Supporting Information for

"*N*-Heterocyclic Carbene Catalysed Aerobic Oxidation of Aromatic Aldehydes to Aryl Esters using Boronic Acids"

Panjab Arde, B T Ramanjaneyulu, Virsinha Reddy, Apurv Saxena and R Vijaya Anand*

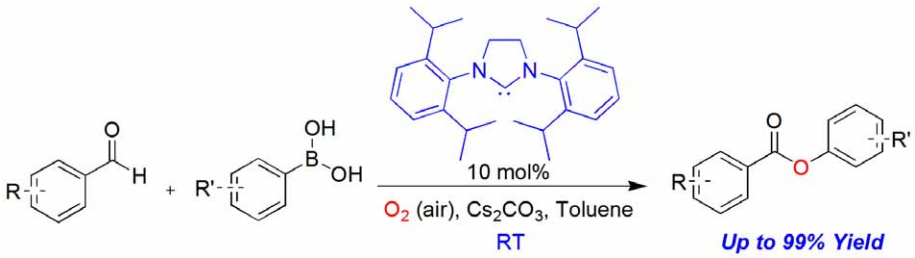
Indian Institute of Science Education and Research (IISER) Mohali, Sector 81, S A S Nagar, Manuali 140 306, Punjab, India

E-Mail: rvijayan@iisermohali.ac.in

Table of Contents

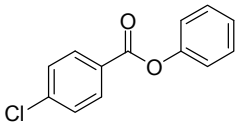
***General Methods*:** All reactions were carried out in open atmosphere. All the reagents including *N*-heterocyclic carbene precursors used were purchased from commercial sources and used as such. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ using 400 MHz Bruker FT-NMR spectrometer. Chemical shifts values are reported in parts per million relative to TMS. High Resolution Mass spectra (HRMS) were recorded on a Bruker maXis spectrometer. The IR spectra were recorded on a Perkin – Elmer FT IR spectrometer. Thin layer chromatography was performed on Merck Silica gel 60 F_{254} TLC plates using Hexane/EtOAc mixture as an eluent. Column chromatography was carried out through silica gel (100-200 mesh).

***Reaction Scheme*:**



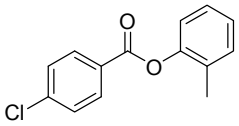
General procedure for NHC catalysed aerobic oxidation of aryl aldehydes with aryl boronic acids: Aromatic aldehyde (0.65 mmol) was added to a suspension of boronic acid (0.5 mmol), NHC **4** (0.05 mmol) and cesium carbonate (0.75 mmol) in Toluene (5 mL) at room temperature. Stirring was continued at room temperature or at 60 ºC (in some cases) under open atmosphere (in the presence of air) until the reaction was complete. The reaction mass was then filtered through a pad of celite®, washed with EtOAc (10 mL) and dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure and the residue was purified through silical gel column using EtOAc/Hexane mixture as an eluent.

Phenyl-4-chloro benzoate (7):[1]



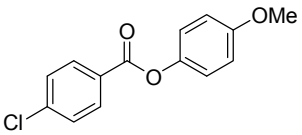
99% Yield. White solid; mp 104 - 106 ºC; FT IR 1732 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 8.6 Hz, 2H), 7.50 (d, J = 8.6 Hz, 2H), 7.47 – 7.43 (m, 2H), 7.32 – 7.28 (m, 1H), 7.24 – 7.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.8, 140.1, 131.6, 129.6, 128.9, 128.1, 126.1, 121.6.

2-Methyl phenyl-4-chloro benzoate (8a):



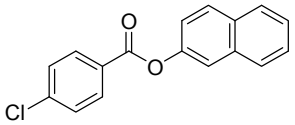
85% Yield. Semi-solid; FT IR 1745 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.6 Hz, 2H), 7.40 (d, J = 8.6 Hz, 2H), 7.29 – 7.24 (m, 2H), 7.21 – 7.17 (m, 1H), 7.13 (d, J = 8.0 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 149.4, 140.2, 131.6, 131.3, 130.2, 129.0, 128.0, 127.1, 126.3, 121.9, 16.3; HRMS (ESI) calcd for $C_{14}H_{11}ClO_2Na$ 269.0448, found 269.0345.

4-Methoxy phenyl-4-chloro benzoate (8b):[2]



84% Yield. White solid; mp 103 - 105 ºC; FT IR 1734 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.6 Hz, 2H), 7.49 (d, J = 8.6 Hz, 2H), 7.13 (d, J = 9.0 Hz, 2H), 6.95 (d, J = 9.0 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 157.4, 144.2, 140.1, 131.5, 128.9, 128.1, 122.4, 114.6, 55.6.

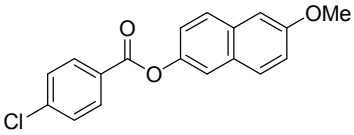
2-Naphthyl-4-chloro benzoate (8c):[3]



84% Yield. White solid; mp 122 - 124 ºC; FT IR 1736 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J = 8.7 Hz, 2H), 7.92 (d, J = 8.9 Hz, 1H), 7.90 – 7.84 (m, 2H), 7.70 (d, J = 2.2 Hz, 1H), 7.55 – 7.48 (m, 4H), 7.36 (dd, J = 8.8, 2.2 Hz, 1H); ^{13}C NMR

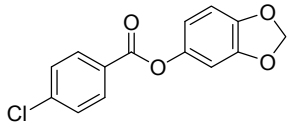
(100 MHz, $CDCl_3$) δ 164.6, 148.4, 140.2, 133.8, 131.6, 131.5, 129.6, 129.0, 128.0, 127.8, 127.7, 126.7, 125.9, 121.1, 118.7.

6-Methoxy naphthyl-4-chloro benzoate (8d):



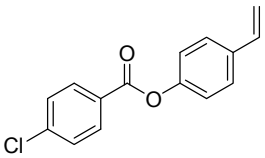
92% Yield. White solid; mp 153 - 155 ºC; FT IR 1732 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 8.9 Hz, 2H), 7.80 (d, J = 8.9 Hz, 1H), 7.73 (d, J = 8.6 Hz, 1H), 7.62 (d, J = 2.4 Hz, 1H), 7.52 (d, J = 8.7 Hz, 2H), 7.31 (dd, J = 8.8, 2.4 Hz, 1H), 7.21 (d, J = 2.5 Hz, 1H), 7.18 (s, 1H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 157.7, 146.8, 140.2, 132.8, 131.6, 129.1, 129.0, 128.9, 128.2, 128.1, 121.4, 119.6, 118.6, 105.8, 55.4; HRMS (ESI) calcd for $C_{18}H_{13}ClO_3Na$ 335.0553, found 335.0445.

Benzo[d][1,3]dioxol-6-yl 4-chlorobenzoate (8e):



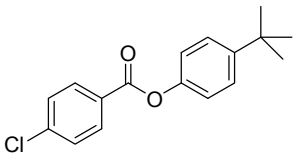
98% Yield. White solid; mp 92 – 94 ºC; FT IR 1729 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.7 Hz, 2H), 7.49 (d, J = 8.7 Hz, 2H), 6.83 (d, J = 8.4 Hz, 1H), 6.73 (d, J = 2.3 Hz, 1H), 6.66 (dd, J = 8.4, 2.3 Hz, 1H), 6.02 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 148.1, 145.6, 145.0, 140.2, 131.5, 128.9, 127.9, 114.0, 108.1, 103.8, 101.8; HRMS (ESI) calcd for $C_{14}H_9ClO_4Na$ 299.0189, found 299.0082.

4-Vinylphenyl-4-chlorobenzoate (8f):[4]



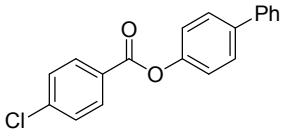
99% Yield. White solid; mp 104 - 106 ºC; FT IR 1732 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.7 Hz, 2H), 7.52 – 7.46 (m, 4H), 7.18 (d, J = 8.6 Hz, 2H), 6.74 (dd, J = 17.6, 10.9 Hz, 1H), 5.74 (dd, J = 7.6, 0.7 Hz, 1H), 5.28 (dd, J = 10.9, 0.7 Hz, 1H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 150.3, 140.2, 135.9, 135.6, 131.6, 129.0, 127.9, 127.3, 121.7, 114.2.

4-tert-Butylphenyl-4-chlorobenzoate (8g):



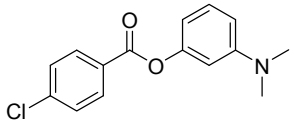
86% Yield. White solid; mp 117 – 118 ºC; FT IR 1747 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.7 Hz, 2H), 7.50 (d, J = 8.7 Hz, 2H), 7.45 (d, J = 8.8 Hz, 2H), 7.14 (d, J = 8.8 Hz, 2H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 148.9, 148.4, 140.0, 131.5, 128.9, 128.2, 126.5, 120.9, 34.5, 31.4; HRMS (ESI) calcd for $C_{17}H_{17}ClO_2Na$ 311.0917, found 311.0809.

(4-Phenyl) phenyl-4-chlorobenzoate (8h):[5]



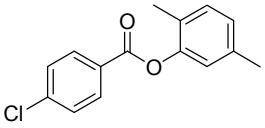
90% Yield. White solid; mp 169 - 171 ºC; FT IR 1732 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 8.7 Hz, 2H), 7.65 (d, J = 8.7 Hz, 2H), 7.62 – 7.60 (m, 2H), 7.52 (d, J = 8.7 Hz, 2H), 7.49 – 7.45 (m, 2H), 7.40 – 7.36 (m, 1H), 7.30 (d, J = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.2, 140.3, 140.2, 139.2, 131.6, 129.0, 128.9, 128.3, 128.0, 127.4, 127.2, 121.9.

3-(Dimethylamino) phenyl-4-chlorobenzoate (8i):



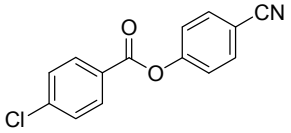
80% Yield. White solid; mp 142 – 144 ºC; FT IR 1731 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.7 Hz, 2H), 7.45 (d, J = 8.7 Hz, 2H), 7.28 (t, J = 8.2 Hz, 1H), 6.64 (dd, J = 8.4, 1.9 Hz, 1H), 6.57 – 6.53 (m, 2H), 2.98 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 151.9, 151.7, 139.9, 131.5, 129.8, 128.9, 128.3, 110.2, 109.3, 105.5, 40.5; HRMS (ESI) calcd for $C_{15}H_{14}ClNO_2Na$ 298.0713, found 298.0605.

2,5-dimethylphenyl-4-chlorobenzoate (8j):



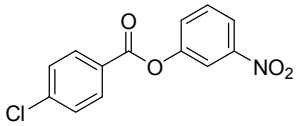
78% Yield. Semi-solid; FT IR 1746 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 8.6 Hz, 2H), 7.51 (d, J = 8.6 Hz, 2H), 7.18 (d, J = 7.7 Hz, 1H), 7.02 (d, J = 7.7 Hz, 1H), 6.98 (s, 1H), 2.37 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 149.2, 140.1, 137.0, 131.5, 130.9, 129.0, 128.0, 127.0, 126.9, 122.4, 20.9, 15.8; HRMS (ESI) calcd for $C_{15}H_{13}ClO_2Na$ 283.0604, found 283.0496.

4-Cyano phenyl-4-chlorobenzoate (8k):[2]



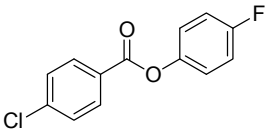
70% Yield. White solid; mp 110 - 112 ºC; FT IR 2360, 1738 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 8.8 Hz, 2H), 7.52 (d, J = 8.8 Hz, 2H), 7.37 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5, 154.0, 140.8, 133.8, 131.7, 129.2, 127.1, 122.9, 118.2, 110.1.

3-Nitro phenyl-4-chlorobenzoate (8l):[6]



68% Yield. White solid; mp 134 - 136 ºC; FT IR 1745, 1523, 1358 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 – 8.14 (m, 2H), 8.15 (d, J = 8.6 Hz, 2H), 7.66 – 7.58 (m, 2H), 7.53 (d, J = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 151.0, 148.9, 140.9, 131.7, 130.2, 129.2, 128.2, 127.0, 121.0, 117.5.

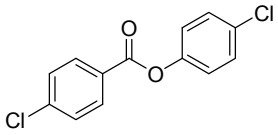
4-Fluoro phenyl-4-chlorobenzoate (8m):[7]



88% Yield. White solid; mp 96 - 98 ºC; FT IR 1734 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.7 Hz, 2H), 7.50 (d, J = 8.7 Hz, 2H), 7.21 – 7.09 (m, 4H); ^{13}C NMR

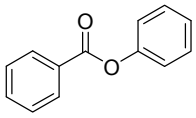
(100 MHz, $CDCl_3$) δ 164.4, 161.6, 146.6, 140.3, 131.6, 129.0, 127.7, 123.1, 123.0, 116.3, 116.1.

4-Chloro phenyl-4-chlorobenzoate (8n):[8]



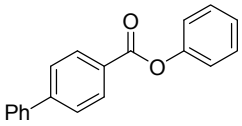
95% Yield. White solid; mp 96 - 98 ºC; FT IR 1744 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.3 Hz, 2H), 7.40 (d, J = 8.6 Hz, 2H), 7.17 (d, J = 8.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 149.2, 140.4, 131.6, 131.5, 129.6, 129.0, 127.6, 123.0.

Phenyl benzoate (9a):[1]



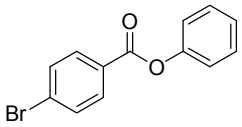
86% Yield. White solid; mp 68 - 70 ºC; FT IR 1731 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.22 (m, 2H), 7.68 – 7.64 (m, 1H), 7.56 – 7.52 (m, 2H), 7.48 – 7.43 (m, 2H), 7.32 – 7.28 (m, 1H), 7.25 – 7.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 151.0, 133.6, 130.2, 129.6, 129.5, 128.6, 125.9, 121.7.

Phenyl-(4-phenyl) benzoate (9b):[9]



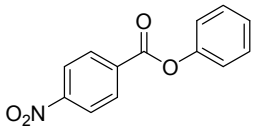
97% Yield. White solid; mp 160 - 162 ºC; FT IR 1730 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 8.5 Hz, 2H), 7.72 (d, J = 8.5 Hz, 2H), 7.66 – 7.63 (m, 2H), 7.50 – 7.38 (m, 5H), 7.29 – 7.21 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 151.0, 146.4, 139.9, 130.7, 129.5, 129.0, 128.4, 128.3, 127.4, 127.3, 125.9, 121.8.

Phenyl-(4-bromo) benzoate (9c):[1]



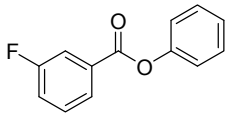
99% Yield. White solid; mp 120 - 122 ºC; FT IR 1731 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 8.6 Hz, 2H), 7.67 (d, J = 8.6 Hz, 2H), 7.48 – 7.42 (m, 2H), 7.32 – 7.28 (m, 1H), 7.23 – 7.20 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 150.8, 131.9, 131.7, 129.6, 128.9, 128.5, 126.1, 121.6.

Phenyl-(4-nitro) benzoate (9d):[10]



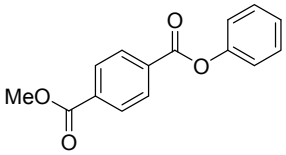
95% Yield. White solid; mp 129 - 131 ºC; FT IR 1741, 1520, 1347 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.36 (m, 4H), 7.50 – 7.45 (m, 2H), 7.35 – 7.31 (m, 1H), 7.26 – 7.23 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 150.9, 150.5, 135.0, 131.3, 129.7, 126.4, 123.7, 121.4.

Phenyl-(3-fluoro) benzoate (9e):[11]



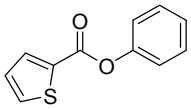
90% Yield. White solid; mp 53 - 55 ºC; FT IR 1734 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 1H), 7.91 – 7.88 (m, 1H), 7.54 – 7.43 (m, 3H), 7.38 – 7.28 (m, 2H), 7.24 – 7.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 150.8, 130.3, 130.2, 129.6, 126.1, 125.9, 121.6, 120.8, 120.6, 117.2, 116.9.

Phenyl-(4-methylester) terephalate (9f):[1]



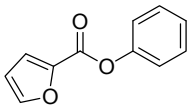
96% Yield. White solid; mp 110 - 112 ºC; FT IR 1734, 1719 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 8.6 Hz, 2H), 8.18 (d, J = 8.6 Hz, 2H), 7.48 – 7.43 (m, 2H), 7.33 – 7.22 (m, 3H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 164.4, 150.8, 134.5, 133.4, 130.2, 129.7, 129.6, 126.2, 121.6, 52.55.

Phenyl thiophene-2-carboxylate (9g):[12]



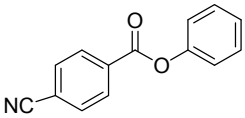
82% Yield. Semi-solid; FT IR 1741 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 3.8, 1.2 Hz, 1H), 7.68 (d, J = 5.0 Hz, 1.3 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.31 – 7.22 (m, 2H), 7.19 (dd, J = 5.0, 3.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 150.6, 134.7, 133.5, 132.9, 129.5, 128.1, 126.0, 121.7.

Phenyl furan-2-carboxylate (9h):[10]



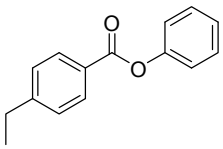
60% Yield. White solid; mp 54 - 56 ºC; FT IR 1738 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.69 (dd, J = 1.7, 0.9 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.40 (dd, J = 3.5, 0.9 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.24 – 7.21 (m, 2H), 6.61 (dd, J = 3.5, 1.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 150.2, 147.1, 144.0, 129.5, 126.1, 121.6, 119.4, 120.2.

Phenyl-(4-cyano) benzoate (9i):[1]



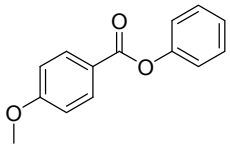
93% Yield. White solid; mp 89 - 91 ºC; FT IR 2233, 1741 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, J = 8.2 Hz, 2H), 7.83 (d, J = 8.2 Hz, 2H), 7.48 – 7.45 (m, 2H), 7.34 – 7.30 (m, 1H), 7.23 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 150.5, 133.4, 132.4, 130.7, 129.7, 126.4, 121.5, 117.9, 117.0.

Phenyl-(4-ethyl) benzoate (9j):[13]



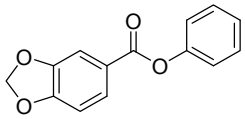
80% Yield. Semi-solid; FT IR 1723 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.3 Hz, 2H), 7.46 – 7.41 (m, 2H), 7.34 (d, J = 8.4 Hz, 2H), 7.32 – 7.20 (m, 3H), 2.76 (q, J = 7.6 Hz, 2H), 1.29 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 151.0, 150.6, 130.4, 129.5, 128.1, 127.0, 125.8, 121.8, 29.1, 15.3.

Phenyl-(4-methoxy) benzoate (9k):[10]



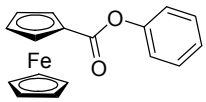
40% Yield. White solid; mp 74 - 76 ºC; FT IR 1727 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 8.6 Hz, 2H), 7.47 – 7.43 (m, 2H), 7.31 – 7.27 (m, 1H), 7.23 (d, J = 8.1 Hz, 2H), 7.01 (d, J = 8.6 Hz, 2H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 163.9, 151.1, 132.3, 129.5, 125.7, 121.9, 121.8, 113.9, 55.5.

Phenyl benzo[d][1,3]dioxole-5-carboxylate (9l):[1]



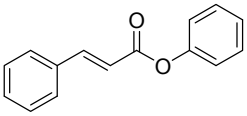
75% Yield. White solid; mp 73 - 75 ºC; FT IR 1724 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, J = 8.2, 1.7 Hz, 1H), 7.63 (d, J = 1.7 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.30 – 7.26 (m, 1H), 7.22 – 7.20 (m, 2H), 6.91 (d, J = 8.2 Hz, 1H), 6.08 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 152.2, 151.0, 147.9, 129.5, 126.2, 125.8, 123.5, 121.8, 109.9, 108.2, 101.9.

Phenyl-(ferrocene)-1-carboxylate (9m):[14]



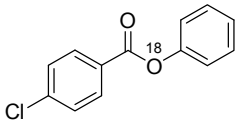
33% Yield. White solid; mp 117 - 119 ºC; FT IR 1723 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.44 (m, 2H), 7.31 – 7.27 (m, 1H), 7.22 (d, J = 8.0 Hz, 2H), 5.00 (s, 2H), 4.53 (s, 2H), 4.34 (s, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 150.9, 129.5, 125.6, 121.8, 71.9, 70.7, 70.1, 69.9.

(E)-Phenyl cinnamate (9n):[10]



25% Yield. White solid; mp 76 - 77 ºC; FT IR 1710 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 16.0 Hz, 1H), 7.63 – 7.59 (m, 2H), 7.46 – 7.39 (m, 5H), 7.29 – 7.22 (m, 1H), 7.20 – 7.17 (m, 2H), 6.65 (d, J = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 150.6, 146.6, 134.2, 130.7, 129.5, 129.0, 128.3, 125.8, 121.6, 117.3.

Isotopic labelling experiment: A solution of *p*-chlorobenzaldehyde (60.0 mg, 0.43 mmol) and phenyl boronic acid (40.0 mg, 0.33 mmol) in toluene (2 mL) was added to a suspension of NHC **4** (14.0 mg, 0.033 mmol) and cesium carbonate (160.0 mg, 0.49 mmol) in Toluene (2 mL) at room temperature. The reaction mixture was stirred under $^{18}O_2$ atmosphere at room temperature for 5 h. The reaction mass was then filtered through a pad of celite®, washed with EtOAc (10 mL) and dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure and the residue was purified through silical gel column using EtOAc/Hexane mixture to give **10** as a white solid.



Yield 92%; White solid; mp 104 - 106 ºC; FT IR 1730 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 8.7 Hz, 2H), 7.50 (d, J = 8.7 Hz, 2H), 7.47 – 7.42 (m, 2H), 7.32 – 7.27 (m, 1H), 7.24 – 7.20 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 150.8, 140.1, 131.6, 129.6, 128.9, 128.0, 126.1, 121.6; HRMS (ES) calcd for $C_{13}H_9ClO_2$ 235.0412 [M+H], found 235.0419; EI MS: *m/z* 234.91 $(M + H)^+$, 141.00, 139.03 (base peak).

References:

1. J. N. Rosa, R. S. Reddy, N. R. Candeias, P. M. S. D. Cal and P. M. P. Gois, *Org. Lett*., 2010, **12**, 2686.
2. H. Neuvonen, K. Neuvonen and P. Pasanen, *J. Org. Chem*., 2004, **69**, 3794.
3. K. Kankanala, V. R. Reddy, K. Mukkanti and S. Pal, *J. Fluorene Chem*., 2009, **130**, 505.
4. B. Sellergren, R. N. Karmalkar and K. J. Shea, *J. Org. Chem*., 2000, **65**, 4009.
5. L. Wu, Z. –W. Li, F. Zhang, Y. –M. He and Q. –H. Fan, *Adv. Synth. Catal*., 2008, **350**, 846.
6. J. H. Bowie and B. Nussey, *Org. Mass Spectrometry,* 1972, **6**, 429.
7. L.Conte, M. Napoli, G. P. Gambaretto, A. Guerrato and F. M. Carlini, *J. Fluorine Chem*., 1994, **67**, 41.
8. A. S. Shawali and N. F. Eweiss, *Can. J. Chem*., 1977, **55**, 3967.
9. C. Ramesh, Y. Kubota, M. Miwa and Y. Sugi, *Synthesis,* 2002, 2171.
10. L. Zhang, G. Zhang, M. Zhang and J. Cheng, *J. Org. Chem*., 2010, **75**, 7472.

11. M. Shibakami, M. Tamura, T. Arimura, S. Kurosawa and A. Sekiya, *Acta Cryst*., 1994, **C-50**, 592.
12. D. A. Watson, X. Fan and S. L. Buchwald, *J. Org. Chem*., 2008, **73**, 7096.
13. C. Qin, H. Wu, J. Chen, M. Liu, J. Cheng, W. Su and J. Ding, *Org. Lett*., 2008, **10**, 1537.
14. C. Imrie, R. T. Elago, N. Williams, C. W. McCleland and P. Engelbrecht, *J. Organomet. Chem*., 2005, **690**, 4959.

