

Supporting Information

New efficient synthesis of benzofuro[2,3-*b*]pyrroles utilizing reactive nitrilium trapping approach by acid-promoted cascade addition/cyclization sequence

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General Information

Chemicals were purchased from Aldrich and Alfa Aesar Chemical Companies and used without further purification. Dried and distilled solvents were used. All reactions involving moisture sensitive reactants were performed using oven dried glassware. Chemicals were purchased from Aldrich and Alfa Aesar Chemical Companies and used without further purification. NMR spectra were recorded in CDCl₃ on a Jeol JNM ECP 400 and 600 NMR instrument. ¹H NMR chemical shifts are reported in ppm relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard (CDCl₃ at 7.26 ppm). Standard abbreviations were used to denote signal multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. ¹³C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard (CDCl₃ at 77.16 ppm). HRMS were obtained by EI on a double-focusing mass analyzer, ESI (positive ion mode) on TOF mass analyzer. All melting points were determined using open capillaries on an Electrothermal-9100 (Japan) instrument and are uncorrected.

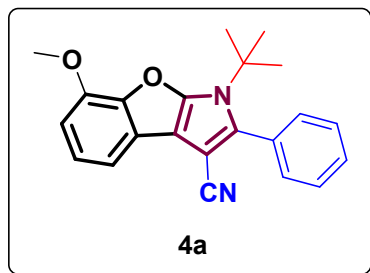
Experimental procedure

General procedure

To a 25 ml oven dried R. B. flask successively added of 2-hydroxybenzaldehydes **1a** (1 mmol), benzoylacetonitrile (**2a**), *tert*-butyl isocyanide (**3a**), *p*-TSA.H₂O (0.04 mmol) and 2.0 mL ethanol. The resulting mixture was stirred at 80 °C for 4-6 h. After completion of the reaction (monitored by TLC), the reaction mixture was cooled to ambient temperature and directly subjected to flash column chromatography on silica gel (60–120 mesh) using petroleum ether/ethylacetate = 80:20 as an eluant to afford the pure product **4a** in good yield.

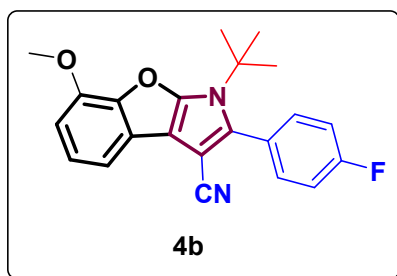
Characterization Data of the compounds

1-(*tert*-Butyl)-7-methoxy-2-phenyl-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4a)



Yield: 91% (314 mg); Yellow solid; Mp: 94-96 °C; ¹H NMR (600 MHz, CDCl₃) δ 7.98 – 7.93 (m, 2H), 7.47 – 7.42 (m, 2H), 7.38 – 7.33 (m, 1H), 7.13 (dd, *J* = 7.9, 1.4 Hz, 1H), 6.97 (t, *J* = 8.0 Hz, 1H), 6.88 (dd, *J* = 8.1, 1.4 Hz, 1H), 3.93 (s, 3H), 1.30 (s, 9H).; ¹³C NMR (150 MHz, CDCl₃) δ 153.3, 151.3, 147.4, 142.4, 129.0, 128.9, 128.7, 124.6, 122.2, 120.5, 116.9, 115.6, 110.0, 104.3, 100.0, 93.8, 56.2, 54.1, 30.1; FT-IR (thin film): ν (cm⁻¹) 3060, 2965, 2921, 2223, 1597, 1561, 1490, 1468, 1438, 1365, 1275, 1250, 1221, 1097, 1090, 1010, 934, 911, 762, 732.; HRMS (ESI, *m/z*): calcd for C₂₂H₂₀N₂O₂ (M+H⁺) 344.1525, found 344.1529.

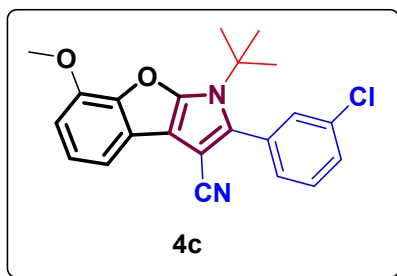
1-(*tert*-Butyl)-2-(4-fluorophenyl)-7-methoxy-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4b)



Yield: 84% (304.4 mg); Yellow solid; Mp: 102-104 °C; ¹H NMR (600 MHz, CDCl₃) δ 7.95 – 7.91 (m, 2H), 7.16 – 7.13 (m, 2H), 7.10 (dd, *J* = 7.9, 1.4 Hz, 1H), 6.97 (t, *J* = 8.0 Hz, 1H), 6.87 (dd, *J* = 8.1, 1.3 Hz, 1H), 3.93 (s, 3H), 1.28 (s, 9H).; ¹³C NMR (150 MHz, CDCl₃) 163.7, 162.1, 152.5, 151.3, 147.4, 142.4, 126.6, 126.6, 125.1, 125.1, 122.1, 120.6, 116.8, 116.3, 116.1, 115.6, 110.1, 104.4, 100.0, 93.5, 56.2, 54.1, 30.1; FT-IR (thin film): ν (cm⁻¹) 3071, 2967, 2932, 2223,

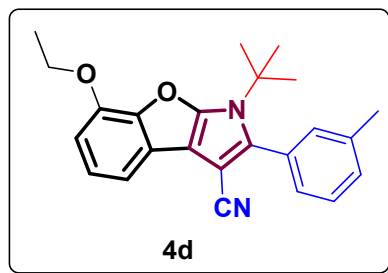
1596, 1567, 1503, 1468, 1438, 1394, 1365, 1277, 1232, 1159, 1088, 1010, 935, 834, 810, 732.; HRMS (ESI, m/z): calcd for $C_{22}H_{19}FN_2O_2$ ($M+H^+$) 362.1431, found: 362.1434.

1-(*tert*-Butyl)-2-(3-chlorophenyl)-7-methoxy-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4c)



Yield: 86% (326 mg); Yellow solid; Mp: 96-98 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.82 (m, 2H), 7.40 – 7.34 (m, 1H), 7.32 – 7.28 (m, 1H), 7.10 (dd, $J = 7.9, 1.4$ Hz, 1H), 6.97 (t, $J = 8.0$ Hz, 1H), 6.87 (dd, $J = 8.1, 1.4$ Hz, 1H), 3.93 (s, 3H), 1.31 (s, 9H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 151.0, 147.3, 142.3, 135.1, 130.3, 128.6, 124.2, 122.4, 122.1, 120.6, 116.5, 115.2, 110.0, 103.5, 95.0, 56.1, 53.9, 30.2; HRMS (ESI, m/z): calcd for $C_{22}H_{19}ClN_2O_2$ ($M+H^+$) 378.1135, found: 378.1139.

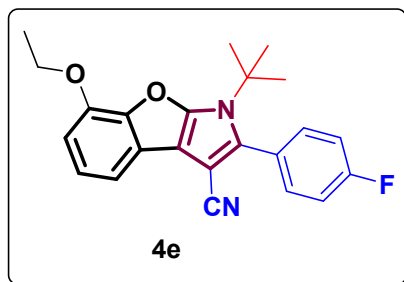
1-(*tert*-Butyl)-7-ethoxy-2-(*m*-tolyl)-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4d)



Yield: 82% (305.7 mg); Brown solid; Mp: 108-110 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.79 – 7.74 (m, 2H), 7.37 – 7.32 (m, 1H), 7.17 (d, $J = 7.9$ Hz, 1H), 7.11 (dd, $J = 7.9, 1.4$ Hz, 1H), 6.95 (t, $J = 8.0$ Hz, 1H), 6.86 (dd, $J = 8.1, 1.4$ Hz, 1H), 4.16 (q, $J = 7.0$ Hz, 2H), 2.42 (s, 3H), 1.48 (t, $J = 7.0$ Hz, 3H), 1.30 (s, 9H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 151.5, 146.5, 142.4, 138.7,

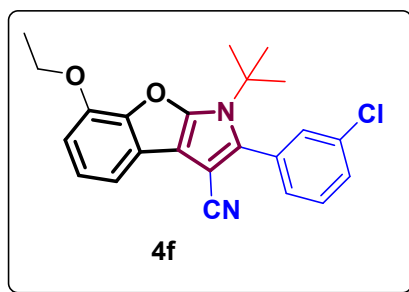
129.7, 128.9, 128.7, 125.1, 122.1, 121.8, 120.5, 116.8, 115.7, 110.9, 103.9, 93.6, 64.8, 53.9, 30.2, 21.6, 15.0; HRMS (ESI, m/z): calcd for $C_{24}H_{24}N_2O_2$ ($M+H^+$) 372.1838, found: 372.1841.

1-(*tert*-Butyl)-7-ethoxy-2-(4-fluorophenyl)-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4e)



Yield: 71% (267.4 mg); Yellow solid; Mp: 100-102 °C; 1H NMR (600 MHz, $CDCl_3$) δ 7.96 – 7.90 (m, 2H), 7.15 – 7.12 (m, 2H), 7.08 (dd, $J = 7.9, 1.4$ Hz, 1H), 6.94 (t, $J = 8.0$ Hz, 1H), 6.85 (dd, $J = 8.1, 1.4$ Hz, 1H), 4.15 (q, $J = 7.0$ Hz, 2H), 1.47 (t, $J = 7.0$ Hz, 3H), 1.29 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.6, 162.0, 152.2, 151.7, 146.4, 142.4, 126.5, 126.5, 125.2, 122.0, 120.5, 116.7, 116.2, 116.1, 115.6, 110.9, 103.6, 93.5, 64.8, 53.8, 30.2, 14.9; HRMS (ESI, m/z): calcd for $C_{23}H_{21}FN_2O_2$ ($M+H^+$) 376.1587, found: 376.1589.

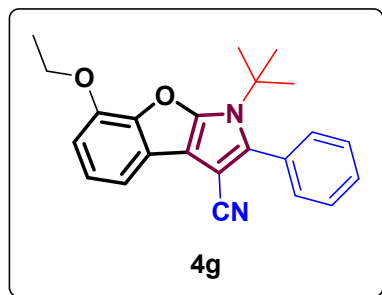
1-(*tert*-Butyl)-2-(3-chlorophenyl)-7-ethoxy-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4f)



Yield: 74% (290.5 mg); Yellow solid; Mp: 111-113°C; 1H NMR (400 MHz, $CDCl_3$) δ 7.90 – 7.81 (m, 2H), 7.40 – 7.35 (m, 1H), 7.32 – 7.28 (m, 1H), 7.09 – 7.04 (m, 1H), 6.95 (t, $J = 8.0$ Hz, 1H), 6.86 (dd, $J = 8.0, 1.0$ Hz, 1H), 4.20 – 4.14 (q, 2H), 1.49 (t, 3H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 150.8, 146.4, 142.4, 135.1, 130.4, 128.6, 124.2, 122.4, 122.1, 120.6,

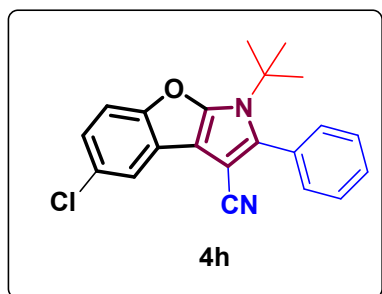
116.5, 115.3, 110.8, 102.9, 95.1, 64.9, 53.8, 30.3, 15.0; HRMS (ESI, m/z): calcd for $C_{23}H_{21}ClN_2O_2$ ($M+H^+$) 392.1292, found: 392.1295.

1-(*tert*-Butyl)-7-ethoxy-2-phenyl-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4g)



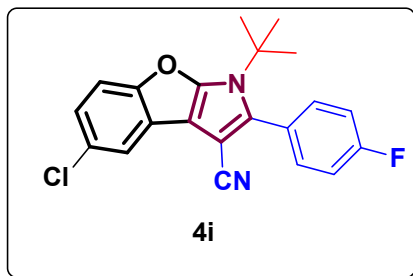
Yield: 80% (285.2 mg); Brown solid; Mp: 90-92 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.93 (m, 2H), 7.47 – 7.42 (m, 2H), 7.38 – 7.32 (m, 1H), 7.10 (dd, $J = 7.9, 1.4$ Hz, 1H), 6.95 (t, $J = 8.0$ Hz, 1H), 6.85 (dd, $J = 8.1, 1.4$ Hz, 1H), 4.16 (q, 2H), 1.48 (t, 3H), 1.31 (s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 151.7, 146.5, 142.4, 129.0, 128.8, 124.5, 122.1, 120.5, 116.8, 115.7, 110.8, 103.5, 93.8, 64.8, 53.8, 30.2, 15.0; HRMS (ESI, m/z): calcd for $C_{23}H_{22}N_2O_2$ ($M+H^+$) 358.1681, found: 358.1684.

1-(*tert*-Butyl)-5-chloro-2-phenyl-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4h)



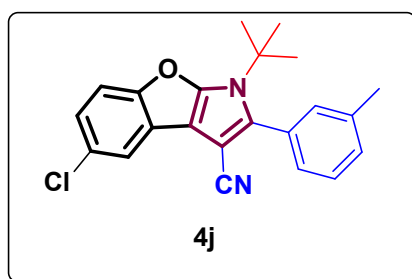
Yield: 86% (299.8 mg); Brown solid; Mp: 106-108 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.95 (m, 2H), 7.64 (d, $J = 2.5$ Hz, 1H), 7.53 – 7.45 (m, 3H), 7.24 (dd, $J = 8.7, 2.5$ Hz, 1H), 6.95 (d, $J = 8.7$ Hz, 1H), 1.18 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 152.9, 146.1, 130.3, 129.9, 129.3, 128.7, 127.8, 125.6, 125.4, 120.4, 118.3, 114.8, 114.0, 93.4, 57.3, 29.4; HRMS (ESI, m/z): calcd for $C_{21}H_{17}ClN_2O$ ($M+H^+$) 348.1029, found: 348.1032.

