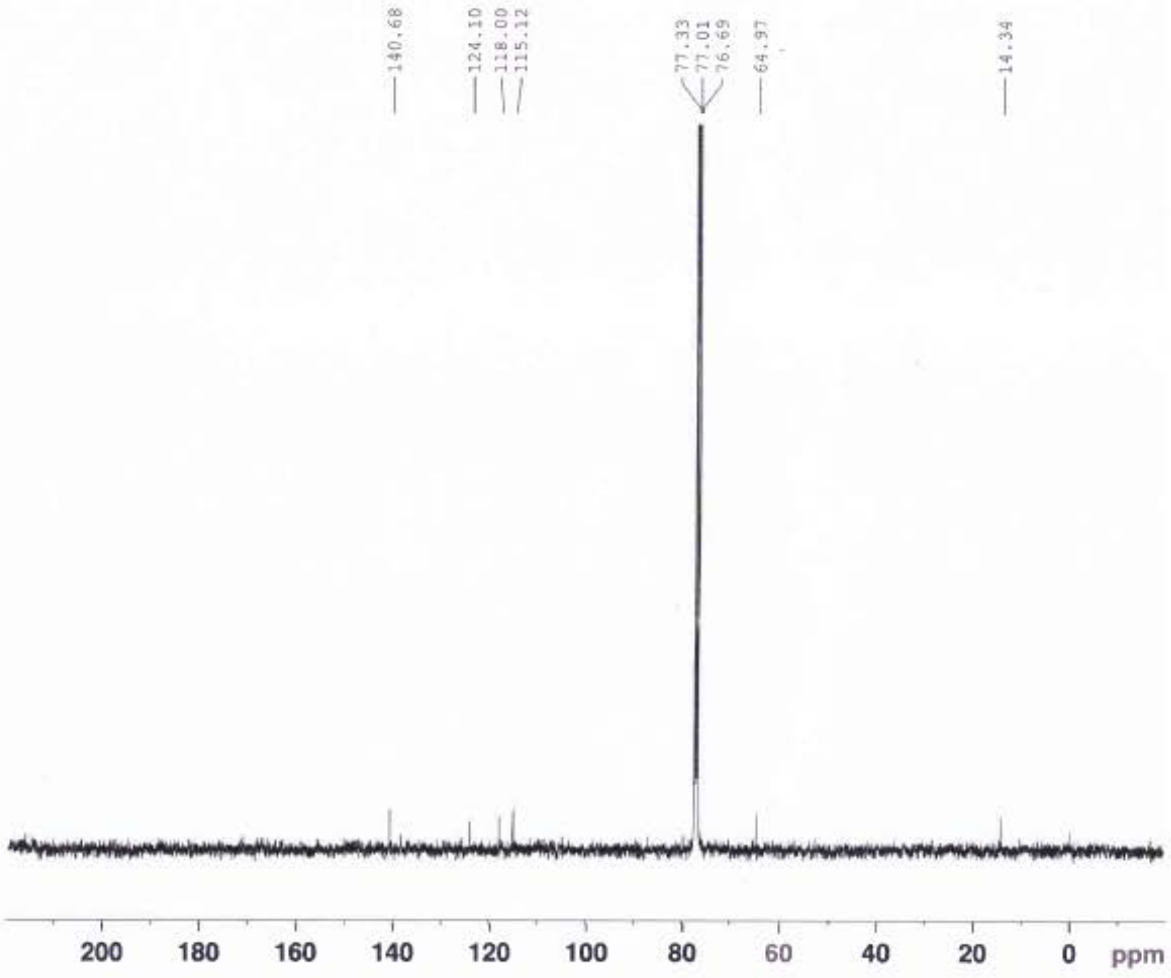
# $^1$H NMR – 2n



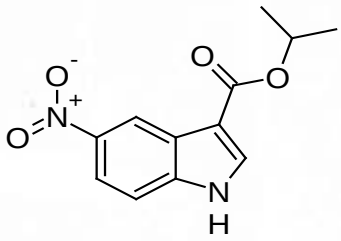



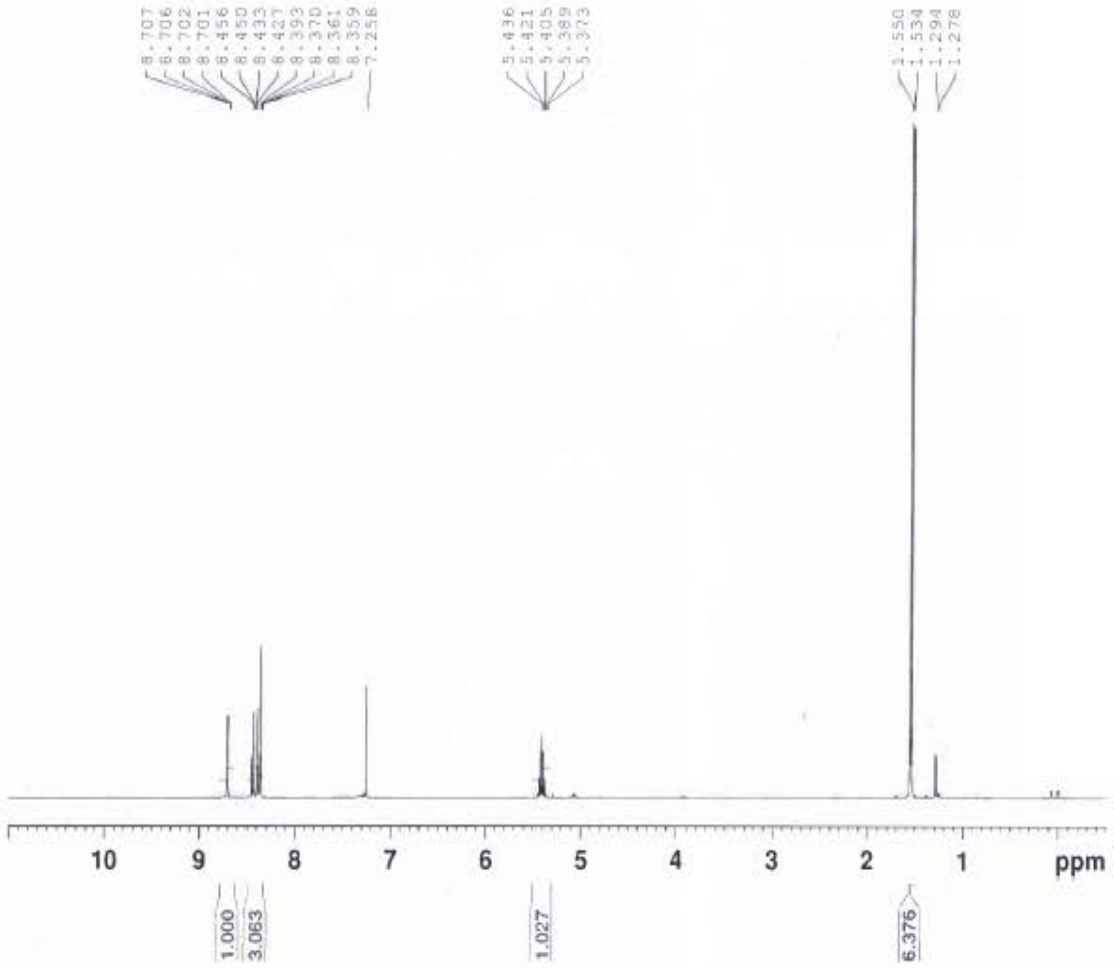
# $^{13}$C NMR – 2n



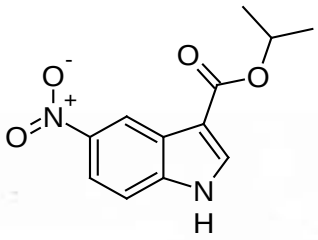



