

Supporting Information

Synthesis of Novel Fluorescent Bicyclic amidines and Evaluation of their Photophysical Properties

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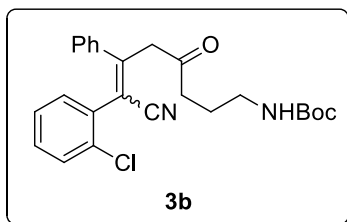
1. Experimental procedures

1.1 Preparation of Michael adducts

A solution of internal alkyne **1** (1.0 mmol) in DMF (1 mL) were added to a mixture of nitrile **2** (1.1 equiv) and KO^tBu (1.1 equiv) in DMF (1 mL) at room temperature. The reaction was stirred at room temperature for 2 h. Then, the mixture was cooled down under ice-bath and neutralized with 1 N HCl. The products were extracted with EtOAc. The combined organic layers were washed with water, successively, dried over Na₂SO₄, and the solvent was concentrate under reduced pressure. Crude products were purified by column chromatography on silica gel using hexanes and an increasing proportion of EtOAc as eluents to afford compound **3** or **4**. For the synthesis of nitro compounds, K₂CO₃ was used as base, instead of KO^tBu, and the reaction was stirred at room temperature for 4 h.

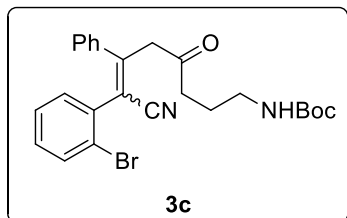
*** Unless otherwise noted, all known compounds **1**, **3** and **4** were prepared according to our previous literatures.^{1,2}

tert-Butyl (7-(2-chlorophenyl)-7-cyano-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3b)



85% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 46:54) 7.57–7.29 (m, 10H), 7.23–7.10 (m, 4H), 7.07–6.96 (m, 4H), 4.72 (br s, 1H), 4.56 (br s, 1H), 4.07 (s, 2H), 3.36 (br d, $J = 16.5$ Hz, 1H), 3.42 (br d, $J = 16.5$ Hz, 1H), 3.10 (br q, $J = 6.3$ Hz, 2H), 2.92 (br q, $J = 6.3$ Hz, 2H), 2.62 (t, $J = 7.1$ Hz, 2H), 2.20 (t, $J = 7.1$ Hz, 2H), 1.78 (quint, $J = 7.0$ Hz, 2H), 1.60–1.50 (m, 2H), 1.43 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 46:54) 204.61, 204.30, 155.98, 155.86, 154.85, 154.43, 138.05, 137.18, 133.90, 133.53, 132.39, 132.29, 132.08, 131.07, 130.77, 130.11, 130.07, 129.66, 129.63, 128.91, 128.68, 128.21, 127.84, 127.70, 127.42, 126.93, 117.03, 113.16, 112.18, 79.11, 51.14, 48.40, 40.08, 39.91, 39.52, 39.42, 28.29, 28.26, 23.82, 23.68; IR (UATR) ν_{max} 3378, 2977, 2212, 1702, 1609, 1513, 1473, 1444, 1392, 1366, 1268, 1250, 1166, 1062, 1035, 860, 759, 732, 699 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{25}\text{H}_{27}\text{Cl}_1\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 461.1602, found 461.1603.

tert-Butyl (7-(2-bromophenyl)-7-cyano-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3c)

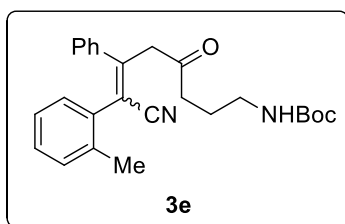


87% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 44:56) 7.69 (d, $J = 8.0$ Hz, 1H), 7.60–7.25 (m, 10H), 7.18–6.95 (m, 7H), 4.66 (br s, 1H), 4.50 (br s, 1H), 4.07 (s, 2H), 3.58 (d, $J = 16.8$ Hz, 1H), 3.40 (d, $J = 16.8$ Hz, 1H), 3.11 (br q, $J = 6.4$ Hz, 2H), 2.93 (br q, $J = 6.5$ Hz, 2H), 2.64 (t, $J = 7.1$ Hz, 2H), 2.30–2.10 (m, 2H), 1.79 (quint, $J = 7.0$ Hz, 2H), 1.60–1.50 (m, 2H), 1.43 (s, 9H), 1.41 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 44:56) 204.55, 204.30, 155.95, 155.83, 154.53, 154.04, 138.02, 137.06, 134.34, 134.23, 133.28, 132.81, 132.23, 131.13, 130.88, 130.15, 129.65, 128.89, 128.68, 128.20, 128.03, 127.82, 127.66, 127.55, 123.90, 123.41, 116.92, 116.87, 115.04, 113.97, 79.09, 51.11, 48.39, 40.10, 39.91, 39.52, 39.41, 28.29, 28.26, 23.81, 23.68; IR (UATR) ν_{max} 3379, 2977, 2212, 1705, 1608, 1510, 1444, 1392, 1366, 1268, 1250, 1166, 1027, 860, 758, 727, 699 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{25}\text{H}_{27}\text{Br}_1\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 505.1097, found 505.1090.

tert-Butyl (7-cyano-7-(2-iodophenyl)-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3d)

82% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 43:57) 7.95 (dd, $J = 8.0, 0.9$ Hz, 1H), 7.82 (dd, $J = 8.0, 1.0$ Hz, 1H), 7.59–7.31 (m, 8H), 7.18–6.88 (m, 8H), 4.72 (br s, 1H), 4.57 (br s, 1H), 4.06 (dd, $J = 3.0$ Hz, 2H), 3.54 (d, $J = 16.8$ Hz, 1H), 3.36 (d, $J = 16.8$ Hz, 1H), 3.10 (br q, $J = 6.3$ Hz, 2H), 2.92 (br q, $J = 6.4$ Hz, 2H), 2.64 (t, $J = 7.1$ Hz, 2H), 2.23 (dt, $J = 17.9, 7.2$ Hz, 1H), 2.15 (dt, $J = 17.9, 7.2$ Hz, 1H), 1.77 (quint, $J = 7.0$ Hz, 2H), 1.60–1.50 (m, 2H), 1.43 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 43:57) 204.44, 204.28, 155.89, 155.78, 154.16, 153.50, 139.59, 139.20, 138.06, 137.99, 137.96, 136.83, 131.71, 130.72, 130.39, 129.96, 129.61, 128.86, 128.82, 128.63, 128.33, 128.13, 127.80, 127.57, 118.19, 117.19, 116.81, 116.72, 99.22, 98.75, 79.01, 51.07, 48.36, 40.10, 39.95, 39.47, 39.35, 28.27, 28.23, 23.73, 23.62; IR (UATR) ν_{max} 3384, 2976, 2211, 1705, 1600, 1509, 1444, 1392, 1366, 1268, 1250, 1165, 1015, 860, 758, 724, 698 cm^{-1} ; HRMS (ESI^+) calcd for $\text{C}_{25}\text{H}_{27}\text{I}_1\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 553.0959, found 553.0963.

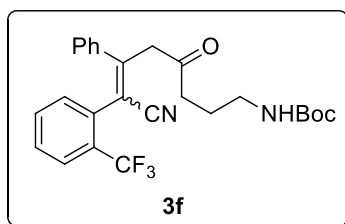
tert-Butyl (7-cyano-4-oxo-6-phenyl-7-(o-tolyl)hept-6-en-1-yl)carbamate (3e)



78% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 76:24) 7.56–6.91 (m, 18H), 4.80 (br s, 1H), 4.62 (br s, 1H), 4.05 (s, 2H), 3.59 (br d, $J = 14.6$ Hz, 1H), 3.39 (br d, $J = 14.6$ Hz, 1H), 3.08 (br q, $J = 6.3$ Hz, 2H), 2.88 (br q, $J = 6.3$ Hz, 2H), 2.59 (t, $J = 7.1$ Hz, 2H), 2.38 (s, 3H), 2.28 (s, 3H), 2.12 (t, $J = 7.1$ Hz, 2H), 1.76 (quint, $J = 7.0$ Hz, 2H), 1.58–1.45 (m, 2H), 1.42 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 76:24) 204.82, 204.51, 155.89, 155.75, 153.67, 152.34, 138.36, 137.42, 136.59, 136.49, 132.91, 132.56, 130.67, 130.25, 130.13, 129.25, 129.03, 128.57, 128.50, 128.46, 127.94, 127.84, 127.59, 126.30, 125.84, 117.88, 117.45, 114.59, 114.01, 78.83, 50.93, 47.91, 39.94, 39.86, 39.35, 39.24, 28.16, 28.13, 23.71, 23.50, 19.49, 19.17; IR (UATR) ν_{max} 3373, 2977, 2210, 1706, 1600, 1512, 1445, 1392, 1366, 1268, 1250, 1167, 1038, 860, 759, 729, 698 cm^{-1} ; HRMS (ESI^+) calcd for $\text{C}_{26}\text{H}_{30}\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 441.2149, found 441.2149.

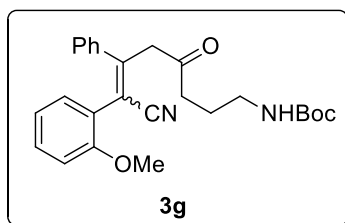
tert-Butyl (7-cyano-4-oxo-6-phenyl-7-(2-(trifluoromethyl)phenyl)hept-6-en-1-yl) carbamate

(3f)



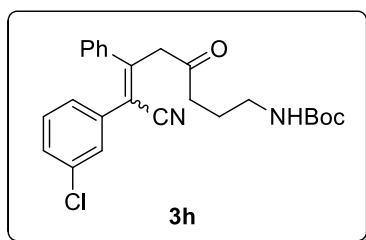
89% yield, yellow oil. ¹H NMR (300 MHz, CDCl₃) δ (isomeric ratio 31:69) 7.78 (d, J = 7.6 Hz, 1H), 7.68–7.34 (m, 14H), 7.19–7.10 (m, 2H), 7.14–6.95 (m, 1H), 4.68 (br s, 1H), 4.51 (br s), 3.6 (d, J = 17.0 Hz, 1H), 3.29 (d, J = 17.0 Hz, 3.09 (br q, J = 5.9 Hz, 2H), 2.90 (br q, J = 6.4 Hz, 2H), 2.60 (t, J = 6.7 Hz, 2H), 2.30–2.07 (m, 2H), 1.78 (quint, J = 7.0 Hz, 2H), 1.60–1.50 (m, 2H), 1.43 (s, 9H), 1.40 (s, 9H); ¹³C NMR (75 MHz, CDCl₃) δ (isomeric ratio 31:69) 204.50, 204.24, 155.99, 155.85, 155.18, 154.50, 138.02, 136.94, 133.10, 132.62, 131.94, 131.84, 131.81, 131.59, 129.68, 129.59, 129.05, 128.72, 128.67, 128.13, 127.90, 127.52, 126.82, 126.75, 126.68, 126.61, 125.42, 125.36, 121.79, 121.73, 117.24, 117.12, 112.83, 111.52, 79.06, 51.36, 48.60, 40.03, 39.95, 39.48, 39.33, 28.25, 28.21, 23.79, 23.70; IR (UATR) ν_{max} 3384, 2978, 2216, 1706, 1603, 1513, 1446, 1393, 1366, 1315, 1269, 1250, 1171, 1128, 1112, 1065, 1035, 860, 771, 698 cm⁻¹; HRMS (ESI⁺) calcd for C₂₆H₂₇F₃N₂Na₁O₃ (M+Na)⁺ 495.1866, found 495.1867.

tert-Butyl (7-cyano-7-(2-methoxyphenyl)-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3g)



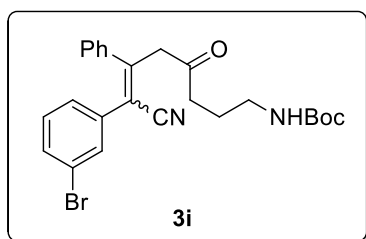
85% yield, yellow oil. ¹H NMR (300 MHz, CDCl₃) δ (isomeric ratio 42:58) 7.54 (dd, J = 8.0, 1.8 Hz, 2H), 7.548–7.34 (m, 4H), 7.28–7.18(m, 3H), 7.14 (dd, J = 5.2, 1.7 Hz, 2H), 7.04–6.93 (m, 4H), 6.90 (dd, J = 7.6, 1.7 Hz, 1H), 6.81 (d, J = 8.0 Hz, 1H), 6.72 (t, J = 7.5 Hz, 1H), 4.70 (br s, 1H), 4.55 (br s, 1H), 4.04 (s, 2H), 3.85 (s, 3H), 3.74 (s, 3H), 3.55 (s, 2H), 3.09 (br q, J = 6.4 Hz, 2H), 2.92 (br q, J = 6.4 Hz, 2H), 2.61 (t, J = 7.1 Hz, 2H), 2.21 (t, J = 7.1 Hz, 2H), 1.76 (quint, J = 7.0 Hz, 2H), 1.60–1.50 (m, 2H), 1.43 (s, 9H), 1.41 (s, 9H); ¹³C NMR (75 MHz, CDCl₃) δ (isomeric ratio 42:58) 205.25, 204.82, 156.94, 156.69, 155.93, 155.82, 153.34, 152.27, 138.60, 137.98, 131.36, 130.90, 130.43, 130.18, 129.27, 128.52, 128.47, 128.00, 127.88, 127.86, 122.47, 120.84, 120.47, 118.12, 118.05, 111.45, 110.98, 79.01, 55.61, 55.38, 51.28, 48.59, 39.85, 39.71, 39.54, 39.48, 28.25, 23.77, 23.63; IR (UATR) ν_{max} 3359, 2976, 2212, 1694, 1597, 1513, 1494, 1454, 1392, 1366, 1252, 1166, 1025, 859, 757, 698 cm⁻¹; HRMS (ESI⁺) calcd for C₂₆H₃₀N₂Na₁O₄ (M+Na)⁺ 457.2098, found 457.2101.

tert-Butyl (7-(3-chlorophenyl)-7-cyano-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3h)



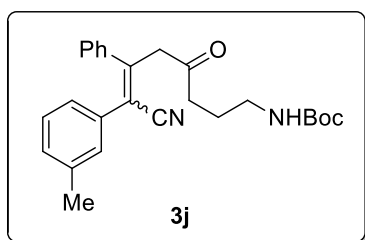
89% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 52:48) 7.51–7.28 (m, 8H), 7.28–7.13 (m, 6H), 7.10 (d, $J = 7.8$ Hz, 1H), 7.08–7.01 (m, 2H), 6.98 (dt, $J = 7.8, 1.3$ Hz, 1H), 4.77 (br s, 1H), 4.66 (br s, 1H), 4.04 (s, 2H), 3.68 (s, 2H), 3.08 (br q, $J = 6.4$ Hz, 2H), 2.96 (br q, $J = 6.4$ Hz, 2H), 2.57 (t, $J = 7.2$ Hz, 2H), 2.30 (t, $J = 7.1$ Hz, 2H), 1.75 (quint, $J = 7.0$ Hz, 2H), 1.61 (quint, $J = 7.0$ Hz, 2H), 1.43 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 52:48) 205.24, 204.15, 155.97, 155.89, 153.70, 152.72, 138.51, 137.32, 135.48, 134.72, 134.09, 130.26, 129.55, 129.46, 129.27, 129.19, 128.99, 128.64, 128.54, 128.51, 128.46, 128.13, 127.56, 127.50, 126.70, 118.02, 117.96, 114.04, 113.84, 78.97, 52.01, 48.47, 40.25, 40.04, 39.40, 39.31, 28.20, 28.18, 23.77, 23.73; IR (UATR) ν_{max} 3367, 2977, 2214, 1706, 1595, 1513, 1445, 1392, 1366, 1250, 1167, 882, 787, 698 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{25}\text{H}_{27}\text{Cl}_1\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 461.1602, found 461.1606.

tert-Butyl (7-(3-bromophenyl)-7-cyano-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3i)



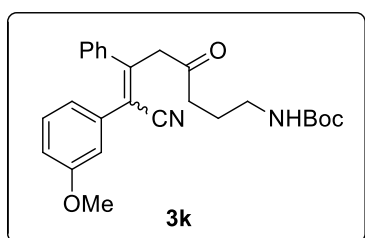
84% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 52:48) 7.57–7.19 (m, 14H), 7.08–6.95 (m, 4H), 4.79 (br s, 1H), 4.69 (br s, 1H), 4.03 (s, 2H), 3.67 (s, 2H), 3.08 (br q, $J = 6.4$ Hz, 2H), 2.96 (br q, $J = 6.4$ Hz, 2H), 2.57 (t, $J = 7.2$ Hz, 2H), 2.30 (t, $J = 7.2$ Hz, 2H), 1.75 (quint, $J = 7.0$ Hz, 2H), 1.61 (quint, $J = 7.0$ Hz, 2H), 1.42 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 52:48) 205.22, 204.12, 155.92, 155.85, 153.74, 152.75, 138.47, 137.25, 135.70, 134.94, 132.15, 132.01, 131.33, 131.31, 130.47, 129.66, 129.52, 128.97, 128.60, 128.51, 128.10, 127.92, 127.52, 127.12, 122.72, 122.08, 117.98, 117.93, 113.88, 113.67, 78.93, 51.97, 48.46, 40.21, 40.01, 39.36, 39.28, 28.18, 28.16, 23.74, 23.71; IR (UATR) ν_{max} 3381, 2977, 2213, 1706, 1513, 1444, 1366, 1250, 1167, 1075, 997, 882, 785, 697 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{25}\text{H}_{27}\text{Br}_1\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 505.1097, found 505.1090.

tert-Butyl (7-cyano-4-oxo-6-phenyl-7-(*m*-tolyl)hept-6-en-1-yl)carbamate (3j)



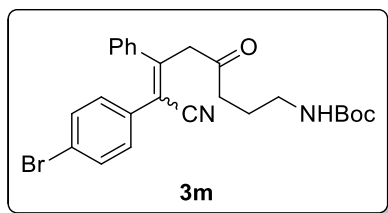
79% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 45:55) 7.53–7.39 (m, 5H), 7.35–7.15 (m, 8H), 7.09–7.03 (m, 2H), 7.02 (s, 2H), 6.86 (dt, $J = 6.9, 2.0$ Hz, 1H), 4.57 (br s, 1H), 4.45 (br s, 1H), 4.04 (s, 2H), 3.68 (s, 2H), 3.10 (br q, $J = 6.6$ Hz, 2H), 2.97 (br q, $J = 6.4$ Hz, 2H), 2.58 (t, $J = 7.1$ Hz, 2H), 2.38 (s, 3H), 2.29 (t, $J = 7.2$ Hz, 2H), 2.21 (s, 3H), 1.75 (quint, $J = 7.0$ Hz, 2H), 1.61 (quint, $J = 7.0$ Hz, 2H), 1.43 (s, 9H), 1.41 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 45:55) 205.47, 204.50, 155.93, 155.84, 152.38, 150.94, 138.94, 138.77, 137.99, 137.94, 133.86, 132.88, 129.86, 129.32, 129.10, 129.06, 128.80, 128.62, 128.38, 128.31, 128.04, 127.69, 126.44, 125.48, 118.66, 118.53, 115.60, 115.36, 79.03, 52.11, 48.54, 40.20, 39.98, 39.46, 28.26, 28.24, 23.82, 23.77, 21.21, 21.06; IR (UATR) ν_{max} 3372, 2977, 2212, 1705, 1605, 1509, 1445, 1392, 1366, 1269, 1250, 1166, 1042, 1000, 859, 784, 765, 700 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{26}\text{H}_{30}\text{N}_2\text{Na}_1\text{O}_3$ (M+Na) $^+$ 441.2149, found 441.2149.

tert-Butyl (7-cyano-7-(3-methoxyphenyl)-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3k)



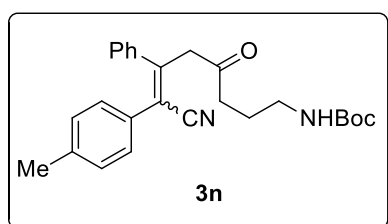
89% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 50:50) 7.52–7.38 (m, 5H), 7.33 (dd, $J = 9.0, 7.6$ Hz, 1H), 7.26–7.20 (m, 3H), 7.13–7.05 (m, 3H), 7.00–6.90 (m, 3H), 6.80–6.71 (m, 2H), 6.62 (dd, $J = 2.2, 1.9$ Hz, 1H), 4.68 (br s, 1H), 4.58 (br s, 1H), 4.04 (s, 2H), 3.81 (s, 3H), 3.69 (s, 2H), 3.55 (s, 3H), 3.08 (br q, $J = 6.4$ Hz, 2H), 2.96 (br q, $J = 6.5$ Hz, 2H), 2.57 (t, $J = 7.1$ Hz, 2H), 2.29 (t, $J = 7.1$ Hz, 2H), 1.76 (quint, $J = 7.0$ Hz, 2H), 1.60 (quint, $J = 7.0$ Hz, 2H), 1.43 (s, 9H), 1.41 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 50:50) 205.54, 204.49, 159.81, 159.16, 155.97, 155.89, 152.73, 151.37, 138.85, 138.02, 135.14, 134.13, 130.06, 129.44, 129.32, 128.74, 128.68, 128.53, 128.25, 127.71, 121.77, 120.71, 118.49, 118.40, 114.96, 114.89, 114.21, 113.88, 79.11, 55.27, 54.95, 52.16, 48.63, 40.25, 40.05, 39.52, 39.44, 28.28, 28.63, 23.85, 23.72; IR (UATR) ν_{max} 3385, 2976, 2212, 1708, 1599, 1580, 1513, 1489, 1445, 1392, 1366, 1287, 1252, 1167, 1041, 995, 857, 782, 699 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{26}\text{H}_{30}\text{N}_2\text{Na}_1\text{O}_4$ (M+Na) $^+$ 457.2098, found 457.2103

tert-Butyl (7-(4-bromophenyl)-7-cyano-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3m)



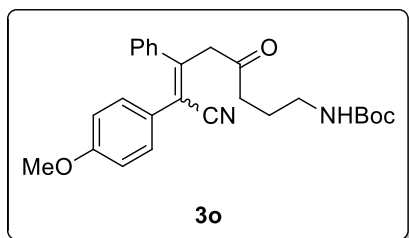
91% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 54:46) 7.56 (d, $J=8.4$ Hz, 2H), 7.50–7.39 (m, 5H), 7.34–7.21 (m, 7H), 7.08–7.02 (m, 2H), 7.00 (d, $J=8.6$ Hz, 2H), 4.68 (br s, 1H), 4.56 (br s, 1H), 4.03 (s, 2H), 3.67 (s, 2H), 3.08 (br q, $J=6.4$ Hz, 2H), 2.97 (br q, $J=6.4$ Hz, 2H), 2.57 (t, $J=7.1$ Hz, 2H), 2.31 (t, $J=7.1$ Hz, 2H), 1.76 (quint, $J=7.0$ Hz, 2H), 1.60 (quint, $J=7.0$ Hz, 2H), 1.43 (s, 9H), 1.41 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 54:46) 205.27, 204.23, 155.96, 155.91, 153.16, 152.05, 138.64, 137.56, 132.79, 132.19, 132.01, 131.51, 130.88, 130.20, 129.58, 128.97, 128.72, 128.67, 128.21, 127.62, 123.52, 122.65, 118.14, 118.08, 114.43, 114.35, 79.10, 52.16, 48.50, 40.37, 40.11, 39.49, 39.36, 28.28, 28.26, 23.86, 23.78; IR (UATR) ν_{max} 3372, 2976, 2213, 1698, 1587, 1511, 1487, 1444, 1393, 1366, 1268, 1250, 1166, 1073, 1011, 828, 765, 699 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{25}\text{H}_{27}\text{Br}_1\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 505.1097, found 505.1098.

tert-Butyl (7-cyano-4-oxo-6-phenyl-7-(p-tolyl)hept-6-en-1-yl)carbamate (3n)



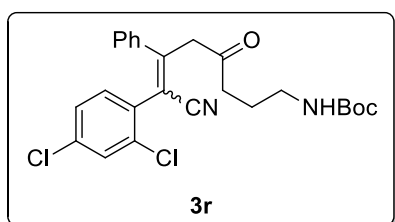
81% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 45:55) 7.48 (dd, $J=8.0, 1.9$ Hz, 2H), 7.46–7.37 (m, 4H), 7.28 (d, $J=8.2$ Hz, 2H), 7.25–7.18 (m, 5H), 7.08–7.03 (m, 1H), 7.02 (d, $J=8.4$ Hz, 2H), 6.96 (d, $J=8.4$ Hz, 2H), 4.72 (br s, 1H), 4.60 (br s, 1H), 4.02 (s, 2H), 3.68 (s, 2H), 3.07 (br q, $J=6.4$ Hz, 2H), 2.95 (br q, $J=6.4$ Hz, 2H), 2.56 (t, $J=7.1$ Hz, 2H), 2.37 (s, 3H), 2.28 (t, $J=7.1$ Hz, 2H), 2.24 (s, 3H), 1.74 (quint, $J=7.0$ Hz, 2H), 1.59 (quint, $J=7.0$ Hz, 2H), 1.42 (s, 9H), 1.41 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 45:55) 205.52, 204.54, 155.87, 155.81, 152.08, 150.35, 139.09, 138.93, 138.29, 137.94, 130.96, 130.00, 129.53, 129.21, 129.07, 128.88, 128.53, 128.39, 128.26, 128.25, 127.63, 118.64, 118.55, 115.18, 78.91, 52.07, 48.45, 40.12, 39.91, 39.42, 39.36, 28.19, 28.17, 23.73, 23.63, 21.07, 20.97; IR (UATR) ν_{max} 3376, 2977, 2212, 1706, 1607, 1510, 1444, 1392, 1366, 1268, 1250, 1166, 1042, 858, 820, 765, 735, 699 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{26}\text{H}_{30}\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 441.2149, found 441.2150.

tert-Butyl (7-cyano-7-(4-methoxyphenyl)-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3o)



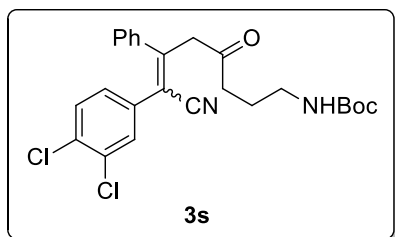
85% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 60:40) 7.50–7.38 (m, 7H), 7.33 (d, $J = 8.8$ Hz, 2H), 7.26–7.20 (m, 2H), 7.11–7.03 (m, 1H), 7.06 (d, $J = 8.8$ Hz, 2H), 6.94 (d, $J = 8.8$ Hz, 2H), 6.70 (d, $J = 8.8$ Hz, 2H), 4.63 (br s, 1H), 4.52 (br s, 1H), 4.01 (s, 2H), 3.83 (s, 3H), 3.74 (s, 3H), 3.70 (s, 2H), 3.08 (br q, $J = 6.4$ Hz, 2H), 2.97 (br q, $J = 6.4$ Hz, 2H), 2.57 (t, $J = 7.1$ Hz, 2H), 2.30 (t, $J = 7.1$ Hz, 2H), 1.75 (quint, $J = 7.0$ Hz, 2H), 1.61 (quint, $J = 7.0$ Hz, 2H), 1.43 (s, 9H), 1.41 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 60:40) 205.65, 204.67, 160.04, 159.36, 155.91, 155.85, 151.65, 149.48, 139.02, 138.06, 130.59, 129.81, 129.23, 128.58, 128.53, 128.48, 128.28, 127.68, 126.10, 125.20, 118.72, 118.66, 114.99, 114.26, 113.63, 78.99, 55.20, 55.04, 52.09, 48.52, 40.26, 39.93, 39.42, 28.23, 28.21, 23.78, 23.70; IR (UATR) ν_{max} 3387, 2976, 2213, 1710, 1607, 1511, 1444, 1366, 1290, 1252, 1176, 1031, 836, 767, 700 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{26}\text{H}_{30}\text{N}_2\text{Na}_1\text{O}_4$ ($\text{M}+\text{Na}$) $^+$ 457.2098, found 457.2096.

tert-Butyl (7-cyano-7-(2,4-dichlorophenyl)-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3r)



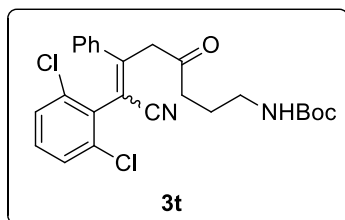
92% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 51:49) 7.55–7.49 (m, 3H), 7.47–7.41 (m, 3H), 7.38 (d, $J = 2.0$ Hz, 1H), 7.35–7.32 (m, 2H), 7.22–7.15 (m, 3H), 7.03 (dd, $J = 8.3, 2.0$ Hz, 1H), 7.01–6.96 (m, 1H), 6.98 (dd, $J = 7.0, 1.6$ Hz, 1H), 6.92 (d, $J = 8.3$ Hz, 1H), 4.72 (br s, 1H), 4.57 (br s, 1H), 4.06 (s, 2H), 3.63 (br d, $J = 16.2$ Hz, 1H), 3.40 (br d, $J = 16.2$ Hz, 1H), 3.10 (br q, $J = 6.3$ Hz, 2H), 2.94 (br q, $J = 6.4$ Hz, 2H), 2.62 (t, $J = 7.1$ Hz, 2H), 2.25 (t, $J = 7.1$ Hz, 2H), 1.78 (quint, $J = 7.0$ Hz, 2H), 1.56 (quint, $J = 6.9$ Hz, 2H), 1.43 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 51:49) 204.39, 204.11, 155.98, 155.88, 155.43, 155.25, 137.80, 136.98, 136.18, 135.37, 134.67, 134.43, 132.90, 131.95, 131.00, 130.76, 129.96, 129.77, 129.55, 129.09, 128.69, 128.36, 127.82, 127.71, 127.61, 127.36, 116.67, 116.63, 112.09, 111.26, 79.10, 51.09, 48.38, 40.12, 39.97, 39.47, 39.29, 28.26, 28.23, 23.82, 23.73; IR (UATR) ν_{max} 3367, 2977, 2215, 1706, 1512, 1431, 1392, 1366, 1250, 1167, 1093, 1014, 834, 782, 734, 700 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{25}\text{H}_{26}\text{Cl}_2\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 495.1213, found 495.1215.

tert-Butyl (7-cyano-7-(3,4-dichlorophenyl)-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3s)



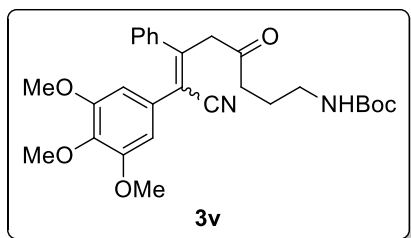
89% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 59:41) 7.54 (d, $J = 2.2$ Hz, 1H), 7.52 (d, $J = 8.4$ Hz, 1H), 7.49–7.41 (m, 4H), 7.32–7.25 (m, 5H), 7.23 (d, $J = 8.4$ Hz, 2H), 7.08–7.03 (m, 2H), 6.92 (dd, $J = 8.4, 2.2$ Hz, 1H), 4.66 (br s, 1H), 4.55 (br s, 1H), 4.04 (s, 2H), 3.68 (s, 2H), 3.09 (br q, $J = 6.5$ Hz, 2H), 2.99 (br q, $J = 6.5$ Hz, 2H), 2.58 (t, $J = 7.1$ Hz, 2H), 2.33 (t, $J = 7.1$ Hz, 2H), 1.77 (quint, $J = 7.0$ Hz, 2H), 1.63 (quint, $J = 6.9$ Hz, 2H), 1.43 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 59:41) 205.19, 204.05, 156.00, 155.95, 154.11, 153.28, 138.42, 137.26, 133.69, 133.21, 133.00, 132.69, 132.60, 131.09, 131.04, 130.49, 130.24, 129.79, 129.27, 128.82, 128.81, 128.64, 128.12, 127.98, 127.60, 117.81, 113.30, 113.23, 79.16, 52.17, 48.60, 40.44, 40.19, 39.50, 39.33, 28.29, 28.26, 23.91; IR (UATR) ν_{max} 3374, 2977, 2216, 1705, 1510, 1470, 1366, 1250, 1167, 1032, 884, 824, 765, 700 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{25}\text{H}_{26}\text{Cl}_2\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 495.1213, found 495.1216.

tert-Butyl (7-cyano-7-(2,6-dichlorophenyl)-4-oxo-6-phenylhept-6-en-1-yl)carbamate (3t)



92% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 35:65) 7.62–7.56 (m, 2H), 7.52–7.42 (m, 7H), 7.34 (dd, $J = 9.0, 7.0$ Hz, 1H), 7.28–7.12 (m, 5H), 7.11–7.05 (m, 1H), 4.64 (br s, 1H), 4.46 (br s, 1H), 4.10 (s, 2H), 3.49 (s, 2H), 3.08 (br q, $J = 6.5$ Hz, 2H), 2.89 (br q, $J = 6.5$ Hz, 2H), 2.63 (t, $J = 7.1$ Hz, 2H), 2.20 (t, $J = 7.1$ Hz, 2H), 1.76 (quint, $J = 7.0$ Hz, 2H), 1.50 (quint, $J = 7.0$ Hz, 2H), 1.43 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 35:65) 203.79, 203.60, 156.38, 156.35, 155.94, 155.82, 137.42, 136.87, 135.52, 135.43, 131.25, 131.02, 130.87, 130.69, 129.99, 129.24, 128.76, 128.59, 128.09, 127.76, 126.96, 116.23, 116.15, 110.00, 109.47, 79.08, 51.21, 48.11, 39.94, 39.89, 39.56, 39.37, 28.29, 28.27, 23.72, 23.53; IR (UATR) ν_{max} 3367, 2977, 2215, 1705, 1511, 1430, 1366, 1250, 1167, 1040, 862, 781, 733, 700 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{25}\text{H}_{26}\text{Cl}_2\text{N}_2\text{Na}_1\text{O}_3$ ($\text{M}+\text{Na}$) $^+$ 495.1213, found 495.1219.

tert-Butyl (7-cyano-4-oxo-6-phenyl-7-(3,4,5-trimethoxyphenyl)hept-6-en-1-yl)carbamate (3v)



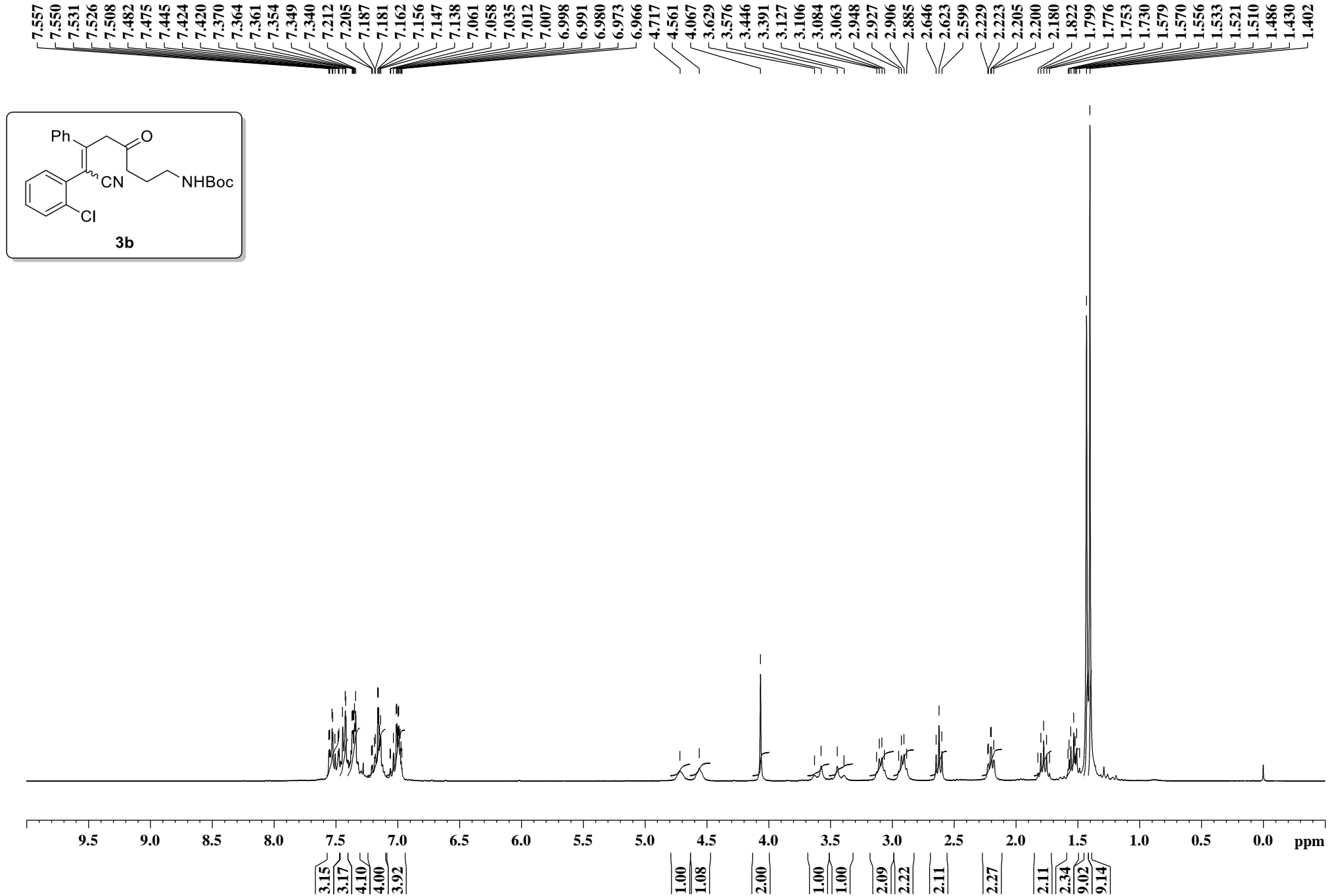
79% yield, yellow oil. ^1H NMR (300 MHz, CDCl_3) δ (isomeric ratio 56:44) 7.51–7.40 (m, 4H), 7.30–7.23 (m, 4H), 7.13–7.08 (m, 2H), 6.68 (s, 2H), 6.34 (s, 2H), 4.63 (br s, 1H), 4.51 (br s, 1H), 4.03 (s, 2H), 3.88 (s, 3H), 3.86 (s, 6H), 3.79 (s, 3H), 3.72 (s, 2H), 3.57 (s, 6H), 3.10 (br q, $J = 6.5$ Hz, 2H), 2.97 (br q, $J = 6.5$ Hz, 2H), 2.59 (t, $J = 7.2$ Hz, 2H), 2.32 (t, $J = 7.2$ Hz, 2H), 1.77 (quint, $J = 7.0$ Hz, 2H), 1.60 (quint, $J = 7.0$ Hz, 2H), 1.43 (s, 9H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ (isomeric ratio 56:44) 205.90, 204.52, 155.97, 153.44, 152.74, 152.33, 150.70, 138.76, 138.63, 138.42, 138.07, 129.54, 129.24, 128.78, 128.69, 128.15, 127.99, 127.72, 118.44, 118.42, 115.59, 115.49, 106.75, 105.76, 79.21, 60.83, 60.78, 56.17, 55.78, 52.26, 48.82, 40.70, 40.13, 39.57, 39.46, 28.31, 28.28, 23.90; IR (UATR) ν_{max} 3393, 2937, 2213, 1709, 1592, 1513, 1456, 1425, 1366, 1251, 1206, 1156, 1062, 1037, 927, 841, 766, 698 cm^{-1} ; HRMS (ESI $^+$) calcd for $\text{C}_{28}\text{H}_{34}\text{N}_2\text{Na}_1\text{O}_6$ (M+Na) $^+$ 517.2315, found 517.2318.

1.2 References

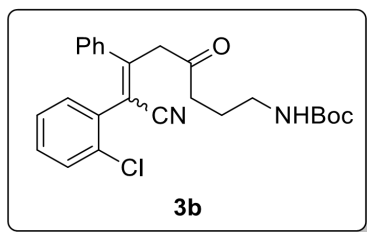
1. S. Ruchirawat and W. Disadee, *Org. Chem. Front.*, 2017, **4**, 2026;
2. W. Disadee and S. Ruchirawat, *J. Org. Chem.*, 2020, **85**, 1802.

1.3 Copies of ^1H and ^{13}C NMR spectra for all new compounds

¹H NMR (300 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)

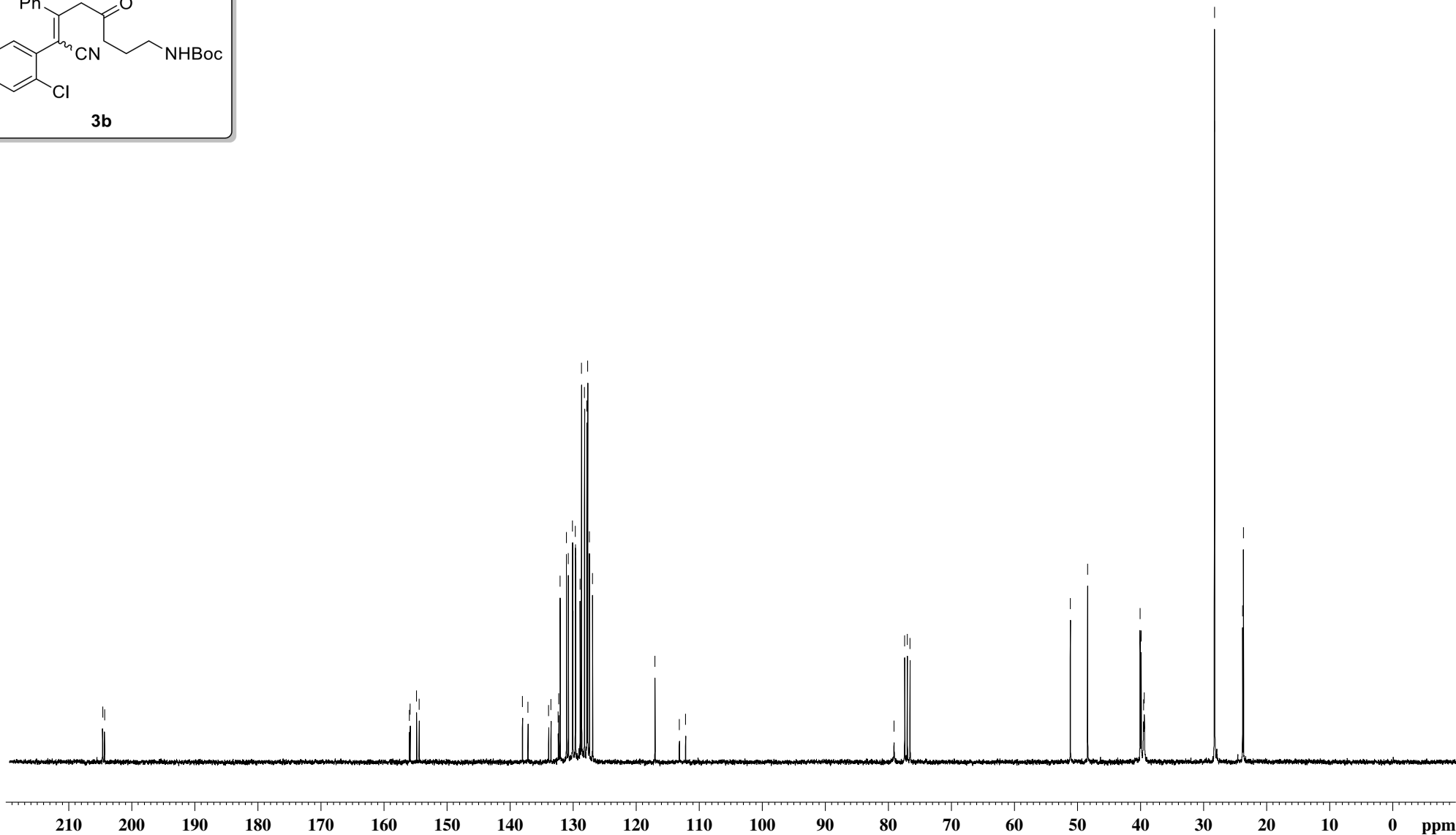


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204.303

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154.426
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132.075
131.068
130.774
130.112
130.066
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112.176

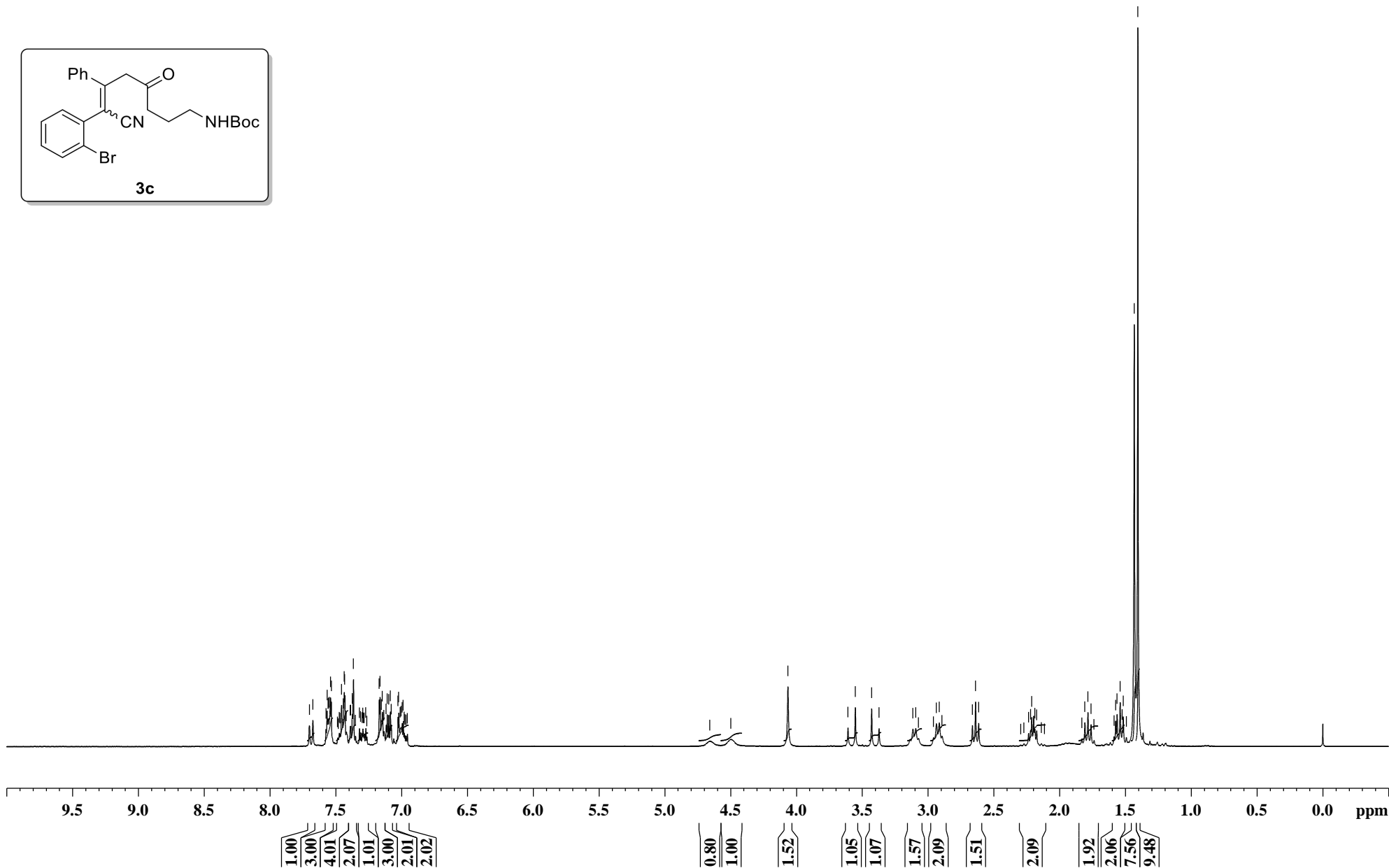
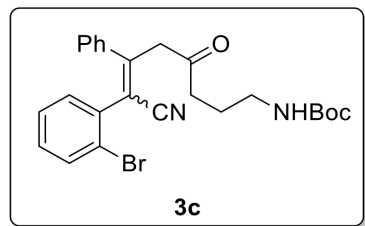
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23.820
23.679

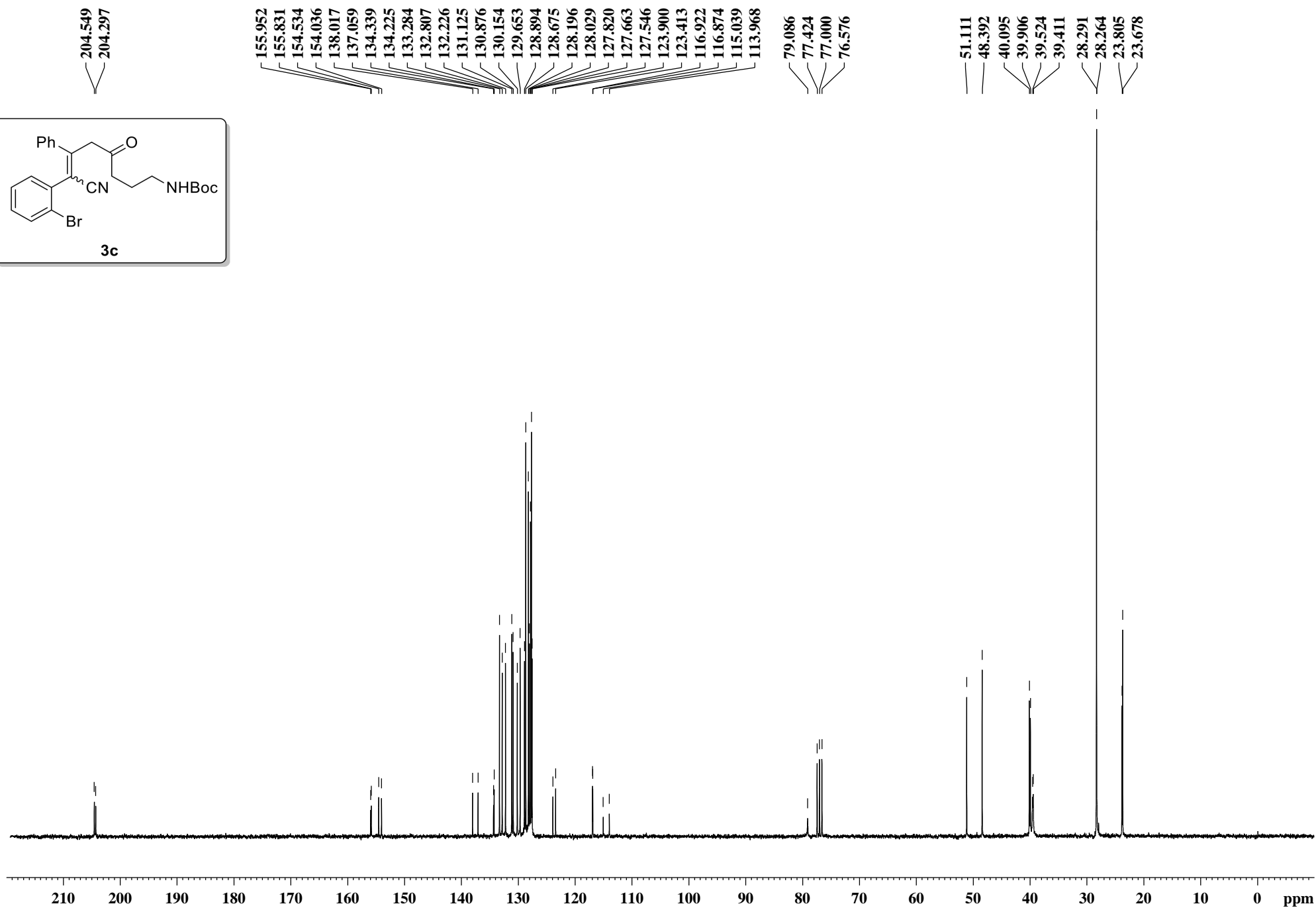
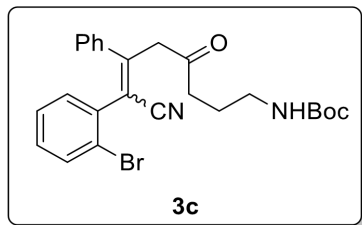


1H NMR (300 MHz, CDCl3)

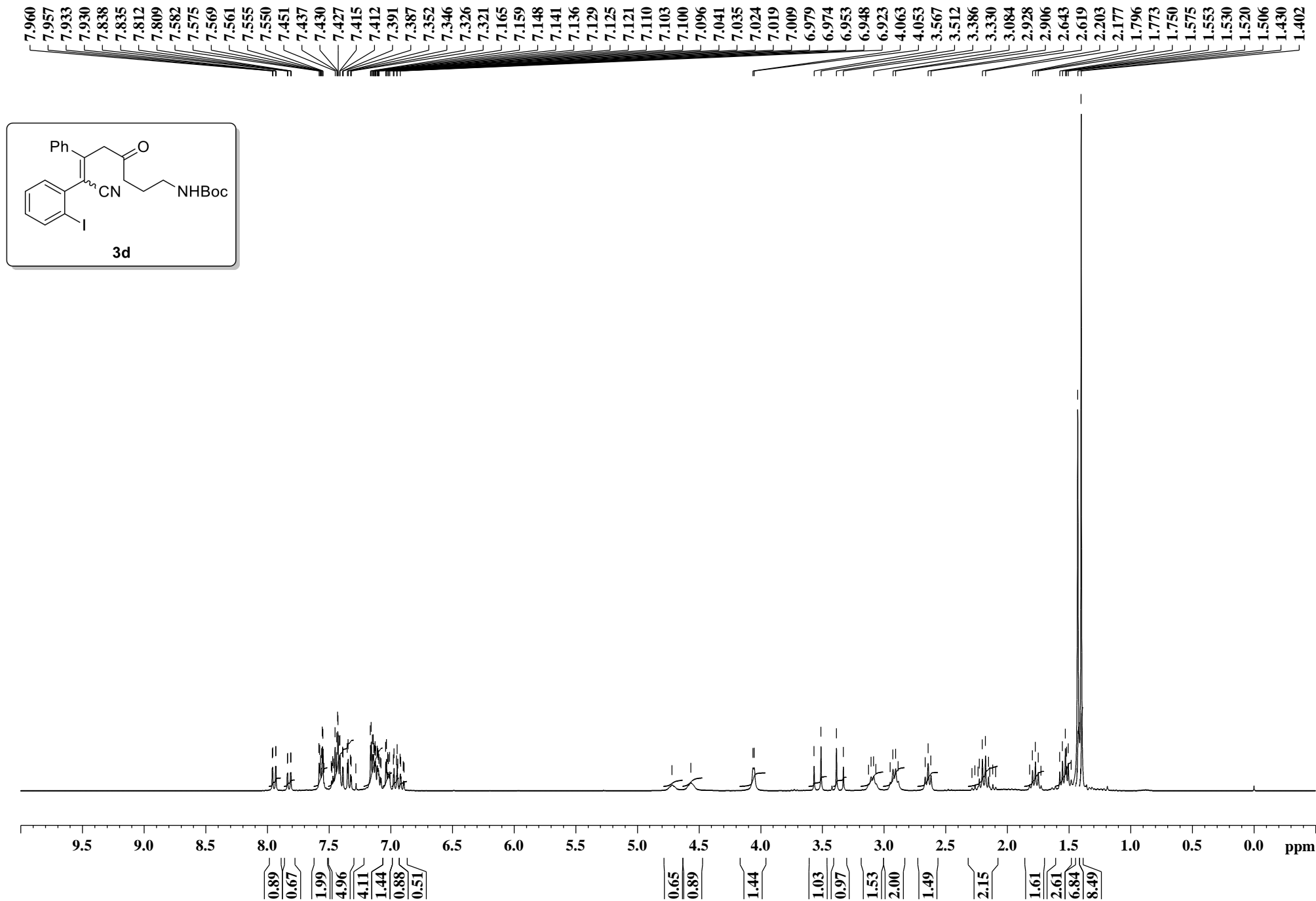
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7.436
7.432
7.420
7.391
7.387
7.375
7.366
7.321
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7.300
7.295
7.291
7.284
7.272
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7.154
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3.115
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2.615
2.236
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2.212
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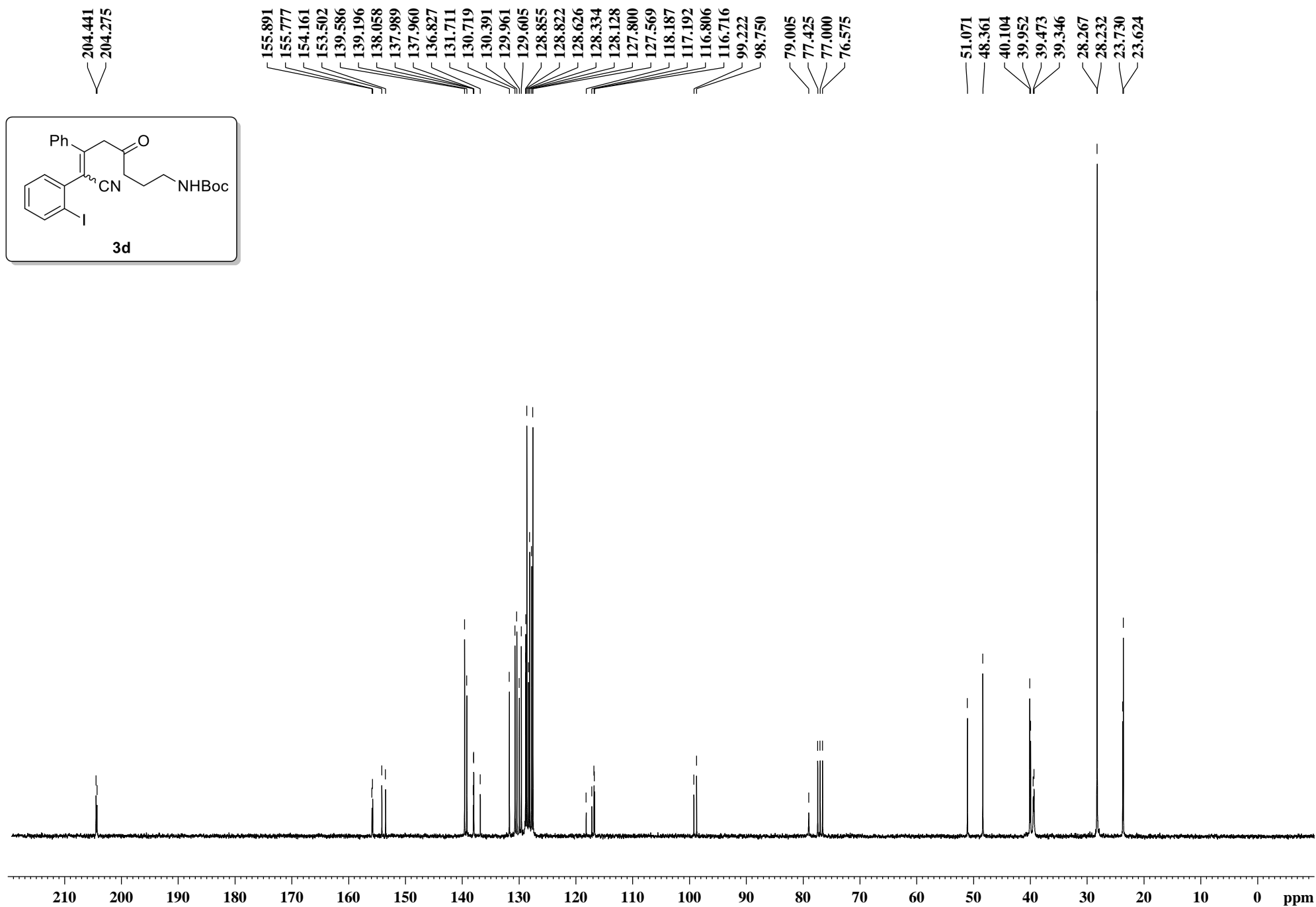
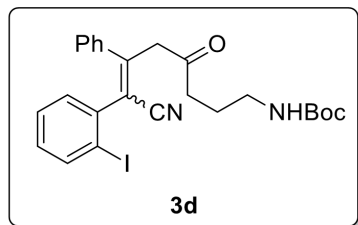
13C NMR (75 MHz, CDCl3)



