

Supporting information

The fast and efficient KI/H₂O₂ mediated 2-sulfonylation of indoles and N-methylpyrrole in water

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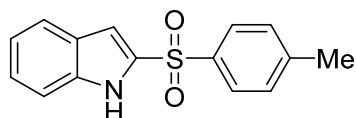
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General Information

Unless otherwise stated, all solvents and reagents were obtained commercially without further purification, all reactions were carried out in air and the reaction was monitored by TLC. All products were isolated by short chromatography on a silica gel (200–300 mesh) column using petroleum ether (60–90 °C) and ethyl acetate. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker Advance III HD 400 MHz spectrometer in CDCl_3 solution. All chemical shifts were reported in ppm (δ) relative to the internal standard TMS (0 ppm). ESI–Mass spectrum was measured on an Agilent 6210 ESI/TOF MS.

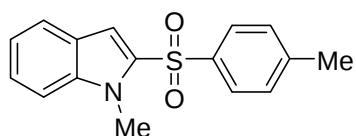
Characterization of compounds

2-tosyl-1H-indole (3a)¹

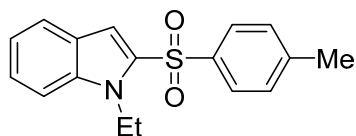


White solid, 110 mg, 81% yield, m.p. 190–192 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.91 (s, 1H), 7.88 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.8 Hz, 1H), 7.43–7.39 (m, 1H), 7.36–7.27 (m, 3H), 7.20–7.14 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.68, 138.68, 137.12, 134.69, 130.12, 127.49, 126.10, 122.81, 121.69, 112.36, 108.98, 21.74.

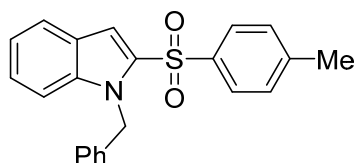
1-methyl-2-tosyl-1H-indole (3b)²



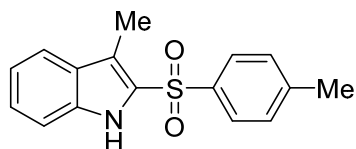
Pale yellow solid, 114 mg, 80% yield, m.p. 124–125 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.84 (d, J = 8.3 Hz, 2H), 7.69 (d, J = 8.1 Hz, 1H), 7.39–7.28 (m, 5H), 7.21–7.14 (m, 1H), 3.84 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.61, 139.56, 138.37, 135.30, 130.07, 127.86, 125.73, 125.31, 122.94, 121.22, 110.54, 110.34, 31.11, 21.74.

1-ethyl-2-tosyl-1H-indole (3c)²

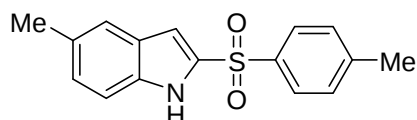
Light yellow liquid, 63 mg, 42% yield. ¹H NMR (400 MHz, CDCl₃): δ 7.84 (d, *J* = 6.8 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.37-7.27 (m, 5H), 7.20-7.13 (m, 1H), 4.37 (q, *J* = 7.2 Hz, 2H), 2.39 (s, 2H), 1.16 (t, *J* = 7.2 Hz, 3H).

1-benzyl-2-tosyl-1H-indole (3d)²

Pale yellow solid, 47 mg, 26% yield. ¹H NMR (400 MHz, CDCl₃): δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 0.8 Hz, 1H), 7.28-7.22 (m, 1H), 7.20-7.07 (m, 3H), 7.07-6.99 (m, 4H), 6.68 (d, *J* = 7.1 Hz, 2H), 5.64 (s, 2H), 2.28 (s, 3H).

3-methyl-2-tosyl-1H-indole (3e)²

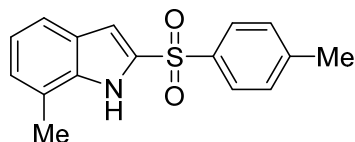
Yellow solid, 115 mg, 80% yield, m.p. 186–187 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.28 (s, 1H), 7.87 (dd, *J* = 8.3, 2.6 Hz, 2H), 7.58 (d, *J* = 8.1 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.33–7.23 (m, 3H), 7.17–7.11 (m, 1H), 2.53 (s, 3H), 2.36 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.38, 139.09, 136.09, 130.02, 129.52, 128.32, 126.12, 118.51, 112.42, 21.65, 9.02.

5-methyl-2-tosyl-1H-indole (3f)³

White solid, 111 mg, 78% yield, m.p. 135–137 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.88 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.42 (s, 1H), 7.29 (dd, *J* = 8.3, 5.3 Hz, 3H), 7.15 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.09–7.07 (m, 1H), 2.41 (s, 3H), 2.38 (s, 3H); ¹³C

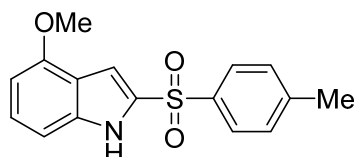
NMR (101 MHz, CDCl₃) δ 144.55, 138.80, 135.61, 134.43, 130.07, 128.03, 127.41, 121.98, 112.03, 108.53, 21.72.

7-methyl-2-tosyl-1H-indole (3g)³



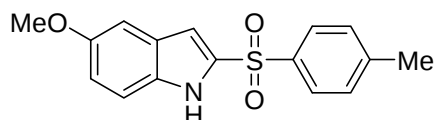
White solid, 116 mg, 82% yield, m.p. 171–173 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.01 (s, 1H), 7.92 (t, *J* = 6.5 Hz, 2H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 2.2 Hz, 1H), 7.13–7.05 (m, 2H), 2.48 (s, 3H), 2.39 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.61, 138.76, 137.21, 134.27, 130.11, 127.44, 126.30, 121.86, 120.26, 109.62, 21.72, 16.89.

4-methoxy-2-tosyl-1H-indole (3h)



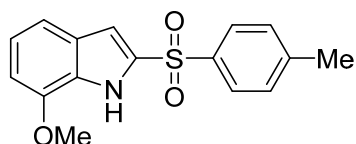
White solid, 123 mg, 82% yield, m.p. 155–158 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.90 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 7.1 Hz, 3H), 7.23 (d, *J* = 8.0 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 1H), 6.52 (d, *J* = 7.8 Hz, 1H), 3.92 (s, 3H), 2.38 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 154.65, 144.52, 130.06, 127.45, 127.20, 106.80, 105.11, 100.55, 55.52, 21.72; HRMS(ESI): *m/z* calcd for C₁₆H₁₅NO₃S (M)⁺: 301.0767, found: 301.0763.

5-methoxy-2-tosyl-1H-indole (3i)²



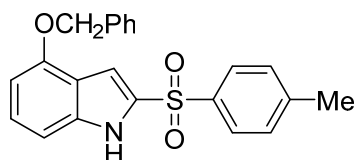
White solid, 134 mg, 89% yield, m.p. 145–147 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.92 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.29 (dd, *J* = 8.5, 4.2 Hz, 3H), 7.08 (dd, *J* = 2.1, 0.9 Hz, 1H), 7.04–6.97 (m, 2H), 3.82 (s, 3H), 2.39 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 155.26, 144.58, 134.74, 132.48, 130.09, 127.73, 127.41, 117.75, 113.35, 108.52, 102.66, 55.83, 21.73.

7-methoxy-2-tosyl-1H-indole (3j)



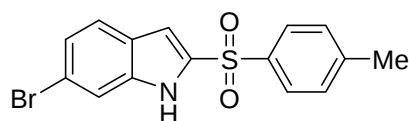
White solid, 123 mg, 82% yield, m.p. 149-151 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.00 (s, 1H), 7.86 (d, $J = 8.3$ Hz, 2H), 7.28 (s, 2H), 7.23 (d, $J = 8.2$ Hz, 1H), 7.16–7.03 (m, 3H), 6.73 (d, $J = 7.7$ Hz, 1H), 3.95 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 146.65, 144.52, 138.77, 134.40, 130.04, 127.47, 122.15, 114.85, 109.09, 104.80, 55.60, 21.71; HRMS(ESI): m/z calcd for $\text{C}_{16}\text{H}_{15}\text{NO}_3\text{S}(\text{M})^+$: 301.0767, found: 301.0769.

4-(benzyloxy)-2-tosyl-1H-indole (3k)



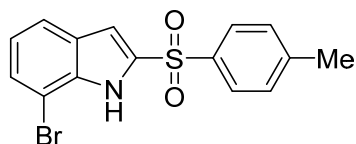
White solid, 113 mg, 60% yield, m.p. 136-139 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.97 (s, 1H), 7.87 (d, $J = 8.3$ Hz, 2H), 7.47 (d, $J = 7.2$ Hz, 2H), 7.37 (dt, $J = 24.0, 7.0$ Hz, 4H), 7.28 (s, 1H), 7.22 (t, $J = 8.1$ Hz, 1H), 6.58 (d, $J = 7.8$ Hz, 1H), 5.18 (s, 2H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.74, 138.79, 138.54, 136.92, 133.16, 130.07, 128.72, 128.15, 127.44, 107.00, 105.38, 101.85, 70.11, 21.72; HRMS(ESI): m/z calcd for $\text{C}_{22}\text{H}_{19}\text{NO}_3\text{S}(\text{M})^+$: 377.1080, found: 377.1075.

6-bromo-2-tosyl-1H-indole (3l)



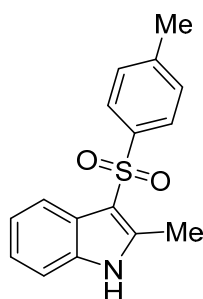
Brown solid, 136 mg, 78% yield, m.p. 181-182 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.25 (s, 1H), 7.88 (d, $J = 8.3$ Hz, 2H), 7.61 – 7.48 (m, 2H), 7.33 – 7.27 (m, 3H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.99, 138.28, 137.75, 135.32, 130.24, 127.50, 126.01, 125.30, 123.96, 119.78, 115.35, 108.91, 21.77; HRMS(ESI): m/z calcd for $\text{C}_{15}\text{H}_{12}\text{BrNNaO}_2\text{S}(\text{M}+\text{Na})^+$: 371.9664, found: 371.9653.

7-bromo-2-tosyl-1H-indole (3m)



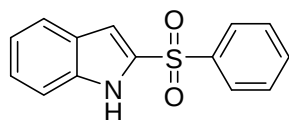
Dark red solid, 91 mg, 52% yield, m.p. 155-158 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.86 (s, 1H), 7.91 (d, $J = 8.3$ Hz, 2H), 7.60 (d, $J = 8.1$ Hz, 1H), 7.51–7.47 (m, 1H), 7.33 (d, $J = 8.1$ Hz, 2H), 7.22 (d, $J = 2.2$ Hz, 1H), 7.06 (t, $J = 7.8$ Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.87, 138.14, 135.77, 135.57, 130.10, 128.20, 128.02, 127.51, 122.67, 121.87, 109.60, 105.32, 21.64; HRMS(ESI): m/z calcd for $\text{C}_{15}\text{H}_{12}\text{BrNNaO}_2\text{S}(\text{M}+\text{Na})^+$: 371.9664, found: 371.9661.

2-methyl-3-tosyl-1H-indole (3n)



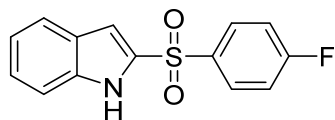
White solid, 125 mg, 88% yield, m.p. 179-181 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.26 (s, 1H), 7.97 (d, $J = 8.5$ Hz, 1H), 7.83 (d, $J = 8.3$ Hz, 2H), 7.24–7.10 (m, 5H), 2.64 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.38, 141.52, 141.19, 134.54, 129.75, 126.15, 125.40, 123.10, 122.17, 119.28, 111.42, 111.27, 21.57, 13.04; HRMS(ESI): m/z calcd for $\text{C}_{16}\text{H}_{16}\text{NO}_2\text{S}(\text{M}+\text{H})^+$: 286.0896, found: 286.0900.

2-(phenylsulfonyl)-1H-indole (3o)¹



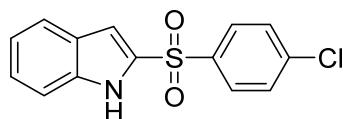
White solid, 104 mg, 81% yield, m.p. 159-161 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.53 (s, 1H), 8.02 (d, $J = 7.7$ Hz, 2H), 7.65 (d, $J = 8.0$ Hz, 1H), 7.53 (t, $J = 7.3$ Hz, 1H), 7.45 (dd, $J = 18.0, 8.4$ Hz, 3H), 7.32–7.28 (m, 1H), 7.22 (s, 1H), 7.15 (t, $J = 7.1$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 141.50, 137.51, 133.93, 133.56, 129.47, 127.32, 127.05, 126.14, 122.68, 121.62, 112.64, 109.39.

2-((4-fluorophenyl)sulfonyl)-1H-indole (3p)¹



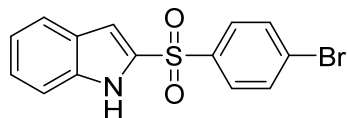
White solid, 88 mg, 65% yield, m.p. 139-141 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.12 (s, 1H), 8.02 (dd, $J = 8.9, 5.0$ Hz, 2H), 7.67 (d, $J = 8.0$ Hz, 1H), 7.42 (d, $J = 7.8$ Hz, 1H), 7.33 (d, $J = 8.3$ Hz, 1H), 7.20–7.15 (m, 4H); ^{13}C NMR (101 MHz, CDCl_3) δ 137.29, 133.98, 130.34, 130.24, 127.21, 126.39, 122.87, 121.88, 116.95, 116.72, 112.45, 109.48.

2-((4-chlorophenyl)sulfonyl)-1H-indole (3q)³



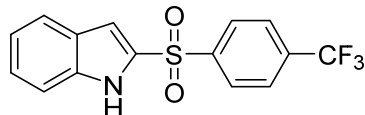
White solid, 104 mg, 71% yield, m.p. 146-148 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.51 (s, 1H), 8.05 (d, $J = 8.7$ Hz, 2H), 7.50 (d, $J = 8.8$ Hz, 3H), 7.44–7.37 (m, 2H), 7.29–7.23 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 140.67, 138.65, 135.98, 133.34, 131.34, 129.58, 129.38, 127.39, 123.24, 122.52, 112.51.

2-((4-bromophenyl)sulfonyl)-1H-indole (3r)¹

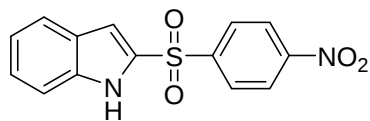


White solid, 97 mg, 58% yield, m.p. 191-193 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.97 (s, 1H), 7.85 (d, $J = 8.7$ Hz, 2H), 7.67 (d, $J = 8.1$ Hz, 1H), 7.63 (d, $J = 8.7$ Hz, 2H), 7.42 (d, $J = 8.4$ Hz, 1H), 7.38–7.33 (m, 1H), 7.21–7.17 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 140.67, 137.31, 133.63, 132.82, 131.77, 128.93, 127.25, 126.51, 122.92, 121.95, 112.42, 109.75.

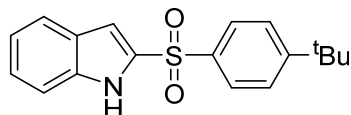
2-((4-(trifluoromethyl)phenyl)sulfonyl)-1H-indole (3s)¹



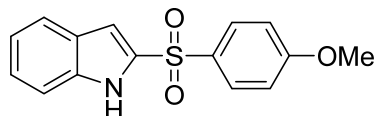
White solid, 109 mg, 67% yield, m.p. 151-153 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.96 (s, 1H), 8.12 (d, $J = 8.2$ Hz, 2H), 7.76 (d, $J = 8.3$ Hz, 2H), 7.68 (d, $J = 8.1$ Hz, 1H), 7.43 (d, $J = 8.4$ Hz, 1H), 7.39–7.35 (m, 1H), 7.24–7.08 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.05, 137.35, 132.82, 127.81, 127.11, 126.61, 122.86, 121.94, 112.33, 110.25, 65.61.

2-((4-nitrophenyl)sulfonyl)-1H-indole (3t)

Light yellow solid, 102 mg, 68% yield, m.p. 129-132 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.90 (s, 1H), 8.36–8.34 (m, 1H), 8.33 (d, *J* = 2.1 Hz, 1H), 8.20–8.15 (m, 2H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.46–7.42 (m, 1H), 7.41–7.37 (m, 1H), 7.29 (dd, *J* = 2.1, 0.8 Hz, 1H), 7.22 (ddd, *J* = 8.0, 6.8, 1.1 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 150.40, 147.18, 137.49, 132.20, 129.24, 128.58, 127.15, 126.92, 124.61, 124.46, 122.97, 122.12, 112.35, 110.85; HRMS(ESI): *m/z* calcd for C₁₄H₁₀N₂NaO₄S(M+Na)⁺: 325.0253, found: 325.0251.

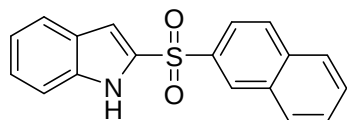
2-((4-(tert-butyl)phenyl)sulfonyl)-1H-indole (3u)¹

White solid, 118 mg, 76% yield, m.p. 192-194 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.50 (s, 1H), 7.94 (d, *J* = 8.7 Hz, 2H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.42 (d, *J* = 7.7 Hz, 1H), 7.29 (ddd, *J* = 8.3, 7.1, 1.0 Hz, 1H), 7.21 (d, *J* = 1.3 Hz, 1H), 7.18 – 7.12 (m, 1H), 1.27 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 157.57, 138.47, 137.38, 134.50, 127.28, 127.12, 126.54, 126.02, 122.67, 121.58, 112.59, 109.01, 35.33, 31.10.

2-((4-methoxyphenyl)sulfonyl)-1H-indole (3v)¹

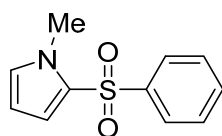
White solid, 73 mg, 51% yield, m.p. 186-187 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.25 (s, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 2.6 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.19 – 7.14 (m, 1H), 7.07 (ddd, *J* = 12.3, 7.3, 1.6 Hz, 3H), 6.69–6.62 (m, 2H), 3.65 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 157.89, 136.57, 130.14, 129.62, 129.12, 128.68, 123.06, 120.89, 119.77, 114.61, 111.64, 104.72, 55.46.

2-(naphthalen-2-ylsulfonyl)-1H-indole (3w)¹



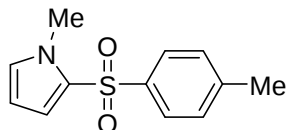
White solid, 124 mg, 81% yield, m.p. 156-158 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.91 (s, 1H), 8.61 (s, 1H), 7.99–7.91 (m, 3H), 7.87 (d, $J = 7.7$ Hz, 1H), 7.68–7.58 (m, 3H), 7.49–7.29 (m, 3H), 7.17 (t, $J = 7.5$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 138.24, 137.07, 135.14, 134.19, 132.18, 129.77, 129.44, 129.30, 128.74, 127.96, 127.74, 127.16, 126.11, 122.73, 122.27, 121.63, 112.22, 109.32.

1-methyl-2-(phenylsulfonyl)-1H-pyrrole (5a)⁴



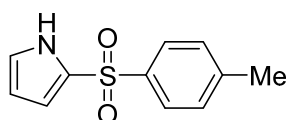
Light yellow viscous solid, 62 mg, 57% yield, m.p. 76-78 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.88 (d, $J = 7.1$ Hz, 2H), 7.57–7.48 (m, 3H), 7.03 (dd, $J = 4.0, 1.9$ Hz, 1H), 6.76 (s, 1H), 6.17 (dd, $J = 4.0, 2.6$ Hz, 1H), 3.70 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 142.25, 132.98, 129.81, 129.31, 127.23, 118.96, 108.45, 35.73.

1-methyl-2-tosyl-1H-pyrrole (5b)⁴

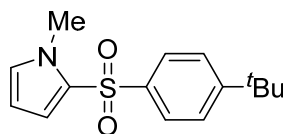


White solid, 55 mg, 47% yield, m.p. 99-101 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.77 (d, $J = 8.3$ Hz, 2H), 7.29 (d, $J = 8.0$ Hz, 2H), 7.00 (dd, $J = 4.0, 1.9$ Hz, 1H), 6.74 (t, $J = 2.2$ Hz, 1H), 6.16 (dd, $J = 4.0, 2.6$ Hz, 1H), 3.70 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.90, 139.36, 129.94, 129.54, 128.44, 118.63, 108.35, 35.72, 21.68.

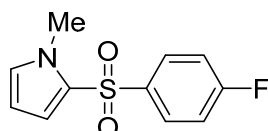
2-tosyl-1H-pyrrole (5b')⁵



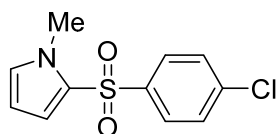
White solid, 20 mg, 18% yield. ^1H NMR (400 MHz, CDCl_3): δ 9.35 (s, 1H), 7.80 (d, $J = 8.4$ Hz, 2H), 7.28 (d, $J = 8.0$ Hz, 2H), 6.95 (td, $J = 2.8, 1.6$ Hz, 1H), 6.85 (ddd, $J = 4.0, 2.4, 1.6$ Hz, 1H), 6.28 (dt, $J = 3.6, 2.4$ Hz, 1H), 2.39 (s, 3H).

2-((4-(tert-butyl)phenyl)sulfonyl)-1-methyl-1H-pyrrole (5c)

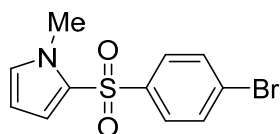
Pale yellow solid, 58 mg, 42% yield, m.p. 59-61 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.80 (d, $J = 8.7$ Hz, 2H), 7.50 (d, $J = 8.7$ Hz, 2H), 7.02 (dd, $J = 4.0, 1.9$ Hz, 1H), 6.75 (t, $J = 2.2$ Hz, 1H), 6.16 (dd, $J = 4.0, 2.6$ Hz, 1H), 3.72 (s, 3H), 1.32 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 156.84, 139.25, 129.56, 128.43, 127.16, 126.33, 118.64, 108.33, 35.79, 35.30, 31.18; HRMS(ESI): m/z calcd for $\text{C}_{15}\text{H}_{20}\text{NO}_2\text{S}(\text{M}+\text{H})^+$: 278.1209, found: 278.1208.

2-((4-fluorophenyl)sulfonyl)-1-methyl-1H-pyrrole (5d)⁴

Pale yellow solid, 59 mg, 50% yield, m.p. 61-63 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.90 (dd, $J = 8.9, 5.1$ Hz, 2H), 7.17 (t, $J = 8.6$ Hz, 2H), 7.01 (dd, $J = 4.0, 1.9$ Hz, 1H), 6.78 (t, $J = 2.1$ Hz, 1H), 6.17 (dd, $J = 4.0, 2.6$ Hz, 1H), 3.71 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.49, 163.95, 138.35, 130.07, 129.97, 127.72, 118.97, 116.67, 116.44, 108.52, 35.69.

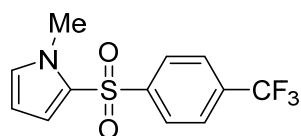
2-((4-chlorophenyl)sulfonyl)-1-methyl-1H-pyrrole (5e)⁴

Yellow solid, 66 mg, 52% yield, m.p. 73-75 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.82 (d, $J = 8.8$ Hz, 2H), 7.47 (d, $J = 8.8$ Hz, 2H), 7.03 (dd, $J = 4.1, 1.9$ Hz, 1H), 6.78 (t, $J = 2.2$ Hz, 1H), 6.18 (dd, $J = 4.1, 2.6$ Hz, 1H), 3.71 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 140.87, 139.57, 130.13, 129.65, 128.77, 127.54, 119.30, 108.70, 35.80.

2-((4-bromophenyl)sulfonyl)-1-methyl-1H-pyrrole (5f)⁴

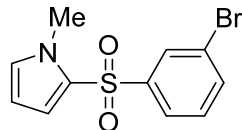
Pale yellow solid, 70 mg, 47% yield, m.p. 90-92 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.74 (d, *J* = 8.7 Hz, 2H), 7.64 (d, *J* = 8.7 Hz, 2H), 7.03 (dd, *J* = 4.1, 1.9 Hz, 1H), 6.78 (t, *J* = 2.2 Hz, 1H), 6.18 (dd, *J* = 4.1, 2.6 Hz, 1H), 3.71 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 141.39, 132.62, 130.16, 128.83, 128.07, 127.45, 119.32, 35.79.

1-methyl-2-((4-(trifluoromethyl)phenyl)sulfonyl)-1H-pyrrole (5g)



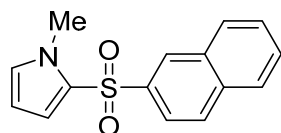
Pale yellow solid, 62 mg, 43% yield, m.p. 66-68 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.01 (d, *J* = 8.2 Hz, 2H), 7.77 (d, *J* = 8.3 Hz, 2H), 7.09 (dd, *J* = 4.1, 1.9 Hz, 1H), 6.81 (t, *J* = 2.2 Hz, 1H), 6.21 (dd, *J* = 4.1, 2.6 Hz, 1H), 3.73 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 145.96, 134.76, 134.43, 130.61, 127.77, 126.85, 126.53, 126.50, 124.63, 121.92, 119.92, 108.94, 35.87; HRMS(ESI): *m/z* calcd for C₁₂H₁₁F₃NO₂S (M+H)⁺: 290.0457, found: 290.0457.