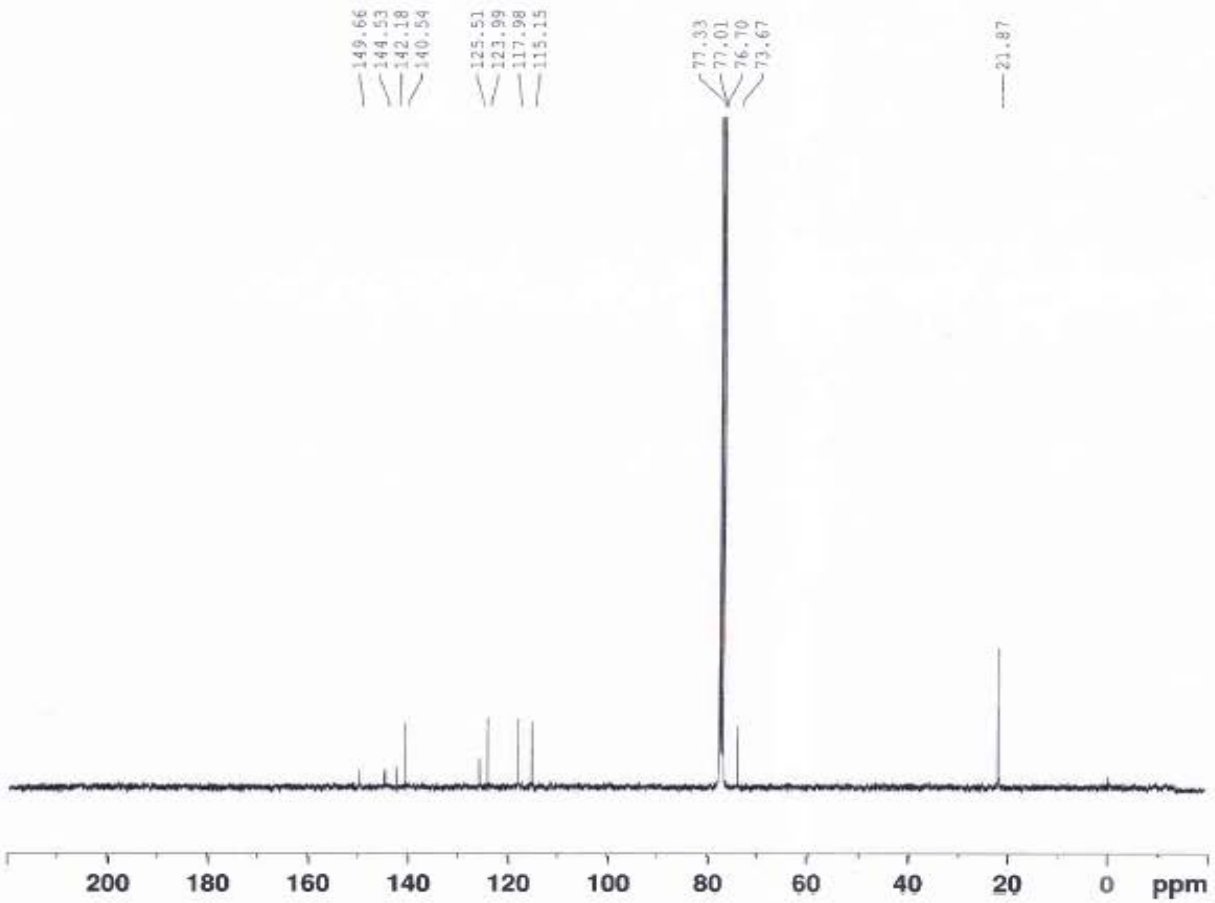
# $^{1}$H NMR – 2º



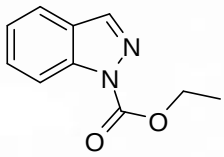



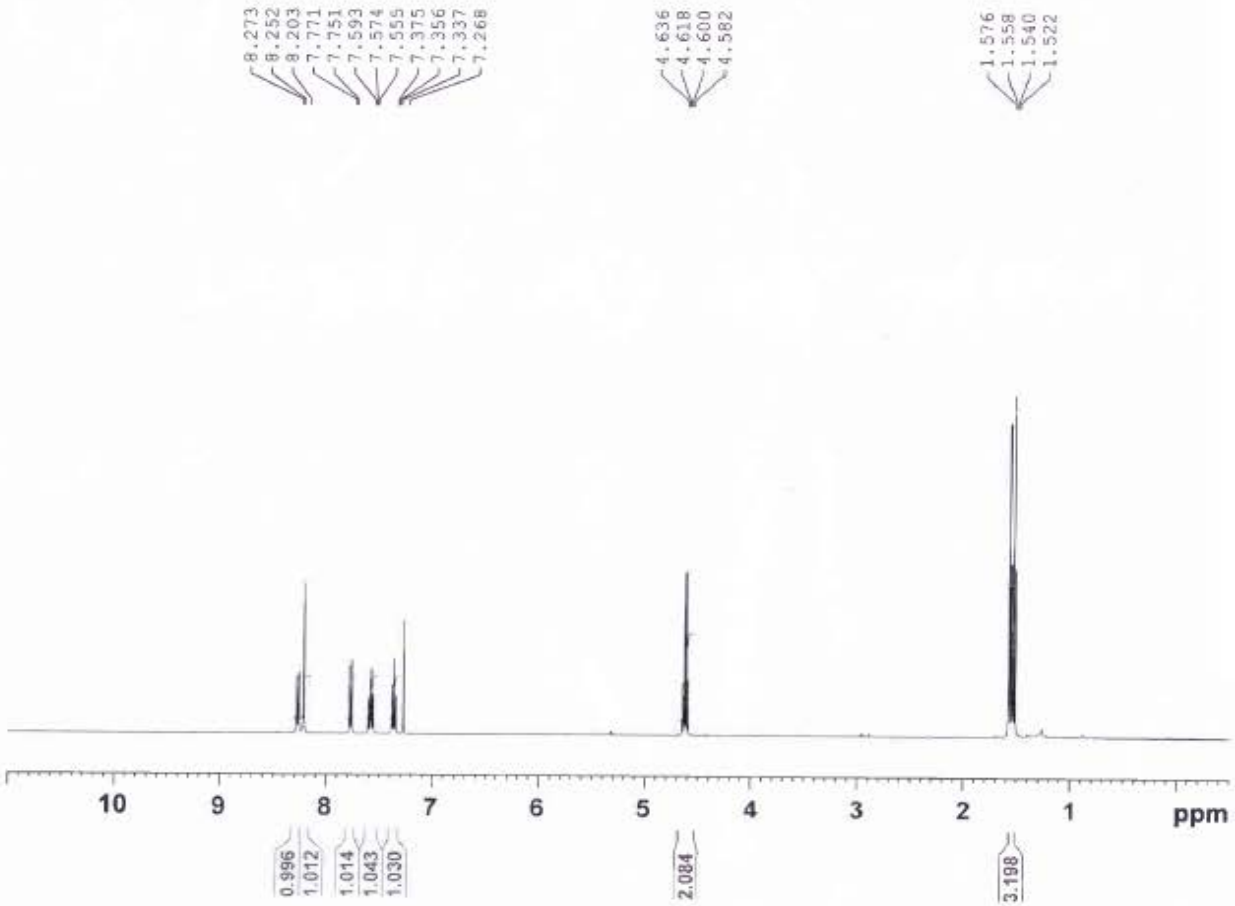
# $^{13}$C NMR – 2o



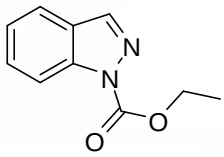



