Supporting Information for

Regio- and Diastereoselective Pd-Catalyzed Aminochlorocyclization of Allylic Carbamates: Scope, Derivatization, and Mechanism

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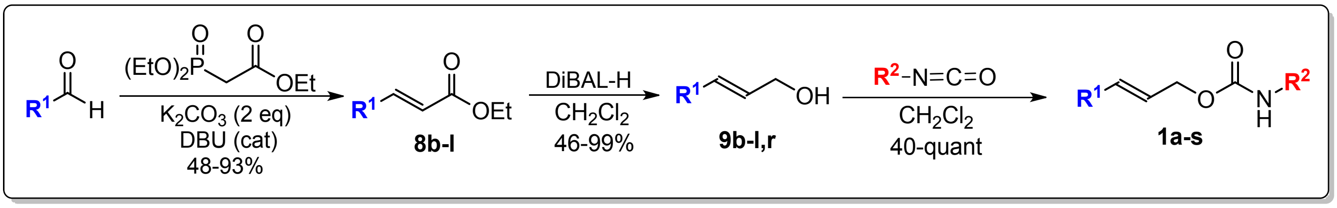
1. General Experimental Details:

Reactions were performed in oven-dried glassware using syringe-septum cap techniques under an inert atmosphere of Ar. Reaction mixtures were magnetically stirred unless otherwise stated. All commercially obtained reagents were used as received. The solvents were obtained from commercial suppliers and used as received or were treated when necessary according to the literature.[1] All substrates whose syntheses were not described were either obtained from commercial suppliers or prepared using the referenced literature procedures. Analytical thin layer chromatography was performed on pre-coated silica gel 60 F-254 plates (particle size 40-55 micron, 230-400 mesh) and visualized by a UV lamp, by staining with iodine, or by ninhydrin, or by sulfuric vanillin followed by a heating using a heat gun. Column chromatography was performed using silica gel (Silicycle - SiliaFlash®) P60, 230-400 mesh and compressed by air pressure with commercial grade solvents. Melting points were recorded with a Büchi M-569 apparatus in open capillary tubes and are uncorrected. NMR spectra were recorded at 300 MHz (^{1}H) and 75 MHz (^{13}C) on a Bruker Avance III 300 MHz spectrometer at 298 K. Chemical shifts are reported in ppm relative to tetramethylsilane (TMS) as internal standard. The following abbreviations are used in reporting NMR data: s, singlet; brs, broad singlet; d, doublet; t, triplet; q, quartet; p, pentet; dd, doublet of doublets; ddd, doublet of doublets of doublets; dt, doublet of triplets; appt, apparent triplet; m, multiplet. Infrared spectra were measured on a Shimadzu FT/IR Prestige-21 spectrometer using KBr pellets in 4000-400 cm^{-1} region. High-resolution mass spectra (HRMS) were measured on a Bruker micrOTOF-QII by ESI spectrometer.

2. Reaction Sequence for the Preparation of Allylic Carbamates 1a-s.

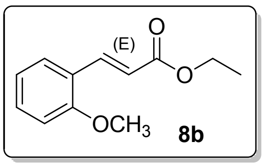
Scheme S1 represents the synthetic route for the preparation of starting materials. For detailed experimental procedures, characterization data and yields, see the below.



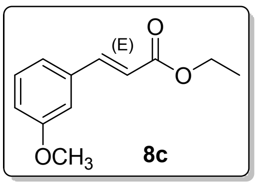
Scheme S1. Synthesis of oxazolidinones (**1a-s**) from corresponding aldehydes.

3. Experimental Procedures:

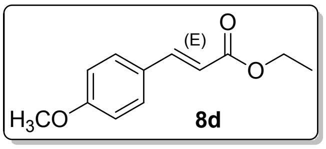
3.1. General Procedure for the Preparation of Substrates Allylic Esters 8b-l. Esters (**8b-l**) were prepared according to the previously reported procedure by Ando and Yamada.[2] A 25 mL round bottom flask equipped with a stir bar was charged with the corresponding aldehyde (30.0 mmol, 1.0 equiv), triethyl phosphonoacetate (7.40 g, 33.0 mmol, 1.1 equiv) and DBU (1,8-diazabicyclo[5.4.0]undec-7-ene) (137 mg, 0.9 mmol, 0.03 equiv), the reaction mixture was stirred vigorously by 10 minutes. Potassium carbonate (8.29 g, 60.0 mmol, 2.0 equiv) was added, and the resulting mixture was stirred for 24 h at room temperature. Then, the reaction was quenched with water (30 mL) and extracted with EtOAc (3x50 mL). The combined extracts were washed with brine, dried (Na_2SO_4), and concentrated to provide the crude allylic ester. Purification was carried out by flash column chromatography (silica gel, hexanes/EtOAc).



(2*E*)-3-(2-Methoxyphenyl) ethyl ester **(8b)** - (CAS: 24393-54-2). Compound **8b** was obtained in 93% (5.75 g) yield according to the general procedure as a colorless oil; *E*:*Z* = 98:2; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.99 (d, *J* = 16.1 Hz, 1H), 7.51 (d, *J* = 7.7 Hz, 1H), 7.35 (t, *J* = 7.7 Hz, 1H), 6.98-6.90 (m, 2H), 6.53 (d, *J* = 16.1 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.89 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 167.53, 158.33, 140.02, 131.41, 128.92, 123.45, 120.69, 118.80, 111.12, 60.34, 55.45, 14.37; IR (neat): 2978, 1703, 1629, 1590, 1157, 1024, 748 cm^{-1}. Consistent with published data.[3]

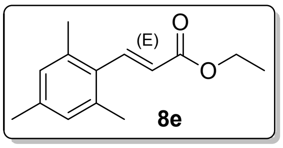


(2*E*)-3-(3-Methoxyphenyl) ethyl ester **(8c)** - (CAS: 24393-55-3). Compound **8c** was obtained in 86% (5.32 g) yield according to the general procedure as a colorless oil; *E*:*Z* = 99:1; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.64 (d, *J* = 16.0 Hz, 1H), 7.28 (t, *J* = 7.9 Hz, 1H), 7.10 (d, *J* = 7.9 Hz, 1H), 7.03 (s, 1H), 6.92 (dd, *J* = 8.2, 2.4 Hz, 1H), 6.42 (d, *J* = 16.0 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.80 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 166.91, 159.92, 144.50, 135.85, 129.87, 120.74, 118.58, 116.10, 112.93, 60.50, 55.25, 14.33; IR (neat): 3059, 2980, 1712, 1639, 1598, 1178, 1041, 785, 680 cm^{-1}. Consistent with published data.[4]



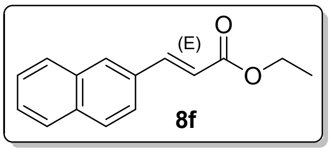
8d

(2*E*)-3-(4-Methoxyphenyl) ethyl ester **(8d)** - (CAS: 24393-56-4). Compound **8d** was obtained in 93% (5.75 g) yield according to the general procedure as a colorless solid; mp: 47-49 °C; *E*:*Z* = 99:1; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.64 (d, *J* = 16.0 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 2H), 6.90 (d, *J* = 7.6 Hz, 2H), 6.31 (d, *J* = 16.0 Hz, 2H), 4.25 (q, *J* = 7.1 Hz, 2H), 3.83 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 167.37, 161.34, 144.26, 129.70, 127.21, 115.76, 114.32, 60.34, 55.37, 14.36; IR (KBr): 2976, 1707, 1629, 1602, 1174, 1005, 831 cm^{-1}. Consistent with published data.[3]



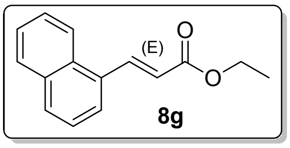
8e

(2*E*)-2-Propanoic acid, 3-(2,4,6-trimethylphenyl) ethyl ester **(8e)** - (CAS: 84001-90-1). Compound **8e** was obtained in 48% (3.14 g) yield according to the general procedure as a white solid; mp: 35-36 °C; *E*:*Z* = 99:1; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.84 (d, *J* = 16.4 Hz, 1H), 6.89 (s, 2H), 6.05 (d, *J* = 16.4 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 2.33 (s, 6H), 2.28 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 167.06, 143.20, 138.28, 136.83, 130.98, 129.14, 123.21, 60.49, 21.10, 21.04, 14.33; IR (KBr): 2980, 2968, 1705, 1622, 1606, 1176, 852 cm^{-1}. Consistent with published data.[5]



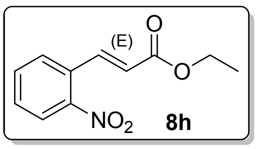
8f

(2*E*)-3-(2-Naphthalenyl)-2-propenoic acid ethyl ester **(8f)** - (CAS: 114833-06-6). Compound **8f** was obtained in 92% (6.24 g) yield according to the general procedure as a white solid; mp: 67-68 °C; *E*:*Z* = 99:1; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.92 (s, 1H), 7.84 (d, *J* = 16.0 Hz, 1H), 7.87-7.79 (m, 3H), 7.66 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.54-7.46 (m, 2H), 6.54 (d, *J* = 16.0 Hz, 1H), 4.29 (q, *J* = 7.1 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 167.03, 144.60, 134.18, 133.27, 131.94, 129.87, 128.65, 128.54, 127.75, 127.18, 126.67, 123.47, 118.41, 60.50, 14.35; IR (KBr): 3055, 2976, 1707, 1633, 1593, 1037, 860, 821 cm^{-1}. Consistent with published data.[5]



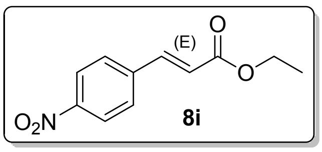
8g

(2*E*)-3-(1-Naphthalenyl)-2-propenoic acid ethyl ester **(8g)** - (CAS: 98978-43-9). Compound **8g** was obtained in 73% (4.95 g) yield according to the general procedure as a colorless oil; *E*:*Z* = 99:1; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.48 (d, *J* = 15.8 Hz, 1H), 8.10 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.75 (d, *J* = 7.9 Hz, 2H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.48-7.38 (m, 2H), 7.33 (dd, *J* = 7.9 Hz, 1H), 6.46 (d, *J* = 15.8 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 1.32 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 166.51, 141.18, 133.34, 131.38, 131.08, 130.15, 128.39, 126.50, 125.86, 125.10, 124.63, 123.01, 120.51, 60.25, 14.09; IR (neat): 3059, 2980, 2968, 1712, 1683, 800, 775 cm^{-1}. Consistent with published data.[3]



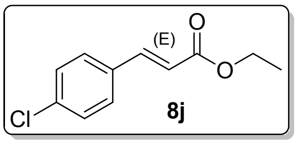
8h

(2*E*)-3-(2-Nitrophenyl) acrylic acid ethyl ester **(8h)** - (CAS: 24393-59-7). Compound **8h** was obtained in 73% (4.84 g) yield according to the general procedure as a yellow solid; mp: 40-42 °C; *E*:*Z* = 92:8; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.09 (d, *J* = 15.7 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.67-7.64 (m, 2H), 7.58-7.53 (m, 1H), 6.37 (d, *J* = 15.7 Hz, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 1.34 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 165.78, 148.32, 139.80, 133.62, 130.50, 130.38, 129.14, 124.88, 123.29, 60.90, 14.27; IR (KBr): 3060, 2998, 1712, 1580, 1519, 1344, 758 cm^{-1}. Consistent with published data.[6]

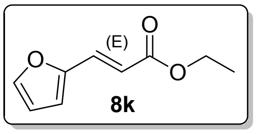


8i

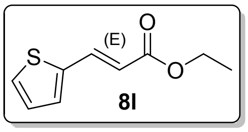
(2*E*)-3-(4-Nitrophenyl) acrylic acid ethyl ester **(8i)** - (CAS: 953-26-4). Compound **8i** was obtained in 82% (5.44 g) yield according to the general procedure as a brown solid; mp: 138-140 °C; *E*:*Z* = 93:7; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.25 (d, *J* = 8.3, 2H), 7.72 (d, *J* = 16.2 Hz, 1H), 7.67 (d, *J* = 8.3 Hz, 2H), 6.56 (d, *J* = 16.2 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 166.02, 148.54, 141.61, 140.65, 128.65, 124.18, 122.66, 61.01, 14.28; IR (KBr): 2997, 1712, 1610, 1593, 1514, 1340, 832 cm^{-1}. Consistent with published data.[3]



(E)-Ethyl 4-chlorocinnamate **(8j)** - (CAS: 24393-52-0). Compound **8j** was obtained in 86% (5.43 g) yield according to the general procedure as a colorless oil; E:Z = 99:1; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.61 (d, J = 16.0 Hz, 1H), 7.43 (d, J = 8.5 Hz, 2H), 7.33 (d, J = 8.5 Hz, 2H), 6.33 (d, J = 16.0 Hz, 1H), 4.26 (q, J = 7.1 Hz, 2H), 1.33 (t, J = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 166.69, 143.09, 136.10, 132.96, 129.20, 129.15, 118.87, 60.60, 14.31. IR (neat): 3066, 2981, 1718, 1637, 1490, 821 cm^{-1}. Consistent with published data.[3]

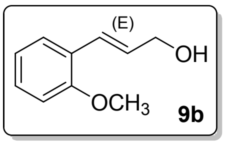


(E)-Ethyl 3-(2-furyl) acrylate **(8k)** - (CAS: 53282-12-5). Compound **8k** was obtained in 92% (4.58 g) yield according to the general procedure as a brown oil; E:Z = 99:1; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.47 (s, 1H) 7.42 (d, J = 15.0 Hz, 1H), 6.66 (d, J = 3.3 Hz, 1H), 6.47-6.45 (m, 1H), 6.31 (d, J = 15.0 Hz, 1H), 4.24 (q, J = 7.1 Hz, 2H), 1.31 (t, J = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 167.08, 150.97, 144.69, 130.98, 115.97, 114.64, 112.25, 60.45, 14.32; IR (neat): 3100, 2981, 1712, 1641, 1590, 748 cm^{-1}. Consistent with published data.[3]

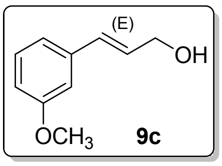


(E)-Ethyl 3-(2-thienyl) acrylate **(8l)** - (CAS: 70326-81-7). Compound **8l** was obtained in 87% (4.76 g) yield according to the general procedure as an orange oil; E:Z = 99:1; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.0 (d, J = 15.6 Hz, 1H), 7.36 (d, J = 5.0 Hz, 1H), 7.24 (d, J = 3.6 Hz, 1H), 7.04 (m, 1H), 6.26 (d, J = 15.6 Hz, 1H), 4.25 (q, J = 7.1 Hz, 2H), 1.31 (t, J = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 166.87, 139.61, 137.04, 130.82, 128.35, 128.06, 117.04, 60.50, 14.33; IR (neat): 3105, 2980, 1712, 1625, 705 cm^{-1}. Consistent with published data.[3]

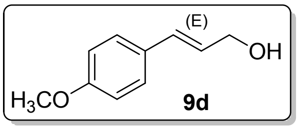
3.2. General Procedure for the Preparation of Substrates of Allylic Alcohols 9b-l,r. Allylic alcohols (**9b-l, r**) were prepared according to the previously reported procedure.[7] A stirred solution of ester (**8b-l**) or aldehyde (**8r** – commercially available) (3.0 mmol, 1.0 equiv.) in anhydrous DCM was cooled in ice-water bath to 0 °C under an argon atmosphere. DIBAL-H (1.0 M in hexane, 5 mL, 5.0 mmol) was added dropwise to the cooled solution, the resultant mixture was stirred for 1 h and the reaction was quenched with saturated aqueous sodium potassium tartrate (15 mL) (Rochelle's salt). The mixture was stirred at ambient temperature for 2 h, and then extracted with Et_2O (3x30 mL). The combined organic layer was washed with brine, dried over Na_2SO_4, and evaporated under reduced pressure. The residue was purified by flash column chromatography (silica gel, 1:1 EtOAc/Hexane) to give the desired allylic alcohol (**9b-l,r**).



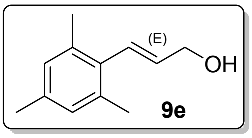
(2E)-3-(2-Methoxyphenyl)-2-propen-1-ol **(9b)** - (CAS: 114568-19-3). Compound **9b** was obtained in 62% (0.30 g) yield according to the general procedure as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.43 (dd, J = 7.6, 1.8 Hz, 1H), 7.22 (dt, J = 7.6, 1.8 Hz, 1H), 6.95-6.85 (m, 3H), 6.37 (dt, J = 16.0, 5.9 Hz, 1H), 4.31 (dd, J = 5.9, 1.8 Hz, 2H), 3.83 (s, 3H), 1.88 (bs, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 156.75, 129.30, 128.76, 127.01, 126.16, 125.74, 120.69, 110.85, 64.19, 55.43; IR (neat): 3358 (brs), 3026, 2935, 1600, 1489, 1244, 752 cm^{-1}. Consistent with published data.[8]



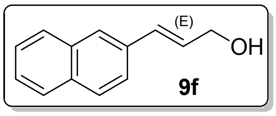
(2E)-3-(3-Methoxyphenyl)-2-propen-1-ol **(9c)** - (CAS: 125617-35-8). Compound **9c** was obtained in 80% (0.39 g) yield according to the general procedure as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.21 (t, J = 7.9 Hz, 1H), 6.97 (d, J = 7.9 Hz, 1H), 6.90 (brs, 1H), 6.79 (dd, J = 7.9, 2.0 Hz, 1H), 6.55 (d, J = 16.0 Hz, 1H), 6.33 (dt, J = 16.0, 5.6 Hz, 1H), 4.27 (d, J = 5.6 Hz, 2H), 3.79 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 159.79, 138.28, 130.74, 129.58, 129.04, 119.16, 113.25, 111.85, 63.37, 55.22; IR (neat): 3352 (brs), 3026, 2937, 1598, 1489, 1257, 1045, 771, 688 cm^{-1}. Consistent with published data.[8]



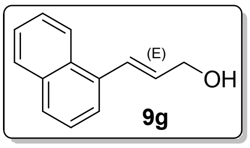
(2*E*)-3-(4-Methoxyphenyl)-2-propen-1-ol **(9d)** - (CAS: 53484-50-7). Compound **9d** was obtained in 53% (0.26 g) yield according to the general procedure as a white solid; mp: 74-76 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.32 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.55 (d, *J* = 15.9 Hz, 1H), 6.24 (dt, *J* = 15.9, 6.0 Hz, 1H), 4.29 (d, *J* = 6.0 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 159.32, 130.94, 129.45, 127.68, 126.29, 114.03, 63.89, 55.30; IR (KBr): 3356 (brs), 2914, 1604, 1512, 1244, 1026, 837 cm^{-1}. Consistent with published data.[8]



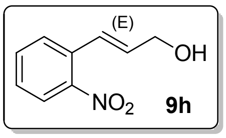
(2*E*)-3-(2,4,6-Trimethylphenyl)-2-propen-1-ol **(9e)** - (CAS: 287929-73-1). Compound **9e** was obtained in 91% (0.48 g) yield according to the general procedure as a white solid; mp: 51-54 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 6.86 (s, 2H), 6.57 (d, *J* = 16.2 Hz, 1H), 5.87 (dt, *J* = 16.2, 5.7 Hz, 1H), 4.33 (d, *J* = 5.7 Hz, 2H), 2.27 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 136.28, 135.87, 133.42, 133.36, 128.84, 128.59, 64.13, 20.92, 20.89; IR (KBr): 3379 (brs), 2935, 1660, 1477, 1375, 974 cm^{-1}. Consistent with published data.[9]



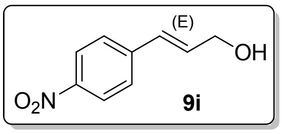
(*E*)-3-(Naphtalen-2-yl)prop-2-en-1-ol **(9f)** - (CAS: 114833-07-7). Compound **9f** was obtained in 97% (0.54 g) yield according to the general procedure as a white solid; mp: 111-112 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.80-7.76 (m, 3H), 7.72 (s, 1H), 7.59 (d, *J* = 8.5 Hz, 1H), 7.50-7.37 (m, 2H), 6.77 (d, *J* = 15.9 Hz, 1H), 6.48 (dt, *J* = 15.9, 5.7 Hz, 1H), 4.37 (dd, *J* = 5.7, 5.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 134.12, 133.56, 133.03, 131.23, 128.86, 128.25, 127.98, 127.67, 126.47, 126.29, 125.93, 123.55, 63.80; IR (KBr): 3270, 3020, 1008, 738 cm^{-1}. Consistent with published data.[10]



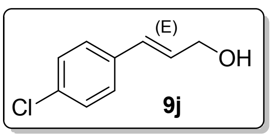
(*E*)-3-(Naphtalen-1-yl)prop-2-en-1-ol **(9g)** - (CAS: 98978-44-0). Compound **9g** was obtained in 99% (0.54 g) yield according to the general procedure as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.14-8.05 (m, 1H), 7.87-7.79 (m, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.56 (d, *J* = 7.1 Hz, 1H), 7.52-7.38 (m, 3H), 7.34 (d, *J* = 15.6 Hz, 1H), 6.36 (dt, *J* = 15.6, 5.6 Hz, 1H), 4.39 (d, *J* = 5.6 Hz, 2H), 1.93 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 134.42, 133.57, 131.76, 131.12, 128.51, 128.07, 127.99, 126.03, 125.77, 125.59, 123.88, 123.72, 63.83; IR (neat): 3352 (brs), 3057, 1585, 1091, 775 cm^{-1}. Consistent with published data.[11]



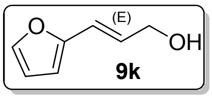
(*E*)-3-(2-Nitrophenyl)-2-propen-1-ol **(9h)** - (CAS: 130489-97-3). Compound **9h** was obtained in 46% (0.25 g) yield according to the general procedure as a brown oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.60-7.52 (m, 2H), 7.40-7.28 (m, 1H), 7.06 (d, *J* = 15.7 Hz, 1H), 6.34 (dt, *J* = 15.7, 5.3 Hz, 1H), 4.36 (d, *J* = 5.3 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 147.78, 134.27, 133.14, 132.55, 128.77, 128.10, 125.65, 124.48, 63.12; IR (neat): 3354, 3070, 2918, 1519, 1346, 736 cm^{-1}. Consistent with published data.[12]



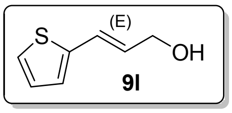
(*E*)-3-(4-Nitrophenyl)-2-propen-1-ol **(9i)** - (CAS: 35271-56-8). Compound **9i** was obtained in 74% (0.40 g) yield according to the general procedure as an orange solid; Compound unstable and was used in the next reaction step immediately after isolated; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.19 (d, *J* = 8.8 Hz, 2H), 7.52 (d, *J* = 8.8 Hz, 2H), 6.75 (d, *J* = 15.9, 1H), 6.54 (dt, *J* = 15.9, 5.0 Hz, 1H), 4.41 (d, *J* = 5.1 Hz, 2H). Consistent with published data.[12]



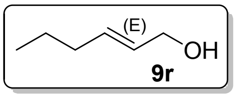
(2*E*)-3-(4-Chlorophenyl)-2-propen-1-ol **(9j)** - (CAS: 24583-70-8). Compound **9j** was obtained in 89% (0.45 g) yield according to the general procedure as a white solid; mp: 45-46 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.40-7.18 (m, 4H), 6.57 (d, *J* = 15.9 Hz, 1H), 6.33 (dt, *J* = 15.9, 5.6 Hz, 1H), 4.32 (d, *J* = 5.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 135.19, 133.30, 129.76, 129.18, 128.76, 127.66, 63.51; IR (KBr): 3323 (brs), 2924, 2870, 1490, 842, 798 cm^{-1}. Consistent with published data.[8]



(*E*)-3-(2-Furanyl)-2-propen-1-ol **(9k)** - (CAS: 79380-02-2). Compound **9k** was obtained in 86% (0.32 g) yield according to the general procedure as a brown oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.35 (brs, 1H), 6.45 (d, *J* = 15.9 Hz, 1H), 6.39-6.35 (m, 1H), 6.35-6.22 (m, 2H), 4.29 (d, *J* = 5.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 152.38, 142.04, 127.19, 119.30, 111.28, 108.01, 63.27; IR (neat): 3342, 2877, 1560, 740 cm^{-1}. Consistent with published data.[13]



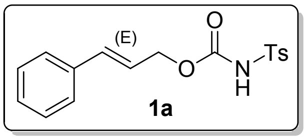
(*E*)-3-(2-Thienyl)-2-propen-1-ol **(9l)** - (CAS: 3216-44-2). Compound **9l** was obtained in 97% (0.41 g) yield according to the general procedure as an orange oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.18-7.13 (m, 1H), 6.96 (d, *J* = 3.3 Hz, 2H), 6.73 (d, *J* = 15.8 Hz, 1H), 6.19 (dt, *J* = 15.8, 5.8 Hz, 1H), 4.26 (d, *J* = 5.8 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 141.77, 128.11, 127.38, 125.83, 124.39, 124.32, 63.31; IR (neat): 3396, 2920, 2883, 1637, 700 cm^{-1}. Consistent with published data.[14]



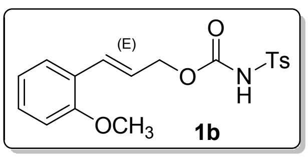
(*E*)-Hex-2-en-1-ol **(9r)** - (CAS: 928-95-0). Compound **9r** was obtained in 71% (0.21 g) yield according to the general procedure as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 5.76-5.57 (m, 2H), 4.08 (d, *J* = 5.1 Hz, 2H), 2.09-1.97 (m, 2H), 1.48-1.34 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 133.28, 129.03, 63.79, 34.30, 22.29, 13.68. Consistent with published data.[15]

3.3. General Procedures for the Preparation of Allylic Carbamates 1a-s.

Carbamates (**1a-l, r,s**) were prepared according to the previously reported procedure.[15] To a stirred solution of allylic alcohol (**9a-l, r,s**) (5.0 mmol, 1.0 equiv.) in anhydrous DCM, *p*-toluenesulfonyl isocyanate (986 mg, 5.0 mmol, 1.0 equiv.) was added dropwise at 0 °C under an argon atmosphere. The reaction mixture was stirred for 2 h at room temperature and was quenched with water (125 mL). The mixture was extracted with DCM (3x50 mL), the combined organic layer was dried over Na_2SO_4, and evaporated under reduced pressure. The residue was purified by flash column chromatography (90:9:1 DCM/MeOH/NH_4OH) to give the desired allylic carbamate (**1a-l**).

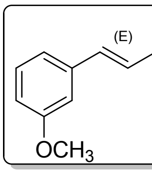


Carbamic acid, [(4-methylphenyl)sulfonyl]-, (2*E*)-3-phenyl-2-propenyl ester **(1a)** - (CAS: 855422-02-5). Compound **1a** was obtained in 95% (1.58 g) yield according to the general procedure as a white solid; mp: 103-105 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.93 (d, *J* = 7.5 Hz, 2H), 7.33-7.32 (m, 7H), 6.58 (d, *J* = 16.0 Hz, 1H), 6.14 (dt, *J* = 16.0, 6.6 Hz, 1H), 4.72 (d, *J* = 6.6 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 150.19, 145.17, 135.75, 135.47, 135.42, 129.64, 128.66, 128.46, 128.40, 126.70, 121.58, 67.38, 21.67; IR (KBr): 3242, 3026, 1755, 1599, 1435, 1163 cm^{-1}. Partially consistent with published data by Cossío, Carreaux and coworkers.[16] Our NMR results do not show evidence for the presence of rotamers.



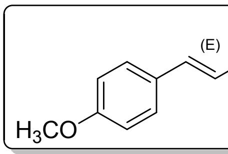
Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(2-methoxyphenyl)-2-propen-1-yl ester **(1b)** - (CAS: 1863094-76-1). Compound **1b** was obtained in 88% (1.59 g) yield according to the general procedure as a white solid; mp: 99-98 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.32-7.14 (m, 4H), 6.90-6.77 (m, 3H), 6.10 (dt, *J* = 16.0, 6.6 Hz, 1H), 4.65 (d, *J* = 6.6 Hz, 2H), 3.76 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 156.94, 150.34, 145.06, 135.48, 130.59, 129.60, 129.48, 128.45, 127.26, 124.77, 122.15, 120.66, 110.89, 67.99, 55.43, 21.65; IR

(KBr): 3234, 1745, 1598, 1436, 1222, 1153, 1059, 750 cm^{-1}. Partially consistent with published data by Cossío, Carreaux and coworkers.[16] Our NMR results do not show evidence for the presence of rotamers.



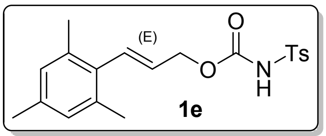
1c

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(3-methoxyphenyl)-2-propen-1-yl ester **(1c)** - (CAS: 1863094-80-7). Compound **1c** was obtained in 88% (1.59 g) yield according to the general procedure as a white solid; mp: 99-98 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.86 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 1H), 6.96-6.77 (m, 3H), 6.51 (d, *J* = 15.9 Hz, 1H), 6.16 (dt, *J* = 15.9, 6.2 Hz, 1H), 4.65 (d, *J* = 6.2 Hz, 2H), 3.81 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 159.74, 152.81, 144.22, 137.39, 136.57, 134.44, 129.54, 129.47, 128.00, 122.66, 119.29, 113.78, 111.95, 66.92, 55.21, 21.51; IR (KBr): 3232, 1745, 1577, 1438, 1265, 1151, 1085, 773, 663 cm^{-1}.



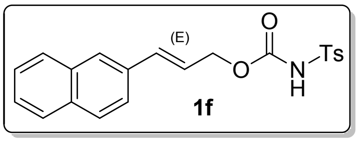
1d

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(4-methoxyphenyl)-2-propen-1-yl ester **(1d)** - (CAS: 1863094-90-9). Compound **1d** was obtained in 90% (1.63 g) yield according to the general procedure as a yellow oil; ^{1}H NMR (300 MHz, CD_3OD, ppm): δ 7.86 (d, *J* = 8.2 Hz, 2H), 7.29 (t, *J* = 8.7 Hz, 4H), 6.85 (d, *J* = 8.7 Hz, 2H), 6.49 (d, *J* = 15.9 Hz, 1H), 6.06 (dt, *J* = 15.9, 6.2 Hz, 1H), 4.59 (d, *J* = 6.2 Hz, 2H), 3.77 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, CD_3OD, ppm): δ 161.01, 156.53, 144.55, 139.85, 134.53, 130.39, 130.18, 128.82, 128.62, 122.04, 114.95, 67.28, 55.69, 21.46; IR (neat): 3184, 1624, 1512, 1292, 1238, 1138, 1062, 813 cm^{-1}. Partially consistent with published data by Cossío, Carreaux and coworkers.[16] Our NMR results do not show evidence for the presence of rotamers.



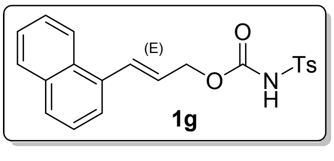
1e

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(2,4,6-trimethylphenyl)-2-propen-1-yl ester **(1e)** - (CAS: 1863094-98-7). Compound **1e** was obtained in a quantitative (1.87 g) yield according to the general procedure as a light yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.78 (d, *J* = 8.2 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 6.74 (s, 2H), 6.34 (d, *J* = 16.2 Hz, 1H), 5.53 (dt, *J* = 16.2, 6.2 Hz, 1H), 4.50 (d, *J* = 6.2 Hz, 2H), 2.21 (s, 3H), 2.19 (s, 3H), 2.05 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 153.49, 143.84, 136.73, 136.29, 135.67, 132.61, 132.40, 129.26, 128.47, 127.75, 127.32, 67.19, 21.31, 20.82, 20.60; IR (neat): 3257, 1720, 1656, 1448, 1384, 975 cm^{-1}.



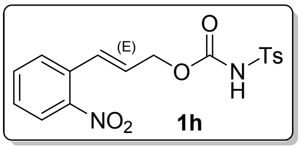
1f

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(2-naphthalenyl)-2-propen-1-yl ester **(1f)** - (CAS: 1863095-02-6). Compound **1f** was obtained in a quantitative (1.91 g) yield according to the general procedure as a white solid; mp: 124-125 °C; ^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.81-7.71 (m, 3H), 7.64 (s, 1H), 7.53-7.42 (m, 3H), 7.22 (d, *J* = 8.1 Hz, 2H), 6.66 (d, *J* = 15.9 Hz, 1H), 6.28 (dt, *J* = 15.9, 6.1 Hz, 1H), 4.68 (d, *J* = 6.1 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6, ppm): δ 157.57, 142.71, 139.79, 134.08, 133.23, 132.53, 130.84, 128.27, 128.18, 127.89, 127.59, 126.84 (2C), 126.42, 125.99, 123.56, 79.22, 63.87, 20.92; IR (KBr): 3184, 3055, 1620, 1450, 1138 cm^{-1}.



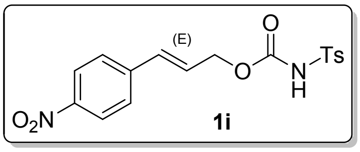
1g

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(1-naphthalenyl)-2-propen-1-yl ester **(1g)** - (CAS: 1863095-00-4). Compound **1g** was obtained in 98% (1.87 g) yield according to the general procedure as a brown oil. ^{1}H NMR (300 MHz, CD_3OD, ppm): δ 8.06-7.98 (m, 1H), 7.83 (d, *J* = 8.3 Hz, 2H), 7.79 (m, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.51-7.41 (m, 4H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.28 (d, *J* = 15.7 Hz, 1H), 7.18 (d, *J* = 8.1 Hz, 1H), 6.18 (dt, *J* = 15.6, 5.7 Hz, 1H), 4.67 (d, *J* = 5.7 Hz, 2H), 2.23 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 159.94, 142.22, 139.04, 133.88, 133.40, 130.93, 130.16, 129.09, 128.27, 127.94, 127.09, 126.82, 125.98, 125.62, 125.45, 123.85, 123.65, 66.36, 21.09; IR (neat): 3207, 3049, 2951, 1745, 1614, 1454, 1273 cm^{-1}.



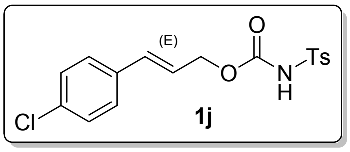
1h

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(2-nitrophenyl)-2-propen-1-yl ester **(1h)**. Compound **1h** was obtained in 40% (0.75 g) yield according to the general procedure as a brown oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.94-7.90 (m, 3H), 7.58-7.48 (m, 2H), 7.43-7.38 (m, 1H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.03 (d, *J* = 15.8 Hz, 1H), 6.13 (dt, *J* = 15.8, 6.0 Hz, 1H), 4.74 (d, *J* = 6.0 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 150.65, 147.66, 145.08, 135.48, 133.35, 131.73, 129.63, 129.56, 128.90, 128.76, 128.32, 127.28, 124.58, 66.42, 21.61; IR (neat): 3269, 2947, 1743, 1523, 1465, 1414, 740 cm^{-1}; HRMS (ESI): m/z $[M+NH_4]^+$ calculated for $C_{17}H_{20}N_3O_6S$: 394.1067; found: 394.1055.



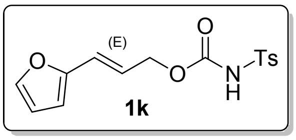
1i

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(4-nitrophenyl)-2-propen-1-yl ester **(1i)** – (CAS 2254190-75-3). Compound **1i** was obtained in 66% (1.24 g) yield according to the general procedure as an orange solid; mp: 120-122 °C; ^{1}H NMR (300 MHz, CD_3OD-d_4, ppm): δ 8.14 (d, *J* = 8.8 Hz, 2H), 7.81 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.8 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 6.62 (d, *J* = 16.0 Hz, 1H), 6.48 (dt, *J* = 16.0, 6.0 Hz, 1H), 4.61 (d, *J* = 6.0 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6, ppm): δ 156.13, 146.42, 143.25, 140.66, 131.28, 128.67, 128.54, 127.29, 126.98, 123.98, 79.22, 63.76, 20.95; IR (KBr): 3471, 2960, 1737, 1597, 1450, 740 cm^{-1}. Partially consistent with published data by Cossío, Carreaux and coworkers.[16] Our NMR results do not show evidence for the presence of rotamers.



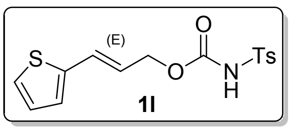
1j

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(4-chlorophenyl)-2-propen-1-yl ester **(1j)** - (CAS: 1863094-84-1). Compound **1j** was obtained in 77% (1.41 g) yield according to the general procedure as a white solid; mp: 138-140 °C; ^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ 7.50 (d, *J* = 8.1 Hz, 2H), 7.31-7.17 (m, 2H), 7.06 (bd, *J* = 8.1 Hz, 2H), 6.33 (d, *J* = 16.0 Hz, 1H), 6.12 (dt, *J* = 16.0, 5.5 Hz, 1H), 4.26 (d, *J* = 5.5 Hz, 2H), 2.16 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6, ppm): δ 156.79, 142.01, 140.25, 135.39, 131.96, 129.68, 128.63, 128.39, 128.01, 126.94, 126.89, 63.85, 20.92; IR (KBr): 3182, 3062, 2976, 1625, 1492, 1300, 1138, 968, 813 cm^{-1}. Partially consistent with published data by Cossío, Carreaux and coworkers.[16] Our NMR results do not show evidence for the presence of rotamers.



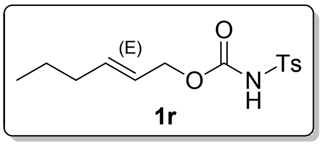
1k

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(2-furanyl)-2-propen-1-yl ester **(1k)**. The compound **1k** is unstable and should be used in the next reaction step immediately after isolated according to the general procedure as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.93 (d, *J* = 8.0 Hz, 2H), 7.35-7.30 (m, 3H), 6.40-6.35 (m, 2H), 6.25 (d, *J* = 3.1 Hz, 1H), 6.06 (dt, *J* = 15.6, 6.1 Hz, 1H), 4.68 (d, *J* = 6.1 Hz, 2H), 2.42 (s, 3H).

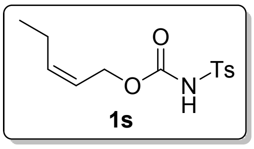


1l

Carbamic acid, *N*-[(4-methylphenyl)sulfonyl]-, (2*E*)-3-(2-thiophenyl)-2-propen-1-yl ester **(1l)**. The compound **1l** is unstable and should be used in the next reaction step immediately after isolated according to the general procedure as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.92 (d, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.21-7.19 (m, 1H), 6.96 (d, *J* = 3.3 Hz, 2H), 6.70 (d, *J* = 15.9 Hz, 1H), 5.95 (dt, *J* = 15.9, 6.6 Hz, 1H), 4.68 (d, *J* = 6.6 Hz, 2H), 2.43 (s, 3H).

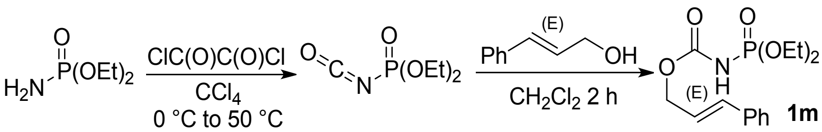


(*E*)-hex-2-en-1-yl tosylcarbamate **(1r)** - (CAS: 1437784-91-2). Compound **1r** was obtained in 89% (1.32 g) yield according to the general procedure as a yellow viscous oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.81 (d, J = 8.0 Hz, 2H), 7.15 (d, J = 8.0 Hz, 2H), 5.63-5.51 (m, 1H), 5.44-5.30 (m, 1H), 4.34 (d, J = 6.3 Hz, 2H), 1.90 (q, J = 7.0 Hz, 2H), 1.39-1.21 (m, 2H), 0.83 (t, J = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 155.59, 142.95, 138.11, 136.15, 129.21, 127.56, 123.87, 66.73, 34.22, 21.98, 21.48, 13.63. Consistent with published data.[17]



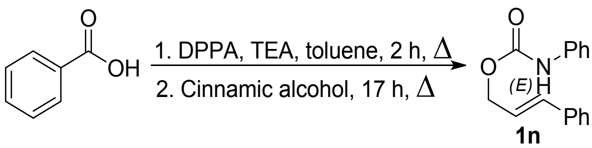
(*Z*)-pent-2-en-1-yl tosylcarbamate **(1s)** - (CAS: 1437784-84-3). Compound **1s** was obtained in a quantitative (1.42 g) yield according to the general procedure as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.92 (d, J = 8.3 Hz, 2H), 7.84 (bs, NH), 7.34 (d, J = 8.3 Hz, 2H), 5.70-5.58 (m, 1H), 5.45-5.33 (m, 1H), 4.62 (d, J = 7.0 Hz, 2H), 2.44 (s, 3H), 2.05 (p, J = 7.5 Hz, 2H), 0.95 (t, J = 7.5 Hz, 3H). Consistent with published data.[18]

Synthesis cinnamyl diethoxyphosphorylcarbamate (1m).



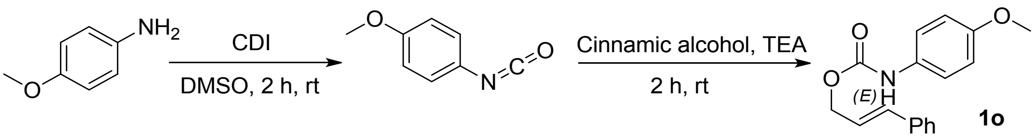
Carbamate **1m** was prepared according to the previously reported procedure.[15,19] A solution of diethyl phosphoramidate (765 mg, 5.0 mmol, 1.0 equiv) in carbon tetrachloride (7.5 mL) was slowly added dropwise to a cooled solution (0 °C) of oxalyl chloride (472 µL, 5.5 mmol, 1.1 equiv) in carbon tetrachloride (7.5 mL). After the addition was completed the temperature of the mixture is slowly raised to 50 °C and maintained for 1 h. The mixture is then cooled to room temperature and evaporated under reduced pressure. The residual liquid was distilled under reduced pressure using a bulb-to-bulb apparatus to afford the corresponding isocyanate, that should be carefully protected from moisture. Then a solution of the obtained isocyanate in anhydrous CH_2Cl_2 (10.0 mL) was added dropwise to a solution of cinnamic alcohol (738 mg, 5.5 mmol, 1.1 equiv) in anhydrous CH_2Cl_2 (10.0 mL) at 0 °C under nitrogen atmosphere. The reaction mixture was stirred for 2 h and solvent was evaporated under reduced pressure. The residue was purified by flash column chromatography (DCM) to give the desired carbamate **1m** in 49% (after 2 steps reactions, 0.77 g) yield as a colorless solid; mp: 59-62 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.39-7.24 (m, 5H), 6.68 (d, J = 15.8 Hz, 1H), 6.27 (dt, J = 15.8, 6.4 Hz, 1H), 4.77 (d, J = 6.4 Hz, 2H), 4.24-4.17 (m, 4H), 1.37-1.32 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 153.40, 136.12, 134.49, 128.63, 128.15, 126.61, 122.72, 66.52, 64.11 (d, J_{CP} = 5.6 Hz), 16.08 (d, J_{CP} = 6.9 Hz); IR (KBr): 3111, 3026, 2983, 1732, 1444, 1029 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{14}H_{20}NO_5P$: 314.1152; found: 314.1147.

Synthesis of cinnamyl phenylcarbamate (1n) – (CAS: 28315-20-0).



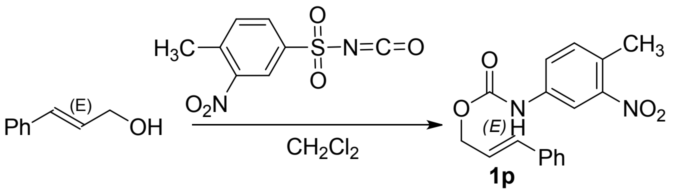
Carbamate **1n** was prepared according to the previously reported procedure.[20] To a stirred solution of benzoic acid (611 mg, 5.0 mmol, 1.0 equiv) in anhydrous toluene (4.0 mL), diphenylphosphoryl azide (DPPA) (1,22 g, 5.0 mmol, 1.0 equiv), triethylamine (0.7 mL, 5.0 mmol, 1.0 equiv) were added respectively. The mixture was stirred for 2 h under reflux after no more gas was formed. The reaction was allowed to cool and a solution of cinnamic alcohol (738 mg, 5.0 mmol, 1.0 equiv) in toluene (4.0 mL) was added slowly. The reaction was stirred overnight under reflux. Solvent was removed under reduced pressure. The residue was purified by flash column chromatography (DCM) to give the carbamate **1n** in 60% (0.76 g) yield as a white solid; mp: 86-88 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.40-7.37 (m, 4H), 7.34-7.24 (m, 4H), 7.08-7.03 (m, 1H), 6.72 (brs, 1H), 6.68 (d, J = 16.0 Hz, 1H), 6.32 (dt, J = 16.0, 6.4 Hz, 1H), 4.82 (d, J= 6.4 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 153.33, 137.79, 136.18, 134.23, 129.07, 128.62, 128.10, 126.64, 123.53, 123.34, 118.77, 65.77; IR (KBr): 3321, 3043, 2974, 1697, 1442, 1236 cm^{-1}. Consistent with published data.[21]

Synthesis of cinnamyl (4-methoxyphenyl)carbamate (1o) – (CAS: 1580503-51-0).



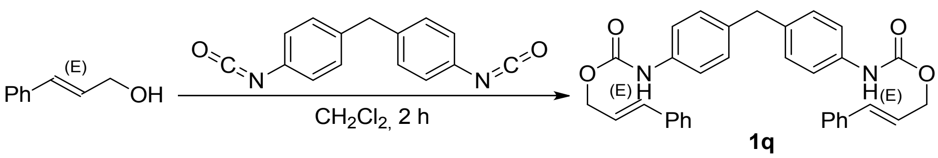
Carbamate **1o** was prepared according to the previously reported procedure.[22] A solution of *p*-anidisine (246 mg, 2.0 mmol, 1.0 equiv) in DMSO (5.0 mL) was treated with 1,1'-carbonyldiimidazole - CDI (389 mg, 2.4 mmol, 1.2 equiv). The mixture was stirred at room temperature for 2 h. Cinnamic alcohol (295 mg, 2.2 mmol, 1.1 equiv) and triethylamine (0.3 mL, 2.2 mmol, 1.1 equiv) were added and the reaction was allowed to stir at room temperature for more 2 h. Ethyl acetate (10 mL) was added, and the solution was washed with water (4 x 10 mL) and then dried over Na_2SO_4. The combined organic extract was filtered and the concentrated under reduced pressure. The residue was purified by flash column chromatography (DCM) to give the carbamate **1o** in 47% (0.66 g) yield as a white solid; mp: 113-114 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.42-7.21 (m, 7H), 6.84 (d, J = 9.0 Hz, 2H), 6.67 (m, 2H), 6.31 (dt, J = 15.9, 6.3 Hz, 1H), 4.80 (d, J = 6.3 Hz, 2H), 3.76 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 156.15, 153.90, 136.33, 134.18, 130.97, 128.72, 128.17, 126.74, 123.62, 120.90 (brs), 114.36, 65.80, 55.59; IR (KBr): 3331, 2924, 1693, 1529, 1238, 1058, 744, 692 cm^{-1}. Consistent with published data.[22]

Synthesis of cinnamyl (4-methyl-3-nitrophenyl)carbamate (1p).



To a stirred solution of cinnamic alcohol (443 mg, 3.3 mmol, 1.1 equiv) in anhydrous DCM, 4-methyl-3-nitrophenyl isocyanate (727 mg, 3.0 mmol, 1.0 equiv) was added dropwise at 0 °C under argon atmosphere. The reaction mixture was stirred for 2 h and solvent was evaporated under reduced pressure. The residue was purified by flash column chromatography (DCM) to give the desired carbamate **1p** in 76% (0.71 g) yield as a yellow solid; mp: 104.5-106.2 °C; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.05 (d, J = 1.9 Hz, 1H), 7.56 (d, J = 7.8 Hz, 1H), 7.40 (d, J = 7.8 Hz, 2H), 7.34 (d, J = 6.8 Hz, 1H), 7.32-7.22 (m, 3H), 6.86 (s, 1H), 6.69 (d, J = 15.9 Hz, 1H), 6.32 (dt, J= 15.9, 6.5 Hz, 1H), 4.82 (d, J = 6.5, 2H), 2.54 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 153.23, 149.36, 136.91, 136.15, 134.86, 133.40, 128.79, 128.38, 128.33, 126.80, 123.15, 122.95 (brs), 114.69, 66.37, 19.98; IR (KBr): 3356, 3016, 2926, 1735, 1344, 1319, 690 cm^{-1}; HRMS (ESI): m/z $[M+NH_4]^+$ calculated for $C_{17}H_{20}N_3O_4$: 330.1448; found: 330.1442.

Synthesis of dicinnamyl (methylenebis(4,1-phenylene))dicarbamate (1q).



To a stirred solution of cinnamic alcohol (6.6 mmol, 2.2 equiv) in anhydrous DCM, 4,4'-methylenebis(phenyl isocyanate) (3.0 mmol, 1.0 equiv) was added dropwise at 0 °C under nitrogen atmosphere. The reaction mixture was stirred for 2 h and solvent was evaporated under reduced pressure. The residue was purified by flash column chromatography (DCM) to give the desired carbamate **1q** in 60% (0.93 g) yield as a white solid; mp: 156-158 °C; ^{1}H NMR (300 MHz, Acetone-d_6, ppm): δ 8.65 (brs, 2H), 7.52-7.16 (m, 18 H), 6.75 (d, J = 15.9 Hz, 2H), 6.41 (dt, J = 15.9, 6.1 Hz, 2H), 4.79 (d, J = 6.1 Hz, 4H), 3.90 (s, 2H); ^{13}C NMR (75 MHz, Acetone-d_6, ppm): δ 154.29, 138.21, 137.47, 136.90, 134.01, 129.95, 129.51, 128.76, 127.38, 125.17, 119.36, 65.61, 41.09; IR (KBr): 3307, 3026, 2958, 1703, 1529, 1415, 867, 854 cm^{-1}; HRMS (ESI): m/z $[M+NH_4]^+$ calculated for $C_{33}H_{34}N_3O_4$: 536.2544; found: 536.2530.

3.4. General Procedures for the Synthesis and Characterization Data of Oxazolidinones 2a-s.

*Synthesis of **2a-l***. A 10 mL vial was charged with AgOAc (33 mg, 0.2 mmol, 1.0 equiv), Bu_4Cl (55 mg, 0.2 mmol, 1.0 equiv) and CH_3CN (2.0 mL), the mixture was allowed to stir for 1 h at room temperature to obtained *in situ* Bu_4NOAc. Next were added $CuCl_2$ (134 mg, 1.0 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (4,6 mg, 0.02 mmol, 10 mol %), LiCl (42 mg, 1.0 mmol, 5.0 equiv) and the corresponding allylic carbamate **1a-l** (0.2 mmol, 1.0 equiv), respectively. The reaction was heated to 60 °C (50 °C to allylic carbamate **1e**) for 2.5 h. The solvent was removed under reduced vacuum. Flash chromatography column (1:1 EtOAc/Hexane) gave the desired product.

*Synthesis of **2m***. A 10 mL vial was charged with AgOAc (66 mg, 0.4 mmol, 4.0 equiv), Bu_4Cl (110 mg, 0.4 mmol, 2.0 equiv) and CH_3CN (2.0 mL), the mixture was allowed to stir for 1 h at room temperature to obtained *in situ* Bu_4NOAc. Next were added $CuCl_2$ (134 mg, 1.0 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (4,6 mg, 0.02 mmol, 10 mol %), LiCl (42 mg, 1.0 mmol, 5.0 equiv) and the corresponding allylic carbamate **1m** (62 mg, 0.2 mmol, 1.0 equiv), respectively. The reaction was heated to 60 °C for 24 h. The solvent was removed under vacuum. Flash chromatography column (1:1 EtOAc/Hexane) gave the desired product.

*Synthesis of **2n***. A 10 mL vial was charged with AgOAc (66 mg, 0.4 mmol, 4.0 equiv), Bu_4Cl (110 mg, 0.4 mmol, 2.0 equiv) and CH_3CN (2.0 mL), the mixture was allowed to stir for 1 h at room temperature to obtained *in situ* Bu_4NOAc. Next were added $CuCl_2$ (134 mg, 1.0 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (4,6 mg, 0.02 mmol, 10 mol %), LiCl (42 mg, 1.0 mmol, 5.0 equiv) and the corresponding allylic carbamate **1n** (51 mg, 0.2 mmol, 1.0 equiv), respectively. The reaction was heated to 80 °C for 24 h. The solvent was removed under reduced vacuum. Flash chromatography column (1:1 EtOAc/Hexane) gave the desired product.

*Synthesis of **2o***. A 10 mL vial was charged with AgOAc (33 mg, 0.2 mmol, 1.0 equiv), Bu_4Cl (55 mg, 0.2 mmol, 1.0 equiv) and CH_3CN (2.0 mL), the mixture was allowed to stir for 1 h at room temperature to obtained *in situ* Bu_4NOAc. Next were added $CuCl_2$ (134 mg, 1.0 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (4,6 mg, 0.02 mmol, 10 mol %), LiCl (42 mg, 1.0 mmol, 5.0 equiv) and the corresponding allylic carbamate **1o** (57 mg, 0.2 mmol, 1.0 equiv), respectively. The reaction was heated to 60 °C for 5 h. The solvent was removed under reduced vacuum. Flash chromatography column (1:1 EtOAc/Hexane) gave the desired product.

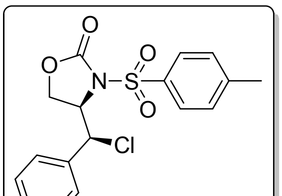
*Synthesis of **2p***. A 10 mL vial was charged with AgOAc (33 mg, 0.2 mmol, 1.0 equiv), Bu_4Cl (55 mg, 0.2 mmol, 1.0 equiv) and CH_3CN:THF (1.0:1.0 mL), the mixture was allowed to stir for 1 h at room temperature to obtained *in situ* Bu_4NOAc. Next were added $CuCl_2$ (134 mg, 1.0 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (4,6 mg, 0.02 mmol, 10 mol %), LiCl (42 mg, 1.0 mmol, 5.0 equiv) and the corresponding allylic carbamate **1p** (62 mg, 0.2 mmol, 1.0 equiv), respectively. The reaction was heated to 80 °C for 24 h. The solvent was removed under reduced vacuum. Flash chromatography column (1:1 EtOAc/Hexane) gave the desired product.

*Synthesis of **2q***. A 10 mL vial was charged with AgOAc (66 mg, 0.4 mmol, 4.0 equiv), Bu_4Cl (110 mg, 0.4 mmol, 2.0 equiv) and CH_3CN:THF (1.0:1.0 mL), the mixture was allowed to stir for 1 h at room temperature to obtained *in situ* Bu_4NOAc. Next were added $CuCl_2$ (134 mg, 1.0 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (4,6 mg, 0.02 mmol, 10 mol %), LiCl (42 mg, 1.0 mmol, 5.0 equiv) and the corresponding allylic carbamate **1q** (104 mg, 0.2 mmol, 1.0 equiv), respectively. The reaction was heated to 60 °C for 24 h. The solvent was removed under reduced vacuum. Flash chromatography column (1:1 EtOAc/Hexane) gave the desired product.

*Tentative synthesis of **2r***. A AgOAc (33 mg, 0.2 mmol, 1.0 equiv), Bu_4Cl (55 mg, 0.2 mmol, 1.0 equiv) and THF (2.0 mL), the mixture was allowed to stir for 1 h at room temperature, then the mixture was centrifugated to obtain Bu_4NOAc. Next were added carbamate $CuCl_2$ (134 mg, 1.0 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (4,6 mg, 0.02 mmol, 10 mol %), LiCl (42 mg, 1.0 mmol, 5.0 equiv) and **1r** (59 mg, 0.2 mmol, 1.0 equiv), respectively. The reaction was stirred at room temperature overnight. The solvent was removed under reduced vacuum. Flash chromatography column (3:7 EtOAc/Hexane) gave the [3,3]-sigmatropic rearrangement product **3r**.

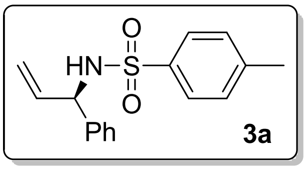
*Synthesis of **2s***. A 10 mL vial was charged with carbamate **1s** (57 mg, 0.2 mmol, 1.0 equiv), $CuCl_2$ (134 mg, 1.0 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (4,6 mg, 0.02 mmol, 10 mol %), LiCl (42 mg, 1.0 mmol, 5.0 equiv) and THF (2.0 mL) respectively. The reaction was stirred at room temperature for 24 h. The reaction was heated to 60 °C for 24 h. The solvent was removed under reduced vacuum. Flash chromatography column (3:7 EtOAc/Hexane) gave the desired product.

*Gram-Scale Preparation of **2a***. A 50 mL round-bottom flask was charged with AgOAc (500 mg, 3.0 mmol, 1.0 equiv), Bu_4Cl (834 mg, 3 mmol, 1.0 equiv) and CH_3CN (30 mL), the mixture was allowed to stir for 1 h at room temperature to obtained *in situ* Bu_4NOAc. Next were added $CuCl_2$ (2.0 g, 15 mmol, 5.0 equiv), $PdCl_2(CH_3CN)_2$ (69 mg, 0.3 mmol for the reaction using 10 mol % and 34.5 mg, 0.15 mmol for the reaction using 5 mol %), LiCl (640 mg, 15 mmol, 5.0 equiv) and the corresponding allylic carbamate **1a** (1.0 g, 3.0 mmol, 1.0 equiv), respectively. The reaction was heated to 60 °C for 2.5 h (24 h for the reaction using $PdCl_2(CH_3CN)_2$ at 5 mol %). The solvent was removed under reduced vacuum. Flash chromatography column (1:1 EtOAc/Hexane) gave the desired product in 65% and 75% yield in reactions using 10 mol % and 5 mol % of the palladium salt, respectively.



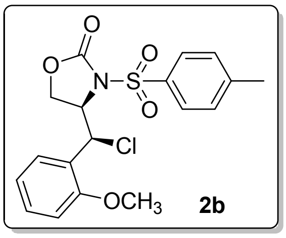
2a

4-(Chloro(phenyl)methyl)-3-tosyloxazolidin-2-one **(2a)**. Compound **2a** was obtained in 65% (47 mg) yield according to the general procedure as a white solid; mp: 86-89 °C; dr = 20:1 [determined by the ratio of area at δ 5.80 (d, J = 2.4 Hz, major isomer) and δ 5.54 (d, J = 3.9 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.02 (d, J = 8.4 Hz, 2H), 7.50-7.34 (m, 7H), 5.80 (d, J = 2.5 Hz, 1H), 4.89 (ddd, J = 8.9, 3.7, 2.5 Hz, 1H), 4.42 (dd, J = 9.3, 3.7 Hz, 1H), 4.13 (appt, J = 9.3 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 151.98, 145.93, 134.74, 134.51, 129.83, 129.18 (2C), 128.65, 127.03, 62.95, 62.75, 61.37, 21.76; IR (KBr): 3030, 2983, 1776, 1595, 1174, 817 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{17}H_{17}ClNO_4S$: 366.0561; found: 366.0566.



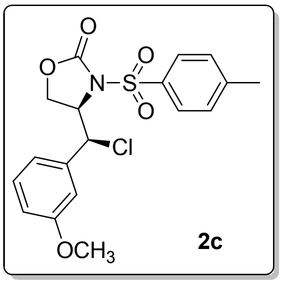
3a

4-Methyl-*N*-(1-phenylallyl)benzenesulfonamide **(3a)** – (CAS: 58567-43-4). Compound **3a** was obtained in 14% (8 mg) yield according to the general procedure as a white solid; mp: 90-91 °C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.21 – 7.07 (m, 7H), 5.84 (ddd, *J* = 17.1, 10.1, 5.9 Hz, 1H), 5.50 (brs, 1H), 5.14 – 5.02 (m, 2H), 4.97 – 4.88 (m, 1H), 2.36 (s, 3H); ^{13}C RMN (75 MHz, $CDCl_3$, ppm): δ 143.19, 139.51, 137.72, 137.18, 129.43, 128.60, 127.68, 127.24, 127.14, 116.73, 59.95, 21.53. Isolated as a by-product. Consistent with published data.[23]



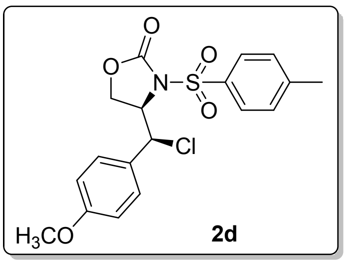
2b

4-(Chloro(2-methoxyphenyl)methyl)-3-tosyloxazolidin-2-one **(2b)**. Compound **2b** was obtained in 65% (51 mg) yield according to the general procedure as a white solid; mp: 167-169 °C; dr = 12:1 [determined by the ratio of area at δ 6.07 (d, *J* = 2.5 Hz, major isomer), 5.95 (d, *J* = 4.7 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.03 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.38-7.32 (m, 3H), 7.01 (t, *J* = 7.5 Hz, 1H), 6.91 (d, *J* = 8.2 Hz, 1H), 6.07 (d, *J* = 2.5 Hz, 1H), 5.00 (ddd, *J* = 8.9, 3.6, 2.5 Hz, 1H), 4.32 (dd, *J* = 9.3, 3.6 Hz, 1H), 4.05 (appt, *J* = 9.3 Hz, 1H), 3.95 (s, 3H), 2.45 (s, 3H); ^{13}C RMN (75 MHz, $CDCl_3$, ppm): δ 155.98, 152.38, 145.73, 135.00, 130.53, 129.84, 129.21, 128.70, 128.60, 122.93, 121.03, 110.67, 63.34, 58.85, 58.83, 55.78, 21.85; IR (KBr): 3003, 2954, 1774, 1597, 1242, 1178, 819 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{18}H_{19}ClNO_5S$: 396.0667; found: 396.0671.



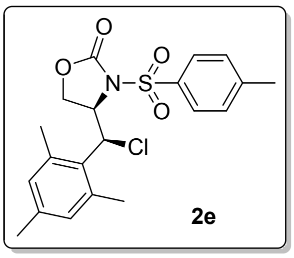
2c

4-(Chloro(3-methoxyphenyl)methyl)-3-tosyloxazolidin-2-one **(2c)**. Compound **2c** was obtained in 60% (47 mg) yield according to the general procedure as a white solid; mp: 126-128 °C; dr = 8:1 [determined by the ratio of area at δ 5.76 (d, *J* = 2.3 Hz, major isomer), 5.52 (d, *J* = 3.8 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.01 (d, *J* = 8.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.04-6.96 (m, 3H), 6.89 (dd, *J* = 8.0, 2.1 Hz, 1H), 5.76 (d, *J* = 2.4 Hz, 1H), 4.89 (ddd, *J* = 9.1, 3.6, 2.4 Hz, 1H), 4.39 (dd, *J* = 9.1, 3.6 Hz, 1H), 4.12 (appt, *J* = 9.1 Hz, 1H), 3.82 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 160.16, 152.04, 145.97, 136.31, 134.56, 130.35, 129.87, 128.67, 119.15, 114.31, 113.13, 63.11, 62.74, 61.37, 55.47, 21.79; IR (KBr): 3089, 2976, 1764, 1583, 1201, 1170, 800, 700 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{18}H_{19}ClNO_5S$: 396.0667; found: 396.0668.



2d

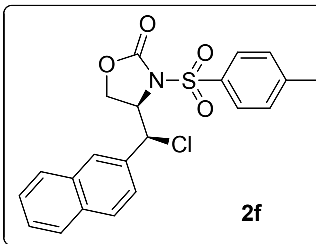
4-(Chloro(4-methoxyphenyl)methyl)-3-tosyloxazolidin-2-one **(2d)**. Compound **2d** was obtained in 55% (43 mg) yield according to the general procedure as a white solid; mp: 148-150 °C; dr = 8:1 [determined by the ratio of area at δ 5.51 (brs, major isomer), 5.14 (d, *J* = 5.4 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.02 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.7 Hz, 2H), 6.92 (d, *J* = 8.7 Hz, 2H), 5.51 (brs, 1H), 4.57 (ddd, *J* = 8.9, 3.8, 2.1 Hz, 1H), 4.37 (dd, *J* = 8.9, 3.8 Hz, 1H), 3.98 (appt, *J* = 8.9 Hz, 1H), 3.81 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 159.71, 152.75, 145.94, 135.01, 130.05, 128.59, 126.88, 114.45, 71.57, 62.52, 62.15, 55.48, 29.84, 21.88; IR (KBr): 3003, 2924, 1770, 1510, 1251, 1172, 817 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{18}H_{19}ClNO_5S$: 396.0667; found: 396.0682.



2e

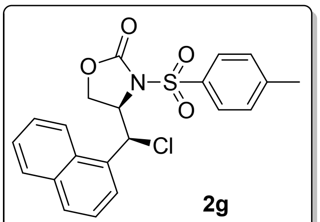
4-(Chloro(mesityl)methyl)-3-tosyloxazolidin-2-one **(2e)**. Compound **2e** was obtained in 50% (40 mg) yield according to the general procedure as a white solid; mp: 116-118 °C; dr = 16:1 [determined by the ratio of area at δ 5.84 (d, *J* = 5.0 Hz, major isomer), 4.91 (d, *J* = 7.1 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.48 (d, *J* = 8.4

Hz, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 6.94 (s, 1H), 6.72 (s, 1H), 5.84 (d, *J* = 5.0 Hz, 1H), 4.59 (ddd, *J* = 5.0, 3.4 Hz, 1H), 3.80 (dd, *J* = 12.2, 5.0 Hz, 1H), 3.68 (dd, *J* = 12.2, 3.4 Hz, 1H), 2.54 (s, 3H), 2.41 (s, 3H), 2.29 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 151.30, 145.57, 139.18, 138.21, 136.90, 134.42, 131.81, 130.20, 129.48, 128.43, 78.00, 58.59, 44.85, 21.83, 20.98, 20.73, 19.32; IR (KBr): 3010, 2951, 1784, 1597, 1190, 667 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{20}H_{23}ClNO_4S$: 408.1031; found: 408.1035.



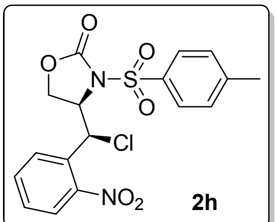
2f

4-(Chloro(naphthalen-2-yl)methyl)-3-tosyloxazolidin-2-one **(2f)**. Compound **2f** was obtained in 53% (44 mg) yield according to the general procedure as a white solid; mp: 180-182 °C; dr >20:1 [determined by the ratio of area at δ 5.93 (d, *J* = 2.5 Hz, major isomer), 5.69 (d, *J* = 4.5 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 8.02 (d, *J* = 8.4 Hz, 2H), 7.92-7.85 (m, 4H), 7.56-7.52 (m, 3H), 7.34 (d, *J* = 8.4 Hz, 2H), 5.92 (d, *J* = 2.5 Hz, 1H), 5.01 (ddd, *J* = 9.1, 3.5 Hz, 1H), 4.49 (dd, *J* = 9.1, 3.5 Hz, 1H), 4.13 (appt, *J* = 9.1 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 152.16, 146.03, 134.66, 133.43, 133.16, 132.17, 129.93, 129.32, 128.76, 128.27, 127.89, 127.29, 127.21, 126.84, 124.24, 63.35, 63.08, 61.42, 21.90; IR (KBr): 3059, 2985, 1768, 1595, 1172, 1085, 758 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{21}H_{19}ClNO_4S$: 416.0718; found: 416.0713.



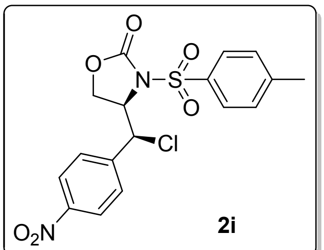
2g

4-(Chloro(naphthalen-1-yl)methyl)-3-tosyloxazolidin-2-one **(2g)**. Compound **2g** was obtained in 55% (45 mg) yield according to the general procedure as a white solid; mp: 175-178 °C; dr >20:1 [determined by the ratio of area at δ 6.70 (brs, major isomer), 6.30 (d, *J* = 4.5 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, DMSO-*d*$_6$, ppm): *δ* 8.29 (d, *J* = 8.6 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 2H), 8.05 (t, *J* = 8.1 Hz, 2H), 7.86 (d, *J* = 7.2 Hz, 1H), 7.76 (t, *J* = 7.2 Hz, 1H), 7.69-7.56 (m, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 6.62 (brs, 1H), 5.30 (dt, *J* = 9.0, 3.0 Hz, 1H), 4.47 (dd, *J* = 9.0, 3.0 Hz, 1H), 4.31 (appt, *J* = 9.3 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR (75 MHz, DMSO-*d*$_6$, ppm): *δ* 151.80, 145.91, 134.15, 133.30, 130.10, 129.94, 129.86, 129.64, 129.10, 128.59, 127.50, 126.47, 126.07, 125.47, 122.40, 63.46, 61.46, 59.47, 21.22; IR (KBr): 3041, 2999, 1774, 1595, 1176, 781 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{21}H_{19}ClNO_4S$: 416.0718; found: 416.0713.



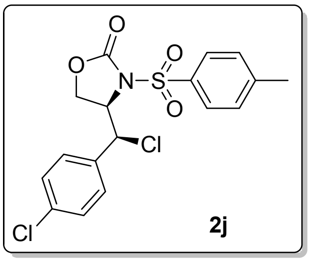
2h

4-(Chloro(2-nitrophenyl)methyl)-3-tosyloxazolidin-2-one **(2h)**. Compound **2h** was obtained in 70% (57 mg) yield according to the general procedure as a brown solid; mp: 174-176 °C; dr >20:1 [determined by the ratio of area at δ 6.38 (d, *J* = 3.6 Hz, major isomer), 6.11 (d, *J* = 4.1 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 8.01 (d, *J* = 8.3 Hz, 3H), 7.90 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.74 (td, *J* = 8.0, 1.2 Hz, 1H), 7.59 (td, *J* = 8.0, 1.2 Hz, 1H), 7.36 (d, *J* = 8.3 Hz, 2H), 6.38 (d, *J* = 3.6 Hz, 1H), 5.11 (ddd, *J* = 8.5, 3.6 Hz, 1H), 4.49 (dd, *J* = 9.0, 3.6 Hz, 1H), 4.17 (appt, *J* = 9.0 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 152.12, 148.54, 146.01, 134.67, 133.87, 130.73, 130.62, 130.00, 129.81, 128.65, 125.60, 63.31, 59.91, 58.03, 21.87; IR (KBr): 3091, 2927, 1791, 1529, 1379, 1350, 1170, 700 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{17}H_{16}ClN_2O_6S$: 411.0412; found: 411.0415.

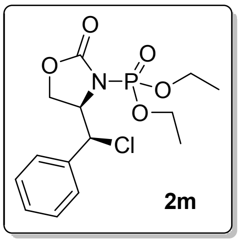


2i

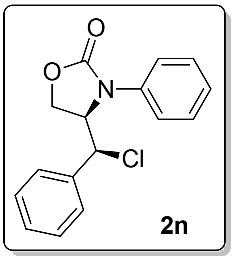
4-(Chloro(4-nitrophenyl)methyl)-3-tosyloxazolidin-2-one **(2i)**. Compound **2i** was obtained in 60% (49 mg) yield according to the general procedure as a light yellow solid; mp: 153-154 °C; dr >20:1 [determined by the ratio of area at δ 5.86 (d, *J* = 2.6 Hz, major isomer), 5.66 (d, *J* = 4.0 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 8.27 (d, *J* = 8.8 Hz, 2H), 7.99 (d, *J* = 8.2 Hz, 2H), 7.69 (d, *J* = 8.8 Hz, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 5.86 (d, *J* = 2.6 Hz, 1H), 4.94 (ddd, *J* = 8.0, 3.2 Hz, 1H), 4.35 (dd, *J* = 9.0, 3.2 Hz, 1H), 4.18 (appt, *J* = 9.0 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 151.79, 148.40, 146.38, 141.74, 134.33, 130.04, 128.72, 128.52, 124.43, 63.01, 61.99, 61.10, 21.89; IR (KBr): 3080, 2981, 1778, 1517, 1377, 1350, 1184, 856 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{17}H_{16}ClN_2O_6S$: 411.0412; found: 411.0401.



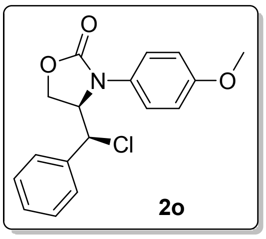
4-(Chloro(4-chlorophenyl)methyl)-3-tosyloxazolidin-2-one **(2j)**. Compound **2j** was obtained in 82% (65 mg) yield according to the general procedure as a white solid; mp: 148-150 °C; dr = 6:1 [determined by the ratio of area at δ 5.74 (d, *J* = 2.7 Hz, major isomer), 5.52 (d, *J* = 3.9 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 7.99 (d, *J* = 8.4 Hz, 2H), 7.41-7.34 (m, 6H), 5.74 (d, *J* = 2.7 Hz, 1H), 4.86 (ddd, *J* = 9.3, 3.6, 2.7 Hz, 1H), 4.35 (dd, *J* = 9.3, 3.6 Hz, 1H), 4.14 (appt, *J* = 9.3 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 151.95, 146.11, 135.33, 134.50, 133.39, 129.94, 129.46, 128.70, 128.59, 63.06, 62.21, 61.28, 21.86; IR (KBr): 3032, 2981, 1776, 1597, 1168, 821 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{17}H_{16}Cl_2NO_4S$: 400.0172; found: 400.0171.



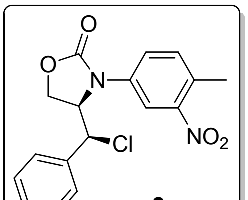
Diethyl (4-(chloro(phenyl)methyl)-2-oxooxazolidin-3-yl)phosphonate **(2m)**. Compound **2m** was obtained in 58% (40 mg) yield according to the general procedure as a light-yellow oil; dr = 10:1 [determined by the ratio of area at δ 5.83 (d, *J* = 2.0 Hz, major isomer), 5.43 (d, *J* = 4.2 Hz, minor isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 7.50-7.31 (m, 5H), 5.83 (d, *J* = 2.3 Hz, 1H), 4.61 (ddd, *J* = 8.6, 3.7, 2.3 Hz, 1H), 4.49 (dd, *J* = 9.3, 3.7 Hz, 1H), 4.42-4.24 (m, 4H), 4.17 (appt, *J* = 9.3 Hz, 1H), 1.51-1.34 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 155.46 (d, J^2_{C-P} = 8.2 Hz), 135.48, 129.14, 129.04, 127.20, 65.40 (d, J^2_{C-P} = 6.6 Hz), 65.14 (d, J^2_{C-P} = 6.4 Hz), 64.10, 63.80 (d, J^3_{C-P} = 8.8 Hz), 61.96 (d, J^3_{C-P} = 5.2 Hz), 16.25 (d, J^3_{C-P} = 2.8 Hz), 16.16 (d, J^3_{C-P} = 3.3 Hz); IR (neat): 3057, 2981, 1778, 1770, 1205, 1192, 732, 702 cm^{-1}. HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{14}H_{20}ClNO_5P$: 448.0762; found: 448.0779.



4-(Chloro(phenyl)methyl)-3-phenyloxazolidin-2-one **(2n)**. Compound **2n** was obtained in 95% (54 mg) yield according to the general procedure as a white solid; mp: 98-100 °C; dr = 6:1 [determined by the ratio of area at δ 5.22 (d, *J* = 3.7 Hz, minor isomer), 5.17 (d, *J* = 3.0 Hz, major isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 7.51-7.16 (m, 10H), 5.17 (d, *J* = 3.2 Hz, 1H), 4.82 (ddd, *J* = 8.3, 4.5 Hz, 1H), 4.60 (dd, *J* = 9.1, 4.5 Hz, 1H), 4.34 (appt, *J* = 9.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 155.92, 135.72, 129.64, 129.16, 129.14, 127.15, 126.58, 123.79, 120.86, 62.64, 62.19, 61.39; IR (KBr): 3022, 2926, 1741, 1500, 1138, 736, 692 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{16}H_{15}ClNO_4$: 288.0786; found: 288.0788.

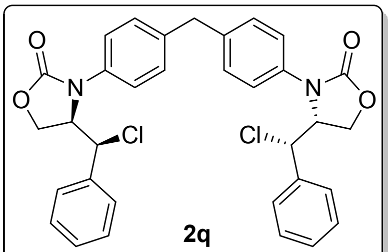


4-(Chloro(phenyl)methyl)-3-(4-methoxyphenyl)oxazolidin-2-one **(2o)** – (CAS: 1948274-67-6). Compound **2o** was obtained in 82% (52 mg) yield according to the general procedure as a brown solid; mp: 80-81.4 °C; dr = 8:1 [determined by the ratio of area at δ 5.14 (d, *J* = 4.1 Hz, minor isomer), 5.10 (d, *J* = 3.1 Hz, major isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 7.39-7.27 (m, 7H), 6.94 (d, *J* = 8.9 Hz, 2H), 5.11 (d, *J* = 3.2 Hz, 1H), 4.68 (ddd, *J* = 9.1, 4.8, 3.2 Hz, 1H), 4.58 (dd, *J* = 9.1, 4.8 Hz, 1H), 4.33 (appt, *J* = 9.1 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 158.44, 156.43, 135.79, 129.10, 129.05, 128.30, 127.15, 126.32, 114.93, 62.92, 62.70, 61.64, 55.63; IR (KBr): 3070, 2999, 1749, 1514, 1251, 748, 705 cm^{-1}; HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{17}H_{17}ClNO_3$: 318.0891; found:318.0921. Consistent with published data.[24]



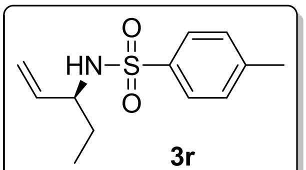
2p

4-(Chloro(phenyl)methyl)-3-(4-methyl-3-nitrophenyl)oxazolidin-2-one **(2p)**. Compound **2p** was obtained in 86% (59 mg) yield according to the general procedure as light-yellow solid; mp: 132-134 °C; dr = 6:1 [determined by the ratio of area at δ 5.18 (d, *J* = 4.3 Hz, minor isomer), 5.15 (d, *J* = 4.2 Hz, major isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 7.92 (d, *J* = 2.4 Hz, 1H), 7.73 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.36-7.24 (m, 6H), 5.16 (d, *J* = 4.3 Hz, 1H), 4.88 (ddd, *J* = 9.1, 4.3 Hz, 1H), 4.63 (dd, *J* = 9.1, 4.3 Hz, 1H), 4.43 (appt, *J* = 9.1 Hz, 1H), 2.56 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 155.41, 149.01, 135.28, 134.82, 133.74, 131.15, 129.20, 129.10, 127.76, 127.26, 118.63, 63.43, 61.52, 61.37, 20.11; IR (KBr): 3028, 2991, 1735, 1531, 1355, 1332, 727 cm^{-1}; HRMS (ESI): m/z [M+H]$^+$ calculated for $C_{17}H_{16}ClN_2O_4$: 347.0793; found: 347.0796.



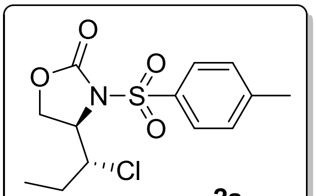
2q

3,3'-(Methylenebis(4,1-phenylene))bis(4-(chloro(phenyl)methyl)oxazolidin-2-one) **(2q)**. Compound **2q** was obtained in 44% (52 mg) yield according to the general procedure as a light brown oil; dr = 8:1 [determined by the ratio of area at δ 5.20 (d, *J* = 3.9 Hz, minor isomer), 5.16 (d, *J* = 3.0 Hz, major isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 7.51-7.06 (m, 18H), 5.22-5.10 (m, 2H), 4.78 (ddd, *J* = 9.1, 4.5 Hz, 2H), 4.58 (dd, *J* = 9.1, 4.5 Hz, 2H), 4.33 (appt, *J* = 9.1 Hz, 2H), 4.01-3.90 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 156.09, 139.14, 135.66, 133.85, 130.09, 129.12, 127.16, 124.13, 62.72, 62.28, 61.48, 40.97; IR (neat): 3030, 2918, 1747, 1716, 1514, 754, 731 cm^{-1}. HRMS (ESI): m/z [M+H]$^+$ calculated for $C_{33}H_{29}Cl_2N_2O_4$: 587.1499; found: 587.1492.



3r

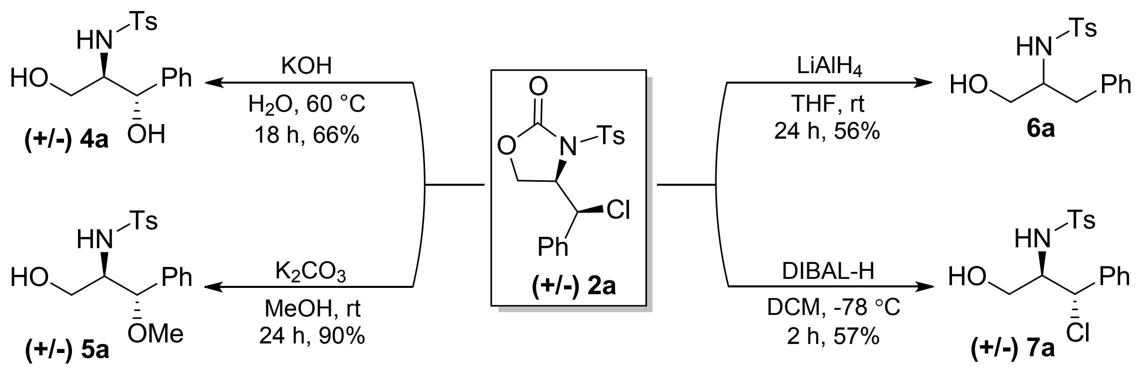
N-(Hex-1-en-3-yl)-4-methylbenzenesulfonamide **(3r)** – (CAS: 57981-16-5). Compound **3r** was obtained in 23% (11 mg) yield according to the general procedure as a white solid; mp: 54-56 °C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 7.73 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 5.53 (ddd, *J* = 17.0, 10.3, 6.6 Hz, 1H), 4.96 (m, 2H), 4.50 (d, *J* = 7.7 Hz, 1H), 3.76 (m, 1H), 2.41 (s, 3H), 1.49–1.38 (m, 1H), 1.30–1.21 (m, 1H), 0.83 (t, *J* = 7.2 Hz, 2H). Consistent with published data.[17]



2s

4-(1-Chloropropyl)-3-tosyloxazolidin-2-one **(2s)**. Compound **2s** was obtained in 60% (38 mg) yield according to the general procedure as a white solid; mp: 175-176 °C; dr >20:1 [determined by the ratio of area at δ 4.94 – 4.84 (m, minor isomer), 4.82 – 4.67 (m, major isomer) in ^{1}H NMR]. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): *δ* 7.95 (d, *J* = 8.3 Hz, 2H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.69 (d, *J* = 8.8 Hz, 2H), 4.77–4.72 (m, 1H), 4.47–4.41 (dd, *J* = 3.3, 9.7 Hz, 1H), 4.41–4.31 (m, 2H), 2.47 (s, 3H), 1.77–1.59 (m, 2H), 1.03 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): *δ* 151.92, 146.16, 134.42, 129.96, 128.42, 64.13, 62.45, 59.83, 22.78, 21.75, 10.91. HRMS (ESI): m/z [M+H]$^+$ calculated for $C_{13}H_{17}ClNO_4S$: 318.0561; found: 318.0569.

4. Derivatization Reactions of 2a and Characterization Data



Synthesis of *N*-(1,3-dihydroxy-1-phenylpropan-2-yl)-4-methylbenzenesulfonamide **(4a)**. In a 10 mL vial oxazolidinone **2a** (36.6 mg, 0.1 mmol, 1.0 equiv), KOH (28 mg, 0.5 mmol, 5.0 equiv) and 1.0 mL of water were added. The reaction was allowed to stir at 60 °C overnight. Then, the reaction was diluted with water (5 mL) and extracted with DCM (3x10 mL). The combined extracts were dried with Na_2SO_4, concentrated under vacuum, and purified by flash chromatography column to give the desired aminodiol **4a** in 66% (21 mg) yield as a white solid; mp: 90-93 °C. ^1H NMR (300 MHz, $CDCl_3$, ppm): δ 7.72 (d, J = 8.3 Hz, 2H), 7.33-7.18 (m, 7H), 5.98 (brs, OH), 4.89 (d, J = 3.7 Hz, 1H), 3.79-3.65 (m, 1H), 3.46-3.32 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 143.83, 140.26, 137.41, 129.98, 128.79, 128.07, 127.17, 125.76, 76.36, 61.44, 59.00, 21.68; IR (KBr): 3508, 3406, 1598, 1450, 1091, 750, 694 cm^{-1}. Consistent with published data.[25]

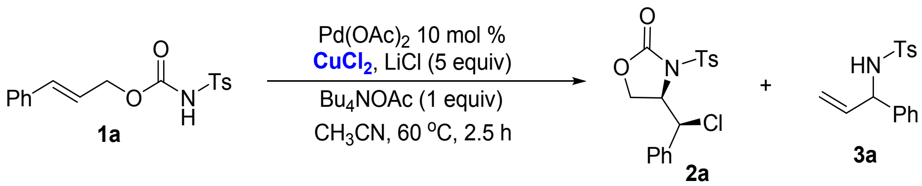
Synthesis of *N*-(3-hydroxy-1-methoxy-1-phenylpropan-2-yl)-4-methylbenzenesulfonamide **(5a)**. In a 20 mL vial oxazolidinone **2a** (110 mg, 0.3 mmol, 1.0 equiv.), K_2CO_3 (207 mg, 1.5 mmol, 5.0 equiv.) and 3.0 mL of MeOH were added. The reaction was allowed to stir at room temperature for 24 h. Then, the reaction was diluted with water (5 mL) and extracted with DCM (3x10 mL). The combined extracts were dried with Na_2SO_4, concentrated under vacuum and purified by flash chromatography column to give the desired product **5a** in 90% (90 mg) yield as a colorless oil; ^1H NMR (300 MHz, $CDCl_3$, ppm): δ 7.72 (d, J = 8.3 Hz, 2H), 7.37-7.12 (m, 7H), 5.58 (d, J = 8.5 Hz, 1H), 4.40 (d, J = 3.8 Hz, 1H), 3.72 (dd, J = 11.6, 3.3 Hz, 1H), 3.40-3.30 (m, 1H), 3.22 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 143.58, 137.77, 137.49, 129.85, 128.87, 128.25, 127.12, 126.53, 86.06, 60.66, 59.03, 58.15, 21.62; IR (neat): 3500, 3277, 1598, 1454, 1091, 759, 704 cm^{-1}. Consistent with published data.[25]

Synthesis of *N*-(1-hydroxy-3-phenylpropan-2-yl)-4-methylbenzenesulfonamide **(6a)** – (CAS: 170304-98-0). In a 10 mL vial oxazolidinone **2a** (73 mg, 0.2 mmol, 1.0 equiv.) was solubilized in 2.0 mL of anhydrous THF. $LiAlH_4$ (76 mg, 2.0 mmol, 10 equiv.) was added under nitrogen atmosphere. The reaction was allowed to stir at room temperature for 24 h. Then, the reaction was quenched with water (5 mL) and extracted with DCM (3x10 mL). The combined extracts were dried with Na_2SO_4, concentrated under vacuum and purified by flash chromatography column (7:3 hexane/AcOEt) to give the desired product **6a** in 57% (34 mg) yield as a white solid; mp: 70-74 °C; ^1H NMR (300 MHz, $CDCl_3$, ppm): δ 7.58 (d, J = 8.3 Hz, 2H), 7.24-7.14 (m, 5H), 7.03-6.94 (m, 2H), 4.72 (d, J = 7.1 Hz, 1H), 3.71-3.39 (m, 3H), 2.84-2.62 (m, 2H), 2.42 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 143.59, 136.92, 136.72, 129.85, 129.28, 128.86, 127.19, 126.93, 64.20, 56.65, 37.96, 21.68; IR (KBr): 3462, 3147, 1598, 1467, 1095, 746, 700 cm^{-1}. Consistent with published data.[26]

Synthesis of *N*-(1-chloro-3-hydroxy-1-phenylpropan-2-yl)-4-methylbenzenesulfonamide **(7a)**. In a 10 mL vial oxazolidinone **2a** (73 mg, 0.2 mmol, 1.0 equiv.) was solubilized in 2.0 mL of anhydrous DCM. The solution was cooled at -78 °C and DIBAL-H (2.0 mL, 1.0 M in Hexane) was added dropwise under nitrogen atmosphere. The reaction was allowed to stir at -78 °C for 2 h. After 1 h at room temperature a saturated solution of Rochelle's salt (10 mL) was slowly added, the mixture was allowed to stir for 1 h. Then, the reaction was extracted with DCM (3x10 mL). The combined extracts were dried with Na_2SO_4, concentrated under vacuum, and purified by flash chromatography column (7:3 hexane/AcOEt) to give the desired product **7a** in 56% (38 mg) yield as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.83 (d, J = 8.3 Hz, 2H), 7.33-7.27 (m, 5H), 7.19-7.11 (m, 2H), 4.33 (ddd, J = 13.1, 9.9, 3.0 Hz, 1H), 4.18 (ddd, J = 13.1, 8.5, 4.9 Hz, 1H), 4.03 (d, J = 4.4 Hz, 1H), 3.19 (ddd, J = 8.5, 4.4, 3.0 Hz, 1H), 3.12 (dd, J = 9.9, 4.9 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (300 MHz, $CDCl_3$, ppm): δ 144.55, 137.21, 134.72, 129.84, 128.78, 128.55, 127.30, 126.55, 60.83, 54.92, 46.46, 21.76; IR (neat): 3522, 3064, 1597, 1450, 1087, 813, 759, 698 cm-1; HRMS (ESI): m/z $[M-Cl^-]^+$ calculated for $C_{16}H_{18}NO_3S$: 304.1007; found: 304.1012; m/z $[M+NH_4]^+$ calculated for $C_{16}H_{22}ClN_2O_3S$: 357.1034; found: 357.1040.

5. Complete Details of Optimization of Reaction Conditions

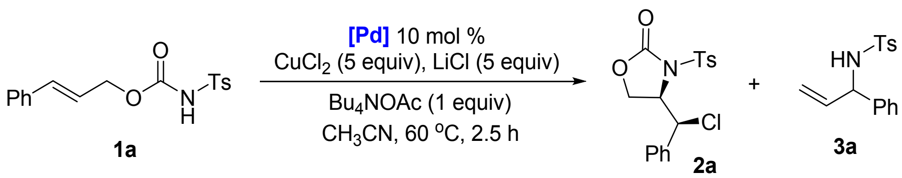
Table S1. Screening of Oxidant Loading[a]



Entry	$CuCl_2$	1a[b]	2a[b]	3a[b]
1	2 equiv	26%	30%	44%
2	3 equiv	10%	70%	20%
3	4 equiv	10%	75%	15%
4	***5 equiv***	***9%***	***76%***	***15%***

[a]Reactions conditions: **1a** (0.20 mmol), $Pd(OAc)_2$ (10 mol %), $CuCl_2$ (x mmol), Bu_4NOAc (0.2 mmol), LiCl (1.0 mmol) in CH_3CN (2.5 mL). [b]Compounds distribution determined by ^1H NMR spectroscopy of the crude reaction mixtures.

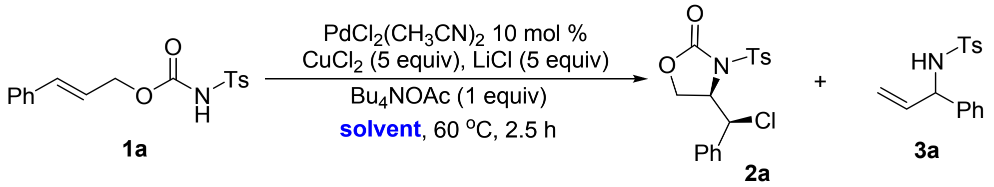
Table S2. Screening of Palladium Catalyst[a]



Entry	[Pd]	1a[b]	2a[b]	3a[b]
1	$PdCl_2$	10%	76%	14%
2	$Pd(OAc)_2$	6%	79%	15%
3	$Pd(TFA)_2$	14%	72%	14%
4	***$PdCl_2(CH_3CN)_2$***	***8%***	***79%***	***13%***
5	$PdCl_2(PhCN)_2$	9%	76%	15%
6	$Pd(NO_3)_2$	18%	68%	14%
7	$PdCl_2$(TMEDA)	61%	39%	-
8	$PdCl_2(PPh_3)_2$	39%	61%	-
9	$Pd(PPh_3)_4$	17%	68%	15%

[a]Reactions conditions: **1a** (0.20 mmol), [Pd] (10 mol %), $CuCl_2$ (1.0 mmol), Bu_4NOAc (0.2 mmol), LiCl (1.0 mmol) in CH_3CN (2.5 mL). [b]Compounds distribution determined by ^1H NMR spectroscopy of the crude reaction mixtures.

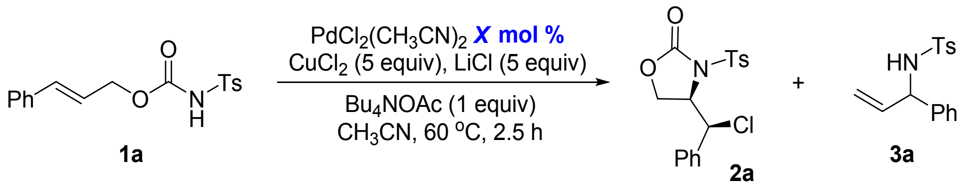
Table S3. Screening of Solvents[a]



Entry	Solvent	1a[b]	2a[b]	3a[b]
1	***CH_3CN***	***8%***	***79%***	***13%***
2	THF	16%	68%	16%
3	Toluene	10%	56%	17%
4	DCM	9%	47%	24%
5	Hexane	18%	63%	19%
6	MeOH	77%	23%	-
7	AcOEt	11%	62%	27%
8	DMF	63%	31%	6%
9	DMSO	51%	42%	7%
10	1,4-Dioxane	100%	-	-

[a]Reactions conditions: **1a** (0.20 mmol), $PdCl_2(CH_3CN)_2$ (10 mol %), $CuCl_2$ (1.0 mmol), Bu_4NOAc (0.2 mmol), LiCl (1.0 mmol) in solvent (2.5 mL). [b]Compounds distribution determined by ^1H NMR spectroscopy of the crude reaction mixtures.

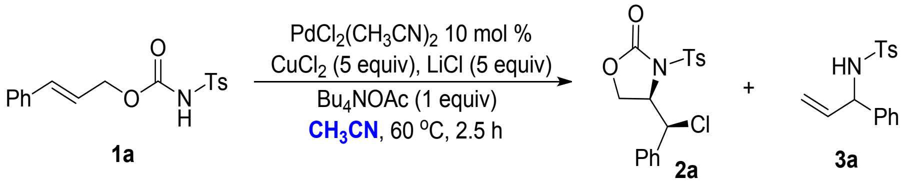
Table S4. Screening of Catalyst Loading[a]



Entry	$PdCl_2(CH_3CN)_2$	1a[b]	2a[b]	3a[b]
1	***10 mol %***	***8%***	***79%***	***13%***
2	5 mol %	54%	46%	-
3	1 mol %	85%	15%	-
4	0.1 mol %	99%	1%	-

[a]Reactions conditions: **1a** (0.20 mmol), $PdCl_2(CH_3CN)_2$ (*x* mol %), $CuCl_2$ (1.0 mmol), Bu_4NOAc (0.2 mmol), LiCl (1.0 mmol) in CH_3CN (2.5 mL). [b]Compounds distribution determined by ^1H NMR spectroscopy of the crude reaction mixtures.

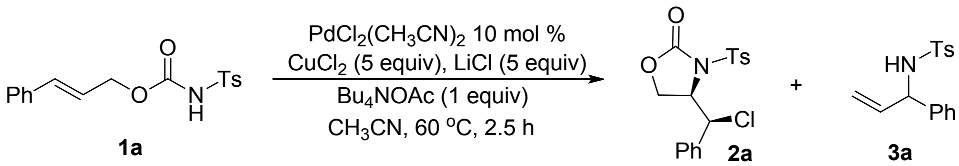
Table S5. Screening of Concentration of Substrate[a]



Entry	Concentration	1a[b]	2a[b]	3a[b]
1	0.08 M	25%	66%	9%
2	0.10 M	9%	77%	14%
3	0.15 M	8%	77%	15%

[a]Reactions conditions: **1a** (0.20 mmol), $PdCl_2(CH_3CN)_2$ (10 mol %), $CuCl_2$ (1.0 mmol), Bu_4NOAc (0.2 mmol), LiCl (1.0 mmol) in CH_3CN (*x* mL). [b]Compounds distribution determined by ^1H NMR spectroscopy of the crude reaction mixtures.

Table S6. Control Experiments of Synthesis of **2a**[a]



Entry	$PdCl_2(CH_3CN)_2$	$CuCl_2$	LiCl	Bu_4NOAc	1a[b]	2a[b]	3a[b]
1[c]	-	+	+	+	100%	-	-
2[d]	+	-	+	+	13%	-	87%
6[d]	+[e]	-	+	+	60%	-	40%
3[f]	+	+	-	+	100%	-	-
4[g]	+	+	+	-	85%	10%	5%
5	+	+	+	+	8%	80%	12%

[a]Reaction conditions: **1a** (0.20 mmol), $PdCl_2(CH_3CN)_2$ (10 mol %), $CuCl_2$ (1.0 mmol), Bu_4NOAc (0.2 mmol), LiCl (1.0 mmol) in CH_3CN. [b]Compounds distribution determined by ^1H NMR spectroscopy of the crude reaction mixtures. [c]Without $PdCl_2(CH_3CN)_2$. [d]Without $CuCl_2$. [e]$PdCl_2(CH_3CN)_2$ (100 mol %). [f]Without LiCl. [g]Without Bu_4NOAc.