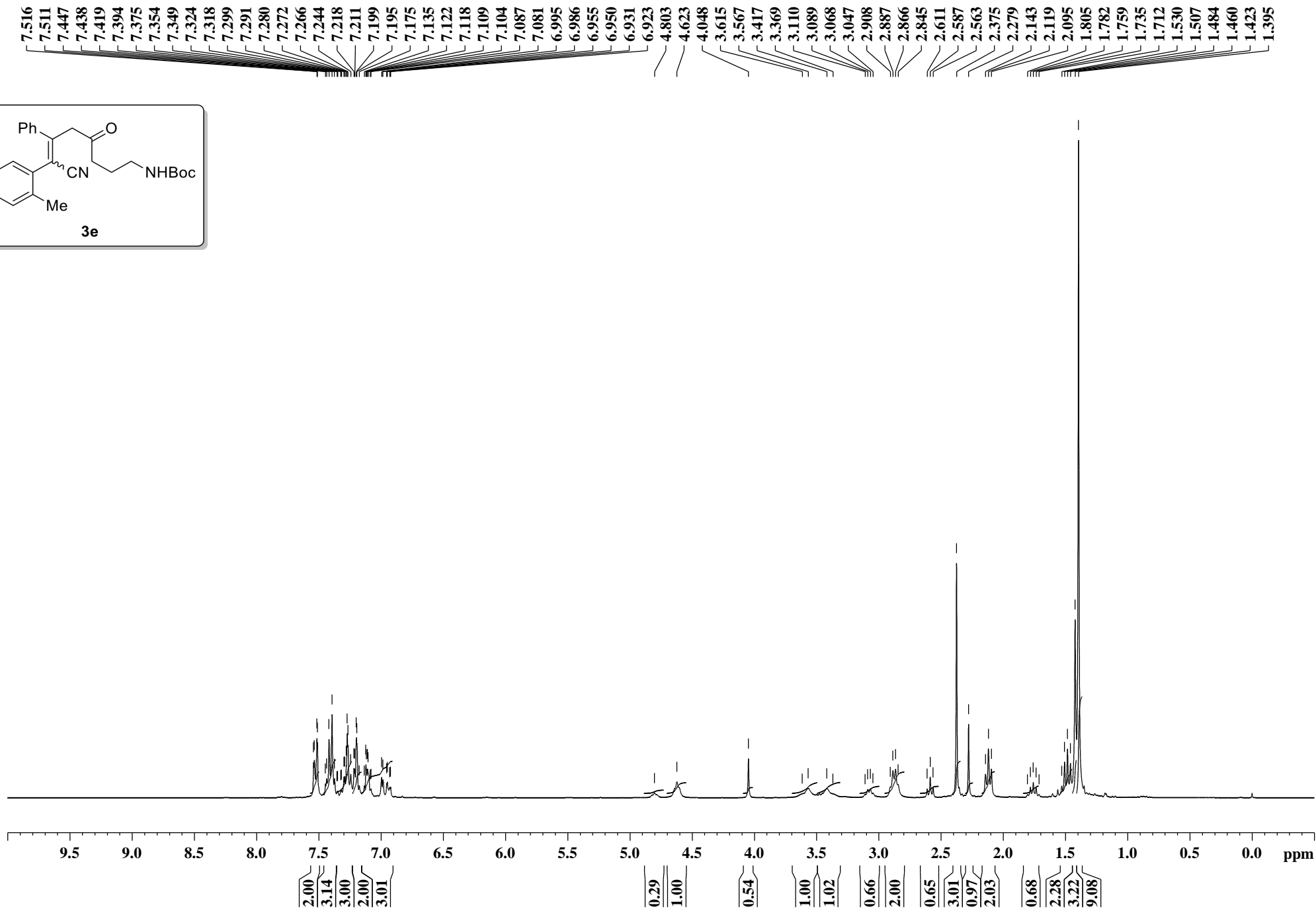
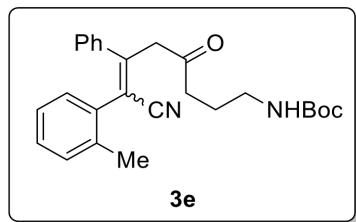
¹H NMR (300 MHz, CDCl₃)



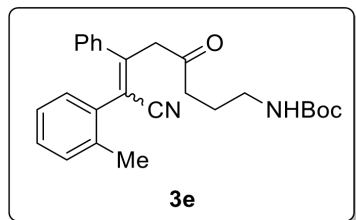
13C NMR (75 MHz, CDCl₃)



1H NMR (300 MHz, CDCl3)



¹³C NMR (75 MHz, CDCl₃)

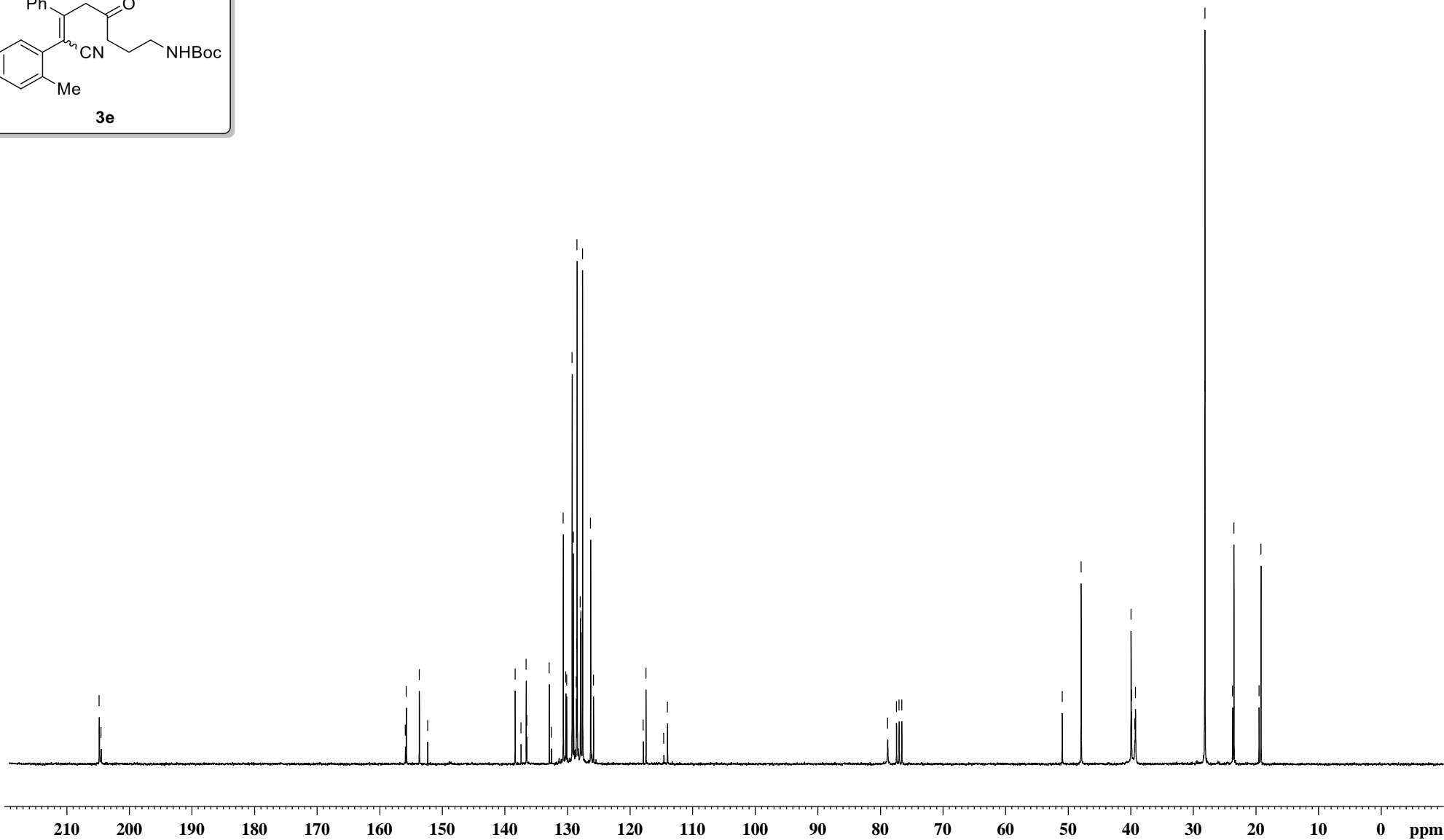


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204.514

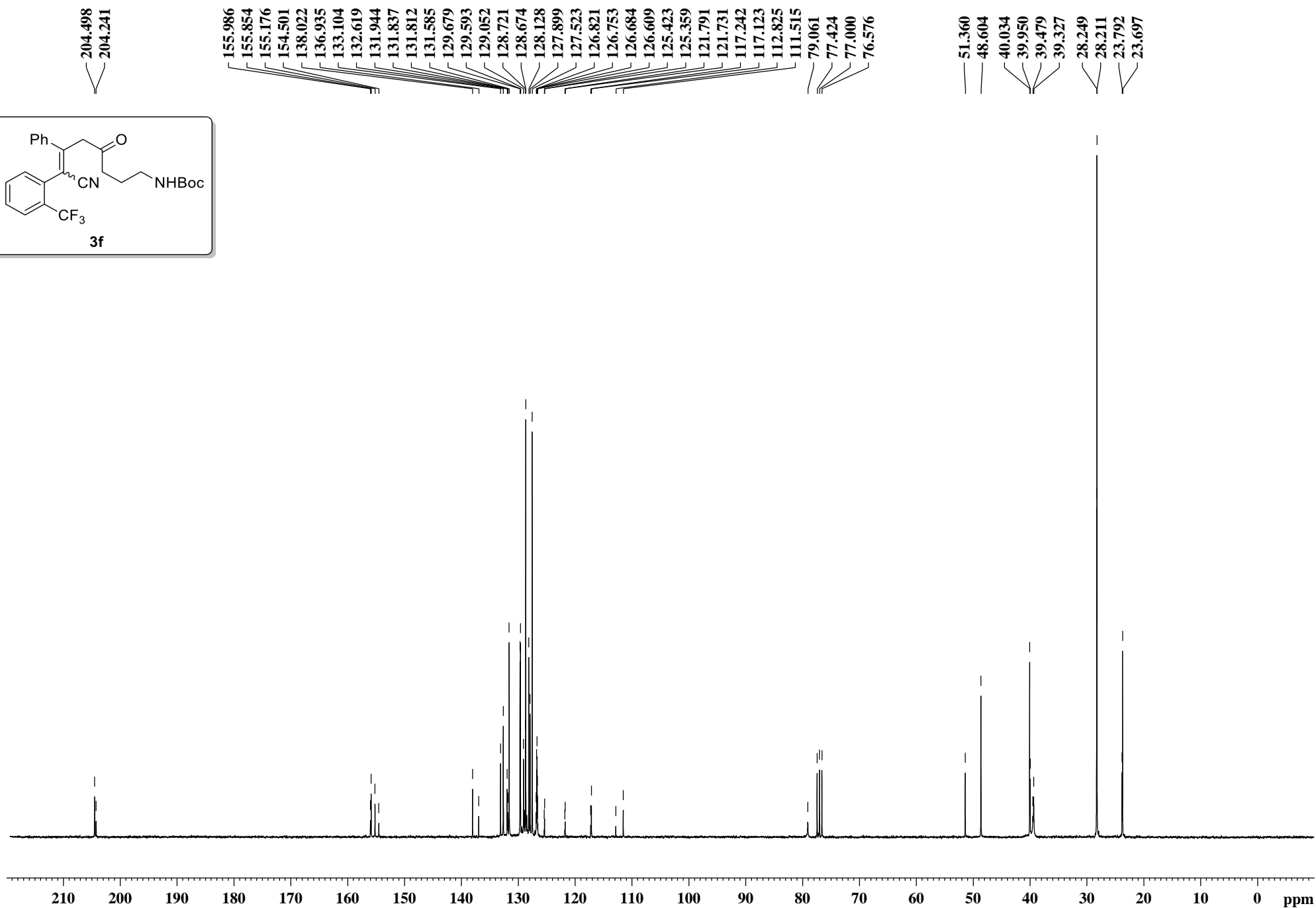
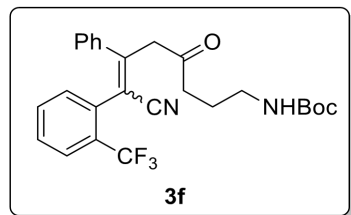
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129.250
129.026
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128.461
127.935
127.843
127.586
126.295
125.842
117.875
117.452
114.592
114.005

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77.426
77.000
76.574

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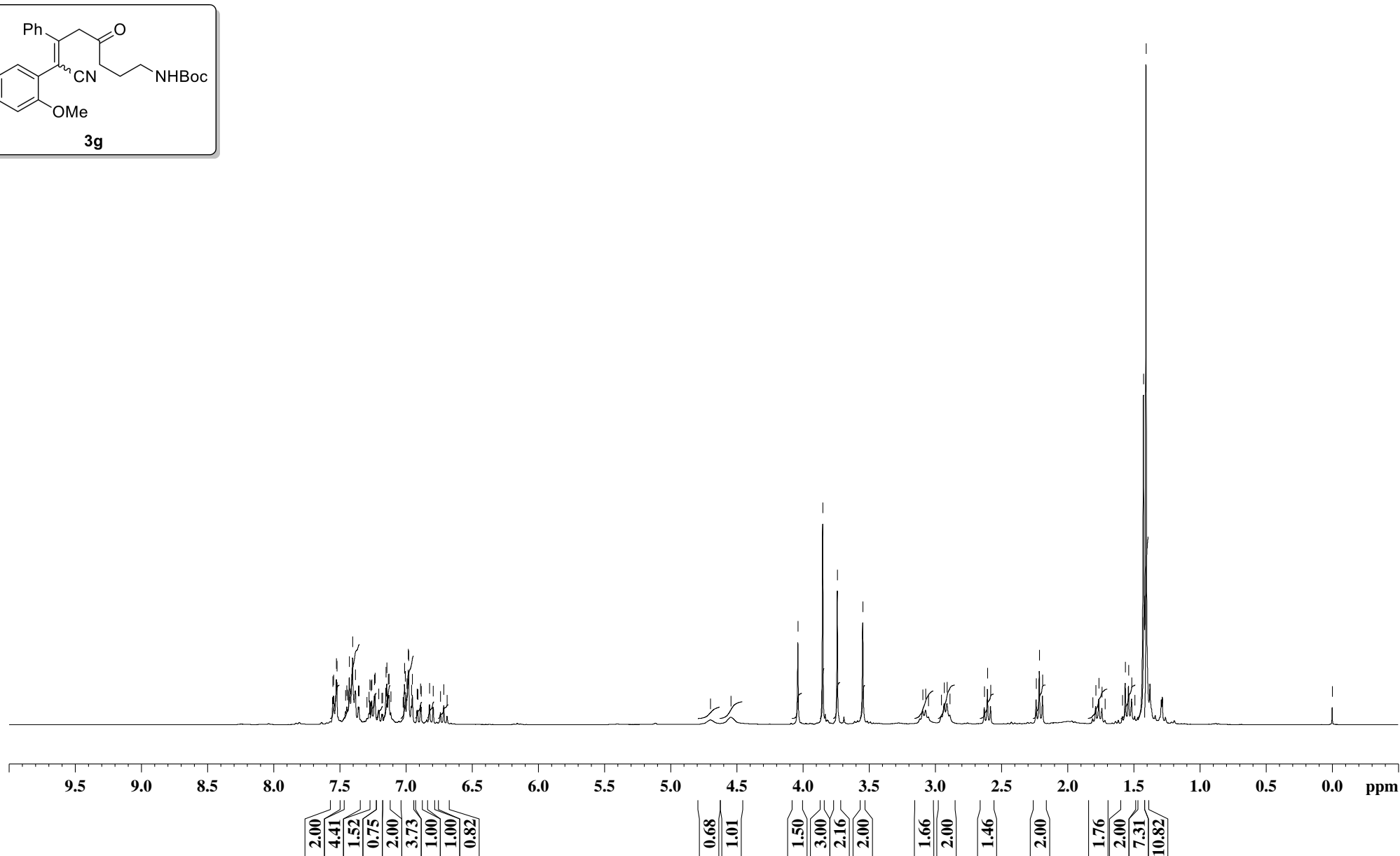
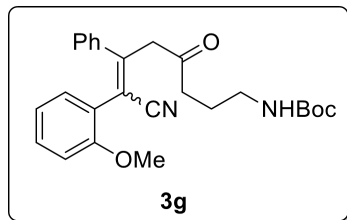


13C NMR (75 MHz, CDCl3)



¹H NMR (300 MHz, CDCl₃)

7.553
7.548
7.527
7.522
7.457
7.448
7.442
7.429
7.404
7.383
7.361
7.355
7.280
7.274
7.264
7.259
7.239
7.234
7.207
7.183
7.178
7.152
7.145
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7.006
6.994
6.983
6.980
6.959
6.952
6.916
6.911
6.891
6.885
6.823
6.795
6.740
6.715
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2.213
2.190
1.787
1.764
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¹³C NMR (75 MHz, CDCl₃)

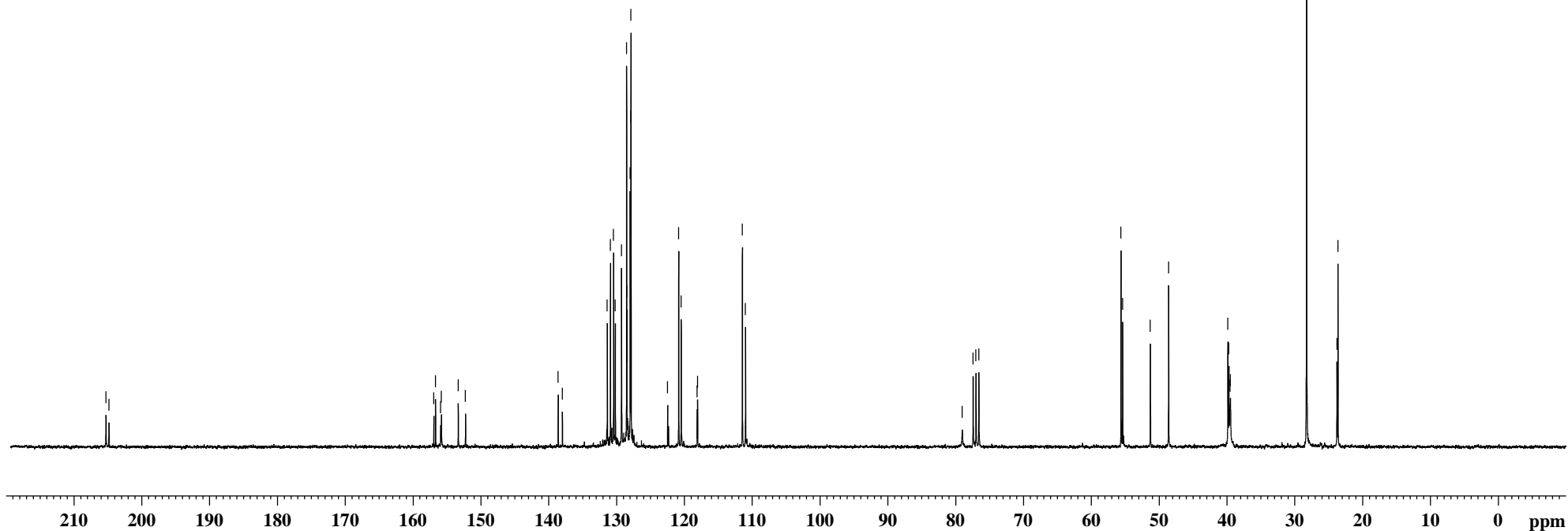
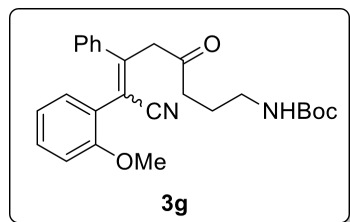
205.253
204.815

156.938
156.690
155.926
155.818
153.337
152.270
138.602
137.981
131.362
130.895
130.429
130.180
129.272
128.517
128.472
127.996
127.879
127.860
122.466
120.837
120.468
118.115
118.054
111.448
110.980

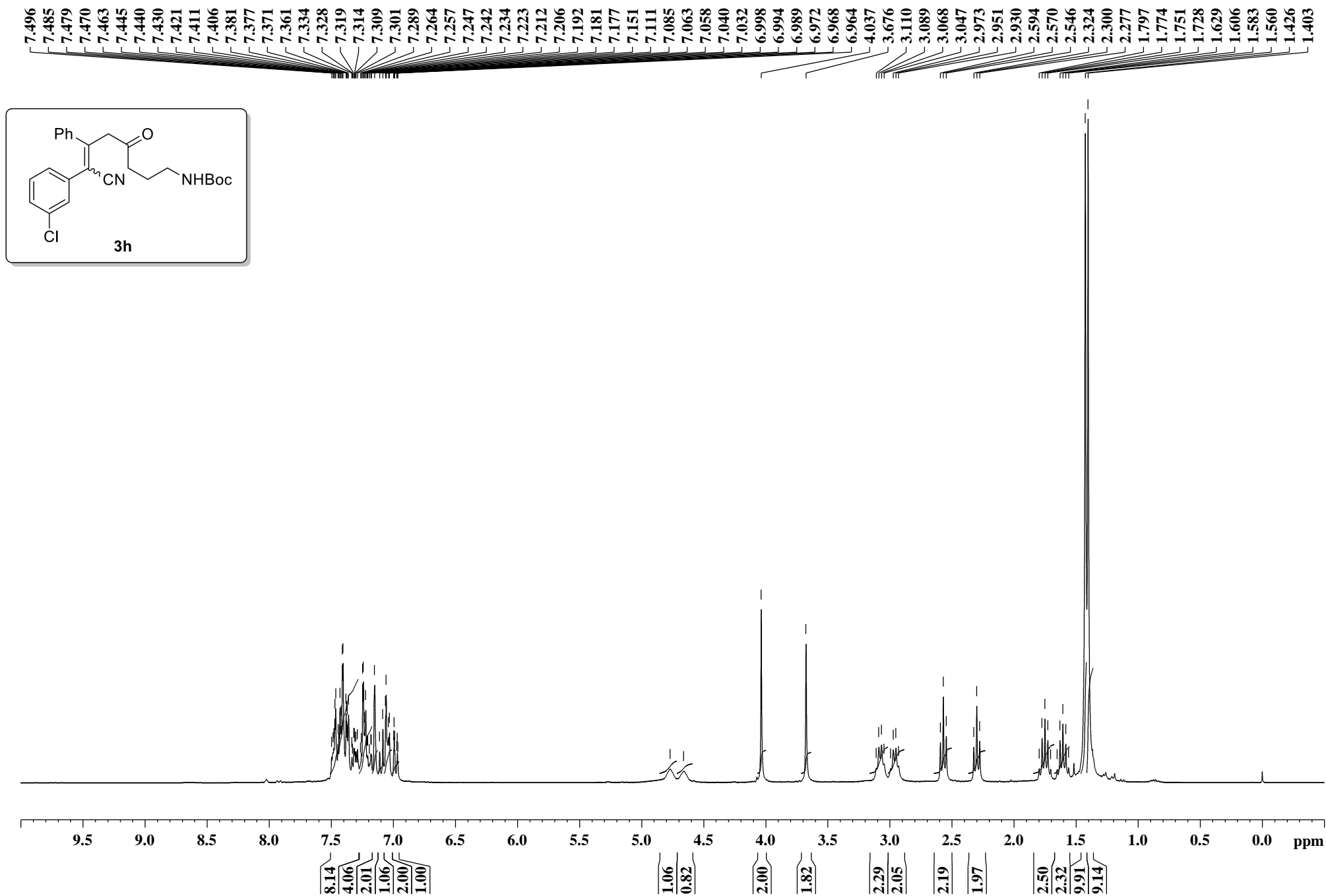
79.010
77.424
77.000
76.577

55.614
55.380
51.284
48.594
39.851
39.707
39.542
39.482

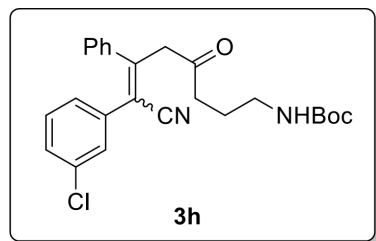
28.247
23.770
23.628



1H NMR (300 MHz, CDCl3)



¹³C NMR (75 MHz, CDCl₃)

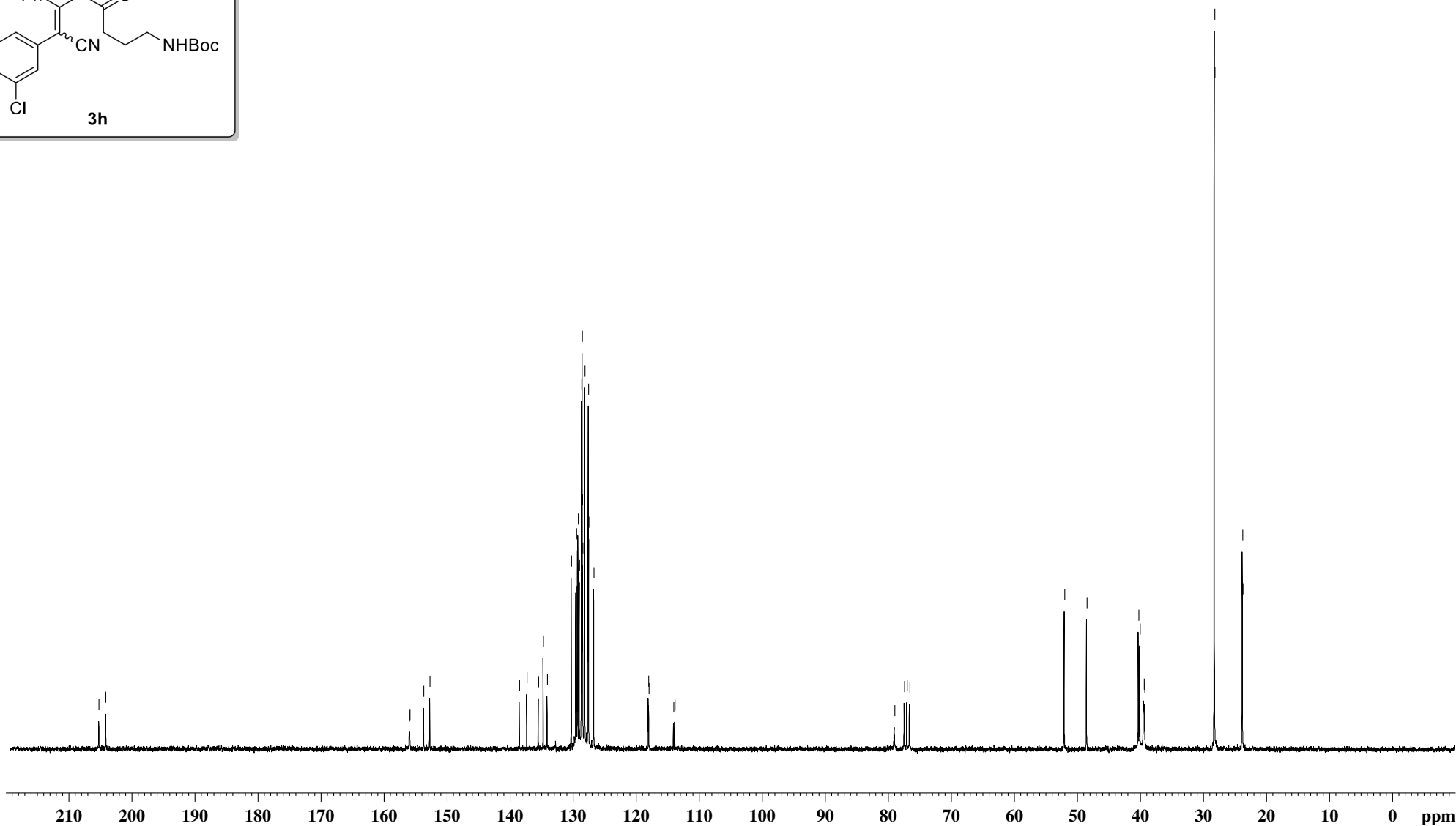


205.237
204.153

155.968
155.887
153.702
152.722
138.506
137.316
135.482
134.723
134.087
130.260
129.546
129.456
129.266
129.187
128.988
128.635
128.541
128.509
128.457
128.125
127.556
127.504
126.700
118.019
117.964
114.037
113.839

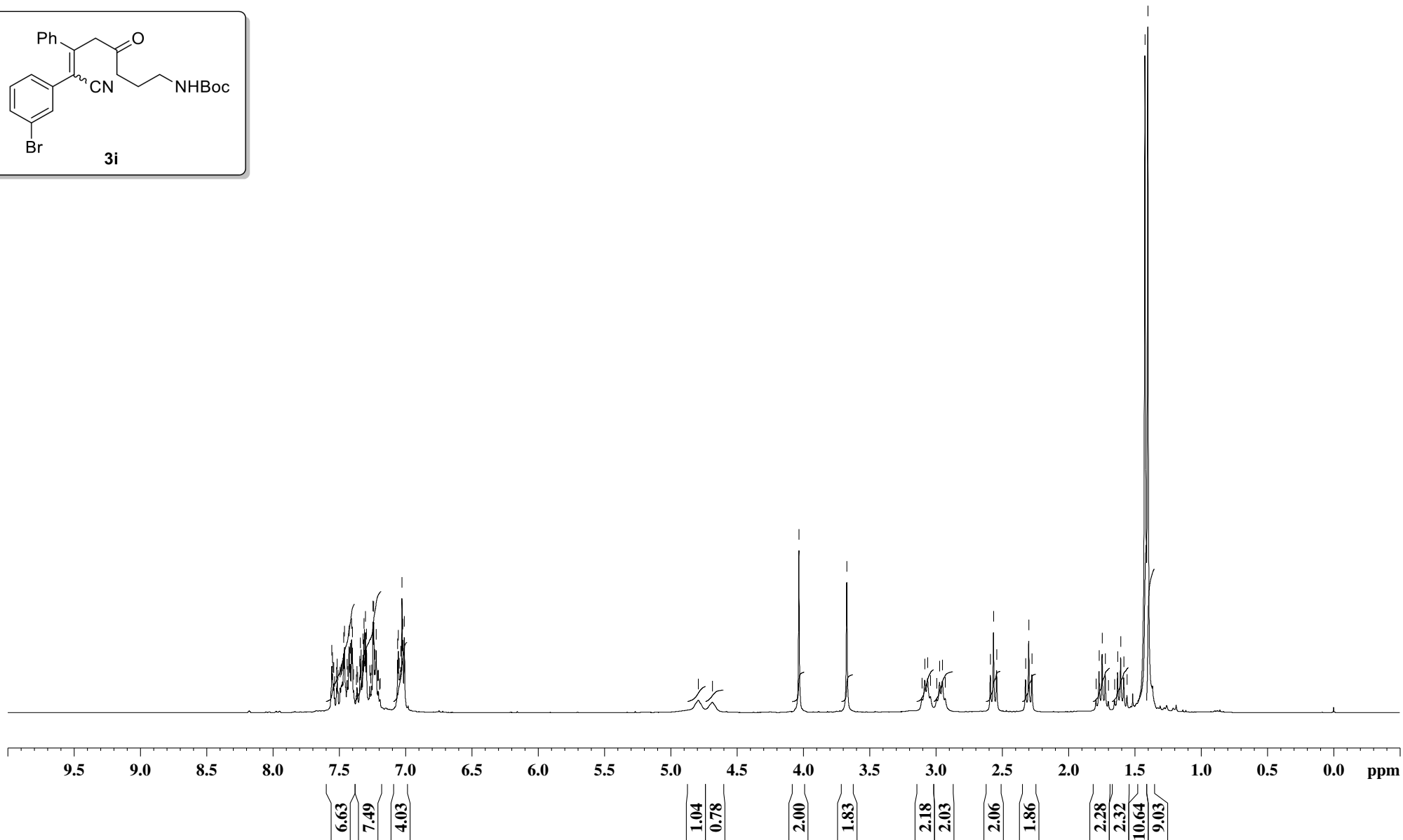
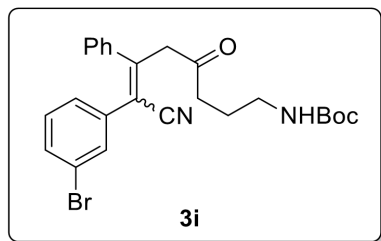
78.967
77.425
77.000
76.575

52.007
48.473
40.252
40.035
39.398
39.311
28.200
28.177
23.769
23.730

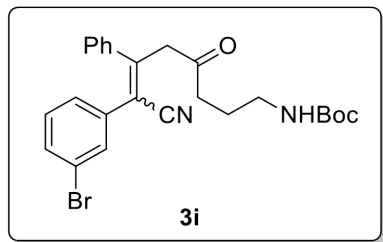


¹H NMR (300 MHz, CDCl₃)

7.557
7.552
7.548
7.543
7.536
7.522
7.517
7.511
7.494
7.487
7.483
7.477
7.468
7.461
7.441
7.436
7.426
7.417
7.408
7.402
7.393
7.372
7.367
7.362
7.346
7.341
7.336
7.329
7.321
7.314
7.311
7.303
7.296
7.270
7.263
7.256
7.247
7.241
7.233
7.222
7.211
7.206
7.061
7.056
7.049
7.037
7.028
7.022
7.010
4.034
3.673
3.084
3.063
3.042
2.973
2.952
2.590
2.566
2.542
2.324
2.300
2.276
1.770
1.746
1.723
1.630
1.607
1.583
1.559
1.424
1.402



13C NMR (75 MHz, CDCl3)

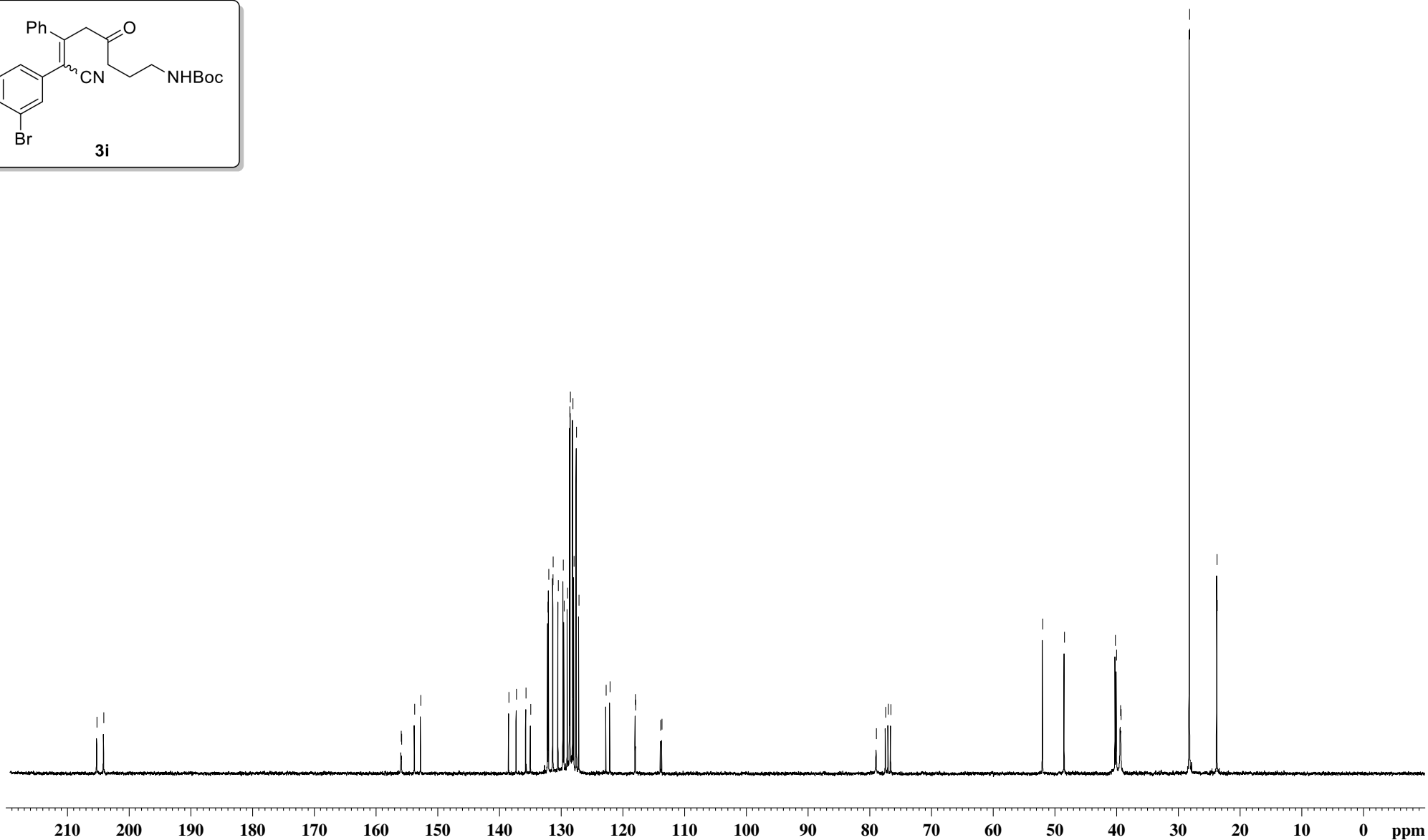


205.220
204.115

155.921
155.850
153.743
152.747
138.472
137.249
135.702
134.935
132.145
132.010
131.328
131.305
130.468
129.660
129.519
128.968
128.600
128.511
128.099
127.915
127.524
127.119
122.718
122.083
117.975
117.933
113.875
113.671

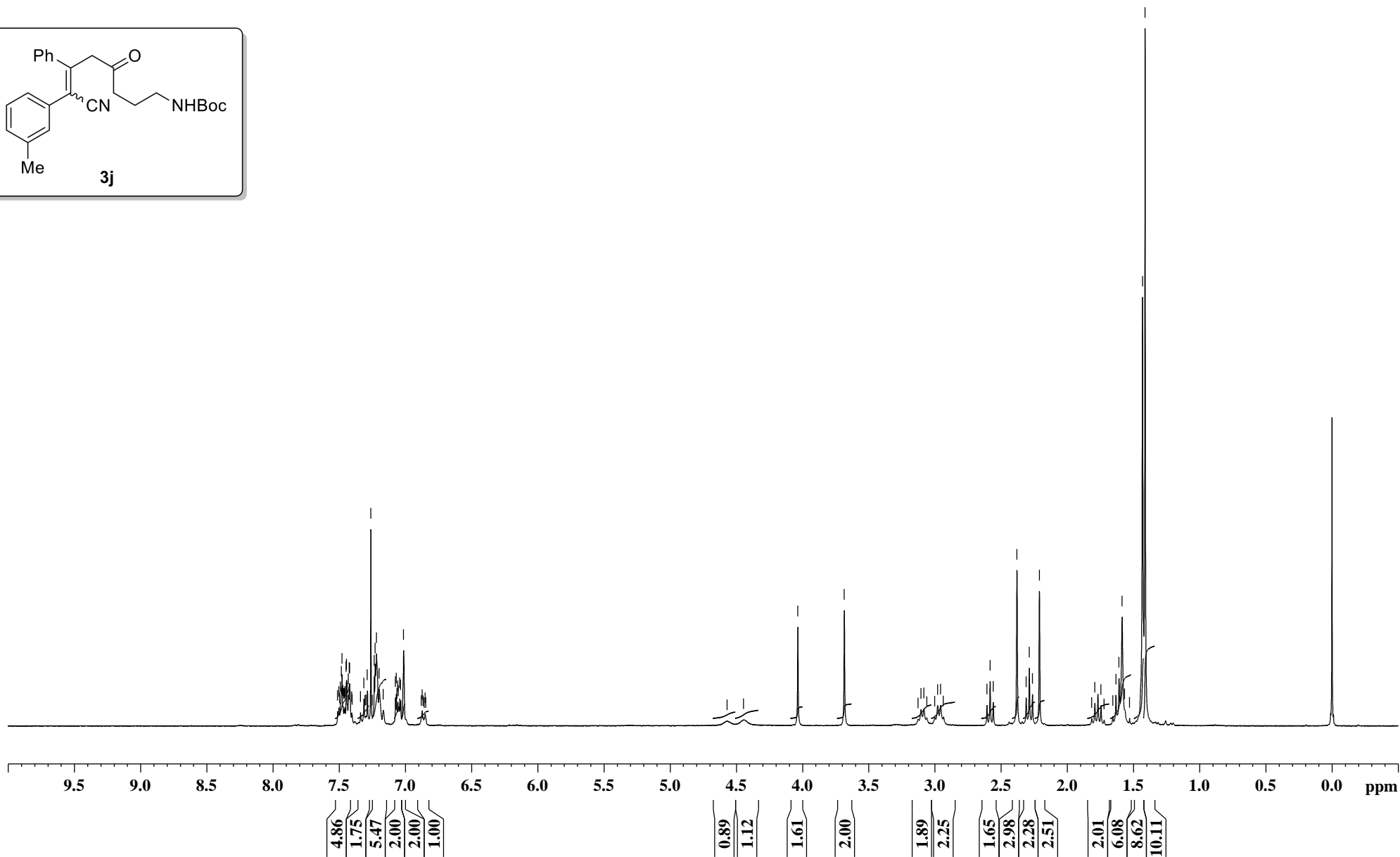
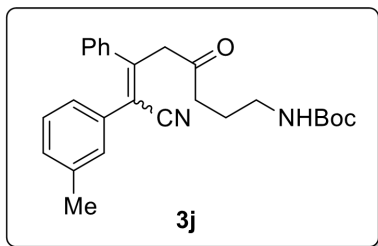
78.928
77.425
77.000
76.575

51.965
48.455
40.205
40.008
39.361
39.278
28.180
28.161
23.736
23.707

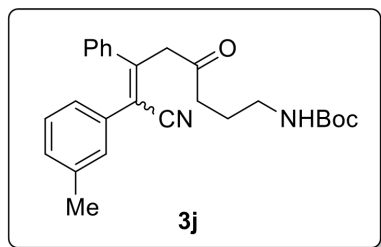


¹H NMR (300 MHz, CDCl₃)

7.512
7.503
7.497
7.491
7.484
7.479
7.471
7.465
7.460
7.457
7.447
7.445
7.439
7.431
7.424
7.421
7.406
7.402
7.339
7.313
7.304
7.297
7.287
7.261
7.250
7.236
7.229
7.219
7.197
7.166
7.075
7.069
7.064
7.058
7.053
7.042
7.036
7.014
6.880
6.874
6.866
6.857
6.851
6.845
4.035
3.684
3.105
3.083
3.061
3.001
2.979
2.958
2.937
2.607
2.583
2.559
2.380
2.311
2.287
2.263
2.211
1.792
1.745
1.656
1.633
1.609
1.586
1.567
1.530
1.432
1.412



13C NMR (75 MHz, CDCl3)

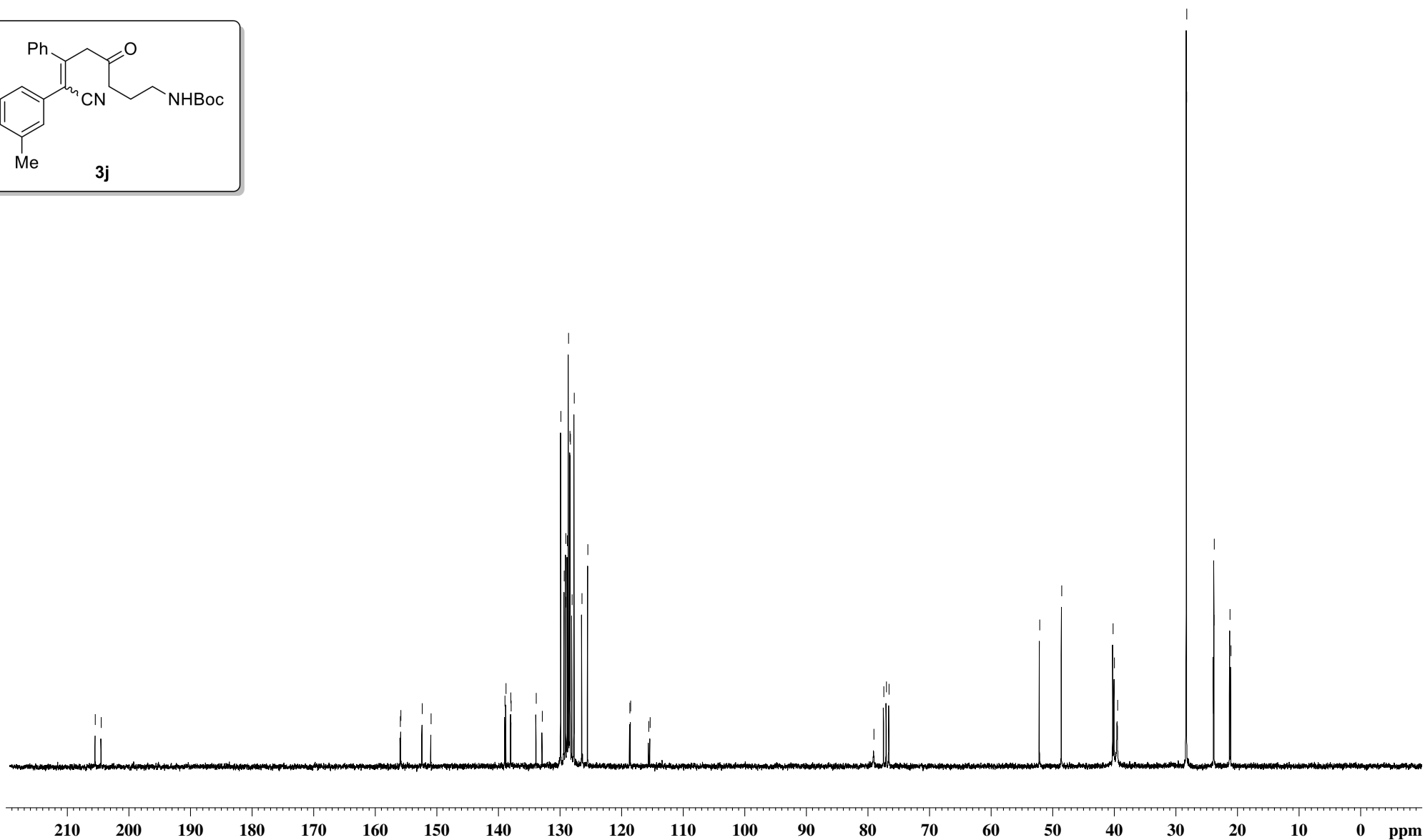


205.465
204.501

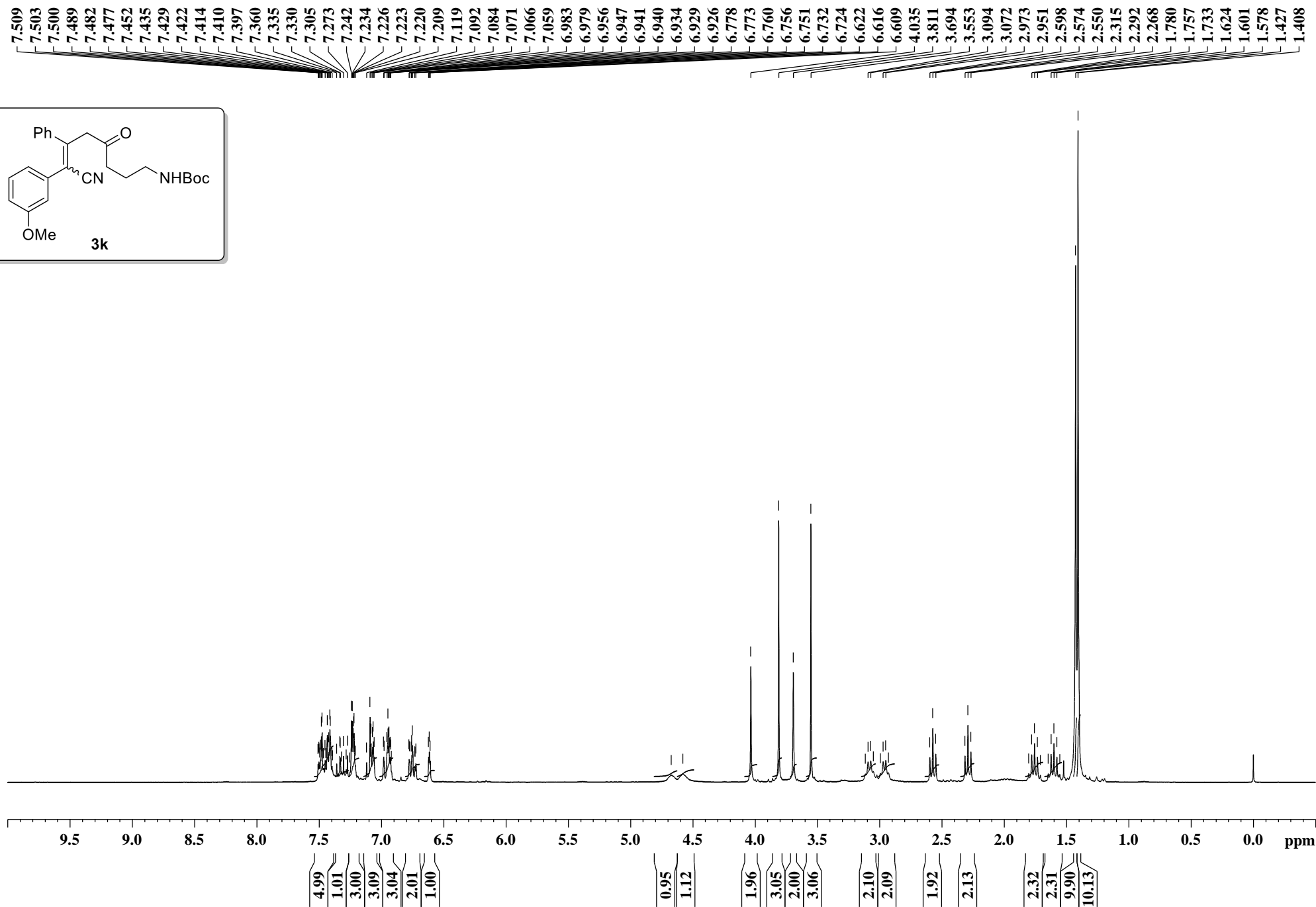
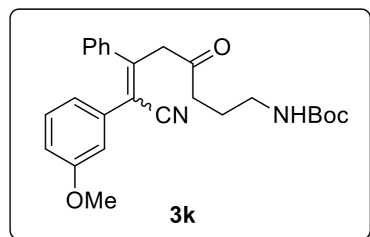
155.929
155.844
152.377
150.938
138.941
138.771
137.992
137.936
133.863
132.876
129.859
129.323
129.095
129.057
128.801
128.615
128.383
128.307
128.038
127.689
126.436
125.483
118.660
118.533
115.595
115.364

79.029
77.424
77.000
76.575

52.110
48.539
40.199
39.983
39.456
28.257
28.235
23.818
23.766
21.214
21.061



¹H NMR (300 MHz, CDCl₃)



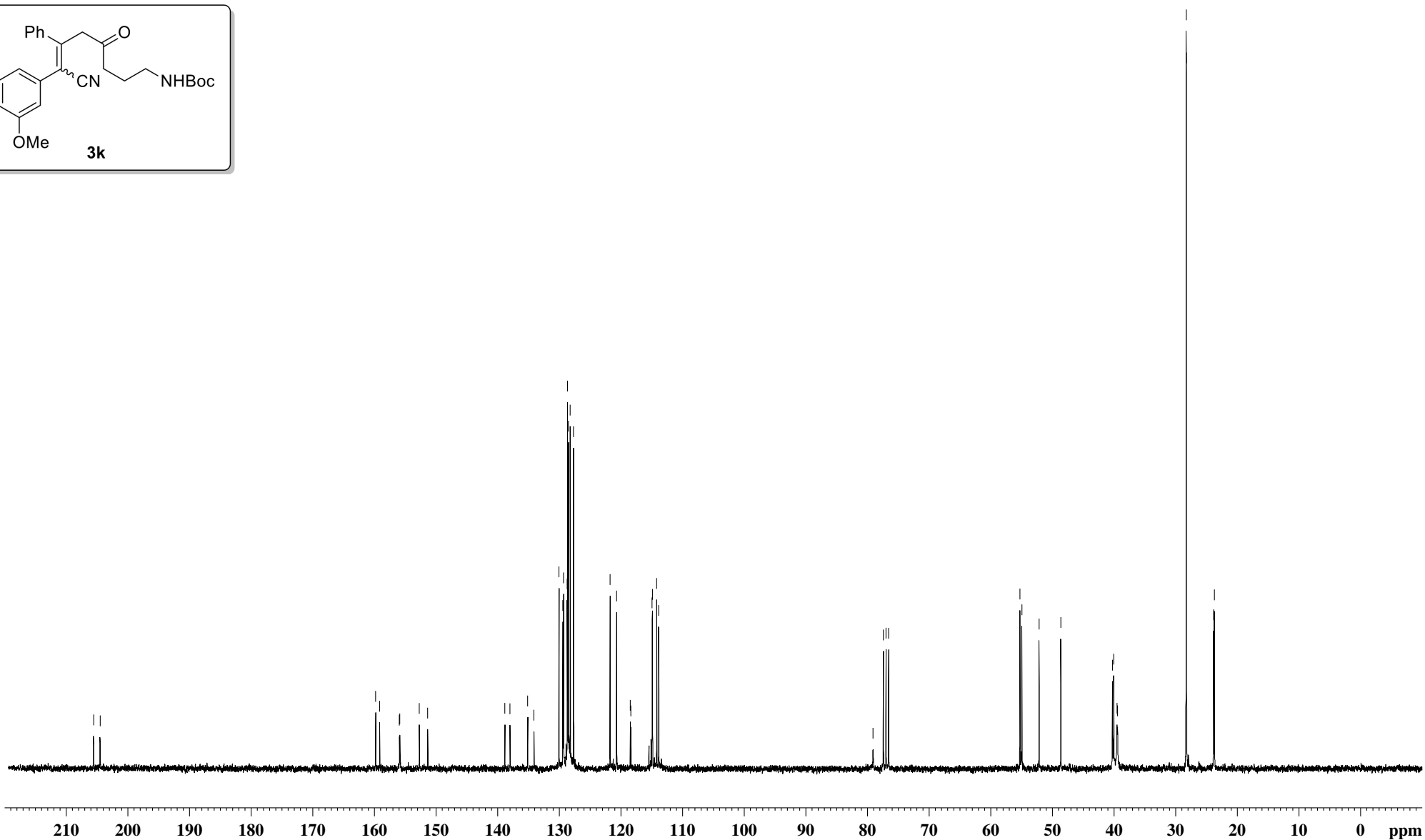
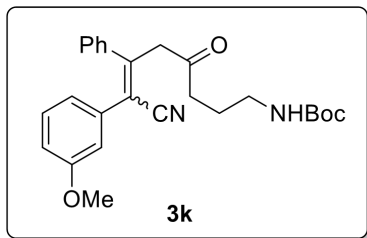
13C NMR (75 MHz, CDCl3)

205.540
204.487

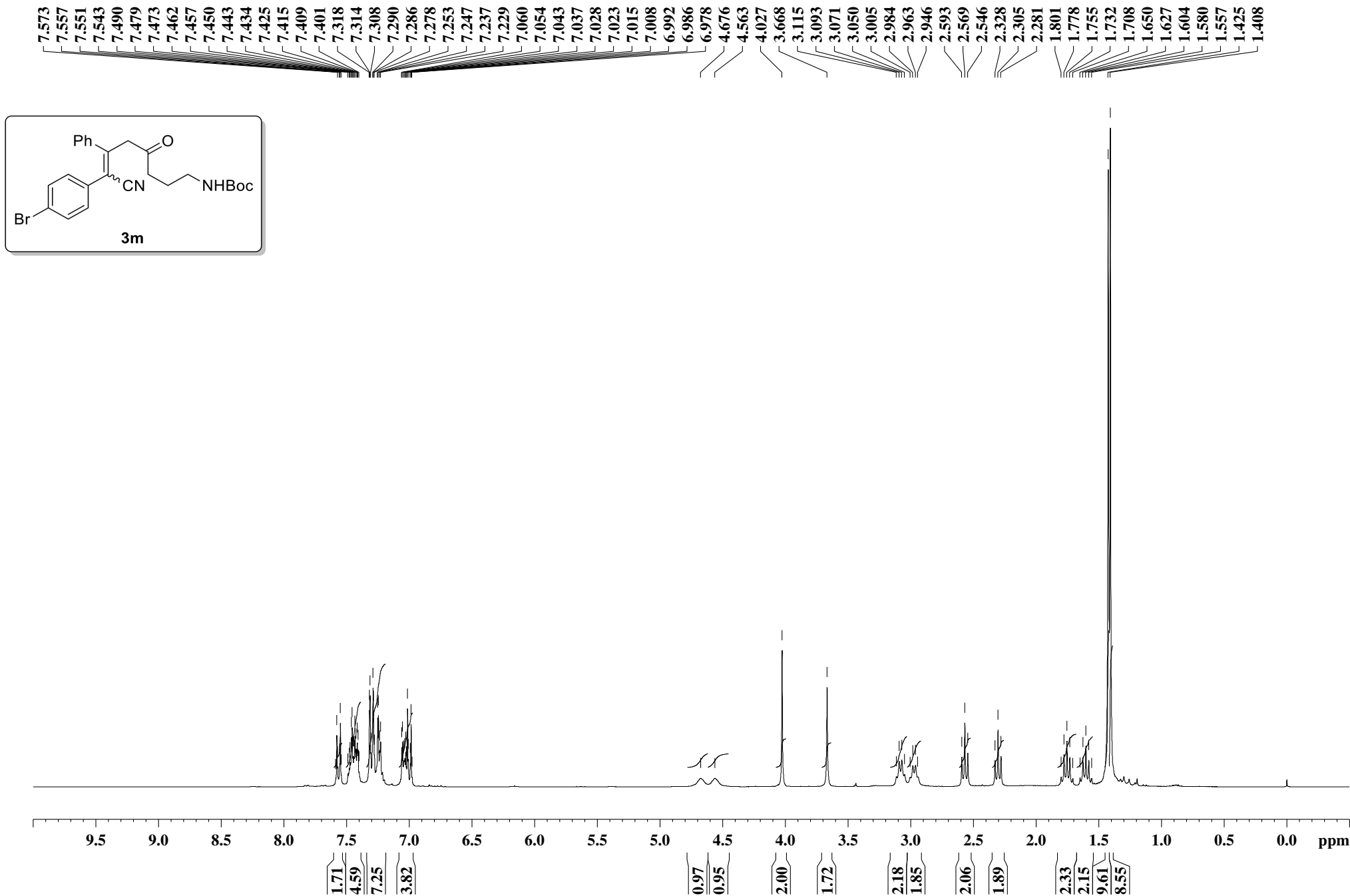
159.809
159.162
155.967
155.887
152.730
151.367
138.846
138.015
135.144
134.132
130.064
129.440
129.322
128.735
128.678
128.528
128.247
127.705
121.768
120.713
118.494
118.397
114.963
114.894
114.214
113.884

79.111
77.424
77.000
76.576

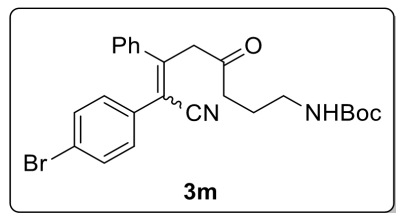
55.272
54.947
52.161
48.632
40.247
40.054
39.517
39.436
28.280
28.263
23.845
23.721



¹H NMR (300 MHz, CDCl₃)



13C NMR (75 MHz, CDCl3)