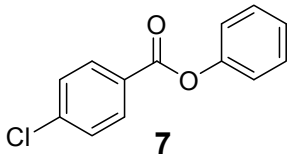
Supporting Information for

"*N*-Heterocyclic Carbene Catalysed Aerobic Oxidation of Aromatic Aldehydes to Aryl Esters using Boronic Acids"

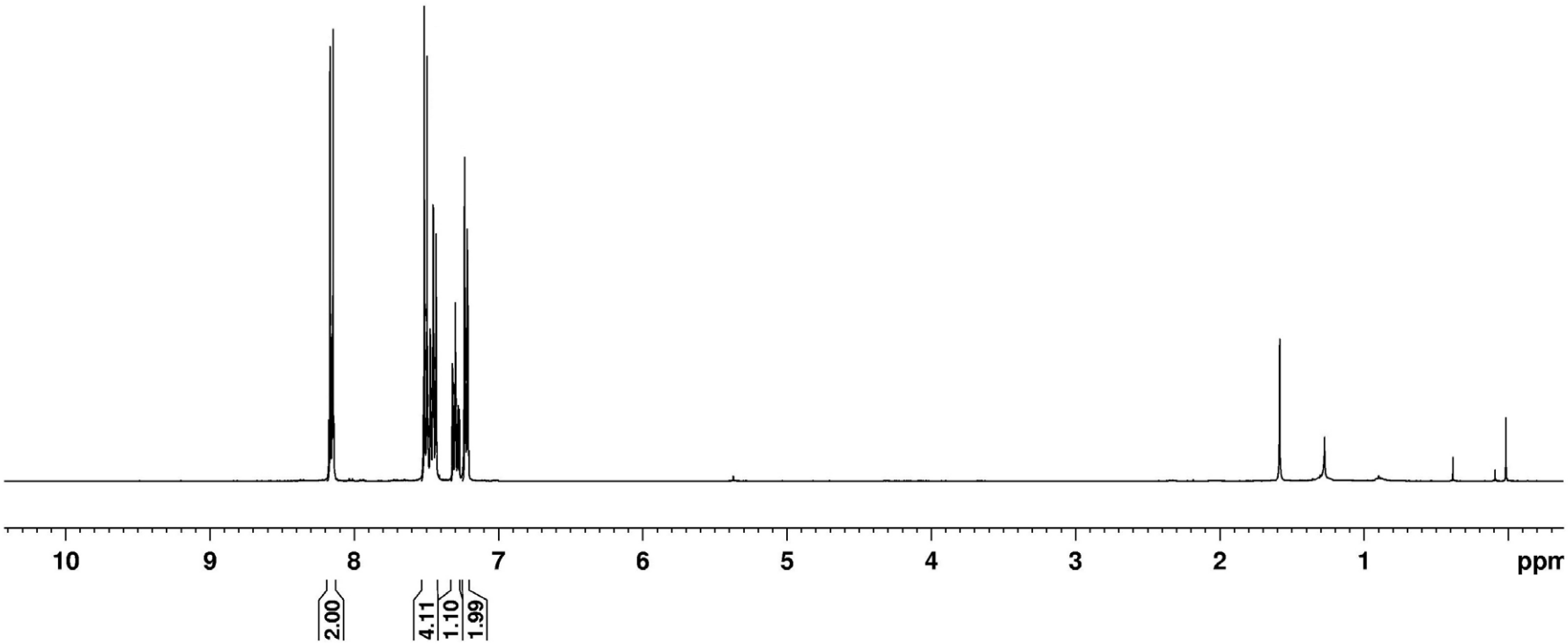
Panjab Arde, B T Ramanjaneyulu, Virsinha Reddy, Apurv Saxena and R Vijaya Anand*
Indian Institute of Science Education and Research (IISER) Mohali, Sector 81, S A S Nagar, Manuali 140 306, Punjab, India
E-Mail: rvijayan@iisermohali.ac.in