1-(*tert*-Butyl)-5-chloro-2-(4-fluorophenyl)-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4i)



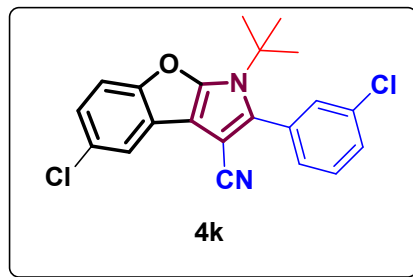
Yield: 78% (287 mg); Yellow solid; Mp: 98-100 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.97 – 7.92 (m, 2H), 7.60 (d, *J* = 2.6 Hz, 1H), 7.22 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.20 – 7.15 (m, 2H), 6.94 (d, *J* = 8.7 Hz, 1H), 1.18 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 164.9, 162.4, 156.0, 152.9, 146.4, 129.9, 128.7, 127.6, 127.5, 125.6, 124.2, 120.3, 118.3, 116.6, 116.4, 114.7, 113.3, 93.1, 57.1, 29.4.; HRMS (ESI, *m/z*): calcd for C₂₁H₁₆ClFN₂O (M+H⁺) 366.0935, found: 366.0937.

1-(*tert*-Butyl)-5-chloro-2-(*m*-tolyl)-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4j)



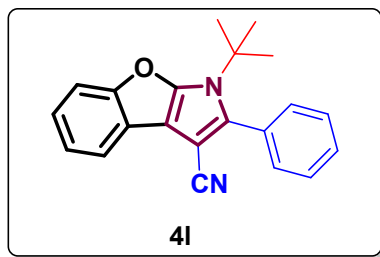
Yield: 79% (386.4 mg); Brown solid; Mp: 110-112 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.80 – 7.73 (m, 2H), 7.63 (d, *J* = 2.5 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.27 – 7.25 (m, 1H), 7.23 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.95 (d, *J* = 8.7 Hz, 1H), 2.43 (s, 3H), 1.18 (s, 9H).; ¹³C NMR (100 MHz, CDCl₃) δ 157.3, 152.9, 146.1, 139.0, 131.2, 129.8, 129.1, 127.7, 125.9, 125.5, 122.6, 120.3, 118.4, 114.8, 113.7, 93.2, 57.2, 29.4, 21.6; HRMS (ESI, *m/z*): calcd for C₂₂H₁₉ClN₂O (M+H⁺) 362.1186, found: 362.1189.

1-(*tert*-Butyl)-5-chloro-2-(3-chlorophenyl)-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4k)



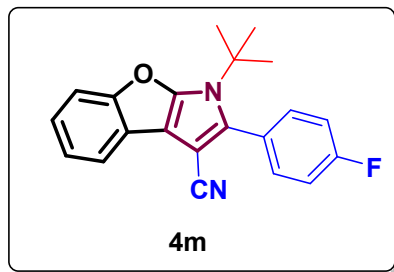
Yield: 82% (314.2 mg); Yellow solid; Mp: 120-121 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.91 (dt, *J* = 7.1, 1.9 Hz, 1H), 7.85 (d, *J* = 1.7 Hz, 1H), 7.59 (d, *J* = 2.5 Hz, 1H), 7.44 – 7.39 (m, 2H), 7.25 – 7.21 (m, 1H), 6.94 (d, *J* = 8.7 Hz, 1H), 1.19 (s, 9H).; ¹³C NMR (100 MHz, CDCl₃) δ 154.9, 152.8, 147.1, 135.3, 130.6, 130.2, 130.0, 129.4, 128.8, 125.7, 125.1, 123.4, 120.3, 118.1, 114.3, 113.0, 94.5, 57.1, 29.5; HRMS (ESI, *m/z*): calcd for C₂₁H₁₆Cl₂N₂O (M+H⁺) 382.0640, found: 382.0644.

1-(*tert*-Butyl)-2-phenyl-1H-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4l)



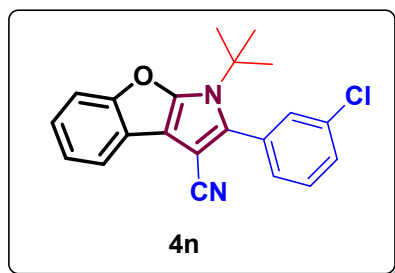
Yield: 90% (283 mg); Yellow solid; Mp: 88-90 °C; ¹H NMR (600 MHz, CDCl₃) δ 7.99 – 7.95 (m, 2H), 7.67 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.50 – 7.47 (m, 2H), 7.45 – 7.41 (m, 1H), 7.31 – 7.27 (m, 1H), 7.06 – 7.01 (m, 2H), 1.18 (s, 9H).; ¹³C NMR (150 MHz, CDCl₃) δ 156.6, 154.1, 146.2, 130.0, 129.9, 129.7, 129.4, 129.2, 128.7, 128.1, 125.3, 120.8, 118.9, 116.9, 115.3, 114.4, 93.7, 56.8, 29.4; HRMS (ESI, *m/z*): calcd for C₂₁H₁₈N₂O (M+H⁺) 314.1419, found: 314.1422.

1-(*tert*-Butyl)-2-(4-fluorophenyl)-1H-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4m)



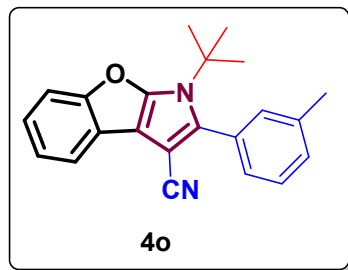
Yield: 79% (263 mg); Yellow solid; Mp: 94-96 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.00 – 7.94 (m, 2H), 7.65 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.32 – 7.27 (m, 1H), 7.20 – 7.16 (m, 2H), 7.05 – 7.01 (m, 2H), 1.18 (s, 9H); ¹³C NMR (150 MHz, CDCl₃) δ 162.7, 155.7, 154.1, 146.3, 130.0, 129.4, 127.5, 127.4, 120.9, 118.9, 116.8, 116.5, 116.4, 115.2, 93.5, 56.8, 29.4; HRMS (ESI, *m/z*): calcd for C₂₁H₁₇FN₂O (M+H⁺) 332.1325, found: 332.1328.

1-(*tert*-Butyl)-2-(3-chlorophenyl)-1H-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4n)



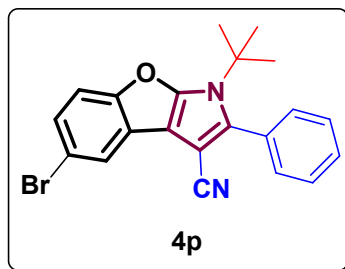
Yield: 88% (307 mg); Yellow solid; Mp: 109-111 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.91 (dt, *J* = 7.3, 1.7 Hz, 1H), 7.86 (t, *J* = 1.7 Hz, 1H), 7.63 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.42–7.38 (m, 2H), 7.32 – 7.26 (m, 1H), 7.06 – 7.00 (m, 2H), 1.19 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 154.5, 154.0, 147.0, 135.3, 130.5, 130.1, 129.9, 129.6, 129.5, 125.0, 123.3, 121.0, 118.8, 116.7, 114.8, 113.9, 94.8, 56.8, 29.5; HRMS (ESI, *m/z*): calcd for C₂₁H₁₇ClN₂O (M+H⁺) 348.1029, found: 348.1032.

1-(*tert*-Butyl)-2-(*m*-tolyl)-1H-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4o)



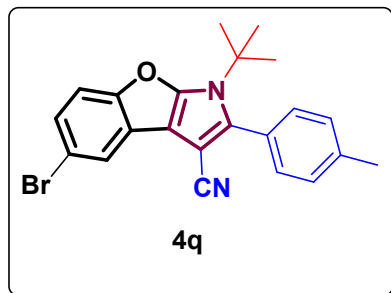
Yield: 91% (299 mg); Yellow solid; Mp: 91-93 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.83 – 7.75 (m, 2H), 7.67 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.31 – 7.27 (m, 1H), 7.26 – 7.22 (m, 1H), 7.08 – 6.99 (m, 2H), 2.43 (s, 3H), 1.18 (s, 9H).; ¹³C NMR (100 MHz, CDCl₃) δ 156.9, 154.1, 145.9, 138.9, 130.9, 129.9, 129.4, 129.1, 128.0, 125.8, 122.6, 118.9, 116.9, 115.3, 114.7, 93.5, 56.9, 29.4, 21.6; HRMS (ESI, *m/z*): calcd for C₂₂H₂₀N₂O (M+H⁺) 328.1576, found: 328.1579.

5-bromo-1-(*tert*-Butyl)-2-phenyl-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4p)



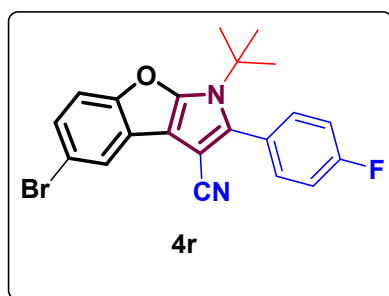
Yield: 76% (298.8 mg); Brown solid; Mp: 104-106 °C; ¹H NMR (600 MHz, CDCl₃) δ 7.83 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.57 – 7.53 (m, *J* = 10.7, 5.1 Hz, 2H), 7.45 – 7.41 (m, *J* = 7.5 Hz, 2H), 7.35 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.93 (d, *J* = 8.7 Hz, 1H), 1.26 (s, 9H).; ¹³C NMR (150 MHz, CDCl₃) δ 157.1, 153.4, 146.2, 132.8, 131.7, 130.3, 127.8, 125.4, 120.8, 120.2, 118.9, 114.7, 113.5, 112.8, 93.5, 57.2, 29.4; HRMS (ESI, *m/z*): calcd for C₂₁H₁₇BrN₂O (M+H⁺) 392.0524, found: 392.0528.

5-bromo-1-(*tert*-Butyl)-2-(*p*-tolyl)-1*H*-benzofuro[2,3-*b*]pyrrole-3-carbonitrile (4q)



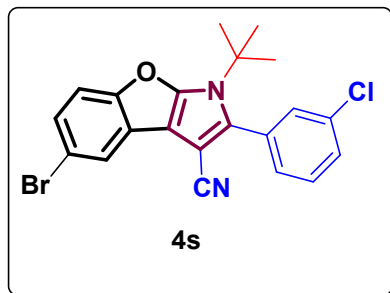
Yield: 68% (277 mg); Brown solid; Mp: 119-121 °C; ¹H NMR (600 MHz, CDCl₃) δ 7.84 (d, *J* = 8.2 Hz, 2H), 7.75 (d, *J* = 2.4 Hz, 1H), 7.33 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.27 (d, *J* = 8.3 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 1H), 2.40 (s, 3H), 1.17 (s, 9H).; ¹³C NMR (150 MHz, CDCl₃) δ 157.2, 153.4, 146.2, 140.6, 132.5, 131.6, 129.9, 127.9, 125.3, 120.6, 119.0, 115.0, 112.6, 92.5, 56.8, 29.4, 21.6; HRMS (ESI, *m/z*): calcd for C₂₂H₁₉BrN₂O (M+H⁺) 406.0681, found: 406.0685.

5-bromo-1-(tert-Butyl)-2-(4-fluorophenyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4r)



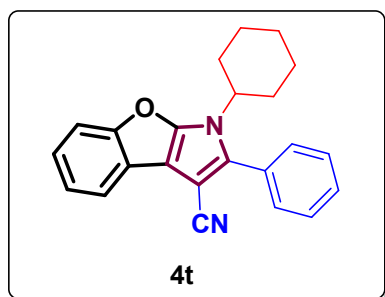
Yield: 70% (287.3 mg); Brown solid; Mp: 130-132 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.99 – 7.94 (m, 2H), 7.76 (d, *J* = 2.4 Hz, 1H), 7.38 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.19 (t, *J* = 8.7 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 1H), 1.18 (s, 9H).; ¹³C NMR (100 MHz, CDCl₃) δ 165.0, 162.4, 156.2, 153.5, 146.1, 132.9, 131.6, 127.6, 127.6, 124.2, 120.9, 118.8, 116.7, 116.4, 114.7, 113.8, 112.8, 93.3, 57.3, 29.4; HRMS (ESI, *m/z*): calcd for C₂₁H₁₆BrFN₂O (M+H⁺) 410.0430, found: 410.0434.

5-bromo-1-(tert-Butyl)-2-(3-chlorophenyl)-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4s)



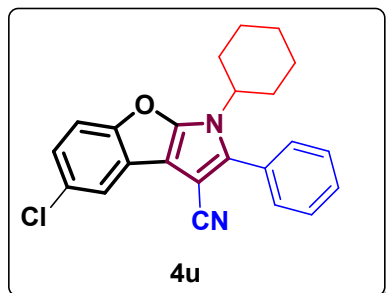
Yield: 72% (308 mg); Brown solid; Mp: 138-140 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.88 (dt, *J* = 7.1, 1.9 Hz, 1H), 7.83 (td, *J* = 1.8, 0.7 Hz, 1H), 7.71 (d, *J* = 2.4 Hz, 1H), 7.43 – 7.38 (m, 2H), 7.35 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.89 (d, *J* = 8.7 Hz, 1H), 1.19 (s, 9H).; ¹³C NMR (100 MHz, CDCl₃) δ 154.6, 153.3, 147.4, 135.3, 132.7, 131.7, 130.6, 130.0, 129.4, 125.0, 123.2, 120.5, 118.7, 114.4, 112.7, 112.2, 94.4, 56.9, 29.4; HRMS (ESI, *m/z*): calcd for C₂₁H₁₆BrClN₂O (M+H⁺) 426.0135, found: 426.0139.