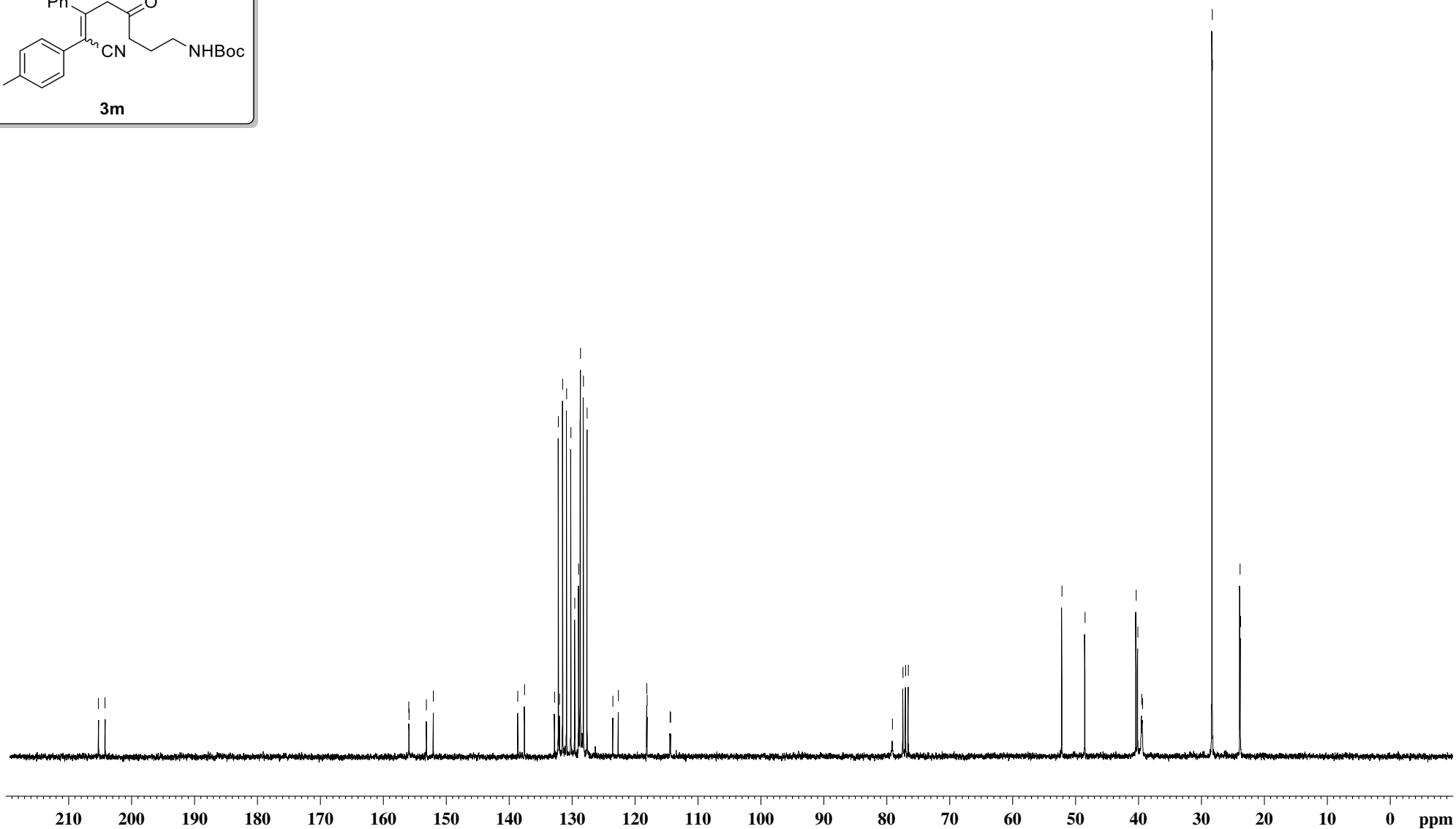


205.272
204.230

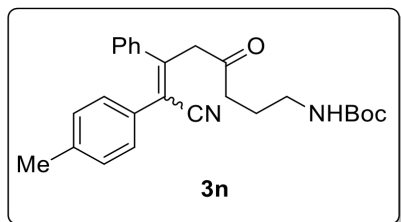
155.955
155.911
153.160
152.053
138.641
137.561
132.789
132.187
132.006
131.506
130.880
130.196
129.584
128.972
128.720
128.674
128.207
127.618
123.522
122.649
118.135
118.075
114.428
114.347

79.101
77.424
77.000
76.576

52.161
48.496
40.369
40.107
39.491
39.358
28.276
28.256
23.864
23.779

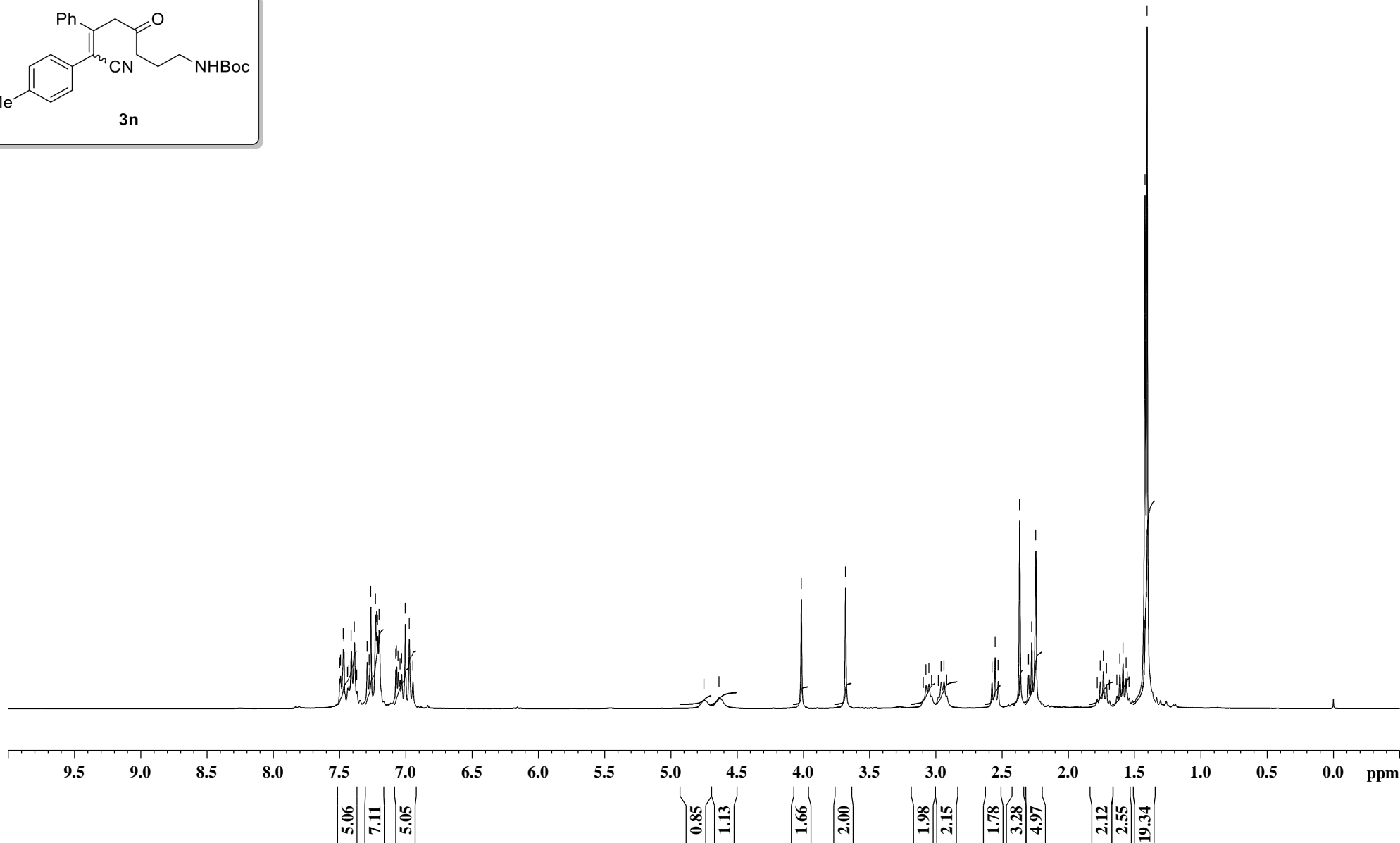


1H NMR (300 MHz, CDCl3)

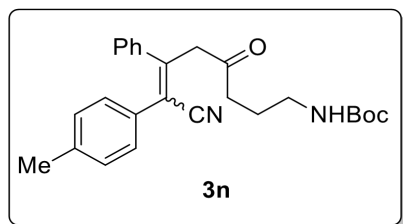


7.499
7.493
7.472
7.467
7.439
7.430
7.412
7.388
7.369
7.292
7.276
7.265
7.229
7.220
7.212
7.202
7.076
7.069
7.058
7.043
7.032
7.004
6.974
6.946

4.749
4.636
4.015
3.682
3.095
3.074
3.053
3.032
2.981
2.960
2.938
2.918
2.577
2.553
2.529
2.368
2.300
2.276
2.245
1.782
1.759
1.736
1.712
1.689
1.634
1.611
1.588
1.564
1.556
1.541
1.422
1.406



13C NMR (75 MHz, CDCl3)

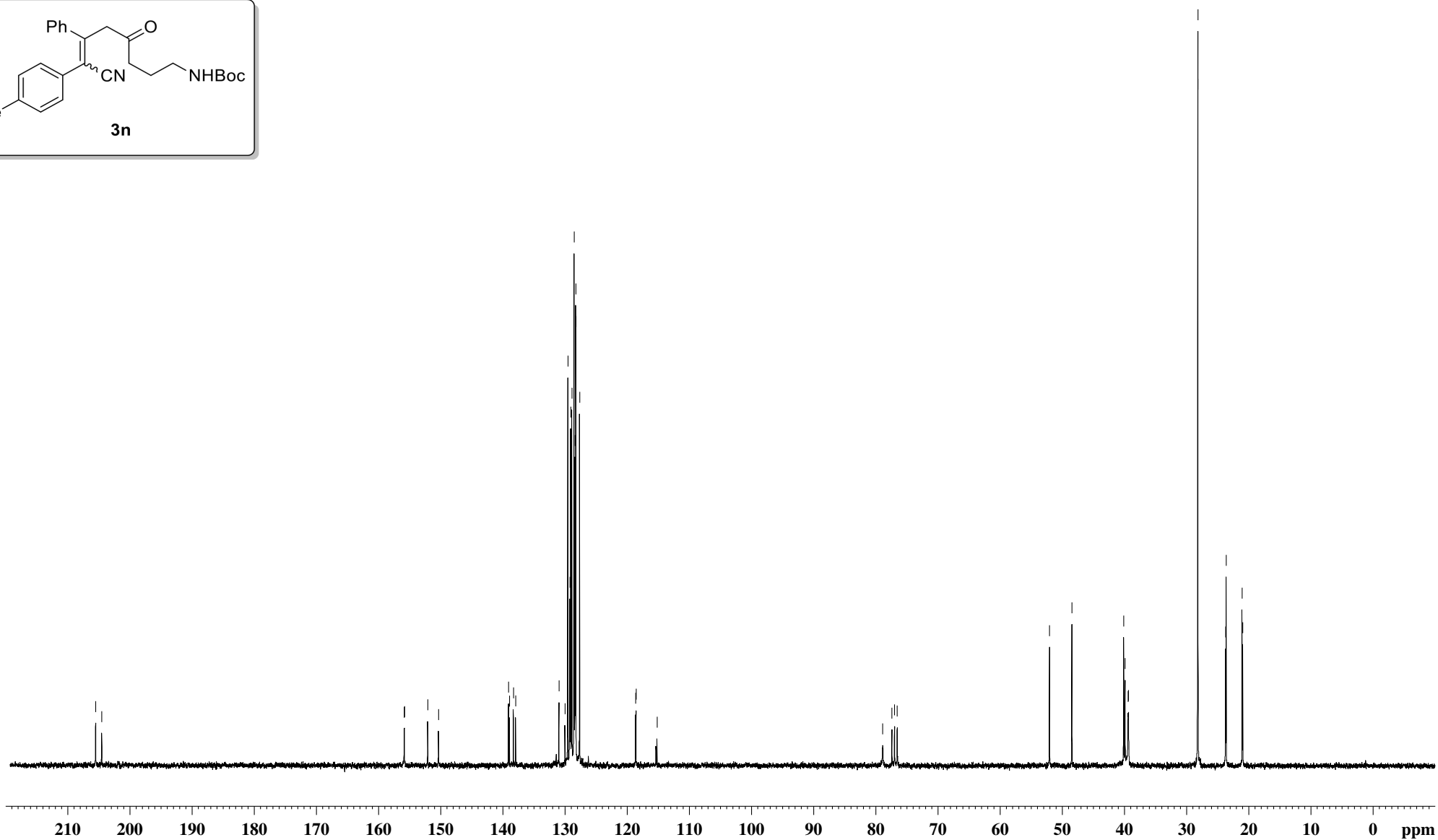


205.515
204.541

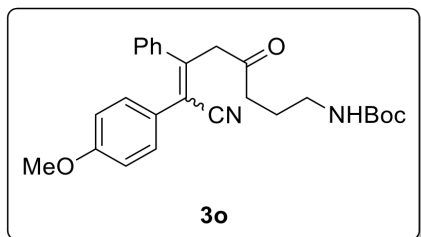
155.874
155.809
152.080
150.346
139.089
138.933
138.287
137.940
130.961
129.998
129.525
129.213
129.073
128.884
128.526
128.386
128.257
128.245
127.634
118.641
118.554
115.178

78.908
77.425
77.000
76.574

52.065
48.454
40.124
39.907
39.415
39.356
28.192
28.173
23.728
23.631
21.072
20.974

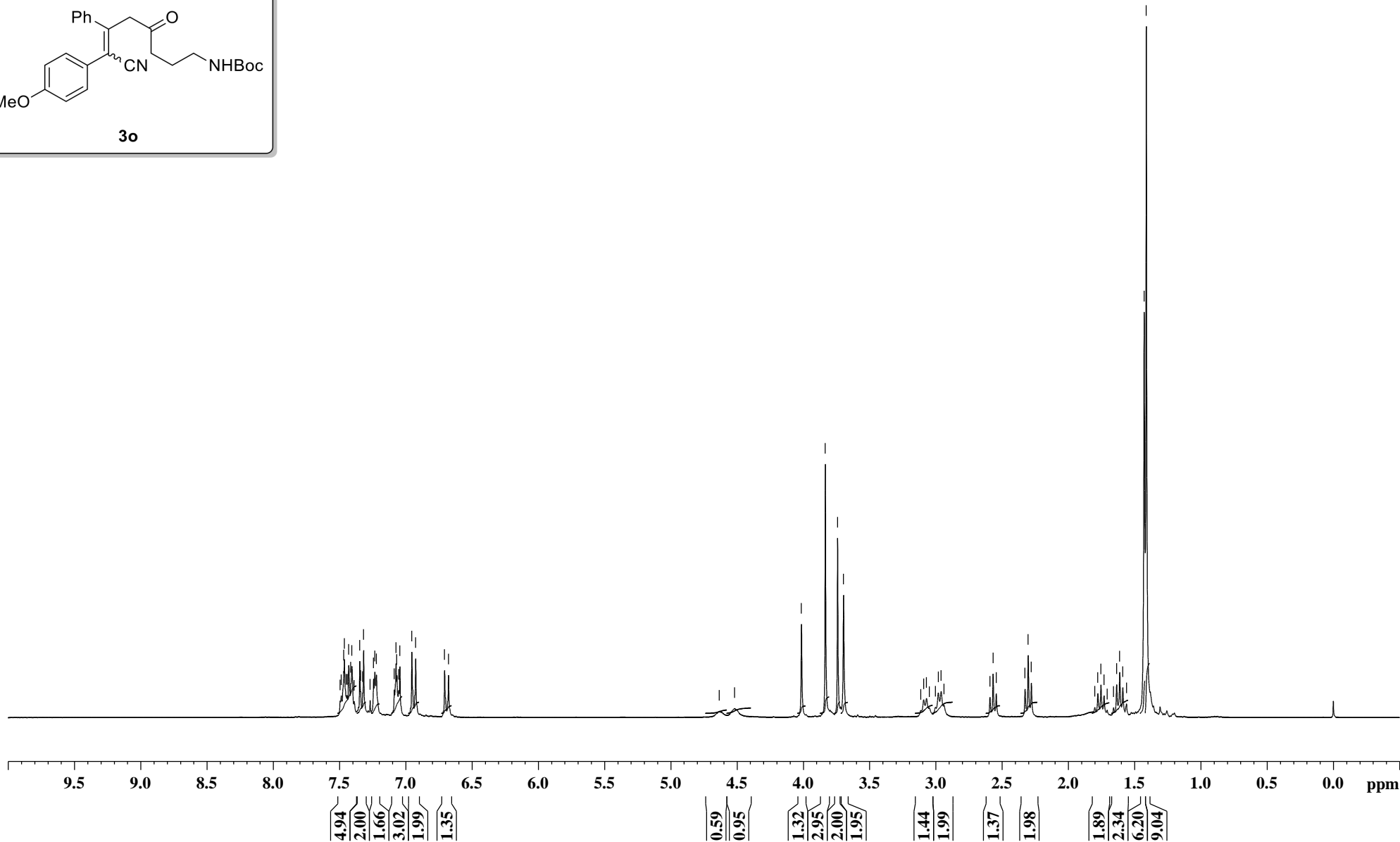


1H NMR (300 MHz, CDCl3)

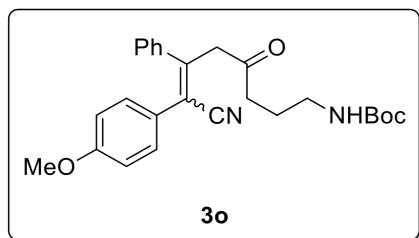


7.496
7.487
7.468
7.464
7.450
7.442
7.431
7.415
7.407
7.391
7.348
7.341
7.325
7.319
7.270
7.243
7.234
7.222
7.087
7.074
7.068
7.052
7.045
6.955
6.926
6.707
6.678

4.634
4.518
4.014
3.834
3.741
3.697
3.113
3.092
3.071
3.050
3.003
2.982
2.960
2.939
2.592
2.568
2.544
2.327
2.303
2.279
1.801
1.777
1.754
1.731
1.707
1.659
1.636
1.612
1.589
1.561
1.428
1.412



13C NMR (75 MHz, CDCl₃)



205.649
204.669

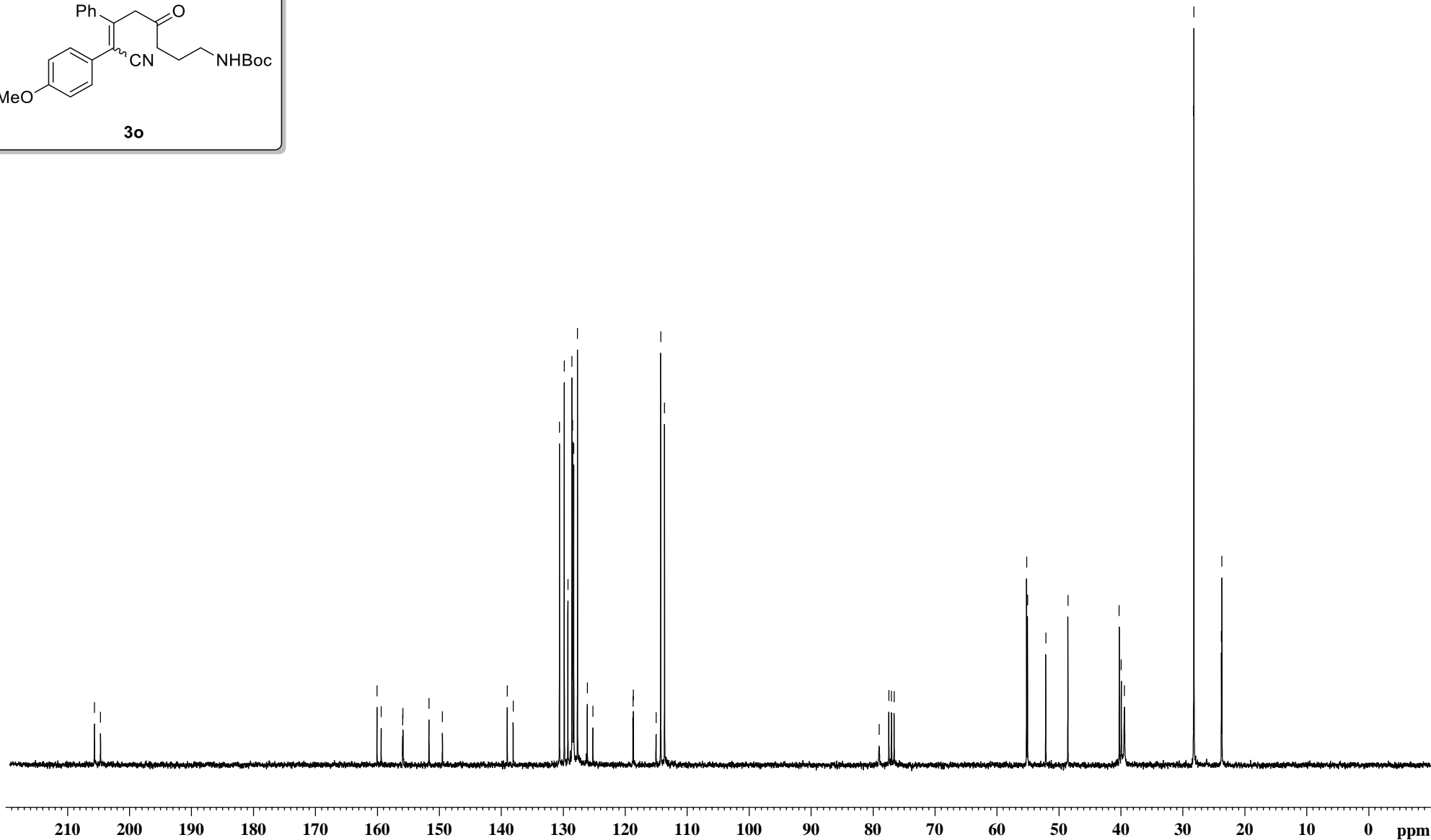
160.037
159.363
155.905
155.845
151.654
149.484
139.017
138.063
130.591
129.810
129.231
128.580
128.526
128.483
128.284
127.676
126.096
125.204
118.723
118.664
114.992
114.255
113.628

78.986
77.423
77.000
76.576

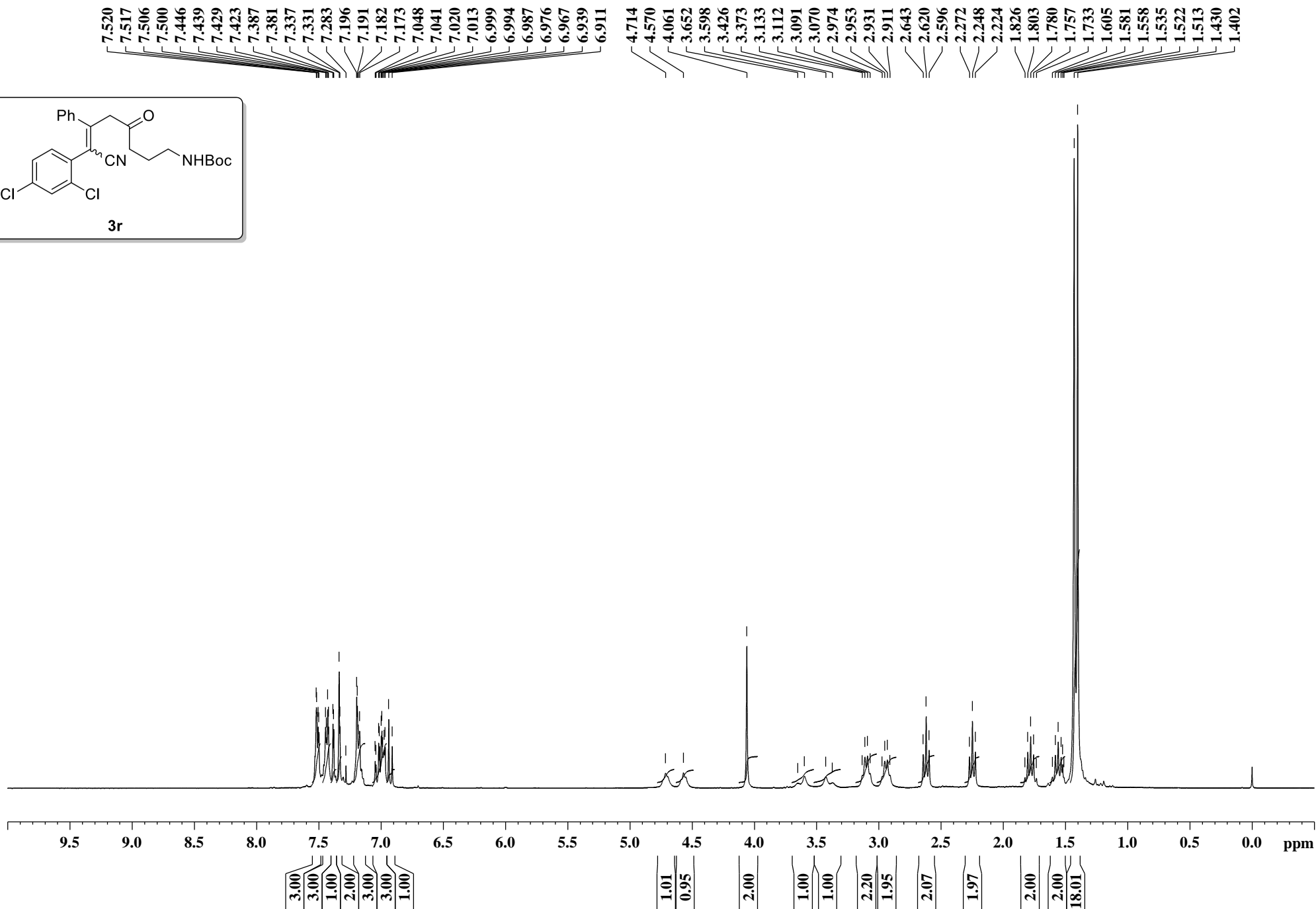
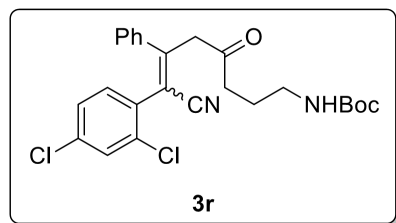
55.196
55.035
52.094
48.524

40.256
39.930
39.416

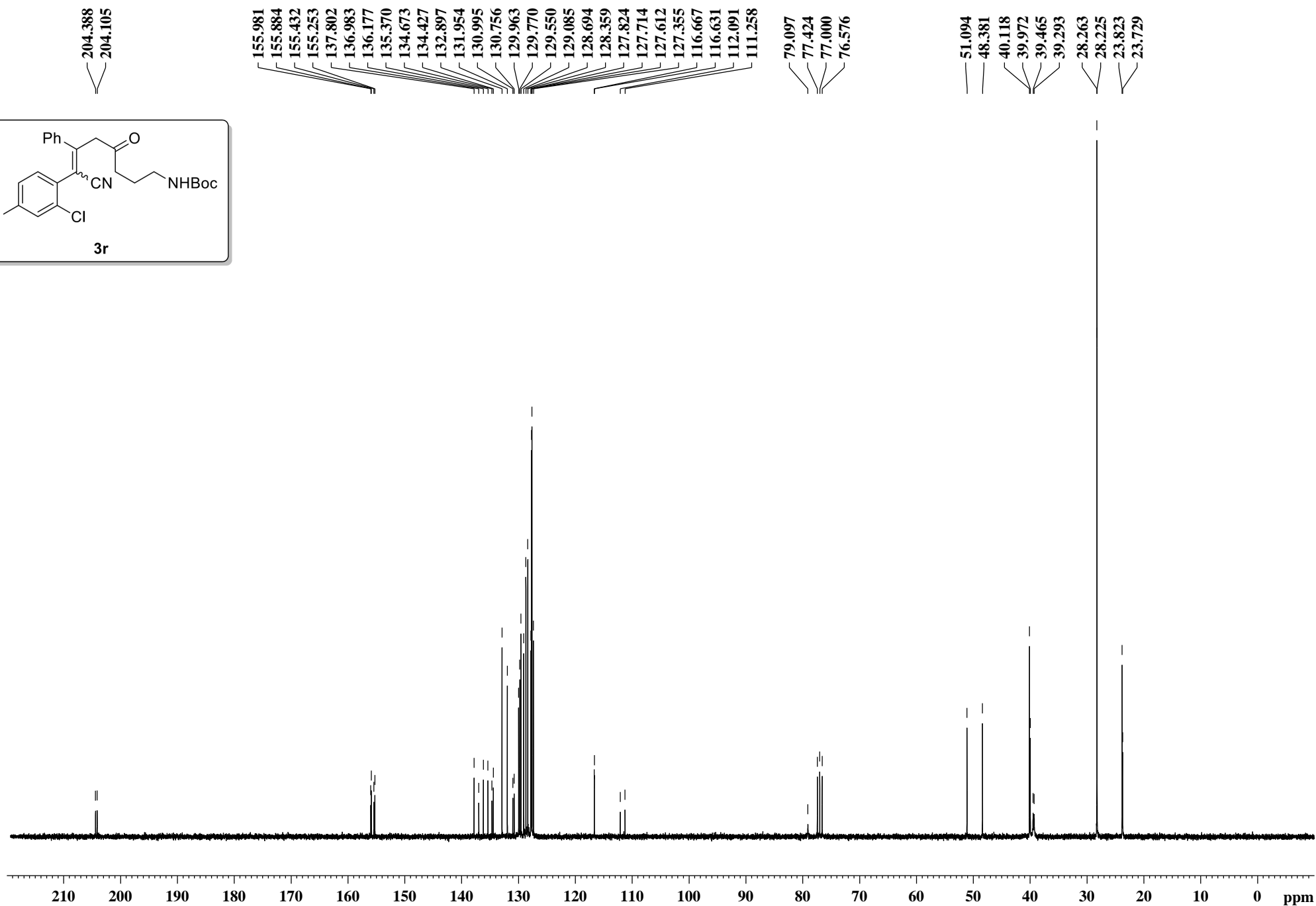
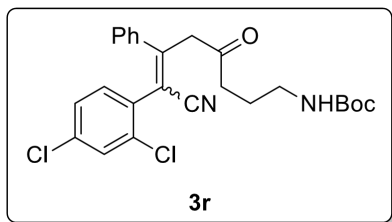
28.226
28.208
23.775
23.696



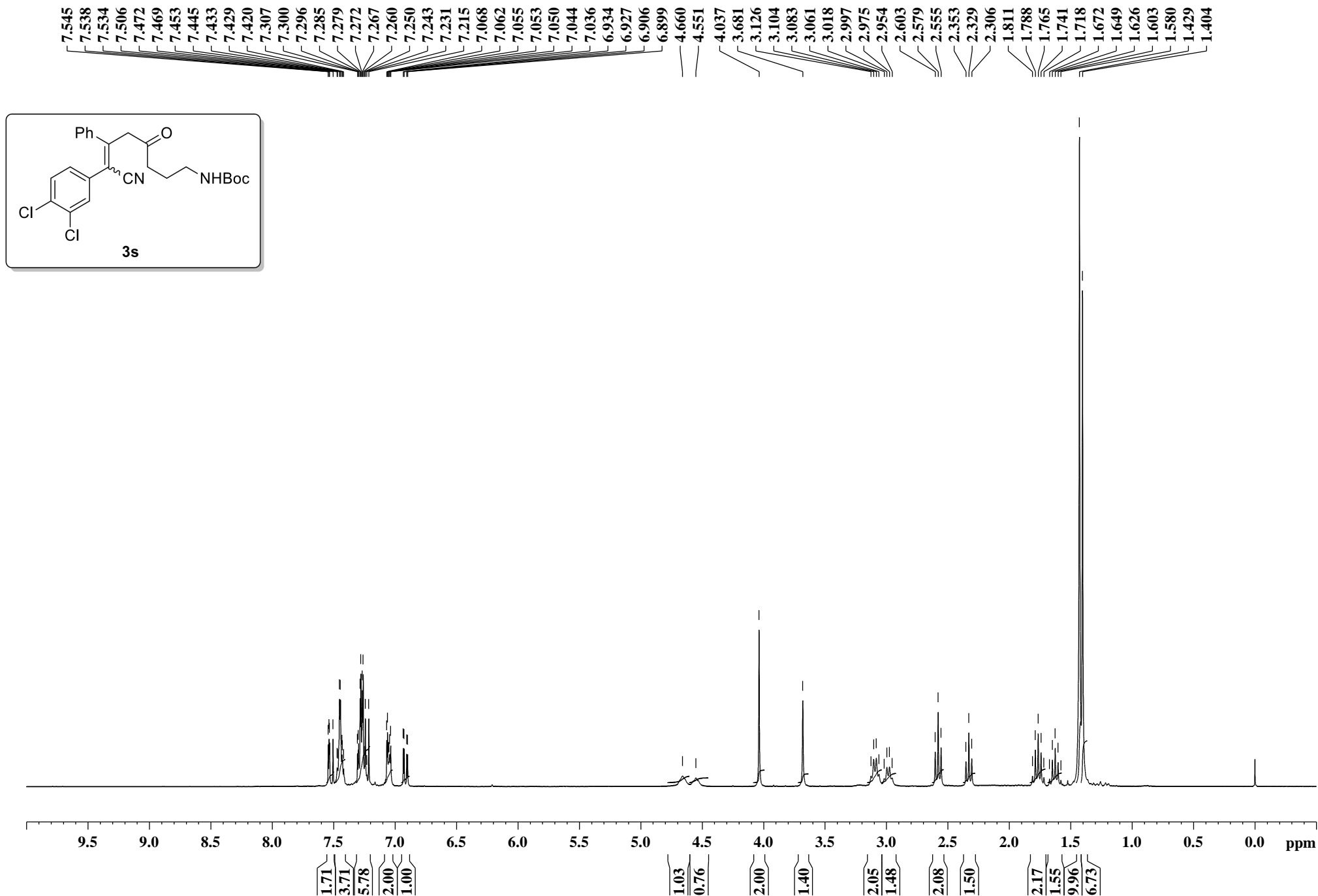
¹H NMR (300 MHz, CDCl₃)



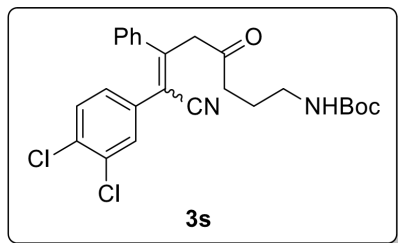
¹³C NMR (75 MHz, CDCl₃)



¹H NMR (300 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)

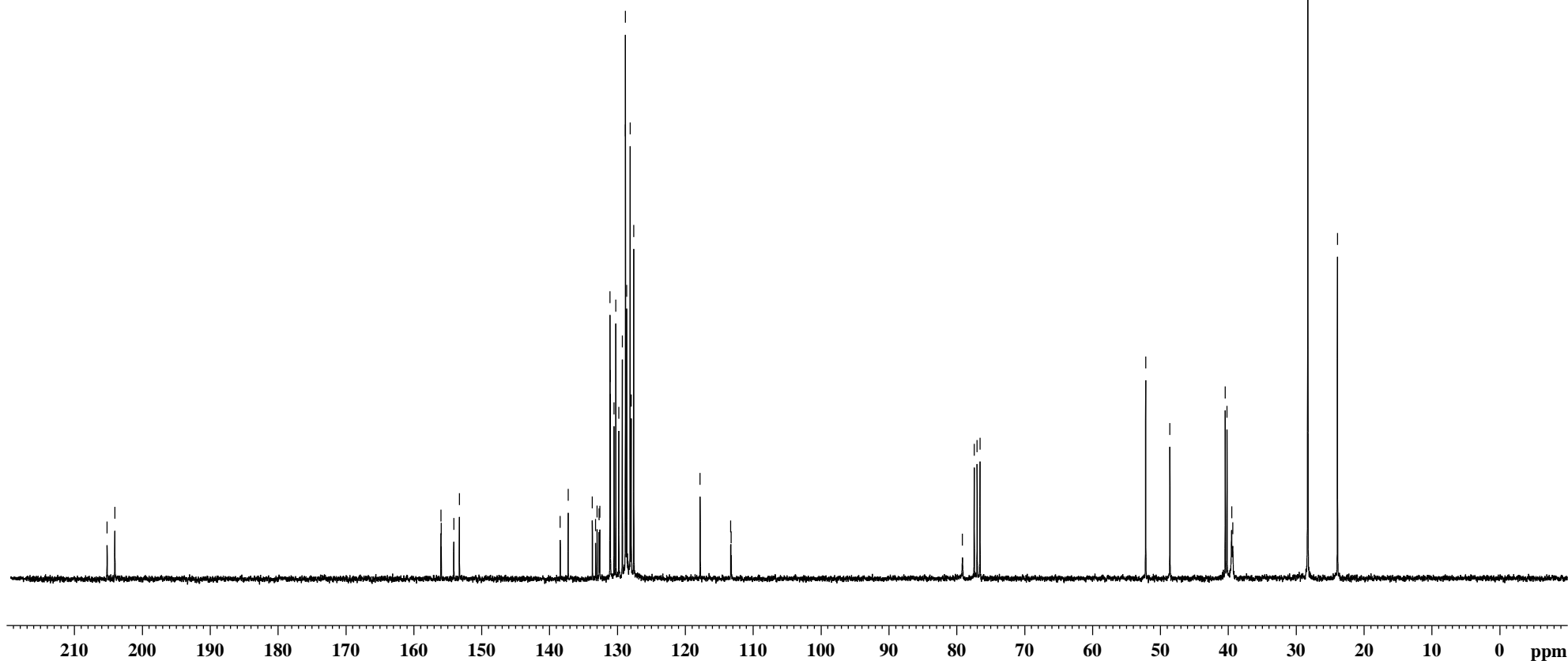


205.187
204.047

156.003
155.949
154.108
153.278
138.418
137.258
133.688
133.214
132.995
132.688
132.601
131.092
131.042
130.491
130.238
129.793
129.273
128.824
128.807
128.636
128.115
127.977
127.600
117.810
113.300
113.228

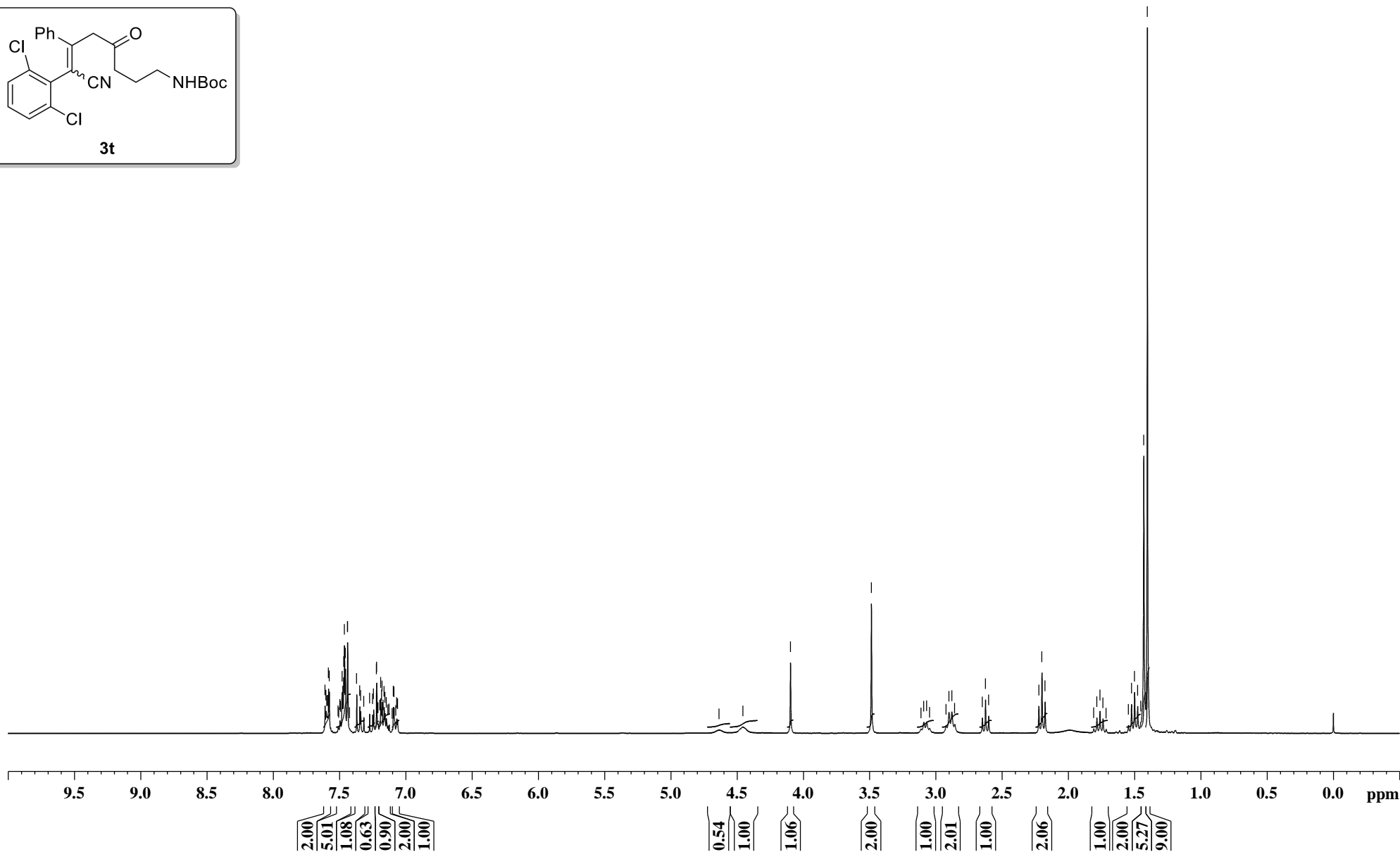
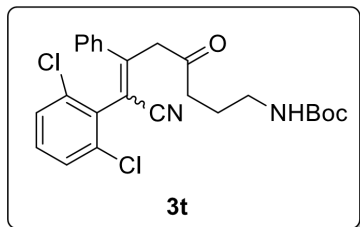
79.155
77.424
77.000
76.576

52.167
48.595
40.442
40.187
39.496
39.330
28.293
28.259
23.907

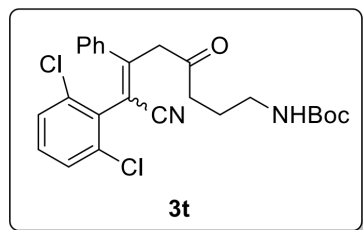


¹H NMR (300 MHz, CDCl₃)

7.610
7.602
7.596
7.593
7.591
7.583
7.578
7.511
7.505
7.497
7.492
7.480
7.474
7.469
7.464
7.456
7.440
7.439
7.371
7.347
7.340
7.317
7.273
7.250
7.243
7.221
7.219
7.213
7.209
7.196
7.190
7.183
7.178
7.170
7.164
7.157
7.147
7.135
7.126
7.094
7.090
7.075
7.068
7.062
4.456
4.097
3.486
3.091
3.069
3.048
2.923
2.901
2.879
2.857
2.649
2.625
2.602
2.223
2.199
2.176
1.808
1.785
1.762
1.738
1.546
1.523
1.500
1.477
1.453
1.431
1.404



13C NMR (75 MHz, CDCl3)

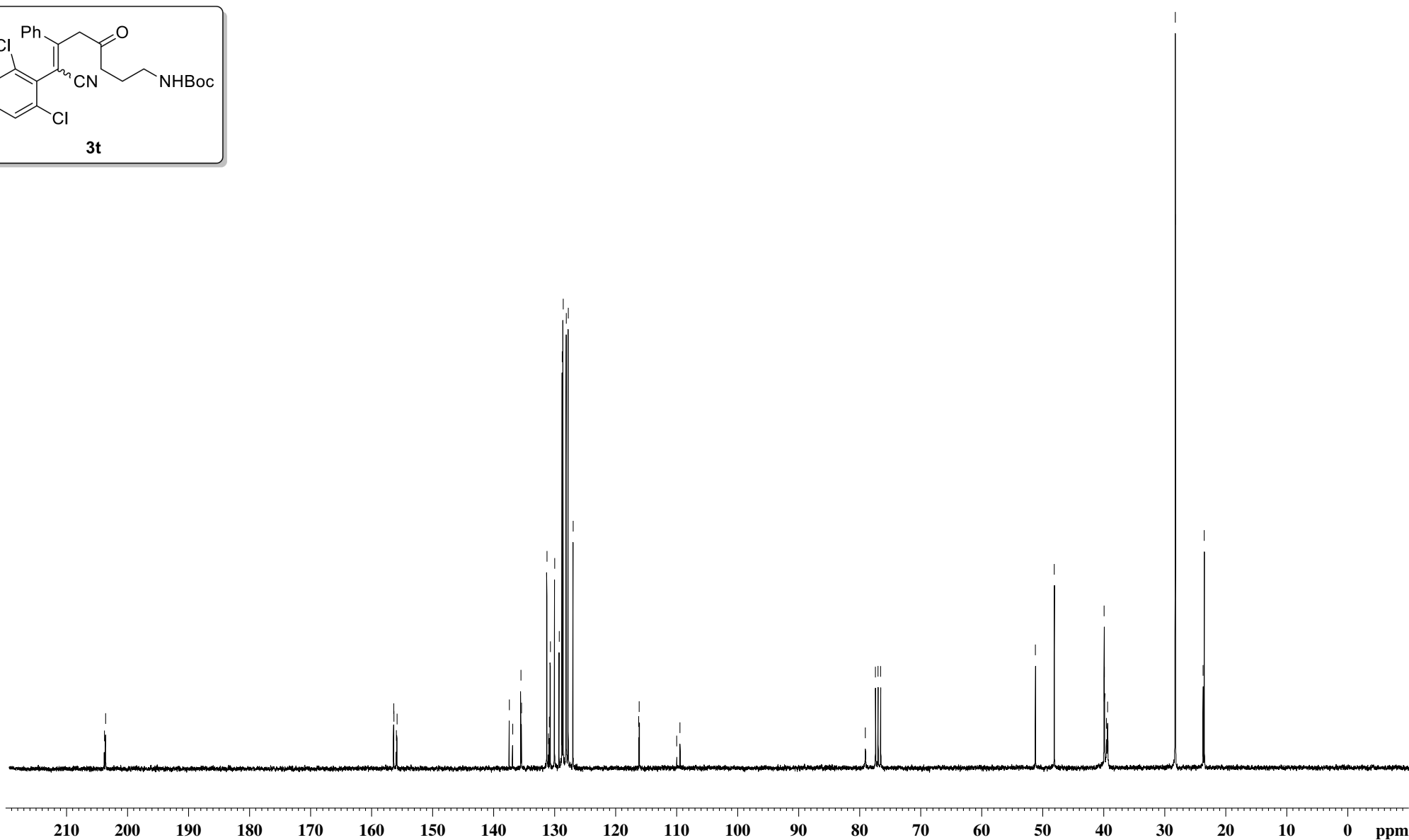


203.790
203.595

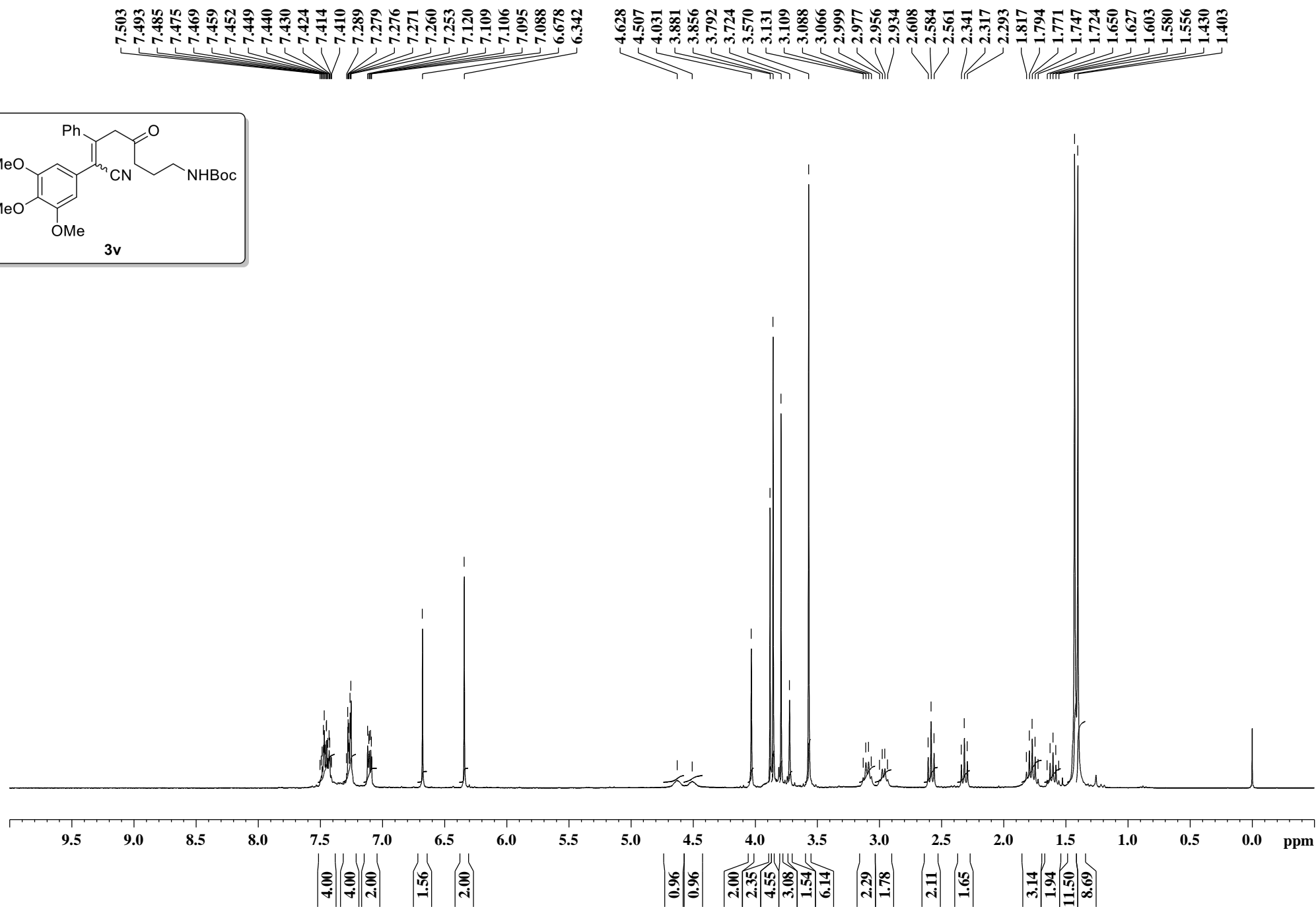
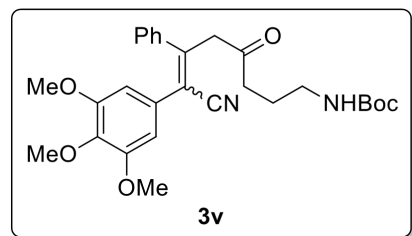
156.376
156.345
155.941
155.823
137.424
136.872
135.522
135.427
131.254
131.017
130.869
130.692
129.993
129.244
128.759
128.594
128.091
127.763
126.964
116.229
116.147
109.997
109.465

79.082
77.424
77.000
76.576

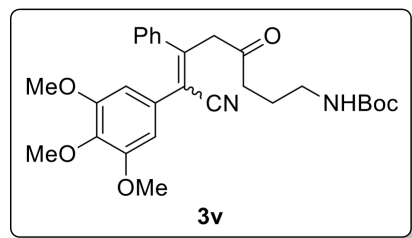
51.206
48.113
39.943
39.892
39.557
39.372
28.289
28.273
23.723
23.533



¹H NMR (300 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)

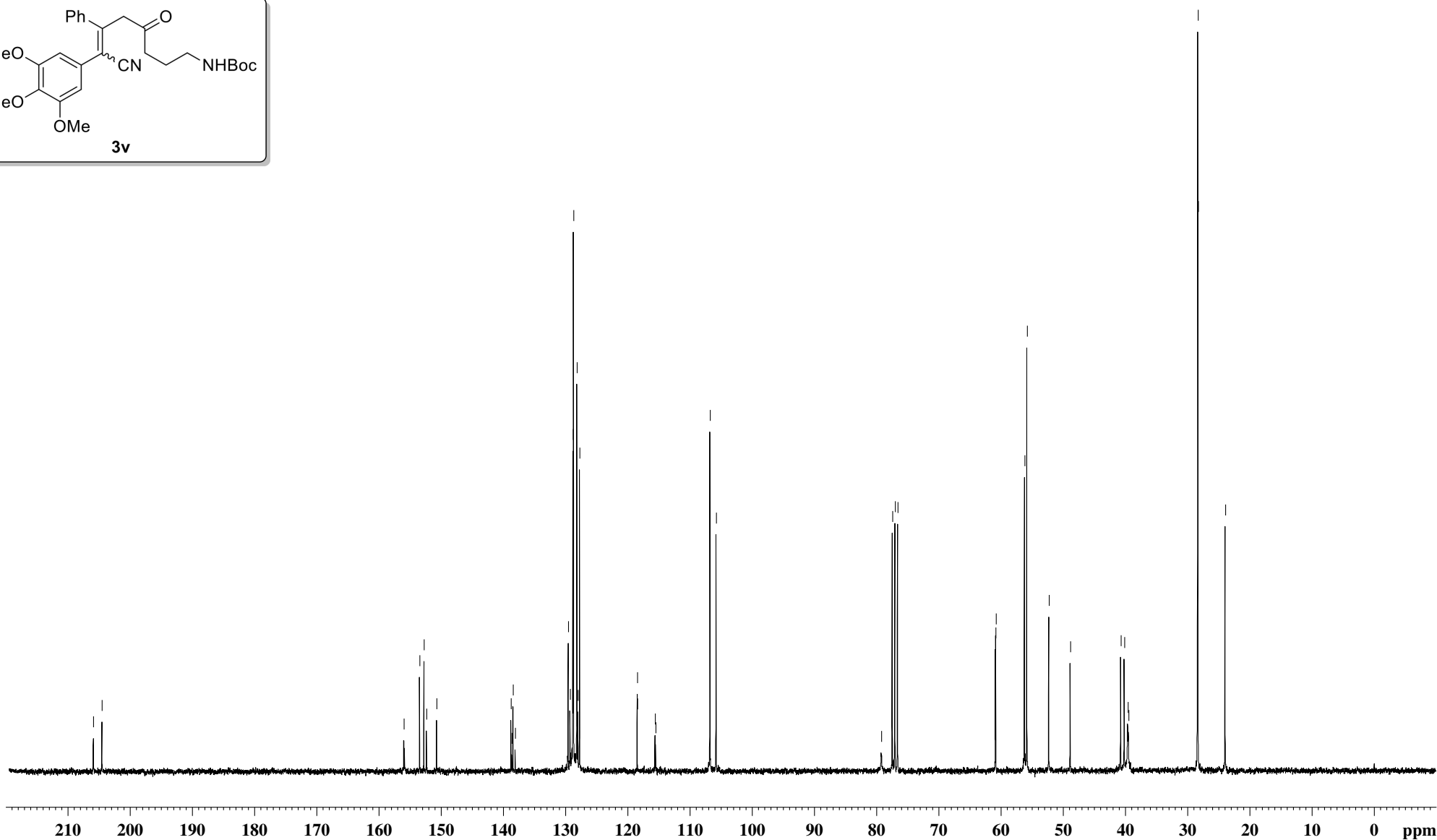


205.896
204.518

155.972
153.438
152.743
152.329
150.701
138.755
138.629
138.424
138.070
129.542
129.244
128.782
128.693
128.150
127.988
127.716
118.444
118.424
115.585
115.487
106.750
105.762

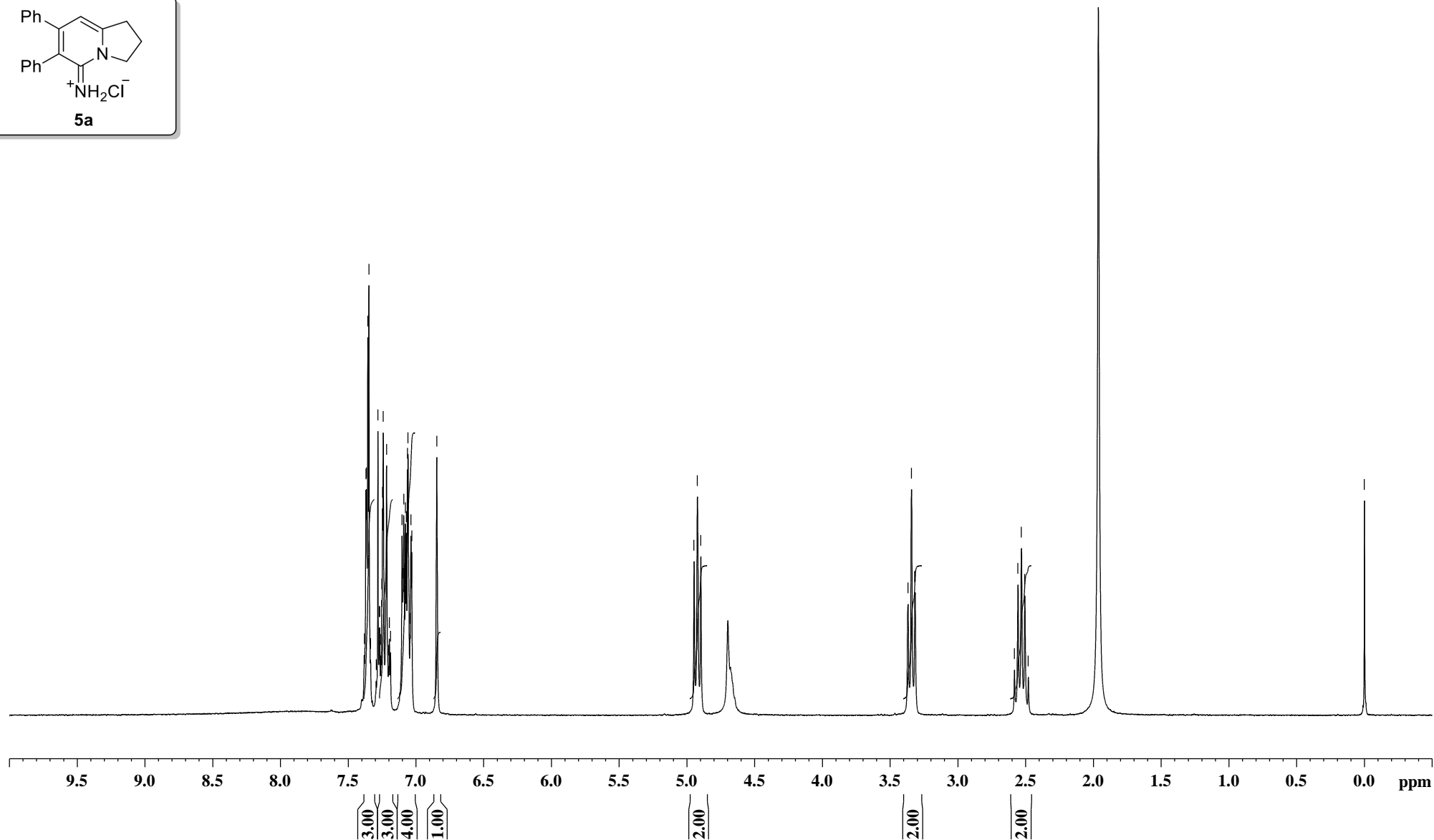
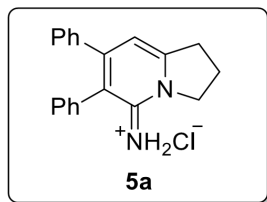
79.208
77.424
77.000
76.576

60.834
60.781
56.171
55.776
52.262
48.823
40.702
40.131
39.570
39.459
28.307
28.272
23.904