Table of Contents

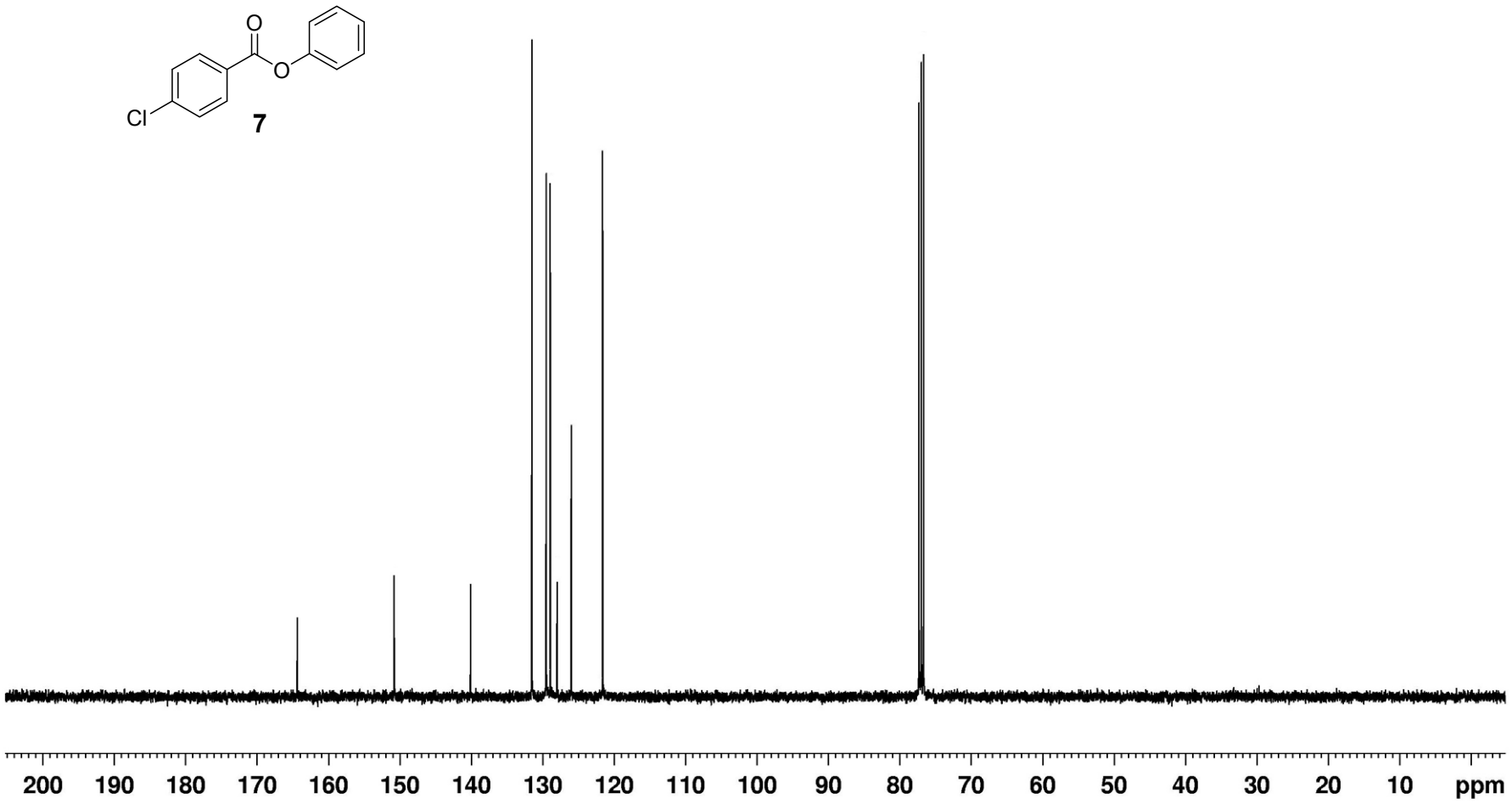
^{1}H NMR Spectrum of **7**



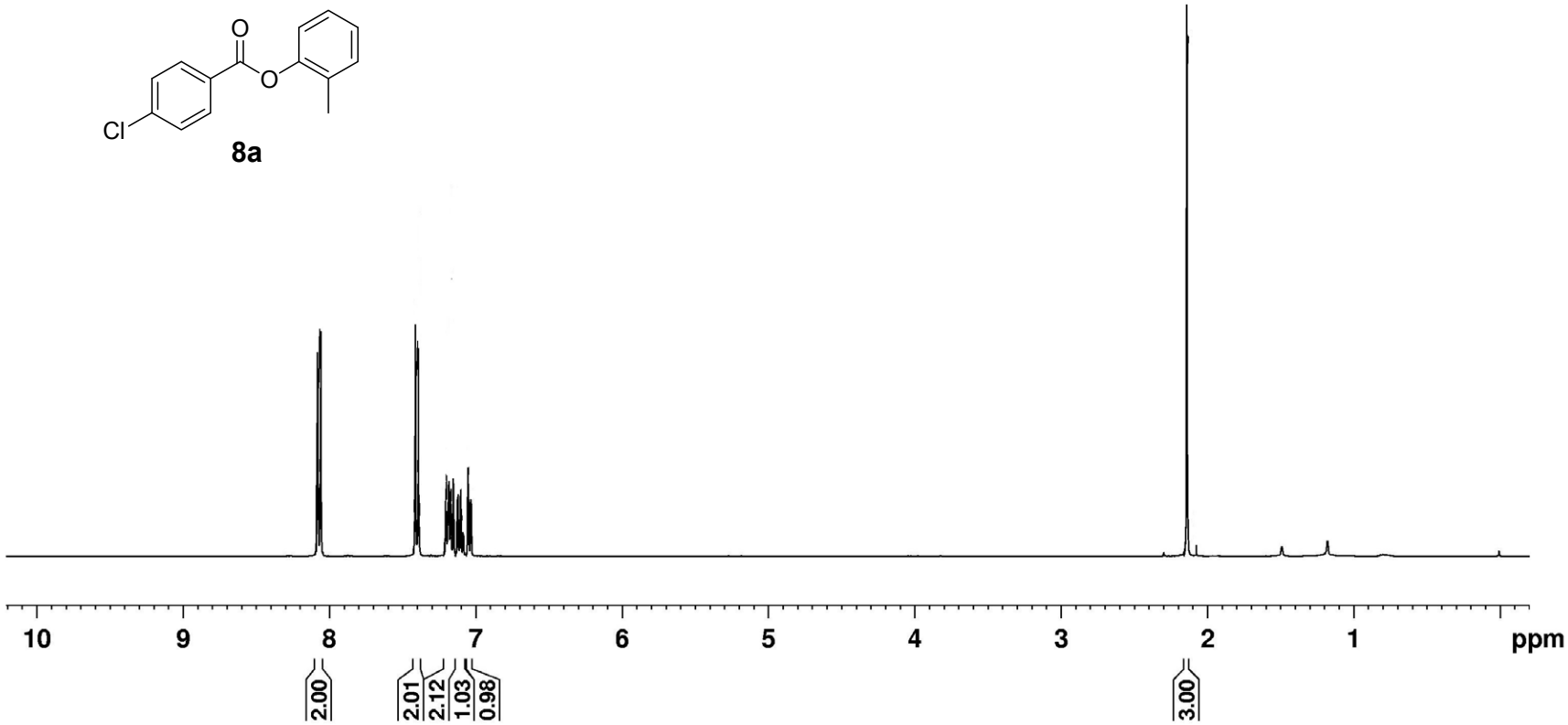
7



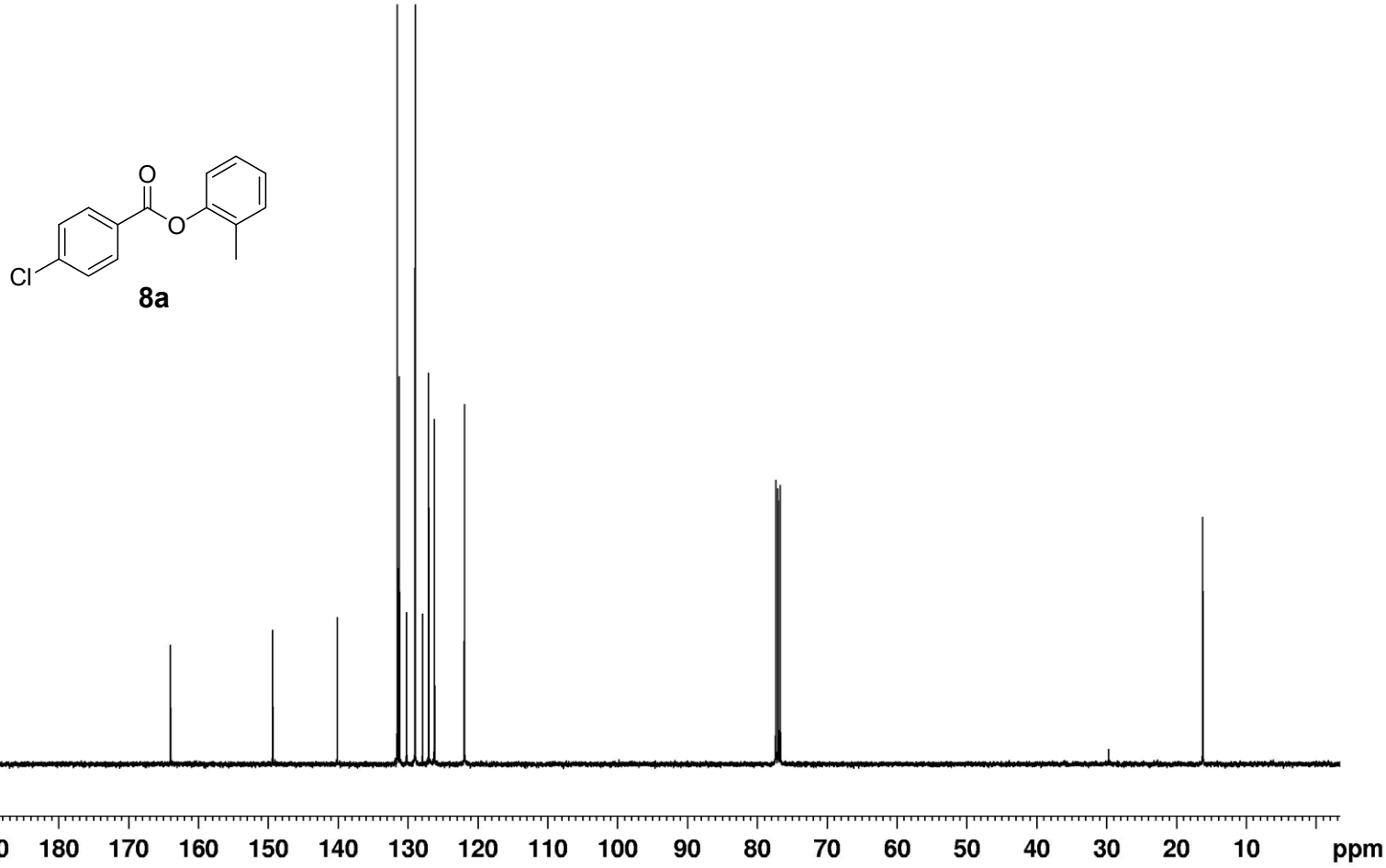
^{13}C NMR Spectrum of **7**



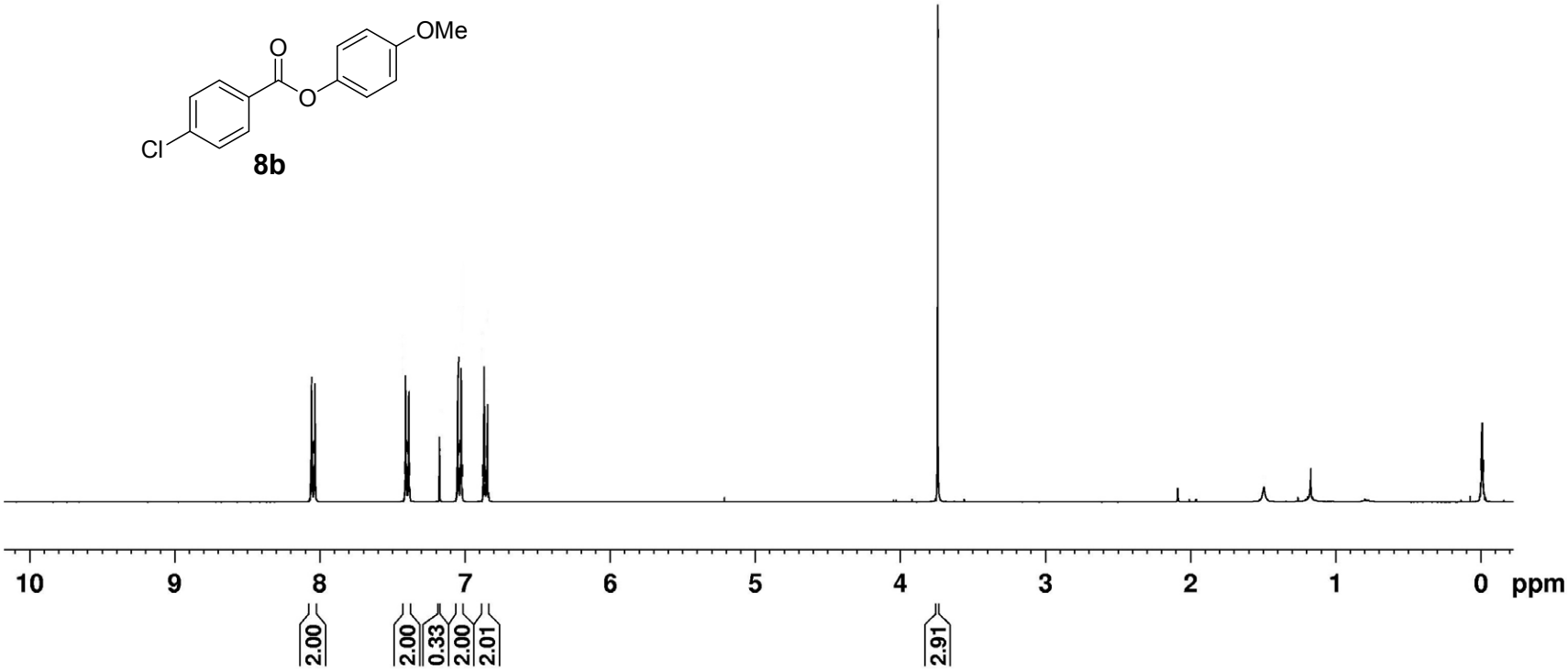
^{1}H NMR Spectrum of **8a**



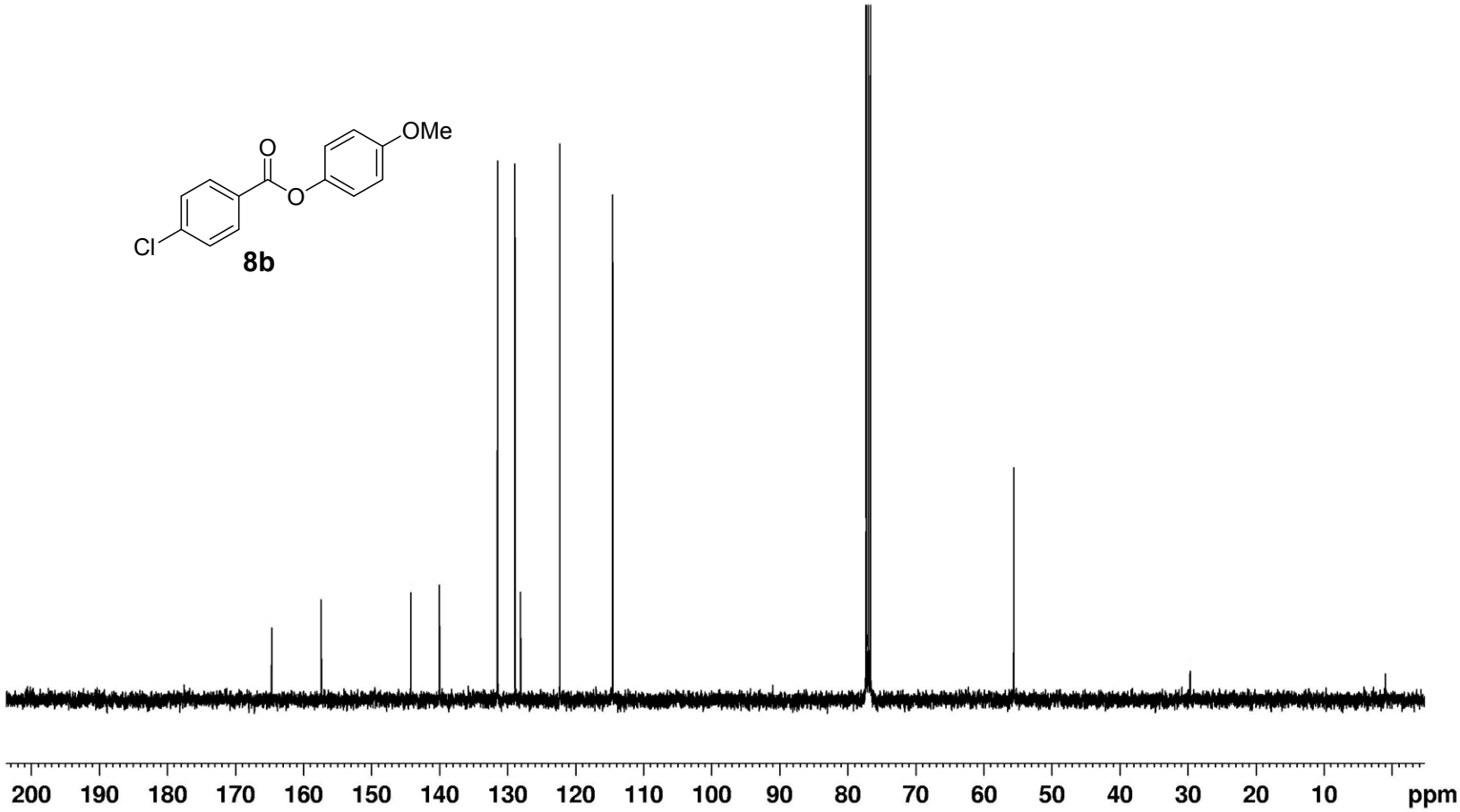
^{13}C NMR Spectrum of **8a**



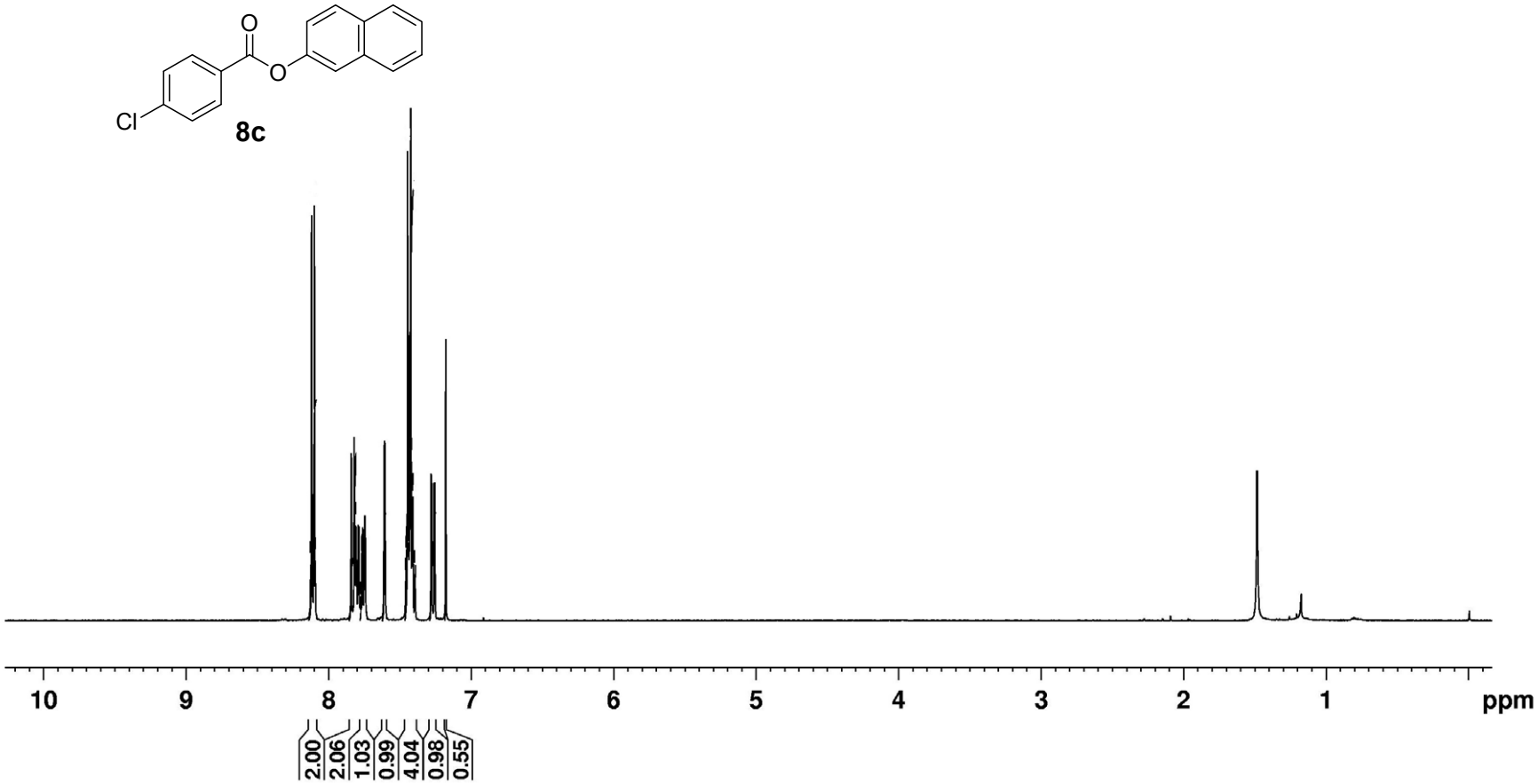
^{1}H NMR Spectrum of **8b**



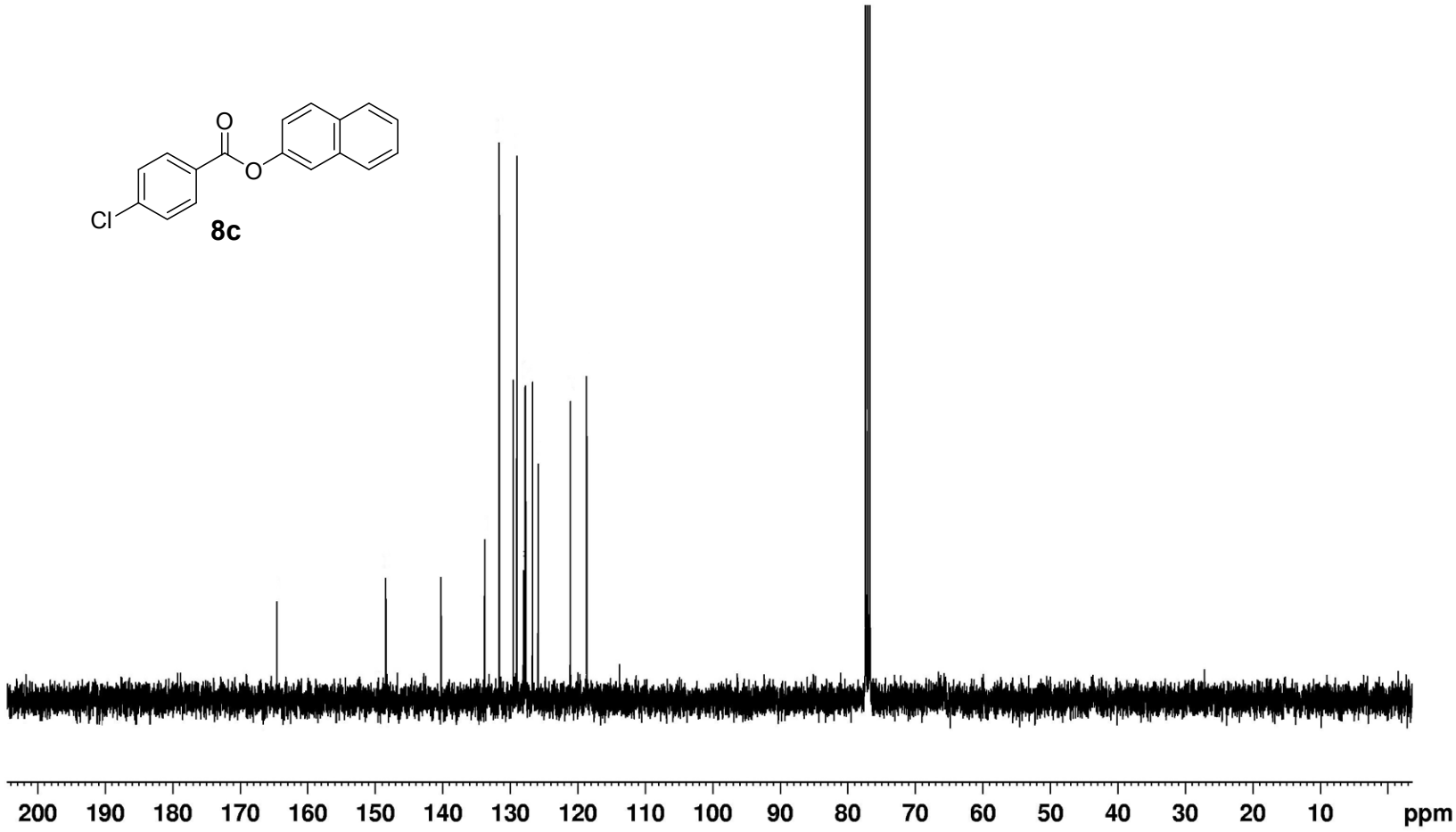
^{13}C NMR Spectrum of **8b**



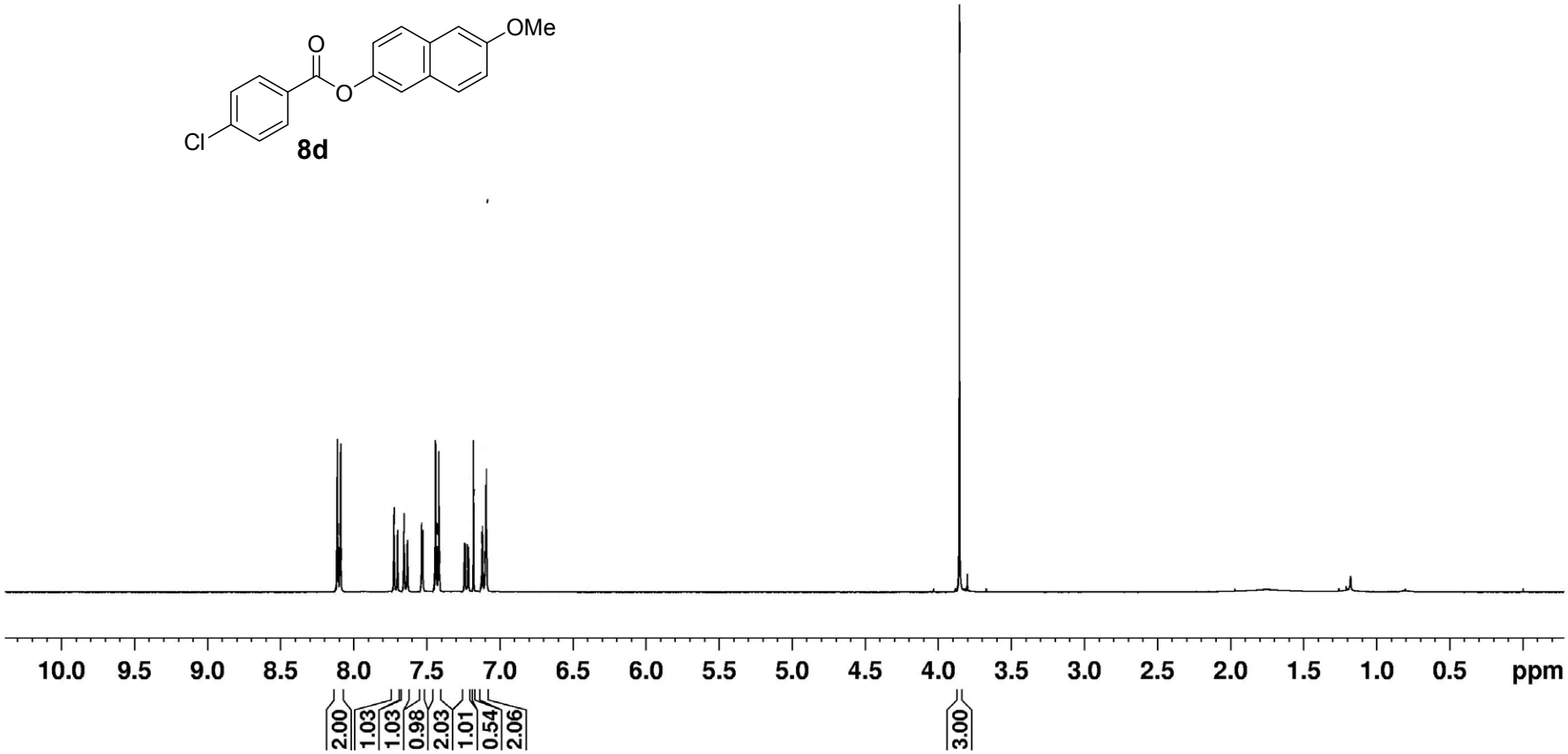
^{1}H NMR Spectrum of **8c**



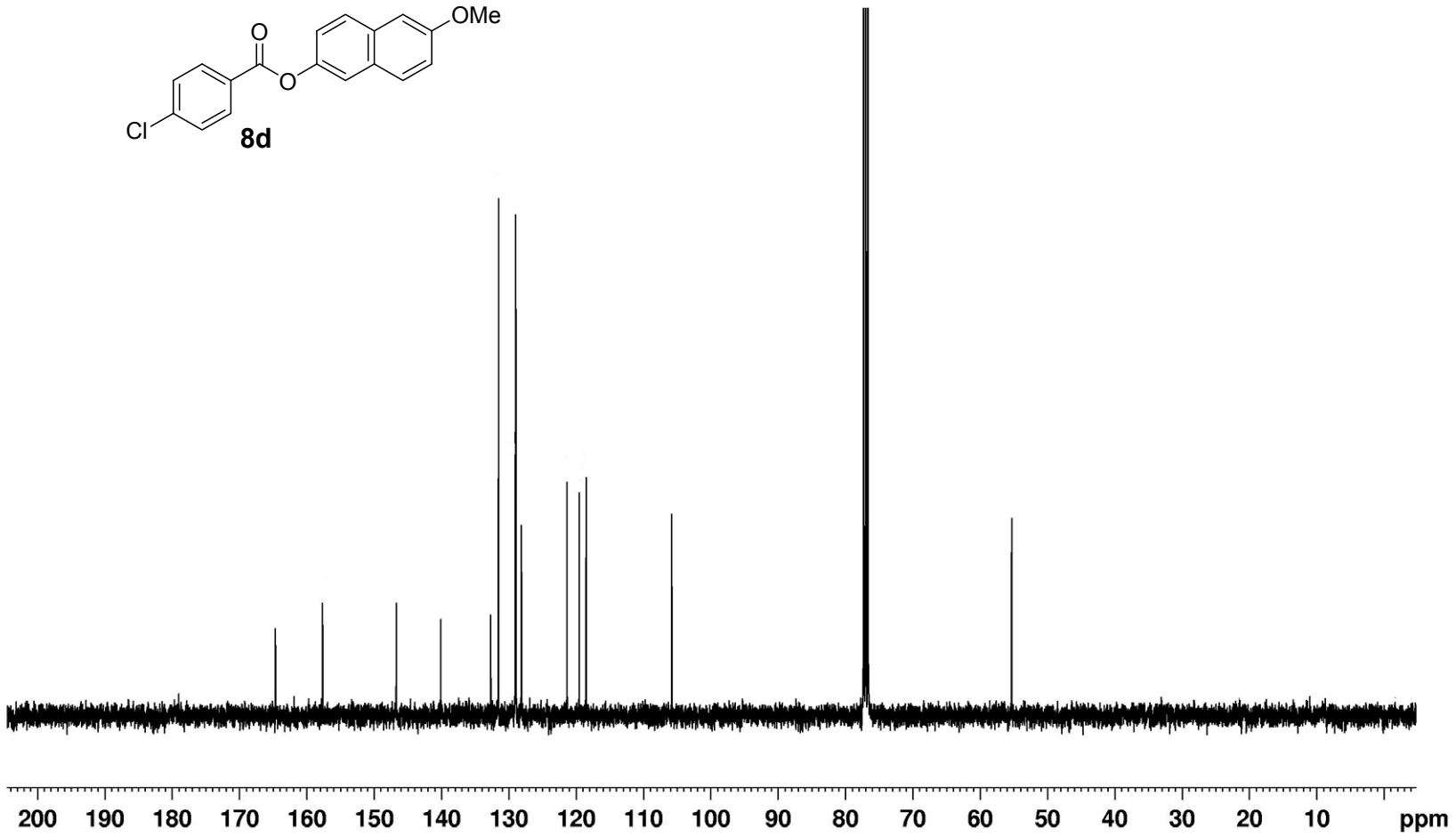
^{13}C NMR Spectrum of **8c**



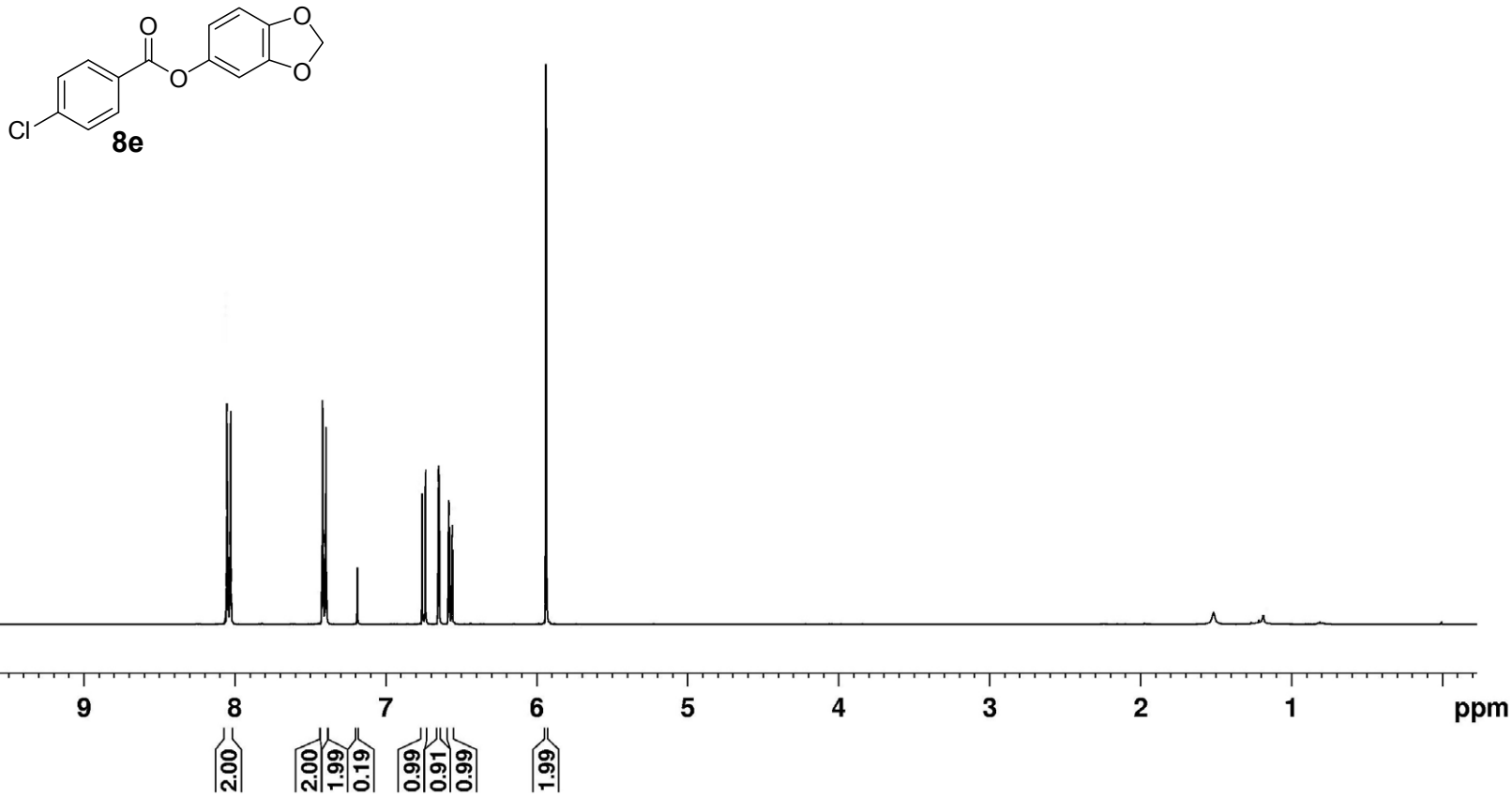
^{1}H NMR Spectrum of **8d**



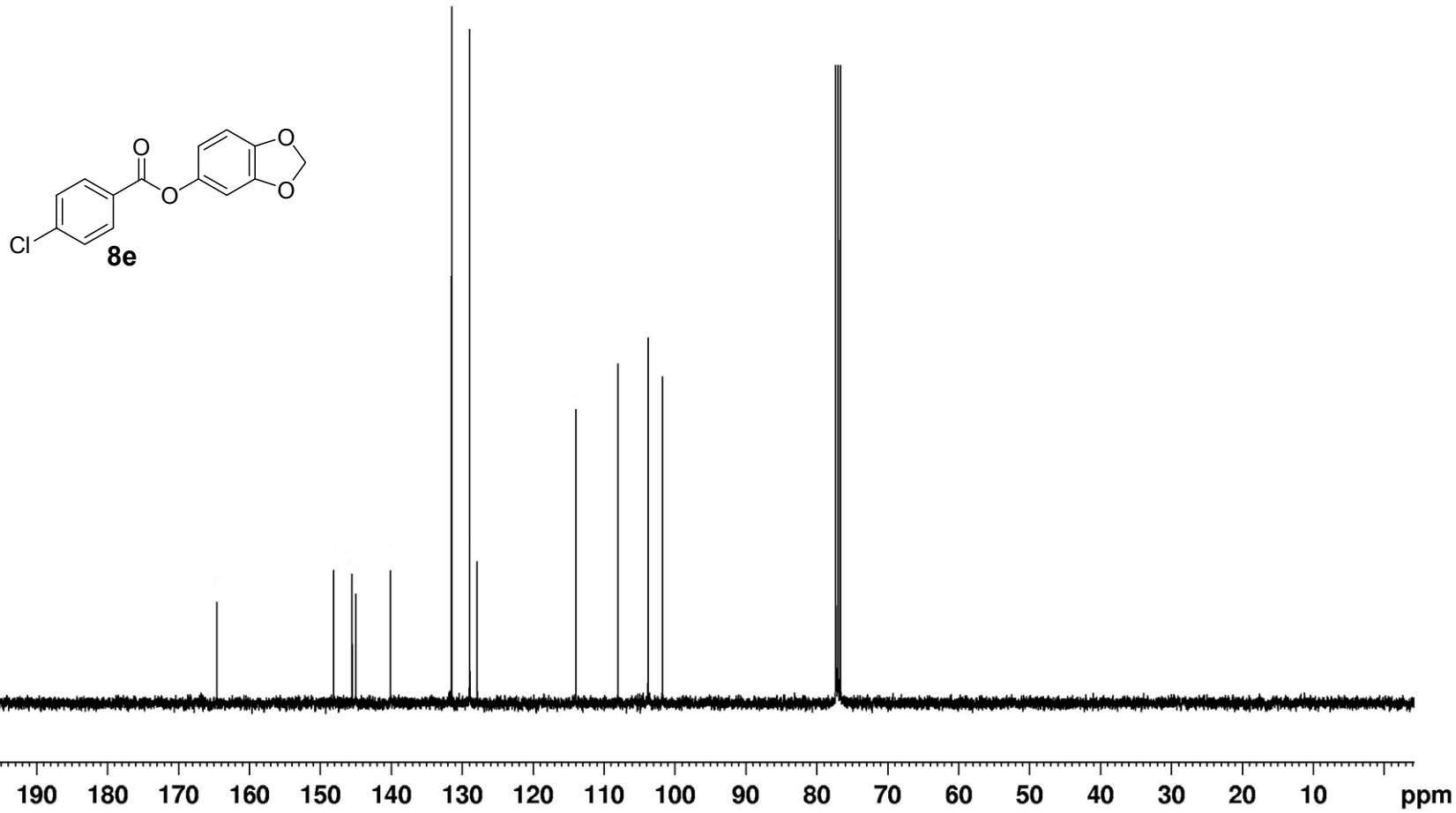
^{13}C NMR Spectrum of **8d**



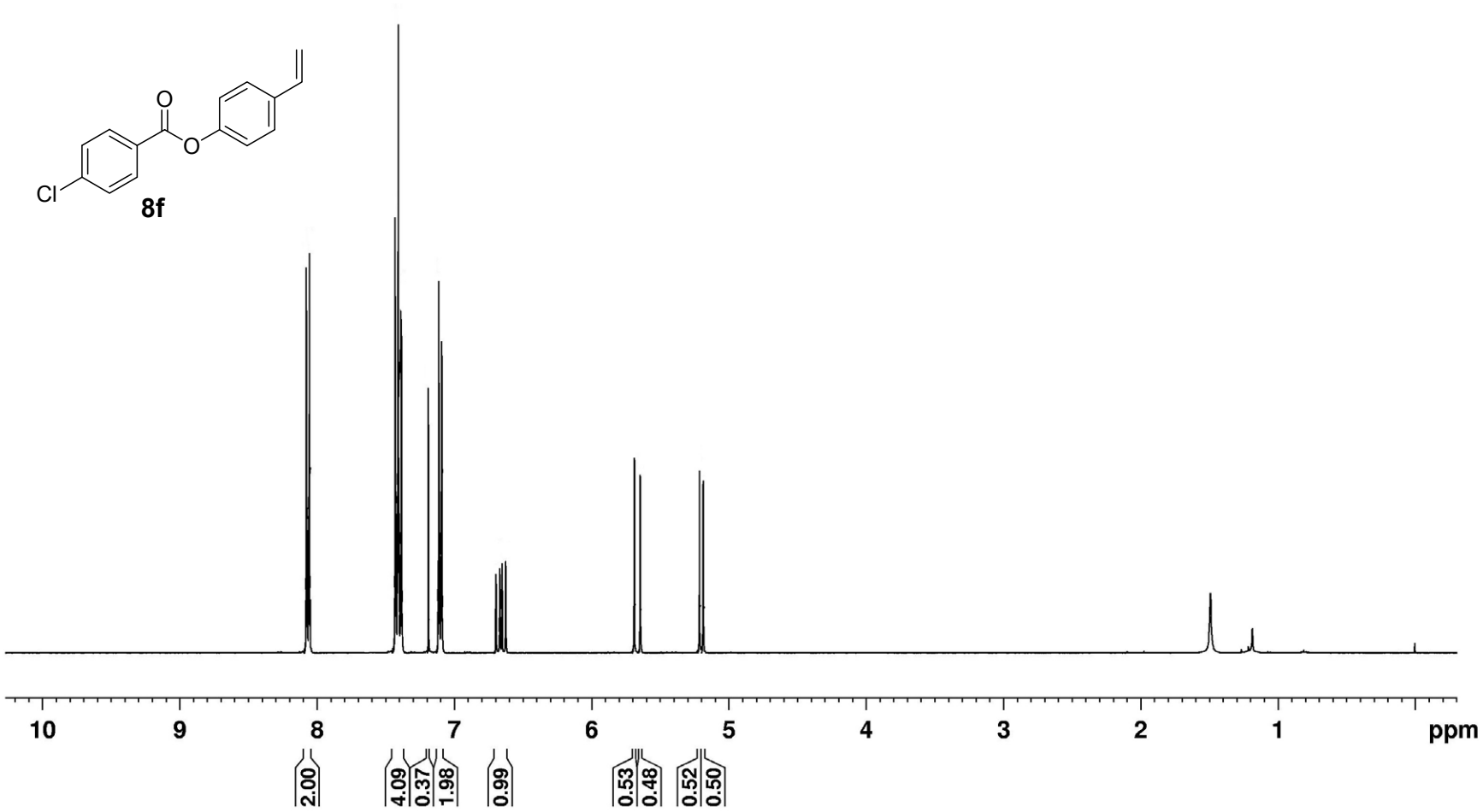
^{1}H NMR Spectrum of **8e**



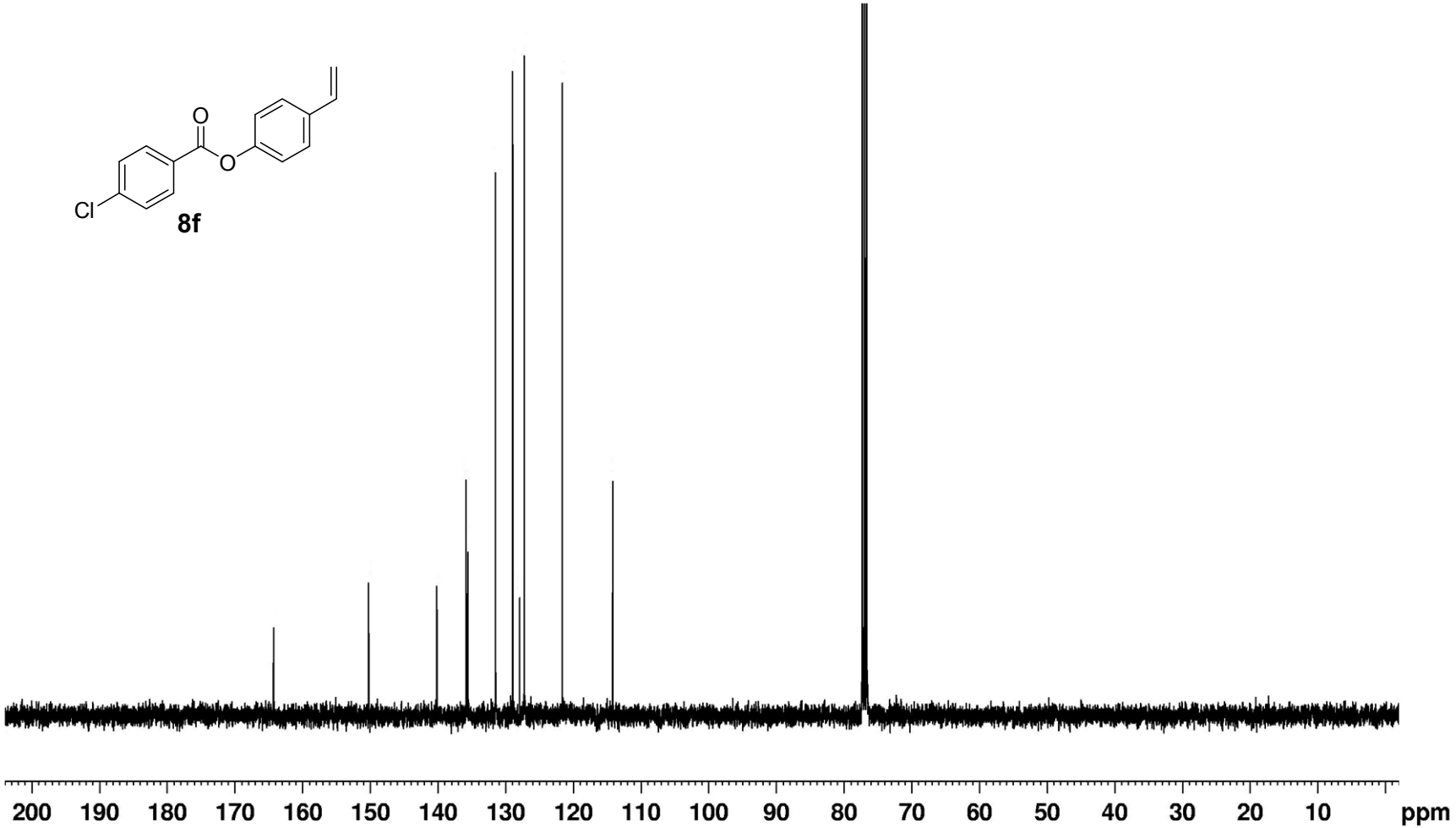
^{13}C NMR Spectrum of **8e**



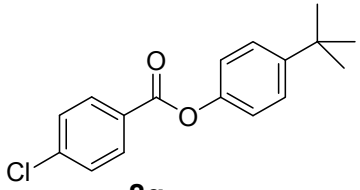