2-((3-bromophenyl)sulfonyl)-1-methyl-1H-pyrrole (5h)



Pale yellow solid, 79 mg, 53% yield, m.p. 55-58 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.01 (t, *J* = 1.8 Hz, 1H), 7.81 (d, *J* = 7.9 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.05 (dd, *J* = 4.1, 1.9 Hz, 1H), 6.80 (t, *J* = 2.2 Hz, 1H), 6.20 (dd, *J* = 4.1, 2.6 Hz, 1H), 3.72 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 144.26, 136.02, 130.86, 130.36, 130.09, 127.11, 125.78, 123.25, 119.62, 108.77, 35.85; HRMS(ESI): *m/z* calcd for C₁₁H₁₁BrNO₂S(M)⁺: 299.9688, found: 298.9690.

1-methyl-2-(naphthalen-2-ylsulfonyl)-1H-pyrrole (5i)



Pale yellow solid, 60 mg, 45% yield, m.p. 60-63 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.50 (s, 1H), 7.93 (td, *J* = 17.0, 16.6, 7.8 Hz, 3H), 7.80 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.66-7.57 (m, 2H), 7.10 (dd, *J* = 4.0, 1.9 Hz, 1H), 6.75 (t, *J* = 2.2 Hz, 1H), 6.19 (dd, *J*

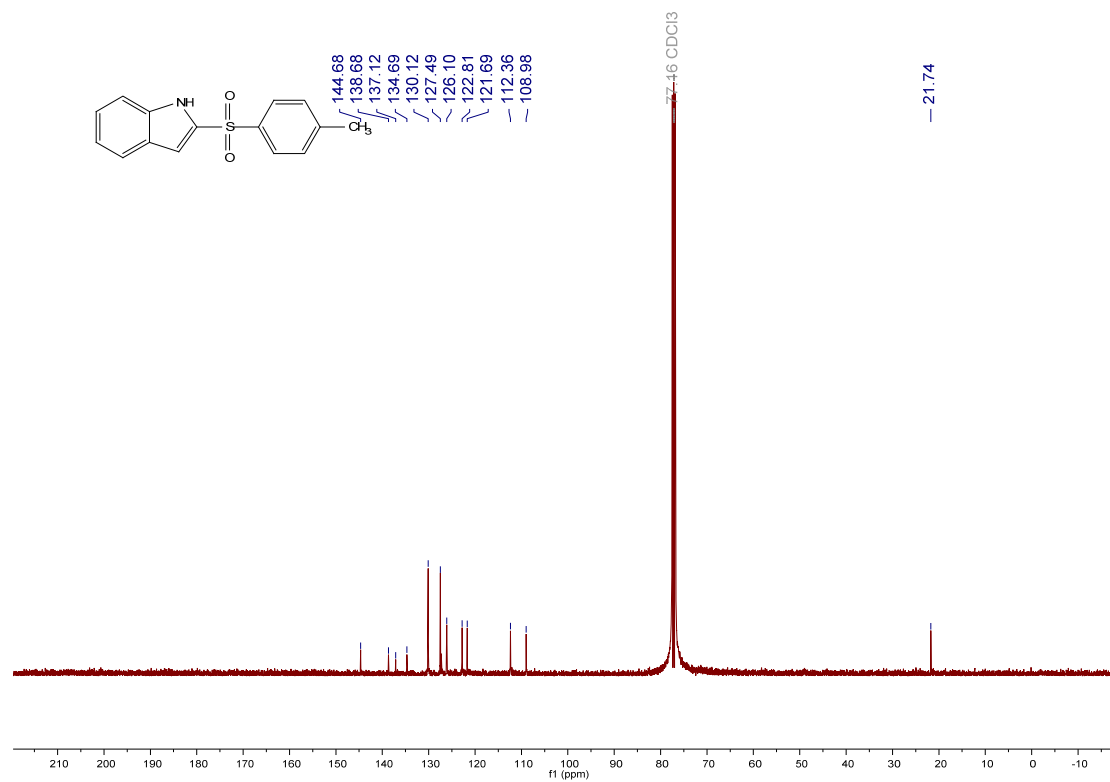
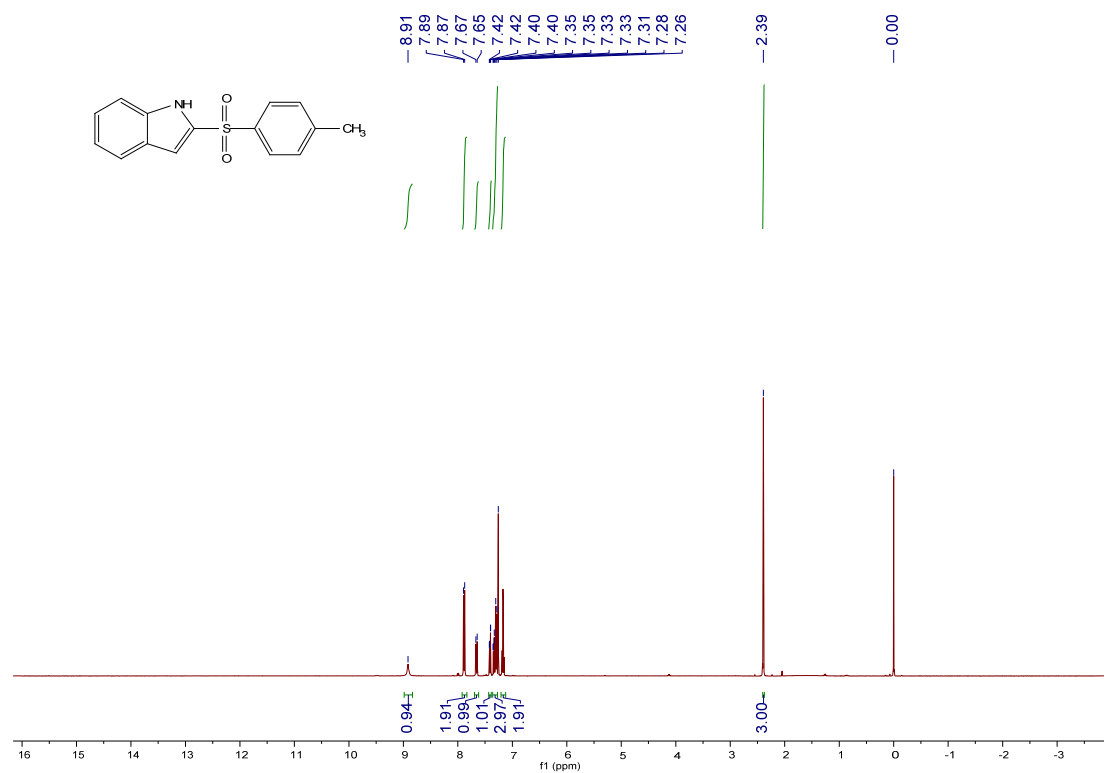
= 4.0, 2.6 Hz, 1H), 3.72 (s, 3H), ¹³C NMR (101 MHz, CDCl₃) δ 139.13, 135.02, 132.30, 129.85, 129.73, 129.47, 129.15, 128.33, 128.06, 127.72, 122.71, 119.14, 108.54, 35.81; HRMS(ESI): m/z calcd for C₁₅H₁₄NO₂S(M+H)⁺: 272.0740, found: 272.0745.

References

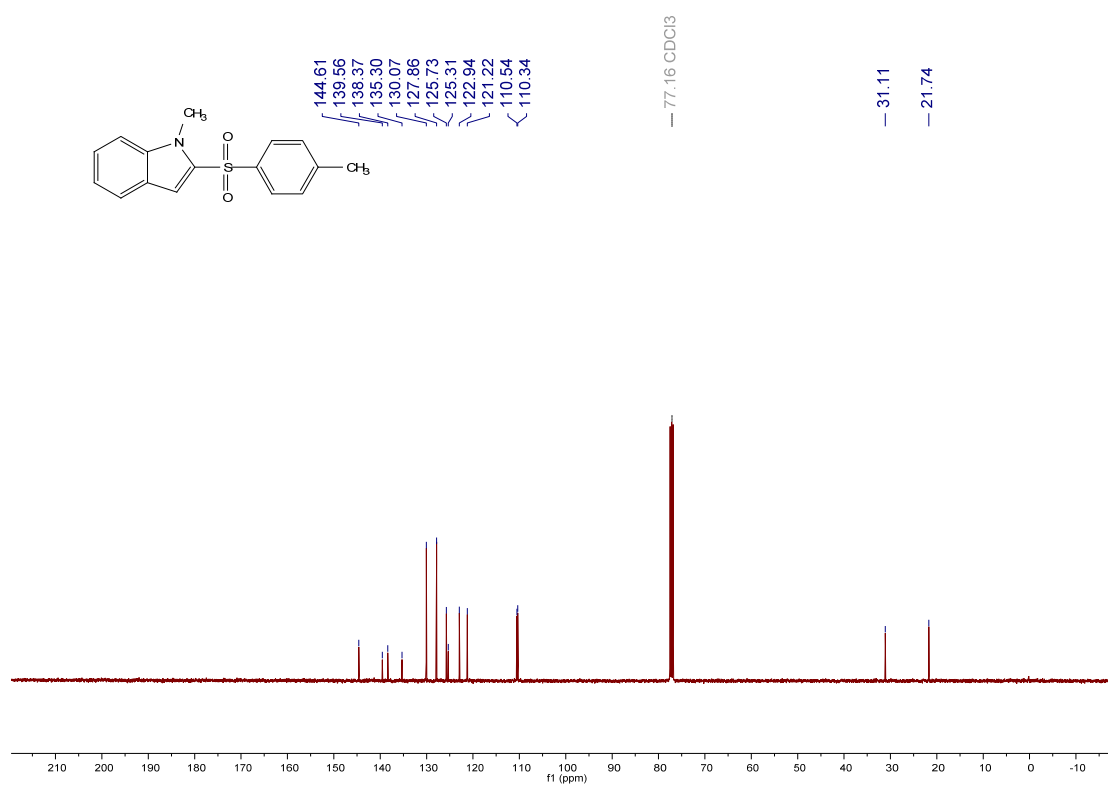
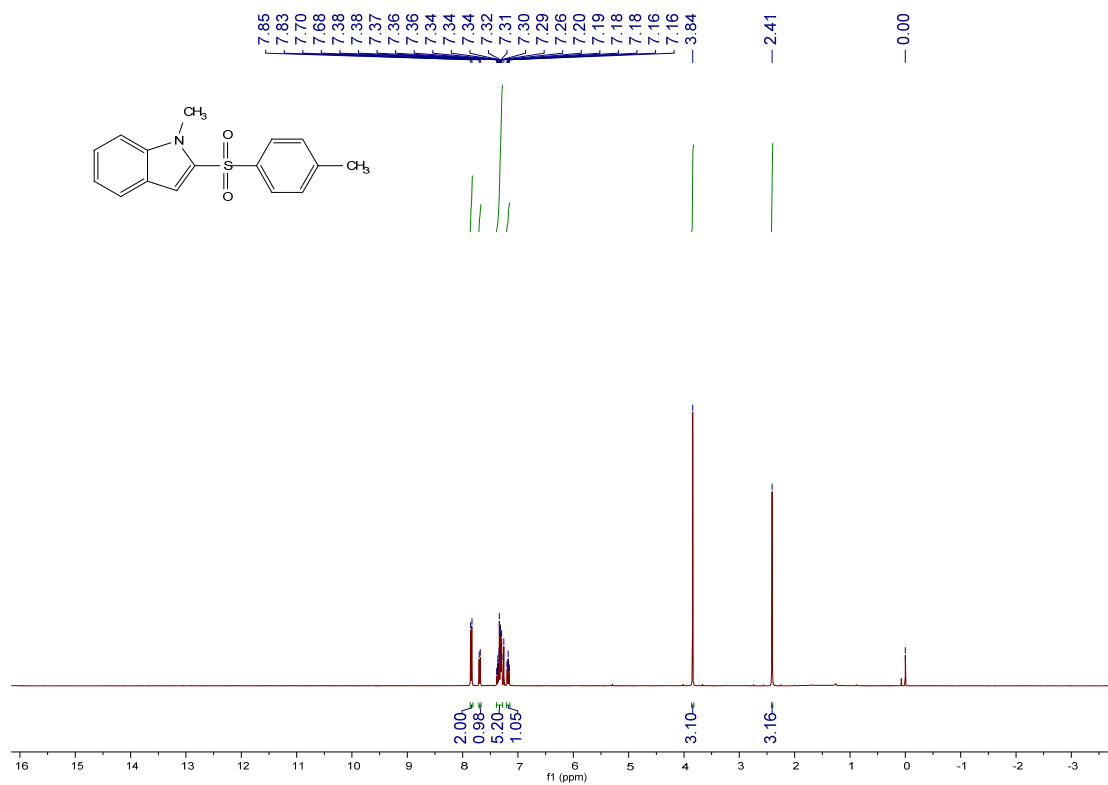
- 1 F. Xiao, H. Chen, H. Xie, S. Chen, L. Yang, G.-J. Deng, *Org. Lett.* **2014**, *16*, 50.
- 2 Katrun, P.; Mueangkaew, C.; Pohmakotr, M.; Reutrakul, V.; Jaipetch, T.; Soorukram, D.; Kuhakarn, C. *J. Org. Chem.* **2014**, *79*, 1778.
- 3 Yang, Y.; Li, W. M.; Xia, C. C.; Ying, B. B.; Shen, C.; Zhang, P. F. *ChemCatChem.* **2016**, *8*, 304.
- 4 Santosh K. Pagire, Asik Hossain, and Oliver Reiser, *Org. Lett.* **2018**, *20*, 648.
- 5 Yadav, J. S., Reddy, B. V. S., Kondaji, G., Rao, R. S., Kumar, S. P. *Tetrahedron lett.*, **2002**, *43*, 8133.

^1H and ^{13}C NMR spectra

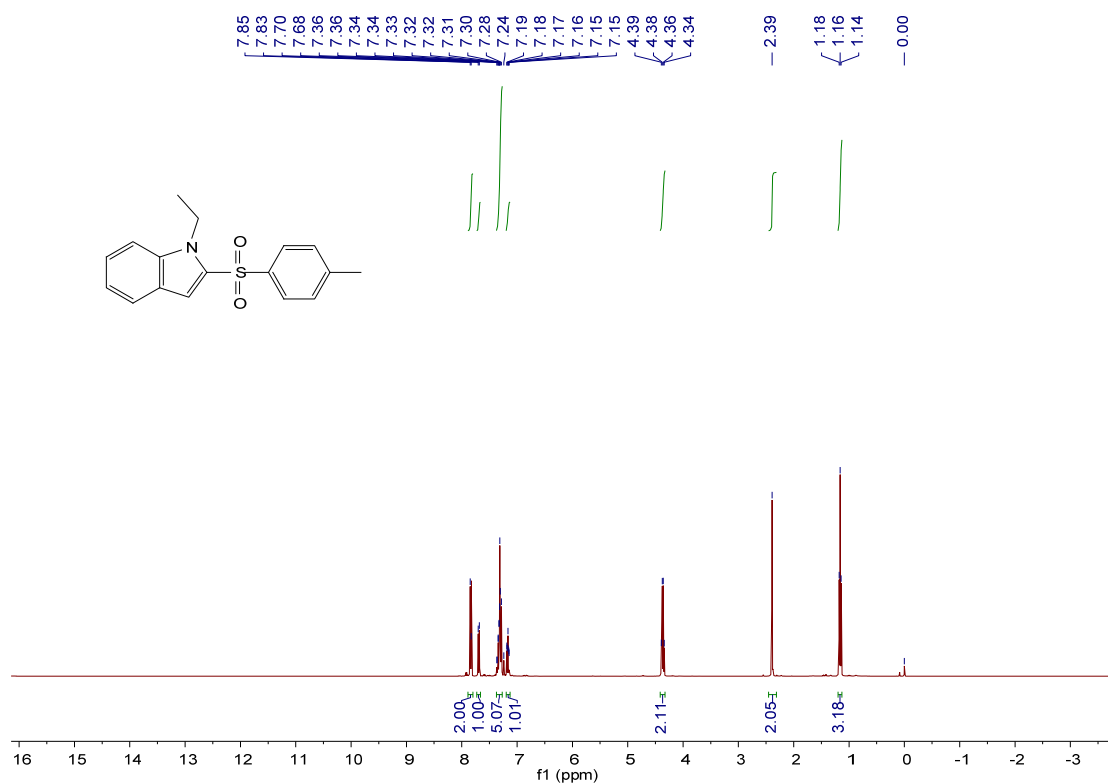
2-tosyl-1H-indole (3a)



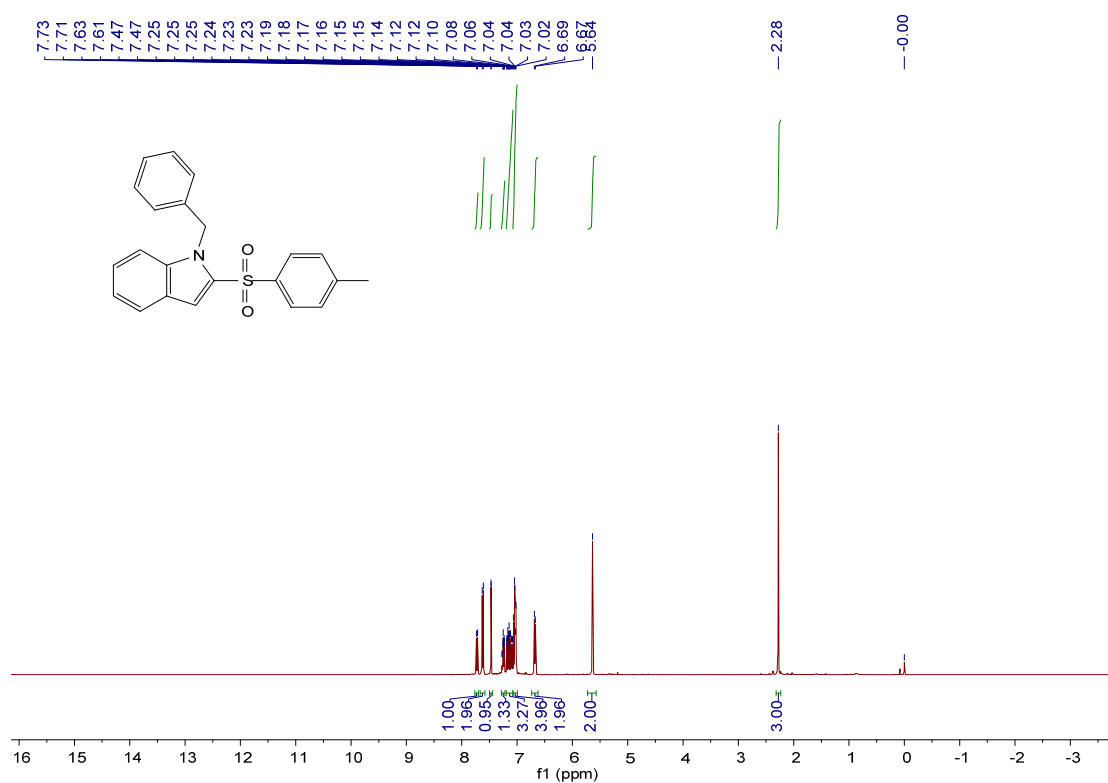
1-methyl-2-tosyl-1H-indole (3b)



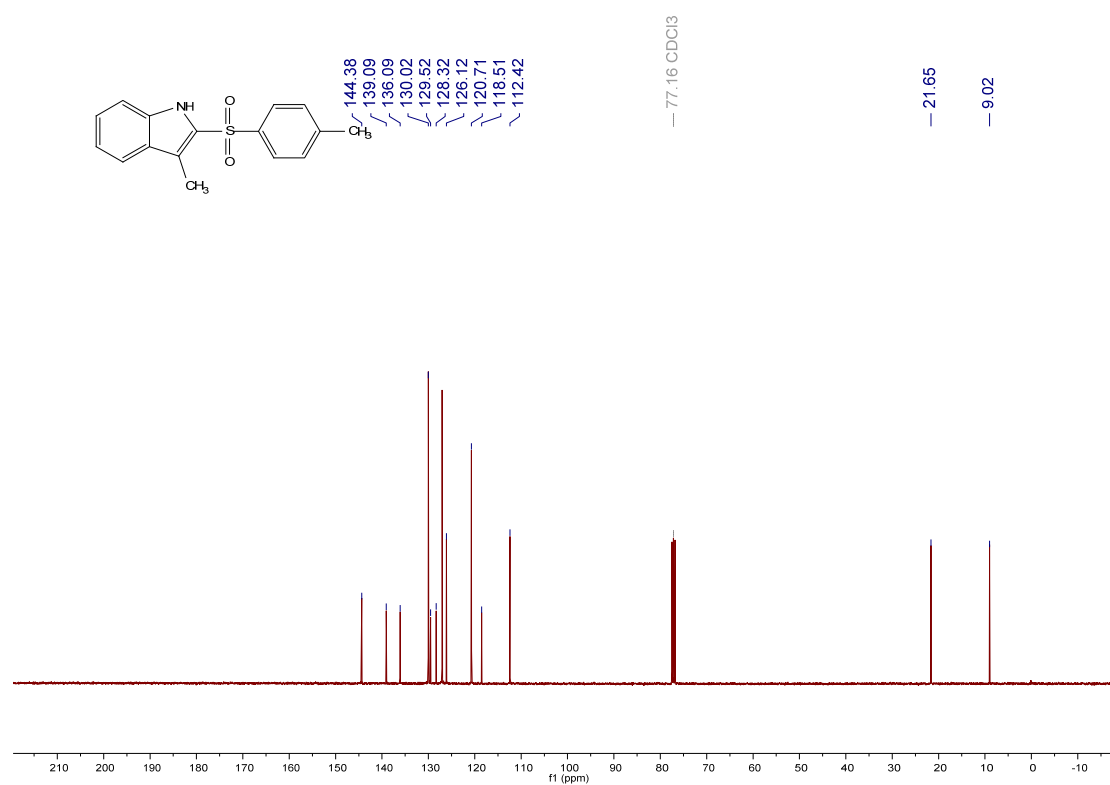
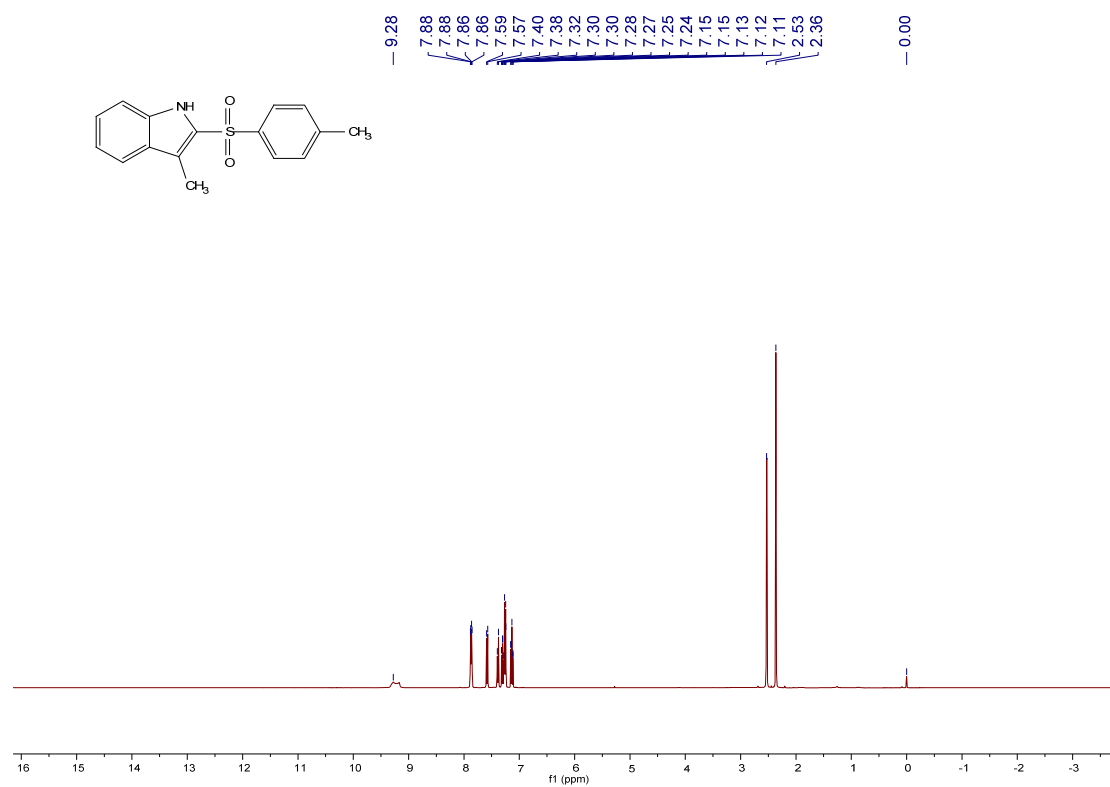
1-ethyl-2-tosyl-1H-indole (3c)