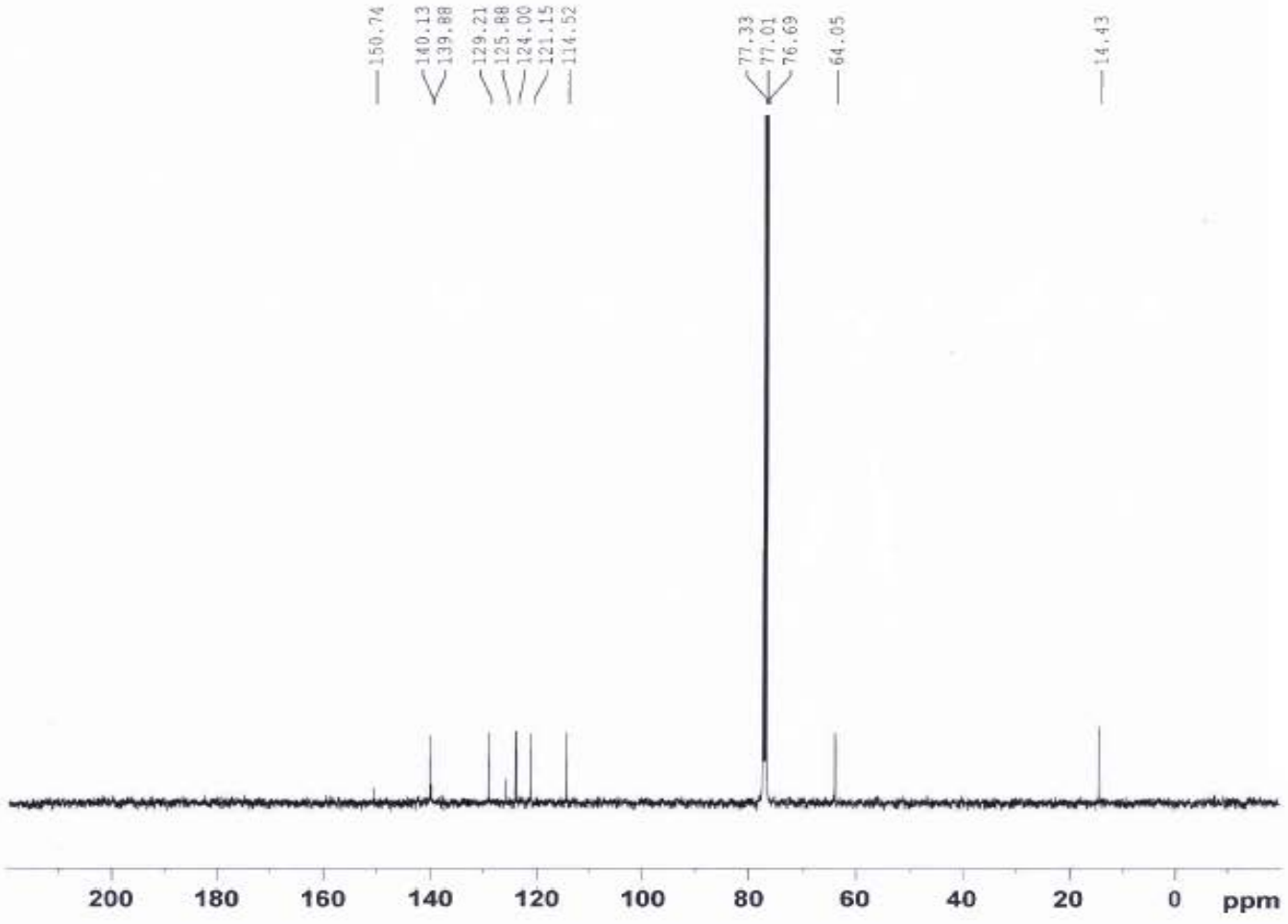
# $^{1}$H NMR – 2p



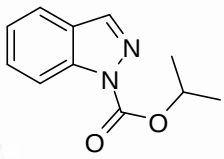



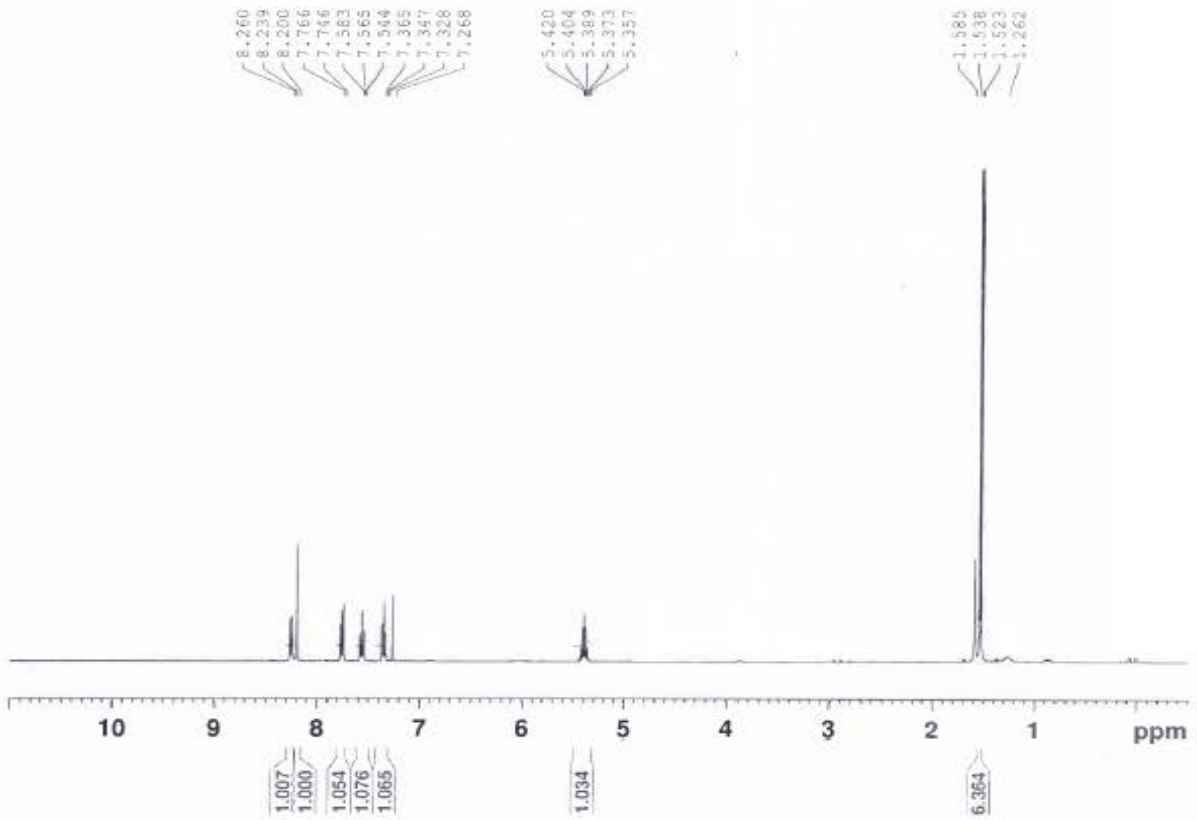
# $^{13}$C NMR – 2p



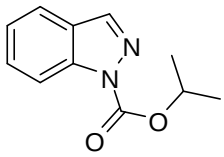