6. ^{1}H NMR Titration Experiments Procedure (at 25 °C)

A solution (A) of $PdCl_2(CH_3CN)_2$ (5.2 mg, 0.02 mmol, 1.0 equiv) and carbamate **1a** (6.63 mg, 0.02 mmol, 1.0 equiv) in CD_3CN (1.0 mL, *c* = 0.02 M) was prepared. A solution (B) of tetrabuthylammonium acetate (Bu_4NOAc, 6.0 mg, 0.02 mmol, 1.0 equiv) in CD_3CN (1.0 mL, *c* = 0.02 M) was prepared.

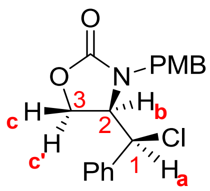
Figure 2 presents the titration of a 1:1 mixture of **1a** and $PdCl_2(CH_3CN)_2$ up to an equimolar amount of Bu_4NOAc leading to the gradual formation of two new sets of signals. After 10 minutes from the solution (A) preparation a ^{1}H NMR spectrum was recorded and showed no reaction (bottom spectrum – 0 mol % of Bu_4NOAc). Then to 0.4 mL of solution (A) were added stepwise 20 µL of solution (B) (0.05 equiv Bu_4NOAc). After each addition, a ^{1}H NMR spectra was recorded at 10-minutes intervals. After the addition of 20 mol % Bu_4NOAc (80 µL of solution B in total) addition was continued in 40 µL steps (0.10 equiv Bu_4NOAc) up to 1.0 equiv of tetrabuthylammonium acetate was added in total.

7. Relative Stereochemistry Determination

Compound 2o

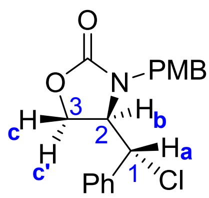
The relative stereochemistry of the major and minor **2o** diastereomers was determined by comparing the NMR data with those described by Xu and co-workers[24] for the characterization of both diastereomers. The main aspects of the ^{1}H and ^{13}C NMR to differentiate both **2o** diastereomers involve the signals of the hydrogens designated as Ha; Hb; Hc; and Hc' as well as carbons C_1; C_2; and C_3. The Table S7 below collect the data related to these hydrogens and carbons obtained for the major and minor **2o** diastereomers and compared to those described in the literature. A determining feature in the differentiation between **2o** diastereomers involves the coupling constant data between Ha and Hb; for the major diastereomer (*anti*-addition product) J_{HaHb} = 3.2 Hz, while for the minor diastereomer (*syn*-addition product) J_{HaHb} = 4.0 Hz. The determined trend for the J_{HaHb} coupling constants for the **2a-s** diastereomers products, follow, in general, the same diagnostic described above for the **2o** diastereomers.

Table S7. Selected relevant NMR signals data (δ in ppm) of major and minor **2o** diastereomers[a]



2o (maj diast)

2o (maj diast)		
Hydrogen	**2o** (maj diast)	Literature data[24]
Ha	5.11 (d, *J* = 3.2 Hz)	5.11 (d, *J* = 3.2 Hz)
Hb	4.68 (ddd, *J* = 9.1, 4.8, 3.2 Hz)	4.68 (ddd, *J* = 8.8, 4.8, 3.2 Hz)
Hc	4.58 (dd, *J* = 9.1, 4.8 Hz)	4.60 (dd, *J* = 9.2, 4.8 Hz)
Hc’	4.33 (appt, *J* = 9.1 Hz)	4.34 (t, *J* = 9.0 Hz)
Carbon		
C_1	61.64	61.6
C_2	62.92	63.0
C_3	62.70	62.7

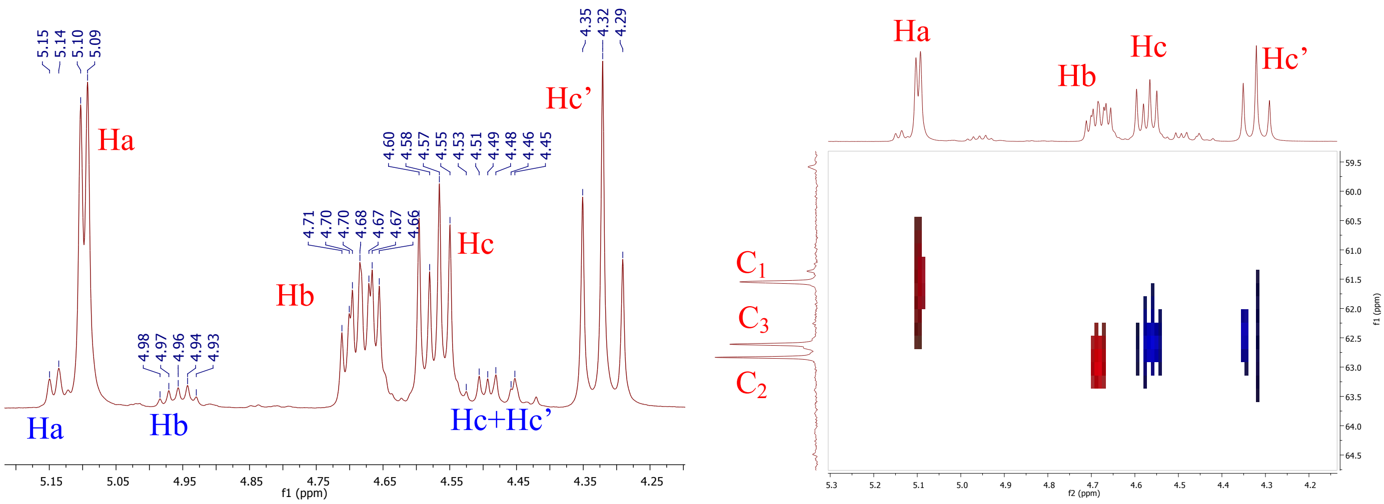


2o (min diast)

2o (min diast)		
Hydrogen	**2o** (min diast)	Literature data[24]
Ha	5.14 (d, *J* = 4.0 Hz)	5.15 (d, *J* = 4.0 Hz)
Hb	4.96 (dt, *J* = 8.1, 4.0 Hz)	4.98-4.93 (m Hz)
Hc	4.53-4.48 (m)	4.53 (dd, *J* = 9.6, 3.7 Hz)
Hc’	4.46-4.45 (m)	4.46 (t, *J* = 9.1 Hz)
Carbon		
C_1	59.7	59.6
C_2	61.5	61.5
C_3	62.7	62.7

[a] ^{1}H (300 MHz) and ^{13}C NMR (75 MHz) NMR (in $CDCl_3$)

The Figure S1 illustrates the partial spectra of ^{1}H NMR (image on the left) and 2D HSQC NMR (image on the right) used for the chemical shift assignments and, consequently, for the designation of the relative stereochemistry of the major and minor **2o** diastereomer. To analyze the complete ^{1}H, ^{13}C, COSY and HSQC NMR spectra obtained for compound **2o**, see pages S185-S188.



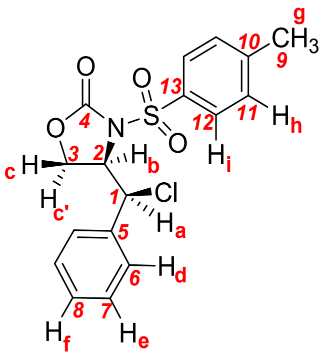
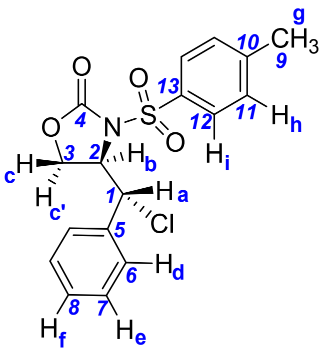
(a) **(b)**

Figure S1. (a) Partial ^{1}H NMR spectra (5.2 – 4.2 ppm) of compound **2o**; (b) Partial 2D HSQC NMR spectra (δ_C/δ_H 65.0 – 59.0/5.3 – 4.1 ppm) of compound **2o**.

Compound 2a

The relative stereochemistry of **2a** diastereomers was designed based on ^{1}H, ^{13}C, COSY, HSQC, HMBC, and NOESY NMR analysis data. Table S8 shows the chemical shift assignments for major and minor **2a** diastereomers. The determined trend of the ^{1}H and ^{13}C NMR data for the **2a** diastereomers products, follow, in general, the same diagnostic described above for the **2o** diastereomers. The main aspects of the ^{1}H and ^{13}C NMR to differentiate both **2a** diastereomers involve the signals of the hydrogens designated as Ha; Hb; Hc; and Hc' as well as carbons C_1; C_2; and C_3. As for **2o** diastereomers, the determining feature in the differentiation between **2a** diastereomers involves the coupling constant data between Ha and Hb; for the major diastereomer (*anti*-addition product) J_{HaHb} = 2.5 Hz, while for the minor diastereomer (*syn*-addition product) J_{HaHb} = 4.0 Hz. Also, the NOE's between hydrogens **Ha-Hb**, **Ha-Hd**, **Ha-Hi**, **Ha-Hc'**, and **Ha-Hd**, were valuable in establishing the **2a** major diastereomer relative stereochemistry.

Table S8. Complete assigned hydrogens and carbons of the ^{1}H and ^{13}C NMR signals data (δ in ppm) of major and minor **2a** diastereomers[a]

		2a (maj diast)		
 **2a** (maj diast)	Hg	2.47 (s)	C9	21.76
	Hc’	4.13 (appt, *J* = 9.3 Hz)	C2	61.37
	Hc	4.42 (dd, *J* = 9.3, 3.7 Hz)	C1	62.75
	Hb	4.89 (ddd, *J* = 8.9, 3.7, 2.5 Hz)	C3	62.95
	Ha	5.80 (d, *J* = 2.5 Hz)	C6	127.03
	Hd+He+Hf+Hh	7.50-7.34 (m)	C12	128.65
	Hi	8.02 (d, *J* = 8.4 Hz)	C7	129.18
			C8	129.18
			C11	129.83
			C13	134.51
			C5	134.74
			C10	145.93
			C4	151.98
		2a (min diast)		
 **2a** (min diast)	Hg	2.40 (s)	C9	21.49
	Hc’	4.26 (dd, *J* = 9.4, 8.6 Hz)	C2	61.01
	Hc	4.50 (dd, *J* = 9.7, 2.8 Hz)	C1	60.46
	Hb	4.78 (ddd, *J* = 6.4, 4.0, 2.8 Hz)	C3	63.40
	Ha	5.55 (d, *J* = 4.0 Hz)	C6	127.21
	Hd+He+Hf+Hh	7.50-7.34 (m)	C12	128.79
	Hi	7.97 (d, *J* = 8.3 Hz)	C7	128.16
			C8	128.36
			C11	130.04
			C13	132.51
			C5	137.11
			C10	146.18
			C4	151.34

[a] ^{1}H (300 MHz) and ^{13}C NMR (75 MHz) NMR (in $CDCl_3$)

The Figures S2-S4 illustrates the partial spectra of COSY, HSQC and NOESY NMR, respectively used for the chemical shift assignments and, consequently, for the designation of the relative stereochemistry of the major and minor **2a** diastereomer. To analyze the complete ^{1}H, ^{13}C, COSY, HSQC, HMBC, and NOESY NMR spectra obtained for compound **2a**, see pages S133-S138.

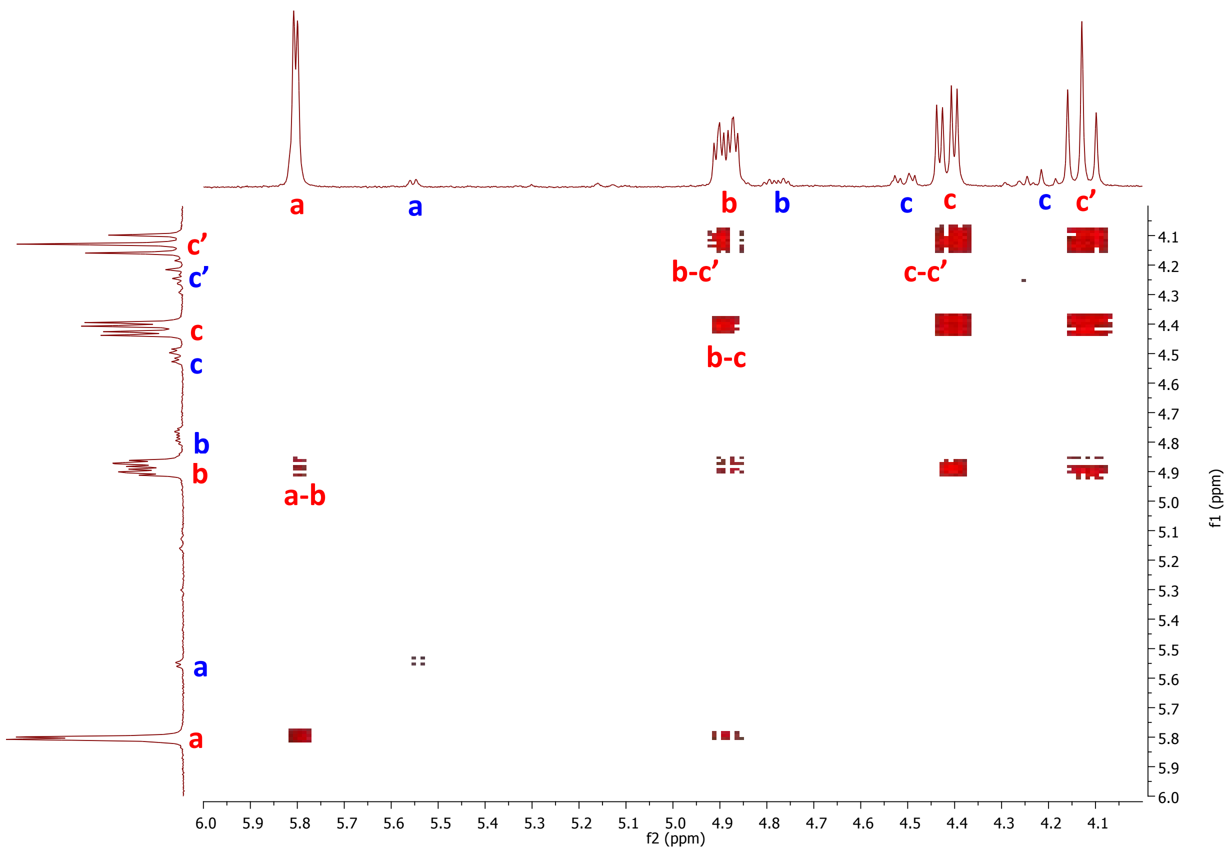


Figure S2. Partial COSY NMR spectra of compound **2a**

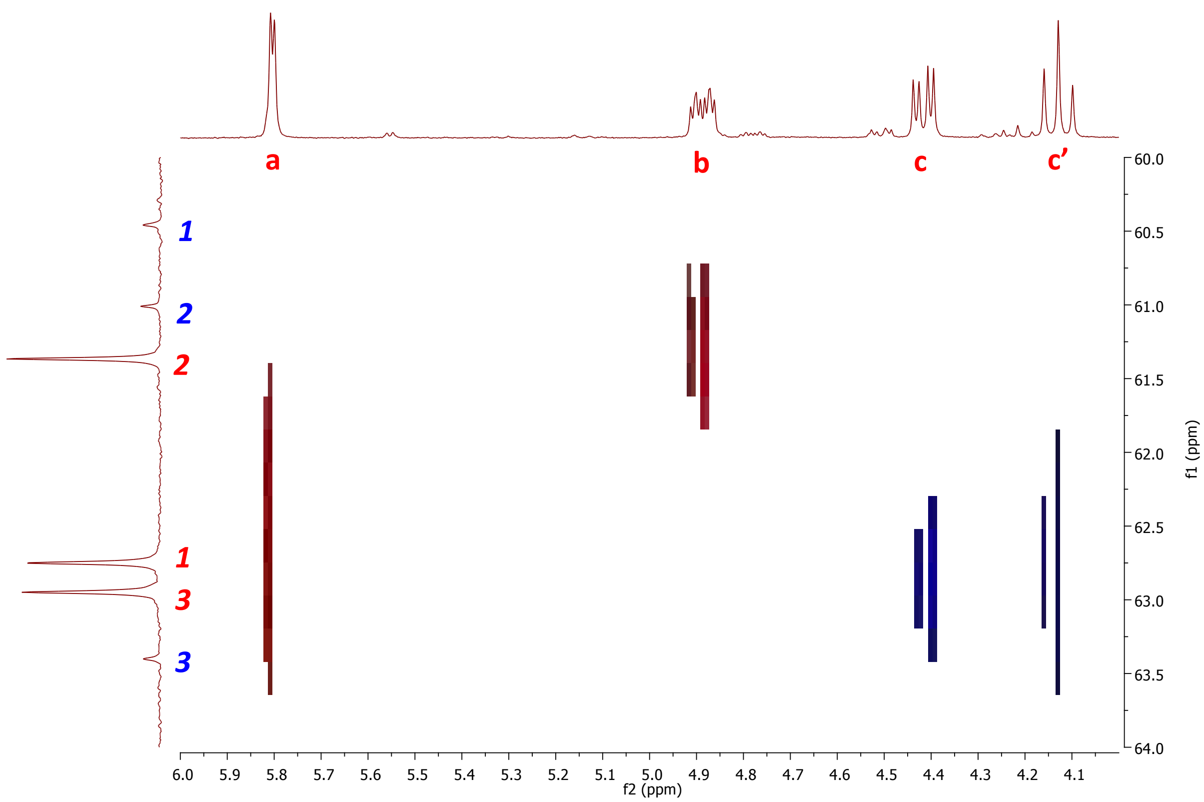


Figure S3. Partial HSQC NMR spectra of compound **2a**

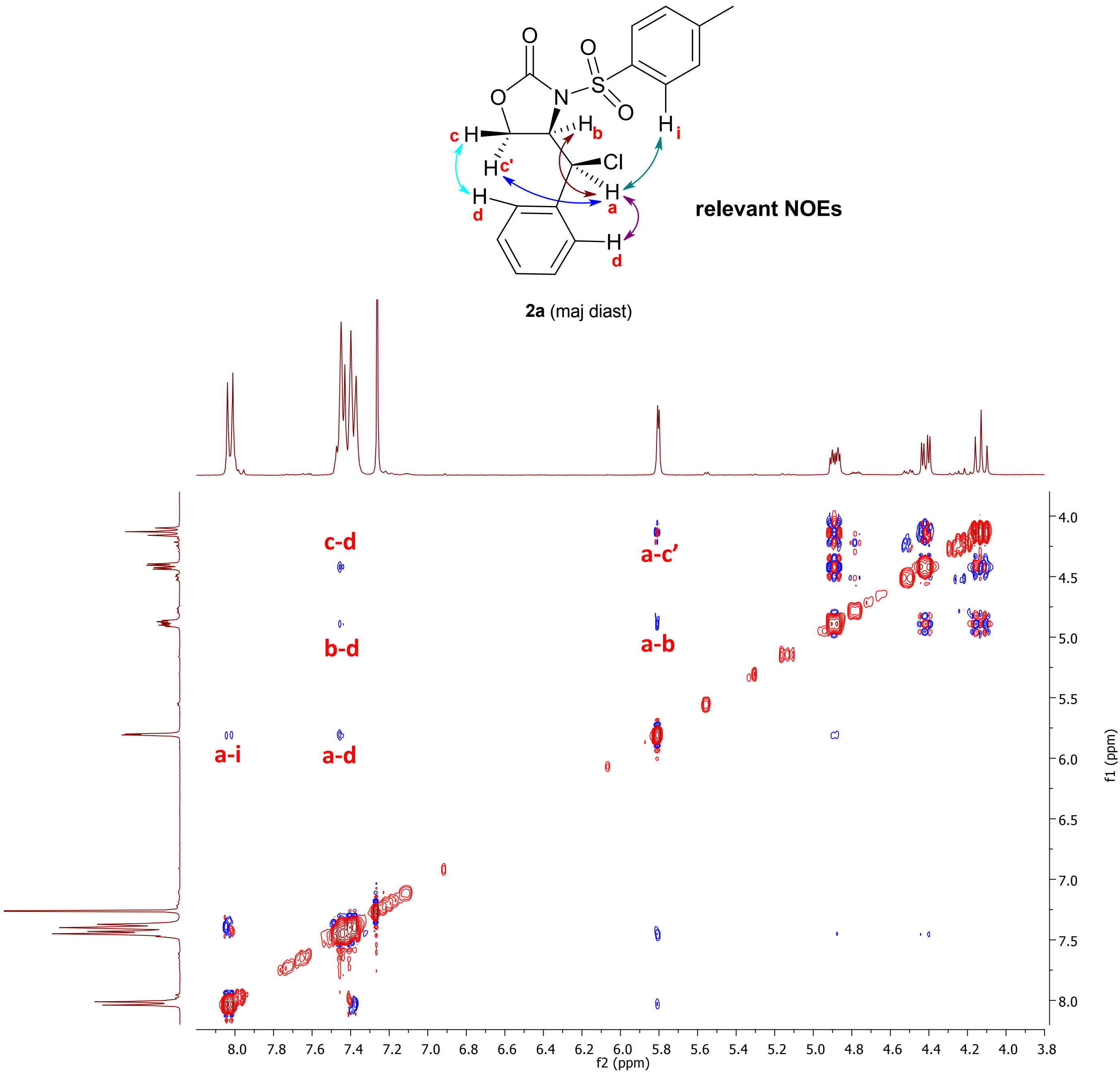
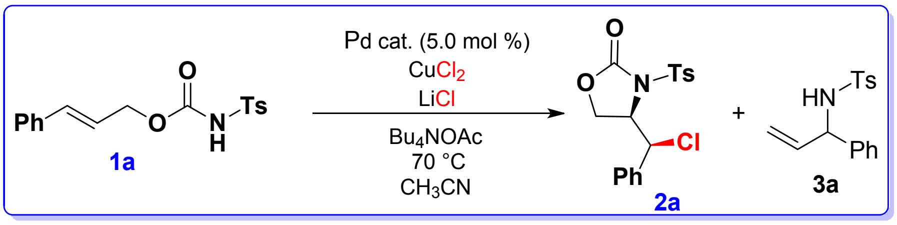


Figure S4. Partial NOESY NMR spectra of compound **2a**

8. Real-time Reaction Monitoring

The reaction was studied by electrospray ionization mass spectrometry (ESI-MS) coupled with pressurized sample infusion (PSI), using a Waters Acquity Triple Quadrupole Detector (TQD) mass spectrometer. PSI-ESI-MS allowed real-time analysis of reaction by applying 5 psi of N_2 to the reaction vessel which enabled transfer of the reaction mixture to the ESI source via a PEEK tubing at an estimated flow rate of 40 µL/min. The MS parameters used were as follows: capillary voltage 3.0 kV; cone voltage 15 V; extraction voltage 3.0 V; temperature source 90 °C; cone gas flow rate 100 L/h; desolvation gas flow rate, 100 L/h; scan time was set to 5 s. MS/MS experiments were carried out with high purity argon (99.999%) and the collision energy ranged from 5 to 40 V.

For these experiments, the specific substrate and reaction conditions described in Scheme S2 was carried out by adding the reagents under magnetic stirring separately every 2 minutes, allowing the reaction evolution after each addition. Therefore, to a flask containing 10 mL of CH_3CN, 0.02 mol/L (1.0 mL) of carbamate was added (0 min) and then, after 2 min, a solution of the $PdCl_2(CH_3CN)_2$ catalyst (0.004 mmol in 1.0 mL of CH_3CN diluted to a final carbamate concentration of 5%). Then, 20 nmol/L (1.0 mL) of tetrabutylammonium acetate were added at 4 min and 30.0 µmol/L (1.0 mL) of $CuCl_2$ were added at 6 min. Finally, 0.07 mol/L (1.0 mL) of LiCl was added at 8 min. The reaction was kept at 70 °C for a total time of 20 min.



Scheme S2. Specific Pd-mediated carbamate cyclization reaction and reaction conditions used for the ESI-PSI-MS experiments

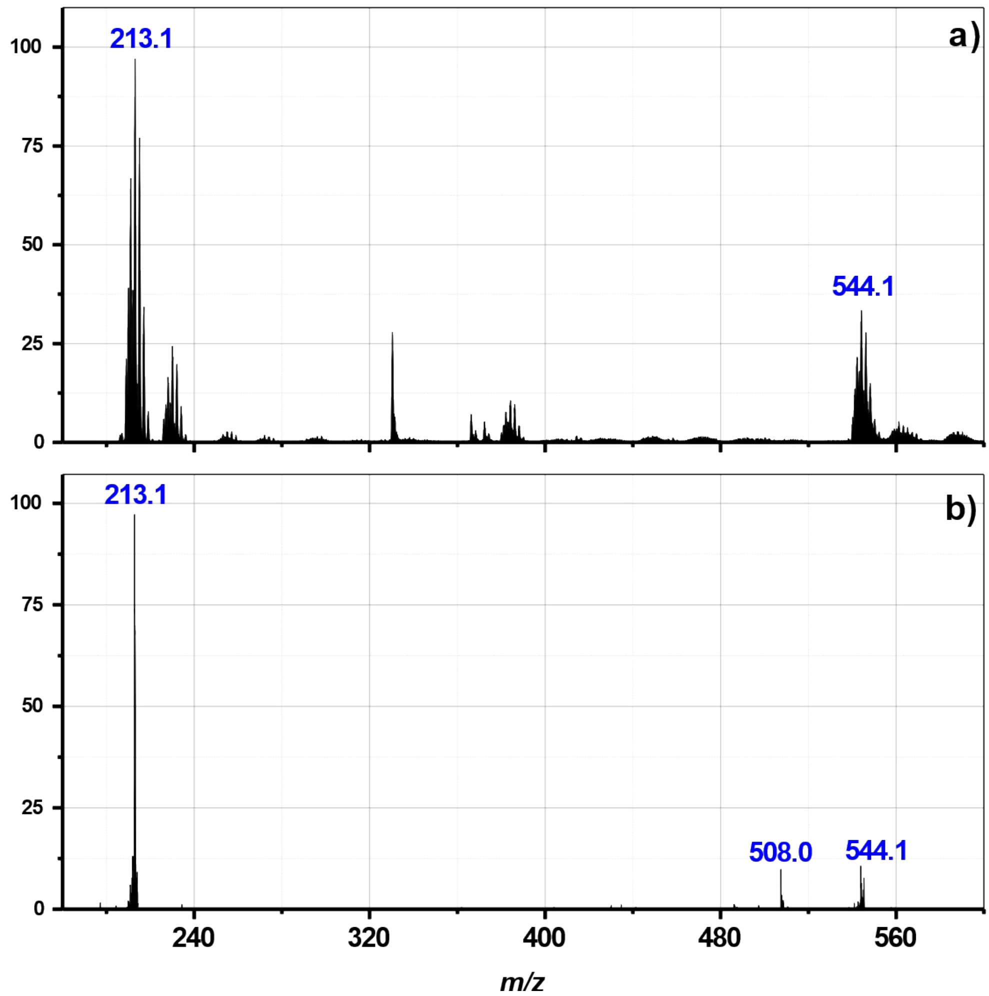


Figure S5. Mass spectra, a) online reaction, b) CID of intermediate *m/z* 544

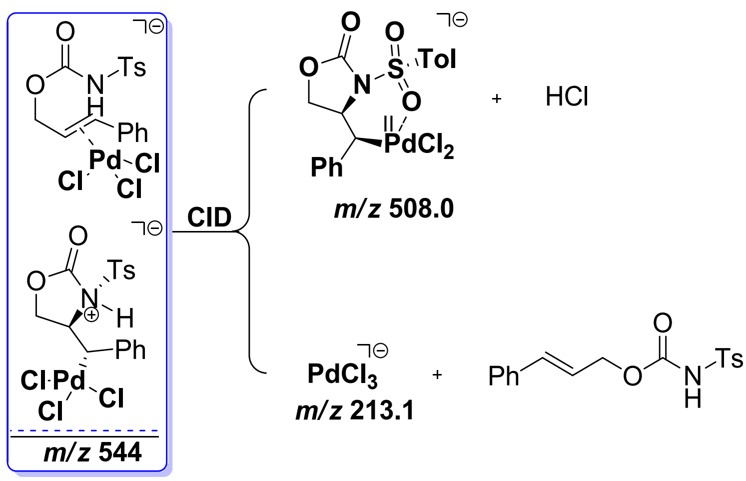


Figure S6. CID of the intermediate (**XIVb**, **XVb**; isomers)

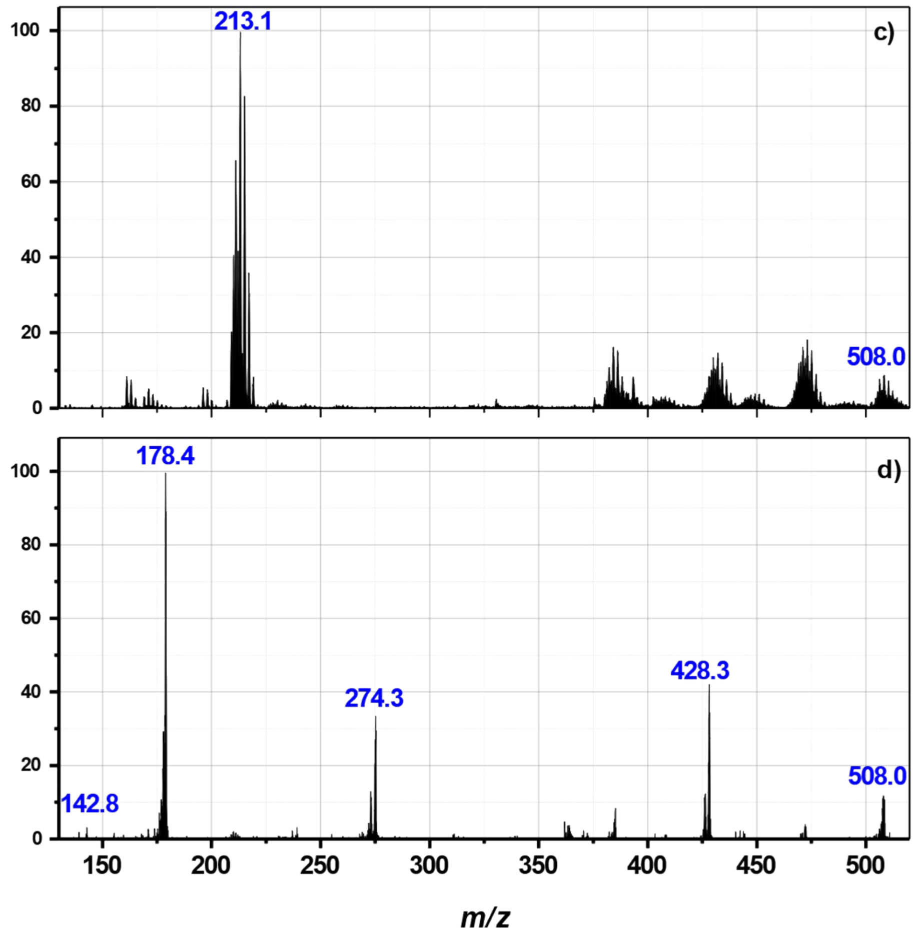


Figure S7. Mass spectra, c) online reaction (3 min), d) CID of intermediate *m/z* 508

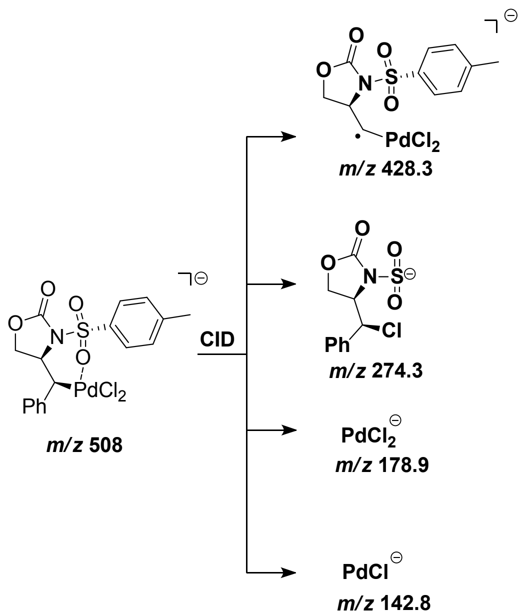


Figure S8. Intermediate CID (**XVIa**)

9. Computational Details

All quantum mechanical calculations were carried out using GAUSSIAN-09 (Revision *C.01*)[27] employing the empirically parameterized hybrid PBE1PBE[28–31] functional for optimizations at the 6-31G(d,p)[32–34] level for the non-metal atoms and Def2-TZVPP[35] level for palladium and copper atoms. The standard Berny algorithm in redundant coordinates and default criteria of convergence were employed. For each optimized ground state, the frequency analysis showed the absence of imaginary frequencies, whereas each transition state showed a single imaginary frequency. All transition structures (TSs) were obtained using the QST2 or QST3 (as implemented in GAUSSIAN) depending on the necessity. All transition states were confirmed following the reaction coordinate in both directions. Solvation obtained with the polarizable continuum model (PCM) on the electronic density (SMD),[36] with CH_3CN as solvent at 333.15 K were included in all single point calculations. All the energies are relative Gibbs energies in kcal mol^{-1}, obtained from single point calculations on the SMD continuum model utilizing M06-2X[37] functional at the 6-311++g(2df,2pd) basis set for the non-metal atoms and Def2-TZVPP level for palladium and copper atoms. We selected combinations of theory levels commonly employed in the literature to study similar mechanisms reactions that has been shown to deliver good results. Thus, we employed theory levels commonly utilized in the literature to study similar reaction mechanisms, for example, analogous to those reported by Poli, Calhorda and,[38,39] Houk and collaborators[40] as well as those compiled by Schoenebeck and collaborators.[41,42] Other works follow the similar methodology as studies of Xue Li and collaborators,[43] Tai-Yuan Lai and collaborators.[44] An extensive analysis of the various possibilities of conformational arrangements and different orientations of reactants that are aligned with the mechanistic proposals presented in this paper were conducted. The 3D structural representations were generated using CYLview software (Legault, C. Y. CYLview version 1.0 BETA, Université de Sherbrooke, 2009 (http://www.cylview.org).

10. References

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11. Cartesian Coordinates (Å) and Energies (hartree) of all the Structures.

Li_2PdCl_4:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -1983.376454
Thermal correction to Gibbs Free Energy = -0.030004
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -1984.03147834

46	0.000001000	0.000007000	-0.000016000
17	-1.627941000	-1.686821000	-0.000259000
17	1.627912000	-1.686846000	0.000230000
17	1.628032000	1.686798000	0.000264000
17	-1.627999000	1.686819000	-0.000293000
3	-3.039438000	0.000118000	0.001872000
3	3.039402000	0.000061000	-0.001303000

LiCl:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -467.620671
Thermal correction to Gibbs Free Energy = -0.019286
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -467.832346279

3	0.000000000	0.000000000	-1.747009000
17	0.000000000	0.000000000	0.308296000

2LiCl:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -935.310031
Thermal correction to Gibbs Free Energy = -0.023554
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -935.703763390

17	0.000000000	1.795396000	-0.000039000
17	0.000000000	-1.795396000	-0.000039000
3	-1.321027000	0.003145000	0.000219000
3	1.321027000	-0.003145000	0.000219000

AcOH:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -228.802122
Thermal correction to Gibbs Free Energy = 0.036477
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -229.087660858

6	1.387035000	-0.154814000	0.000003000
1	1.609907000	-1.221324000	0.000015000
1	1.830295000	0.318112000	0.879786000
1	1.830316000	0.318096000	-0.879778000
6	-0.090396000	0.115779000	-0.000019000
8	-0.596289000	1.212100000	0.000005000
8	-0.816979000	-1.017697000	0.000002000
1	-1.744212000	-0.735892000	0.000011000

$2CuCl_2$:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -5120.841370
Thermal correction to Gibbs Free Energy = -0.033118
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -5121.91060845

29	2.246639000	0.000105000	0.000500000
29	-0.666470000	0.000021000	-0.000430000
17	0.879298000	1.707326000	-0.000192000
17	0.879606000	-1.707296000	-0.000668000
17	-2.227387000	1.467304000	0.000093000
17	-2.227101000	-1.467547000	0.000647000

2CuCl:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -0.029806
Thermal correction to Gibbs Free Energy = -4200.796992
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -4201.55905977

29	0.000001000	-1.210774000	-0.000001000
29	-0.000001000	1.210780000	-0.000001000
17	-1.918802000	-0.000007000	0.000001000
17	1.918802000	-0.000004000	0.000001000

TMA-AcO:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -442.162843
Thermal correction to Gibbs Free Energy = 0.176230
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -442.829264690

6	2.185551000	0.047342000	0.000596000
6	3.698271000	-0.165367000	0.000451000
1	3.984354000	-0.769857000	0.866917000
1	3.987642000	-0.733699000	-0.889322000
1	4.233693000	0.785426000	0.019527000
8	1.761331000	1.225675000	-0.000210000
8	1.480140000	-1.007816000	-0.000328000
7	-1.723534000	-0.005007000	0.000011000
6	-1.221778000	-0.727977000	-1.211284000
1	-0.129614000	-0.828027000	-1.087410000
1	-1.694975000	-1.711956000	-1.241879000
1	-1.497439000	-0.151461000	-2.096129000
6	-1.220618000	-0.723150000	1.213677000
1	-0.128697000	-0.824325000	1.088956000
1	-1.494697000	-0.142690000	2.096433000
1	-1.694343000	-1.706710000	1.249100000
6	-1.170525000	1.386958000	-0.003020000
1	-1.541152000	1.897668000	0.888723000
1	-0.054977000	1.333602000	-0.002778000
1	-1.541267000	1.893824000	-0.896903000
6	-3.205318000	0.034549000	0.000665000
1	-3.593442000	-0.985769000	0.002693000
1	-3.547371000	0.562605000	0.892593000
1	-3.548239000	0.559423000	-0.892804000

TMA-Cl:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -674.024242
Thermal correction to Gibbs Free Energy = 0.133188
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -674.590282473

7	-1.006227000	0.000021000	-0.000036000
6	-0.487550000	-0.870639000	-1.103491000
1	-0.857608000	-1.885022000	-0.942894000
1	-0.858903000	-0.479760000	-2.052738000
1	0.613911000	-0.827664000	-1.049926000
6	-2.488619000	-0.000289000	0.000366000
1	-2.846144000	-1.020667000	0.149768000
1	-2.846495000	0.638998000	0.809400000
1	-2.846927000	0.380380000	-0.957768000
6	-0.486922000	-0.520325000	1.305515000
1	-0.857622000	0.125079000	2.104099000
1	-0.857592000	-1.538157000	1.440963000
1	0.614555000	-0.494590000	1.240809000
6	-0.487927000	1.391186000	-0.202325000
1	-0.858367000	1.759790000	-1.160813000
1	-0.859375000	2.017328000	0.611147000
1	0.613578000	1.323763000	-0.192058000
17	2.505687000	0.000046000	-0.000008000

1a:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -1410.284937
Thermal correction to Gibbs Free Energy = 0.260272
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -1411.81643219

6	-0.583333000	1.990307000	0.192099000
8	0.249045000	2.786298000	-0.511693000
6	1.196222000	2.245469000	-1.442593000
1	2.865433000	2.262390000	-0.015104000
1	0.705843000	1.523547000	-2.107429000
1	1.480155000	3.115833000	-2.042983000
1	2.388818000	-0.115157000	-1.900408000
16	-1.095438000	-0.511063000	1.118373000
8	-1.205503000	-0.036794000	2.483535000
8	-0.367207000	-1.729873000	0.791151000
6	-2.710650000	-0.583945000	0.401321000
6	-2.967928000	-1.547377000	-0.569704000
6	-3.702640000	0.286316000	0.846644000
6	-4.244108000	-1.627353000	-1.112176000
1	-2.181247000	-2.230571000	-0.872542000
6	-4.969864000	0.190168000	0.287760000
1	-3.470392000	1.023724000	1.606035000
6	-5.259598000	-0.759753000	-0.697818000
1	-4.459044000	-2.381551000	-1.864540000
1	-5.752426000	0.863689000	0.626823000
8	-1.531723000	2.455219000	0.768528000
1	0.660399000	0.328929000	-0.071163000
6	4.129245000	-0.167599000	-0.614189000
6	4.358472000	-1.521718000	-0.891213000
6	5.074942000	0.525896000	0.154916000
6	5.485598000	-2.170677000	-0.401360000
1	3.635161000	-2.071297000	-1.488496000
6	6.200864000	-0.121646000	0.643468000
1	4.936523000	1.583373000	0.359805000
6	6.409990000	-1.472586000	0.369451000
1	5.641401000	-3.222501000	-0.621654000
1	6.924077000	0.430821000	1.236052000
1	7.293330000	-1.975595000	0.751388000
6	-6.629126000	-0.831265000	-1.309690000
1	-6.830341000	-1.820308000	-1.729248000
1	-6.728820000	-0.102036000	-2.122343000
1	-7.406781000	-0.605906000	-0.574655000

2a – maj diast:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -1869.754087
Thermal correction to Gibbs Free Energy = 0.254240
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -1871.44641308

7	-2.332305000	-0.991961000	1.861791000
6	-1.202916000	-0.244625000	2.189108000
8	-0.963456000	0.294354000	3.232823000
8	-0.376941000	-0.252536000	1.123531000
6	-2.340518000	-1.419437000	0.476140000
6	-3.397096000	-0.712232000	-0.394160000
1	-4.363389000	-0.841689000	0.097742000
1	-2.554637000	-2.490284000	0.409845000
6	-3.449510000	-1.329713000	-1.771483000
6	-4.150157000	-2.533346000	-1.906677000
6	-2.794090000	-0.797718000	-2.881805000
6	-4.186524000	-3.196251000	-3.128046000
1	-4.677159000	-2.944928000	-1.048337000
6	-2.833180000	-1.462498000	-4.104925000
1	-2.275967000	0.152507000	-2.795966000
6	-3.525173000	-2.662510000	-4.231458000
1	-4.740504000	-4.125810000	-3.220052000
1	-2.325057000	-1.033725000	-4.963696000
1	-3.557780000	-3.175613000	-5.187967000
16	-3.603835000	-1.306156000	2.947843000
8	-4.077143000	-0.051778000	3.493552000
8	-4.473083000	-2.183405000	2.169692000
6	-2.845113000	-2.249473000	4.236613000
6	-2.237923000	-1.591665000	5.303990000
6	-2.894305000	-3.639830000	4.168552000
6	-1.659995000	-2.354063000	6.310408000
1	-2.210743000	-0.508478000	5.327144000
6	-2.312995000	-4.380440000	5.188858000
1	-3.396160000	-4.122546000	3.336444000
6	-1.688433000	-3.752025000	6.271634000
1	-1.177250000	-1.852272000	7.144562000
1	-2.348607000	-5.465857000	5.148052000
17	-3.102735000	1.058191000	-0.414721000
6	-1.089451000	-4.561417000	7.385358000
1	-1.829236000	-4.739967000	8.174610000
1	-0.746726000	-5.537484000	7.031879000
1	-0.241877000	-4.045099000	7.843721000

2a – min diast:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -1869.751052
Thermal correction to Gibbs Free Energy = 0.254821
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -1871.44427590

6	4.417171000	-0.082825000	2.521484000
7	2.482720000	1.077019000	2.854207000
6	3.453566000	0.326720000	3.640244000
16	1.915985000	2.632314000	3.313045000
8	2.475059000	2.828357000	4.641860000
6	2.847277000	-0.916819000	4.312422000
8	2.227144000	3.529594000	2.216827000
1	3.917748000	0.972598000	4.387209000
1	4.868869000	-1.064059000	2.671831000
1	5.201539000	0.666817000	2.373132000
6	0.160732000	2.467903000	3.433448000
6	-0.600857000	2.398048000	2.268034000
6	-0.428055000	2.477257000	4.693269000
6	-1.981102000	2.318886000	2.384280000
1	-0.112865000	2.392679000	1.299098000
6	-1.812978000	2.405958000	4.782869000
1	0.195258000	2.549111000	5.577764000
6	-2.607529000	2.320617000	3.636496000
1	-2.586893000	2.261606000	1.483818000
1	-2.285010000	2.419863000	5.761528000
6	3.881239000	-1.688895000	5.087202000
6	4.534230000	-1.115538000	6.182819000
6	4.227647000	-2.980944000	4.688374000
6	5.520018000	-1.822741000	6.859944000
1	4.250884000	-0.121796000	6.519864000
6	5.216960000	-3.688851000	5.366464000
1	3.715266000	-3.438139000	3.845045000
6	5.865653000	-3.109891000	6.451863000
1	6.018306000	-1.370103000	7.712043000
1	5.475121000	-4.694367000	5.047940000
1	6.635327000	-3.661072000	6.983894000
1	2.411930000	-1.553243000	3.536250000
6	2.543111000	0.700653000	1.505911000
8	1.797502000	1.015268000	0.623084000
8	3.595740000	-0.137384000	1.351499000

17	1.464522000	-0.447698000	5.367025000
6	-4.101544000	2.212435000	3.741145000
1	-4.598951000	2.778073000	2.948149000
1	-4.421773000	1.168313000	3.645441000
1	-4.464100000	2.581067000	4.703995000

3a:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -1221.923232
Thermal correction to Gibbs Free Energy = 0.242161
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -1223.23172029

6	0.435780000	0.059100000	-0.962344000
6	-0.218888000	1.075033000	-0.063479000
7	-1.683871000	1.073432000	-0.202960000
6	1.067920000	-1.024226000	-0.520091000
1	0.348469000	0.245454000	-2.033569000
1	1.151076000	-1.234322000	0.543063000
1	1.503591000	-1.747141000	-1.203022000
1	-0.025359000	0.788746000	0.976905000
16	-2.536246000	-0.202069000	0.482548000
8	-1.754533000	-0.636542000	1.634945000
8	-2.956702000	-1.141436000	-0.552236000
6	-3.999026000	0.622166000	1.065892000
6	-5.212369000	0.388281000	0.432173000
6	-3.915160000	1.467895000	2.171401000
6	-6.356344000	1.024224000	0.906881000
1	-5.251324000	-0.293126000	-0.411431000
6	-5.064264000	2.092639000	2.630022000
1	-2.961496000	1.619134000	2.667112000
6	-6.301329000	1.884341000	2.004441000
1	-7.309548000	0.842658000	0.417502000
1	-5.006812000	2.750073000	3.493891000
6	-7.533760000	2.577411000	2.510924000
1	-8.432112000	2.221146000	2.001245000
1	-7.467524000	3.659999000	2.354994000
1	-7.666225000	2.414168000	3.585296000
6	0.301900000	2.489188000	-0.285066000
6	-0.504781000	3.605009000	-0.050341000
6	1.626065000	2.688196000	-0.684096000
6	0.001850000	4.890814000	-0.214596000
1	-1.533479000	3.456100000	0.263049000
6	2.132716000	3.974054000	-0.845448000
1	2.263046000	1.826975000	-0.865737000
6	1.321566000	5.080876000	-0.613786000
1	-0.639565000	5.748066000	-0.029712000
1	3.164660000	4.109811000	-1.156603000
1	1.715149000	6.084808000	-0.744067000
1	-1.994589000	1.209331000	-1.161557000

Int-A:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2925.999942
Thermal correction to Gibbs Free Energy = 0.244419
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2927.99514400

6	17.050485000	0.158729000	-3.307562000
6	15.898249000	-0.029093000	-2.535342000
7	14.916129000	-1.577920000	-5.258359000
6	15.420608000	-0.522509000	-5.997312000
8	16.665350000	-0.101119000	-5.685198000
6	17.390607000	-0.612768000	-4.563019000
1	17.544117000	1.126268000	-3.243408000
1	17.256817000	-1.688551000	-4.444218000
1	18.439075000	-0.443341000	-4.815118000
1	15.296820000	-0.915033000	-2.719905000
16	13.304635000	-2.111950000	-5.391426000
8	12.432968000	-0.955880000	-5.362297000
8	13.253026000	-3.144208000	-4.366736000
6	13.207106000	-2.874703000	-6.983504000
6	13.392611000	-4.251595000	-7.075892000
6	12.916629000	-2.100002000	-8.104485000
6	13.294657000	-4.857918000	-8.322036000
1	13.589265000	-4.830721000	-6.179445000
6	12.826128000	-2.727934000	-9.339684000
1	12.776501000	-1.030524000	-7.998723000
6	13.016333000	-4.108371000	-9.469560000
1	13.428895000	-5.933273000	-8.404468000
1	12.598553000	-2.134738000	-10.221523000
8	14.815072000	0.010009000	-6.891205000
1	15.448880000	-2.121155000	-4.586293000
6	15.252376000	0.947306000	-1.656523000
6	14.165743000	0.504329000	-0.885402000
6	15.628676000	2.297371000	-1.587850000
6	13.484568000	1.381460000	-0.052206000
1	13.861002000	-0.537224000	-0.947929000
6	14.941259000	3.172748000	-0.760079000
1	16.451878000	2.666717000	-2.189762000
6	13.872637000	2.717536000	0.012472000
1	12.646310000	1.025302000	0.538523000
1	15.234336000	4.217464000	-0.720604000
1	13.336617000	3.408515000	0.656668000
46	17.672562000	-0.952867000	-1.580805000
17	16.806198000	-2.937047000	-2.323977000
17	18.708889000	1.061601000	-0.820238000
6	12.941477000	-4.766021000	-10.817636000
1	12.699740000	-5.828720000	-10.732893000
1	13.902052000	-4.687394000	-11.340464000
1	12.187032000	-4.292023000	-11.451766000
17	18.844806000	-2.199210000	0.086574000
3	19.552484000	-0.237893000	0.760506000

Int-B:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2925.980330
Thermal correction to Gibbs Free Energy = 0.247200
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2927.97983676

6	-0.969929000	-1.951202000	1.085448000
1	-0.197156000	-2.207072000	1.814291000
1	-0.927600000	-2.613945000	0.219899000
46	-3.715462000	-2.076913000	-0.928021000
7	-2.718357000	-0.454803000	1.641815000
6	-1.619895000	0.247377000	0.927845000
8	-1.639998000	1.415525000	0.701231000
8	-0.685191000	-0.622128000	0.623852000
6	-2.381014000	-1.914270000	1.705941000
6	-3.467985000	-2.715042000	0.999874000
1	-4.423369000	-2.415356000	1.446073000
1	-2.337199000	-2.198290000	2.765345000
6	-3.352363000	-4.195943000	1.147846000
6	-4.467085000	-4.980167000	0.808852000
6	-2.218990000	-4.853529000	1.640177000
6	-4.443574000	-6.360279000	0.942086000
1	-5.357113000	-4.485650000	0.427010000
6	-2.194352000	-6.239636000	1.778464000
1	-1.334933000	-4.295121000	1.936153000
6	-3.302853000	-7.000081000	1.427063000
1	-5.320139000	-6.941444000	0.669838000

1	-1.301271000	-6.723168000	2.164394000
1	-3.282473000	-8.080718000	1.532873000
16	-3.017291000	0.279927000	3.327658000
8	-3.901772000	-0.700921000	3.920199000
8	-1.680322000	0.536496000	3.823244000
6	-3.874086000	1.756442000	2.964757000
6	-5.258377000	1.700004000	2.791426000
6	-3.159866000	2.951728000	2.878431000
6	-5.932812000	2.880310000	2.520976000
1	-5.787320000	0.756484000	2.868666000
6	-3.862836000	4.116510000	2.613825000
1	-2.084778000	2.958700000	3.015696000
6	-5.250175000	4.099179000	2.423126000
1	-7.009282000	2.855178000	2.380042000
1	-3.324807000	5.057604000	2.547185000
17	-2.112327000	-3.655135000	-1.761322000
1	-3.639532000	-0.316346000	1.054729000
17	-5.111621000	-0.402968000	-0.053576000
6	-5.990827000	5.359852000	2.090899000
1	-5.473625000	6.243130000	2.473633000
1	-6.075373000	5.471731000	1.003537000
1	-7.005393000	5.347174000	2.497495000
17	-4.204947000	-1.246892000	-3.239700000
3	-2.729490000	-2.754974000	-3.675675000

TS_{AB}:

The Number of Imaginary Frequencies = 1 (-339.2475 cm^{-1})
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2925.942615
Thermal correction to Gibbs Free Energy = 0.244406
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2927.93799202

6	16.317373000	0.249255000	-3.950437000
6	15.916064000	-0.303900000	-2.694361000
7	15.446698000	-0.867075000	-5.441869000
6	16.205872000	-0.312864000	-6.528827000
8	17.386476000	0.128435000	-6.091118000
6	17.592809000	-0.053351000	-4.683538000
1	15.913503000	1.235549000	-4.203728000
1	17.962916000	-1.062557000	-4.479375000
1	18.356119000	0.671205000	-4.383947000
1	15.463060000	-1.295441000	-2.818904000
16	13.701606000	-0.954259000	-5.578068000
8	13.295896000	0.351804000	-6.050288000
8	13.322659000	-1.479332000	-4.279953000
6	13.415349000	-2.183146000	-6.805099000
6	13.345850000	-3.518291000	-6.406546000
6	13.244484000	-1.802110000	-8.134470000
6	13.107410000	-4.486608000	-7.371338000
1	13.462787000	-3.783997000	-5.360566000
6	13.001887000	-2.789784000	-9.078878000
1	13.304280000	-0.755862000	-8.410900000
6	12.936099000	-4.140305000	-8.717149000
1	13.047023000	-5.529893000	-7.074092000
1	12.860371000	-2.507367000	-10.118411000
6	12.709487000	-5.200271000	-9.755013000
1	12.167481000	-6.055359000	-9.342600000
1	13.667160000	-5.573211000	-10.137073000
1	12.145594000	-4.812538000	-10.607247000
8	15.823058000	-0.195659000	-7.654875000
1	15.831449000	-1.738242000	-5.019853000
6	15.104428000	0.551709000	-1.798390000
6	14.008405000	-0.000512000	-1.121996000
6	15.391069000	1.910647000	-1.612765000
6	13.215777000	0.785850000	-0.295310000
1	13.770411000	-1.051060000	-1.265188000
6	14.591256000	2.699440000	-0.794146000
1	16.266618000	2.346223000	-2.087872000
6	13.501248000	2.139792000	-0.132331000
1	12.366208000	0.342581000	0.216078000
1	14.828742000	3.750931000	-0.660732000
1	12.880474000	2.754797000	0.512763000
46	17.527363000	-1.440537000	-1.935043000
17	16.854491000	-3.110095000	-3.460156000
17	18.246086000	0.365260000	-0.585222000
17	19.275254000	-2.904764000	-1.090478000
3	19.591506000	-1.191437000	0.209203000

Int-C:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3368.188087
Thermal correction to Gibbs Free Energy = 0.438100
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3370.86521586

6	17.462671000	-0.305463000	-3.014692000
6	16.641579000	-1.005705000	-2.125412000
7	15.163070000	-1.506834000	-4.525910000
6	15.474237000	-0.543347000	-5.406807000
8	16.759970000	-0.086951000	-5.312287000
6	17.666352000	-0.757929000	-4.440172000
1	17.610694000	0.762681000	-2.865405000
1	17.556831000	-1.838746000	-4.517889000
1	18.659654000	-0.466848000	-4.791280000
1	16.353042000	-2.005655000	-2.431120000
16	13.683790000	-2.168790000	-4.546310000
8	13.627631000	-2.993682000	-3.319847000
8	13.436577000	-2.896442000	-5.808173000
6	12.440448000	-0.911079000	-4.363544000
6	11.987089000	-0.193365000	-5.468479000
6	11.944886000	-0.657021000	-3.086352000
6	11.030083000	0.795570000	-5.278302000
1	12.396601000	-0.368215000	-6.454977000
6	10.979906000	0.329367000	-2.920000000
1	12.313711000	-1.233522000	-2.244560000
6	10.508863000	1.068259000	-4.009804000
1	10.707271000	1.371751000	-6.141069000
1	10.588106000	0.531470000	-1.925848000
6	9.451985000	2.121117000	-3.827857000
1	8.458790000	1.725574000	-4.072610000
1	9.628545000	2.978103000	-4.484492000
1	9.416531000	2.481495000	-2.795830000
8	14.768705000	-0.020105000	-6.266893000
6	15.897263000	-0.483864000	-0.980691000
6	15.113573000	-1.393870000	-0.253007000
6	15.865698000	0.873310000	-0.623597000
6	14.338768000	-0.966211000	0.817362000
1	15.103588000	-2.437363000	-0.554258000
6	15.088621000	1.298302000	0.444048000
1	16.444699000	1.597167000	-1.186003000
6	14.328899000	0.381086000	1.170546000
1	13.736487000	-1.681044000	1.369980000
1	15.067743000	2.351377000	0.708107000
1	13.720780000	0.720409000	2.004363000
46	18.824290000	-1.284151000	-1.676099000
17	18.611080000	-3.377188000	-2.610281000
17	19.238031000	0.878375000	-0.754240000
1	14.789184000	1.288311000	-7.255733000
8	14.789176000	2.083045000	-7.857046000
6	13.575612000	2.301676000	-8.341105000

8	12.594346000	1.626556000	-8.100194000
6	13.552494000	3.508467000	-9.246222000
1	13.882988000	4.393404000	-8.694799000
1	14.252530000	3.365323000	-10.074332000
1	12.545228000	3.662737000	-9.631564000
6	14.600580000	-5.850079000	-5.747217000
1	14.013159000	-4.926026000	-5.701186000
1	14.824893000	-6.097266000	-6.786642000
1	14.070967000	-6.677985000	-5.272677000
6	15.612913000	-5.386682000	-3.571934000
1	15.174648000	-6.294613000	-3.152663000
1	16.554528000	-5.147458000	-3.073921000
1	14.913942000	-4.546945000	-3.477015000
6	16.757444000	-6.836661000	-5.157181000
1	16.979741000	-7.001908000	-6.212735000
1	17.682433000	-6.667578000	-4.603666000
1	16.232552000	-7.701699000	-4.748569000
7	15.891136000	-5.636135000	-5.023017000
6	16.593785000	-4.453496000	-5.611038000
1	17.523848000	-4.294795000	-5.062134000
1	16.793539000	-4.661257000	-6.663779000
1	15.952511000	-3.575155000	-5.512500000
17	20.717978000	-2.164984000	-0.455408000
3	20.823012000	-0.153717000	0.382154000

Int-D:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3368.211902
Thermal correction to Gibbs Free Energy = 0.444617
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3370.89603790

6	-3.348501000	-1.890652000	1.869132000
6	-4.038729000	-3.254267000	1.844550000
7	-3.813149000	-0.999510000	0.787558000
6	-2.812812000	-0.738345000	-0.128017000
8	-1.691996000	-1.342108000	0.262270000
6	-1.834358000	-1.811598000	1.613587000
1	-3.579079000	-1.418132000	2.834235000
1	-1.338198000	-2.777114000	1.677826000
1	-1.349756000	-1.078531000	2.267891000
1	-5.101329000	-3.046129000	1.704265000
16	-5.240061000	-0.077607000	0.897651000
8	-6.081015000	-0.803031000	1.830404000
8	-5.656928000	0.215665000	-0.463023000
6	-4.702653000	1.417497000	1.681016000
6	-4.165353000	2.452026000	0.915551000
6	-4.825125000	1.521315000	3.065473000
6	-3.733337000	3.600011000	1.567112000
1	-4.100731000	2.383437000	-0.166940000
6	-4.384903000	2.680945000	3.692456000
1	-5.282680000	0.714761000	3.629394000
6	-3.828089000	3.732066000	2.957368000
1	-3.322942000	4.414563000	0.976028000
1	-4.484708000	2.774863000	4.770615000
6	-3.331691000	4.973636000	3.640994000
1	-3.593137000	5.871479000	3.073360000
1	-2.239374000	4.955459000	3.732919000
1	-3.746334000	5.071796000	4.647450000
8	-2.872879000	-0.075391000	-1.145025000
6	-3.883972000	-4.073152000	3.081749000
6	-4.863819000	-5.044170000	3.352843000
6	-2.842328000	-3.922349000	4.006805000
6	-4.798671000	-5.834118000	4.491625000
1	-5.678896000	-5.170062000	2.644060000
6	-2.779494000	-4.710366000	5.153370000
1	-2.060866000	-3.185590000	3.842757000
6	-3.753457000	-5.671620000	5.400853000
1	-5.570321000	-6.576832000	4.675465000
1	-1.960684000	-4.571678000	5.854369000
1	-3.701476000	-6.287312000	6.294354000
46	-3.658911000	-4.426828000	0.220675000
17	-5.875929000	-4.087169000	-0.416723000
17	-1.434913000	-5.054745000	0.973888000
1	-3.946941000	0.720353000	-2.269032000
8	-4.338152000	0.984479000	-3.137587000
6	-4.451199000	2.316020000	-3.190322000
8	-4.121165000	3.052787000	-2.288559000
6	-5.032069000	2.779885000	-4.497045000
1	-4.416070000	2.427195000	-5.329185000
1	-6.034466000	2.361317000	-4.627183000
1	-5.083860000	3.867433000	-4.508410000
6	-5.089907000	-1.901924000	-5.138543000
1	-4.774372000	-0.868581000	-4.984261000
1	-4.326812000	-2.452608000	-5.691271000
1	-6.036299000	-1.932389000	-5.681712000
6	-5.722853000	-3.952719000	-3.962001000
1	-4.964306000	-4.504577000	-4.518232000
1	-5.832789000	-4.385462000	-2.964008000
1	-6.673422000	-3.957355000	-4.499082000
6	-3.972231000	-2.514206000	-3.069367000
1	-3.617024000	-1.486619000	-3.011179000
1	-4.140690000	-2.924083000	-2.071599000
1	-3.260363000	-3.147290000	-3.599714000
6	-6.300462000	-1.772989000	-3.030457000
1	-7.238954000	-1.800791000	-3.588058000
1	-6.414015000	-2.254331000	-2.056875000
1	-5.954400000	-0.747438000	-2.904850000
7	-5.273614000	-2.536454000	-3.807893000
17	-3.303553000	-5.836435000	-1.980824000
3	-1.665881000	-6.422900000	-0.711759000

TS_{CD}:

The Number of Imaginary Frequencies = 1 (-250.3031 cm^{-1})
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3368.174159
Thermal correction to Gibbs Free Energy = 0.436580
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3370.85472786

6	16.499114000	-0.690077000	-3.020143000
6	16.143422000	-1.881182000	-2.363897000
7	14.806268000	-0.248368000	-4.331131000
6	15.398080000	0.548651000	-5.244423000
8	16.751128000	0.535777000	-5.095009000
6	17.245563000	-0.550212000	-4.321158000
1	16.433776000	0.239786000	-2.457780000
1	17.215630000	-1.482913000	-4.891144000
1	18.293870000	-0.307376000	-4.125287000
1	16.021762000	-2.748304000	-3.002809000
16	13.246949000	-0.690546000	-4.491390000
8	13.019854000	-1.706678000	-3.453591000
8	12.987100000	-1.108007000	-5.882737000
6	12.222335000	0.703765000	-4.110375000
6	11.867165000	1.605514000	-5.111355000
6	11.803184000	0.872617000	-2.792000000
6	11.078621000	2.696871000	-4.765855000
1	12.184295000	1.463980000	-6.140849000
6	11.017361000	1.973326000	-2.473521000
1	12.078089000	0.138222000	-2.041182000
6	10.648226000	2.902836000	-3.451294000

1	10.790211000	3.400308000	-5.542788000
1	10.677485000	2.109652000	-1.449774000
6	9.822411000	4.106733000	-3.096372000
1	9.111383000	4.350782000	-3.891029000
1	10.460183000	4.986797000	-2.950949000
1	9.261253000	3.950955000	-2.170937000
8	14.909238000	1.254199000	-6.116387000
6	15.333464000	-1.926587000	-1.127688000
6	15.138870000	-3.169234000	-0.509245000
6	14.728520000	-0.797707000	-0.563484000
6	14.373853000	-3.280827000	0.645209000
1	15.614602000	-4.050057000	-0.935042000
6	13.960507000	-0.910185000	0.589779000
1	14.838438000	0.172756000	-1.036653000
6	13.781480000	-2.149210000	1.200604000
1	14.241033000	-4.252103000	1.113482000
1	13.496423000	-0.023520000	1.012713000
1	13.181407000	-2.232395000	2.102168000
46	18.199876000	-2.074276000	-1.935882000
17	18.187461000	-3.791930000	-3.507618000
17	18.214636000	-0.270886000	-0.366322000
1	14.338244000	0.775094000	-7.657644000
8	14.185327000	0.468636000	-8.585184000
6	13.016667000	0.922151000	-9.020806000
8	12.244262000	1.587295000	-8.361708000
6	12.762969000	0.520294000	-10.450679000
1	13.531104000	0.953992000	-11.097560000
1	12.829846000	-0.566439000	-10.552859000
1	11.778006000	0.866287000	-10.761245000
6	13.233685000	-4.243165000	-6.571256000
1	12.865144000	-3.255214000	-6.278875000
1	13.412871000	-4.268013000	-7.647597000
1	12.528222000	-5.027256000	-6.291101000
6	14.297471000	-4.519186000	-4.389893000
1	13.616814000	-5.343144000	-4.167161000
1	15.259959000	-4.681014000	-3.899345000
1	13.854617000	-3.568865000	-4.071891000
6	15.108096000	-5.794774000	-6.295390000
1	15.276282000	-5.774746000	-7.373286000
1	16.054884000	-5.945339000	-5.773603000
1	14.410320000	-6.594733000	-6.042542000
7	14.529038000	-4.492190000	-5.869149000
6	15.488622000	-3.394588000	-6.207532000
1	16.405478000	-3.546465000	-5.631954000
1	15.693736000	-3.433964000	-7.278826000
1	15.020605000	-2.440946000	-5.959127000
17	20.474018000	-2.706821000	-1.325146000
3	20.215066000	-1.074815000	0.085780000

Int-E:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2465.345777

Thermal correction to Gibbs Free Energy = 0.239922

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2467.16434406

6	-2.045794000	0.286110000	-1.091346000
1	-1.451953000	0.119287000	-1.988809000
1	-3.035442000	0.682813000	-1.344377000
46	-5.005533000	-1.433994000	0.244492000
7	-2.301730000	-0.223988000	1.084744000
6	-1.589559000	0.989009000	1.020577000
8	-1.218328000	1.672363000	1.932331000
8	-1.352399000	1.244055000	-0.276937000
6	-2.154876000	-0.948572000	-0.202345000
6	-3.216025000	-1.999939000	-0.511483000
1	-3.045000000	-2.825782000	0.190203000
1	-1.172570000	-1.449594000	-0.187639000
6	-3.126775000	-2.591623000	-1.882437000
6	-3.006326000	-3.985633000	-1.990778000
6	-3.143932000	-1.849472000	-3.073634000
6	-2.892596000	-4.613461000	-3.225891000
1	-3.000191000	-4.585949000	-1.083723000
6	-3.022225000	-2.473283000	-4.309854000
1	-3.301739000	-0.777672000	-3.045573000
6	-2.892449000	-3.857140000	-4.394034000
1	-2.800365000	-5.694831000	-3.274047000
1	-3.043686000	-1.873111000	-5.215108000
1	-2.801368000	-4.341372000	-5.361931000
16	-3.016682000	-0.742673000	2.505800000
8	-3.506004000	0.418144000	3.208369000
8	-3.946750000	-1.816046000	2.069839000
6	-1.761169000	-1.539357000	3.454901000
6	-0.842936000	-0.732526000	4.129118000
6	-1.704323000	-2.928401000	3.518386000
6	0.153683000	-1.347252000	4.872517000
1	-0.909450000	0.348476000	4.052960000
6	-0.699976000	-3.518264000	4.277495000
1	-2.444383000	-3.527898000	2.999365000
6	0.239585000	-2.742738000	4.962766000
1	0.878916000	-0.731874000	5.398143000
1	-0.648934000	-4.601705000	4.341967000
17	-5.963394000	-0.862798000	-1.819876000
6	1.305688000	-3.385632000	5.801631000
1	1.044922000	-3.331232000	6.864936000
1	1.436815000	-4.440063000	5.546723000
1	2.267836000	-2.880070000	5.678060000
17	-7.105635000	-0.955291000	1.514026000
3	-7.707998000	-0.484266000	-0.507699000

Int-F:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2933.020120

Thermal correction to Gibbs Free Energy = 0.229000

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2935.03274935

6	4.398569000	-2.870376000	2.132046000
1	4.904586000	-3.515106000	2.855965000
1	5.094477000	-2.109752000	1.770073000
46	0.916529000	-1.811776000	4.463309000
7	1.881913000	-0.594679000	3.181316000
6	2.948994000	-1.045731000	2.430396000
8	3.450395000	-0.464754000	1.489371000
8	3.362301000	-2.233897000	2.904428000
6	3.823951000	-3.658873000	1.003154000
6	4.062116000	-3.364016000	-0.280581000
1	4.701880000	-2.506827000	-0.490696000
1	3.187591000	-4.496970000	1.281367000
6	3.564650000	-4.074569000	-1.461961000
6	2.581855000	-5.074236000	-1.398344000
6	4.087596000	-3.742795000	-2.719280000
6	2.152152000	-5.722654000	-2.547968000
1	2.139483000	-5.335186000	-0.441421000
6	3.659286000	-4.392588000	-3.871811000
1	4.844195000	-2.964659000	-2.786728000
6	2.690159000	-5.387803000	-3.790455000
1	1.388017000	-6.491860000	-2.477518000
1	4.082506000	-4.119997000	-4.834497000
1	2.350825000	-5.896866000	-4.687967000

16	1.335027000	0.923298000	2.839867000
8	0.225306000	1.116926000	3.824210000
8	2.396934000	1.915690000	2.864095000
6	0.566044000	0.925386000	1.247394000
6	-0.773767000	0.566659000	1.128499000
6	1.327531000	1.282485000	0.136920000
6	-1.357704000	0.575590000	-0.132066000
1	-1.344215000	0.291604000	2.008486000
6	0.722465000	1.281680000	-1.112346000
1	2.372459000	1.540377000	0.263256000
6	-0.623522000	0.931818000	-1.267253000
1	-2.403537000	0.299158000	-0.236283000
1	1.307766000	1.555601000	-1.986264000
17	-0.209076000	-3.233938000	5.983071000
6	-1.266682000	0.961209000	-2.624122000
1	-1.509383000	1.989201000	-2.918015000
1	-0.598521000	0.554482000	-3.388951000
1	-2.195253000	0.384944000	-2.640795000
17	-0.156791000	-2.802737000	2.597758000
17	1.959750000	-0.776914000	6.280840000
3	-0.941113000	-4.159877000	4.136814000
3	0.620467000	0.850518000	5.587248000

Int-G:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2465.338218

Thermal correction to Gibbs Free Energy = 0.236013

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2467.15229144

7	-0.631312000	-2.492037000	1.337001000
6	-1.120637000	-2.232376000	0.076926000
8	-2.067568000	-2.784348000	-0.430289000
8	-0.411656000	-1.313798000	-0.636151000
6	0.113123000	-0.136898000	-0.028459000
6	0.060358000	-0.101069000	1.470429000
1	1.143847000	-0.020272000	-0.377611000
1	-0.477557000	0.704878000	-0.417484000
1	-0.926345000	-0.170099000	1.920998000
6	1.102162000	0.367627000	2.244226000
1	2.022817000	0.653530000	1.736947000
6	1.010268000	0.768611000	3.651080000
6	-0.027964000	0.348168000	4.497049000
6	-0.083001000	0.802866000	5.806875000
6	0.888114000	1.679012000	6.291953000
6	1.929472000	2.089515000	5.464264000
6	1.995312000	1.628710000	4.154967000
1	-0.767450000	-0.367870000	4.150293000
1	-0.884404000	0.463601000	6.456003000
1	0.837644000	2.031539000	7.318094000
1	2.694337000	2.762693000	5.839647000
1	2.813515000	1.937594000	3.509851000
46	1.183707000	-1.929524000	1.965220000
17	3.450042000	-1.424407000	2.621523000
16	-1.703993000	-2.996924000	2.527025000
8	-0.908432000	-2.935692000	3.754683000
8	-2.920175000	-2.197250000	2.419742000
6	-2.112114000	-4.692956000	2.217780000
6	-1.408920000	-5.684953000	2.894196000
6	-1.752877000	-7.014630000	2.681662000
6	-2.786775000	-7.362350000	1.807917000
6	-3.475339000	-6.340147000	1.144530000
6	-3.149889000	-5.005430000	1.342166000
1	-0.612216000	-5.408990000	3.575820000
1	-1.208992000	-7.796815000	3.205052000
1	-4.279518000	-6.594910000	0.458933000
1	-3.671152000	-4.212089000	0.819914000
6	-3.171308000	-8.799670000	1.601386000
1	-4.051745000	-9.057837000	2.201812000
1	-3.423193000	-8.998095000	0.555449000
1	-2.363977000	-9.476710000	1.892639000
17	1.773798000	-4.246930000	1.844156000
3	3.655961000	-3.612492000	2.757497000

Int-H:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2465.354486

Thermal correction to Gibbs Free Energy = 0.238203

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2467.16698862

6	3.629647000	-0.449453000	2.307980000
7	2.238927000	1.459104000	2.354372000
6	3.396205000	0.833352000	3.102967000
46	1.129824000	1.590473000	4.161413000
16	2.795704000	2.880083000	1.416010000
8	3.396244000	3.732838000	2.428466000
6	2.874831000	0.663105000	4.520388000
8	3.596295000	2.292940000	0.349102000
1	4.263218000	1.496170000	3.062651000
1	3.852797000	-1.303269000	2.949060000
1	4.408889000	-0.334227000	1.548671000
6	1.381274000	3.663192000	0.739620000
6	0.949391000	3.296271000	-0.534644000
6	0.782180000	4.699700000	1.451765000
6	-0.114094000	3.985863000	-1.094629000
1	1.439702000	2.490096000	-1.067416000
6	-0.277738000	5.376500000	0.866389000
1	1.141855000	4.965130000	2.439000000
6	-0.741583000	5.031870000	-0.406795000
1	-0.466866000	3.707459000	-2.083644000
1	-0.760398000	6.180675000	1.414046000
6	3.675273000	1.257872000	5.619053000
6	4.321818000	2.497758000	5.491268000
6	3.796792000	0.566741000	6.833038000
6	5.074470000	3.014341000	6.539885000
1	4.217195000	3.074018000	4.575707000
6	4.550507000	1.084992000	7.878896000
1	3.287440000	-0.385927000	6.952588000
6	5.196009000	2.310940000	7.736008000
1	5.565496000	3.976309000	6.422078000
1	4.634087000	0.529389000	8.808698000
1	5.786016000	2.717182000	8.552488000
1	2.602064000	-0.375757000	4.735627000
17	0.331716000	1.191063000	6.361606000
6	1.679150000	0.418921000	1.499892000
8	0.731959000	0.551636000	0.787189000
8	2.389949000	-0.703815000	1.639576000
6	-1.874263000	5.788273000	-1.037079000
1	-1.496075000	6.646907000	-1.604754000
1	-2.437450000	5.158864000	-1.730931000
1	-2.565396000	6.172640000	-0.282496000
17	-0.998846000	2.752827000	3.472774000
3	-1.446147000	2.163834000	5.510278000

TS_{GH}:

The Number of Imaginary Frequencies = 1 (-291.5561 cm^{-1})

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2465.323392

Thermal correction to Gibbs Free Energy = 0.237270

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2467.13654456

7	-0.608370000	-2.212469000	1.289145000
6	-1.049886000	-2.210214000	-0.036484000
8	-1.785311000	-3.023805000	-0.530887000
8	-0.615052000	-1.151981000	-0.751767000
6	0.036157000	-0.117976000	-0.039363000
6	-0.172143000	-0.211177000	1.447481000
1	1.106767000	-0.144763000	-0.269944000
1	-0.379377000	0.829381000	-0.404419000
1	-1.179417000	-0.034574000	1.819598000
6	0.940346000	0.030582000	2.281538000
1	1.843468000	0.348488000	1.755456000
6	0.854479000	0.495796000	3.677261000
6	-0.303222000	0.374556000	4.458801000
6	-0.334529000	0.883979000	5.750828000
6	0.783301000	1.518348000	6.288488000
6	1.940921000	1.638122000	5.523903000
6	1.975708000	1.130702000	4.231346000
1	-1.174129000	-0.145053000	4.075164000
1	-1.238251000	0.777423000	6.343539000
1	0.753082000	1.913151000	7.299916000
1	2.819393000	2.127623000	5.934141000
1	2.882307000	1.219252000	3.638965000
46	1.319970000	-2.063611000	1.967329000
17	3.552728000	-1.689650000	2.693082000
17	1.766212000	-4.416595000	1.504844000
3	3.721279000	-3.849201000	2.285772000
16	-1.738922000	-2.753502000	2.452681000
8	-1.022445000	-2.601177000	3.714893000
8	-2.965782000	-2.001364000	2.208498000
6	-2.058046000	-4.473490000	2.201377000
6	-1.286785000	-5.401995000	2.893907000
6	-1.576511000	-6.752910000	2.746761000
6	-2.623147000	-7.181944000	1.926340000
6	-3.383787000	-6.220542000	1.249248000
6	-3.111201000	-4.867201000	1.378040000
1	-0.480367000	-5.066202000	3.535349000
1	-0.978033000	-7.486840000	3.279662000
1	-4.200384000	-6.539693000	0.606984000
1	-3.691173000	-4.121381000	0.848068000
6	-2.946526000	-8.641825000	1.788105000
1	-3.820114000	-8.906126000	2.395632000
1	-3.183255000	-8.899473000	0.751494000
1	-2.113986000	-9.269889000	2.114939000

Int-I:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -2465.360387
Thermal correction to Gibbs Free Energy = 0.239189
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -2467.17646082

6	3.048134000	-1.831453000	2.737048000
7	1.944079000	0.182096000	2.731034000
6	3.195912000	-0.385969000	3.253640000
46	2.960056000	1.469706000	5.548119000
16	1.881639000	1.867478000	2.536844000
8	2.793032000	2.338040000	3.611204000
6	3.352262000	-0.343103000	4.767798000
8	2.223309000	2.233820000	1.177572000
1	4.047877000	0.100122000	2.764655000
1	2.674615000	-2.494213000	3.524280000
1	3.980443000	-2.232027000	2.337249000
6	0.225714000	2.352909000	2.891265000
6	-0.713881000	2.300638000	1.861171000
6	-0.095512000	2.833108000	4.159197000
6	-2.008956000	2.720007000	2.128444000
1	-0.434896000	1.920567000	0.885827000
6	-1.399048000	3.250513000	4.394978000
1	0.656588000	2.908914000	4.938989000
6	-2.372237000	3.199729000	3.392174000
1	-2.753028000	2.675592000	1.337911000
1	-1.658901000	3.632107000	5.378501000
6	4.733042000	-0.752076000	5.168369000
6	5.863227000	-0.077424000	4.677453000
6	4.934021000	-1.830349000	6.040901000
6	7.144934000	-0.473127000	5.041953000
1	5.736057000	0.783060000	4.024316000
6	6.216302000	-2.228577000	6.402297000
1	4.070471000	-2.350776000	6.446042000
6	7.327180000	-1.553476000	5.902771000
1	8.004523000	0.067343000	4.655892000
1	6.347998000	-3.068180000	7.078993000
1	8.328824000	-1.863449000	6.186119000
1	2.601718000	-0.999173000	5.224129000
17	2.888422000	0.443822000	7.684668000
6	1.416100000	-0.623122000	1.703568000
8	0.519278000	-0.338665000	0.960445000
8	2.081295000	-1.787668000	1.686904000
6	-3.768606000	3.683917000	3.654044000
1	-3.857091000	4.749822000	3.412711000
1	-4.499239000	3.148490000	3.041948000
1	-4.043922000	3.562626000	4.704939000
17	2.581436000	3.780992000	6.519803000
3	2.877472000	2.564168000	8.292361000

Int-J:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -7118.584484
Thermal correction to Gibbs Free Energy = 0.231640
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -7121.27903995

6	-1.472994000	-0.078313000	-1.059907000
1	-0.866509000	-0.472440000	-1.874344000
1	-2.224093000	0.623963000	-1.423983000
46	-5.189736000	-1.294709000	-0.000763000
7	-2.130164000	-0.430984000	1.075594000
6	-1.080707000	0.511116000	1.099335000
8	-0.650025000	1.086551000	2.056065000
8	-0.604907000	0.614933000	-0.150687000
6	-2.085841000	-1.177276000	-0.191237000
6	-3.289133000	-1.994226000	-0.659629000
1	-3.347307000	-2.884027000	-0.032747000
1	-1.312788000	-1.957661000	-0.074648000
6	-3.252600000	-2.392601000	-2.082466000
6	-3.266286000	-3.763591000	-2.385124000
6	-3.193885000	-1.471253000	-3.141761000
6	-3.175058000	-4.201990000	-3.700625000
1	-3.349944000	-4.484972000	-1.577034000
6	-3.107821000	-1.911748000	-4.454417000
1	-3.279949000	-0.409094000	-2.938492000
6	-3.088876000	-3.277102000	-4.737918000
1	-3.176724000	-5.266266000	-3.915588000
1	-3.073826000	-1.187538000	-5.262616000
1	-3.023917000	-3.617676000	-5.767075000
16	-3.148014000	-0.598028000	2.385905000
8	-3.409334000	0.700076000	2.949002000
8	-4.254862000	-1.448656000	1.850186000
6	-2.340095000	-1.627095000	3.565496000
6	-1.420261000	-1.024736000	4.424509000

6	-2.621621000	-2.990805000	3.620869000
6	-0.766059000	-1.823597000	5.351526000
1	-1.218969000	0.038984000	4.351302000
6	-1.956756000	-3.763357000	4.564352000
1	-3.363521000	-3.426542000	2.959669000
6	-1.024039000	-3.196922000	5.440196000
1	-0.042957000	-1.370271000	6.023845000
1	-2.173411000	-4.826210000	4.626880000
17	-7.317108000	-0.460658000	1.293414000
17	-5.772296000	-3.577376000	0.338828000
17	-4.653350000	0.888414000	-0.404058000
6	-0.338036000	-4.037609000	6.476855000
1	-0.906808000	-4.029249000	7.414087000
1	-0.251159000	-5.078814000	6.155971000
1	0.663371000	-3.660035000	6.699495000
17	-6.271603000	-1.347751000	-2.021427000
29	-8.847071000	-1.782772000	0.556300000
17	-9.739230000	-3.361926000	-0.669100000
29	-7.555285000	-3.058240000	-1.160657000

Int-K:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -7118.609348

Thermal correction to Gibbs Free Energy = 0.229103

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -7121.33391591

6	-2.235824000	0.116247000	-0.660121000
1	-1.457297000	-0.184076000	-1.359988000
1	-3.032034000	0.681874000	-1.155235000
46	-6.594724000	-1.058296000	1.217098000
7	-3.175140000	-0.315807000	1.351368000
6	-2.261449000	0.774722000	1.507084000
8	-2.017471000	1.362740000	2.516852000
8	-1.648170000	0.953404000	0.333819000
6	-2.804647000	-1.057782000	0.141020000
6	-3.866509000	-1.901467000	-0.565866000
1	-4.173399000	-2.712565000	0.094273000
1	-1.998738000	-1.773396000	0.375095000
6	-3.339183000	-2.472877000	-1.858225000
6	-2.837658000	-3.776593000	-1.844771000
6	-3.294543000	-1.732898000	-3.043738000
6	-2.284260000	-4.330247000	-2.995204000
1	-2.884612000	-4.364115000	-0.930745000
6	-2.749000000	-2.292095000	-4.194215000
1	-3.706599000	-0.728103000	-3.079474000
6	-2.239043000	-3.588111000	-4.171530000
1	-1.899674000	-5.345341000	-2.973751000
1	-2.727568000	-1.713371000	-5.112479000
1	-1.815897000	-4.021615000	-5.072593000
16	-3.909112000	-0.957251000	2.714912000
8	-4.363629000	0.123333000	3.548047000
8	-4.899017000	-1.924423000	2.139109000
6	-2.710946000	-1.943820000	3.545088000
6	-1.809836000	-1.285085000	4.384618000
6	-2.662136000	-3.322400000	3.347977000
6	-0.839411000	-2.038822000	5.028312000
1	-1.873174000	-0.209625000	4.517317000
6	-1.682563000	-4.052083000	4.010134000
1	-3.394353000	-3.812213000	2.715102000
6	-0.760018000	-3.426629000	4.855604000
1	-0.131134000	-1.539716000	5.683776000
1	-1.639224000	-5.129204000	3.874592000
17	-4.669557000	2.519447000	-0.147436000
17	-7.757751000	-1.038729000	3.192084000
17	-5.403185000	-0.974892000	-0.860198000
6	0.275637000	-4.226262000	5.590002000
1	-0.046838000	-4.416479000	6.620236000
1	0.448989000	-5.194525000	5.114301000
1	1.228149000	-3.691662000	5.641785000
17	-8.397055000	-0.206894000	0.165333000
29	-6.352883000	2.838183000	1.122387000
17	-8.089873000	3.241815000	2.381898000
29	-8.051300000	1.050155000	2.417232000

TS_{JK}:

The Number of Imaginary Frequencies = 1 (-171.172 cm^{-1})

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -7118.559903

Thermal correction to Gibbs Free Energy = 0.227423

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -7121.28003953

6	-1.102445000	-0.084352000	-1.012148000
1	-0.372695000	-0.456516000	-1.731742000
1	-1.800526000	0.616525000	-1.479431000
46	-5.500911000	-1.636073000	-0.039713000
7	-2.057952000	-0.536595000	0.998340000
6	-1.050566000	0.423214000	1.194912000
8	-0.772112000	0.984597000	2.213631000
8	-0.397125000	0.586150000	0.027634000
6	-1.854647000	-1.203246000	-0.289400000
6	-3.000129000	-1.911183000	-0.949426000
1	-3.431568000	-2.653992000	-0.284453000
1	-1.152506000	-2.047886000	-0.132727000
6	-3.055391000	-2.295942000	-2.329008000
6	-3.713496000	-3.516324000	-2.611912000
6	-2.494440000	-1.564391000	-3.398914000
6	-3.747641000	-4.017306000	-3.901763000
1	-4.207170000	-4.050840000	-1.803791000
6	-2.544985000	-2.065515000	-4.687022000
1	-2.057720000	-0.588394000	-3.231270000
6	-3.160710000	-3.294634000	-4.939551000
1	-4.249189000	-4.957946000	-4.103703000
1	-2.118109000	-1.494497000	-5.505188000
1	-3.200122000	-3.677714000	-5.955047000
16	-3.202311000	-0.804033000	2.235227000
8	-3.622267000	0.484963000	2.713043000
8	-4.146947000	-1.773720000	1.634345000
6	-2.368017000	-1.703956000	3.499728000
6	-1.625458000	-0.990277000	4.440776000
6	-2.483635000	-3.092300000	3.549655000
6	-0.971485000	-1.699852000	5.437926000
1	-1.557756000	0.089807000	4.377327000
6	-1.823164000	-3.774952000	4.562602000
1	-3.104086000	-3.617830000	2.831441000
6	-1.058452000	-3.094897000	5.516693000
1	-0.385693000	-1.157690000	6.175059000
1	-1.912860000	-4.856208000	4.619630000
17	-7.245990000	-0.182539000	1.838183000
17	-6.152841000	-3.810598000	0.547797000
17	-4.441943000	0.236301000	-0.885886000
6	-0.373806000	-3.839694000	6.625152000
1	-0.993359000	-3.834960000	7.529543000
1	-0.192403000	-4.883314000	6.356433000
1	0.583085000	-3.378296000	6.884040000
17	-6.724933000	-1.834910000	-1.966165000
29	-8.879520000	-1.425505000	1.273376000
17	-10.174224000	-2.924508000	0.338738000
29	-8.119092000	-2.992637000	-0.560606000

Int-L:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -7118.601178
Thermal correction to Gibbs Free Energy = 0.230331
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -7121.29241679

6	4.031088000	-1.974008000	2.614747000
7	2.451429000	-0.376558000	2.238212000
6	3.695596000	-0.511636000	2.998871000
16	1.558418000	1.046840000	2.094249000
8	0.156611000	0.712729000	2.113182000
6	3.521556000	-0.404646000	4.502820000
8	2.151339000	1.915188000	3.147173000
1	4.458053000	0.181793000	2.628589000
1	3.663164000	-2.675352000	3.370372000
1	5.099717000	-2.127365000	2.466510000
6	2.004642000	1.828269000	0.584314000
6	3.108059000	2.682000000	0.560028000
6	1.231296000	1.577826000	-0.549152000
6	3.437828000	3.291047000	-0.643214000
1	3.676284000	2.879158000	1.464935000
6	1.586936000	2.200856000	-1.736260000
1	0.383400000	0.905079000	-0.493337000
6	2.687501000	3.064134000	-1.802672000
1	4.289056000	3.965044000	-0.678923000
1	0.997477000	2.014737000	-2.629660000
6	4.623710000	-0.968729000	5.299862000
6	5.976202000	-0.801936000	4.957284000
6	4.300412000	-1.770920000	6.407741000
6	6.968758000	-1.432812000	5.695220000
1	6.247941000	-0.145098000	4.137445000
6	5.295568000	-2.402259000	7.140244000
1	3.257050000	-1.890827000	6.688010000
6	6.632858000	-2.235081000	6.784738000
1	8.010856000	-1.291124000	5.425290000
1	5.029581000	-3.022363000	7.990811000
1	7.413438000	-2.723894000	7.360222000
1	2.558875000	-0.825487000	4.799235000
6	2.363724000	-1.334135000	1.210996000
8	1.569060000	-1.351170000	0.316044000
8	3.353469000	-2.223307000	1.386197000
6	3.033119000	3.758026000	-3.087381000
1	2.837232000	3.117970000	-3.951962000
1	2.426989000	4.663591000	-3.207682000
1	4.083135000	4.059614000	-3.111223000
46	3.071431000	1.640021000	4.984284000
17	2.416945000	4.190078000	5.263923000
17	1.067145000	0.879157000	5.972916000
17	5.026118000	2.351336000	4.002034000
17	4.081725000	1.560089000	7.037571000
29	1.589692000	4.239077000	7.248840000
17	1.010955000	3.465263000	9.211405000
29	1.966458000	1.867865000	7.931367000

Int-M:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -7118.628840
Thermal correction to Gibbs Free Energy = 0.228827
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -7121.33851197

6	4.638697000	-0.870372000	2.441621000
7	2.561436000	0.037480000	2.255940000
6	3.620232000	-0.054831000	3.251926000
16	1.433468000	1.282157000	2.075946000
8	0.093437000	0.748237000	2.158374000
6	3.192608000	-0.835393000	4.497537000
8	1.889139000	2.304843000	3.059669000
1	4.030699000	0.931386000	3.492352000
1	5.194293000	-1.589575000	3.043742000
1	5.328670000	-0.198629000	1.922846000
6	1.746418000	1.990366000	0.501863000
6	2.850833000	2.828223000	0.337500000
6	0.872981000	1.690572000	-0.540550000
6	3.066964000	3.379074000	-0.916813000
1	3.525703000	3.042335000	1.162764000
6	1.116187000	2.259047000	-1.783424000
1	0.033919000	1.024042000	-0.375861000
6	2.207857000	3.109202000	-1.990118000
1	3.922506000	4.032367000	-1.063265000
1	0.447624000	2.034113000	-2.609503000
6	4.265901000	-1.020815000	5.518181000
6	5.039300000	0.054250000	5.969394000
6	4.512141000	-2.302410000	6.020439000
6	6.043477000	-0.150564000	6.907139000
1	4.856814000	1.061448000	5.602370000
6	5.522988000	-2.507446000	6.953833000
1	3.909889000	-3.141245000	5.679375000
6	6.287665000	-1.431930000	7.398093000
1	6.628283000	0.696565000	7.252478000
1	5.709497000	-3.506256000	7.336318000
1	7.073383000	-1.590915000	8.130636000
1	2.769183000	-1.798037000	4.195863000
6	2.696745000	-0.947465000	1.260426000
8	1.927159000	-1.174123000	0.372299000
8	3.854130000	-1.593728000	1.483086000
6	2.444116000	3.741716000	-3.330033000
1	1.997009000	3.154489000	-4.135930000
1	1.998890000	4.743052000	-3.364421000
1	3.512161000	3.853555000	-3.535080000
46	2.037399000	2.333844000	5.139685000
17	5.772001000	2.590205000	2.650881000
17	2.305275000	4.602184000	4.996264000
17	1.696198000	-0.024748000	5.258606000
17	2.394517000	2.471257000	7.374874000
29	5.998945000	3.381642000	4.621156000
17	6.215136000	4.047473000	6.681703000
29	4.016564000	3.967382000	6.381965000

TS_{LM}:

The Number of Imaginary Frequencies = 1 (-180.5573)
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -7118.571974
Thermal correction to Gibbs Free Energy = 0.224045
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -7121.28726954

6	4.442300000	-1.921412000	2.442468000
7	2.575221000	-0.607266000	2.189956000
6	3.802675000	-0.606933000	2.984533000
16	1.409873000	0.659923000	2.083810000
8	0.132328000	0.012442000	1.925671000
6	3.587354000	-0.783634000	4.467569000
8	1.721140000	1.499113000	3.262964000
1	4.428034000	0.263875000	2.766772000
1	4.247939000	-2.765380000	3.111909000
1	5.518548000	-1.818702000	2.297225000
6	1.812806000	1.671595000	0.707158000
6	2.540866000	2.842478000	0.926396000
6	1.340926000	1.308691000	-0.557031000
6	2.816556000	3.651970000	-0.167435000

1	2.830779000	3.154650000	1.927225000
6	1.644351000	2.135294000	-1.628201000
1	0.762393000	0.402132000	-0.688930000
6	2.382957000	3.313024000	-1.453329000
1	3.361341000	4.577380000	-0.003559000
1	1.291476000	1.866563000	-2.619991000
6	4.605541000	-1.252557000	5.358182000
6	5.985235000	-1.099241000	5.092043000
6	4.198914000	-1.936484000	6.522888000
6	6.919626000	-1.656277000	5.942117000
1	6.310277000	-0.512261000	4.238183000
6	5.144348000	-2.488791000	7.373521000
1	3.140773000	-2.007360000	6.755066000
6	6.499701000	-2.353137000	7.082188000
1	7.978900000	-1.537252000	5.738793000
1	4.826606000	-3.012753000	8.268782000
1	7.240552000	-2.777725000	7.753314000
1	2.575912000	-1.101067000	4.726213000
6	2.684499000	-1.467003000	1.081036000
8	1.925823000	-1.561751000	0.162416000
8	3.826603000	-2.172166000	1.195634000
6	2.662407000	4.218153000	-2.616869000
1	2.717449000	3.660761000	-3.555652000
1	1.863051000	4.961175000	-2.721671000
1	3.599032000	4.764978000	-2.481709000
46	1.873427000	1.111635000	5.306541000
17	2.644284000	5.095998000	3.630856000
17	-0.427184000	0.691612000	5.475303000
17	4.078847000	1.664905000	5.073862000
17	2.123173000	0.710772000	7.496020000
29	1.186218000	4.906426000	5.163491000
17	-0.319731000	4.842705000	6.746514000
29	-0.324755000	2.768670000	6.143499000

Int-N:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3385.406022

Thermal correction to Gibbs Free Energy = 0.241942

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3387.55296916

6	-1.531064000	-0.086412000	-1.060150000
1	-0.910217000	-0.464563000	-1.871173000
1	-2.297297000	0.596333000	-1.429418000
46	-5.219676000	-1.395882000	-0.022963000
7	-2.195623000	-0.450150000	1.069462000
6	-1.168005000	0.514592000	1.100926000
8	-0.755864000	1.099843000	2.060588000
8	-0.685952000	0.629737000	-0.145437000
6	-2.121930000	-1.200248000	-0.196123000
6	-3.310543000	-2.032677000	-0.679748000
1	-3.338454000	-2.940284000	-0.075177000
1	-1.330103000	-1.959014000	-0.069153000
6	-3.245019000	-2.403325000	-2.113348000
6	-3.154592000	-3.763705000	-2.443507000
6	-3.254833000	-1.460360000	-3.154199000
6	-3.028228000	-4.168706000	-3.767263000
1	-3.183530000	-4.505373000	-1.649967000
6	-3.132619000	-1.867117000	-4.475402000
1	-3.421857000	-0.412193000	-2.928386000
6	-3.008829000	-3.220664000	-4.786330000
1	-2.949682000	-5.225992000	-4.002260000
1	-3.152005000	-1.125867000	-5.268703000
1	-2.914559000	-3.534853000	-5.821702000
16	-3.214079000	-0.647464000	2.372405000
8	-3.505026000	0.640038000	2.945842000
8	-4.299840000	-1.520456000	1.832601000
6	-2.385700000	-1.665832000	3.548711000
6	-1.476744000	-1.049738000	4.409212000
6	-2.639940000	-3.034960000	3.598028000
6	-0.805299000	-1.839568000	5.331771000
1	-1.296560000	0.018047000	4.339736000
6	-1.958203000	-3.798669000	4.537003000
1	-3.373607000	-3.481427000	2.934609000
6	-1.035697000	-3.218053000	5.414134000
1	-0.090136000	-1.375224000	6.005138000
1	-2.152871000	-4.866120000	4.594346000
17	-7.451954000	-0.832977000	1.053416000
17	-5.781763000	-3.692626000	0.300982000
17	-4.753068000	0.803375000	-0.414905000
6	-0.330890000	-4.050043000	6.445522000
1	-0.899929000	-4.062311000	7.382575000
1	-0.219141000	-5.086526000	6.116903000
1	0.661366000	-3.650832000	6.671522000
17	-6.321261000	-1.495820000	-2.019462000
3	-7.716776000	-2.521669000	-0.359468000