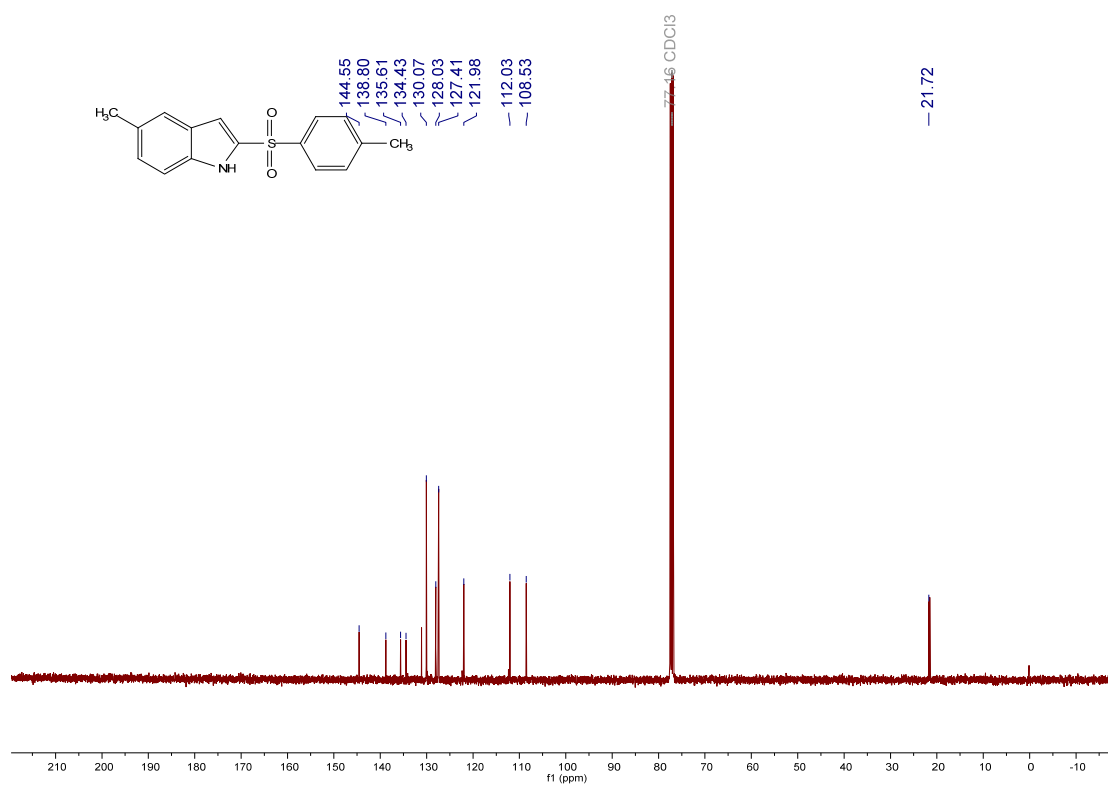
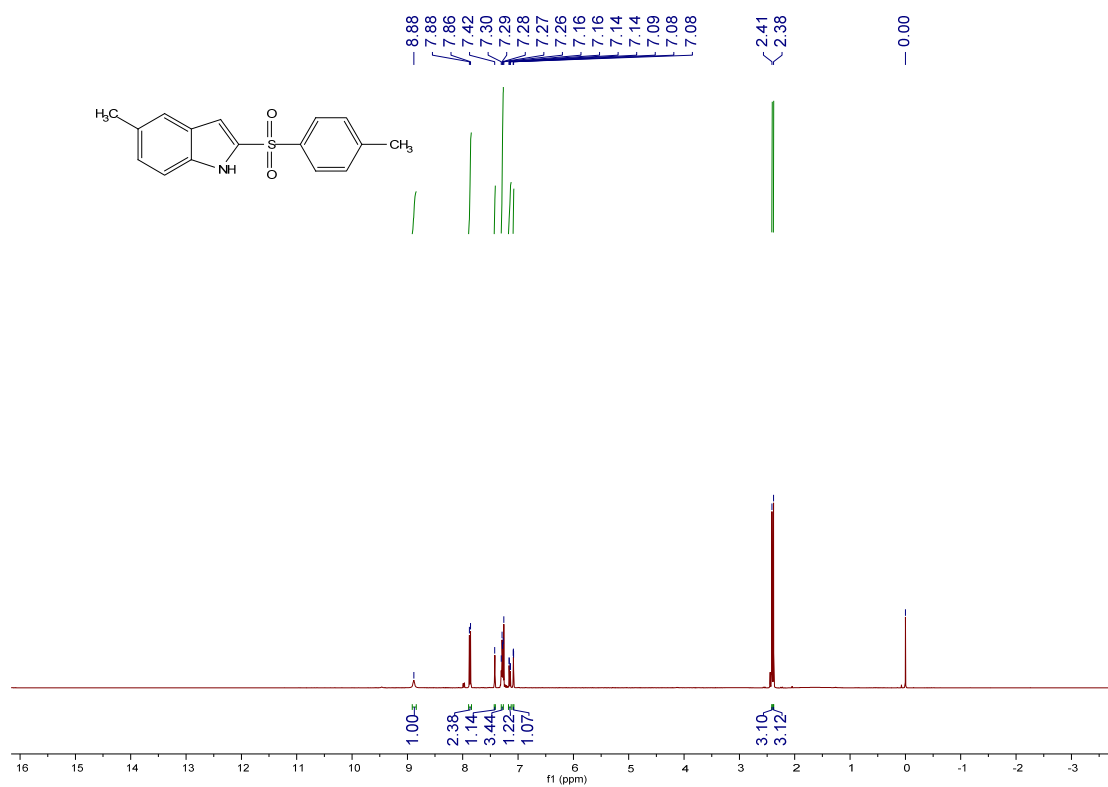
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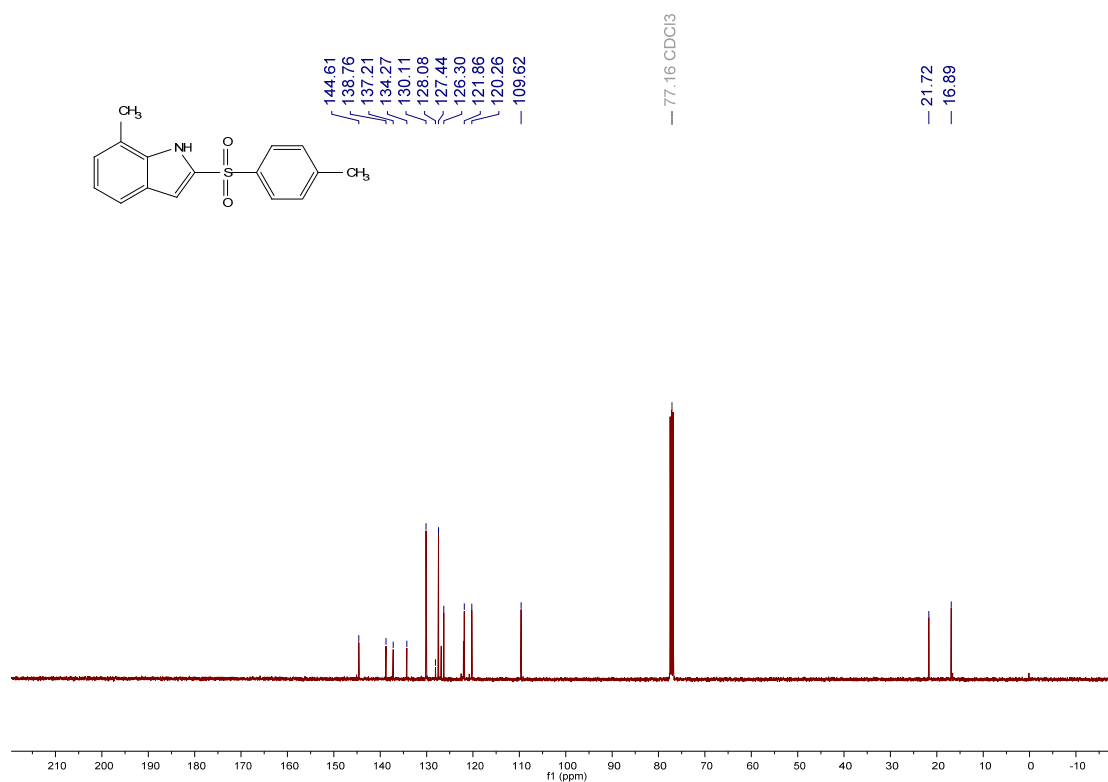
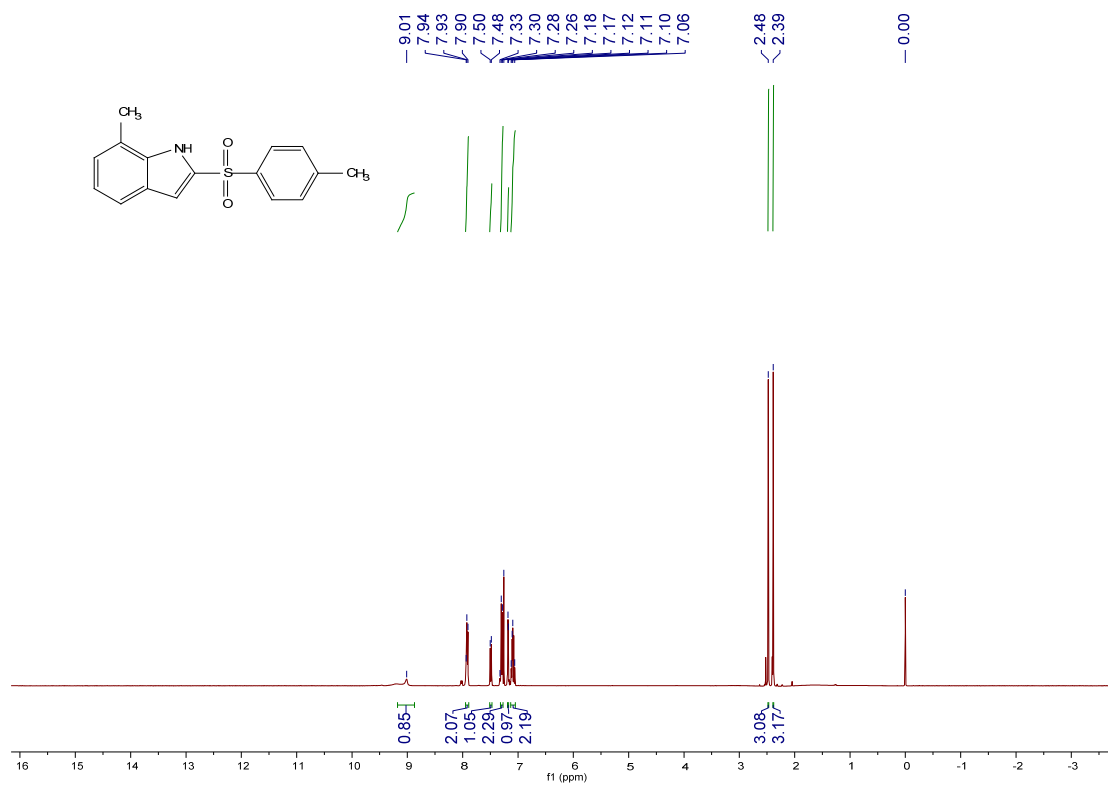
3-methyl-2-tosyl-1H-indole (3e)



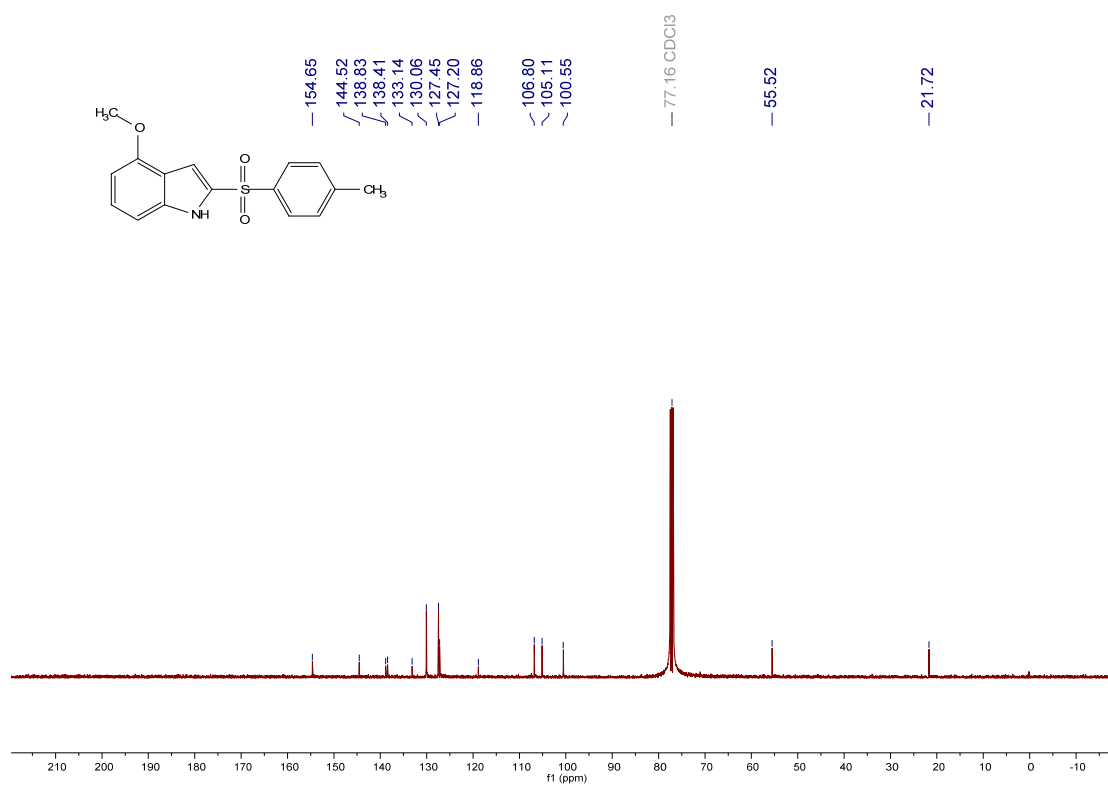
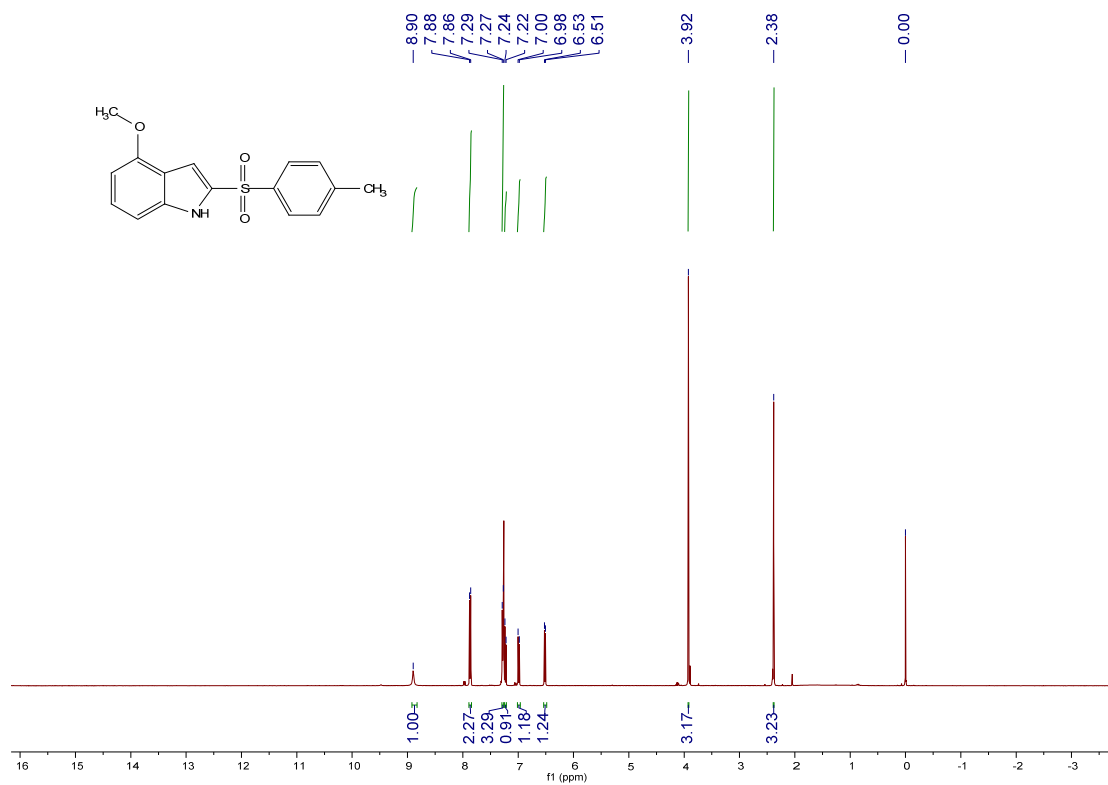
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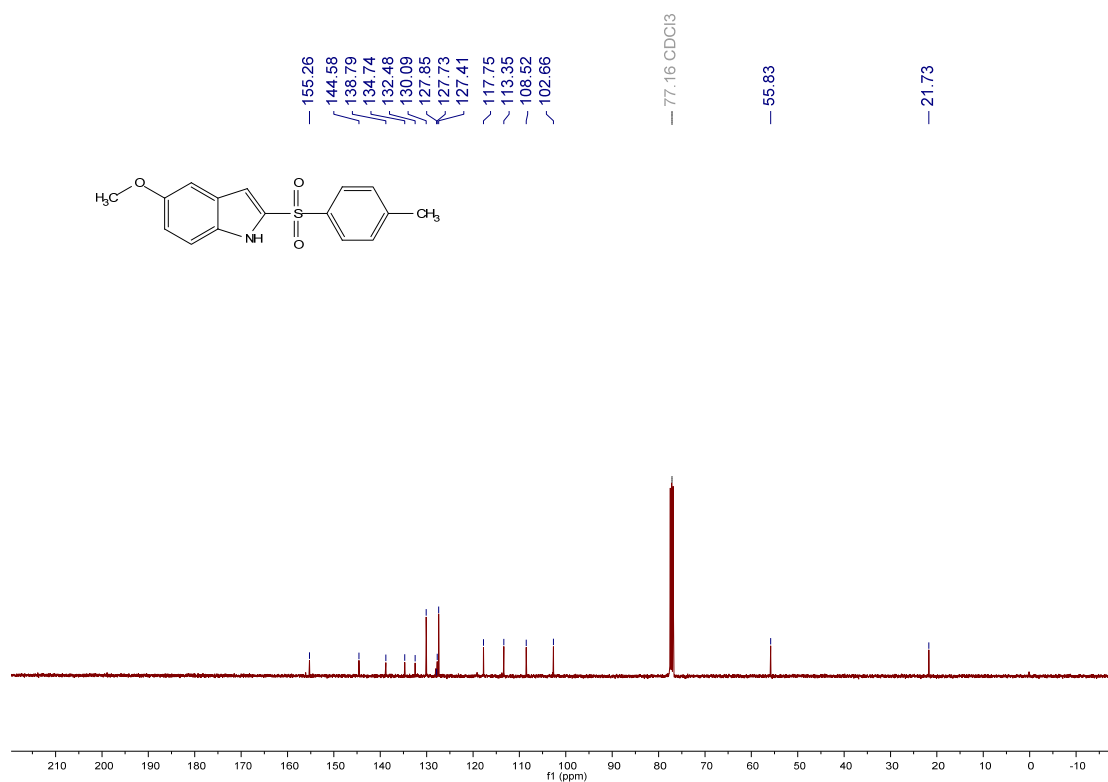
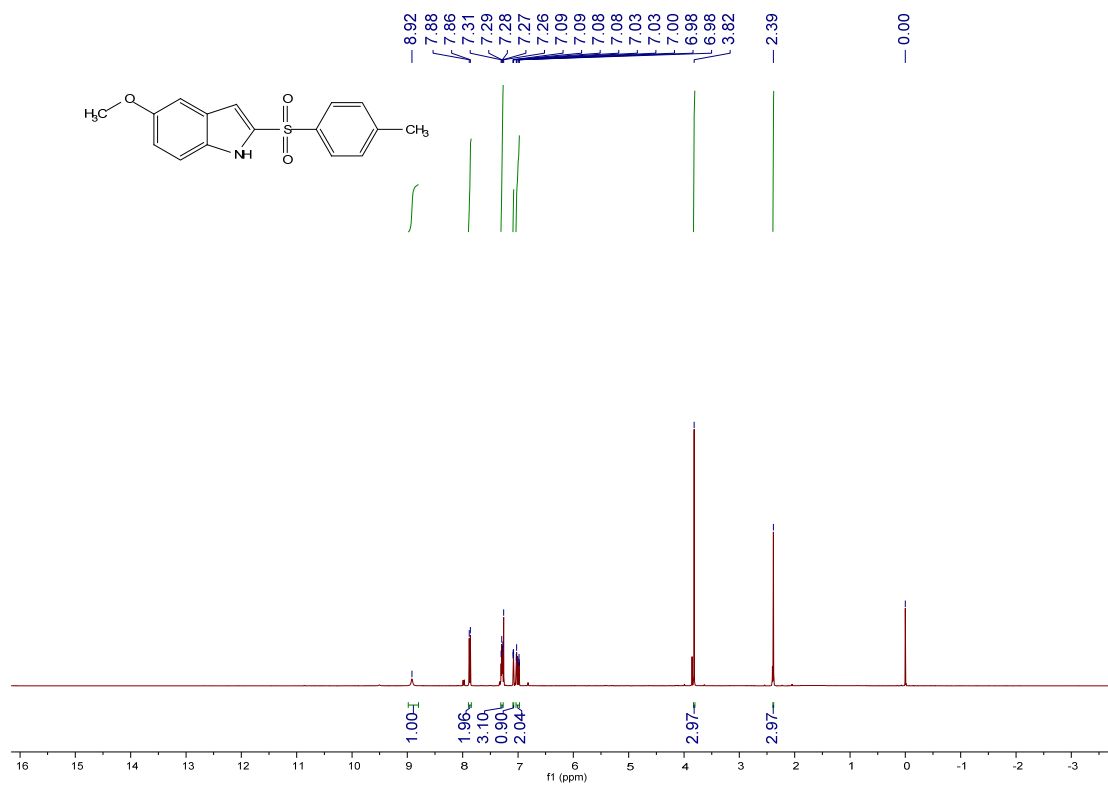
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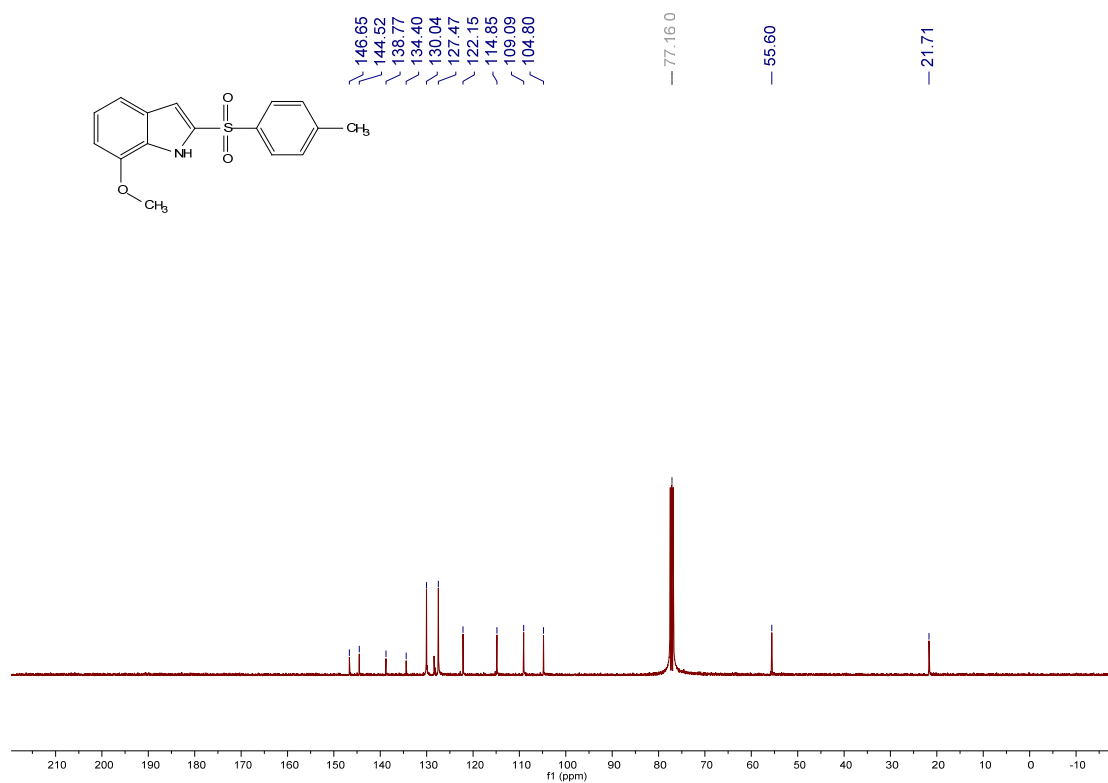
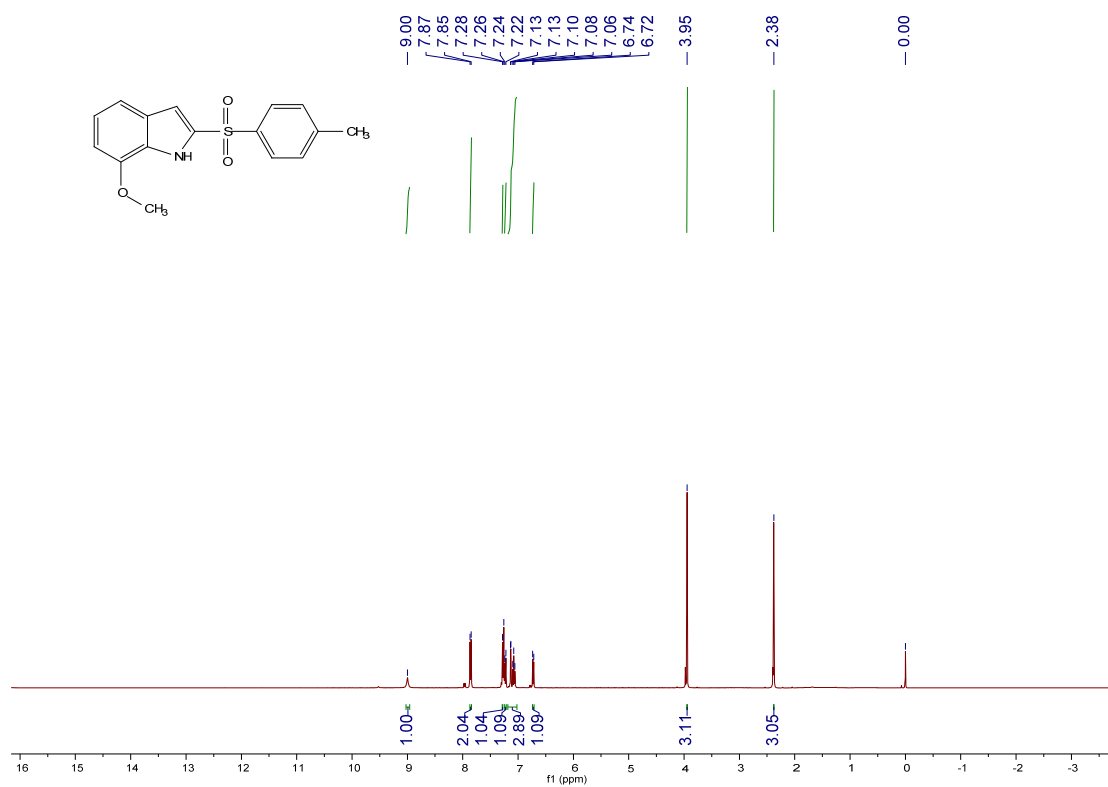
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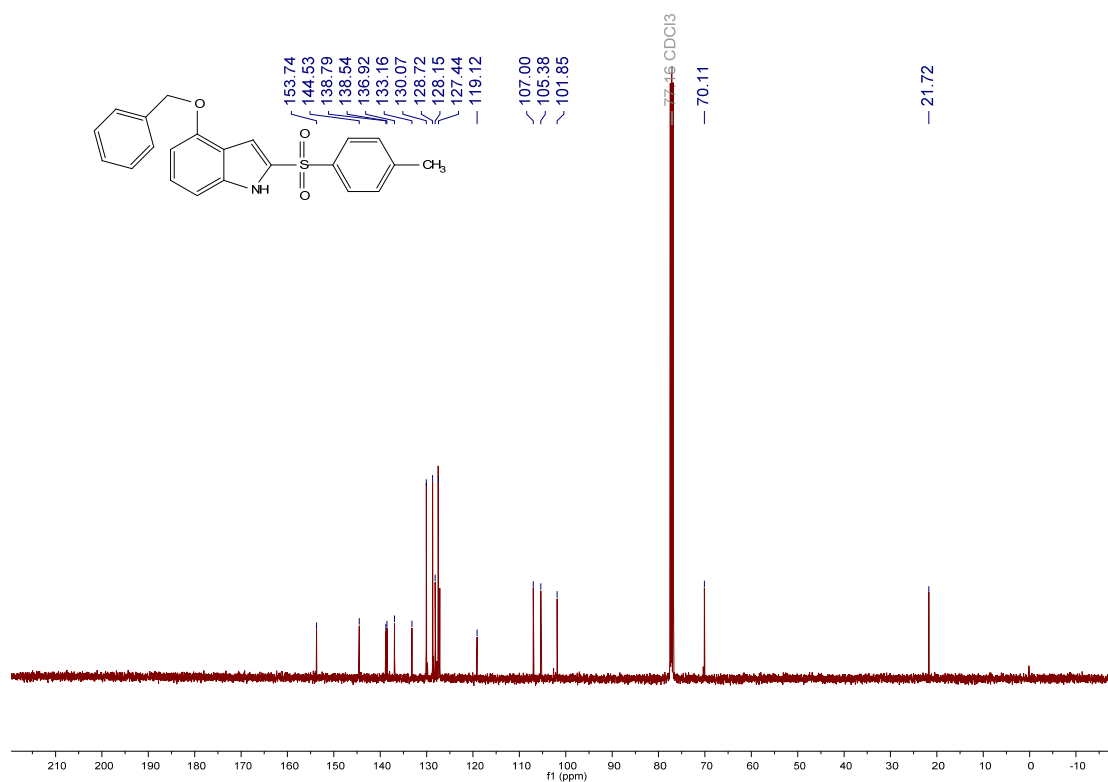
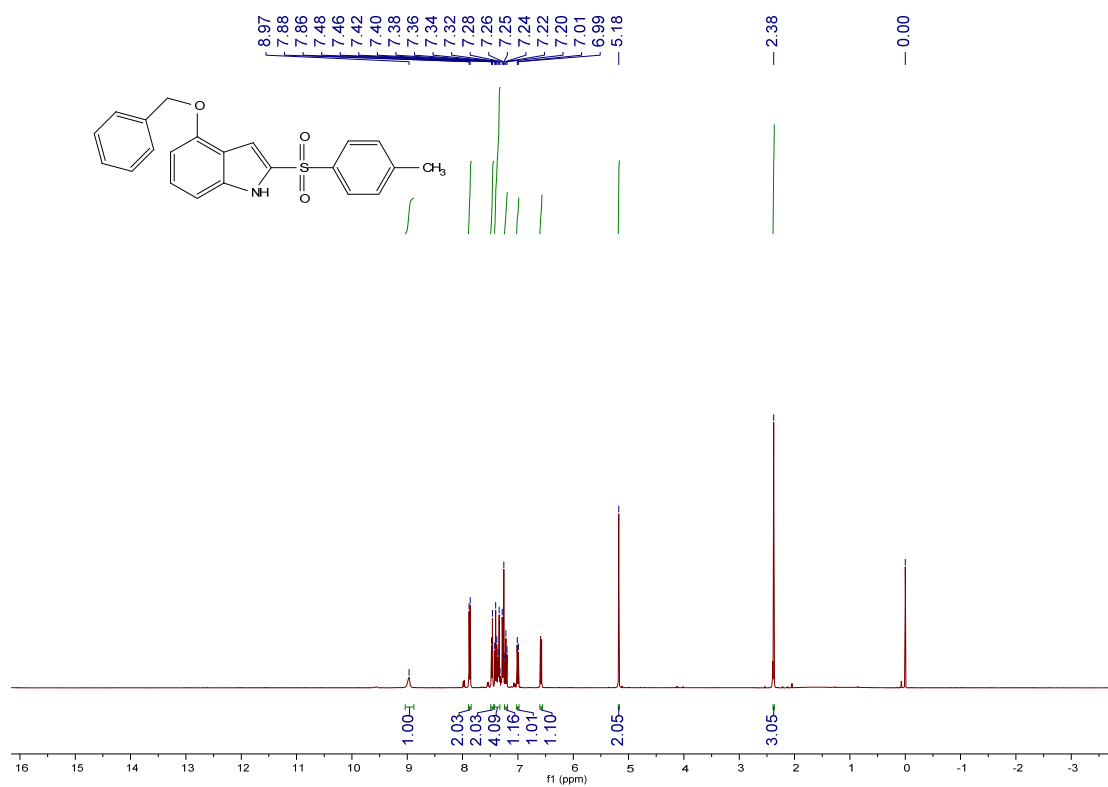
5-methoxy-2-tosyl-1H-indole (3i)