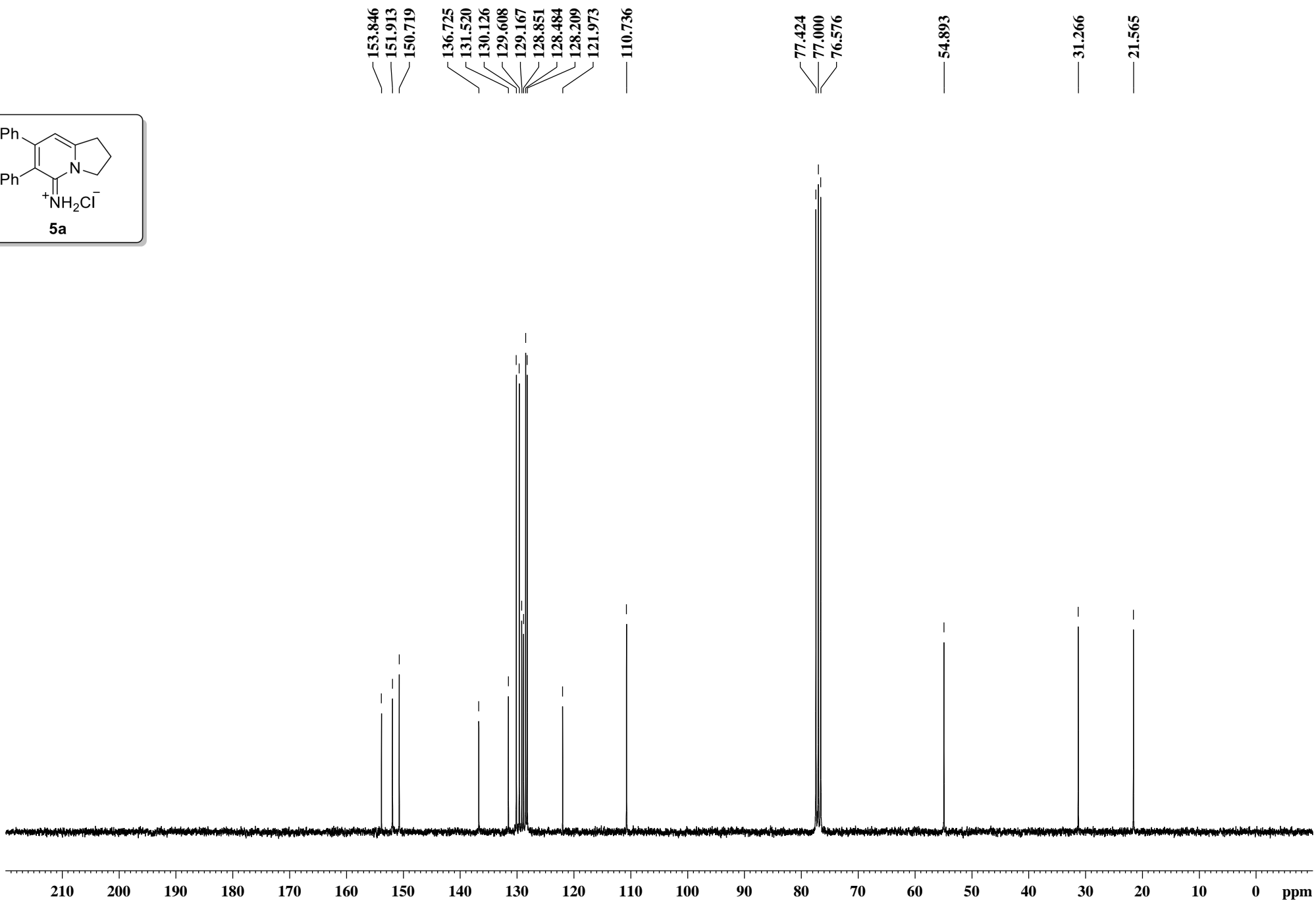
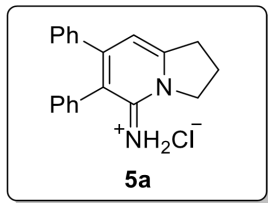


¹H NMR (300 MHz, CDCl₃)

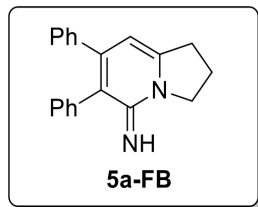
7.381
7.369
7.365
7.354
7.347
7.334
7.293
7.280
7.269
7.267
7.258
7.251
7.246
7.240
7.216
7.201
7.195
7.187
7.102
7.094
7.090
7.077
7.070
7.062
7.058
7.043
7.036
7.030
6.845
4.948
4.923
4.898
3.368
3.343
3.318
3.316
2.583
2.557
2.532
2.507
2.481
-0.000



13C NMR (75 MHz, CDCl3)



1H NMR (300 MHz, CDCl3)



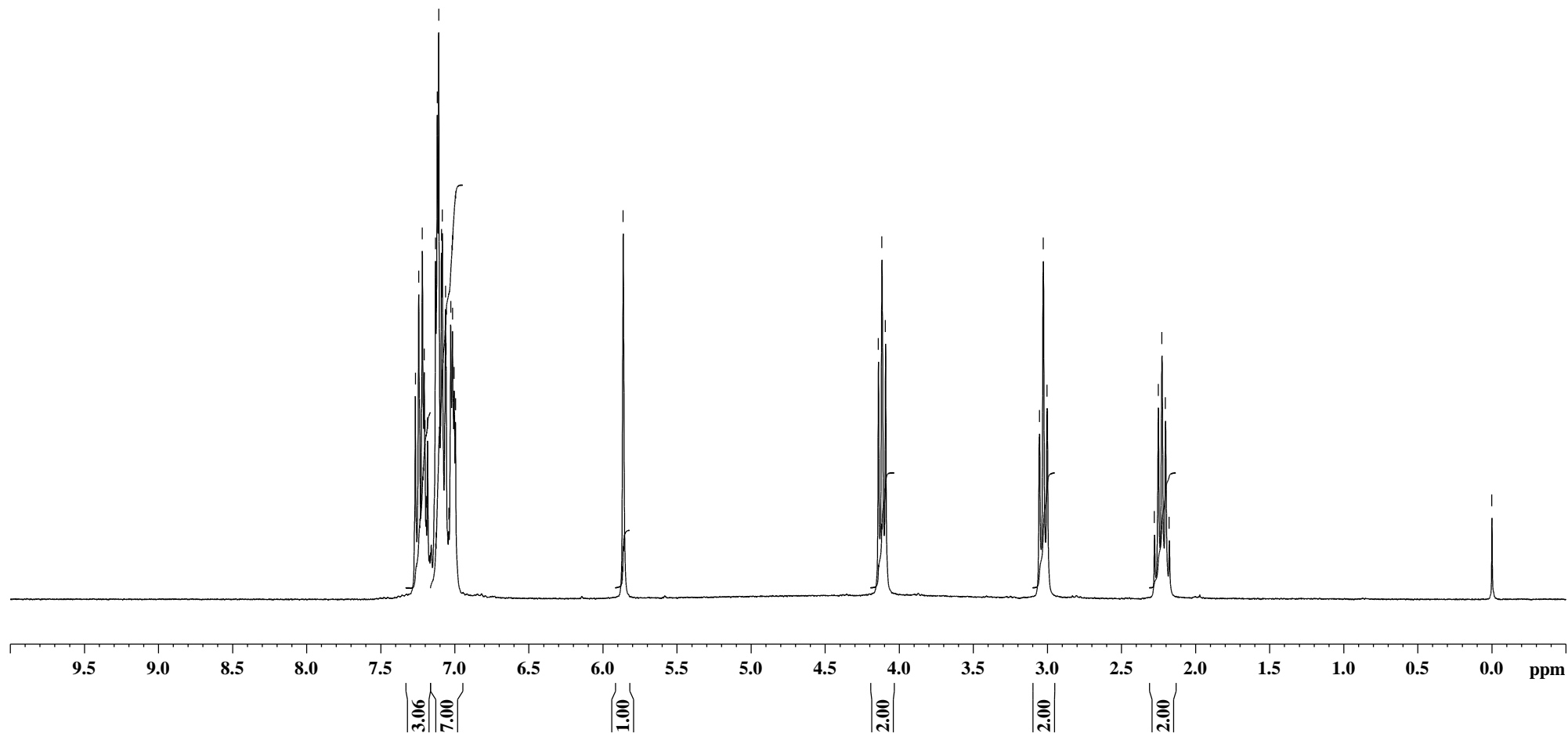
7.265
7.243
7.218
7.206
7.201
7.192
7.183
7.129
7.117
7.108
7.089
7.083
7.062
7.058
7.040
7.027
7.015
7.004
6.995
5.864

4.141
4.117
4.093

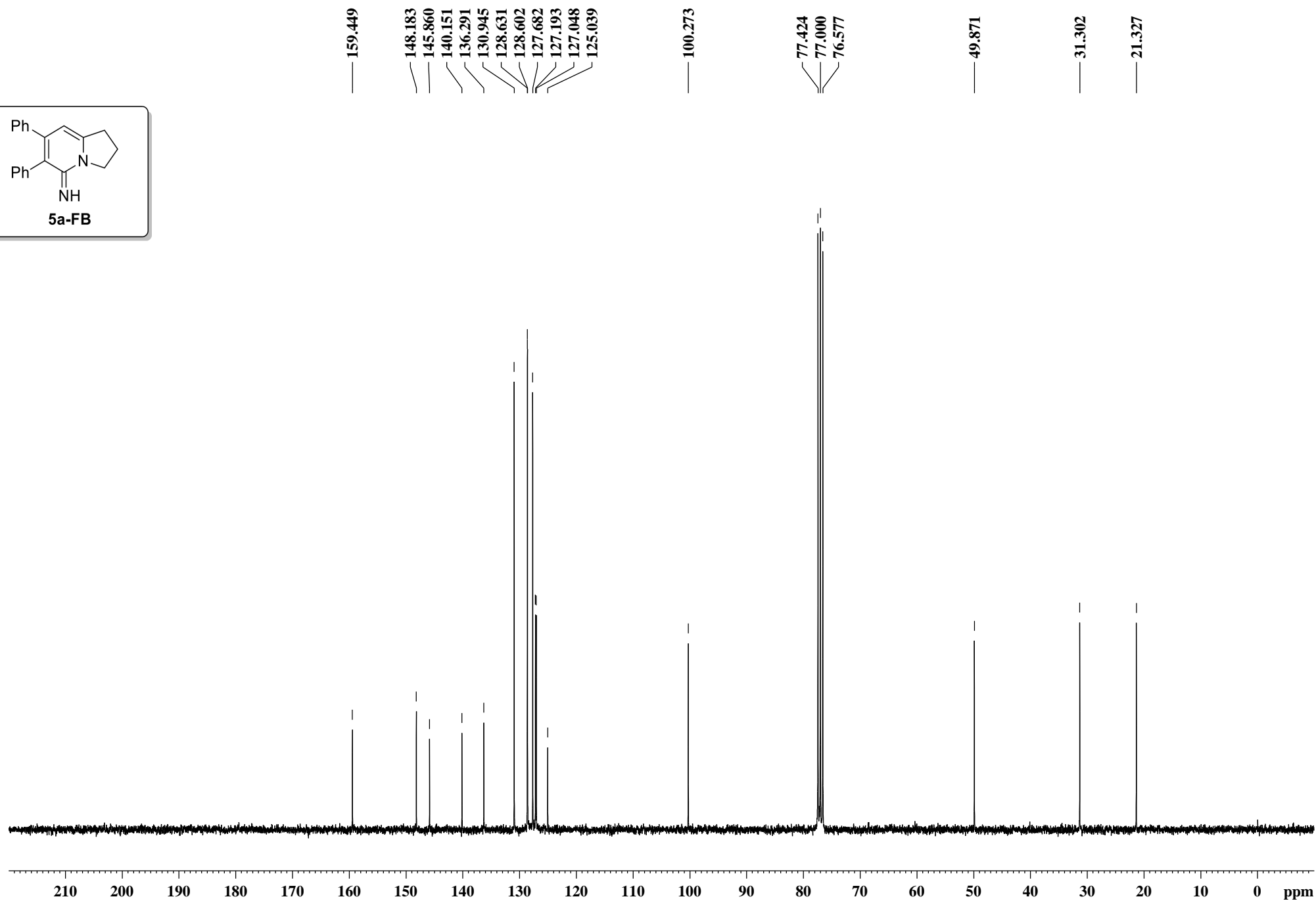
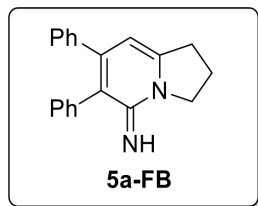
3.054
3.028
3.002

2.278
2.252
2.227
2.203
2.178

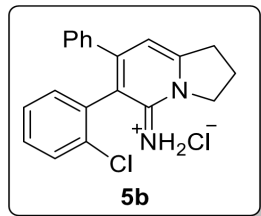
-0.000



13C NMR (75 MHz, CDCl3)



¹H NMR (300 MHz, CDCl₃)



7.453
7.427
7.362
7.338
7.311
7.283
7.257
7.232
7.211
7.112
7.087
7.062
6.848

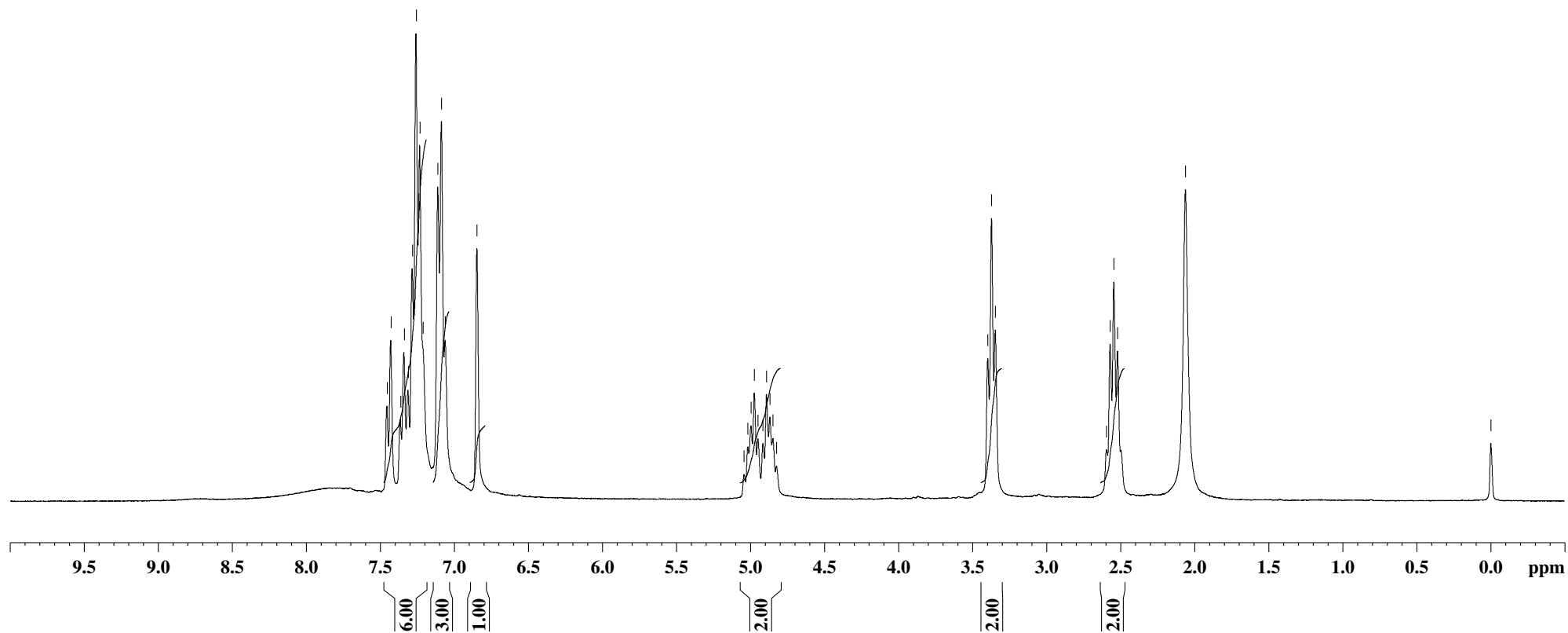
5.044
5.019
4.997
4.974
4.950
4.917
4.892
4.869
4.849
4.824

3.398
3.372
3.347

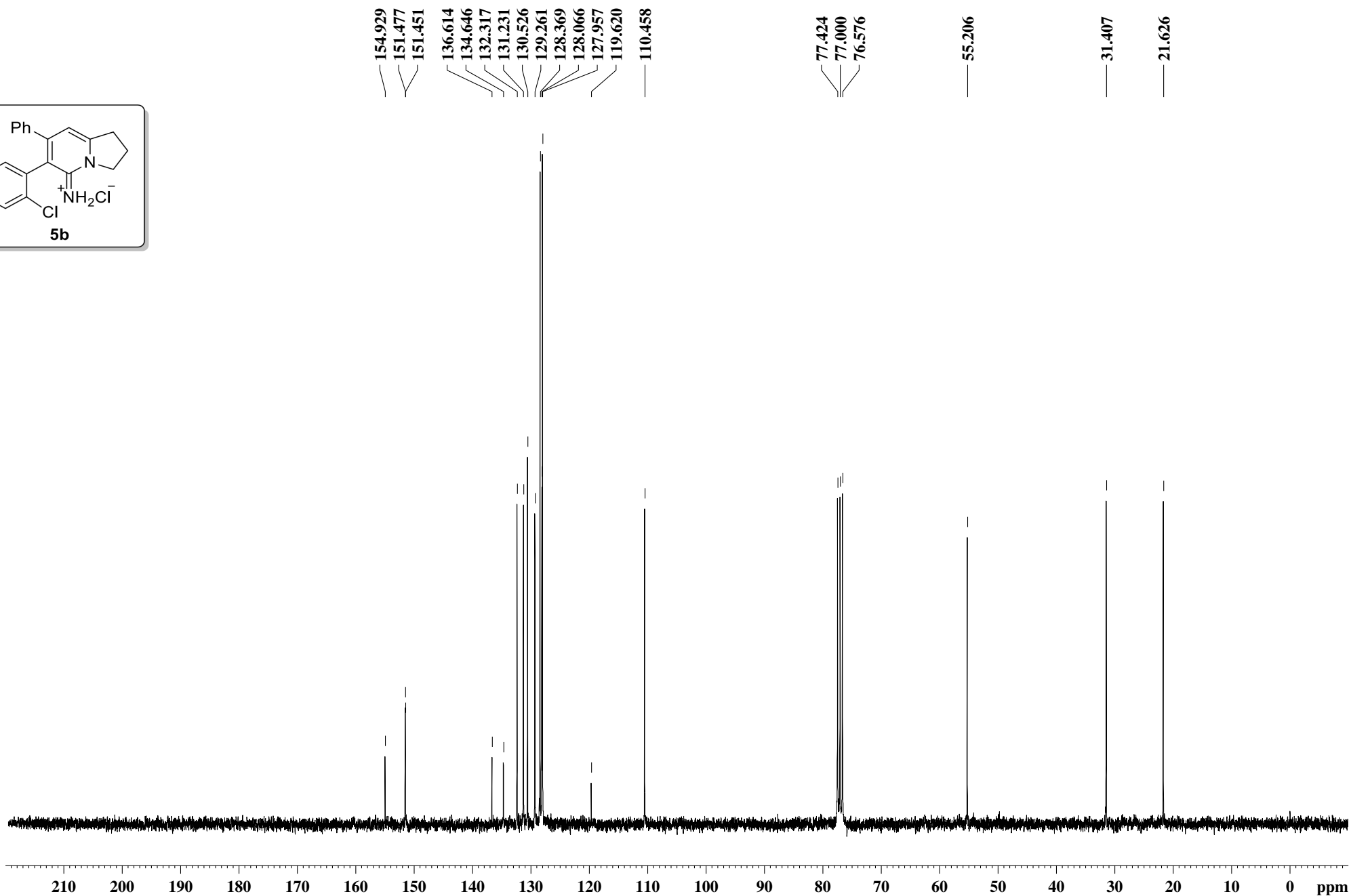
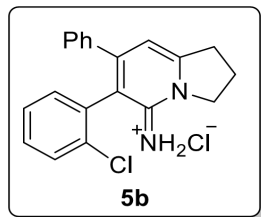
2.596
2.571
2.546
2.521

2.063

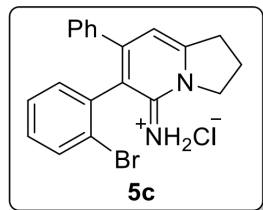
-0.000



¹³C NMR (75 MHz, CDCl₃)



^1H NMR (300 MHz, CDCl_3)



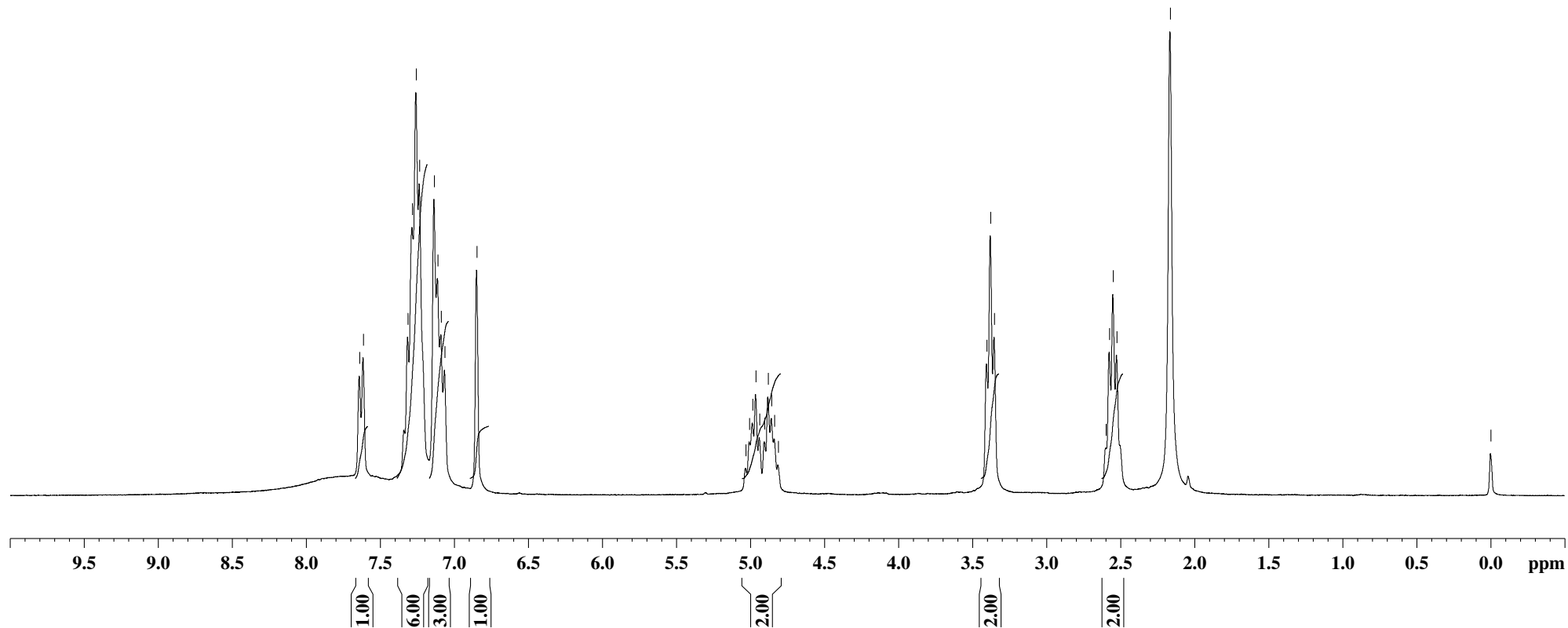
7.640
7.614
7.314
7.283
7.258
7.235
7.135
7.111
7.089
7.064
6.848

5.031
5.007
4.985
4.963
4.938
4.904
4.880
4.857
4.838
4.812

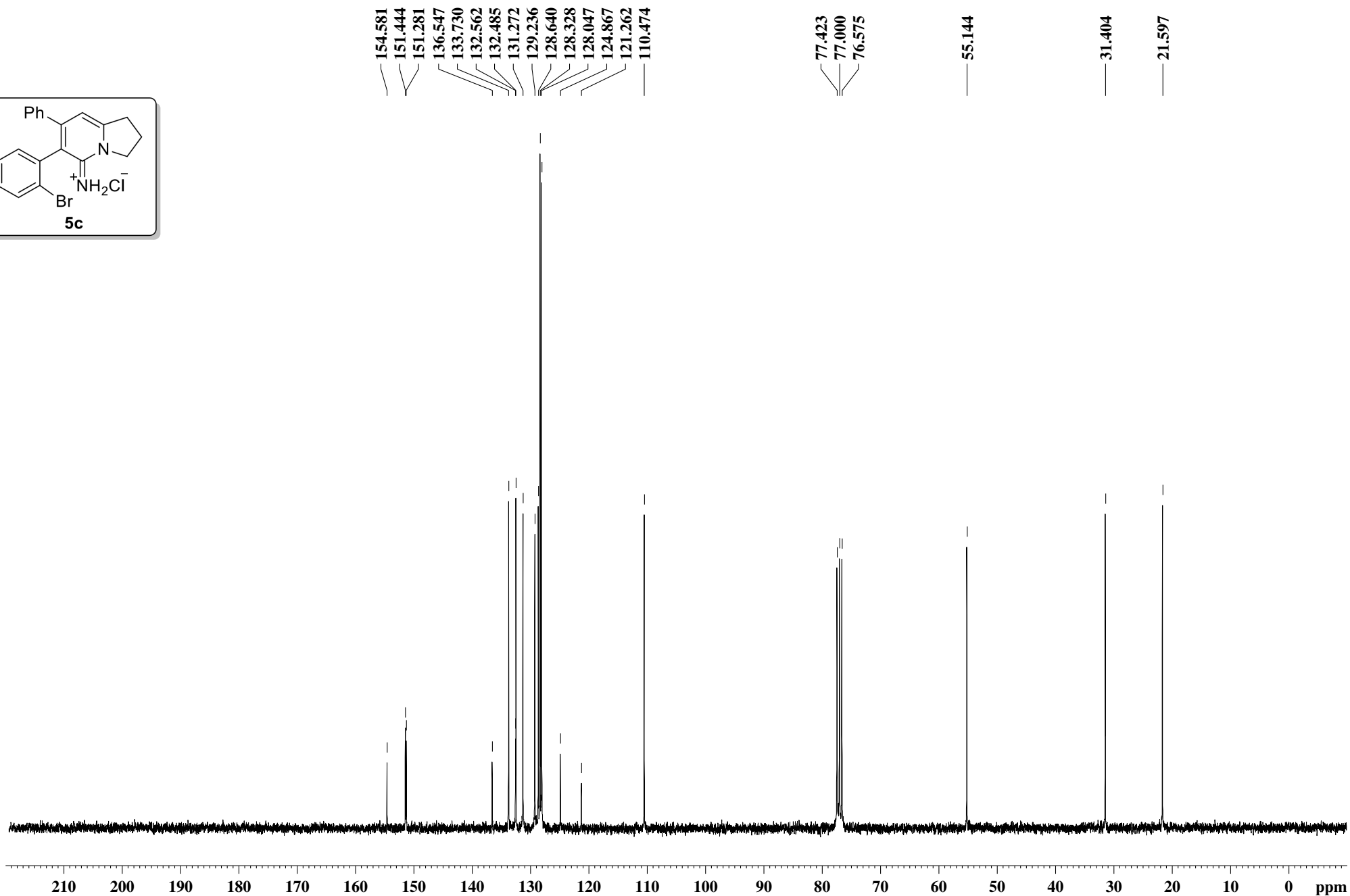
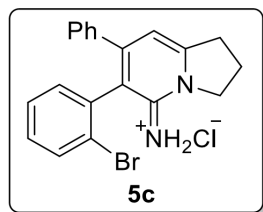
3.404
3.378
3.353

2.599
2.576
2.551
2.526
2.164

-0.000

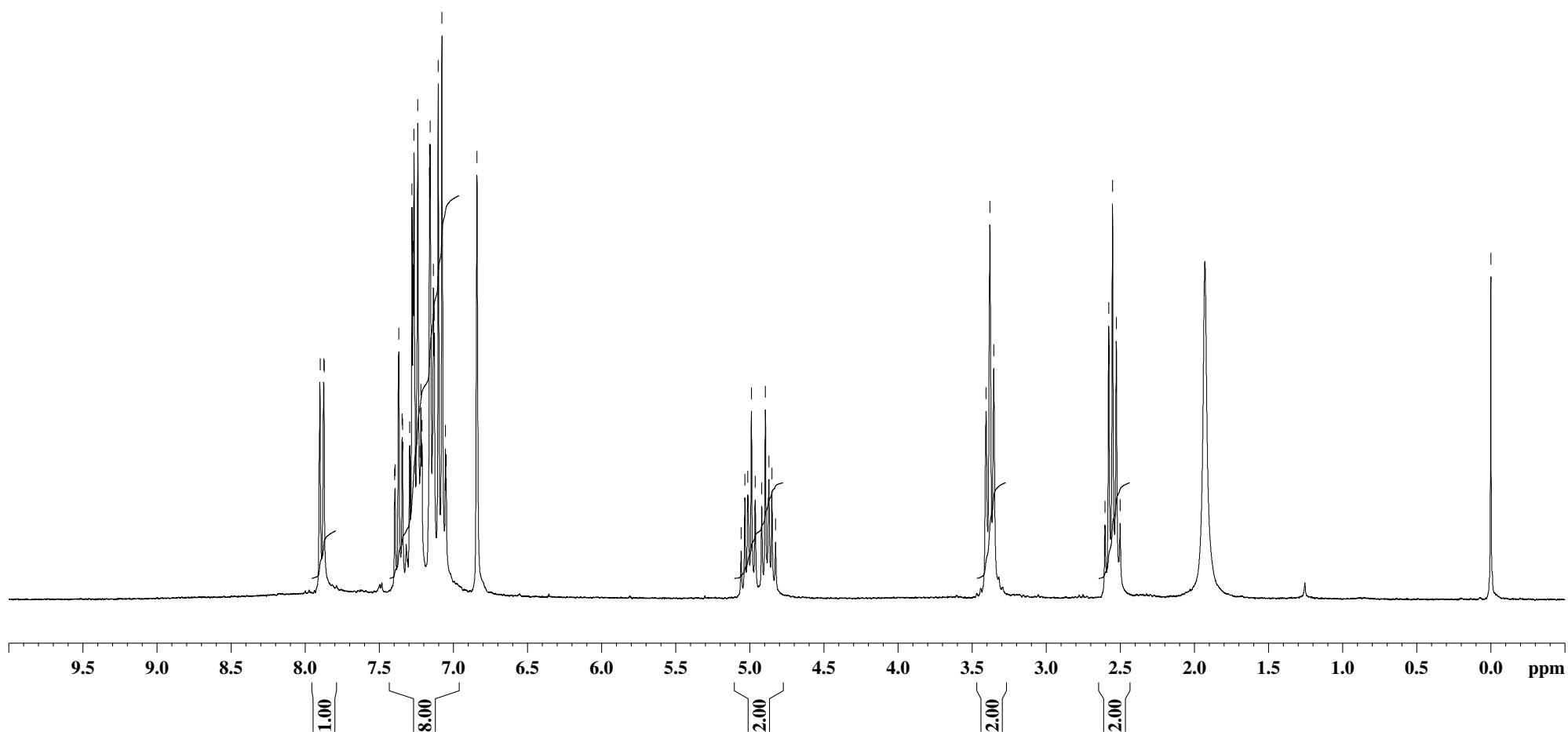
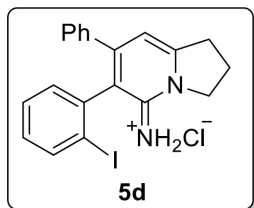


¹³C NMR (75 MHz, CDCl₃)

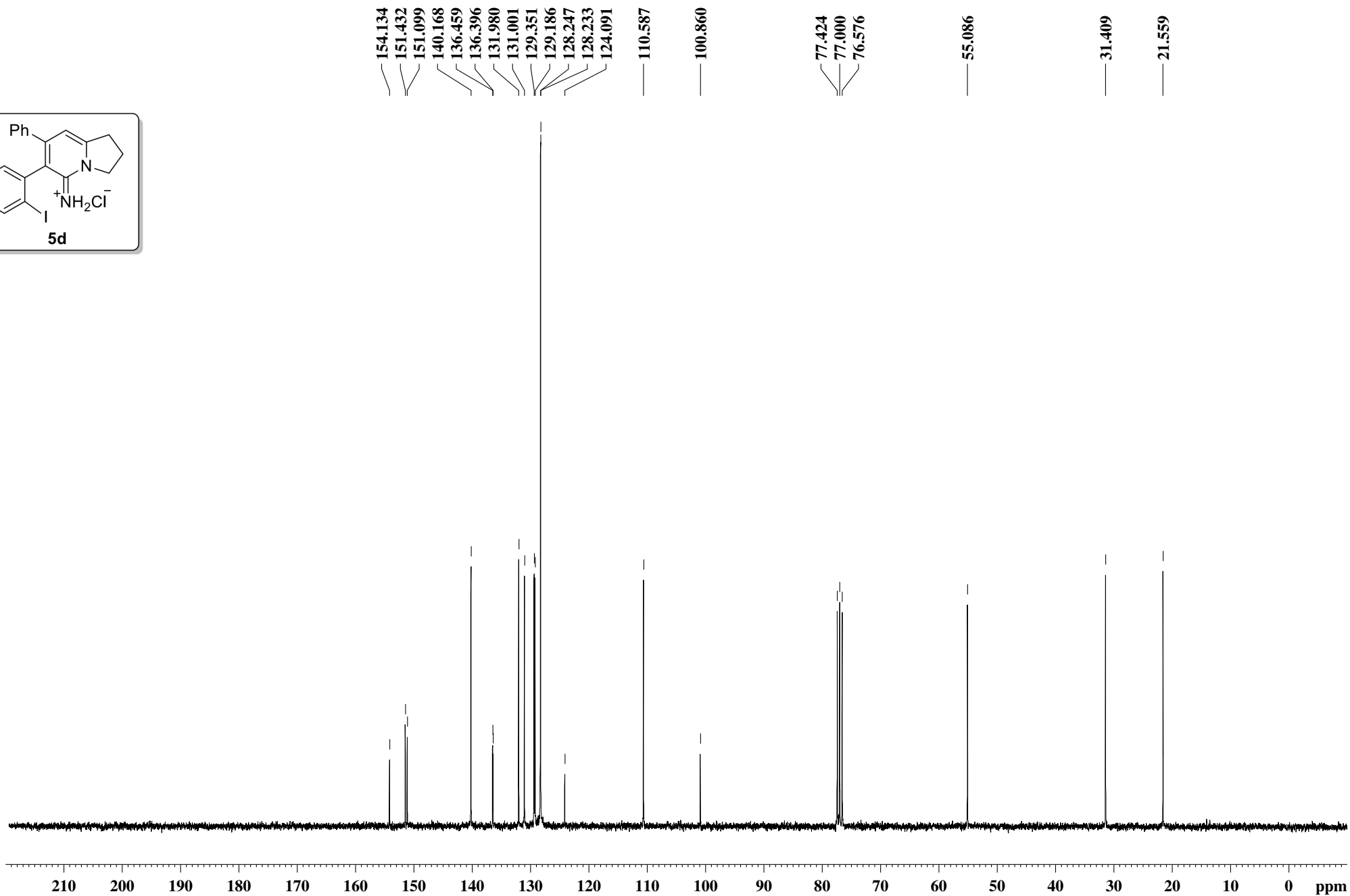
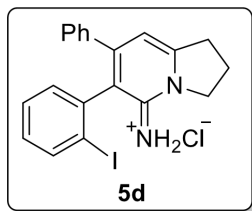


^1H NMR (300 MHz, CDCl_3)

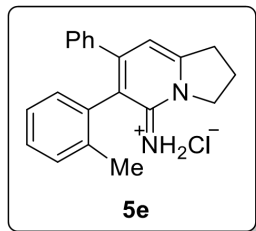
7.901
7.899
7.874
7.872
7.872
7.397
7.394
7.369
7.347
7.343
7.295
7.280
7.273
7.267
7.241
7.226
7.220
7.212
7.161
7.157
7.135
7.130
7.103
7.078
7.054
7.049
6.841
5.059
5.034
5.014
4.989
4.964
4.920
4.895
4.871
4.851
4.826
3.406
3.380
3.354
2.604
2.578
2.553
2.527
2.501
-0.000



¹³C NMR (75 MHz, CDCl₃)



¹H NMR (300 MHz, CDCl₃)

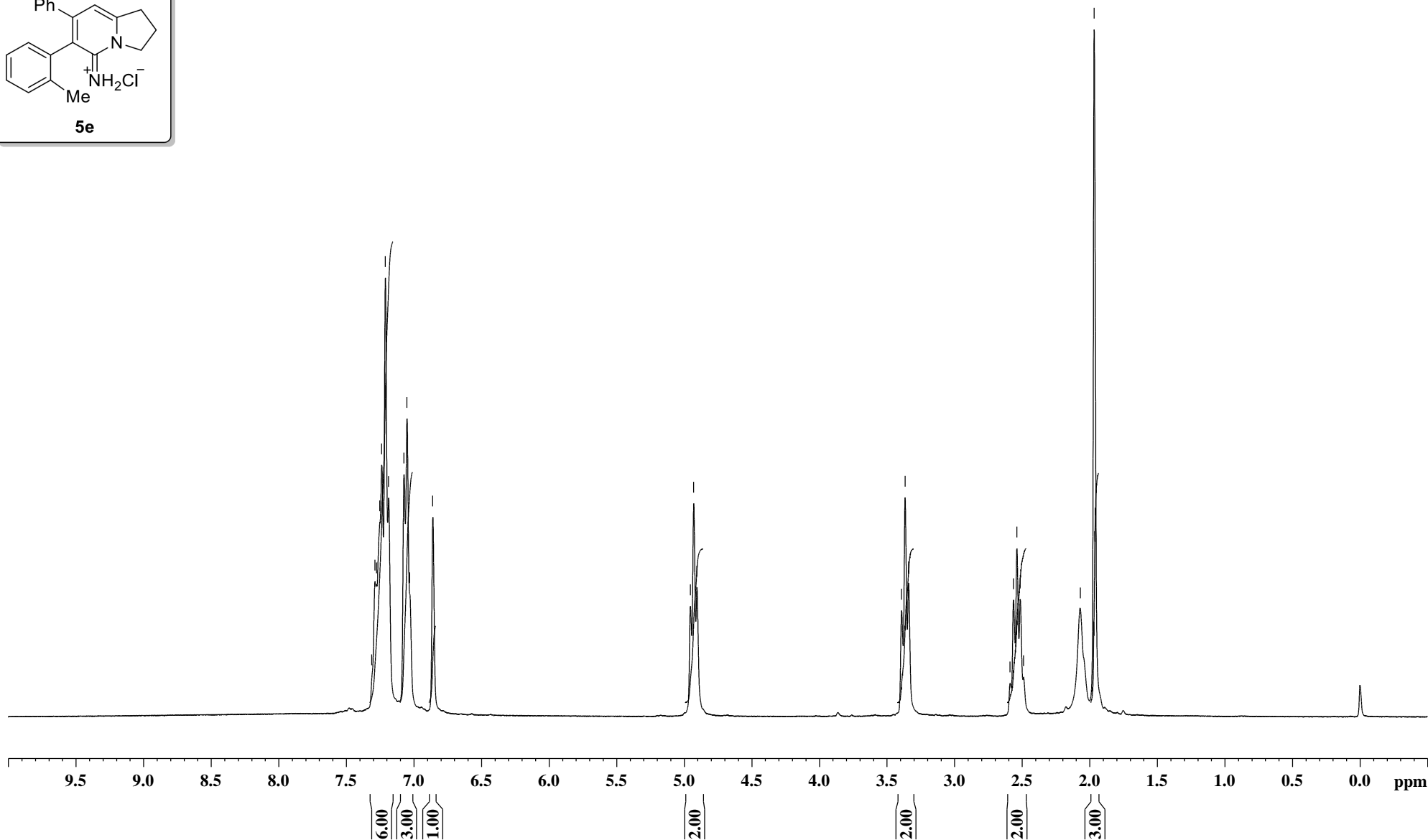


7.312
7.289
7.277
7.253
7.239
7.211
7.187
7.074
7.052
7.031
6.860

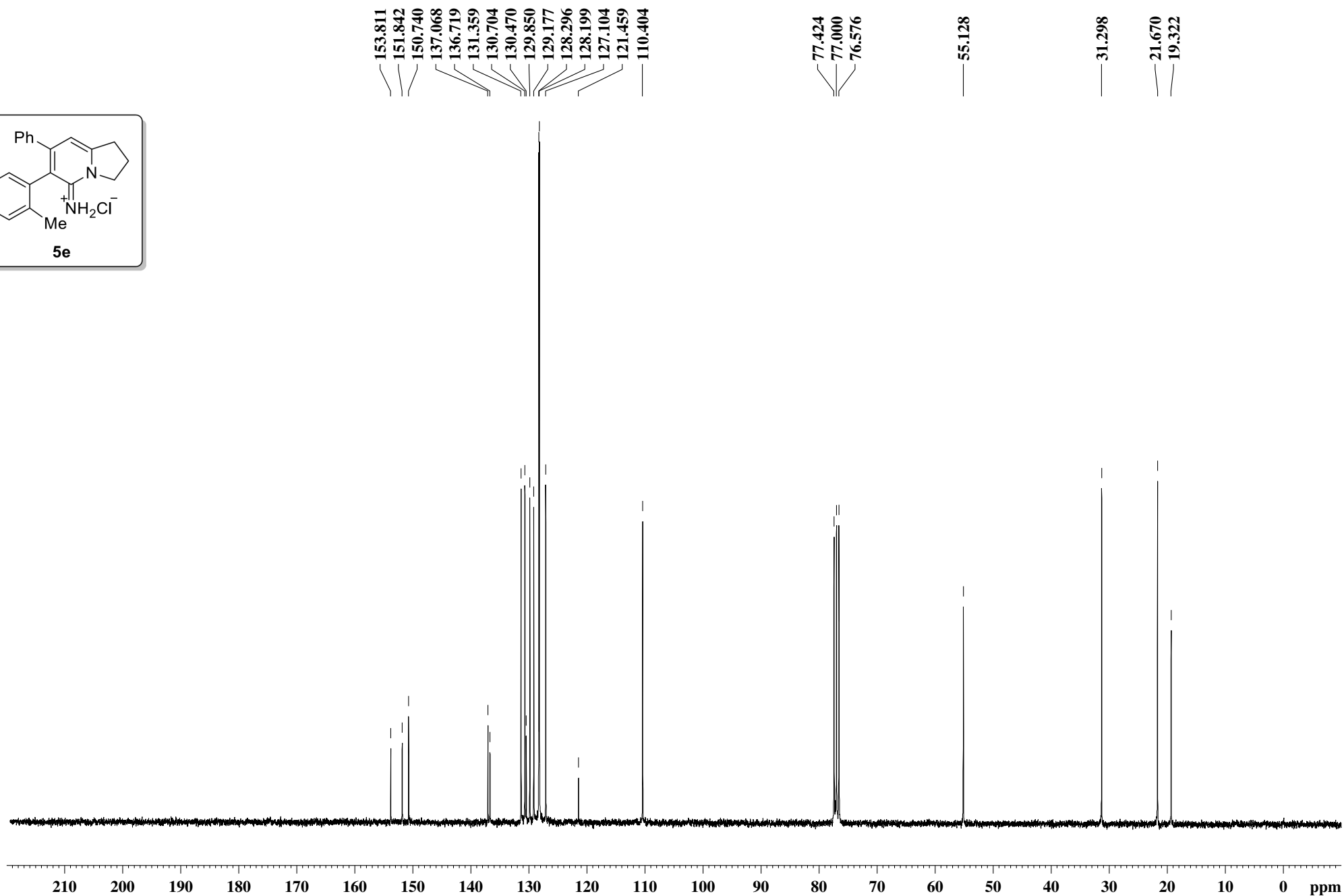
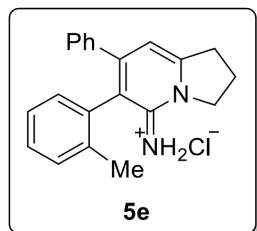
4.955
4.930
4.906

3.392
3.366
3.340

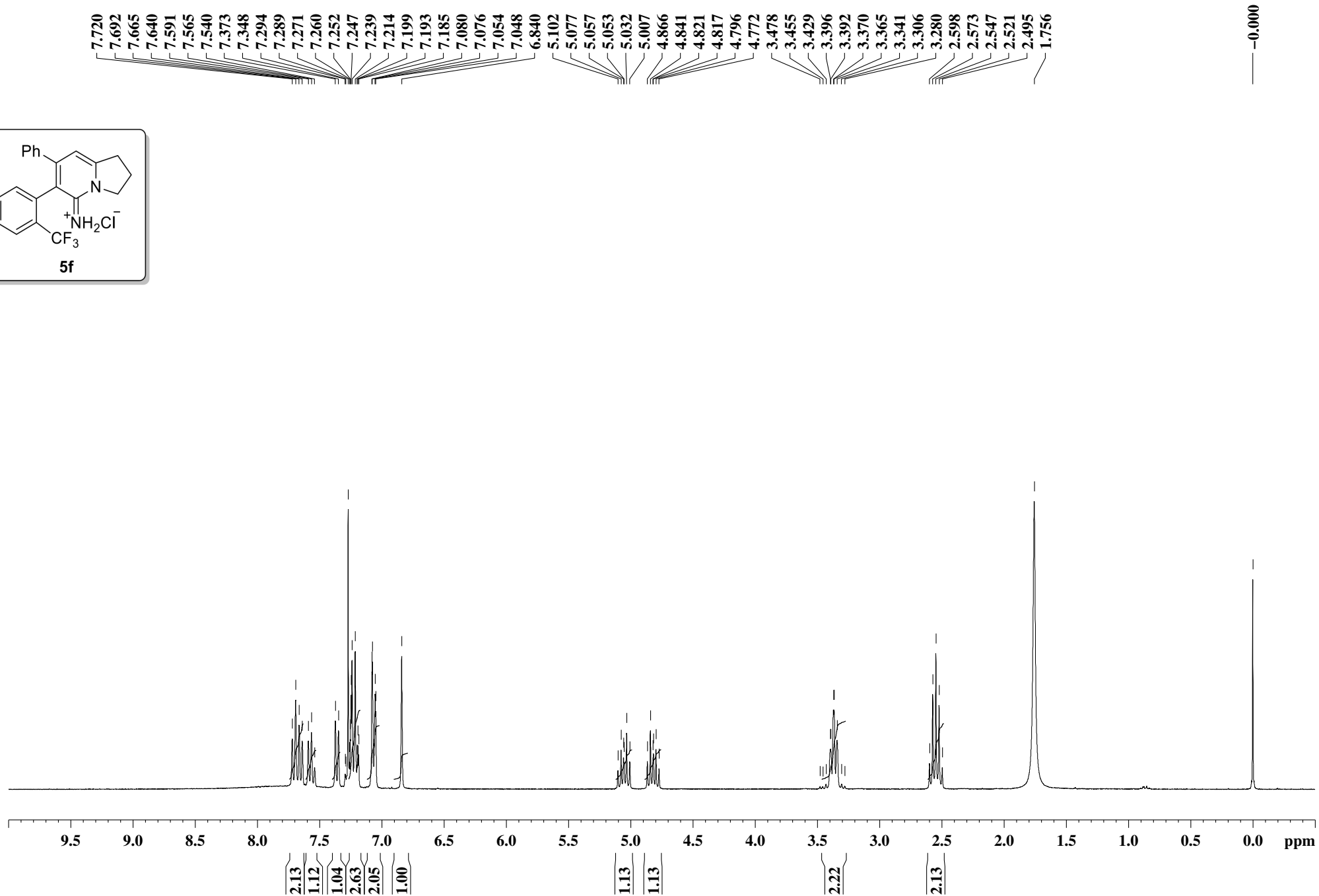
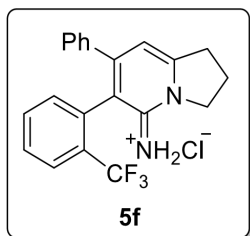
2.589
2.564
2.539
2.514
2.490
2.068
1.967



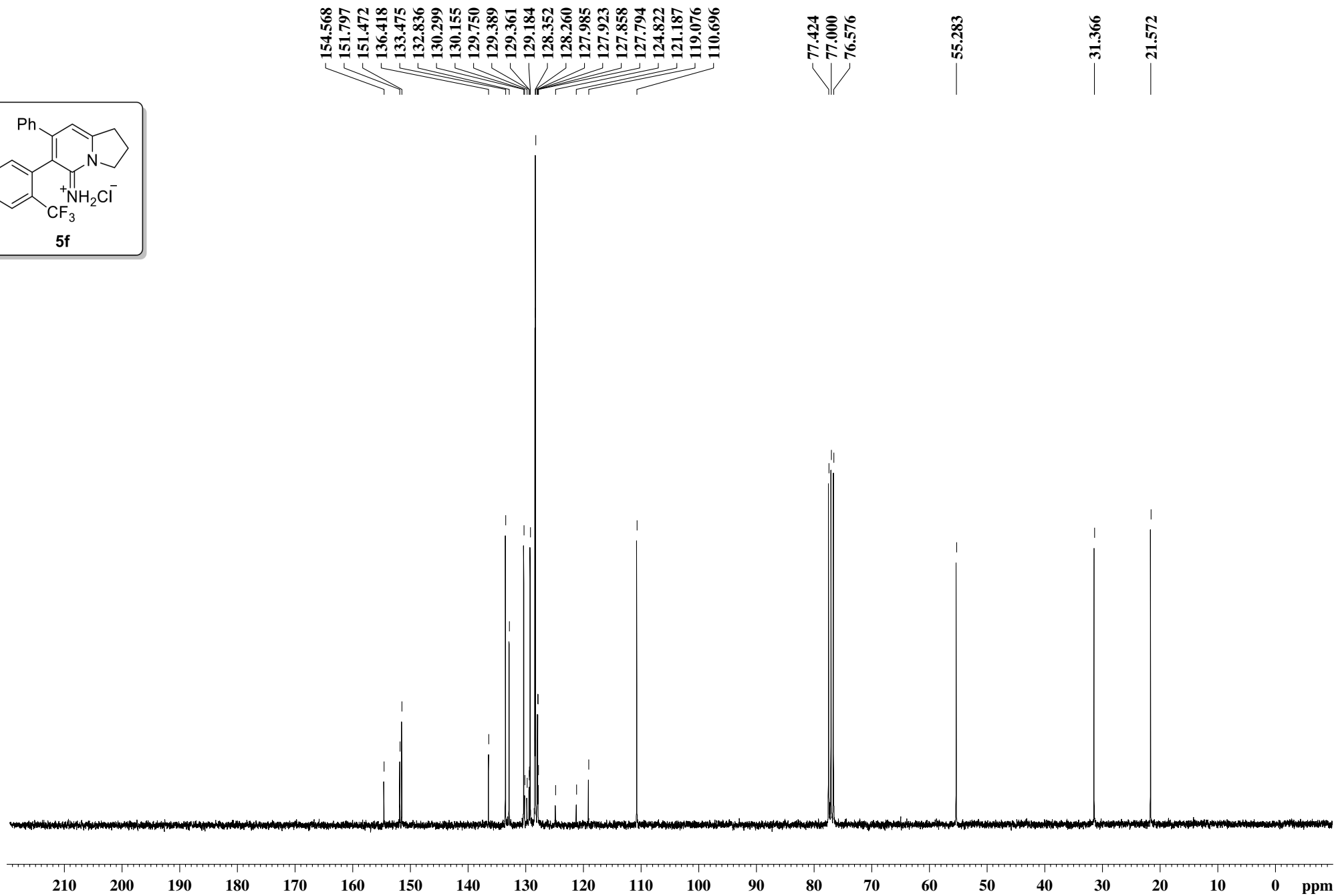
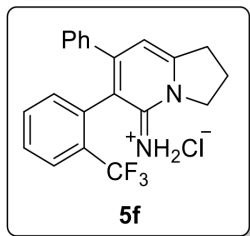
¹³C NMR (75 MHz, CDCl₃)



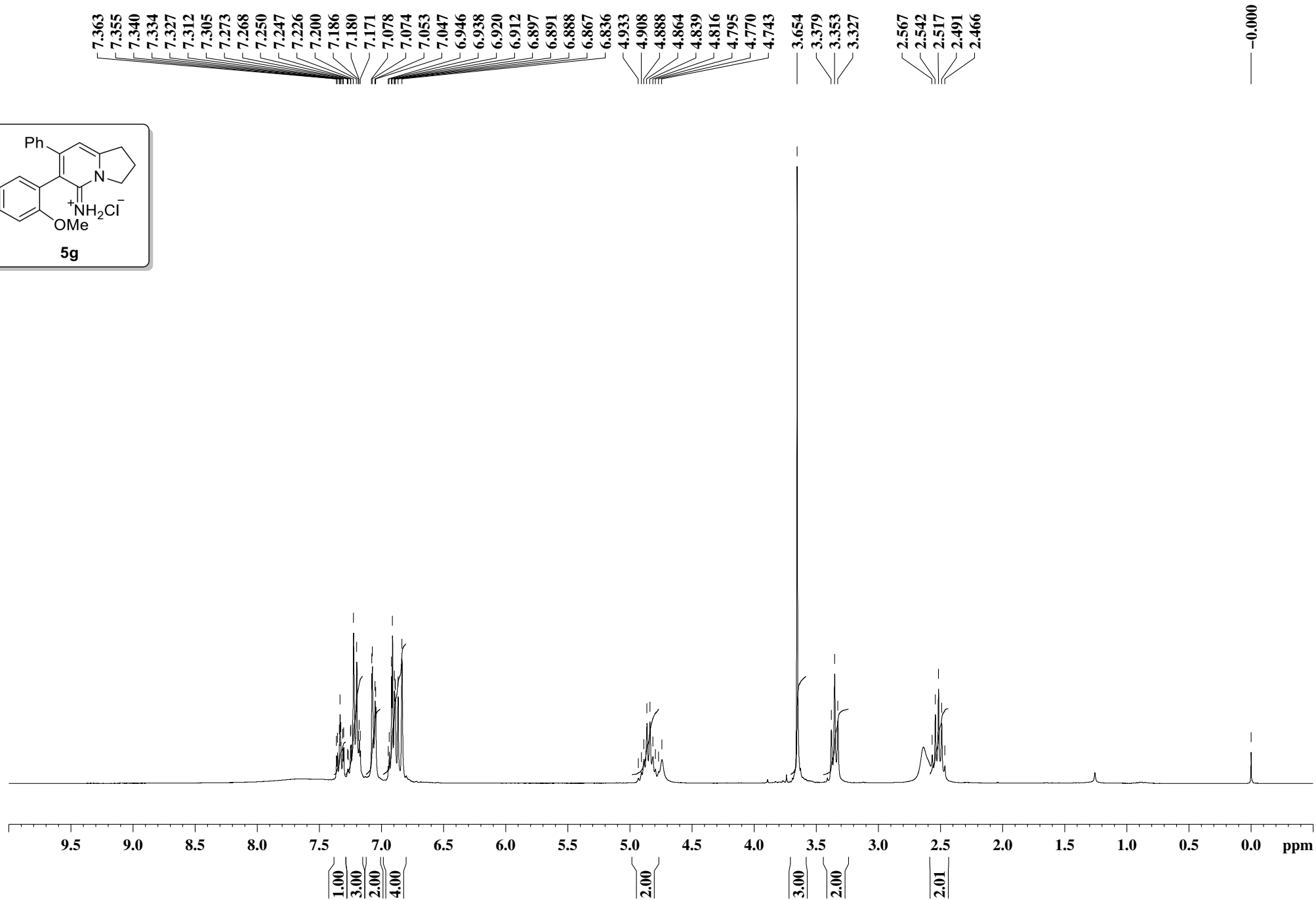
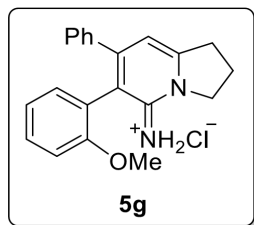
^1H NMR (300 MHz, CDCl_3)



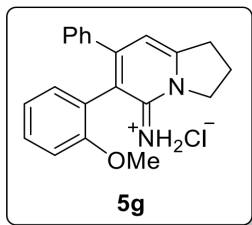
¹³C NMR (75 MHz, CDCl₃)



^1H NMR (300 MHz, CDCl_3)



13C NMR (75 MHz, CDCl3)



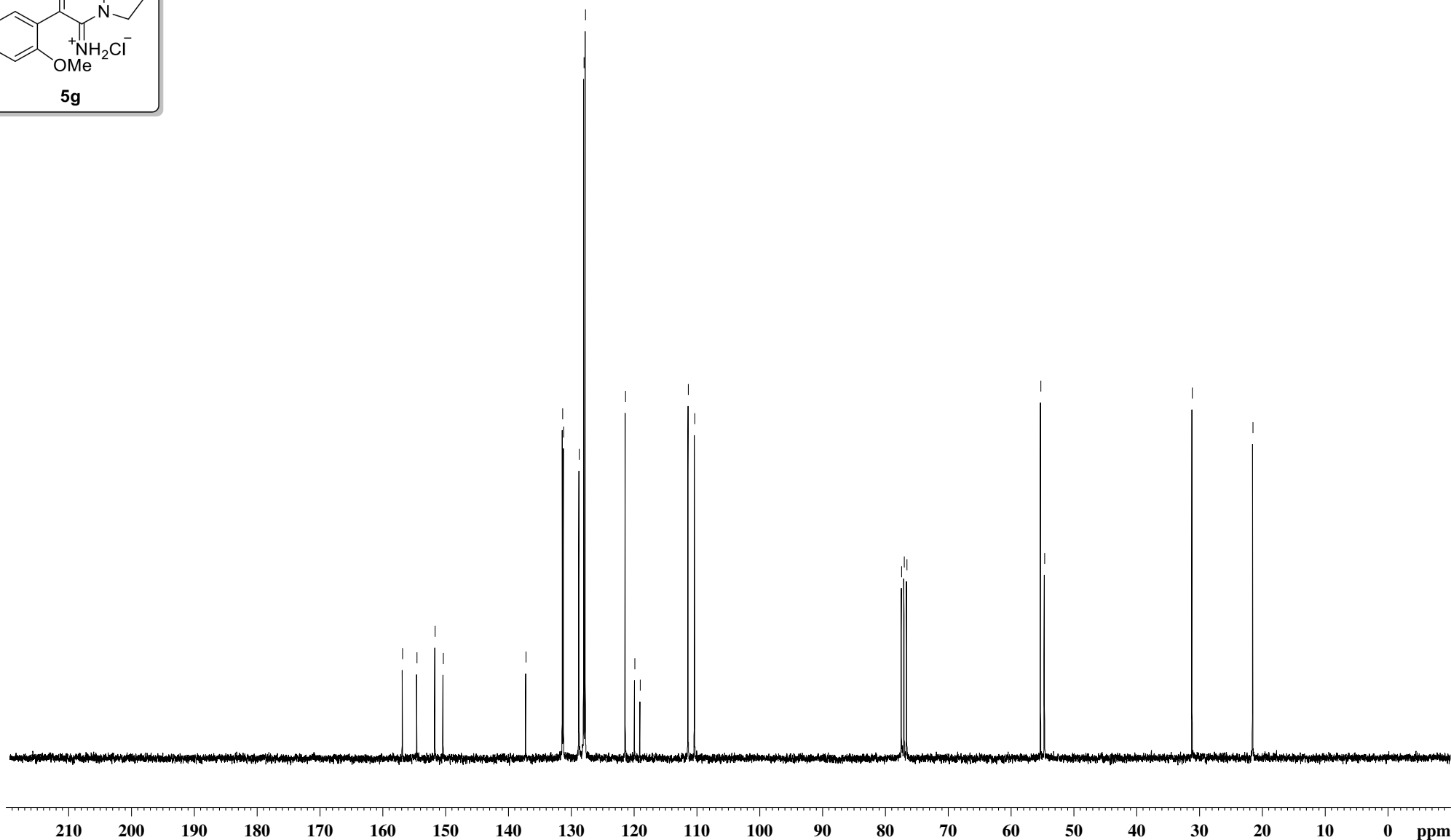
156.854
154.564
151.678
150.369
137.208
131.373
131.211
128.742
127.969
127.737
121.367
119.885
119.025
111.374
110.342

77.425
77.000
76.576

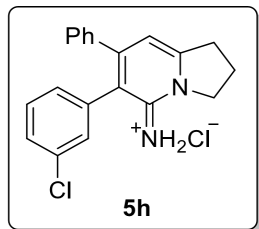
55.264
54.654

31.154

21.500



^1H NMR (300 MHz, CDCl_3)