Int-O:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3385.454590

Thermal correction to Gibbs Free Energy = 0.235722

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3387.62043836

6	-0.921005000	-1.543667000	-0.008294000
1	-0.456714000	-2.532817000	-0.047611000
1	-0.808624000	-1.046028000	-0.972629000
46	-5.392518000	-3.868976000	2.706775000
7	-2.237990000	-1.222360000	1.825313000
6	-0.990669000	-0.634511000	2.085627000
8	-0.639797000	-0.134369000	3.115740000
8	-0.240826000	-0.765965000	0.982148000
6	-2.393080000	-1.628750000	0.433263000
6	-3.359344000	-0.752944000	-0.381453000
1	-4.335341000	-0.784625000	0.108711000
1	-2.770624000	-2.655142000	0.385445000
6	-3.486910000	-1.288307000	-1.790795000
6	-4.209090000	-2.475868000	-1.960968000
6	-2.889935000	-0.689926000	-2.900391000
6	-4.325750000	-3.053083000	-3.220336000
1	-4.673717000	-2.958849000	-1.103708000
6	-3.011425000	-1.270326000	-4.161152000
1	-2.347722000	0.242961000	-2.782241000
6	-3.727078000	-2.451621000	-4.325095000
1	-4.889053000	-3.974324000	-3.335664000
1	-2.547223000	-0.790246000	-5.017817000
1	-3.822474000	-2.900365000	-5.309574000
16	-3.434316000	-1.264784000	2.993263000
8	-3.788182000	0.059165000	3.450669000
8	-4.484673000	-2.044468000	2.273287000
6	-2.737834000	-2.196811000	4.314643000
6	-2.587116000	-1.561984000	5.542930000
6	-2.353258000	-3.523421000	4.114307000
6	-2.048530000	-2.284907000	6.599857000
1	-2.878806000	-0.523608000	5.654037000
6	-1.818641000	-4.221654000	5.186737000
1	-2.473960000	-4.005302000	3.147158000
6	-1.661457000	-3.618616000	6.441851000
1	-1.921024000	-1.800307000	7.563723000
1	-1.516072000	-5.255611000	5.045547000

17	-6.707338000	-2.769666000	4.348824000
17	-4.064796000	-4.845318000	1.130426000
17	-2.847064000	0.966712000	-0.308151000
6	-1.102328000	-4.400427000	7.594466000
1	-1.872162000	-5.048084000	8.030014000
1	-0.278859000	-5.045662000	7.275258000
1	-0.736261000	-3.742344000	8.386143000
17	-6.452423000	-5.887957000	3.049244000
3	-7.760011000	-4.696837000	4.378136000

TS_{NO}:

The Number of Imaginary Frequencies = 1 (-205.4079 cm^{-1})
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3385.373701
Thermal correction to Gibbs Free Energy = 0.237284
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3387.54757873

6	-1.742509000	-0.016860000	-0.887198000
1	-1.116796000	-0.335498000	-1.721093000
1	-2.662778000	0.457075000	-1.240580000
46	-5.325551000	-2.314017000	1.312501000
7	-2.112218000	-0.361431000	1.327336000
6	-1.335685000	0.800772000	1.185637000
8	-0.982858000	1.547566000	2.051422000
8	-1.004161000	0.924900000	-0.113471000
6	-2.050689000	-1.150938000	0.092431000
6	-3.148343000	-2.135682000	-0.203980000
1	-3.219493000	-2.866835000	0.595967000
1	-1.164741000	-1.813157000	0.149810000
6	-3.399329000	-2.722326000	-1.496623000
6	-3.821299000	-4.070203000	-1.500991000
6	-3.243217000	-2.058008000	-2.730468000
6	-4.016942000	-4.745187000	-2.694539000
1	-4.011253000	-4.568567000	-0.553214000
6	-3.448526000	-2.736830000	-3.919490000
1	-3.000018000	-1.003875000	-2.762954000
6	-3.825986000	-4.081320000	-3.905074000
1	-4.337106000	-5.781861000	-2.682093000
1	-3.329900000	-2.216343000	-4.864502000
1	-3.991094000	-4.604752000	-4.842247000
16	-2.863430000	-0.674365000	2.823750000
8	-3.469707000	0.552869000	3.265172000
8	-3.656419000	-1.900734000	2.575701000
6	-1.593373000	-1.183729000	3.934204000
6	-0.861117000	-0.201146000	4.600429000
6	-1.372408000	-2.543342000	4.150019000
6	0.126532000	-0.605129000	5.487810000
1	-1.059329000	0.847938000	4.412713000
6	-0.381102000	-2.917250000	5.047424000
1	-1.987761000	-3.285739000	3.652675000
6	0.381232000	-1.960582000	5.726801000
1	0.707510000	0.149042000	6.011408000
1	-0.204918000	-3.973208000	5.232878000
17	-7.346979000	-1.659592000	3.174160000
17	-5.306548000	-4.479130000	2.237852000
17	-4.936379000	-0.428520000	0.009813000
6	1.424687000	-2.377914000	6.721388000
1	0.999294000	-2.410415000	7.731294000
1	1.816385000	-3.373627000	6.498536000
1	2.261240000	-1.674346000	6.742715000
17	-6.941306000	-3.027314000	-0.111387000
3	-7.529605000	-3.591849000	2.191590000

Int-P:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3853.043834
Thermal correction to Gibbs Free Energy = 0.239343
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3855.39932305

6	-1.523095000	0.019837000	-1.021783000
1	-0.829672000	-0.358467000	-1.774037000
1	-2.295841000	0.669368000	-1.436827000
46	-5.202920000	-1.362101000	-0.047558000
7	-2.222259000	-0.396928000	1.098643000
6	-1.241612000	0.620419000	1.157831000
8	-0.873922000	1.205416000	2.135486000
8	-0.761748000	0.787332000	-0.077621000
6	-2.097226000	-1.121836000	-0.177795000
6	-3.272514000	-1.976956000	-0.649013000
1	-3.292542000	-2.867173000	-0.019326000
1	-1.280136000	-1.858335000	-0.076085000
6	-3.239603000	-2.408708000	-2.070916000
6	-3.297900000	-3.786487000	-2.353047000
6	-3.146378000	-1.516978000	-3.154746000
6	-3.230157000	-4.259773000	-3.664325000
1	-3.384848000	-4.490129000	-1.531685000
6	-3.068240000	-1.987786000	-4.464987000
1	-3.162637000	-0.448352000	-2.976908000
6	-3.103648000	-3.361474000	-4.728560000
1	-3.265338000	-5.328398000	-3.852213000
1	-2.987309000	-1.279483000	-5.283522000
1	-3.046058000	-3.724777000	-5.749877000
16	-3.244750000	-0.647427000	2.382364000
8	-3.576083000	0.615740000	2.987168000
8	-4.321067000	-1.523639000	1.811200000
6	-2.414929000	-1.684321000	3.539638000
6	-1.505764000	-1.074425000	4.404787000
6	-2.650992000	-3.057119000	3.561039000
6	-0.816644000	-1.875007000	5.304268000
1	-1.335540000	-0.003841000	4.352859000
6	-1.951826000	-3.831432000	4.478071000
1	-3.380975000	-3.500341000	2.891805000
6	-1.028265000	-3.257940000	5.358588000
1	-0.098768000	-1.416291000	5.978487000
1	-2.129623000	-4.902731000	4.511958000
17	-7.440611000	-0.824576000	0.966278000
17	-5.768134000	-3.669727000	0.213761000
17	-4.758110000	0.845573000	-0.392016000
6	-0.298557000	-4.103169000	6.361254000
1	-0.849136000	-4.136676000	7.308791000
1	-0.185075000	-5.132218000	6.010885000
1	0.695041000	-3.700543000	6.574796000
17	-6.244357000	-1.429032000	-2.083325000
3	-7.691668000	-2.496526000	-0.472900000
17	0.495546000	-2.742364000	-2.034444000
3	-1.167075000	-3.064110000	-3.288355000

Int-Q:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3853.046474
Thermal correction to Gibbs Free Energy = 0.235344
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3855.44278282

6	-0.842367000	-1.919383000	-0.687789000
1	-0.171177000	-2.514870000	-0.062363000
1	-0.681289000	-2.183448000	-1.733210000
46	-6.109408000	-3.038572000	1.885826000
7	-2.452713000	-0.874225000	0.562215000

6	-1.376105000	0.009411000	0.406556000
8	-1.199075000	1.066890000	0.932474000
8	-0.533323000	-0.536143000	-0.509961000
6	-2.294551000	-2.094685000	-0.224085000
6	-3.409242000	-2.193923000	-1.278461000
1	-4.253256000	-2.734924000	-0.842484000
1	-2.384426000	-3.010253000	0.377073000
6	-3.896079000	-0.947780000	-1.967489000
6	-5.272186000	-0.856833000	-2.233197000
6	-3.017520000	-0.037562000	-2.580239000
6	-5.751272000	0.074853000	-3.160302000
1	-5.946676000	-1.558292000	-1.743448000
6	-3.501122000	0.893534000	-3.502382000
1	-1.952847000	-0.076572000	-2.365886000
6	-4.864859000	0.933730000	-3.816398000
1	-6.815001000	0.120098000	-3.373761000
1	-2.811979000	1.582262000	-3.981694000
1	-5.233808000	1.644736000	-4.549168000
16	-3.652074000	-0.671292000	1.764374000
8	-3.884985000	0.742545000	1.933315000
8	-4.722762000	-1.516187000	1.190968000
6	-2.926482000	-1.366851000	3.204017000
6	-2.505997000	-0.484386000	4.195878000
6	-2.746638000	-2.746321000	3.308277000
6	-1.896389000	-1.008686000	5.327881000
1	-2.662819000	0.582201000	4.078285000
6	-2.128278000	-3.238361000	4.447188000
1	-3.081914000	-3.439857000	2.538472000
6	-1.703665000	-2.386029000	5.473710000
1	-1.569743000	-0.334640000	6.114841000
1	-1.989567000	-4.311730000	4.541016000
17	-3.052229000	-5.310497000	0.765410000
17	-6.353016000	-3.724787000	-0.375667000
17	-6.091638000	-2.269927000	4.010552000
6	-1.082750000	-2.947426000	6.719133000
1	-1.860846000	-3.302584000	7.404784000
1	-0.436148000	-3.799952000	6.492960000
1	-0.492156000	-2.195884000	7.249258000
17	-7.043562000	-5.008826000	2.513062000
3	-5.250438000	-5.424381000	0.939092000
17	-2.911190000	-3.311180000	-2.673401000
3	-4.001039000	-1.559807000	-4.070556000

TS_{PQ}:

The Number of Imaginary Frequencies = 1 (-67.9633 cm^{-1})

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3853.008277

Thermal correction to Gibbs Free Energy = 0.233418

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3855.39065771

6	0.005355000	-1.545896000	-1.124445000
1	0.666579000	-2.377180000	-1.362534000
1	-0.220304000	-0.993043000	-2.039145000
46	-5.734838000	-2.018374000	0.164111000
7	-1.473889000	-0.836066000	0.455304000
6	-0.246860000	-0.195656000	0.690500000
8	-0.006622000	0.630540000	1.523044000
8	0.650340000	-0.684347000	-0.188023000
6	-1.282548000	-2.001338000	-0.405960000
6	-2.470303000	-2.338335000	-1.262828000
1	-2.788912000	-3.373976000	-1.201352000
1	-1.067238000	-2.887904000	0.205176000
6	-3.417801000	-1.441106000	-1.799467000
6	-4.679973000	-1.989032000	-2.192631000
6	-3.146896000	-0.070047000	-2.079493000
6	-5.532868000	-1.235620000	-3.026768000
1	-4.848548000	-3.056355000	-2.075058000
6	-4.012649000	0.656059000	-2.869241000
1	-2.238526000	0.388627000	-1.706203000
6	-5.198850000	0.062957000	-3.367190000
1	-6.465008000	-1.676099000	-3.363643000
1	-3.790819000	1.692128000	-3.103448000
1	-5.861920000	0.644463000	-4.000068000
16	-2.791601000	-0.691806000	1.558469000
8	-3.082194000	0.714796000	1.660684000
8	-3.709673000	-1.676980000	0.951022000
6	-2.295331000	-1.368129000	3.104269000
6	-1.464295000	-0.621337000	3.942254000
6	-2.806616000	-2.611695000	3.477215000
6	-1.115748000	-1.163726000	5.169839000
1	-1.098072000	0.350096000	3.630144000
6	-2.445665000	-3.121417000	4.717663000
1	-3.503841000	-3.138655000	2.832888000
6	-1.598126000	-2.414611000	5.576400000
1	-0.464209000	-0.600203000	5.831986000
1	-2.847330000	-4.081507000	5.028868000
17	-6.538793000	-2.502457000	2.794868000
17	-5.132807000	-4.330810000	0.183545000
17	-6.255809000	0.182851000	0.033640000
6	-1.247895000	-2.964839000	6.927870000
1	-1.973975000	-2.626909000	7.676603000
1	-1.260517000	-4.057798000	6.930928000
1	-0.260162000	-2.629080000	7.254771000
17	-7.773864000	-2.622012000	-0.699061000
3	-7.228954000	-3.926492000	1.266541000
17	-1.397179000	-3.016030000	-3.525058000
3	-3.052459000	-1.612848000	-3.996362000

Int-R:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3385.421393

Thermal correction to Gibbs Free Energy = 0.240577

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3387.56466930

6	3.469314000	-1.176981000	2.662175000
7	2.111160000	0.640691000	2.794162000
6	3.390751000	0.190221000	3.368355000
46	3.234747000	1.922485000	5.827723000
16	1.557399000	2.227489000	2.989335000
8	1.832786000	2.508525000	4.425713000
6	3.385885000	0.018155000	4.873446000
8	2.095875000	3.099136000	1.969669000
1	4.204227000	0.844682000	3.038218000
1	2.991748000	-1.961425000	3.259211000
1	4.493709000	-1.465073000	2.429104000
6	-0.194336000	2.132480000	2.887701000
6	-0.810775000	2.474424000	1.686530000
6	-0.920859000	1.766184000	4.020050000
6	-2.196133000	2.433952000	1.624387000
1	-0.213016000	2.750985000	0.825988000
6	-2.304953000	1.731871000	3.927043000
1	-0.414375000	1.537043000	4.953077000
6	-2.961623000	2.064316000	2.736160000
1	-2.693049000	2.692352000	0.693623000
1	-2.887493000	1.451009000	4.800045000
6	4.499968000	-0.800228000	5.389565000
6	5.817344000	-0.661442000	4.921971000
6	4.223059000	-1.789807000	6.346159000
6	6.818481000	-1.504741000	5.384929000

1	6.061778000	0.136799000	4.227792000
6	5.226874000	-2.632475000	6.804637000
1	3.211112000	-1.884574000	6.731188000
6	6.526752000	-2.494519000	6.322368000
1	7.834176000	-1.382980000	5.020648000
1	4.996085000	-3.395946000	7.541574000
1	7.313570000	-3.150808000	6.682652000
1	2.419618000	-0.372287000	5.200716000
17	4.961463000	2.759570000	4.591509000
6	1.907782000	0.027073000	1.538889000
8	1.121680000	0.359020000	0.699039000
8	2.745839000	-1.015409000	1.442878000
17	1.455900000	1.041887000	7.157500000
17	2.821404000	4.165314000	6.977962000
6	-4.460465000	2.057215000	2.663397000
1	-4.890842000	1.317786000	3.343772000
1	-4.862360000	3.037007000	2.947445000
1	-4.811236000	1.840626000	1.651054000
17	4.655718000	1.433591000	7.546441000
3	2.743210000	2.532542000	8.469056000

Int-S:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3385.454886
Thermal correction to Gibbs Free Energy = 0.233456
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3387.61671360

6	4.355880000	-1.009093000	1.807467000
7	2.417581000	0.137083000	2.127087000
6	3.357725000	-0.662727000	2.914596000
46	3.623252000	3.258144000	4.588445000
16	1.765611000	1.617042000	2.615964000
8	2.272256000	1.762668000	4.008628000
6	2.720112000	-1.927547000	3.501286000
8	2.082378000	2.615897000	1.619899000
1	3.823651000	-0.050371000	3.688343000
1	4.796539000	-2.000653000	1.913875000
1	5.139477000	-0.248468000	1.739144000
6	0.021080000	1.402389000	2.736539000
6	-0.711771000	1.251419000	1.559102000
6	-0.588230000	1.458443000	3.986135000
6	-2.090936000	1.139453000	1.655102000
1	-0.205820000	1.211046000	0.599418000
6	-1.972236000	1.352182000	4.049986000
1	0.010337000	1.595801000	4.879344000
6	-2.741289000	1.186599000	2.894724000
1	-2.676596000	1.020020000	0.747571000
1	-2.463006000	1.403016000	5.017932000
6	3.721452000	-2.750918000	4.264636000
6	4.457884000	-2.195873000	5.316720000
6	3.940234000	-4.082457000	3.905859000
6	5.398860000	-2.964061000	5.991993000
1	4.290941000	-1.164545000	5.616337000
6	4.882995000	-4.850986000	4.583879000
1	3.364871000	-4.521526000	3.094073000
6	5.613928000	-4.292124000	5.627412000
1	5.966967000	-2.523022000	6.805479000
1	5.042924000	-5.886130000	4.296953000
1	6.349763000	-4.889446000	6.157798000
1	2.291140000	-2.522292000	2.689088000
17	5.371348000	1.886947000	4.115131000
6	2.524167000	-0.172913000	0.755896000
8	1.796593000	0.189885000	-0.124835000
8	3.577078000	-0.991745000	0.600018000
17	1.727098000	4.622105000	5.061072000
17	1.314603000	-1.488768000	4.547464000
6	-4.233207000	1.042654000	2.977511000
1	-4.729407000	1.549340000	2.144919000
1	-4.521891000	-0.014115000	2.934047000
1	-4.624478000	1.453088000	3.911700000
17	5.106996000	4.867241000	5.312356000
3	3.298029000	6.135987000	5.326062000

TS_{RS}:

The Number of Imaginary Frequencies = 1 (-199.5886 cm^{-1})
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3385.383595
Thermal correction to Gibbs Free Energy = 0.236417
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3387.55543902

6	-5.191895000	6.350698000	0.451646000
7	-4.157739000	4.335597000	0.362655000
6	-5.361486000	4.949210000	-0.180554000
46	-5.997293000	1.655519000	0.740363000
16	-3.403082000	3.038605000	-0.431636000
8	-4.015917000	1.787879000	0.078836000
6	-6.631563000	4.319391000	0.333626000
8	-3.494517000	3.367772000	-1.841651000
1	-5.318976000	4.982128000	-1.271115000
1	-6.136288000	6.826666000	0.715003000
1	-4.617453000	7.001533000	-0.217028000
6	-1.740079000	3.010347000	0.110813000
6	-0.793729000	3.700907000	-0.643098000
6	-1.397359000	2.261705000	1.236902000
6	0.533945000	3.645722000	-0.242522000
1	-1.092532000	4.249021000	-1.530620000
6	-0.063560000	2.221019000	1.609880000
1	-2.161268000	1.732969000	1.797871000
6	0.917307000	2.909120000	0.883684000
1	1.287439000	4.175479000	-0.818295000
1	0.223510000	1.645049000	2.484970000
6	-7.923077000	4.837279000	-0.026410000
6	-8.156344000	5.508250000	-1.245991000
6	-8.973805000	4.720238000	0.904900000
6	-9.393592000	6.067932000	-1.505492000
1	-7.373331000	5.560346000	-1.996265000
6	-10.213832000	5.281000000	0.634877000
1	-8.802788000	4.175617000	1.828128000
6	-10.423483000	5.955773000	-0.565347000
1	-9.570619000	6.580702000	-2.445635000
1	-11.018905000	5.185758000	1.356283000
1	-11.396022000	6.389476000	-0.779199000
1	-6.555398000	3.940211000	1.352128000
17	-6.752893000	2.401259000	-1.313238000
6	-3.727403000	4.981510000	1.533313000
8	-2.887666000	4.634545000	2.307151000
8	-4.450281000	6.121557000	1.644143000
17	-5.195186000	1.427655000	2.936236000
17	-5.848537000	-1.211227000	0.549497000
6	2.357588000	2.831088000	1.296671000
1	2.956471000	3.610832000	0.820267000
1	2.463726000	2.928932000	2.380942000
1	2.785895000	1.862297000	1.014841000
17	-8.108062000	1.399430000	1.561440000
3	-6.633342000	-0.386555000	2.396135000

Int-T:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3853.055425
Thermal correction to Gibbs Free Energy = 0.237173
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3855.40732158

6	3.401944000	-1.168740000	2.536781000
7	2.074794000	0.652732000	2.795194000
6	3.366502000	0.164238000	3.312332000
46	3.184043000	1.789463000	5.871613000
16	1.521620000	2.219168000	3.087247000
8	1.728173000	2.377131000	4.561622000
6	3.399508000	-0.055085000	4.811419000
8	2.105412000	3.175980000	2.174931000
1	4.173967000	0.827110000	2.983326000
1	2.884493000	-1.969333000	3.075305000
1	4.403732000	-1.515860000	2.286266000
6	-0.225560000	2.150829000	2.921763000
6	-0.797656000	2.632343000	1.746753000
6	-0.992873000	1.665207000	3.979907000
6	-2.180006000	2.613442000	1.634407000
1	-0.168799000	2.995644000	0.942437000
6	-2.372907000	1.655387000	3.837447000
1	-0.520748000	1.325371000	4.896452000
6	-2.985831000	2.127442000	2.670514000
1	-2.642714000	2.978641000	0.722006000
1	-2.987112000	1.281285000	4.651657000
6	4.583204000	-0.782780000	5.329993000
6	5.891450000	-0.534708000	4.875185000
6	4.401088000	-1.744225000	6.342398000
6	6.979447000	-1.202669000	5.437690000
1	6.065798000	0.214067000	4.110405000
6	5.488530000	-2.412072000	6.904762000
1	3.397176000	-1.948026000	6.702985000
6	6.786734000	-2.137217000	6.460650000
1	7.980793000	-0.991789000	5.076160000
1	5.323333000	-3.145224000	7.688048000
1	7.636434000	-2.649797000	6.900579000
1	2.471665000	-0.528172000	5.139541000
17	4.845299000	2.750059000	4.636433000
6	1.872003000	0.135132000	1.488585000
8	1.095399000	0.551090000	0.677697000
8	2.695895000	-0.899458000	1.323051000
17	1.486919000	0.757759000	7.191845000
17	2.713017000	3.931722000	7.103447000
6	-4.480868000	2.141726000	2.545242000
1	-4.939946000	1.343140000	3.133583000
1	-4.886478000	3.092974000	2.909707000
1	-4.795803000	2.029067000	1.504650000
17	4.663968000	1.313223000	7.554163000
3	2.698262000	2.253589000	8.559943000
17	5.160531000	-4.135417000	2.880937000
3	5.653134000	-3.054236000	4.600111000

Int-U:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3853.059040
Thermal correction to Gibbs Free Energy = 0.233281
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3855.45375612

6	4.086629000	-0.288251000	2.641273000
7	2.153046000	0.964101000	2.635755000
6	3.338752000	0.780896000	3.464916000
46	2.857448000	3.826037000	5.421804000
16	1.379989000	2.484422000	2.468032000
8	1.702966000	3.159076000	3.730449000
6	2.973739000	0.428283000	4.905948000
8	1.753901000	3.062107000	1.196864000
1	3.925488000	1.711446000	3.529036000
1	4.409970000	-1.141279000	3.239814000
1	4.943756000	0.147120000	2.118286000
6	-0.345185000	2.141879000	2.507922000
6	-1.010157000	1.897700000	1.307533000
6	-1.011846000	2.171708000	3.732102000
6	-2.377166000	1.663034000	1.348784000
1	-0.462890000	1.880111000	0.372706000
6	-2.379437000	1.934307000	3.741889000
1	-0.481724000	2.408543000	4.650584000
6	-3.080731000	1.676892000	2.558509000
1	-2.908942000	1.466196000	0.422094000
1	-2.912759000	1.960896000	4.688104000
6	4.069205000	0.519974000	5.935398000
6	5.373847000	0.060896000	5.689267000
6	3.712137000	0.870333000	7.246138000
6	6.276807000	-0.101858000	6.744156000
1	5.694563000	-0.194523000	4.685751000
6	4.616235000	0.717655000	8.302356000
1	2.709002000	1.220166000	7.484893000
6	5.893791000	0.205209000	8.055654000
1	7.277411000	-0.470396000	6.539527000
1	4.267518000	1.001255000	9.295713000
1	6.593747000	0.065640000	8.873766000
1	2.130763000	1.049171000	5.217635000
17	4.805318000	3.802368000	4.219184000
6	2.103100000	0.049292000	1.574514000
8	1.265835000	-0.019225000	0.722069000
8	3.161546000	-0.776407000	1.677045000
17	0.861860000	3.675750000	6.624328000
17	2.108510000	1.965964000	10.051031000
6	-4.564993000	1.456375000	2.583020000
1	-4.882788000	0.977105000	3.512740000
1	-5.095827000	2.412979000	2.510660000
1	-4.891884000	0.835694000	1.744772000
17	3.953306000	4.436480000	7.306828000
3	2.127832000	3.611466000	8.612890000
17	2.333642000	-1.300114000	5.050103000
3	4.176964000	-1.331244000	7.153885000

TS_{TU}:

The Number of Imaginary Frequencies = 1 (-218.0154 cm^{-1})
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3853.017144
Thermal correction to Gibbs Free Energy = 0.235670
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3855.41120757

6	4.232895000	-0.383994000	1.897369000
7	2.323745000	0.767970000	2.508228000
6	3.581319000	0.335258000	3.102148000
46	3.334391000	1.953562000	5.916002000
16	1.635908000	2.281435000	2.913871000
8	2.030310000	2.468637000	4.319983000
6	3.355231000	-0.439014000	4.373902000
8	2.014156000	3.252703000	1.911314000
1	4.213065000	1.197113000	3.383386000
1	4.603629000	-1.377380000	2.147176000
1	5.033601000	0.228406000	1.470273000
6	-0.105198000	2.040047000	2.910369000
6	-0.814631000	2.298156000	1.738630000
6	-0.737188000	1.658651000	4.092494000
6	-2.193539000	2.150923000	1.758832000

1	-0.291880000	2.593594000	0.836891000
6	-2.118512000	1.519508000	4.082043000
1	-0.166211000	1.499505000	5.002896000
6	-2.864897000	1.762293000	2.924098000
1	-2.760765000	2.342819000	0.852318000
1	-2.626554000	1.227728000	4.996958000
6	4.452915000	-0.916227000	5.218771000
6	5.772894000	-1.011895000	4.743166000
6	4.129227000	-1.528812000	6.449860000
6	6.718050000	-1.776929000	5.430115000
1	6.066457000	-0.497119000	3.834912000
6	5.071399000	-2.298392000	7.123384000
1	3.123395000	-1.410116000	6.842896000
6	6.364789000	-2.450132000	6.602247000
1	7.730175000	-1.850196000	5.044670000
1	4.801664000	-2.777727000	8.059286000
1	7.096470000	-3.058484000	7.124291000
1	2.385484000	-0.329967000	4.848869000
17	5.171038000	2.710723000	4.772459000
6	2.162880000	0.266451000	1.205792000
8	1.253800000	0.488085000	0.460074000
8	3.208643000	-0.532022000	0.925211000
17	1.511764000	0.882471000	7.013626000
17	2.553527000	4.294548000	7.341096000
6	-4.361072000	1.644891000	2.939527000
1	-4.698615000	0.924201000	3.688829000
1	-4.818550000	2.610919000	3.183876000
1	-4.748517000	1.336944000	1.964699000
17	4.642572000	1.382708000	7.703497000
3	2.621363000	2.452237000	8.471601000
17	2.725977000	-2.526437000	3.606980000
3	4.540364000	-3.137491000	4.838254000

Int-V:

The Number of Imaginary Frequencies = 0
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3368.207509
Thermal correction to Gibbs Free Energy = 0.440939
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3370.89203276

6	1.458993000	0.042567000	-1.313648000
6	0.542806000	0.303401000	-0.113090000
7	-0.809924000	-0.285068000	-0.386667000
6	-1.258189000	-0.704897000	-1.629186000
8	-0.346492000	-1.004346000	-2.535851000
6	1.025321000	-1.177407000	-2.069371000
1	1.413905000	0.898836000	-1.993254000
1	1.065449000	-2.088504000	-1.466310000
1	1.604515000	-1.323370000	-2.980839000
1	0.924921000	-0.229180000	0.757572000
16	-1.923989000	-0.416001000	0.911322000
8	-1.133941000	-0.039524000	2.082486000
8	-2.493781000	-1.760688000	0.862391000
6	-3.204217000	0.779013000	0.692375000
6	-4.353410000	0.446626000	-0.022348000
6	-3.039126000	2.031246000	1.282791000
6	-5.351581000	1.403269000	-0.145673000
1	-4.466603000	-0.519393000	-0.500505000
6	-4.055342000	2.968086000	1.145433000
1	-2.134865000	2.261132000	1.836291000
6	-5.222380000	2.670454000	0.433509000
1	-6.241018000	1.149875000	-0.716040000
1	-3.937198000	3.949331000	1.597391000
6	-6.325769000	3.681708000	0.309776000
1	-6.799136000	3.634211000	-0.675029000
1	-5.958410000	4.699361000	0.466375000
1	-7.108282000	3.494894000	1.054859000
8	-2.449703000	-0.806655000	-1.871893000
6	0.449501000	1.779870000	0.206626000
6	1.098870000	2.286844000	1.332050000
6	-0.240904000	2.658406000	-0.630775000
6	1.063188000	3.649588000	1.615886000
1	1.636444000	1.605947000	1.986498000
6	-0.283457000	4.019472000	-0.346160000
1	-0.756796000	2.276980000	-1.508728000
6	0.369467000	4.519179000	0.778337000
1	1.576251000	4.031011000	2.494269000
1	-0.827025000	4.690577000	-1.005025000
1	0.339295000	5.582423000	0.999405000
46	3.390610000	-0.116291000	-0.734095000
17	2.906784000	-2.035361000	0.529296000
17	3.857573000	1.777480000	-2.113170000
1	-3.461285000	-1.473065000	-3.085492000
8	-4.053703000	-1.838617000	-3.786060000
6	-5.318508000	-1.780752000	-3.387949000
8	-5.685312000	-1.357717000	-2.309471000
6	-6.254788000	-2.308678000	-4.442423000
1	-6.142207000	-1.728518000	-5.362630000
1	-5.998223000	-3.344539000	-4.681739000
1	-7.282579000	-2.250691000	-4.086615000
6	-0.635595000	-4.494426000	3.540323000
1	-1.551744000	-3.912209000	3.431176000
1	-0.798449000	-5.512690000	3.182995000
1	-0.323592000	-4.511354000	4.585993000
6	0.661012000	-2.457347000	3.207124000
1	0.944940000	-2.504646000	4.260145000
1	1.466465000	-2.023625000	2.608372000
1	-0.249957000	-1.871769000	3.074669000
6	1.704709000	-4.622849000	2.838980000
1	1.537542000	-5.642474000	2.487498000
1	2.458960000	-4.126780000	2.223466000
1	2.017107000	-4.633246000	3.884682000
7	0.430078000	-3.856283000	2.723057000
6	0.002617000	-3.831946000	1.287104000
1	0.795496000	-3.343161000	0.714460000
1	-0.133339000	-4.863134000	0.955256000
1	-0.932641000	-3.273615000	1.201650000
17	5.788407000	-0.288543000	0.026944000
3	5.851730000	1.426022000	-1.273468000

TS_{CV}:

The Number of Imaginary Frequencies = 1 (-213.0251 cm^{-1})
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3368.178284
Thermal correction to Gibbs Free Energy = 0.441012
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3370.85633165

6	-1.377704000	-0.042516000	1.363464000
6	-1.057682000	0.573152000	0.112457000
7	1.002650000	-0.159315000	0.028931000
6	1.549461000	-0.617233000	1.183314000
8	0.666419000	-1.097825000	2.083154000
6	-0.687561000	-1.346118000	1.667252000
1	-1.341834000	0.624282000	2.225446000
1	-0.697415000	-2.014548000	0.806079000
1	-1.146433000	-1.851068000	2.518253000
1	-1.143638000	-0.033529000	-0.779195000
16	1.980260000	0.180634000	-1.238929000
8	1.068026000	0.687222000	-2.279724000
8	2.768530000	-1.013093000	-1.596412000

6	3.093847000	1.497378000	-0.825338000
6	4.301150000	1.220117000	-0.187376000
6	2.720081000	2.802159000	-1.139468000
6	5.140177000	2.277548000	0.138326000
1	4.573851000	0.208636000	0.087140000
6	3.579448000	3.843584000	-0.809192000
1	1.774199000	2.989373000	-1.637389000
6	4.798538000	3.598723000	-0.169303000
1	6.069727000	2.056654000	0.655958000
1	3.296910000	4.865199000	-1.051309000
6	5.732518000	4.726556000	0.167181000
1	6.189264000	4.583403000	1.151008000
1	5.216498000	5.690576000	0.166057000
1	6.549278000	4.788139000	-0.561853000
8	2.739673000	-0.627274000	1.475700000
6	-1.019581000	2.017075000	-0.104190000
6	-1.246426000	2.512330000	-1.397243000
6	-0.753959000	2.922254000	0.934130000
6	-1.236834000	3.879206000	-1.641978000
1	-1.422889000	1.811406000	-2.206174000
6	-0.728340000	4.286868000	0.684920000
1	-0.554283000	2.554561000	1.934971000
6	-0.976085000	4.768005000	-0.600409000
1	-1.424656000	4.252036000	-2.644387000
1	-0.514984000	4.978950000	1.493734000
1	-0.960636000	5.837588000	-0.790837000
46	-3.374749000	-0.224480000	0.843719000
17	-2.954204000	-1.992421000	-0.608921000
17	-3.811660000	1.557022000	2.363839000
1	3.804583000	-1.054185000	2.692965000
8	4.447160000	-1.290173000	3.410488000
6	5.681878000	-0.970194000	3.047643000
8	5.987650000	-0.474161000	1.981414000
6	6.677756000	-1.299947000	4.130017000
1	6.430916000	-0.748299000	5.041686000
1	6.623961000	-2.364728000	4.373765000
1	7.682899000	-1.042317000	3.798439000
6	1.487985000	-3.122138000	-3.757004000
1	2.084244000	-2.324163000	-3.305207000
1	1.966247000	-4.088564000	-3.586567000
1	1.355216000	-2.954876000	-4.827310000
6	-0.549830000	-1.833259000	-3.381004000
1	-0.724929000	-1.769255000	-4.456808000
1	-1.495505000	-1.824297000	-2.833250000
1	0.083585000	-1.003866000	-3.051577000
6	-0.683788000	-4.247661000	-3.627323000
1	-0.183691000	-5.194413000	-3.416826000
1	-1.656807000	-4.220760000	-3.133723000
1	-0.808413000	-4.123689000	-4.704321000
7	0.146124000	-3.130396000	-3.102446000
6	0.325664000	-3.304042000	-1.626499000
1	-0.654217000	-3.228545000	-1.150101000
1	0.772004000	-4.284394000	-1.449345000
1	0.992725000	-2.519191000	-1.266485000
17	-5.770456000	-0.492748000	0.351791000
3	-5.882367000	1.183303000	1.719644000

Int-X:

The Number of Imaginary Frequencies = 0

PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3368.173306

Thermal correction to Gibbs Free Energy = 0.432409

E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3370.84878287

6	1.196294000	-0.089977000	-1.832872000
6	0.280997000	0.211646000	-0.655843000
7	-0.650958000	-0.881601000	-0.485890000
6	-1.672270000	-3.513830000	-1.465708000
8	-0.692704000	-4.090898000	-1.211867000
6	1.440668000	-1.355307000	-2.344979000
1	1.457593000	0.772796000	-2.442738000
1	1.014413000	-2.213515000	-1.835191000
1	1.783773000	-1.478095000	-3.369410000
1	0.916335000	0.337280000	0.237398000
16	-1.298403000	-1.009847000	0.939344000
8	-0.442358000	-0.536757000	2.061243000
8	-1.799151000	-2.409461000	1.081710000
6	-2.780128000	-0.006762000	1.072026000
6	-3.976836000	-0.458019000	0.520372000
6	-2.712235000	1.250074000	1.666947000
6	-5.104826000	0.353905000	0.568778000
1	-4.031178000	-1.441910000	0.065944000
6	-3.846405000	2.053860000	1.705422000
1	-1.774162000	1.584288000	2.097145000
6	-5.058095000	1.620836000	1.160183000
1	-6.031122000	-0.007997000	0.129455000
1	-3.788322000	3.037425000	2.166241000
6	-6.288679000	2.481548000	1.233728000
1	-6.963500000	2.286040000	0.395153000
1	-6.034323000	3.545599000	1.226732000
1	-6.852199000	2.287468000	2.154635000
8	-2.680390000	-3.032156000	-1.801953000
6	-0.363758000	1.570125000	-0.933909000
6	0.180536000	2.732233000	-0.384992000
6	-1.482075000	1.671004000	-1.764128000
6	-0.382125000	3.977742000	-0.656119000
1	1.044681000	2.658176000	0.272381000
6	-2.041553000	2.914790000	-2.038571000
1	-1.926496000	0.766923000	-2.169235000
6	-1.495282000	4.071984000	-1.486449000
1	0.045779000	4.873091000	-0.212757000
1	-2.911733000	2.980576000	-2.686773000
1	-1.938168000	5.041466000	-1.698182000
46	3.276249000	-0.771804000	-1.410086000
17	2.741153000	-2.036398000	0.393493000
17	3.903321000	0.441568000	-3.380802000
1	-3.483628000	-1.444474000	-2.611838000
8	-3.800179000	-0.643774000	-3.064914000
6	-5.111354000	-0.521032000	-2.819391000
8	-5.755574000	-1.346718000	-2.212971000
6	-5.653707000	0.772427000	-3.355844000
1	-5.355378000	1.576120000	-2.674047000
1	-5.236210000	0.996476000	-4.339773000
1	-6.741308000	0.725531000	-3.398700000
6	-0.907171000	-3.995616000	3.637604000
1	-1.417203000	-3.275607000	2.989100000
1	-1.359353000	-4.983286000	3.526267000
1	-0.938932000	-3.685953000	4.683698000
6	1.182180000	-2.753866000	3.442956000
1	1.171690000	-2.560140000	4.517649000
1	2.207430000	-2.805879000	3.074654000
1	0.631318000	-1.971798000	2.904930000
6	1.229105000	-5.128629000	3.979949000
1	0.749308000	-6.092049000	3.799080000
1	2.269753000	-5.165893000	3.654215000
1	1.182227000	-4.883964000	5.042541000
7	0.521570000	-4.077315000	3.206489000
6	0.565028000	-4.409528000	1.746860000

1	1.602206000	-4.398099000	1.411747000
1	0.124570000	-5.399163000	1.609889000
1	-0.019481000	-3.662691000	1.205740000
17	5.543935000	-0.675590000	-0.587062000
3	5.883201000	0.471150000	-2.411974000

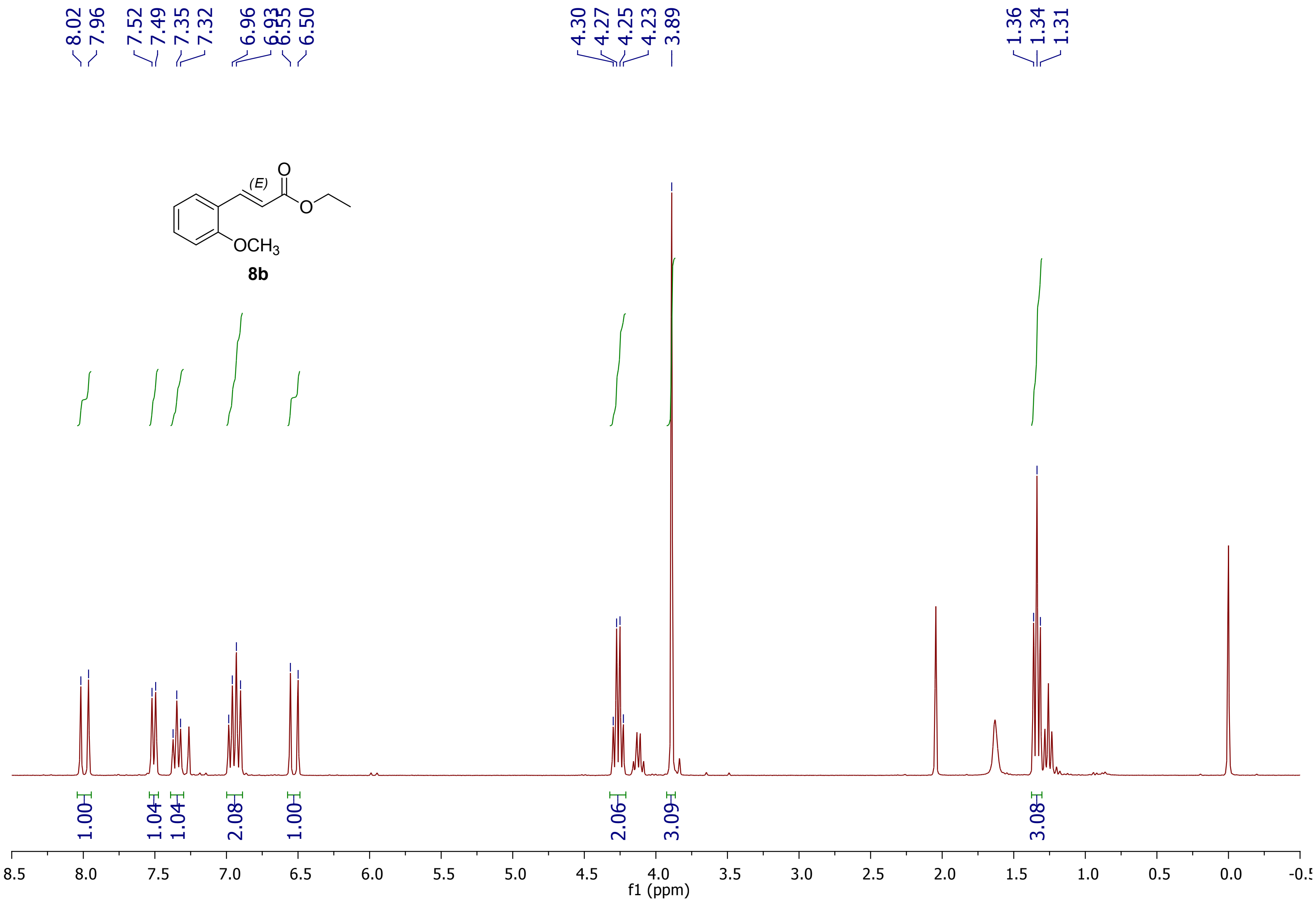
TS_{VX}:

The Number of Imaginary Frequencies = 1 (-376.1913 cm^{-1})
PBE1PBE/6-31G(d,p)/Def2-TZVPP, G = -3368.171925
Thermal correction to Gibbs Free Energy = 0.444053
E(M062X/6-31G(d,p)/Def2-TZVPP,CH_3CN) = -3370.85093243

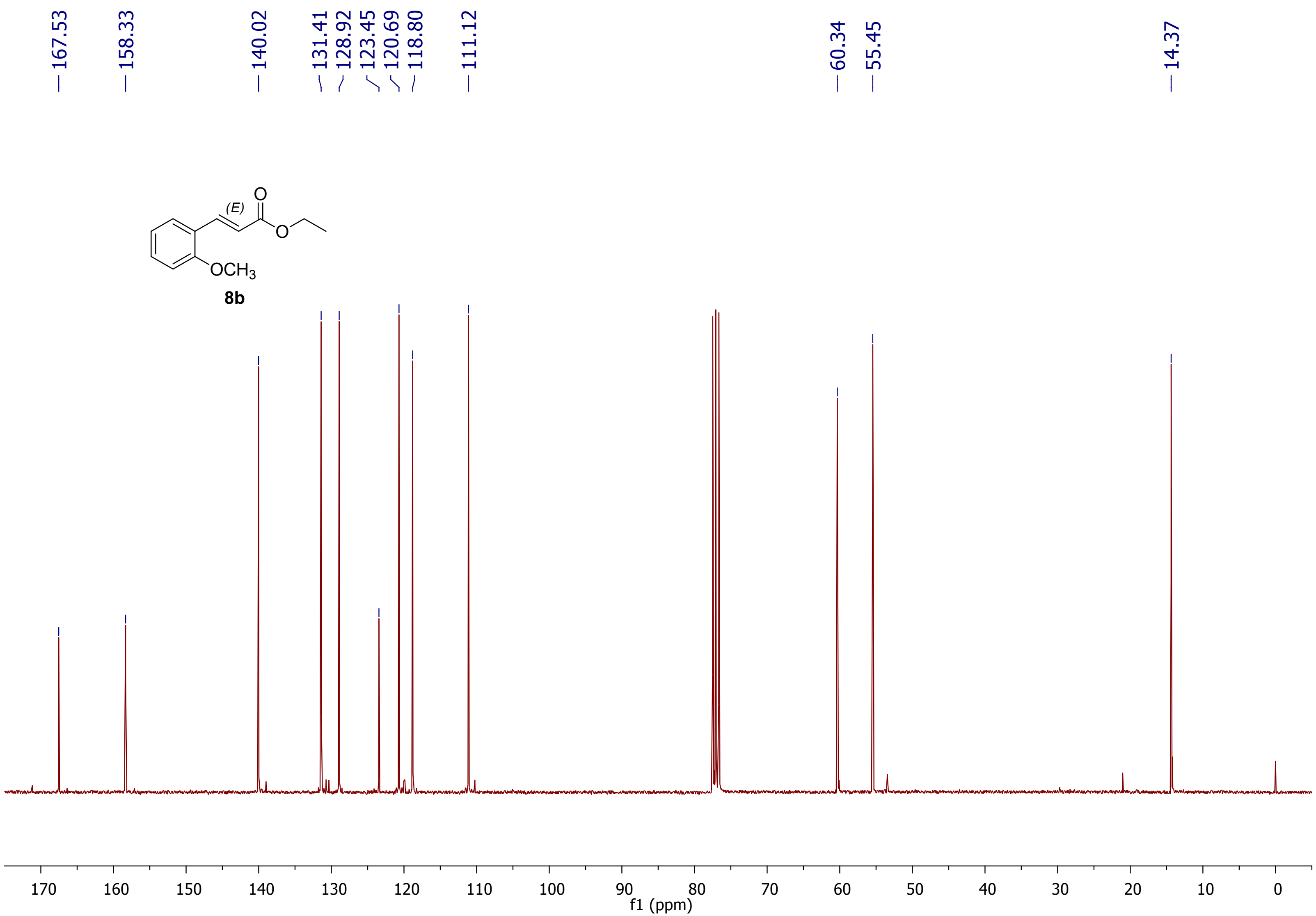
6	1.888511000	-0.951987000	0.836302000
6	0.801153000	-1.237690000	-0.199092000
7	-0.376957000	-0.360655000	0.011438000
6	-0.858196000	0.079341000	1.281661000
8	-0.136481000	-0.125120000	2.298561000
6	1.758132000	0.168215000	1.677509000
1	2.219340000	-1.857117000	1.340598000
1	1.425128000	1.120657000	1.287243000
1	2.224866000	0.170936000	2.656760000
1	1.169107000	-1.003922000	-1.198627000
16	-1.418242000	-0.170848000	-1.321365000
8	-0.720974000	-0.808565000	-2.429773000
8	-1.793027000	1.241187000	-1.453572000
6	-2.909680000	-1.073346000	-0.998392000
6	-4.032995000	-0.402864000	-0.512843000
6	-2.939152000	-2.431799000	-1.296735000
6	-5.202463000	-1.126450000	-0.329320000
1	-3.980682000	0.654634000	-0.269345000
6	-4.122476000	-3.134693000	-1.094819000
1	-2.056196000	-2.928871000	-1.685257000
6	-5.266997000	-2.497061000	-0.611741000
1	-6.085362000	-0.615071000	0.046660000
1	-4.154511000	-4.196934000	-1.321722000
6	-6.546358000	-3.254430000	-0.395863000
1	-7.380360000	-2.776727000	-0.920688000
1	-6.810177000	-3.283107000	0.667282000
1	-6.469308000	-4.285575000	-0.749716000
8	-1.958134000	0.659636000	1.246169000
6	0.421390000	-2.709246000	-0.157132000
6	0.699089000	-3.525372000	-1.254335000
6	-0.207588000	-3.262891000	0.963968000
6	0.354198000	-4.875780000	-1.236645000
1	1.169017000	-3.092629000	-2.133353000
6	-0.557014000	-4.609001000	0.977646000
1	-0.424003000	-2.632439000	1.822844000
6	-0.277147000	-5.419162000	-0.121635000
1	0.573805000	-5.499974000	-2.098402000
1	-1.049372000	-5.027861000	1.850805000
1	-0.549883000	-6.470790000	-0.107595000
46	3.670080000	-0.013909000	0.285685000
17	2.576162000	1.375674000	-1.179987000
17	4.760437000	-1.424368000	1.875680000
1	-2.792413000	1.446080000	2.325704000
8	-3.395120000	1.946780000	2.957869000
6	-4.273030000	2.670297000	2.287569000
8	-4.322755000	2.762699000	1.073089000
6	-5.232431000	3.382246000	3.209035000
1	-5.836505000	2.644261000	3.745454000
1	-4.682392000	3.952864000	3.962233000
1	-5.883161000	4.040329000	2.633928000
6	-1.935152000	4.389126000	-1.568148000
1	-2.362957000	3.388466000	-1.654617000
1	-2.379558000	4.906205000	-0.716416000
1	-2.092792000	4.960259000	-2.484865000
6	0.132720000	3.476791000	-2.481483000
1	-0.053682000	4.029001000	-3.404526000
1	1.202868000	3.361154000	-2.306237000
1	-0.340483000	2.497631000	-2.506555000
6	0.175566000	5.592617000	-1.280023000
1	-0.285206000	6.167657000	-0.475231000
1	1.241476000	5.465125000	-1.084778000
1	0.031804000	6.105215000	-2.232696000
7	-0.461662000	4.251796000	-1.346841000
6	-0.225700000	3.524895000	-0.052420000
1	0.835085000	3.275524000	0.013276000
1	-0.531011000	4.179707000	0.765684000
1	-0.832264000	2.617508000	-0.057292000
17	5.825617000	0.896283000	-0.496237000
3	6.555424000	-0.543095000	0.949905000

12. Copies of NMR Spectra

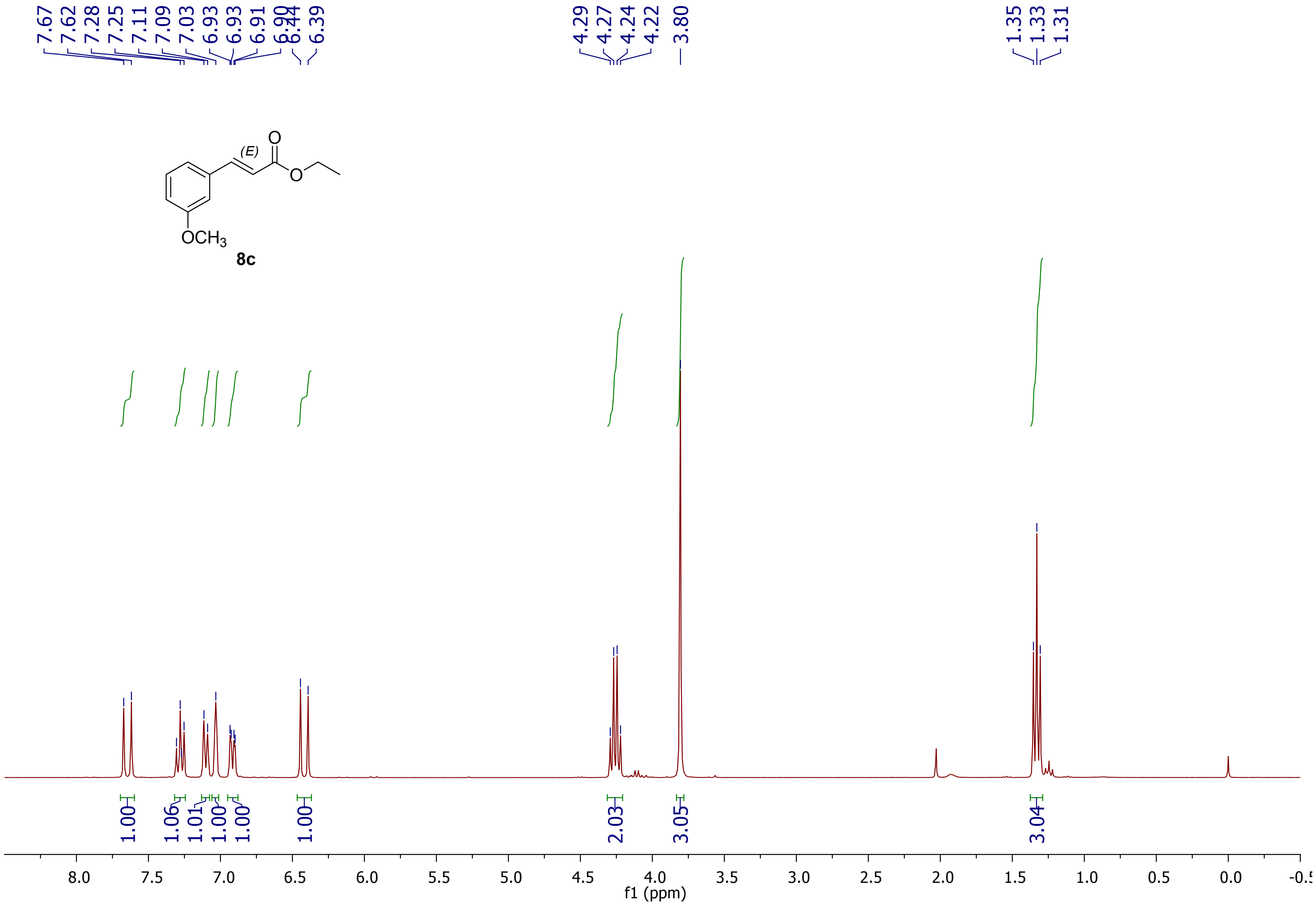
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **8b**



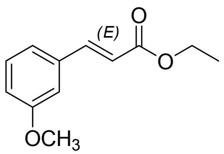
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8b**



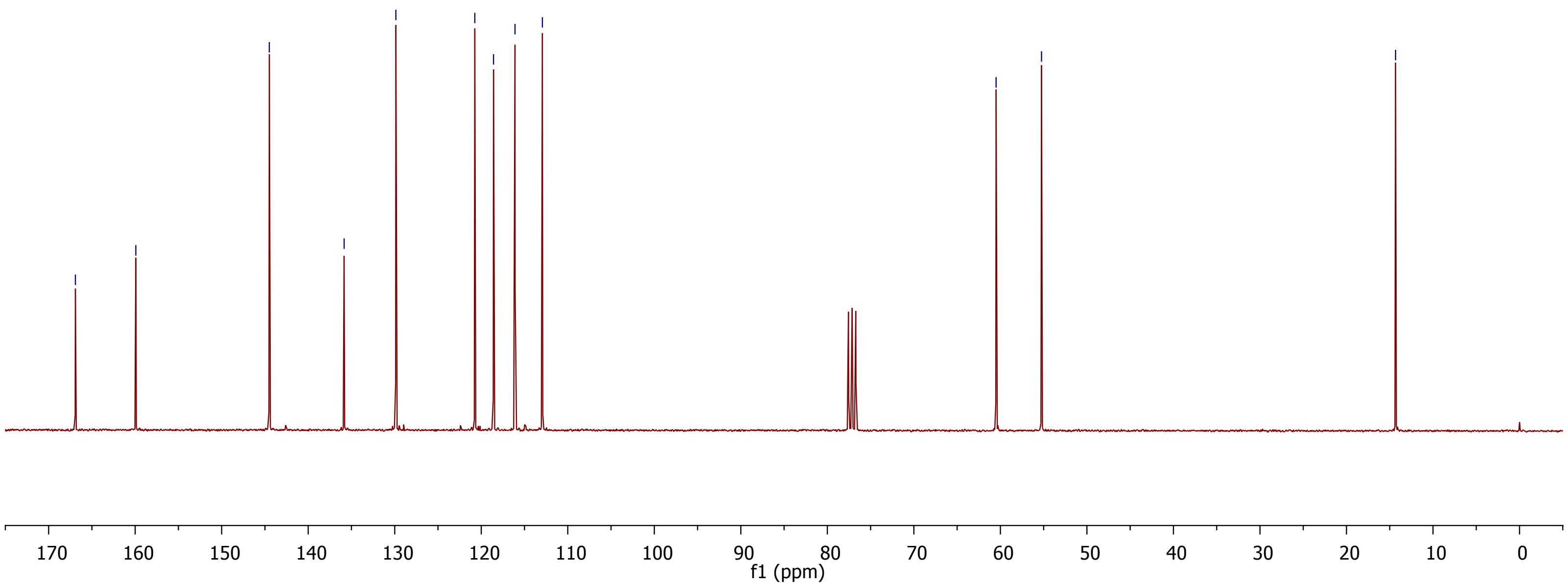
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **8c**



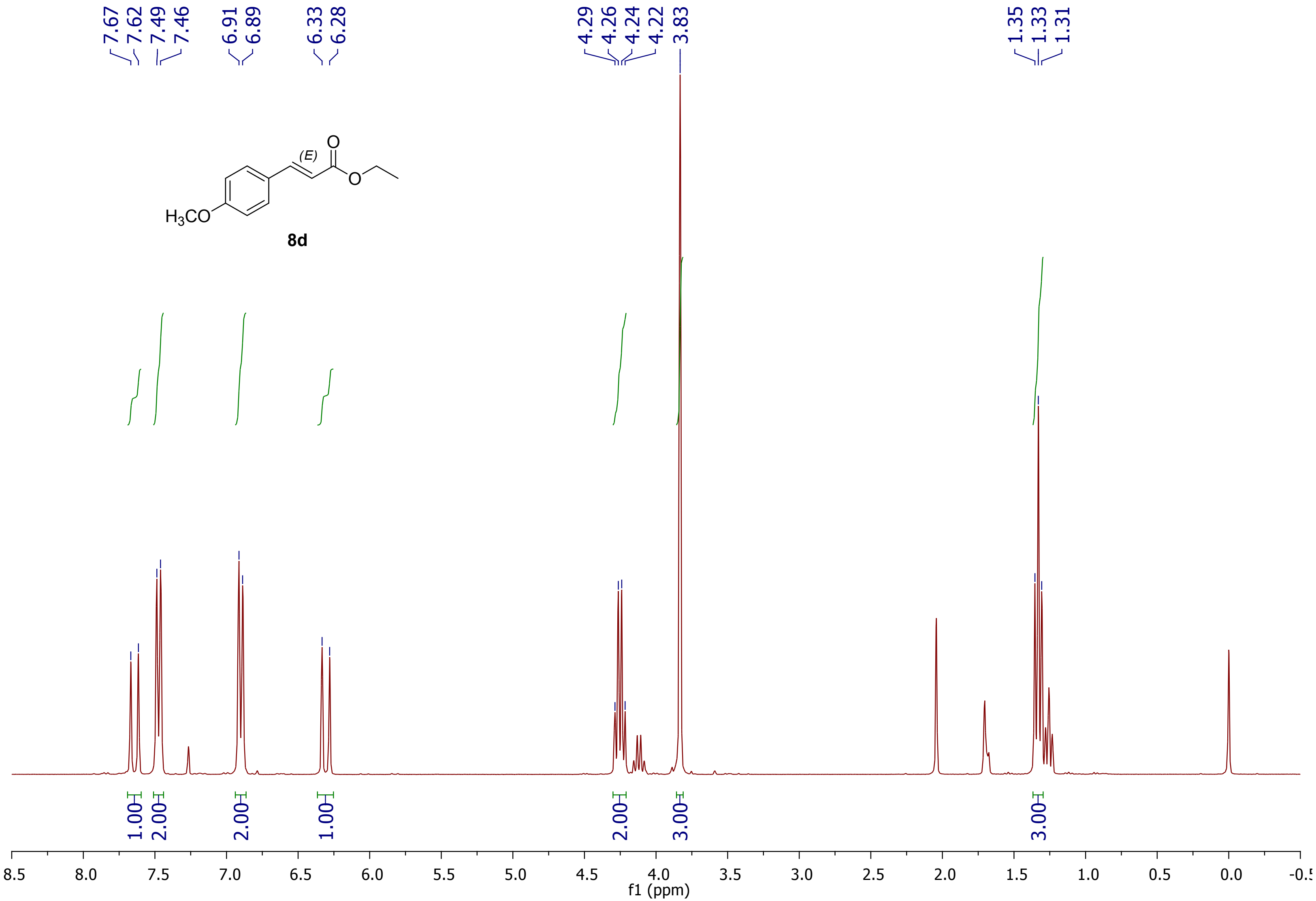
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8c**



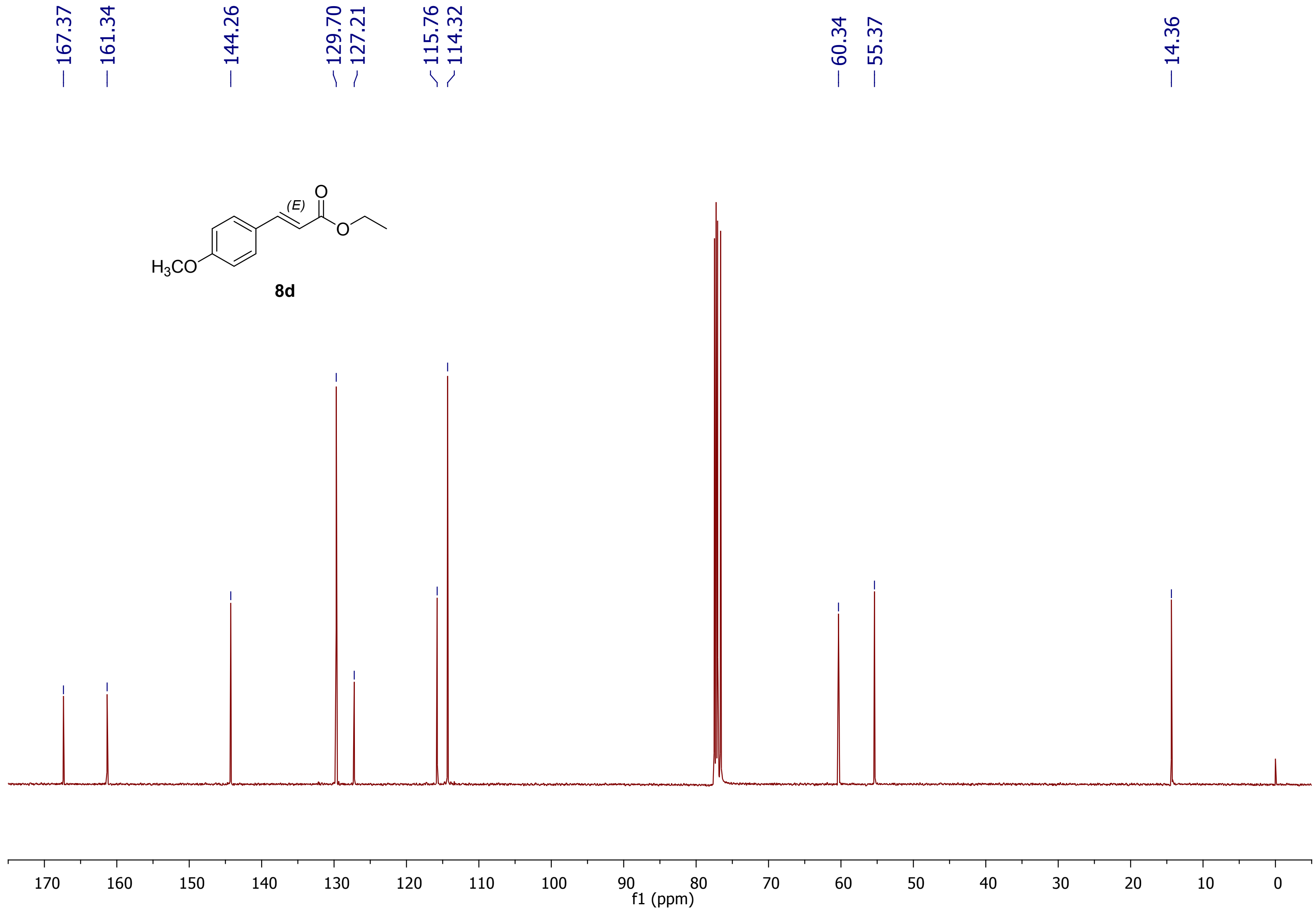
8c



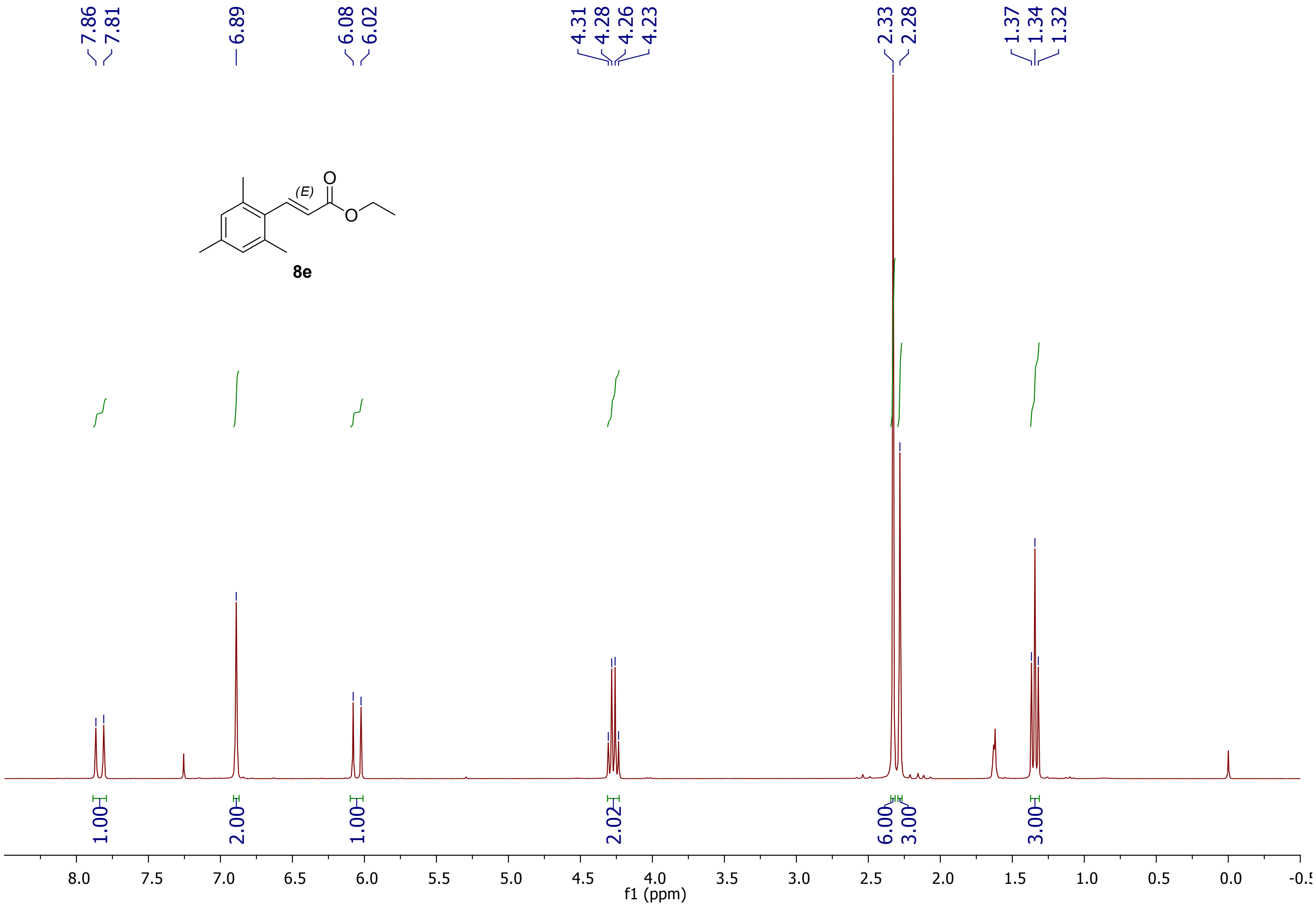
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **8d**



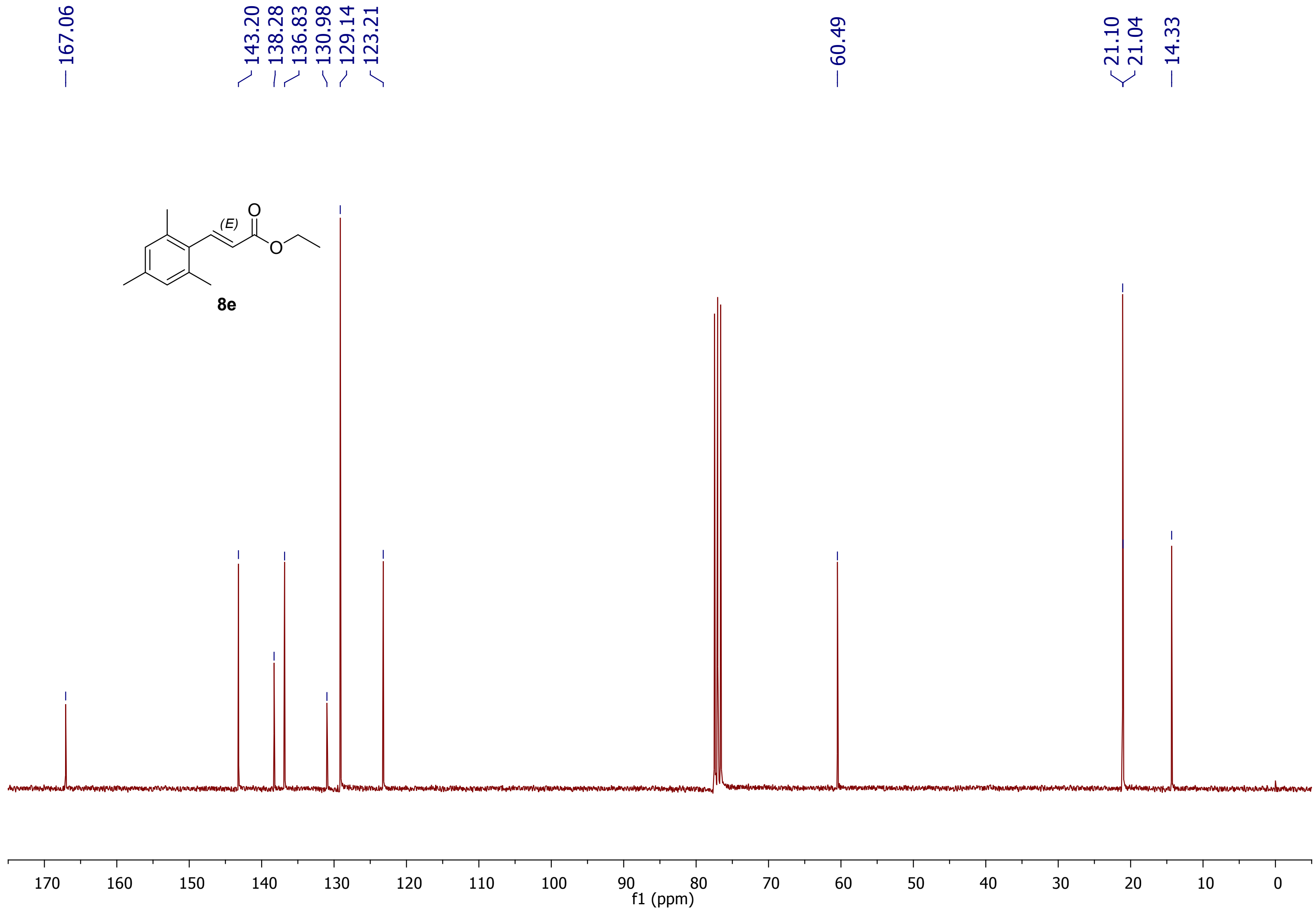
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8d**



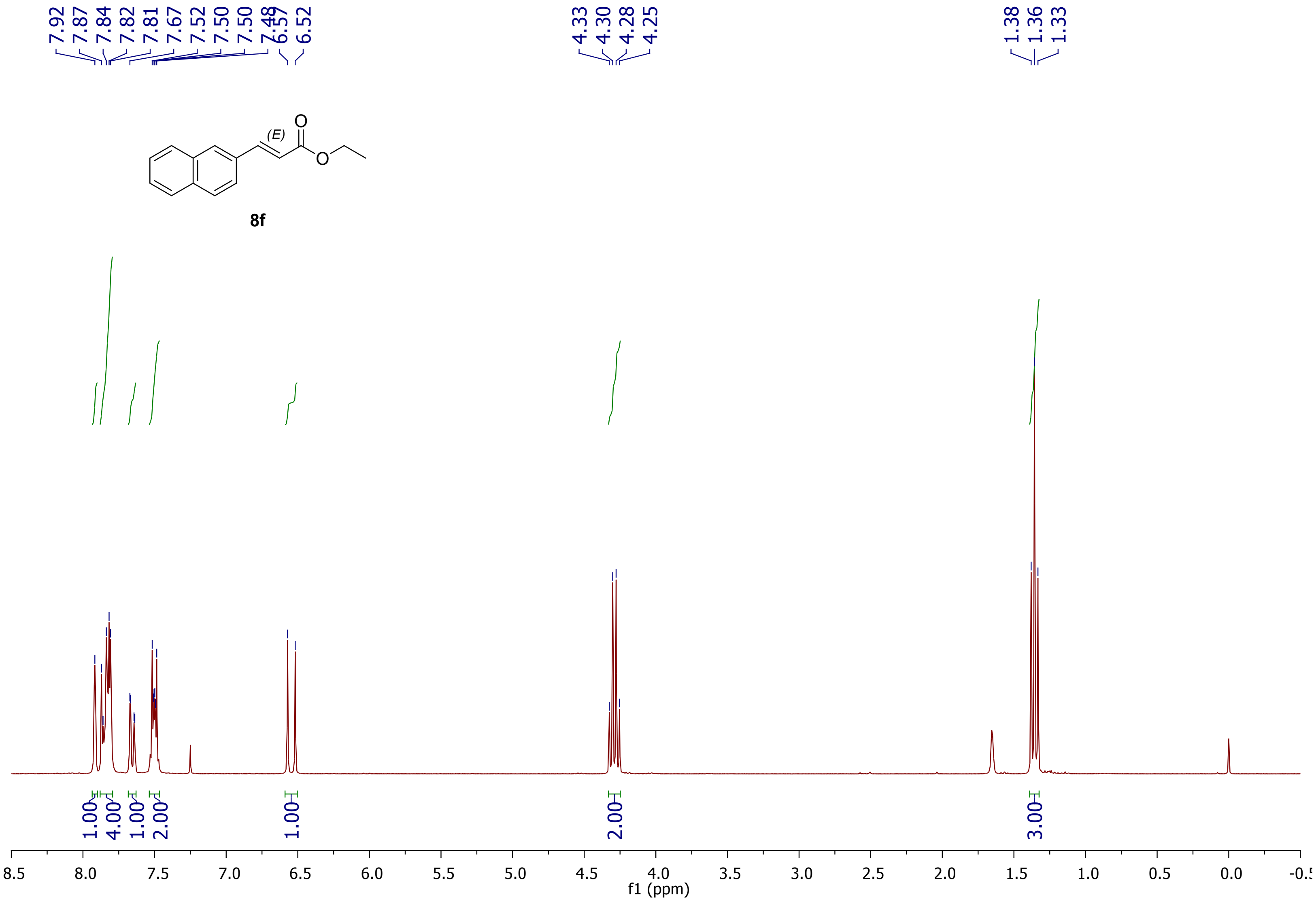
[1]H NMR (300 MHz, $CDCl_3$) of substrate **8e**



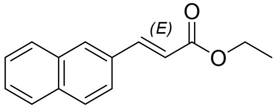
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8e**



[1]H NMR (300 MHz, $CDCl_3$) of substrate **8f**



^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8f**



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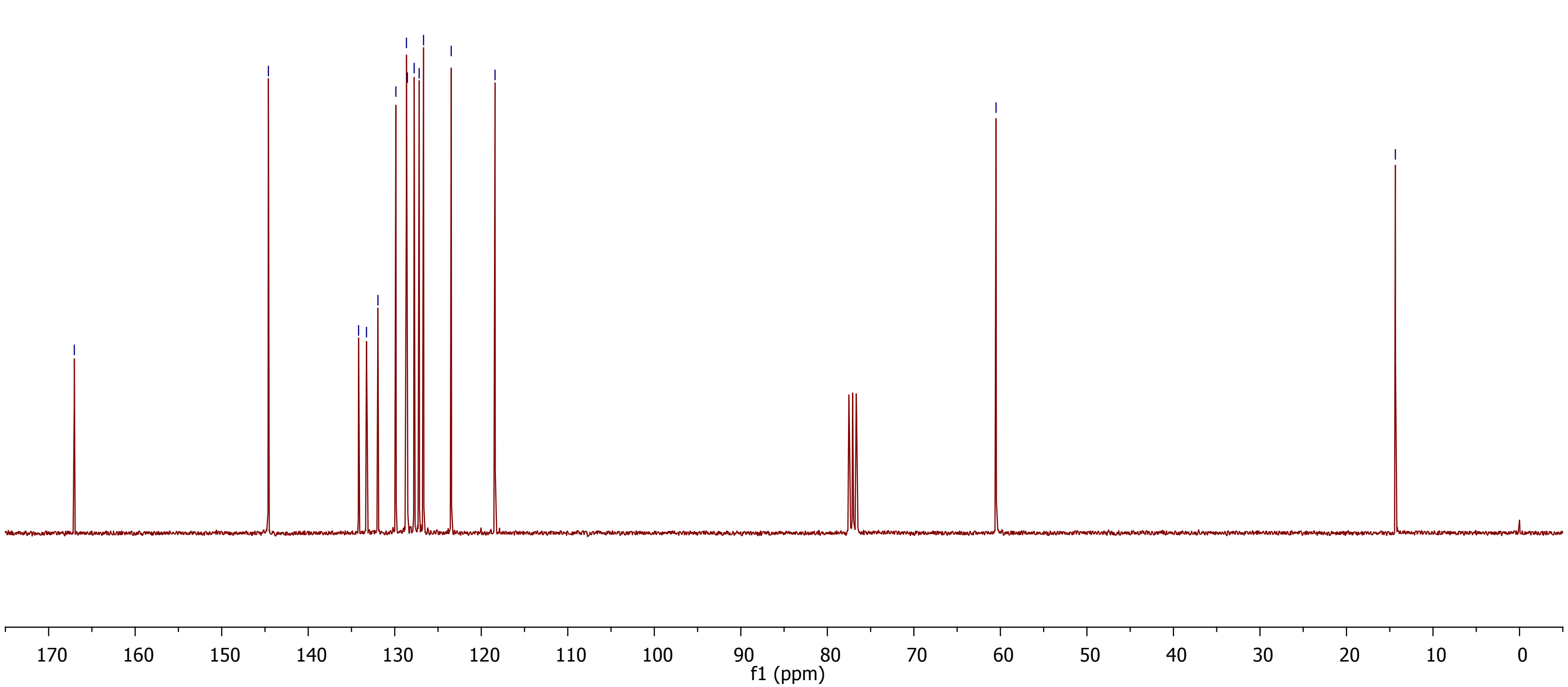
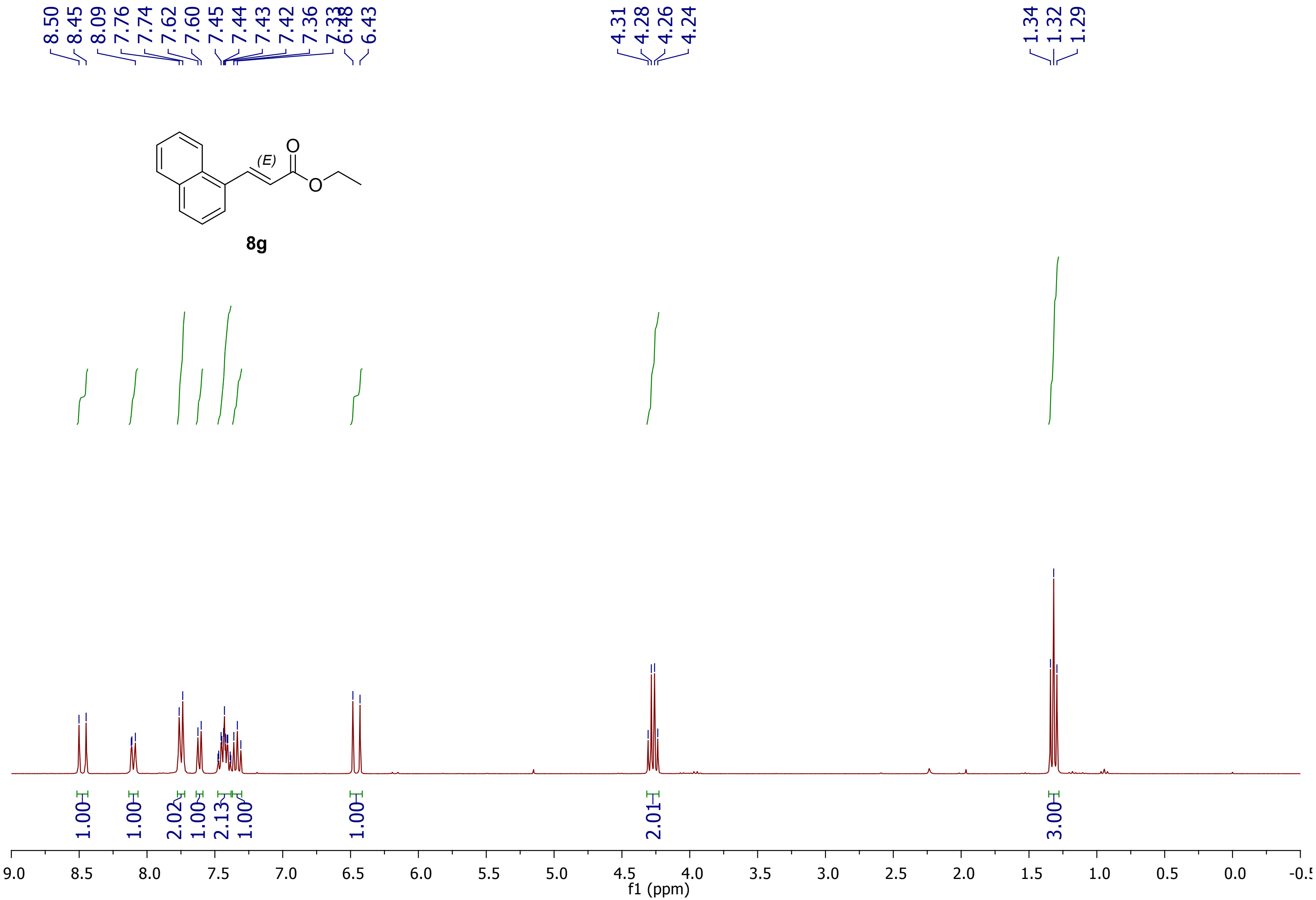
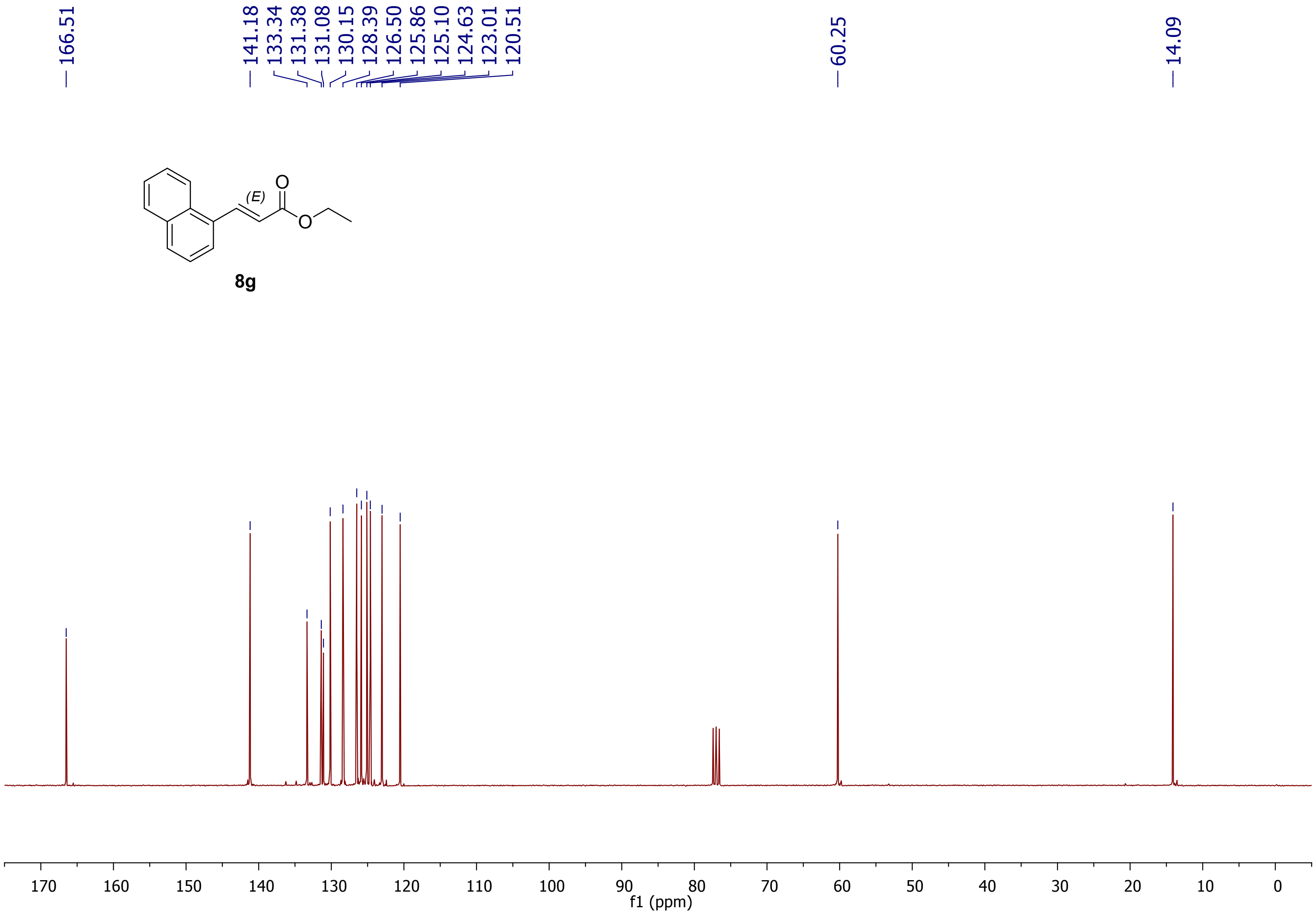


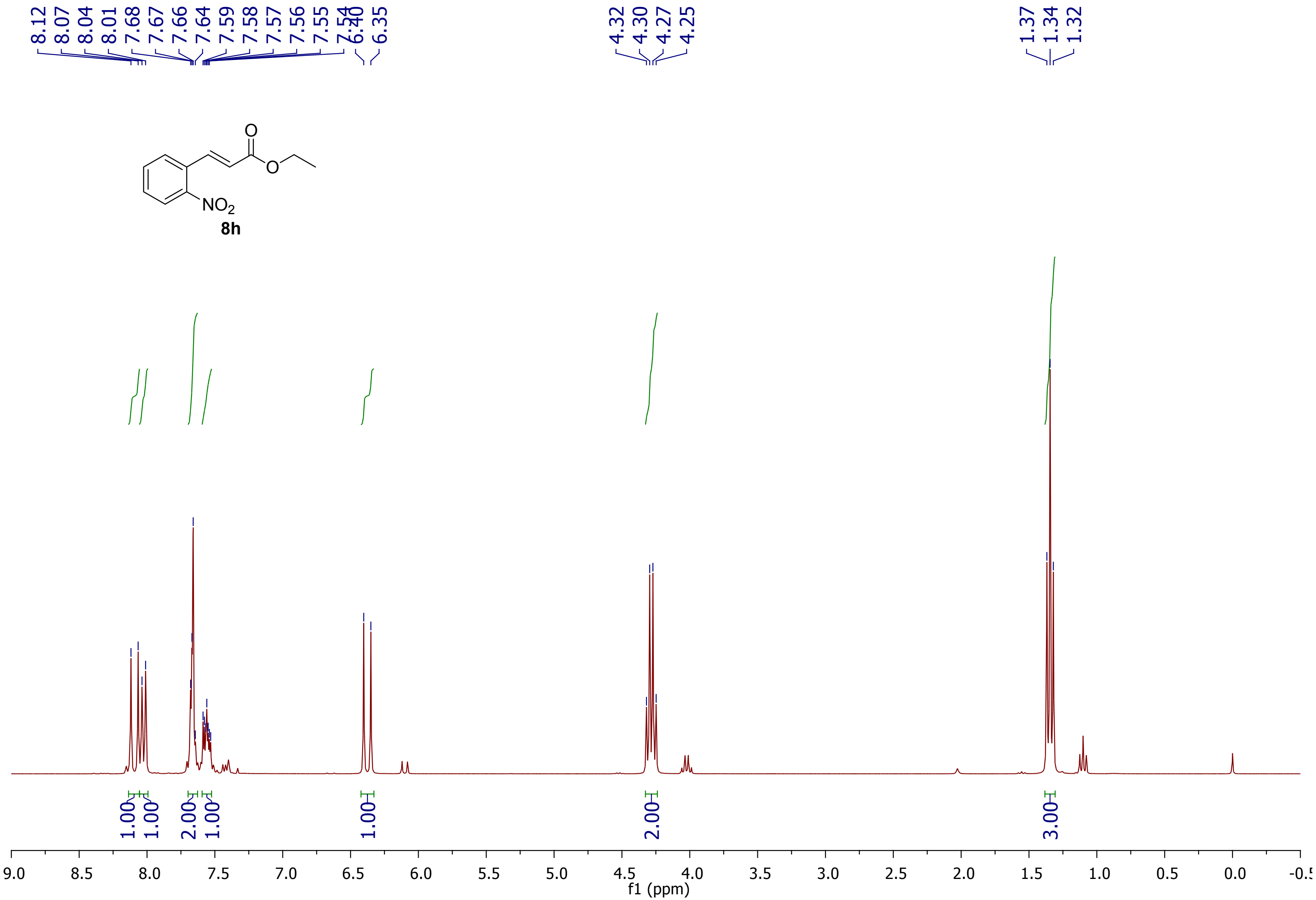
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **8g**



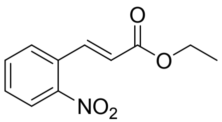
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8g**



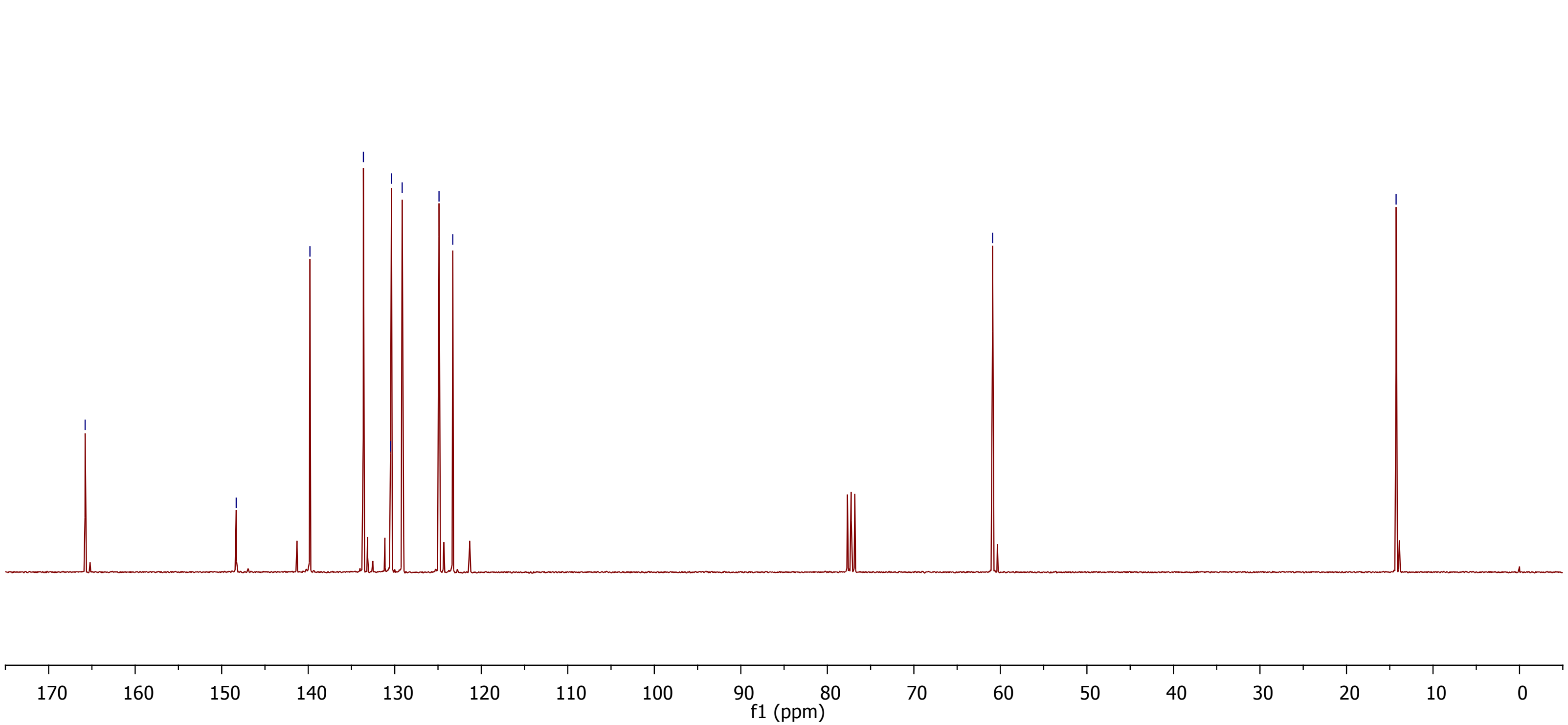
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **8h**



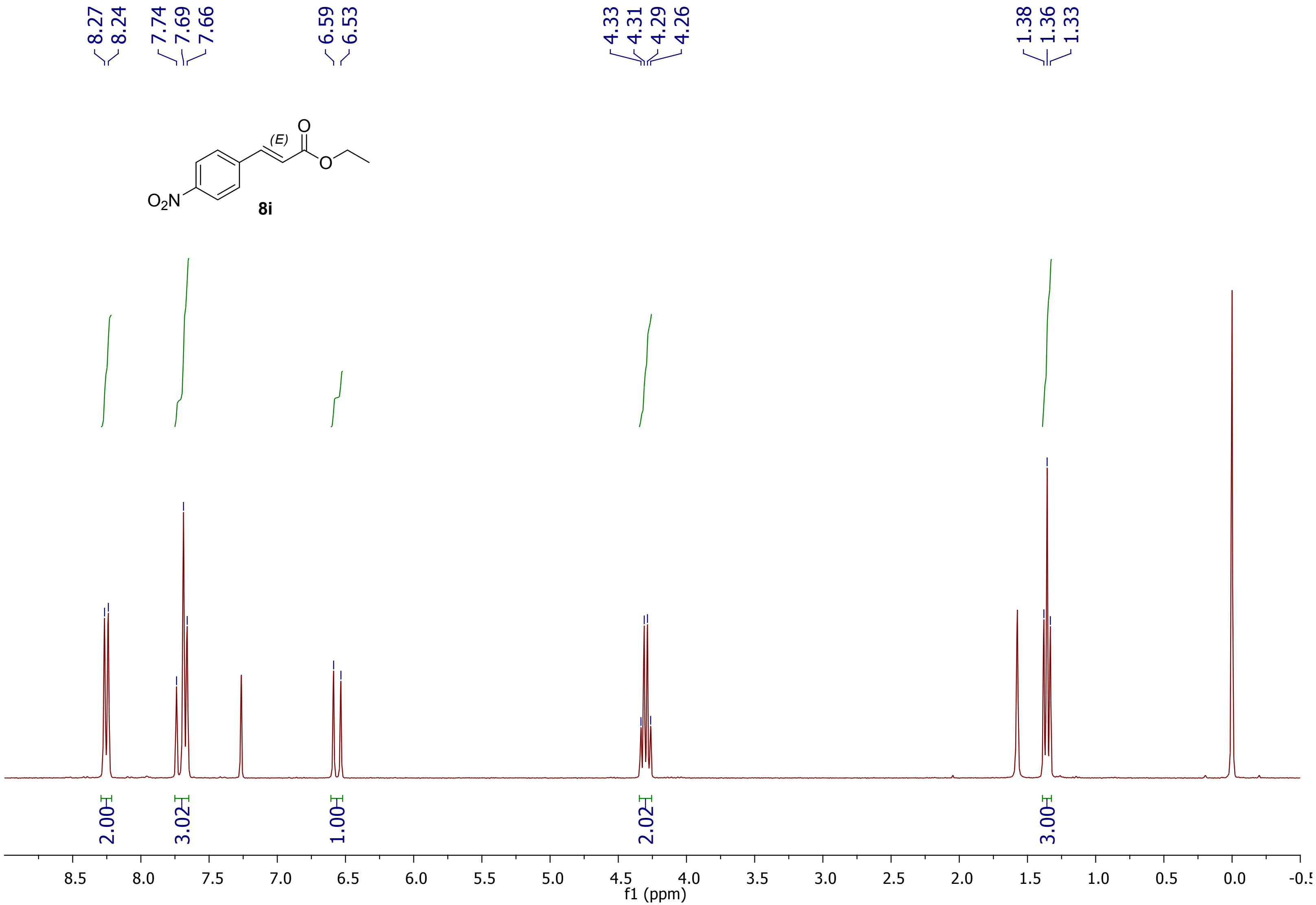
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8h**