1-cyclohexyl-2-phenyl-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4t)



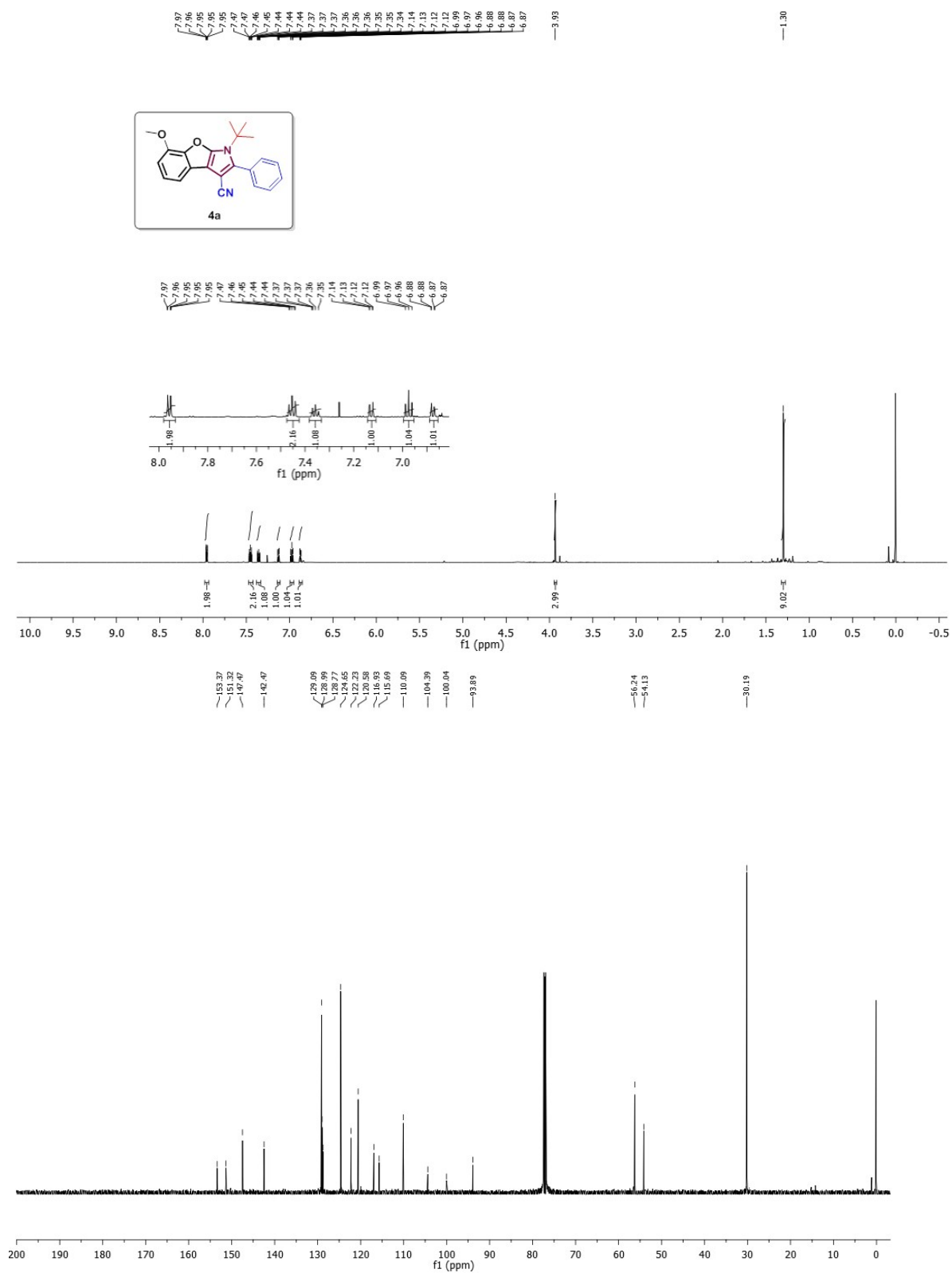
Yield: 61% (207.6 mg); Yellow solid; Mp: 113-115 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.96 – 7.91 (m, 2H), 7.57 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.41 – 7.36 (m, 1H), 7.30 – 7.25 (m, 1H), 7.07 – 6.99 (m, 2H), 3.32 – 3.05 (m, 1H), 1.99 – 1.88 (m, 2H), 1.75 – 1.69 (m, 2H), 1.63 – 1.57 (m, 1H), 1.30 – 1.13 (m, 5H).; ¹³C NMR (100 MHz, CDCl₃) δ 154.2, 153.5, 148.9, 129.8, 129.6, 129.4, 129.1, 128.3, 124.8, 121.1, 118.0, 116.6, 115.3, 105.4, 94.1, 55.8, 33.6, 25.4, 24.7; HRMS (ESI, *m/z*): calcd for C₂₃H₂₀N₂O (M+H⁺) 340.1576, found: 340.1579.

5-chloro-1-cyclohexyl-2-phenyl-1H-benzofuro[2,3-b]pyrrole-3-carbonitrile (4u)

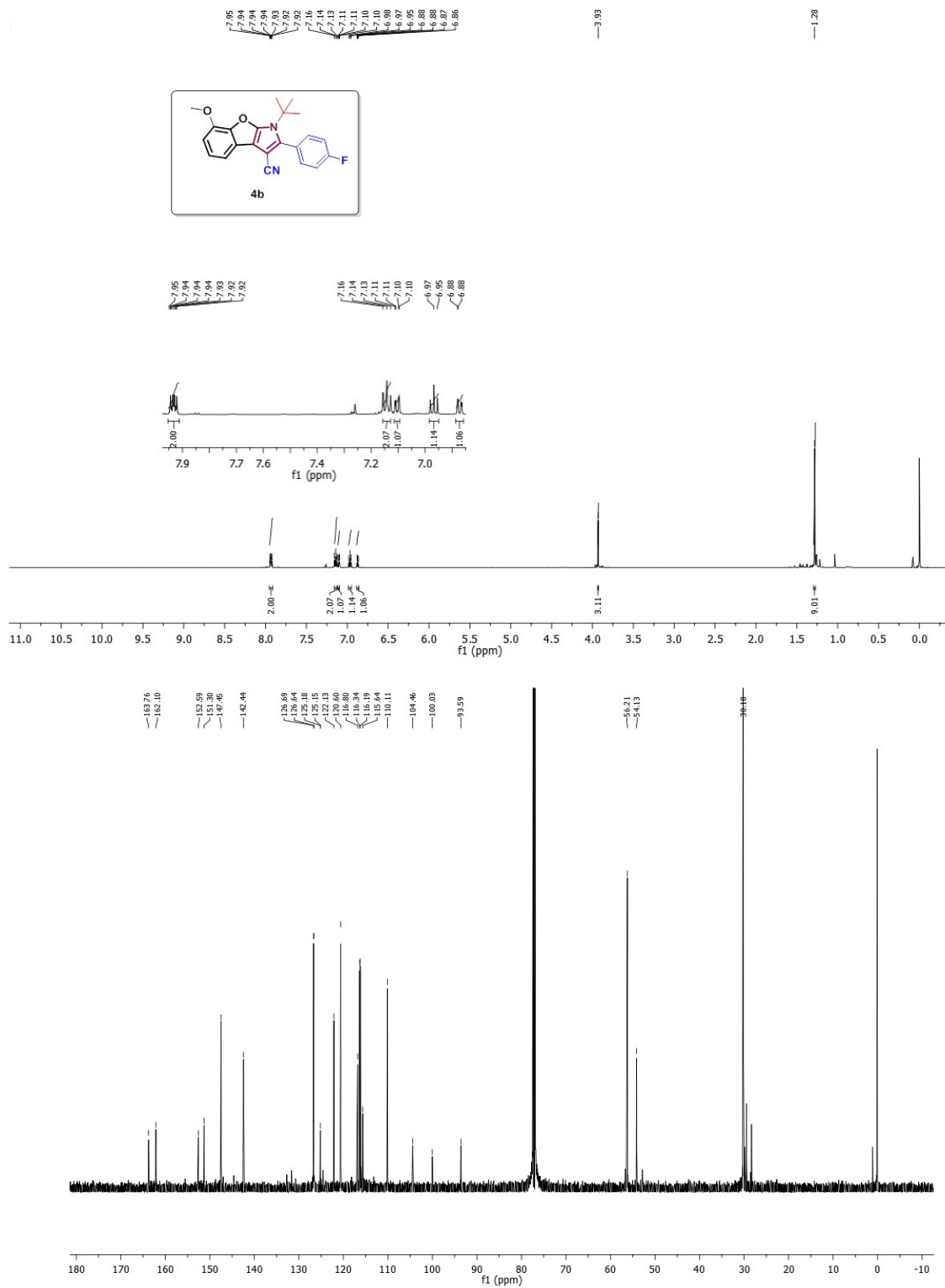


Yield: 58% (217.4 mg); Yellow solid; Mp: 120-122 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.93 – 7.86 (m, 2H), 7.49 – 7.48 (m, 1H), 7.46 – 7.42 (m, 2H), 7.40 – 7.37 (m, 1H), 7.16 (dd, $J = 8.7$, 2.5 Hz, 1H), 6.91 (d, $J = 8.7$ Hz, 1H), 3.26 – 3.15 (m, 1H), 1.98 – 1.90 (m, 2H), 1.75 – 1.70 (m, 2 Hz), 1.62 – 1.56 (m, 1H), 1.30 – 1.16 (m, 5H).; ^{13}C NMR (100 MHz, CDCl_3) δ 153.9, 152.1, 149.7, 129.4, 129.1, 128.4, 128.1, 128.0, 126.8, 125.6, 124.7, 119.1, 115.0, 102.9, 93.6, 55.4, 33.6, 25.4, 24.7; HRMS (ESI, m/z): calcd for $\text{C}_{23}\text{H}_{19}\text{ClN}_2\text{O}$ ($\text{M}+\text{H}^+$) 374.1186, found: 374.1189.

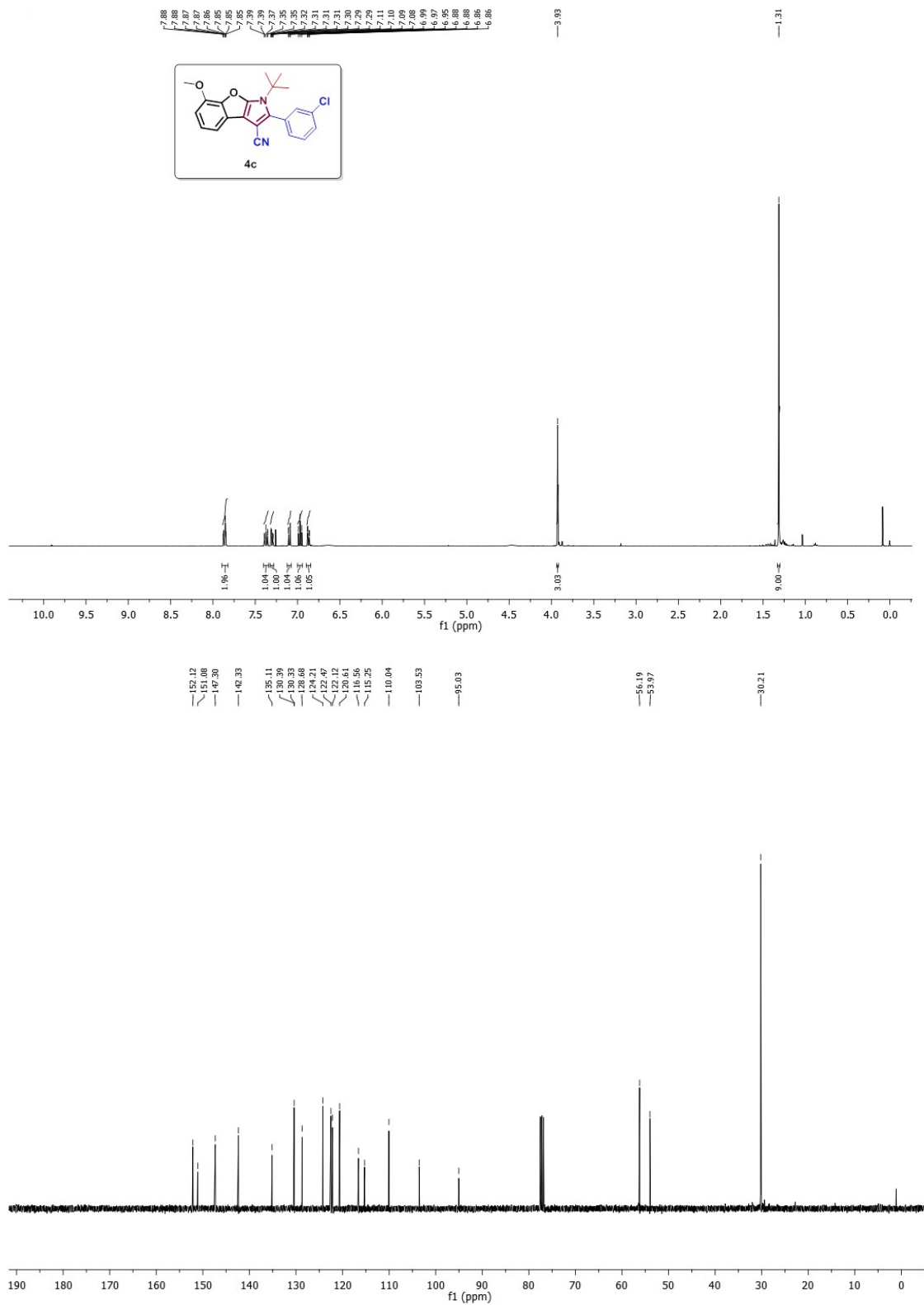
^1H NMR and ^{13}C NMR of compound (4a)



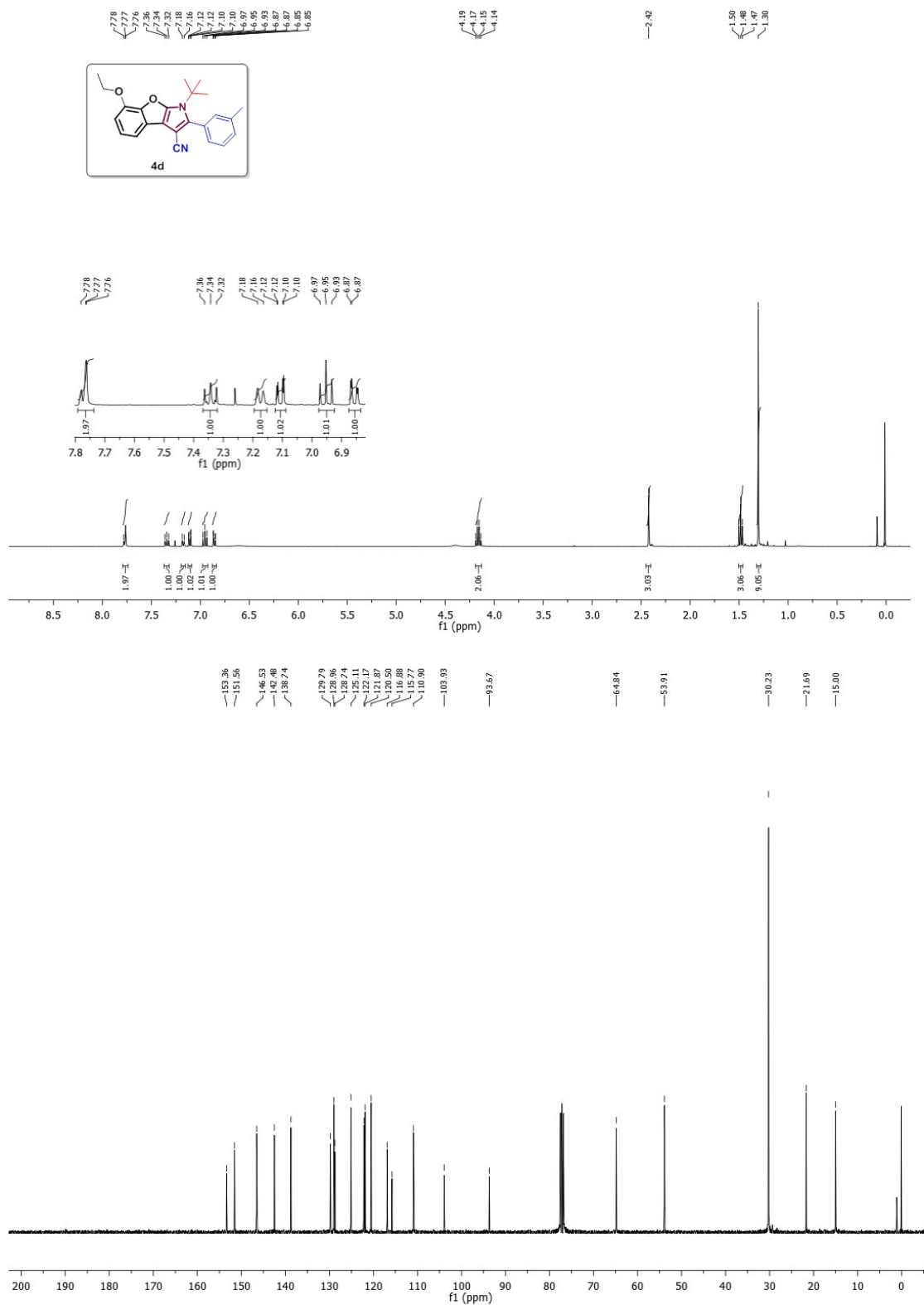
¹H NMR and ¹³C NMR of compound (4b)