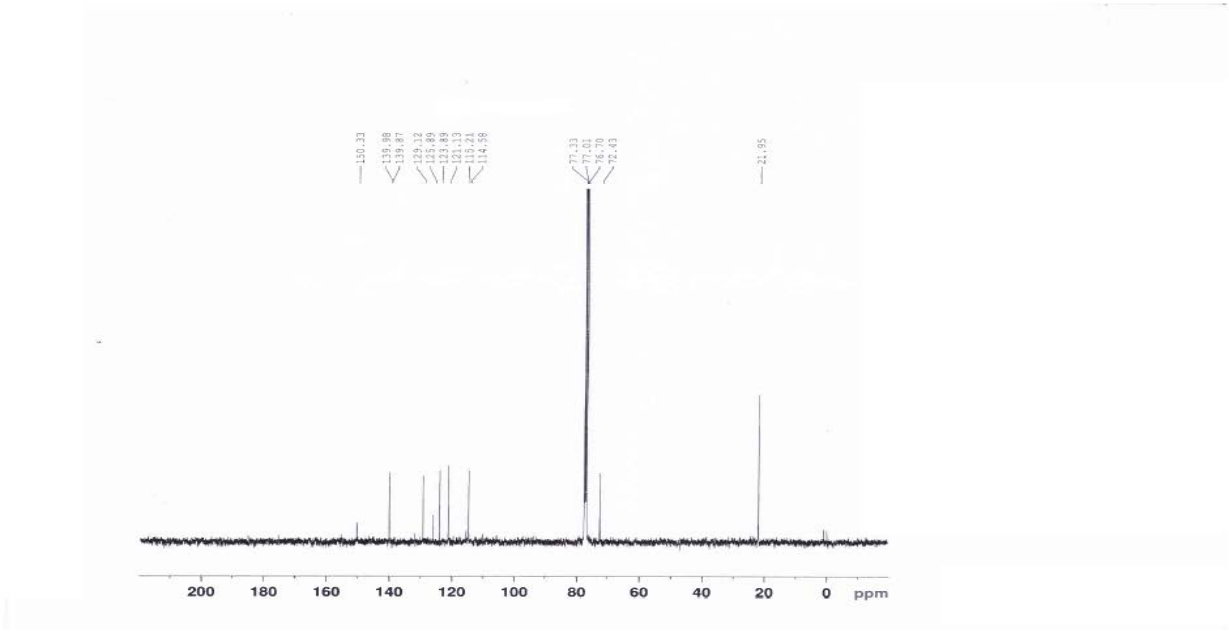
# $^{1}$H NMR – 2q



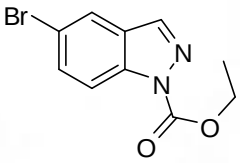



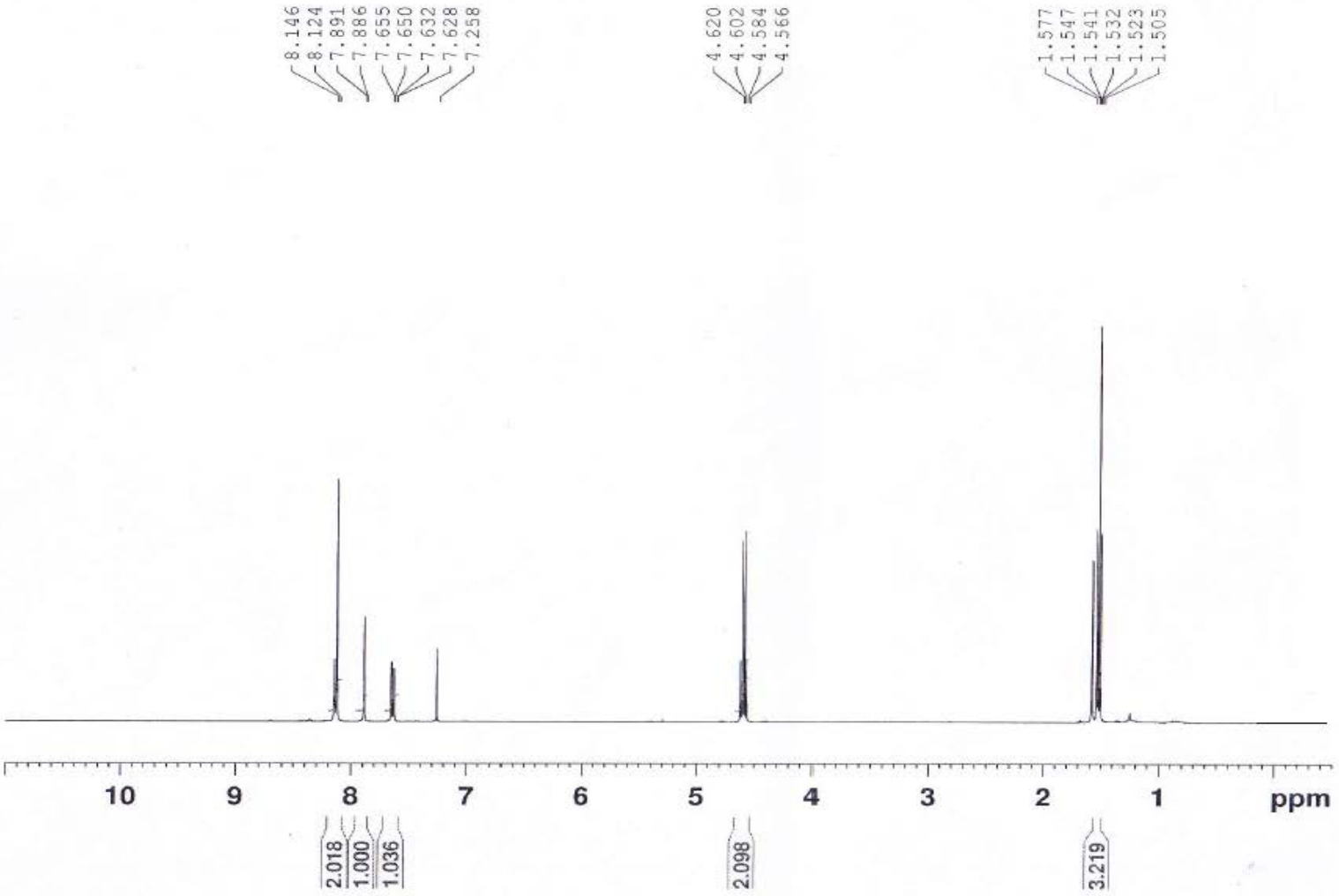
# $^{13}$C NMR – 2q



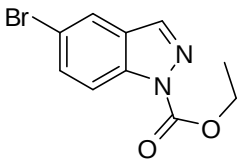