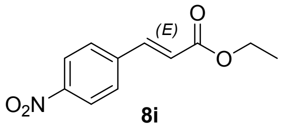
8h



^{1}H NMR (300 MHz, $CDCl_3$) of substrate **8i**



^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8i**



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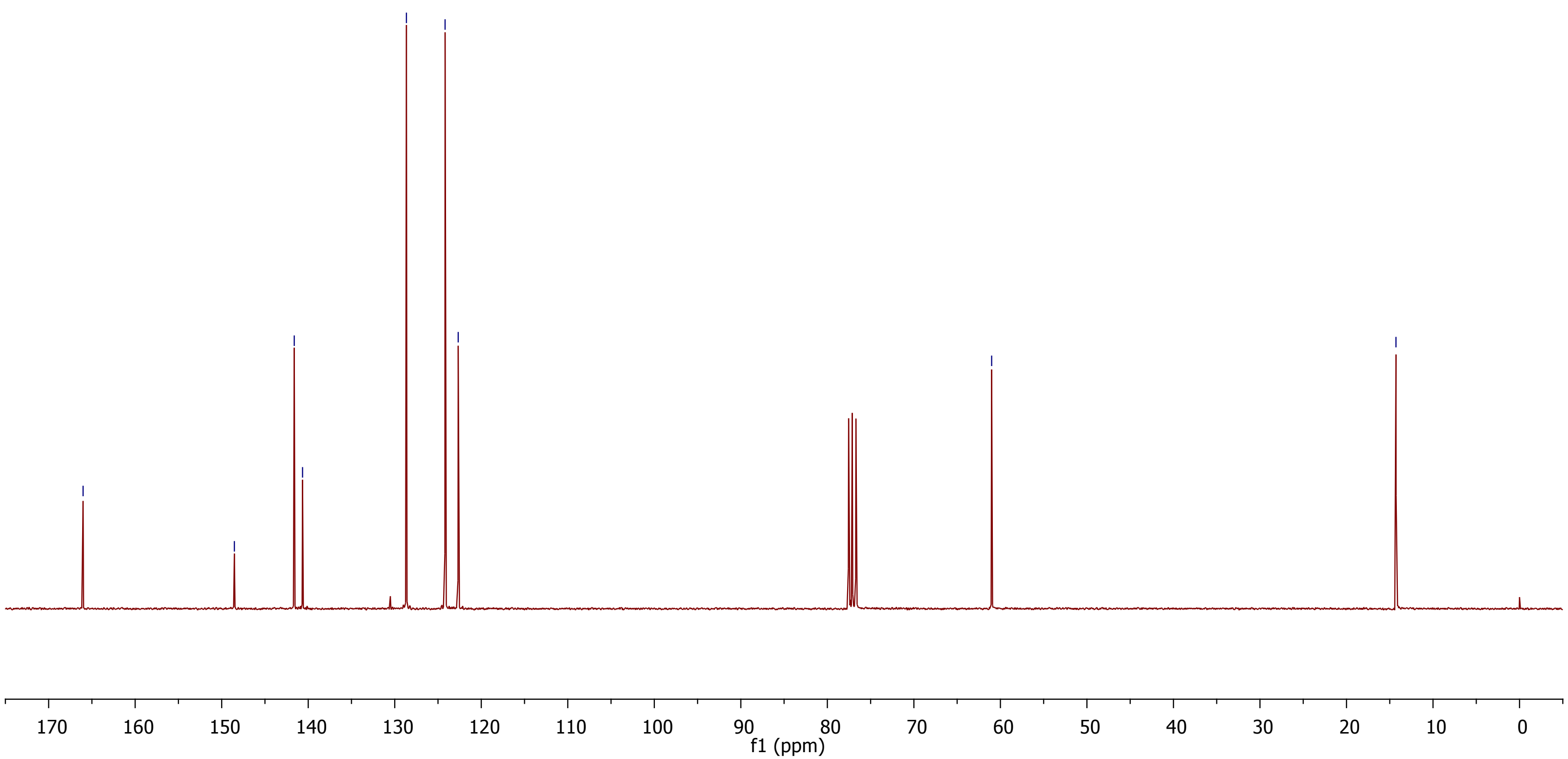

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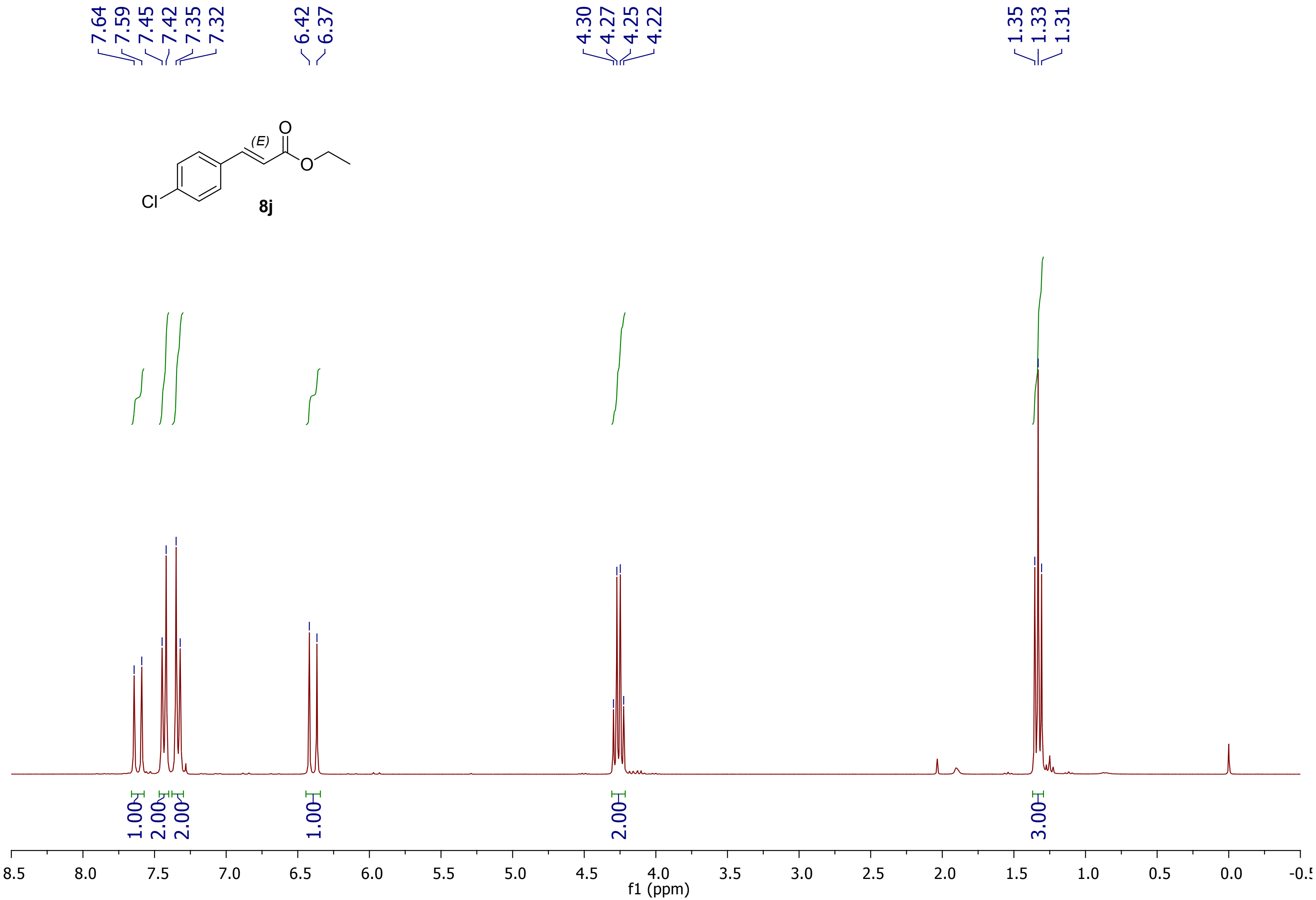
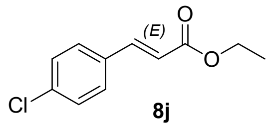


^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8j**



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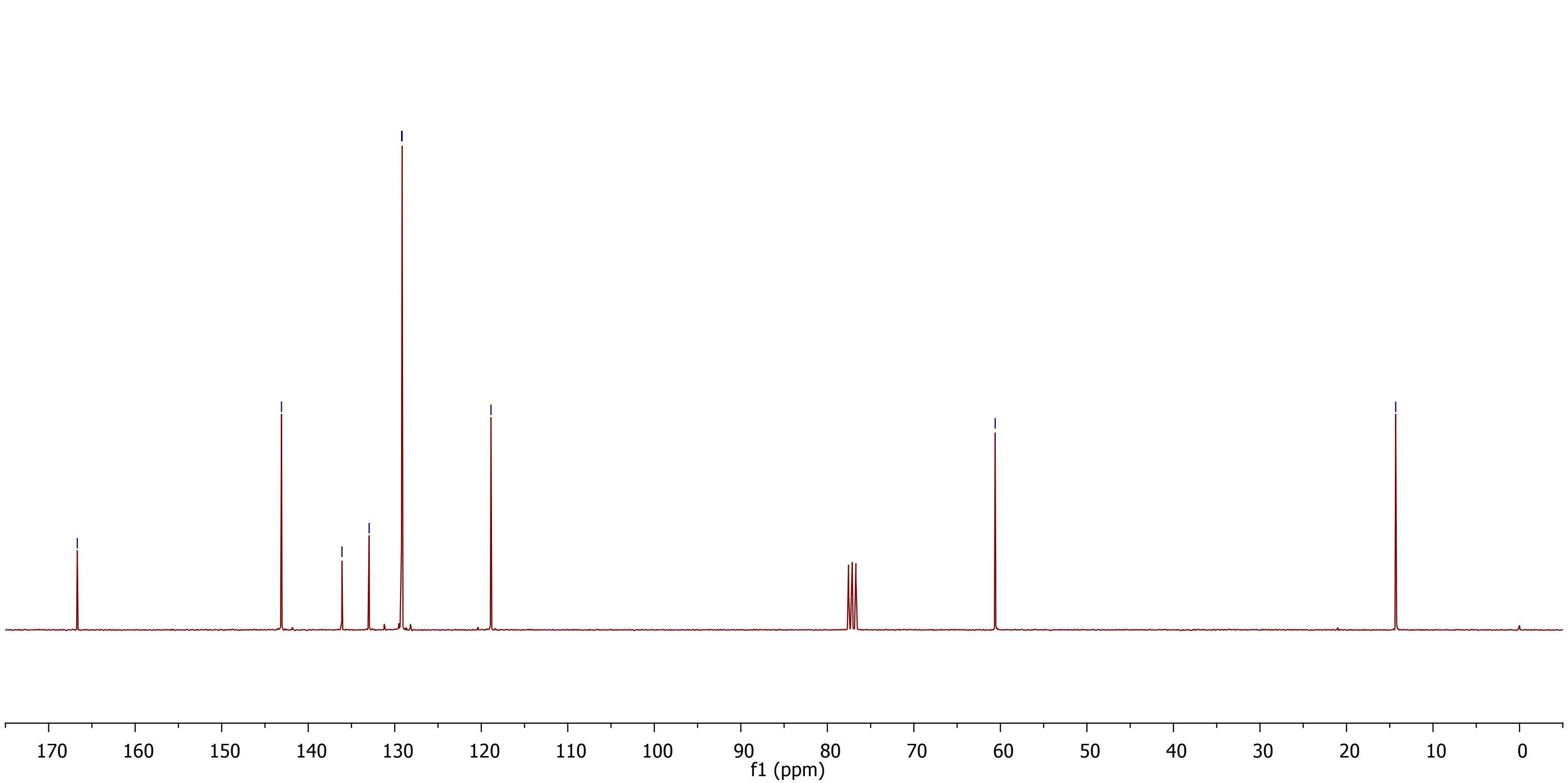
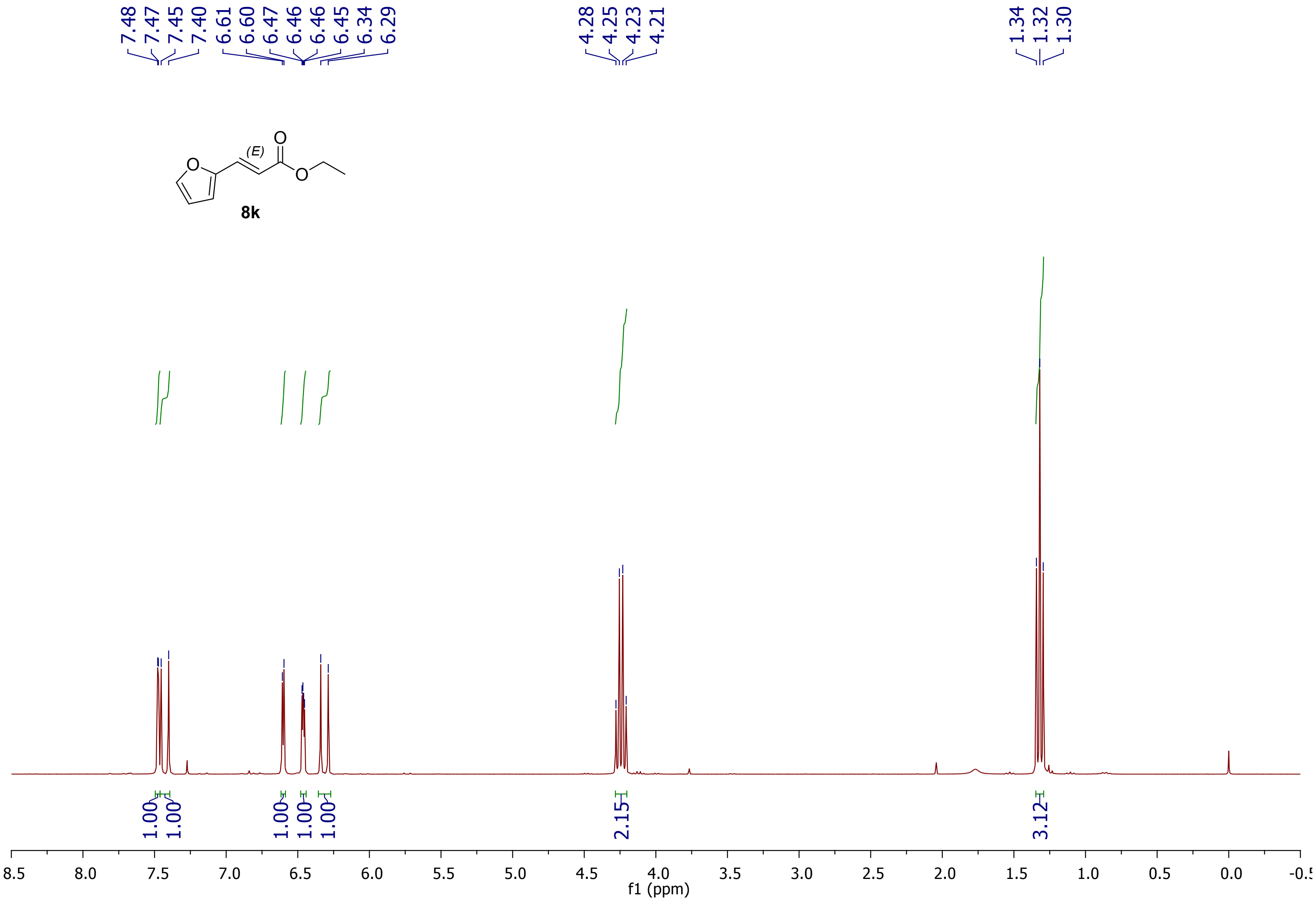
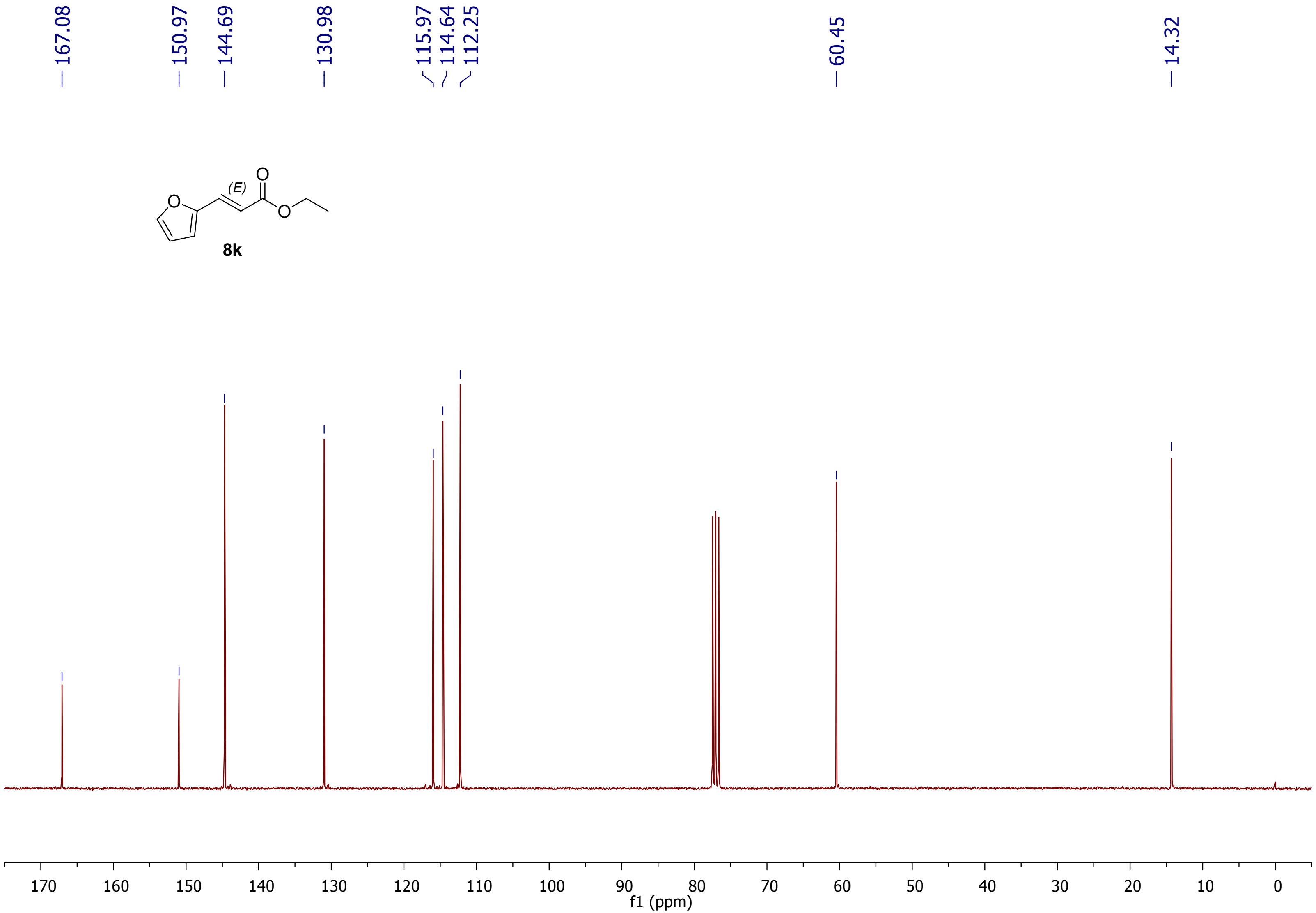


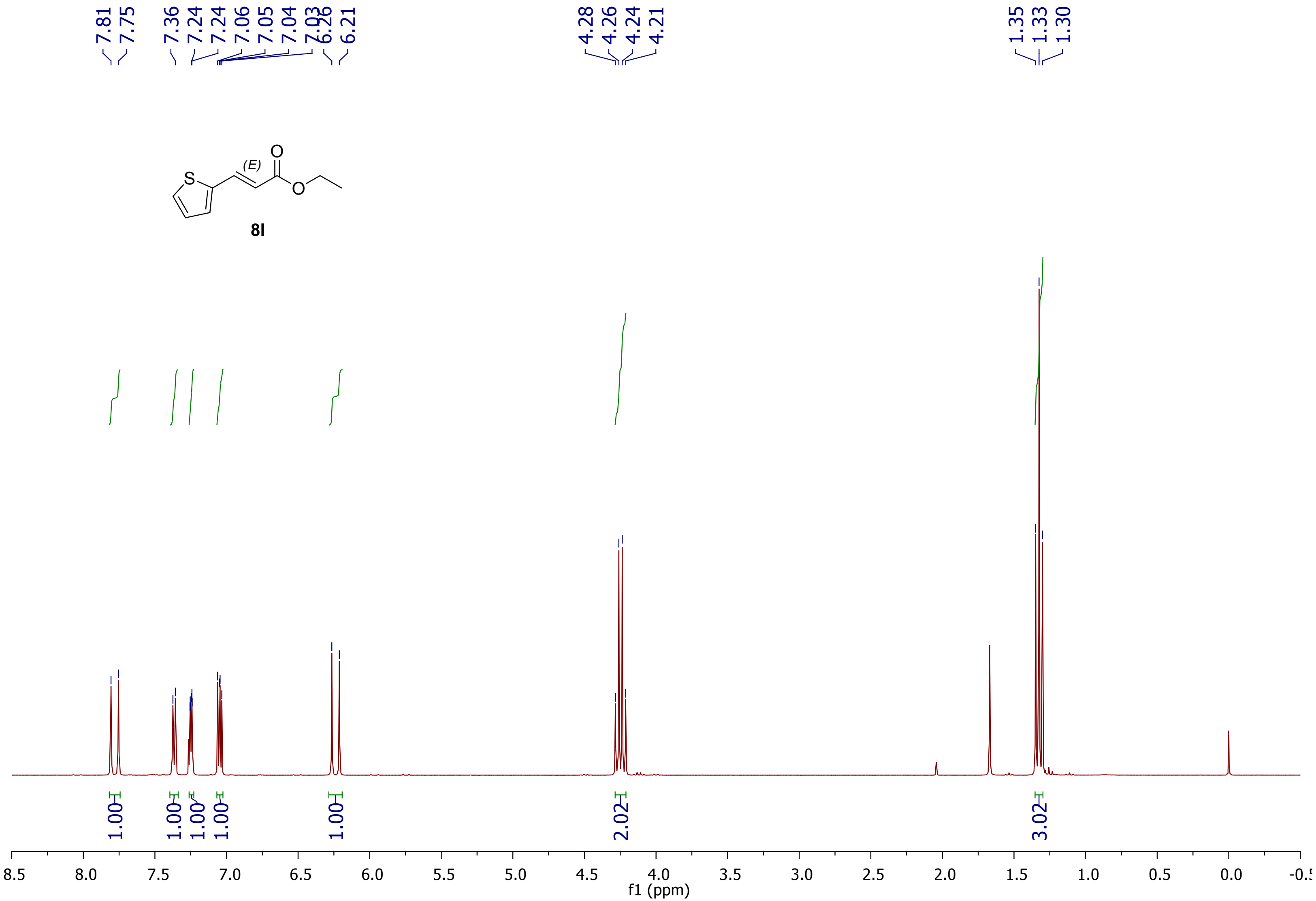
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **8k**



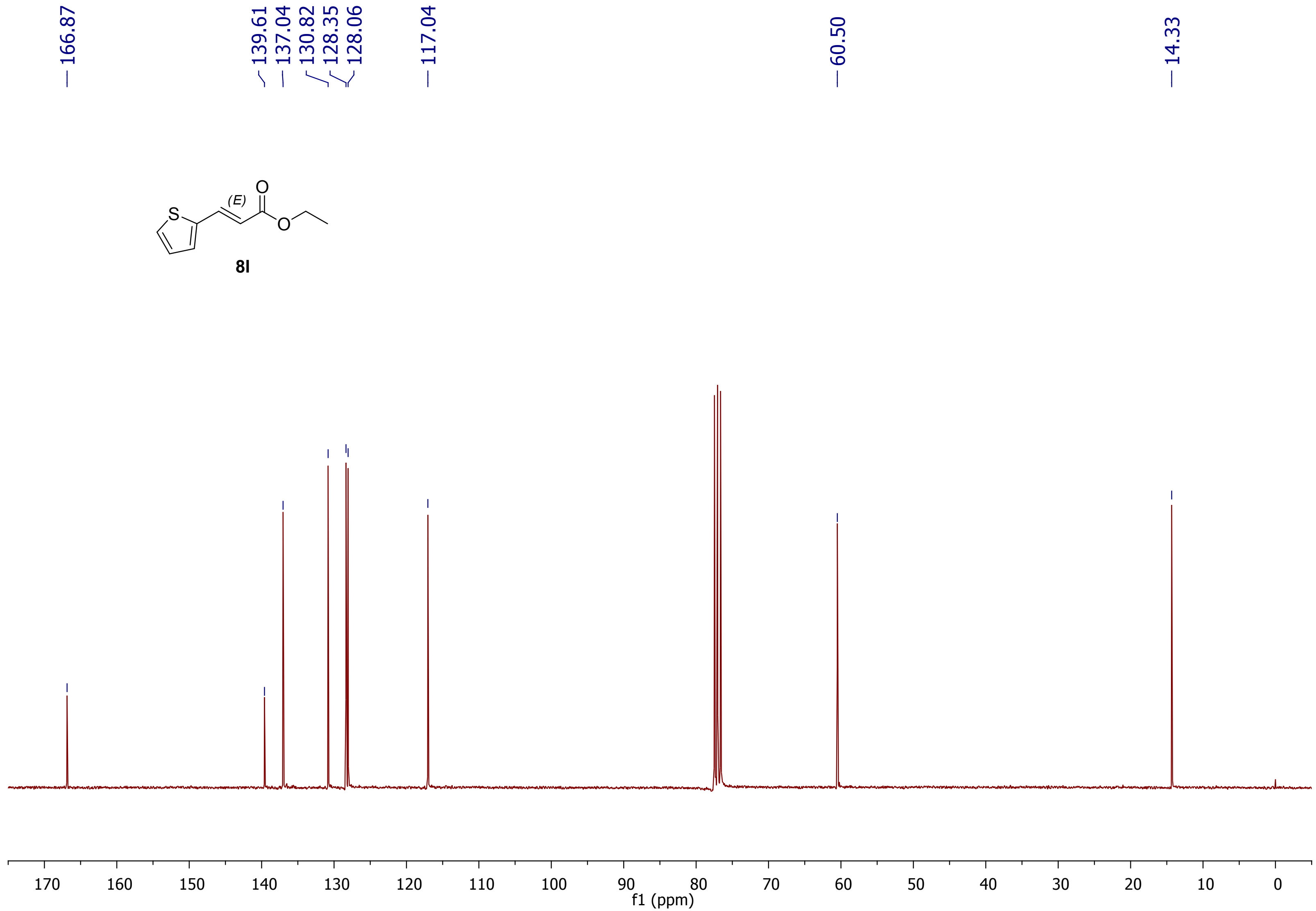
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8k**



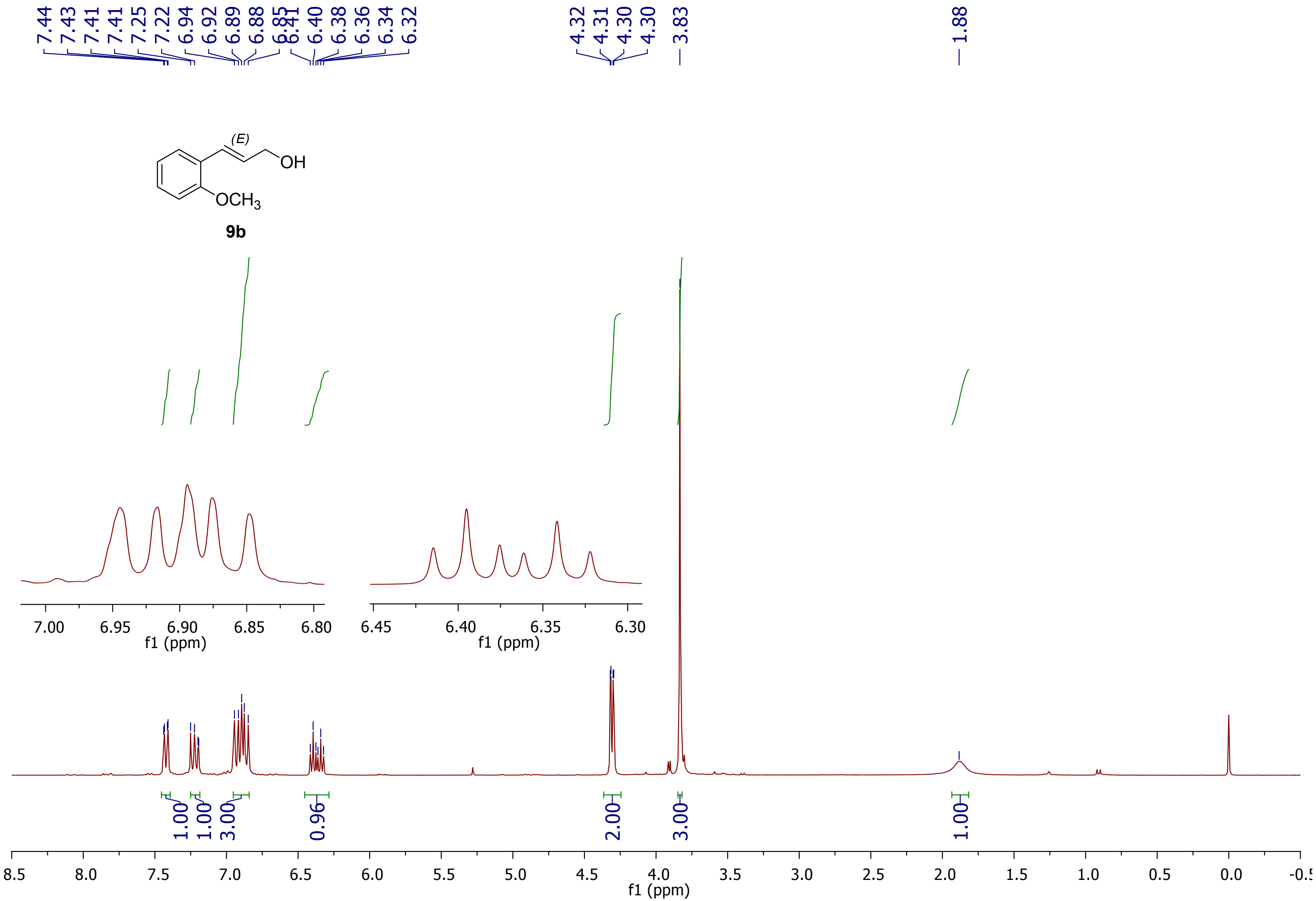
[1]H NMR (300 MHz, $CDCl_3$) of substrate **8l**



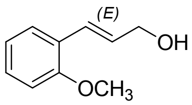
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **8l**



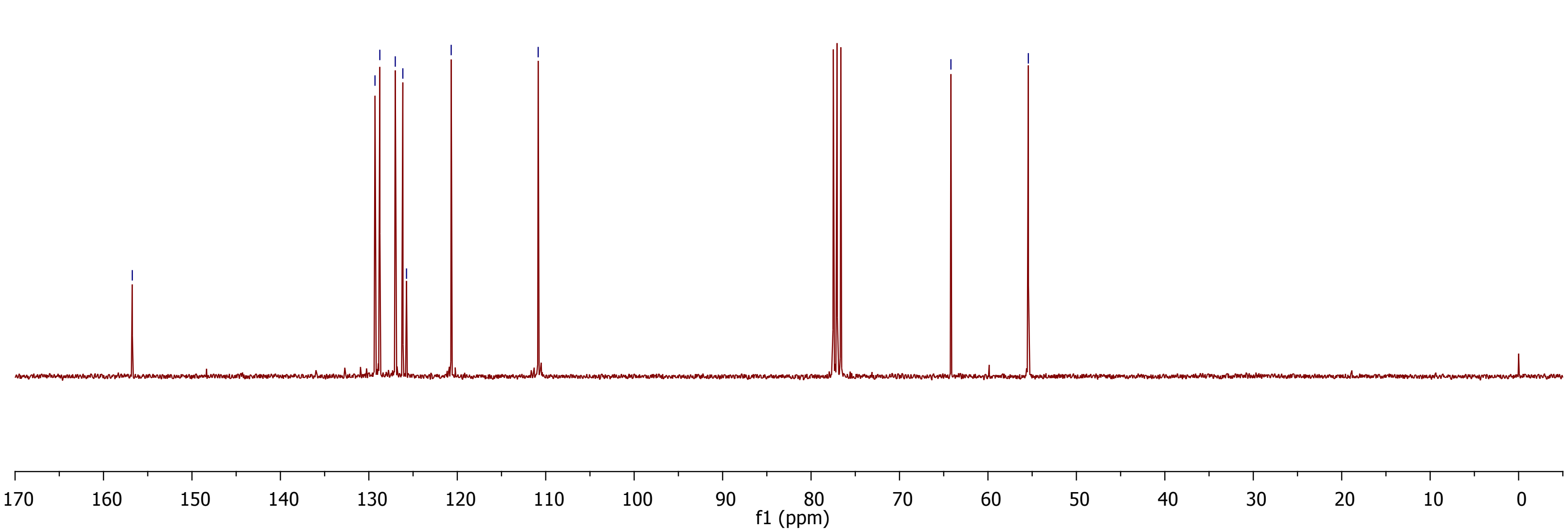
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **9b**



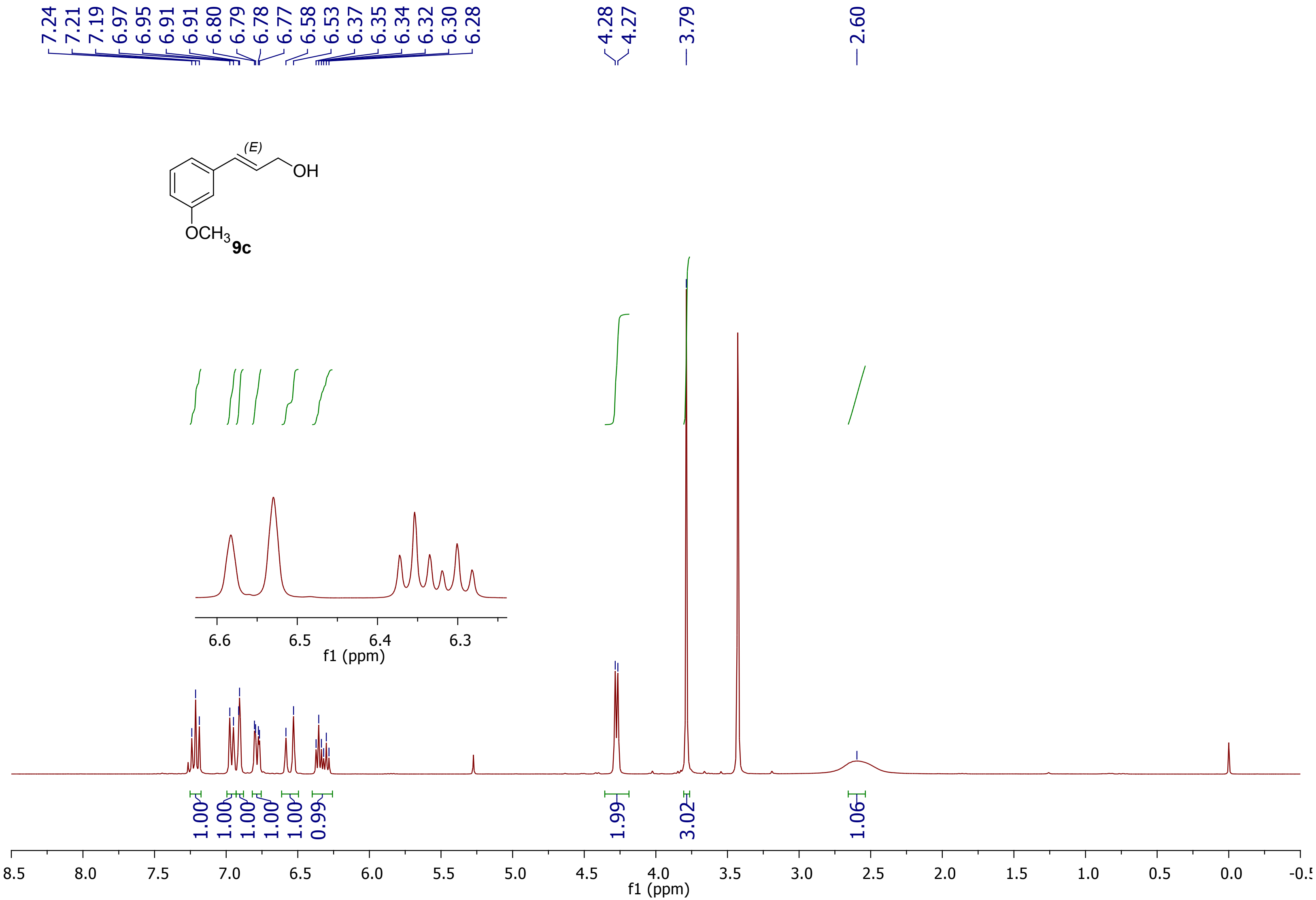
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9b**



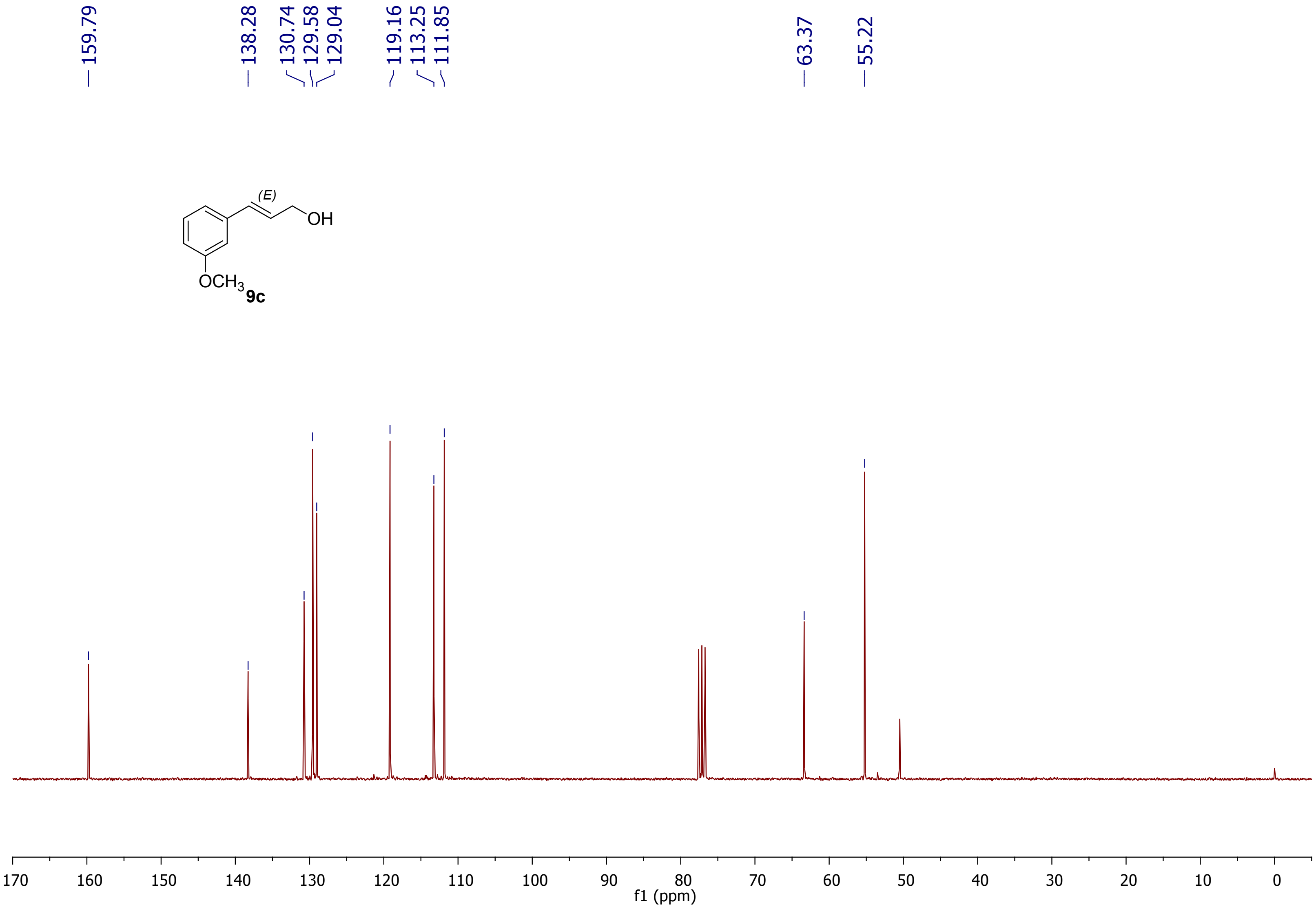
9b



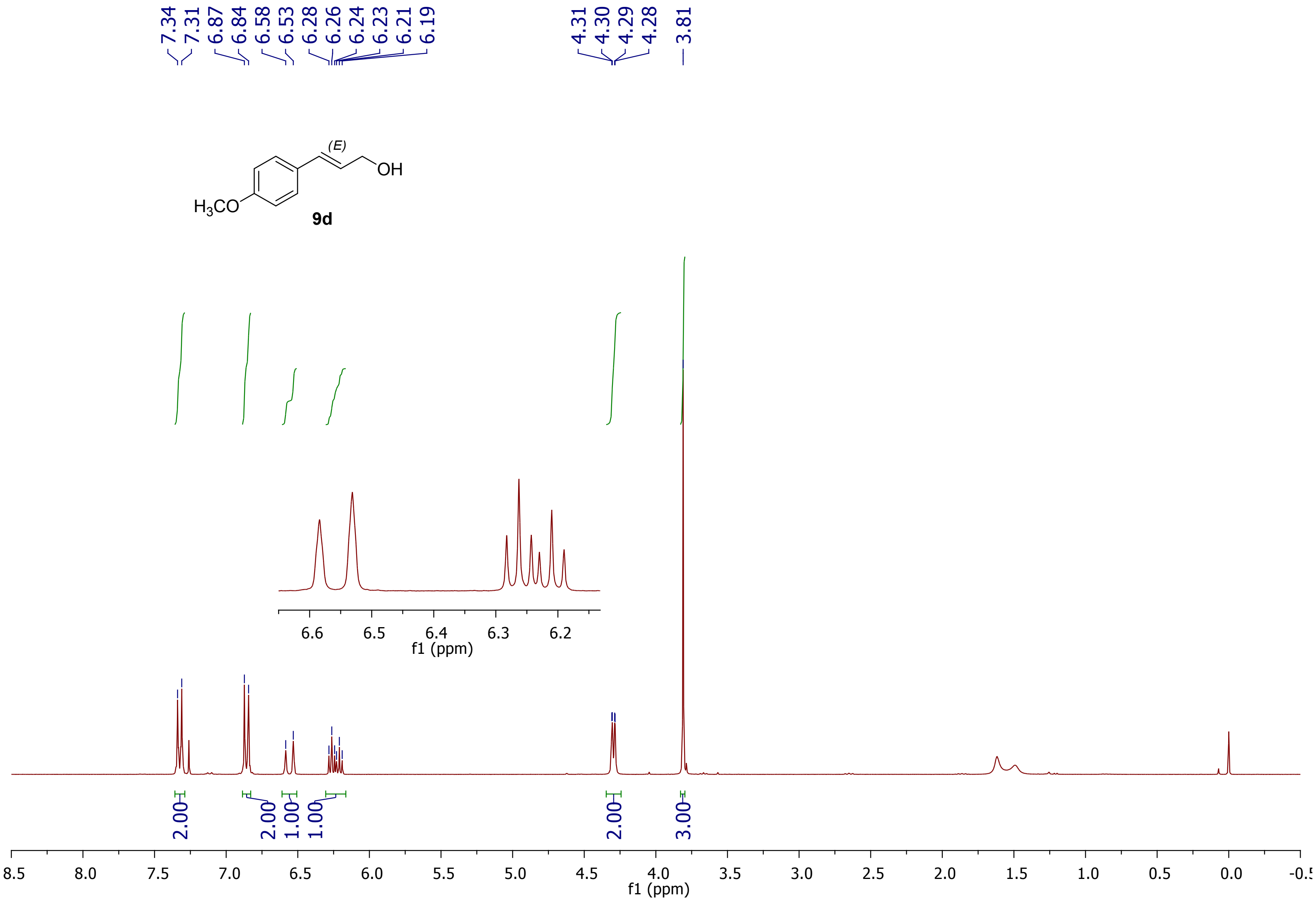
^1H NMR (300 MHz, $CDCl_3$) of substrate **9c**



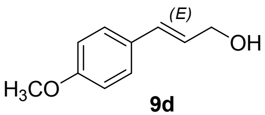
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9c**



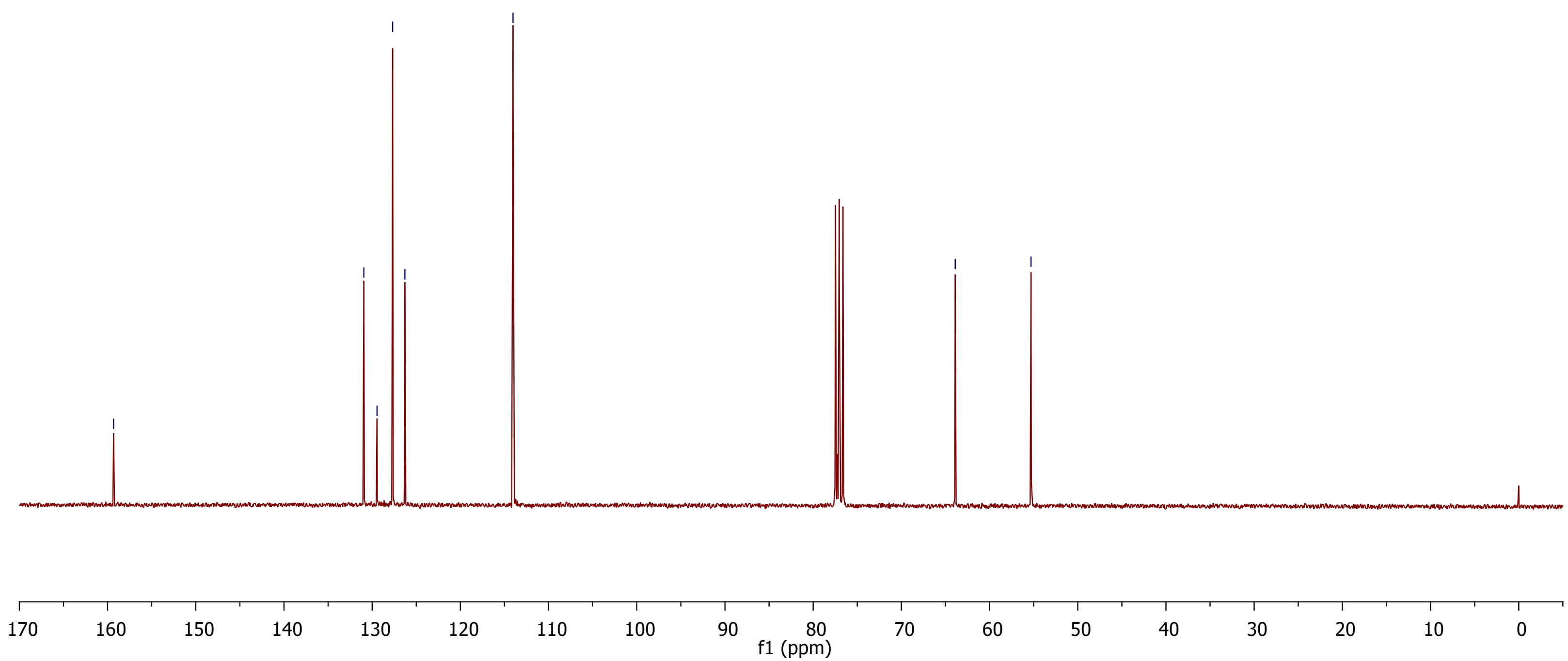
^1H NMR (300 MHz, $CDCl_3$) of substrate **9d**



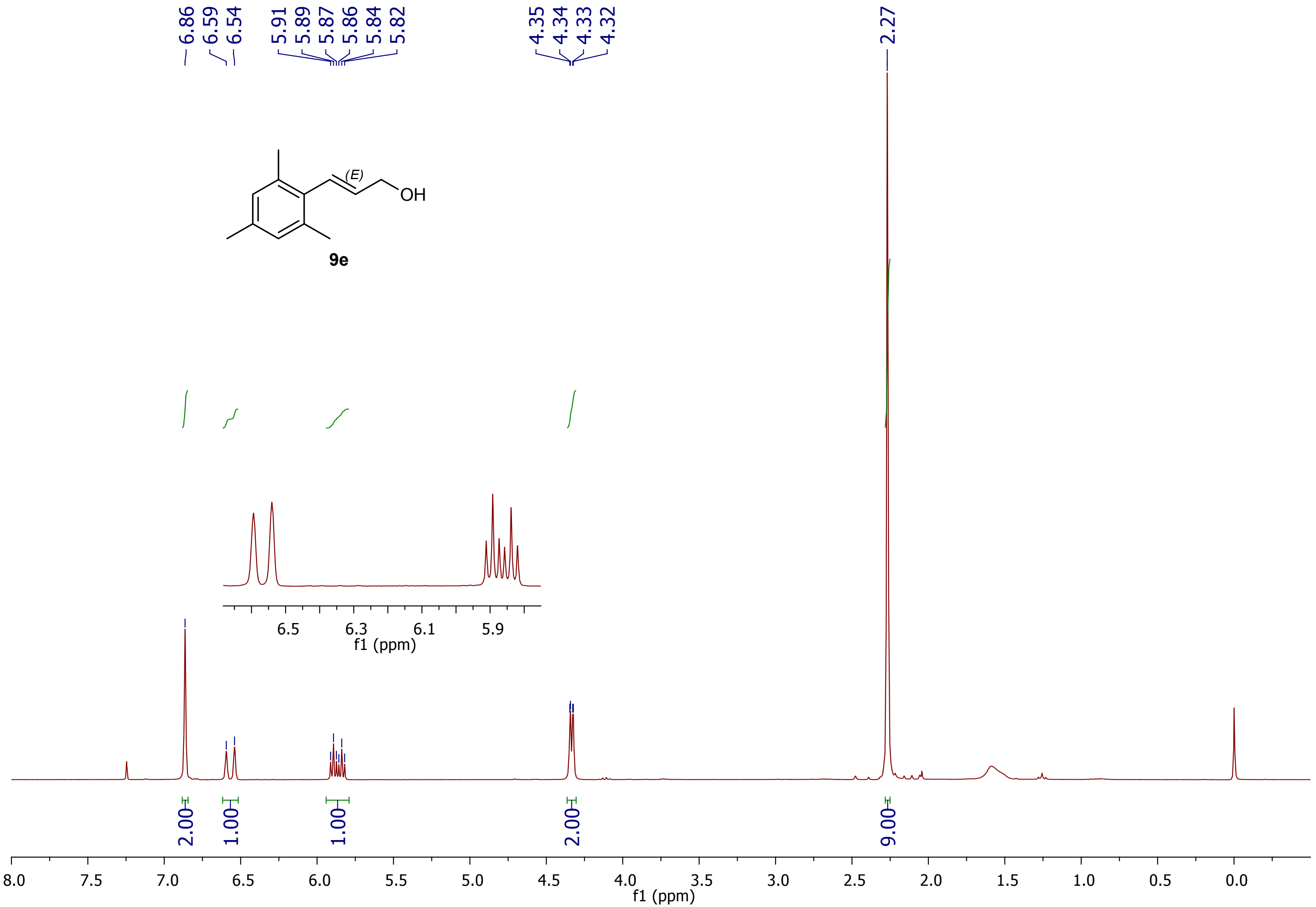
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9d**



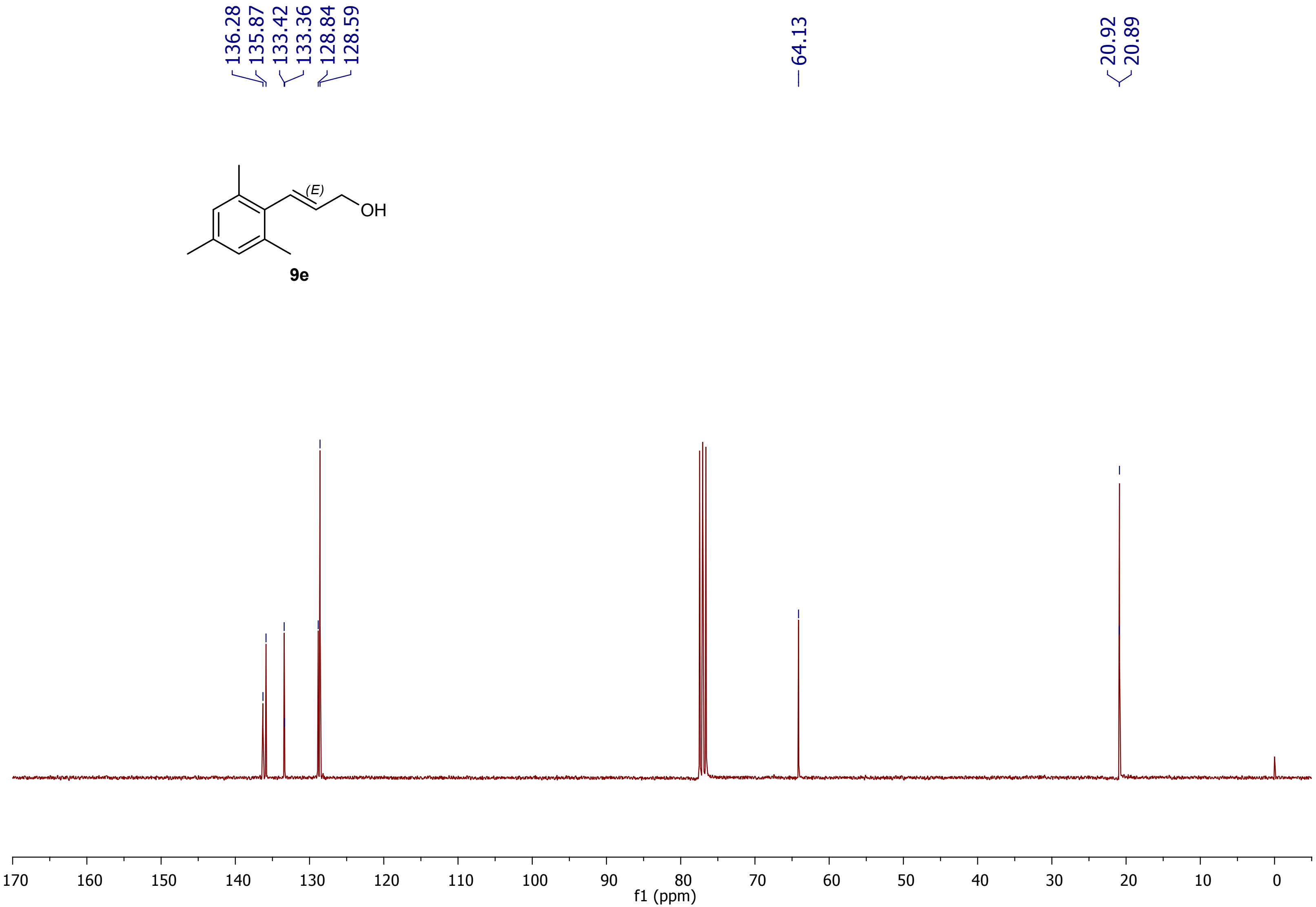
9d



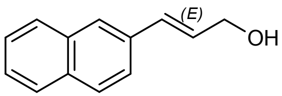
[1]H NMR (300 MHz, $CDCl_3$) of substrate **9e**



^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9e**



^{1}H NMR (300 MHz, $CDCl_3$) of substrate **9f**



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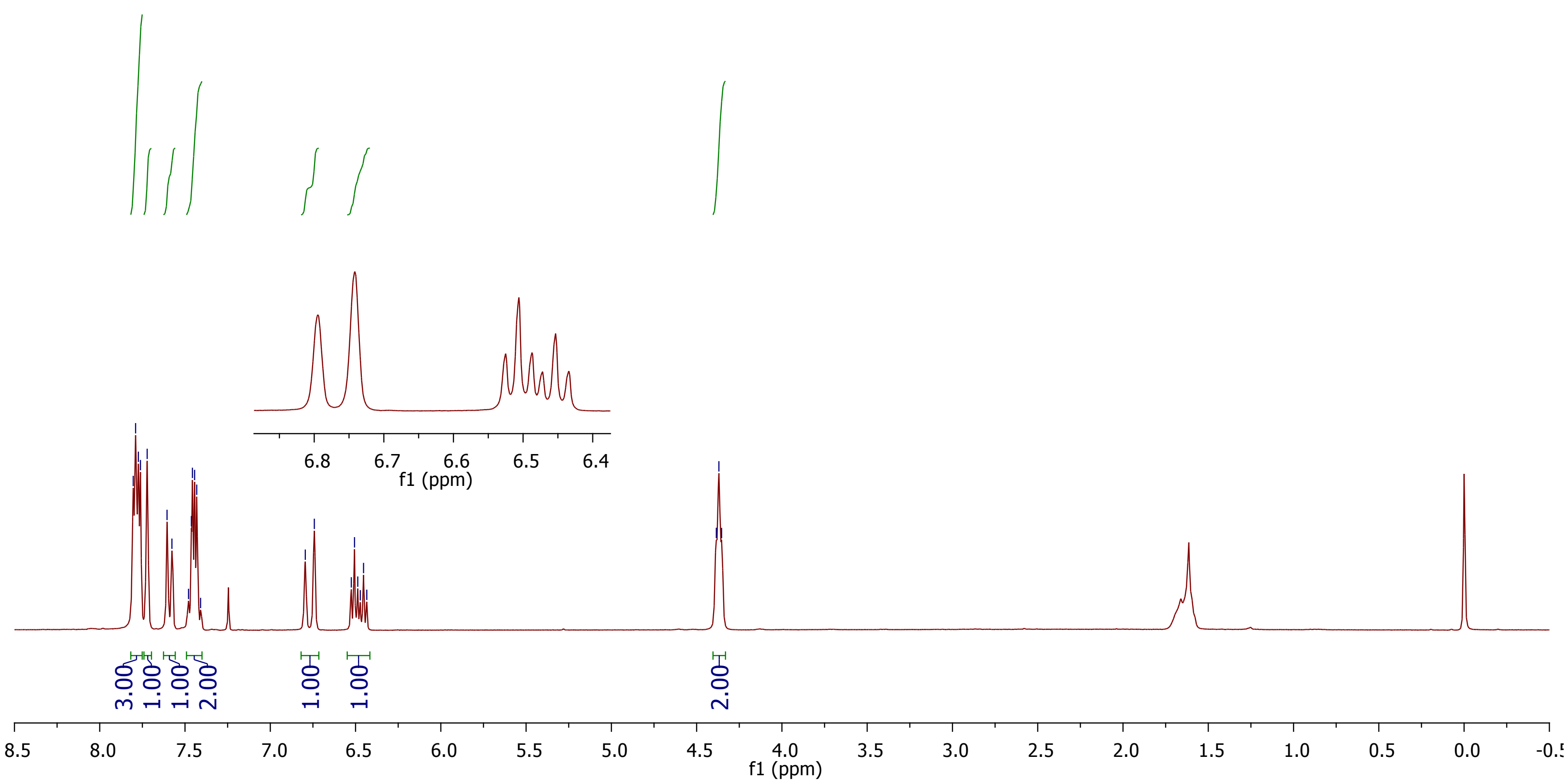
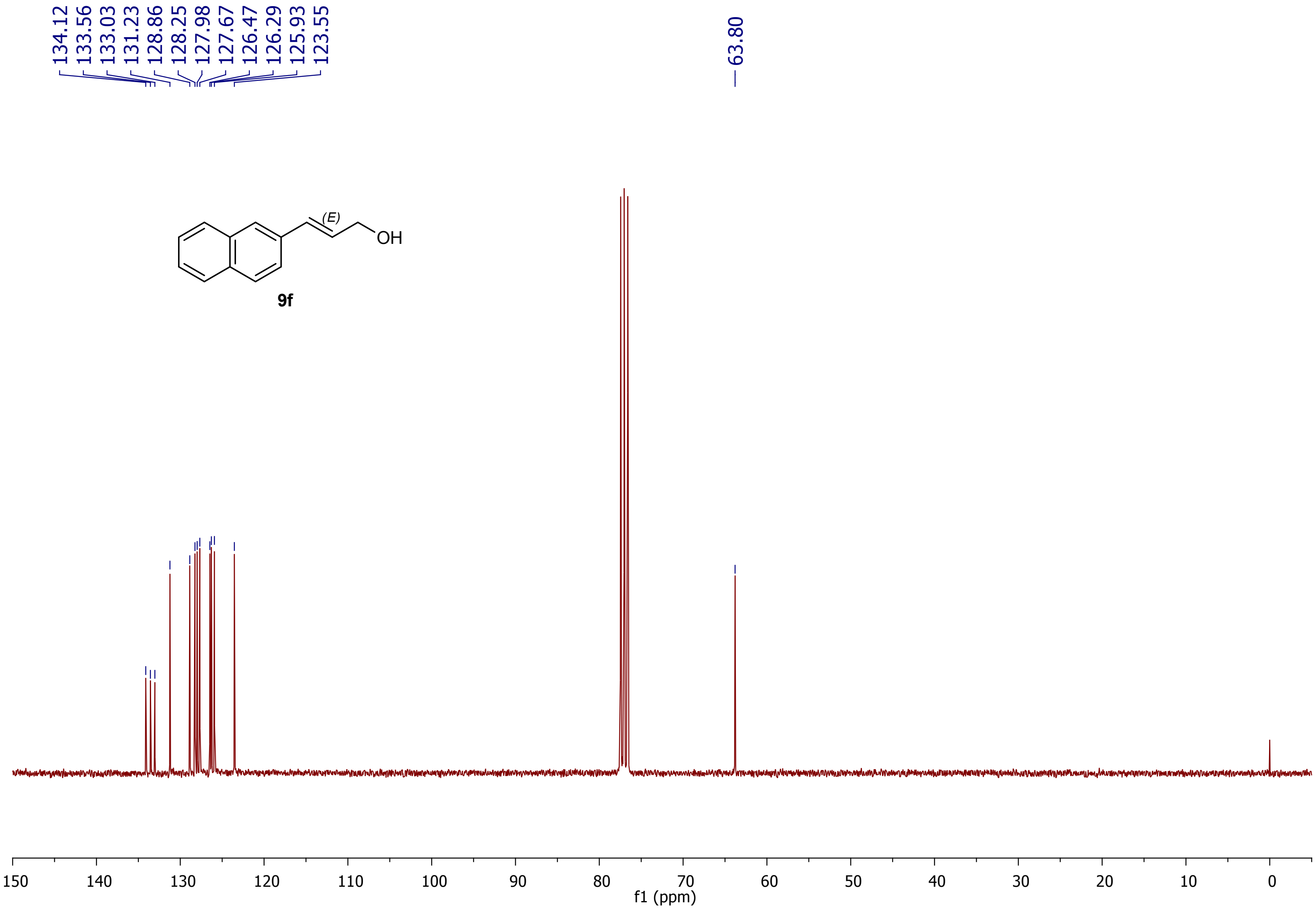
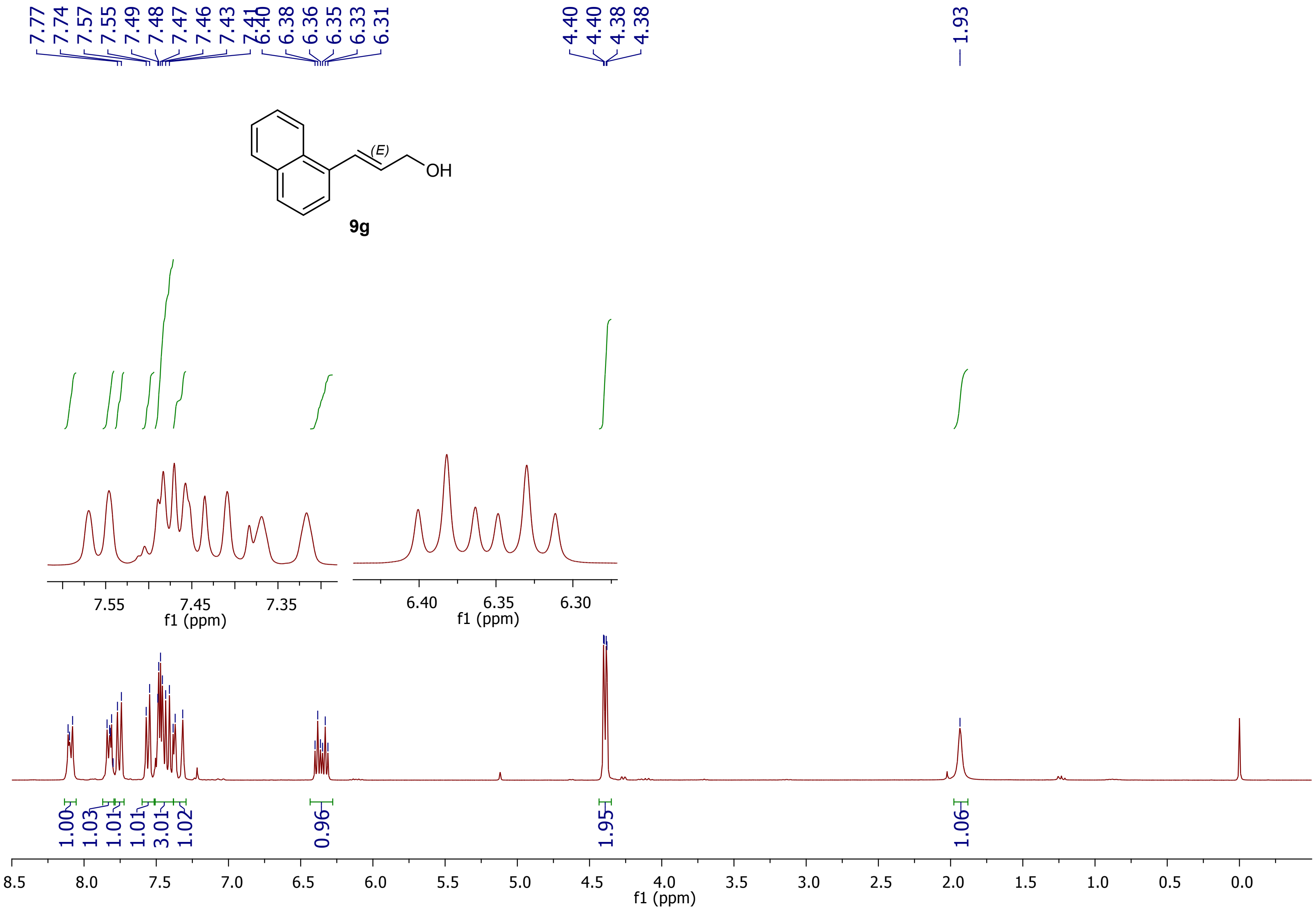


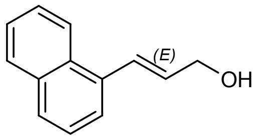
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9f**



^{1}H NMR (300 MHz, $CDCl_3$) of substrate **9g**



^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9g**



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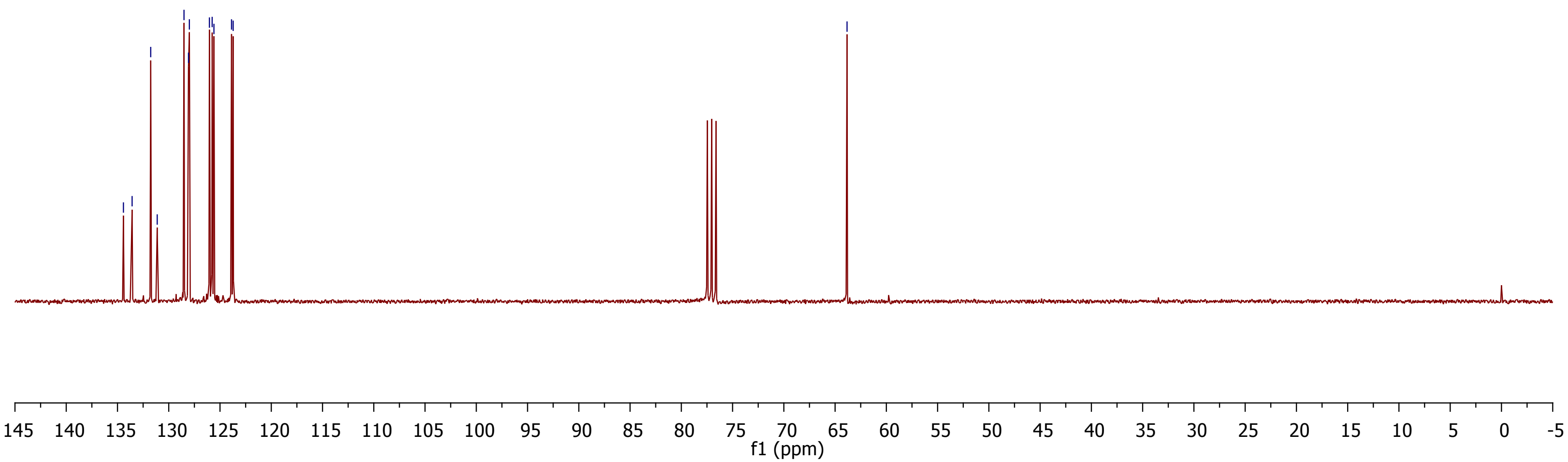
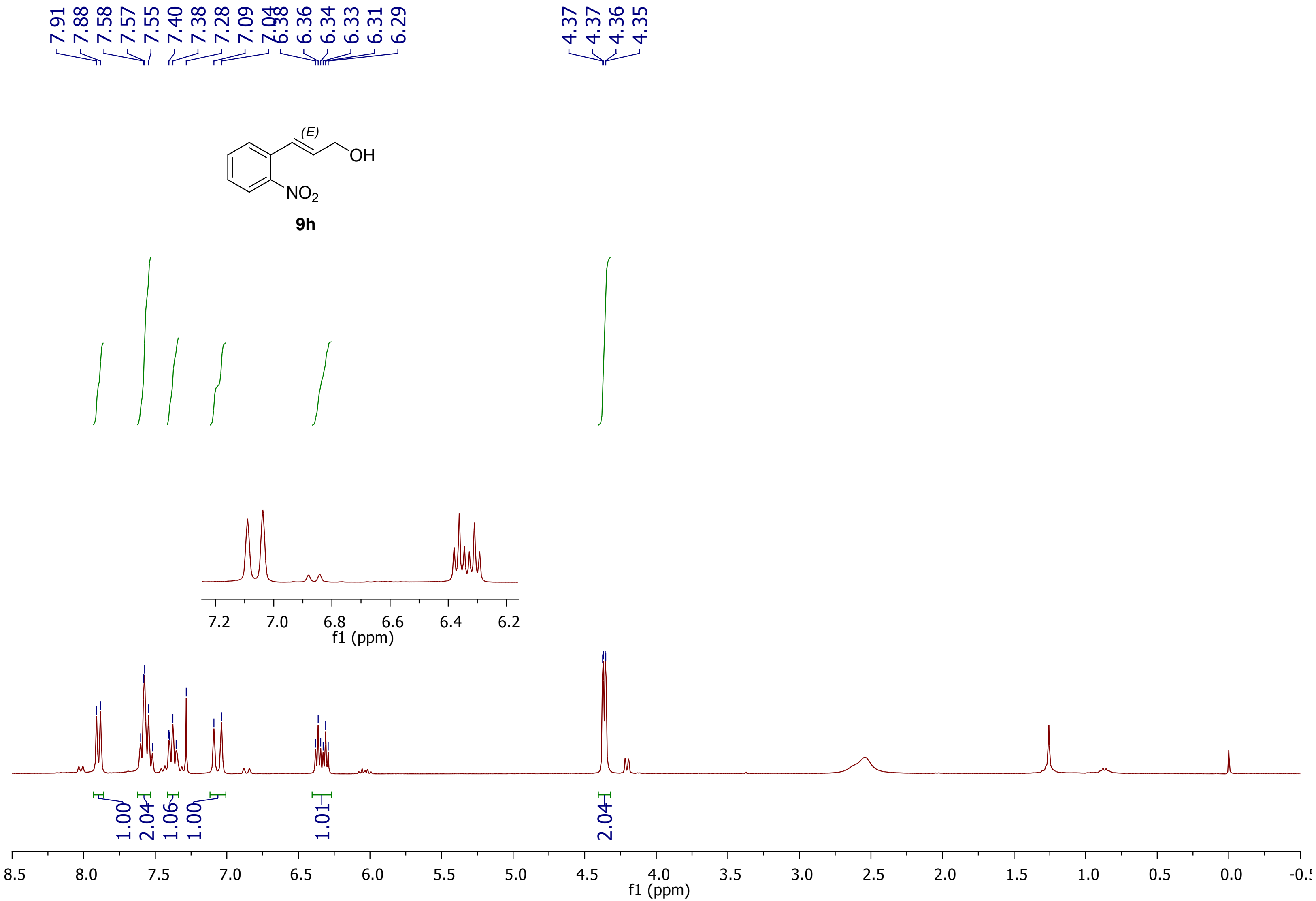
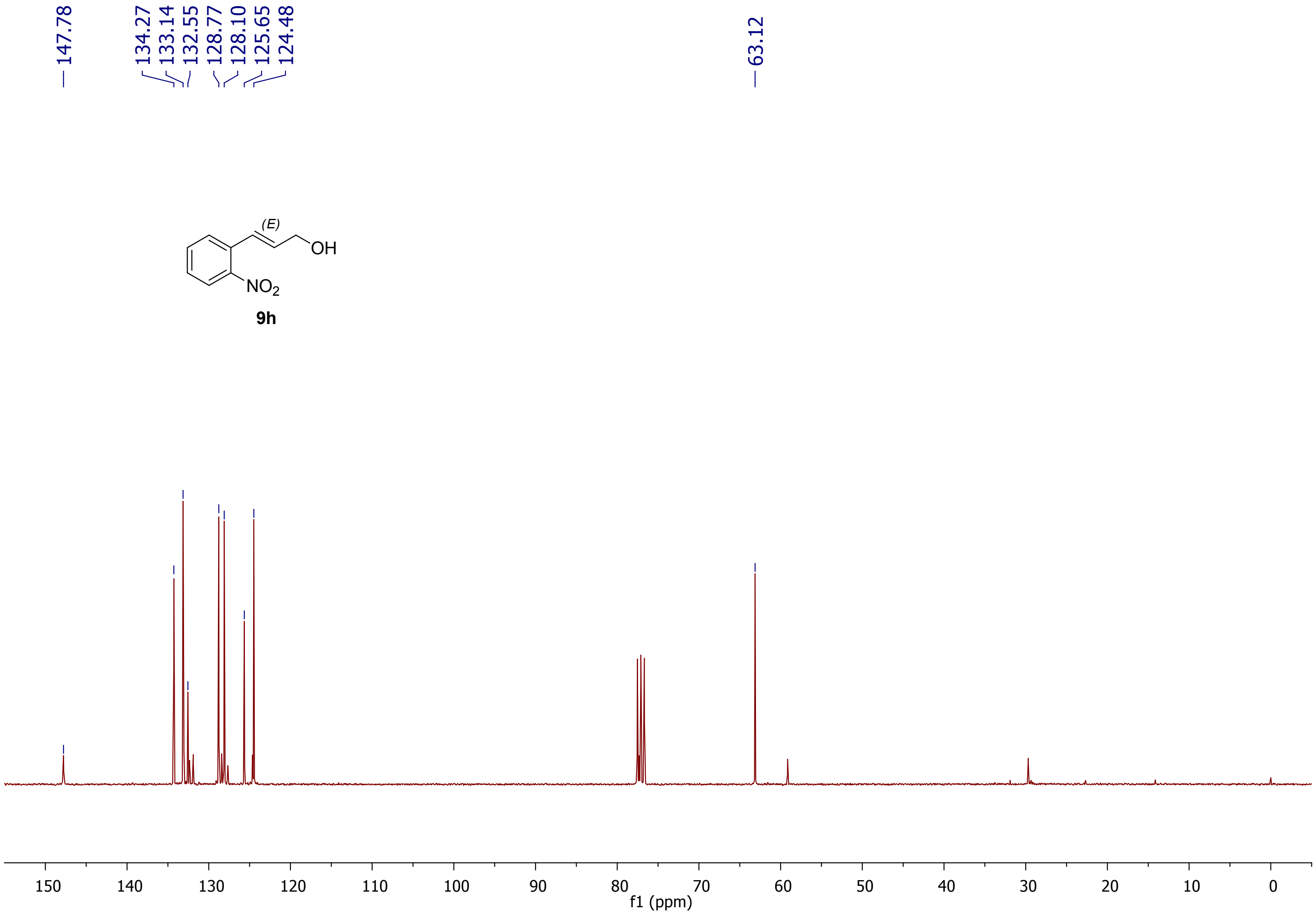


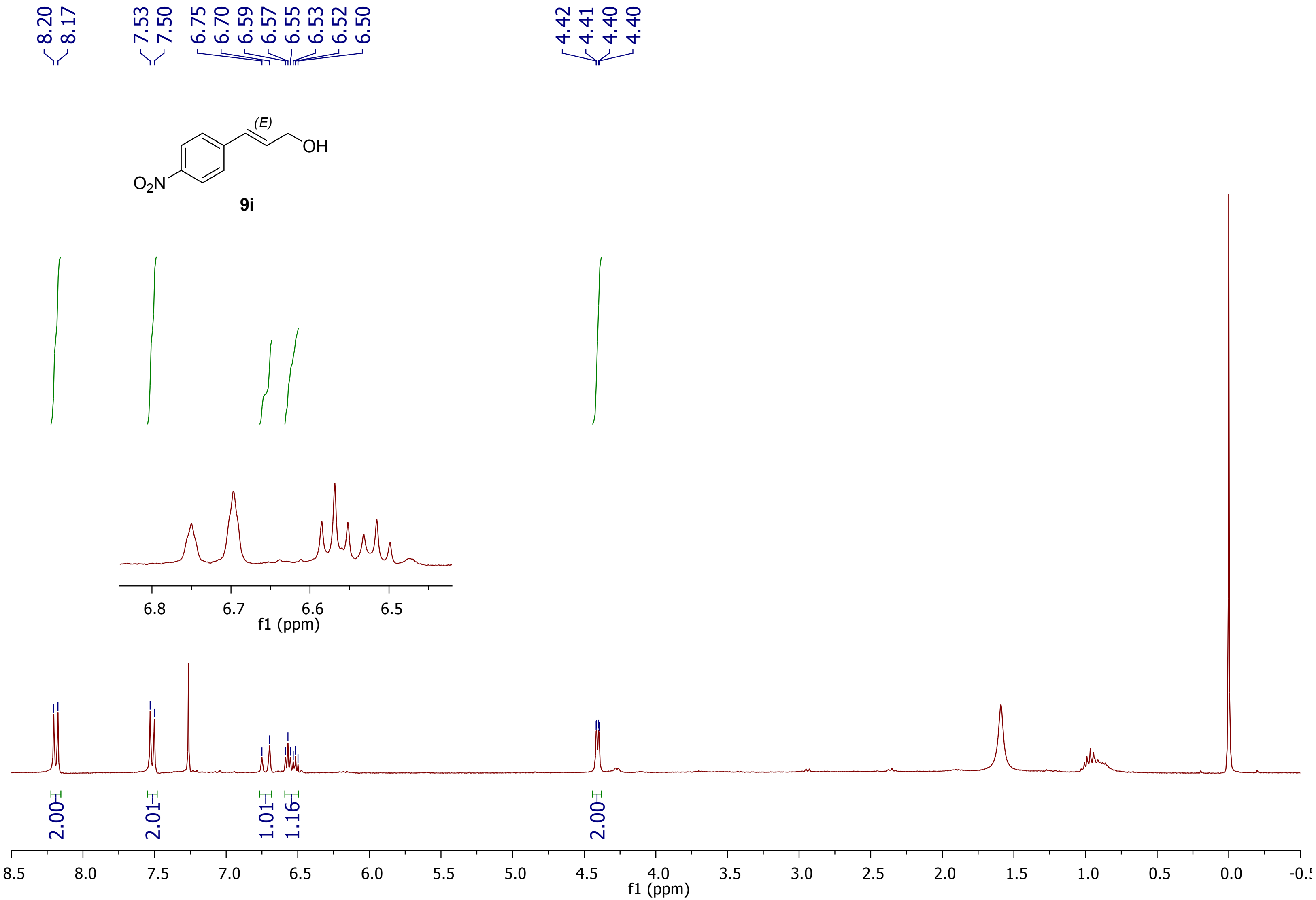
[1]H NMR (300 MHz, $CDCl_3$) of substrate **9h**



^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9h**



[1]H NMR (300 MHz, $CDCl_3$) of substrate **9i**



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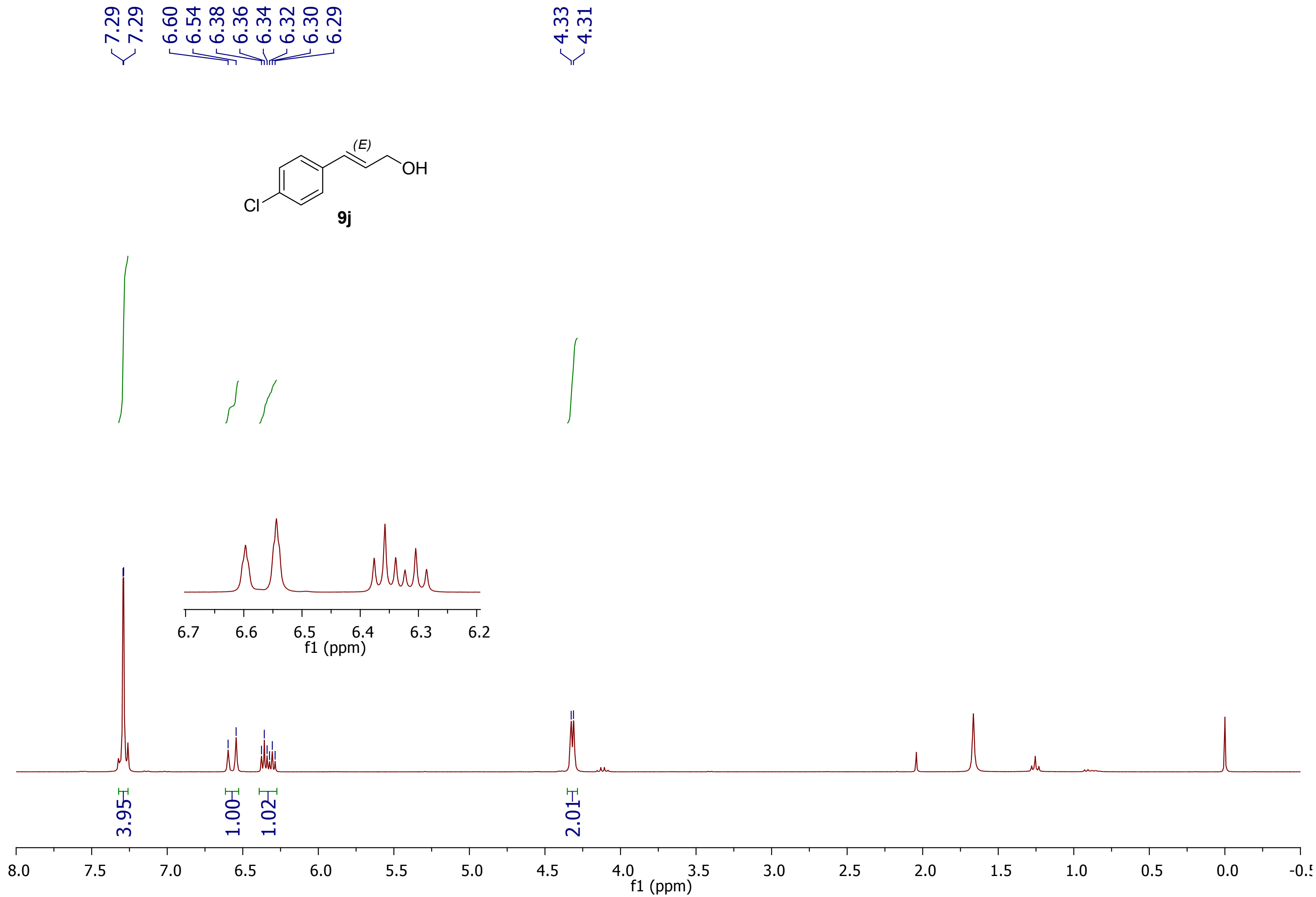
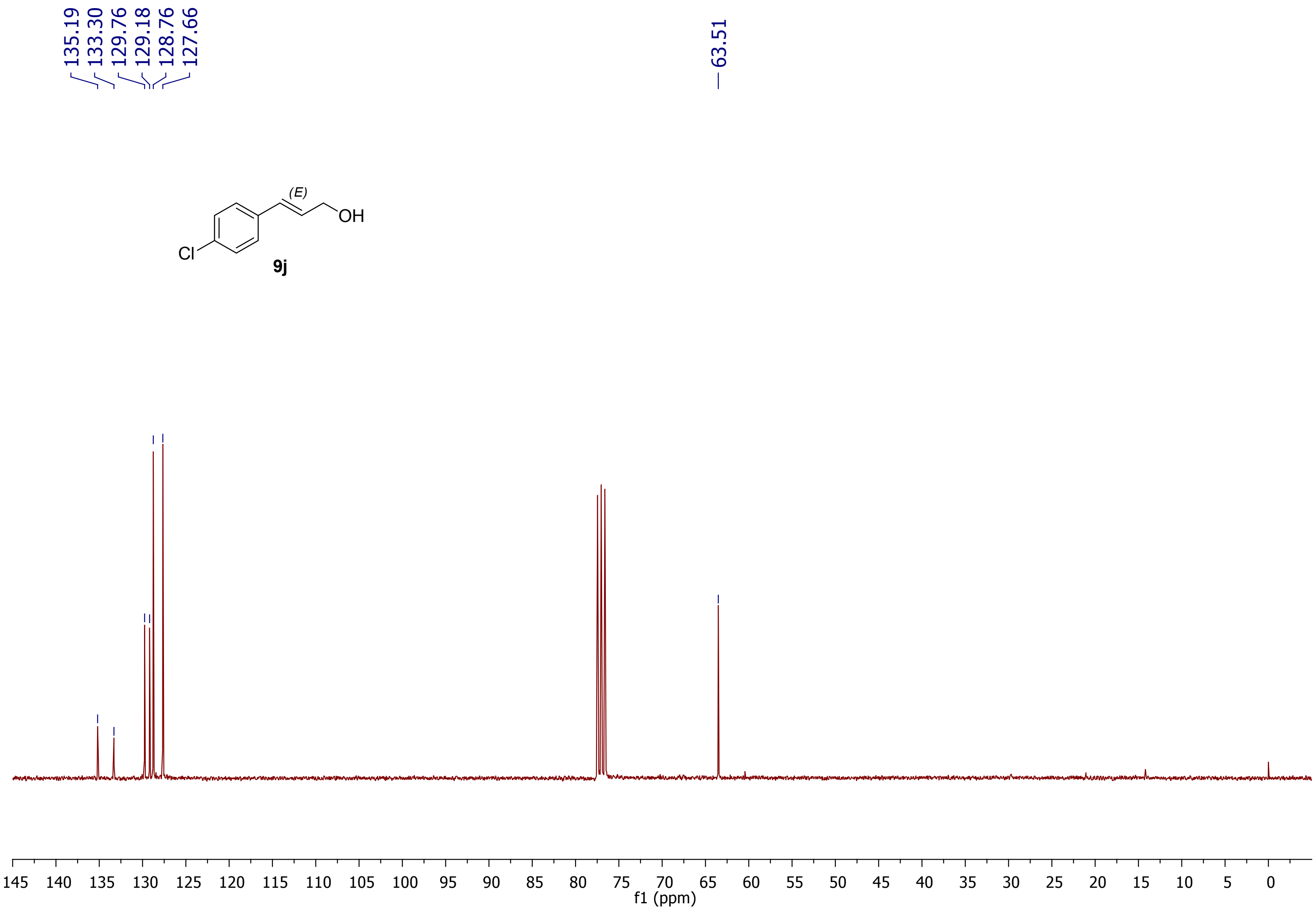
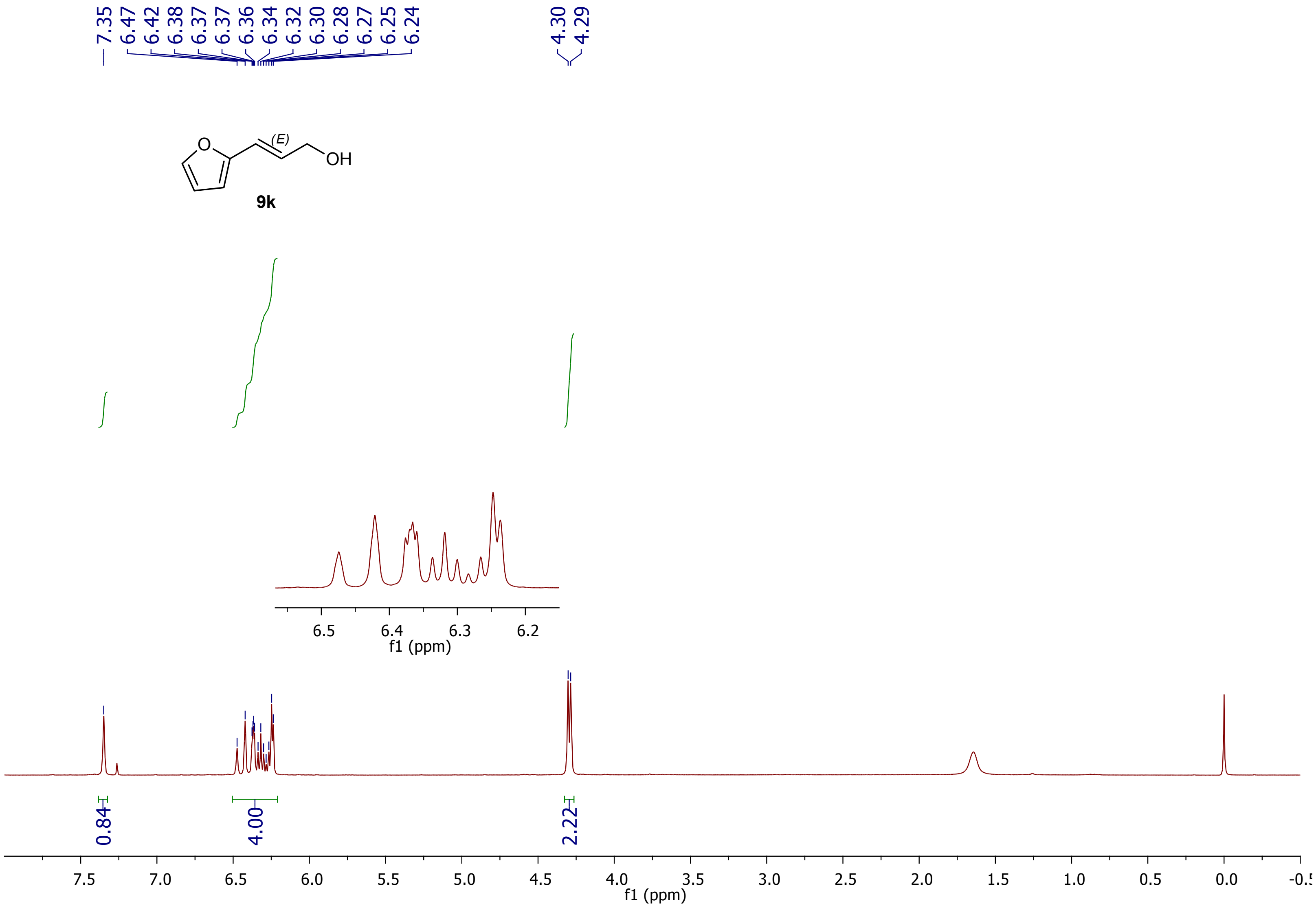


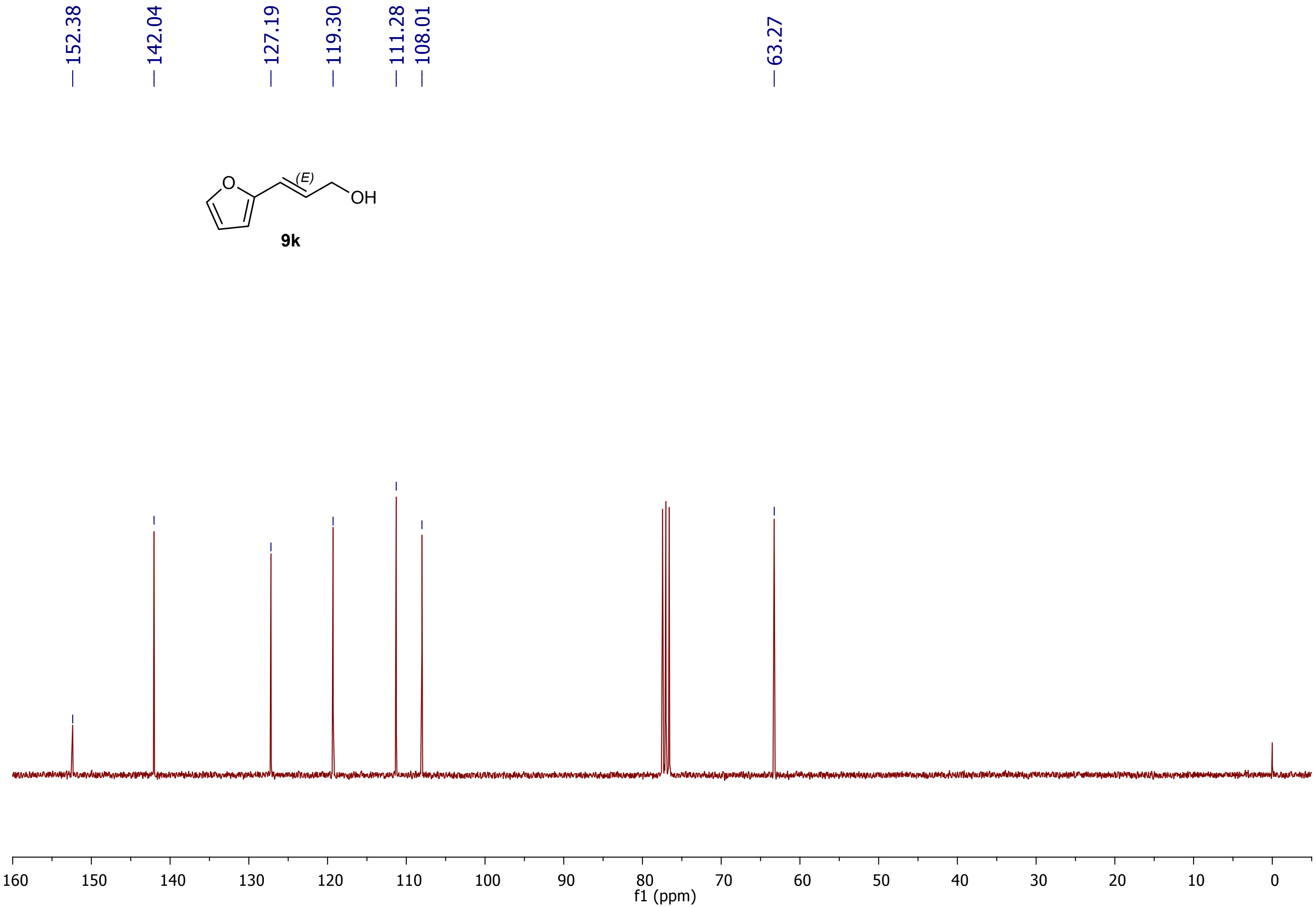
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9j**



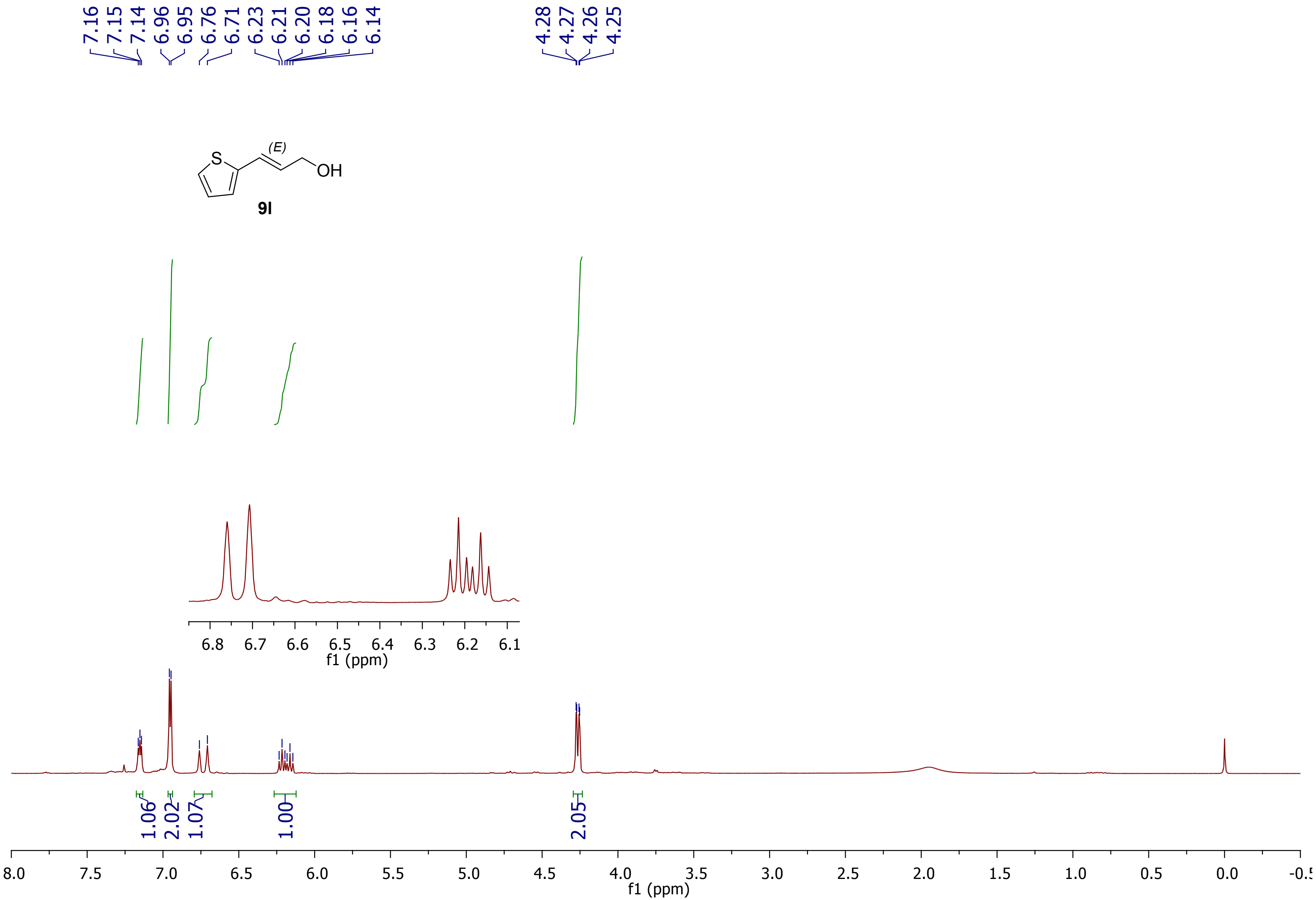
^1H NMR (300 MHz, $CDCl_3$) of substrate **9k**