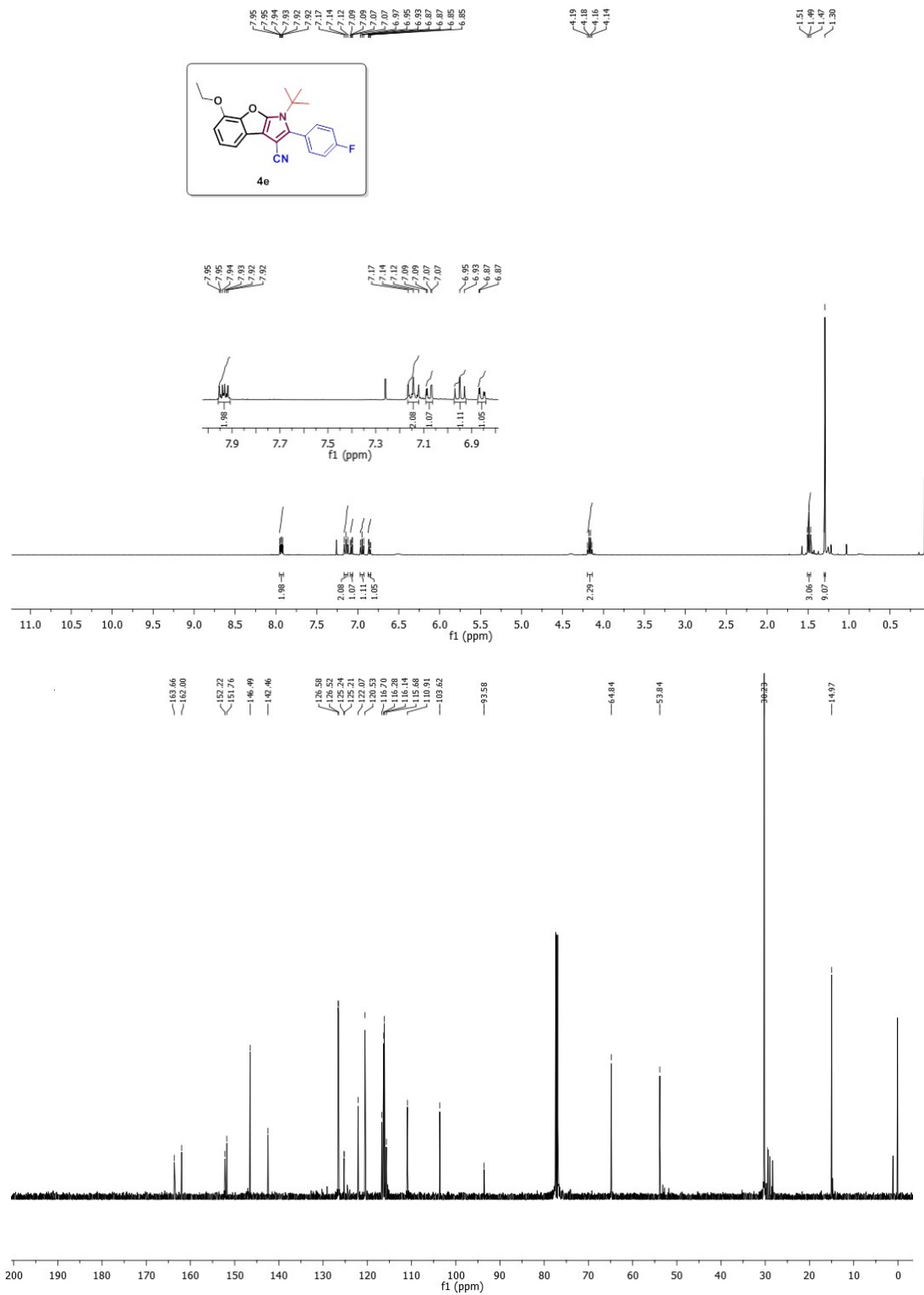
^1H NMR and ^{13}C NMR of compound (4c)



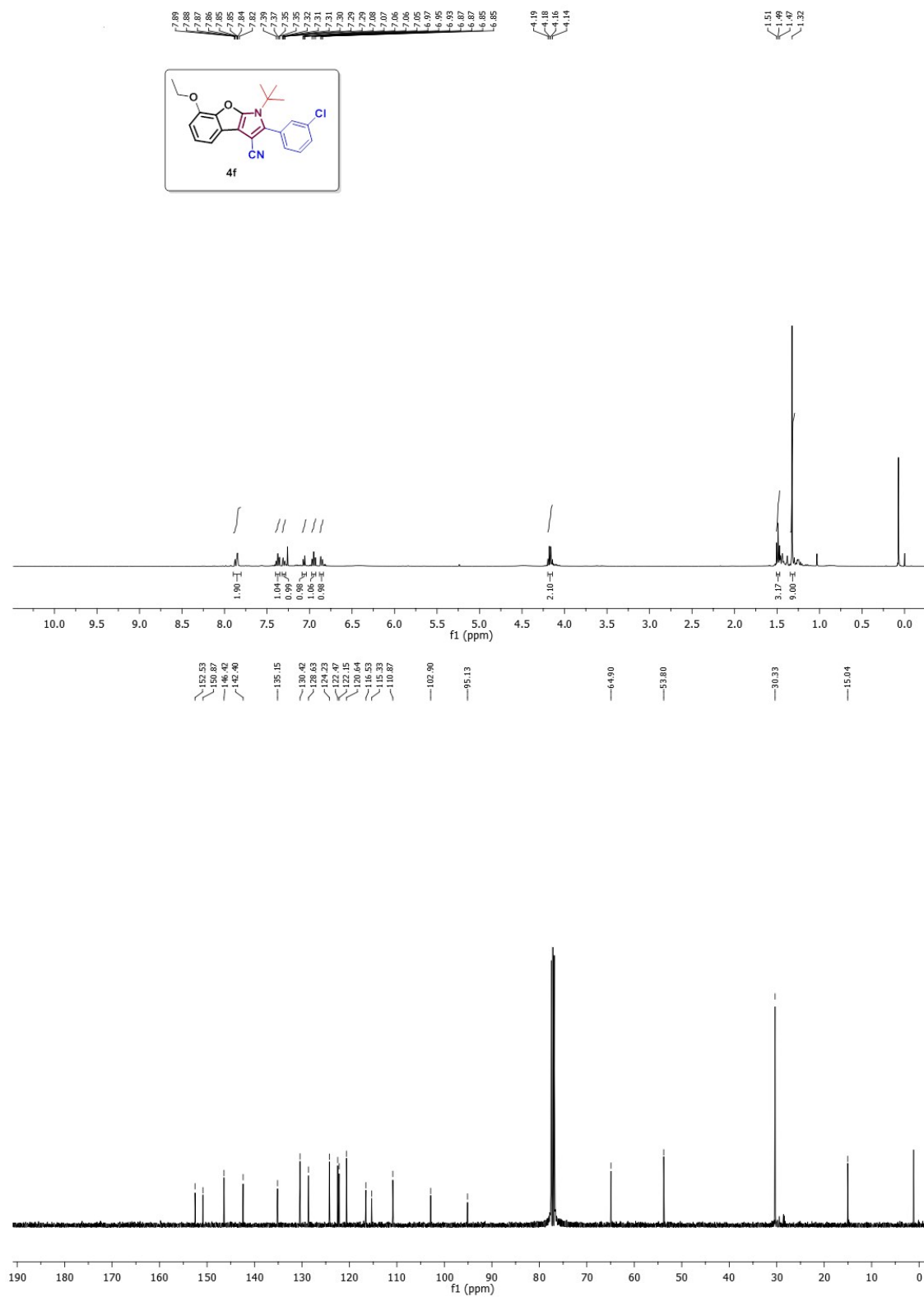
^1H NMR and ^{13}C NMR of compound (4d)



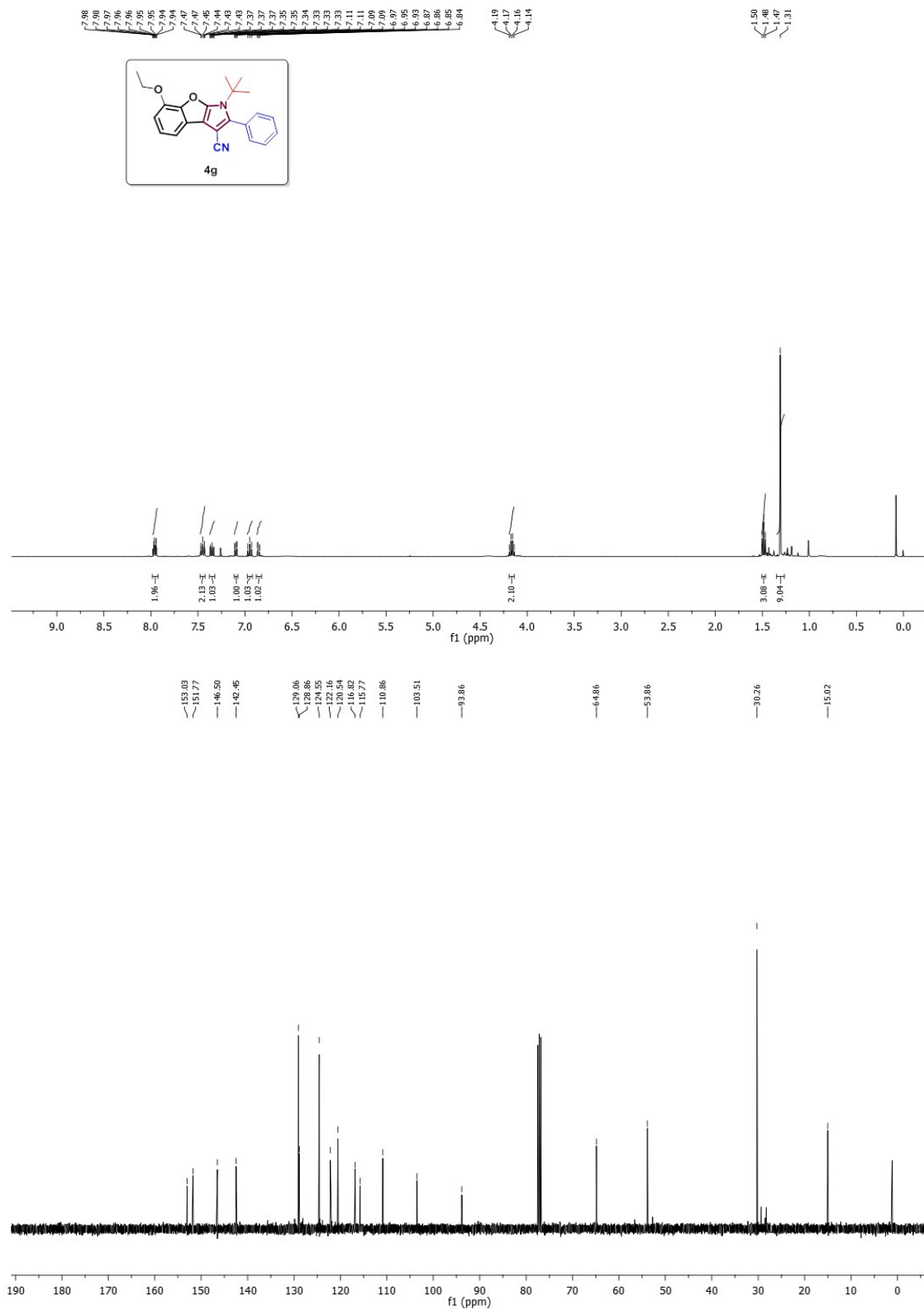
^1H NMR and ^{13}C NMR of compound (4e)