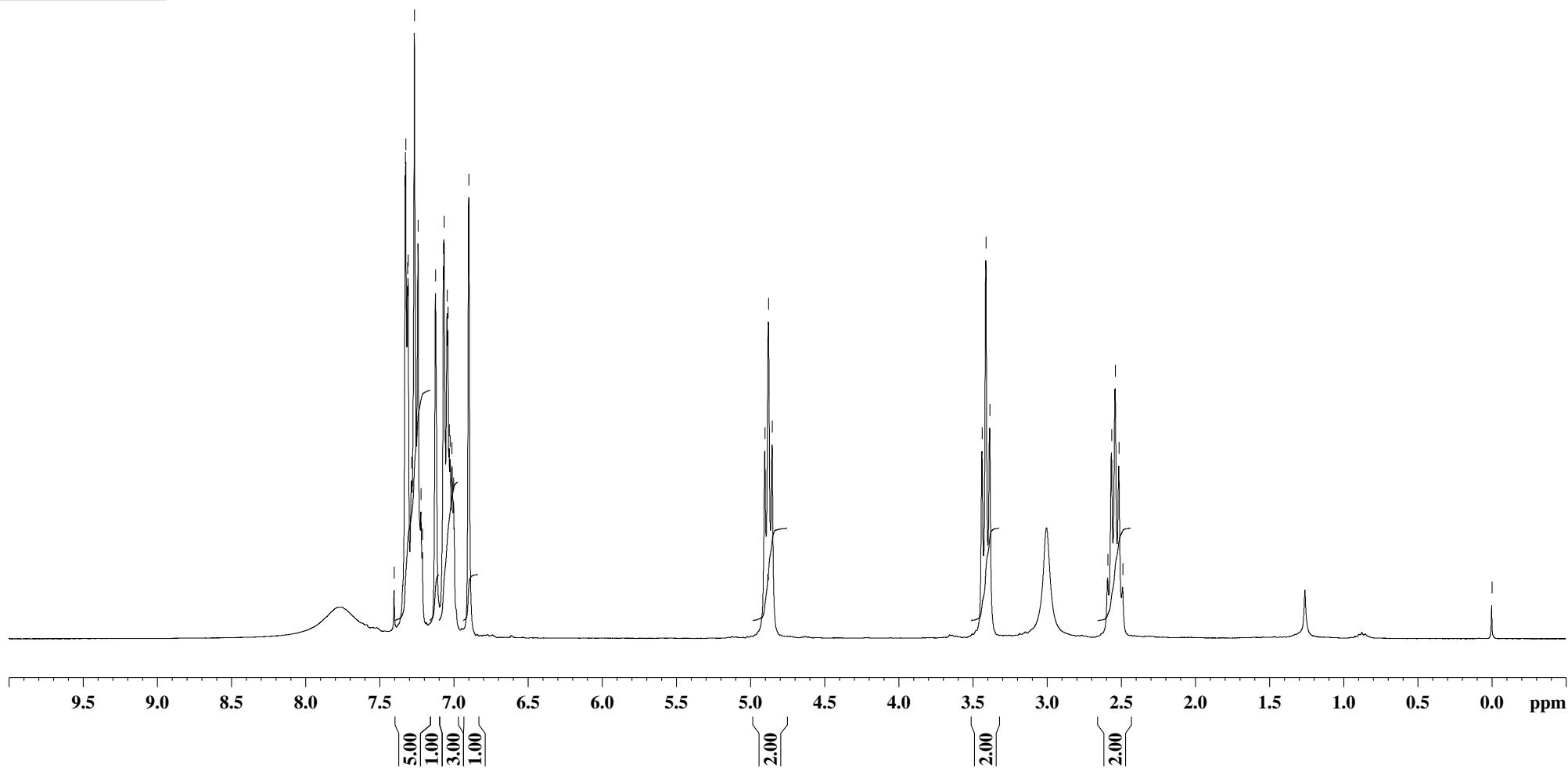
7.403
7.328
7.325
7.313
7.309
7.285
7.266
7.242
7.222
7.212
7.124
7.071
7.066
7.045
7.040
7.032
7.026
7.014
7.003
6.899

4.903
4.879
4.854

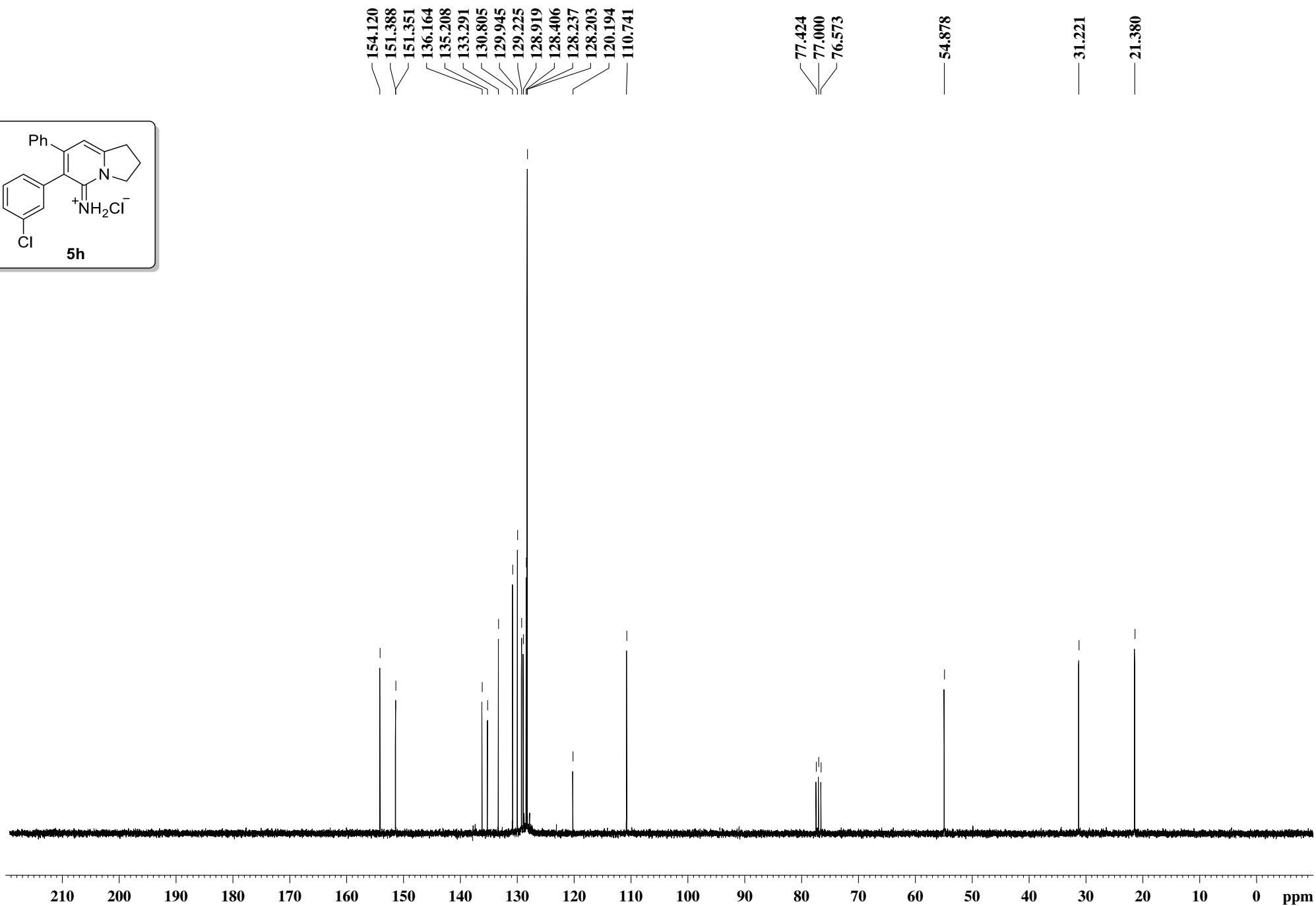
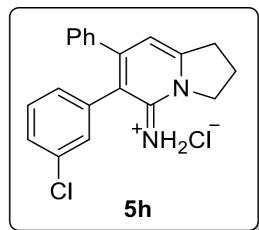
3.438
3.412
3.386

2.591
2.565
2.540
2.515
2.489

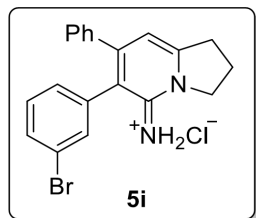
— 0.000



13C NMR (75 MHz, CDCl3)



¹H NMR (300 MHz, CDCl₃)



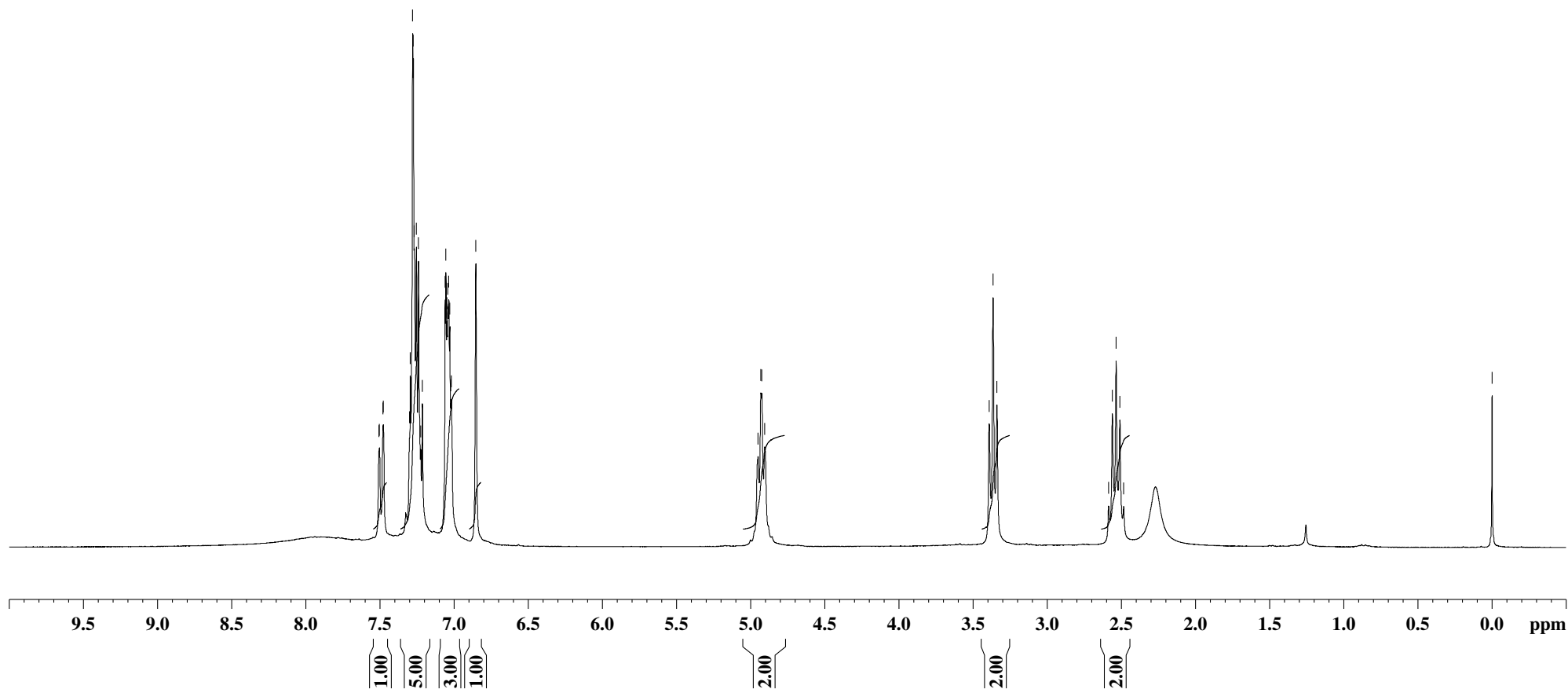
7.507
7.505
7.480
7.478
7.301
7.296
7.281
7.276
7.270
7.255
7.241
7.226
7.214
7.061
7.056
7.049
7.043
7.037
7.029
7.023
7.019
6.854

4.951
4.932
4.925
4.906

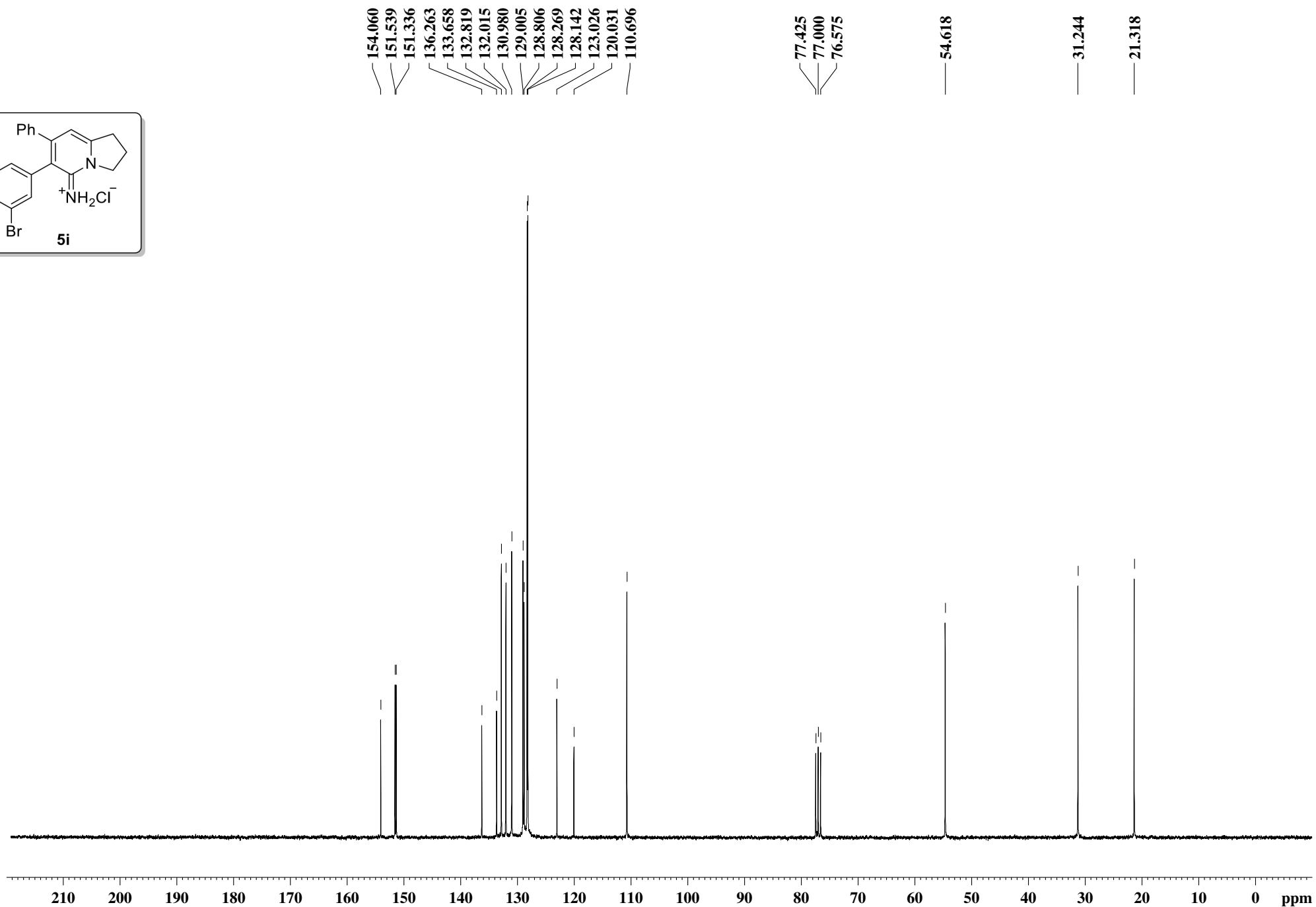
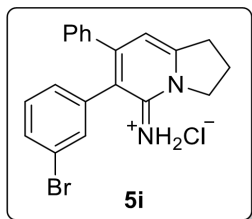
3.392
3.365
3.340

2.586
2.561
2.536
2.510
2.485

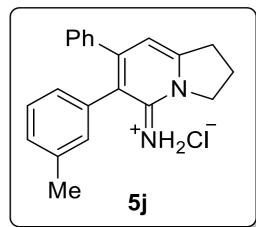
— 0.000



¹³C NMR (75 MHz, CDCl₃)



¹H NMR (300 MHz, CDCl₃)



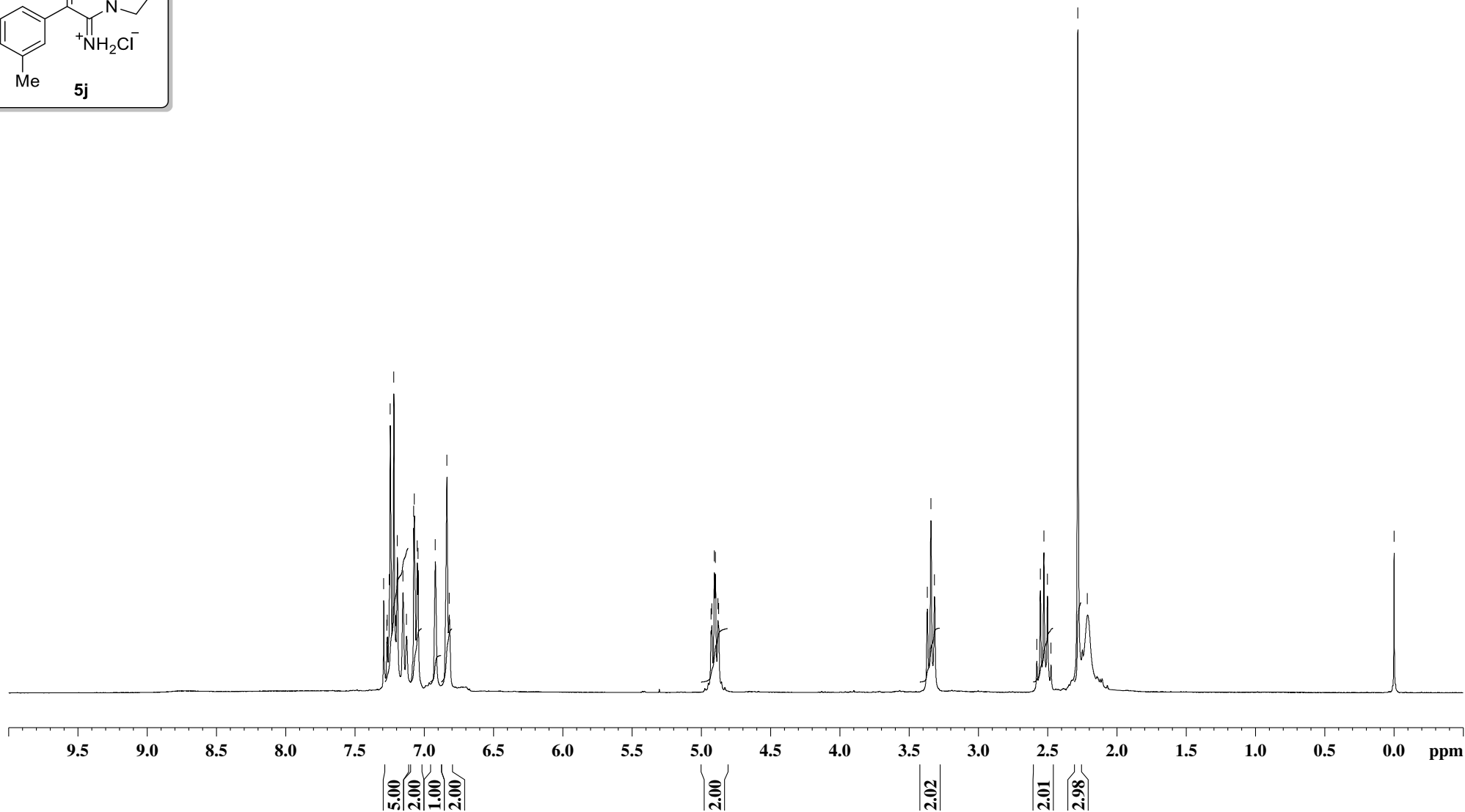
7.294
7.271
7.268
7.253
7.247
7.221
7.207
7.195
7.154
7.129
7.077
7.072
7.051
7.045
6.921
6.837
6.820

4.930
4.925
4.907
4.899
4.881
4.875

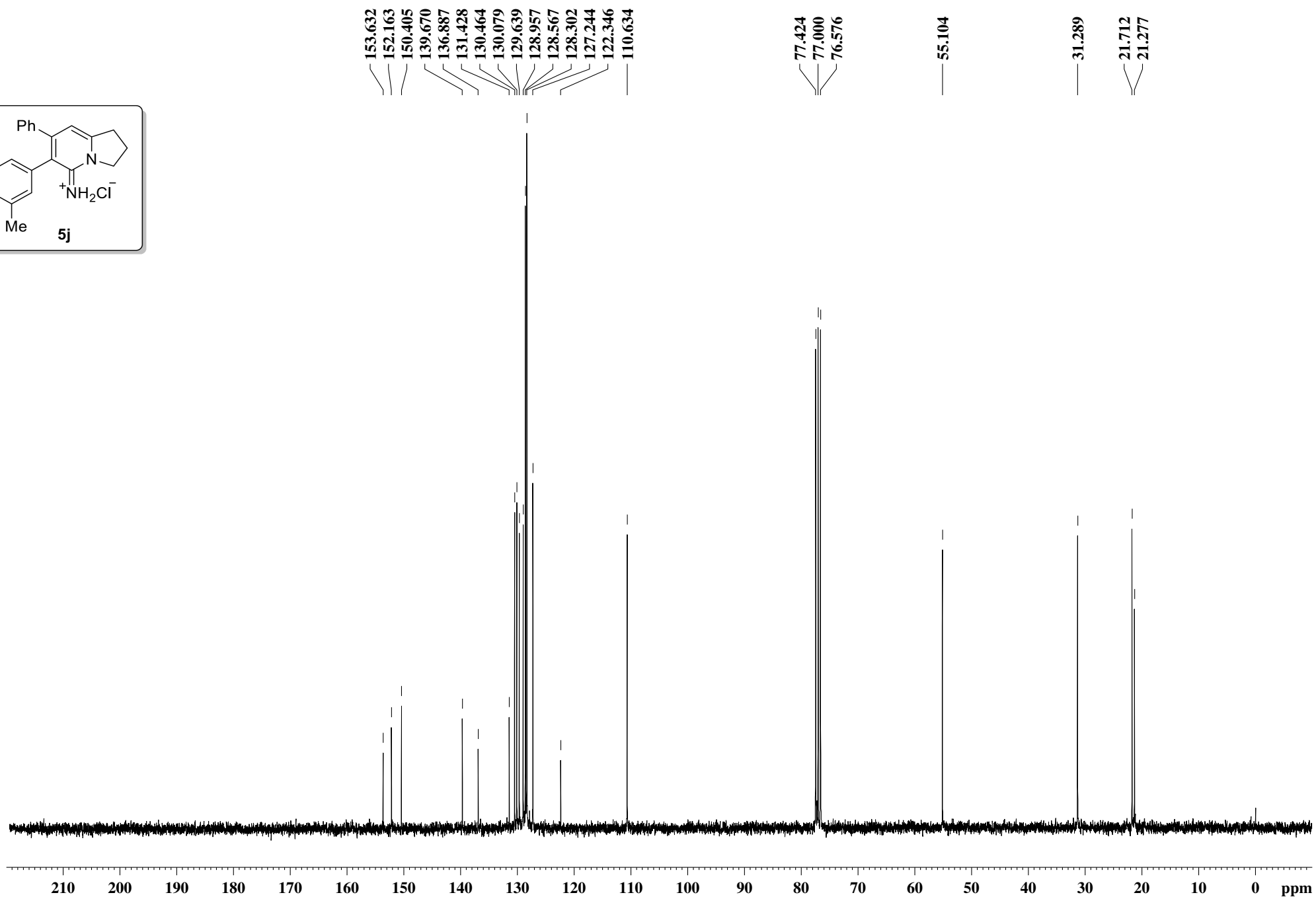
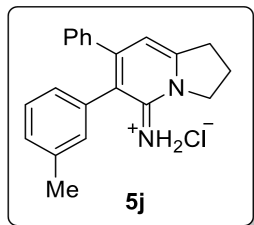
3.369
3.343
3.318

2.579
2.553
2.527
2.502
2.477
2.283
2.214

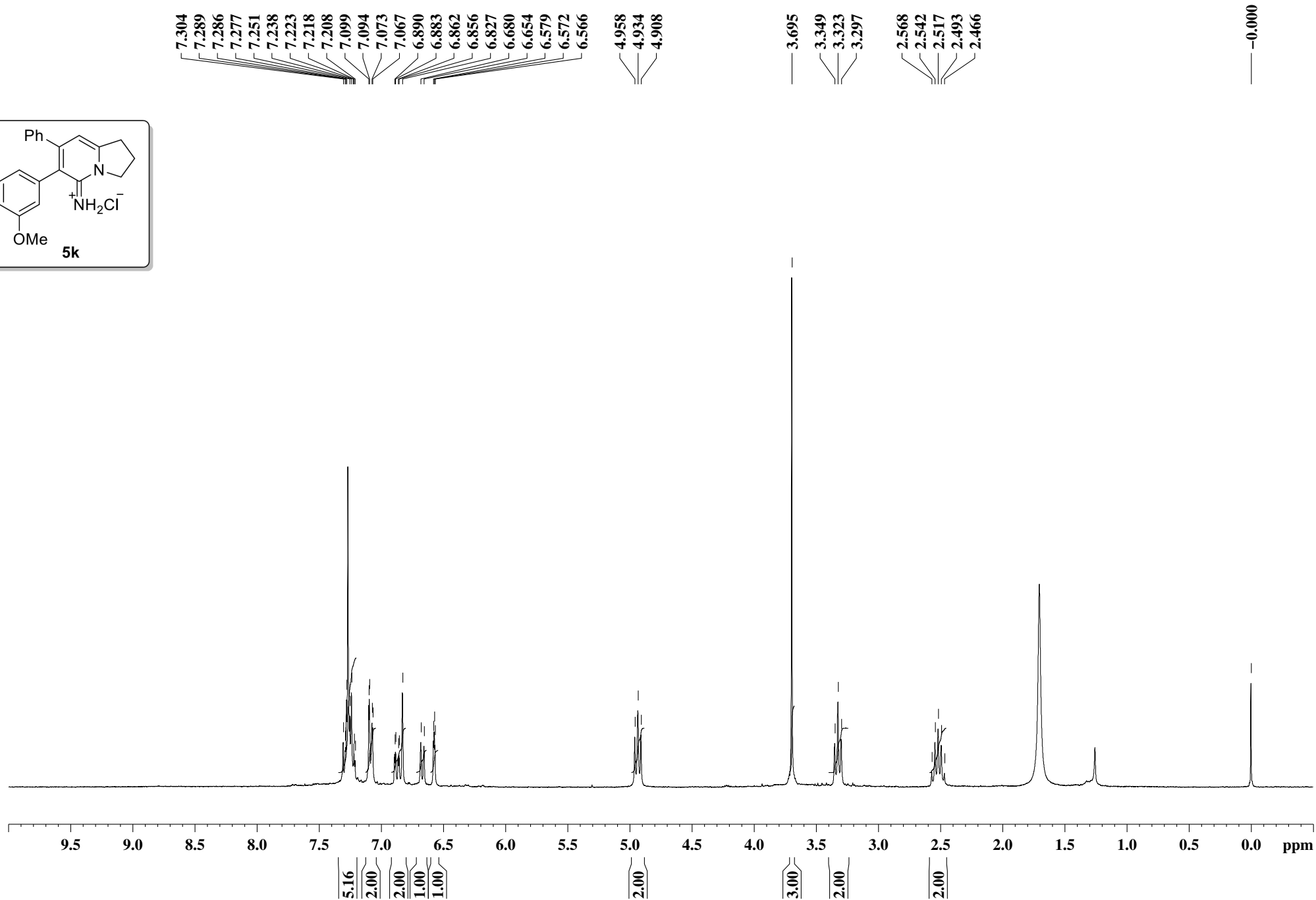
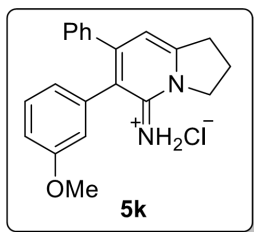
— 0.000



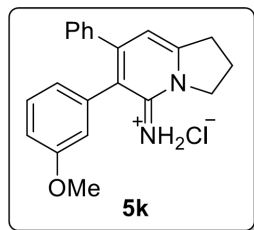
¹³C NMR (75 MHz, CDCl₃)



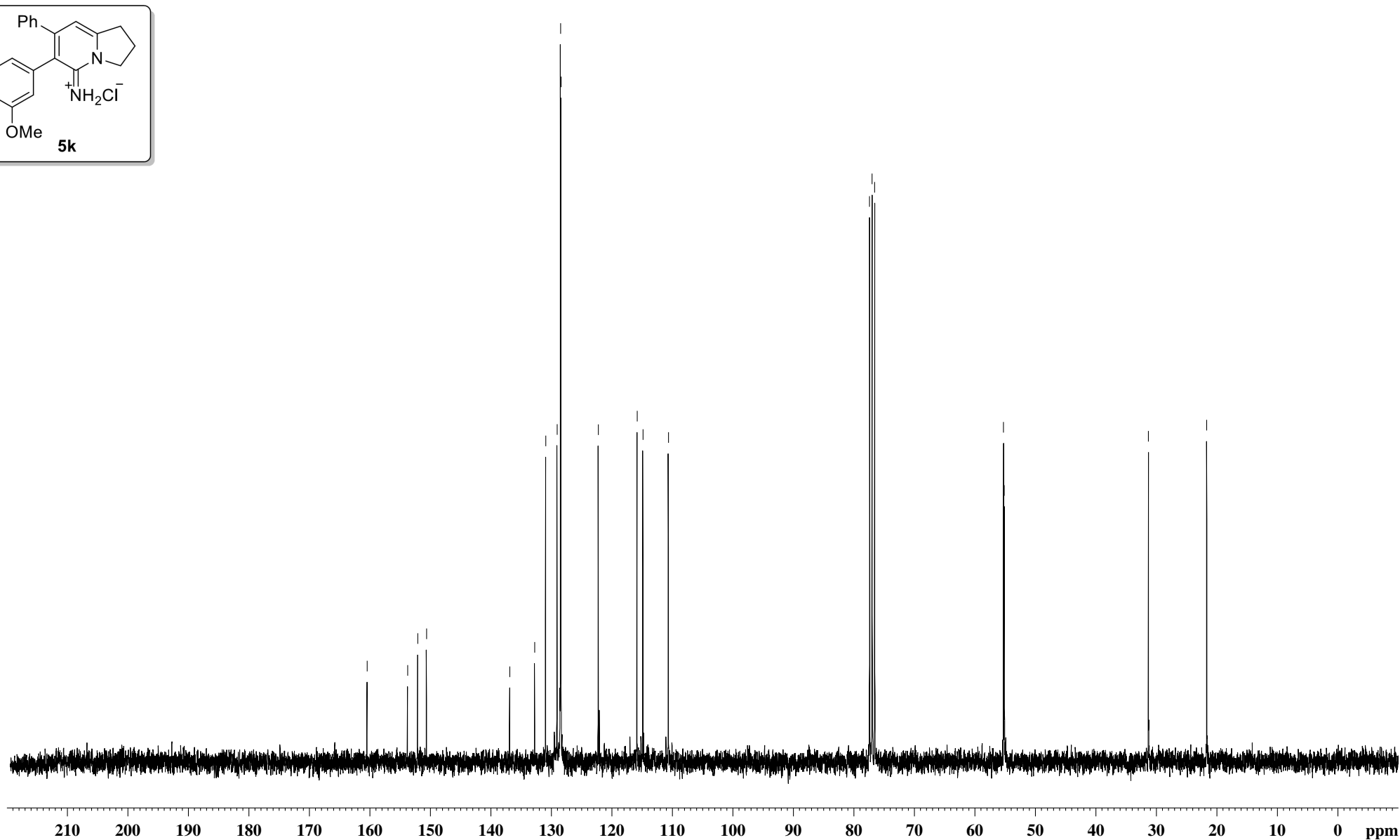
¹H NMR (300 MHz, CDCl₃)



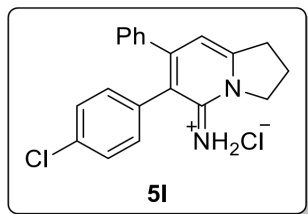
¹³C NMR (75 MHz, CDCl₃)



160.451
153.756
152.085
150.629
136.875
132.762
130.930
129.048
128.476
128.381
122.242
115.816
114.854
110.646
77.424
77.000
76.577
55.282
55.155
31.328
21.694



1H NMR (300 MHz, CDCl3)



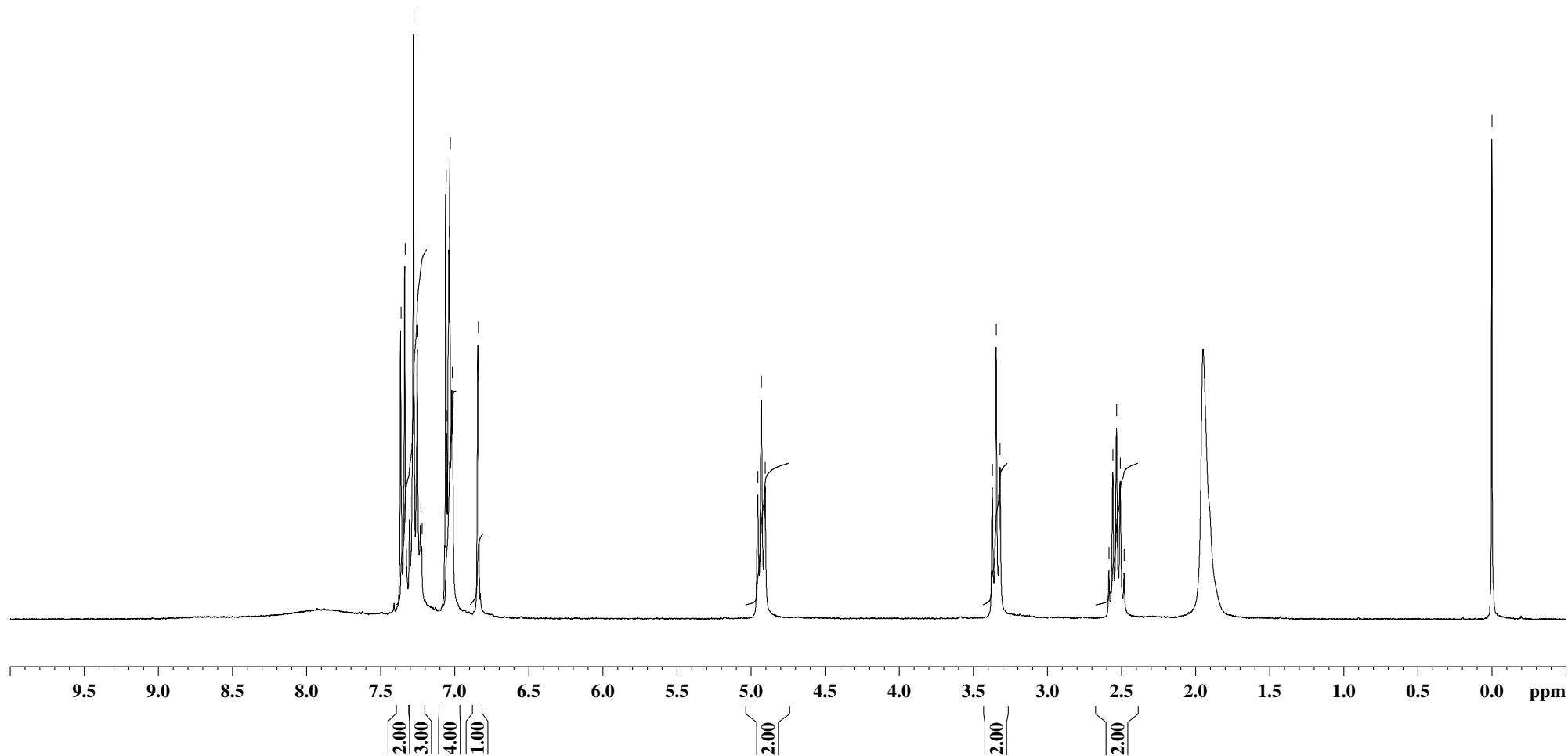
7.362
7.334
7.301
7.275
7.249
7.228
7.220
7.058
7.051
7.036
7.029
7.016
7.011
6.840

4.954
4.930
4.905

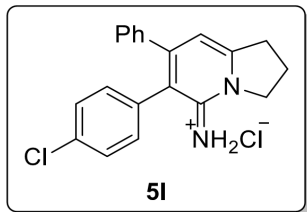
3.371
3.345
3.320

2.584
2.558
2.533
2.508
2.482

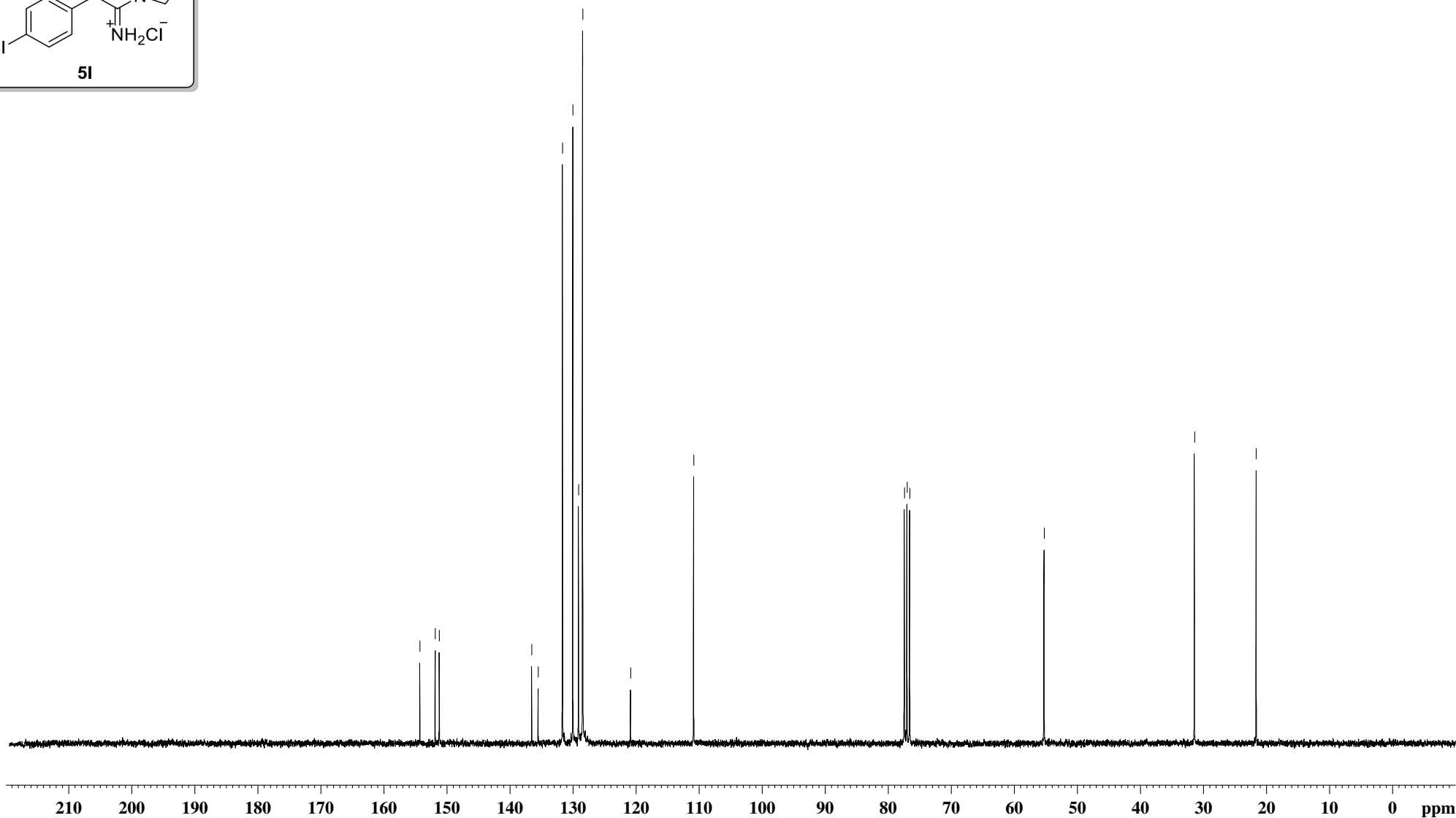
—0.000



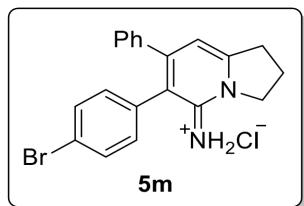
13C NMR (75 MHz, CDCl₃)



154.296
151.866
151.220
136.553
135.525
131.669
130.027
129.123
128.479
128.455
120.857
110.849
77.423
77.000
76.576
55.250
31.391
21.642



¹H NMR (300 MHz, CDCl₃)



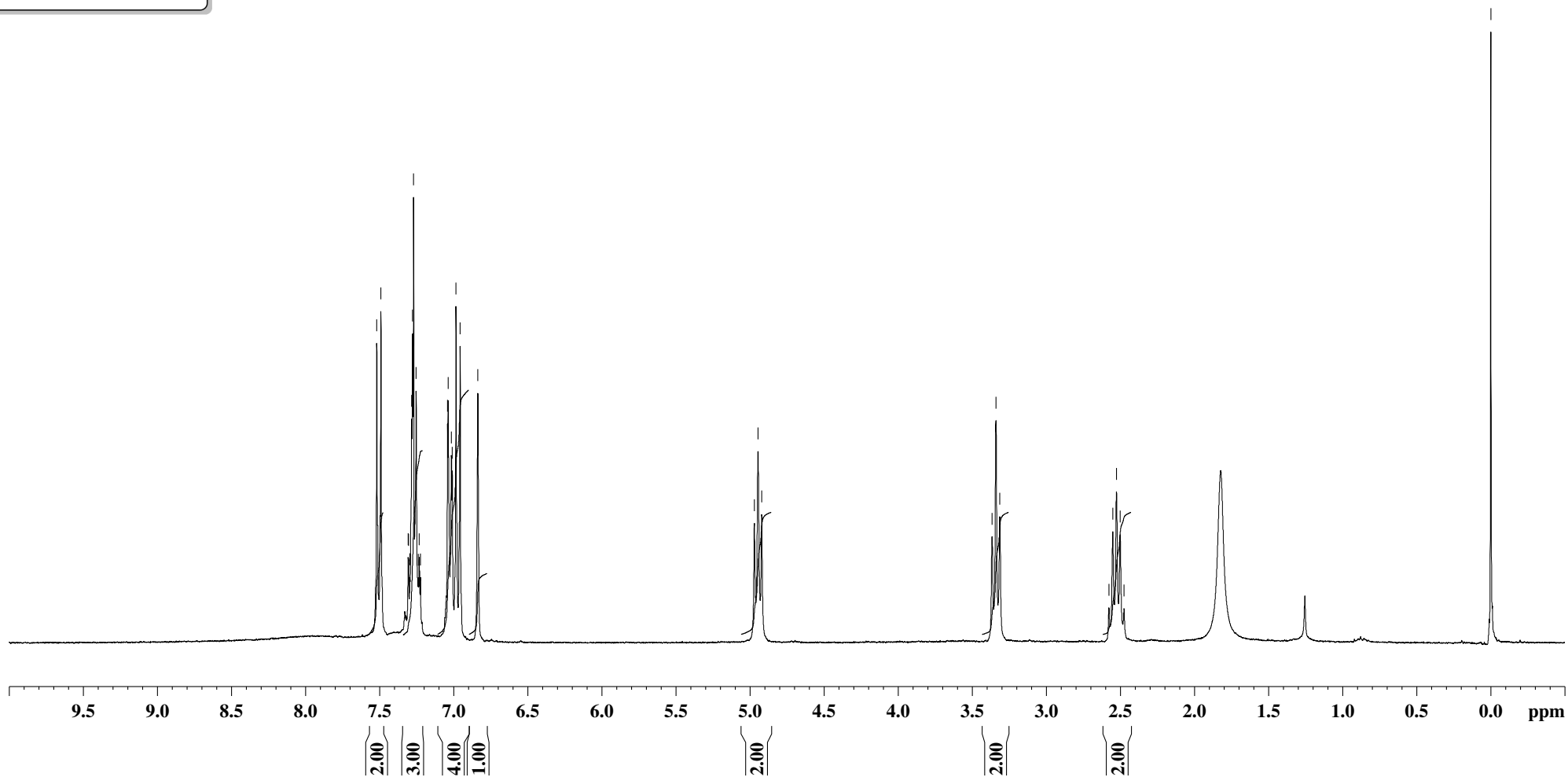
7.520
7.492
7.308
7.305
7.297
7.285
7.279
7.272
7.255
7.240
7.234
7.225
7.042
7.038
7.016
7.011
6.986
6.957
6.838

4.971
4.947
4.922

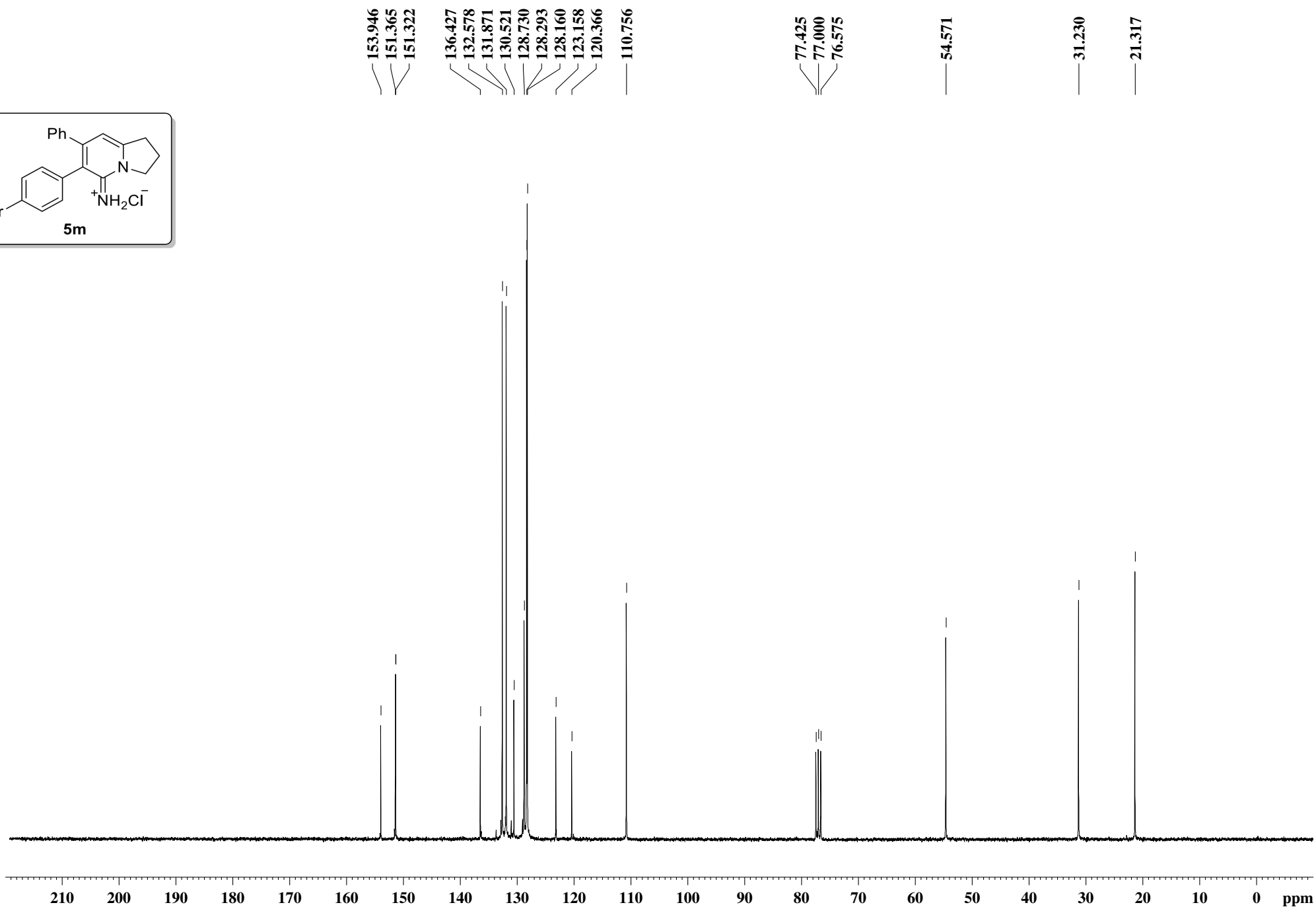
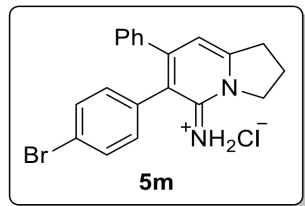
3.367
3.340
3.315

2.578
2.552
2.527
2.502
2.476

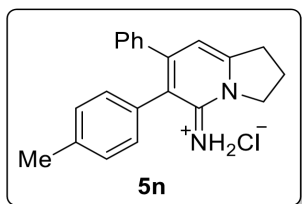
-0.000



¹³C NMR (75 MHz, CDCl₃)



¹H NMR (300 MHz, CDCl₃)



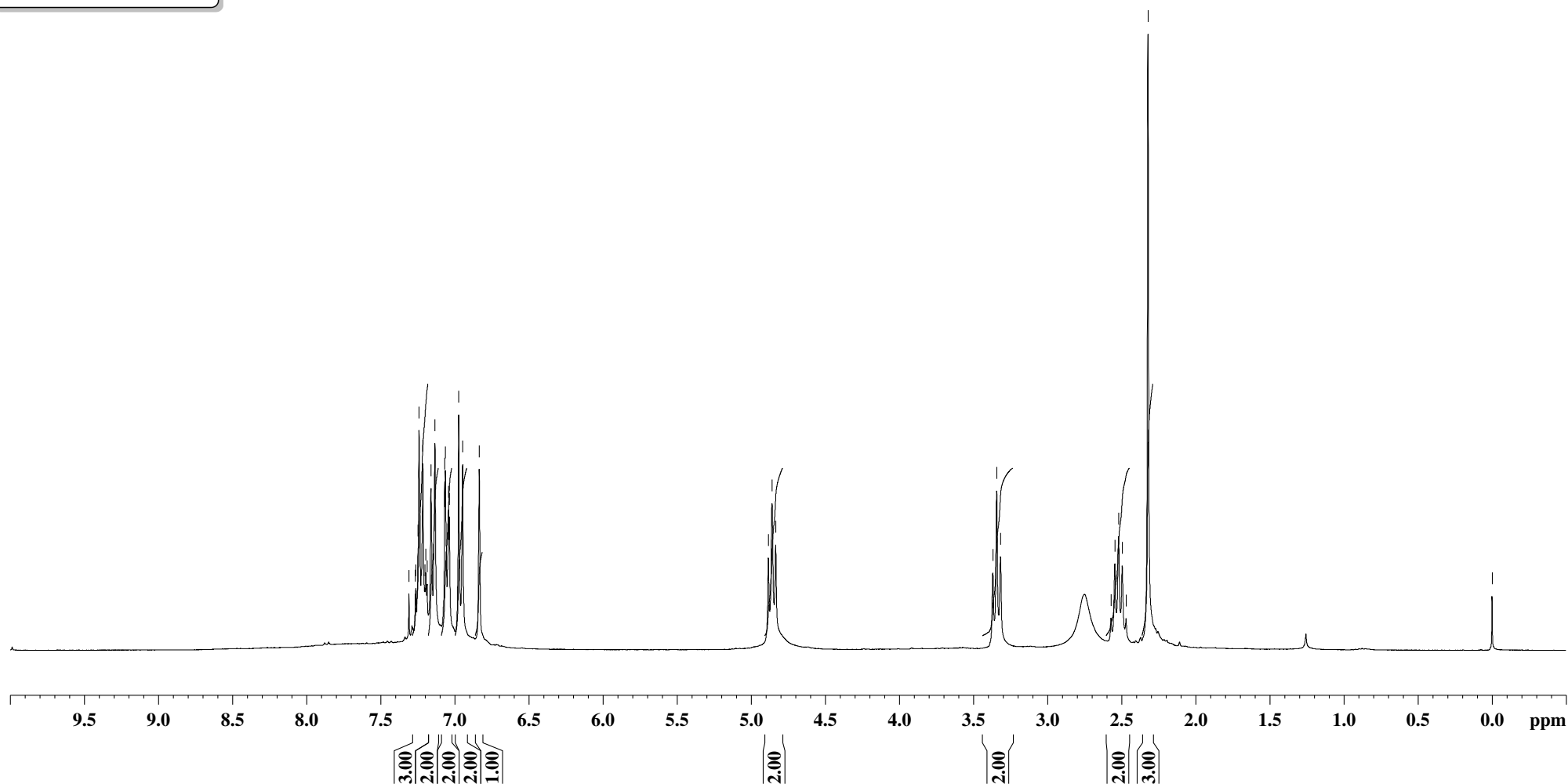
7.310
7.267
7.264
7.249
7.243
7.217
7.202
7.197
7.188
7.162
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6.975
6.948
6.836

4.884
4.860
4.835

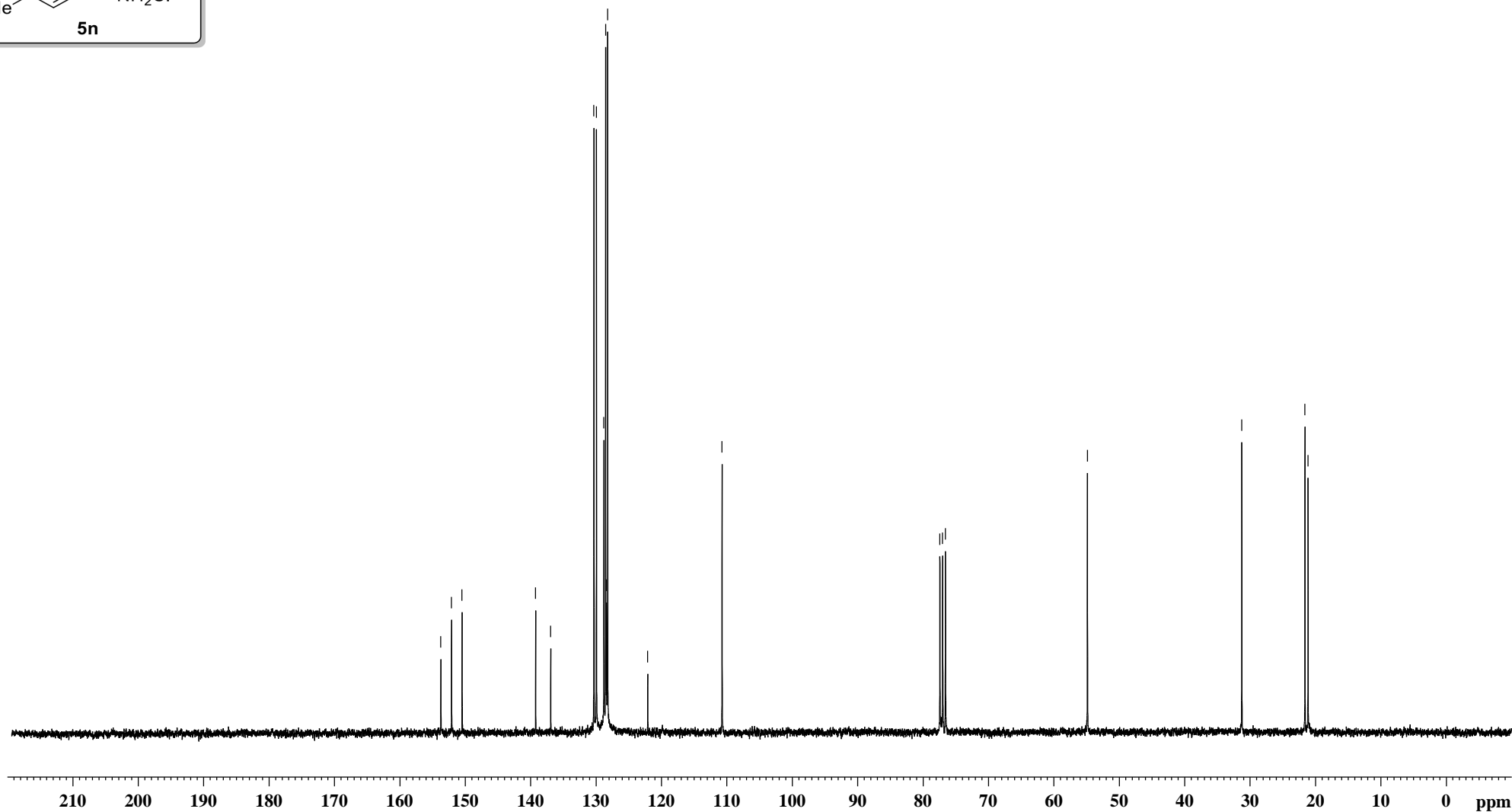
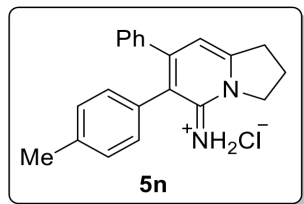
3.369
3.343
3.318

2.572
2.546
2.521
2.496
2.470
2.322

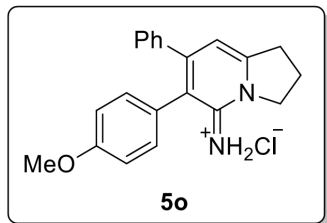
-0.000



¹³C NMR (75 MHz, CDCl₃)



¹H NMR (300 MHz, CDCl₃)



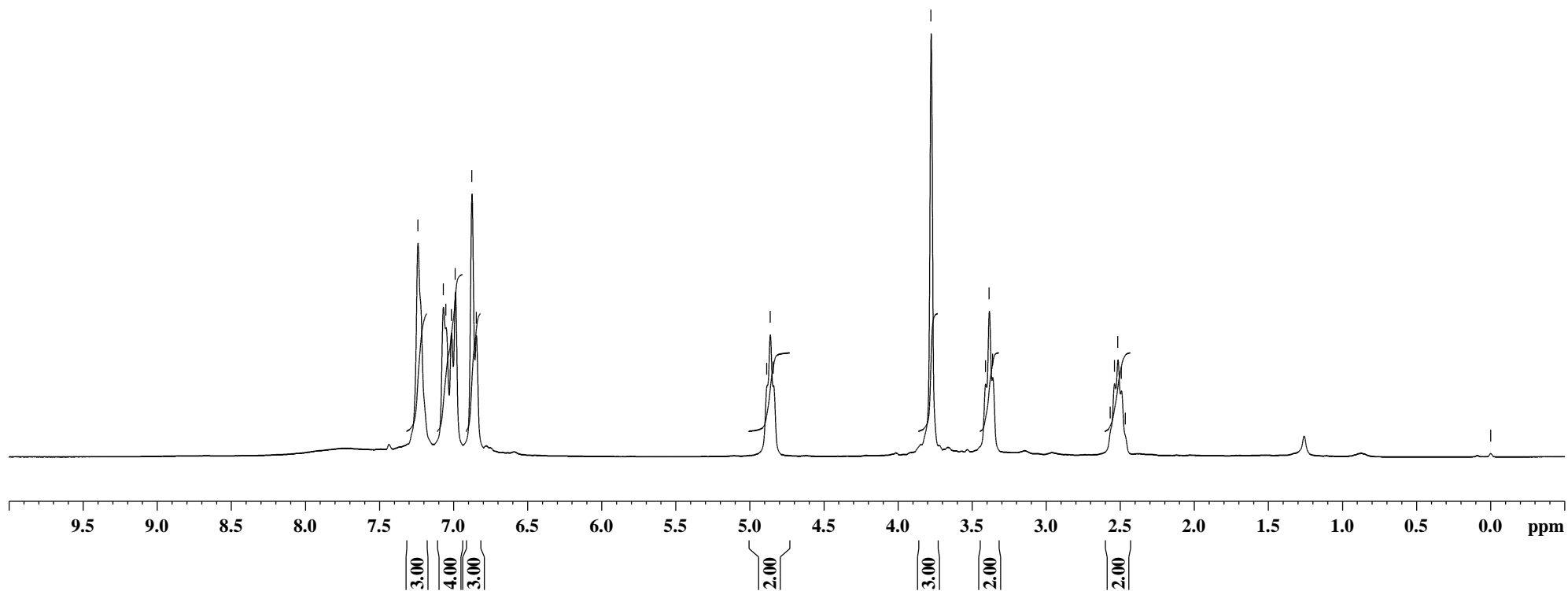
7.241
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7.051
7.015
6.988
6.876
6.847