^{1}H NMR Spectrum of **8f**



^{13}C NMR Spectrum of **8f**

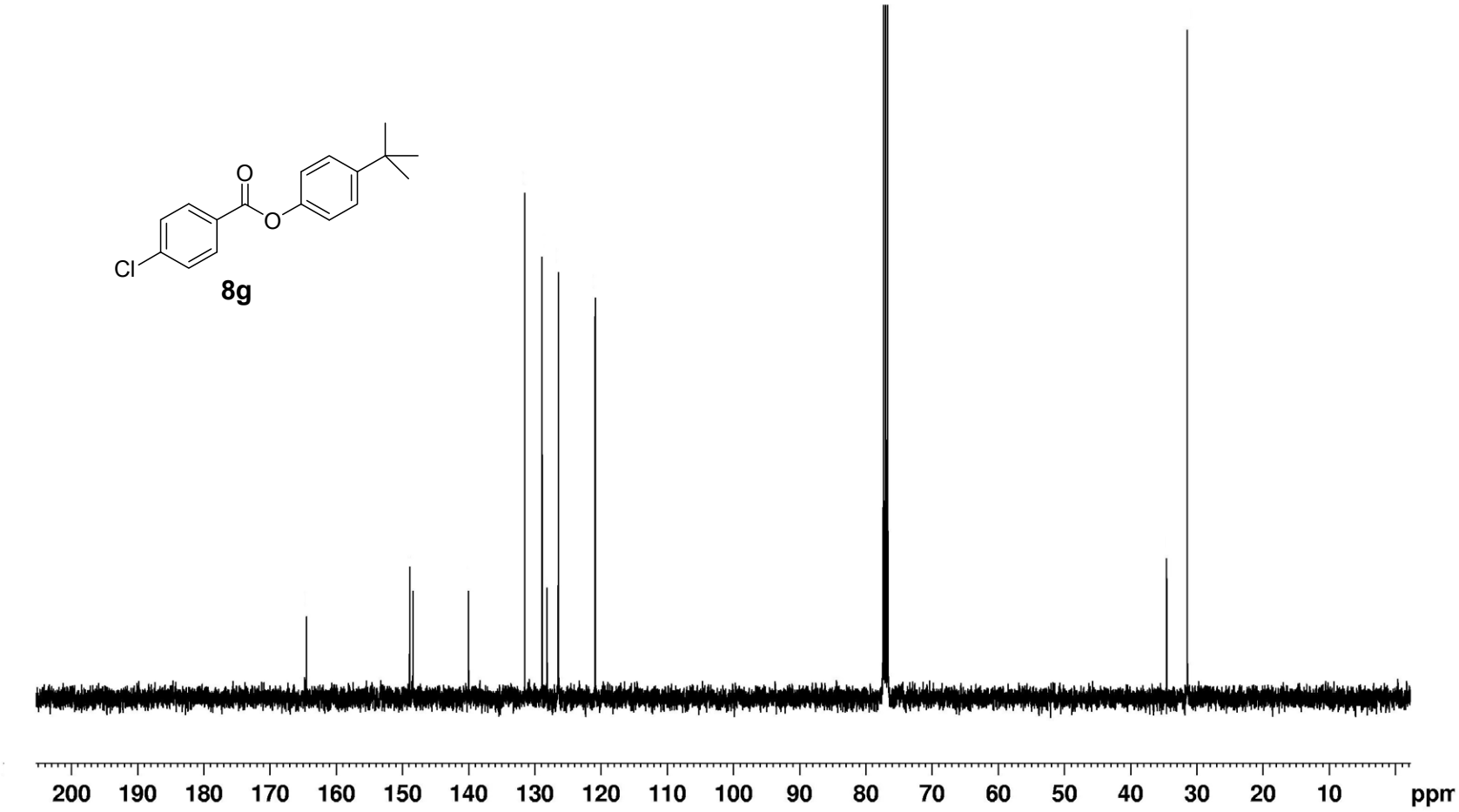


^{1}H NMR Spectrum of **8g**

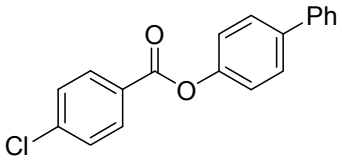


8g

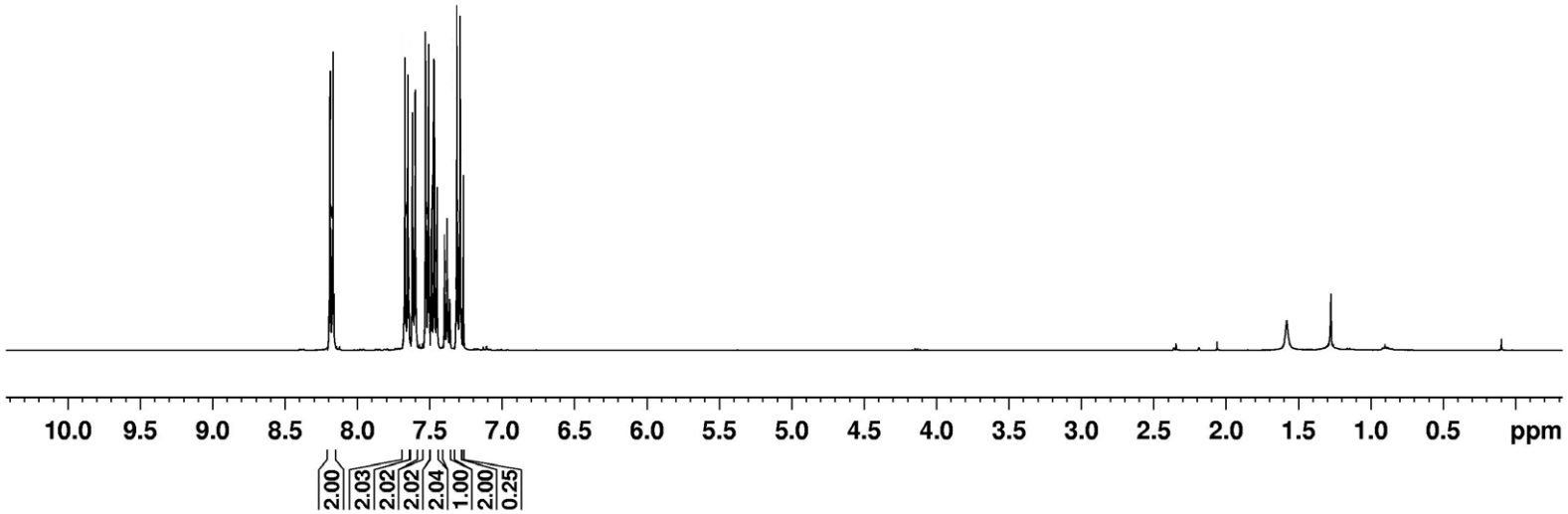
^{13}C NMR Spectrum of **8g**



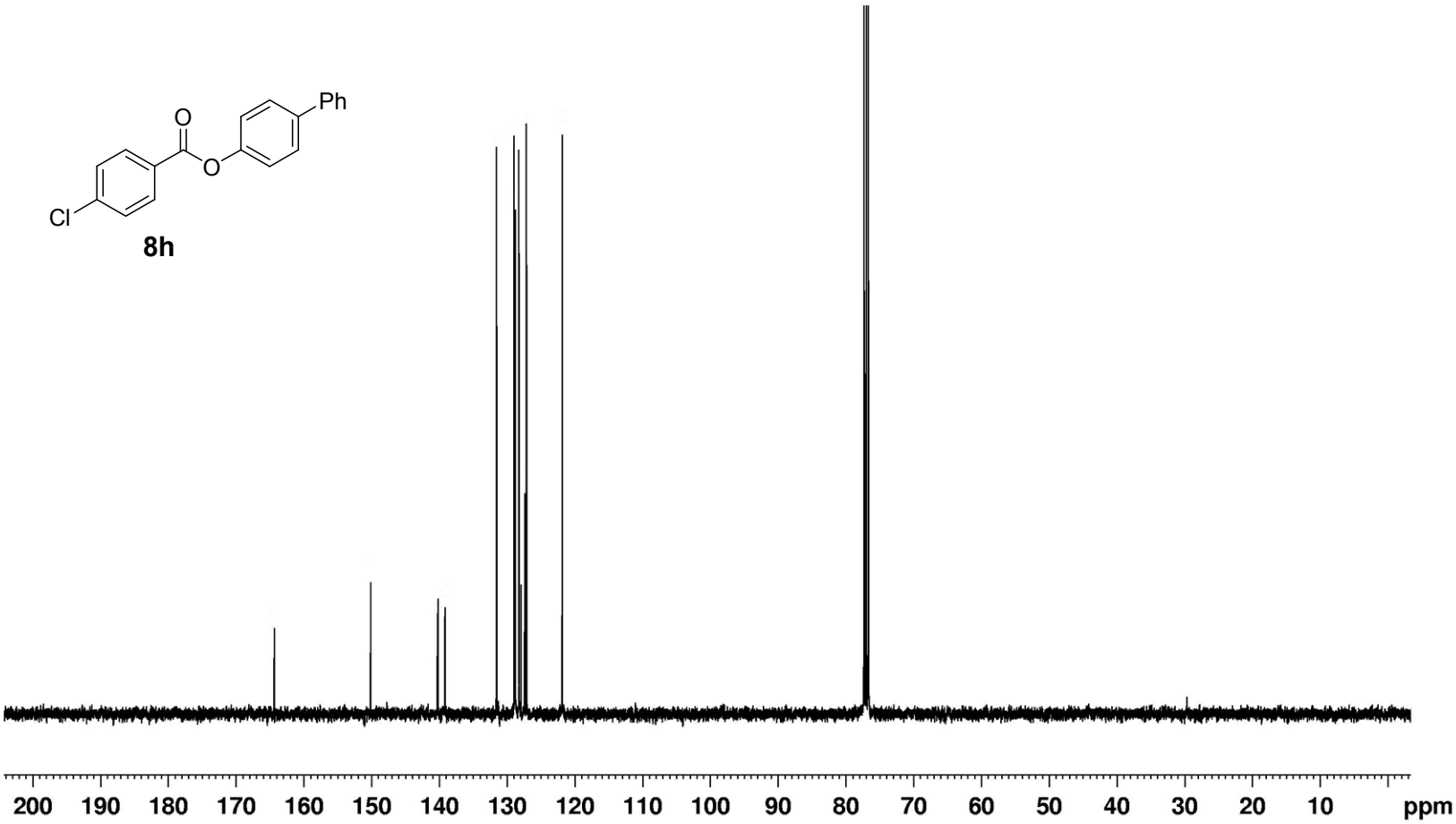
^{1}H NMR Spectrum of **8h**



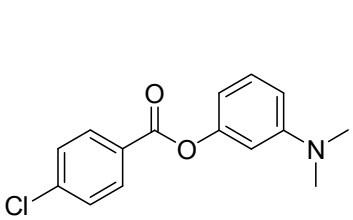
8h



^{13}C NMR Spectrum of **8h**

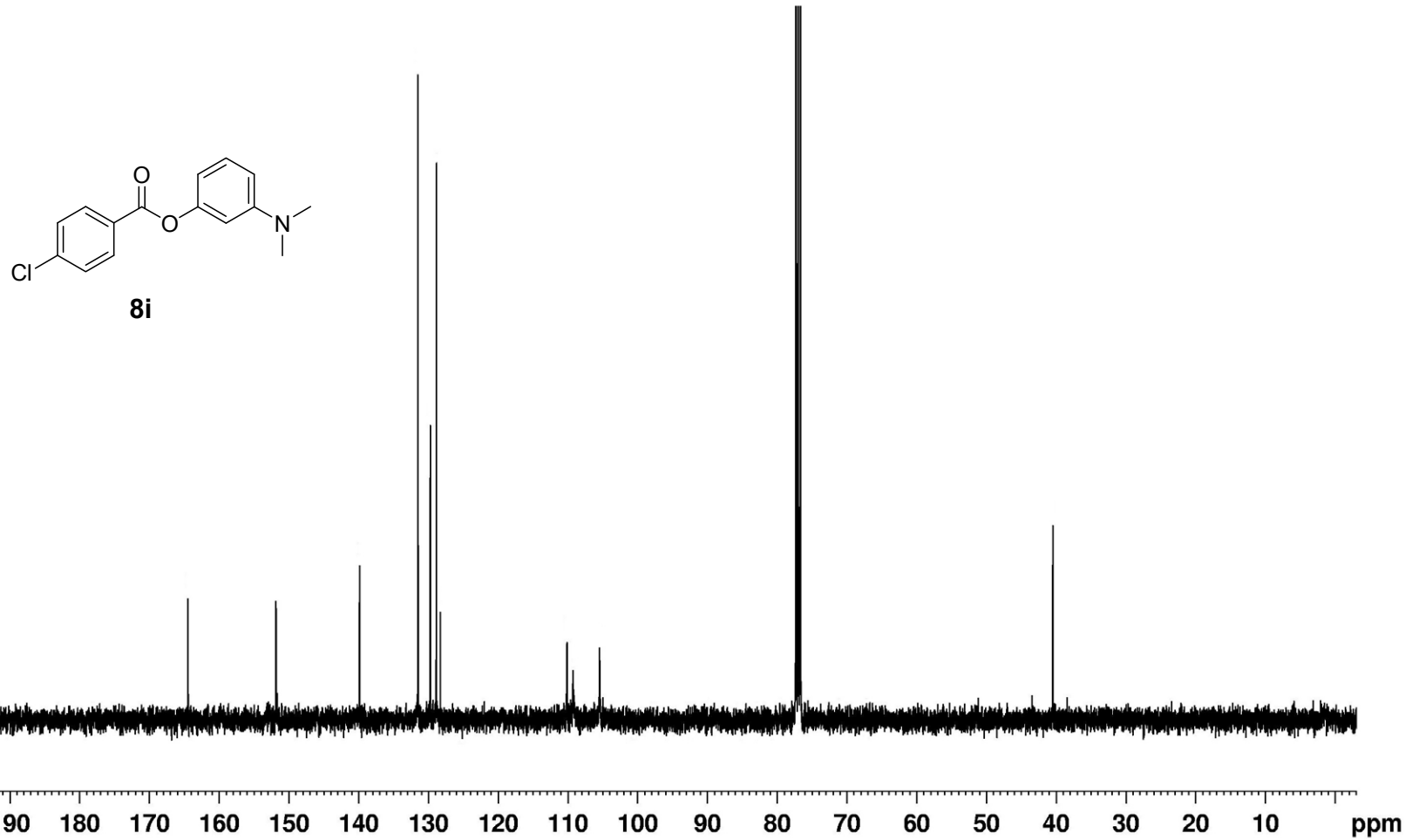


^{1}H NMR Spectrum of **8i**



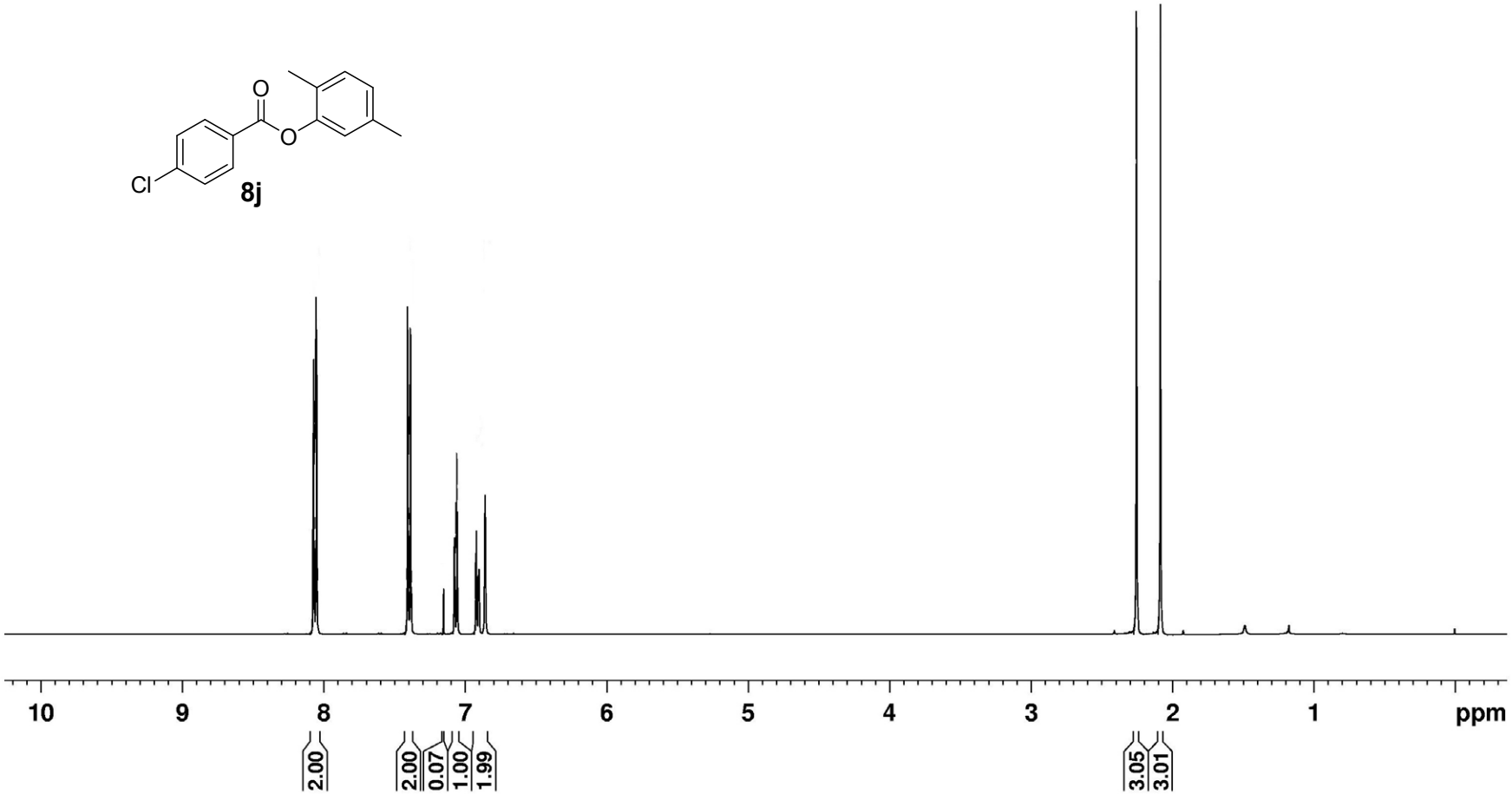
8i

^{13}C NMR Spectrum of **8i**

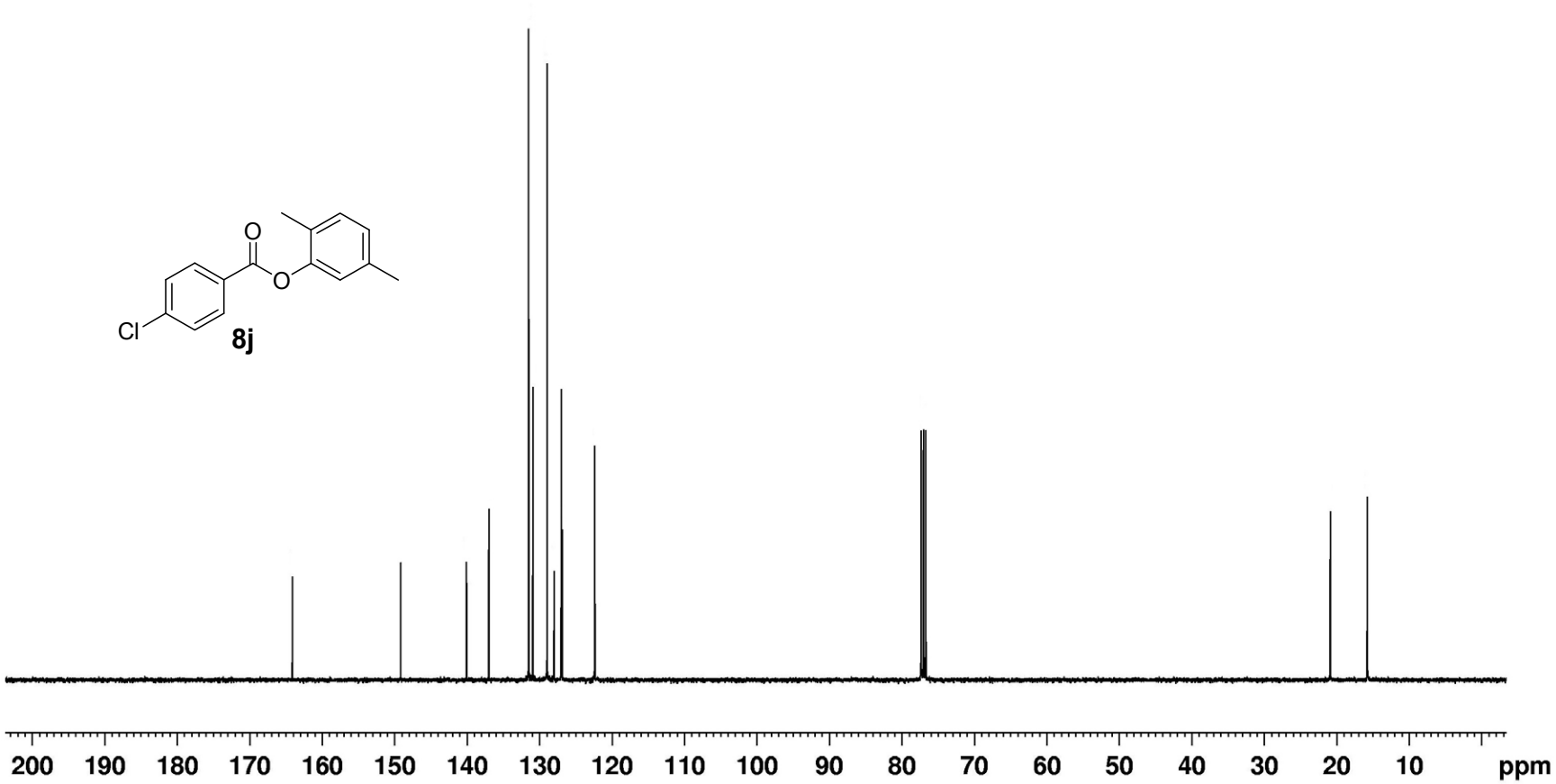


8i

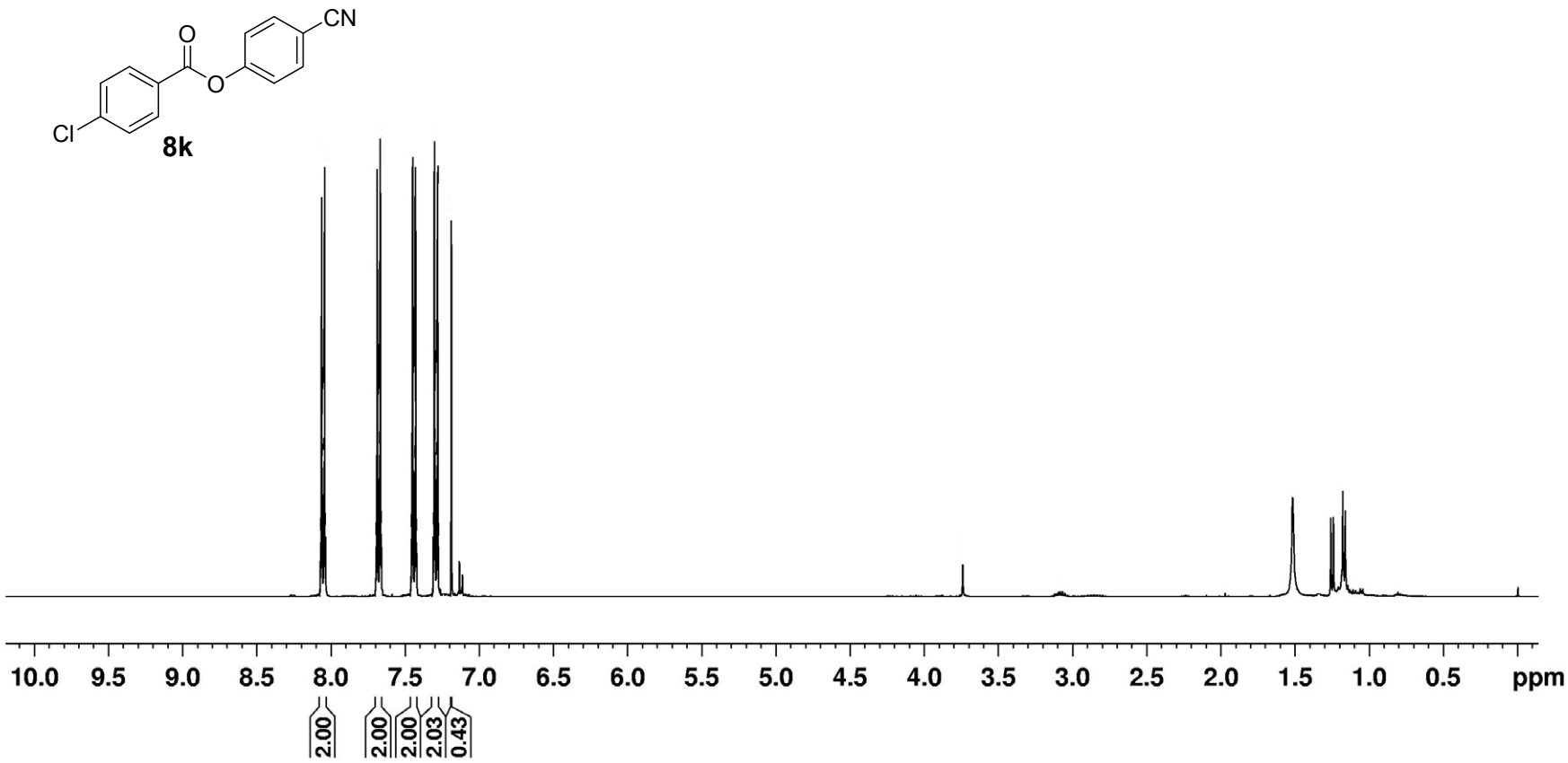
^{1}H NMR Spectrum of **8j**



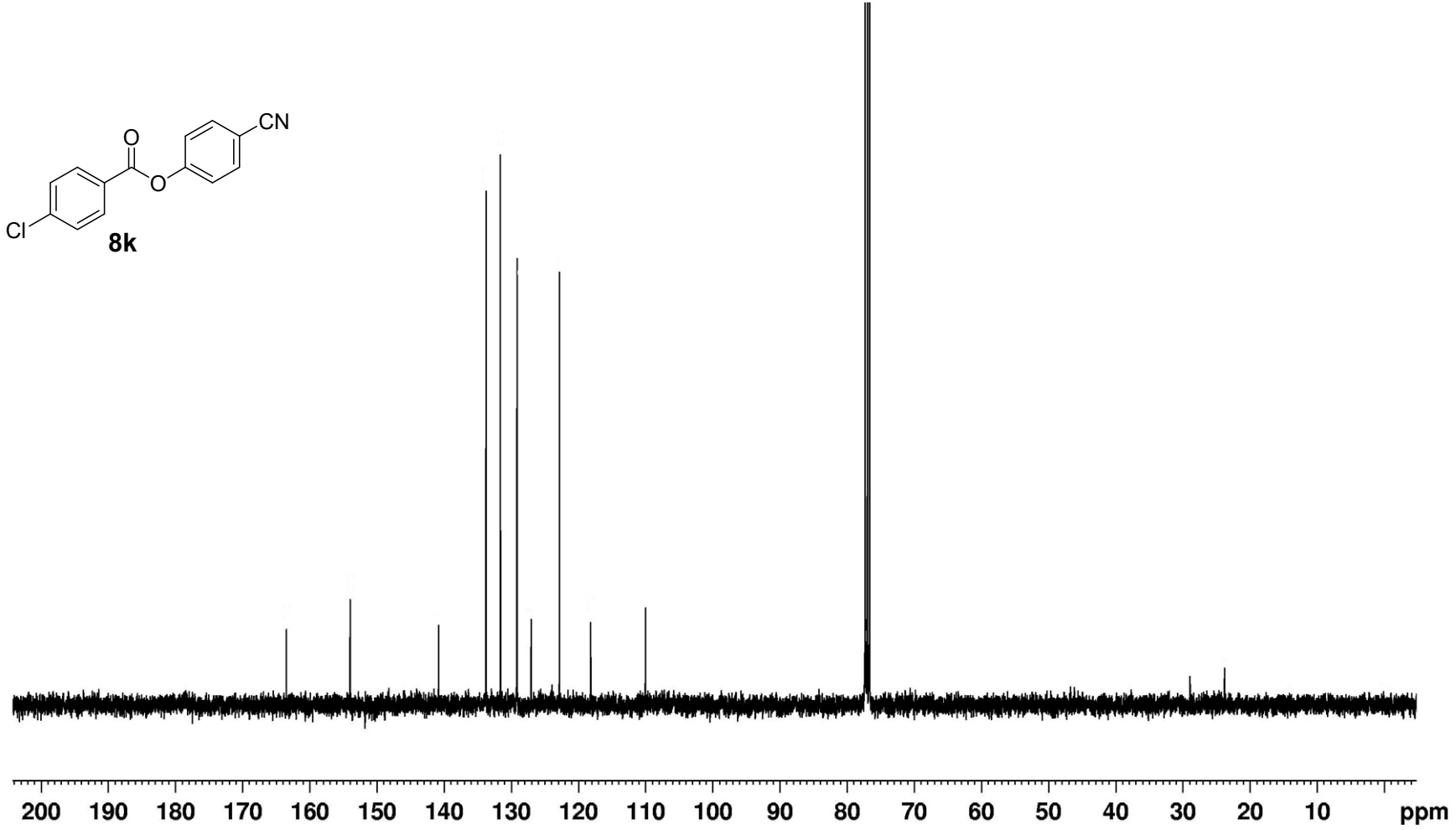
^{13}C NMR Spectrum of **8j**



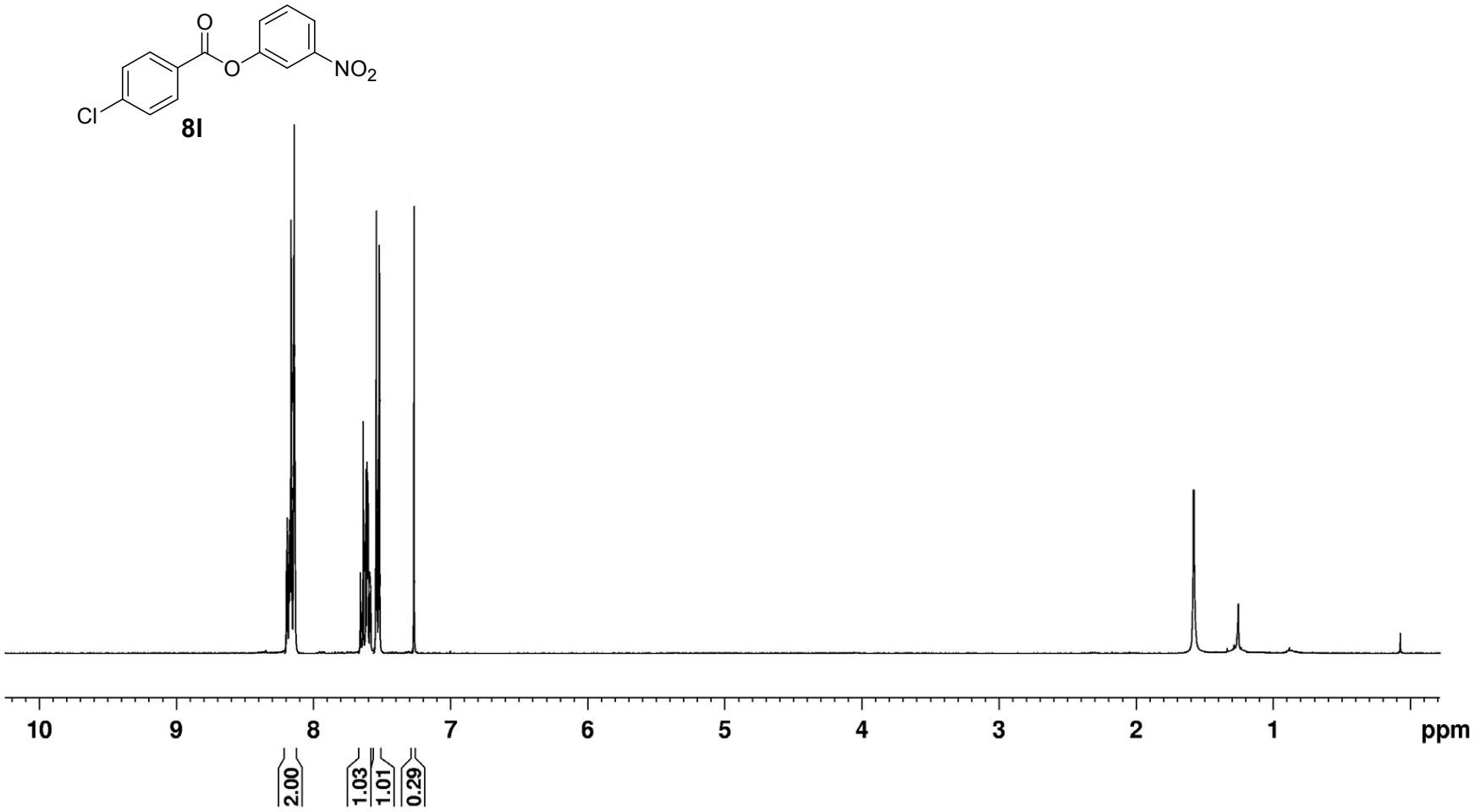
^{1}H NMR Spectrum of **8k**



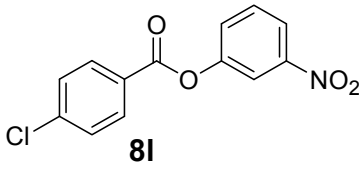
^{13}C NMR Spectrum of **8k**



^{1}H NMR Spectrum of **8l**