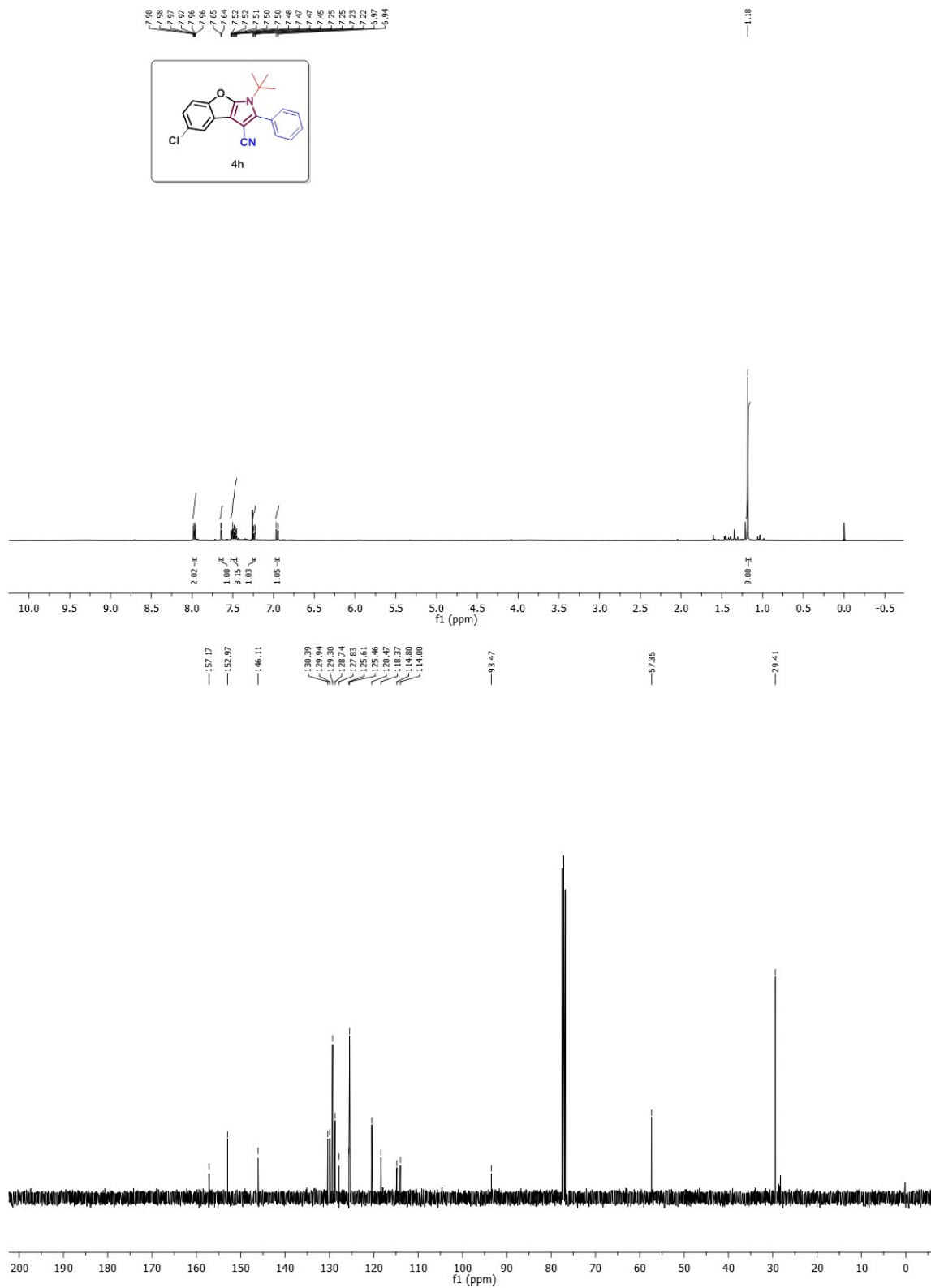
^1H NMR and ^{13}C NMR of compound (**4f**)



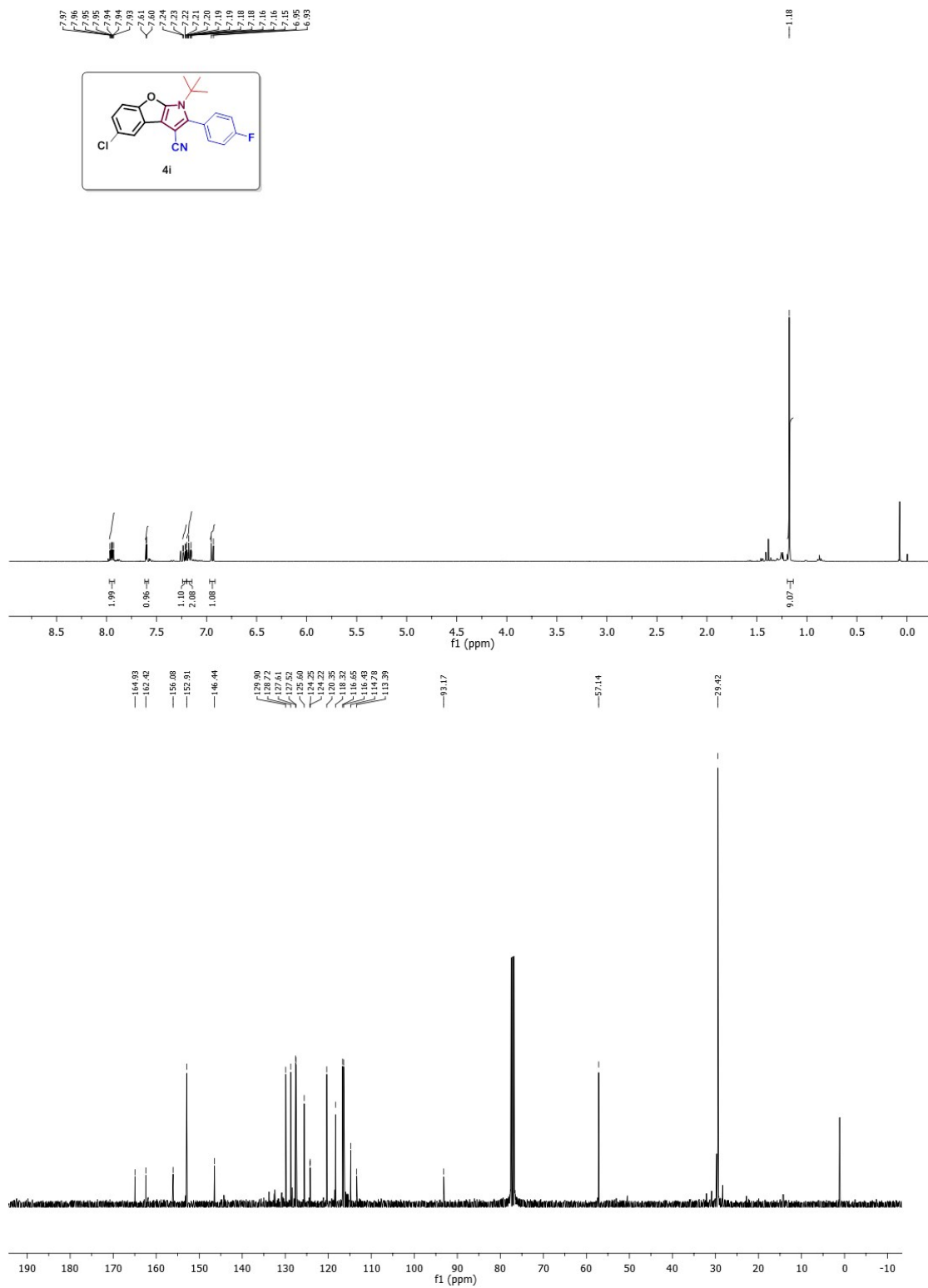
^1H NMR and ^{13}C NMR of compound (4g)



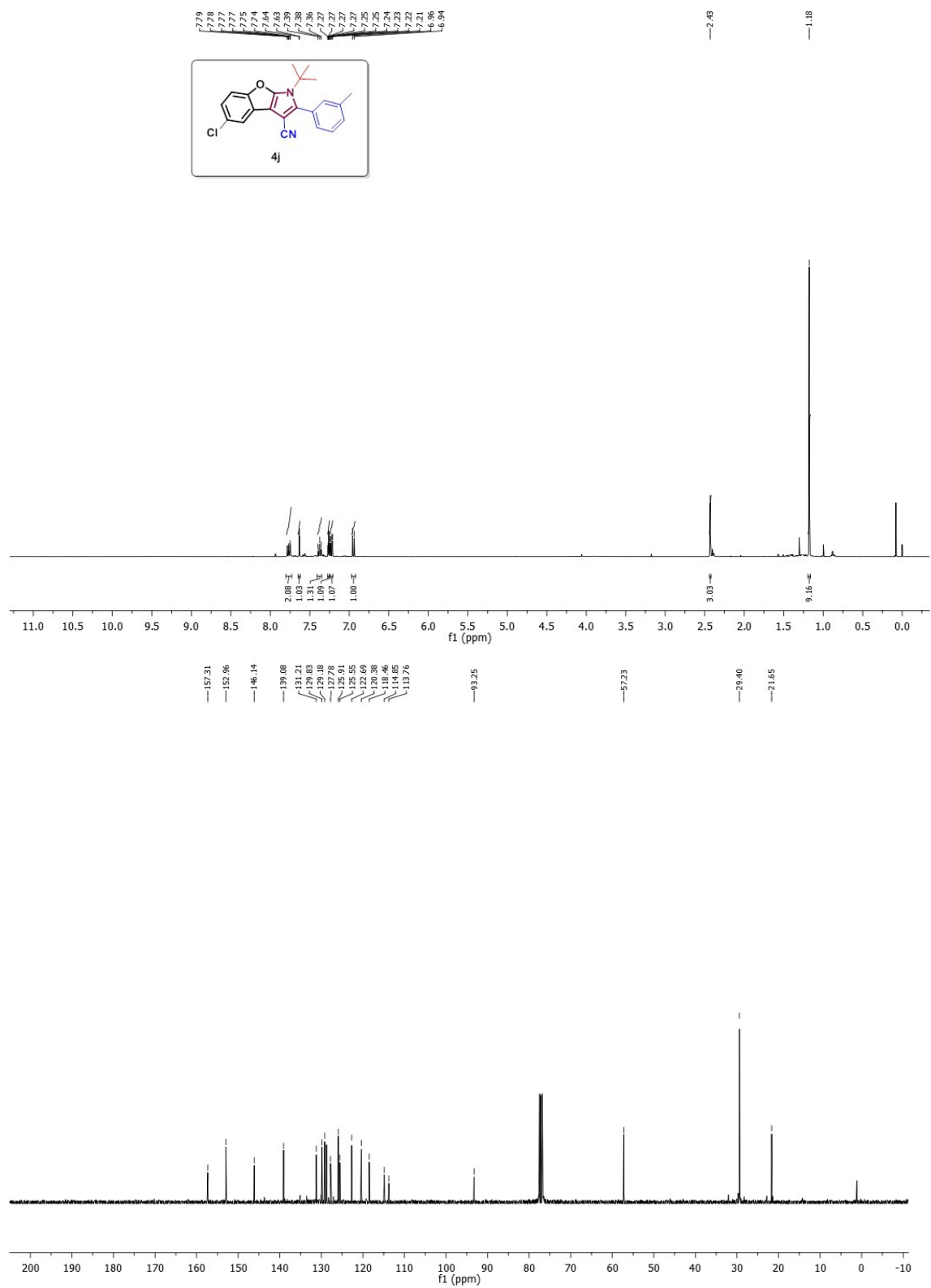
^1H NMR and ^{13}C NMR of compound (**4h**)



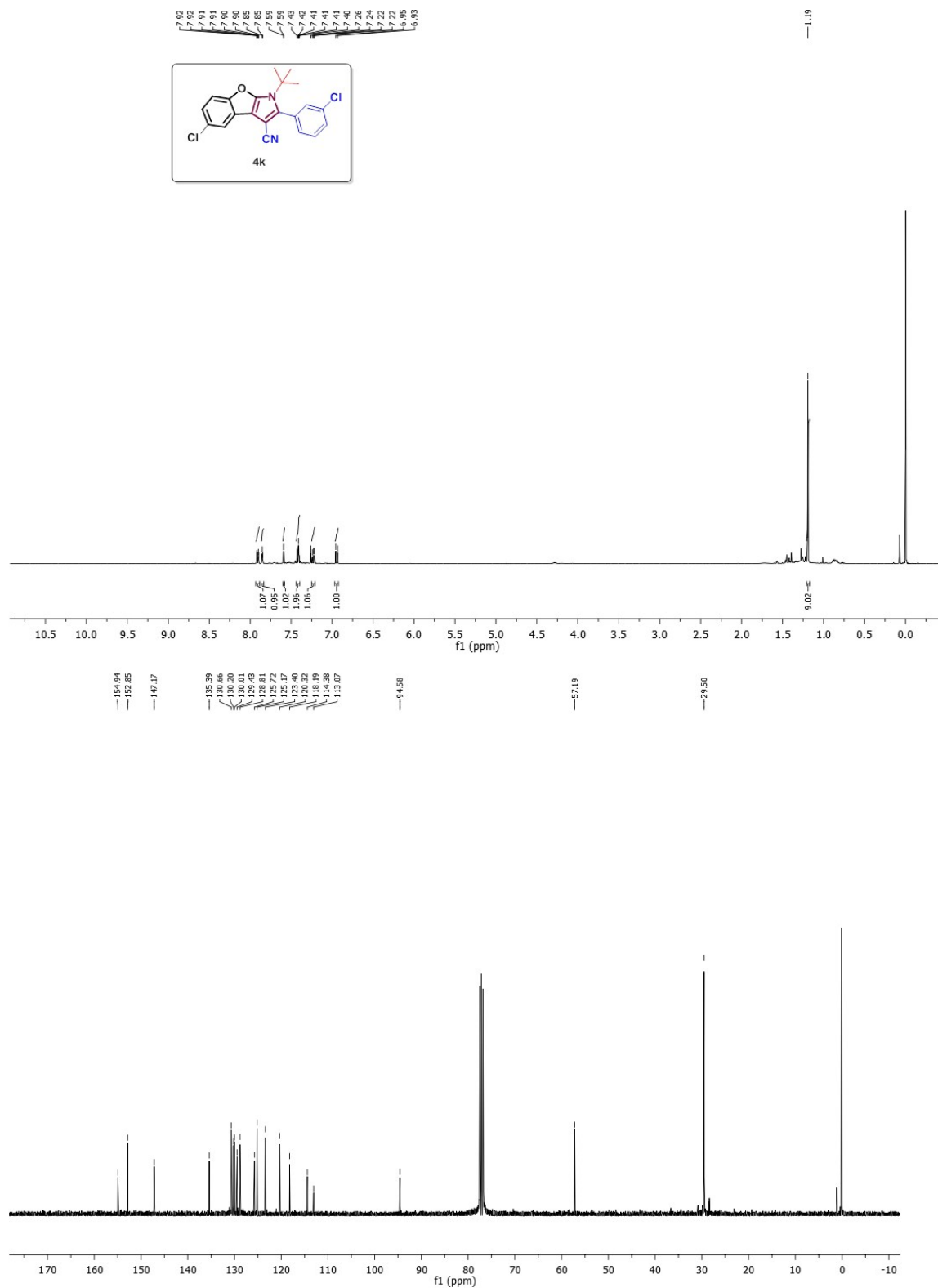
^1H NMR and ^{13}C NMR of compound (**4i**)