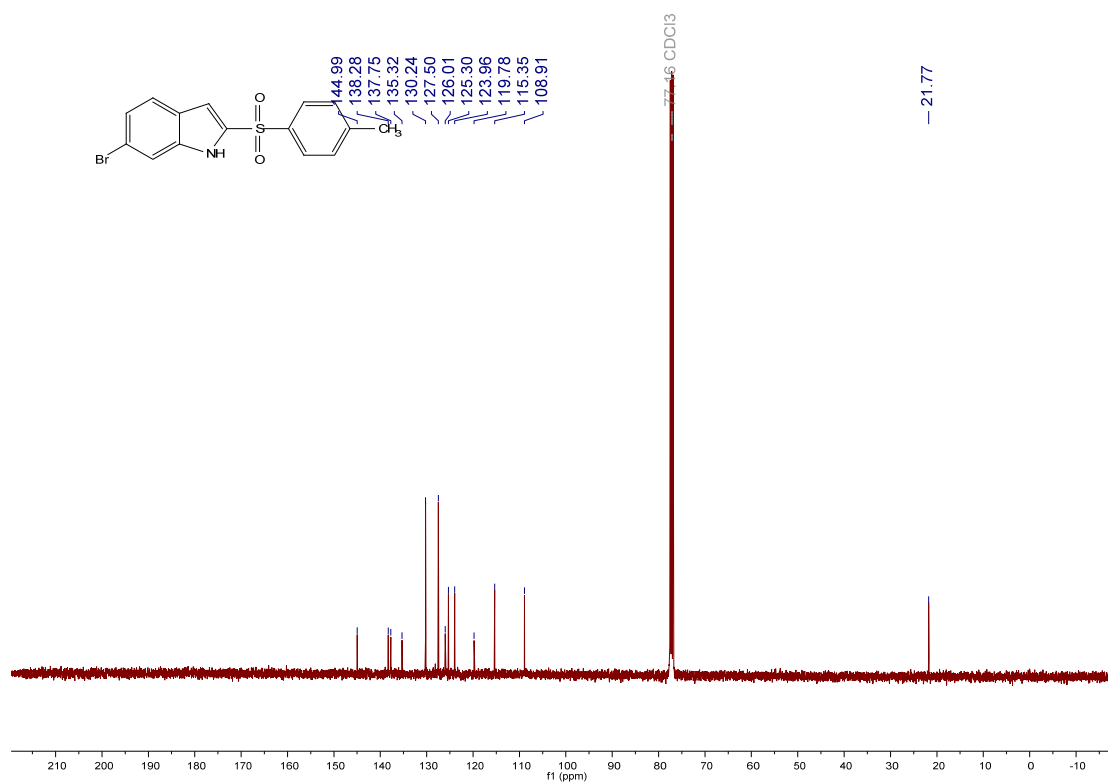
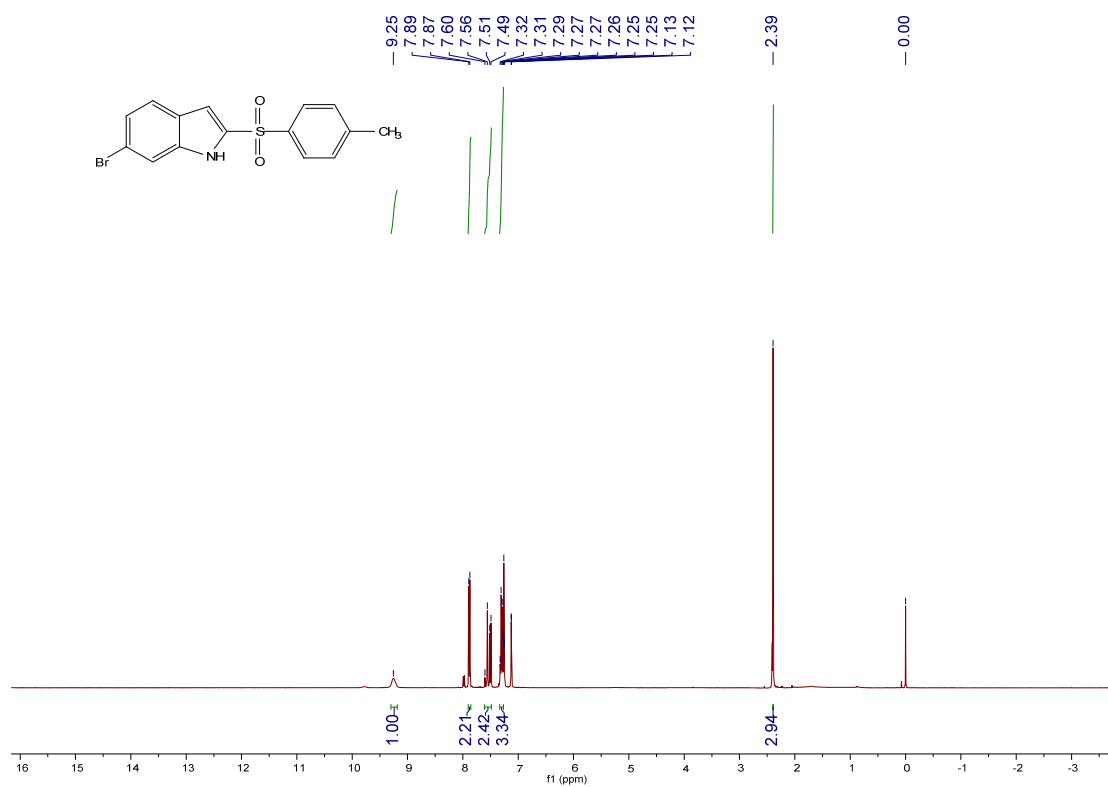
7-methoxy-2-tosyl-1H-indole (3j)