4.887
4.863
4.841

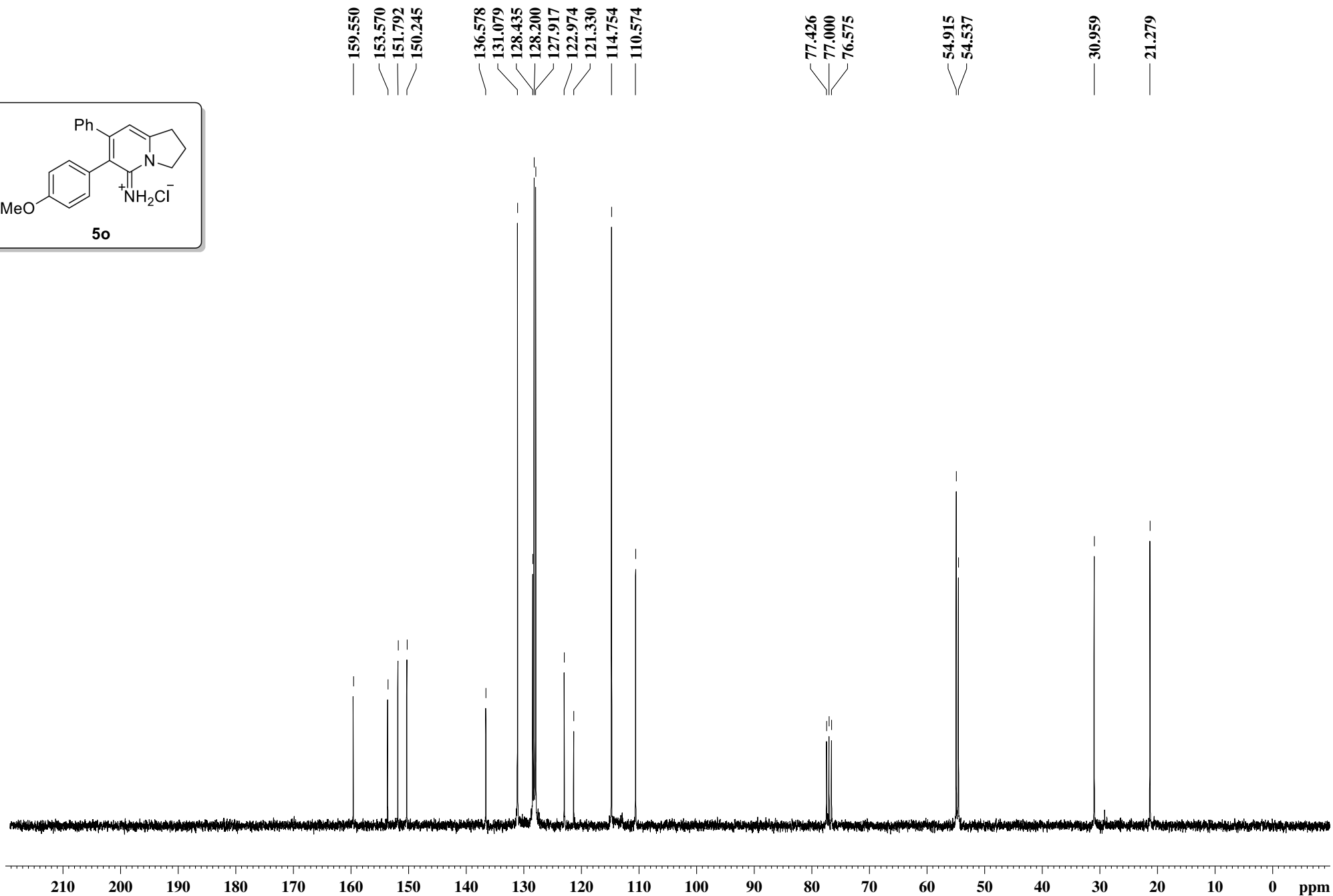
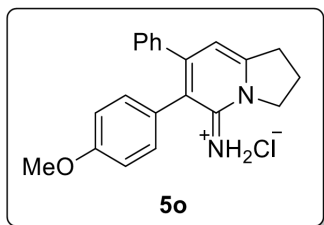
3.777
3.409
3.384
3.361

2.567
2.540
2.516
2.493
2.465

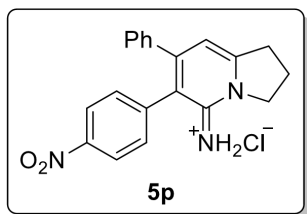
-0.000



¹³C NMR (75 MHz, CDCl₃)



^1H NMR (300 MHz, CDCl_3)



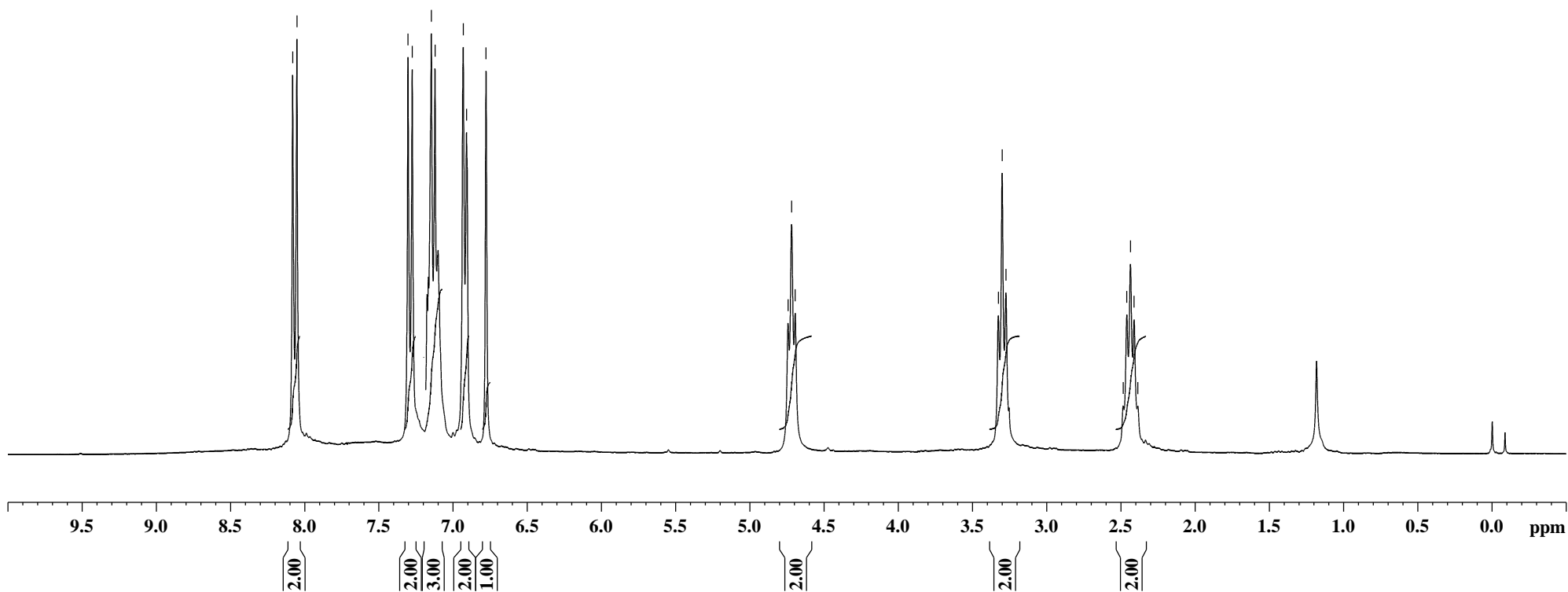
8.081
8.052

7.304
7.275
7.147
7.122
6.932
6.910
6.778

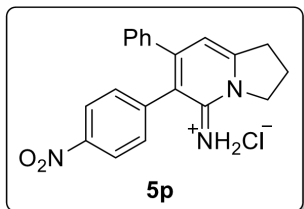
4.743
4.719
4.695

3.326
3.300
3.275

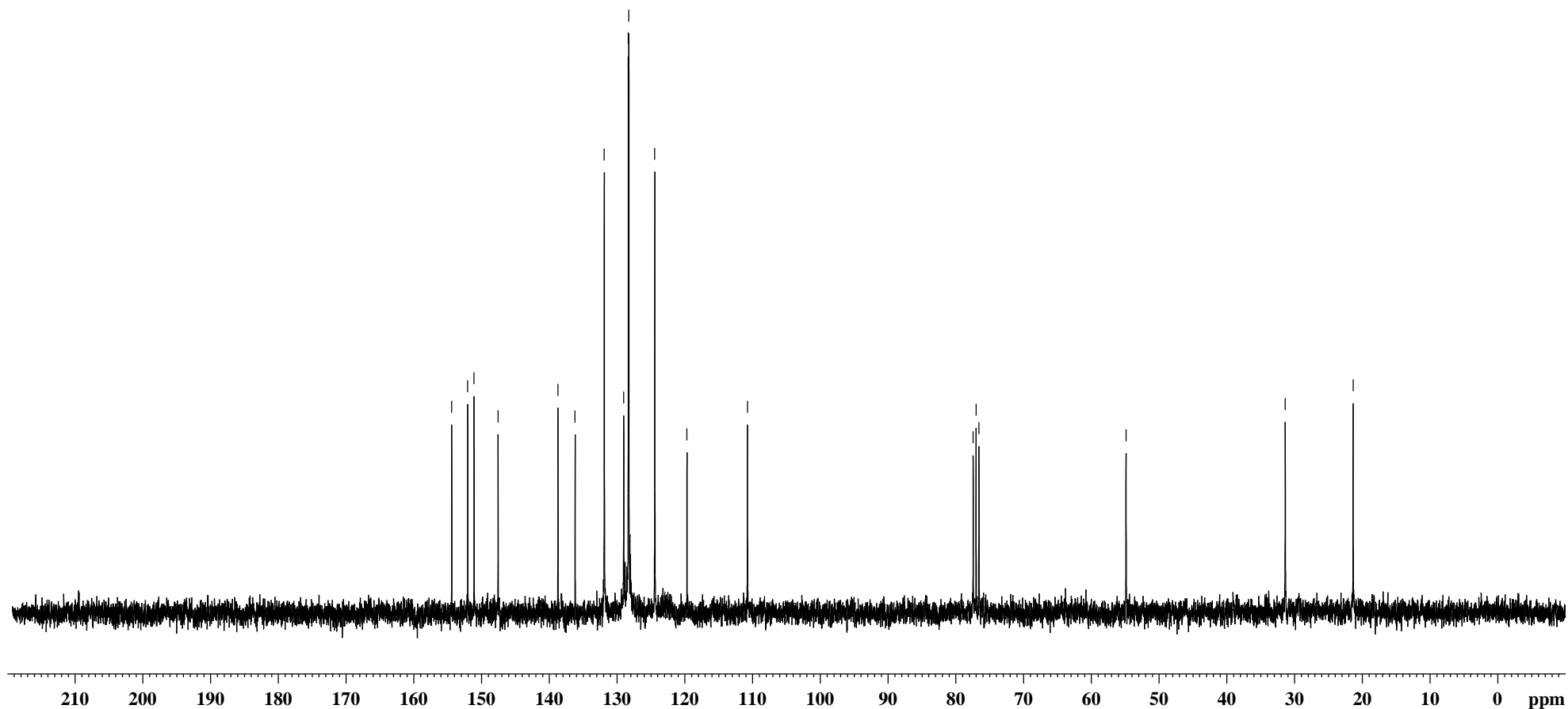
2.485
2.460
2.436
2.411
2.386



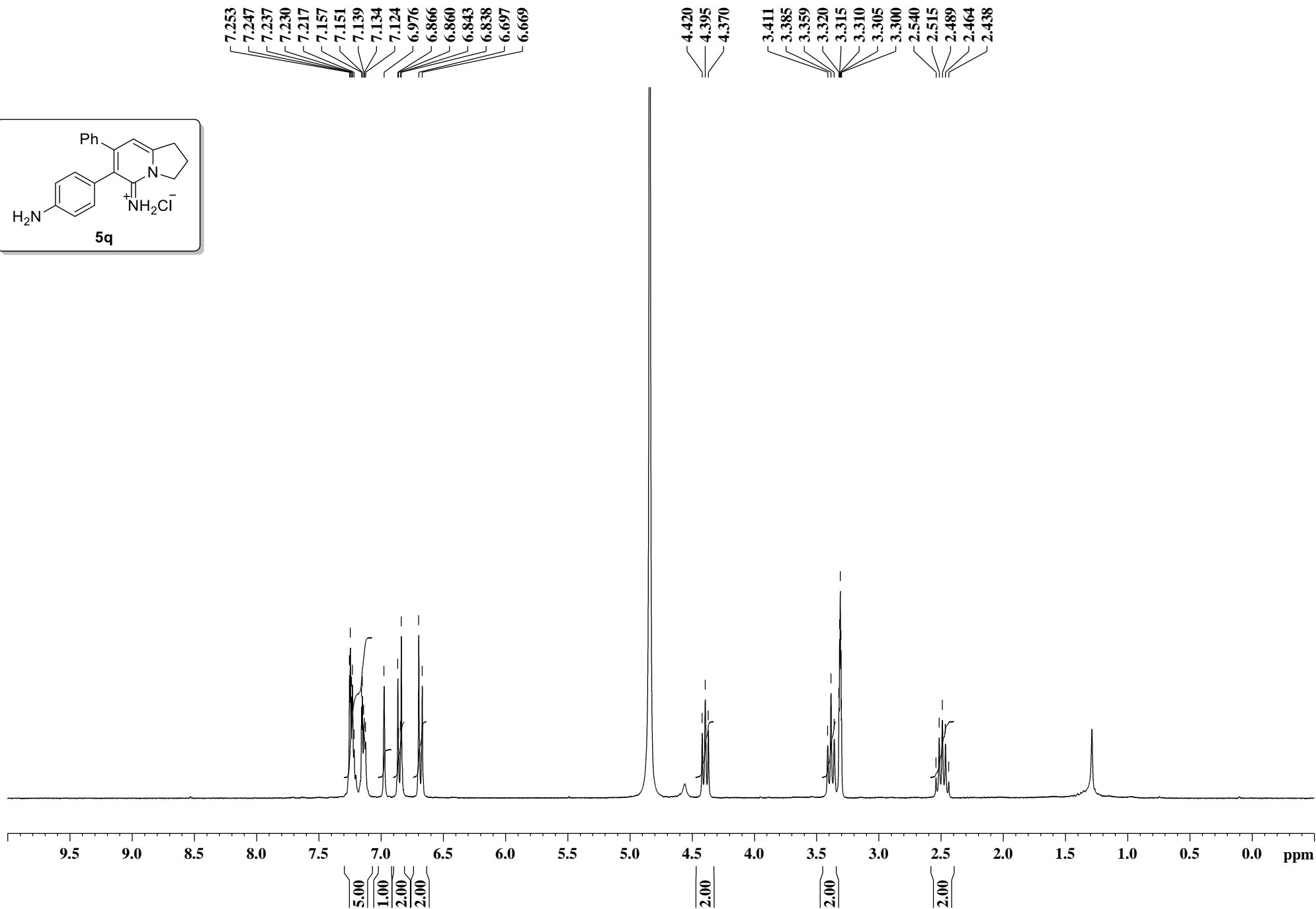
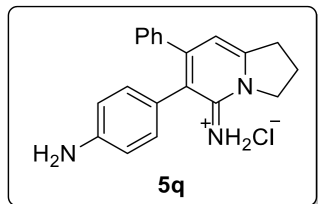
13C NMR (75 MHz, CDCl3)



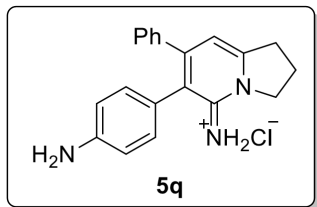
- 154.406
- 152.040
- 151.114
- 147.566
- 138.722
- 136.186
- 131.883
- 129.006
- 128.337
- 128.259
- 124.425
- 119.674
- 110.753
- 77.425
- 77.000
- 76.576
- 54.861
- 31.359
- 21.335



^1H NMR (300 MHz, MeOH- d_4)

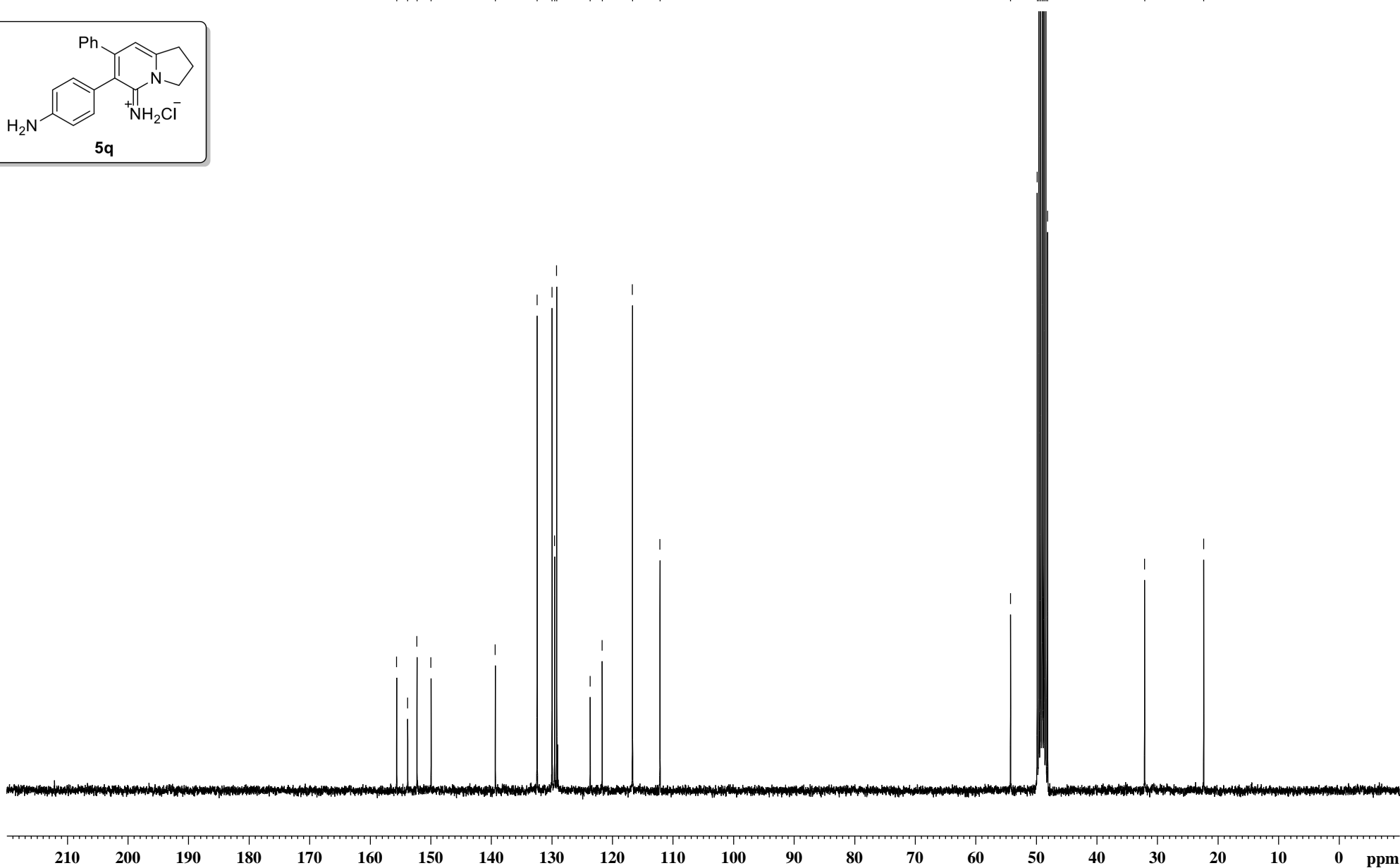


¹³C NMR (75 MHz, MeOH-d₄)



155.635
153.820
152.284
149.959
139.350
132.437
129.979
129.557
129.210
123.681
121.695
116.699
112.150

54.259
49.851
49.567
49.283
49.000
48.716
48.432
48.148
32.119
22.360



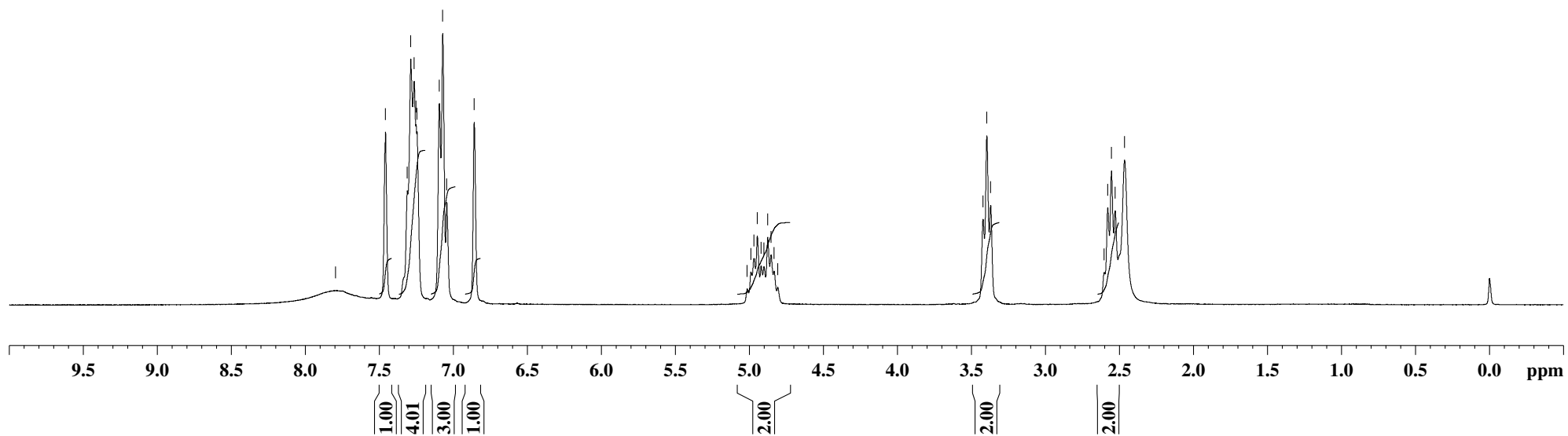
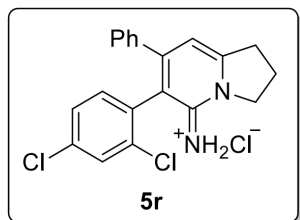
¹H NMR (300 MHz, CDCl₃)

7.796
7.459
7.312
7.289
7.265
7.253
7.246
7.095
7.073
7.045
6.860

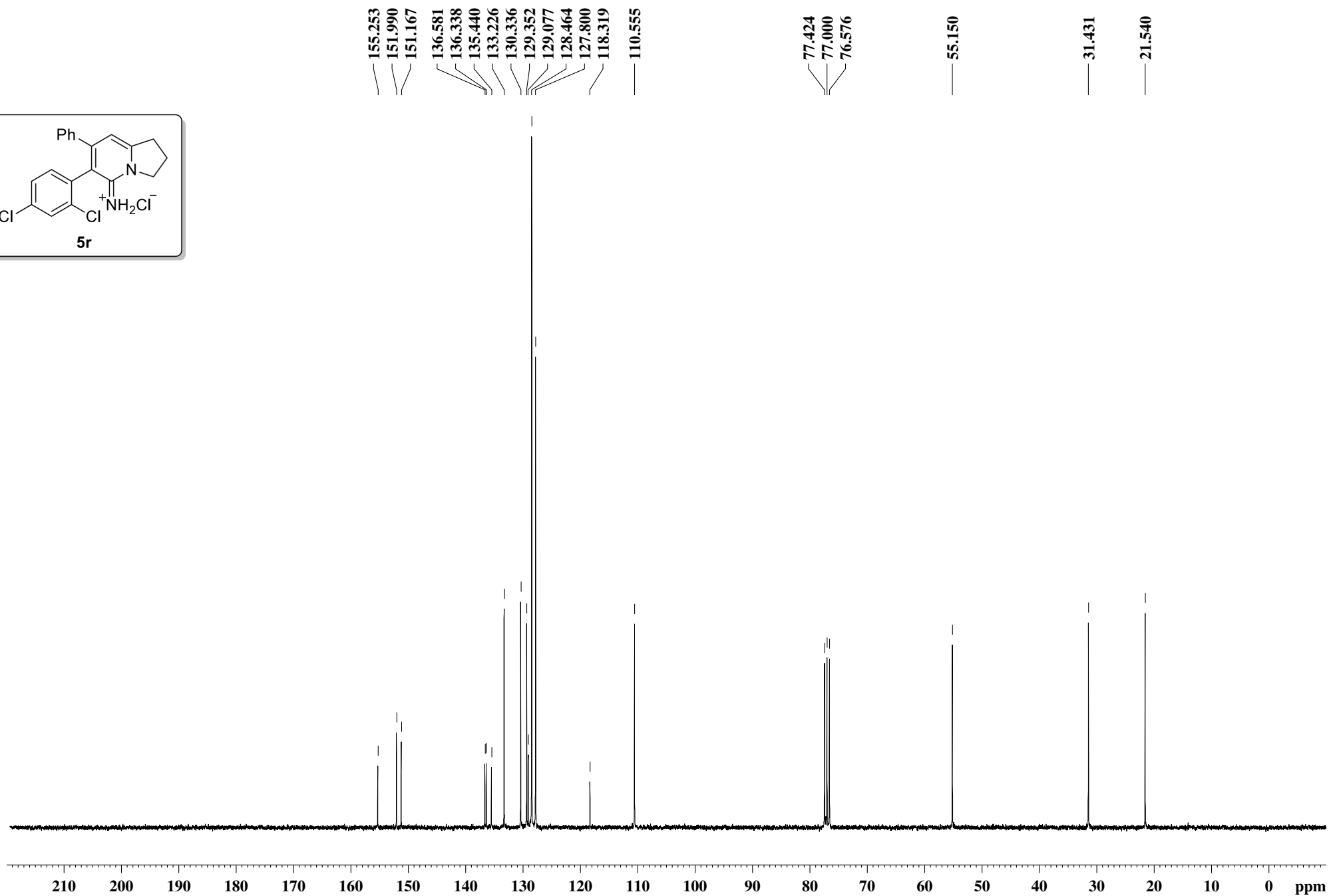
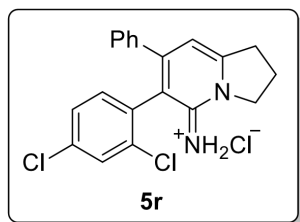
5.016
4.990
4.970
4.947
4.921
4.902
4.877
4.854
4.834
4.809

3.422
3.397
3.371

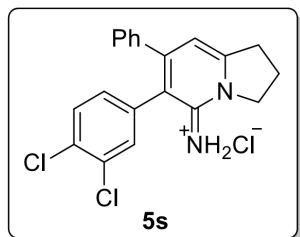
2.604
2.580
2.555
2.530
2.466



¹³C NMR (75 MHz, CDCl₃)



¹H NMR (300 MHz, CDCl₃)



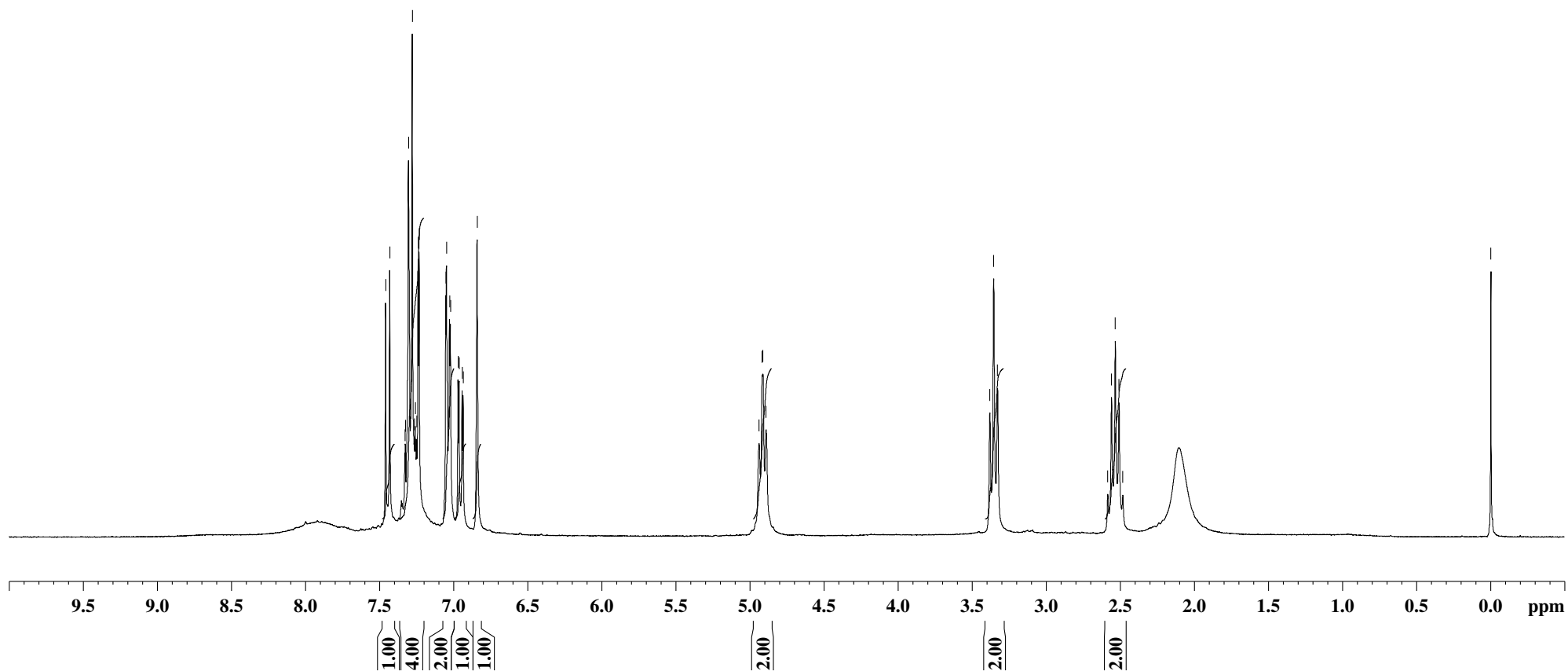
7.458
7.431
7.328
7.325
7.304
7.289
7.279
7.265
7.259
7.249
7.239
7.232
7.052
7.048
7.027
7.021
6.969
6.963
6.942
6.935
6.841

4.939
4.919
4.914
4.893

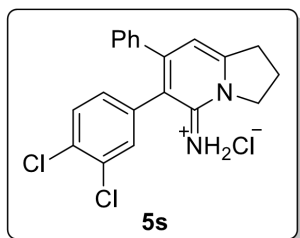
3.382
3.356
3.330

2.586
2.561
2.535
2.510
2.484

— -0.000



¹³C NMR (75 MHz, CDCl₃)



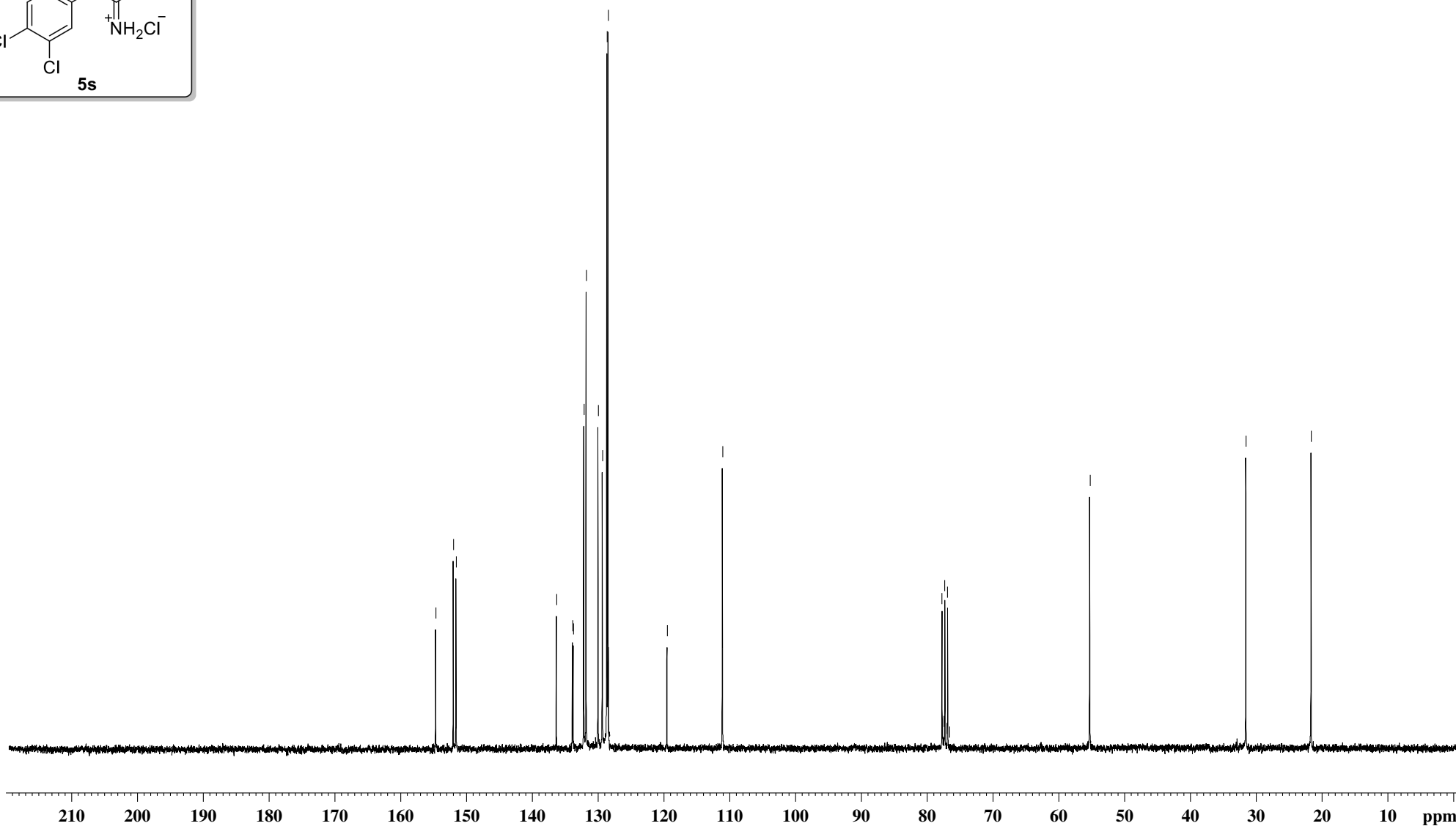
154.654
151.974
151.553
136.298
133.863
133.746
132.134
131.778
129.964
129.317
128.628
128.446
119.482
111.061

77.439
77.000
76.587

55.229

31.549

21.636



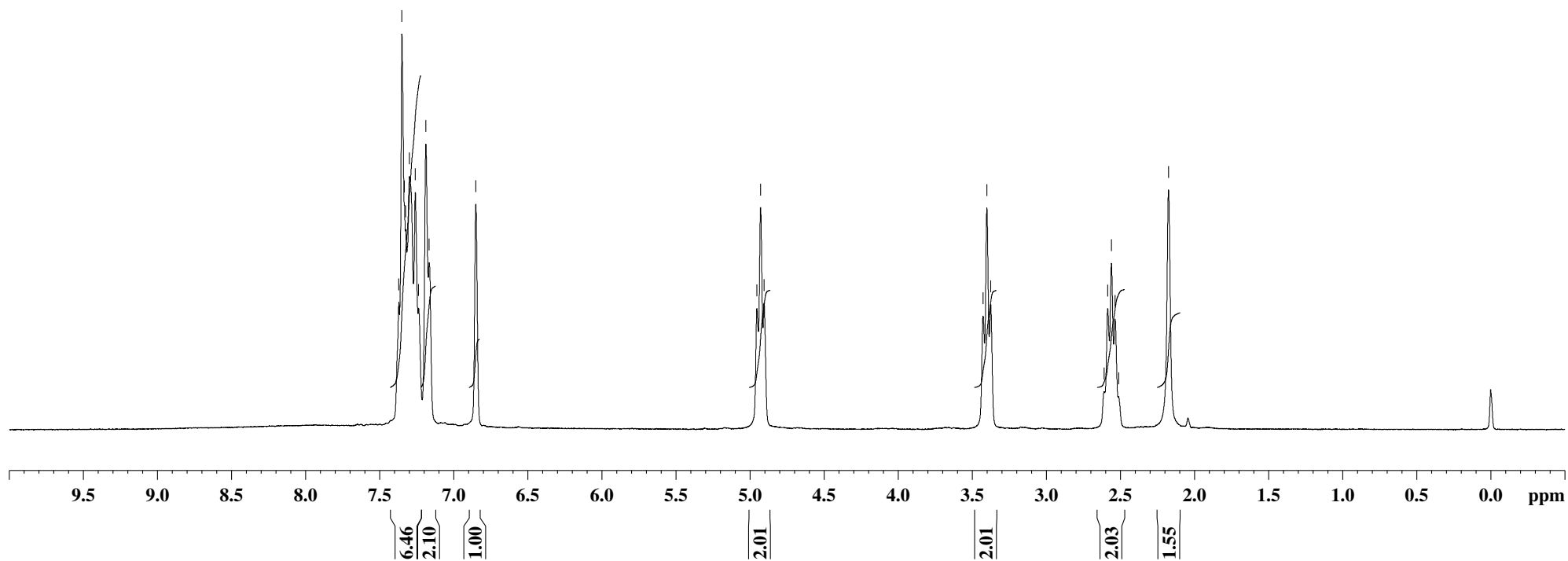
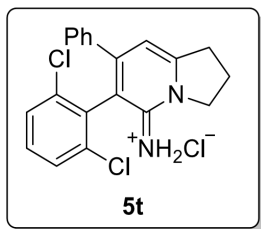
¹H NMR (300 MHz, CDCl₃)

7.372
7.351
7.334
7.325
7.300
7.260
7.238
7.189
7.167
6.851

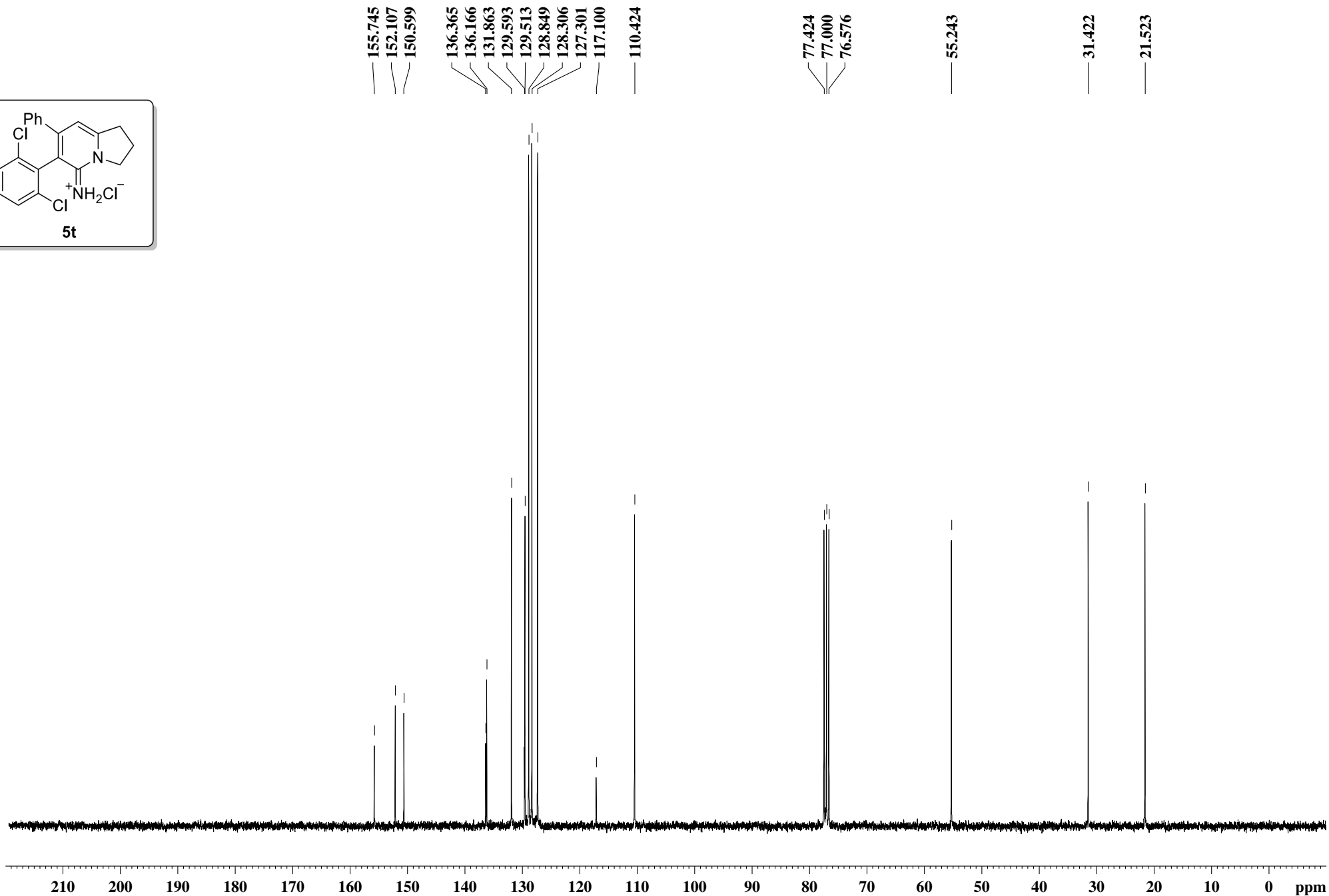
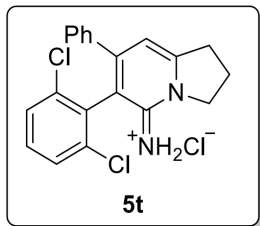
4.954
4.929
4.906

3.428
3.402
3.376

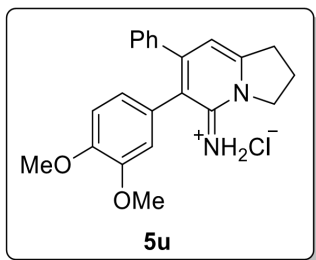
2.611
2.587
2.561
2.537
2.512
2.176



13C NMR (75 MHz, CDCl3)



¹H NMR (300 MHz, CDCl₃)

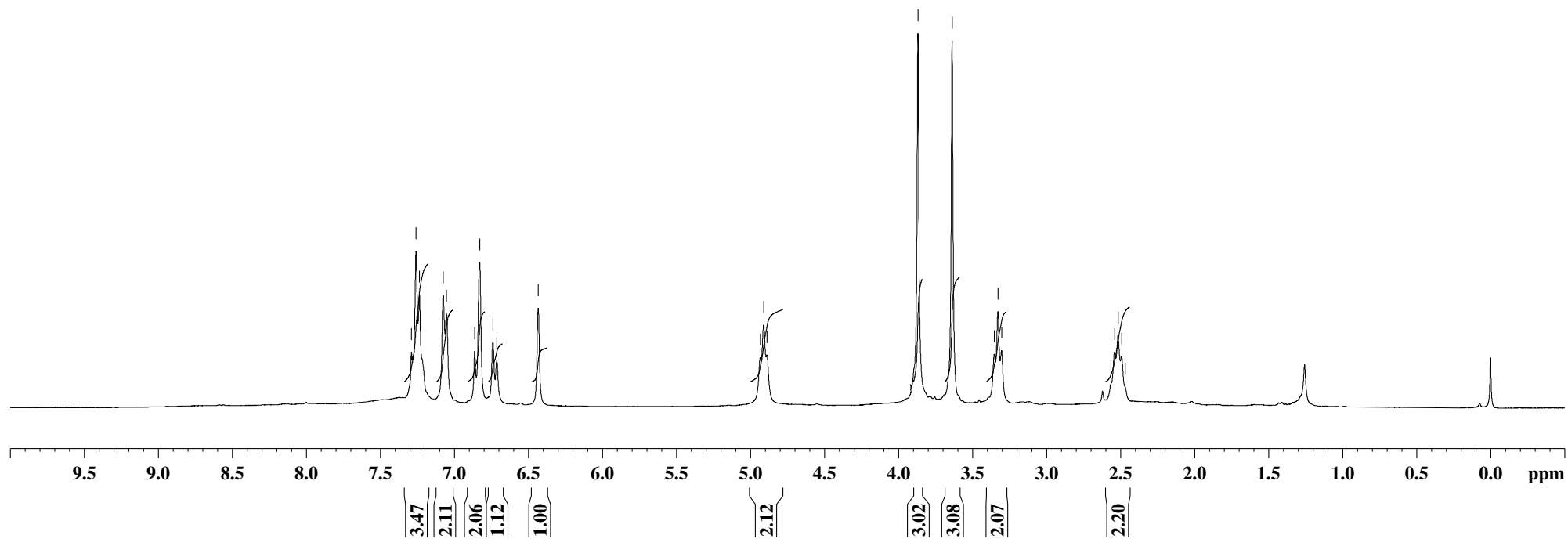


7.291
7.260
7.237
7.076
7.055
6.864
6.829
6.740
6.714
6.434

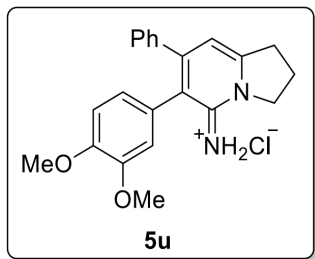
4.934
4.911
4.889

3.869
3.638
3.354
3.329
3.303

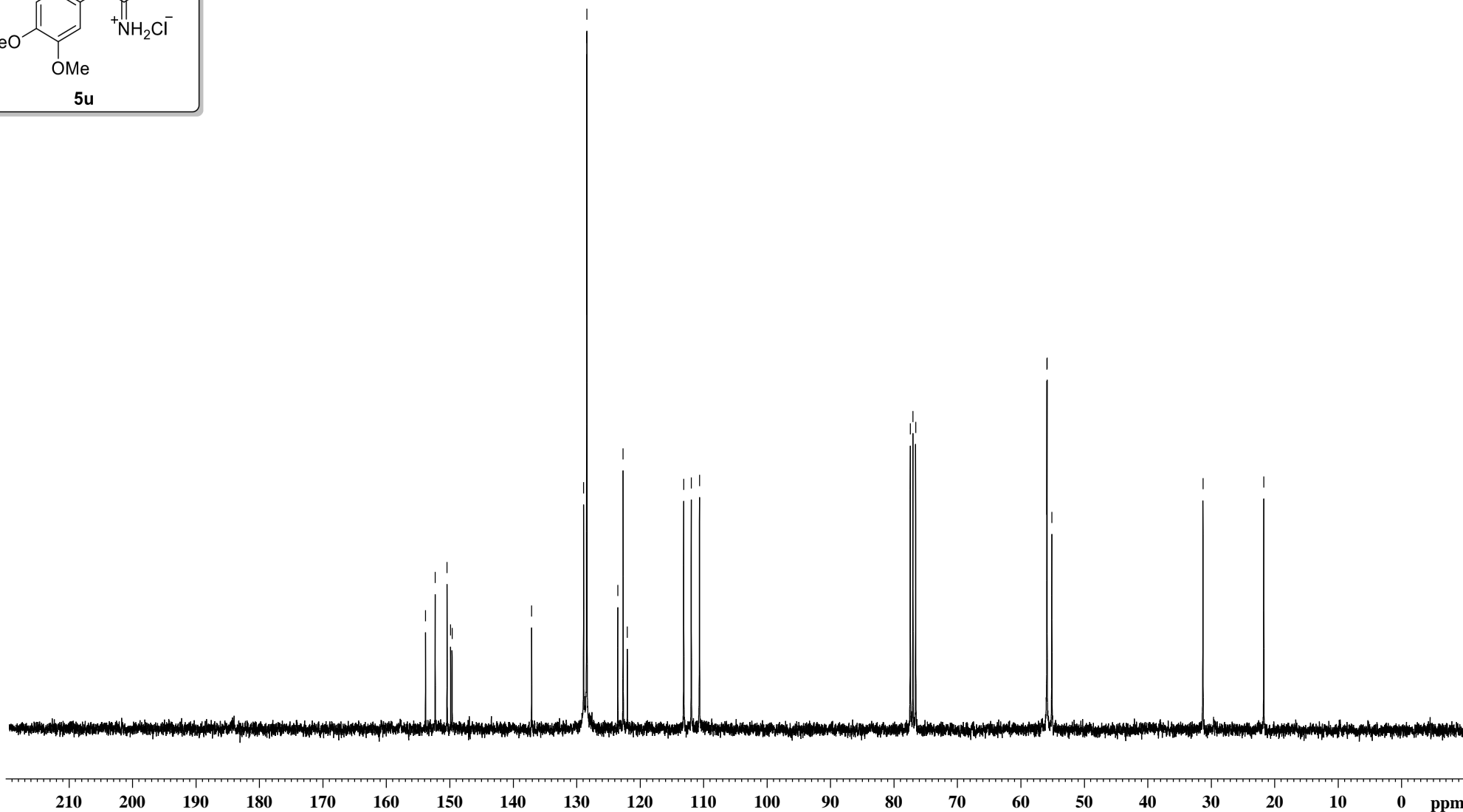
2.566
2.540
2.517
2.493
2.469



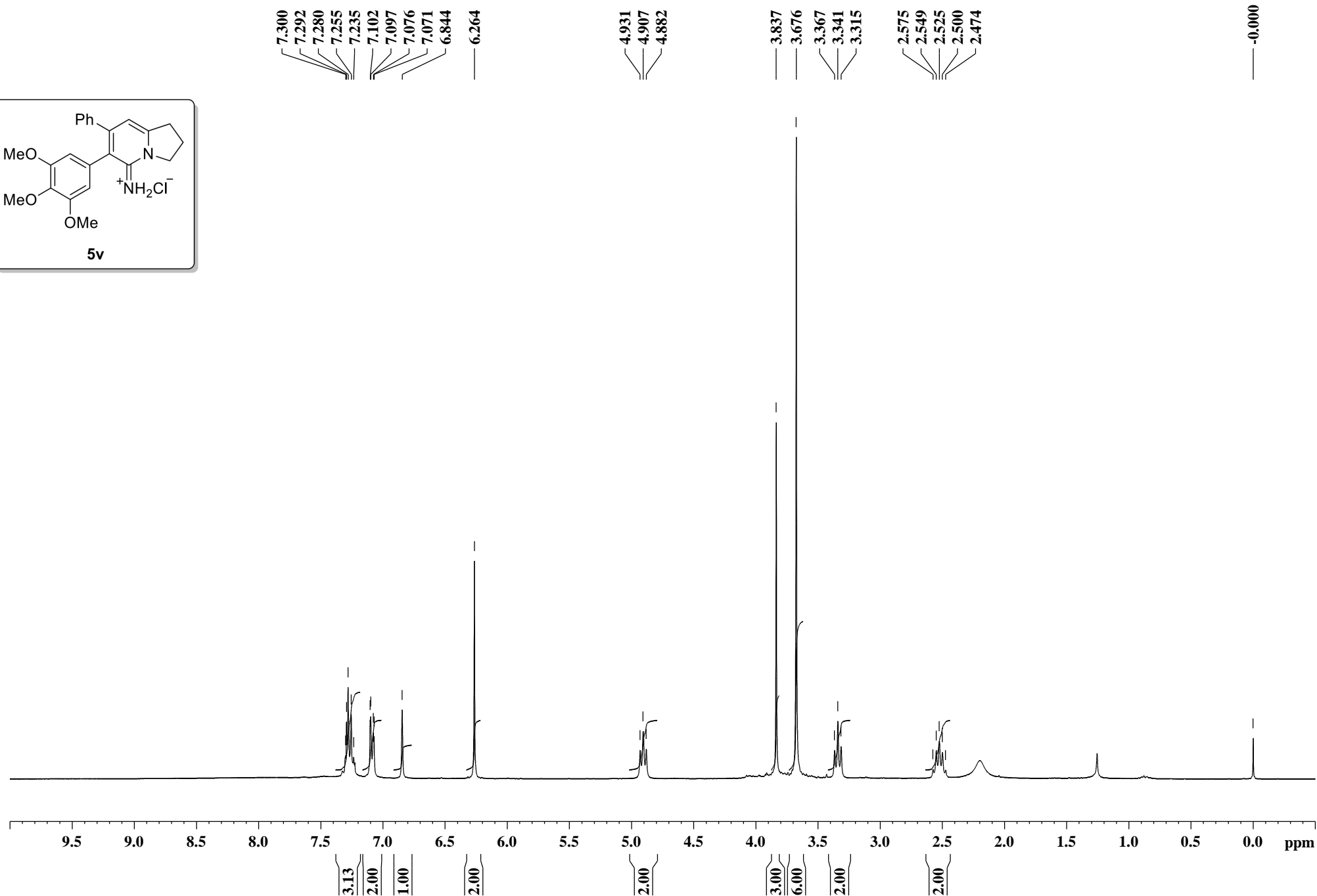
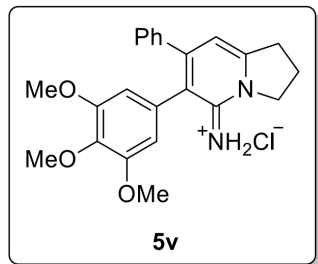
13C NMR (75 MHz, CDCl3)



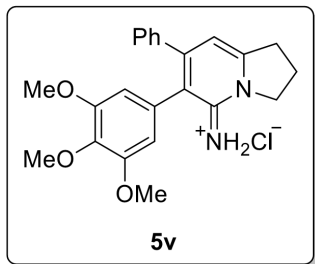
153.817
152.291
150.423
149.858
149.627
137.089
128.901
128.419
128.378
123.520
122.676
122.005
113.127
111.932
110.640
77.424
77.000
76.576
55.891
55.854
55.107
31.291
21.706



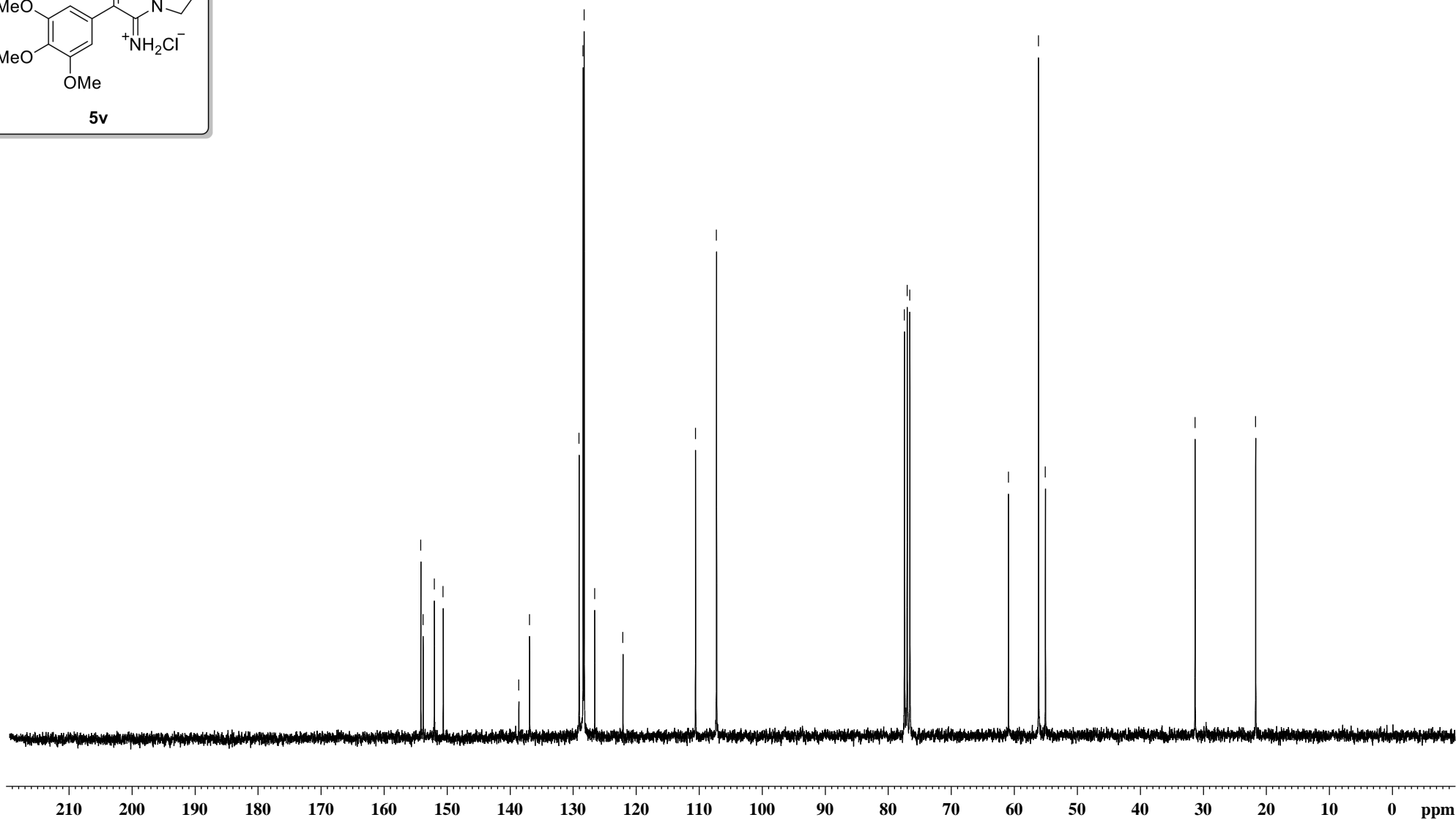
¹H NMR (300 MHz, CDCl₃)



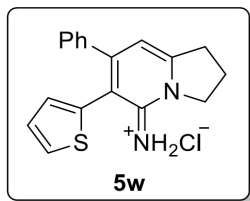
13C NMR (75 MHz, CDCl3)



- 154.179
- 153.815
- 152.032
- 150.628
- 138.631
- 136.923
- 129.060
- 128.430
- 128.257
- 126.581
- 122.104
- 110.591
- 107.256
- 77.424
- 77.000
- 76.576
- 60.929
- 56.156
- 55.062
- 31.308
- 21.694



1H NMR (300 MHz, CDCl3)



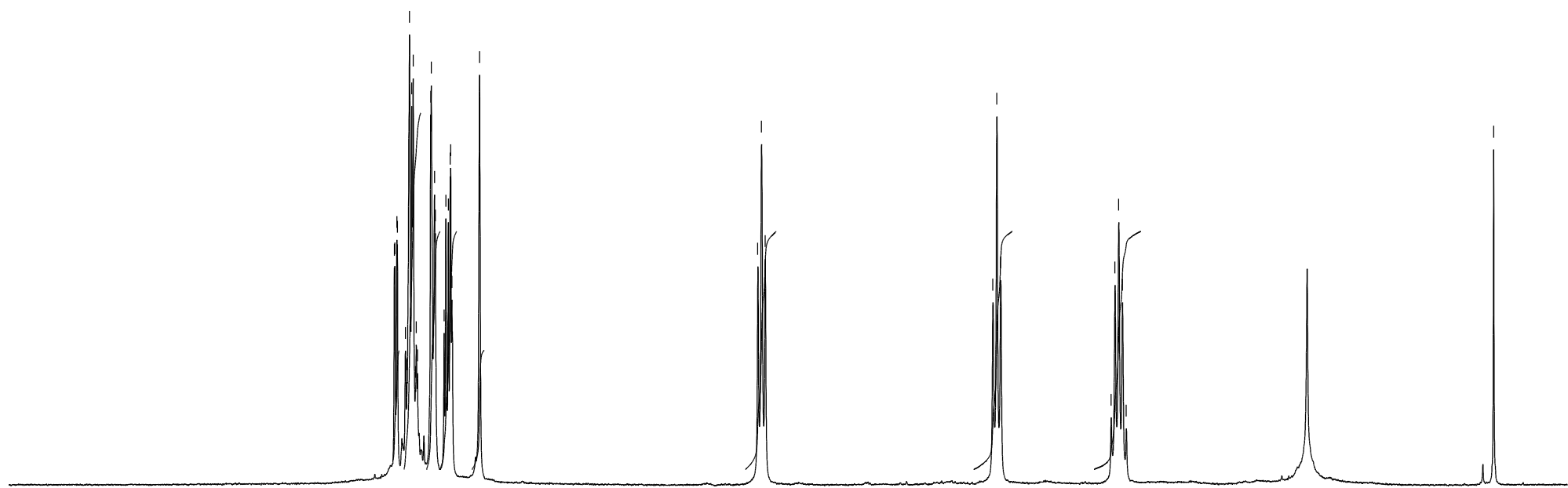
7.402
7.398
7.385
7.381
7.327
7.316
7.300
7.285
7.275
7.260
7.254
7.246
7.157
7.153
7.131
7.126
7.067
7.055
7.038
7.026
7.022
7.014
6.828