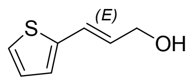
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9k**



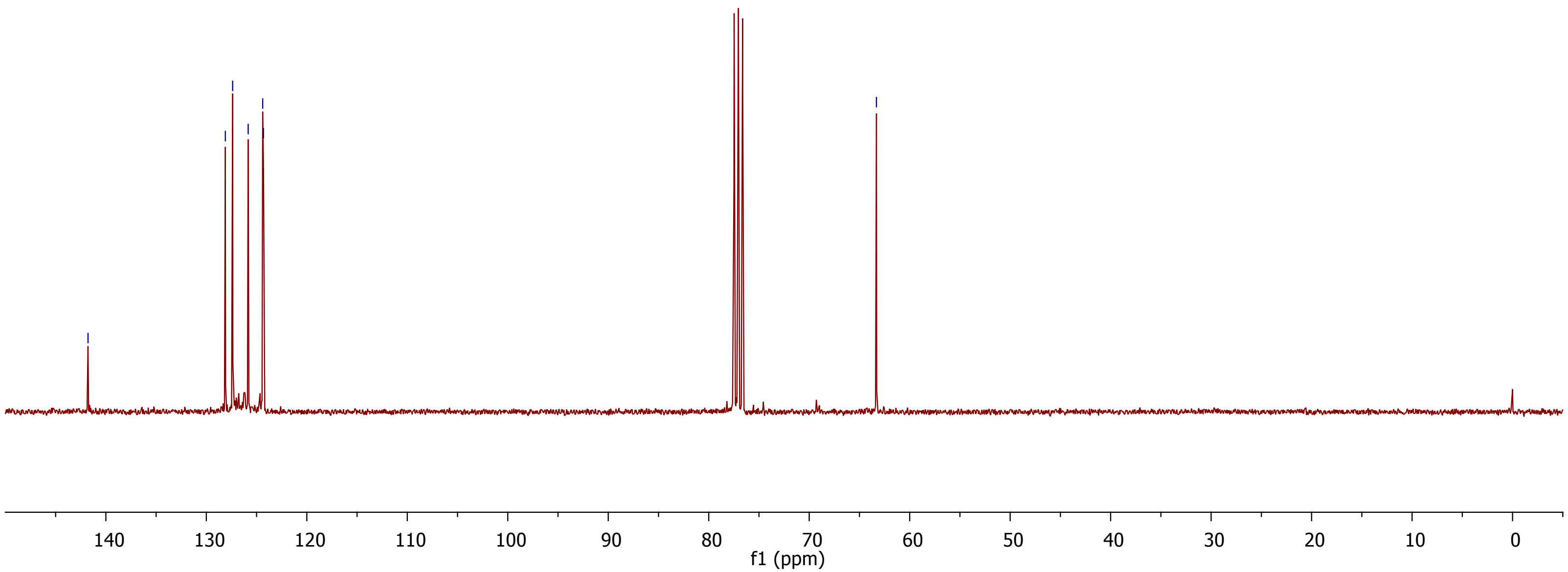
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **9l**



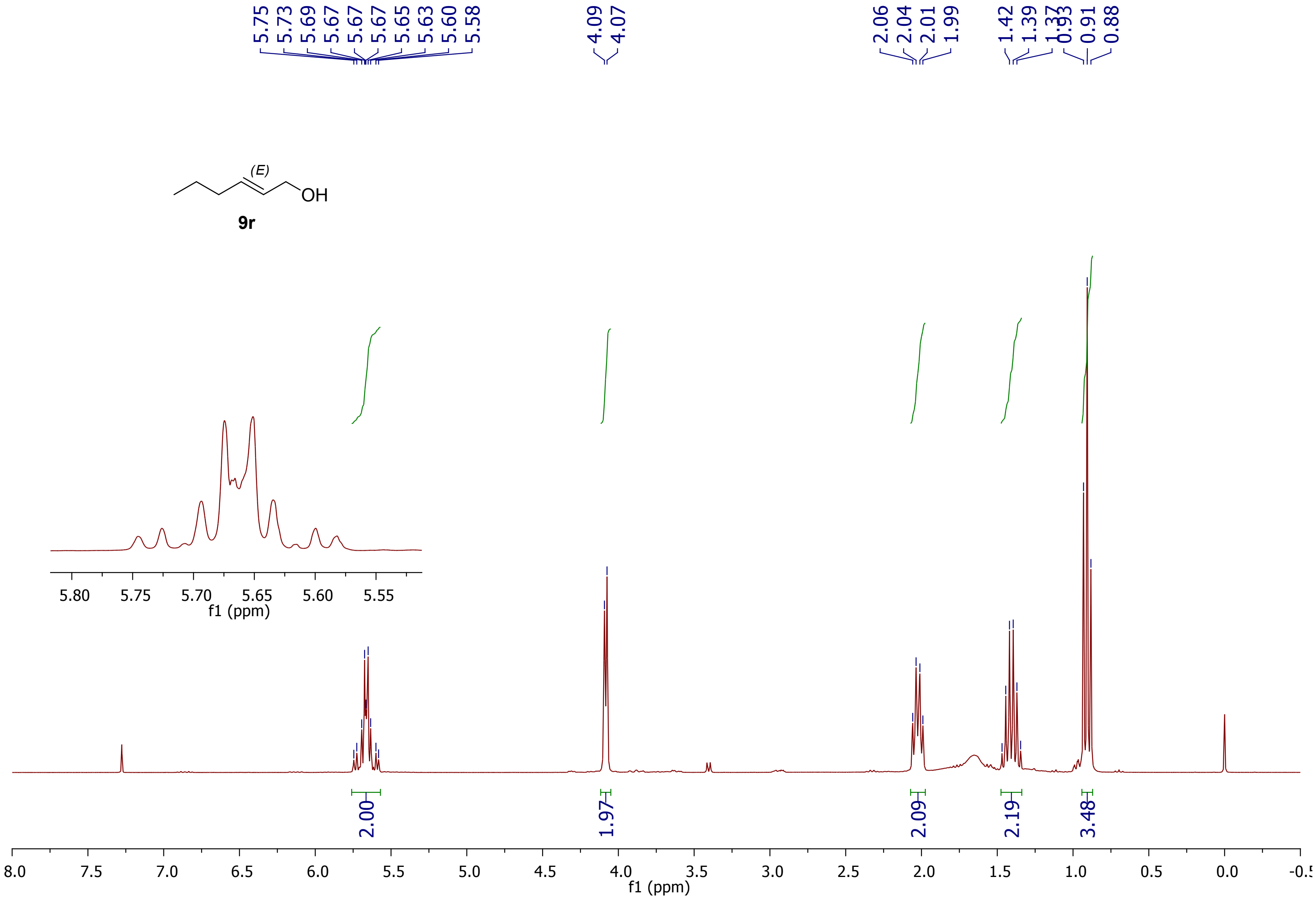
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9l**



9l

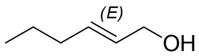


^{1}H NMR (300 MHz, $CDCl_3$) of substrate **9r**

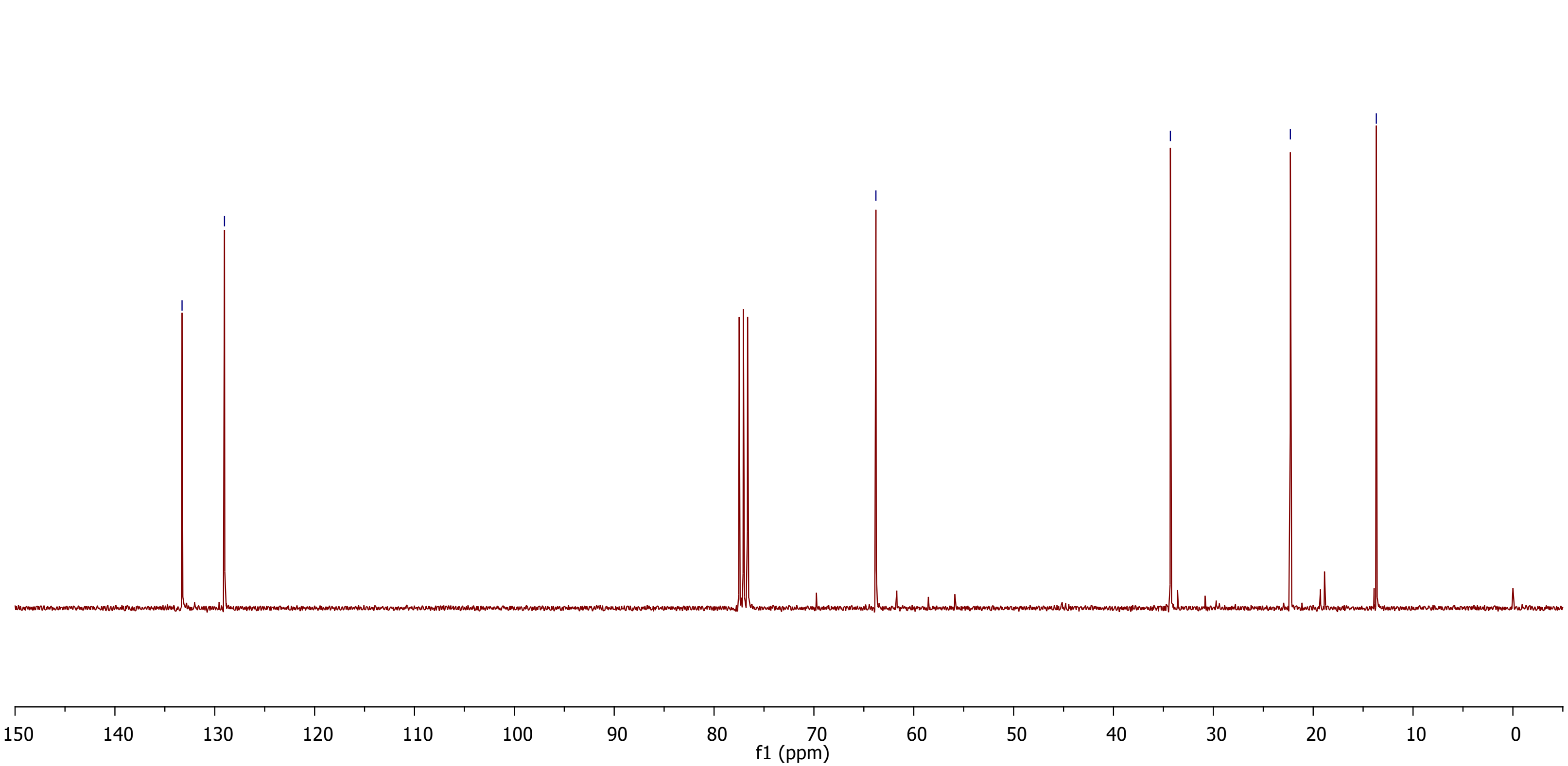


9r

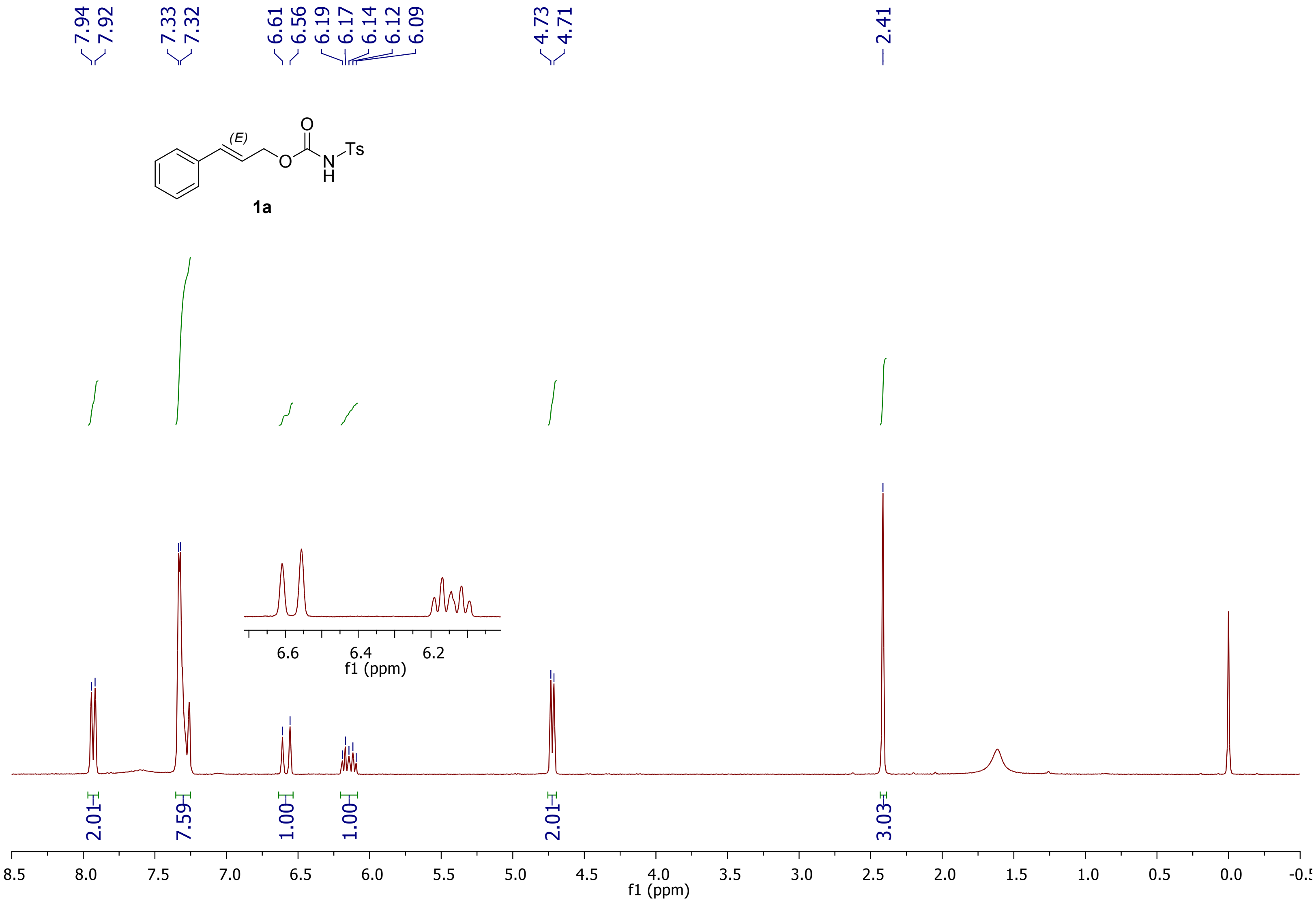
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **9r**



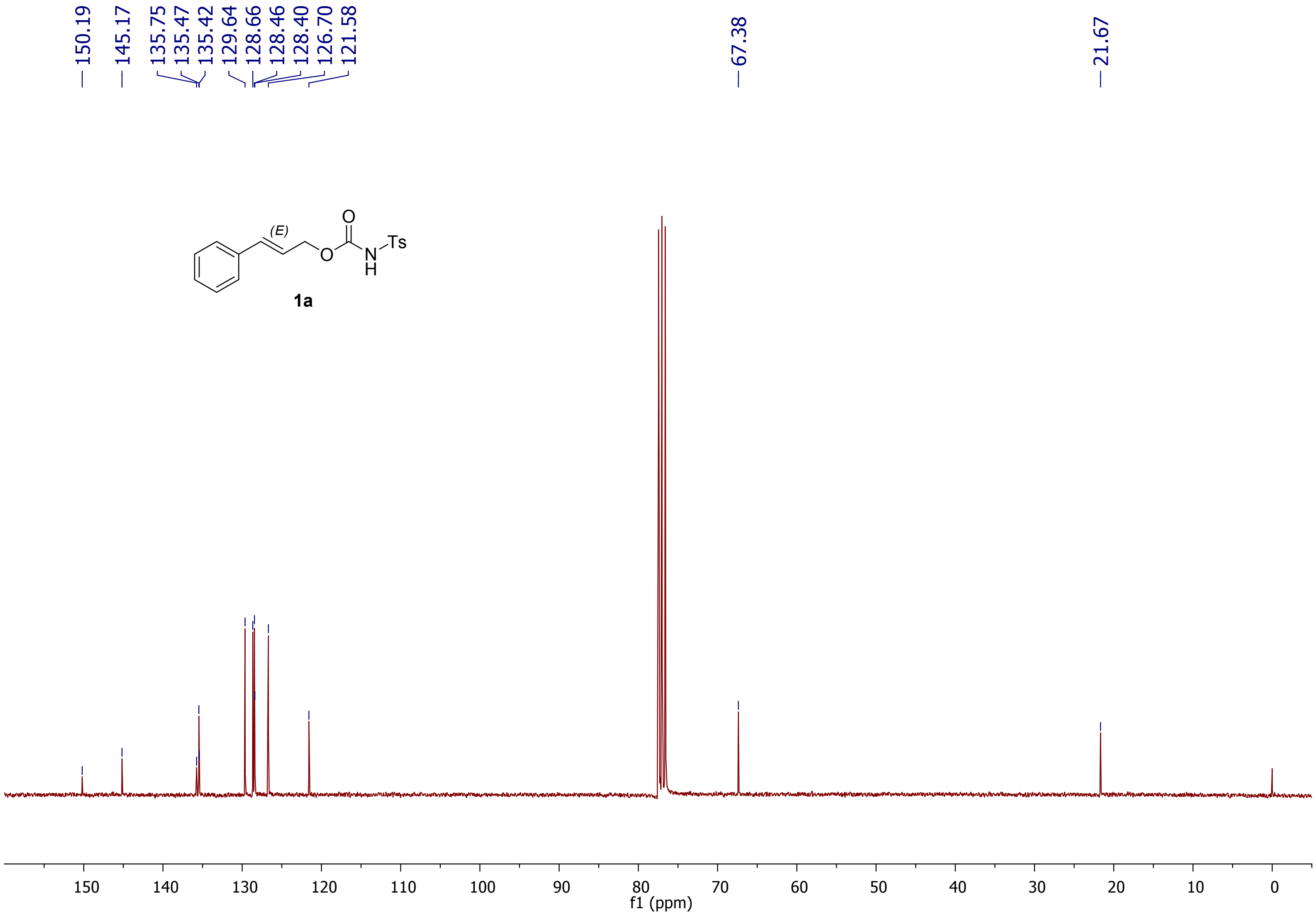
9r



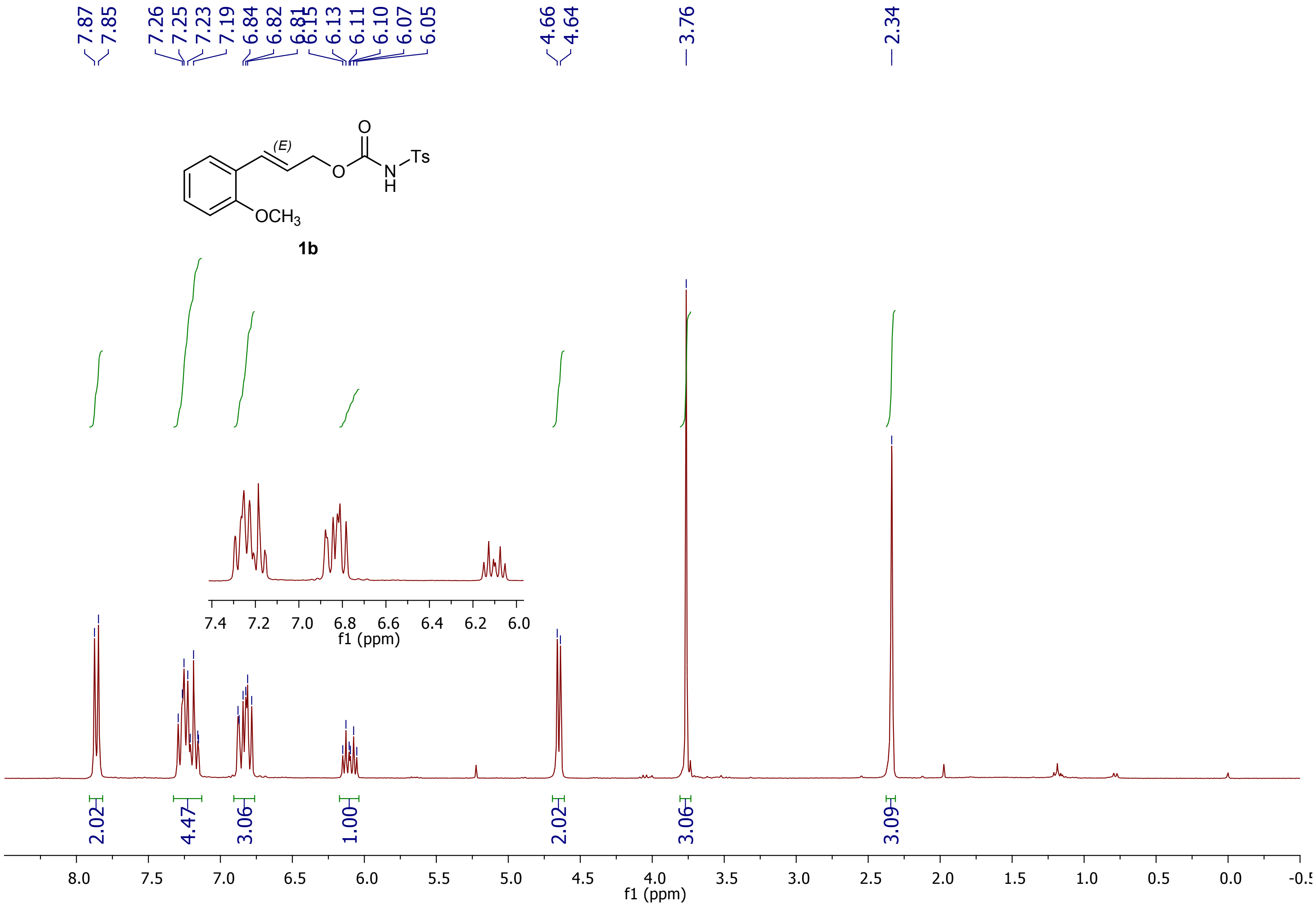
[1]H NMR (300 MHz, $CDCl_3$) of substrate **1a**



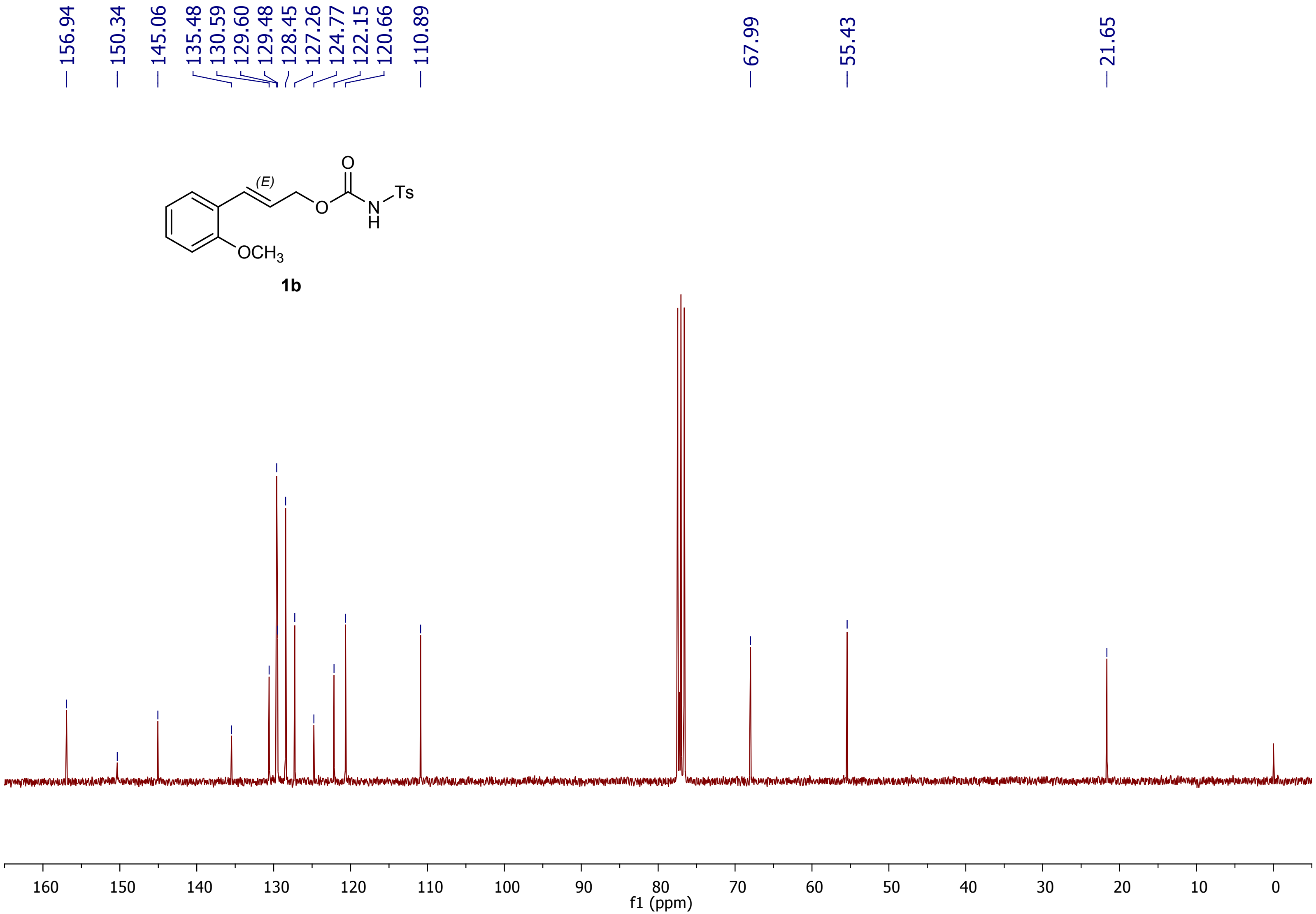
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1a**



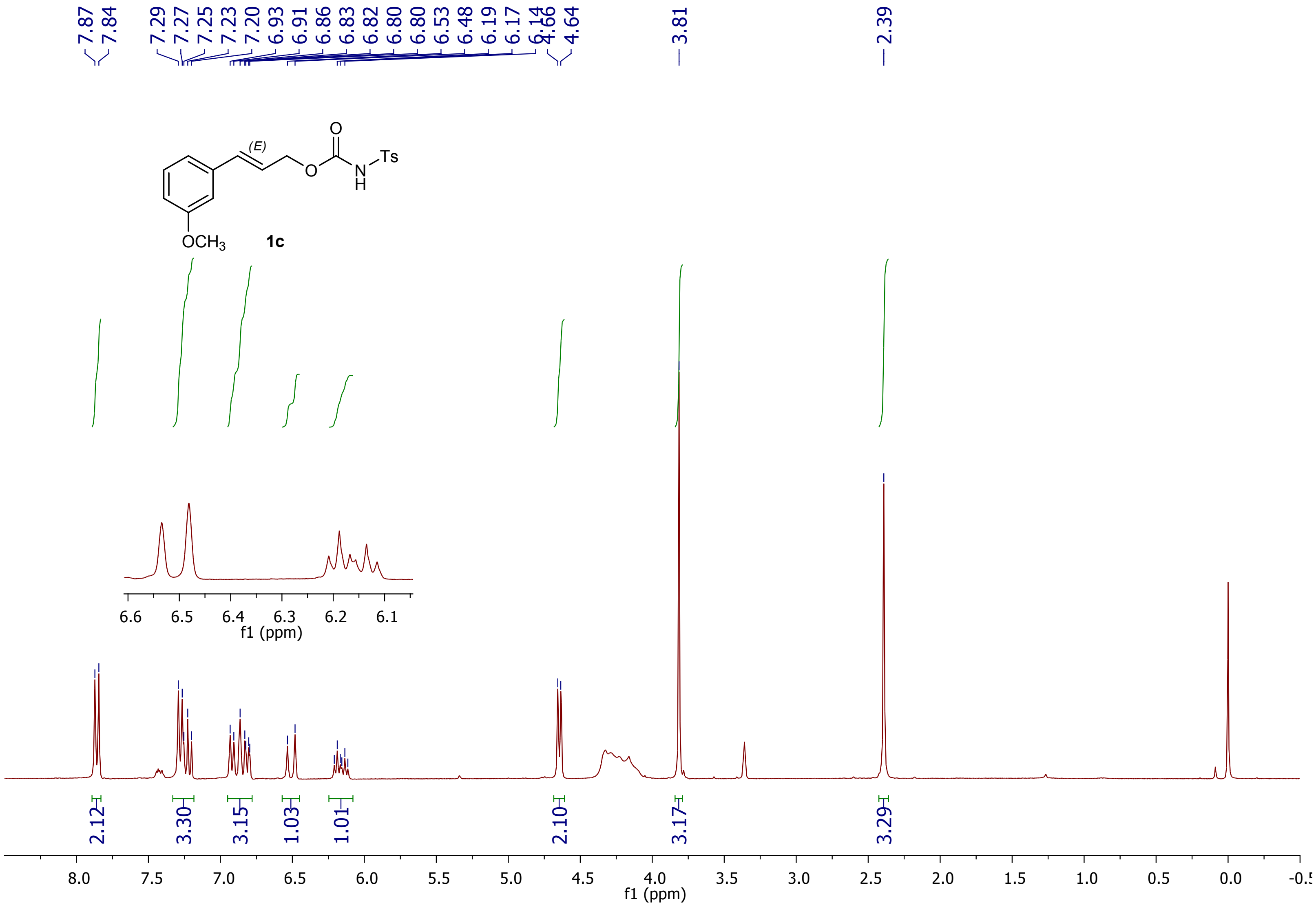
^1H NMR (300 MHz, $CDCl_3$) of substrate **1b**



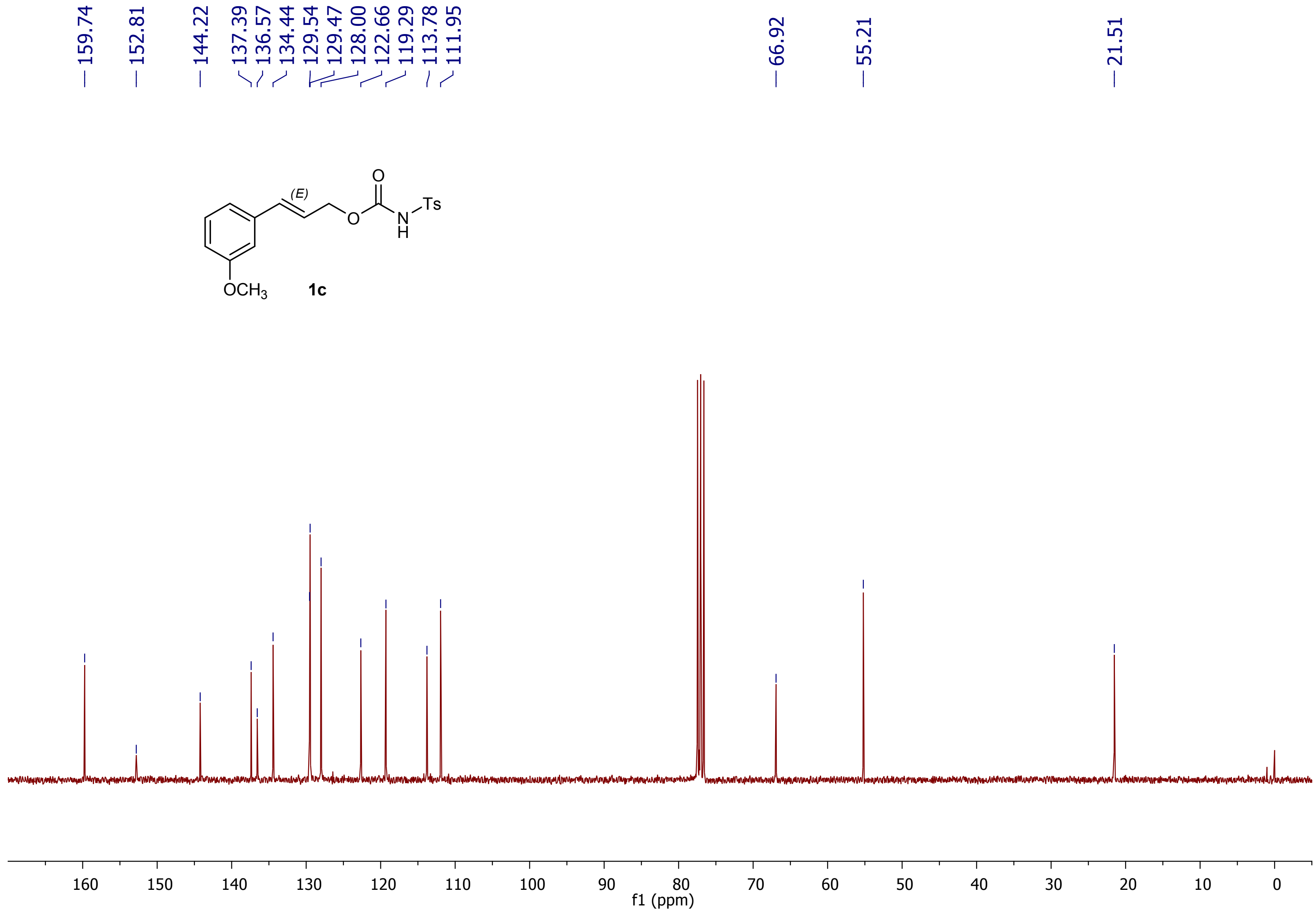
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1b**



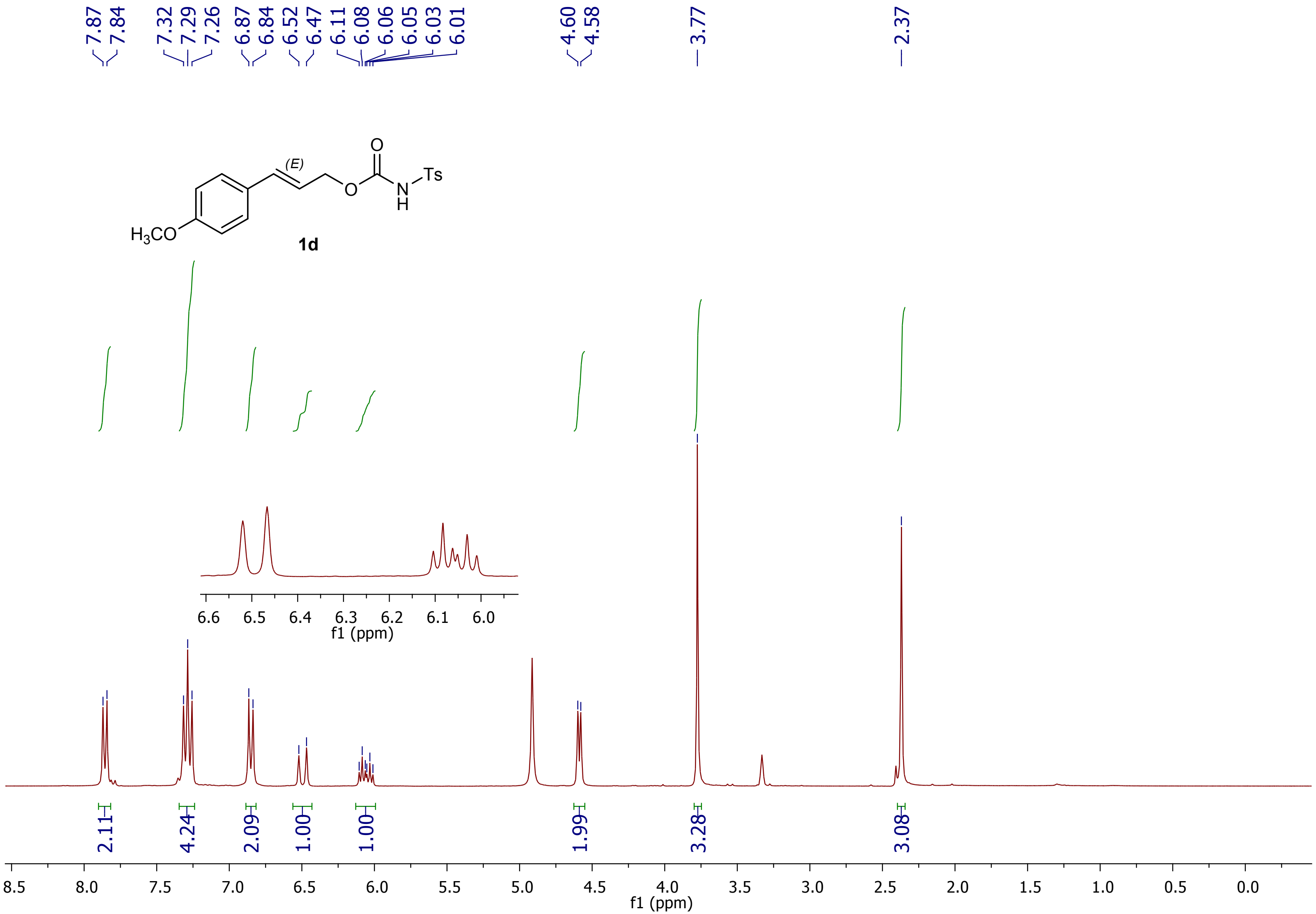
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **1c**



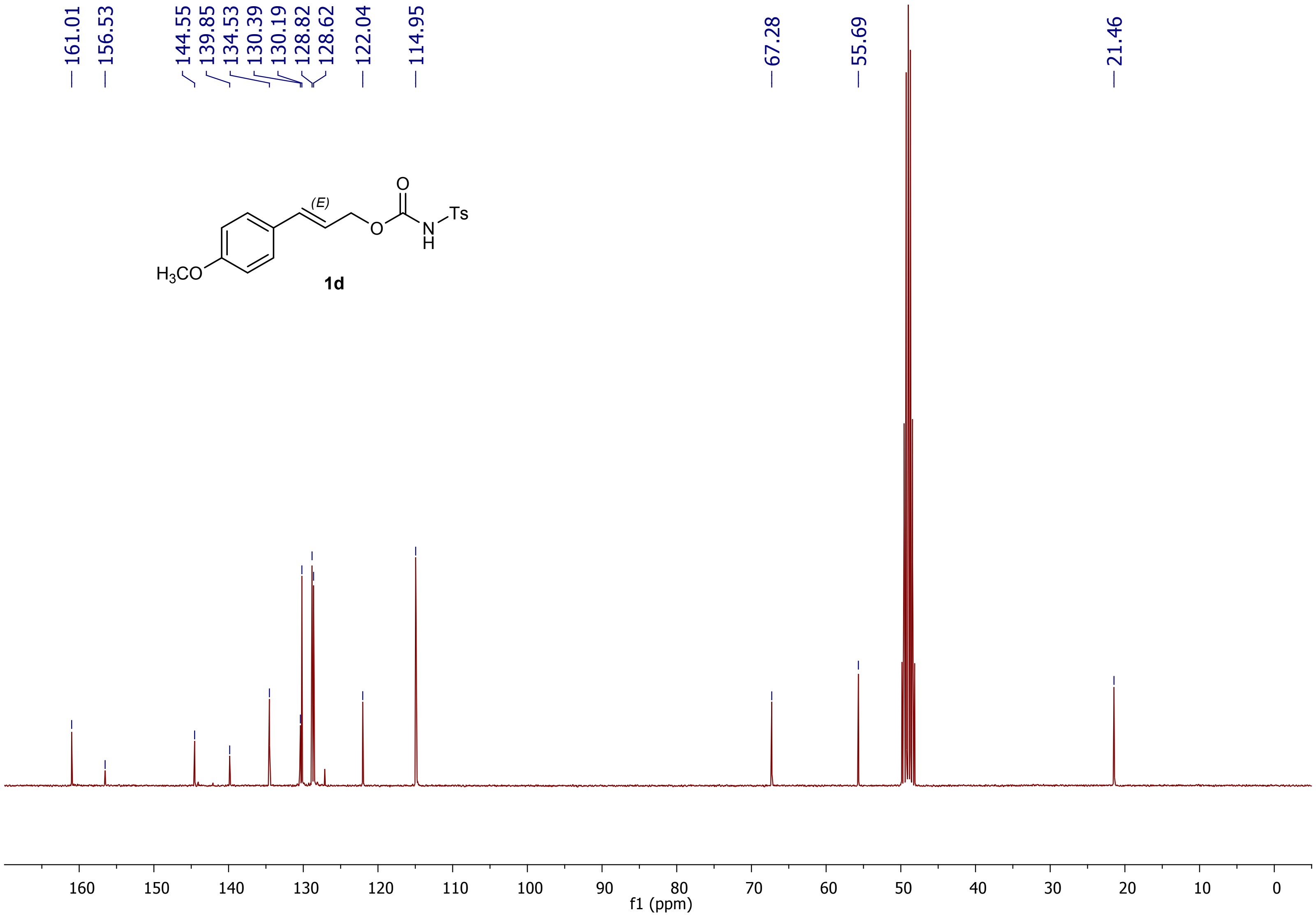
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1c**



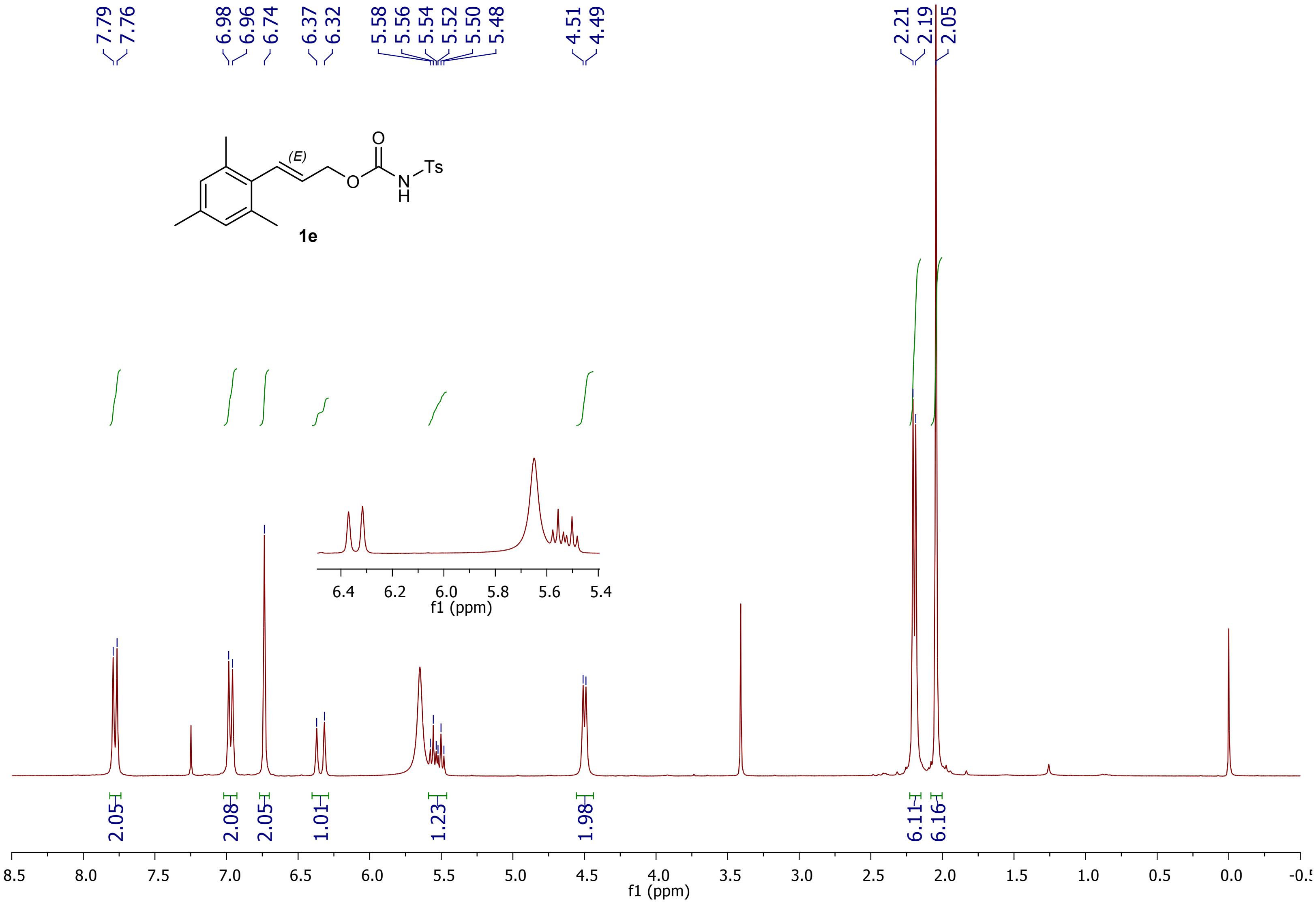
^{1}H NMR (300 MHz, CD_3OD) of substrate **1d**



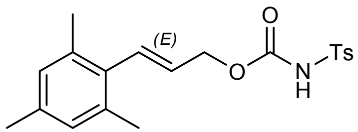
^{13}C NMR (75 MHz, CD_3OD) of substrate **1d**



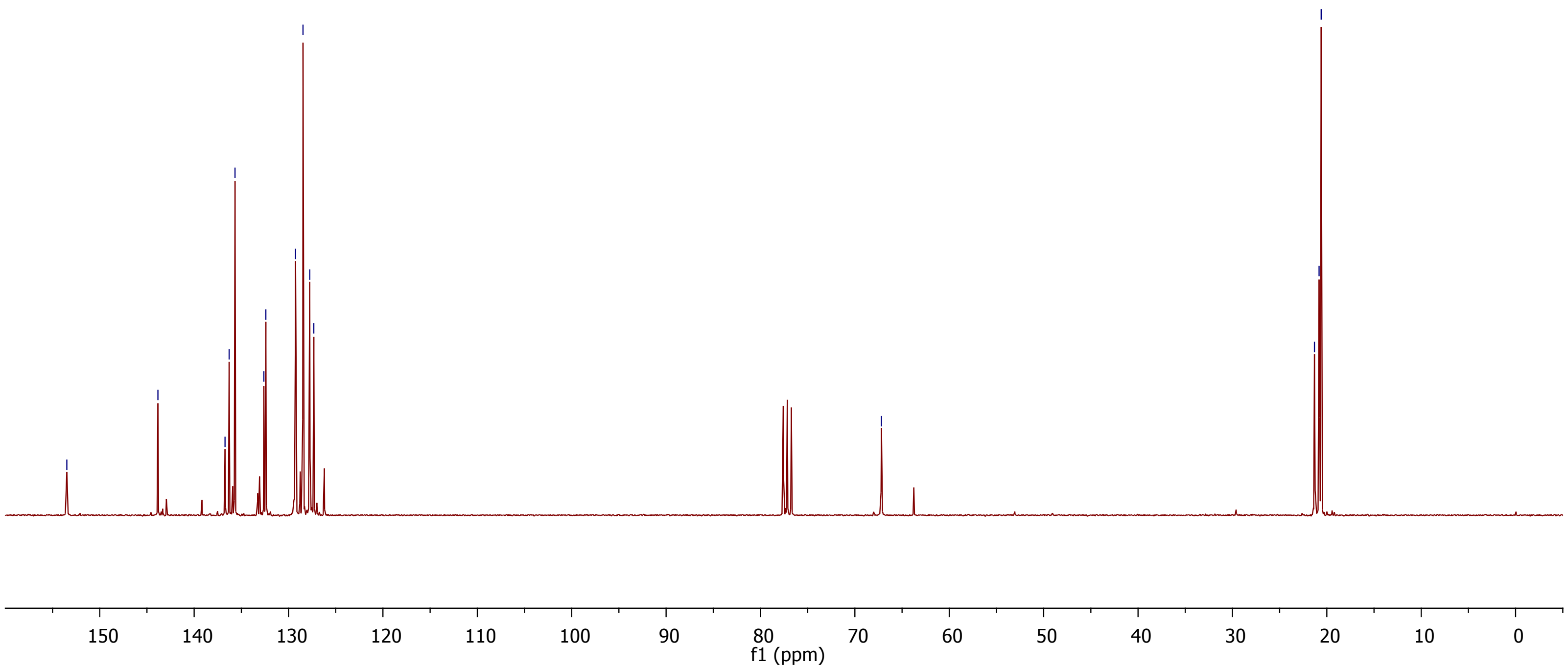
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **1e**



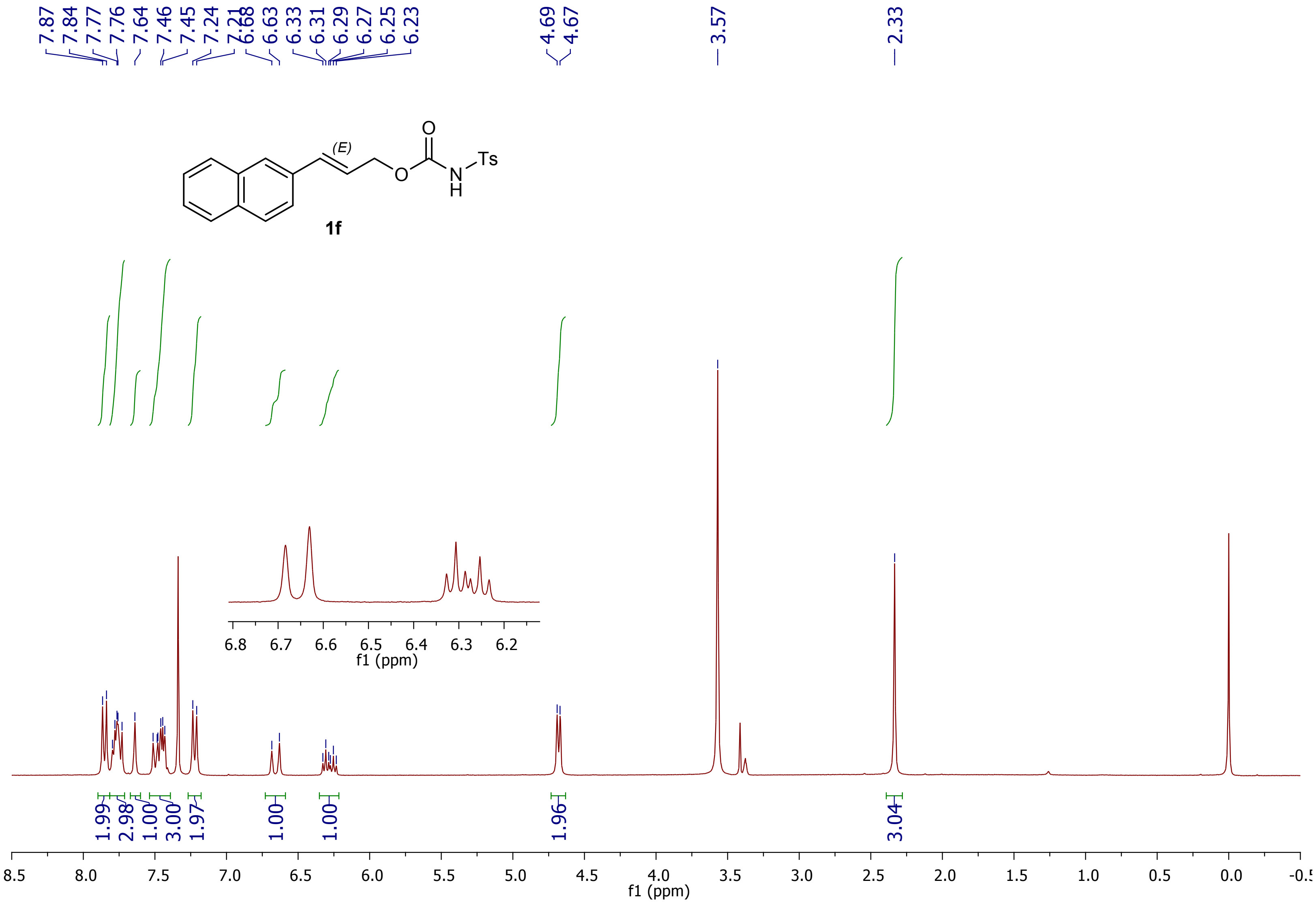
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1e**



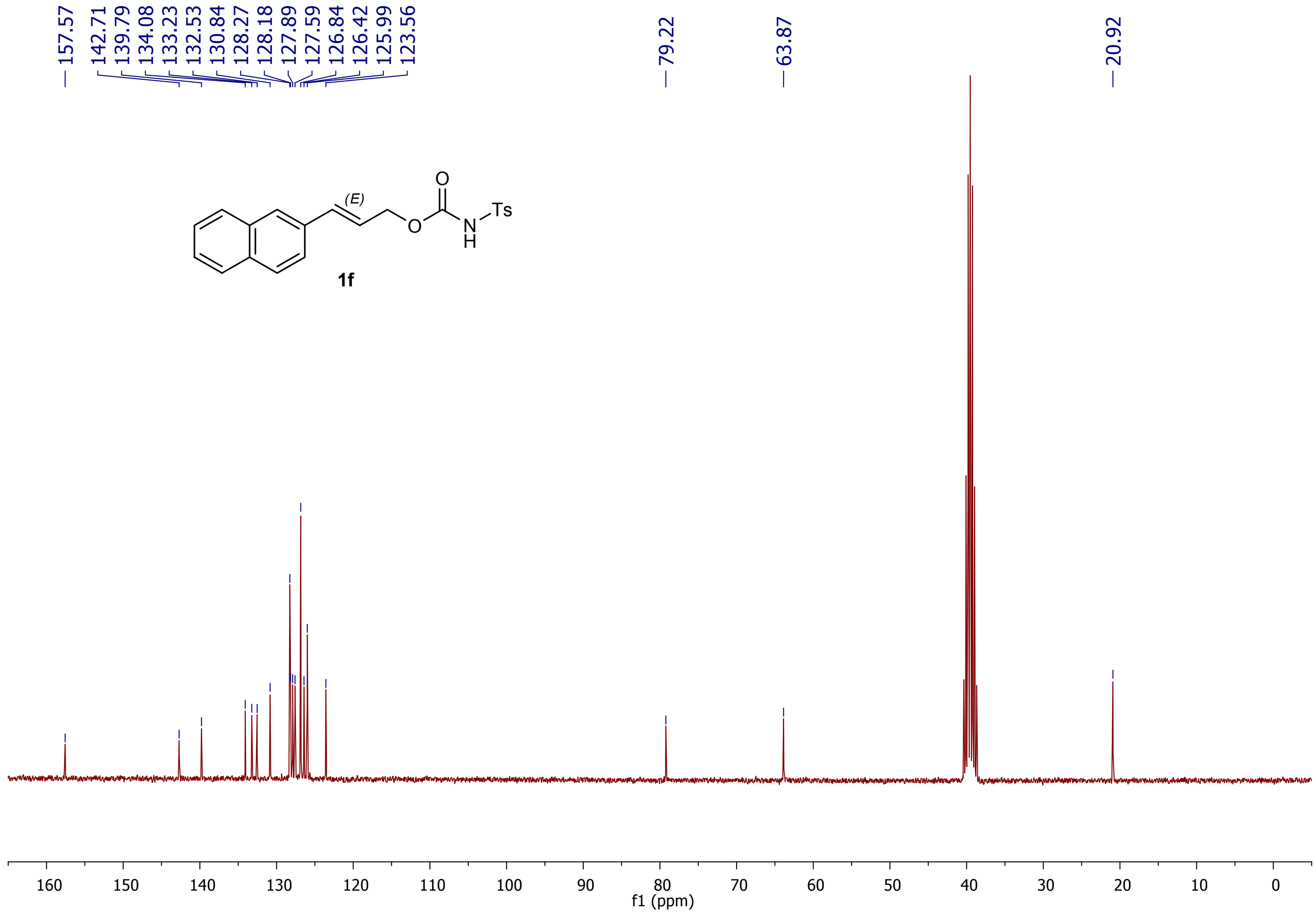
1e



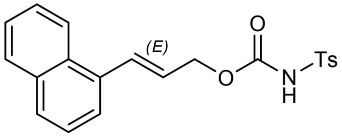
^{1}H NMR (300 MHz, DMSO-d_6) of substrate **1f**



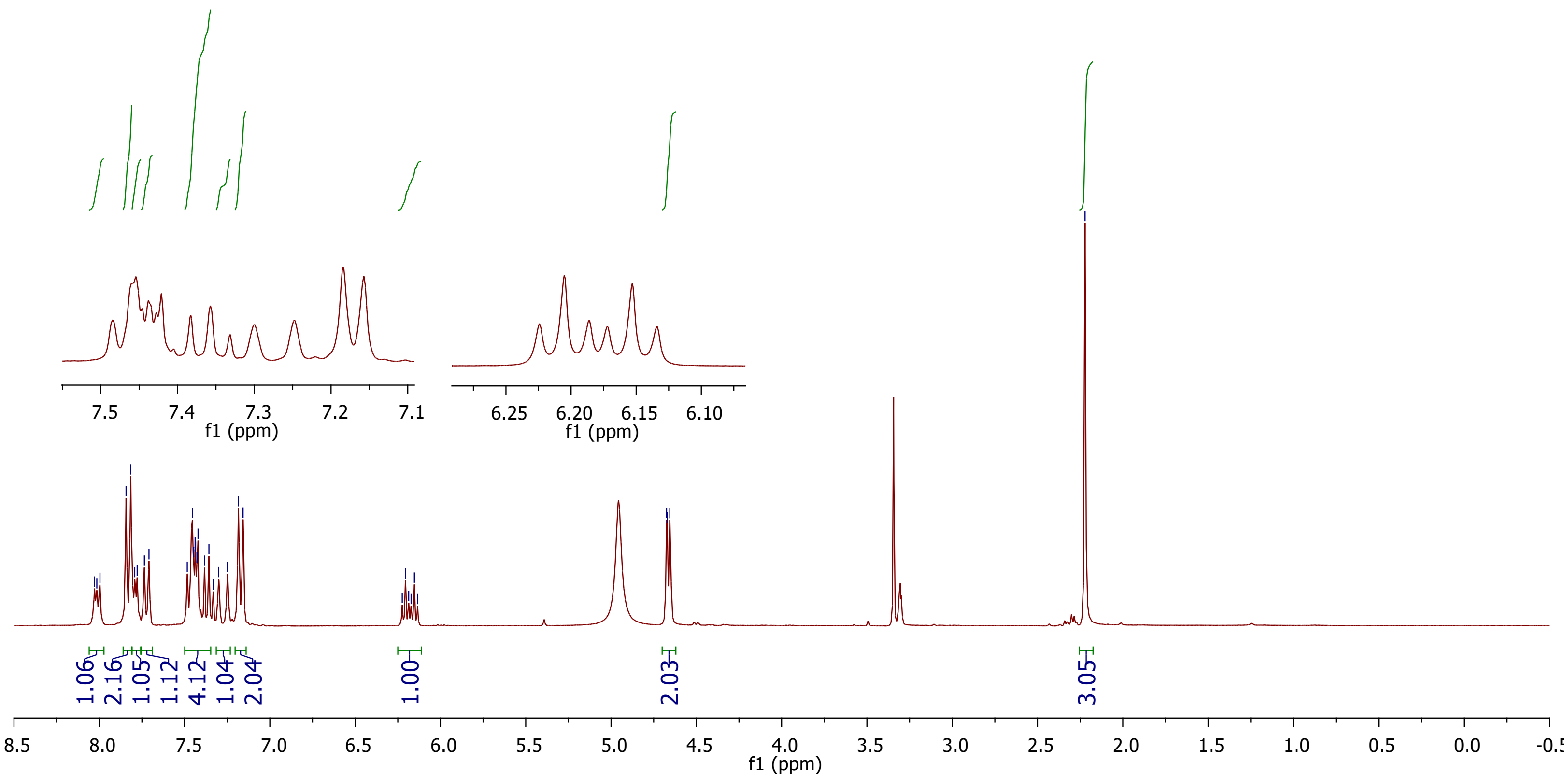
^{13}C NMR (75 MHz, DMSO-d_6) of substrate **1f**



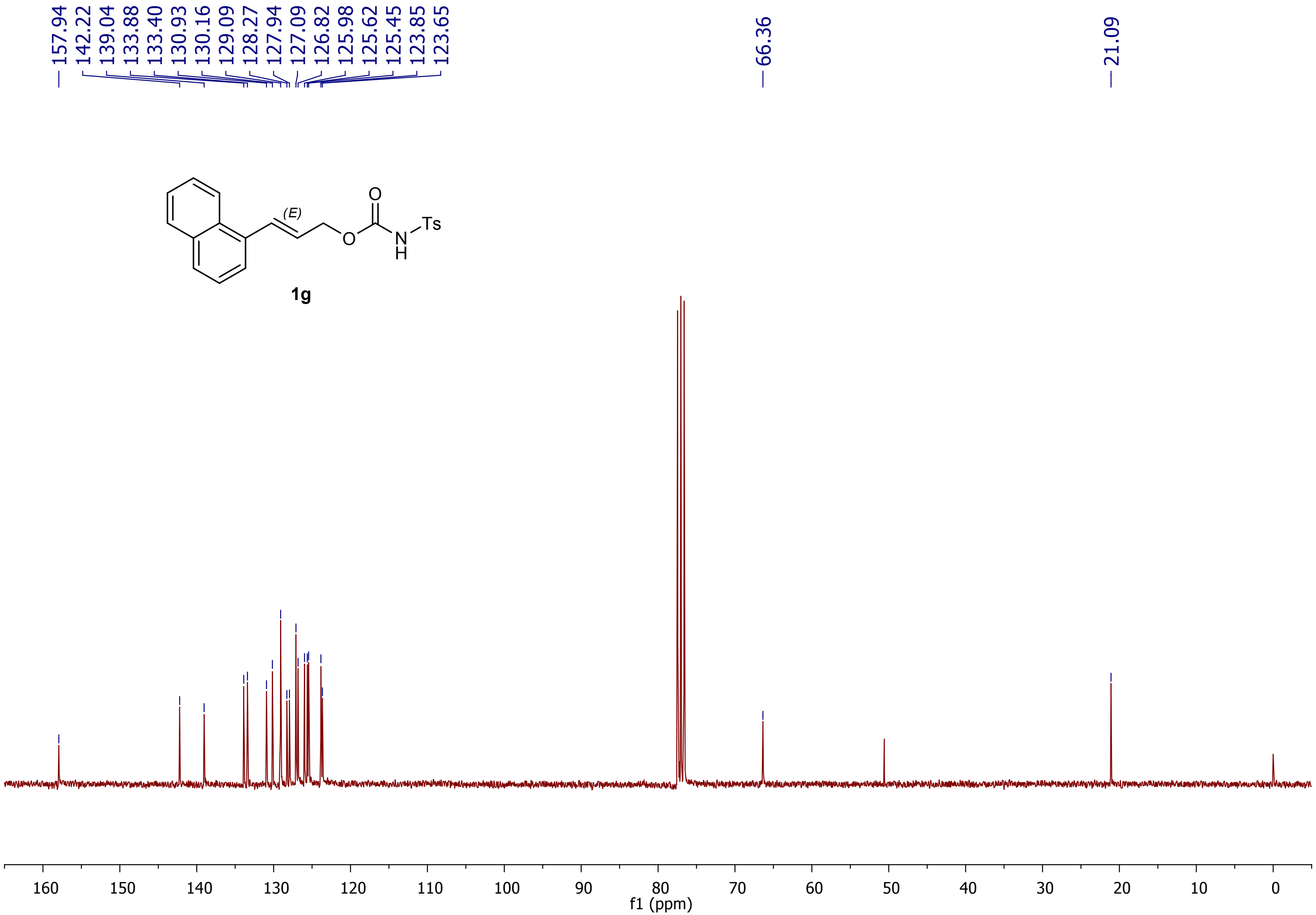
^{1}H NMR (300 MHz, CD_3OD) of substrate **1g**



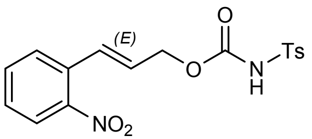
1g



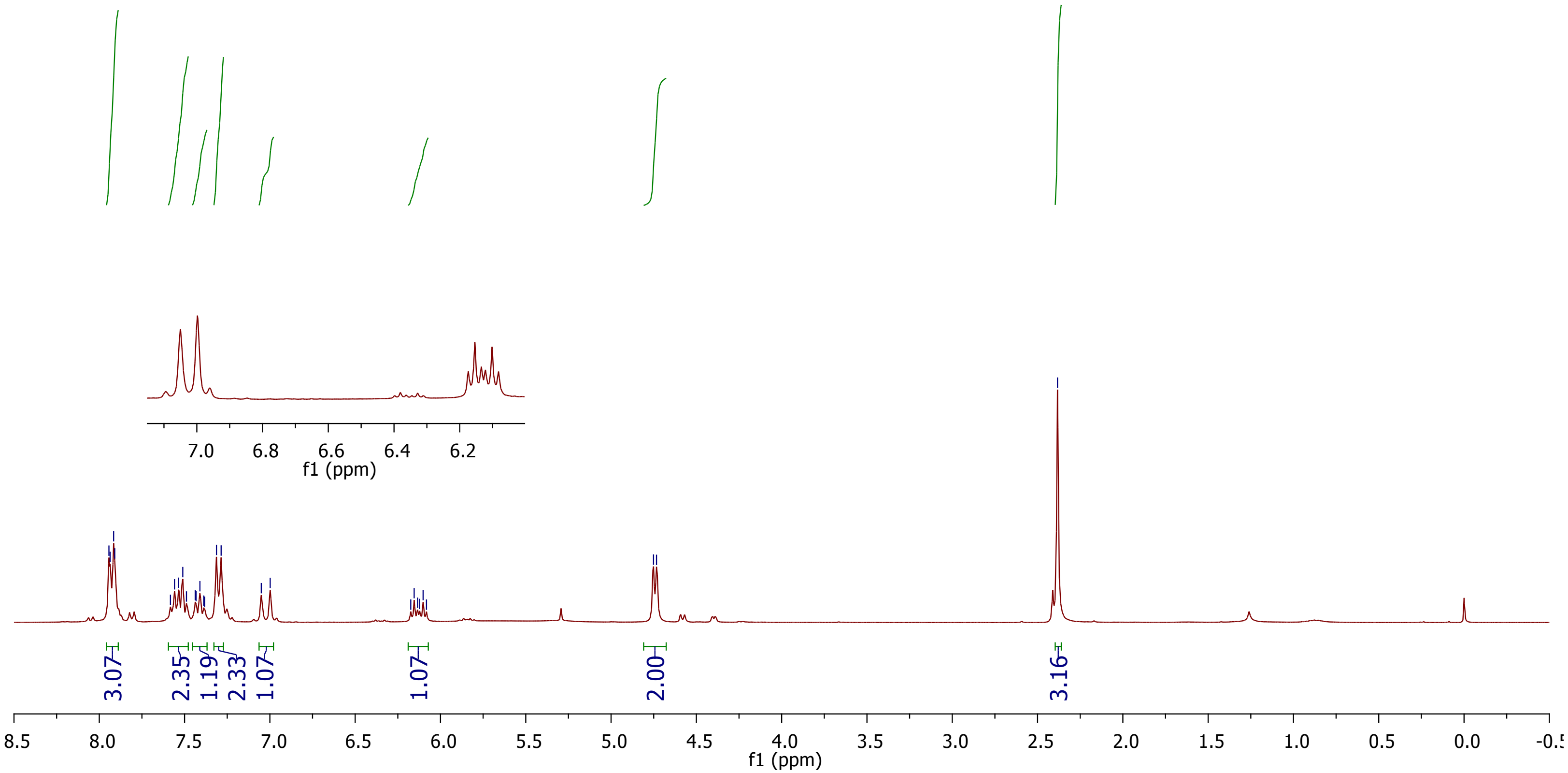
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1g**



^1H NMR (300 MHz, $CDCl_3$) of substrate **1h**



1h



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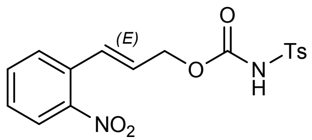
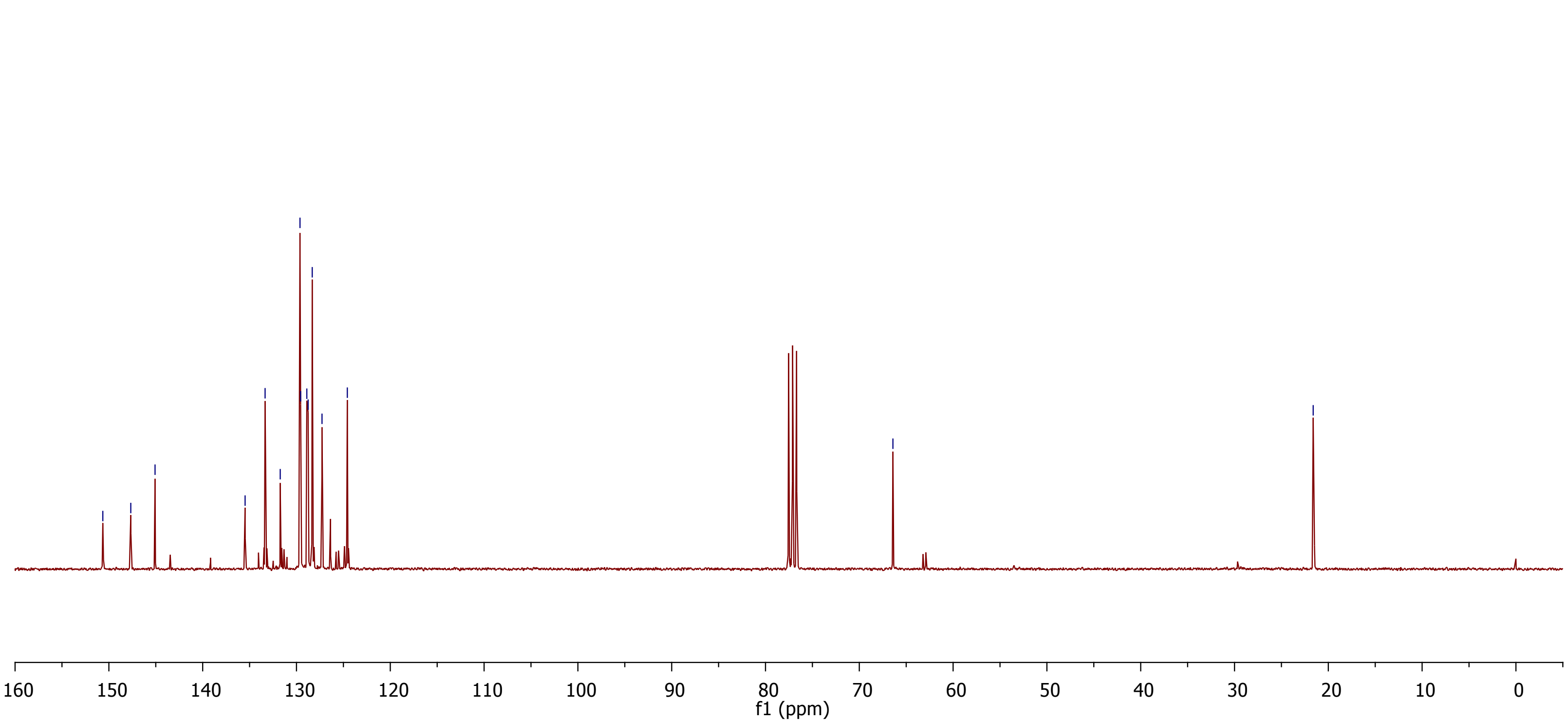
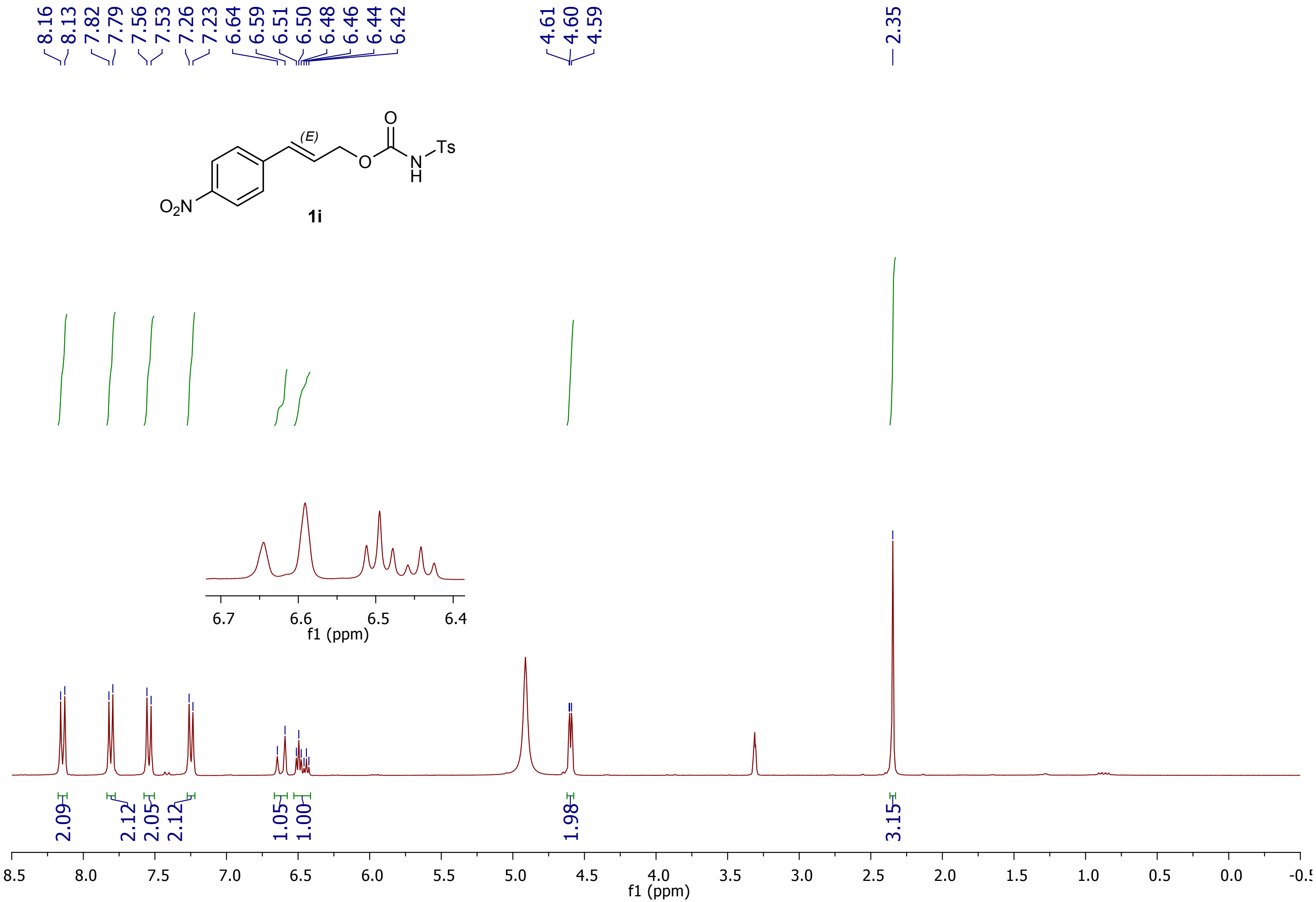


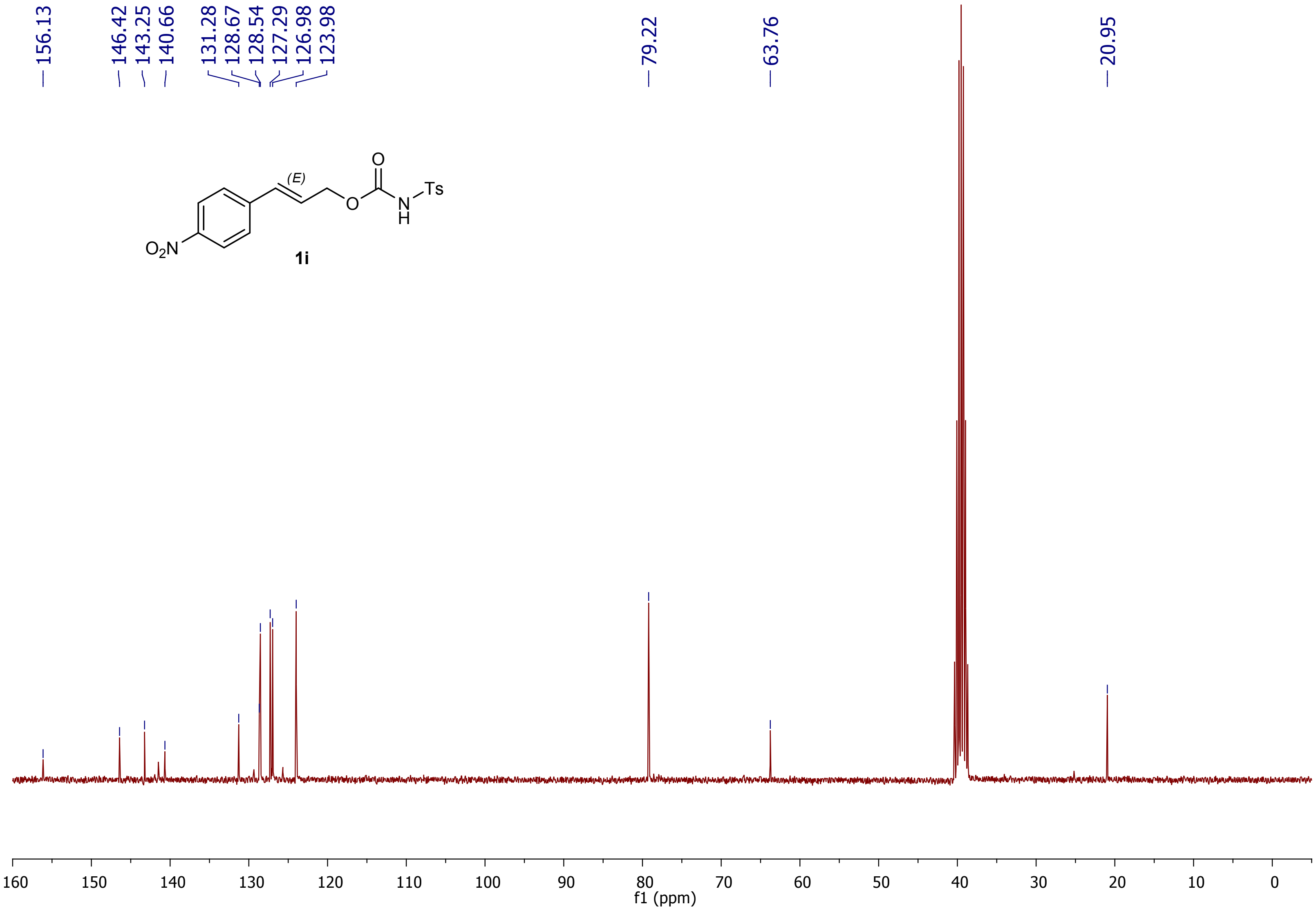
1h



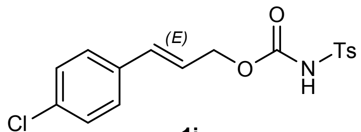
^{1}H NMR (300 MHz, CD_3OD) of substrate **1i**



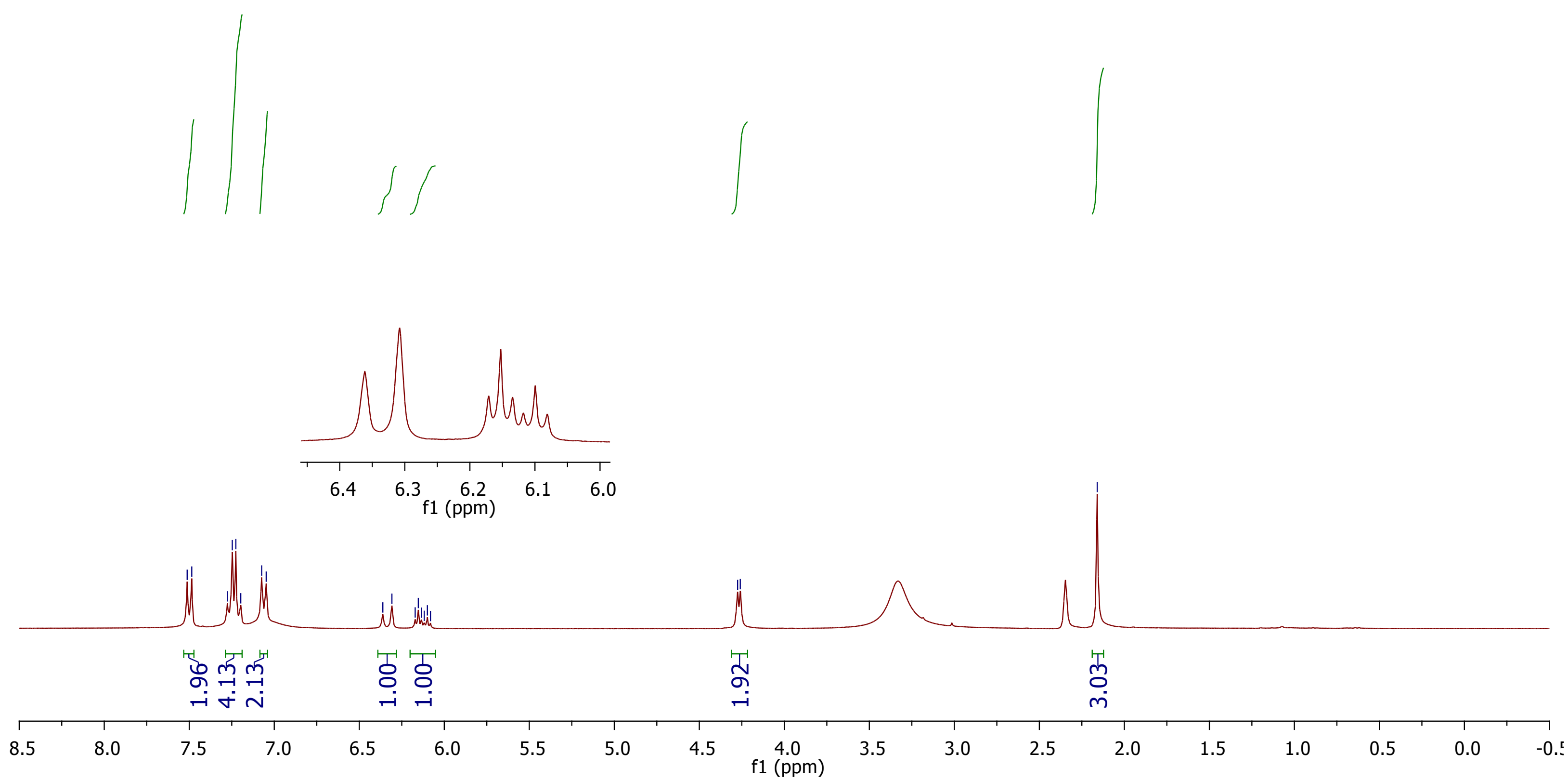
^{13}C NMR (75 MHz, DMSO-d_6) of substrate **1i**



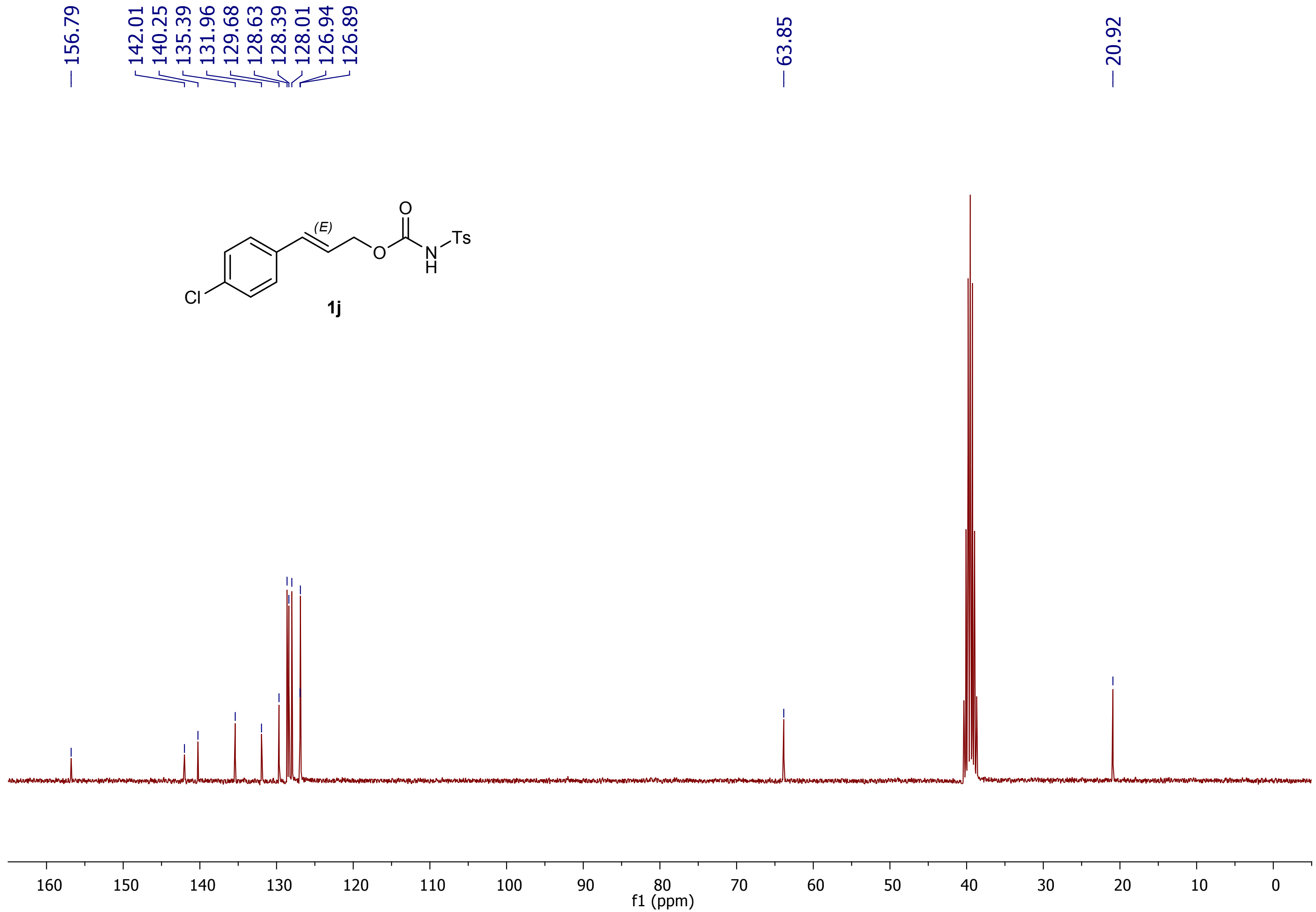
^{1}H NMR (300 MHz, DMSO-d_6) of substrate **1j**



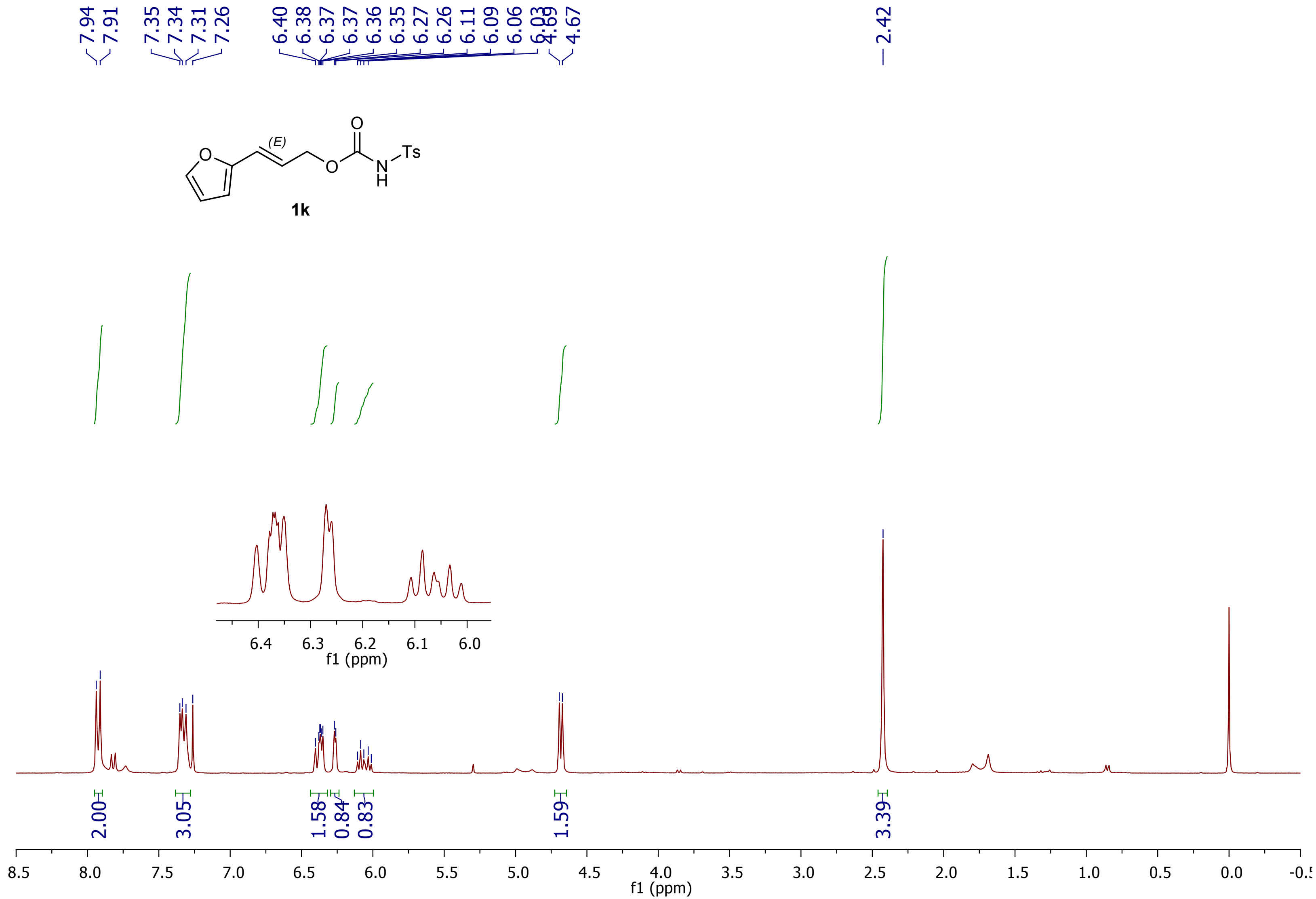
1j



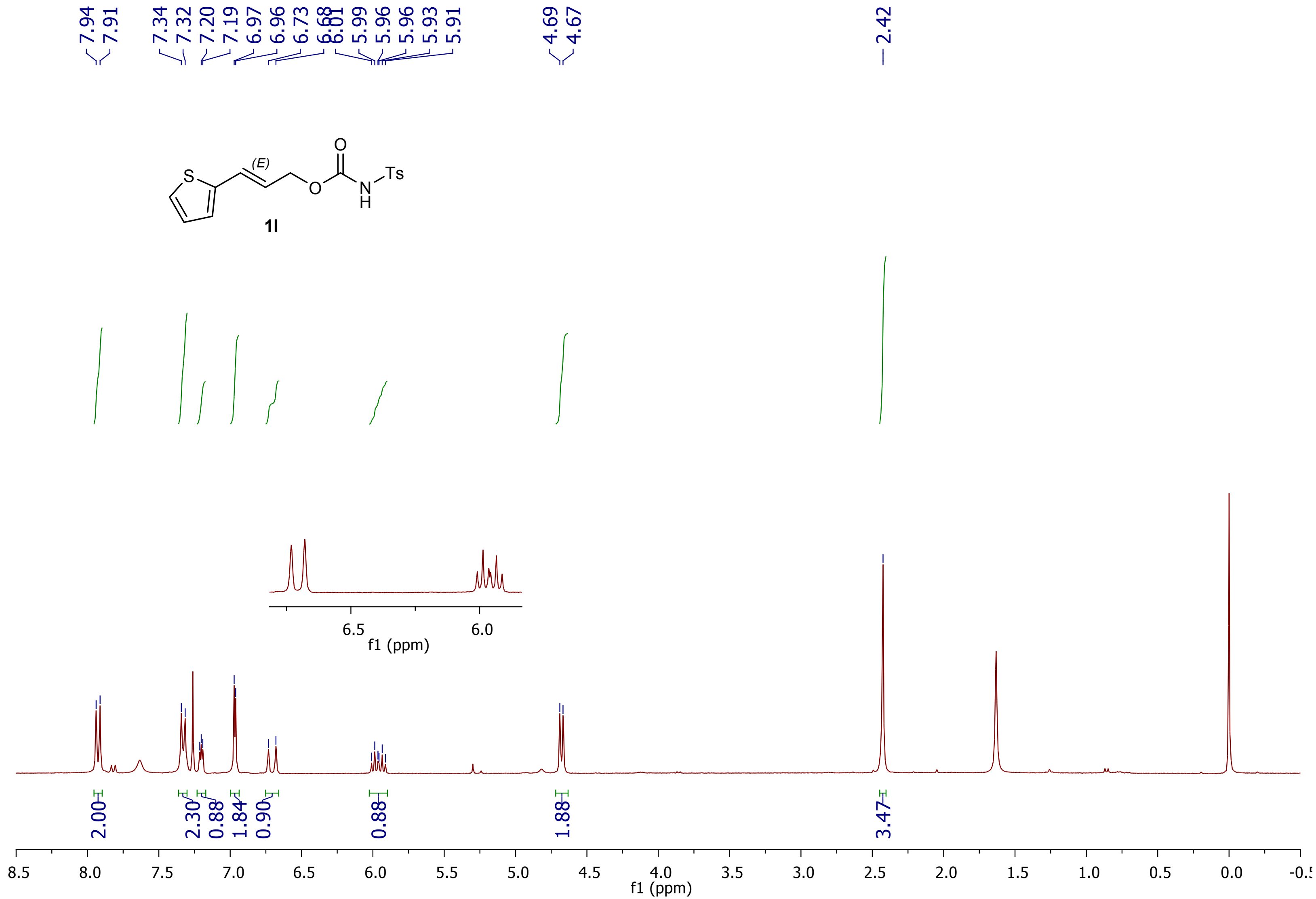
^{13}C NMR (75 MHz, DMSO-d_6) of substrate **1j**



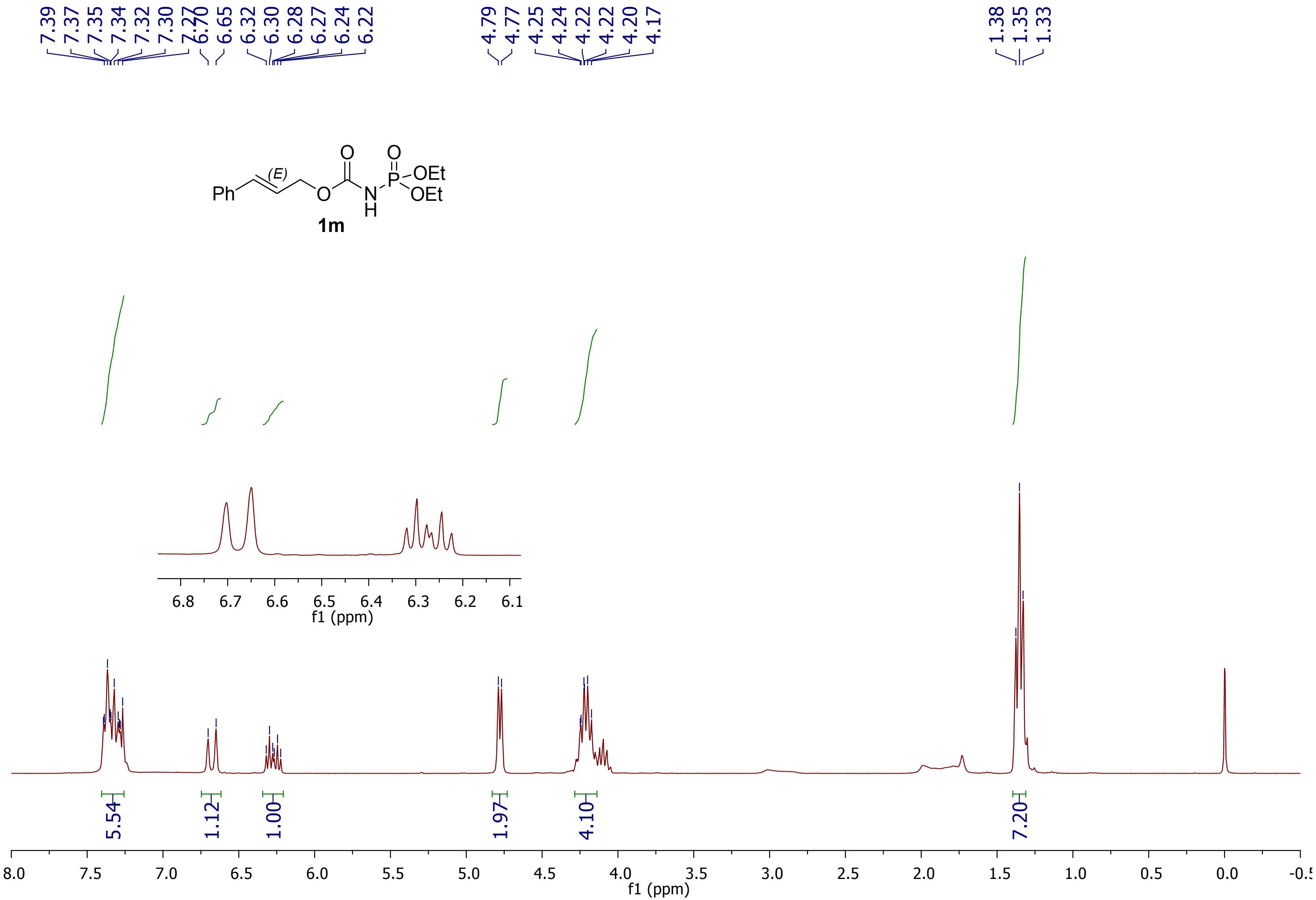
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **1k**