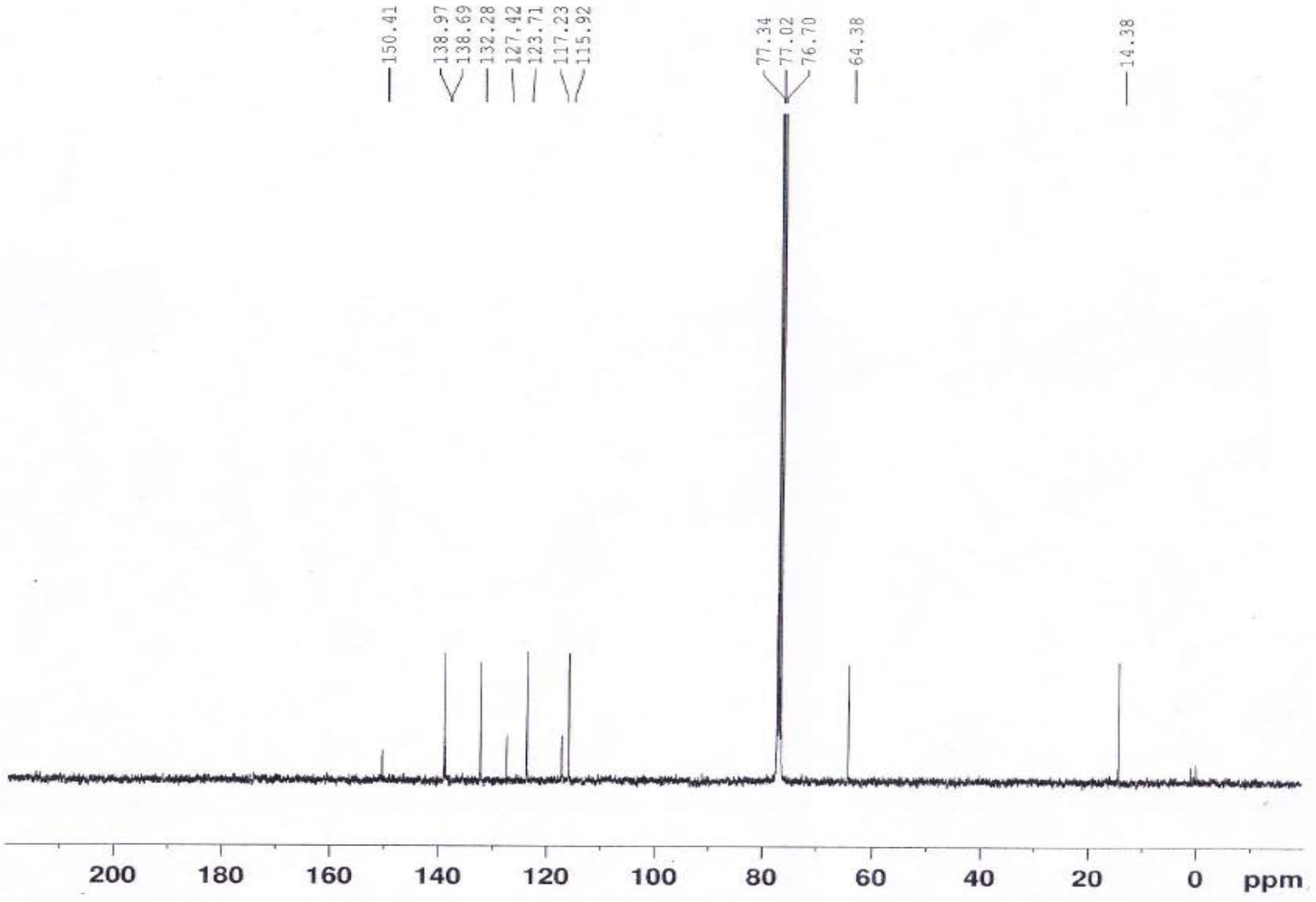
# $^{1}$H NMR – 2r



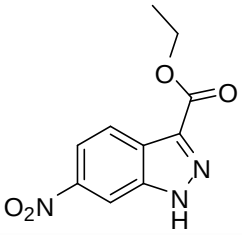



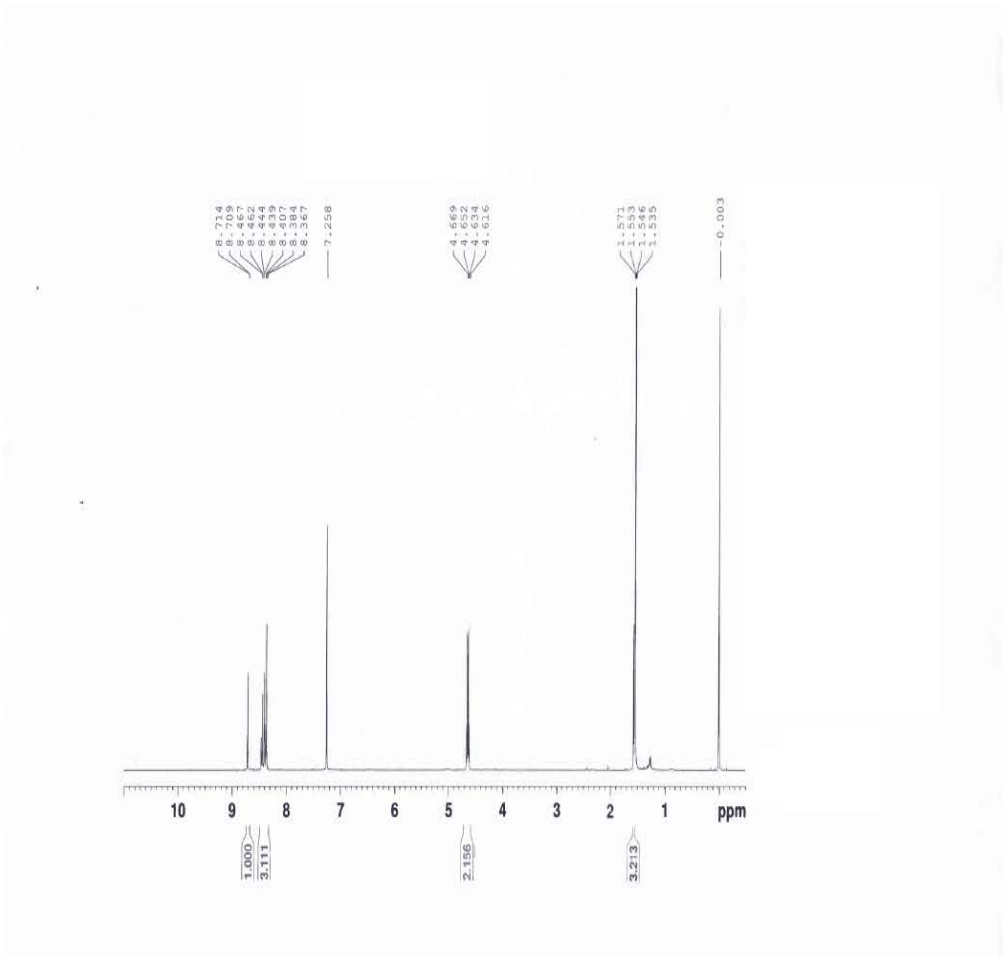
# $^{13}$C NMR – 2r



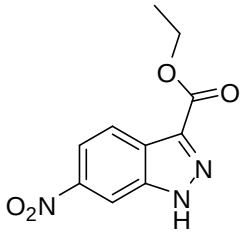