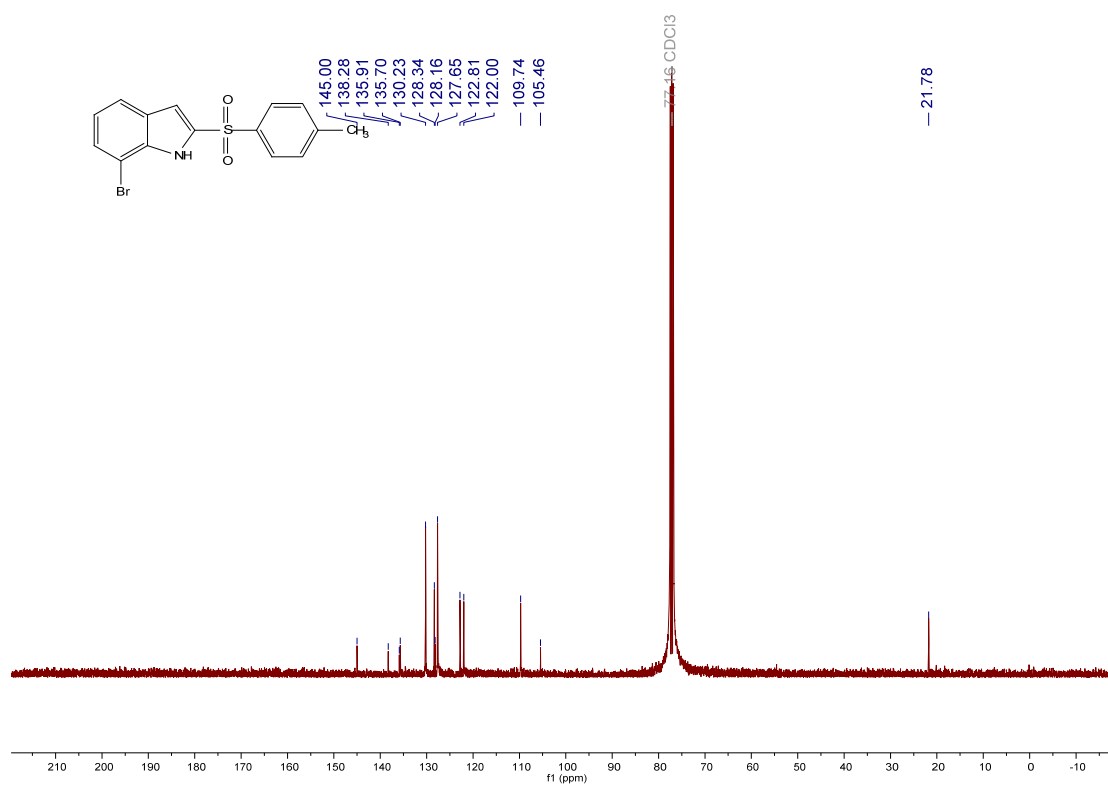
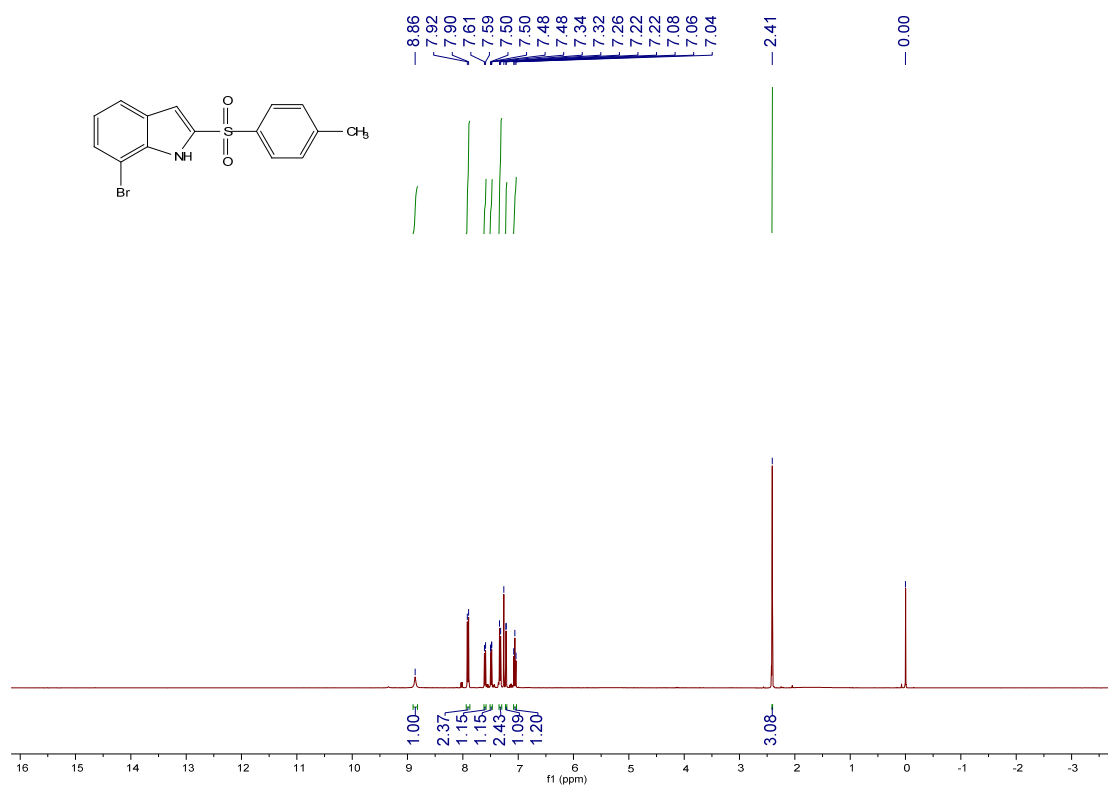
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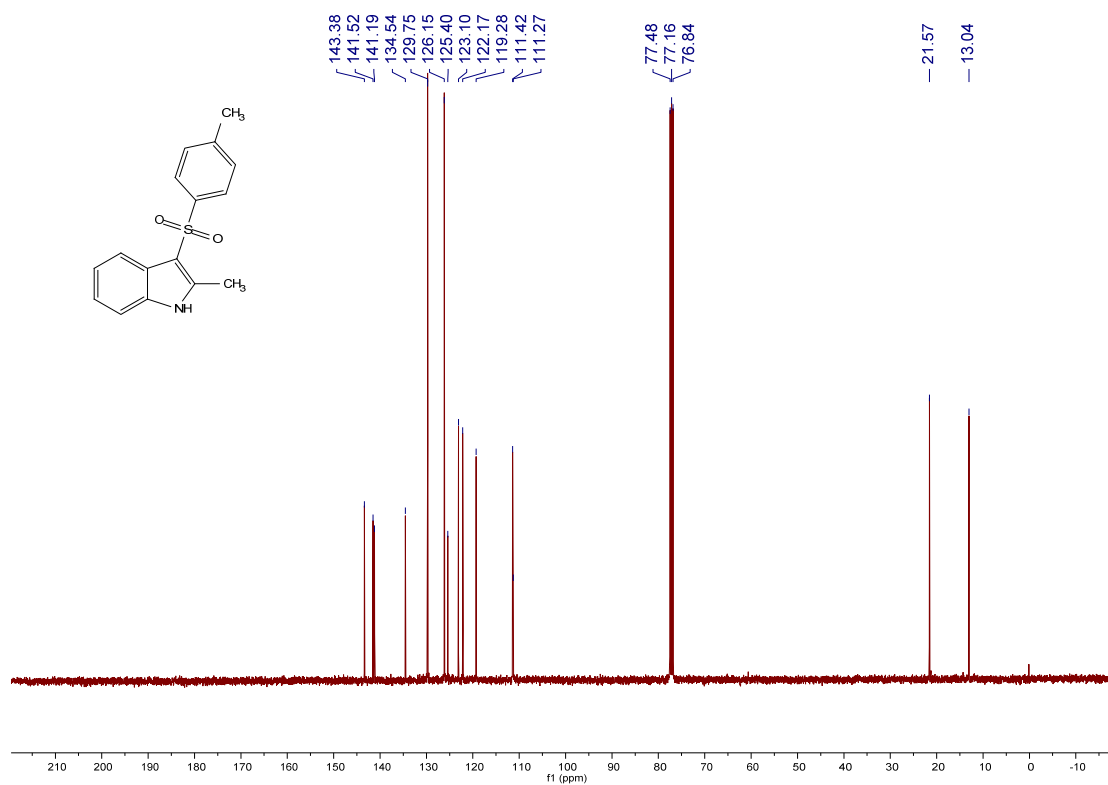
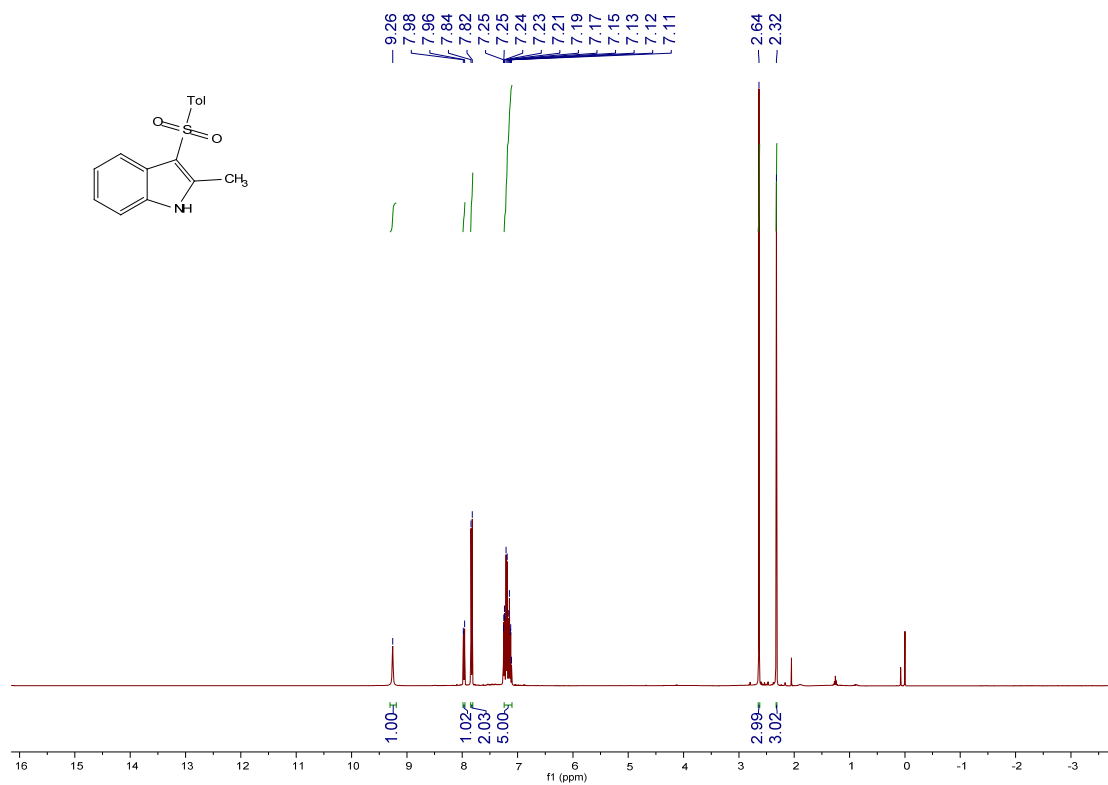
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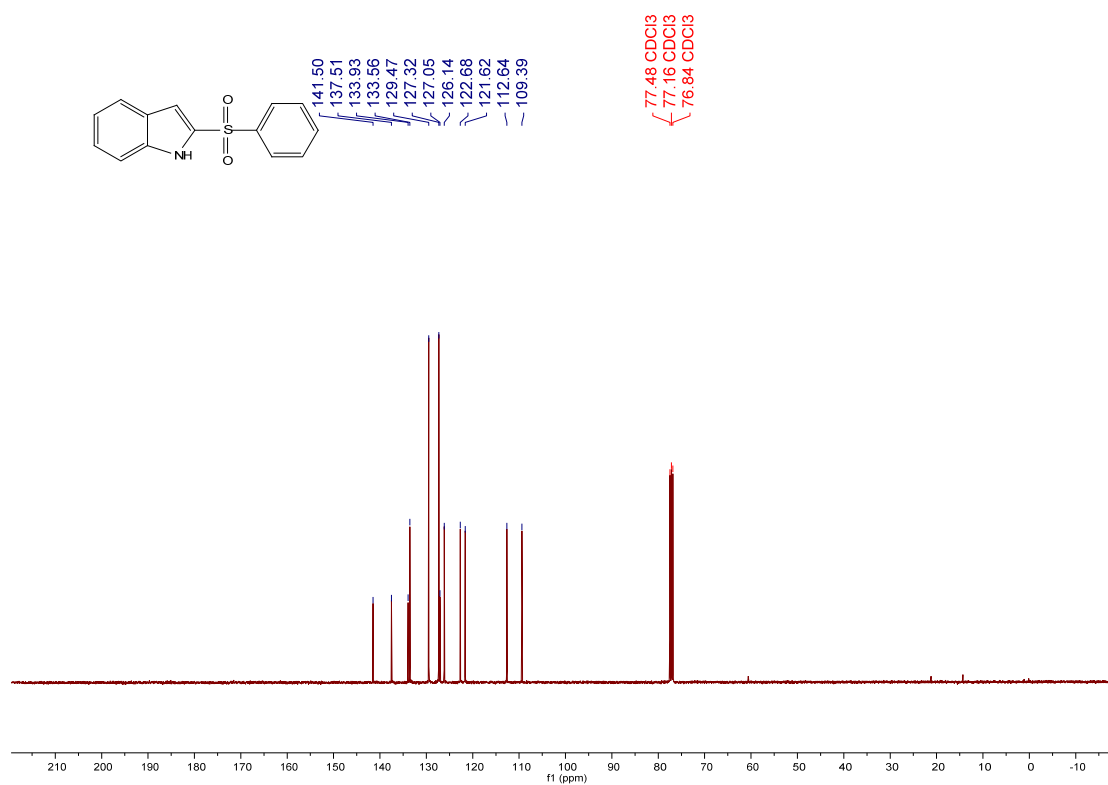
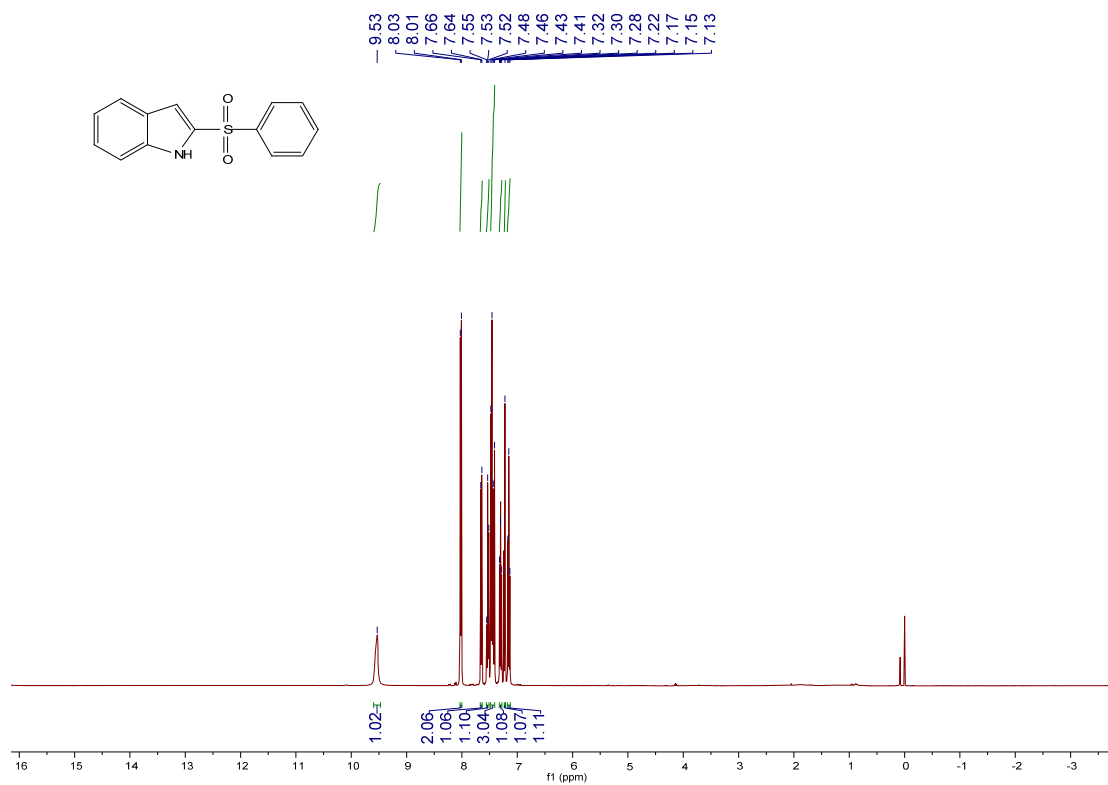
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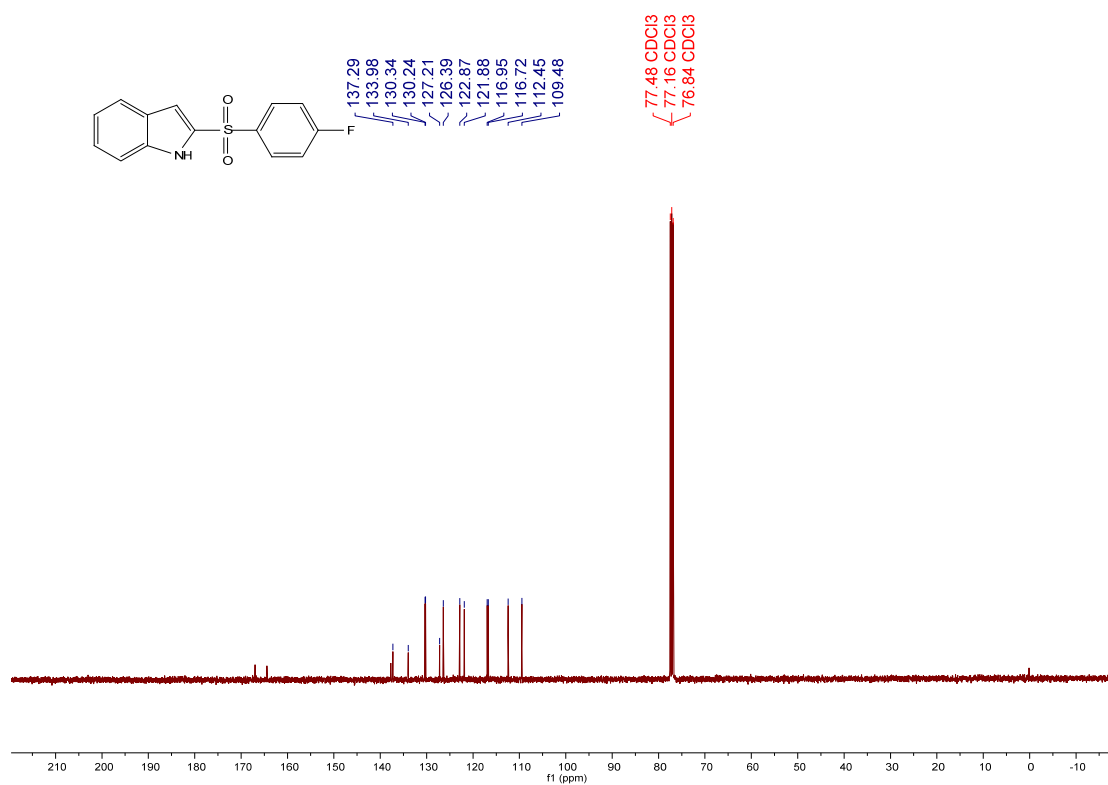
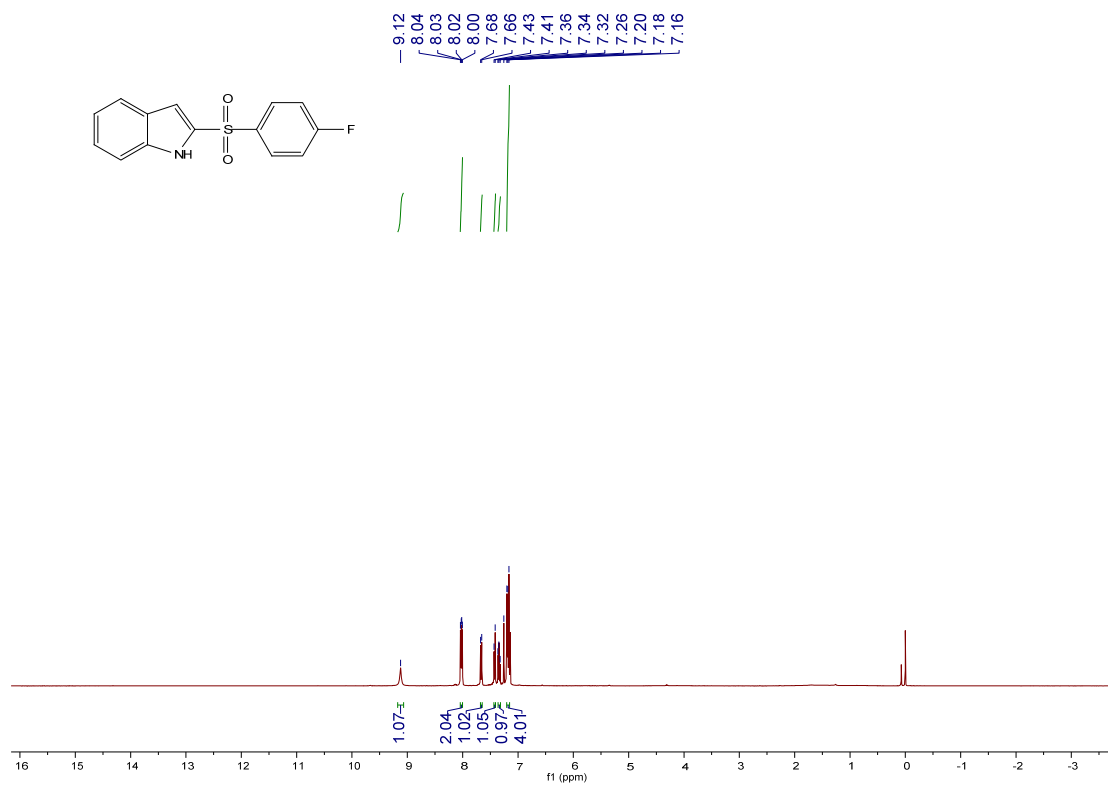
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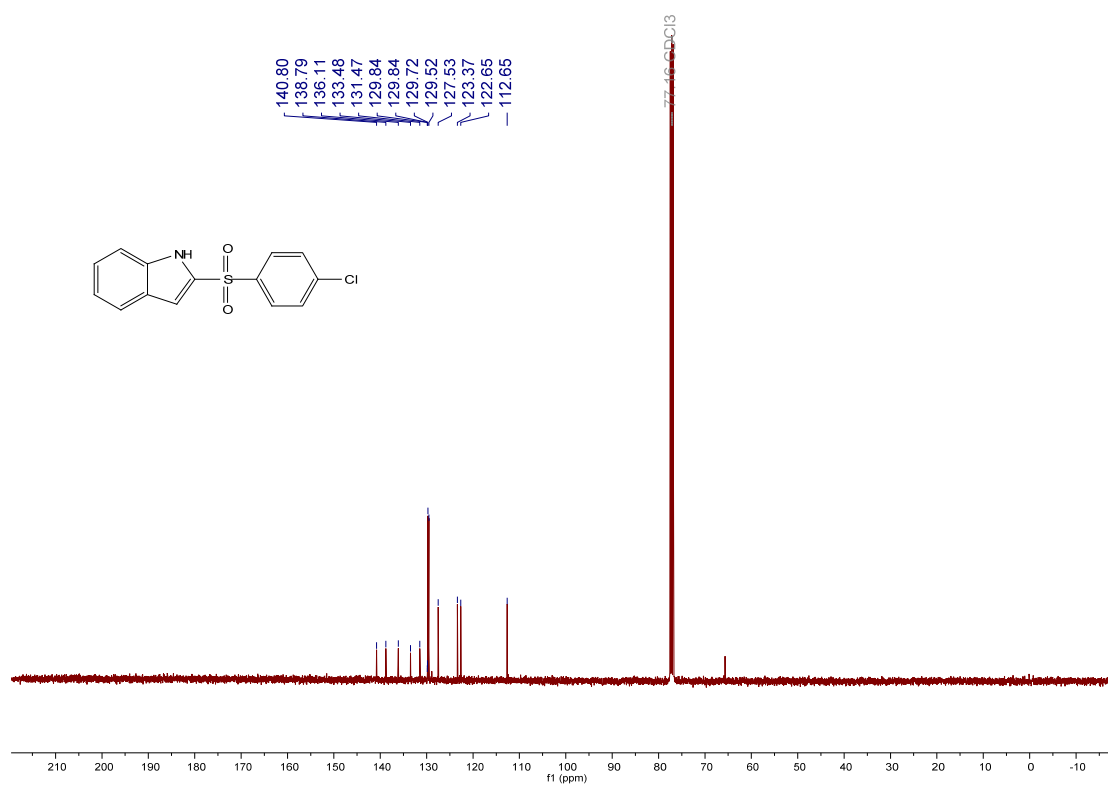
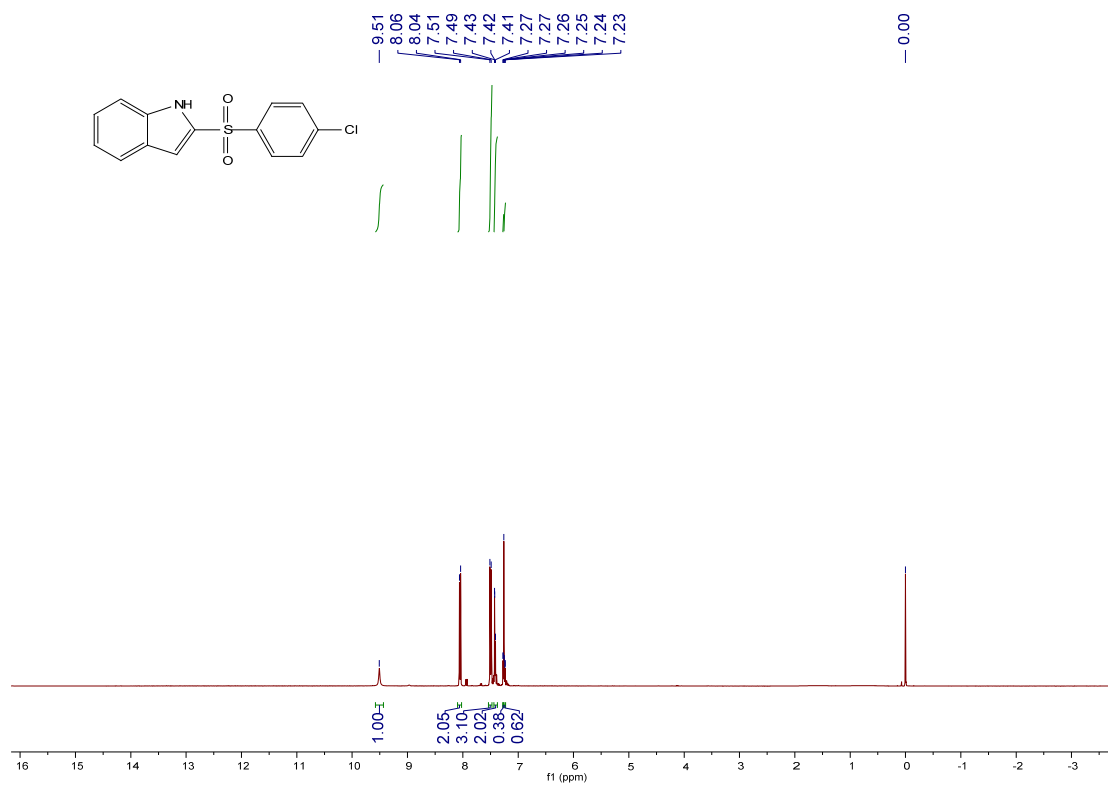
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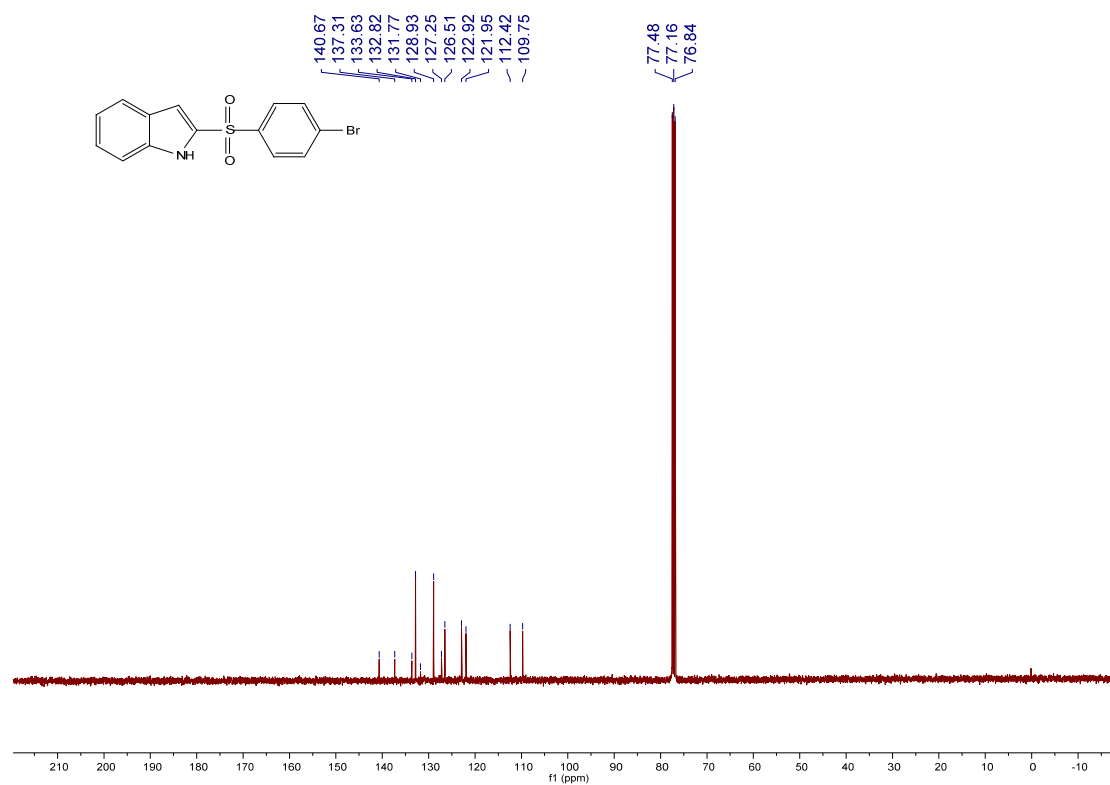
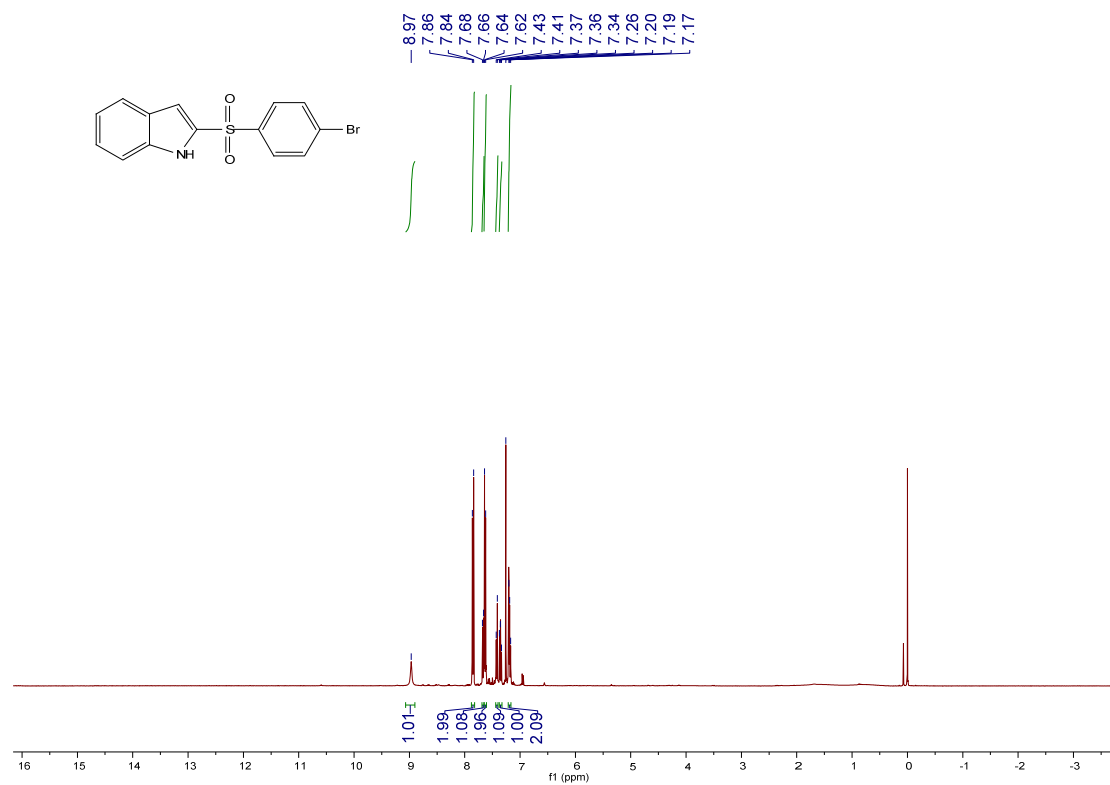
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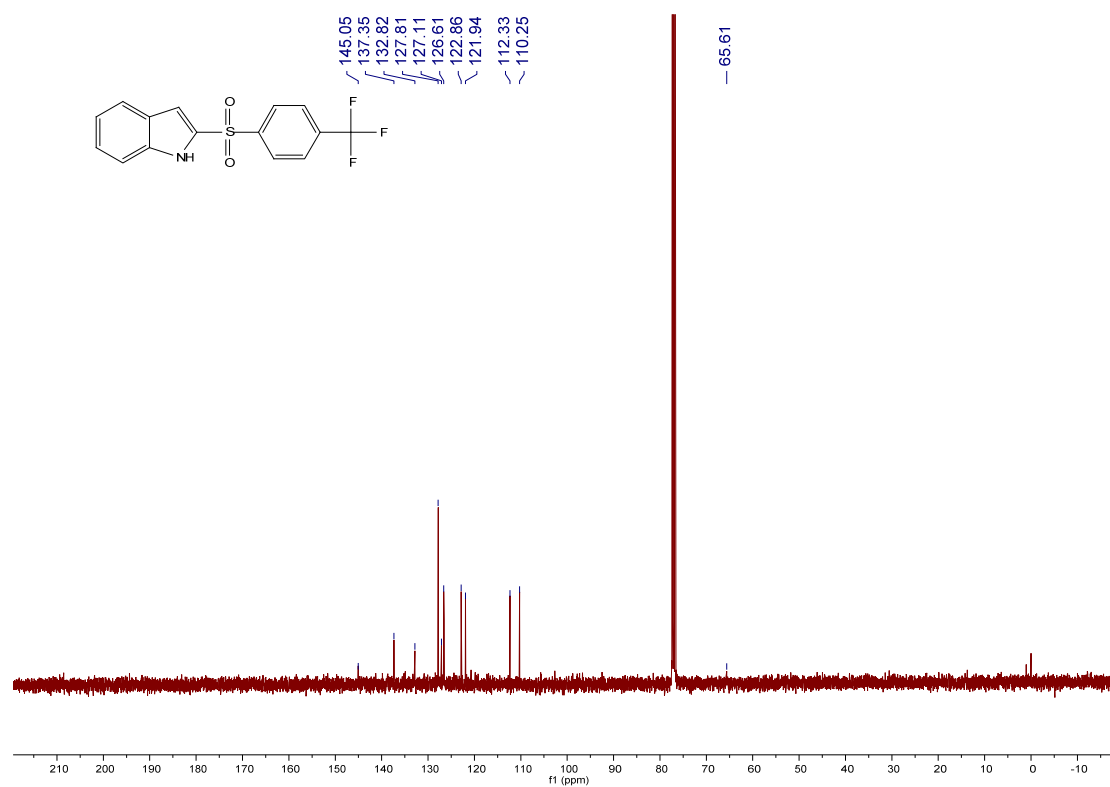
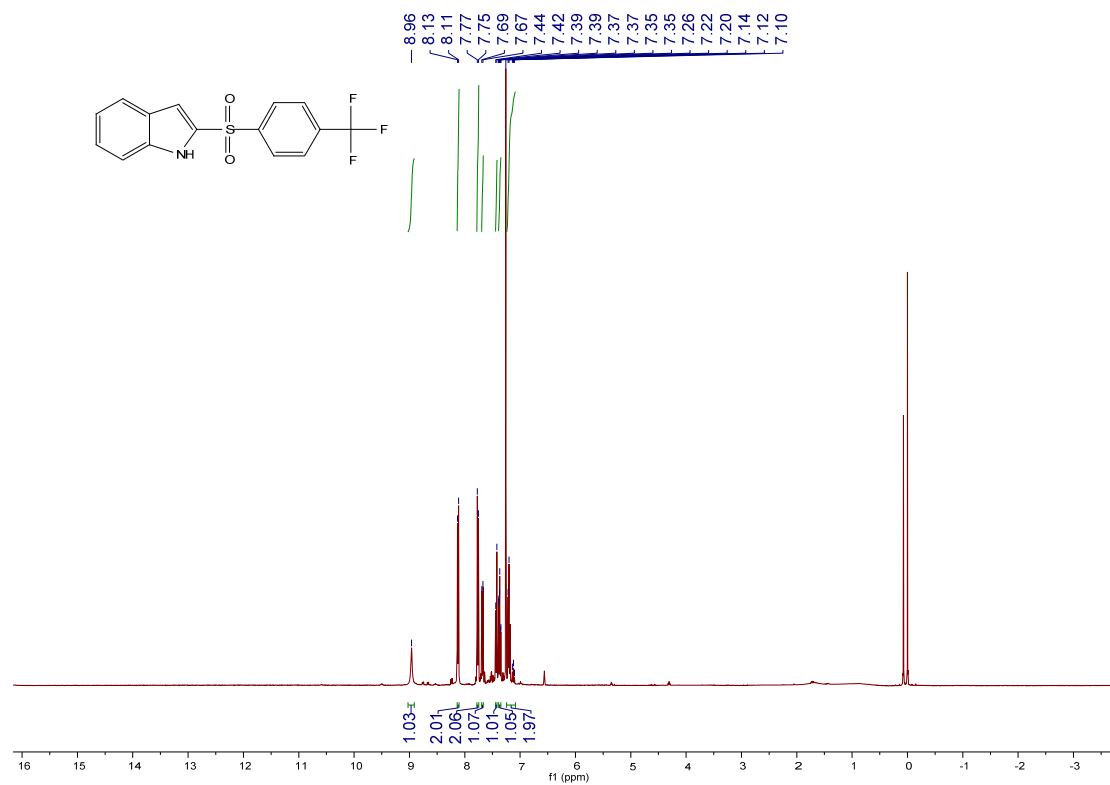
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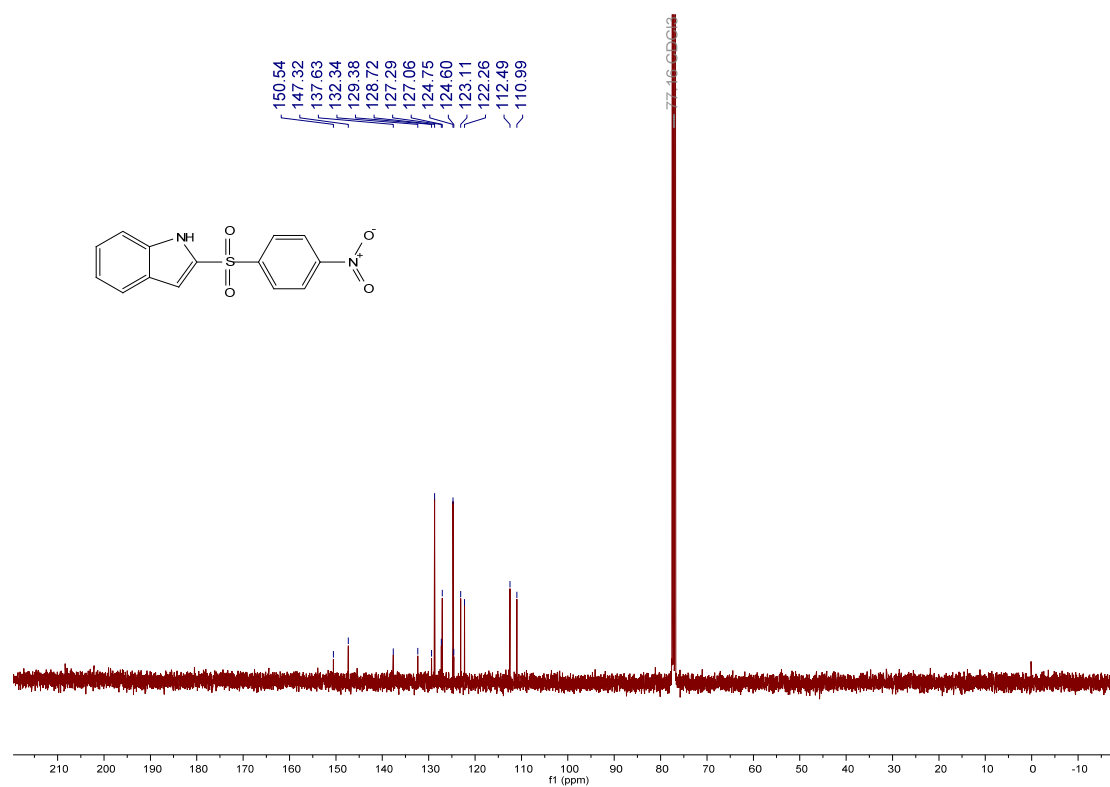
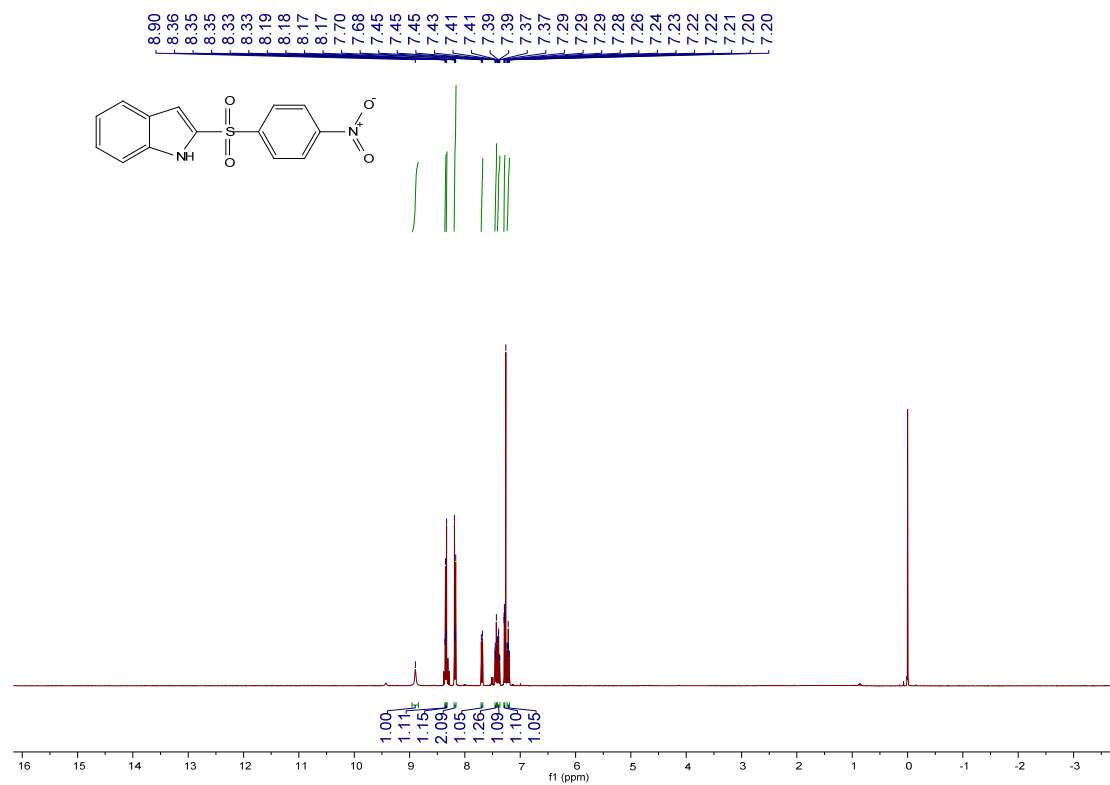
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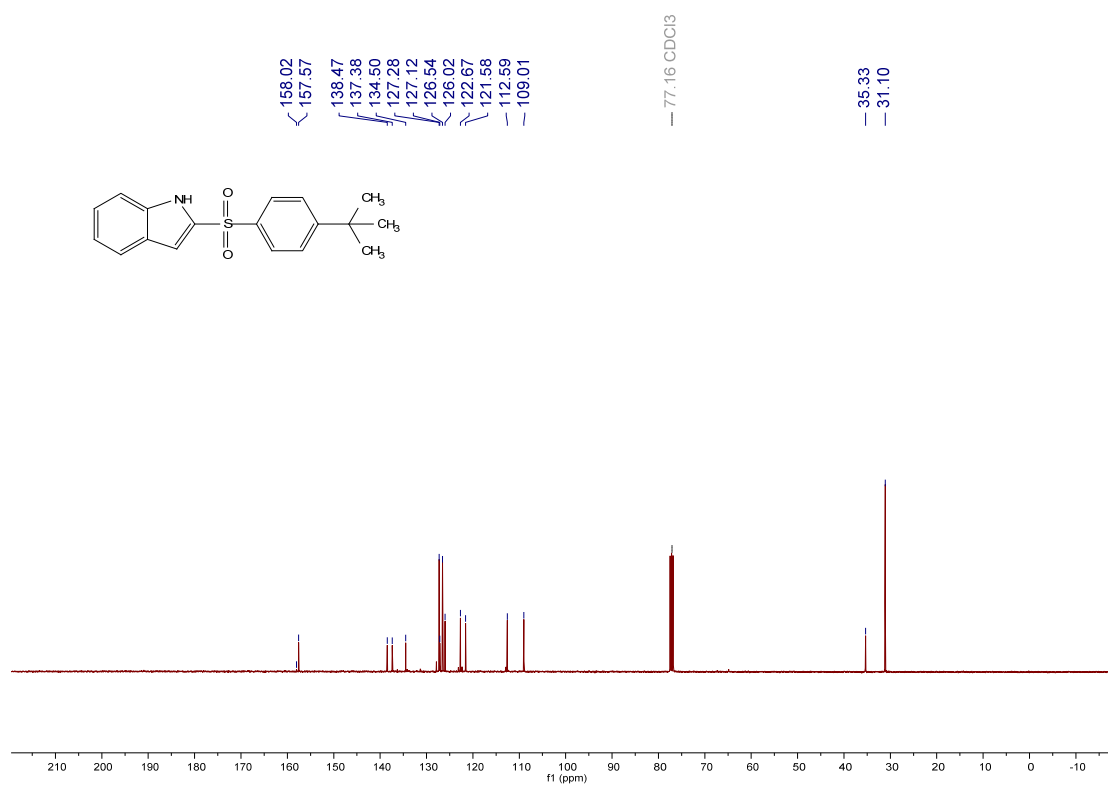
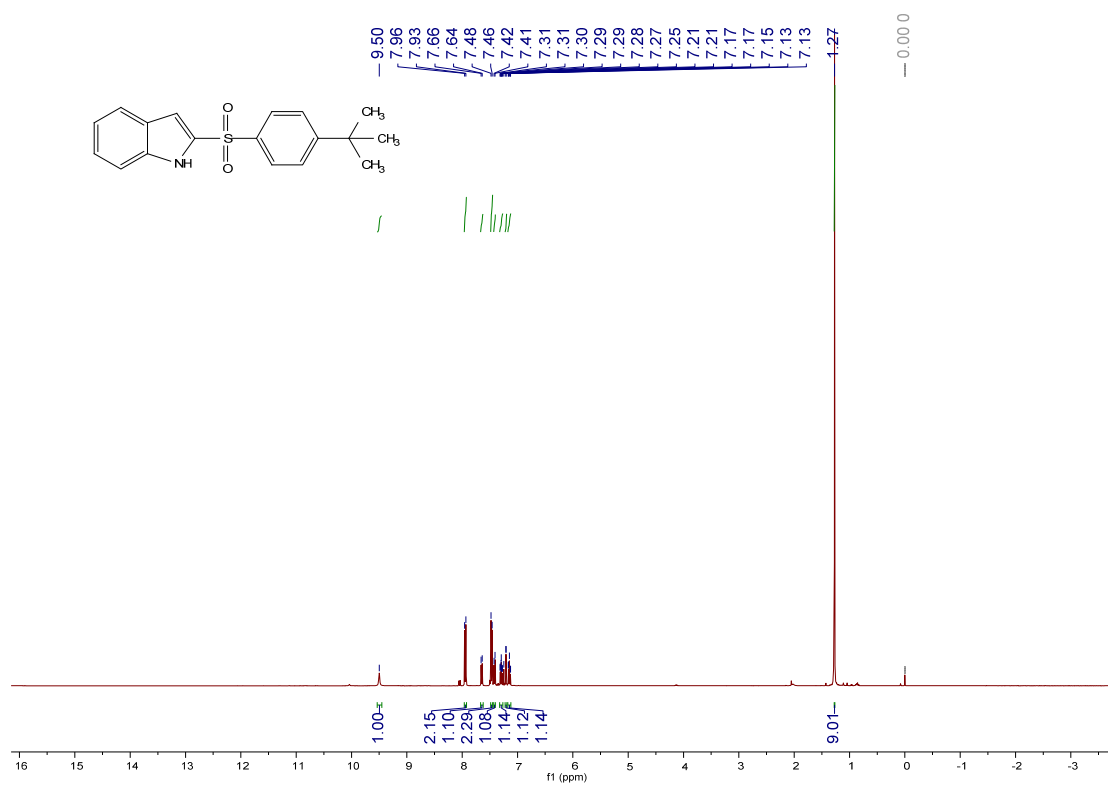
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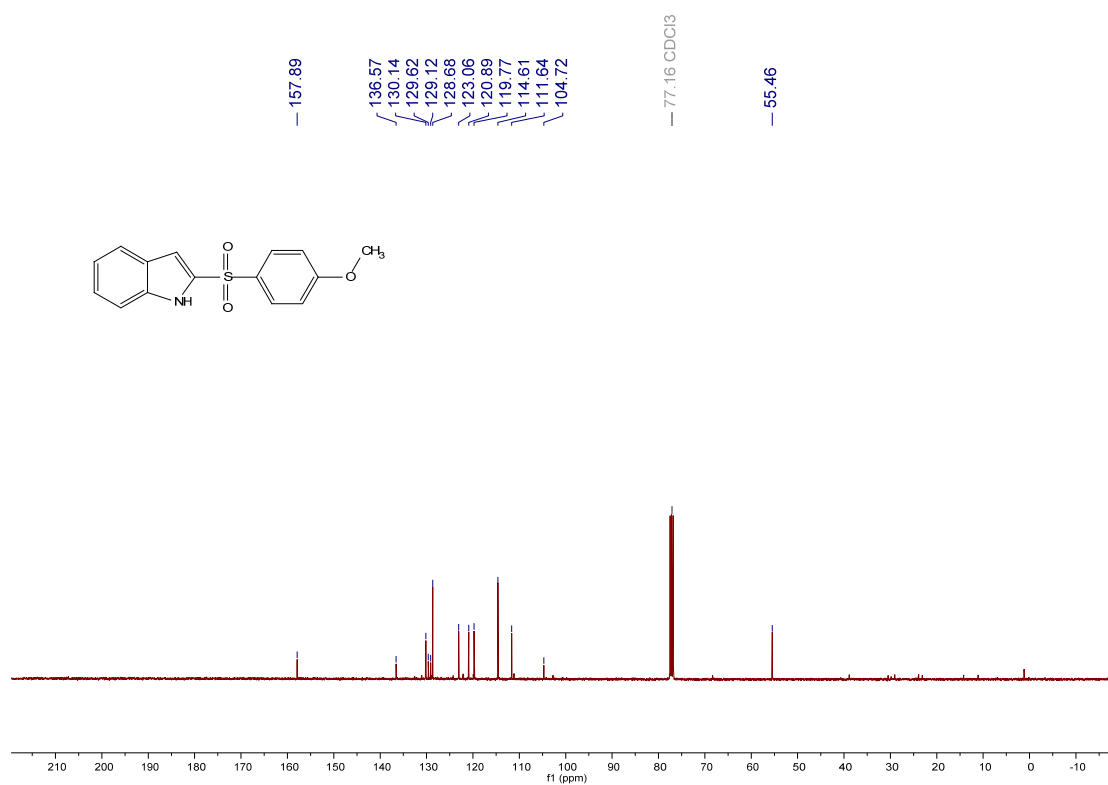
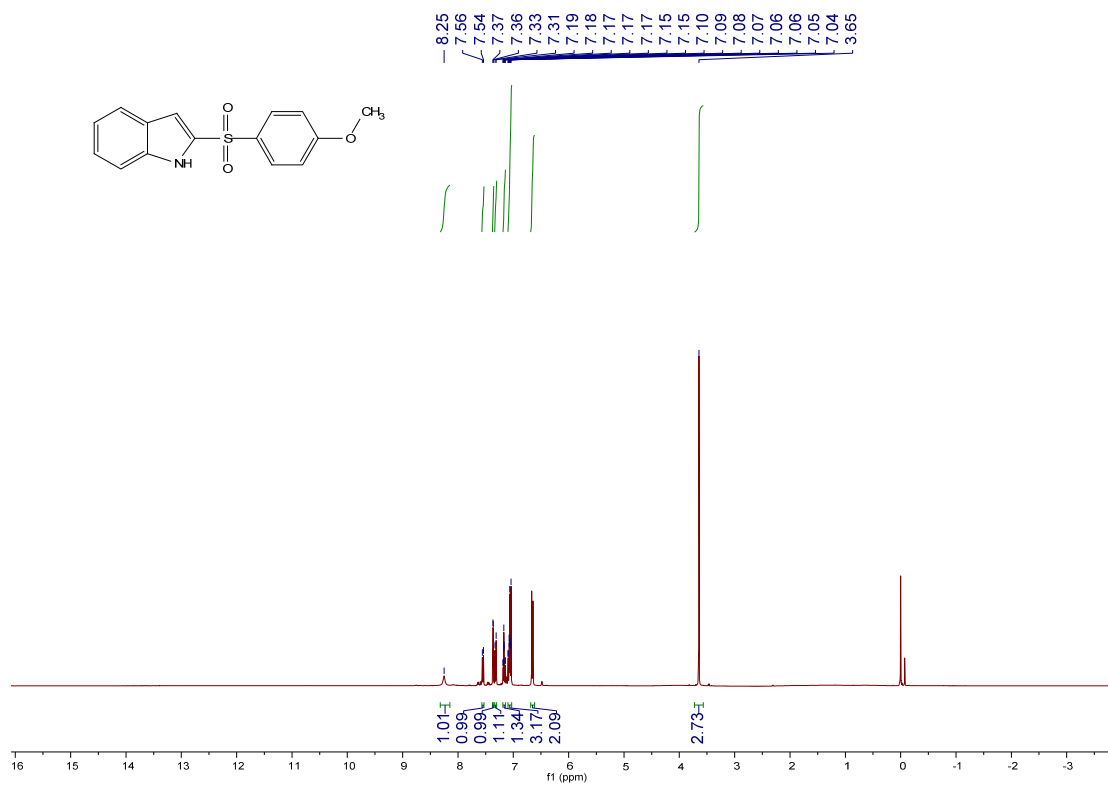
2-((4-nitrophenyl)sulfonyl)-1H-indole (3t)