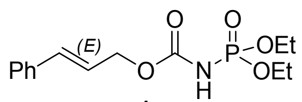
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **1l**



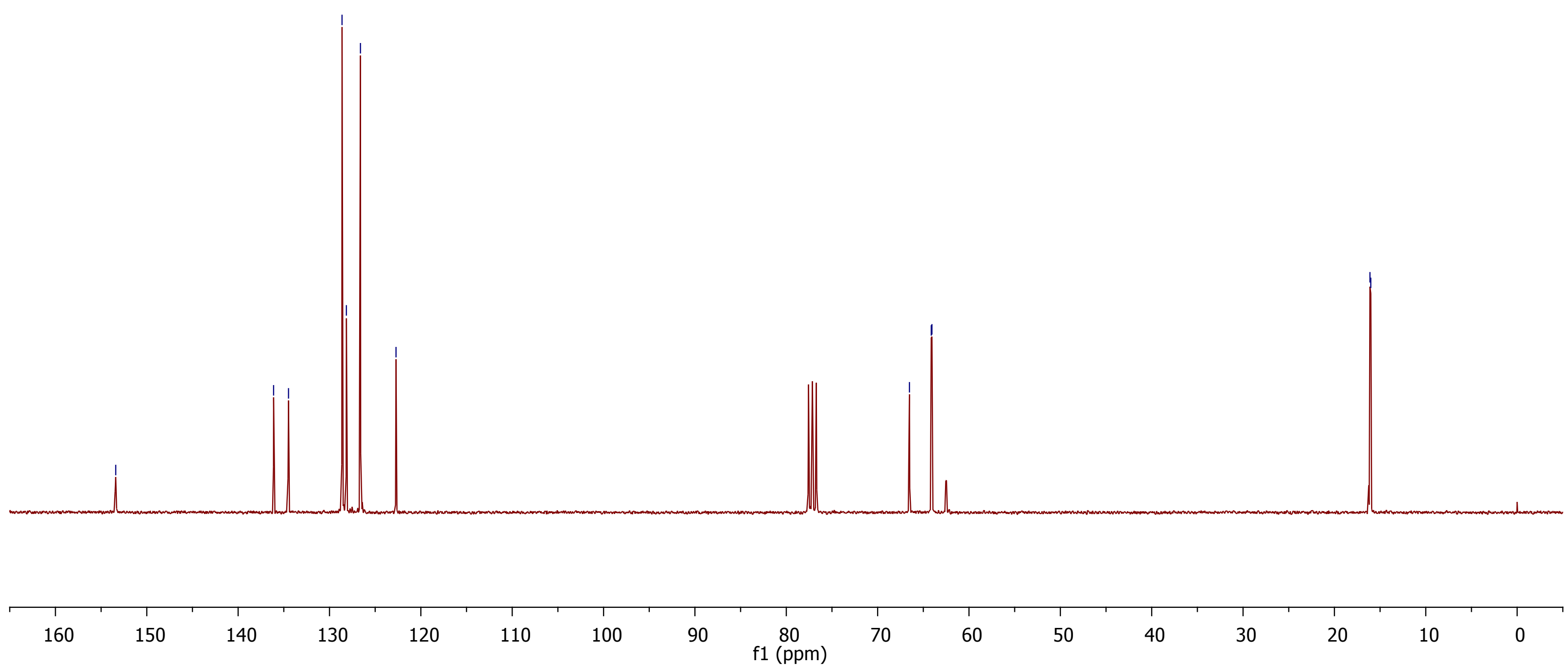
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **1m**



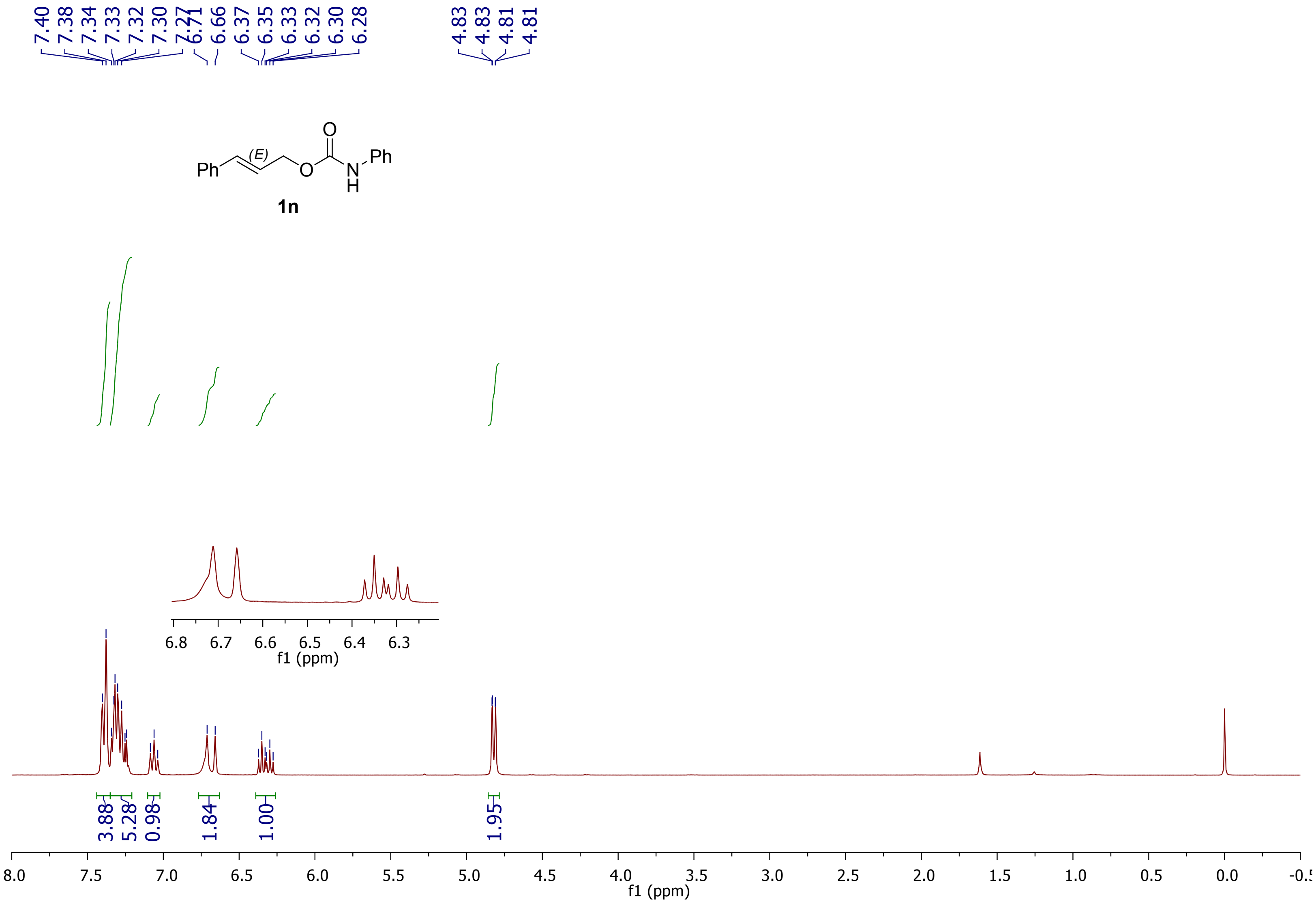
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1m**



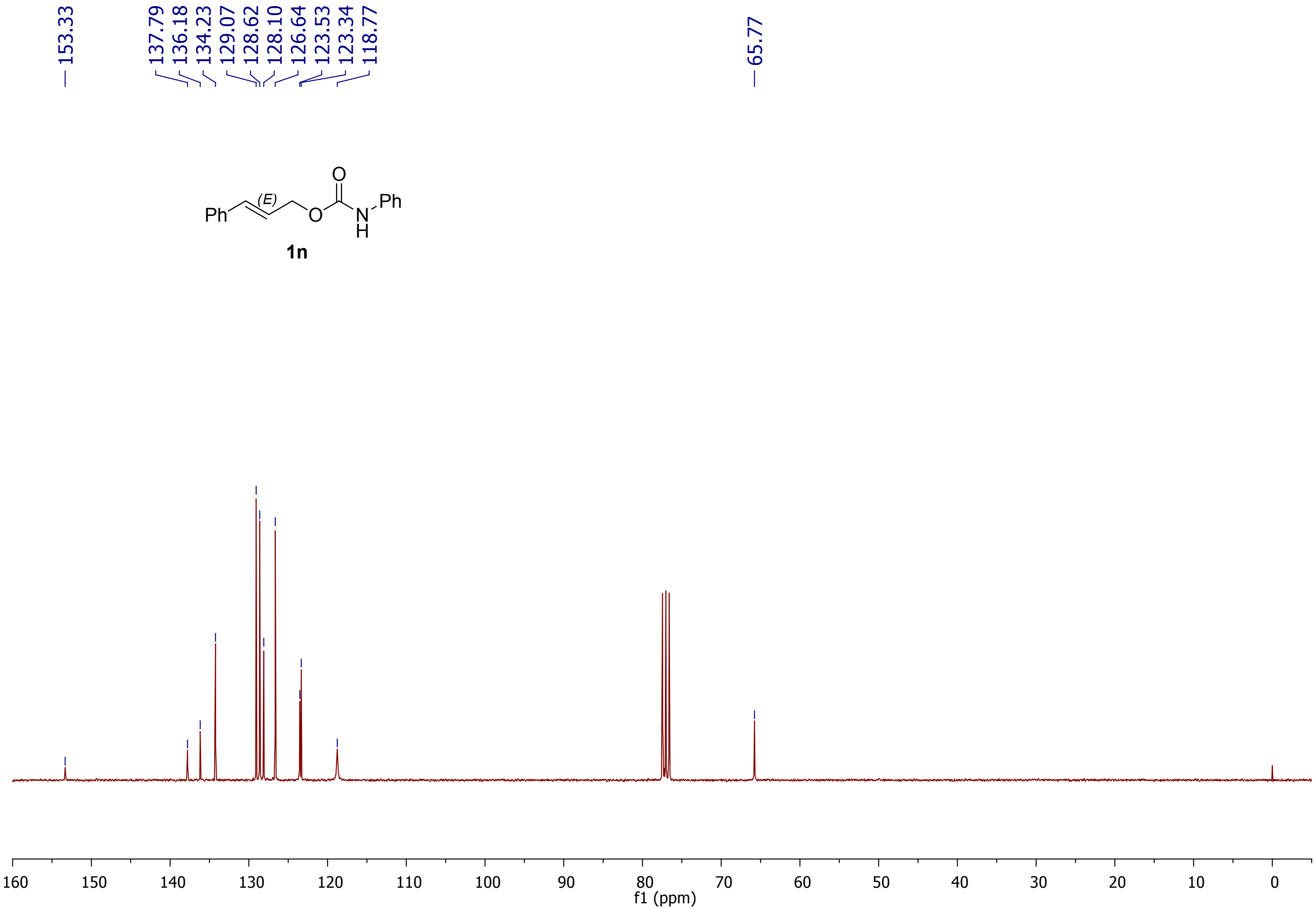
1m



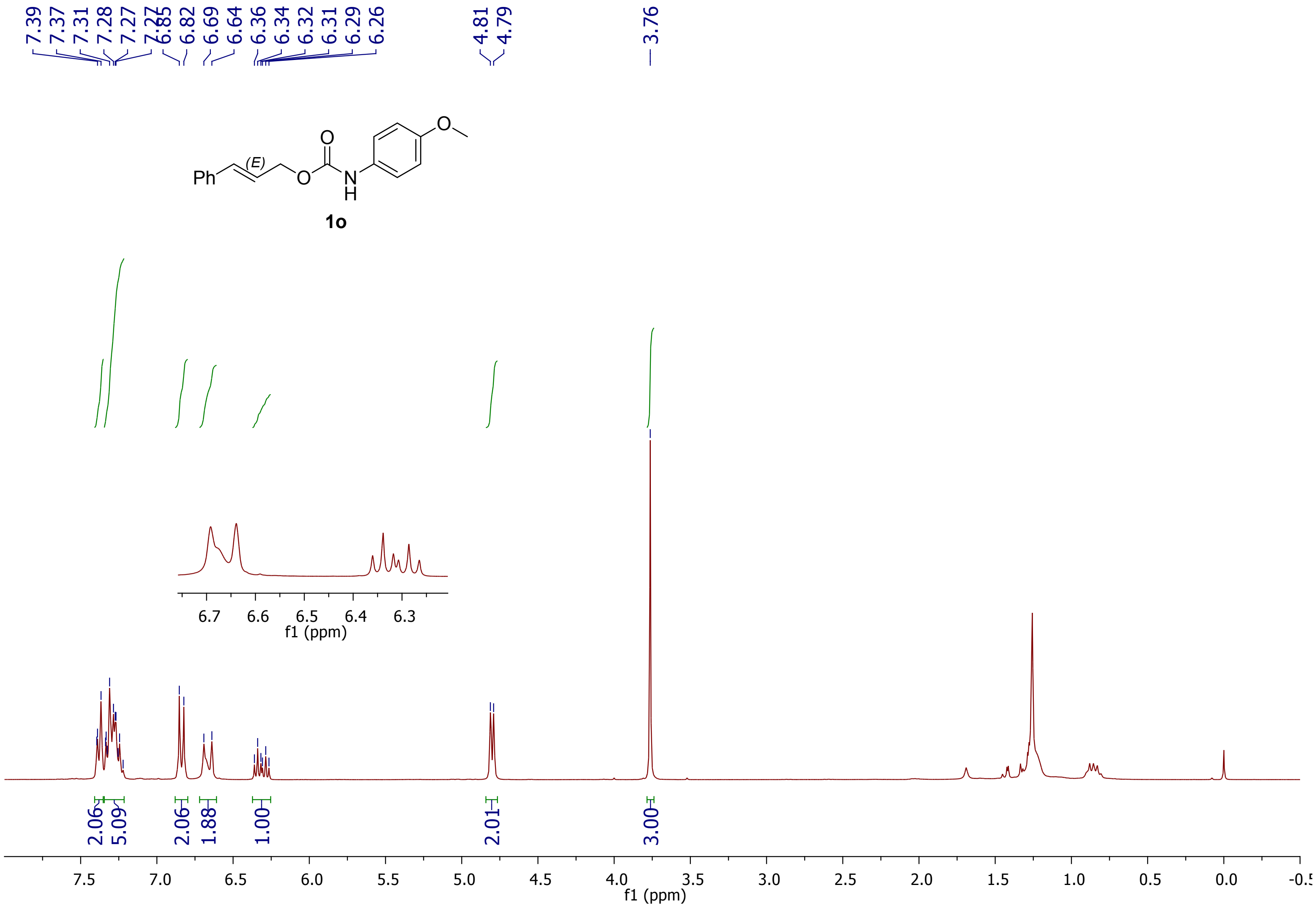
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **1n**



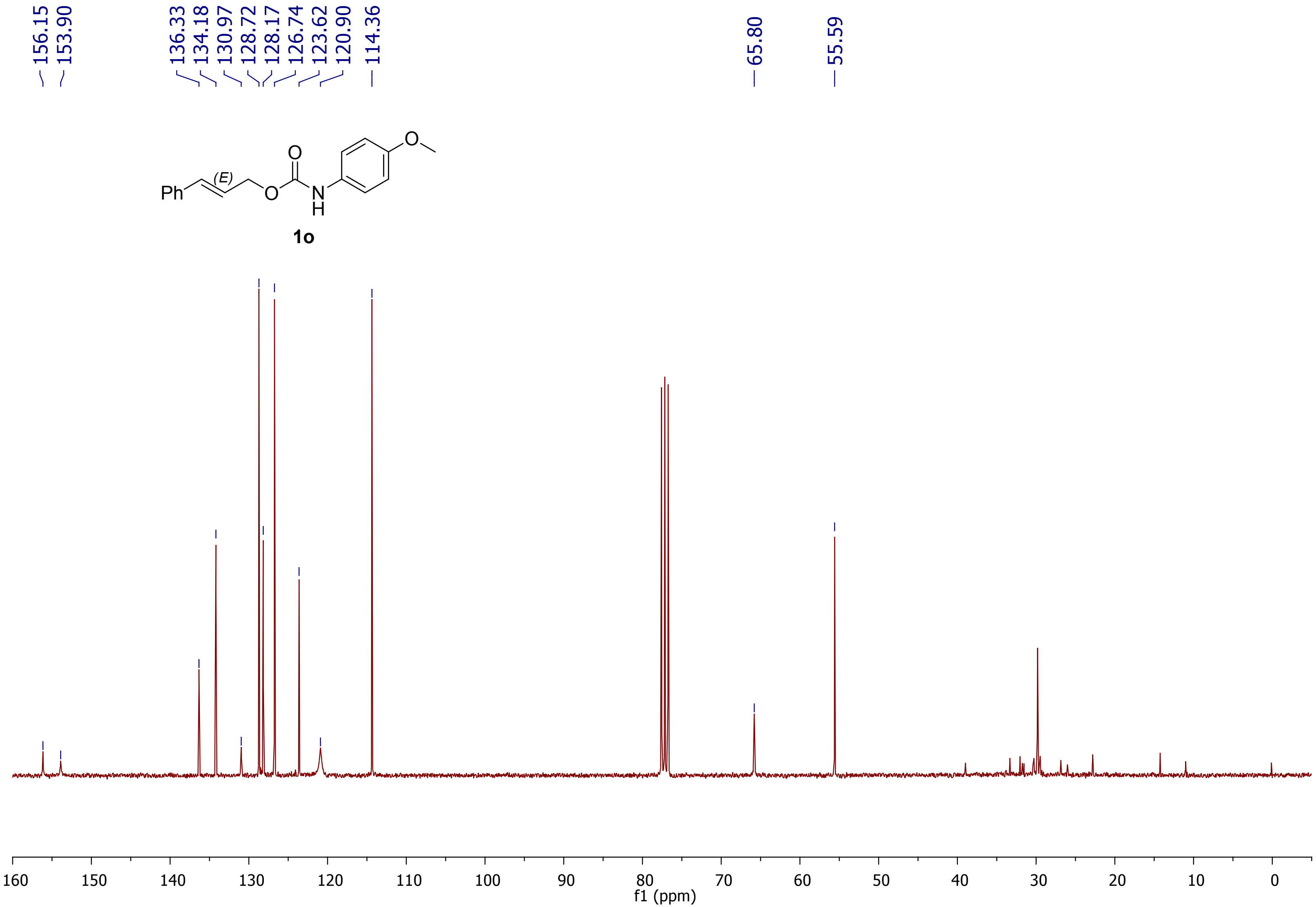
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1n**



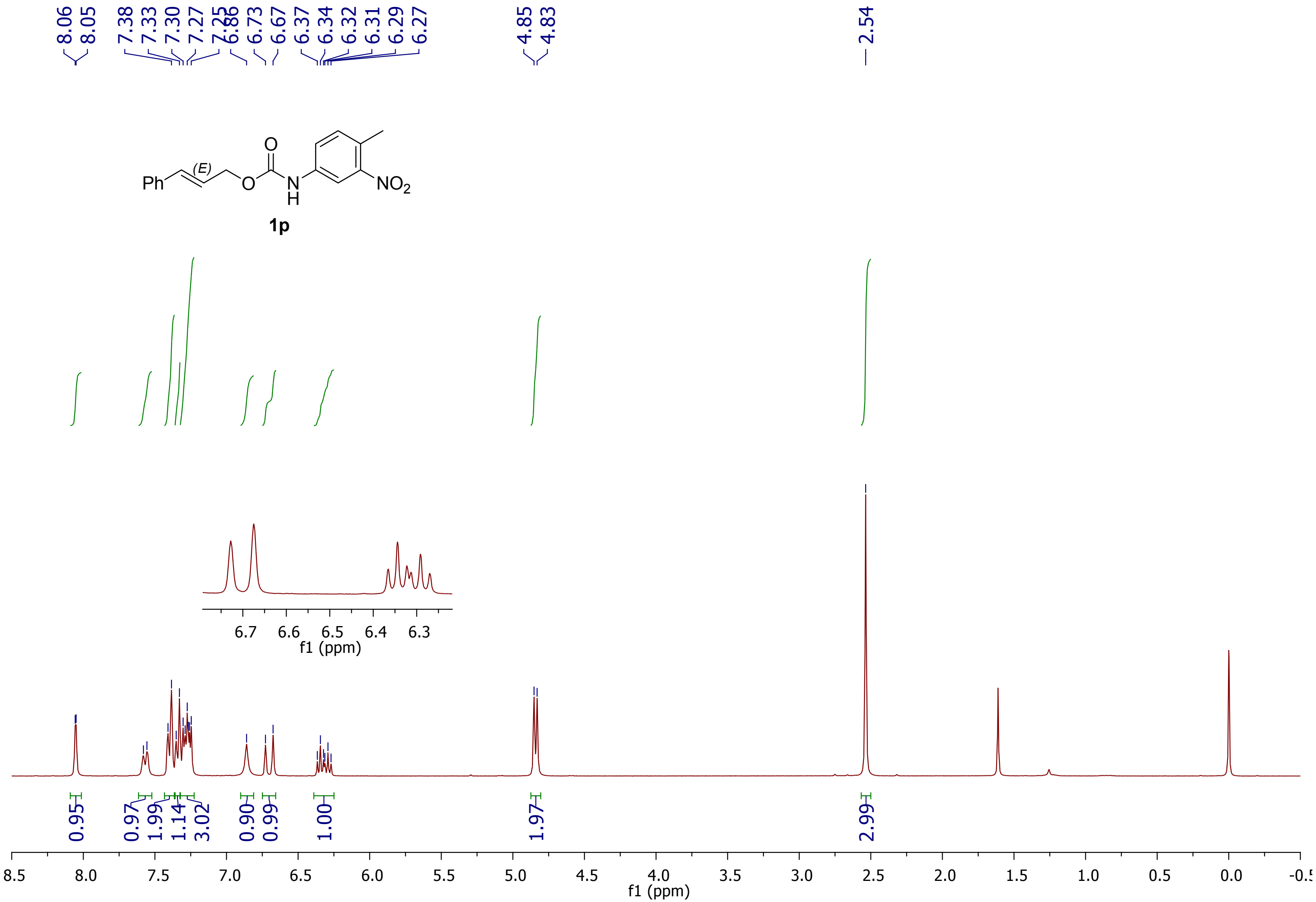
[1]H NMR (300 MHz, $CDCl_3$) of substrate **1o**



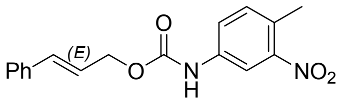
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1o**



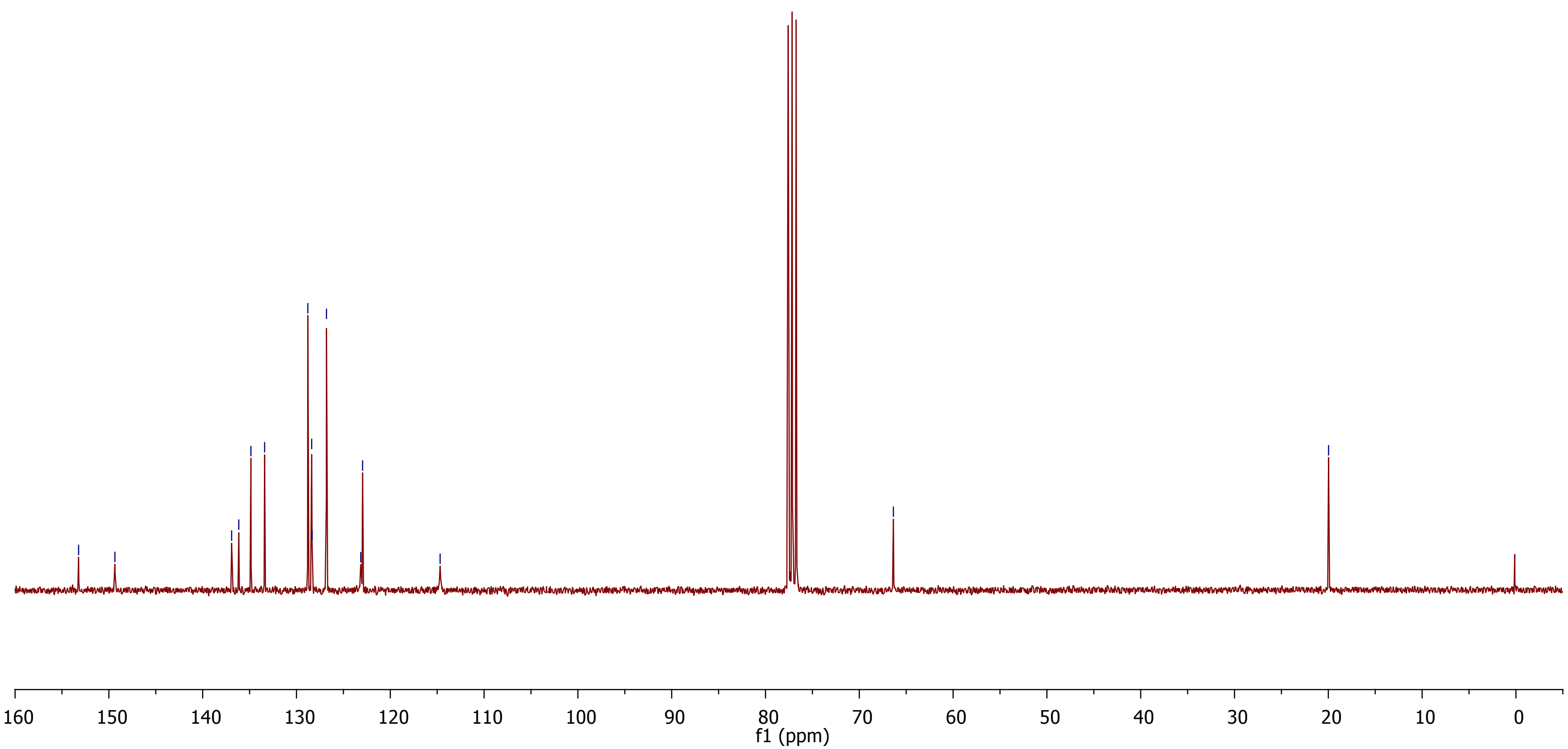
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **1p**



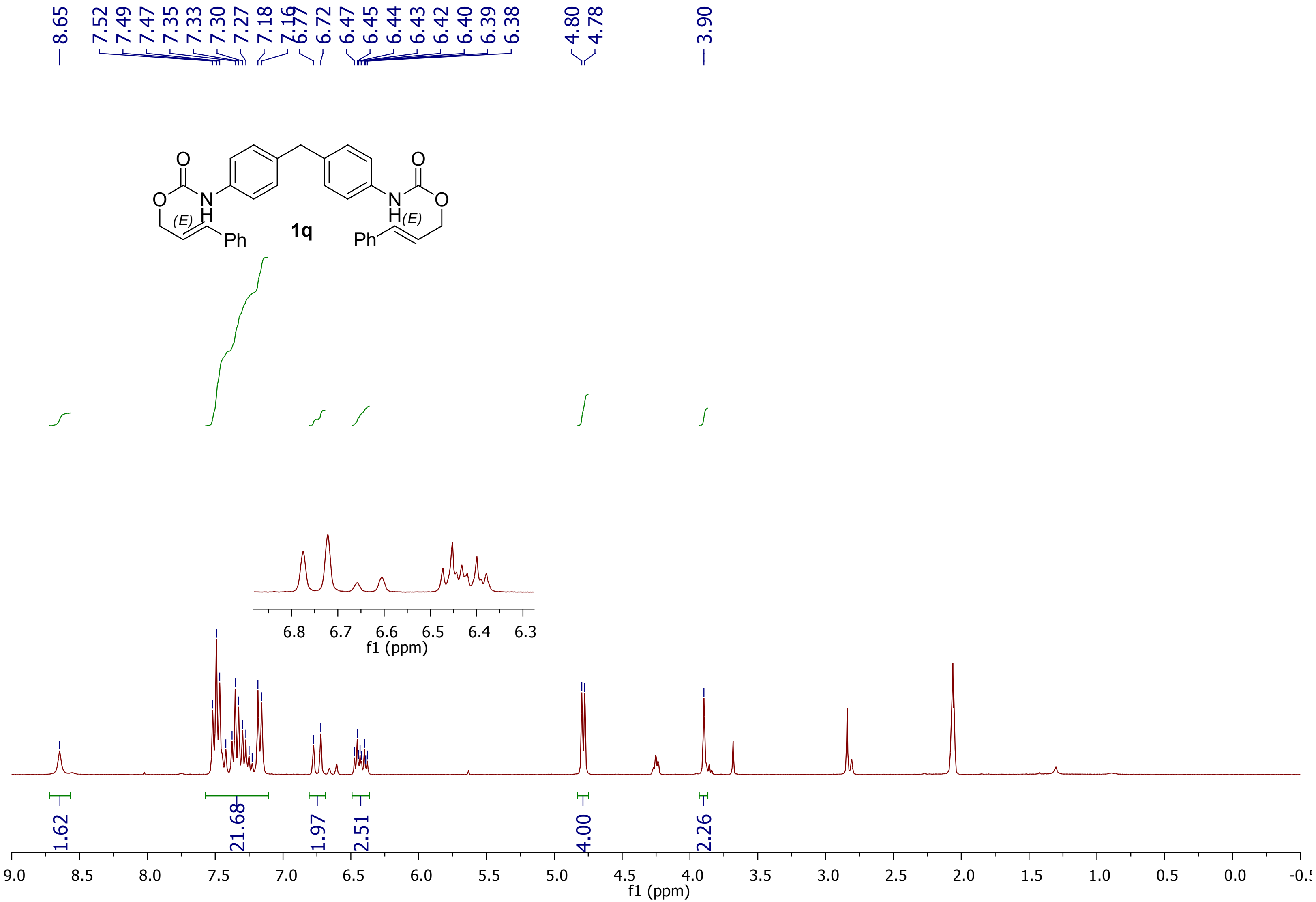
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1p**



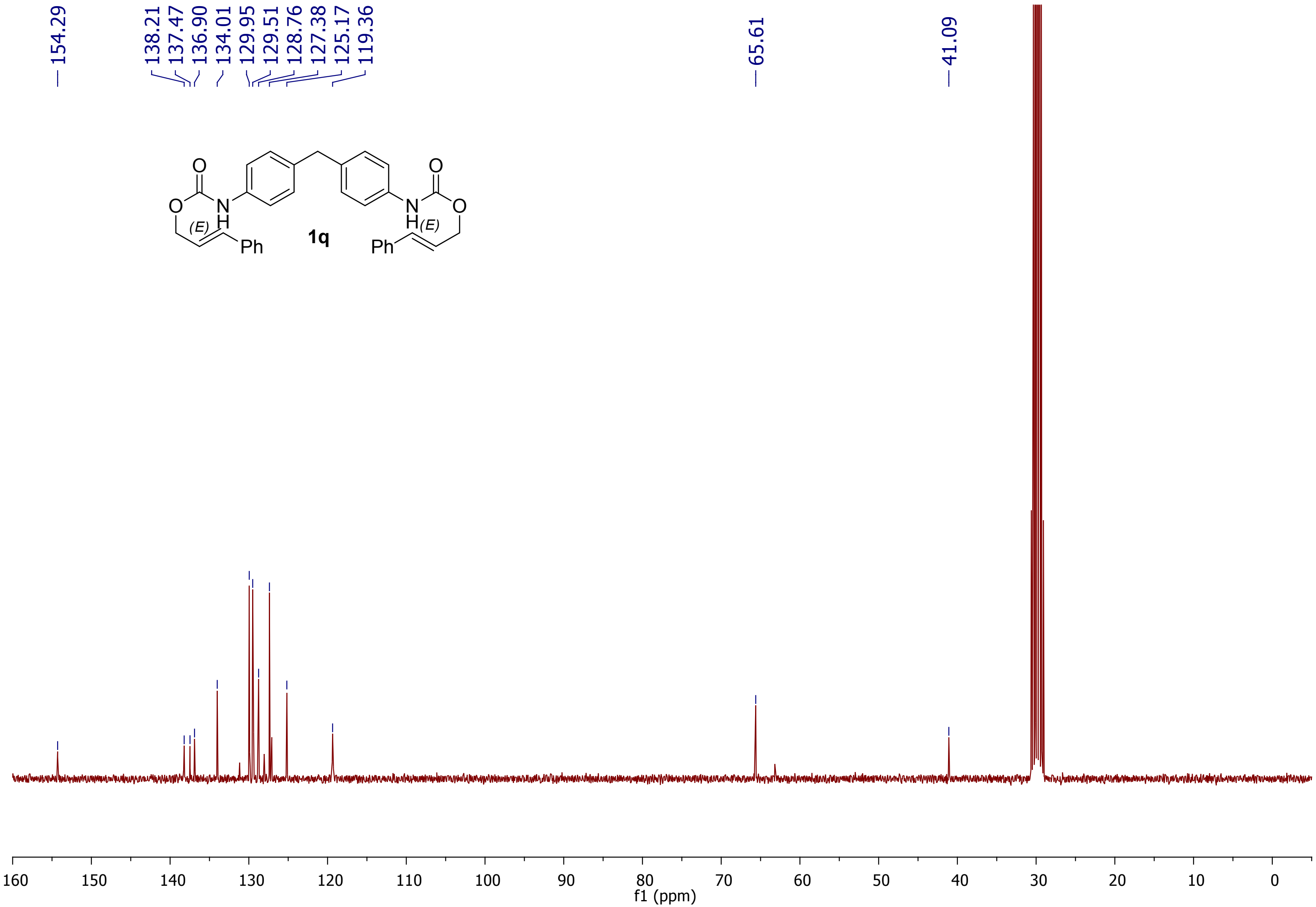
1p



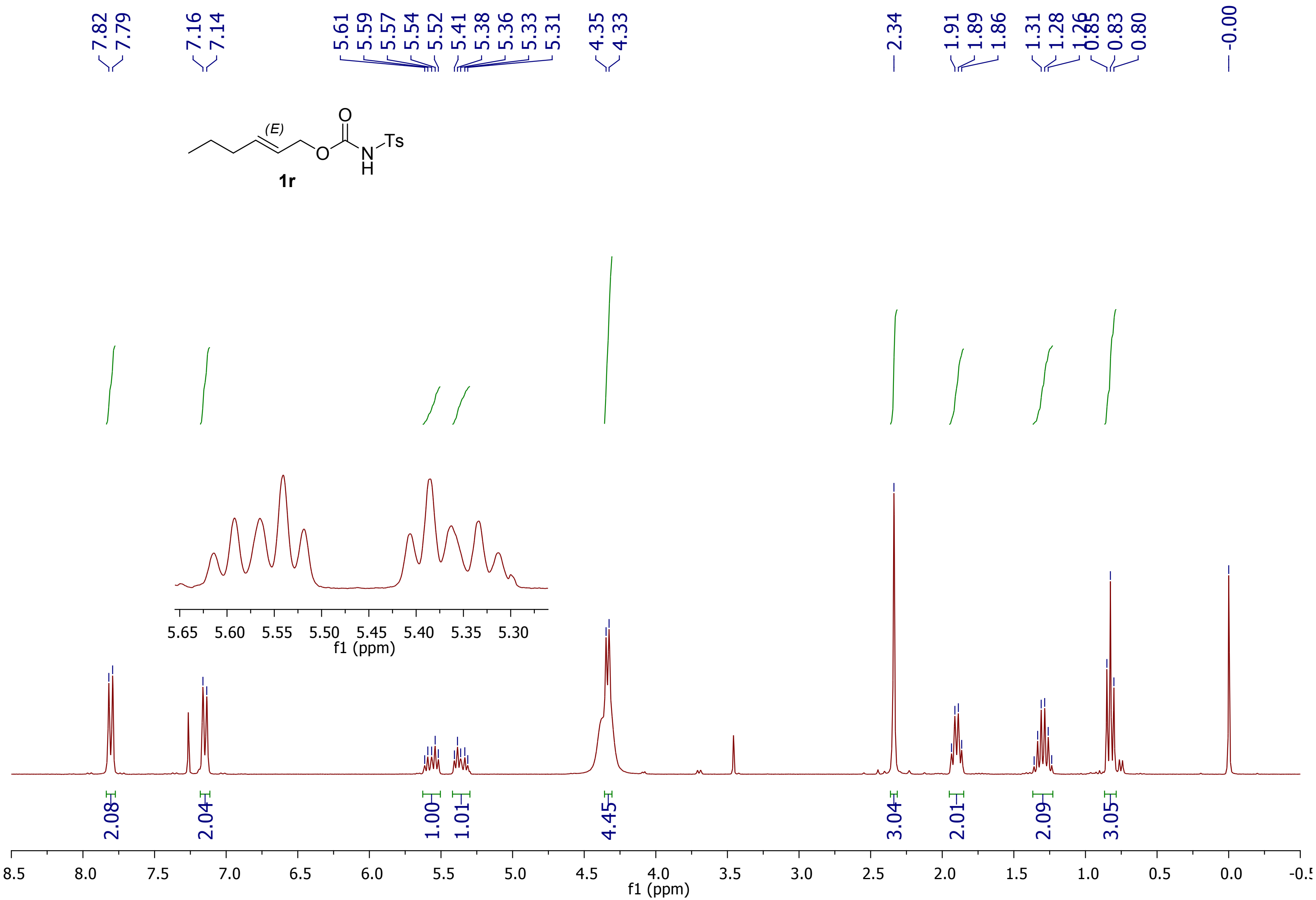
^{1}H NMR (300 MHz, Acetone-d_6) of substrate **1q**



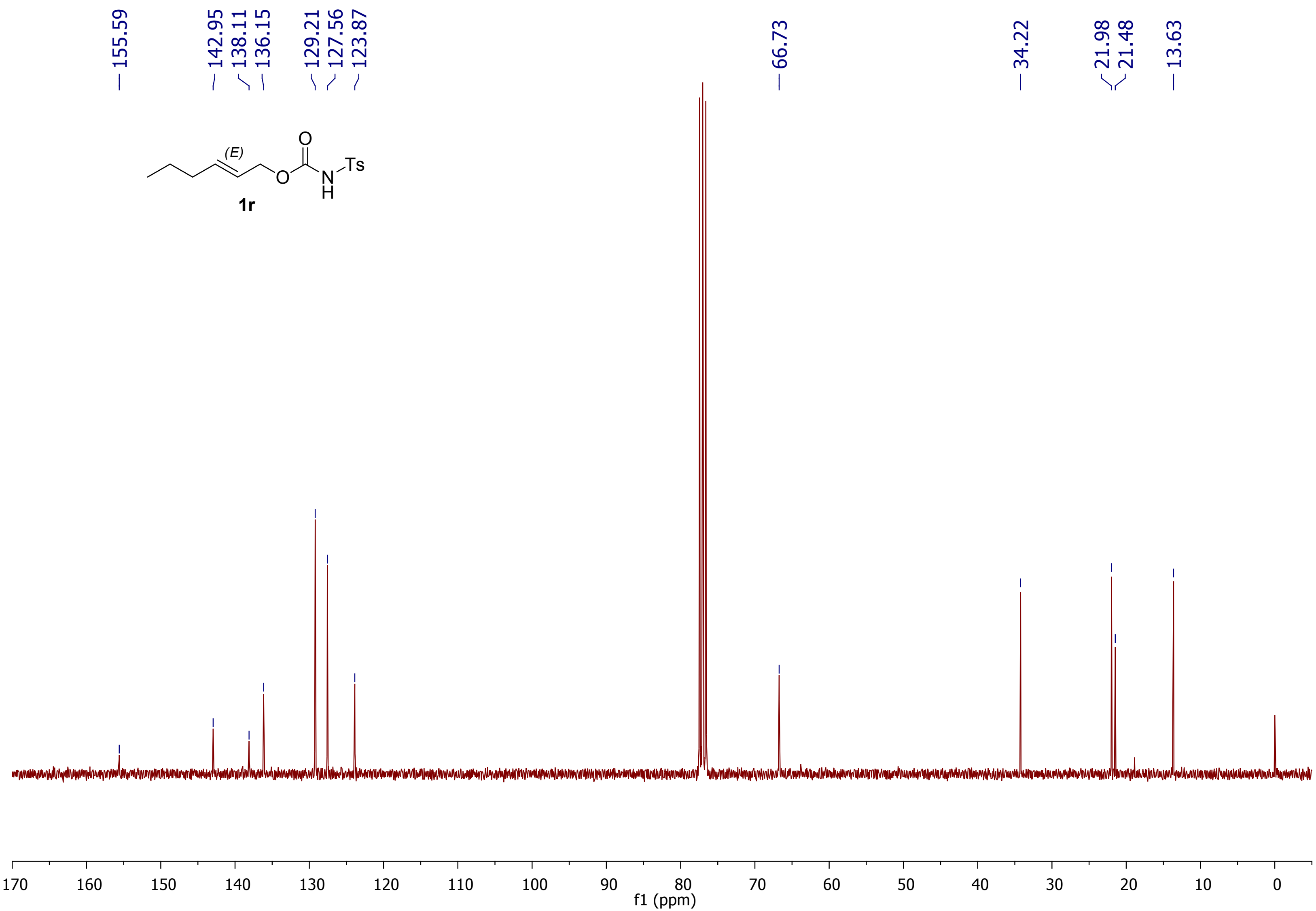
^{13}C NMR (75 MHz, Acetone-d_6) of substrate **1q**



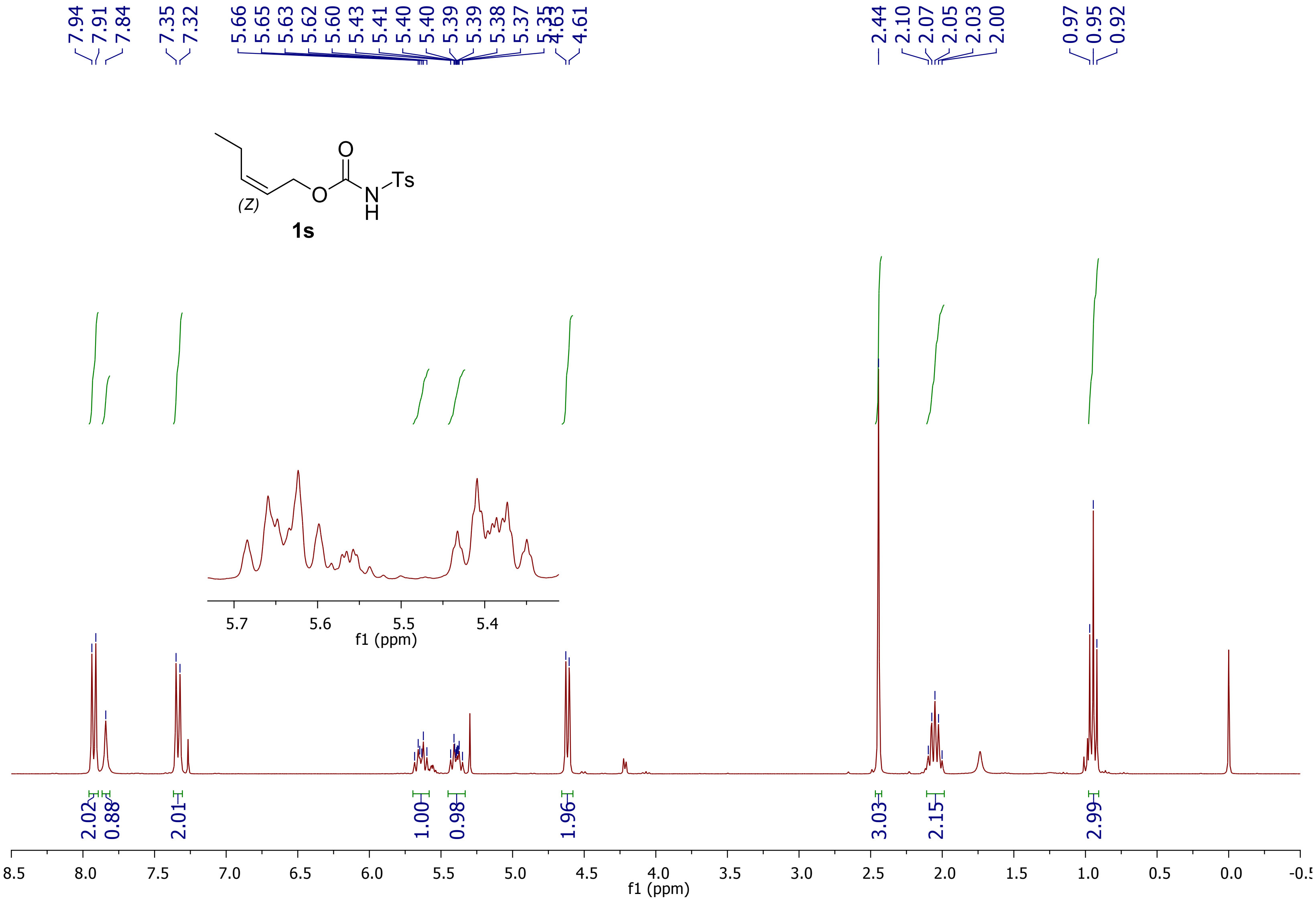
^1H NMR (300 MHz, $CDCl_3$) of substrate **1r**



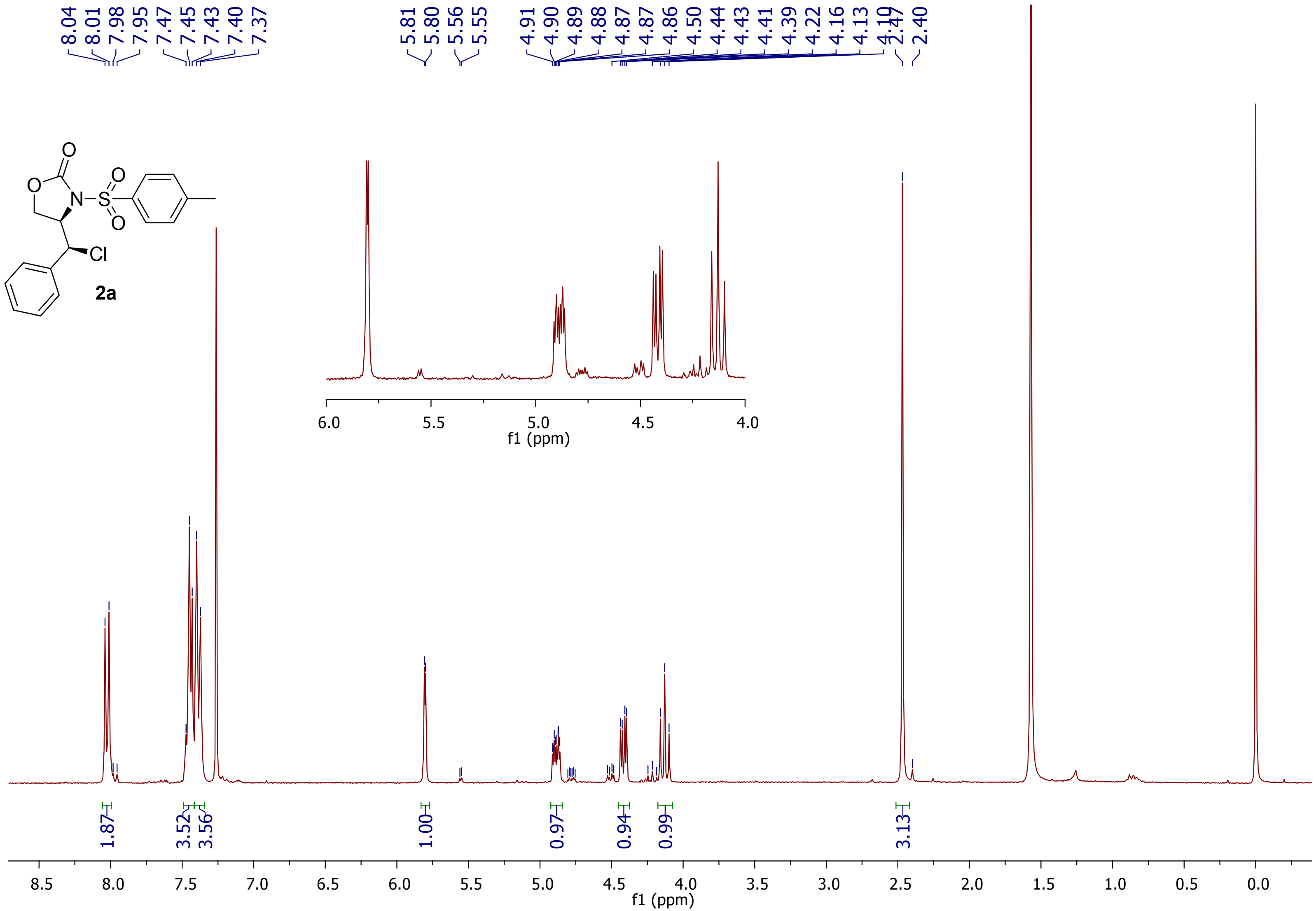
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **1r**



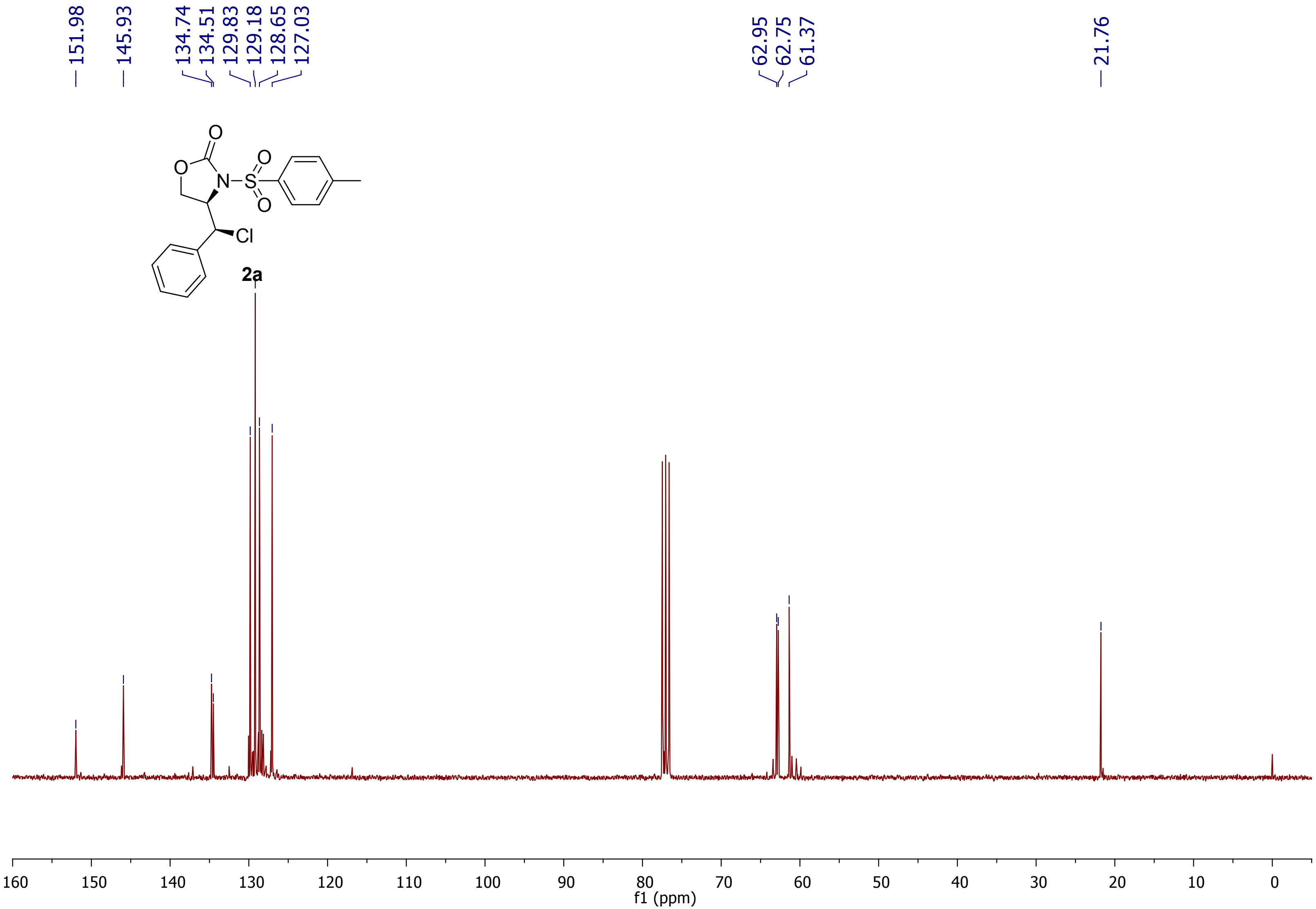
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **1s**



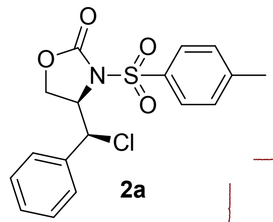
^1H NMR (300 MHz, $CDCl_3$) of substrate **2a**



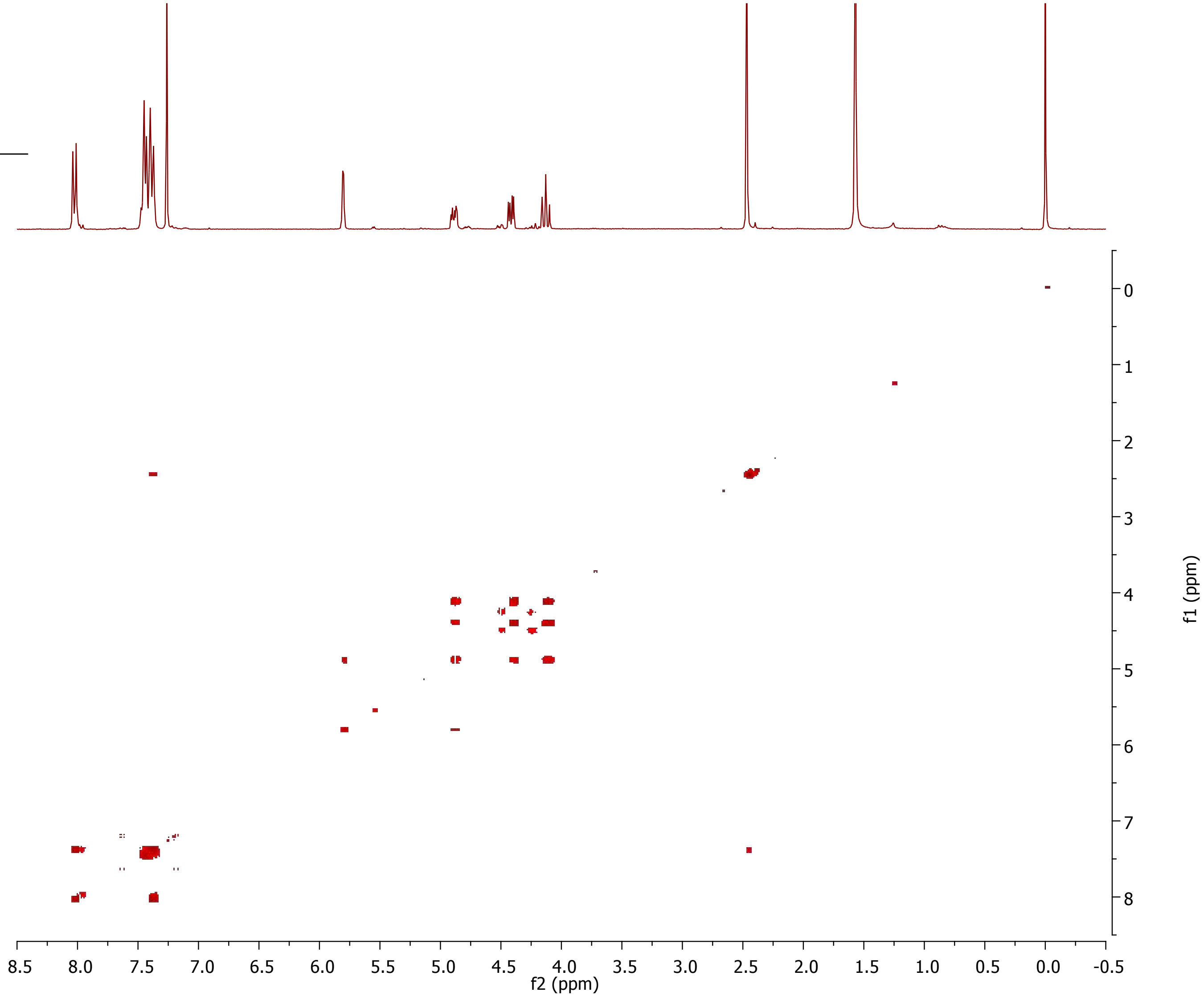
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2a**



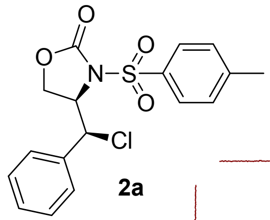
COSY of substrate **2a**



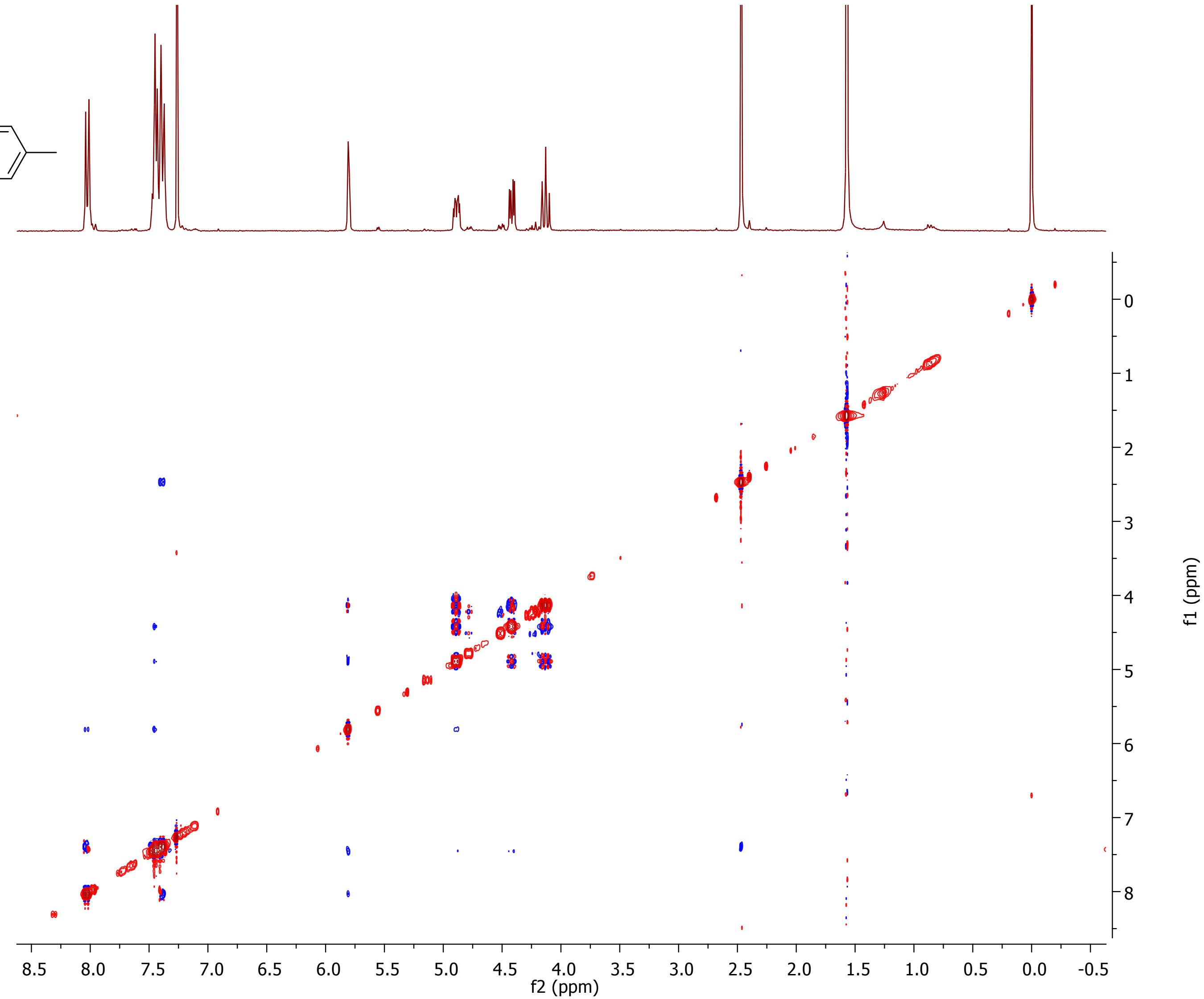
2a



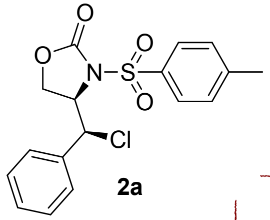
NOESY of substrate **2a**



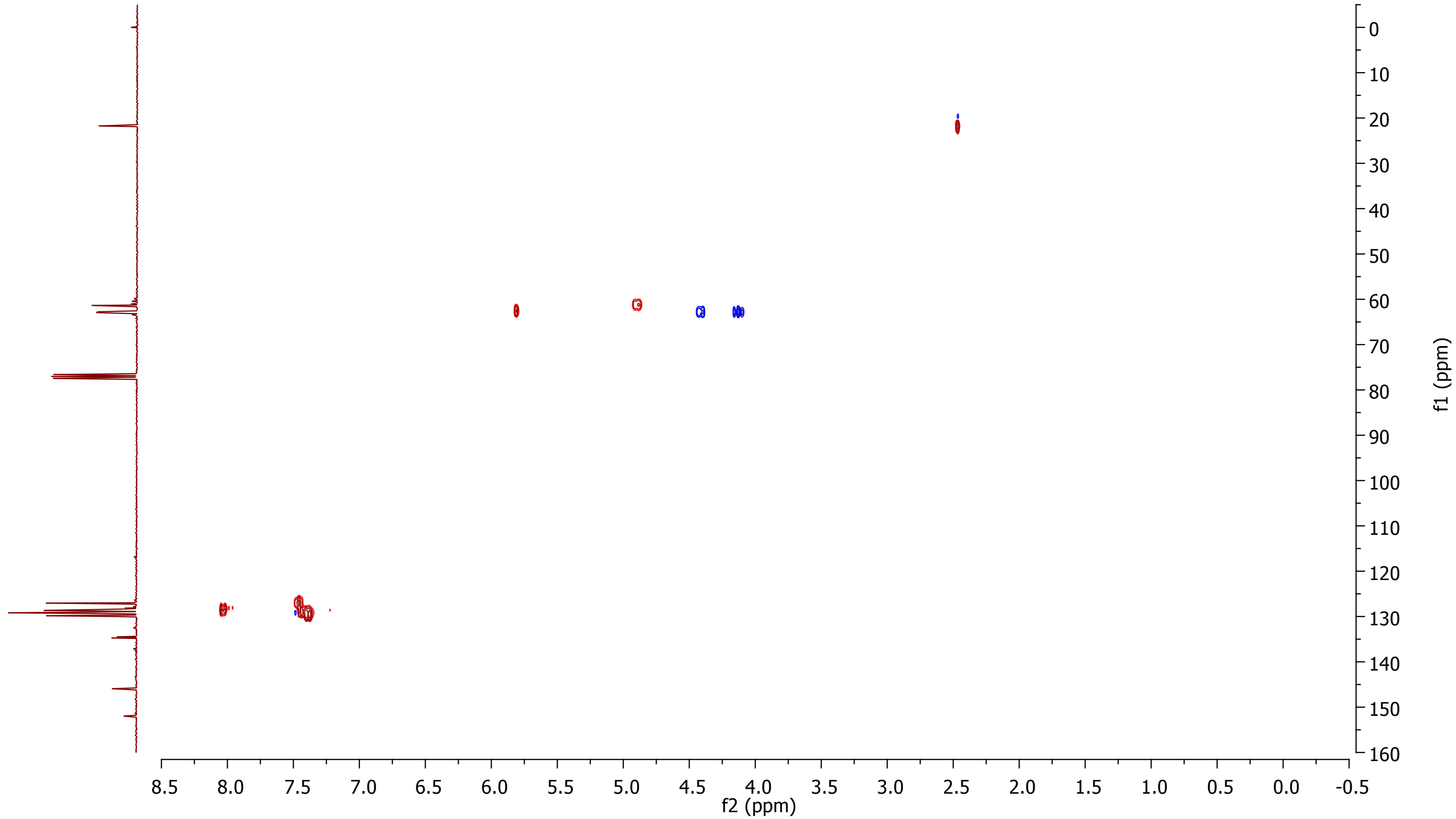
2a



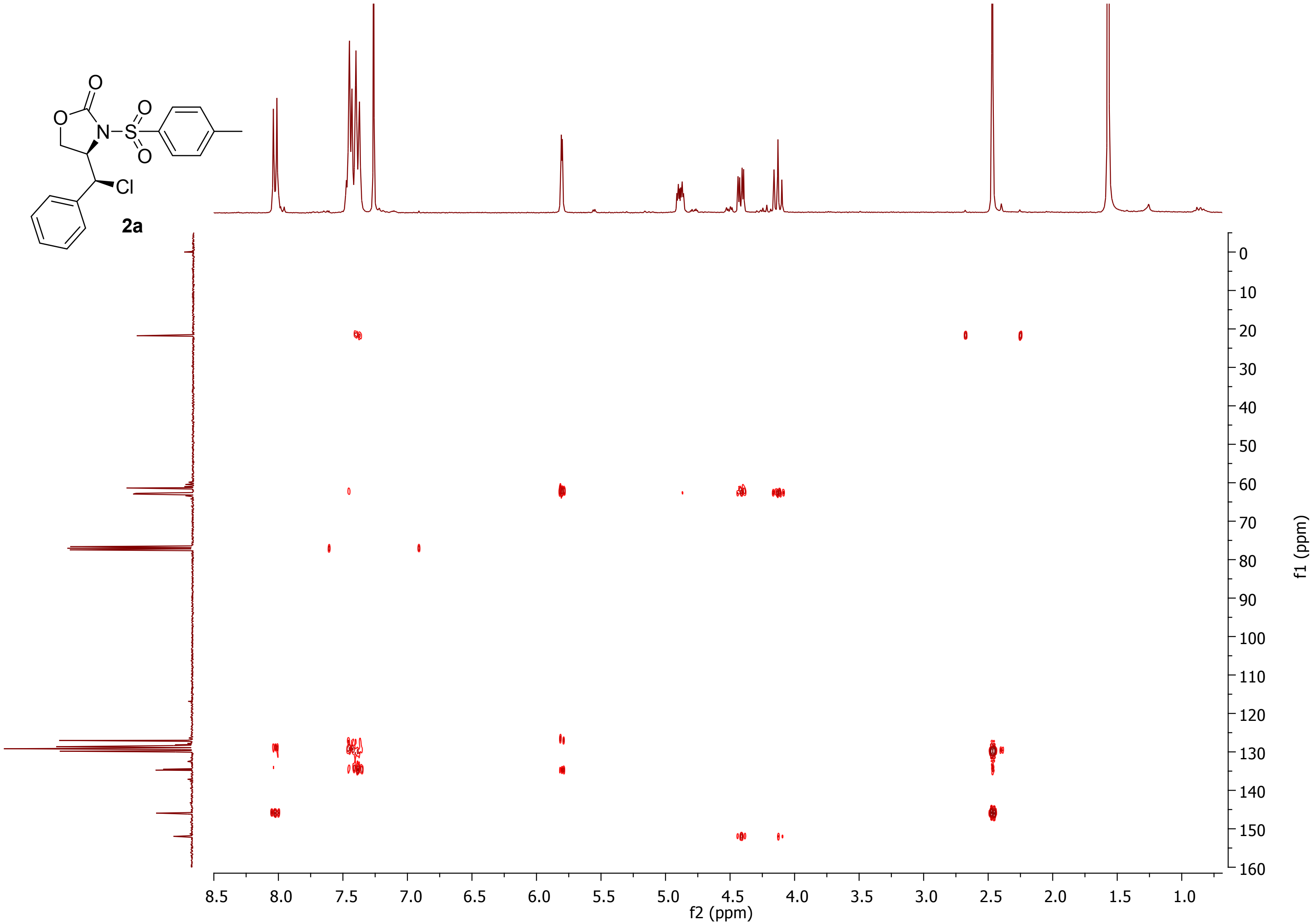
HSQC of substrate **2a**



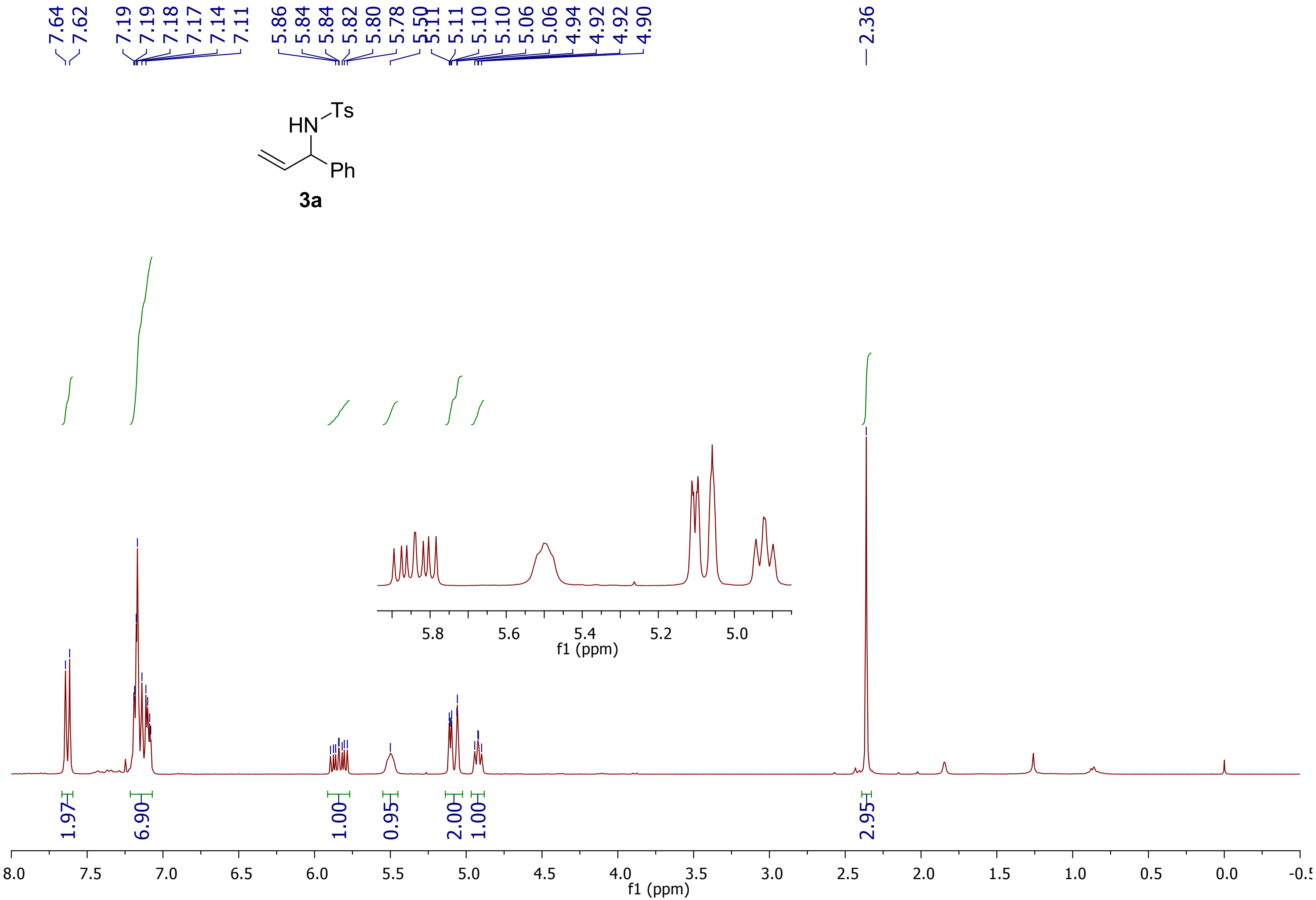
2a



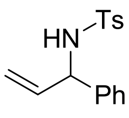
HMBC of substrate **2a**



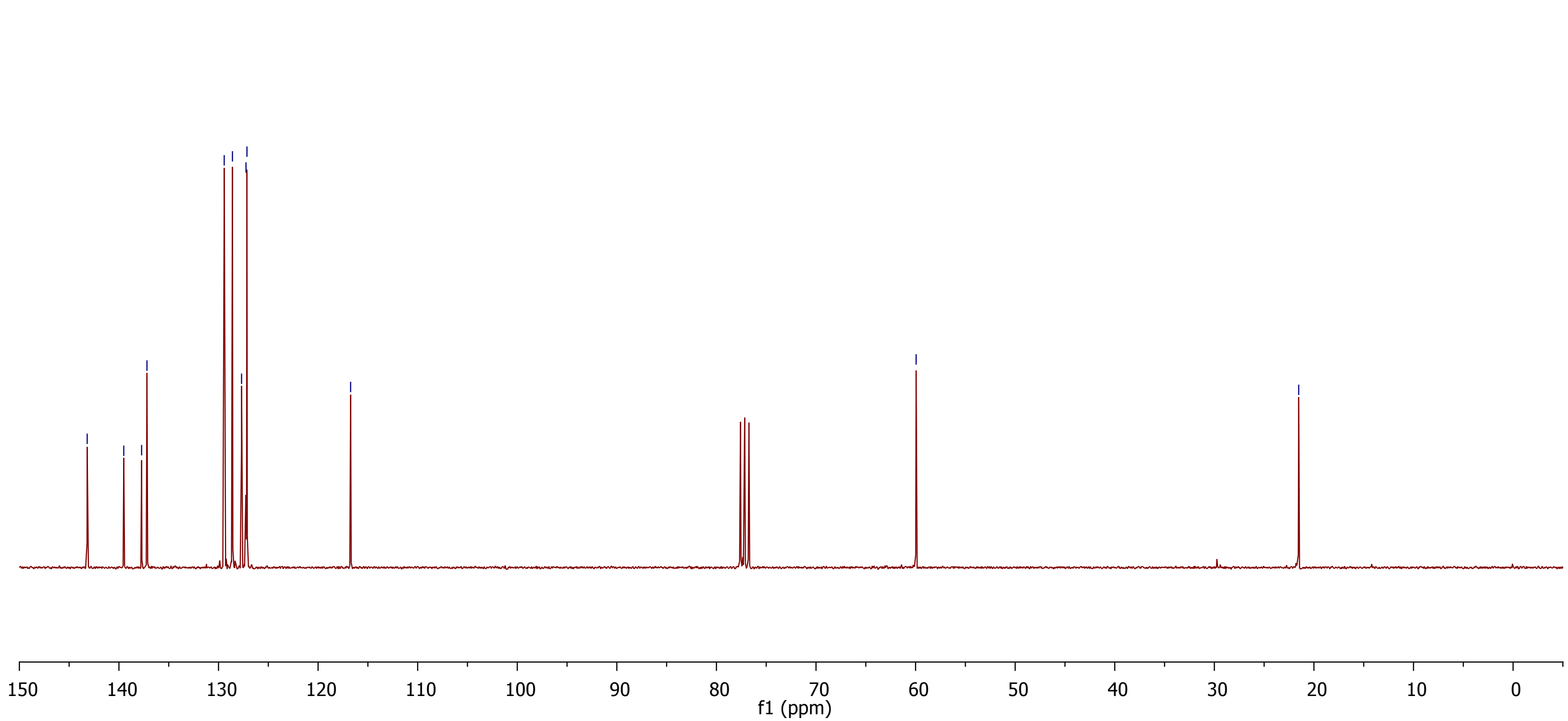
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **3a**



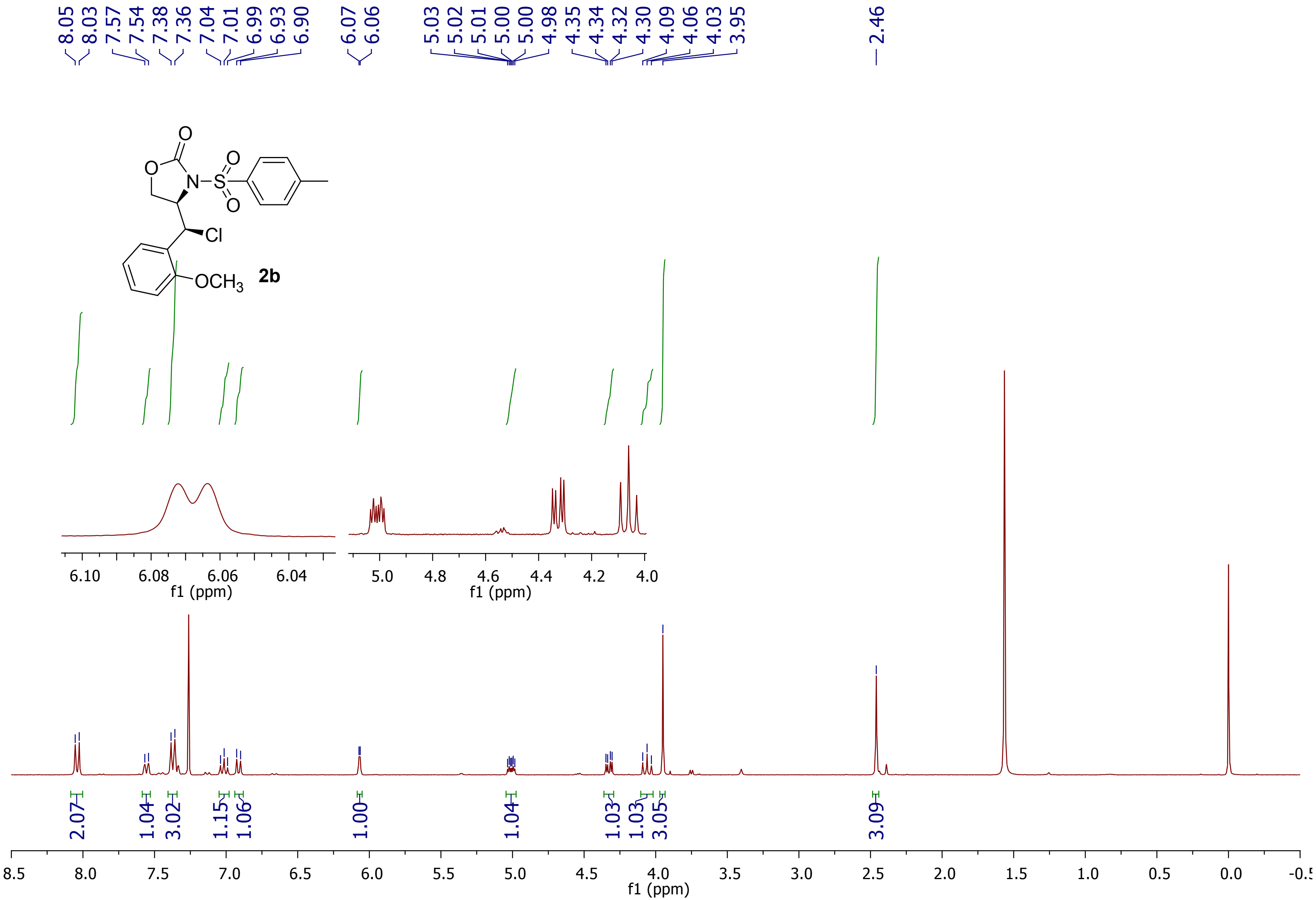
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **3a**



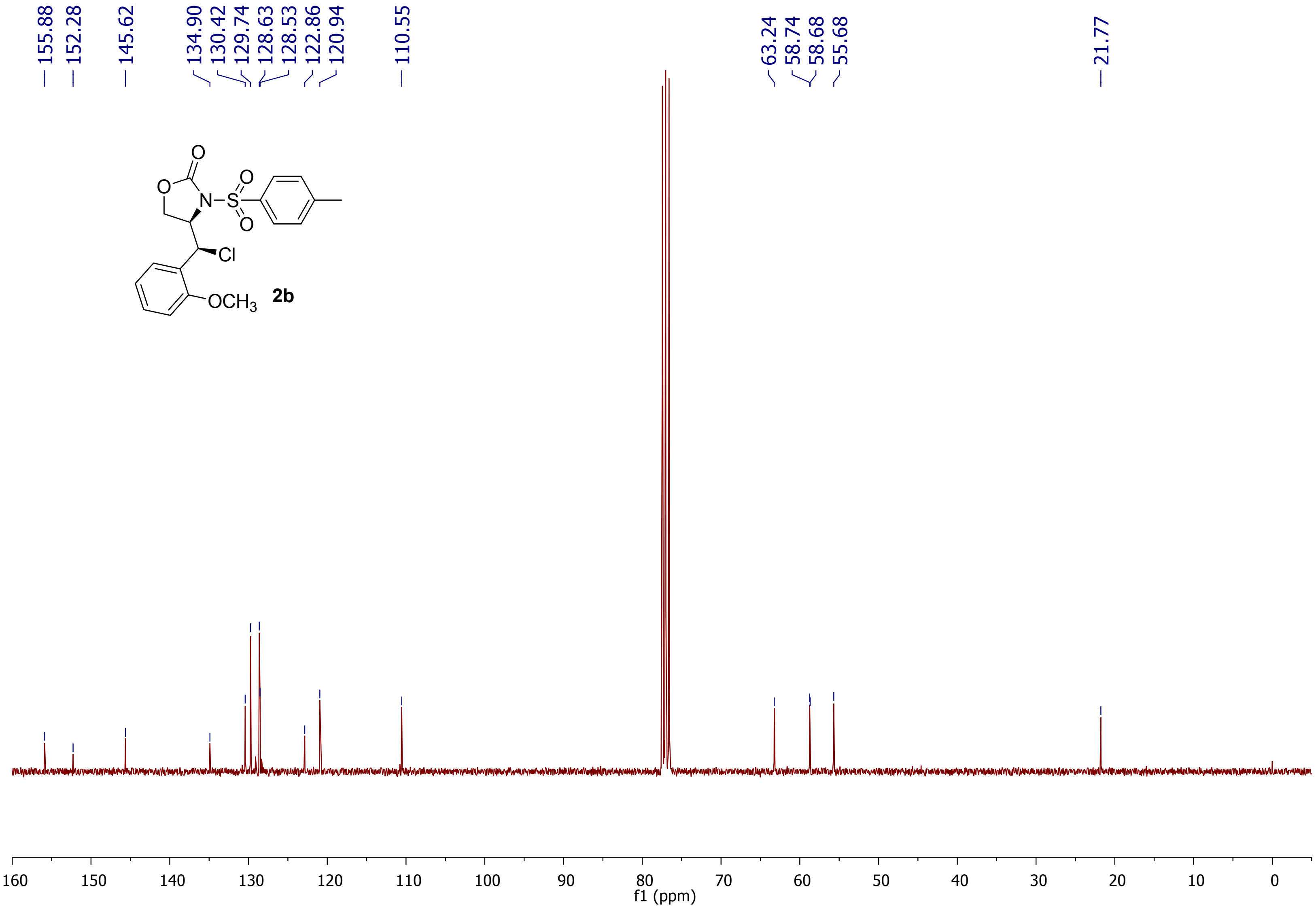
3a



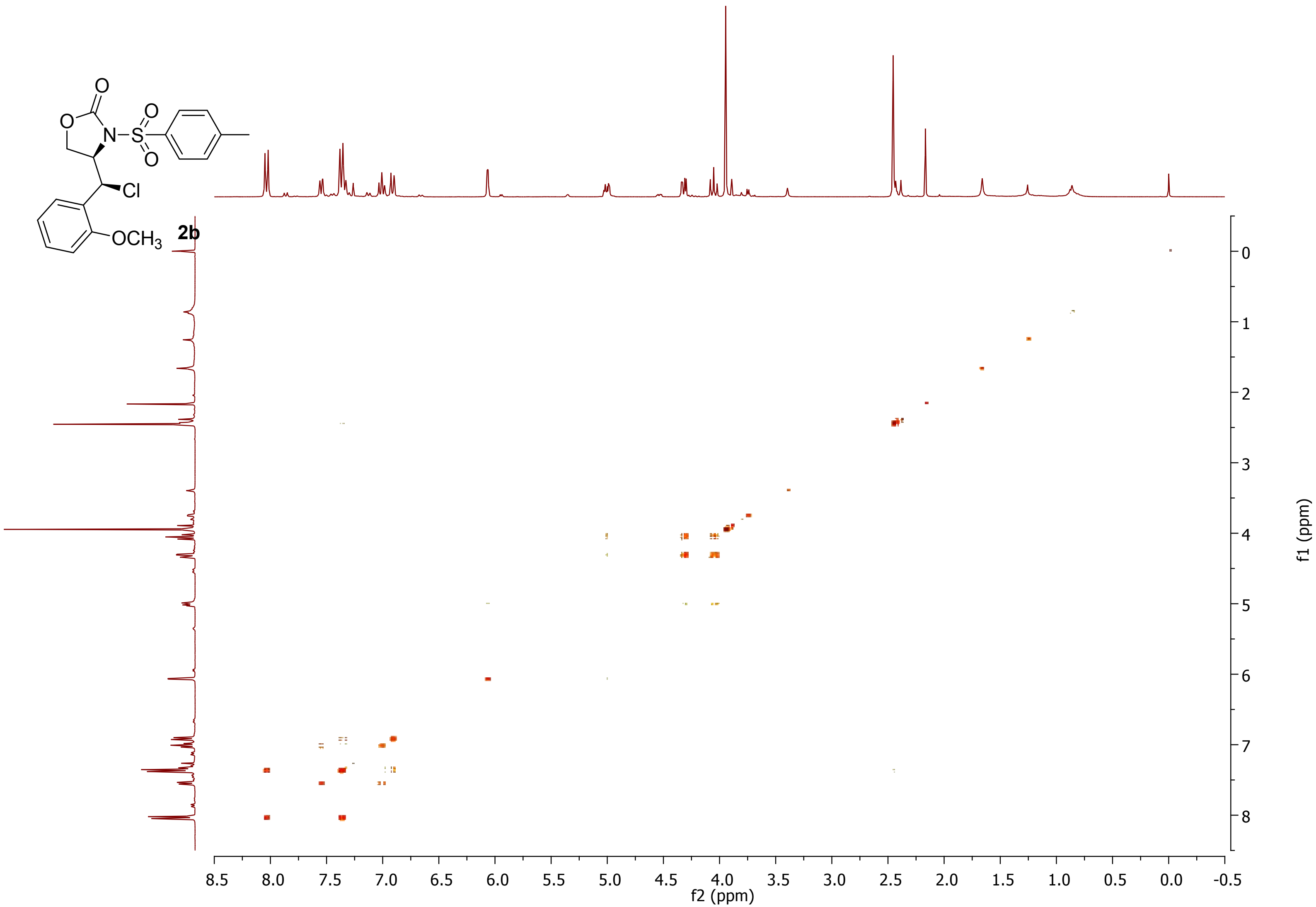
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2b**



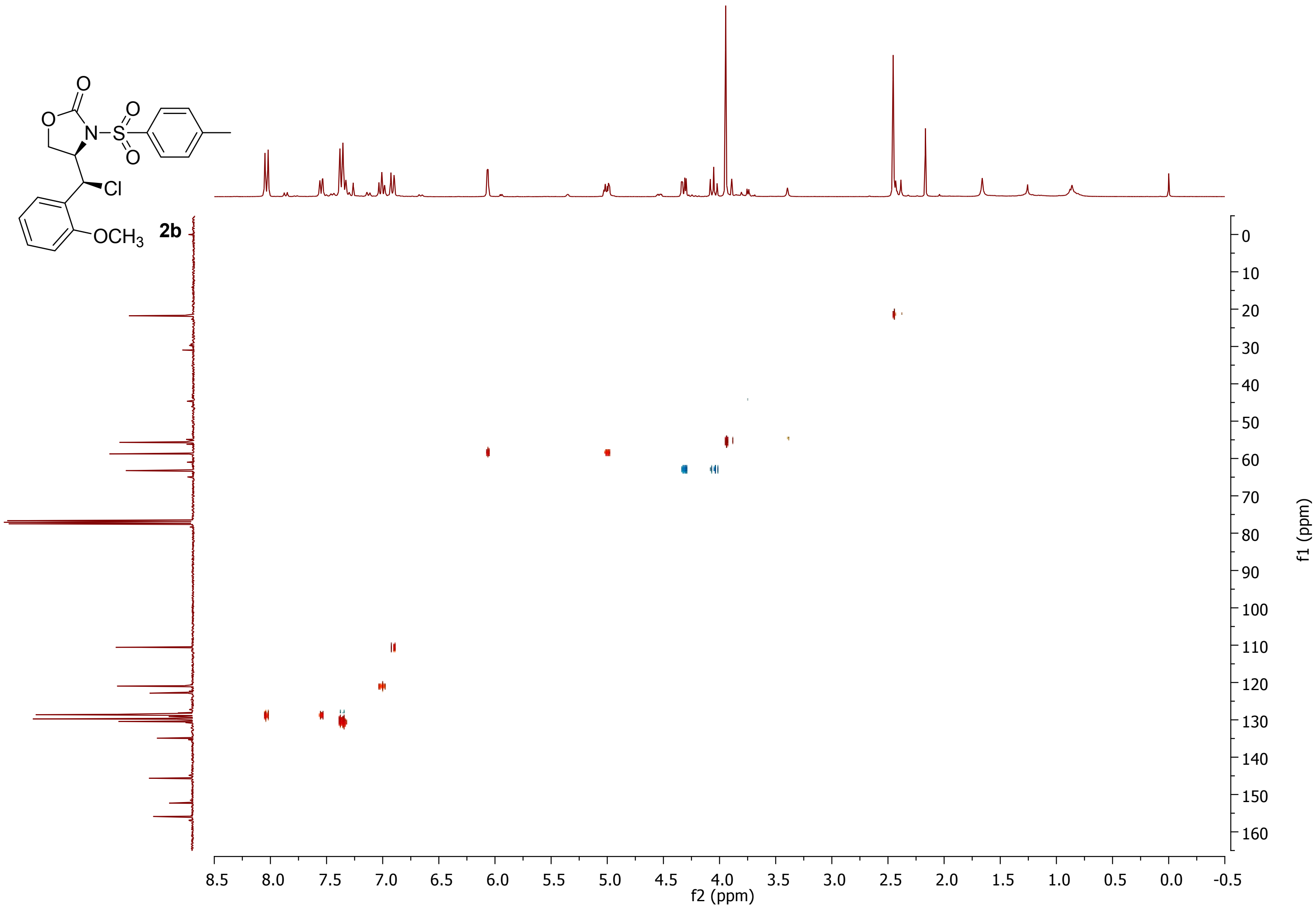
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2b**



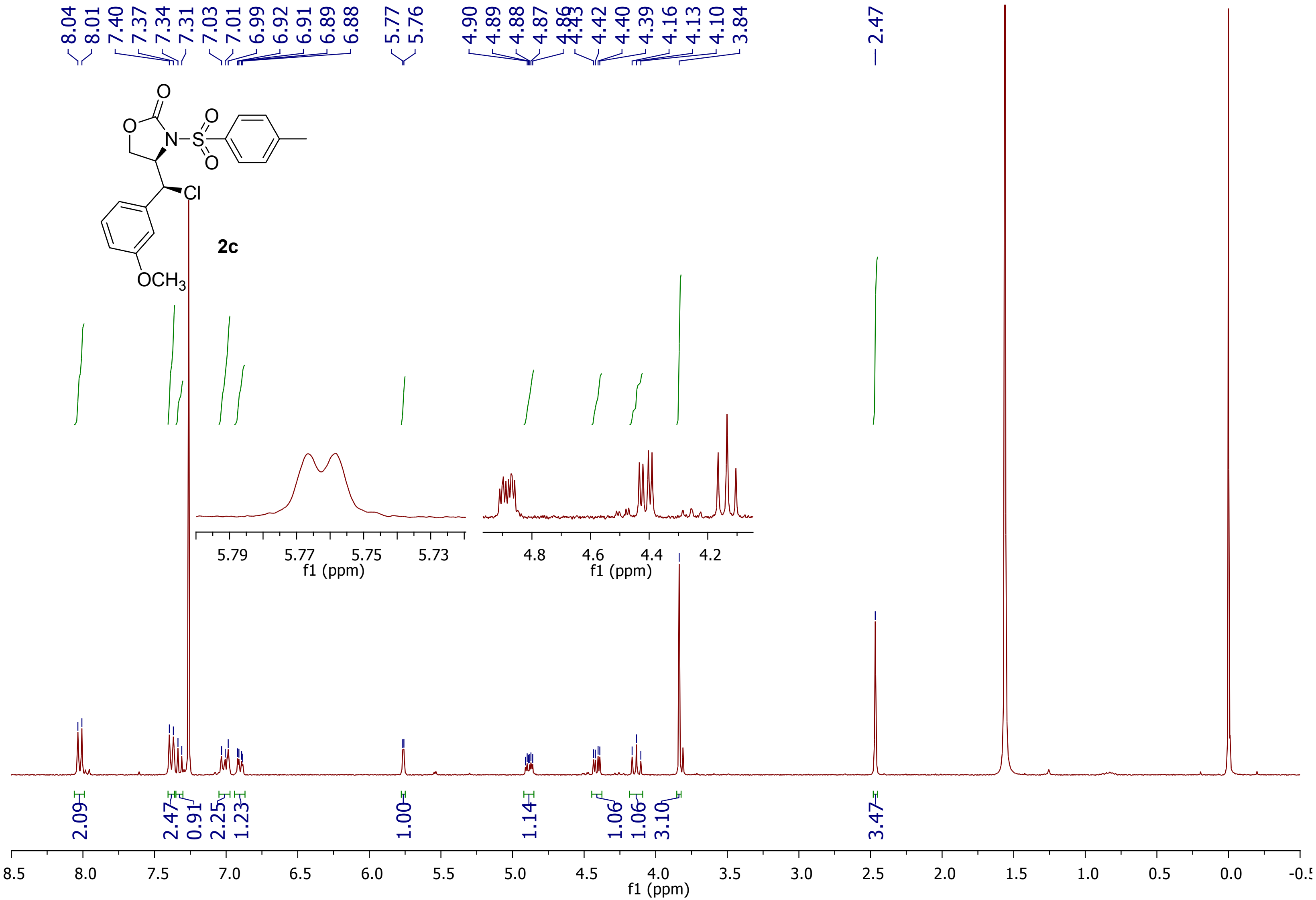
COSY of substrate **2b**



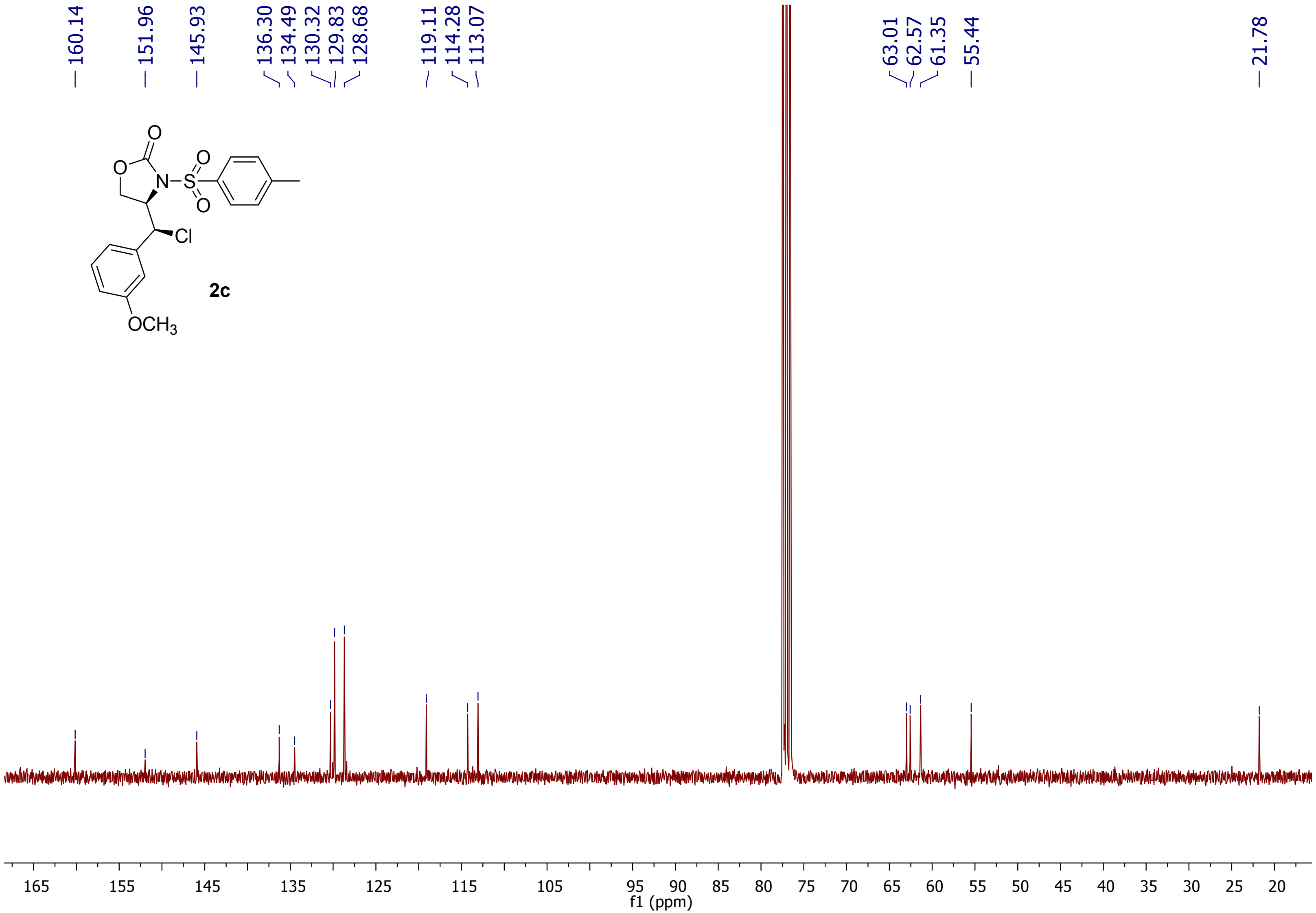
HSQC of substrate **2b**



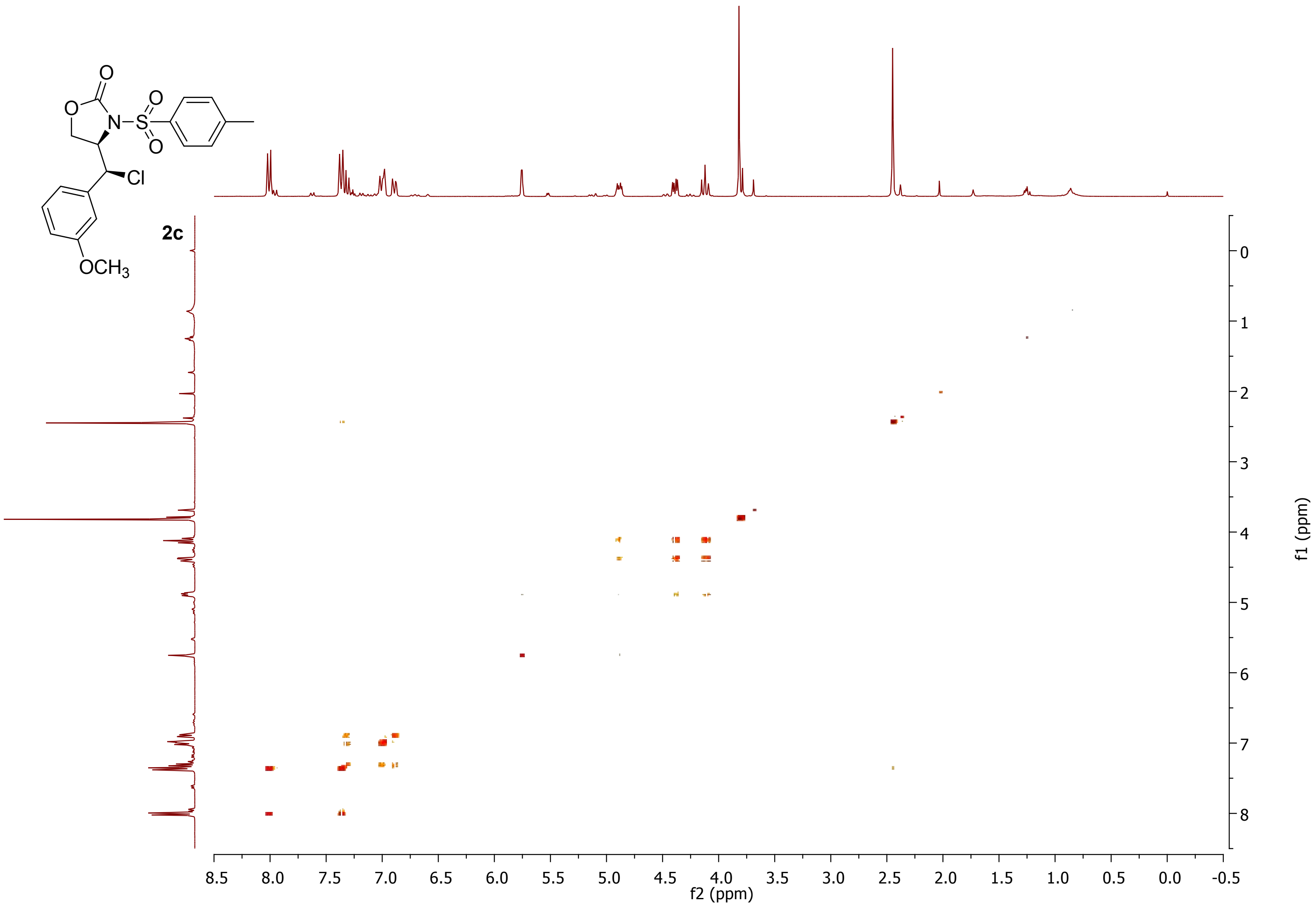
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2c**