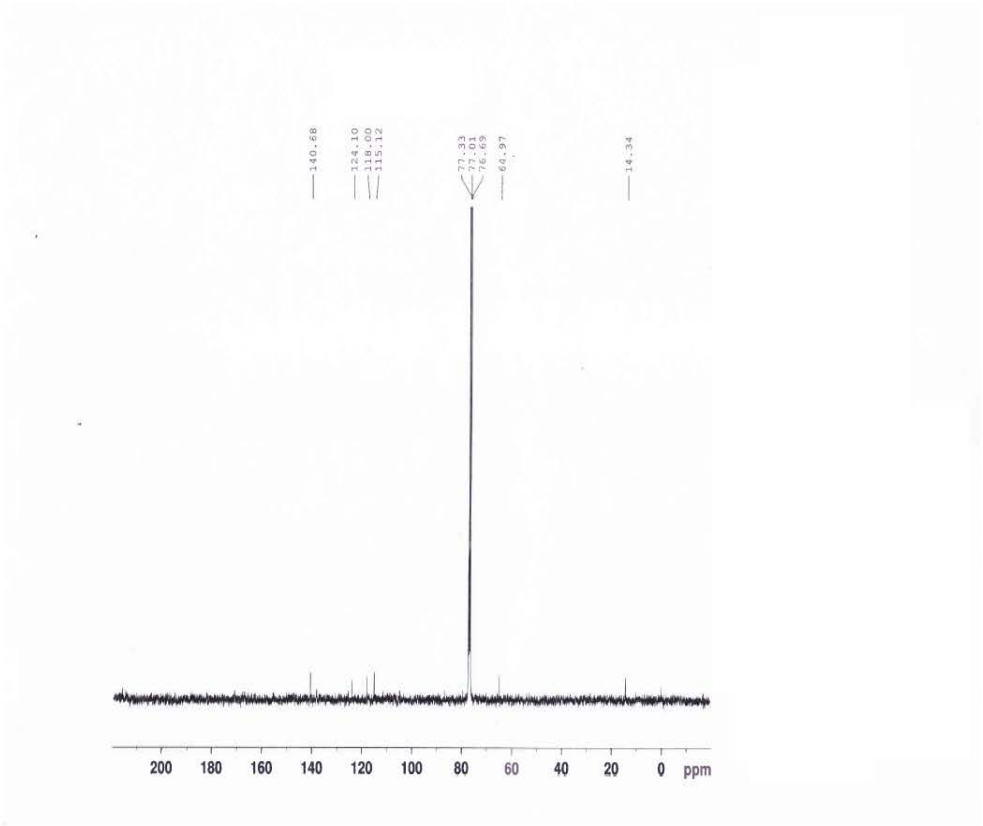
# $^{1}$H NMR – 2s



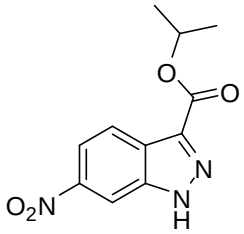



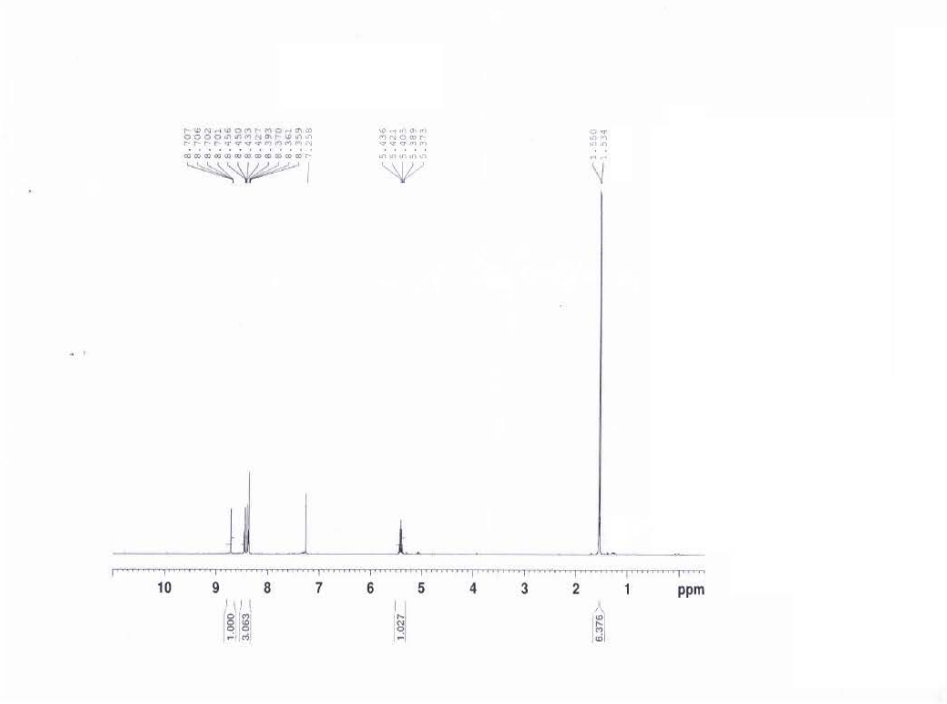
# $^{13}$C NMR – 2s



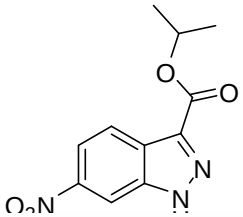