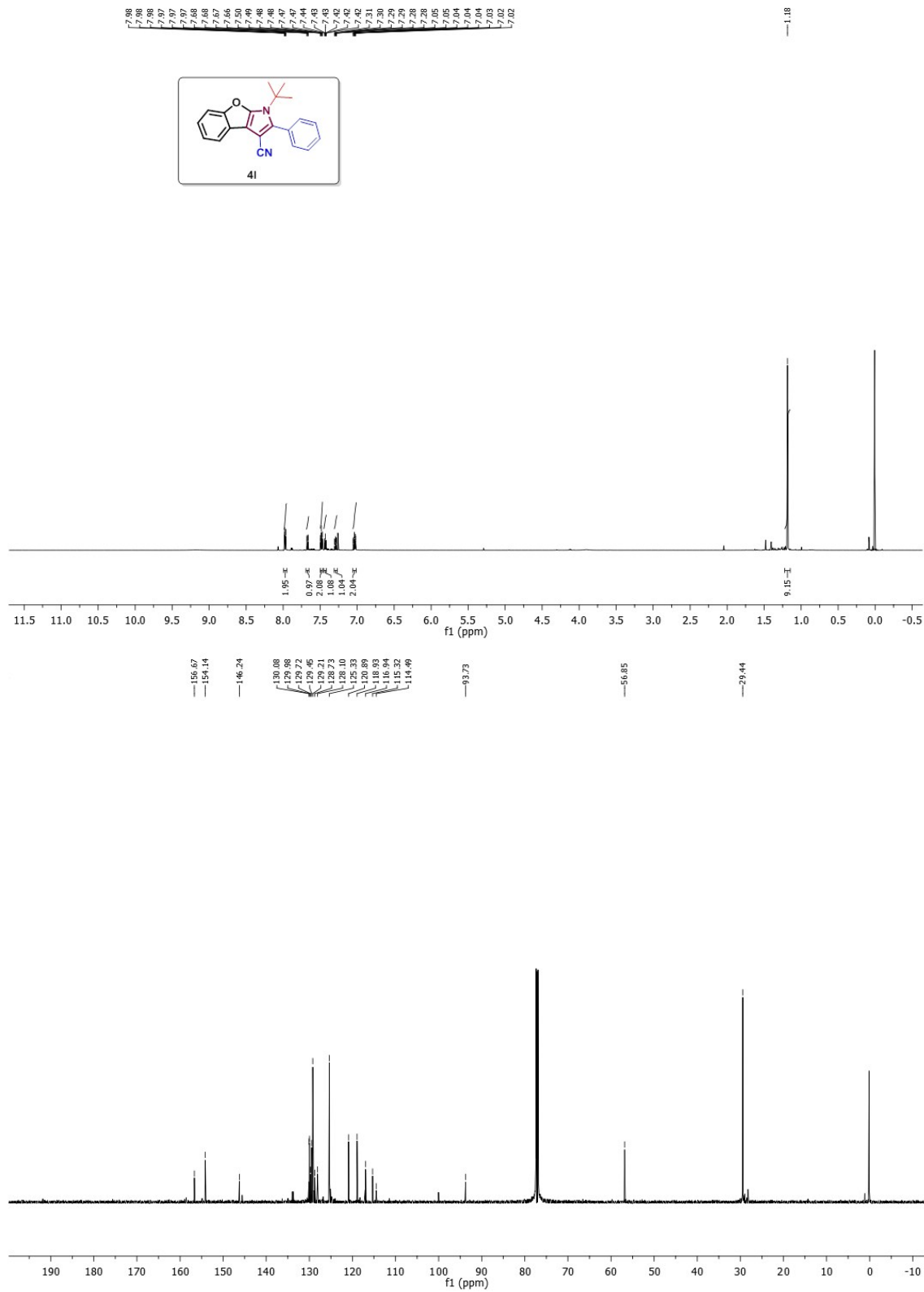
^1H NMR and ^{13}C NMR of compound (4j)



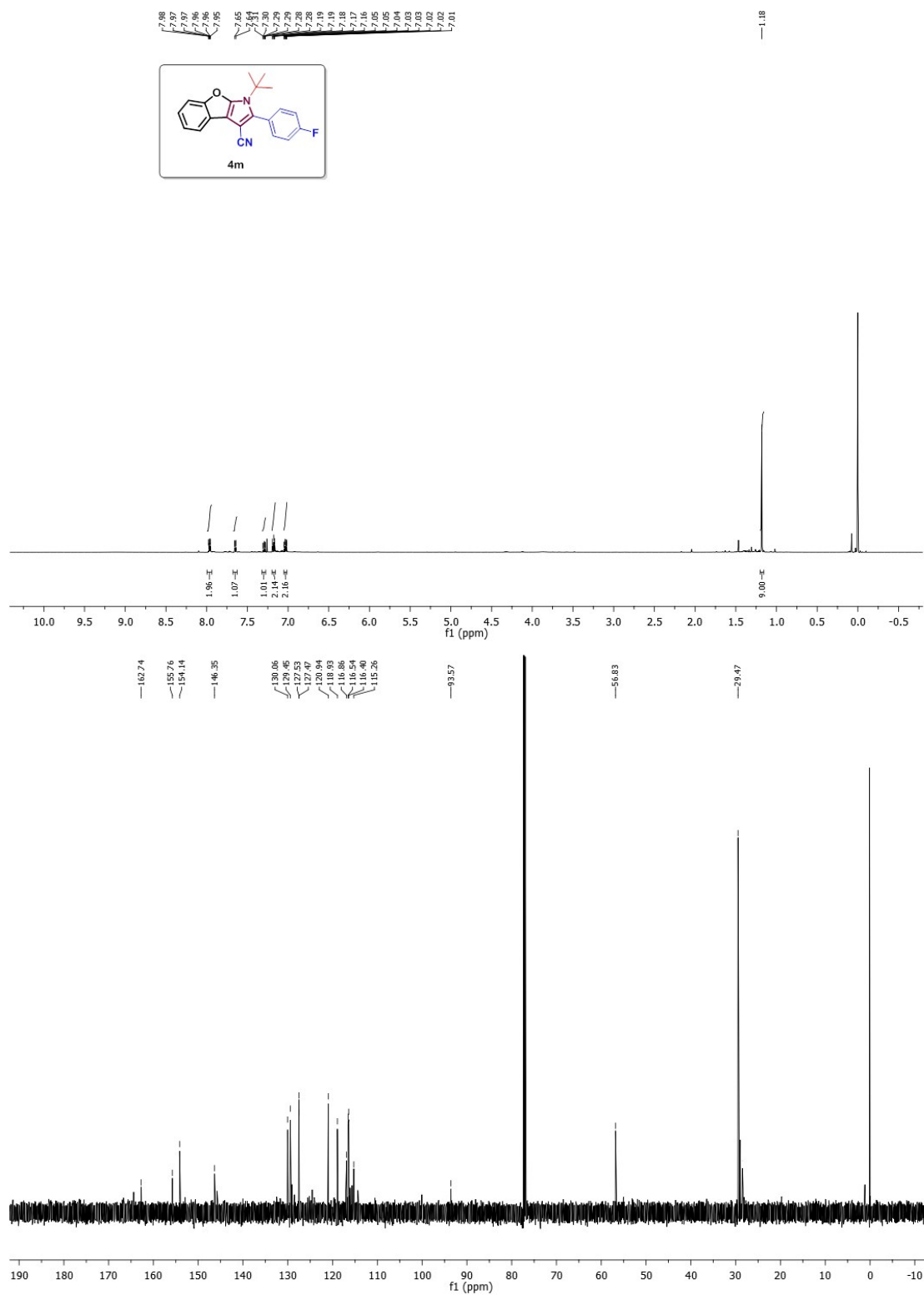
^1H NMR and ^{13}C NMR of compound (**4k**)



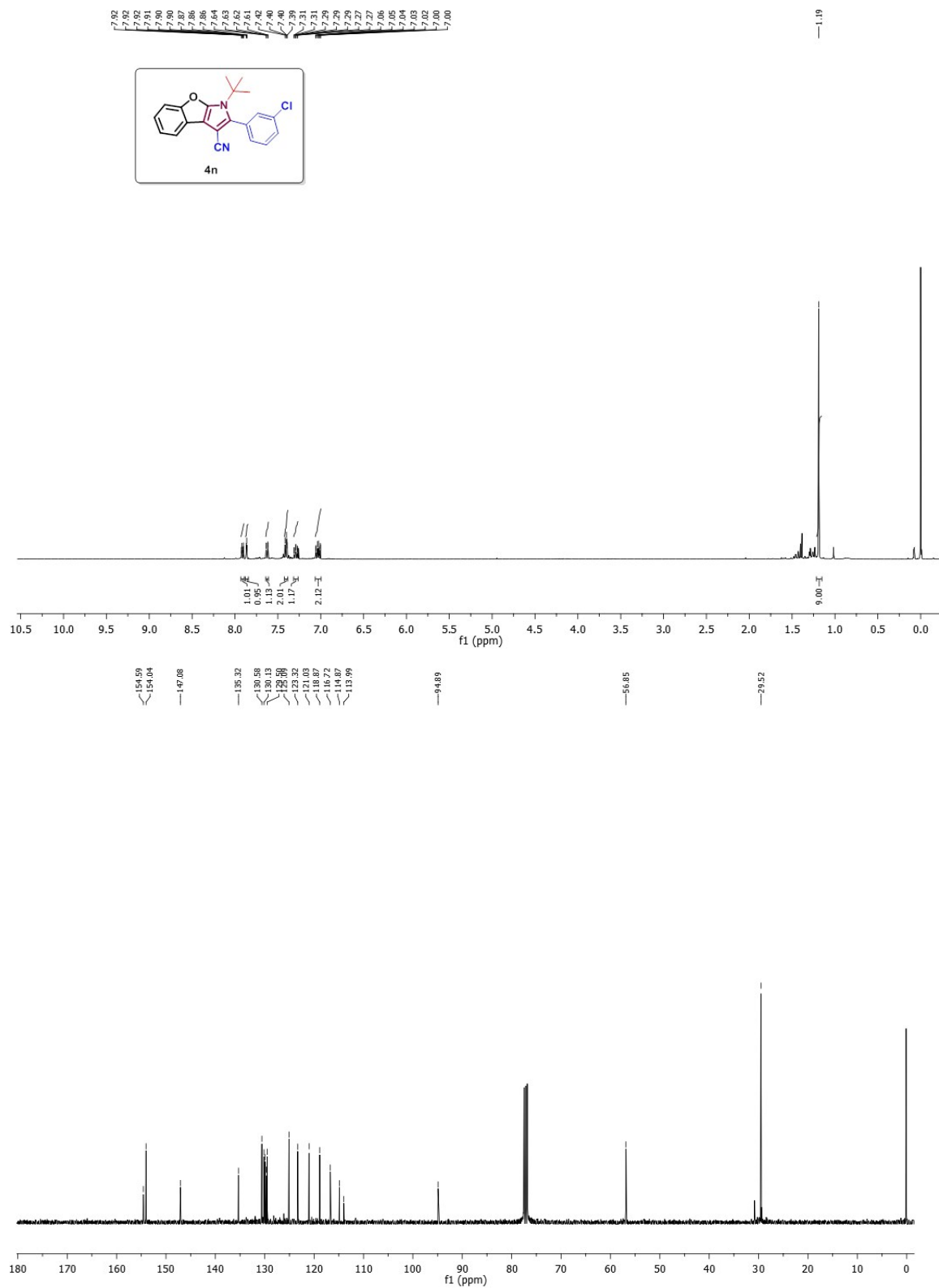
¹H NMR and ¹³C NMR of compound (4I)



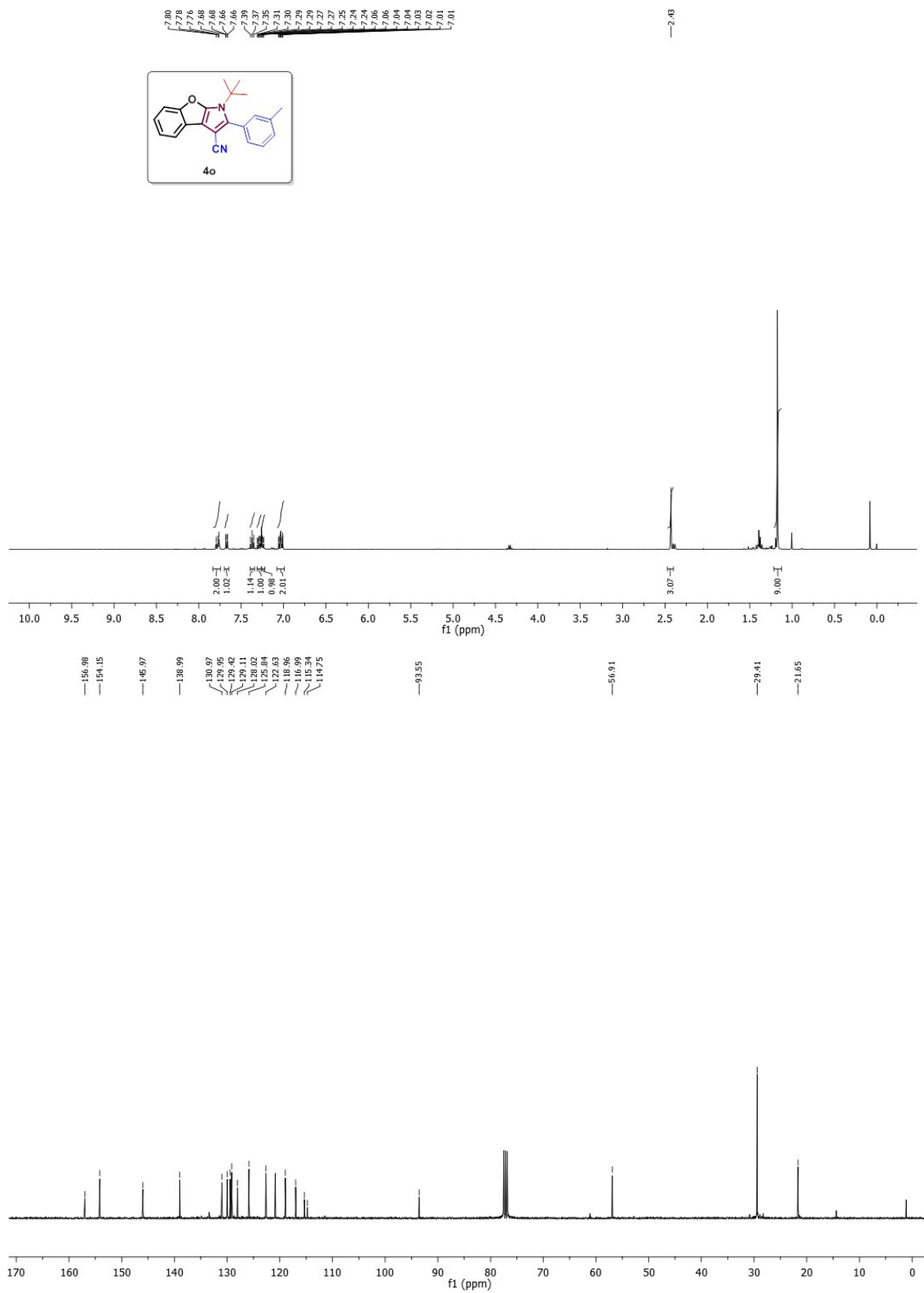
^1H NMR and ^{13}C NMR of compound (4m)