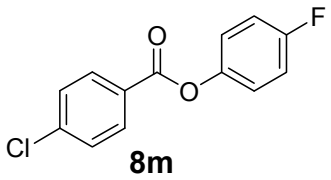


^{13}C NMR Spectrum of **8l**

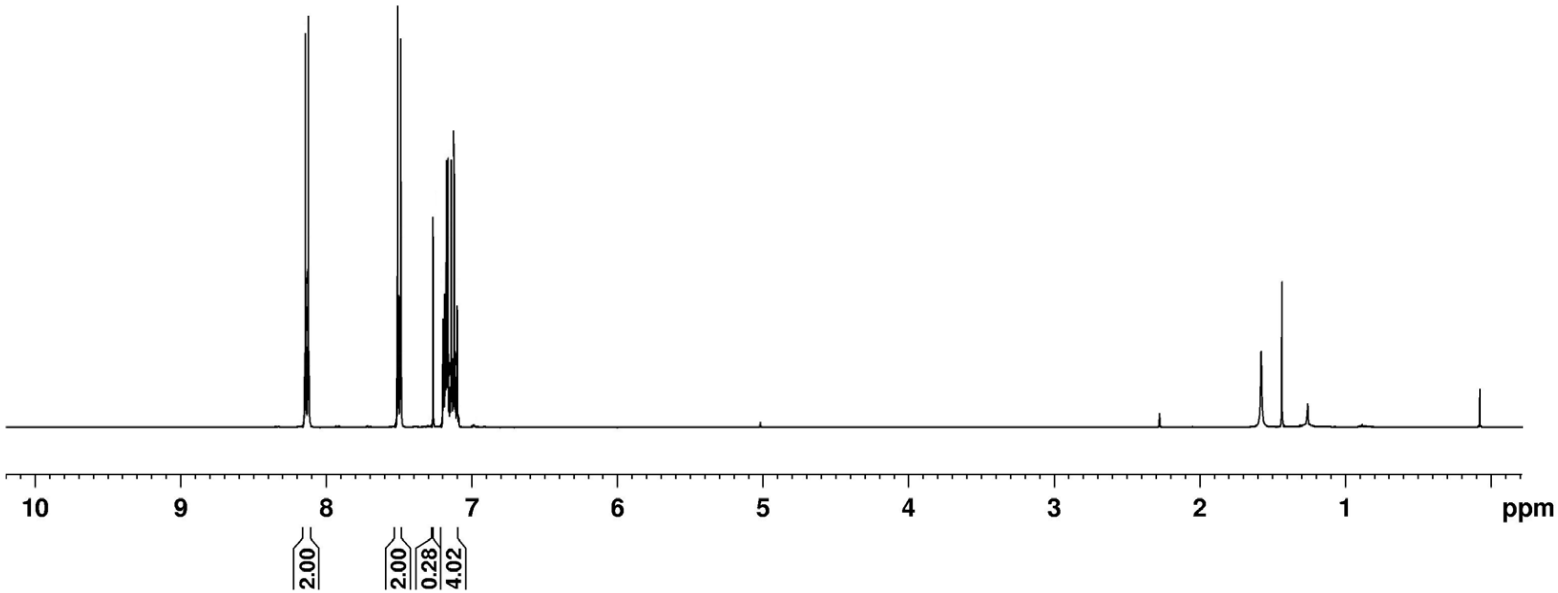


8l

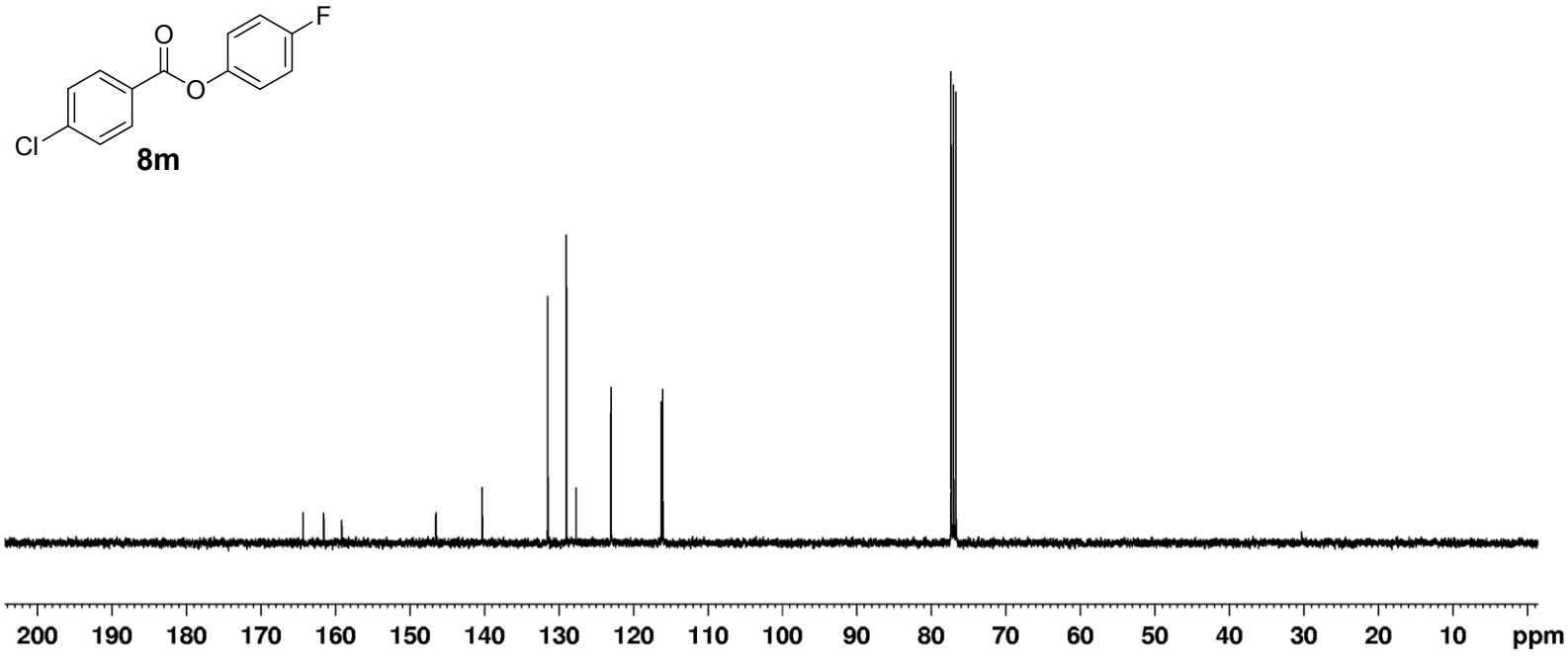
^{1}H NMR Spectrum of **8m**



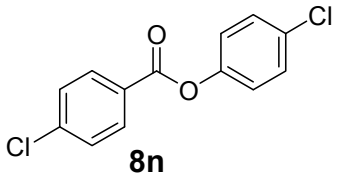
8m



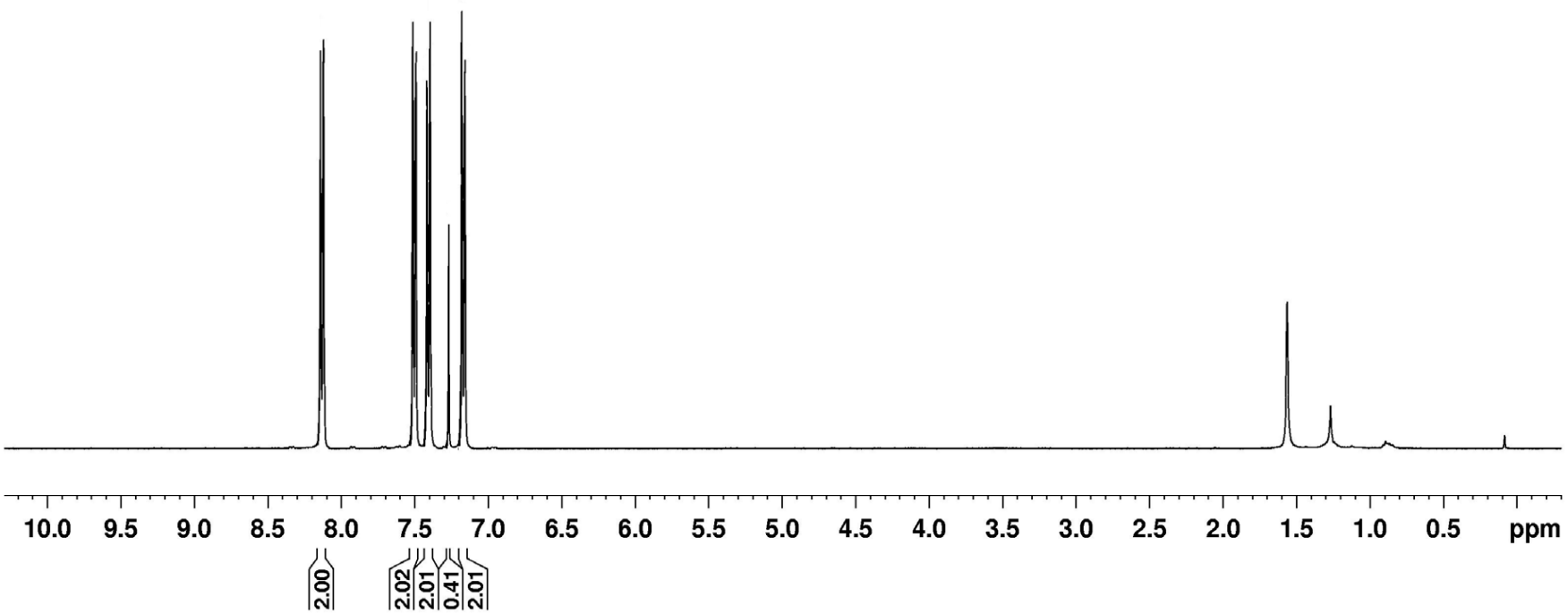
^{13}C NMR Spectrum of **8m**



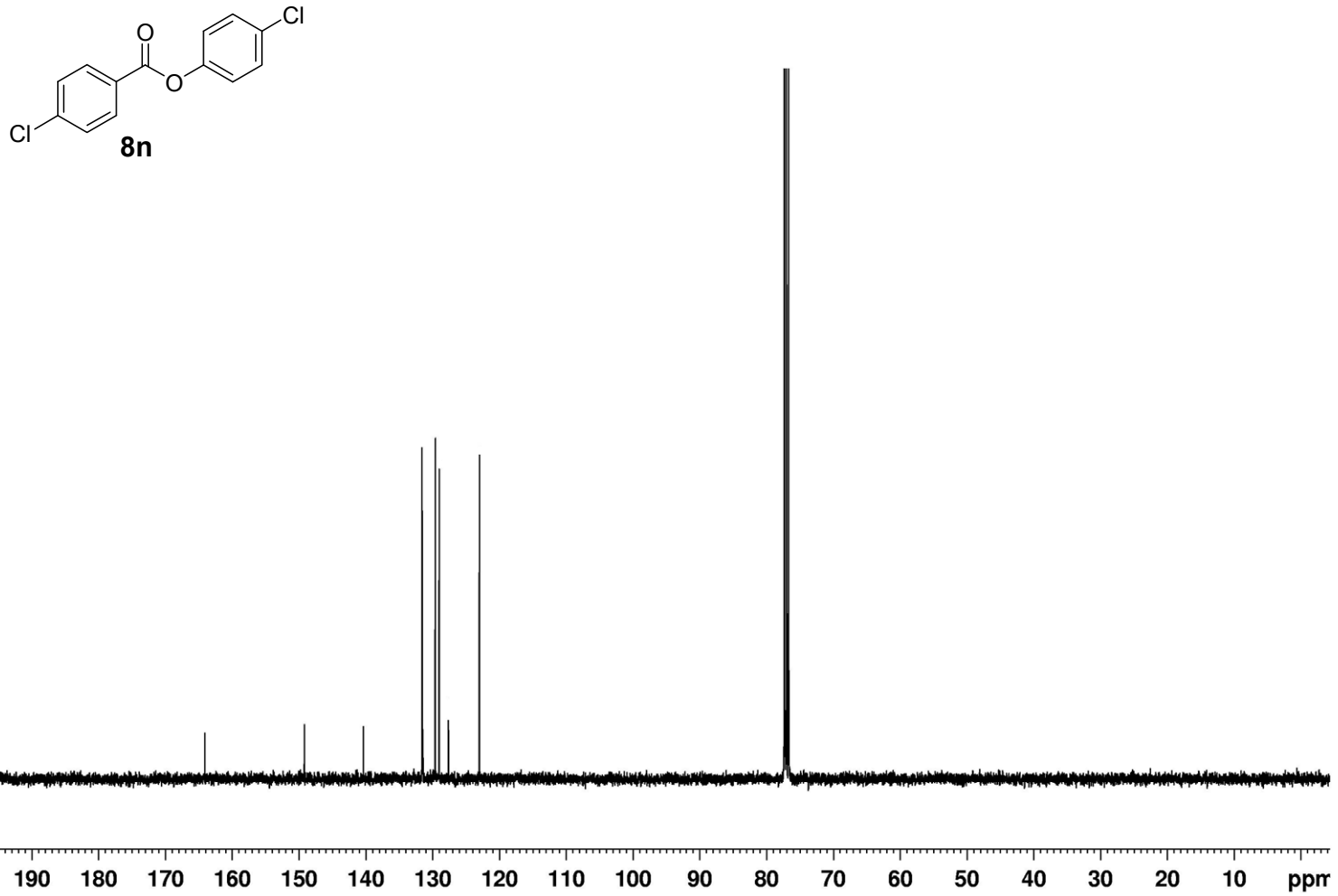
^{1}H NMR Spectrum of **8n**



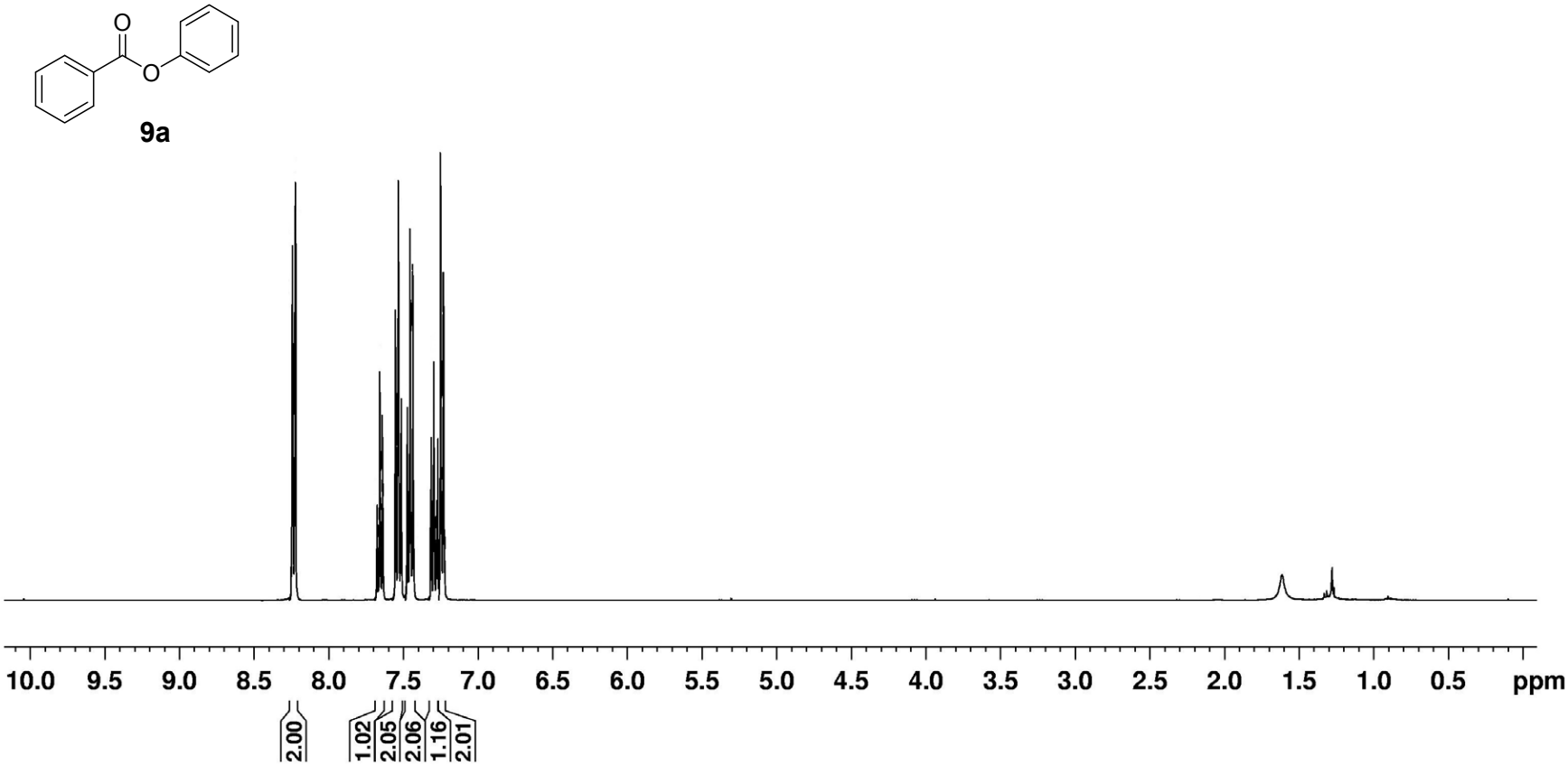
8n



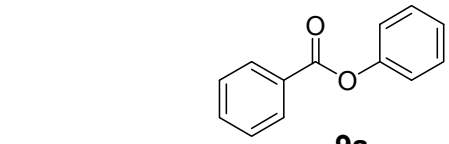
^{13}C NMR Spectrum of **8n**



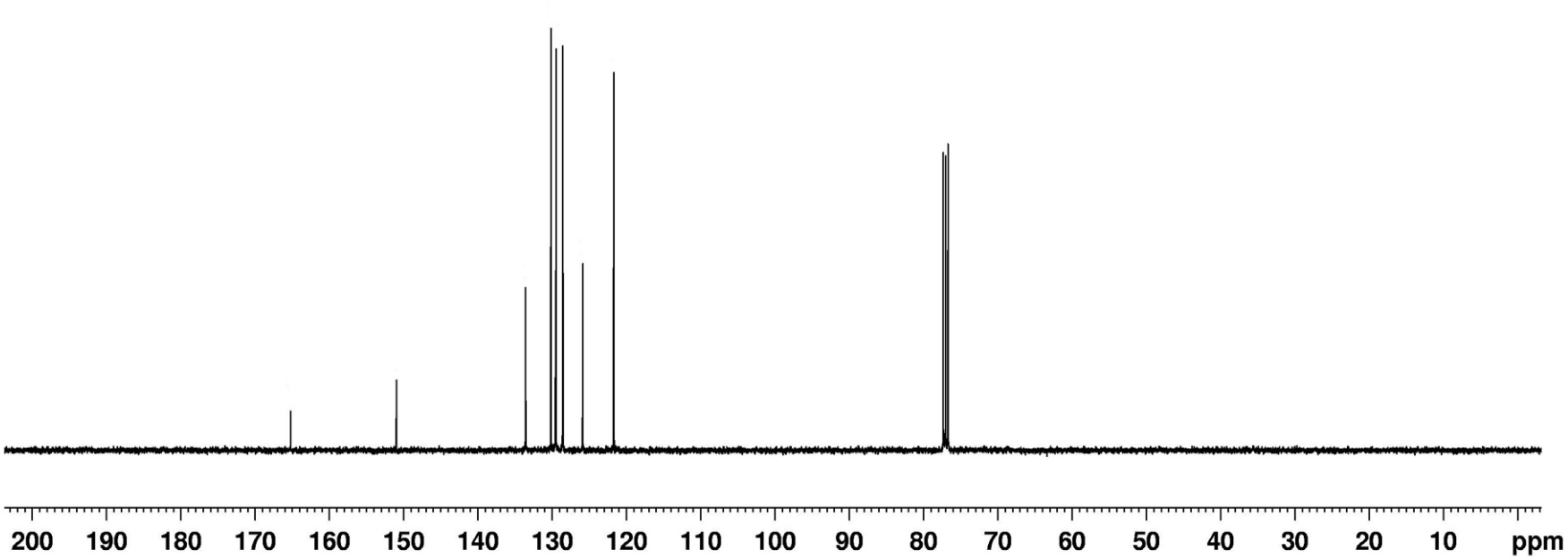
^{1}H NMR Spectrum of **9a**



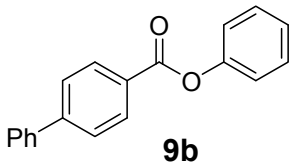
^{13}C NMR Spectrum of **9a**



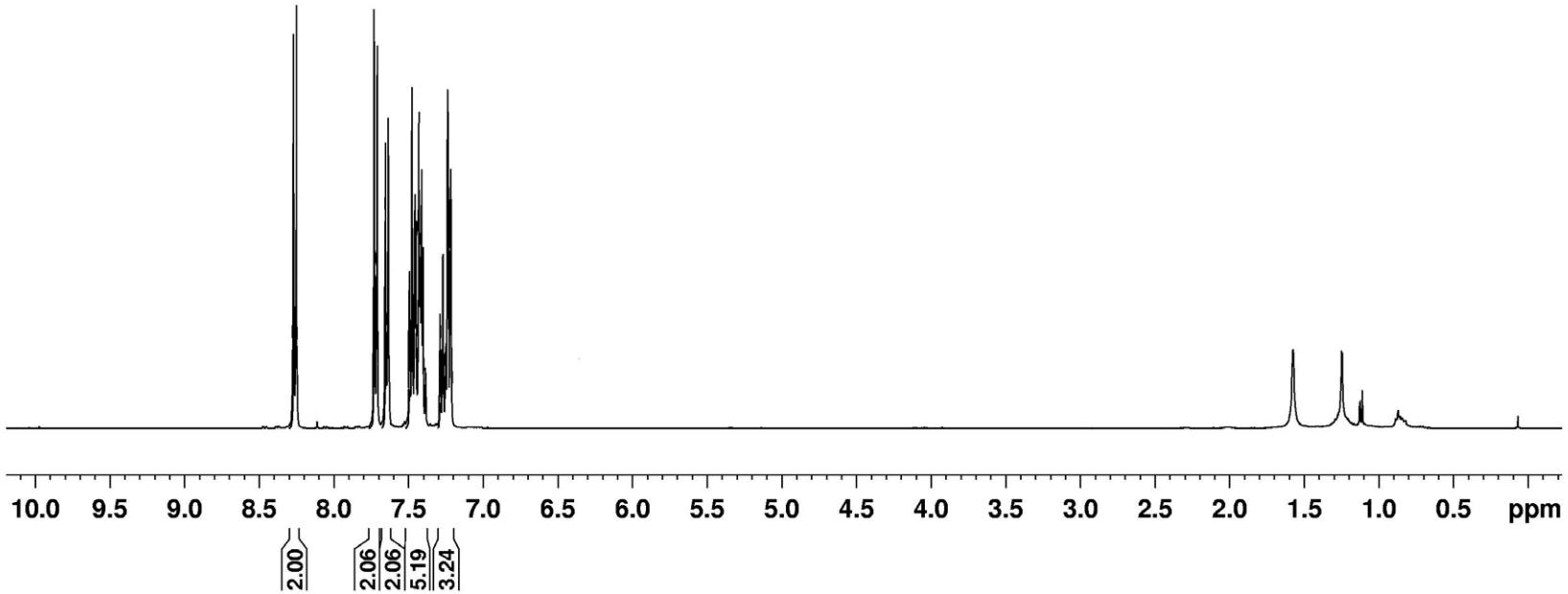
9a



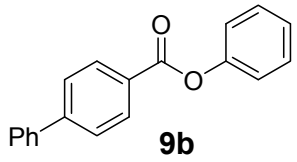
^{1}H NMR Spectrum of **9b**



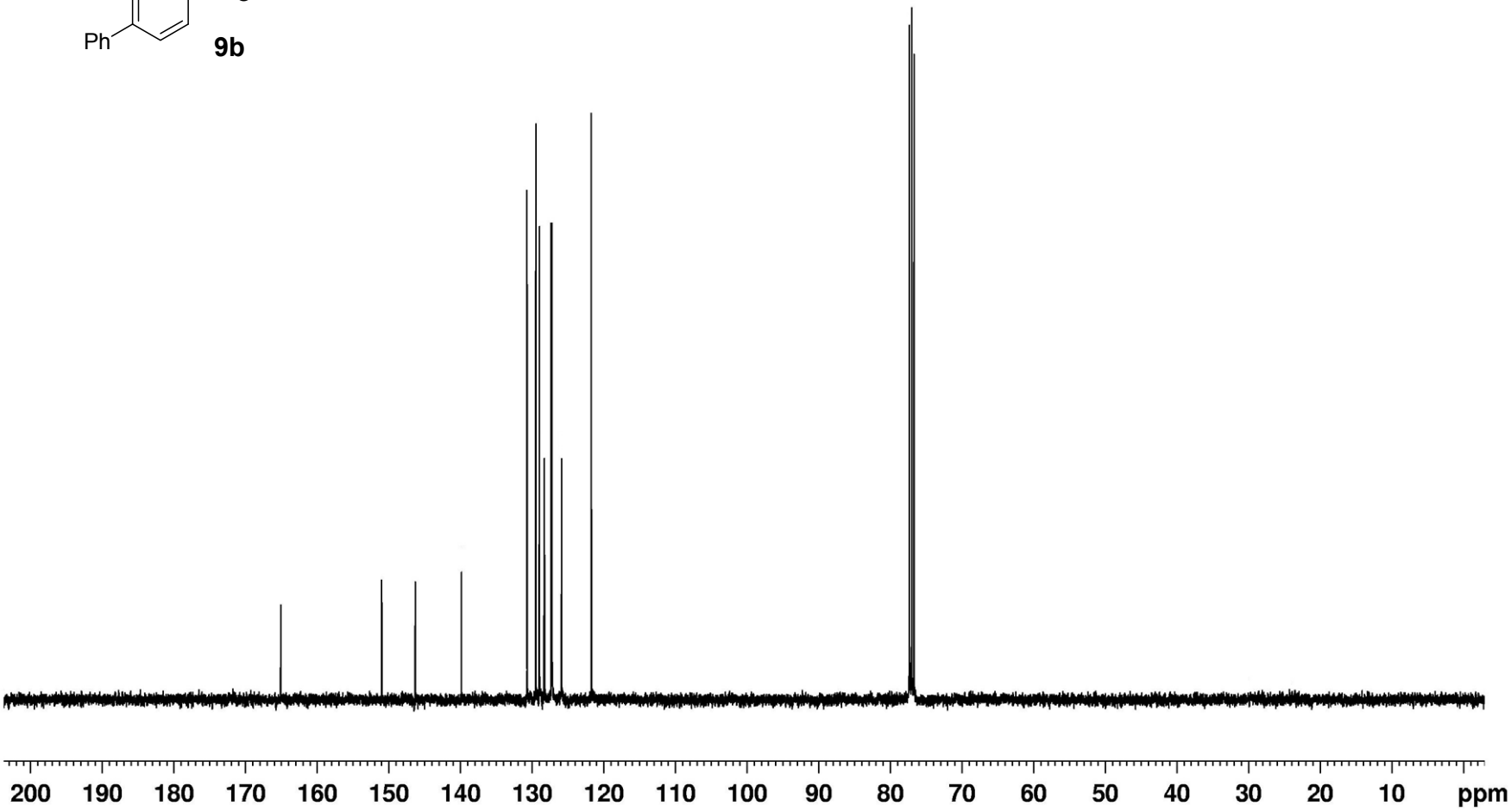
9b



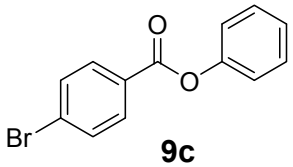
^{13}C NMR Spectrum of **9b**



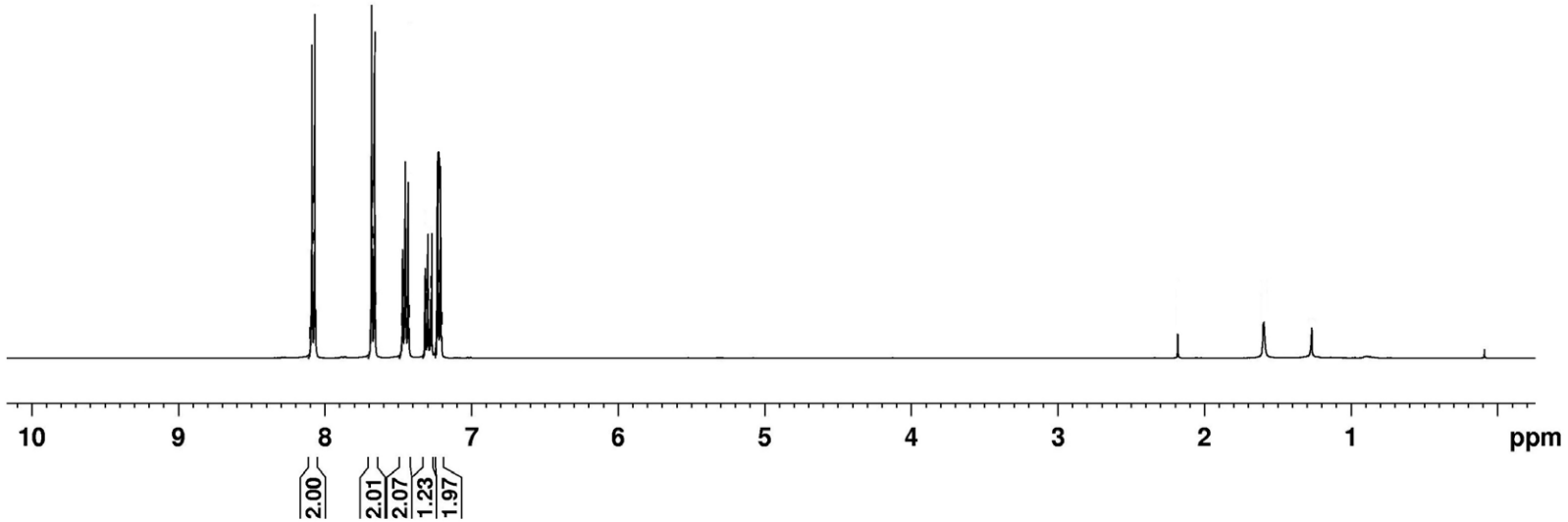
9b



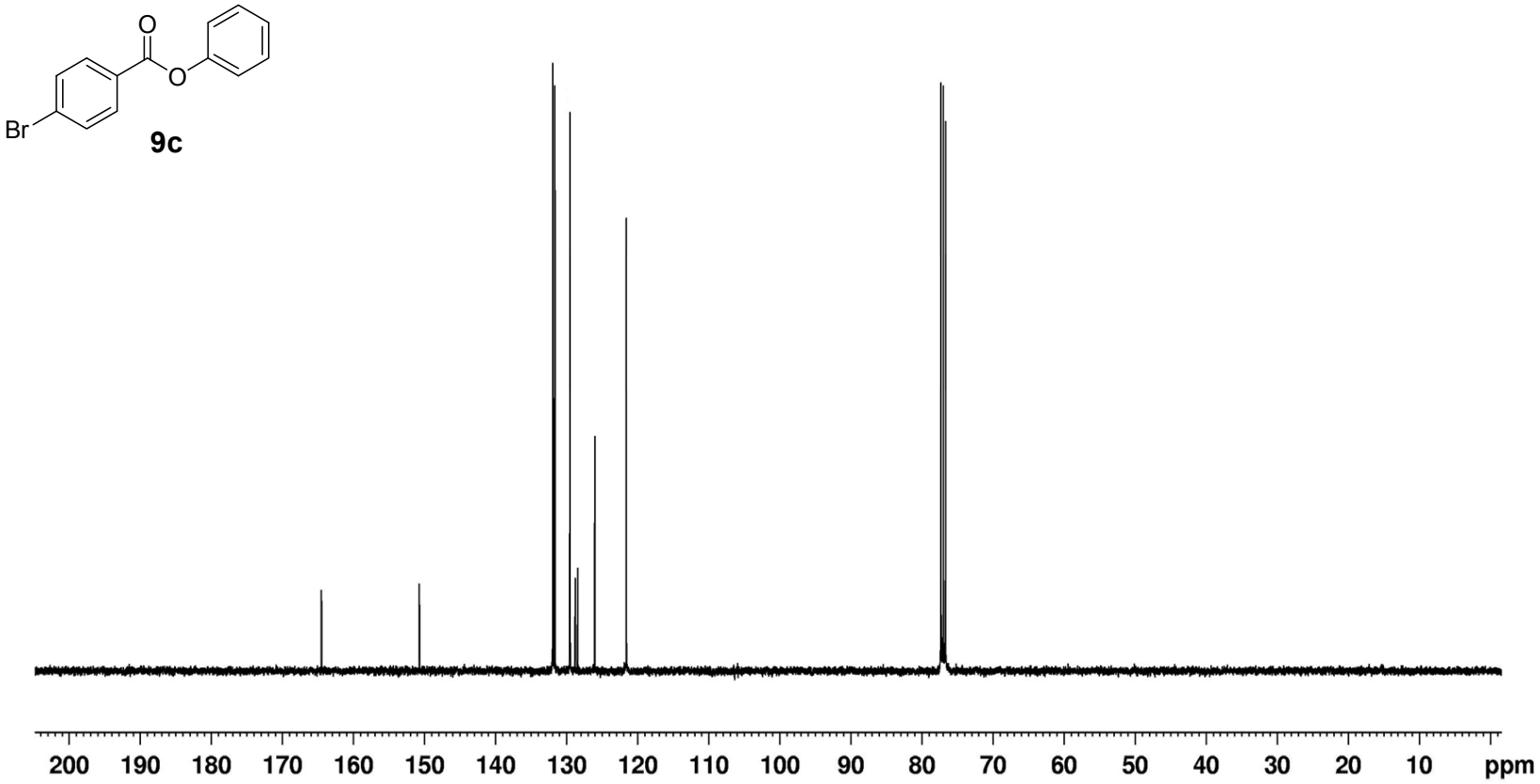