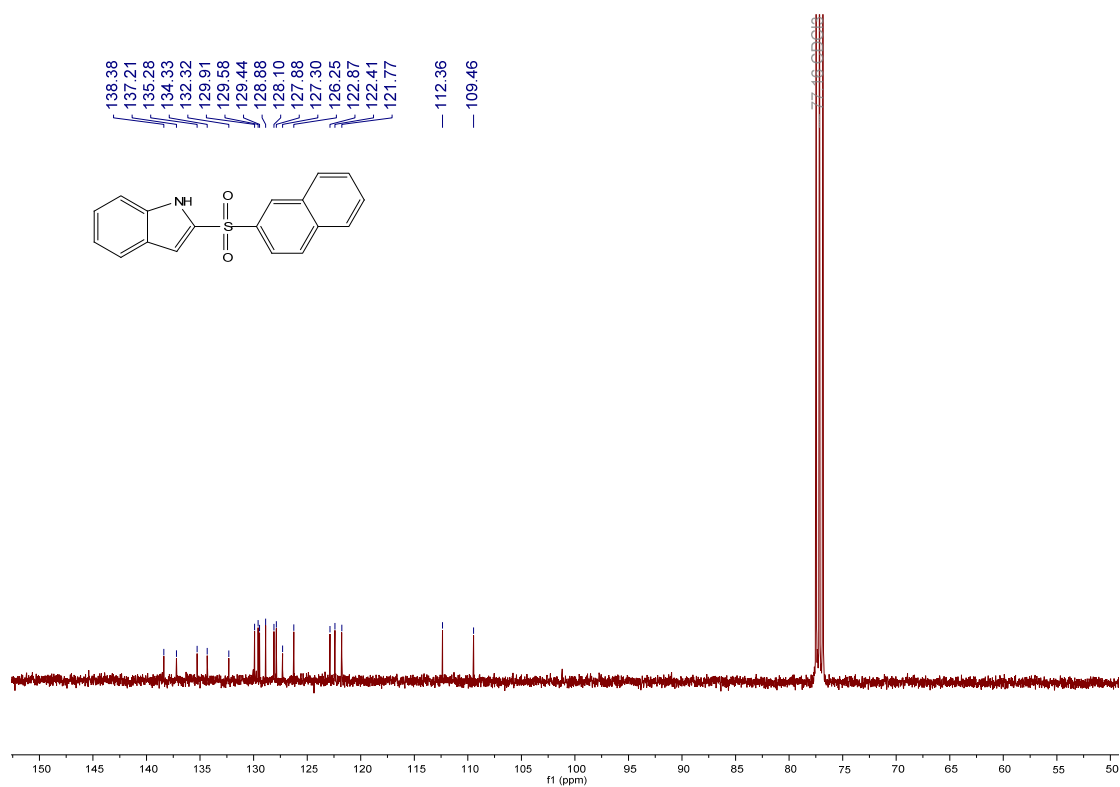
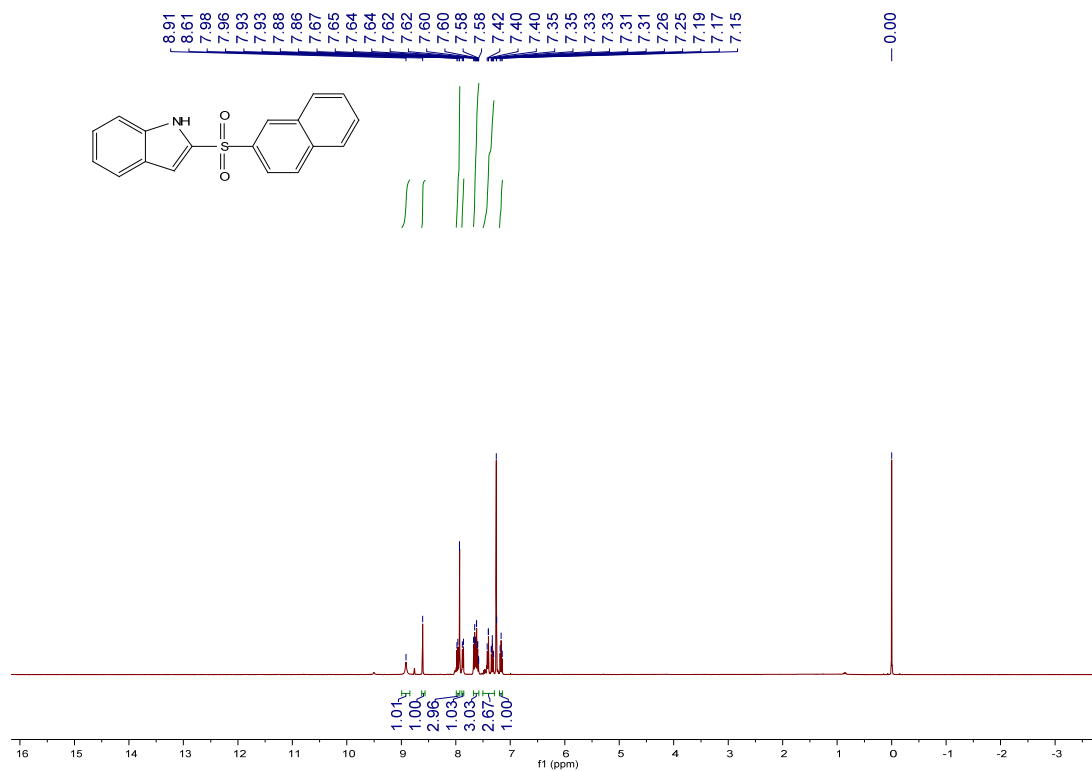
2-((4-(tert-butyl)phenyl)sulfonyl)-1H-indole(3u)