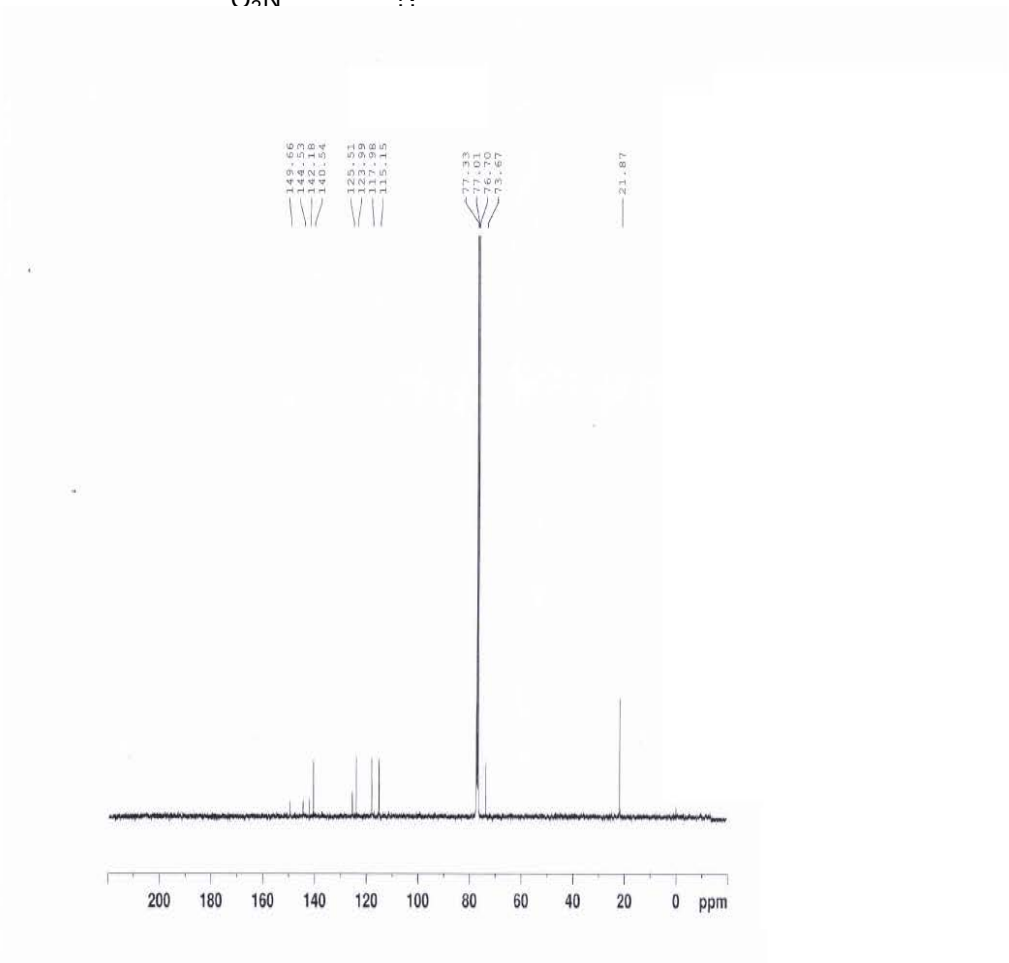
# $^{1}$H NMR – 2t



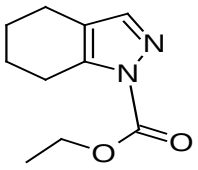



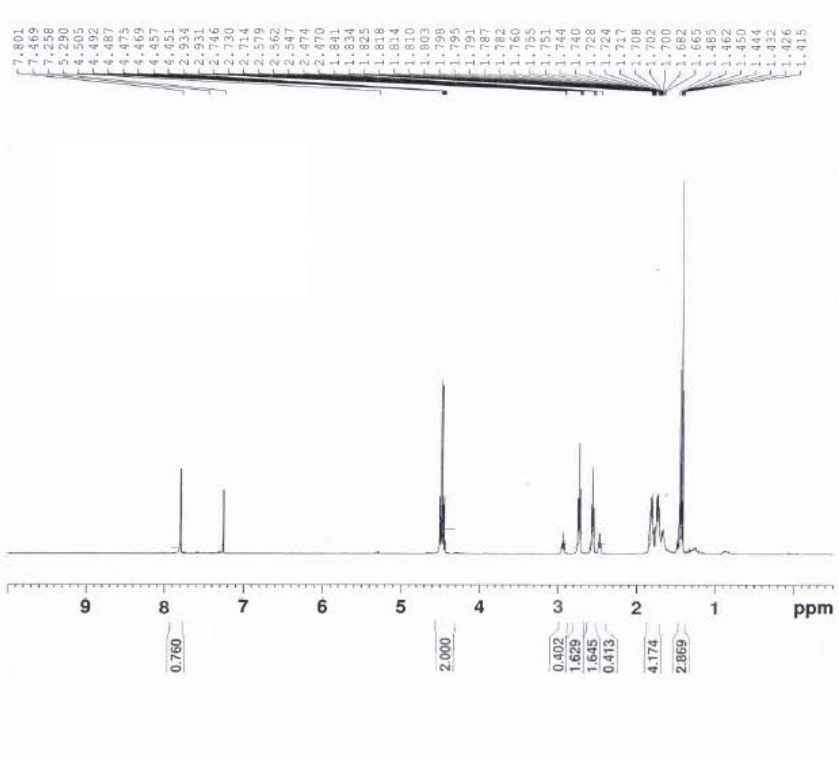
# $^{13}$C NMR – 2t



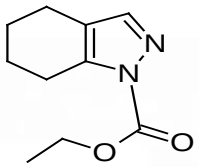