^{1}H NMR Spectrum of **9c**



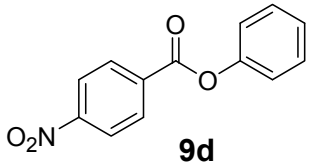
9c



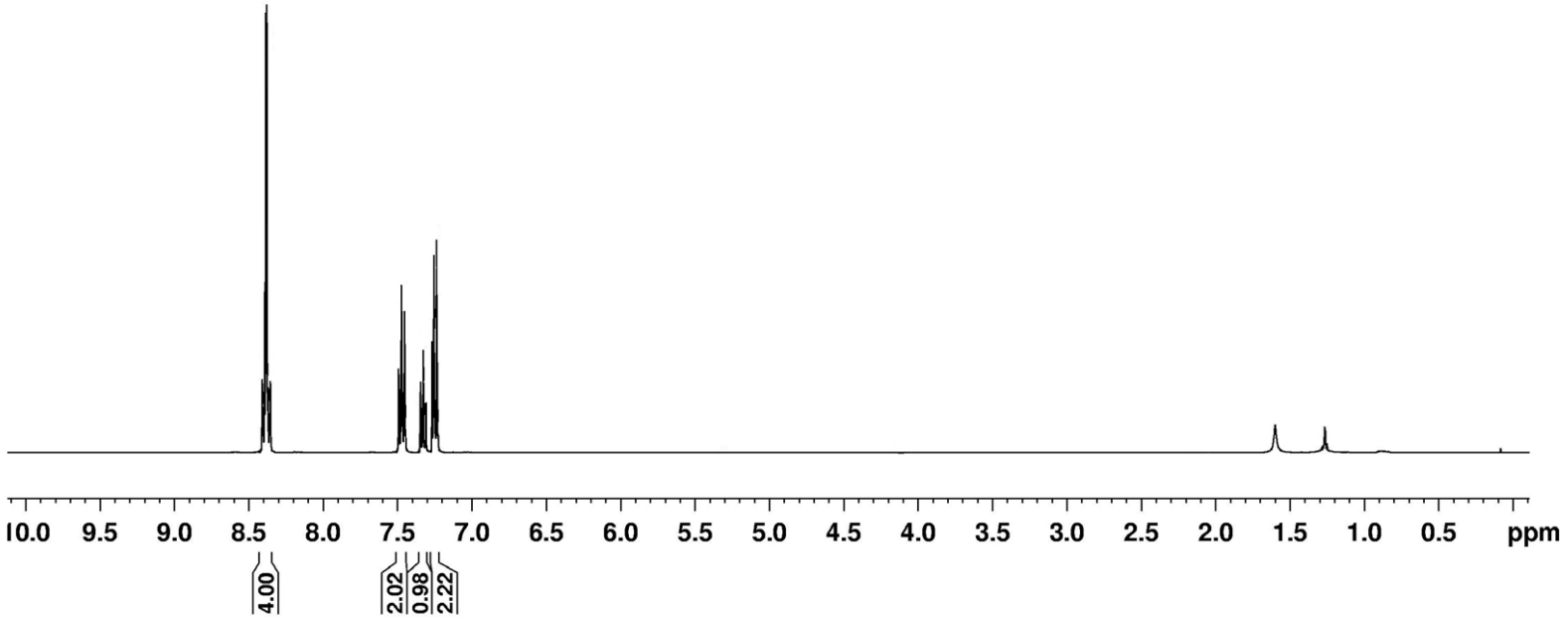
^{13}C NMR Spectrum of **9c**



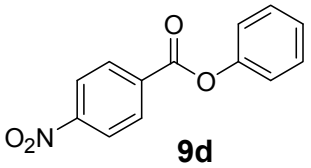
^{1}H NMR Spectrum of **9d**



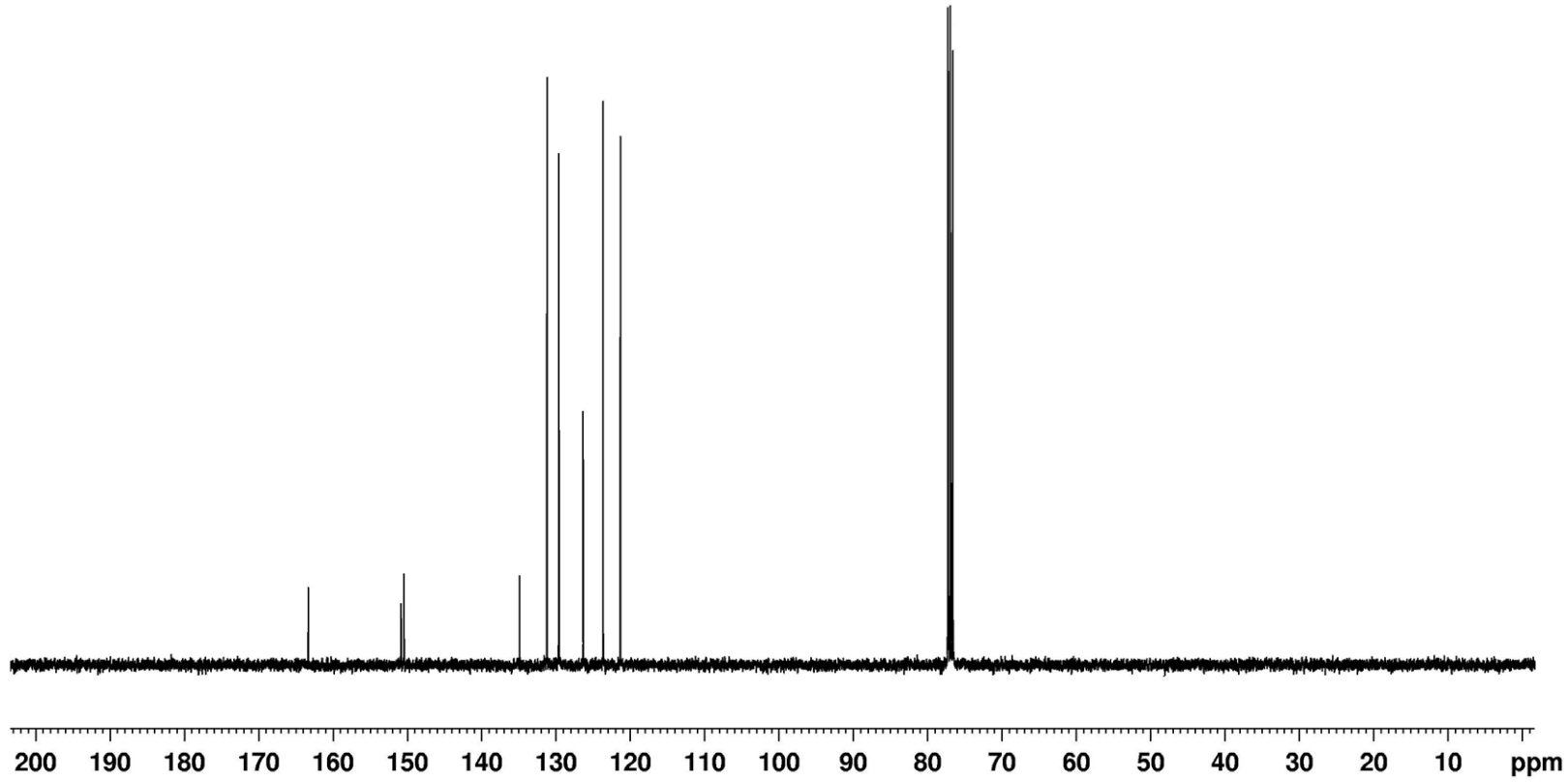
9d



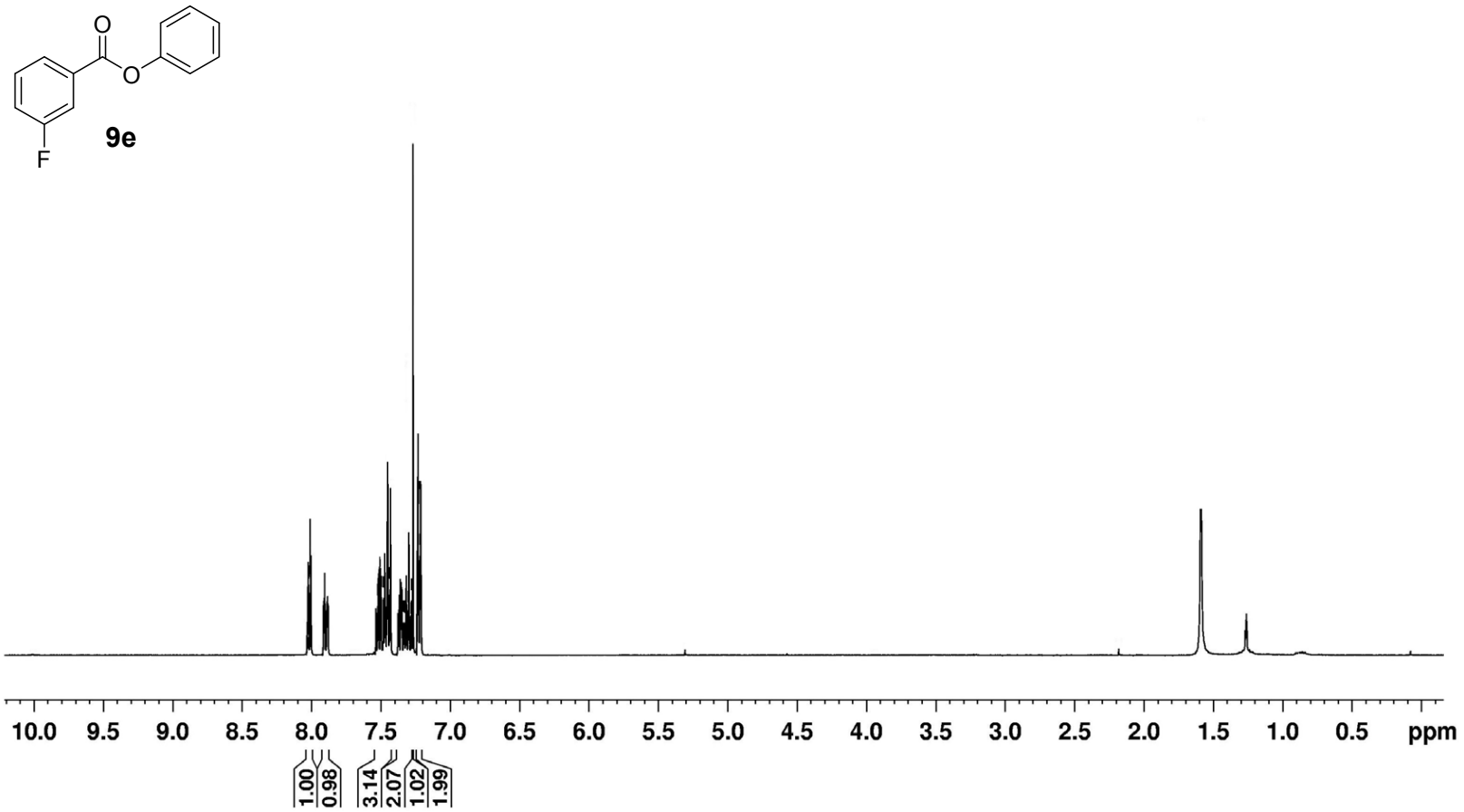
^{13}C NMR Spectrum of **9d**



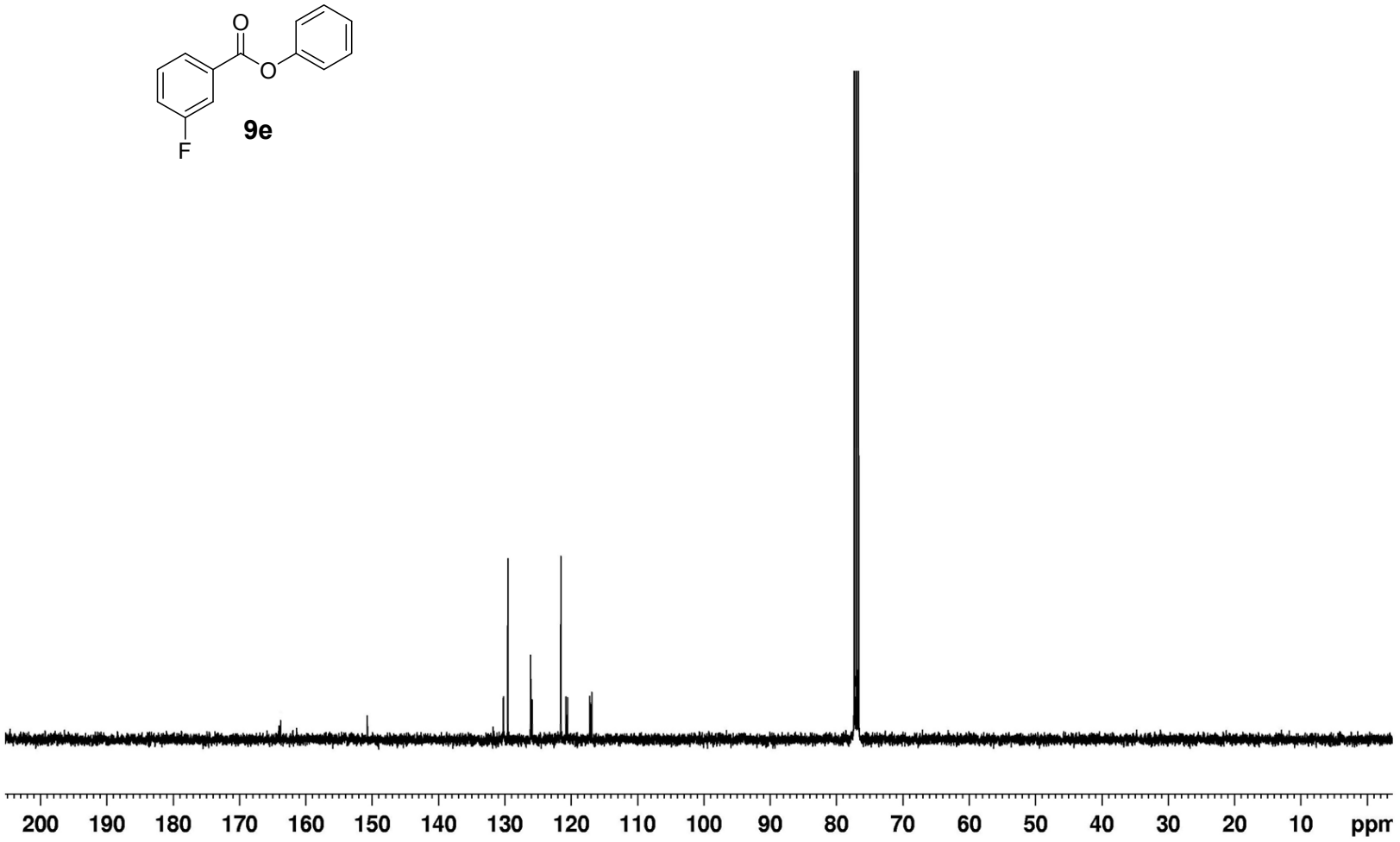
9d



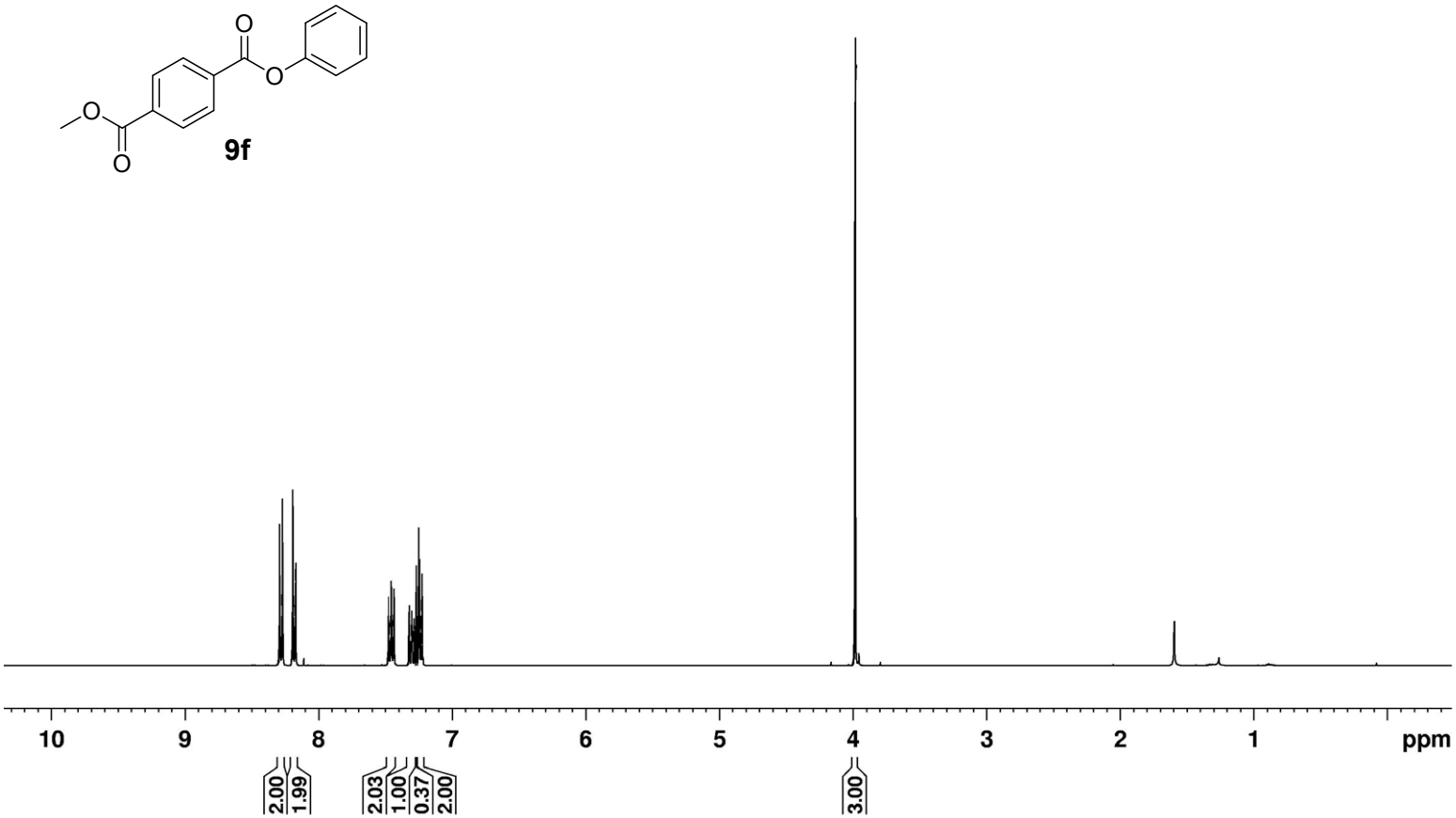
^{1}H NMR Spectrum of **9e**



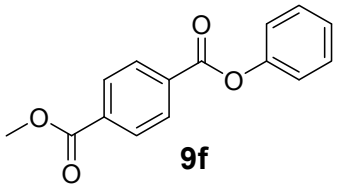
^{13}C NMR Spectrum of **9e**



^{1}H NMR Spectrum of **9f**

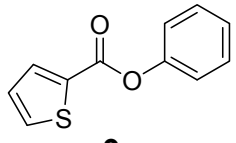


^{13}C NMR Spectrum of **9f**

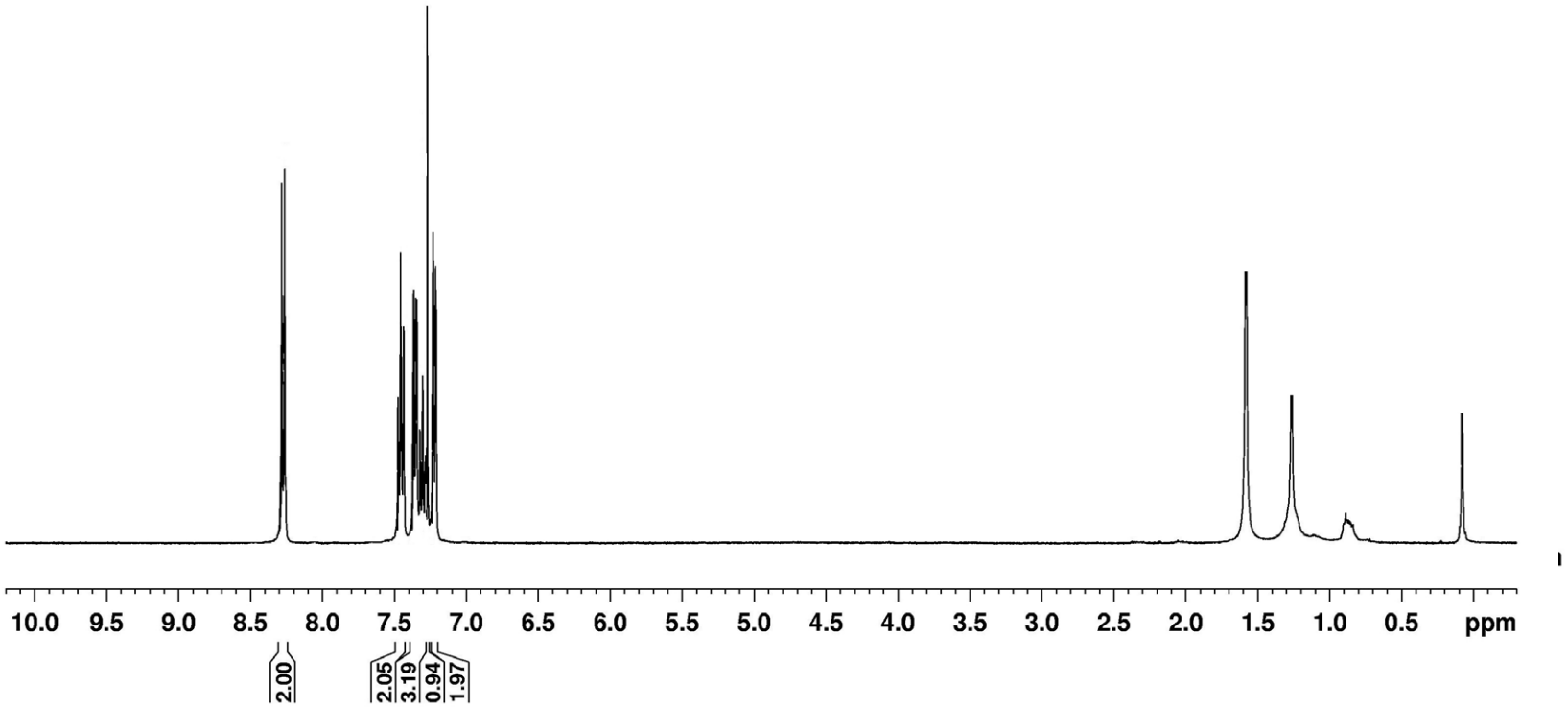


9f

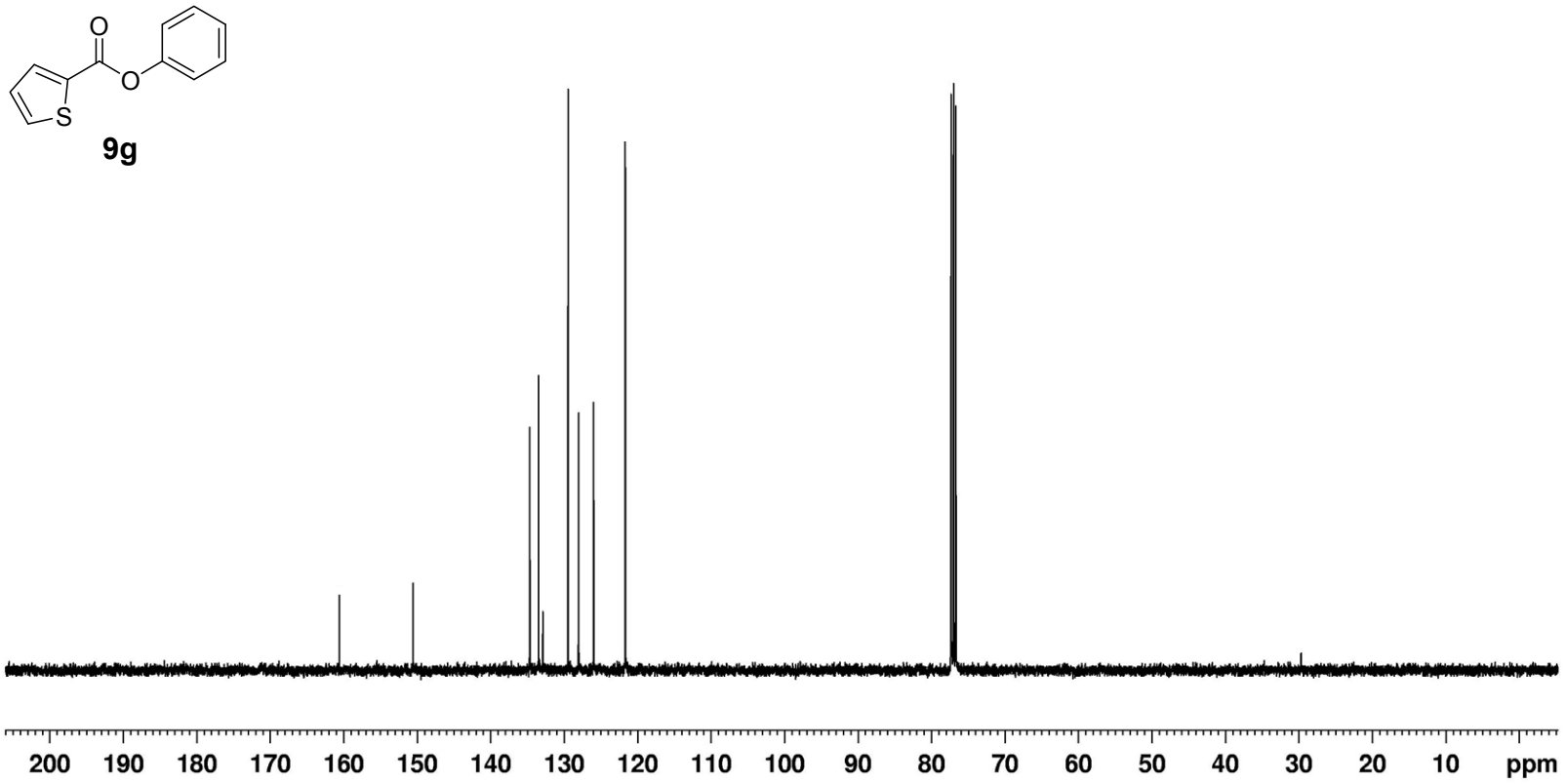
^{1}H NMR Spectrum of **9g**



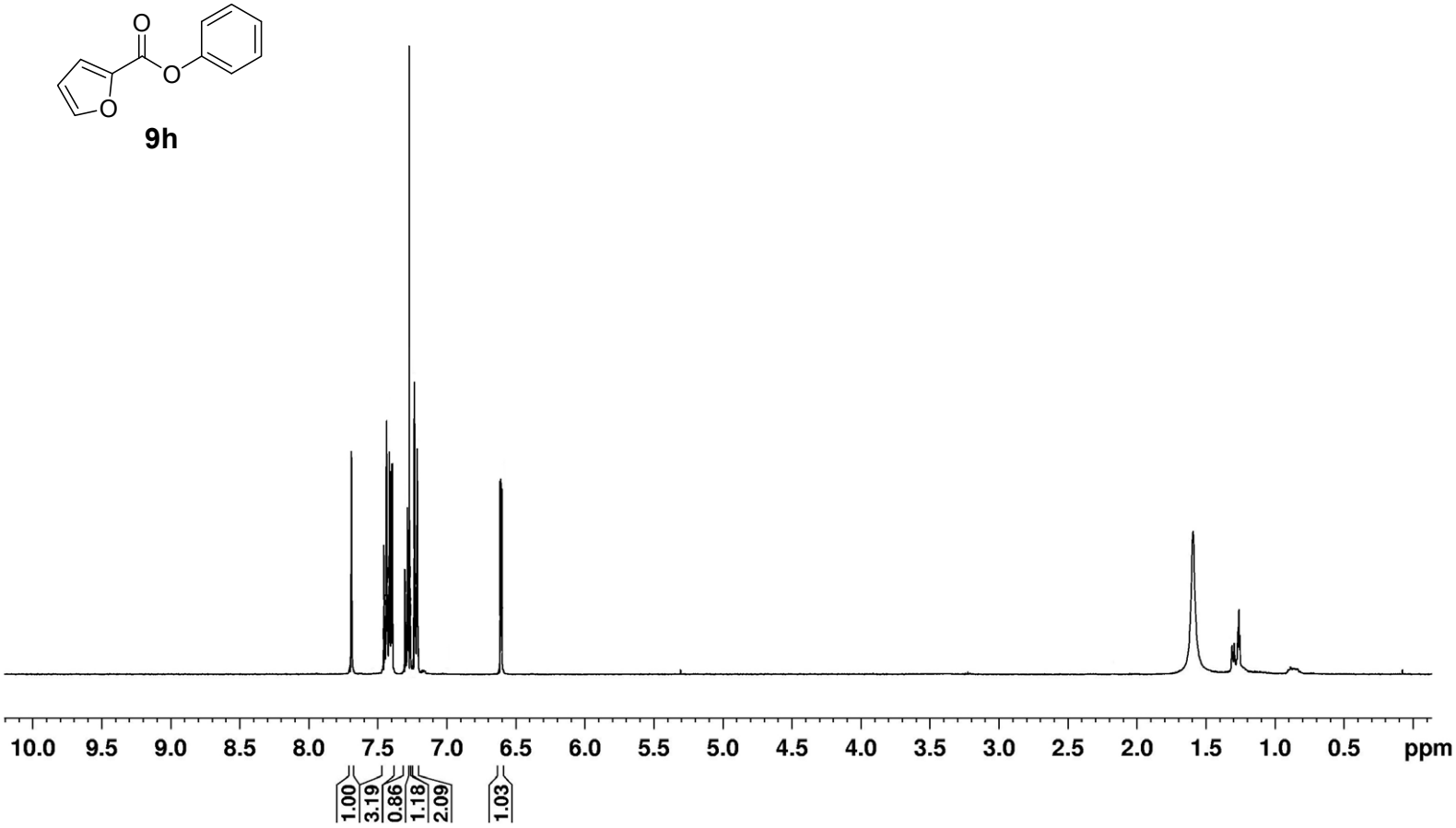
9g



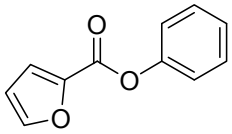
^{13}C NMR Spectrum of **9g**



^{1}H NMR Spectrum of **9h**

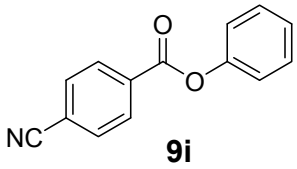