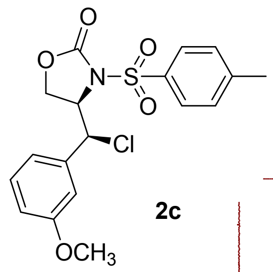
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2c**



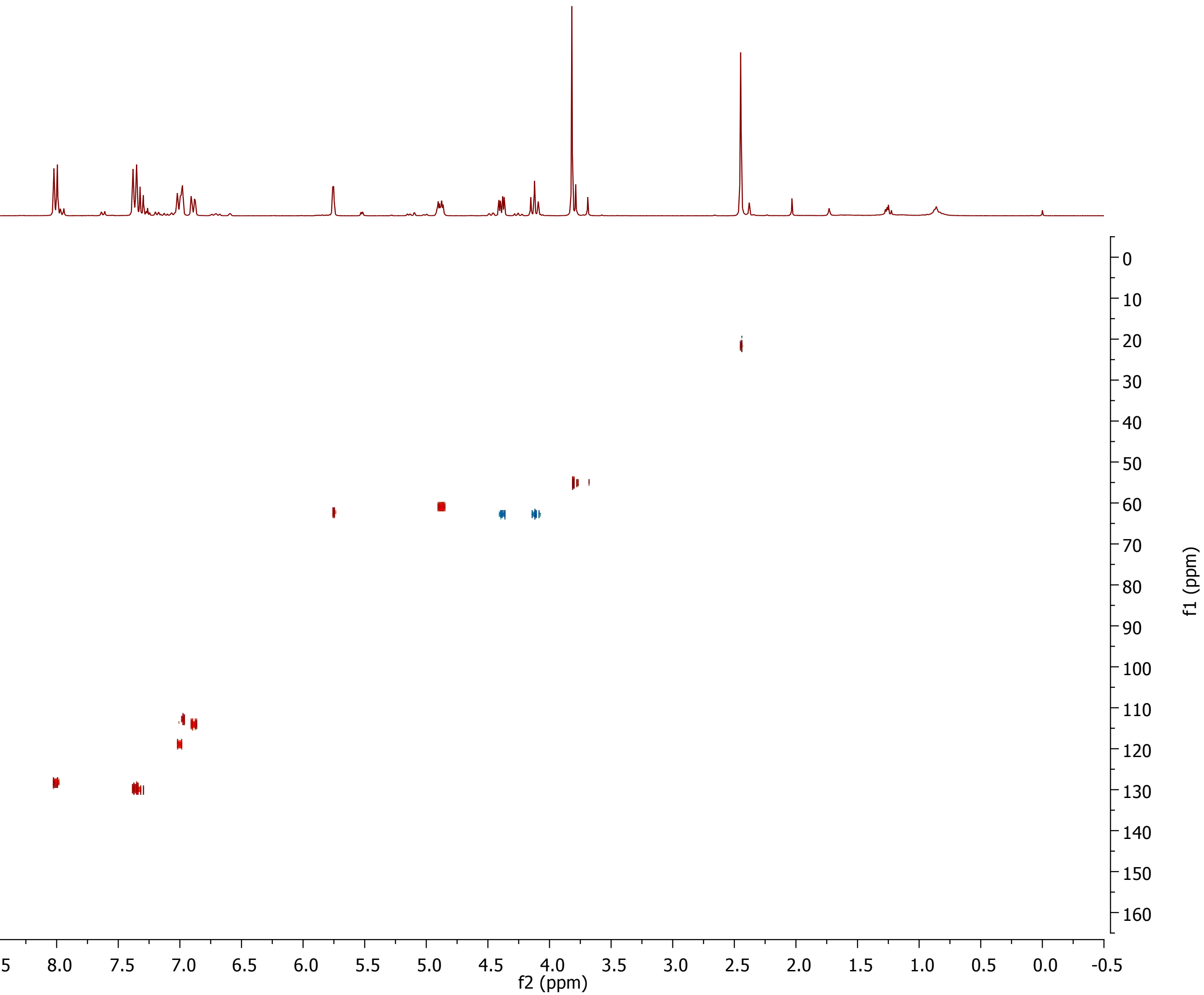
COSY of substrate **2c**



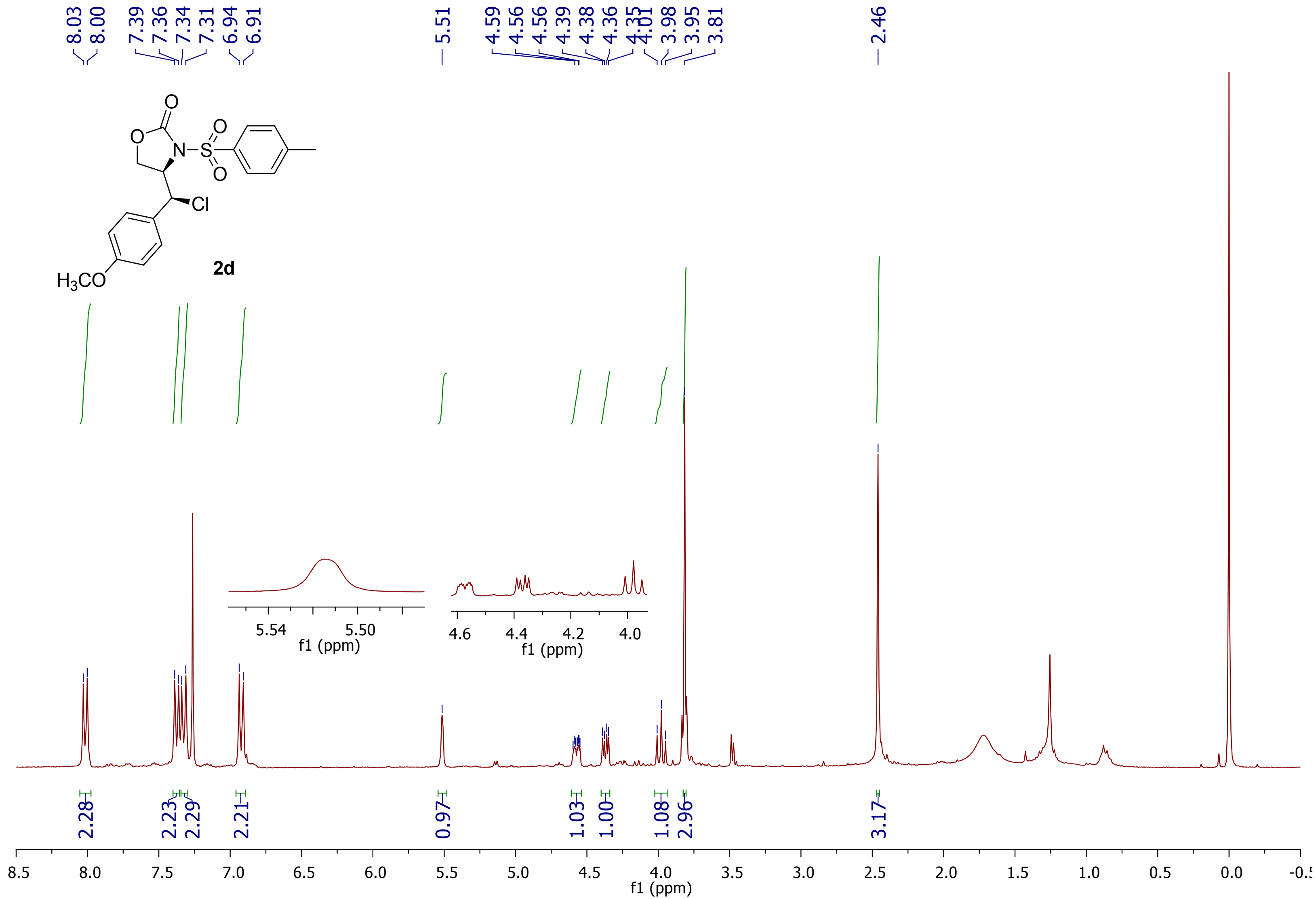
HSQC of substrate **2c**



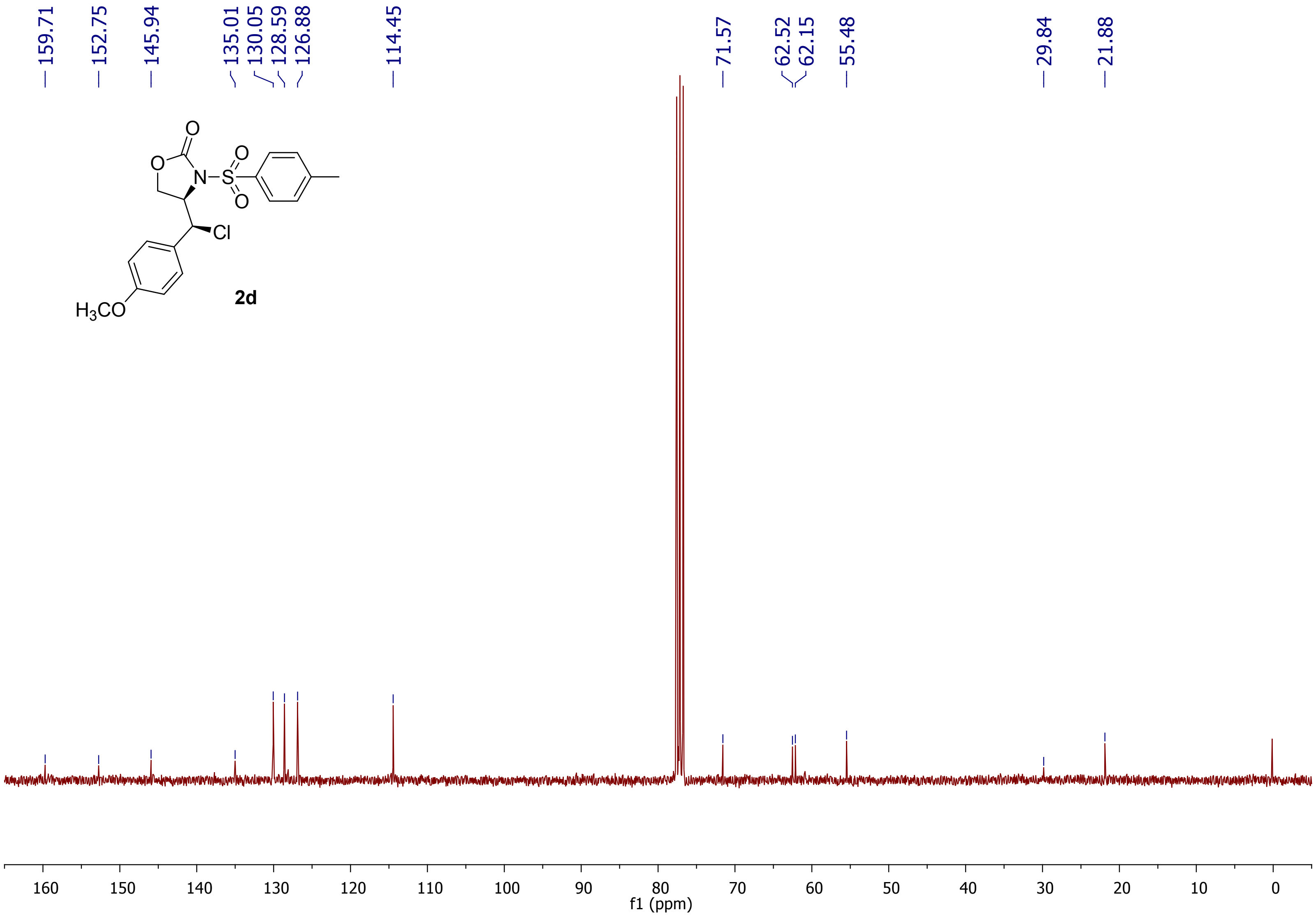
2c



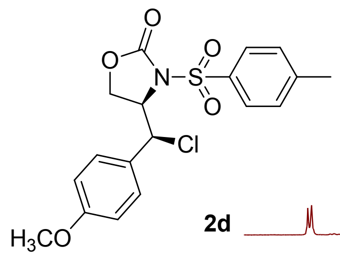
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2d**



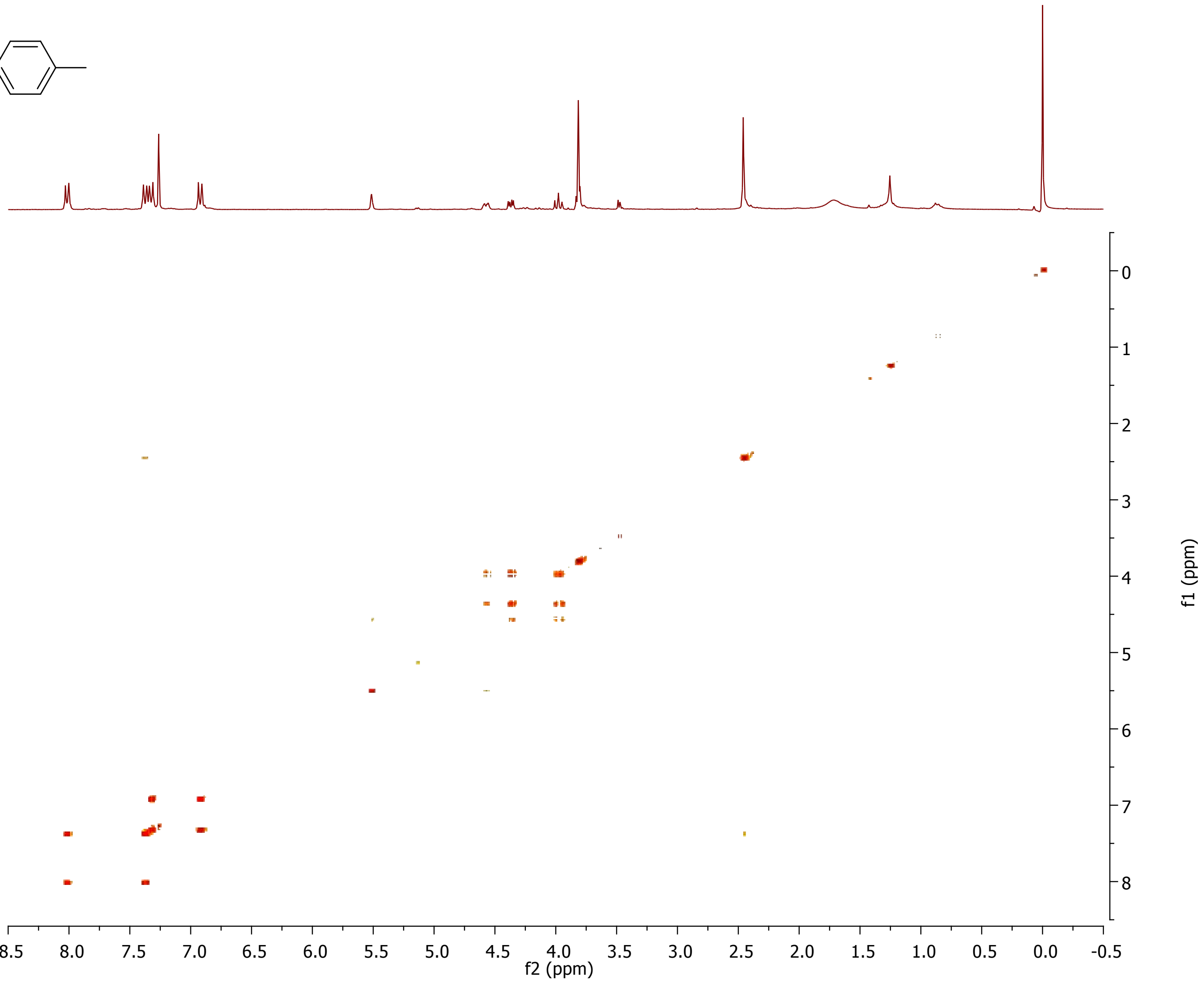
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2d**



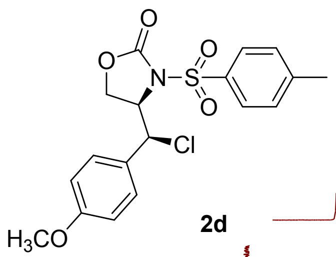
COSY of substrate **2d**



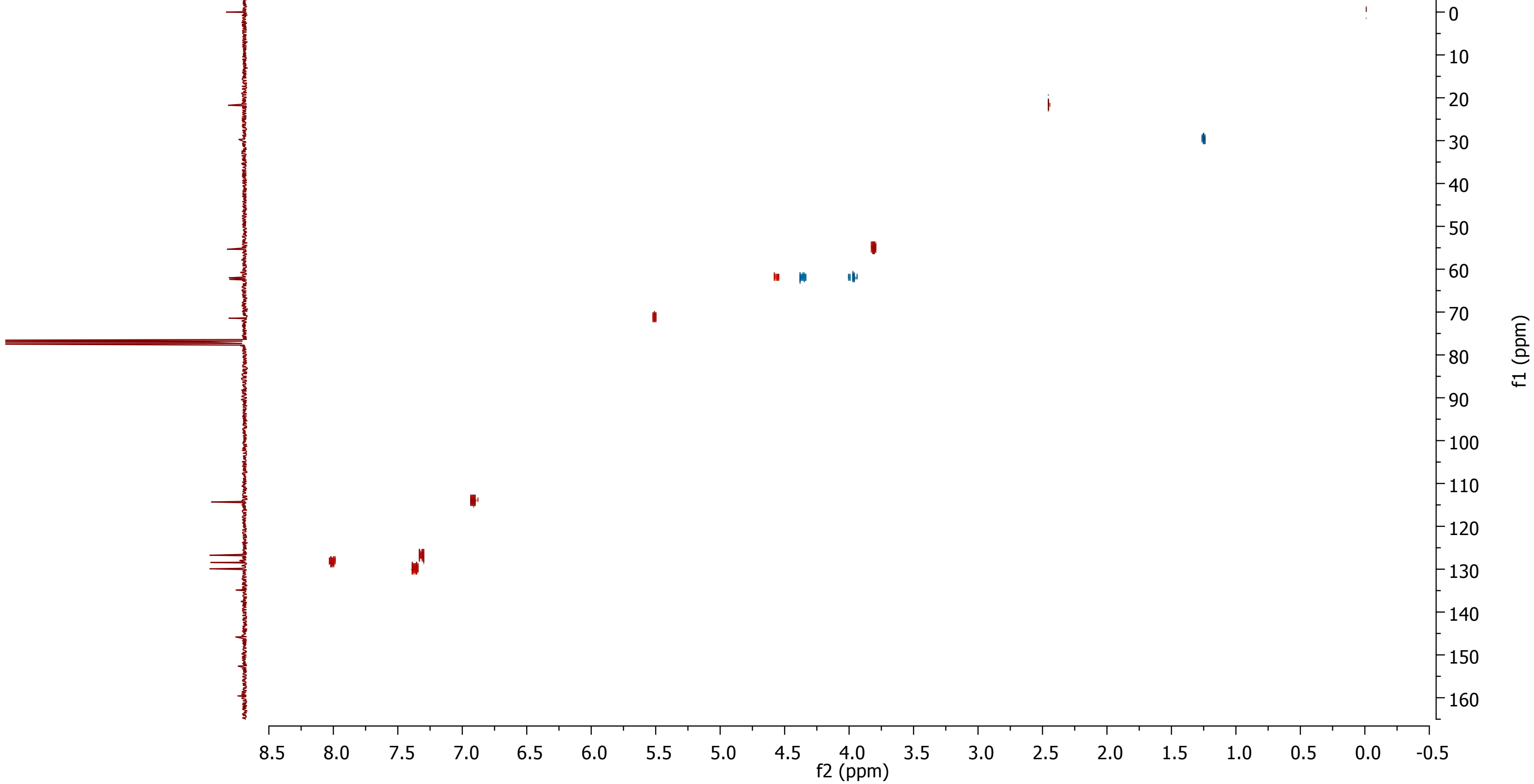
2d



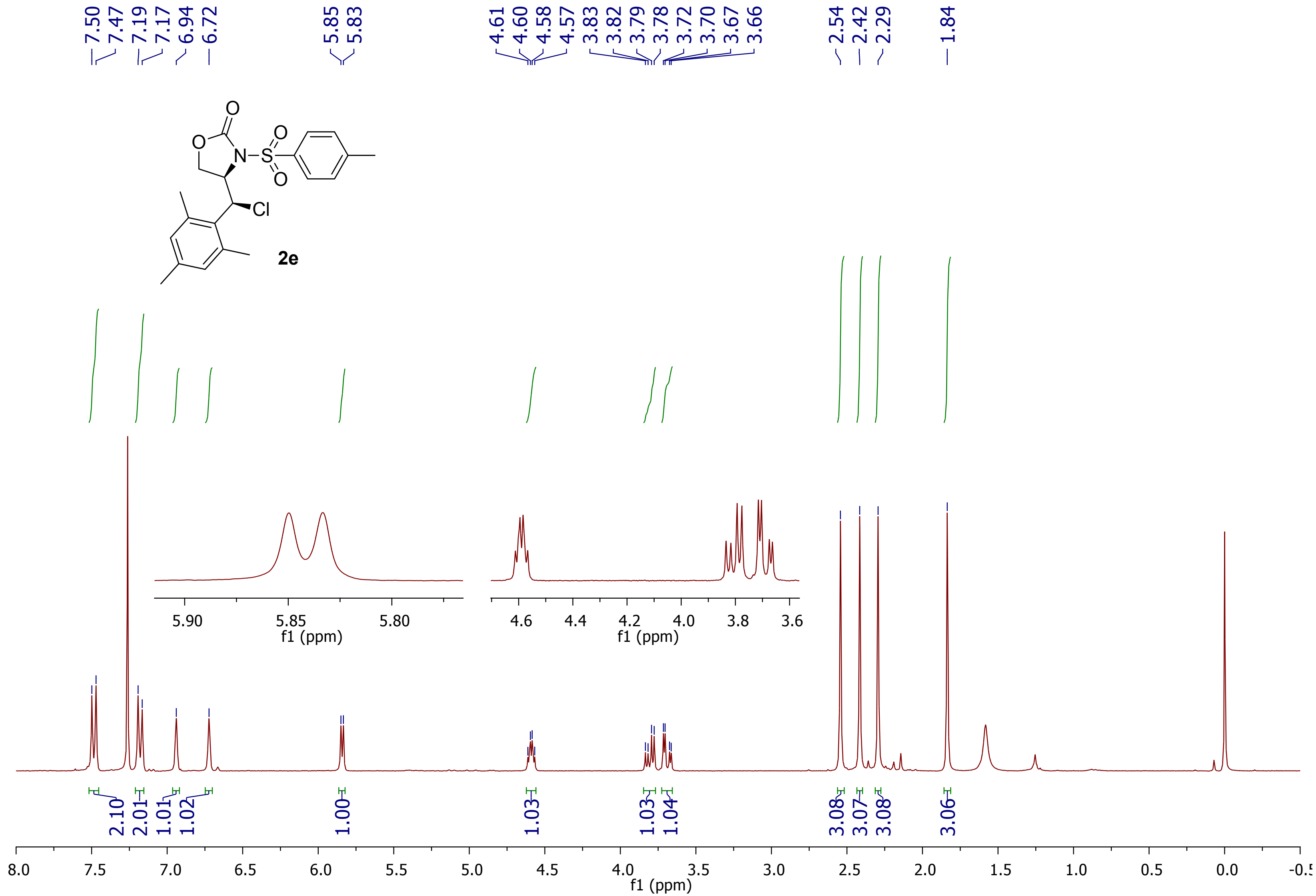
HSQC of substrate **2d**



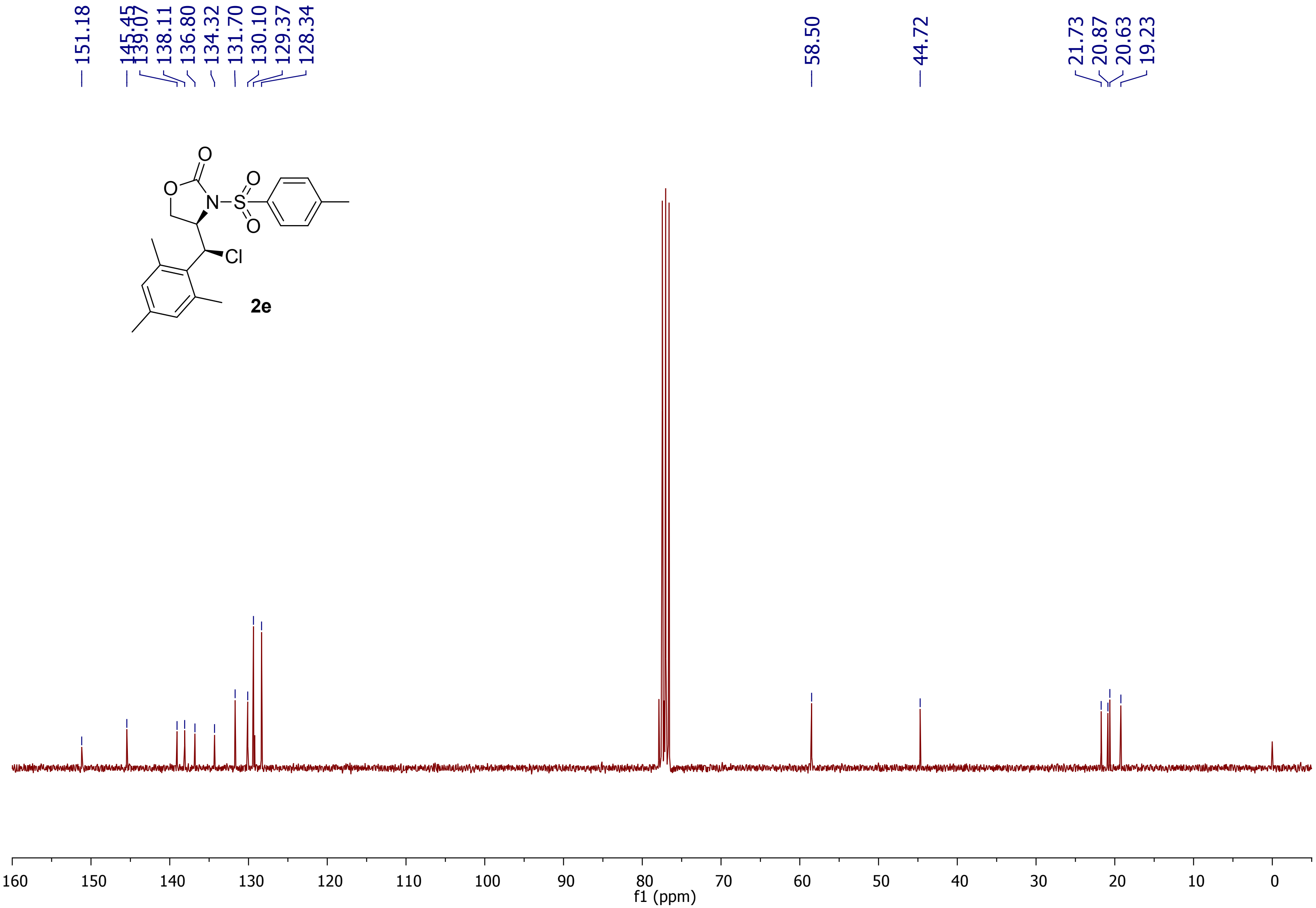
2d



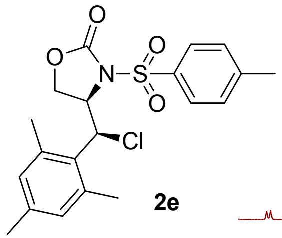
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2e**



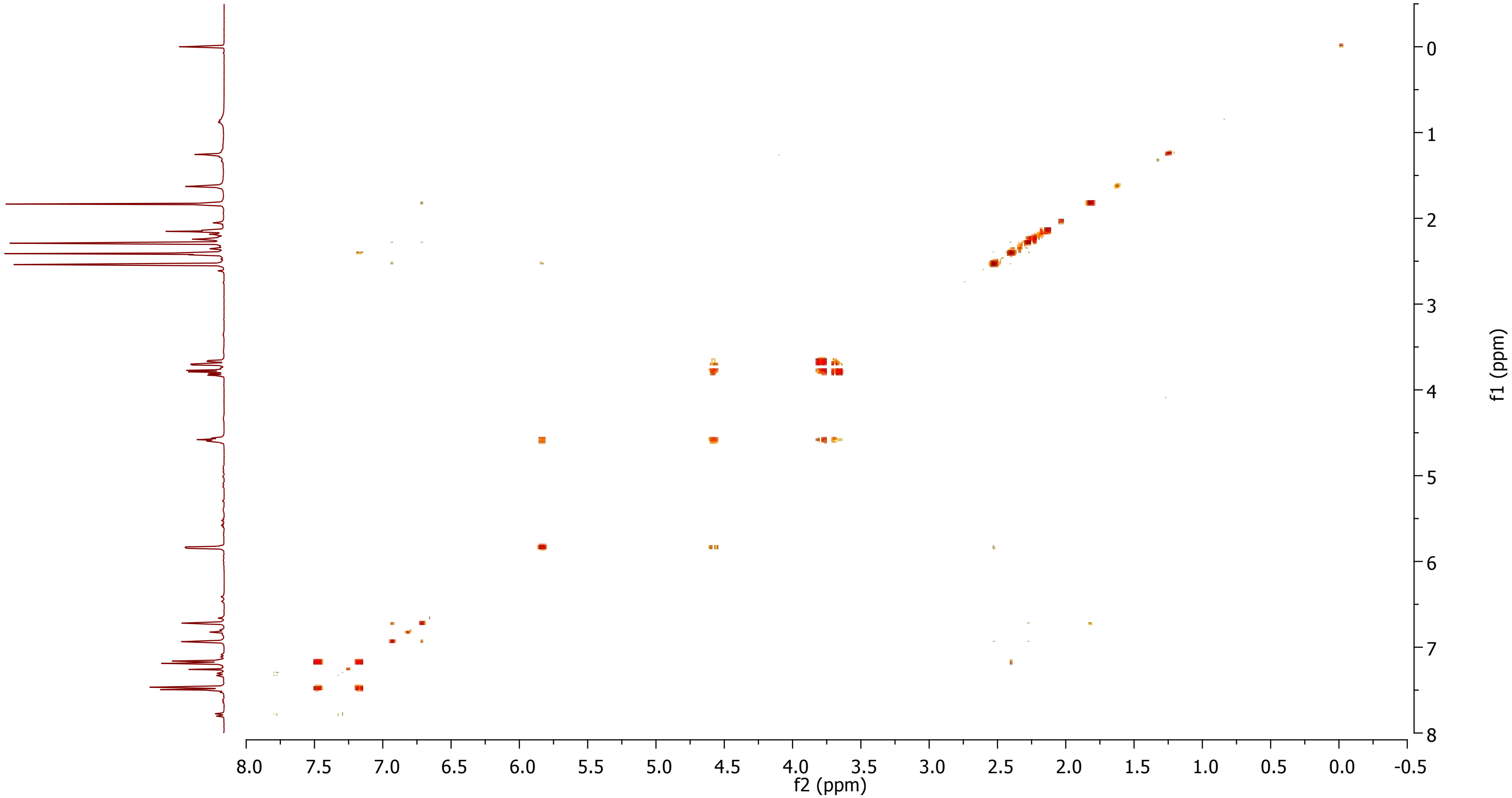
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2e**



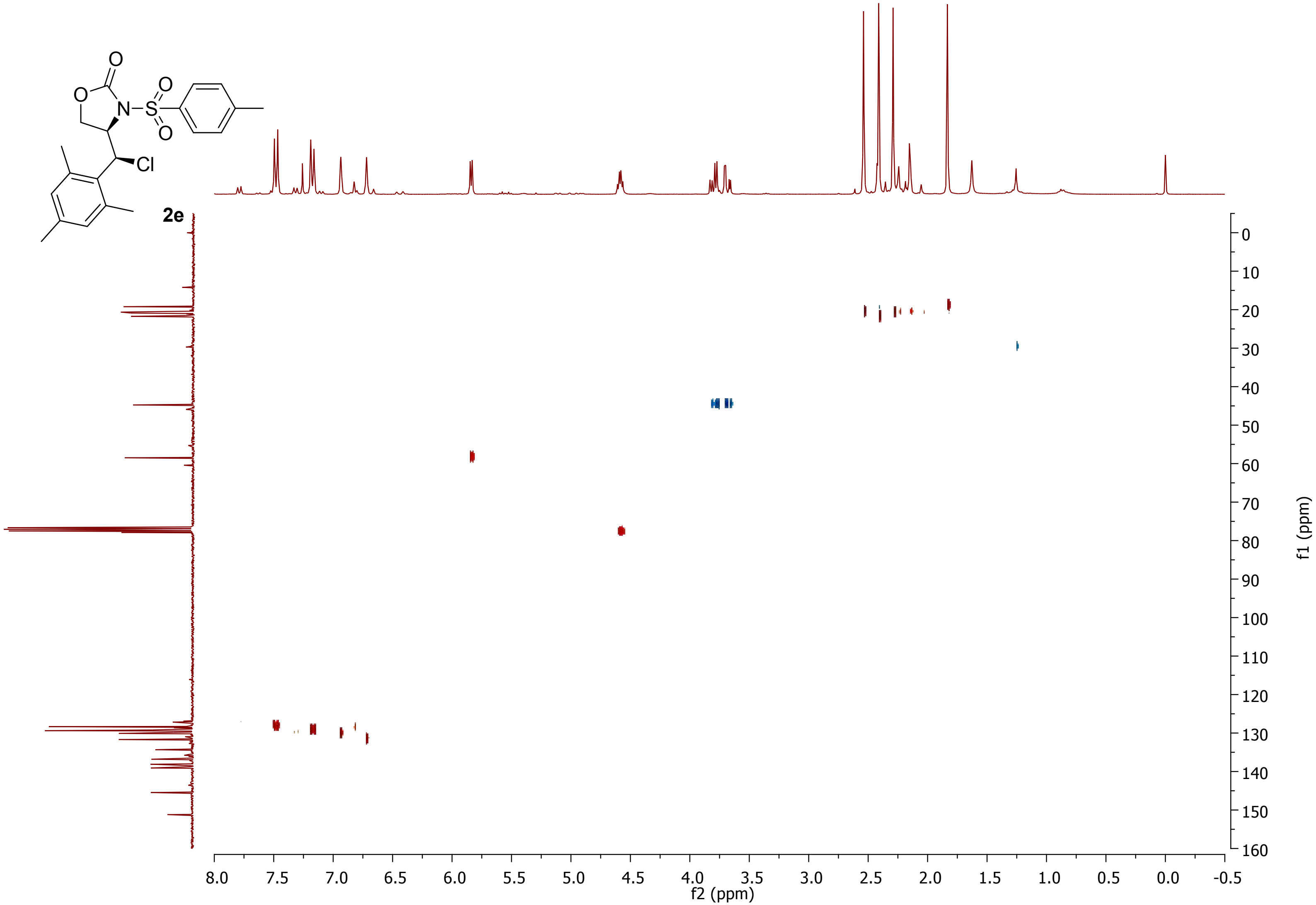
COSY of substrate **2e**



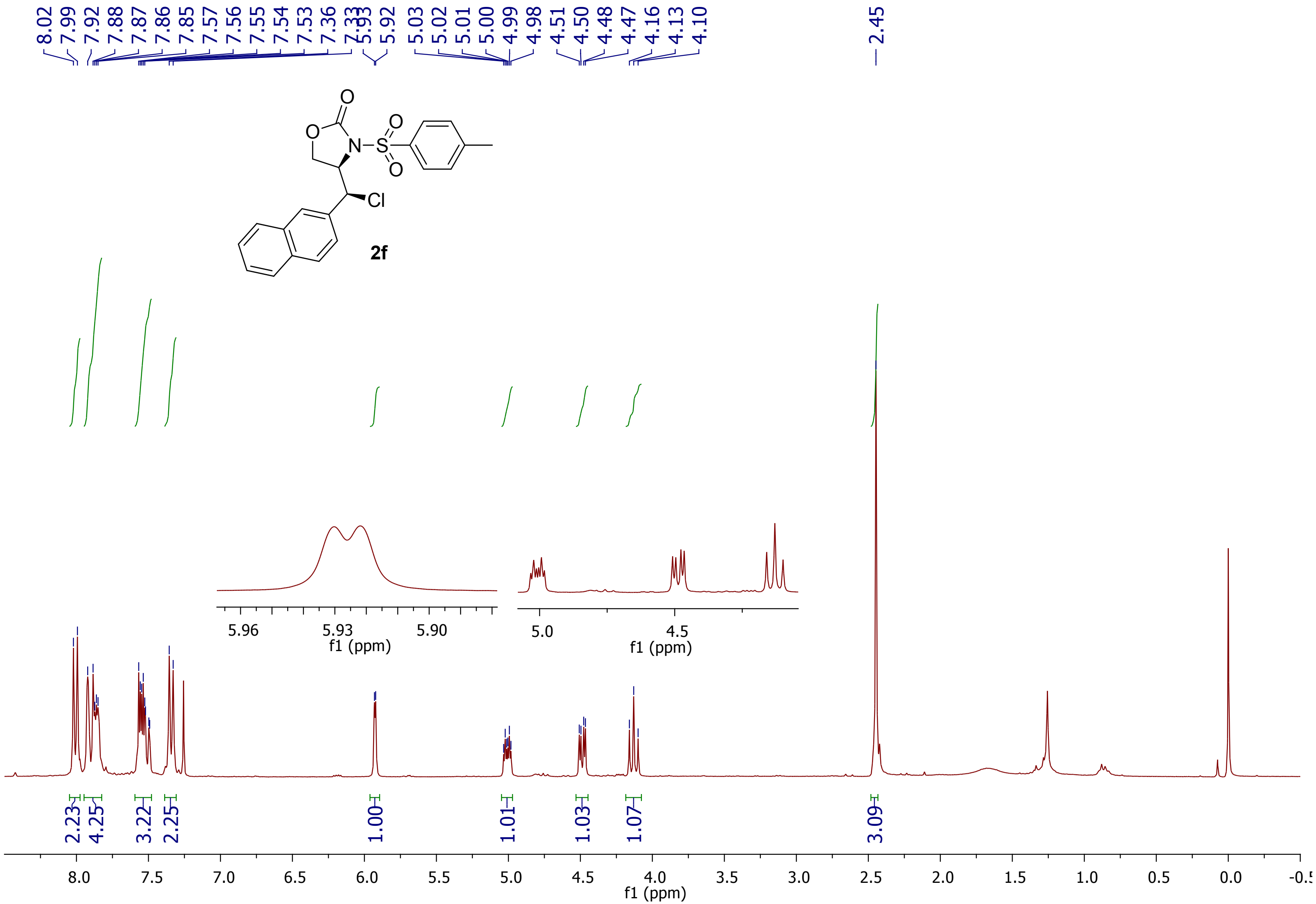
2e



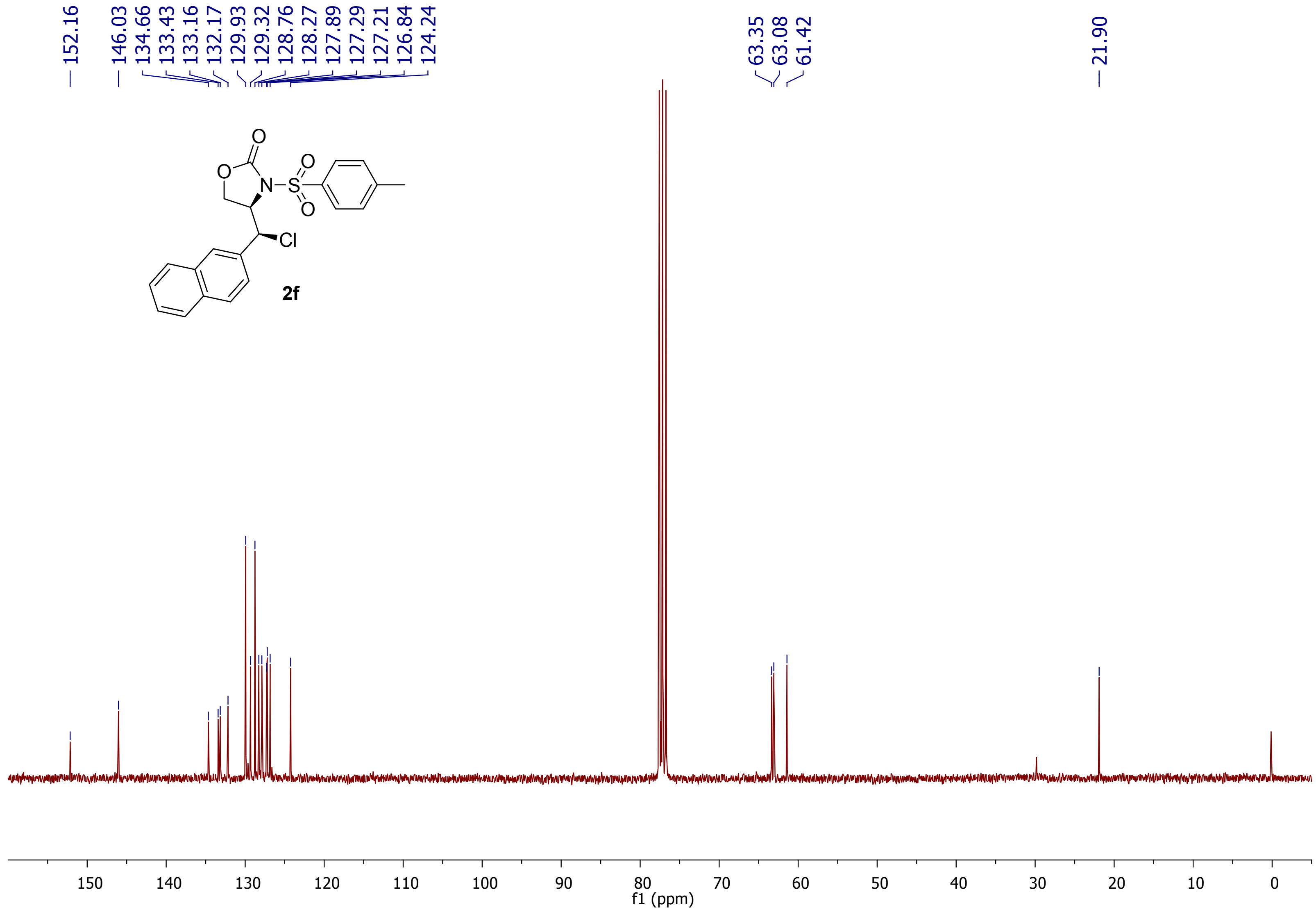
HSQC of substrate **2e**



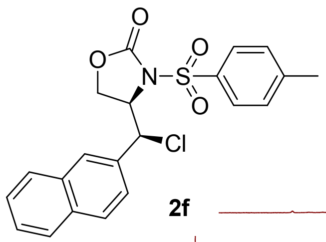
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2f**

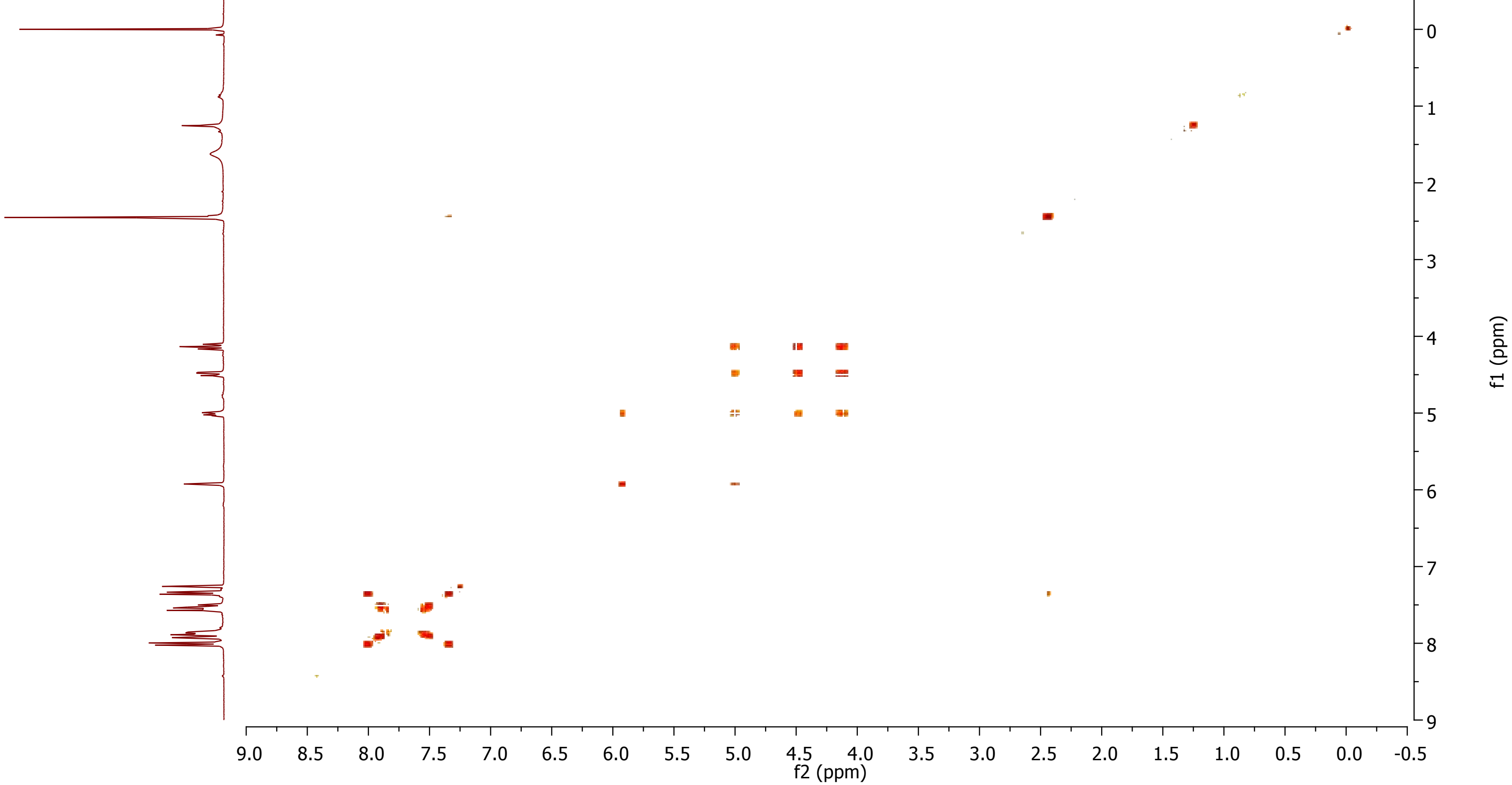


^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2f**

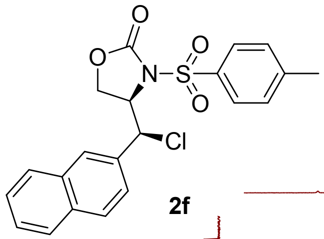


COSY of substrate **2f**

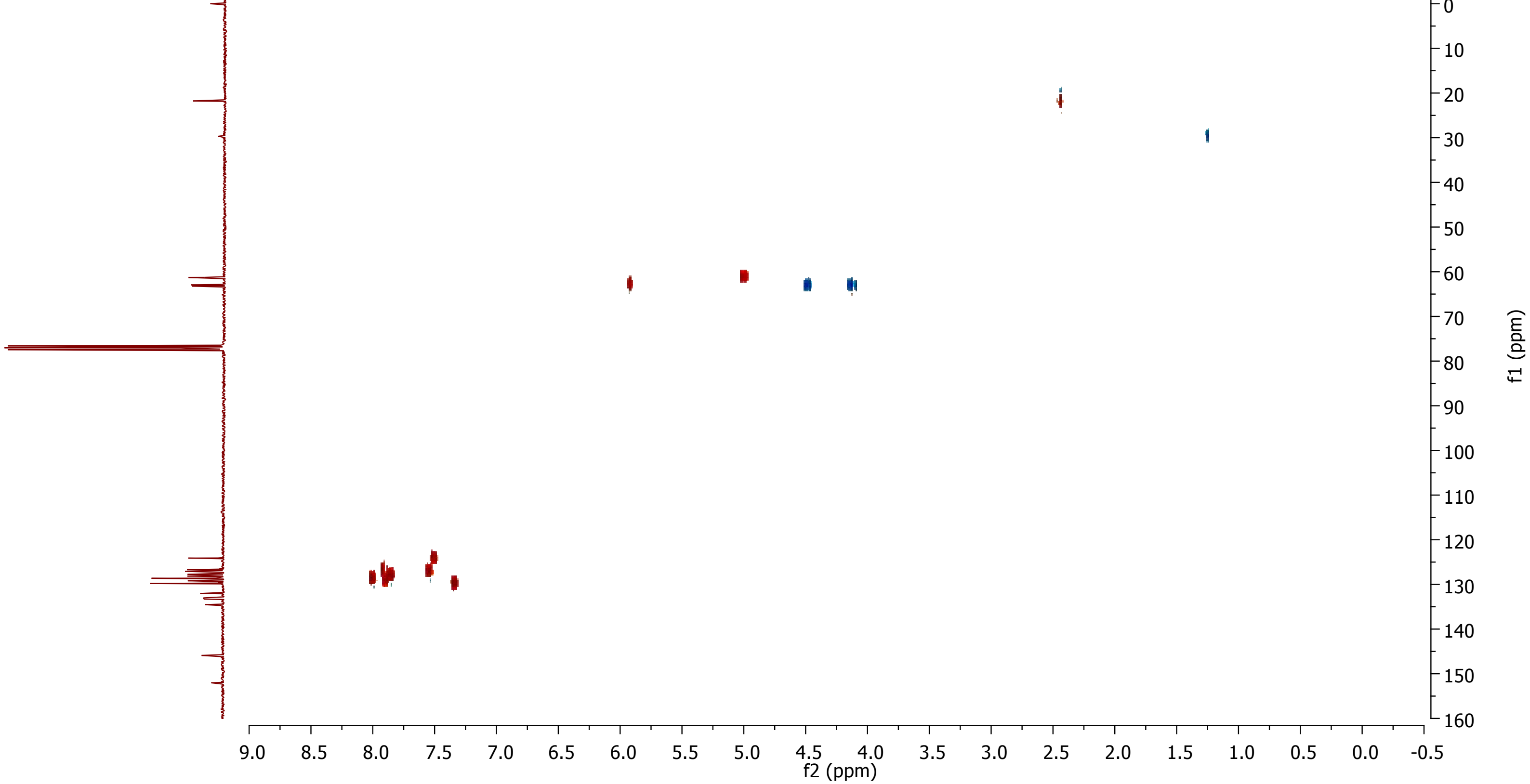




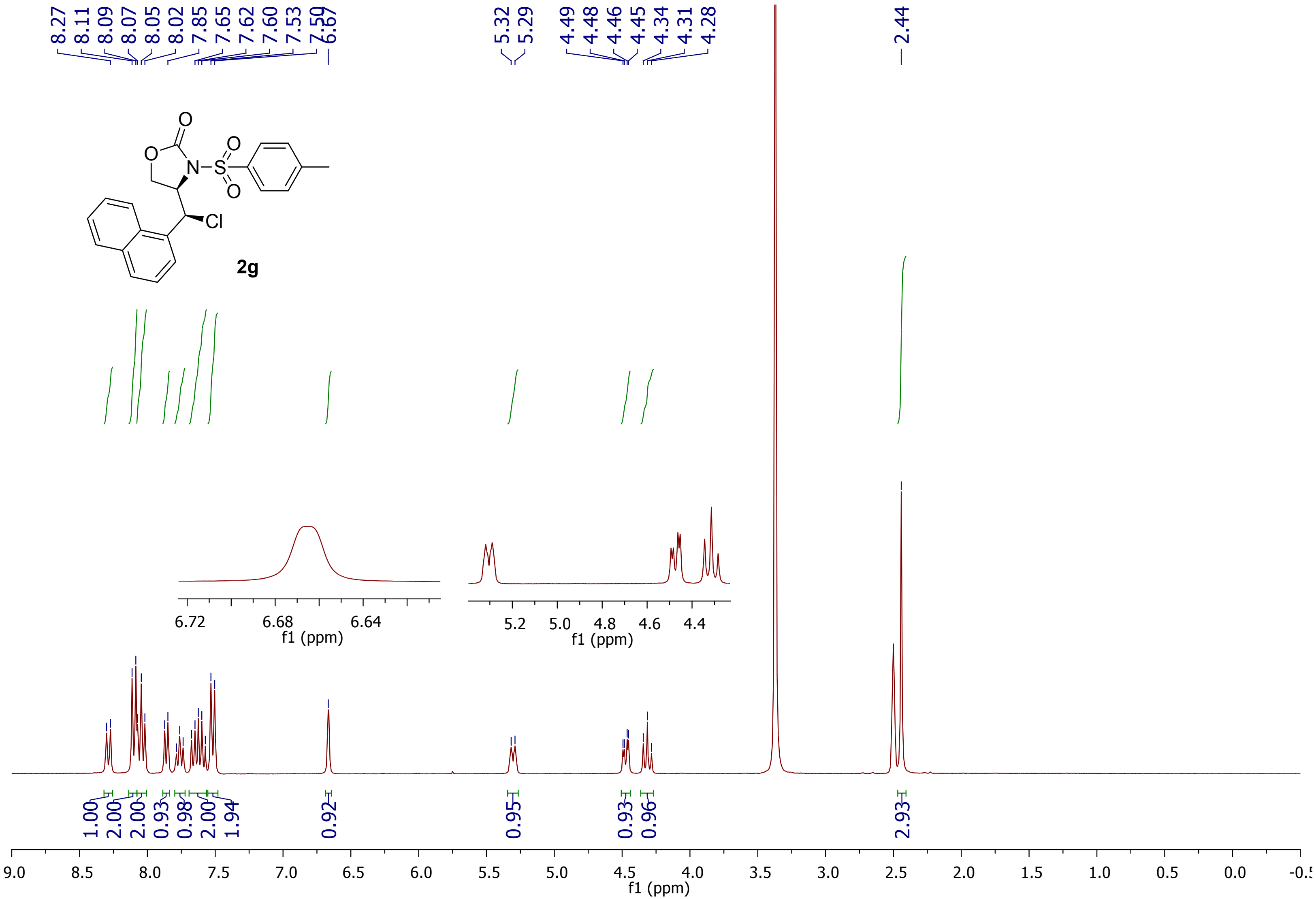
HSQC of substrate **2f**



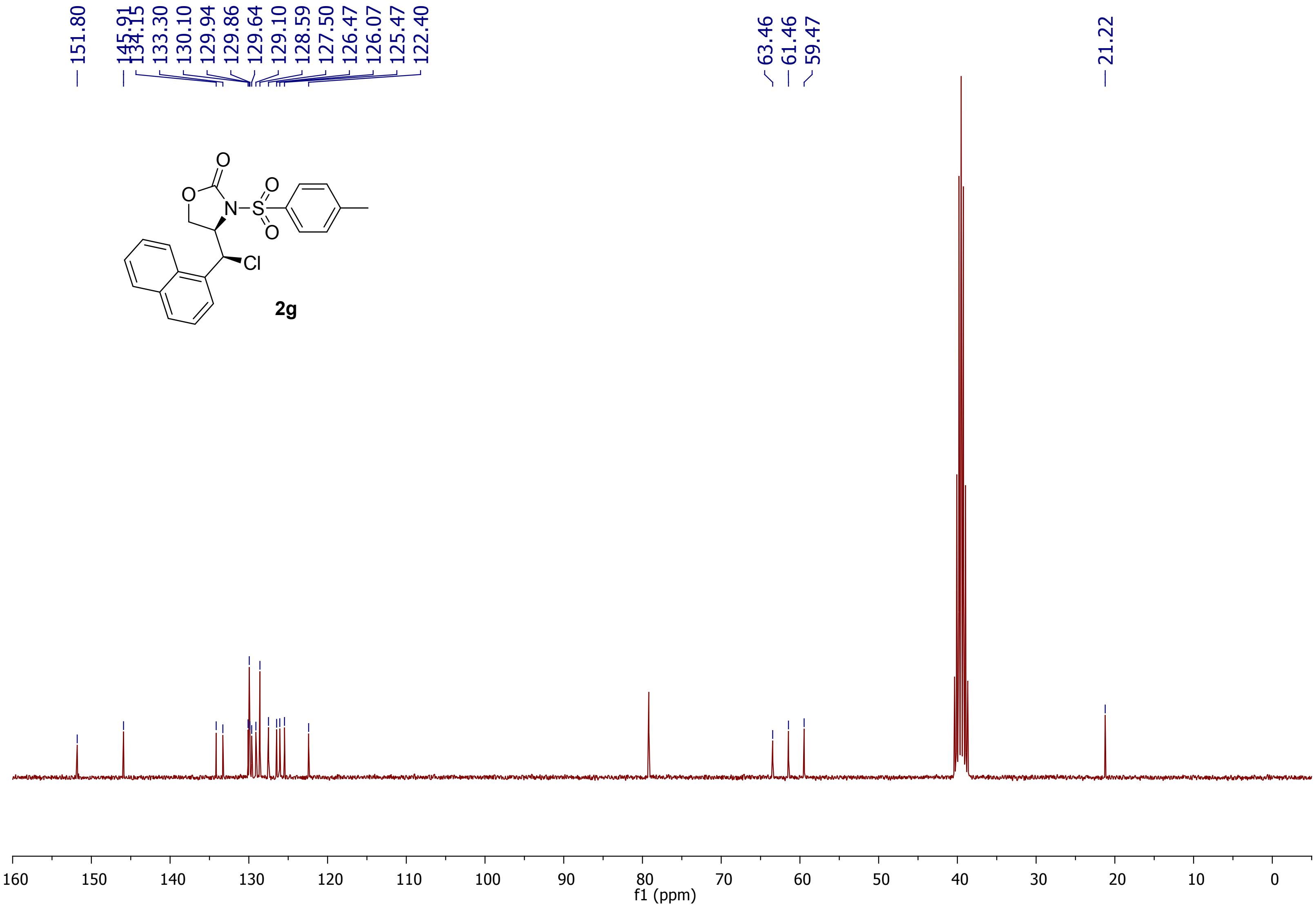
2f



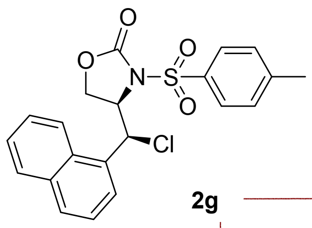
^{1}H NMR (300 MHz, DMSO-d_6) of substrate **2g**



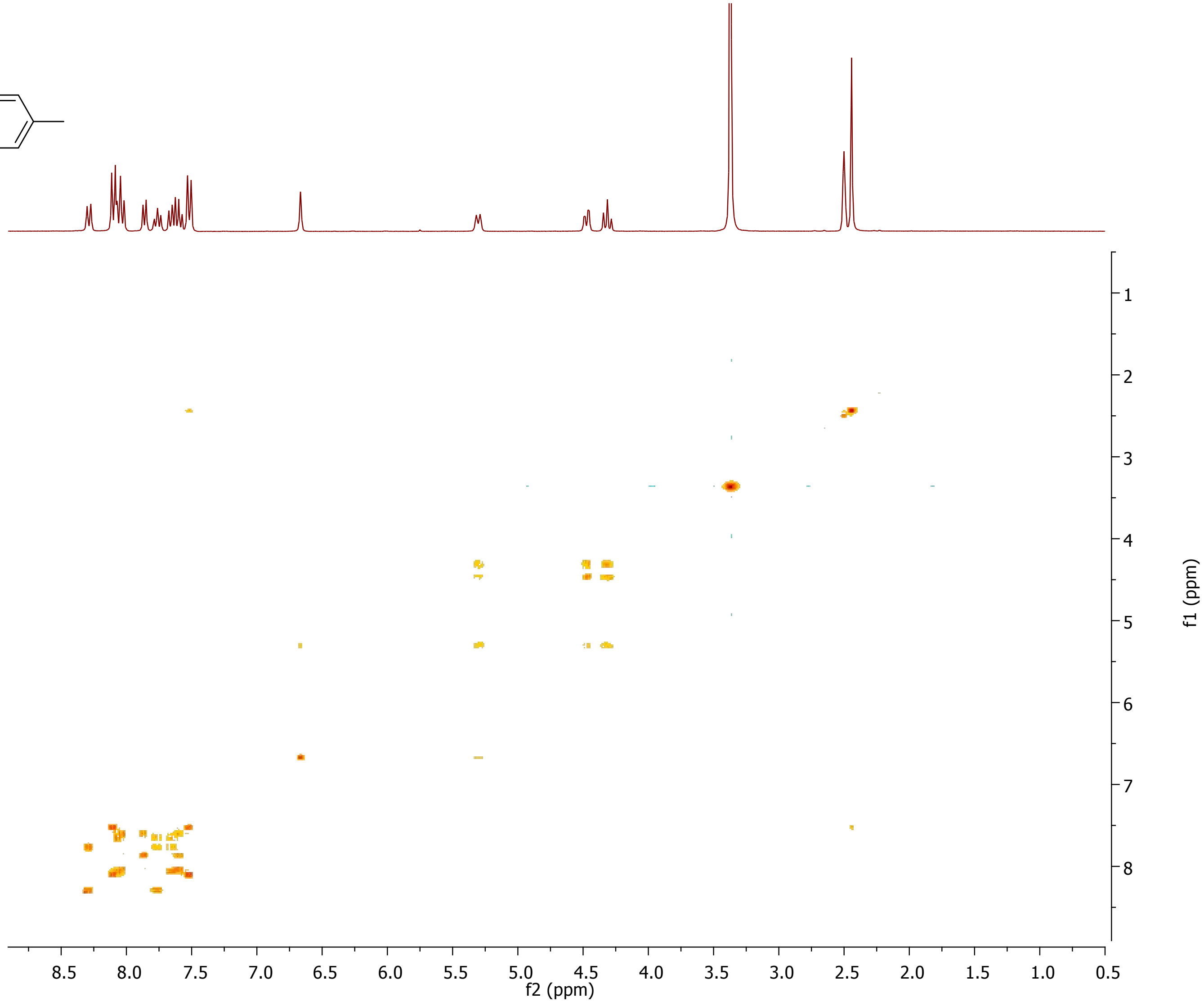
^{13}C NMR (75 MHz, DMSO-d_6) of substrate **2g**



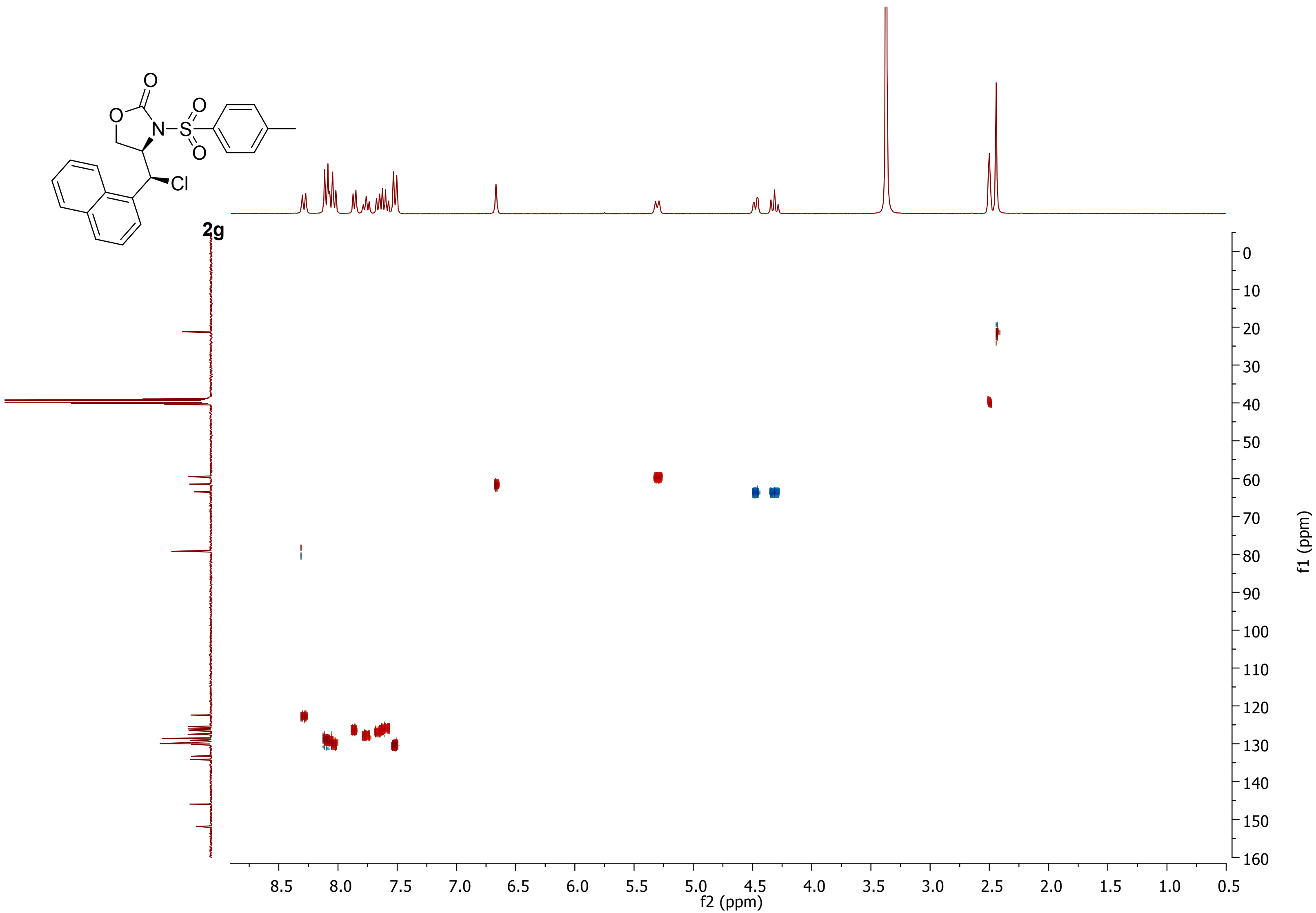
COSY of substrate **2g**



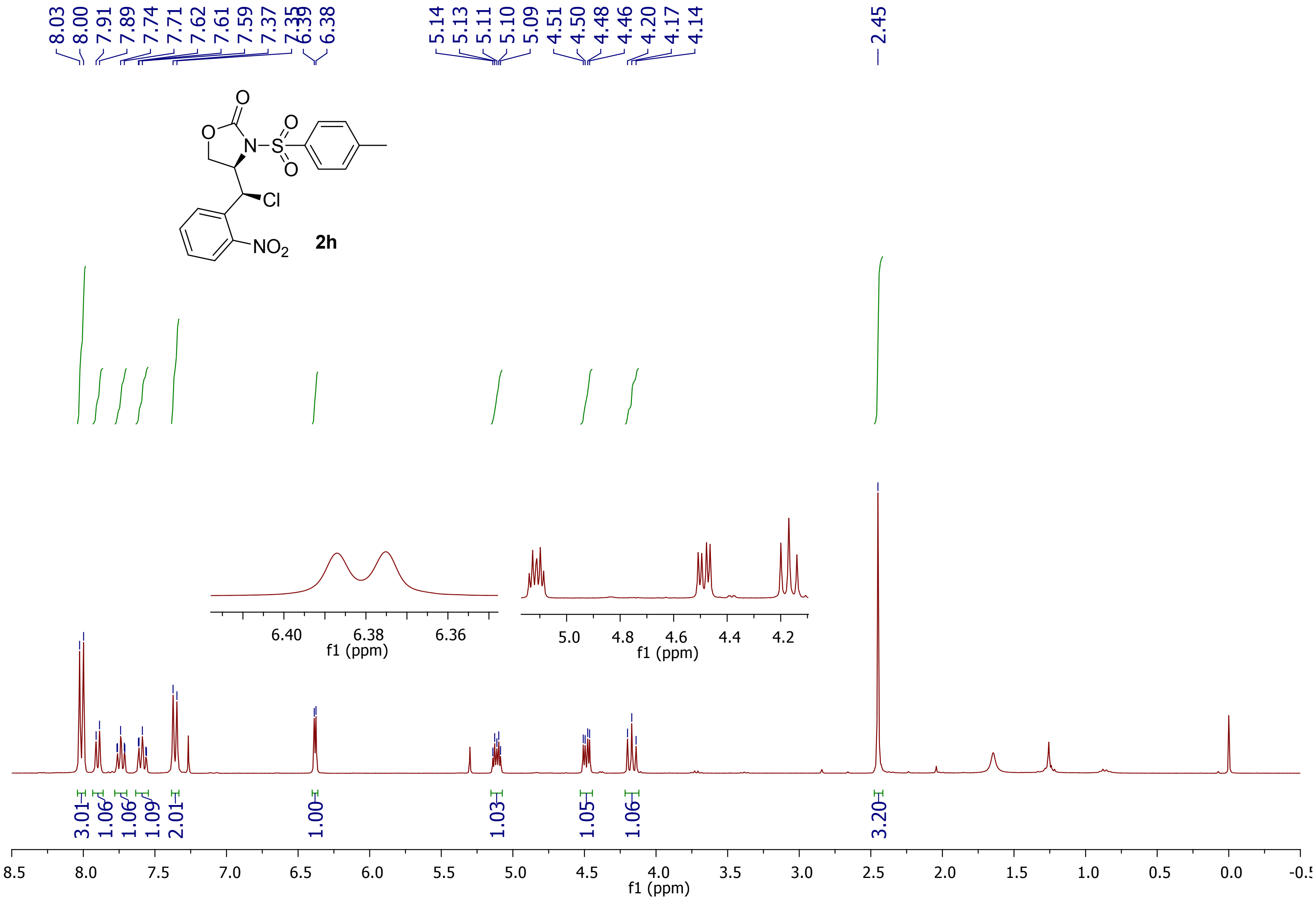
2g



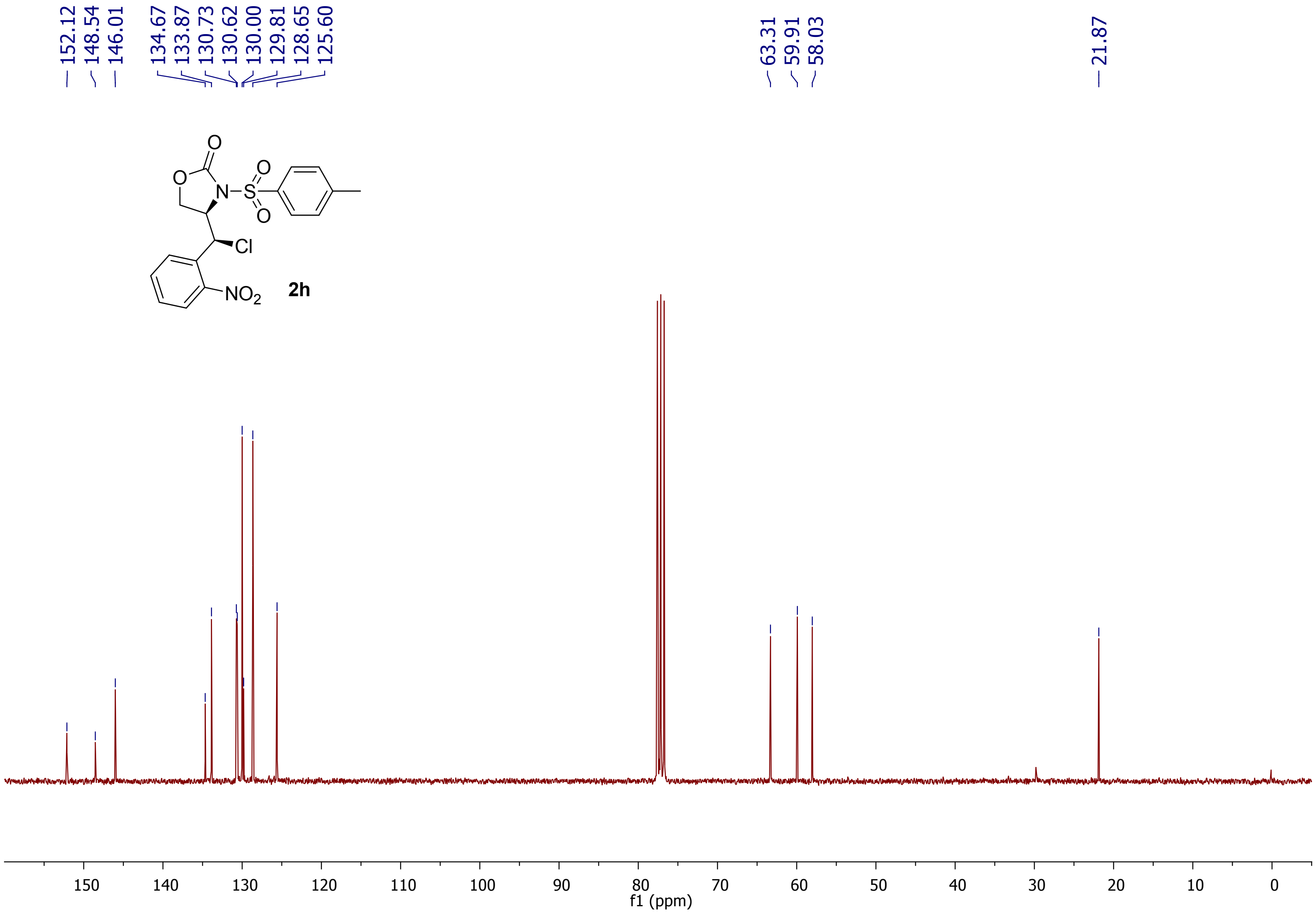
HSQC of substrate **2g**



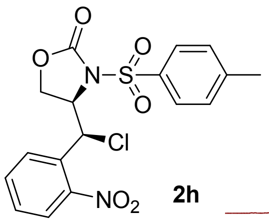
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2h**



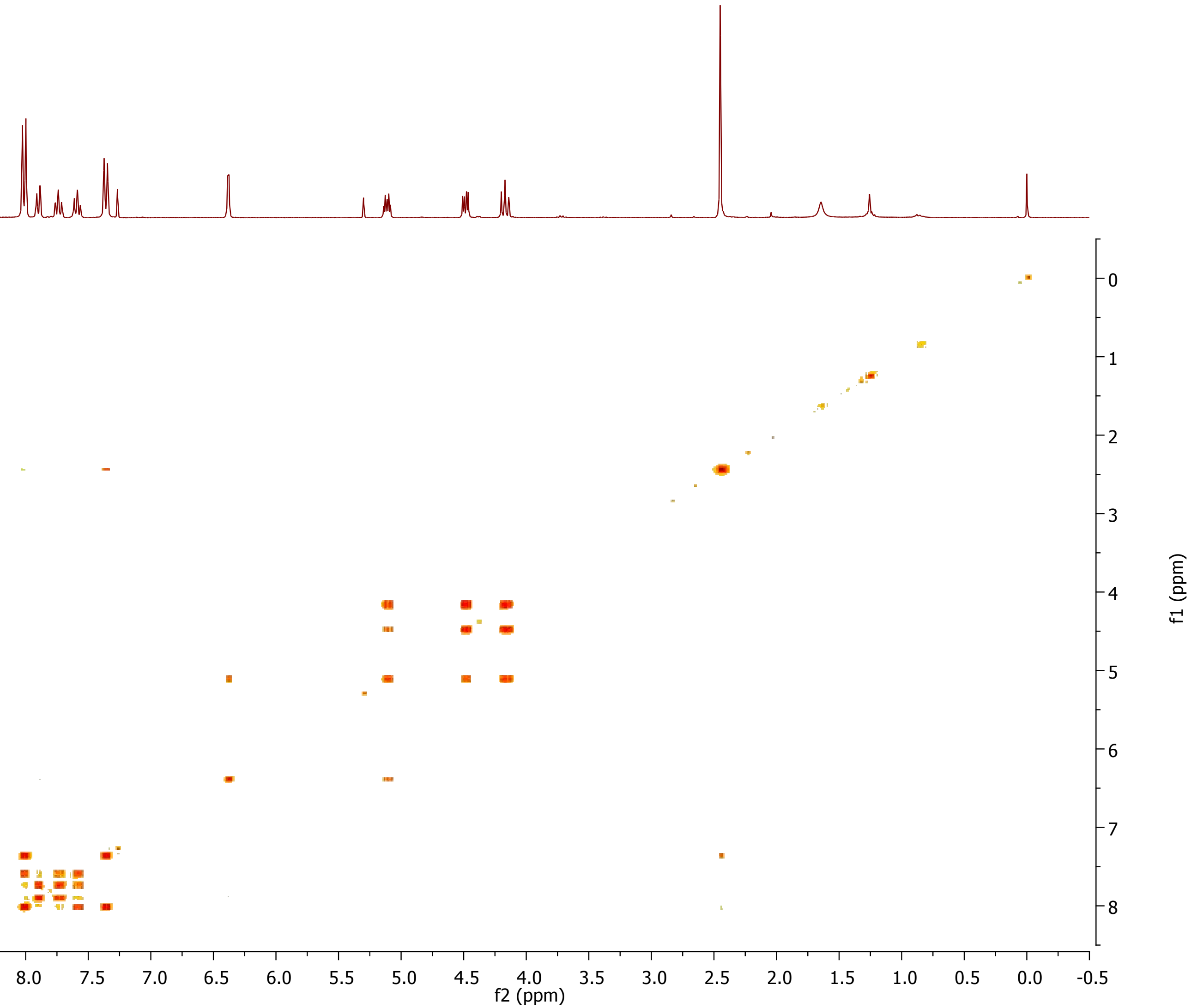
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2h**



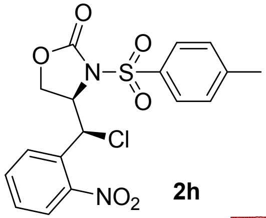
COSY of substrate **2h**



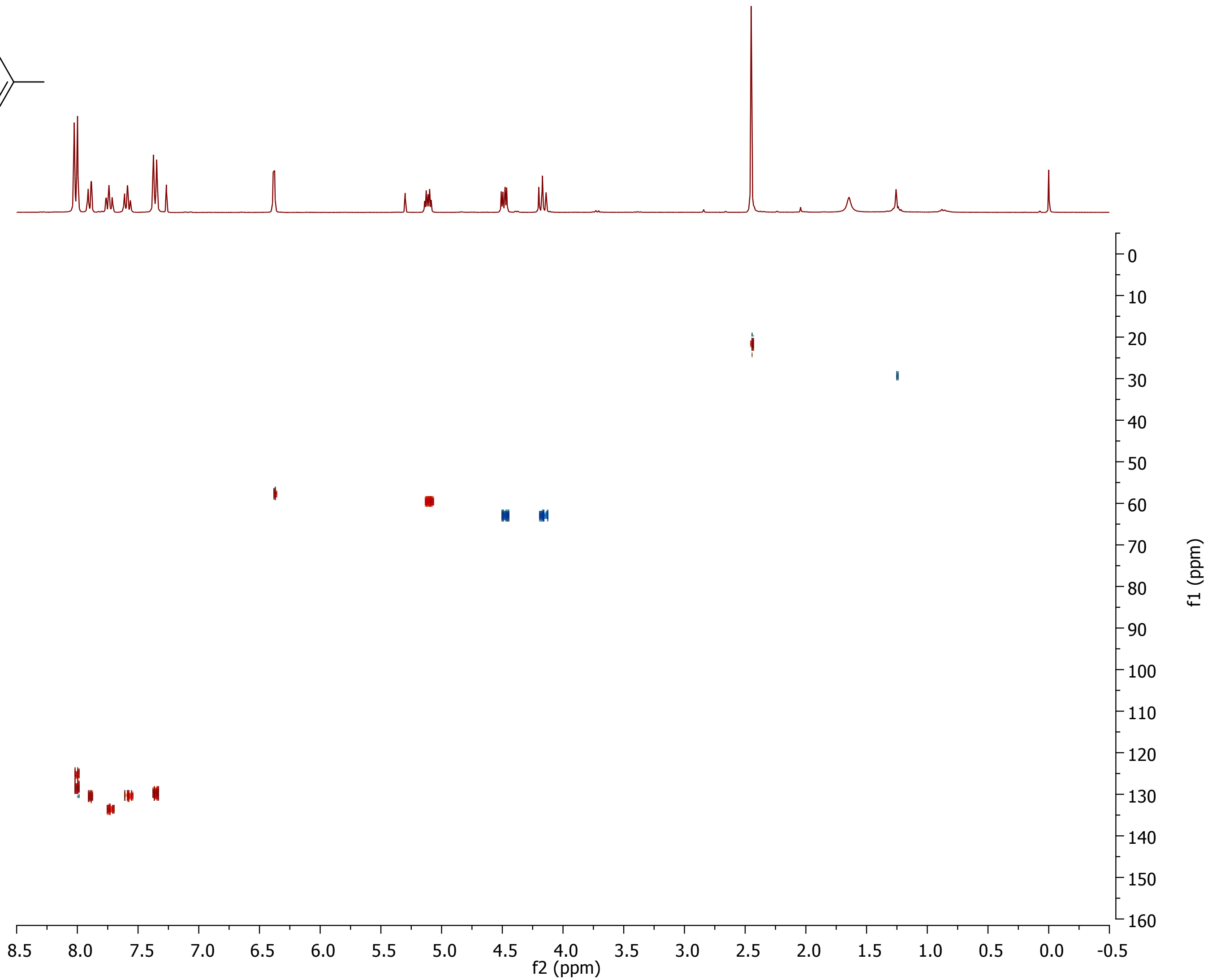
2h



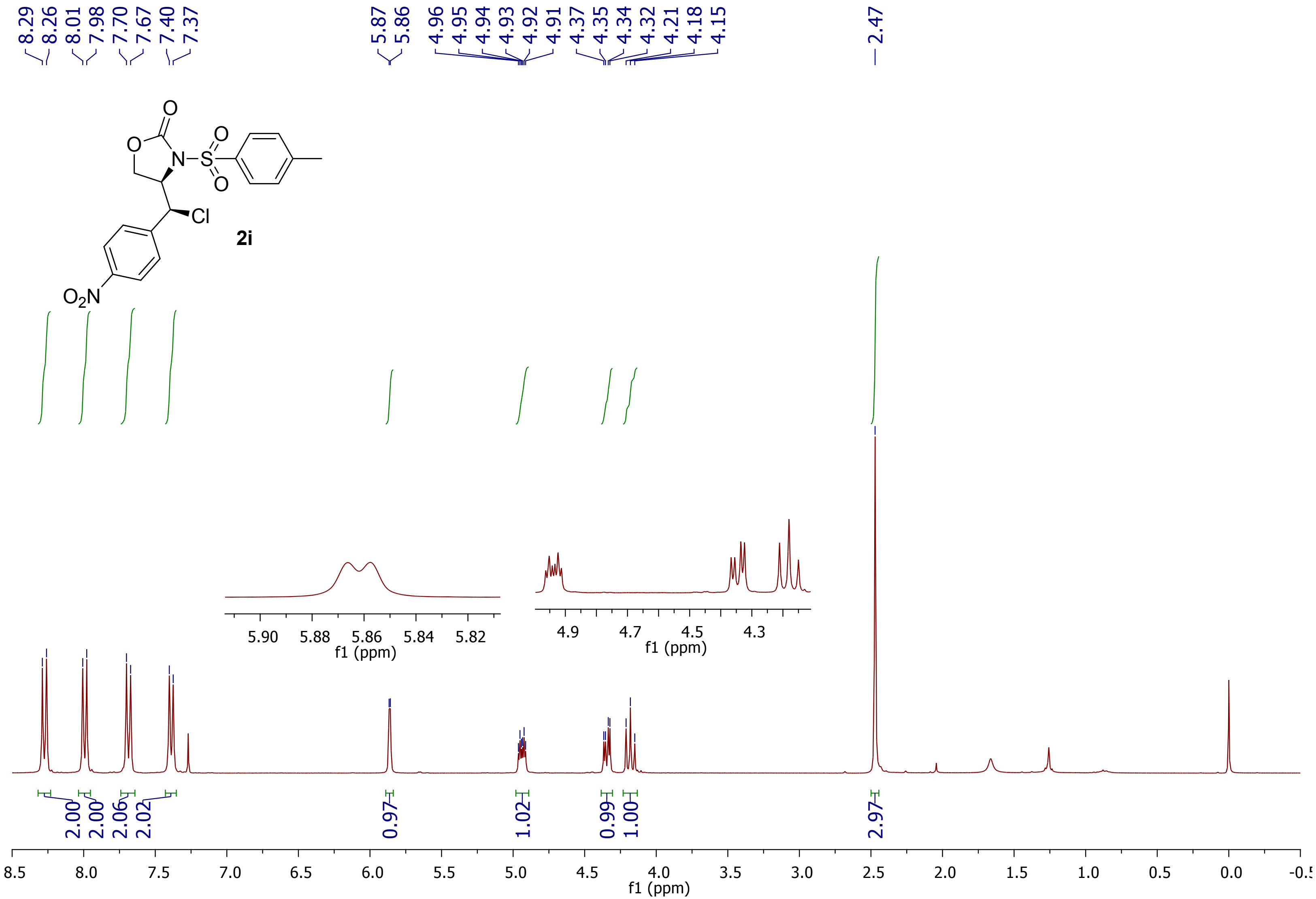
HSQC of substrate **2h**



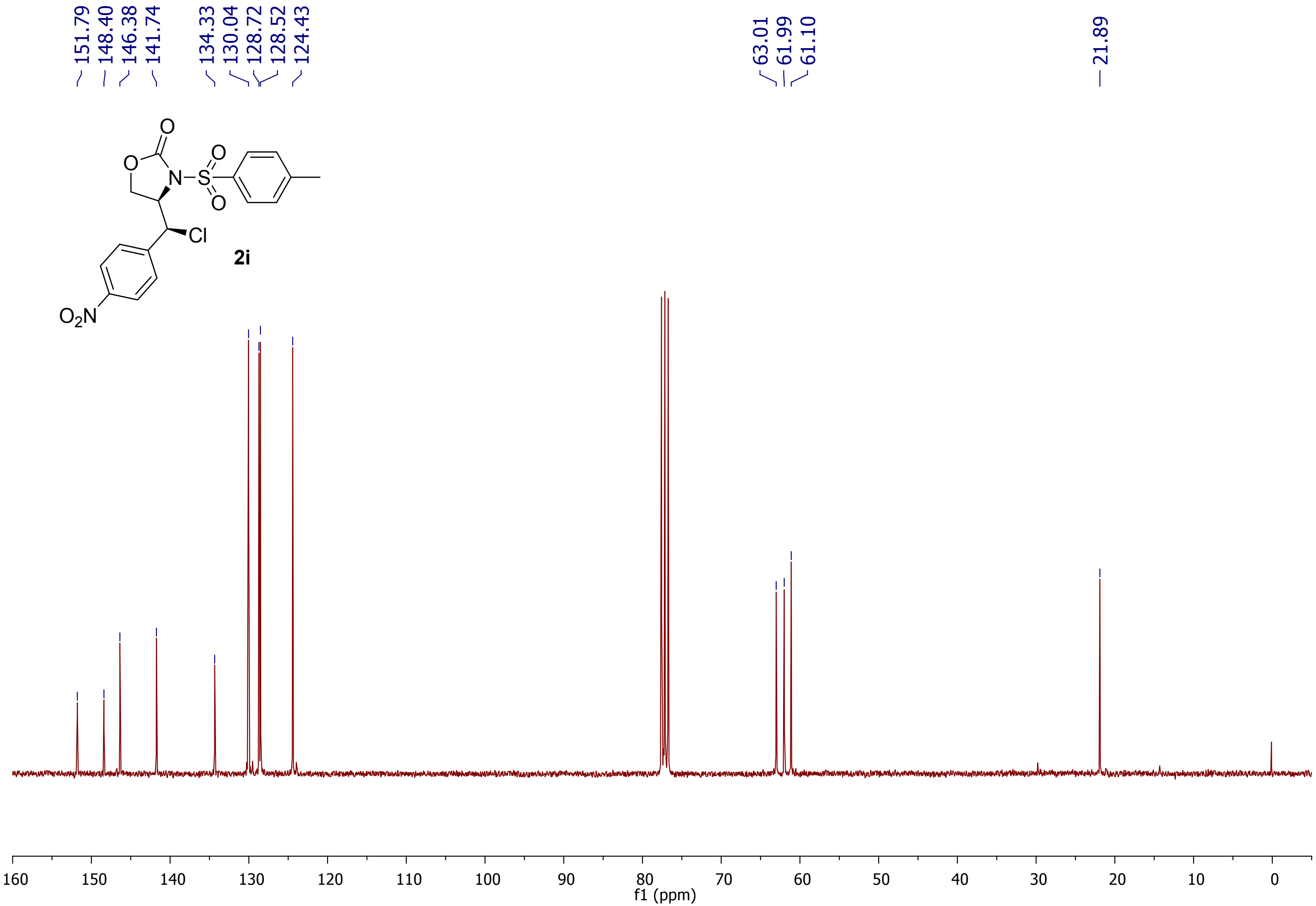
2h



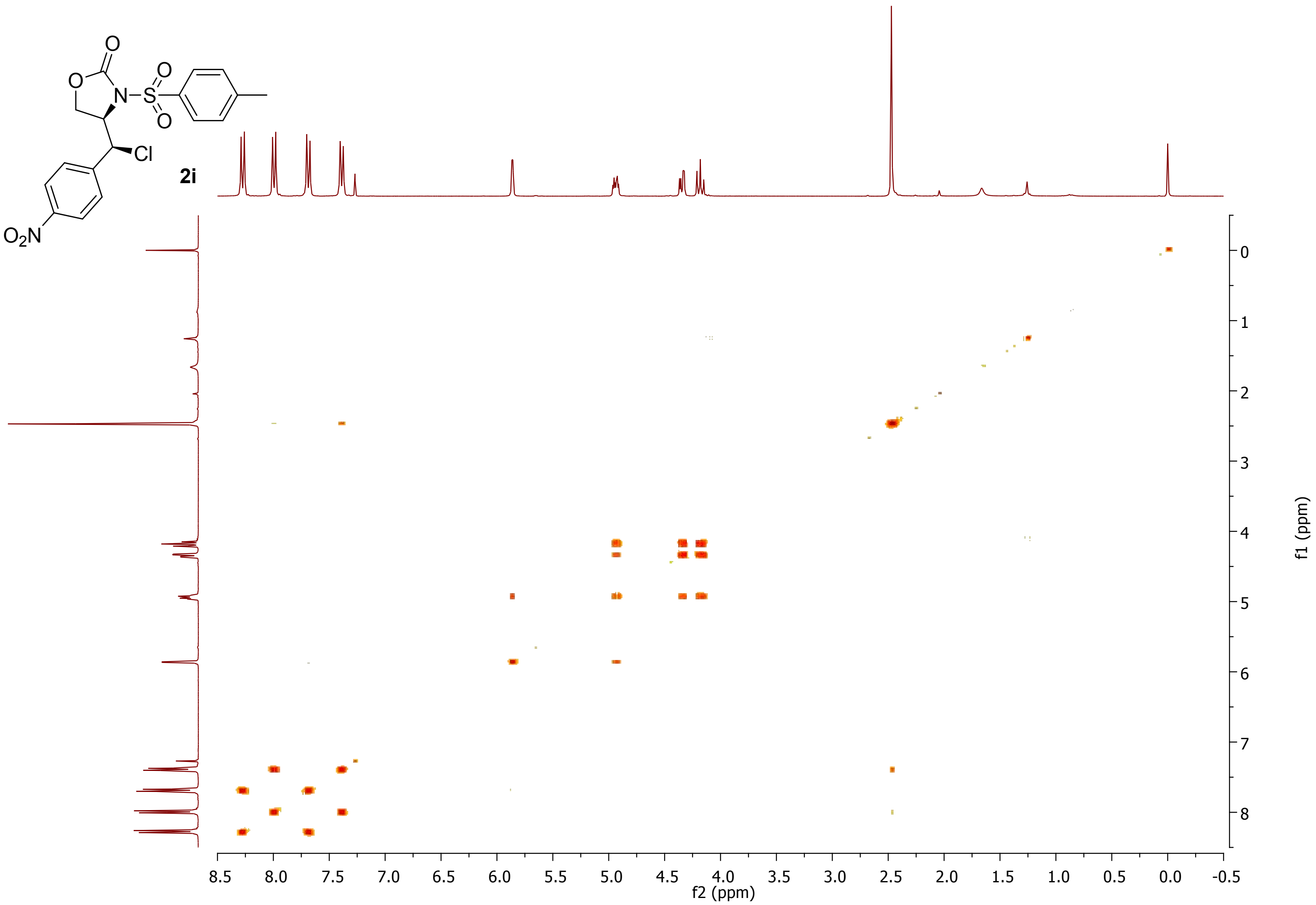
^1H NMR (300 MHz, $CDCl_3$) of substrate **2i**



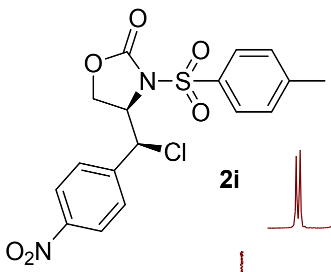
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2i**