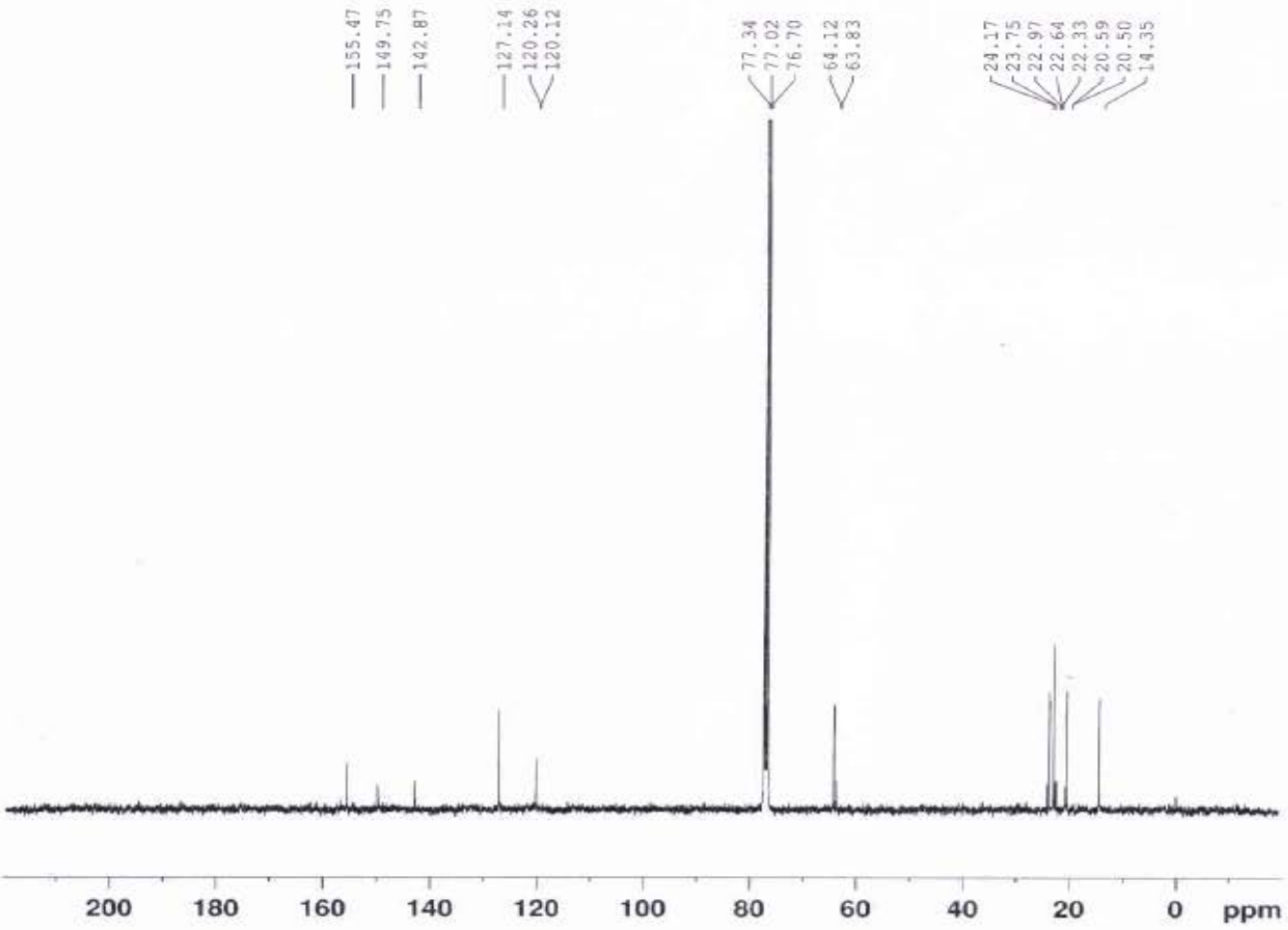
# $^{1}$H NMR – 2u



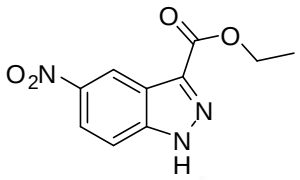



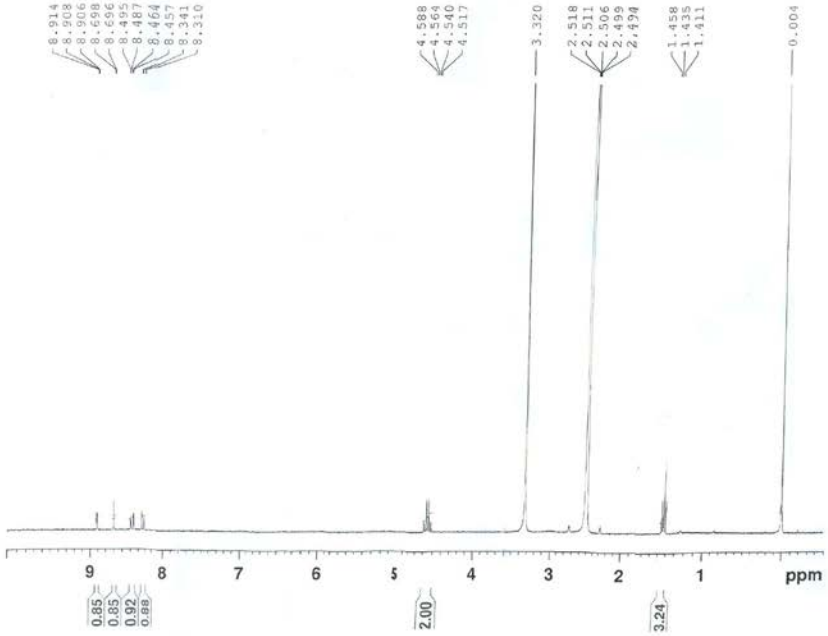
# $^{13}$C NMR – 2u



# $^{1}$H NMR – 2v



# Structure of 2s from X-ray studies