^{13}C NMR Spectrum of **9h**

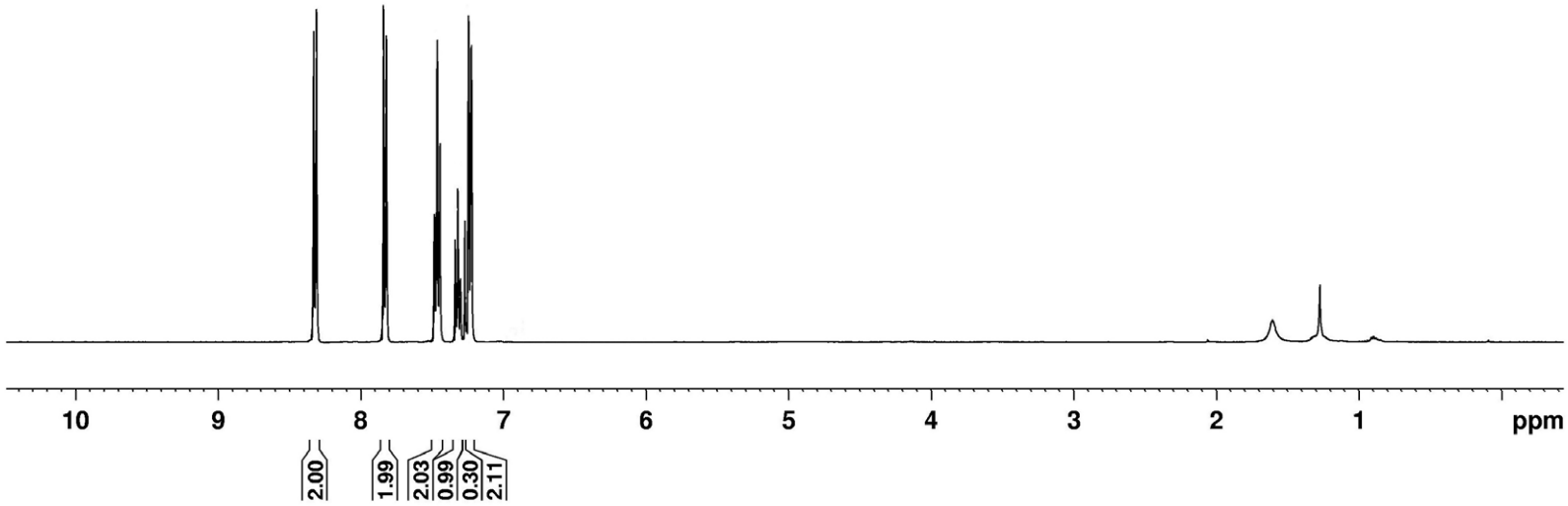


9h

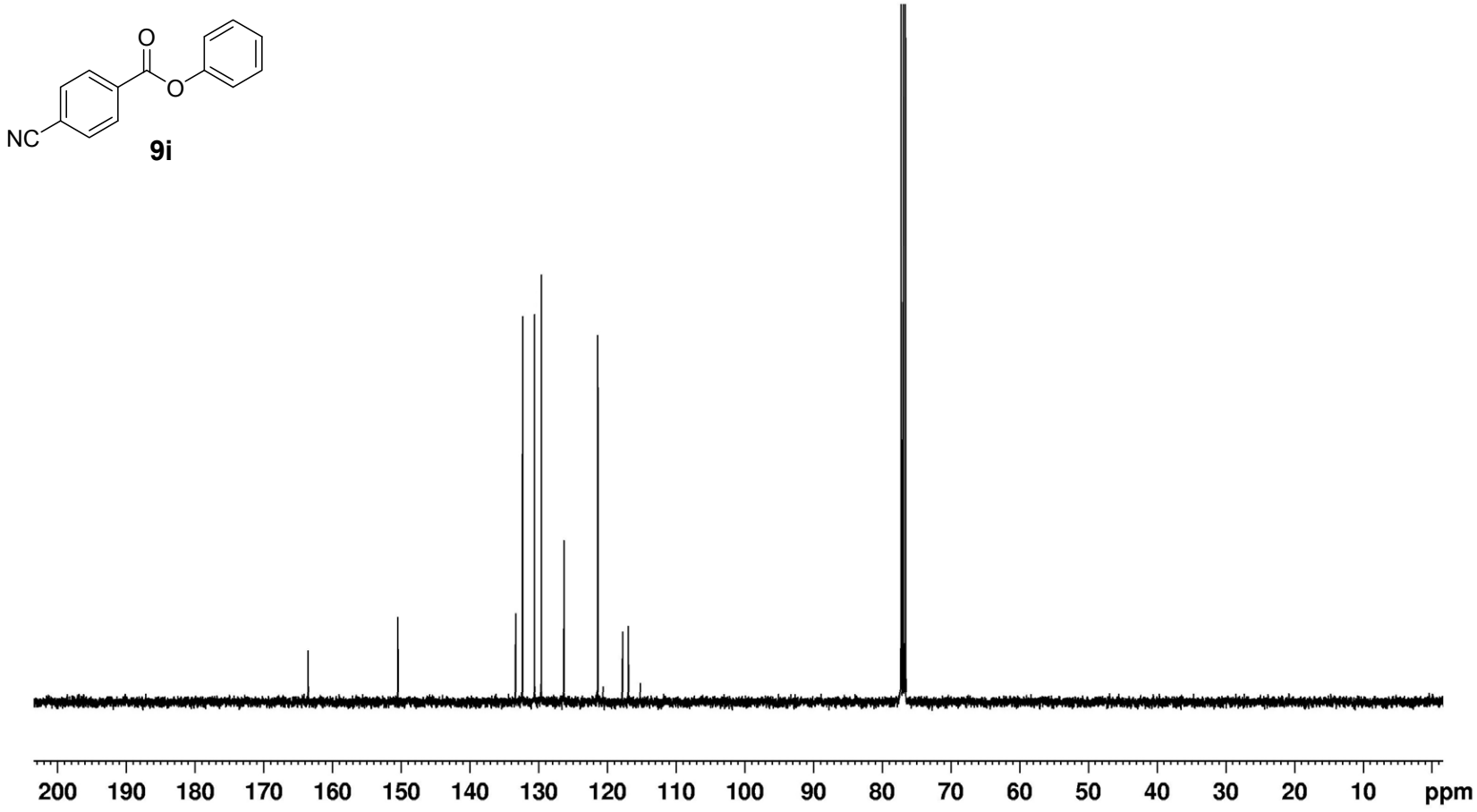
^{1}H NMR Spectrum of **9i**



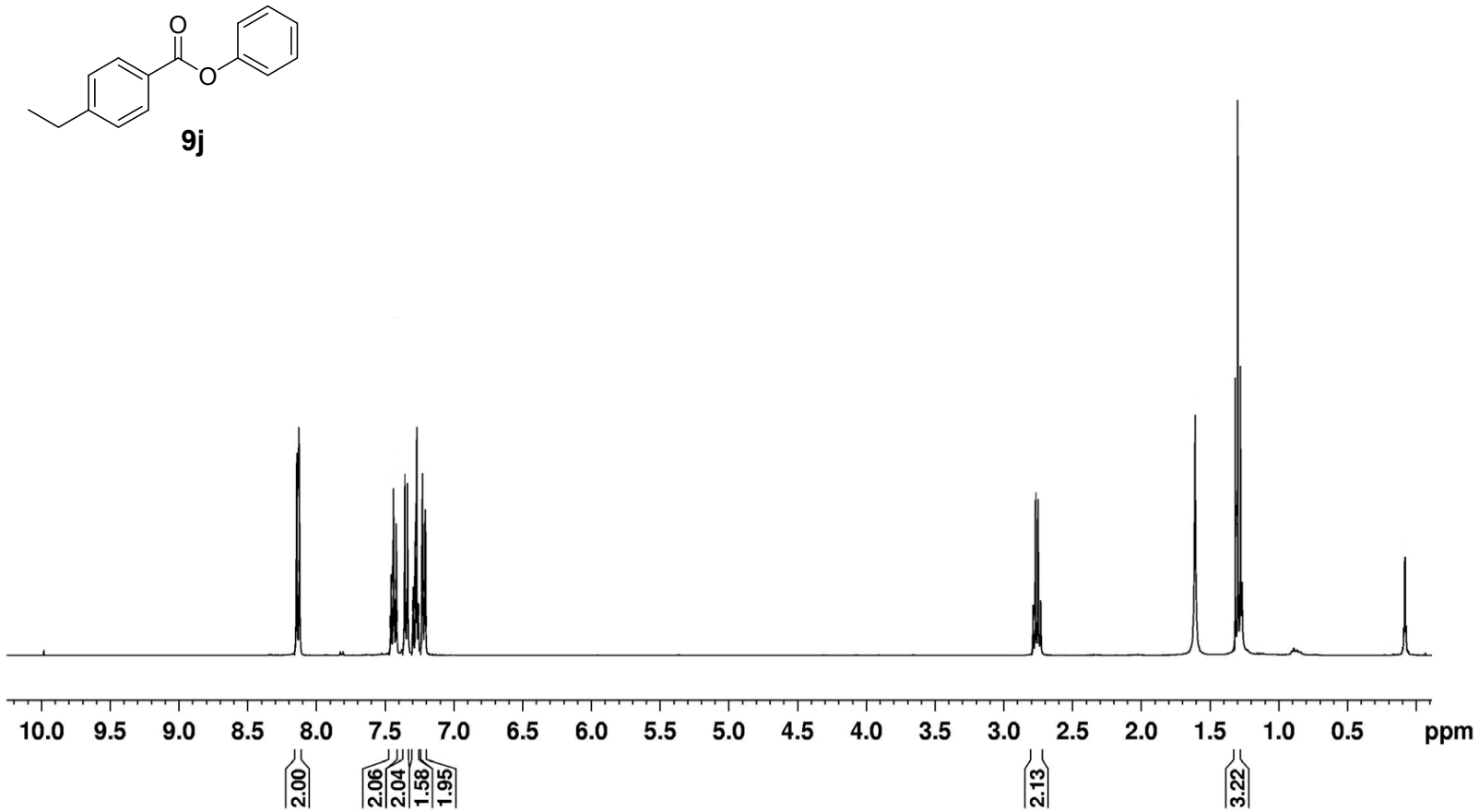
9i



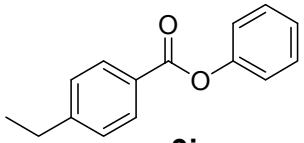
^{13}C NMR Spectrum of **9i**



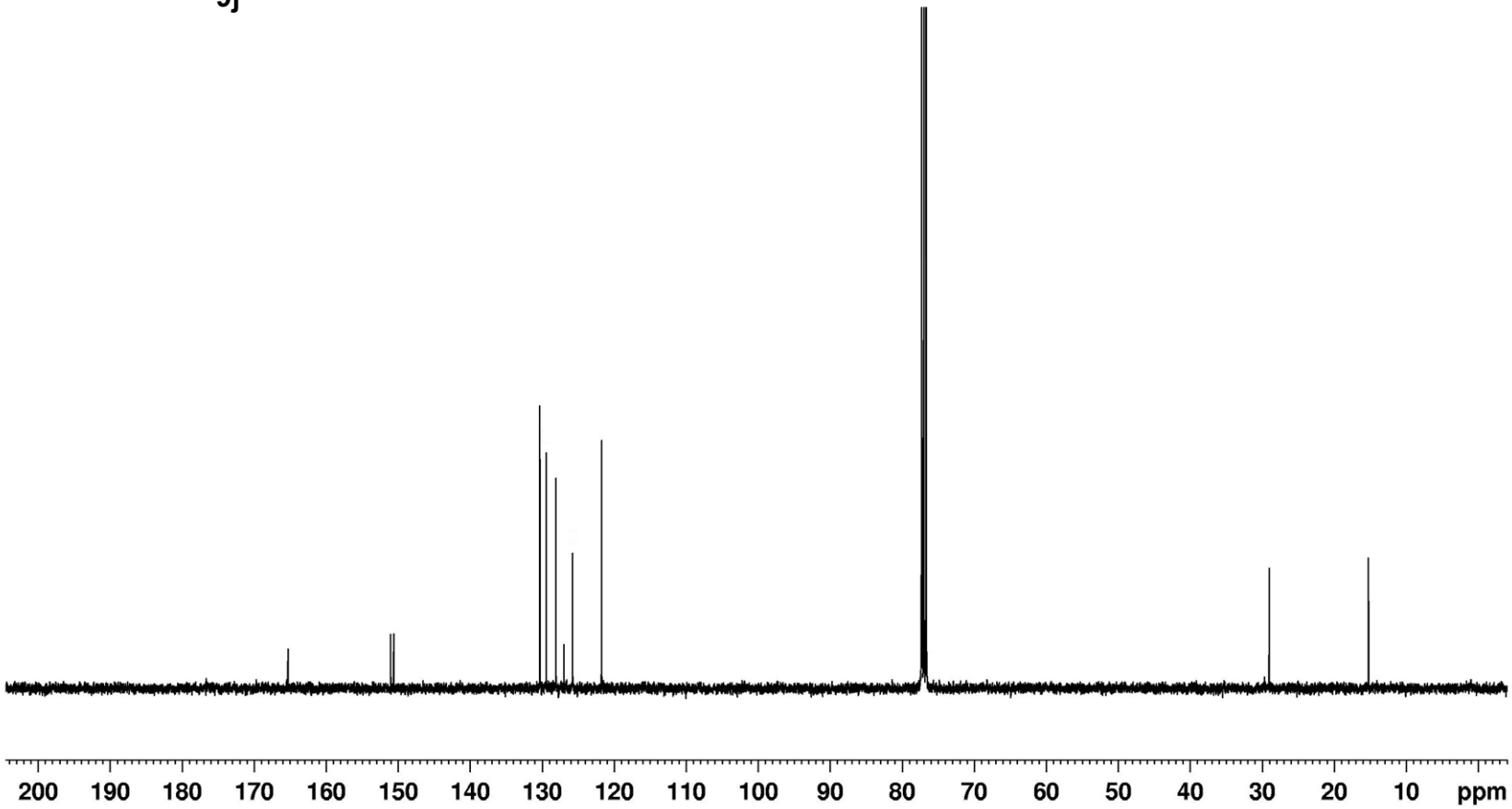
^{1}H NMR Spectrum of **9j**



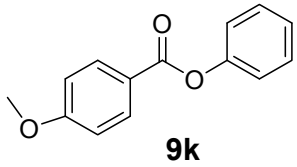
^{13}C NMR Spectrum of **9j**



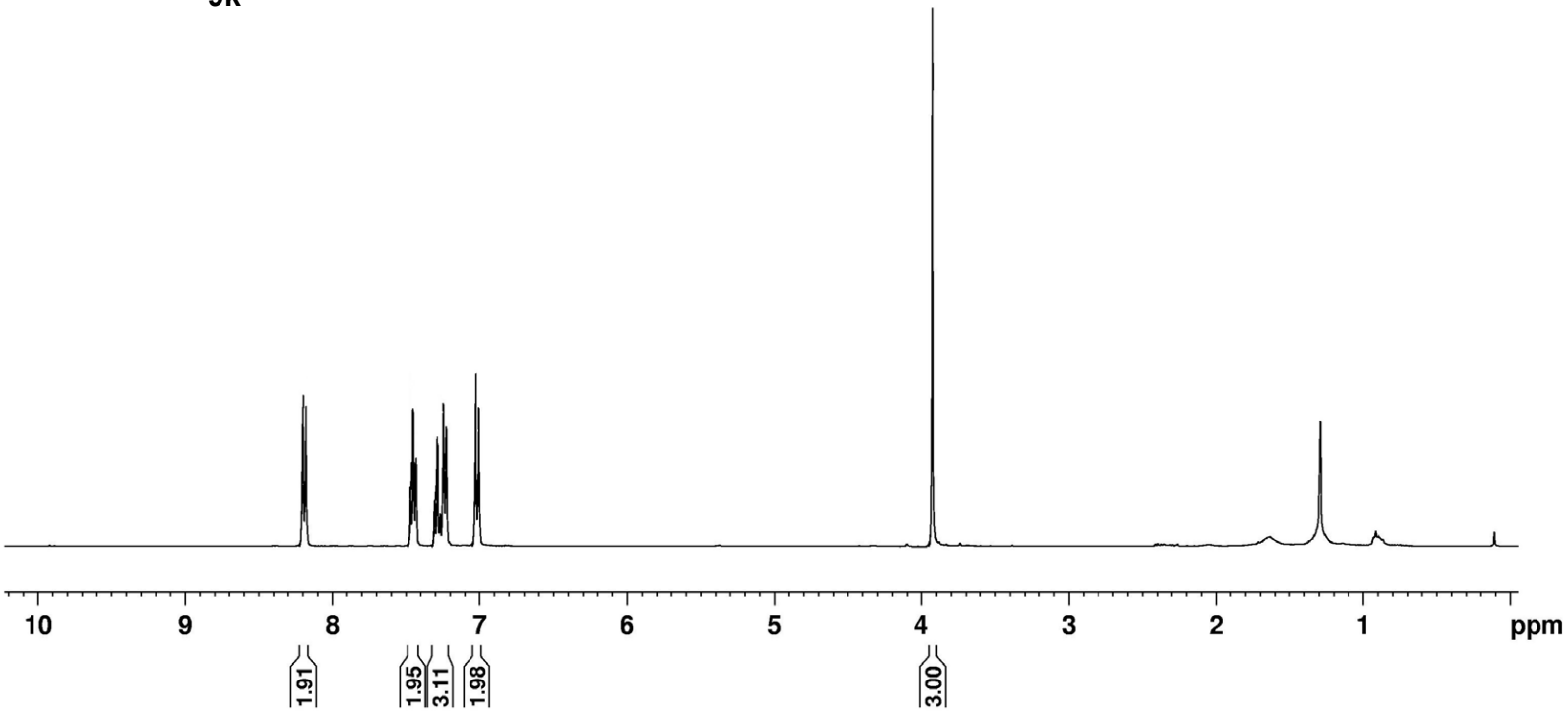
9j



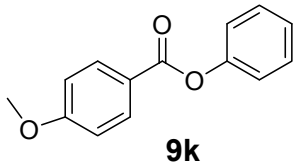
^{1}H NMR Spectrum of **9k**



9k

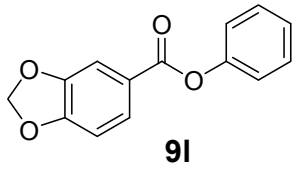


^{13}C NMR Spectrum of **9k**

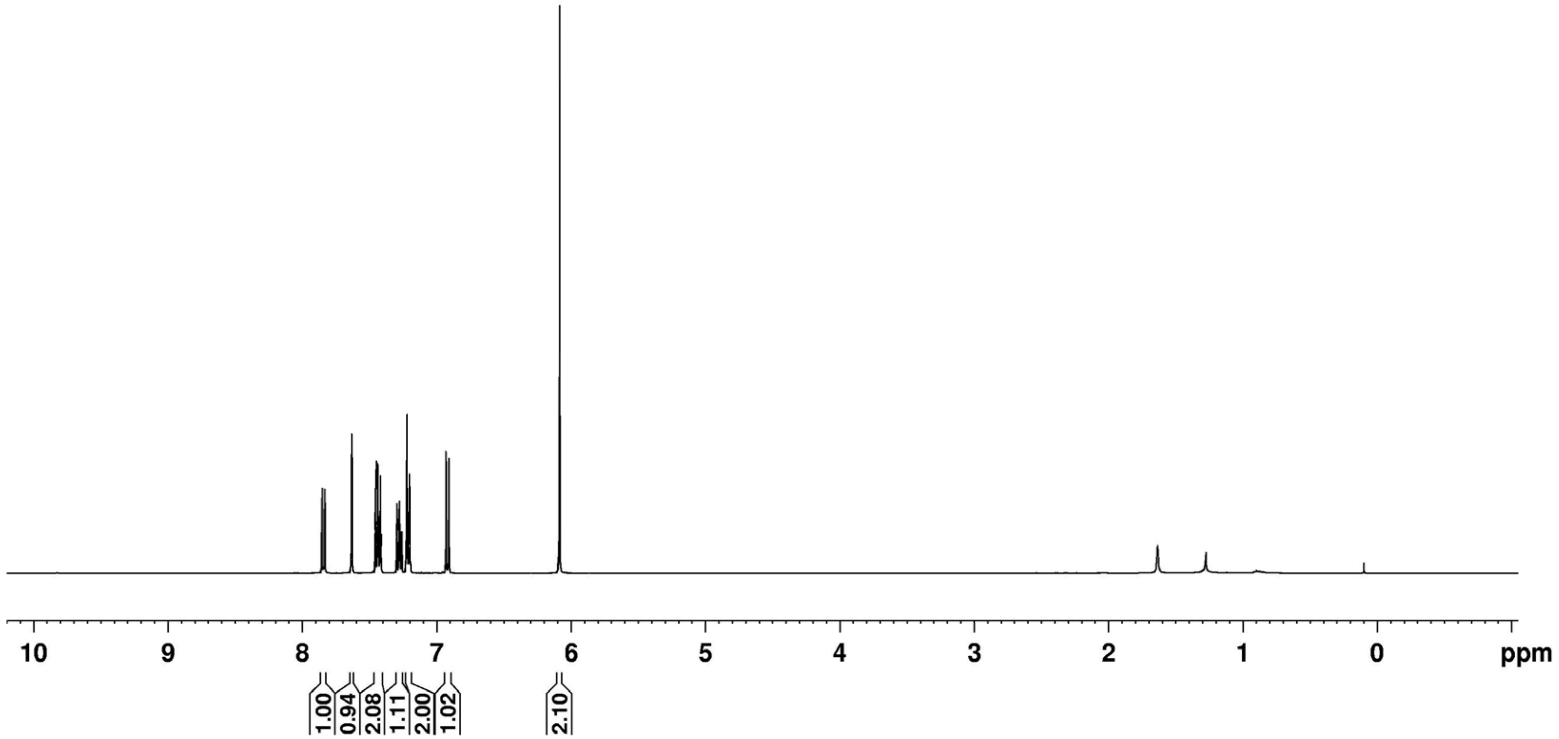


9k

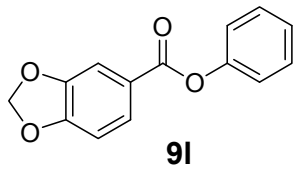
^{1}H NMR Spectrum of **9l**



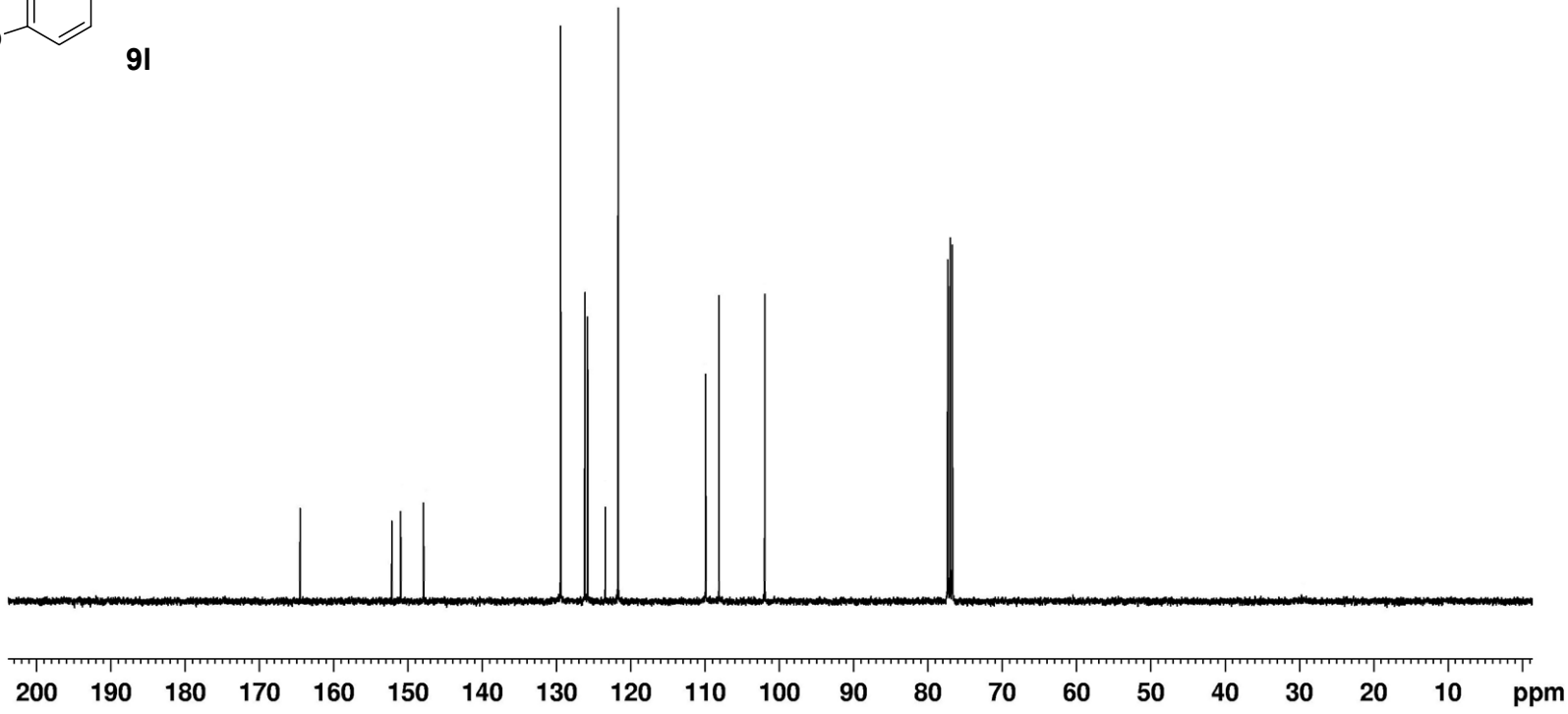
9l



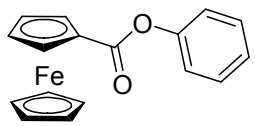
^{13}C NMR Spectrum of **9l**



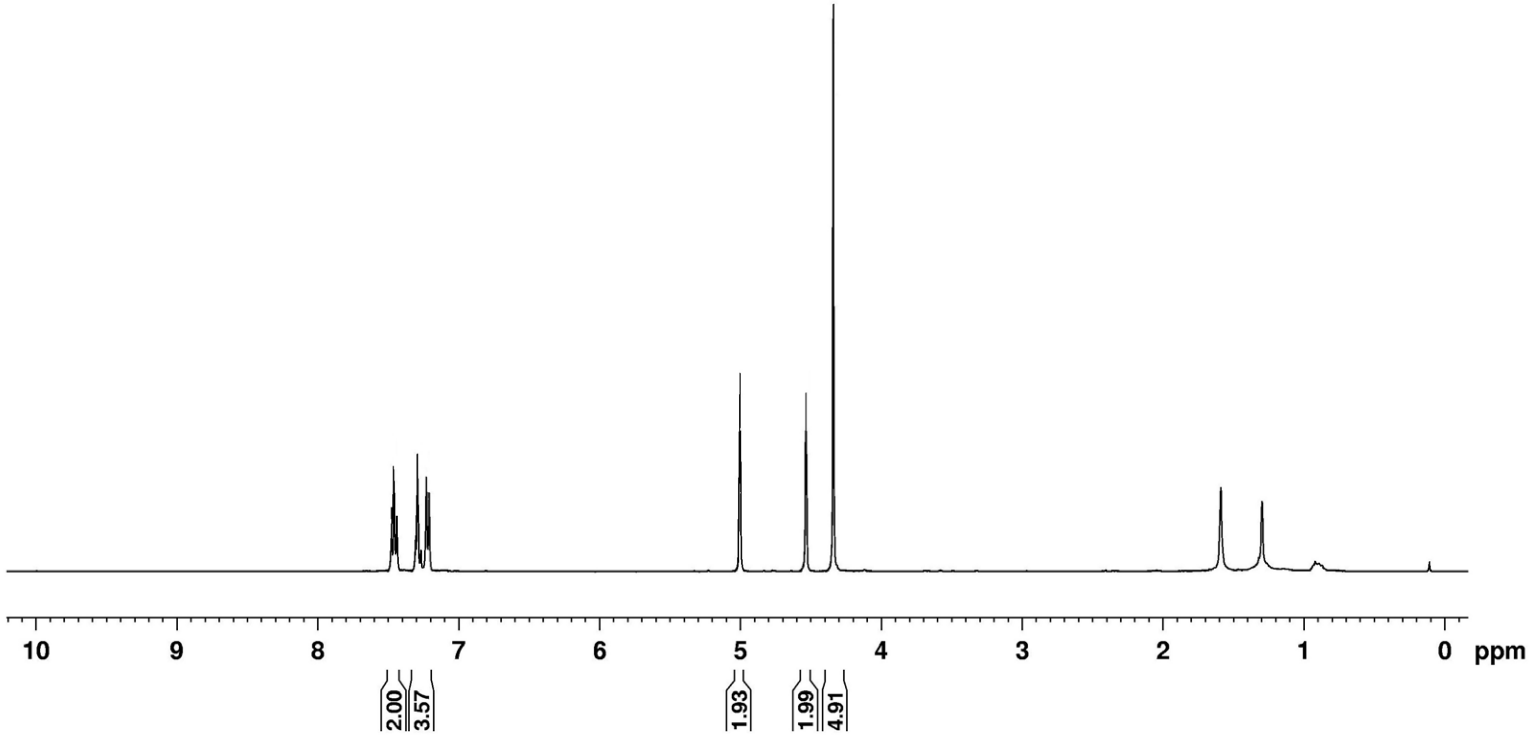
9l



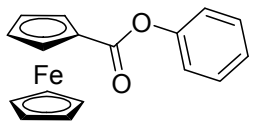
^{1}H NMR Spectrum of **9m**