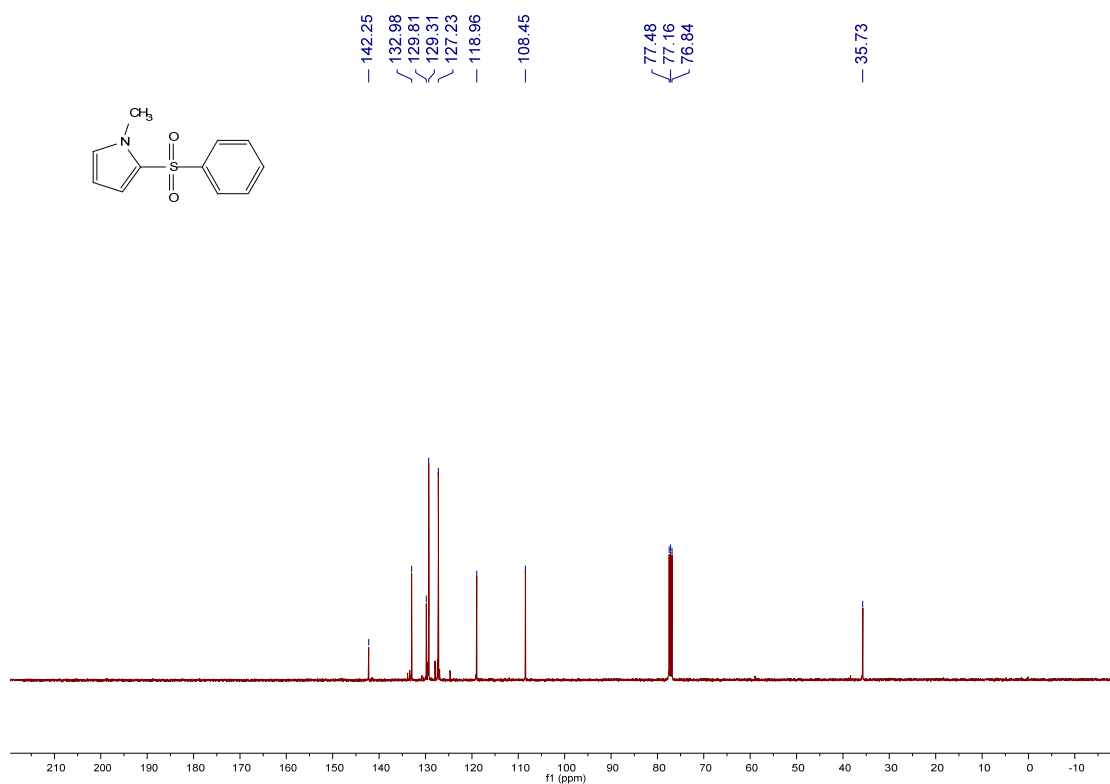
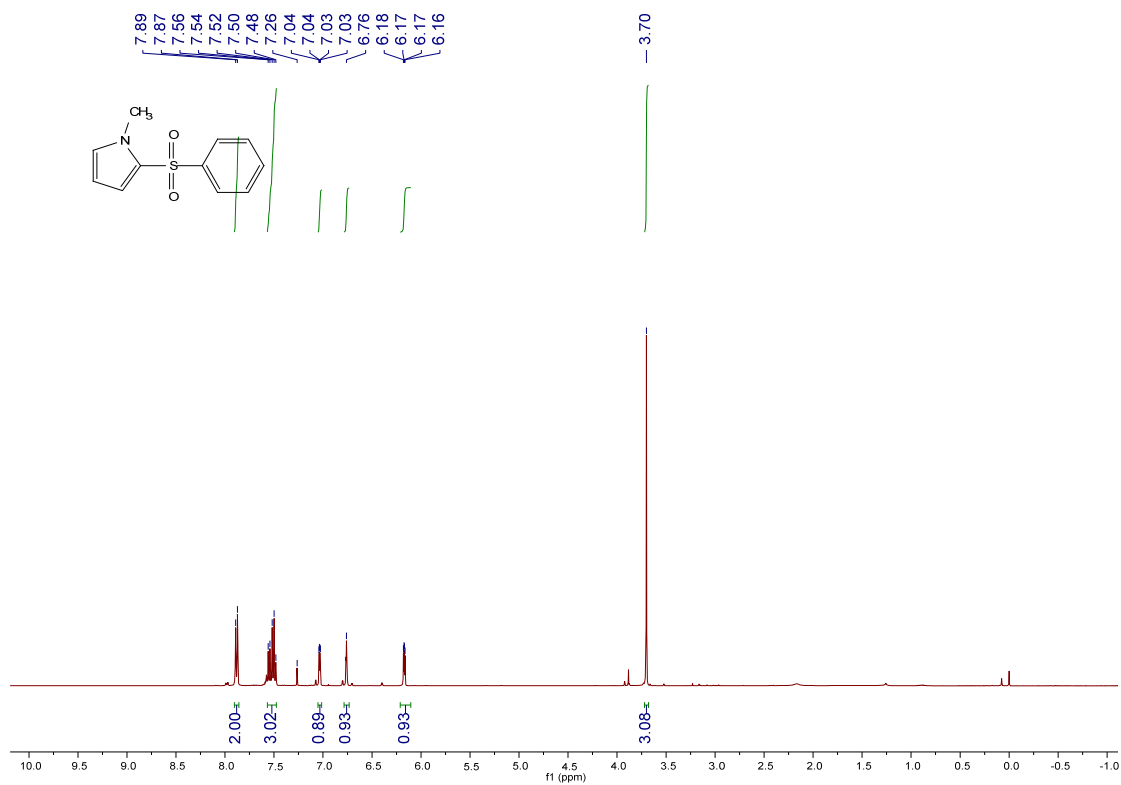
2-((4-methoxyphenyl)sulfonyl)-1H-indole (3v)



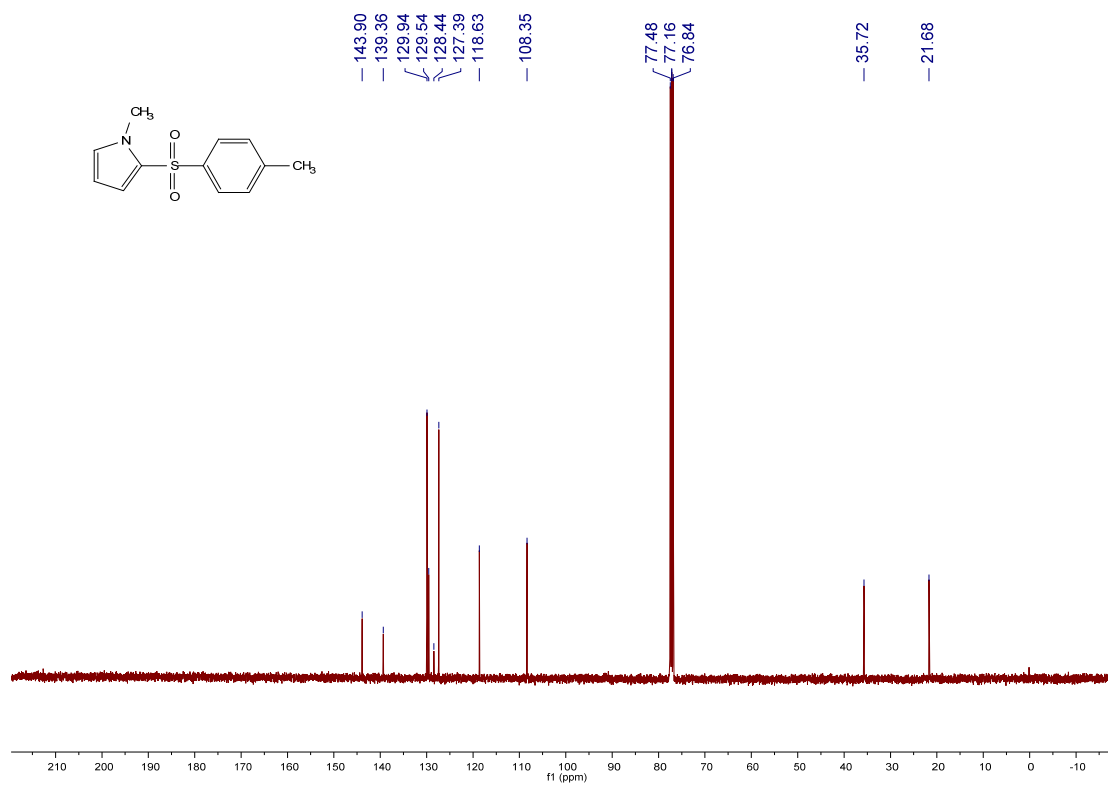
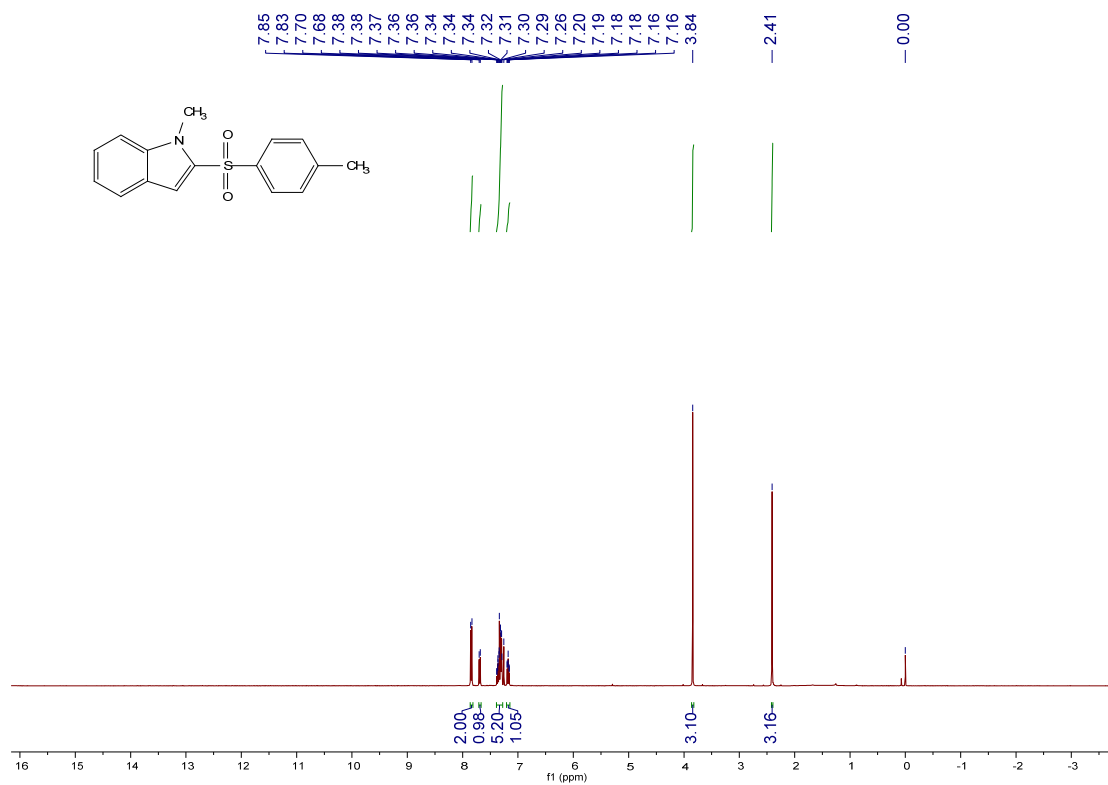
2-(naphthalen-2-ylsulfonyl)-1H-indole (3w)



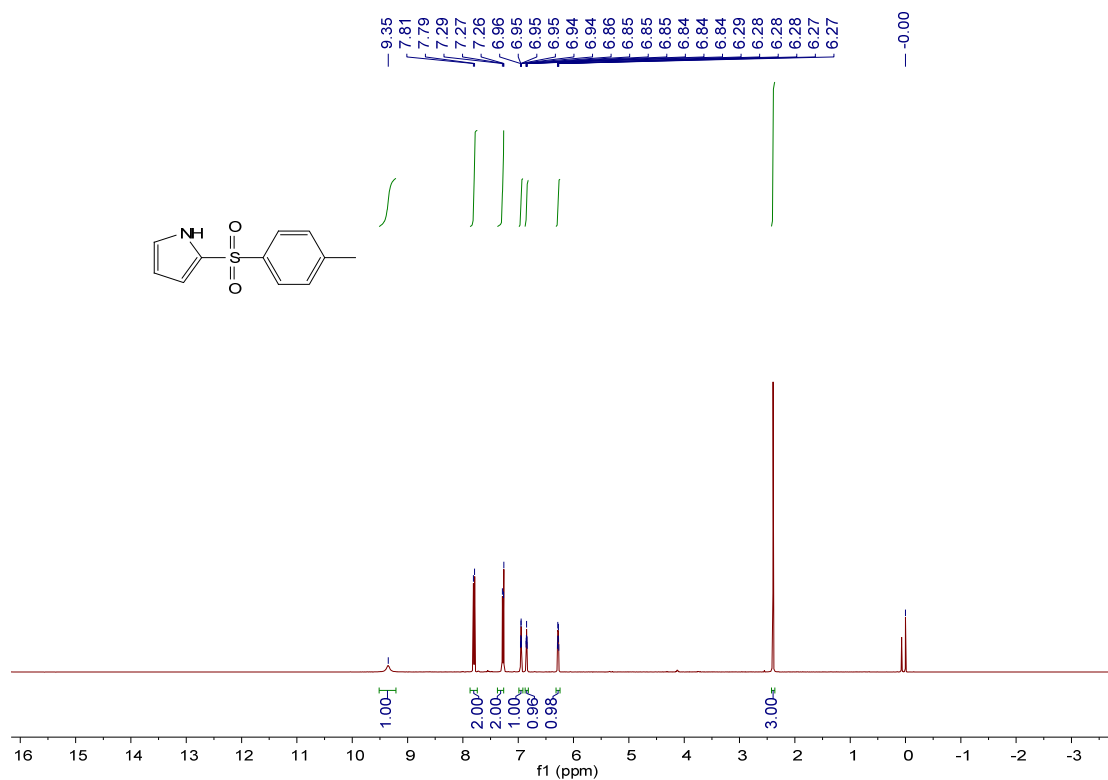
1-methyl-2-(phenylsulfonyl)-1H-pyrrole (5a)



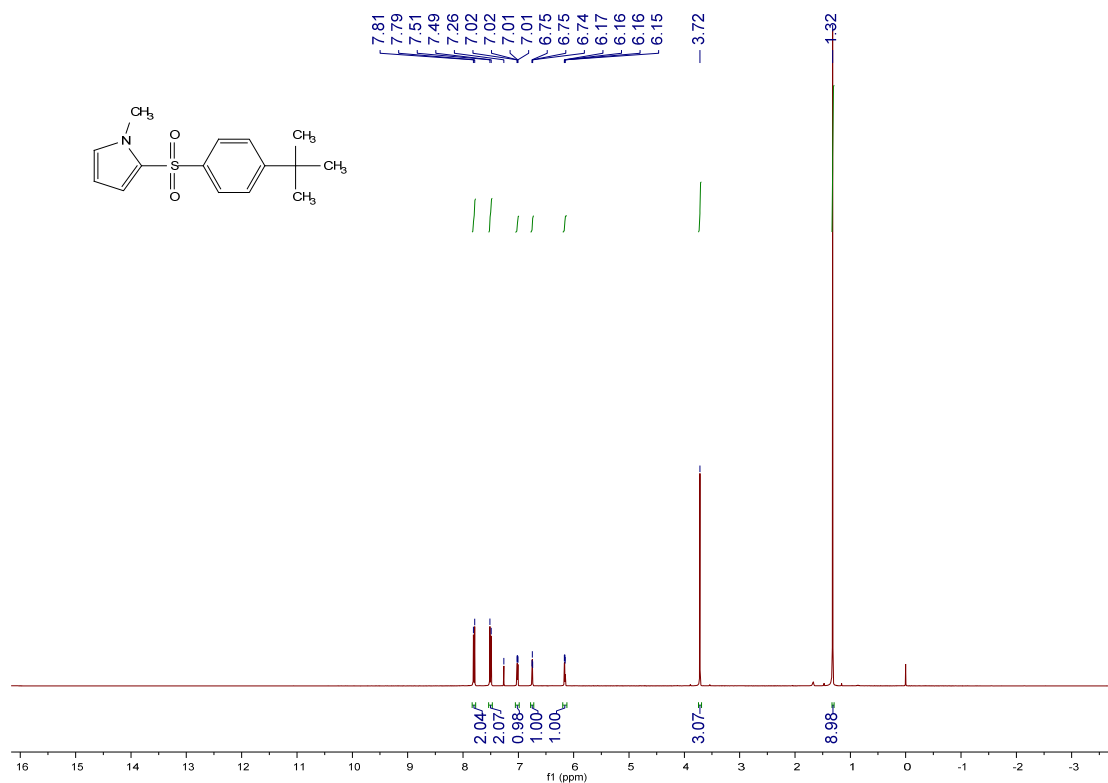
1-methyl-2-tosyl-1H-pyrrole (5b)

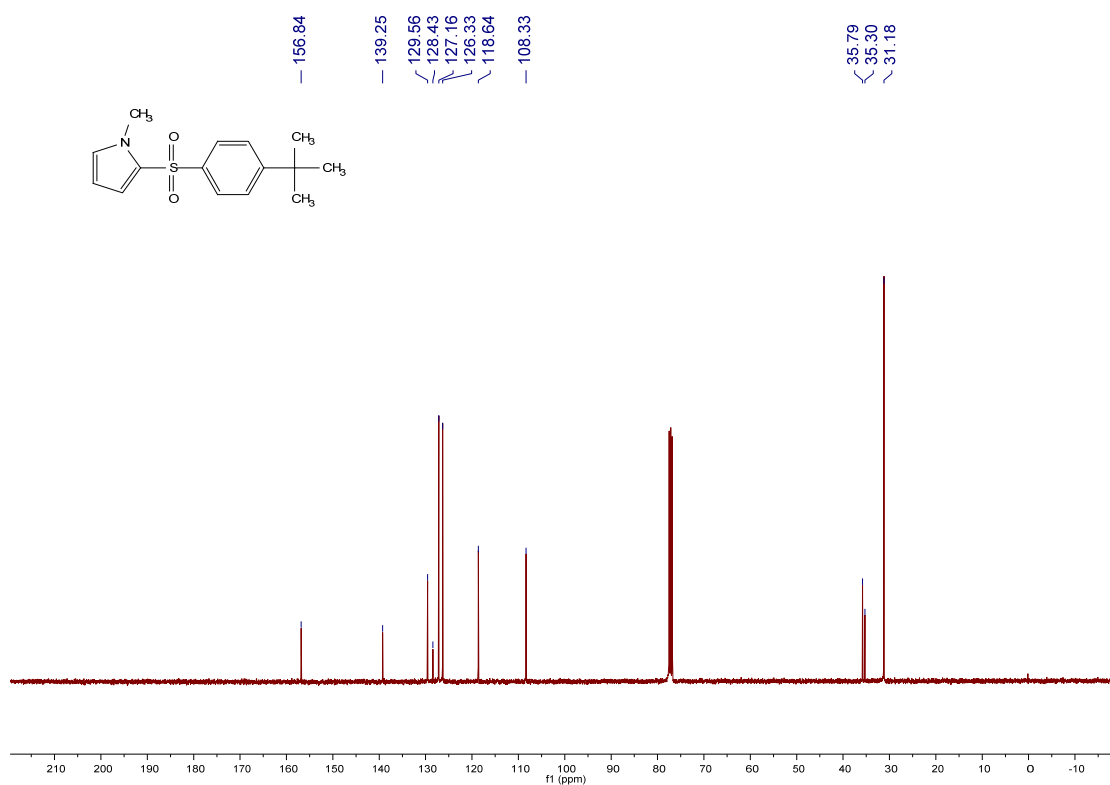


2-tosyl-1H-pyrrole (5b')

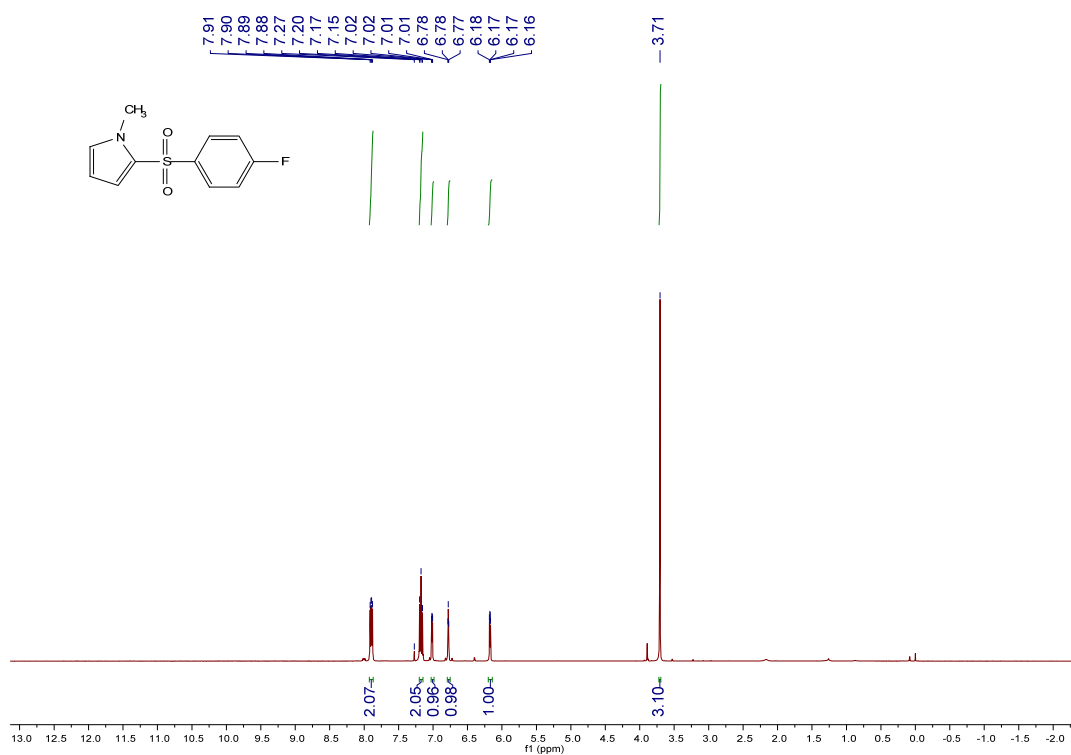


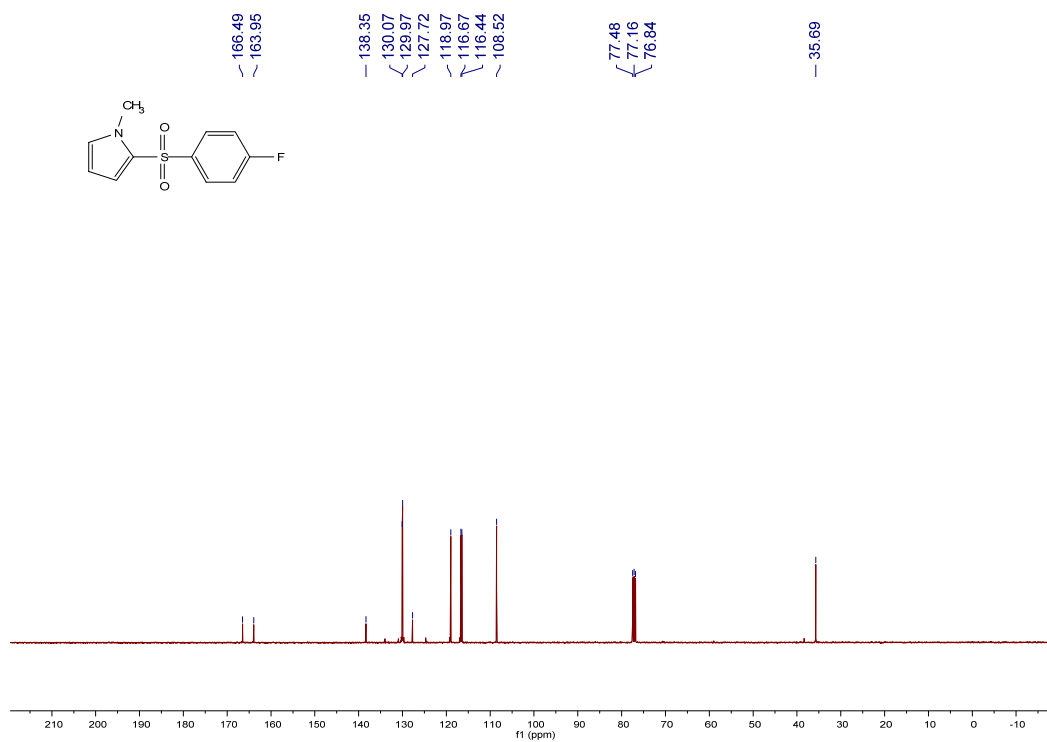
2-((4-(tert-butyl)phenyl)sulfonyl)-1-methyl-1H-pyrrole (5c)