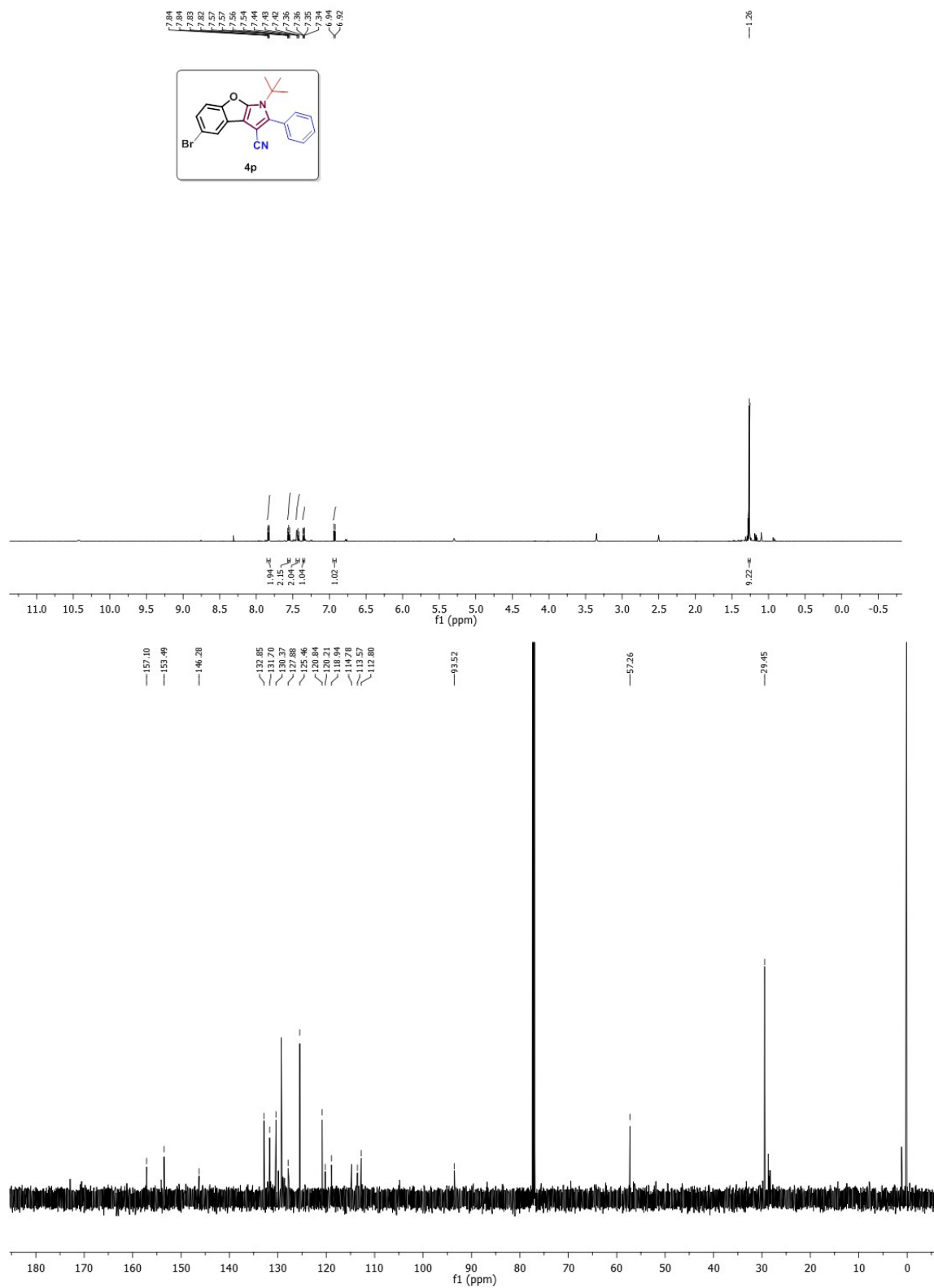
^1H NMR and ^{13}C NMR of compound (4n)



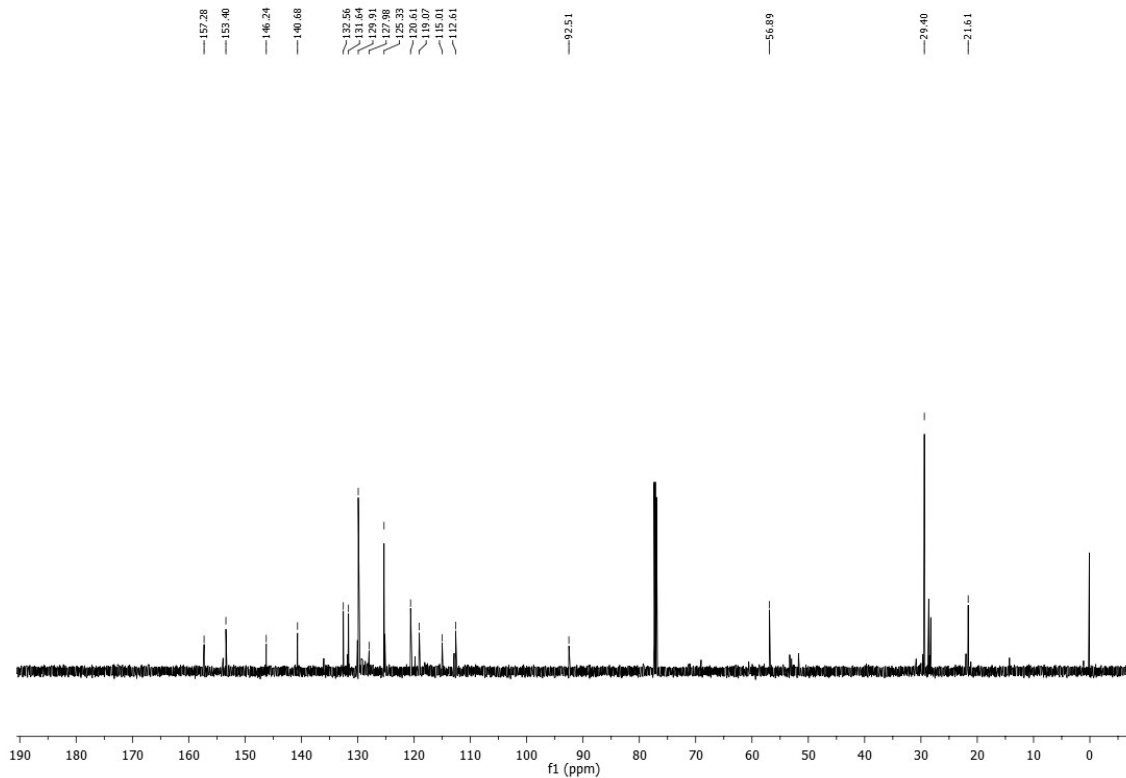
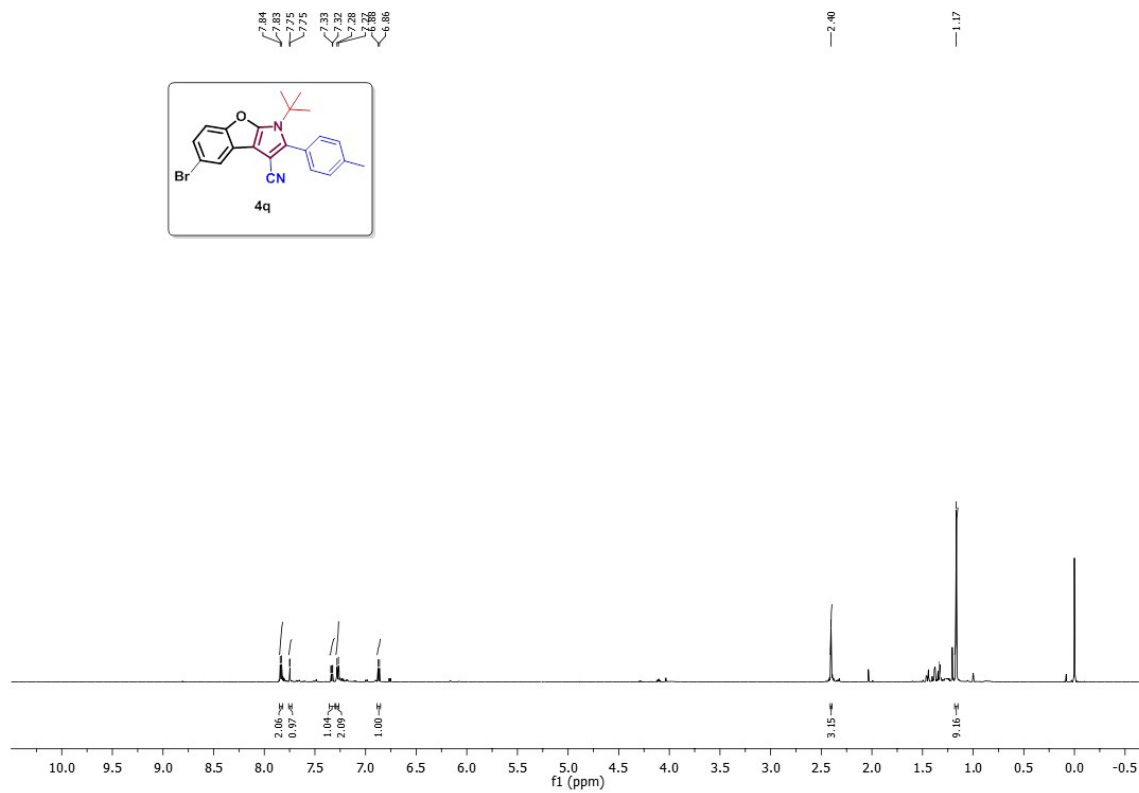
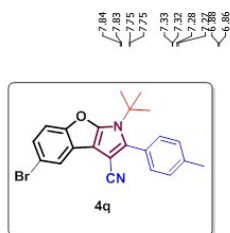
^1H NMR and ^{13}C NMR of compound (**4o**)



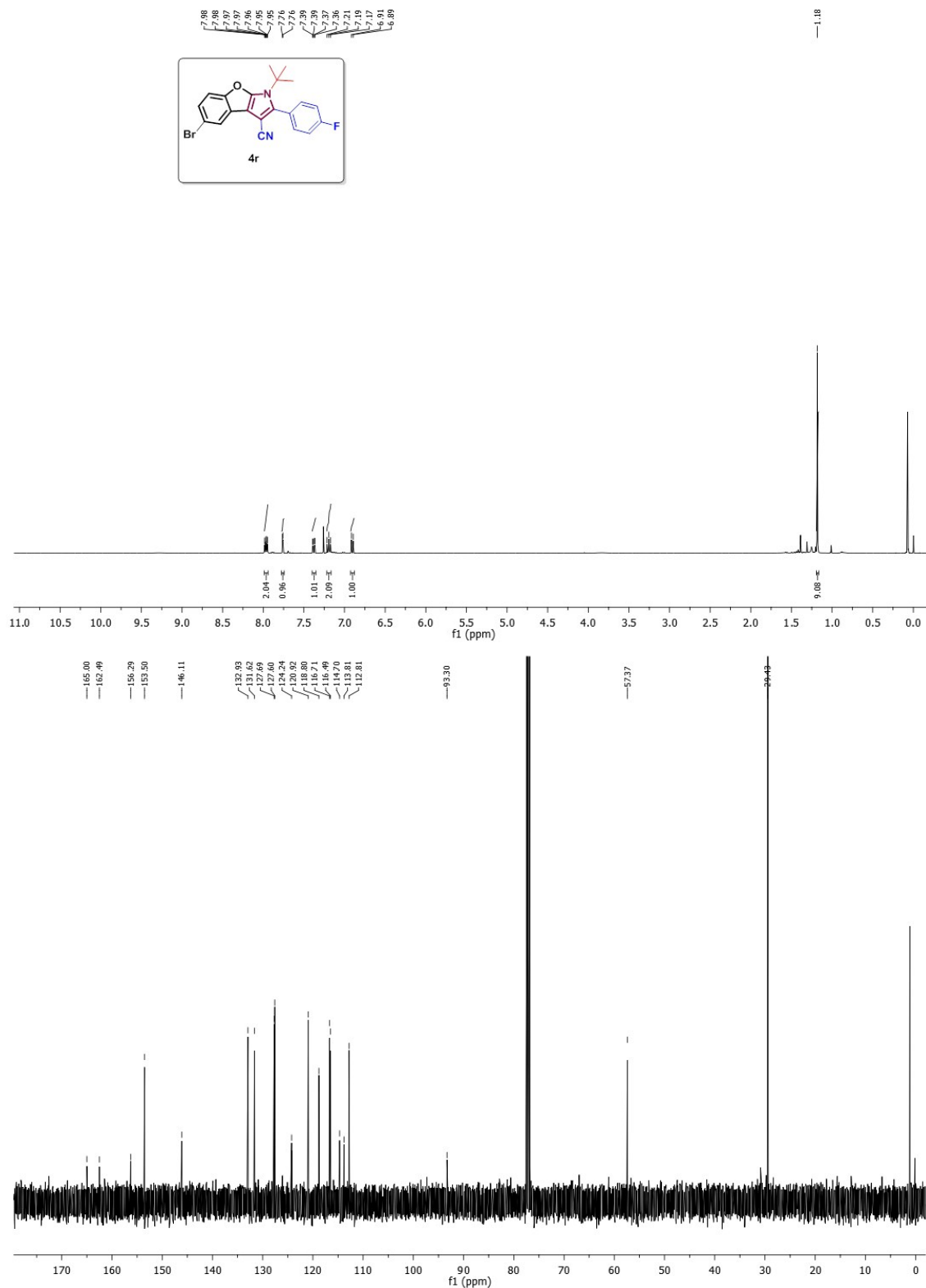
^1H NMR and ^{13}C NMR of compound (**4p**)