4.954
4.930
4.905

3.371
3.345
3.319

2.574
2.548
2.523
2.498
2.472

-0.002



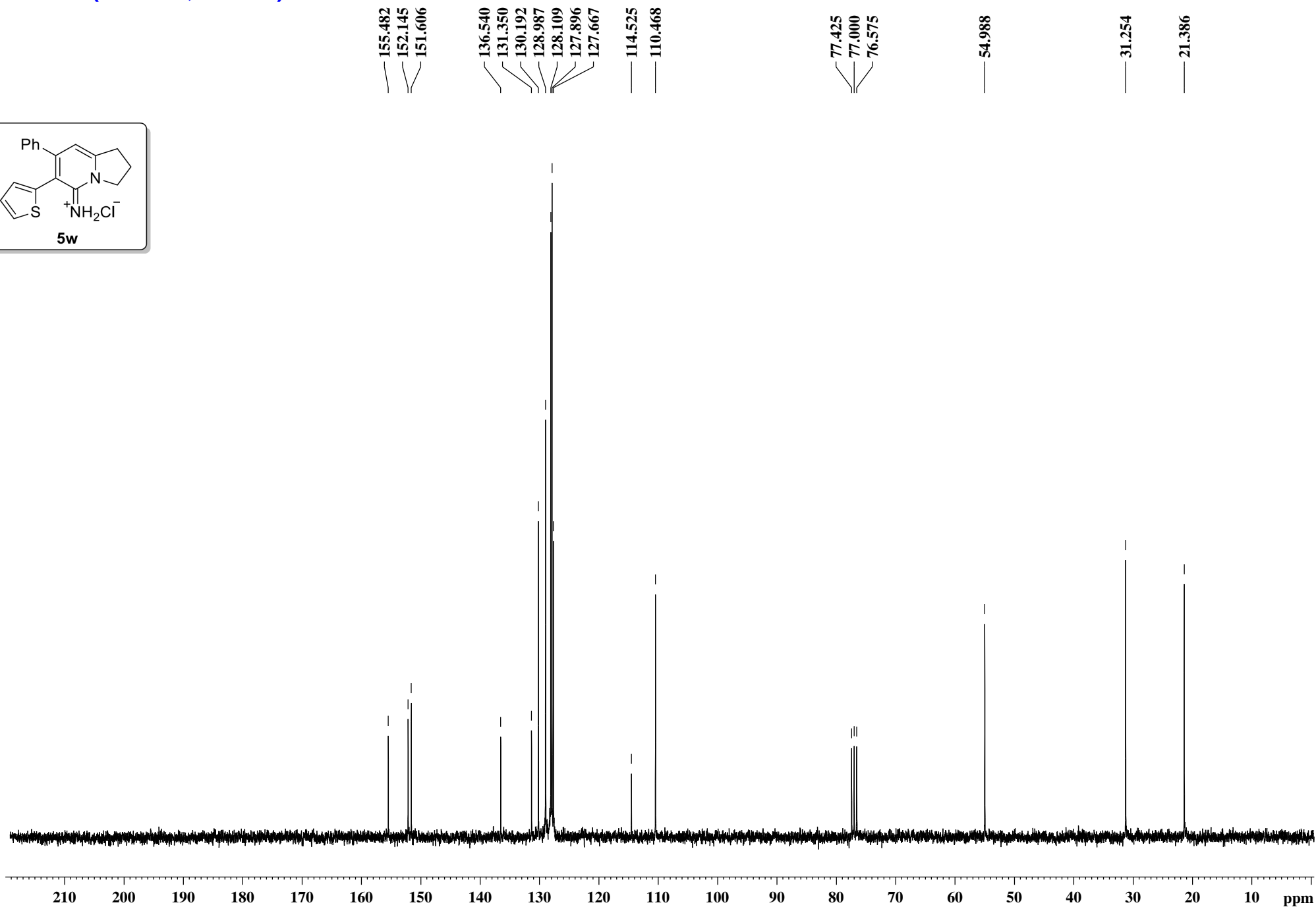
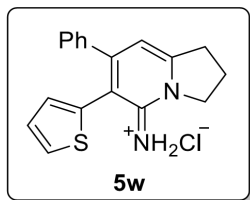
1.00
3.00
2.00
2.00
1.00

2.00

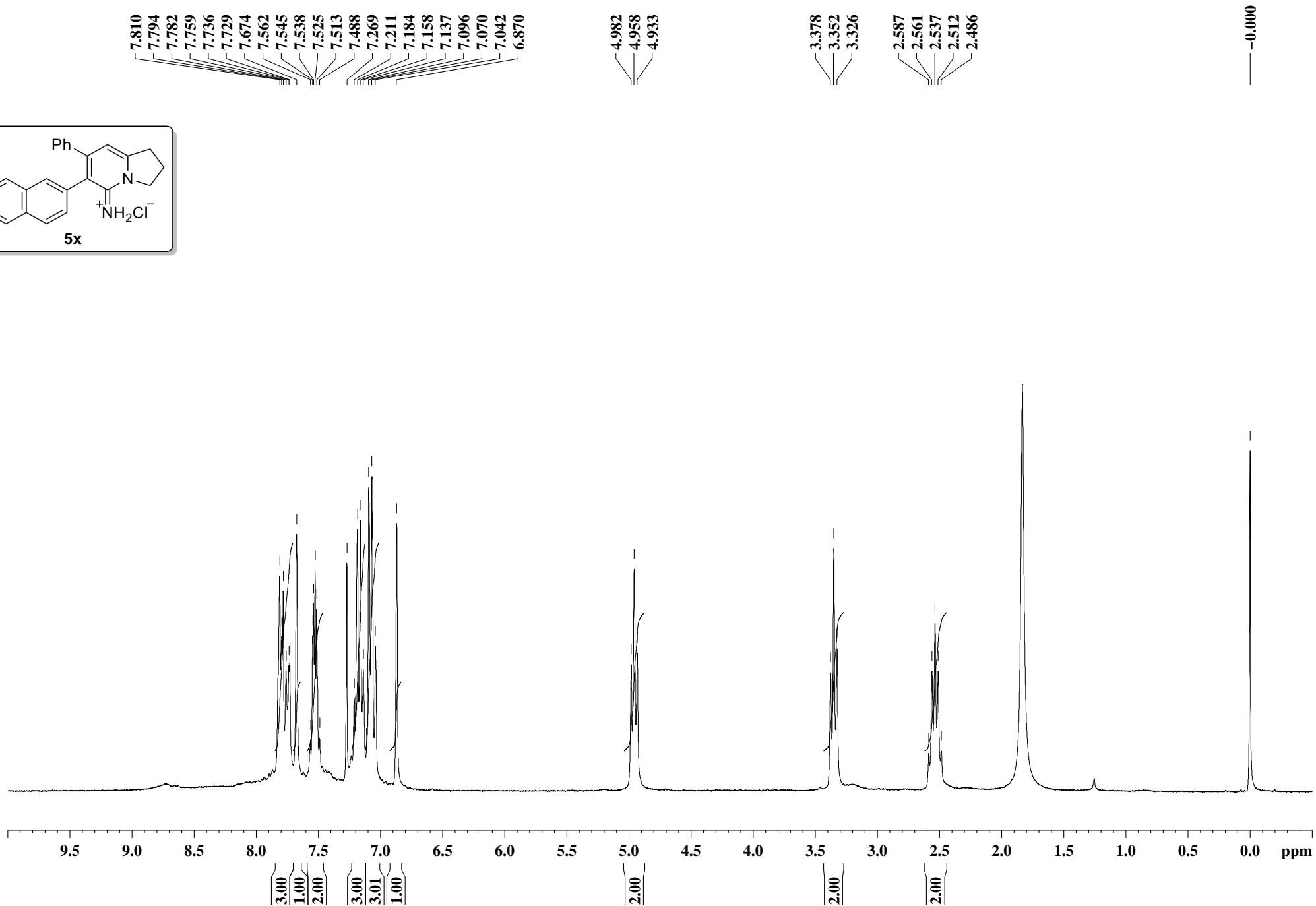
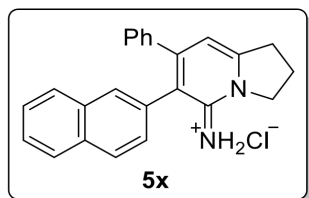
2.00

2.00

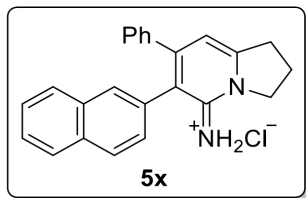
¹³C NMR (75 MHz, CDCl₃)



^1H NMR (300 MHz, CDCl_3)



¹³C NMR (75 MHz, CDCl₃)



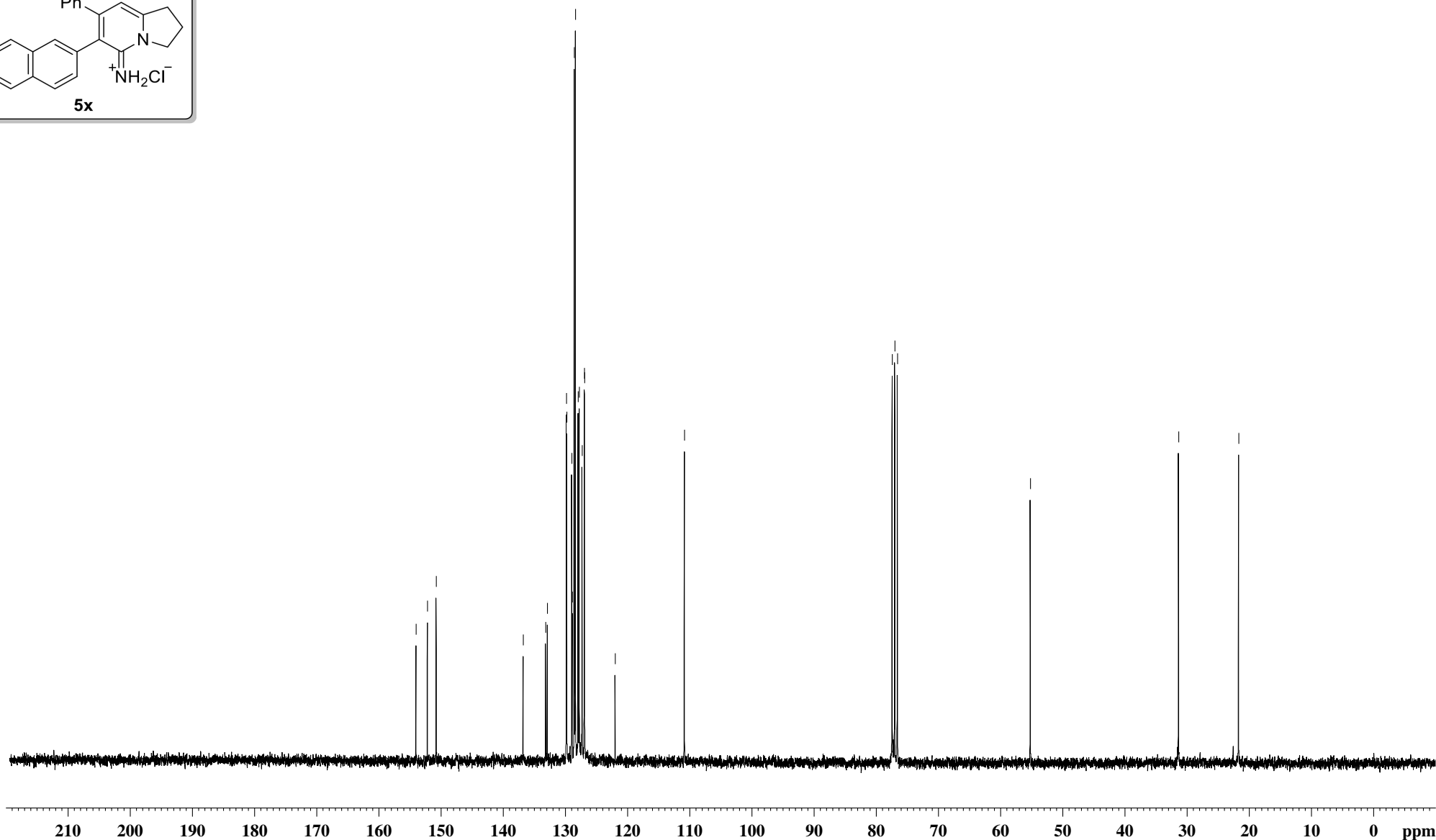
154.018
152.188
150.773
136.779
133.170
132.898
129.828
129.773
128.966
128.886
128.569
128.376
127.946
127.757
127.301
126.940
126.906
121.984
110.843

77.424
77.000
76.576

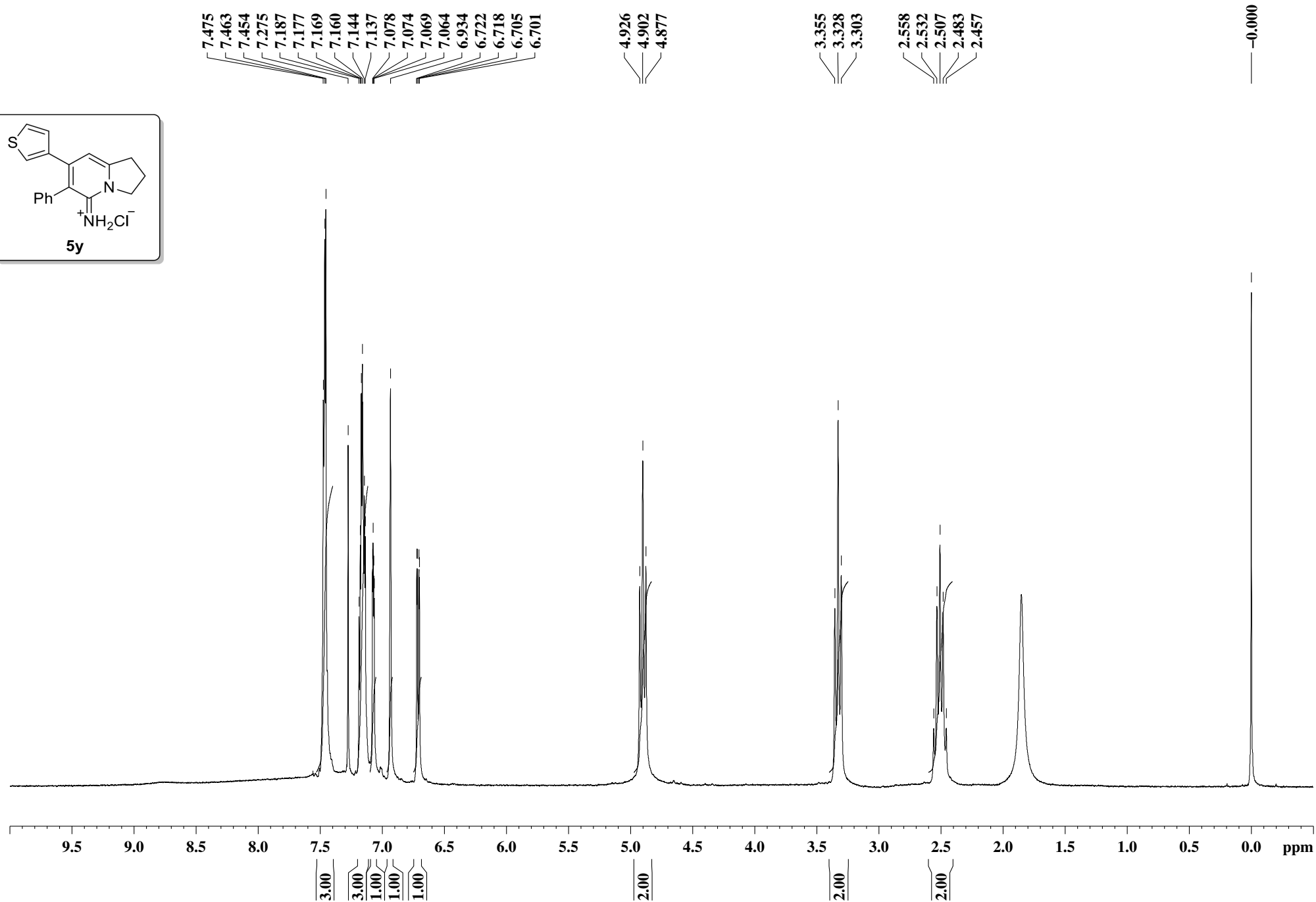
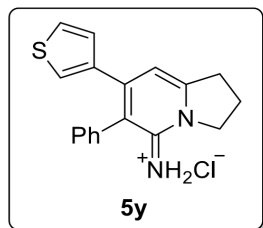
55.197

31.349

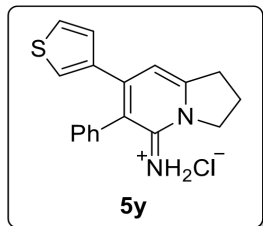
21.686



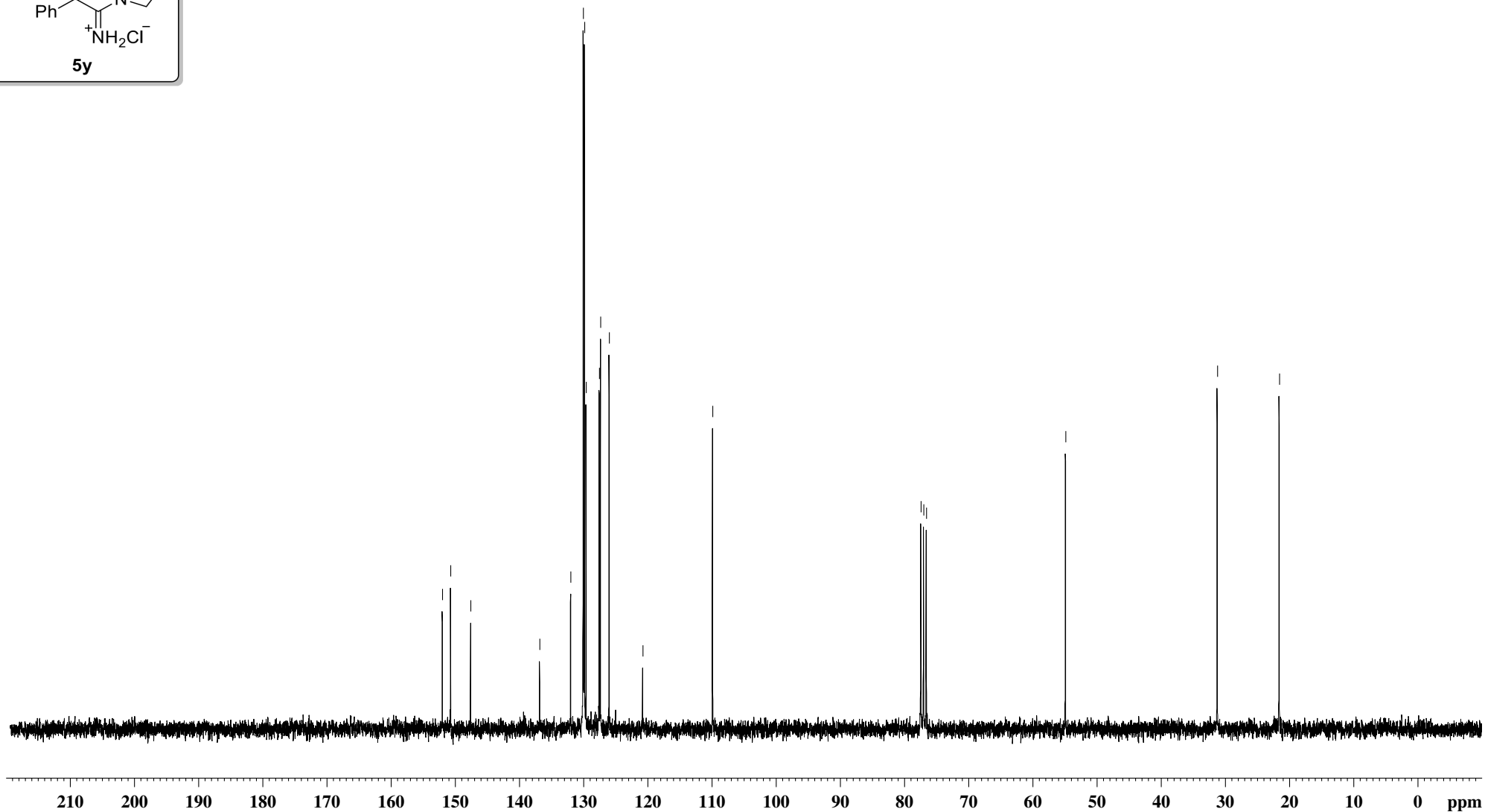
^1H NMR (300 MHz, CDCl_3)



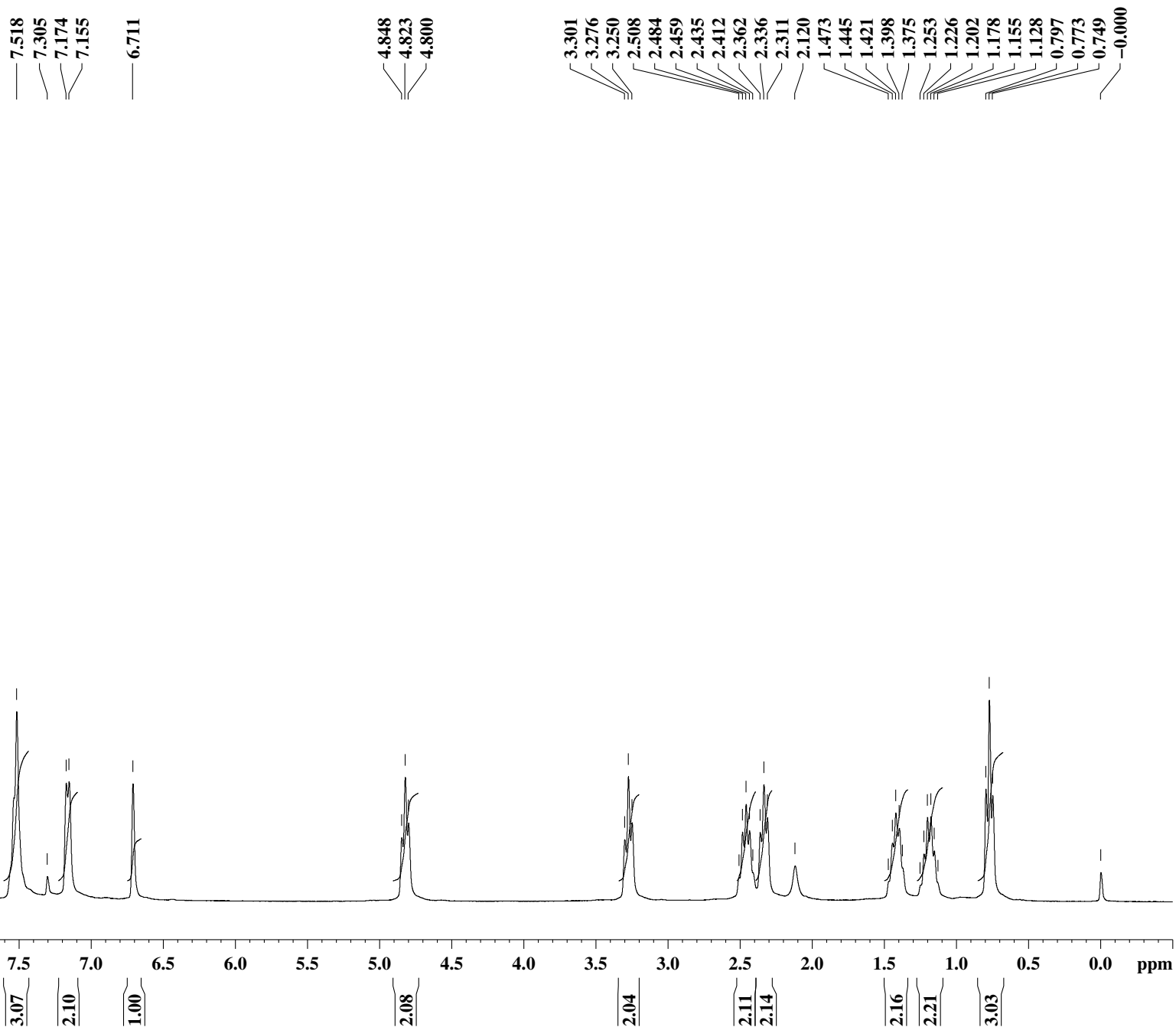
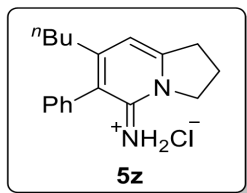
¹³C NMR (75 MHz, CDCl₃)



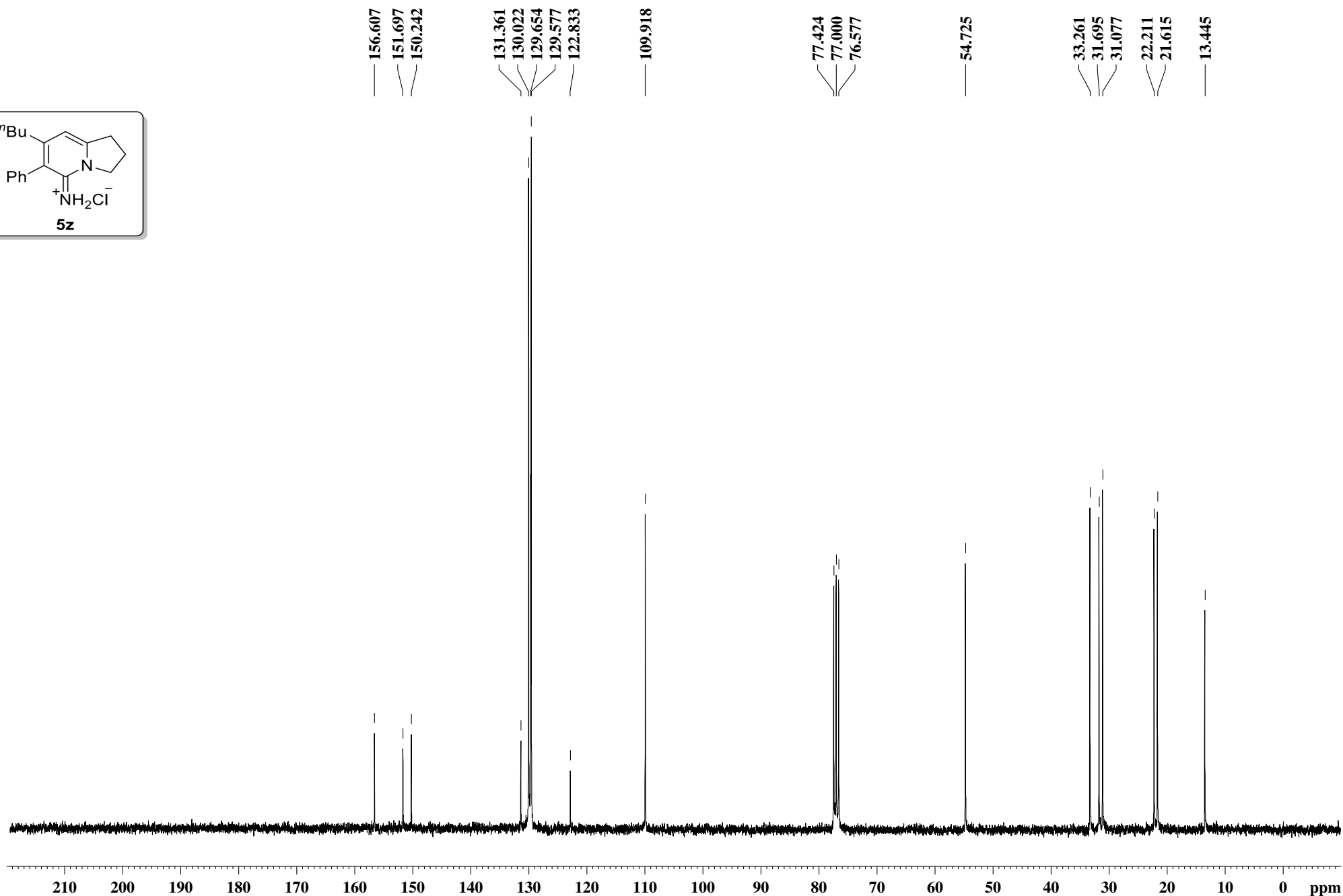
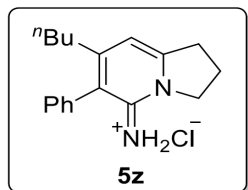
151.999
150.719
147.589
136.836
132.005
130.046
129.841
129.597
127.544
127.351
126.000
120.762
109.886
77.425
77.000
76.575
54.873
31.224
21.564



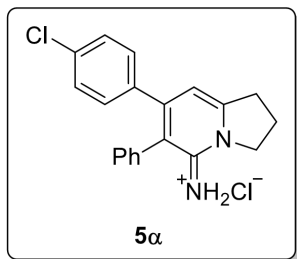
^1H NMR (300 MHz, CDCl_3)



¹³C NMR (75 MHz, CDCl₃)



^1H NMR (300 MHz, CDCl_3)



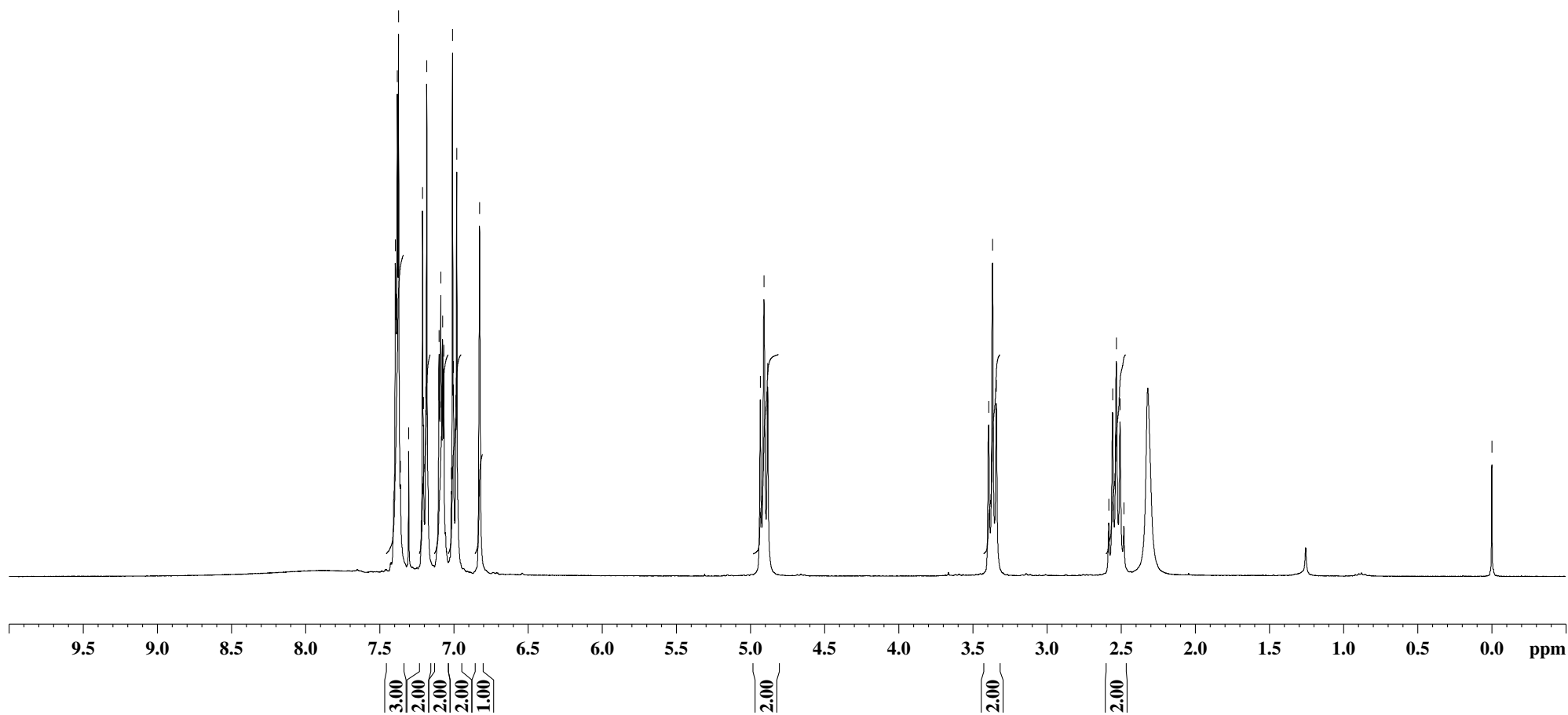
7.395
7.389
7.382
7.374
7.361
7.305
7.212
7.206
7.190
7.184
7.100
7.088
7.076
7.069
7.018
7.010
7.003
6.987
6.981
6.827

4.934
4.909
4.884

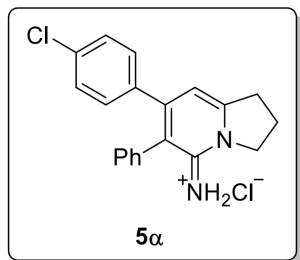
3.393
3.368
3.342

2.584
2.557
2.532
2.508
2.482

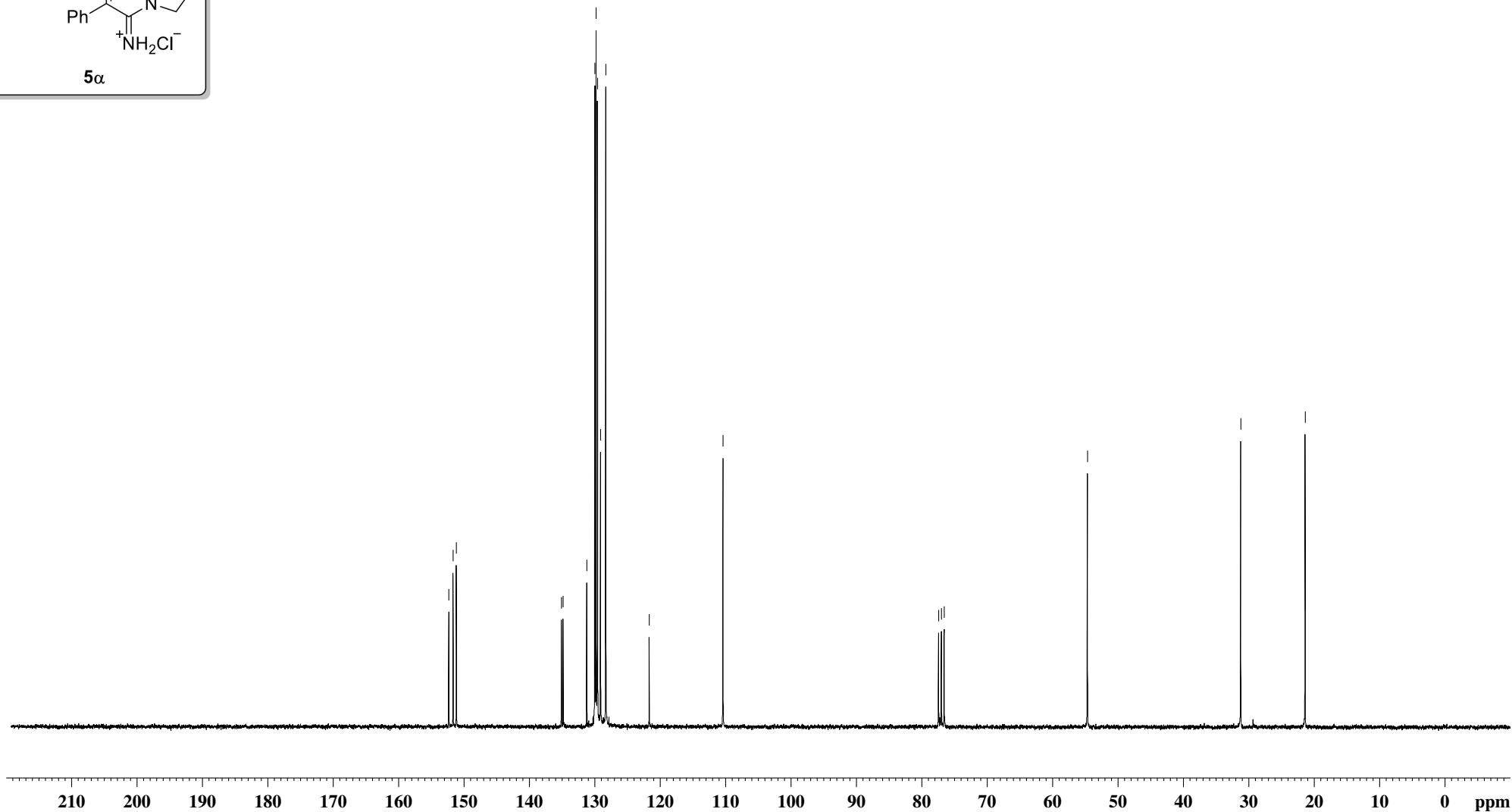
— 0.000



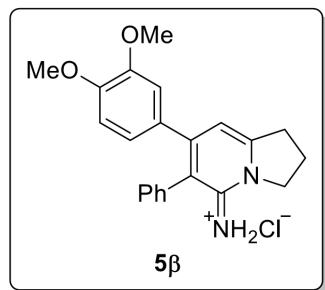
¹³C NMR (75 MHz, CDCl₃)



152.330
151.671
151.175
135.098
134.852
131.223
129.997
129.807
129.582
129.121
128.318
121.681
110.398
77.425
77.000
76.574
54.658
31.217
21.364



¹H NMR (300 MHz, CDCl₃)



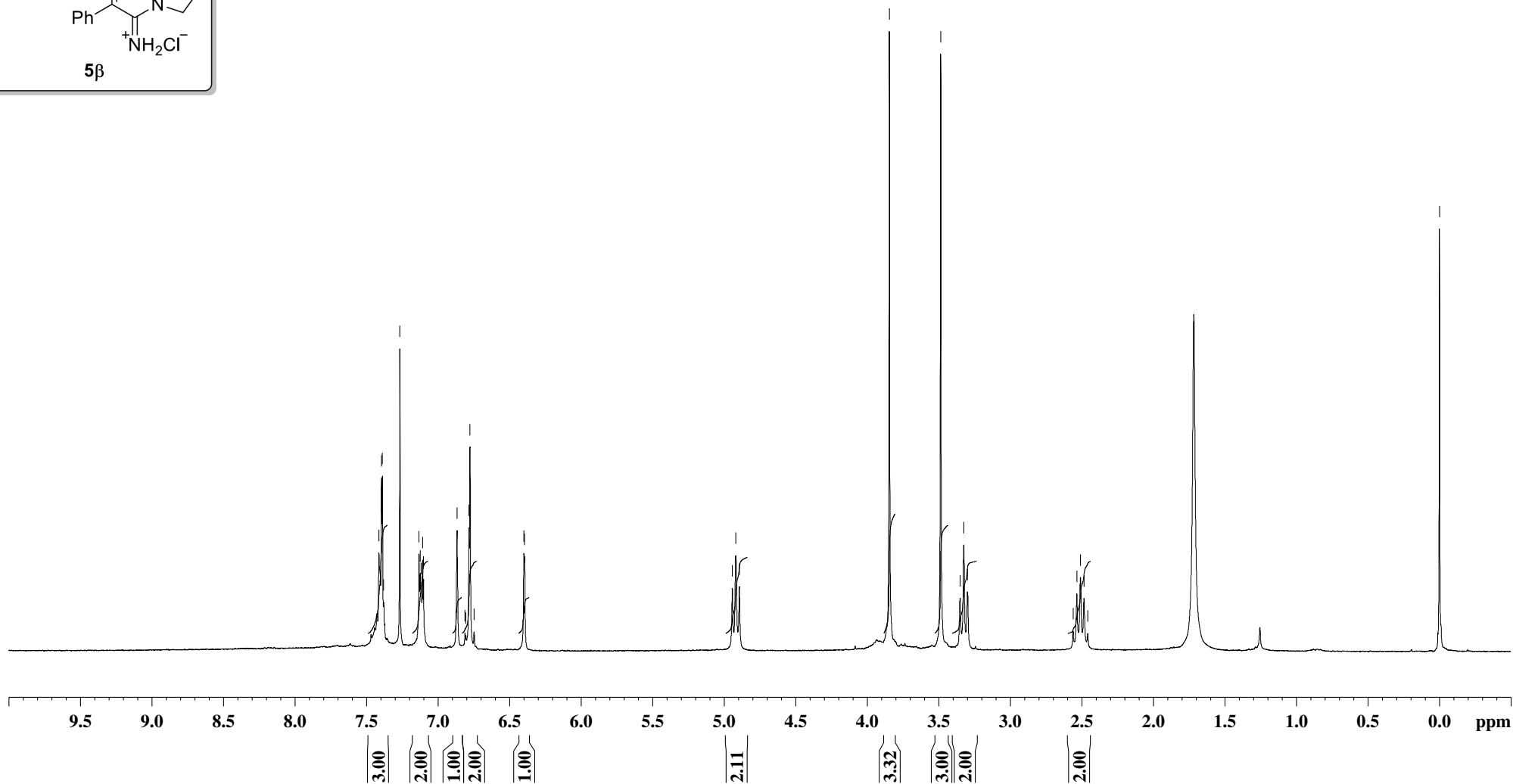
7.414
7.396
7.390
7.382
7.268
7.134
7.125
7.119
7.109
7.103
6.868
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6.807
6.785
6.778
6.749
6.401
6.396

4.944
4.920
4.894

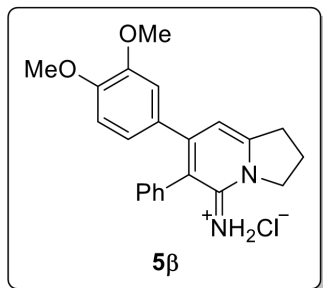
3.846
3.487
3.352
3.325
3.300

2.561
2.535
2.510
2.485
2.459

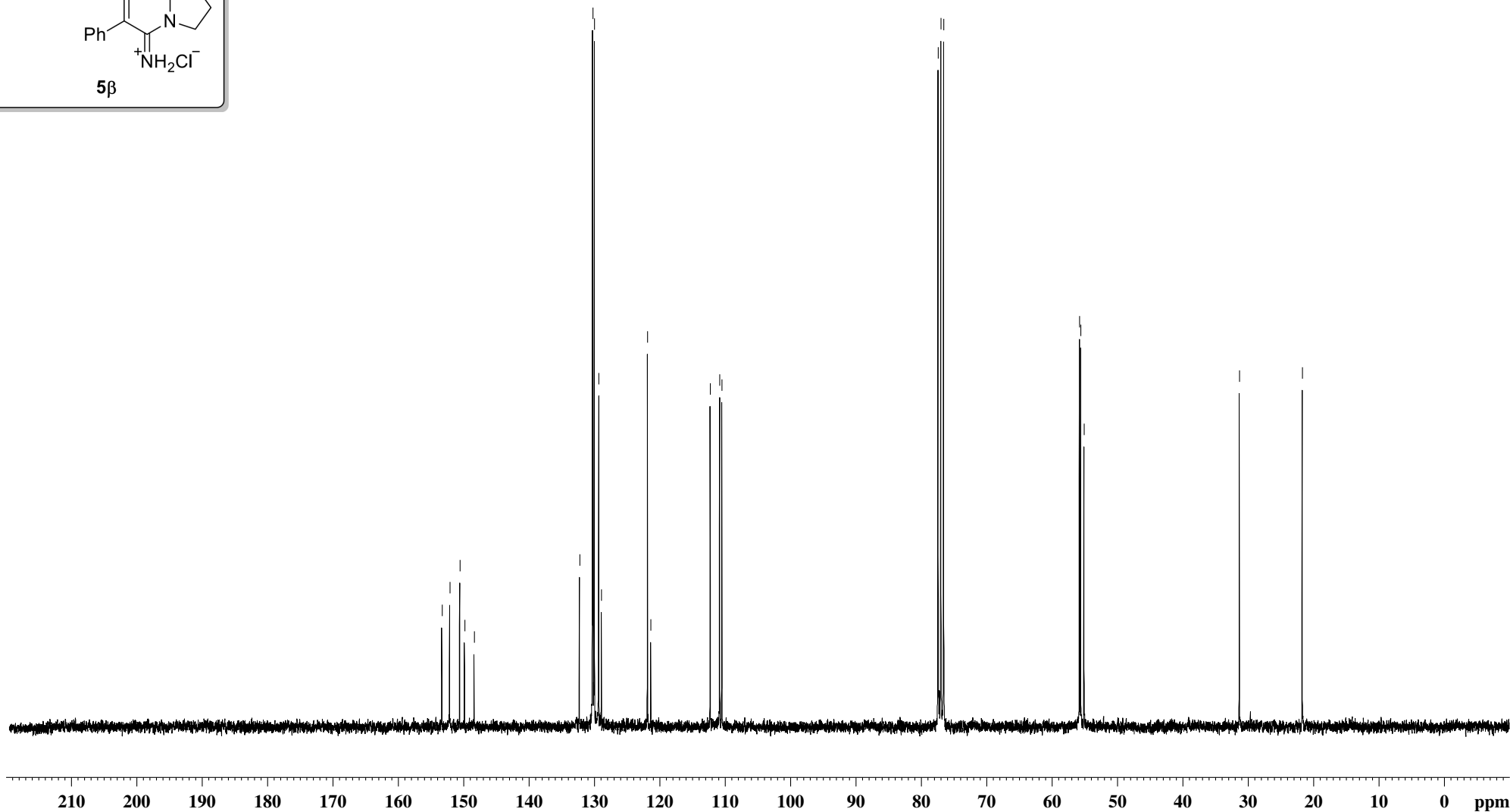
-0.000



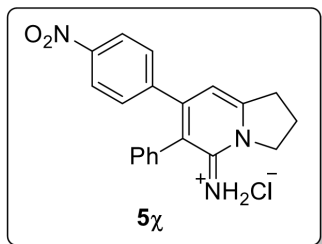
13C NMR (75 MHz, CDCl3)



153.286
152.097
150.559
149.822
148.366
132.238
130.233
130.000
129.337
128.935
121.885
121.382
112.284
110.845
110.505
77.424
77.000
76.576
55.804
55.615
55.099
31.338
21.714



^1H NMR (300 MHz, CDCl_3)



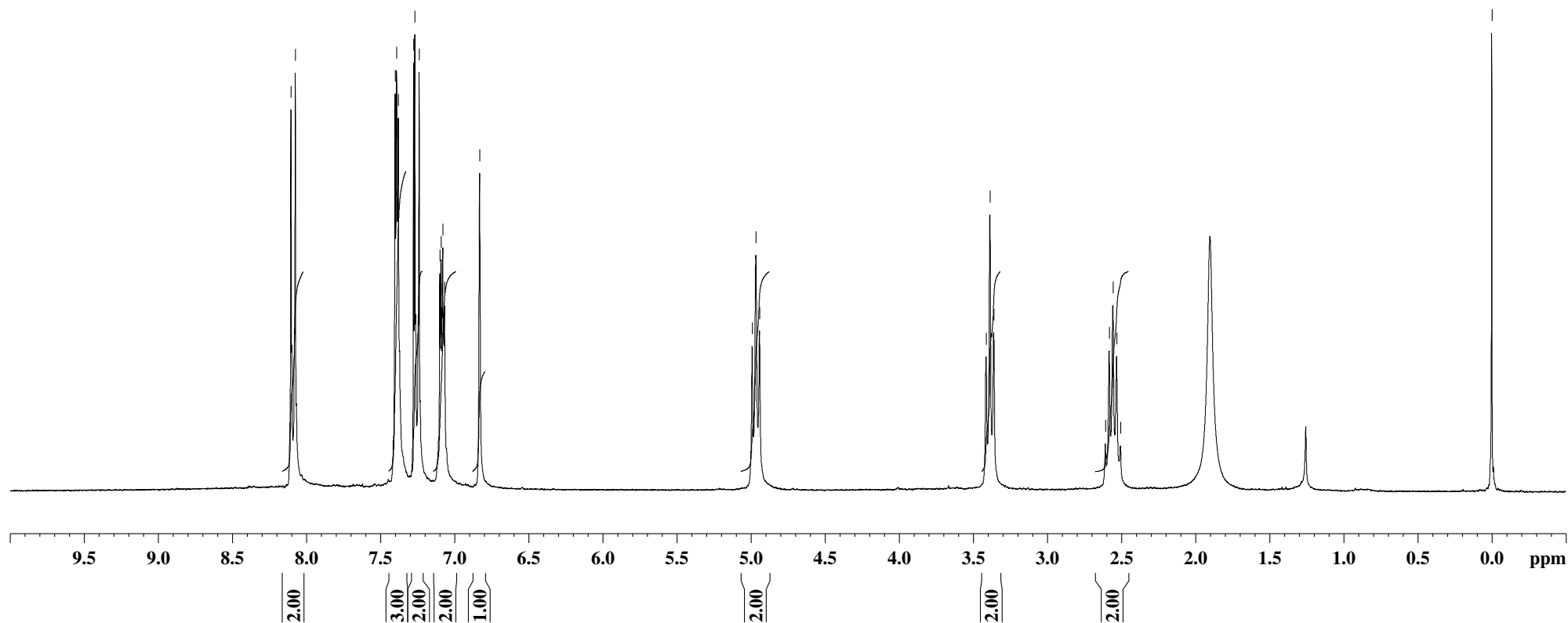
8.105
8.075
7.402
7.392
7.380
7.277
7.269
7.240
7.100
7.092
7.085
7.080
7.068
6.831

4.992
4.967
4.942

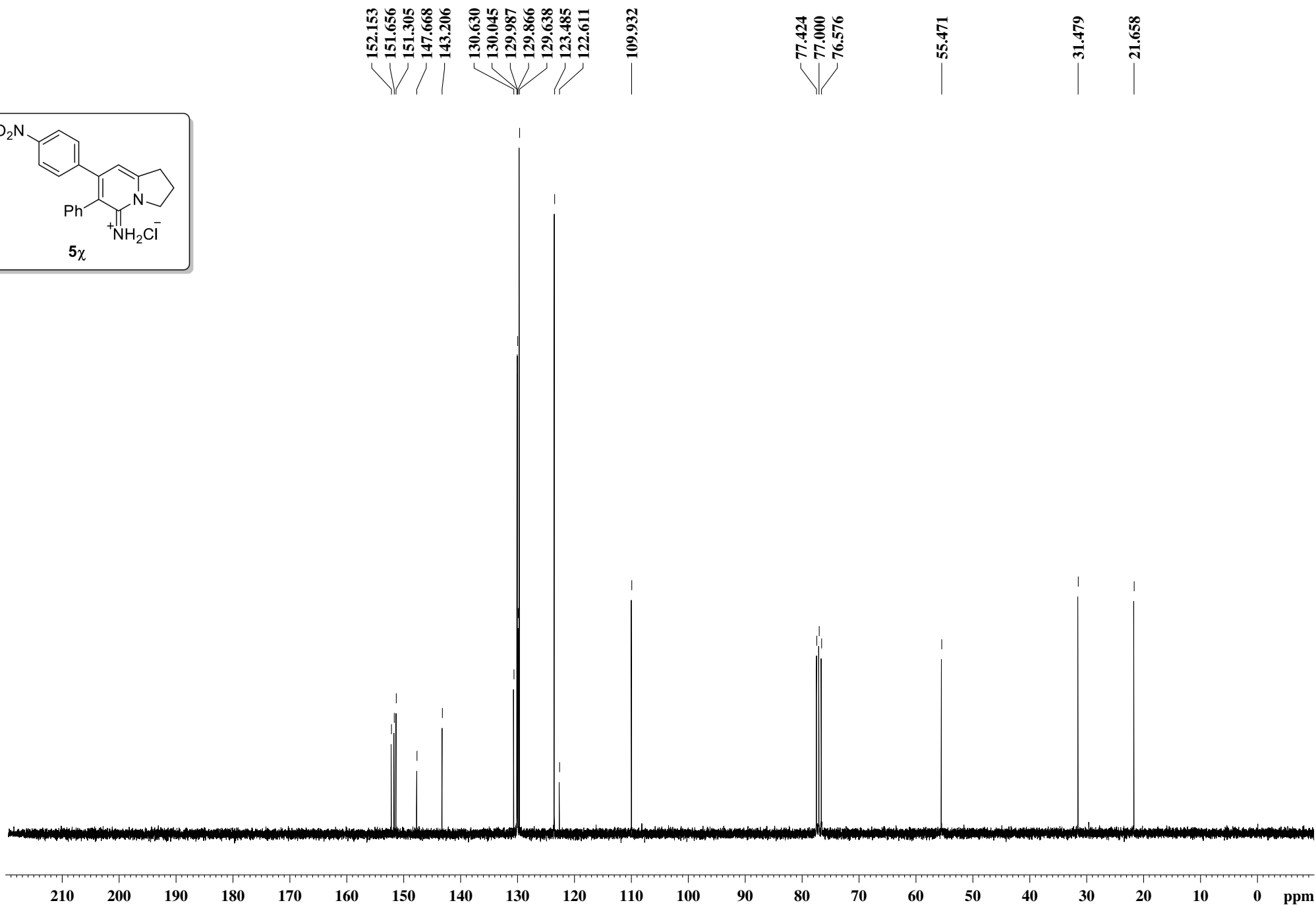
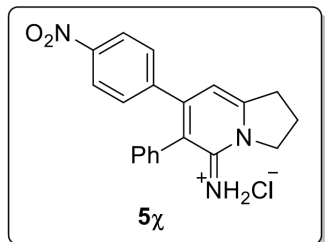
3.413
3.387
3.362

2.608
2.582
2.557
2.532
2.506

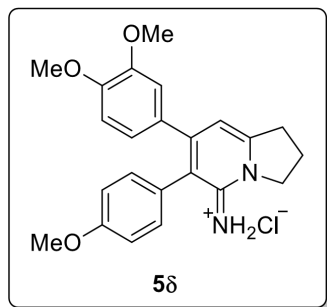
-0.000



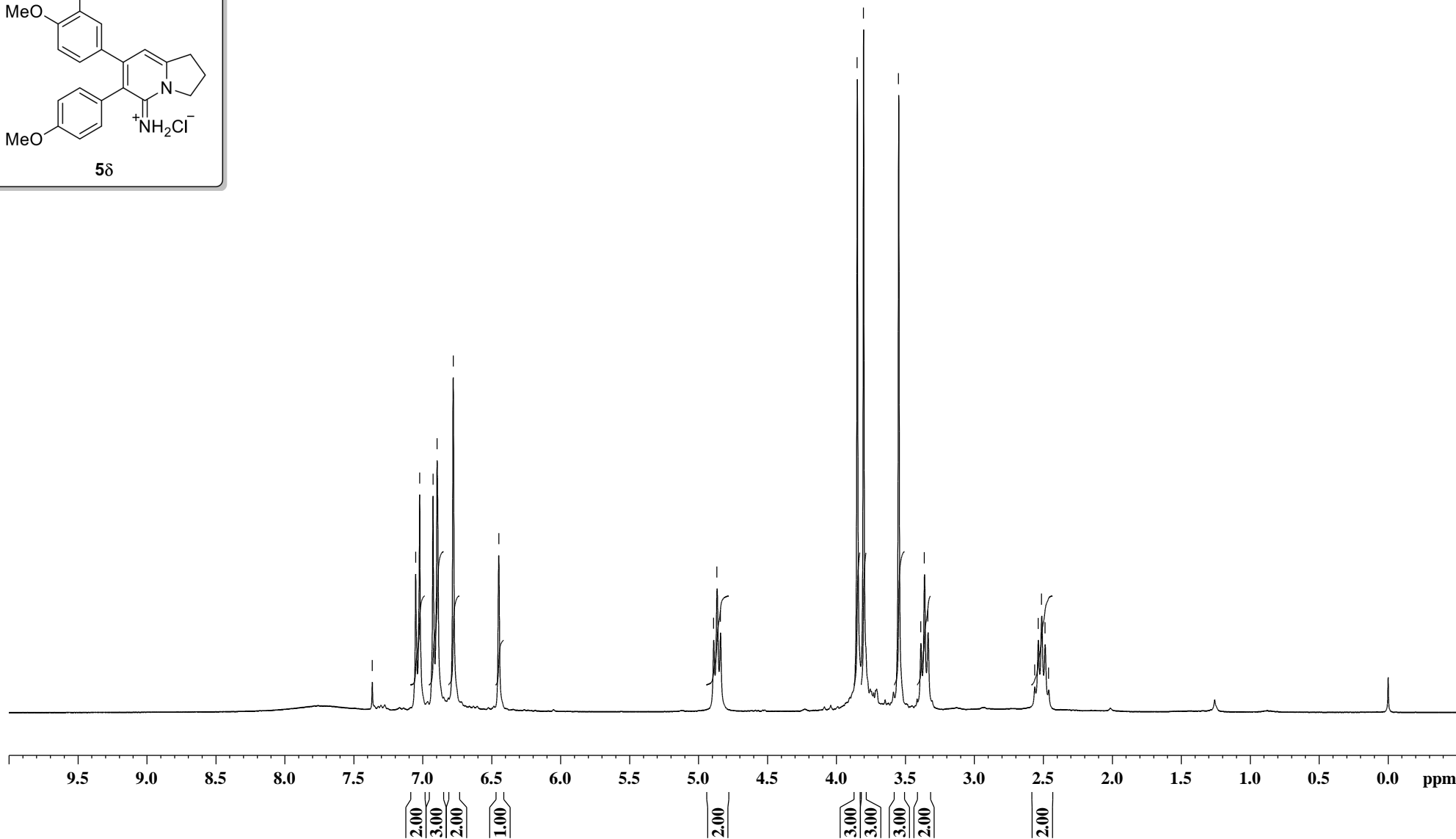
13C NMR (75 MHz, CDCl3)



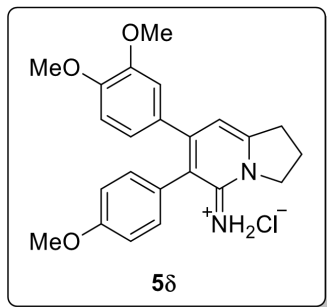
1H NMR (300 MHz, CDCl3)



7.365
7.051
7.022
6.925
6.895
6.779
6.448
4.891
4.867
4.842
3.850
3.804
3.550
3.388
3.362
3.337
2.563
2.537
2.512
2.488
2.462



13C NMR (75 MHz, CDCl3)