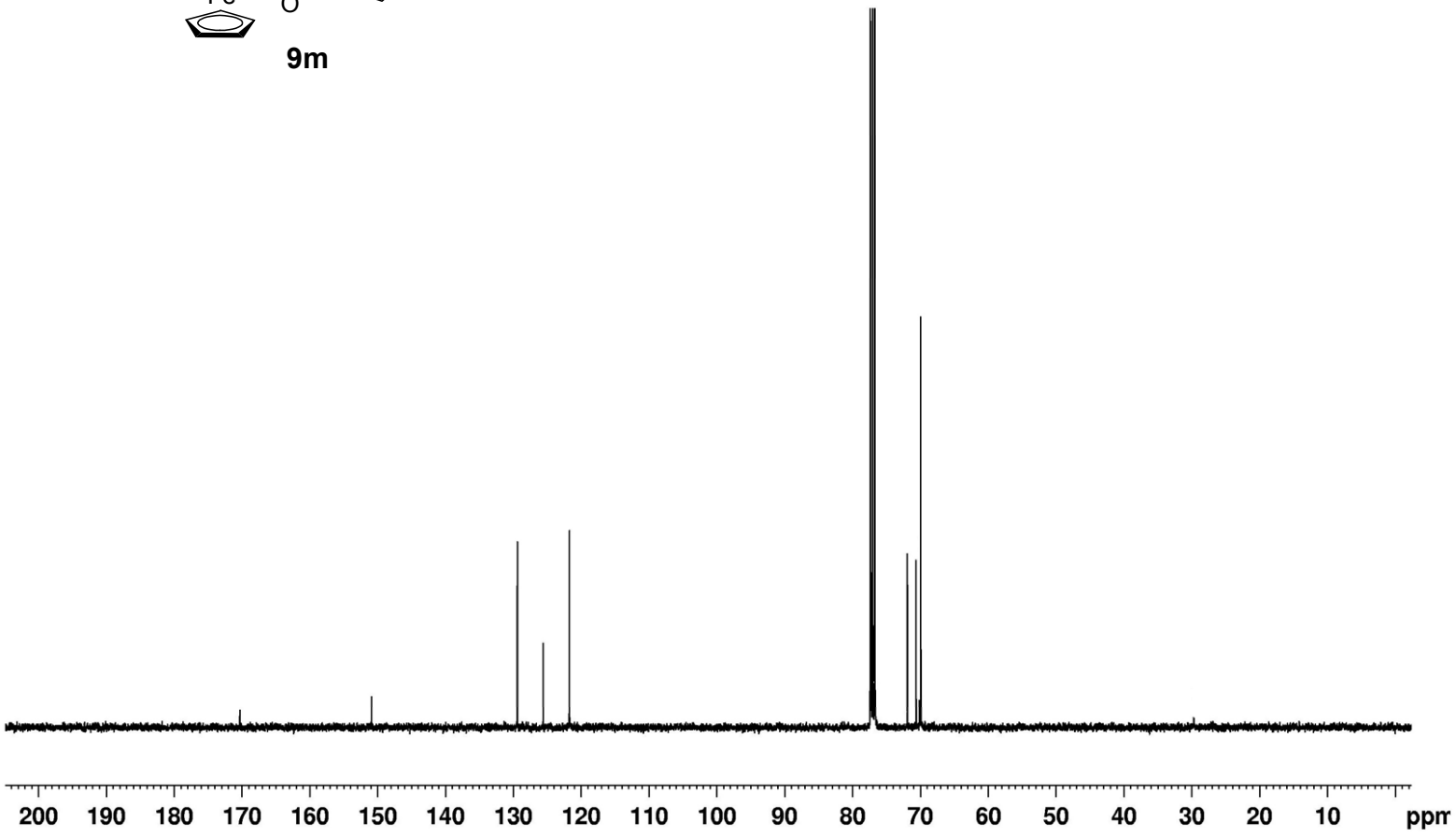
9m



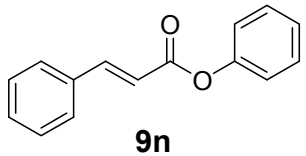
^{13}C NMR Spectrum of **9m**



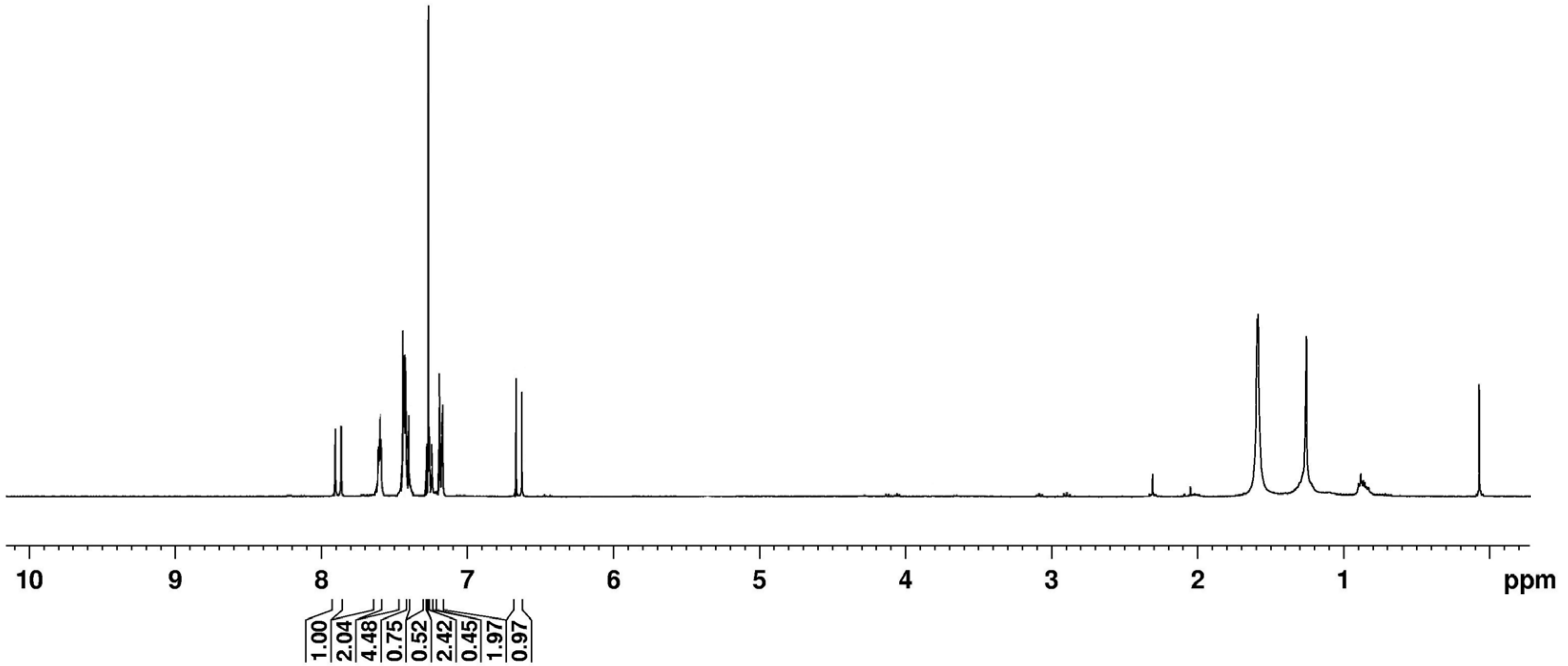
9m



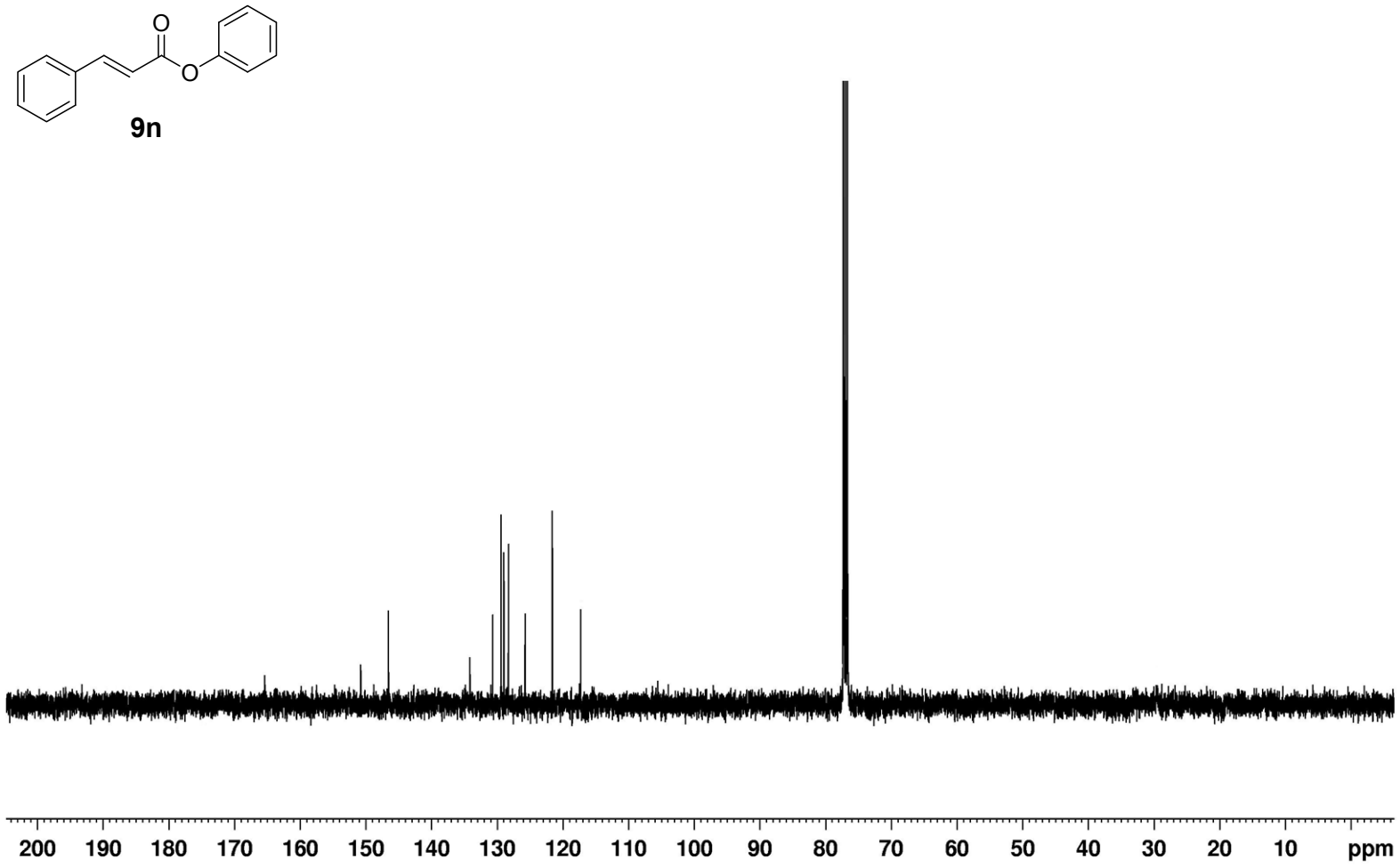
^{1}H NMR Spectrum of **9n**



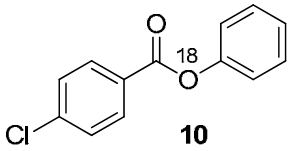
9n



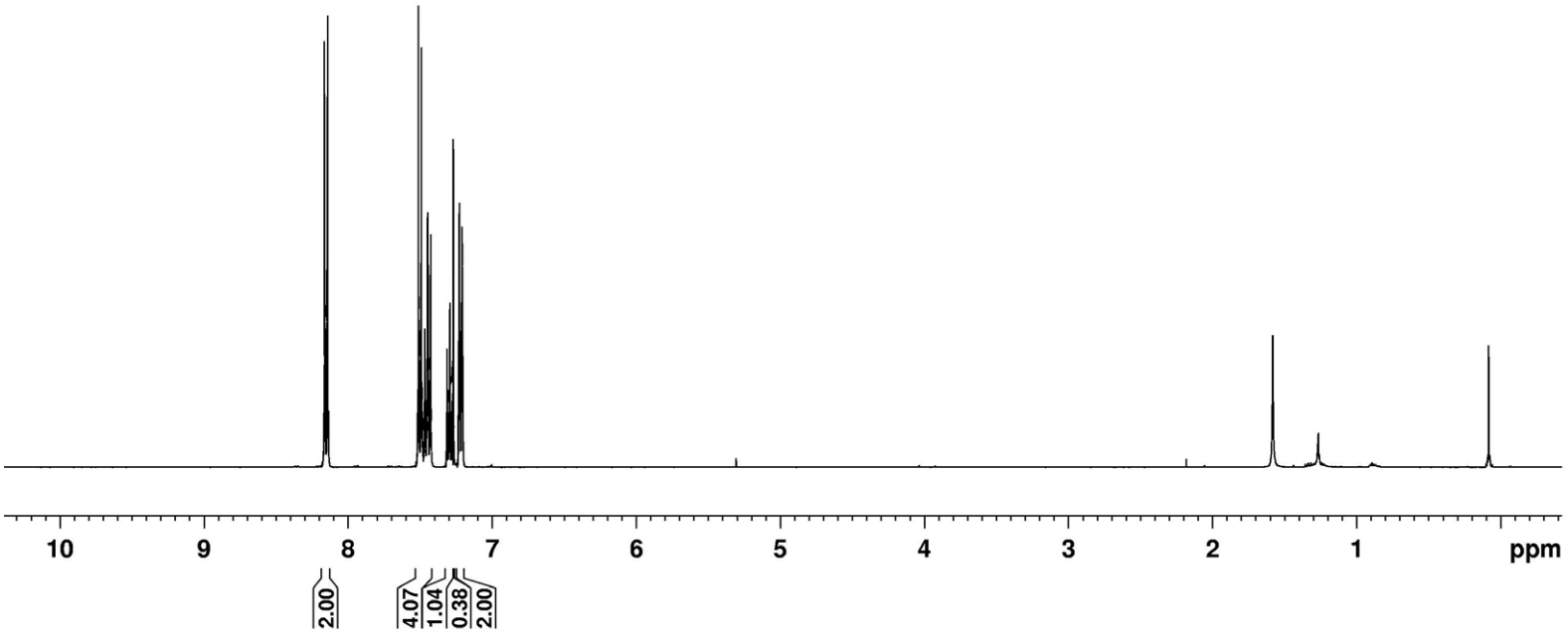
^{13}C NMR Spectrum of **9n**



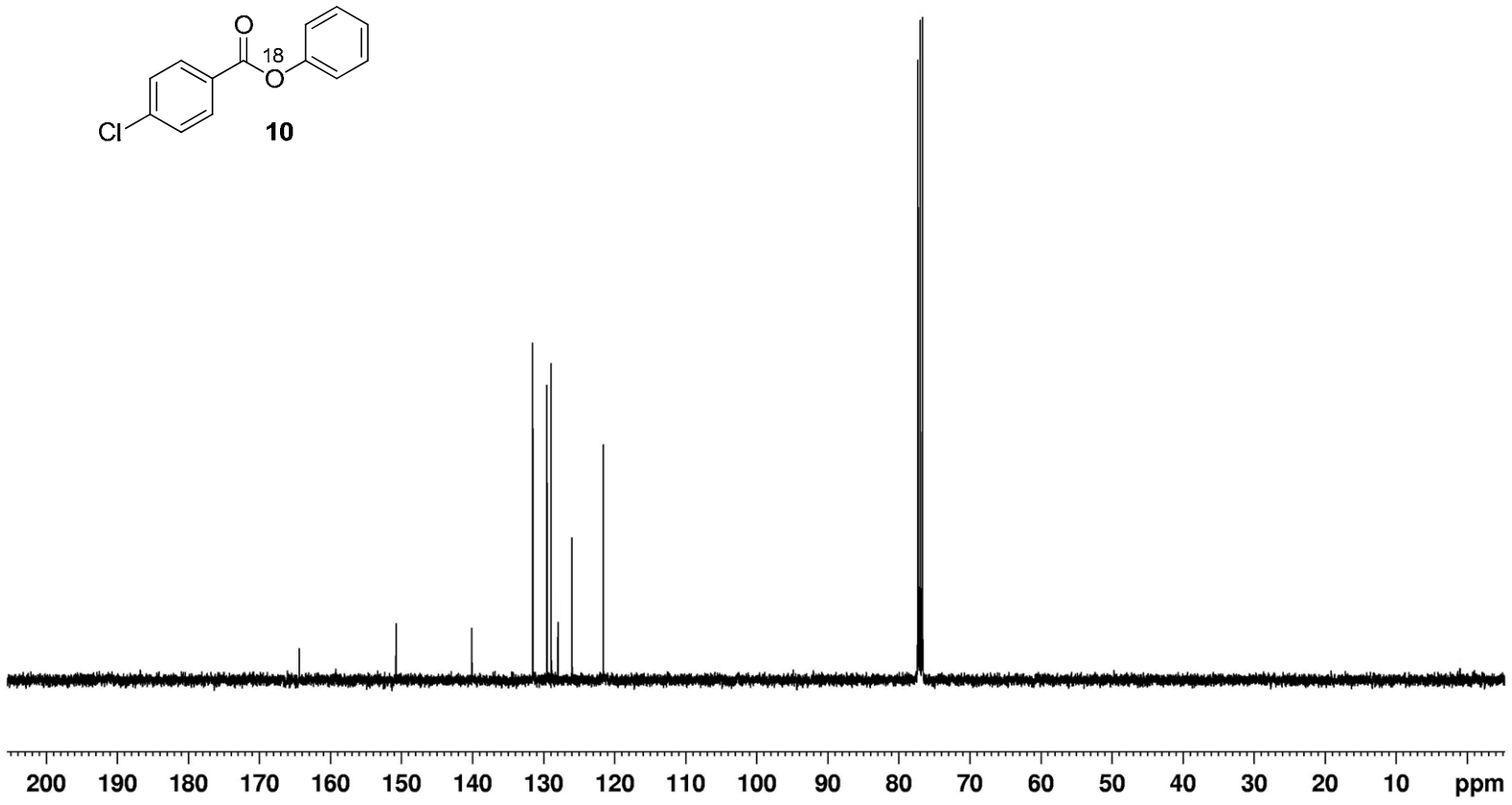
^{1}H NMR Spectrum of **10**



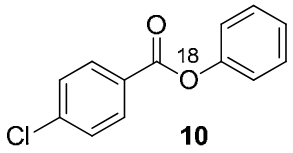
10



^{13}C NMR Spectrum of **10**



HRMS Spectrum of **10**

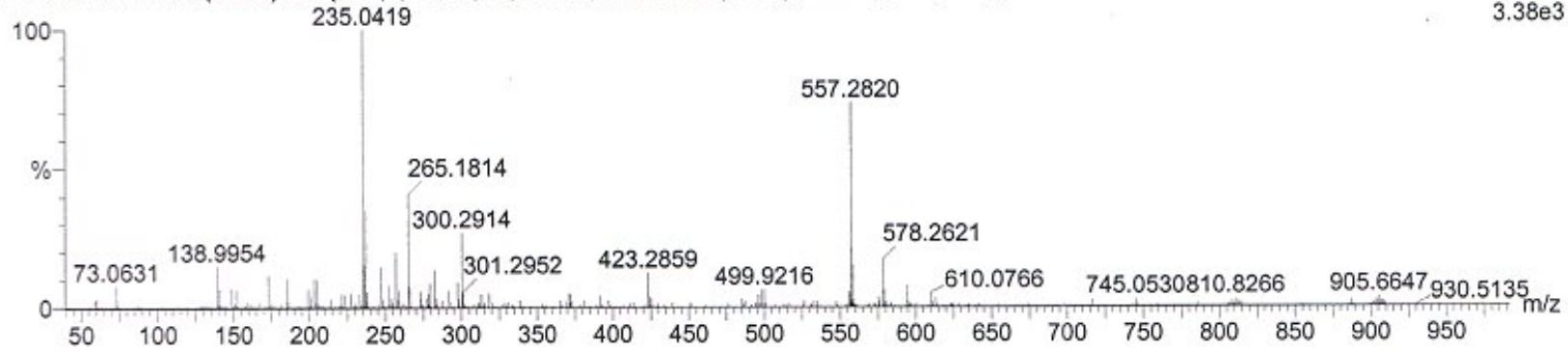


10

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 17-Oct-201111:22:45
C13H9ClO2(O-16; O-18)
SSK-VAS-4-210 3 (0.030) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00); Cm (1:41) TOF MS ES+
3.38e3



Minimum:				-1.5		
Maximum:		200.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
235.0419	235.0412	0.7	3.0	8.5	1	C13 H10 16O 18O Cl

ES-MS Spectrum of **10**