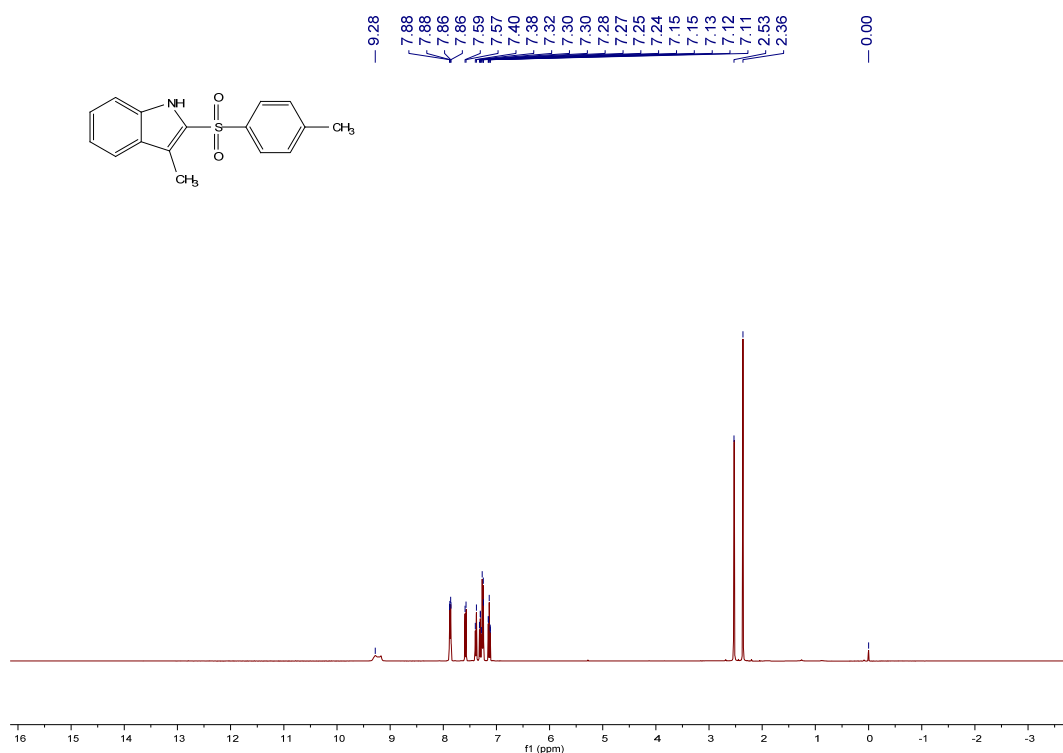


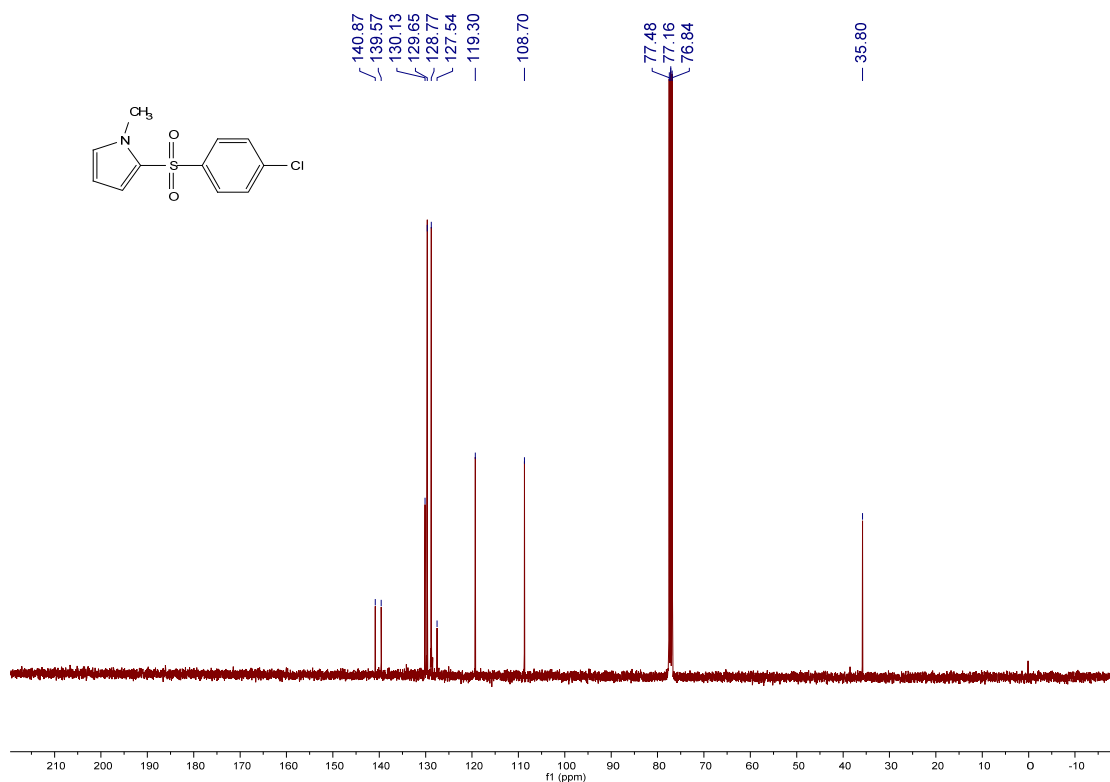
2-((4-fluorophenyl)sulfonyl)-1-methyl-1H-pyrrole (5d)



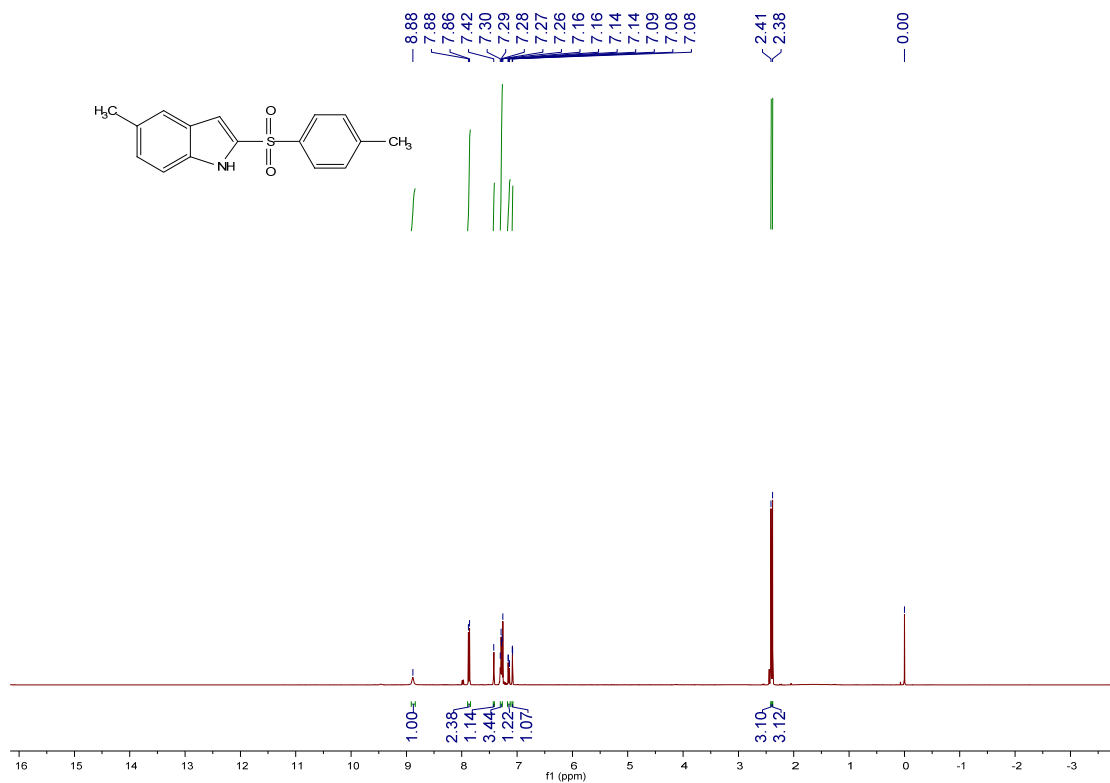


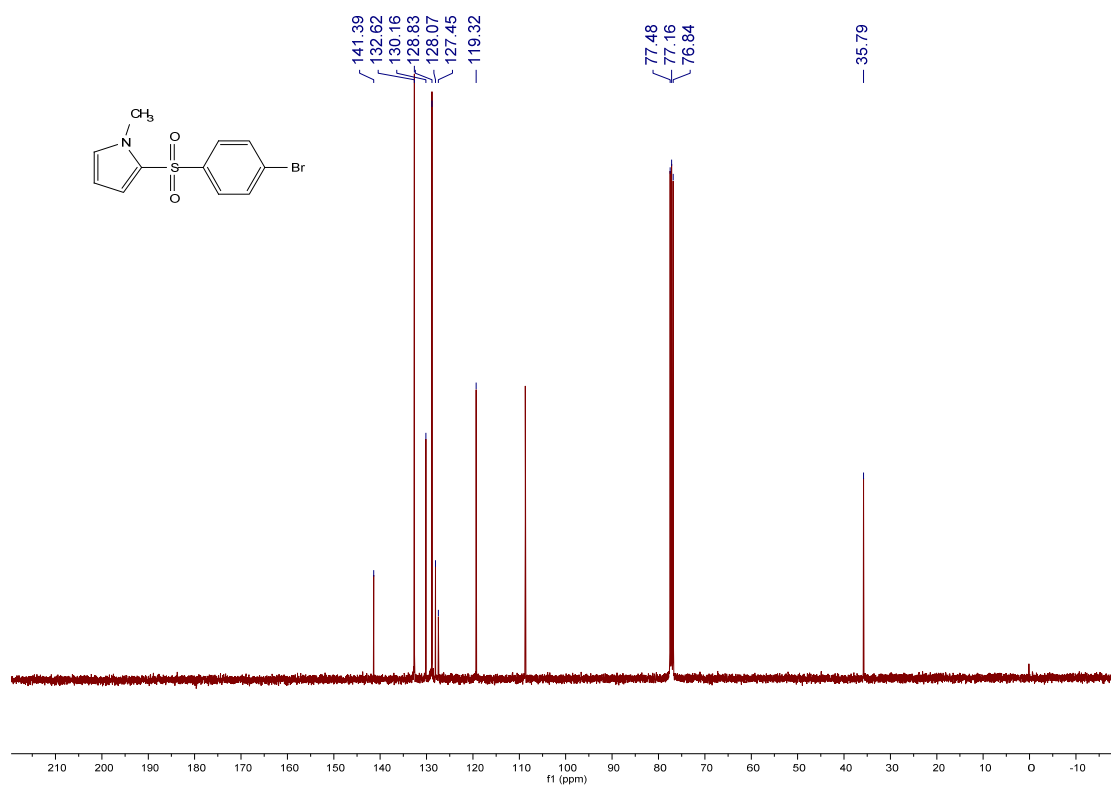
2-((4-chlorophenyl)sulfonyl)-1-methyl-1H-pyrrole (5e)



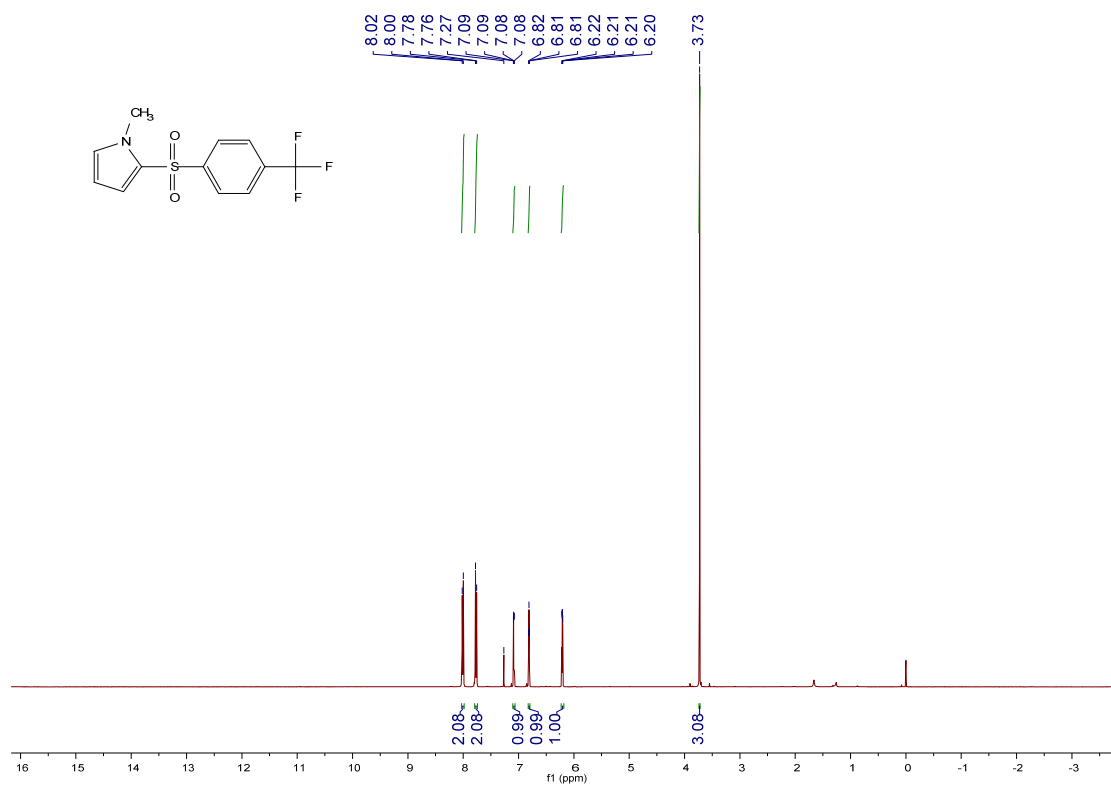


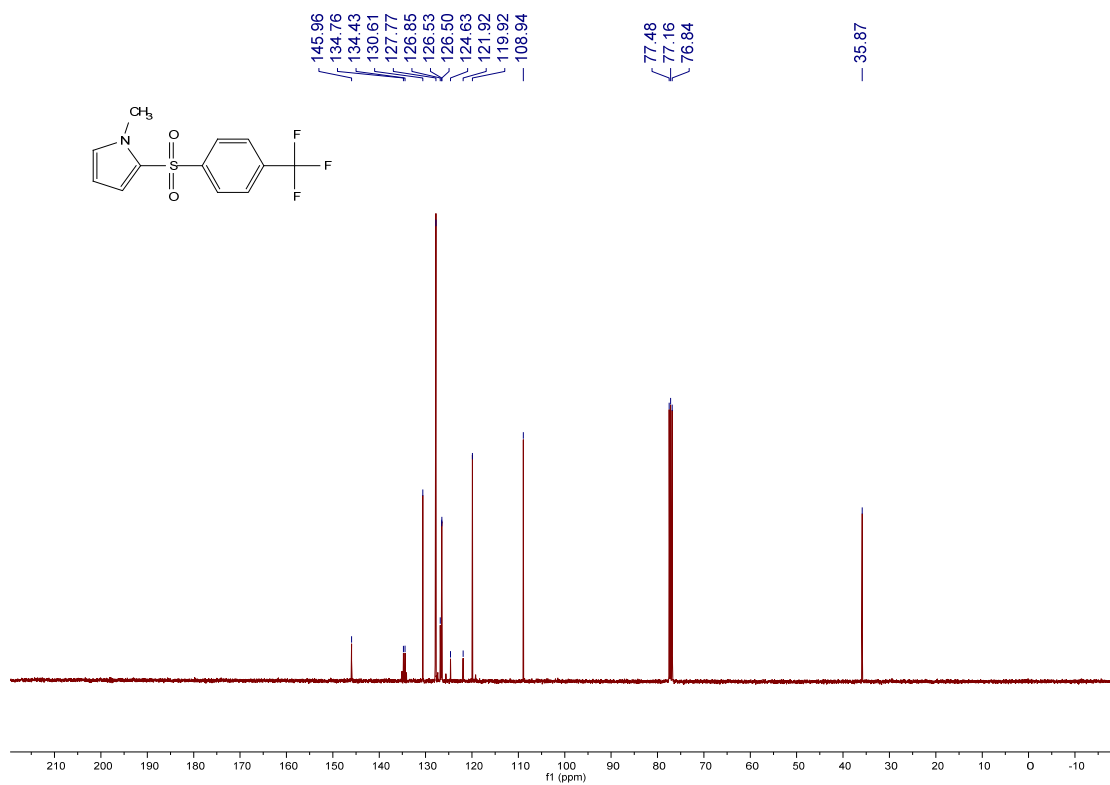
2-((4-bromophenyl)sulfonyl)-1-methyl-1H-pyrrole (5f)



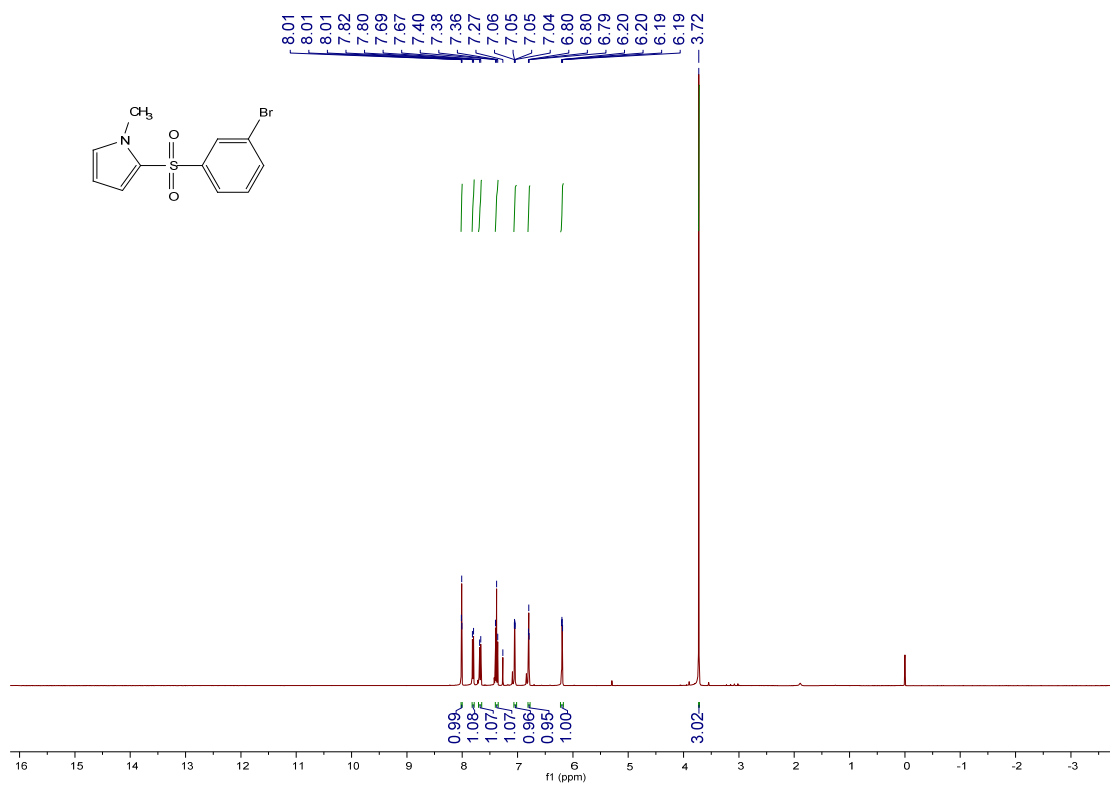


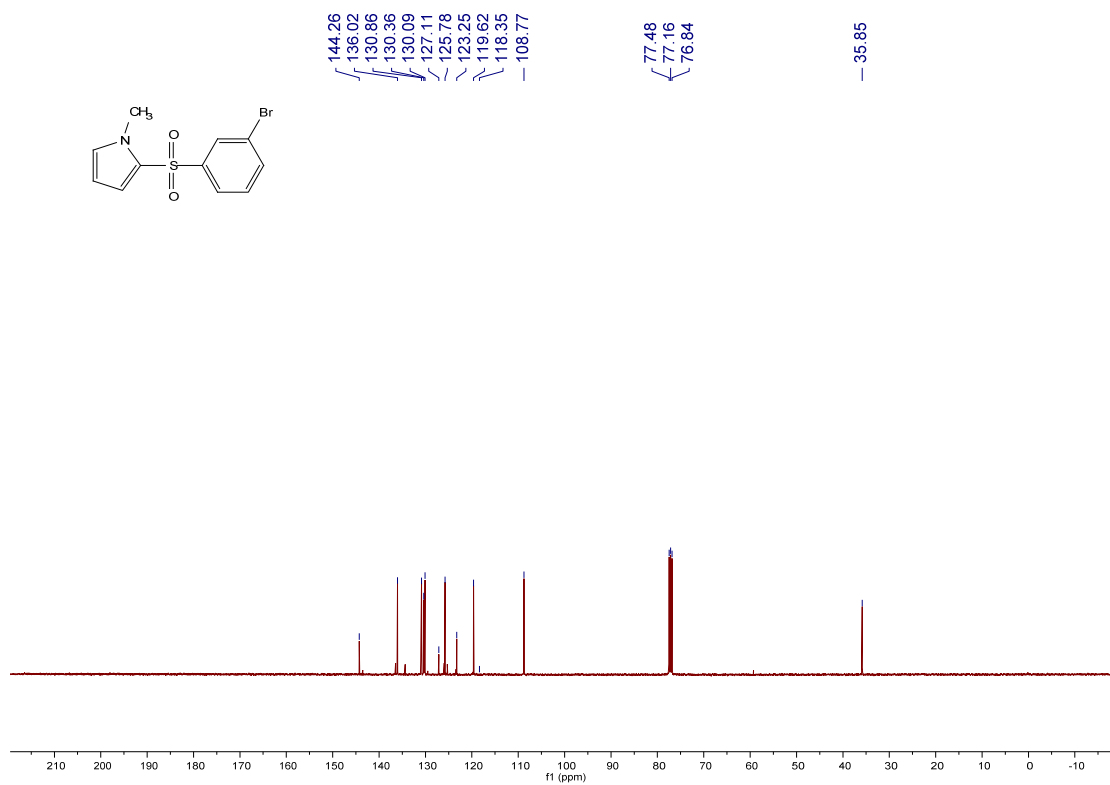
1-methyl-2-((4-(trifluoromethyl)phenyl)sulfonyl)-1H-pyrrole (5g)





2-((3-bromophenyl)sulfonyl)-1-methyl-1H-pyrrole (5h)





1-methyl-2-(naphthalen-2-ylsulfonyl)-1H-pyrrole (5i)