159.862
153.185
152.020
150.234
149.418
148.086

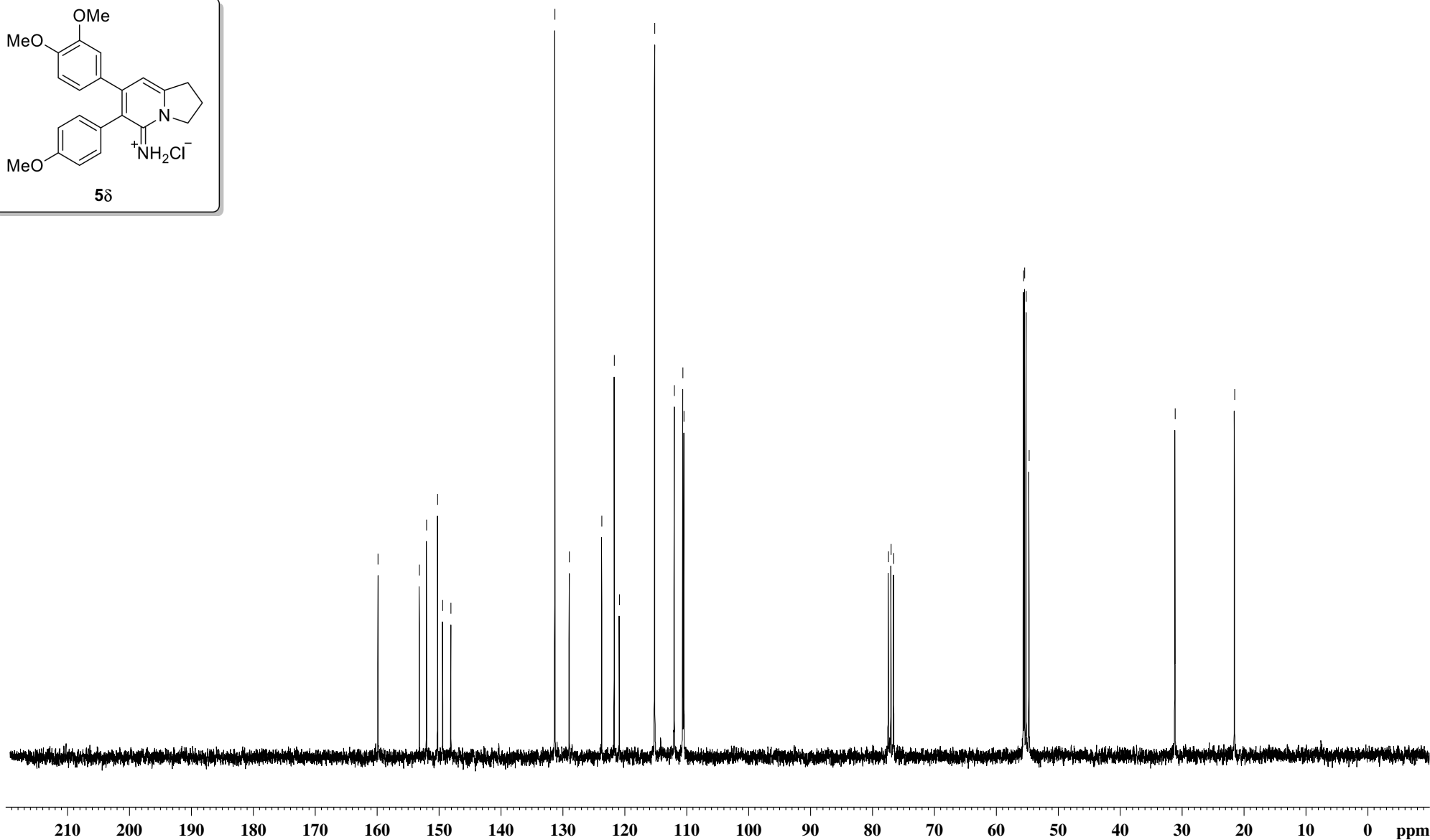
131.294
128.967
123.718
121.701
120.876
115.169
112.002
110.625
110.449

77.424
77.000
76.575

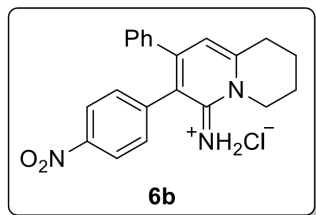
55.597
55.429
55.180
54.705

31.122

21.508



¹H NMR (300 MHz, CDCl₃)



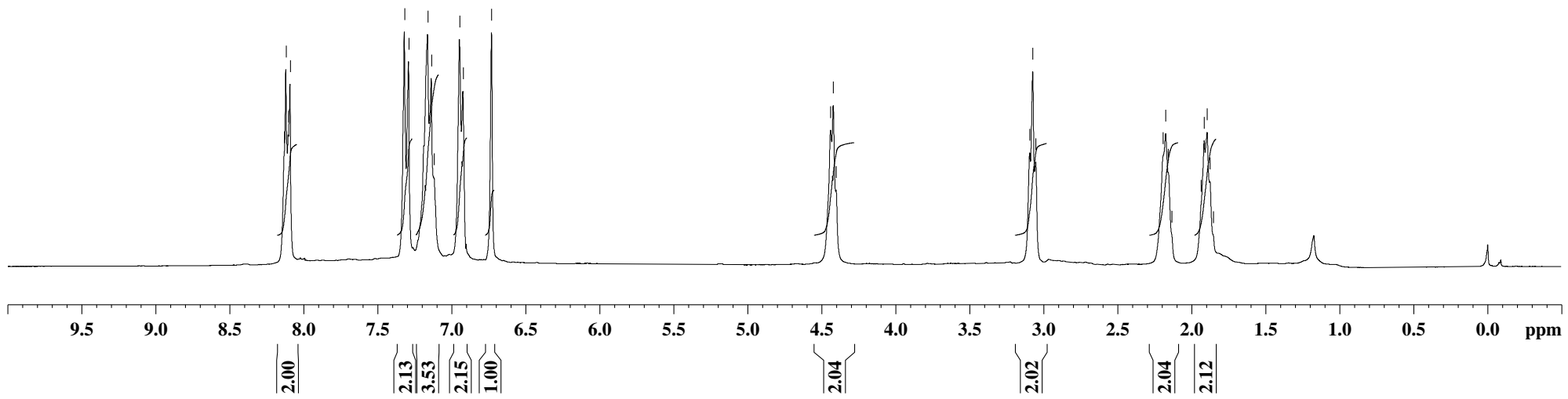
8.131
8.119
8.103
8.090

7.318
7.290
7.161
7.136
7.119
6.946
6.922
6.732

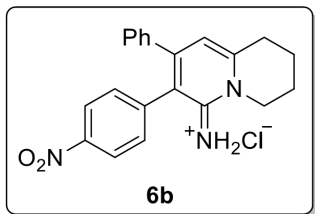
4.441
4.423
4.403

3.095
3.075
3.054

2.194
2.176
2.159
2.135
1.937
1.916
1.896
1.877
1.854



¹³C NMR (75 MHz, CDCl₃)



153.247
152.669
148.692
147.585
138.790
135.554
131.767
129.023
128.294
128.119
124.431
119.713
115.318

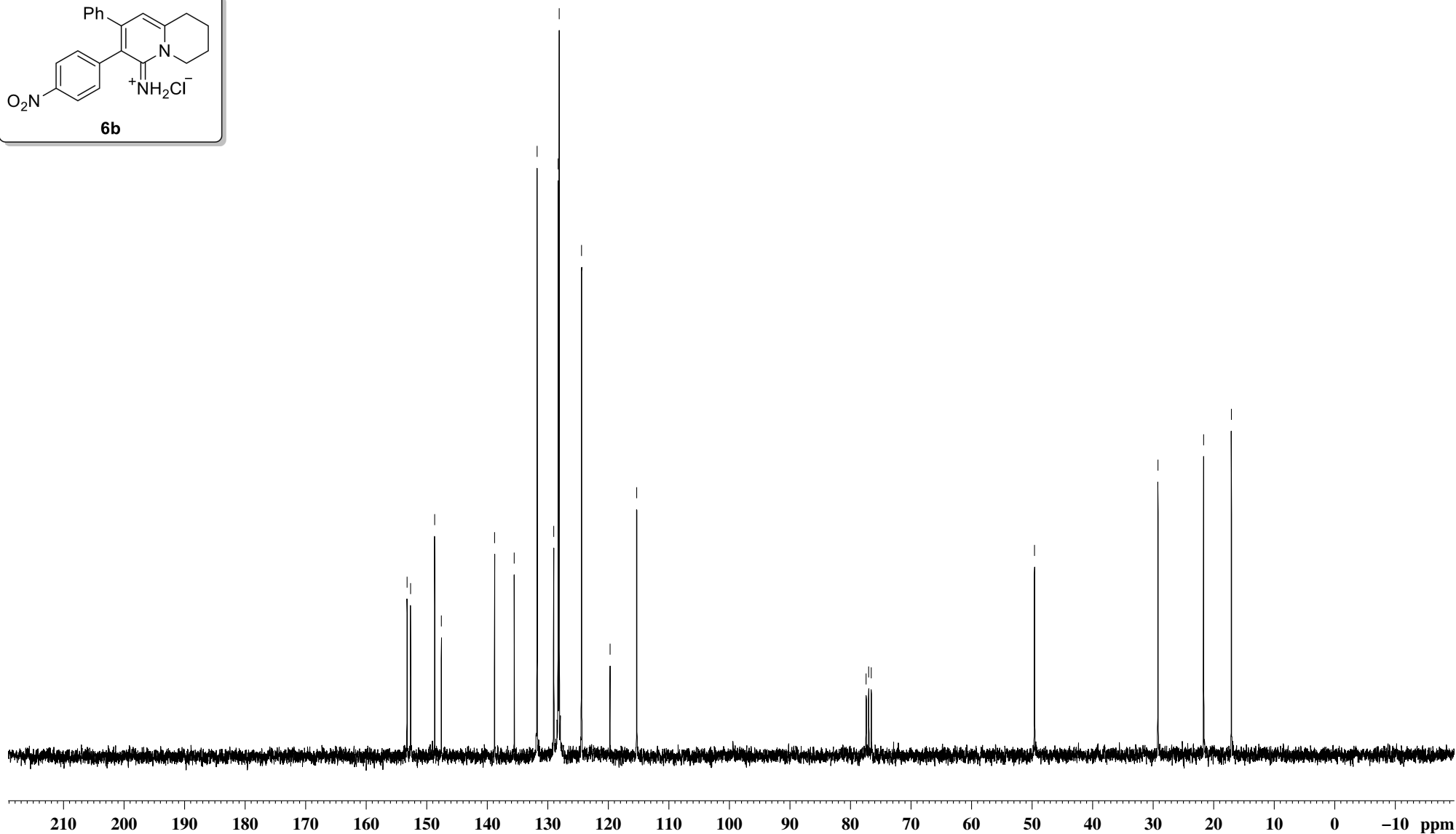
77.427
77.000
76.574

49.604

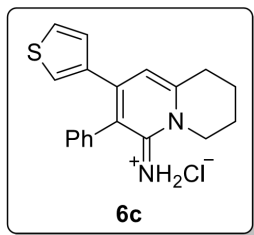
29.207

21.665

17.078



¹H NMR (300 MHz, CDCl₃)

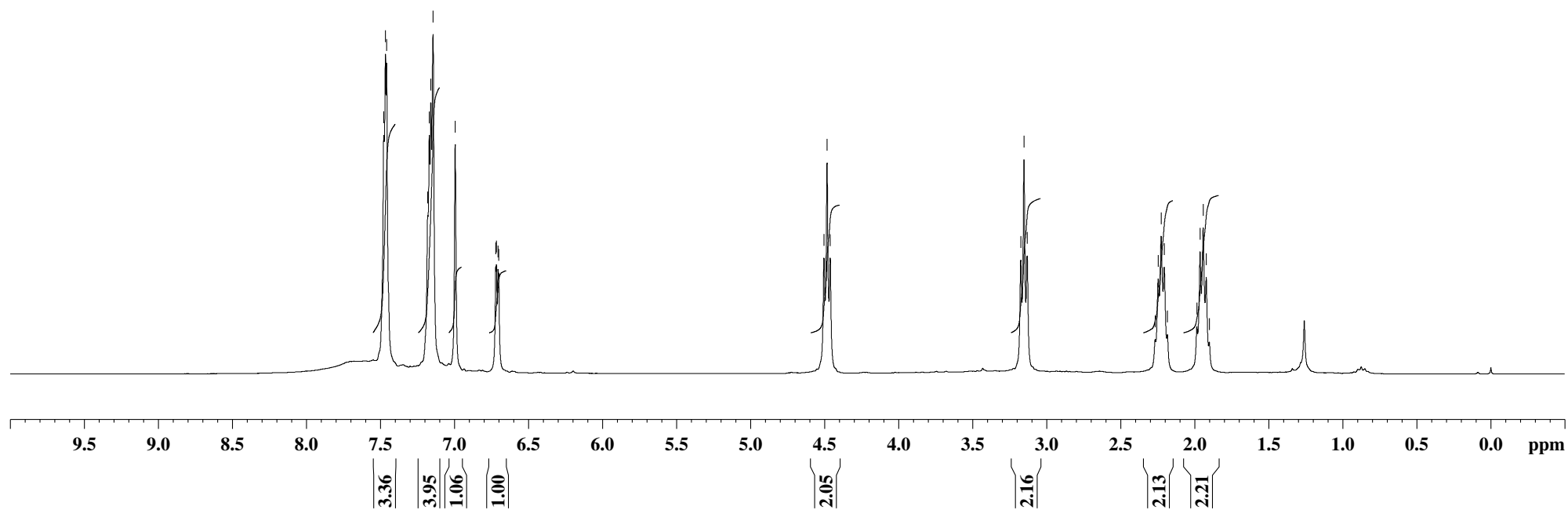


7.478
7.467
7.459
7.181
7.171
7.160
7.145
6.996
6.722
6.717
6.706
6.702

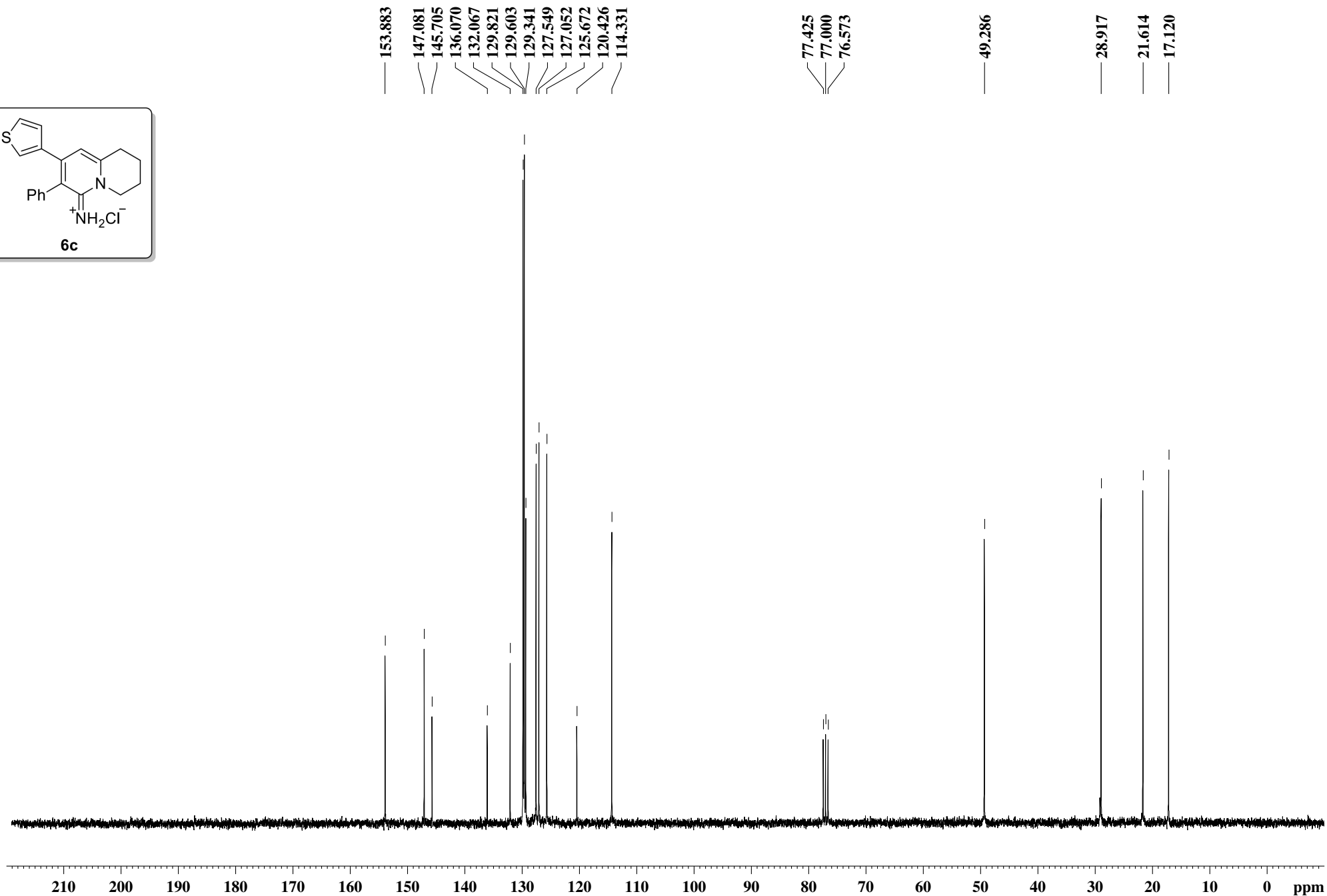
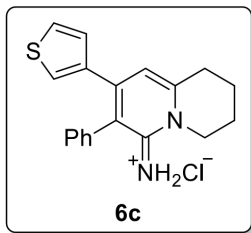
4.505
4.484
4.463

3.175
3.154
3.132

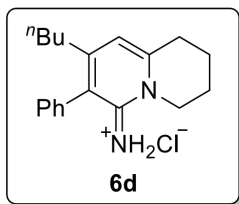
2.268
2.247
2.227
2.206
2.185
1.986
1.964
1.943
1.923
1.902



¹³C NMR (75 MHz, CDCl₃)

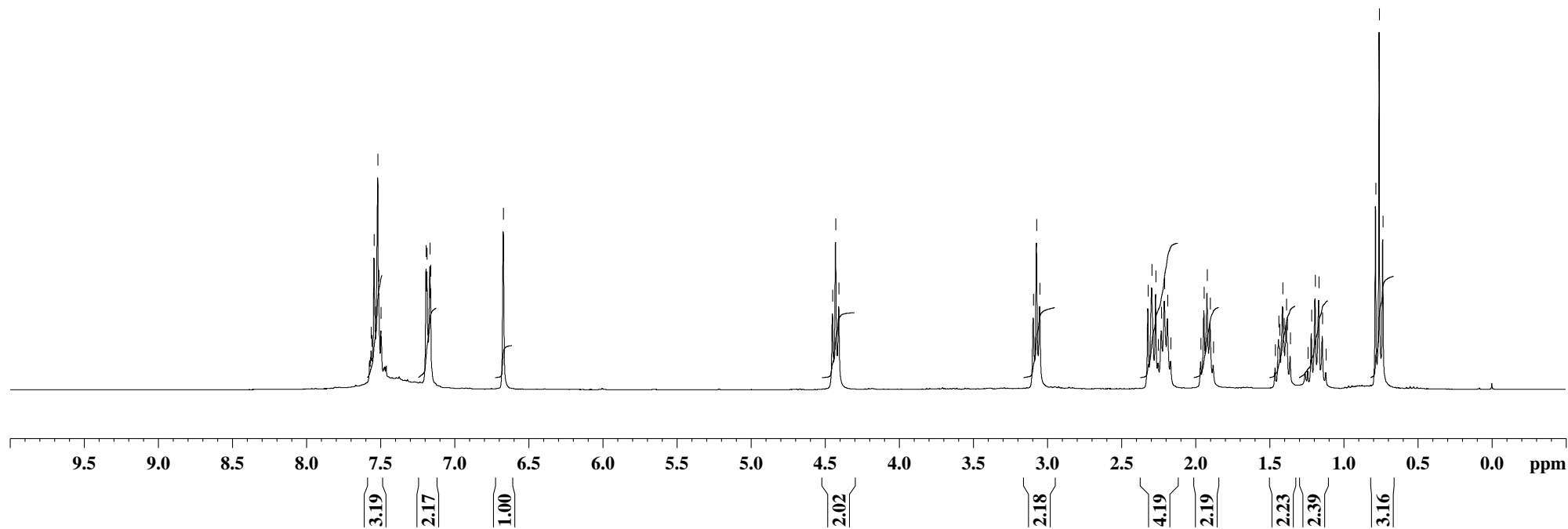


¹H NMR (300 MHz, CDCl₃)

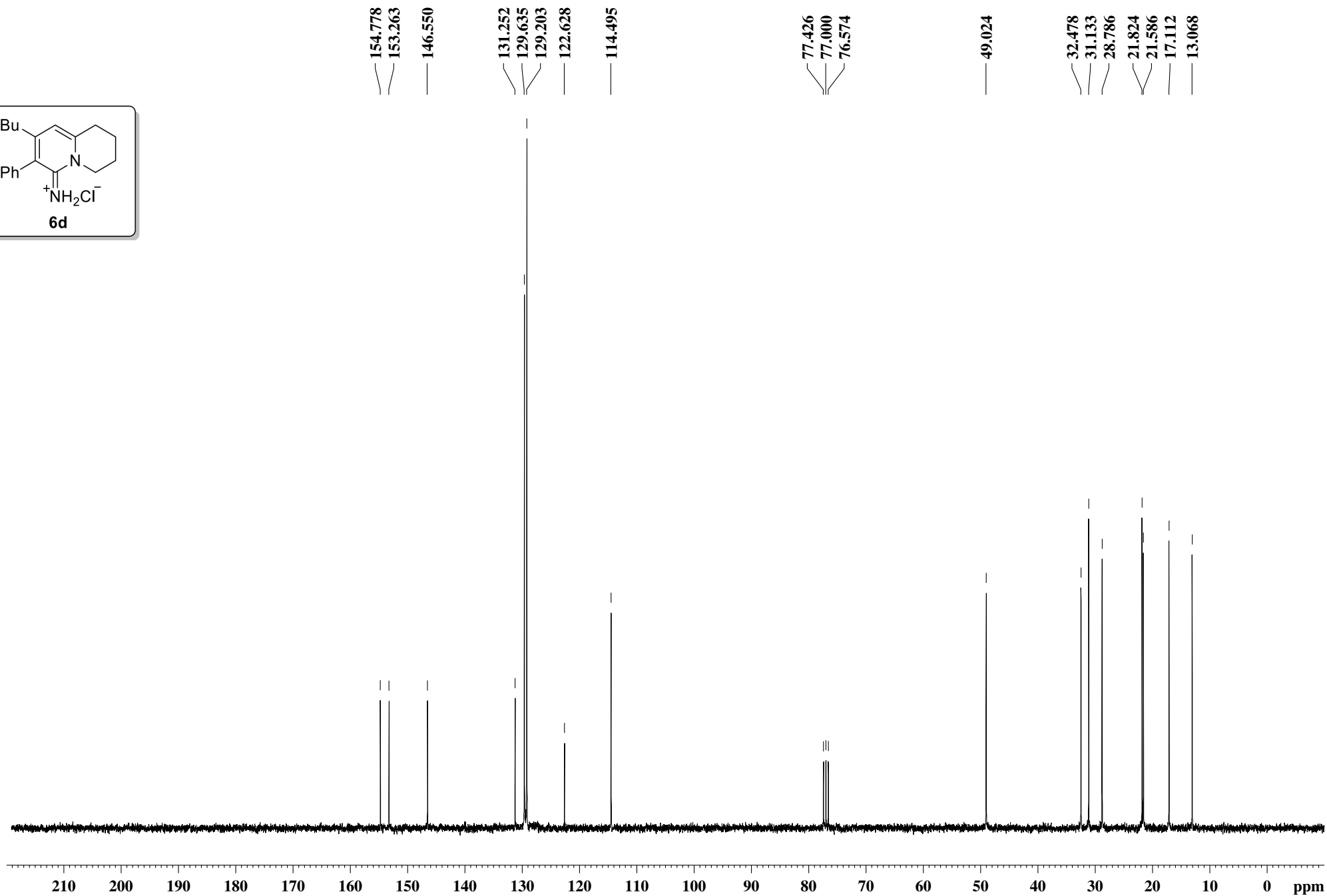
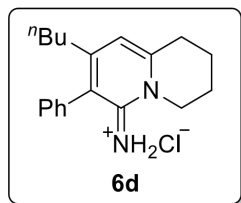


7.564
7.559
7.544
7.534
7.519
7.512
7.498
7.193
7.187
7.167
7.162
6.672

4.450
4.429
4.408
3.095
3.073
3.051
2.321
2.295
2.269
2.252
2.231
2.210
2.189
2.168
1.965
1.943
1.922
1.901
1.880
1.463
1.439
1.433
1.412
1.403
1.387
1.381
1.361
1.242
1.218
1.193
1.168
1.144
1.120
0.785



¹³C NMR (75 MHz, CDCl₃)



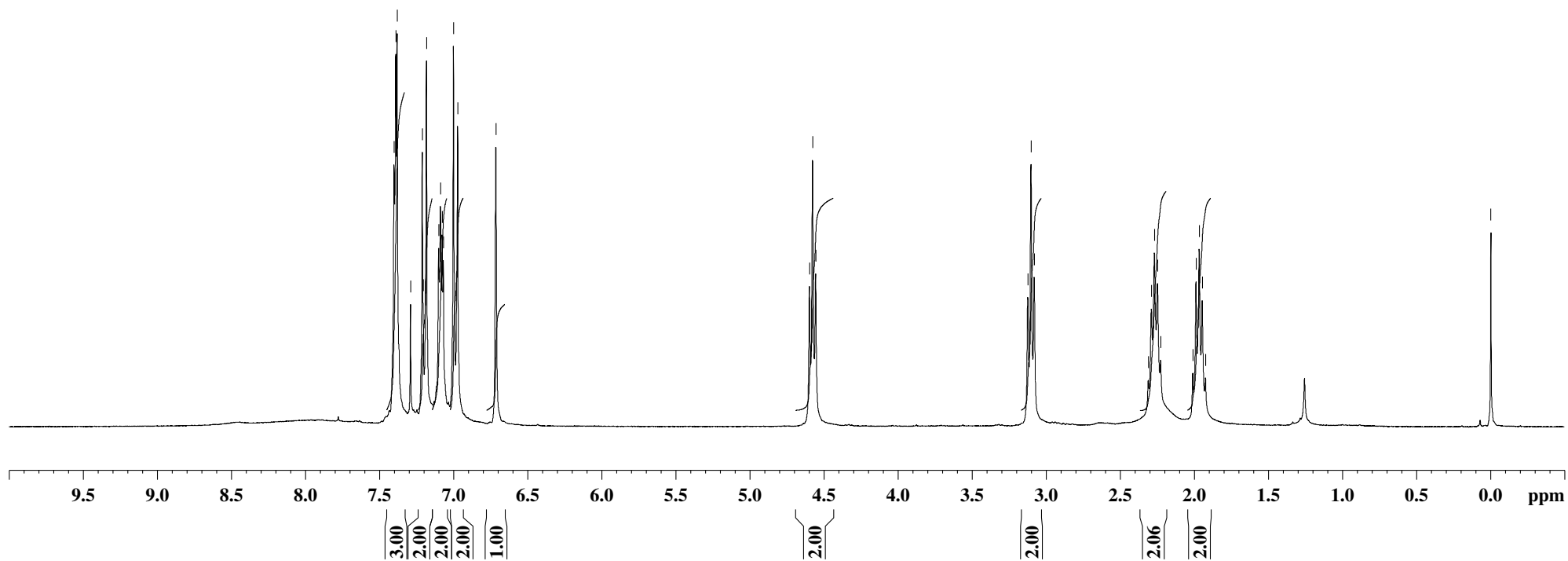
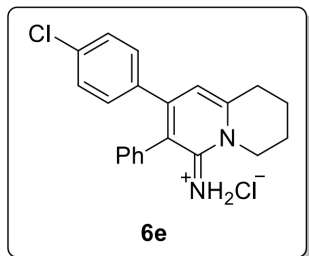
¹H NMR (300 MHz, CDCl₃)

7.402
7.390
7.381
7.290
7.211
7.205
7.183
7.100
7.088
7.077
7.069
7.001
6.972
6.714

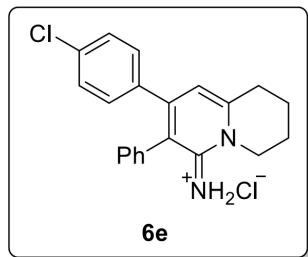
4.597
4.576
4.555

3.124
3.102
3.080
2.310
2.290
2.269
2.248
2.227
2.010
1.988
1.967
1.946
1.924

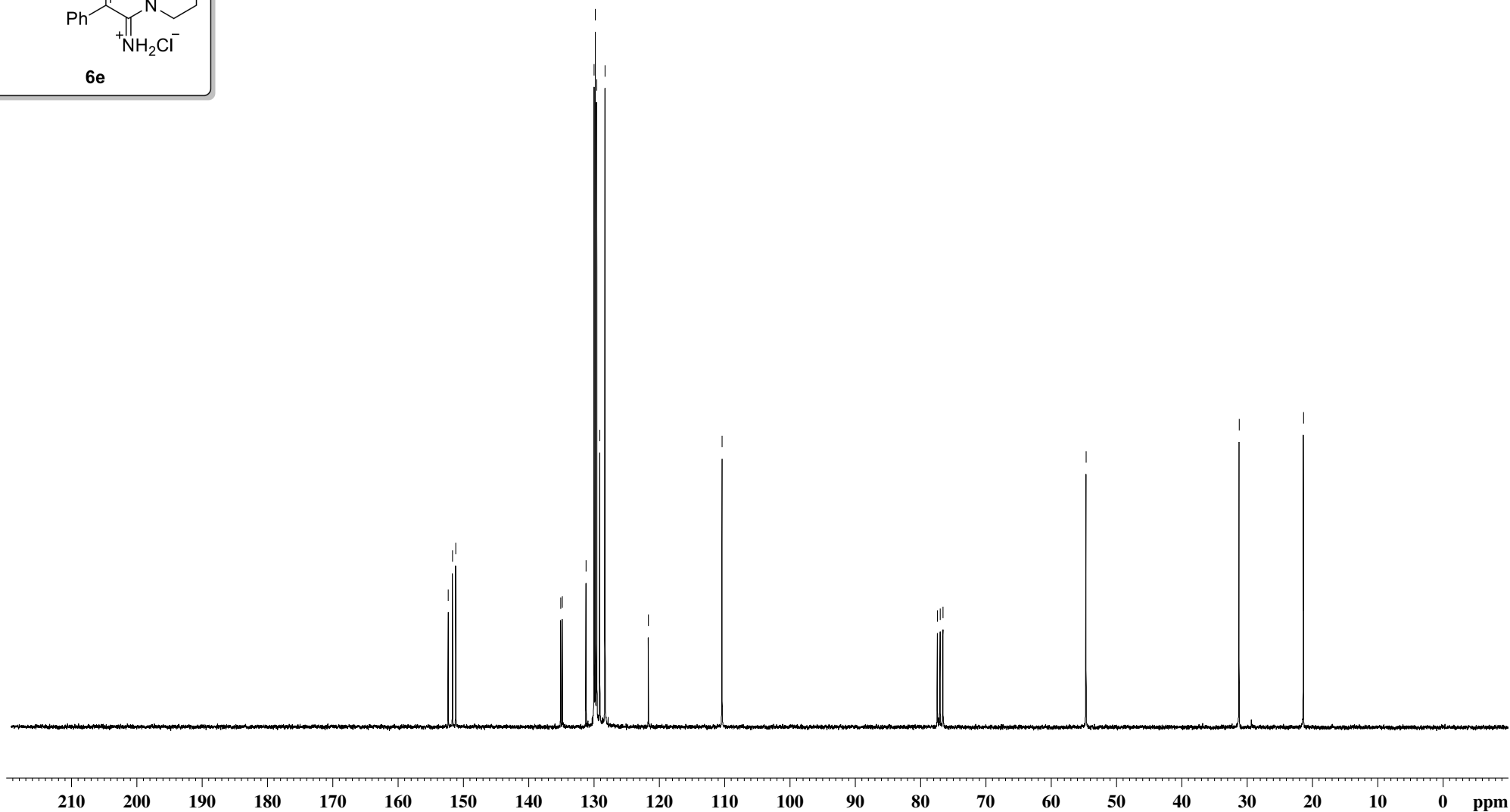
-0.000



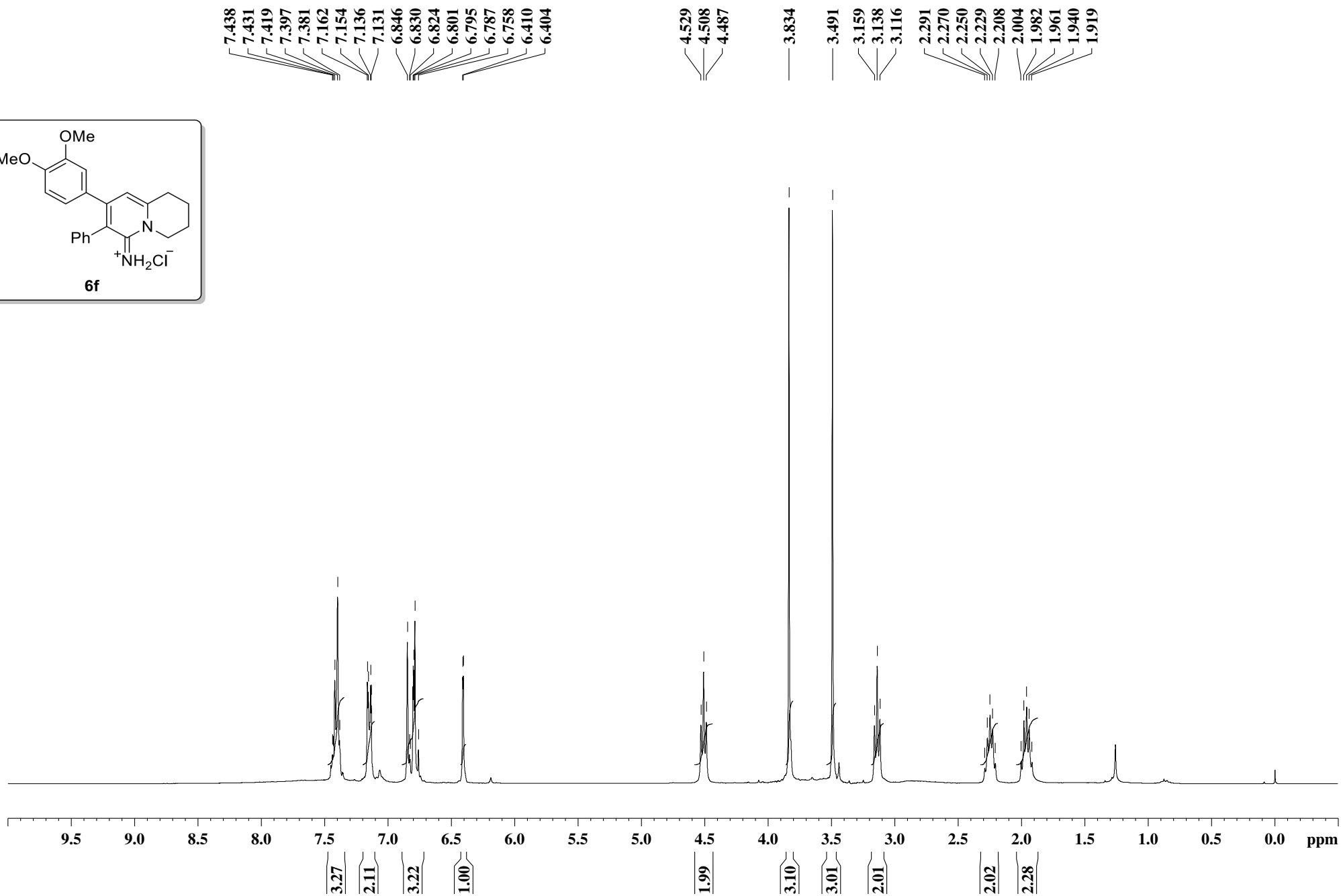
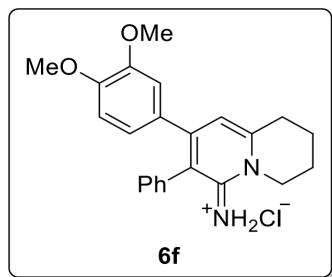
¹³C NMR (75_MHz, CDCl₃)



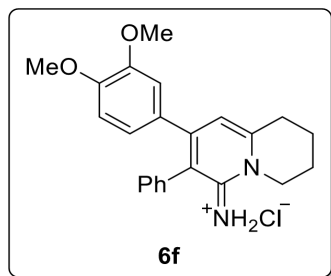
152.330
151.671
151.175
135.098
134.852
131.223
129.997
129.807
129.582
129.121
128.318
121.681
110.398
77.425
77.000
76.574
54.658
31.217
21.364



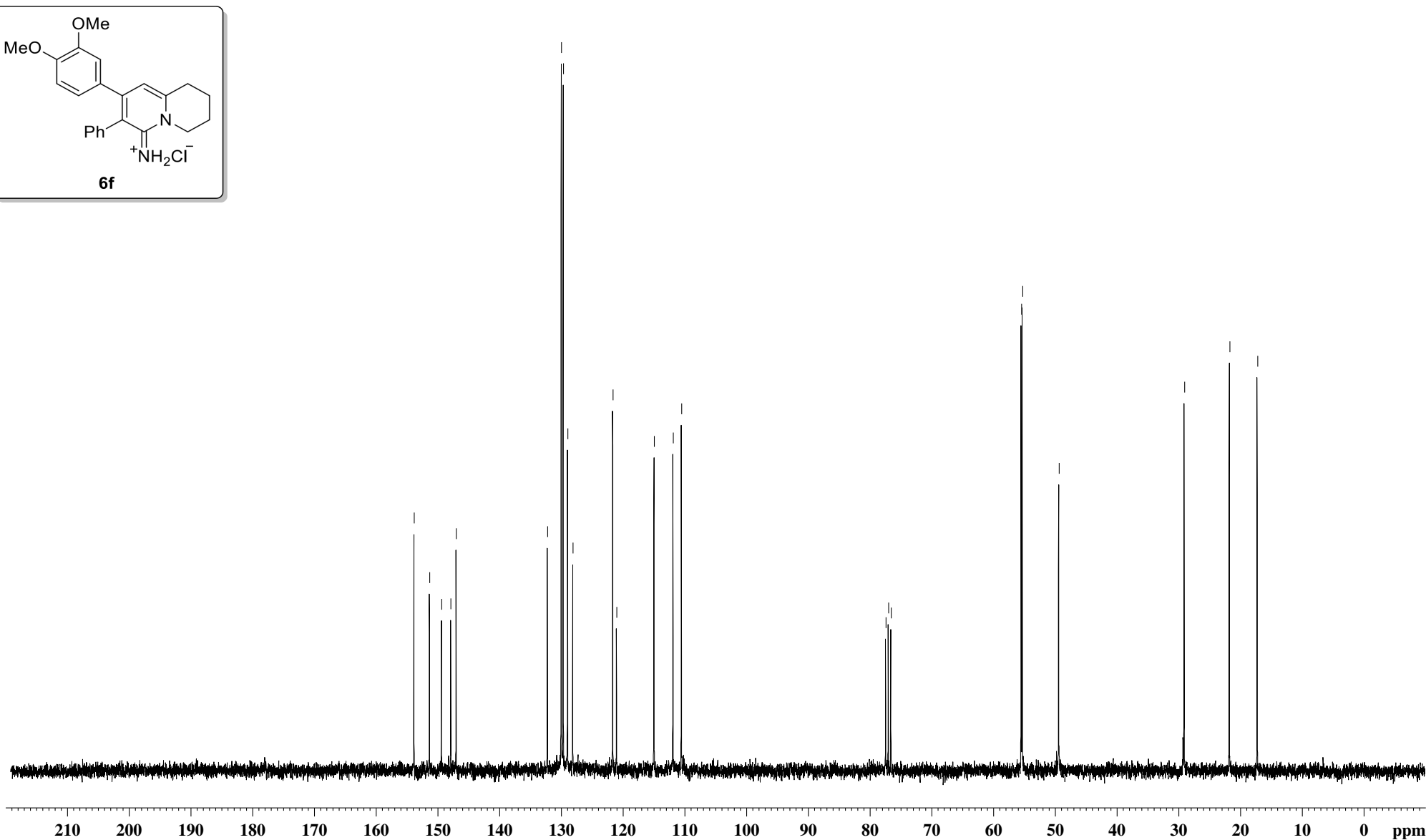
^1H NMR (300 MHz, CDCl_3)



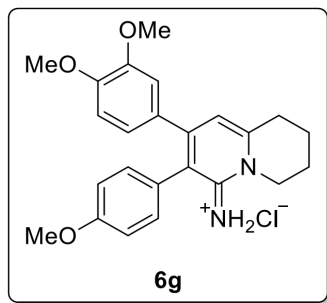
¹³C NMR (75 MHz, CDCl₃)



153.842
151.333
149.387
147.906
147.028
132.234
129.988
129.666
128.958
128.121
121.638
121.030
114.954
111.881
110.521
77.426
77.000
76.576
55.465
55.282
49.380
29.057
21.731
17.218



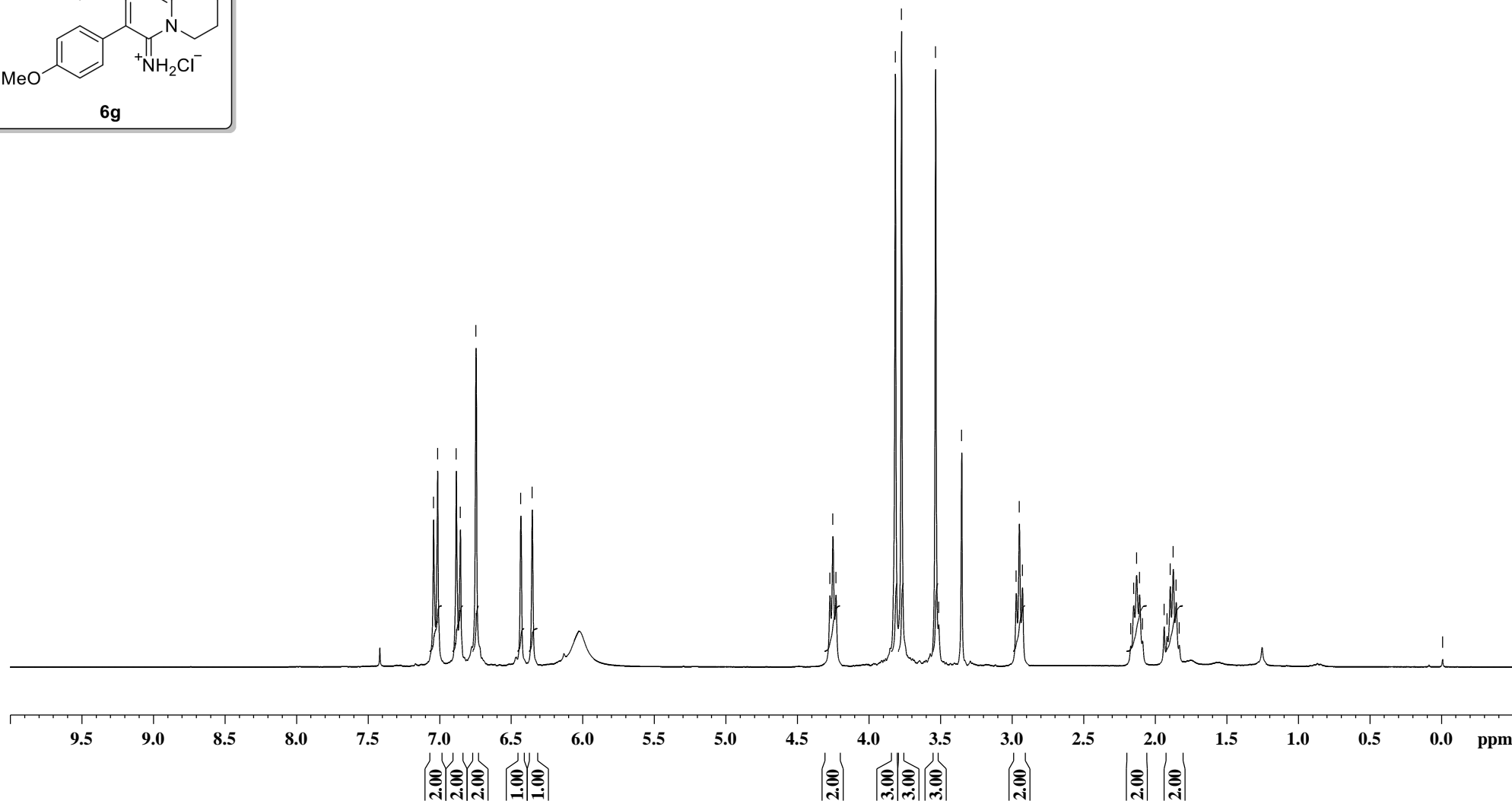
¹H NMR (300 MHz, CDCl₃)



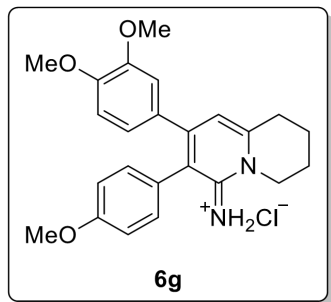
7.043
7.015
6.884
6.856
6.746
6.433
6.354

4.273
4.252
4.231
3.816
3.773
3.535
3.514
3.352
2.971
2.950
2.928
2.171
2.151
2.131
2.110
2.089
1.938
1.917
1.896
1.874
1.854
1.833

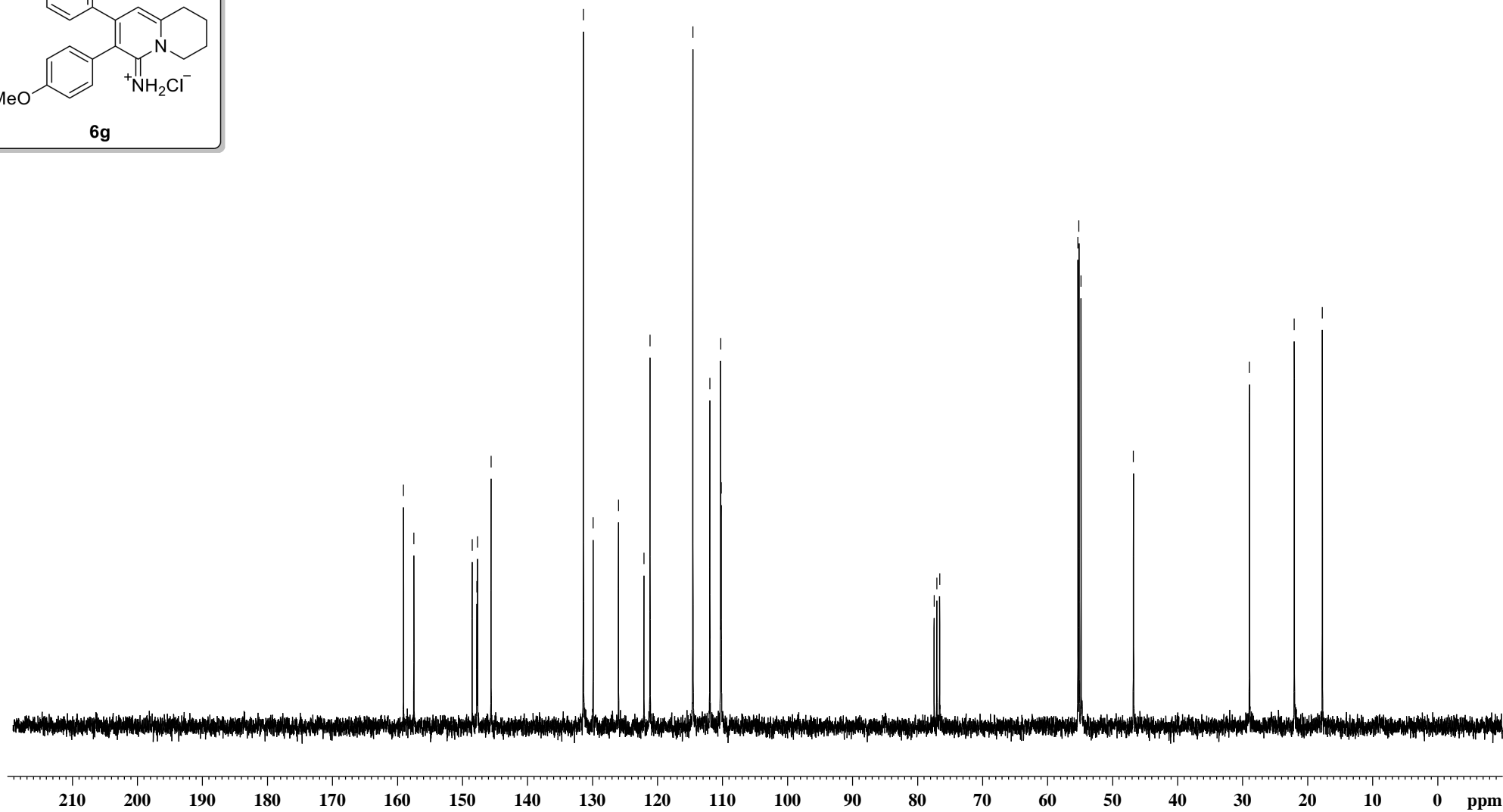
-0.008



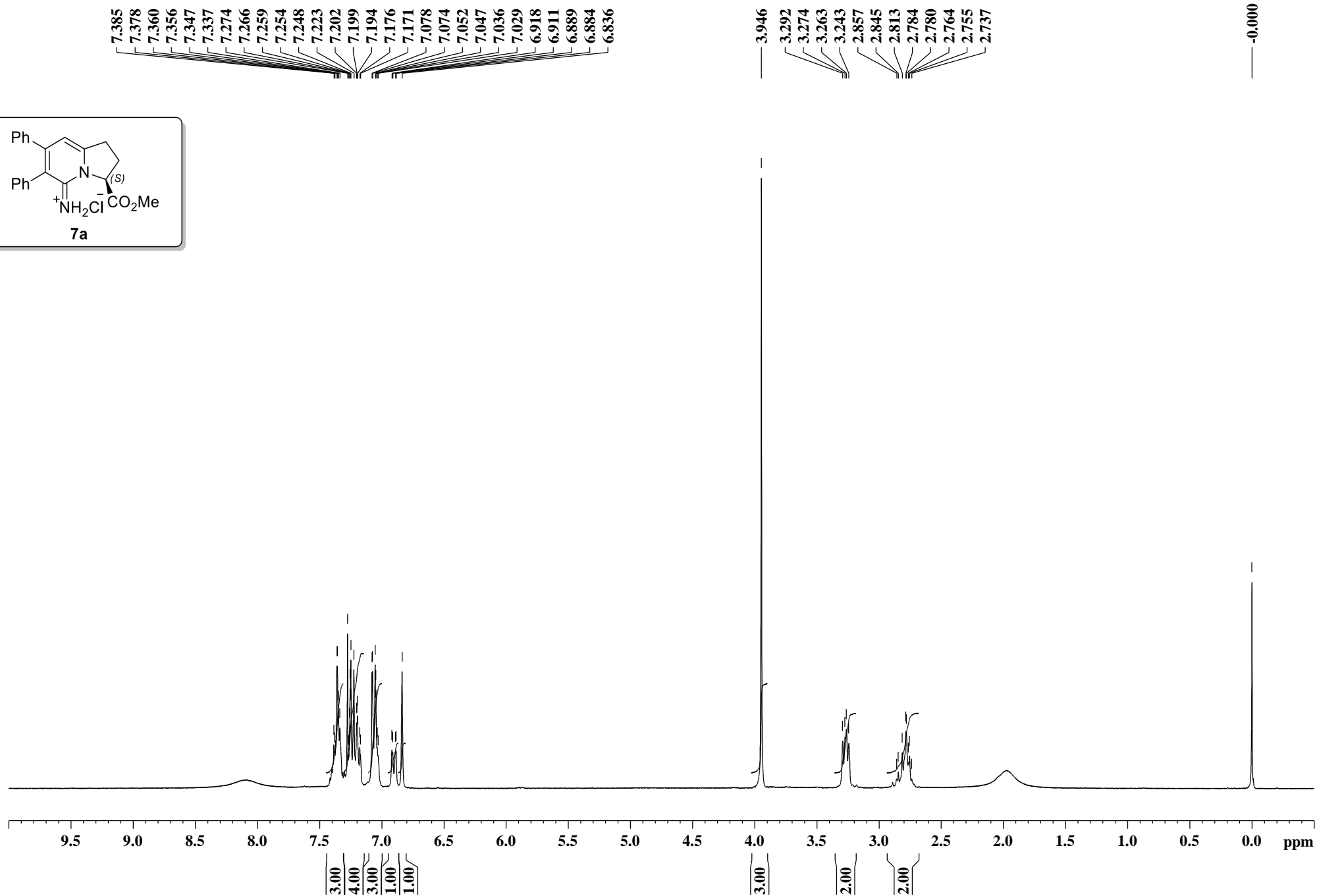
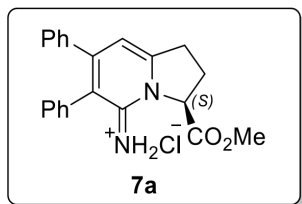
¹³C NMR (75 MHz, CDCl₃)



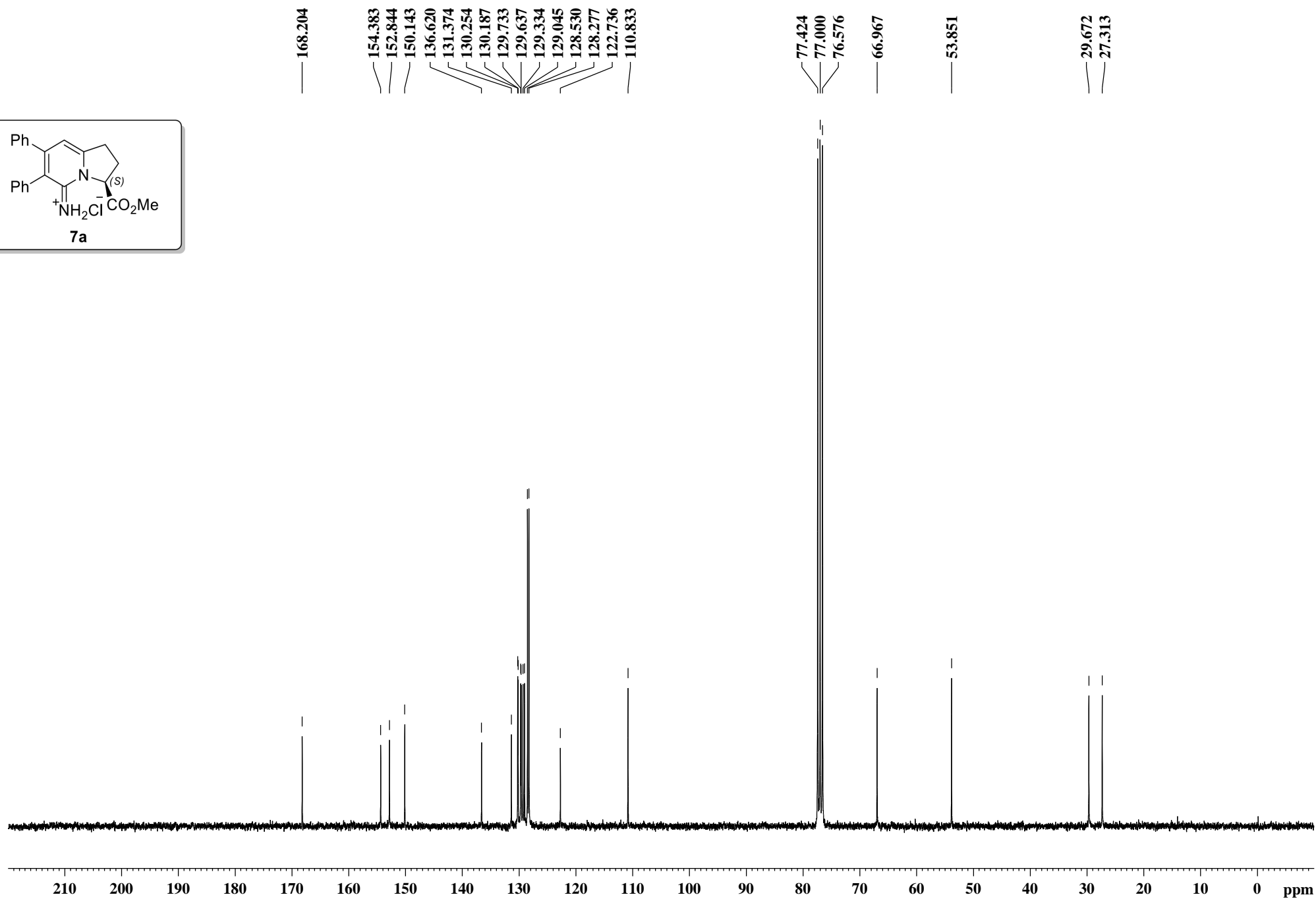
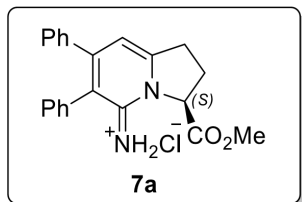
- 159.049
- 157.453
- 148.492
- 147.776
- 147.654
- 145.581
- 131.382
- 129.877
- 125.979
- 122.064
- 121.124
- 114.535
- 111.921
- 110.266
- 110.181
- 77.425
- 77.000
- 76.573
- 55.326
- 55.159
- 54.858
- 46.782
- 28.937
- 22.044
- 17.729



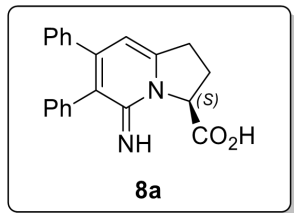
¹H NMR (300 MHz, CDCl₃)



¹³C NMR (75 MHz, CDCl₃)



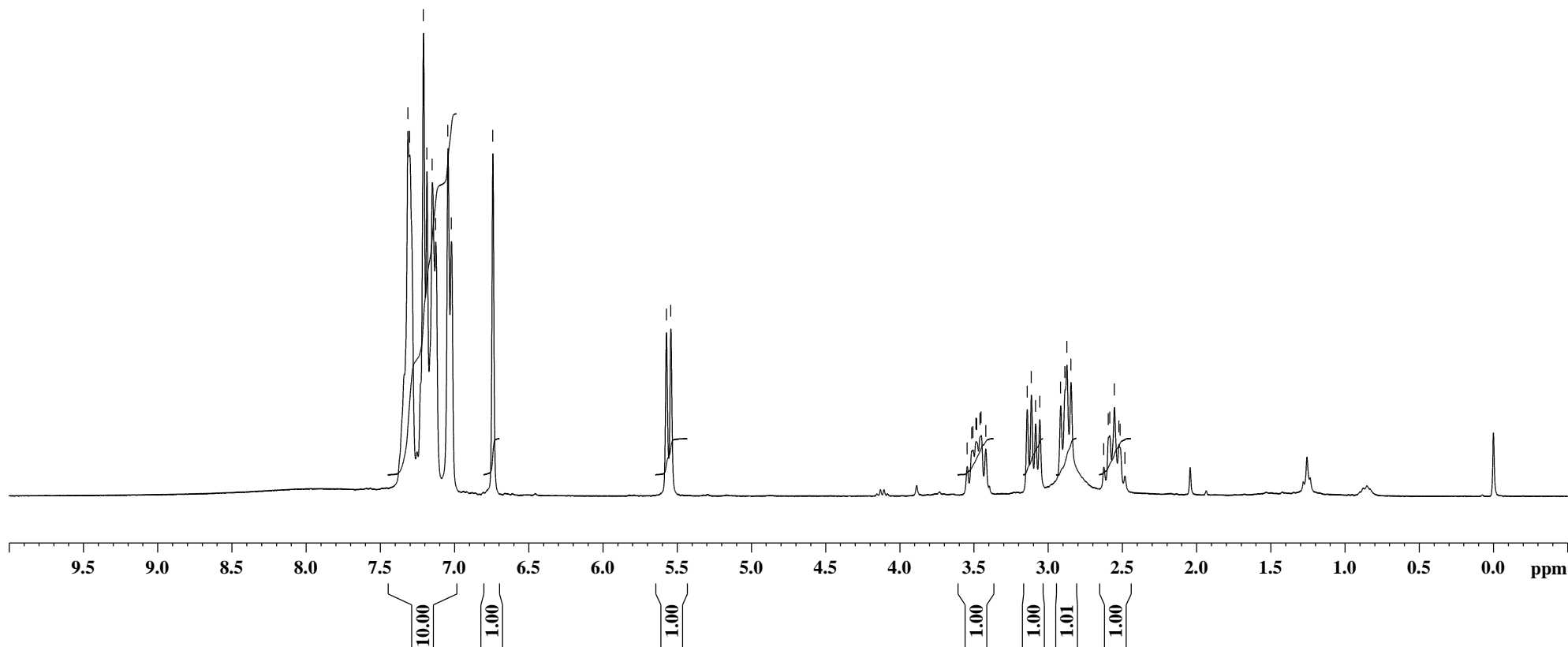
1H NMR (300 MHz, CDCl3)



7.314
7.302
7.210
7.186
7.149
7.127
7.044
7.021
6.742

5.572
5.542

3.546
3.516
3.507
3.487
3.480
3.459
3.452
3.420
3.141
3.113
3.084
3.056
2.915
2.887
2.874
2.846
2.625
2.594
2.585
2.554
2.523
2.514
2.482



¹³C NMR (75 MHz, CDCl₃)