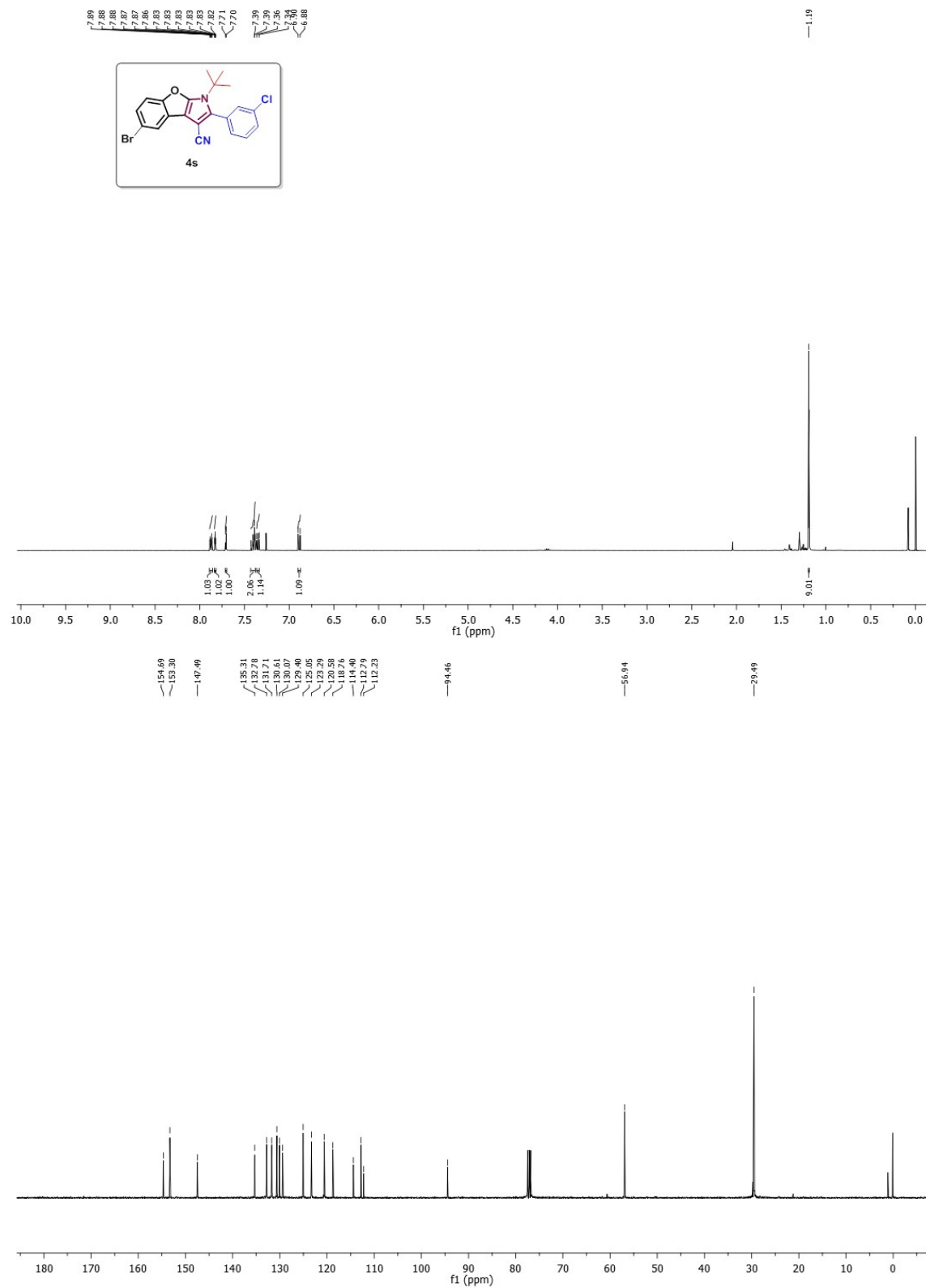
^1H NMR and ^{13}C NMR of compound (4q)



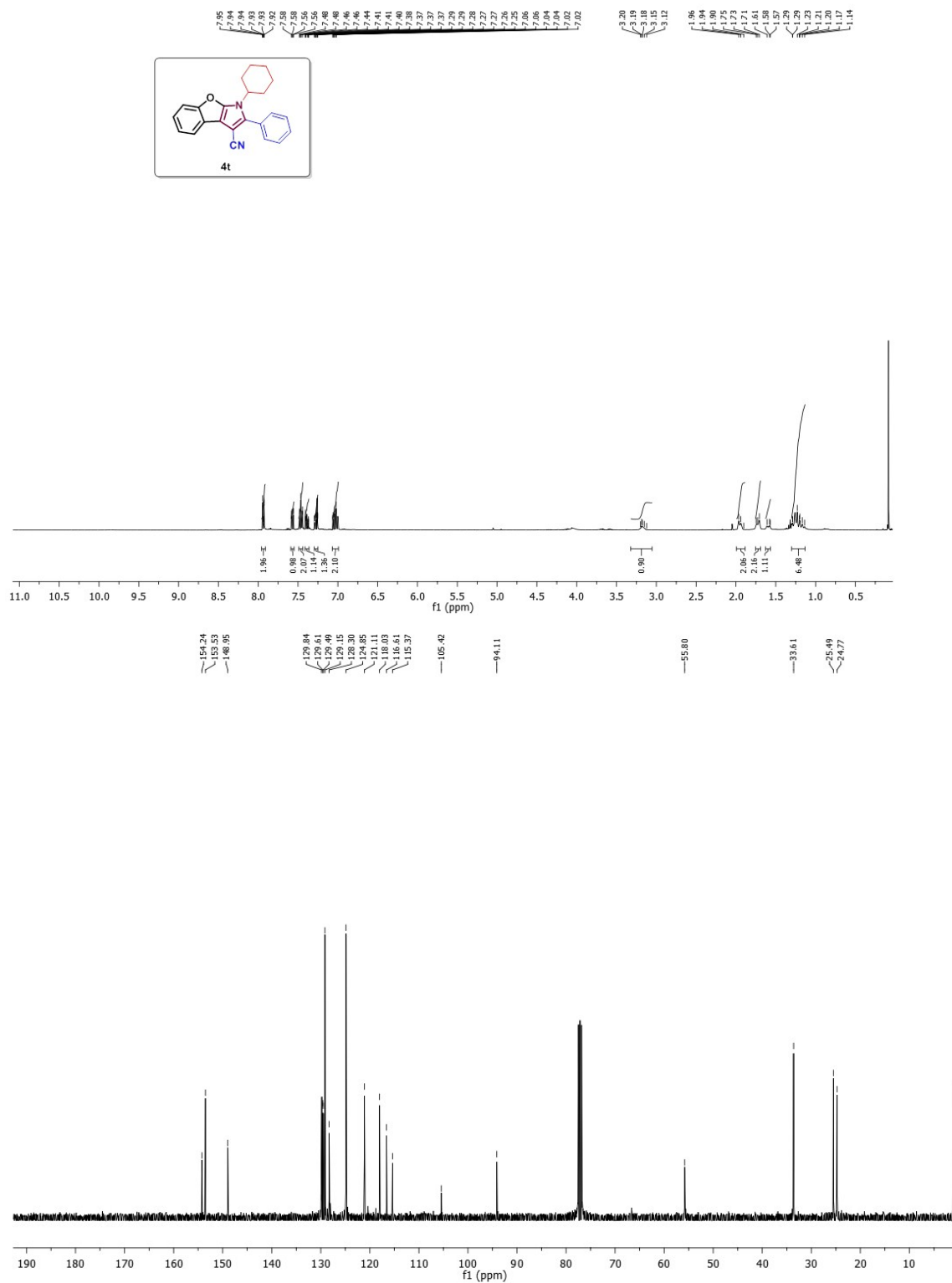
^1H NMR and ^{13}C NMR of compound (**4r**)



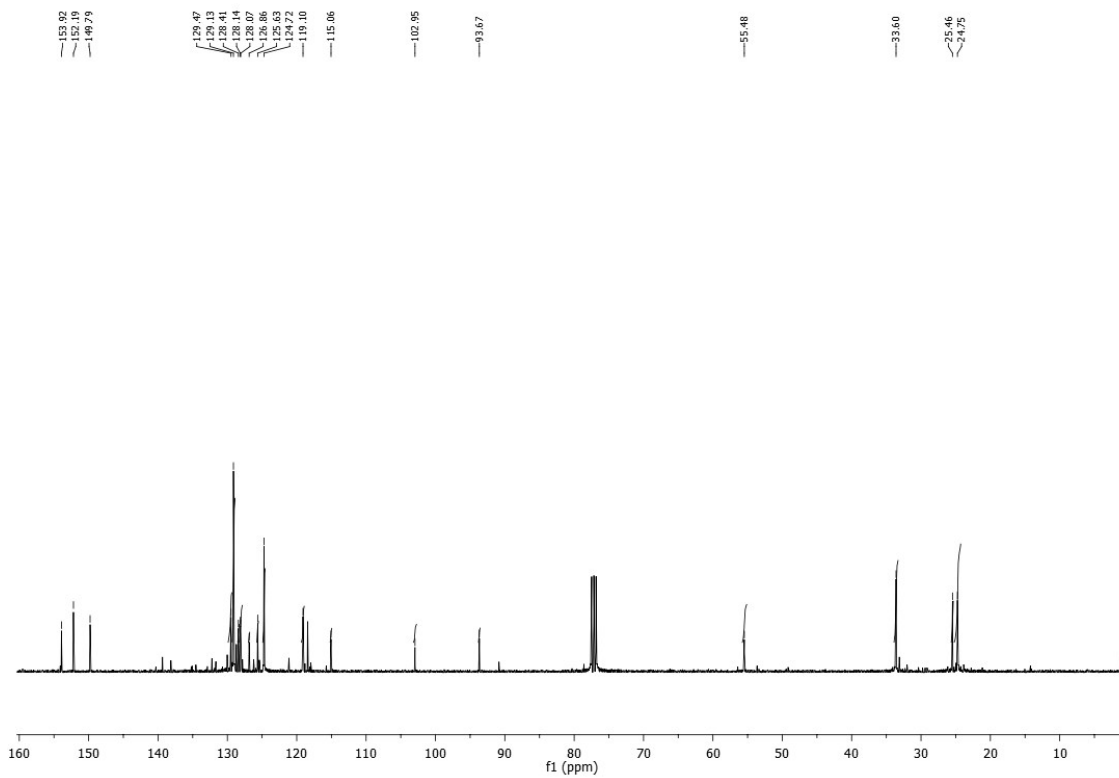
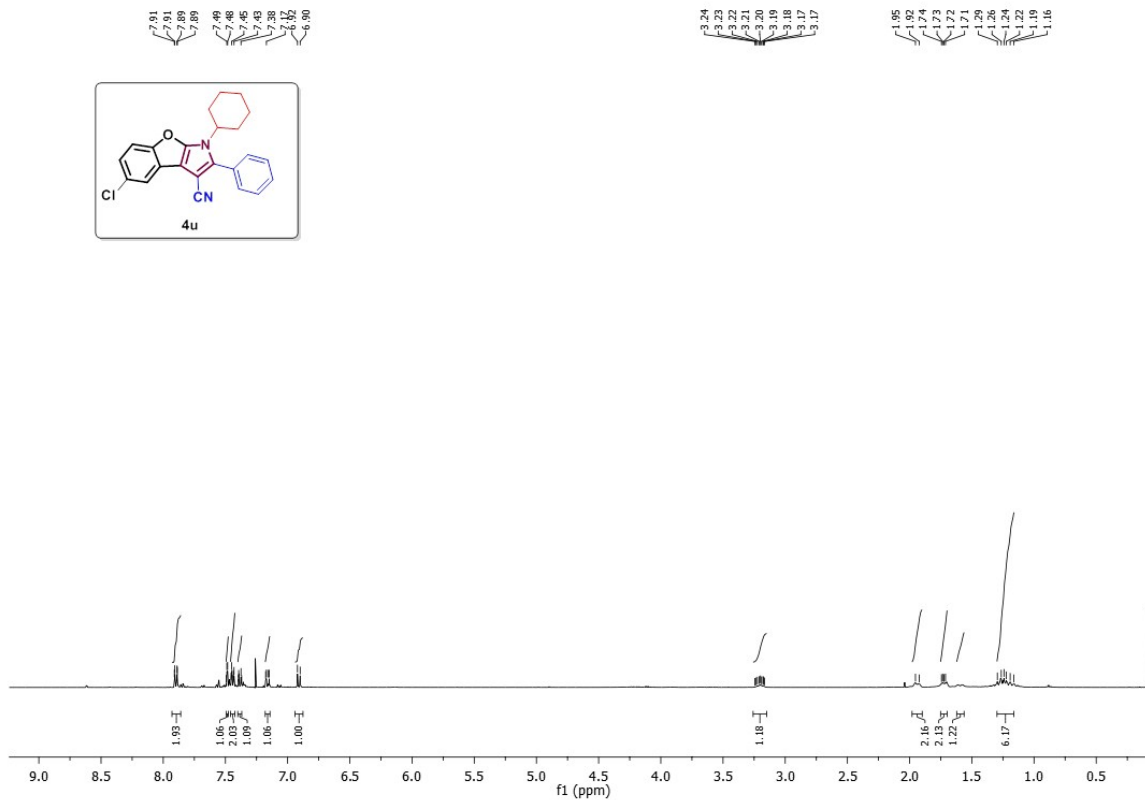
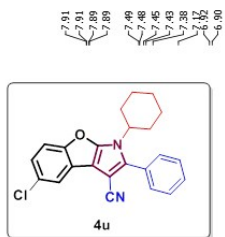
^1H NMR and ^{13}C NMR of compound (4s)



^1H NMR and ^{13}C NMR of compound (**4t**)



^1H NMR and ^{13}C NMR of compound (4u)



^1H NMR and ^{13}C NMR of compound (5)