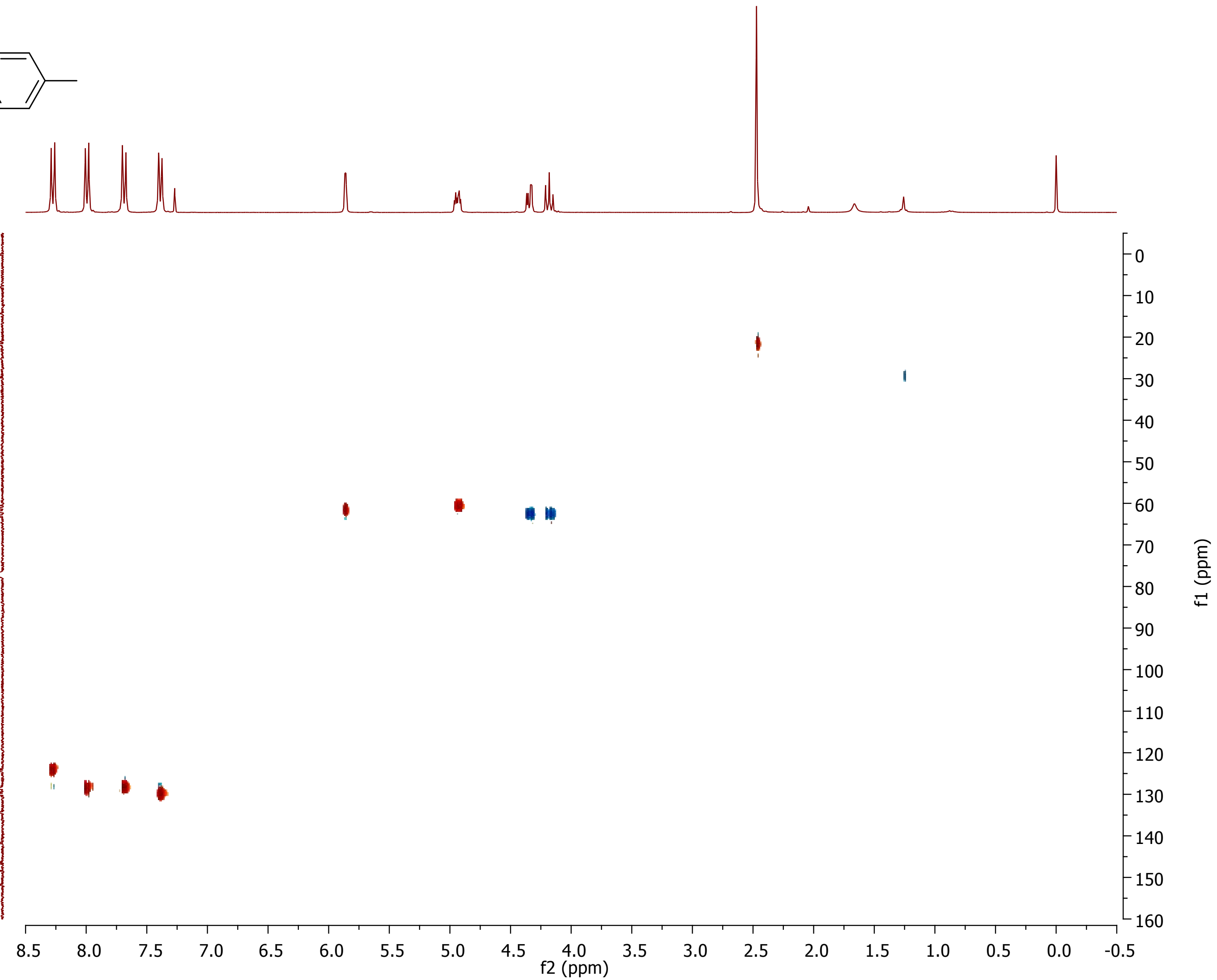


COSY of substrate **2i**

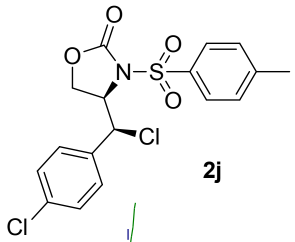


HSQC of substrate **2i**

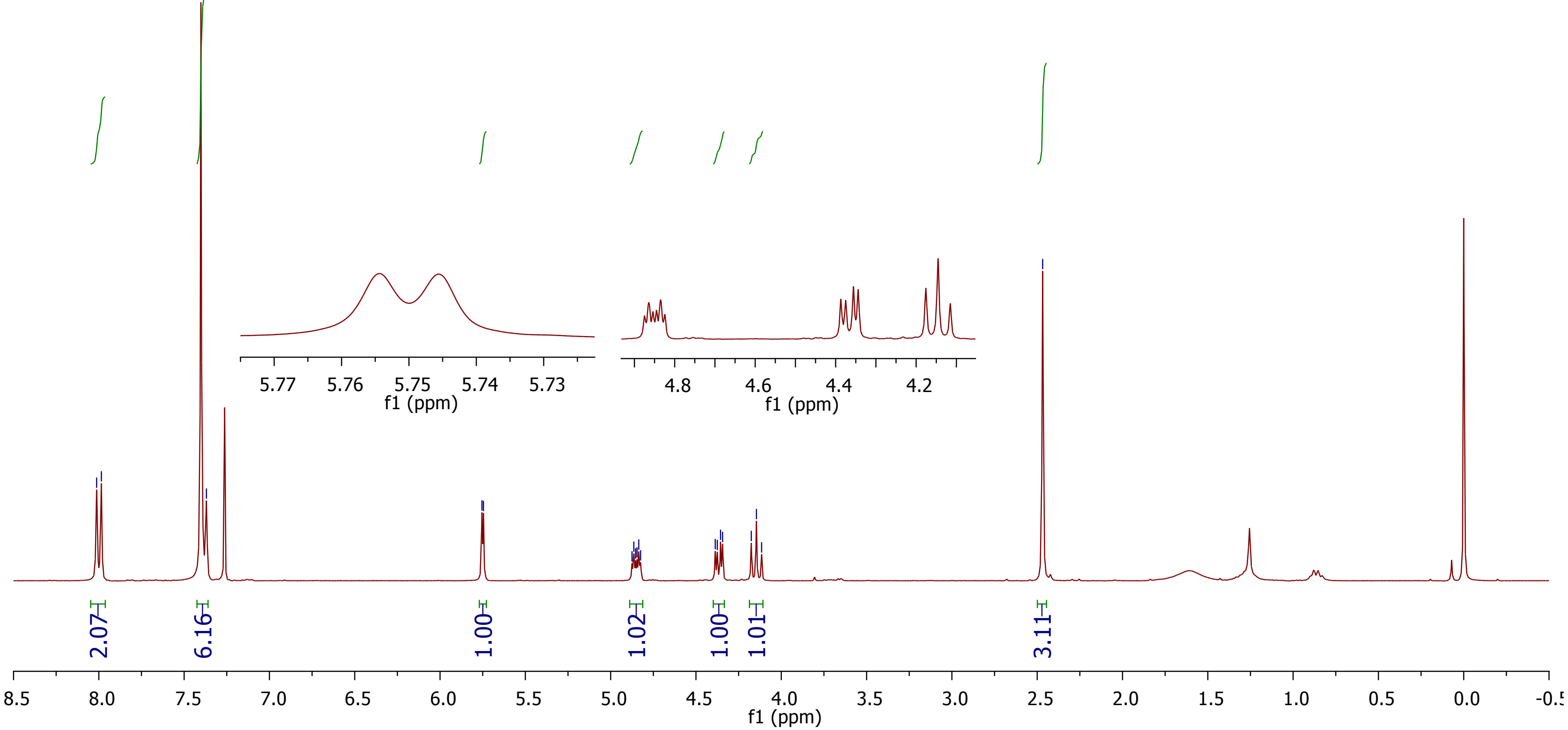




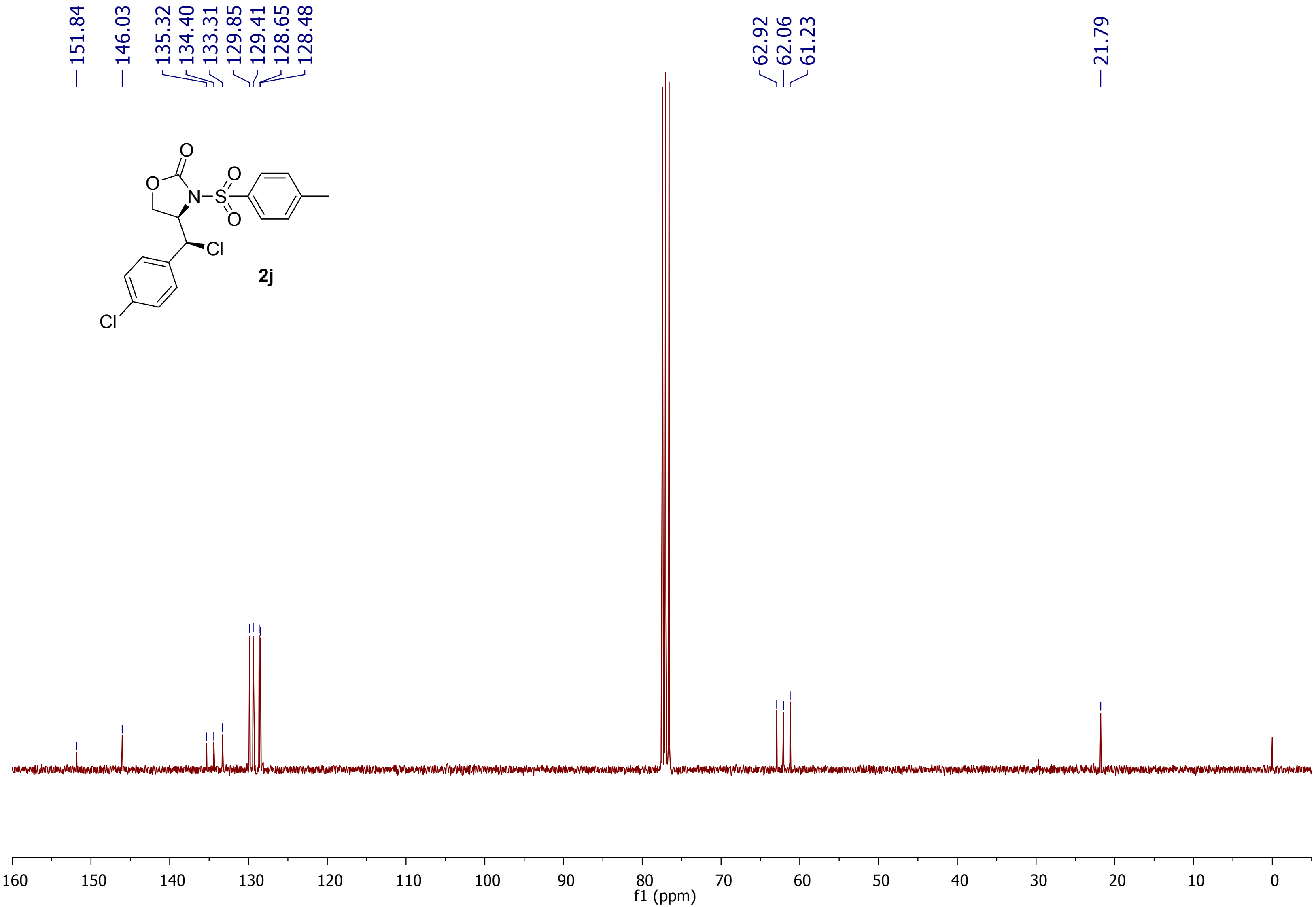
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2j**



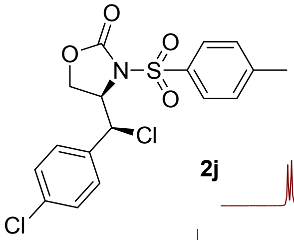
2j



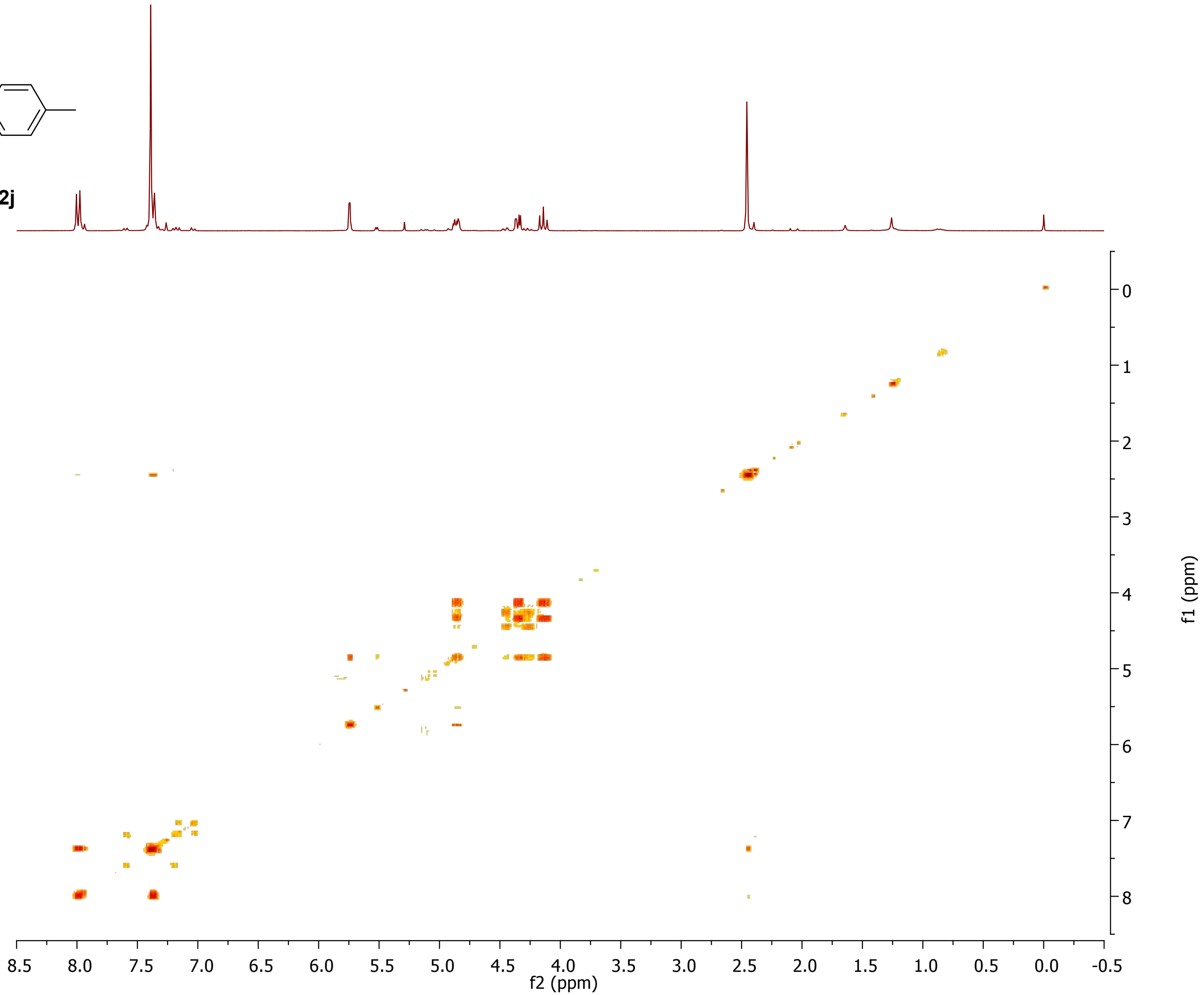
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2j**



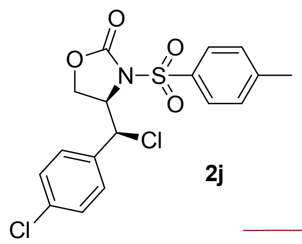
COSY of substrate **2j**



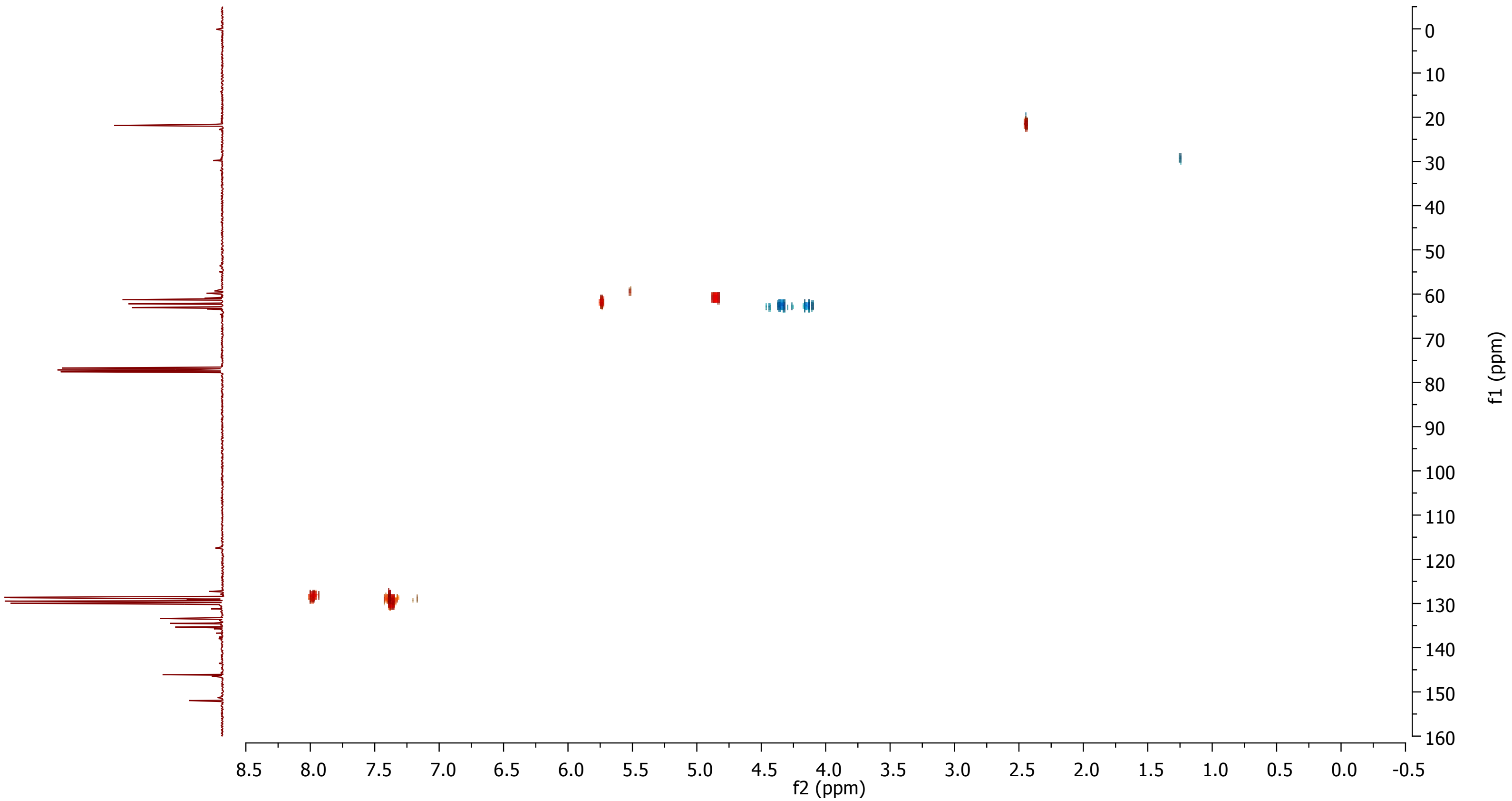
2j



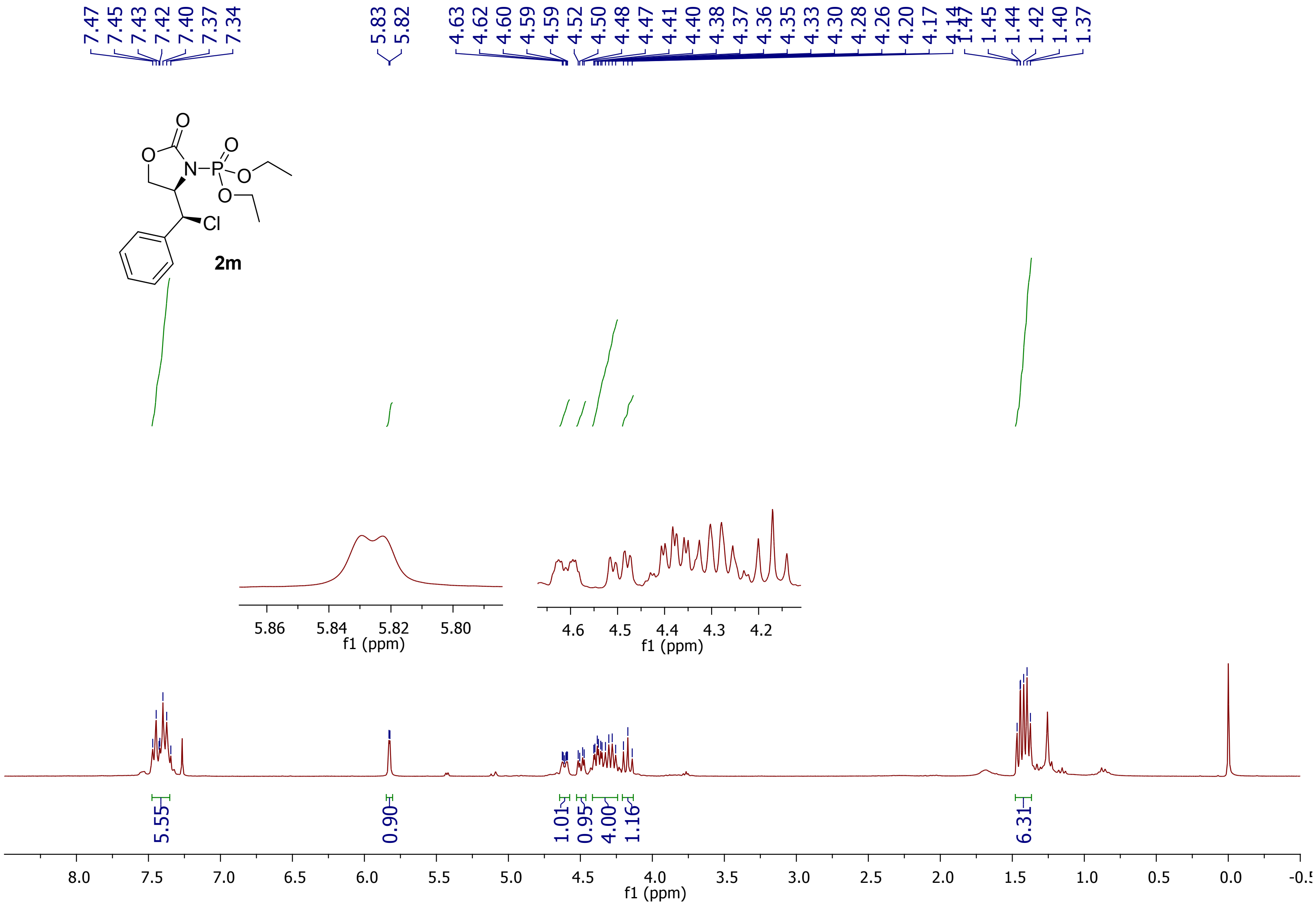
HSQC of substrate **2j**



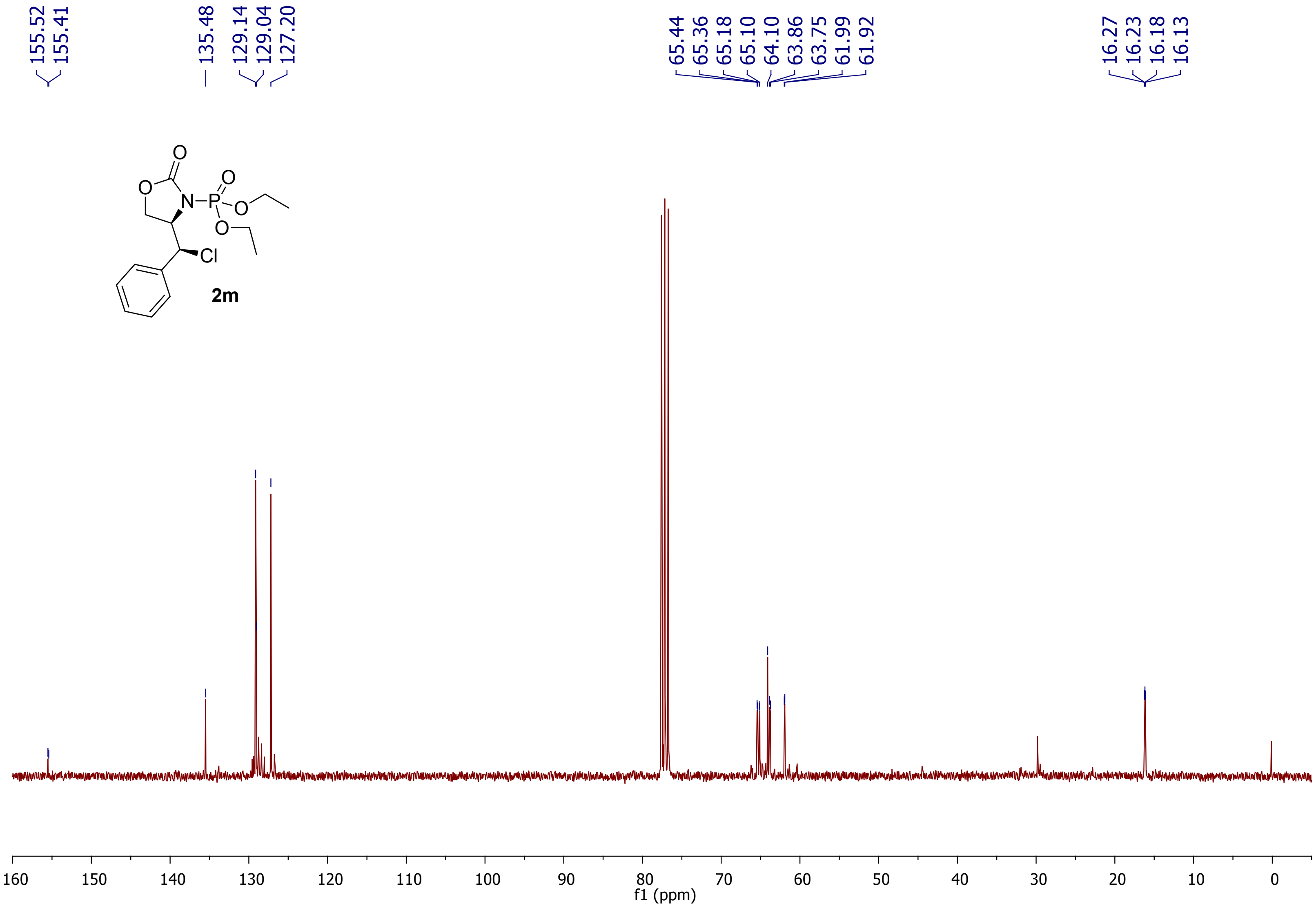
2j



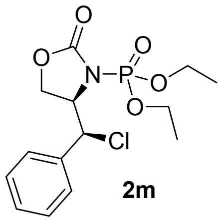
[1]H NMR (300 MHz, $CDCl_3$) of substrate **2m**



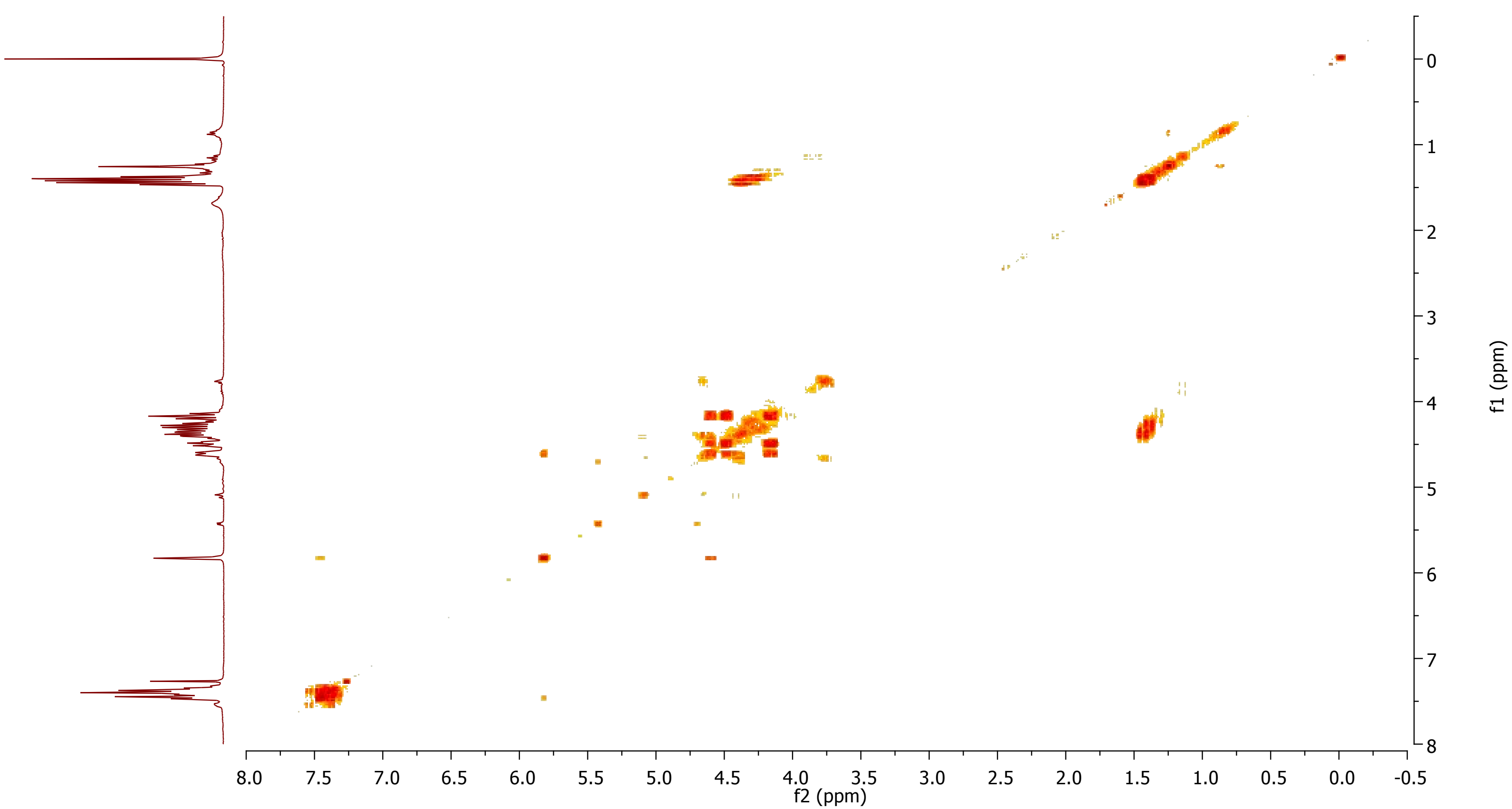
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2m**



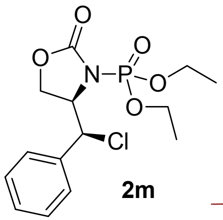
COSY of substrate **2m**



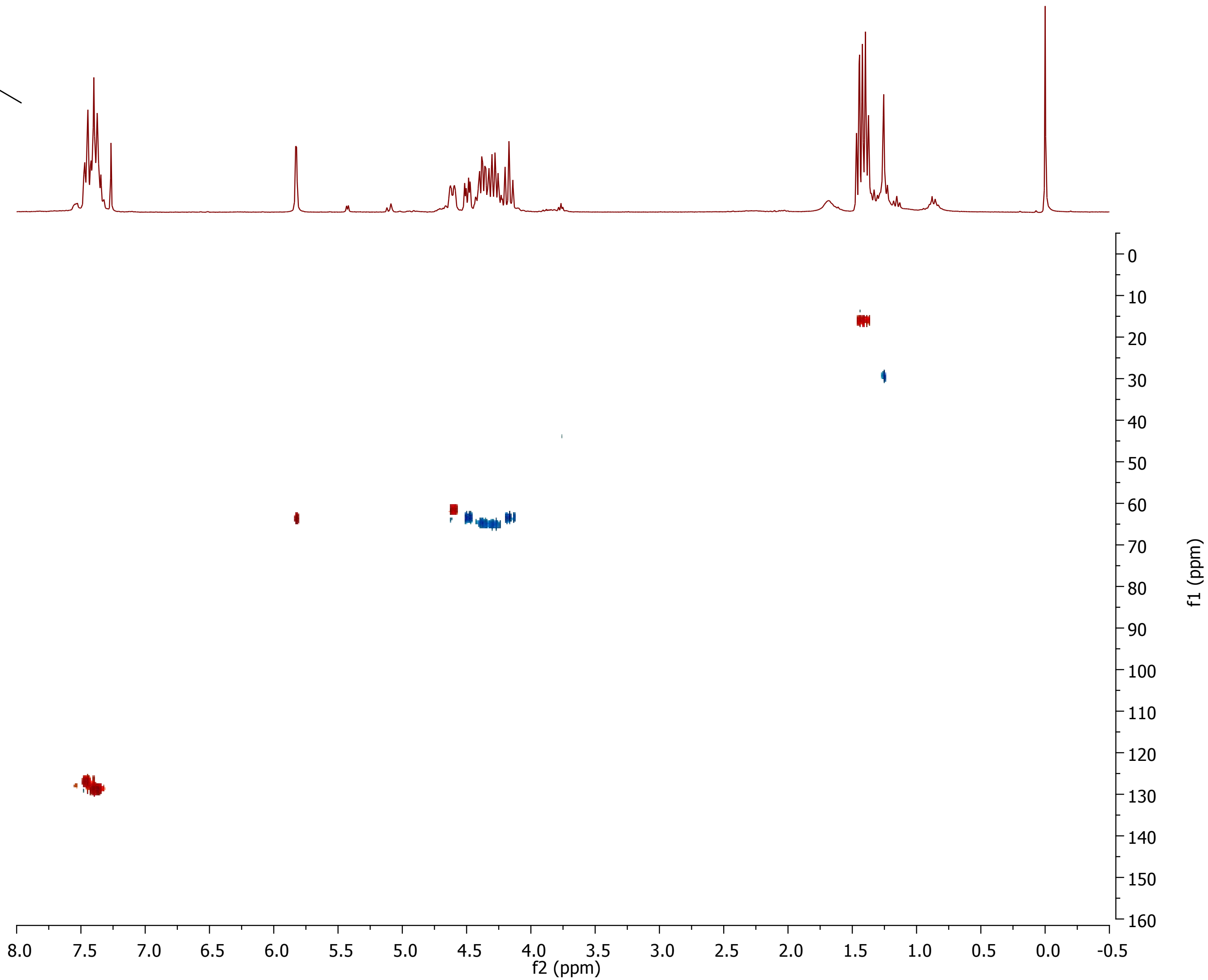
2m



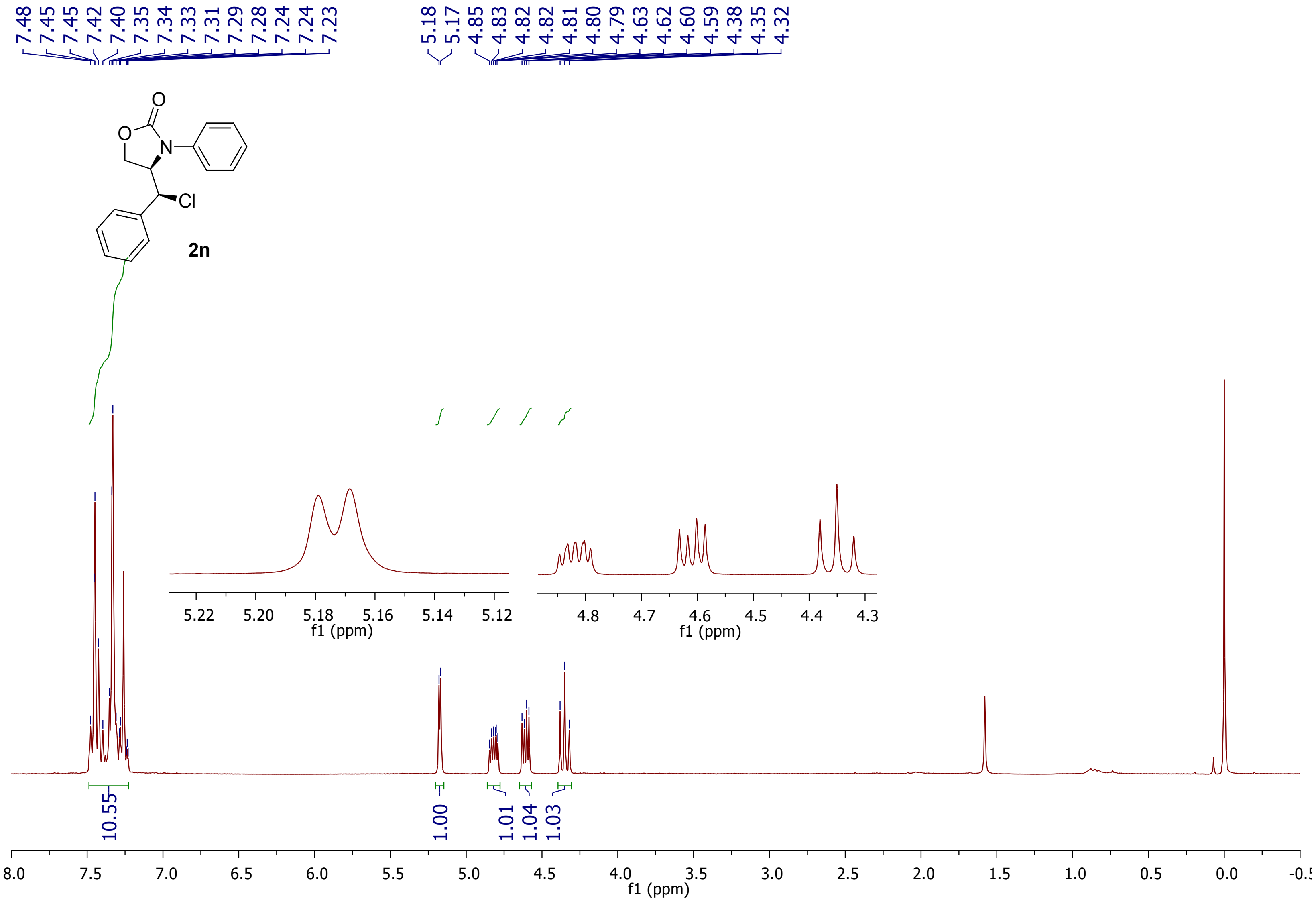
HSQC of substrate **2m**



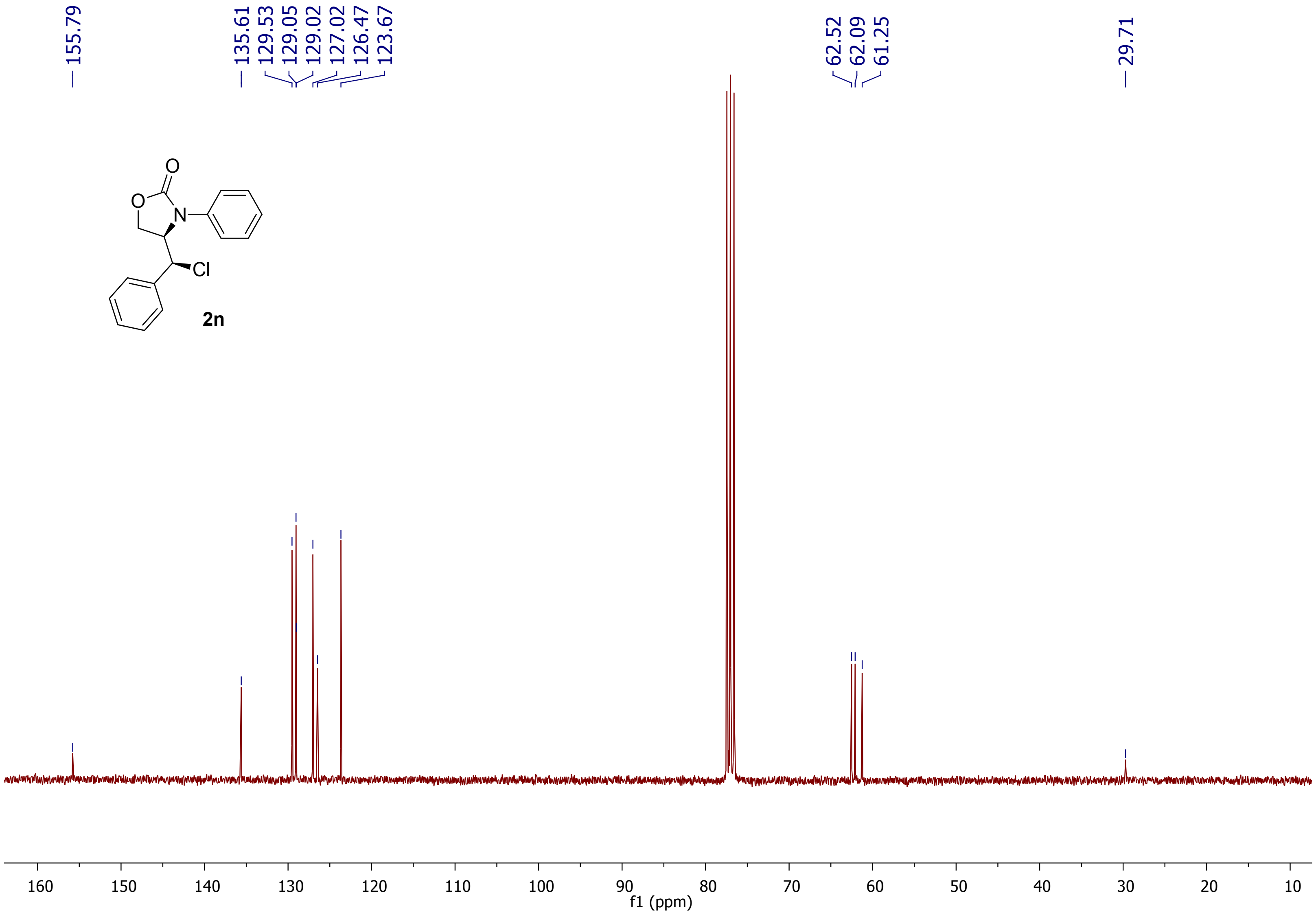
2m



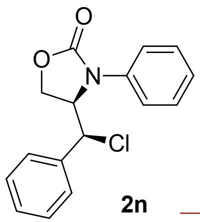
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2n**



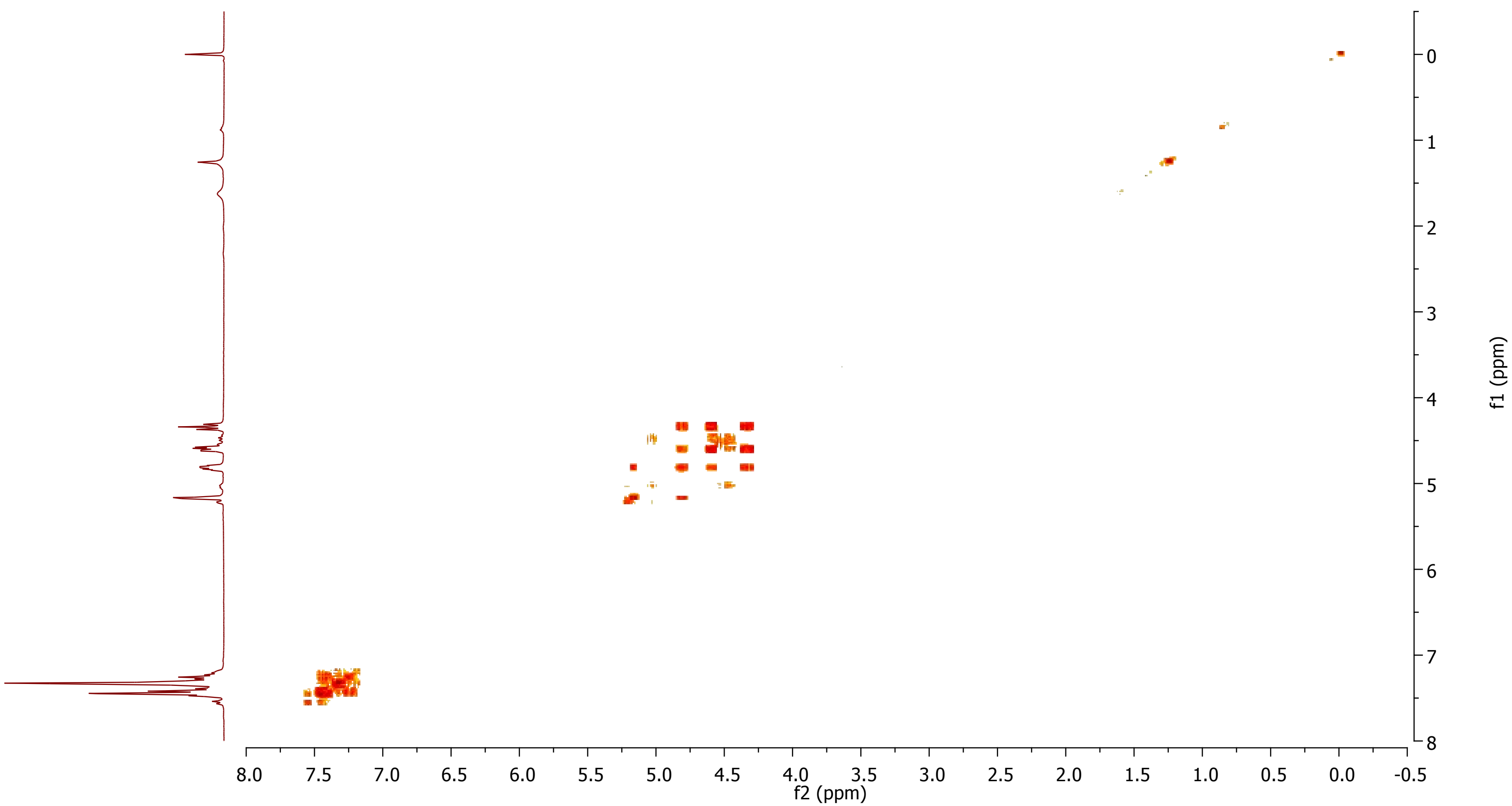
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2n**



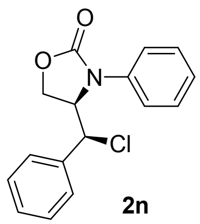
COSY of substrate **2n**



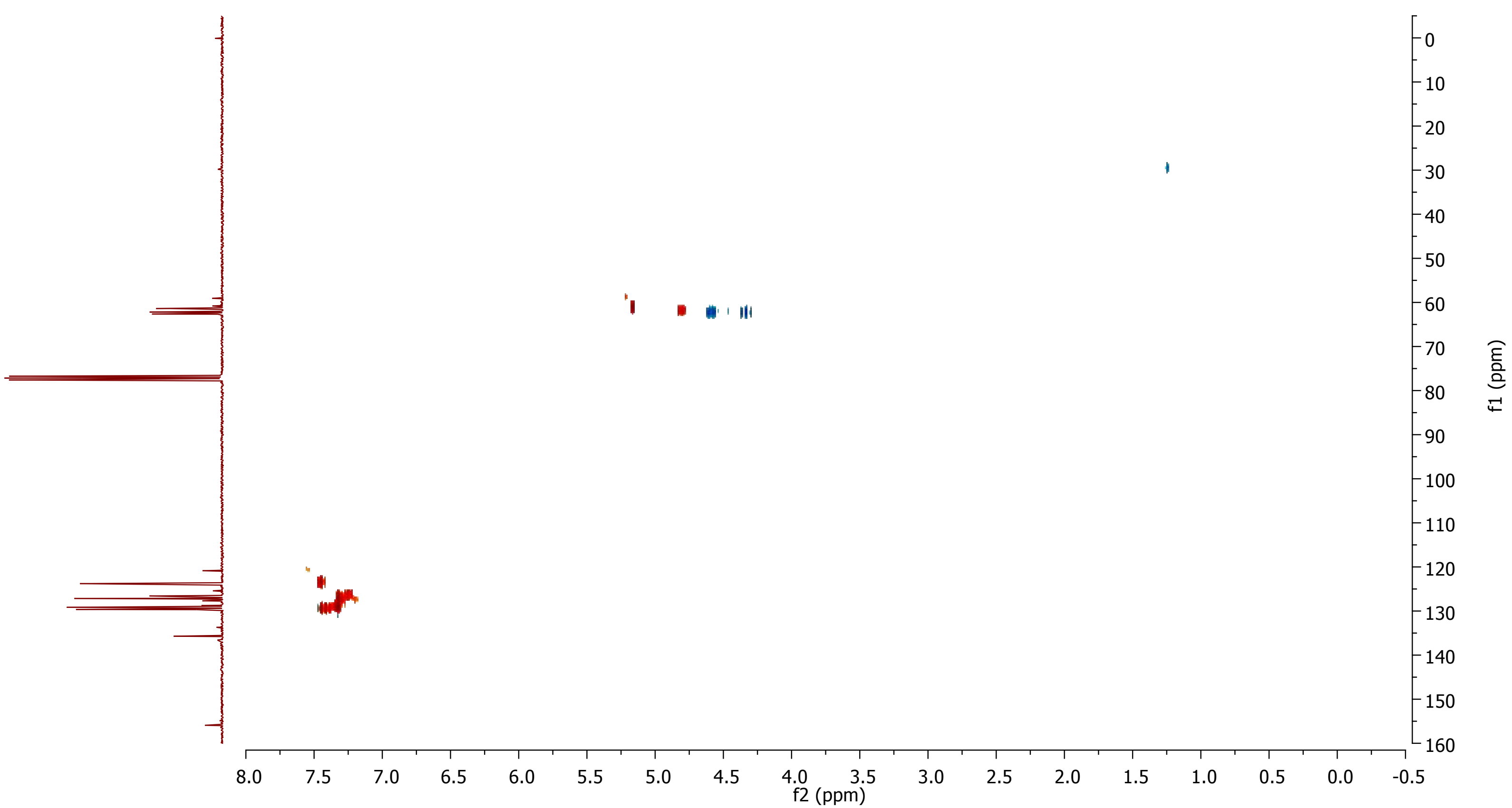
2n



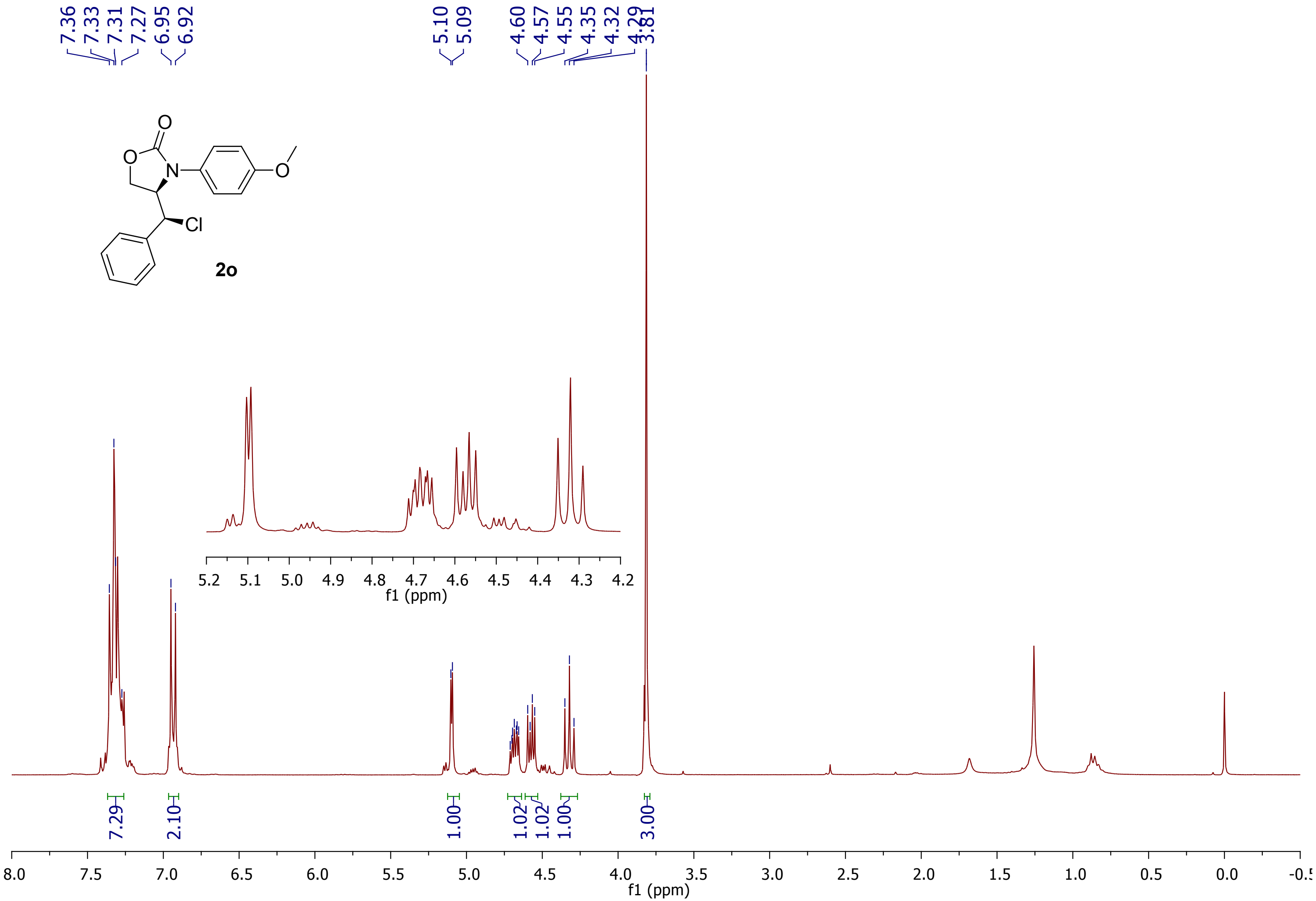
HSQC of substrate **2n**



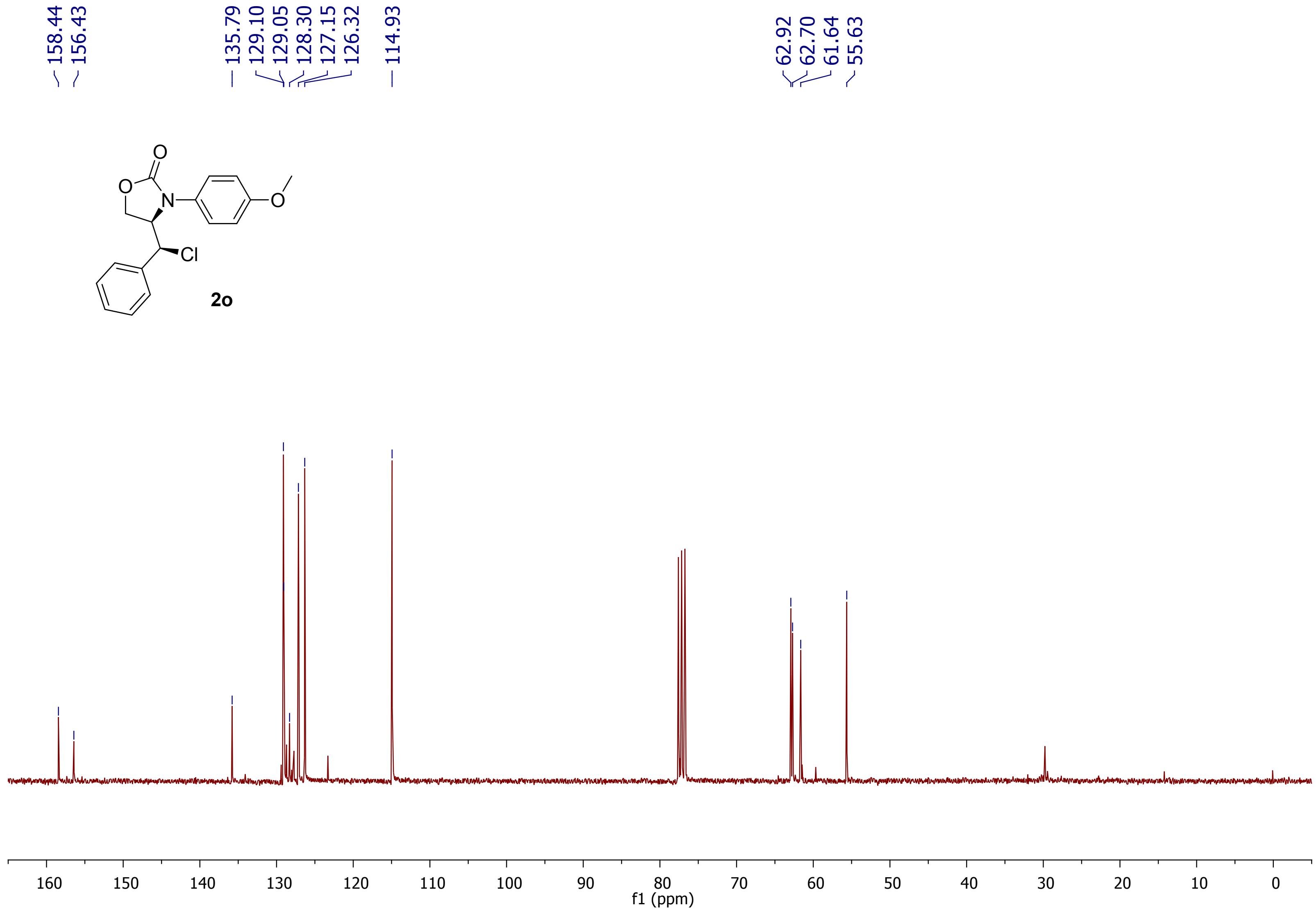
2n



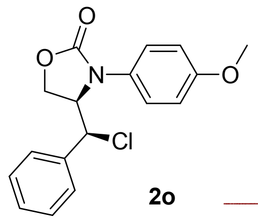
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2o**



^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2o**



COSY of substrate **2o**



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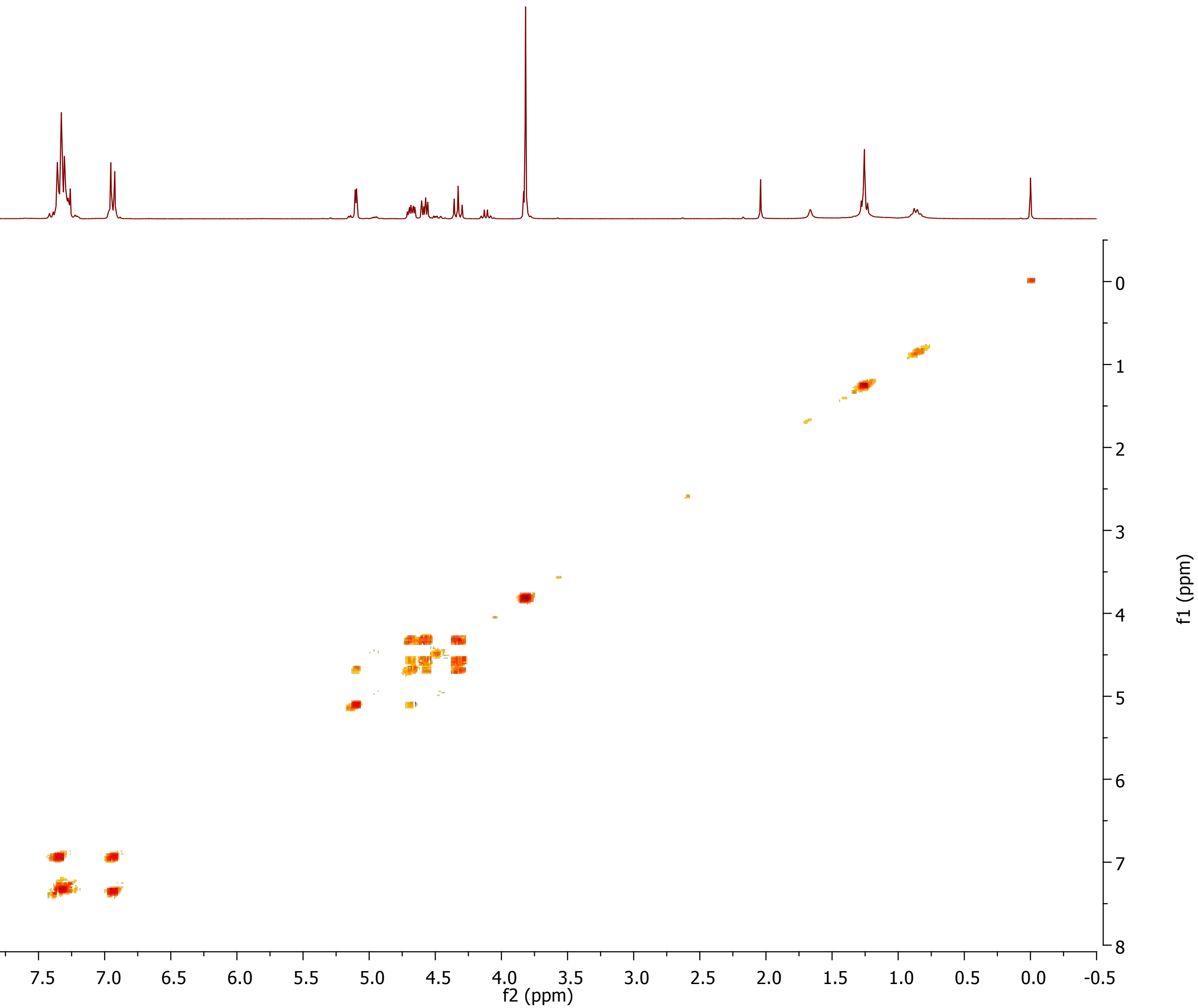
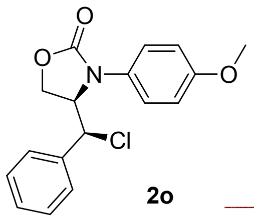
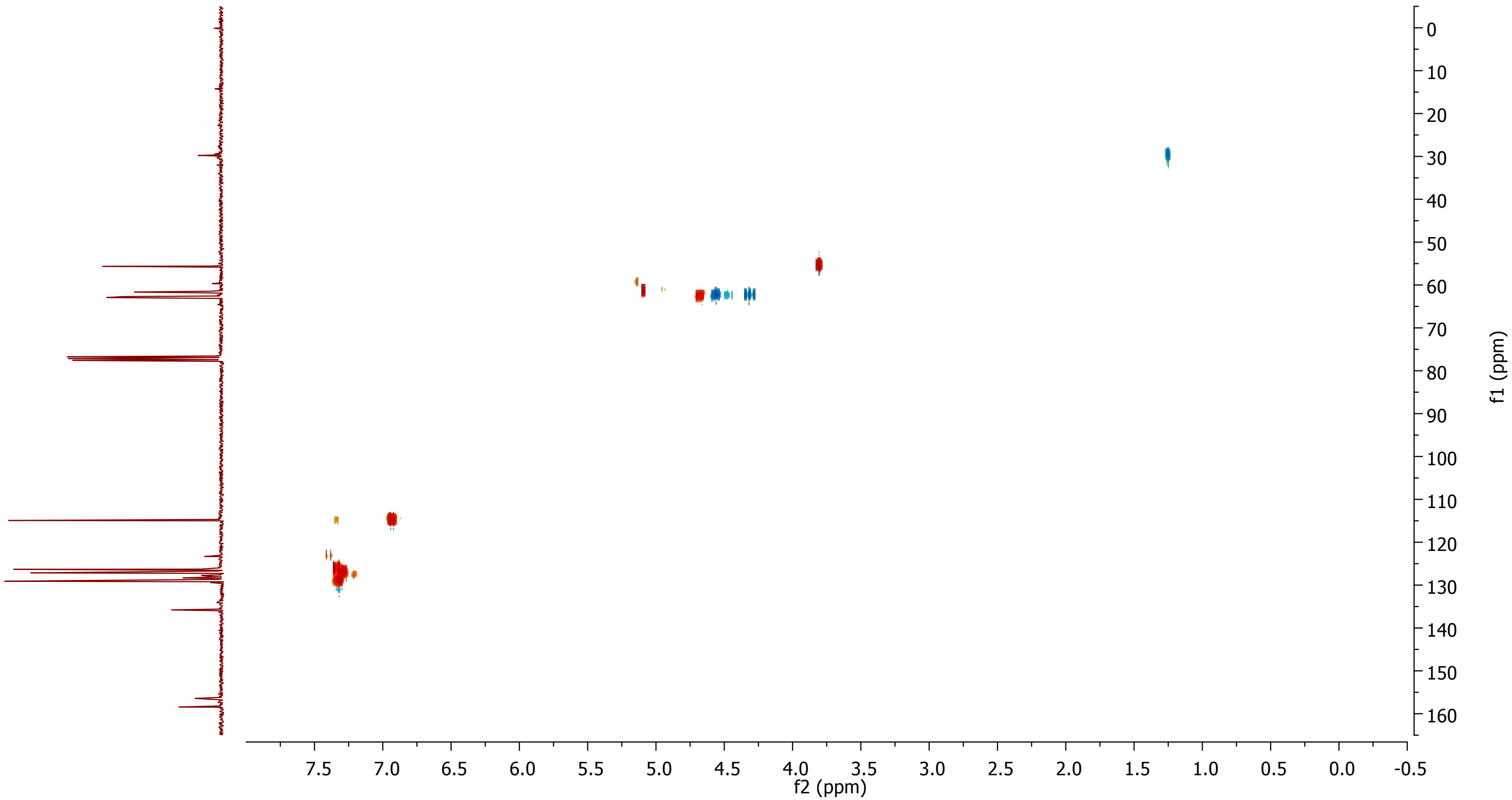


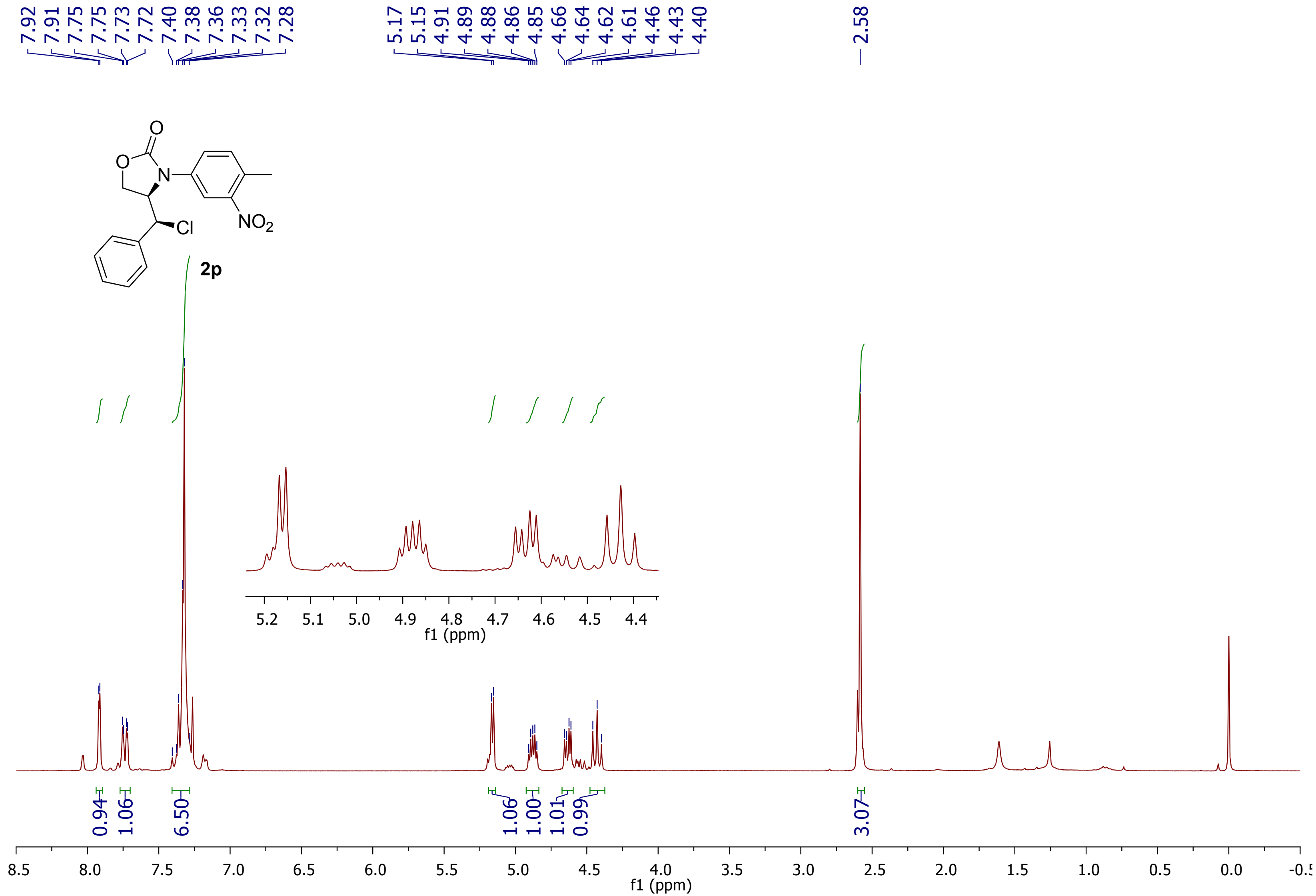
HSQC of substrate **2o**



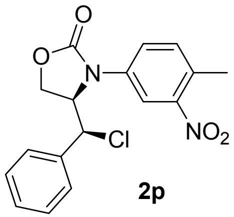
2o



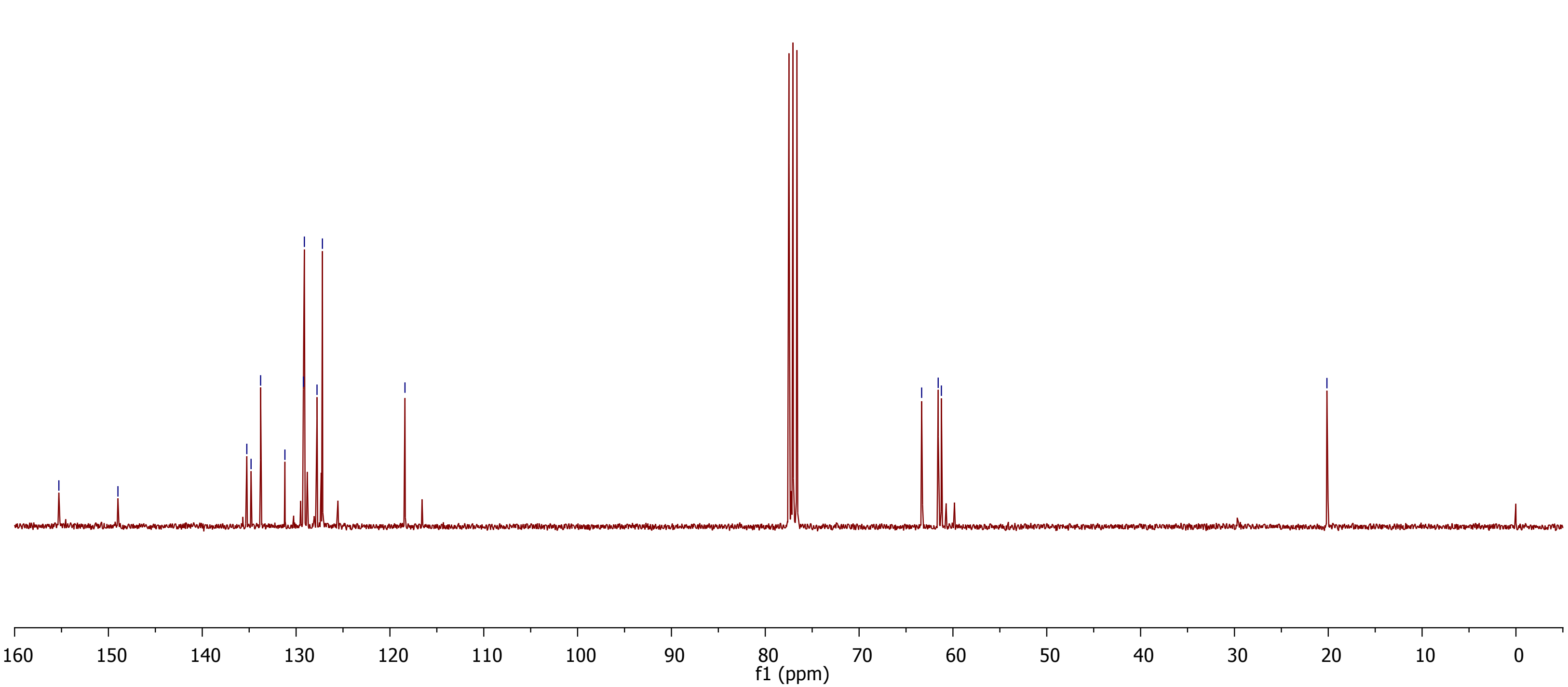
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2p**



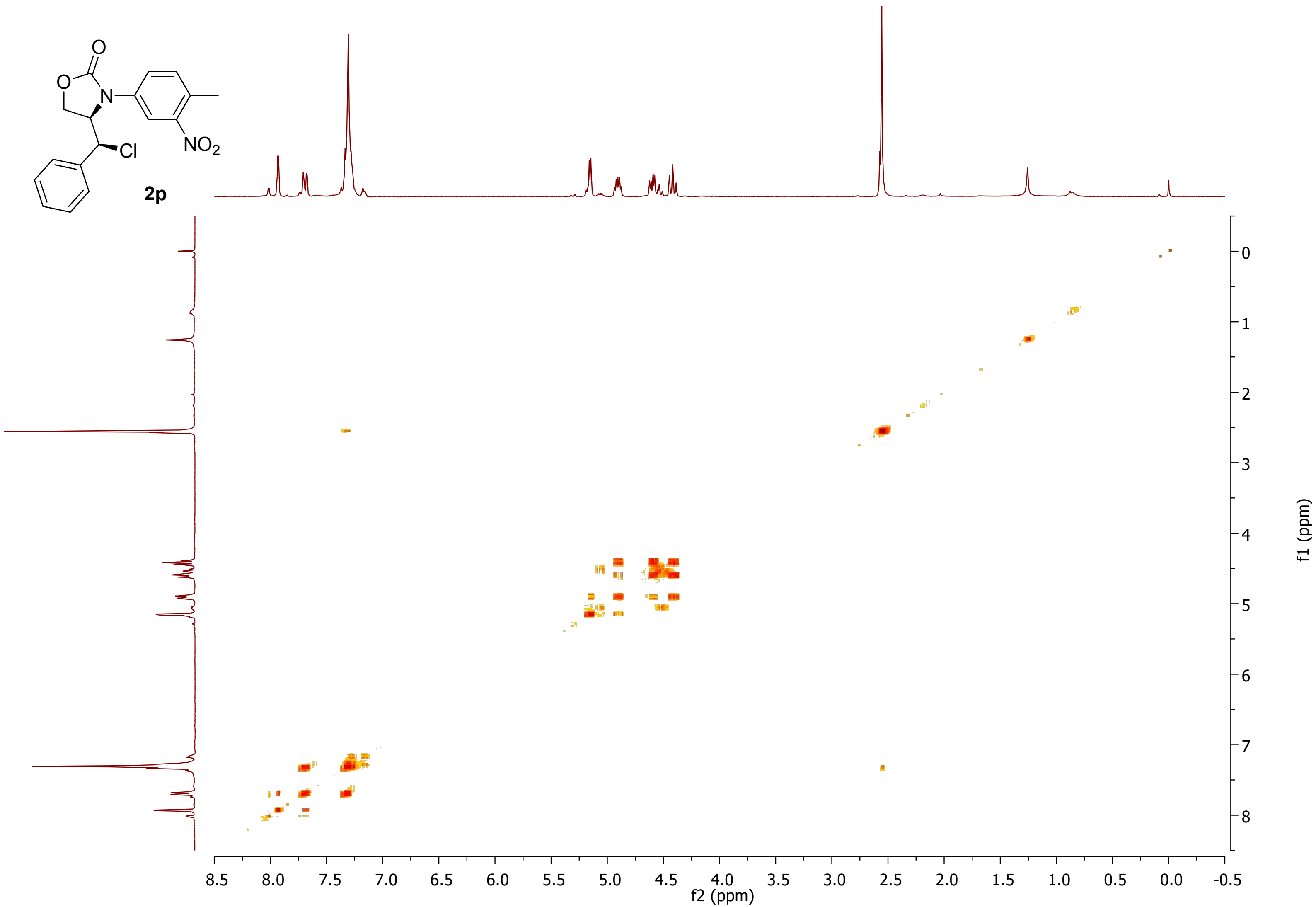
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2p**



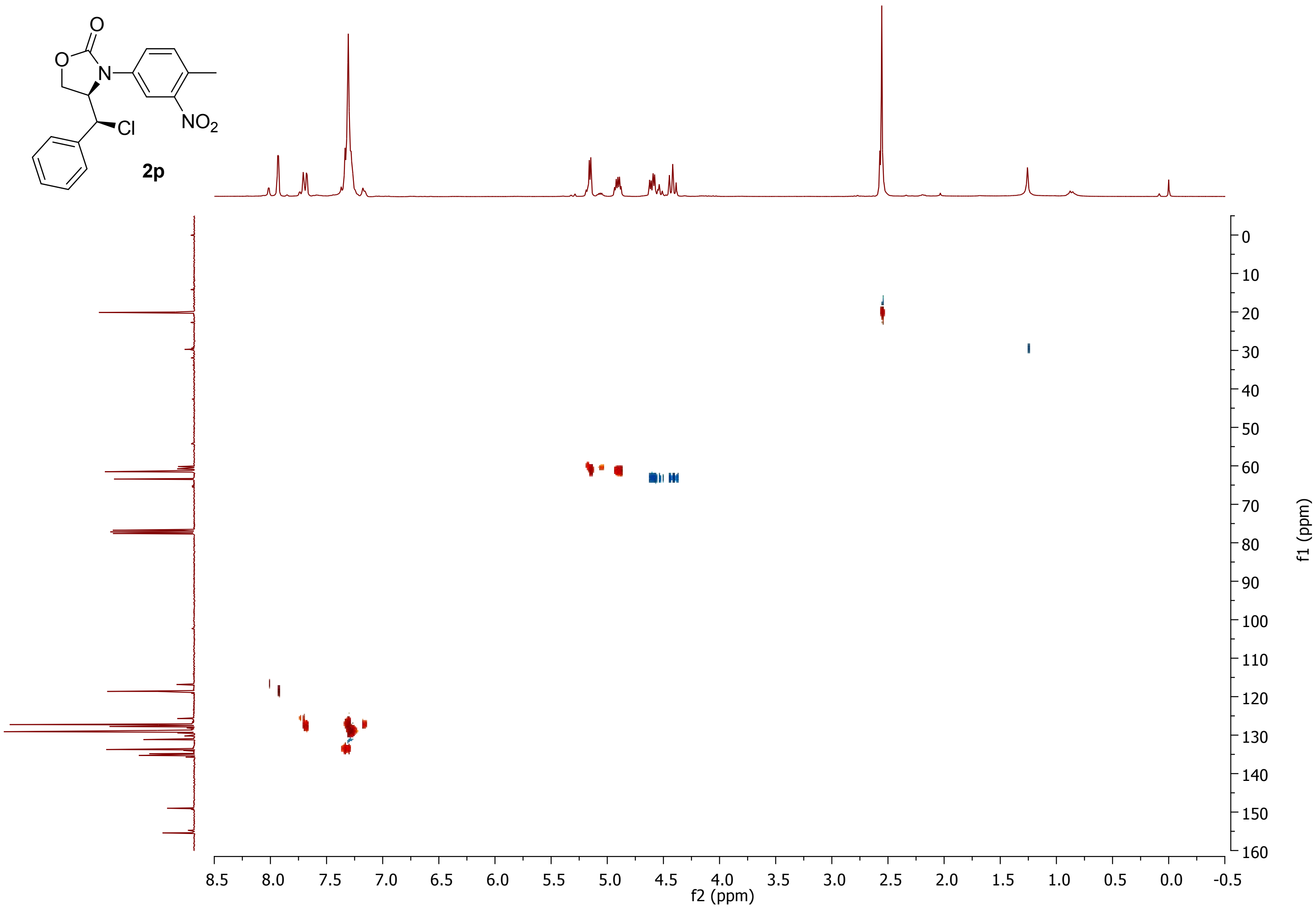
2p



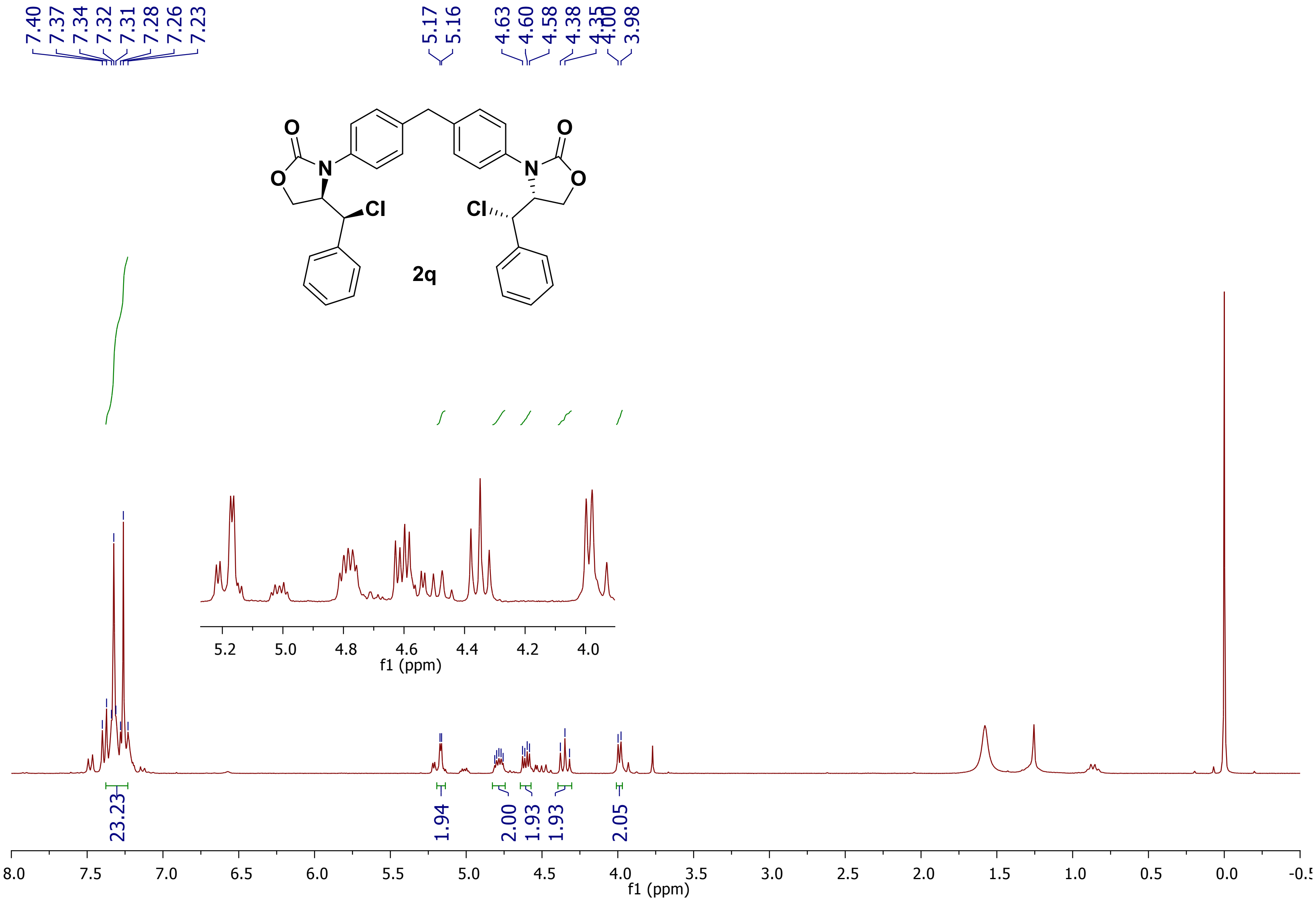
COSY of substrate **2p**



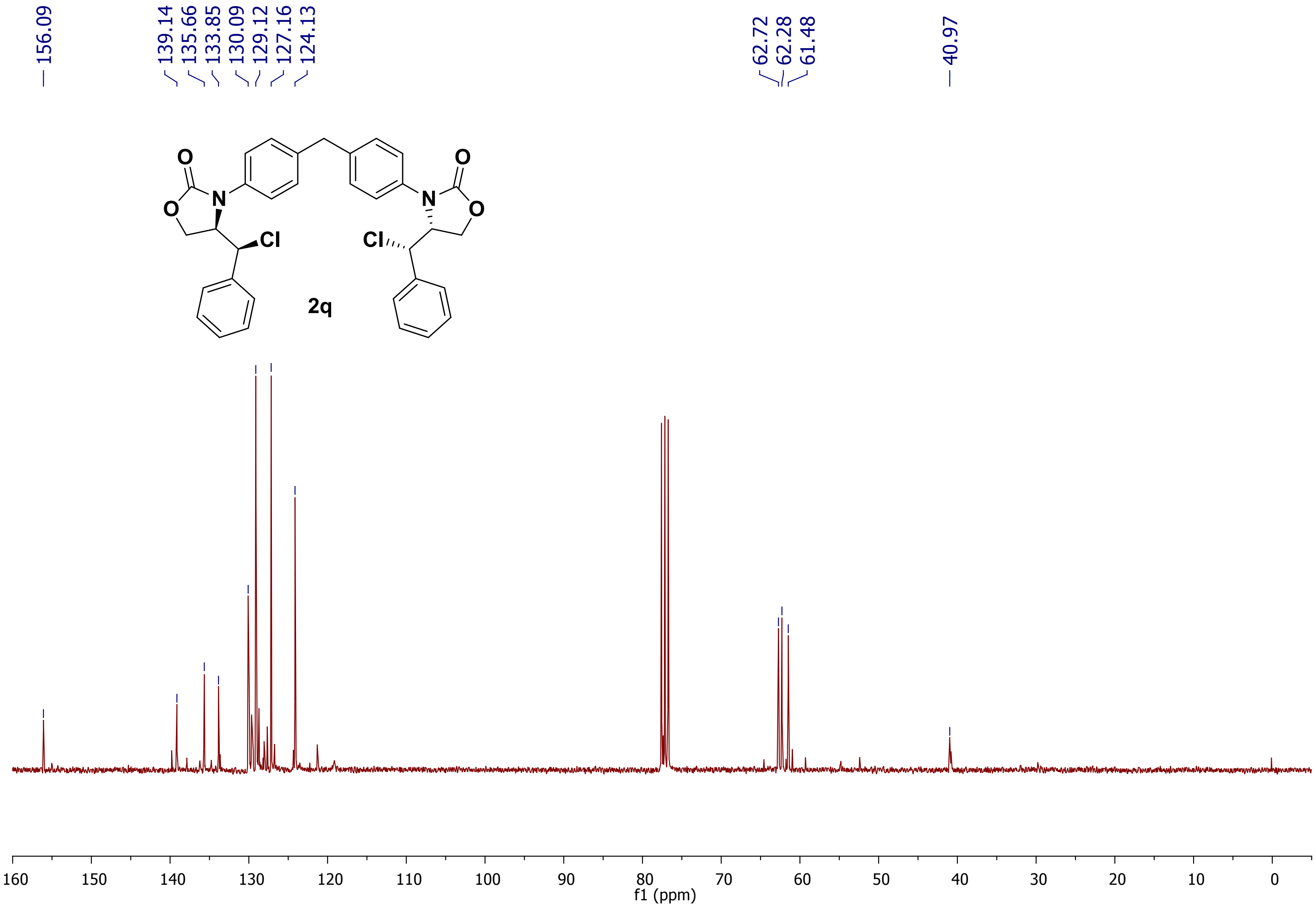
HSQC of substrate **2p**



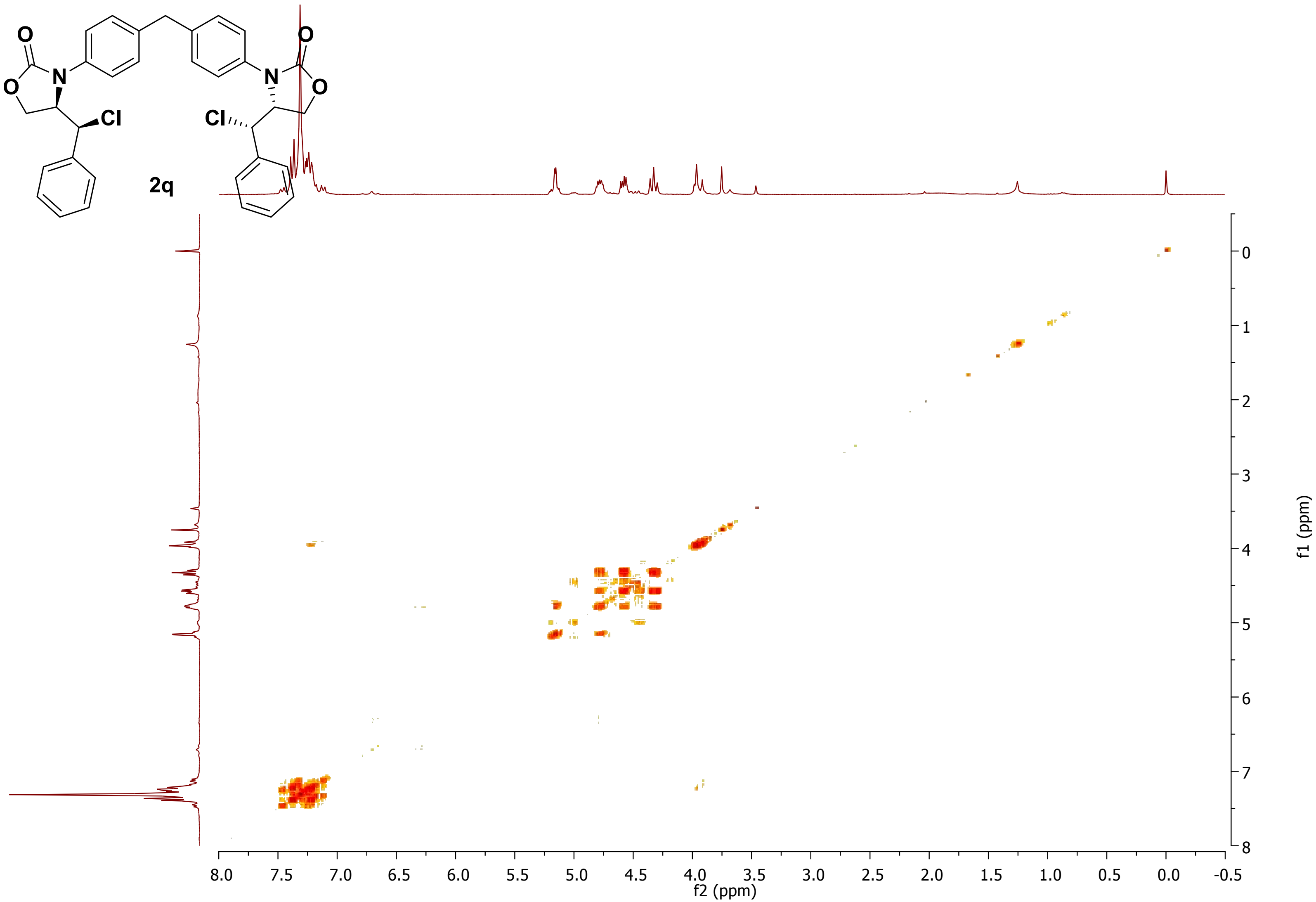
^{1}H NMR (300 MHz, $CDCl_3$) of substrate **2q**



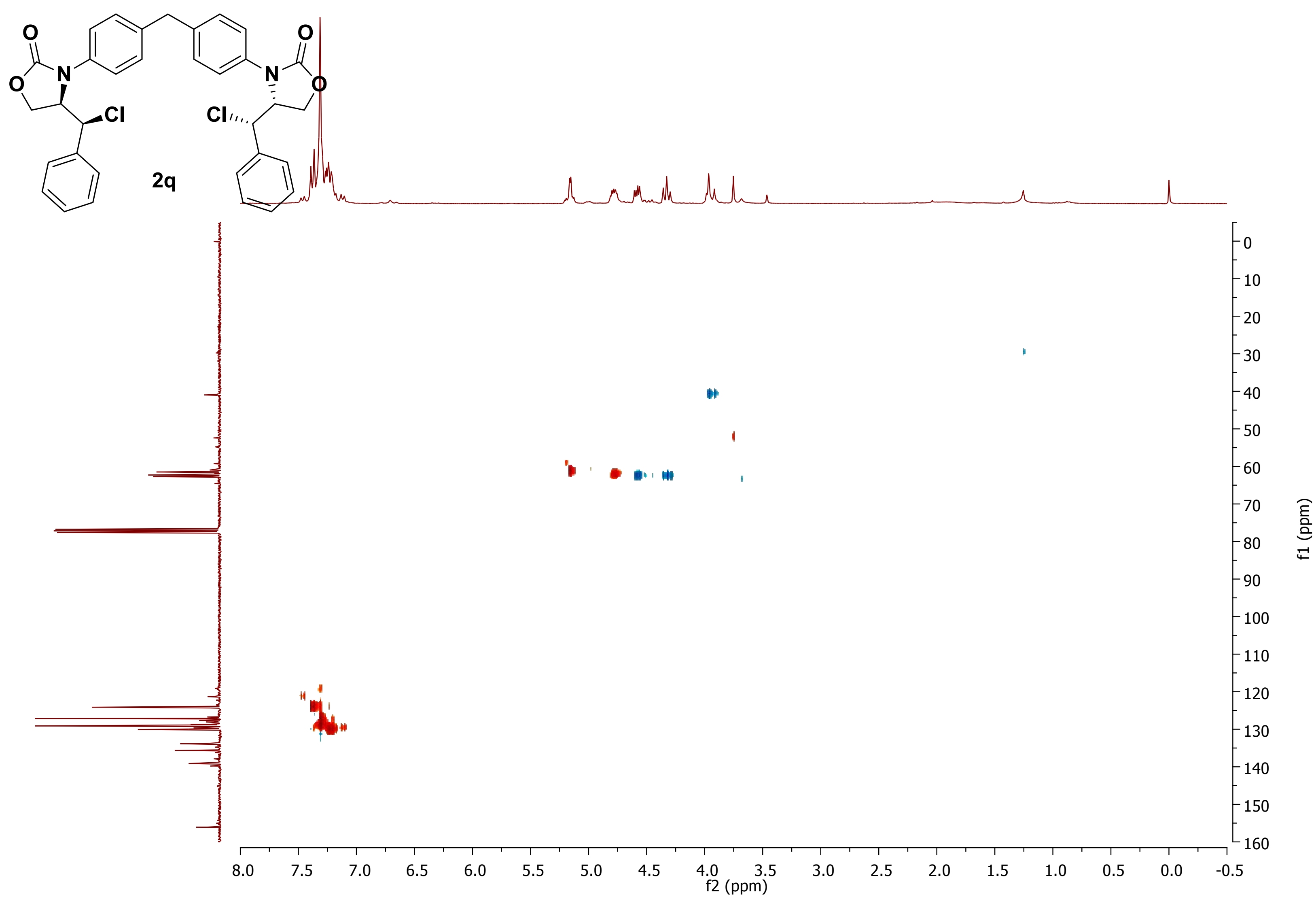
^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2q**



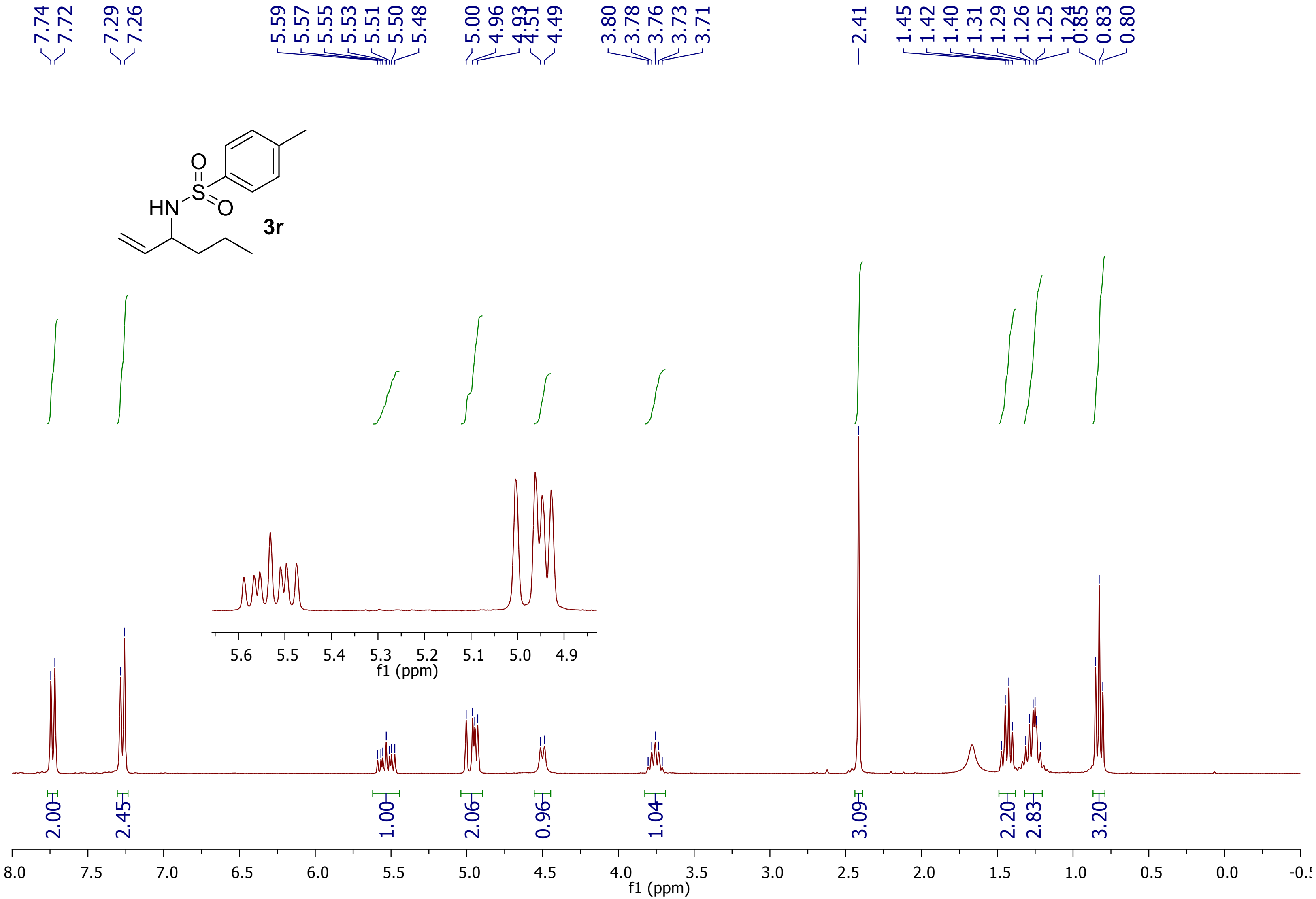
COSY of substrate **2q**



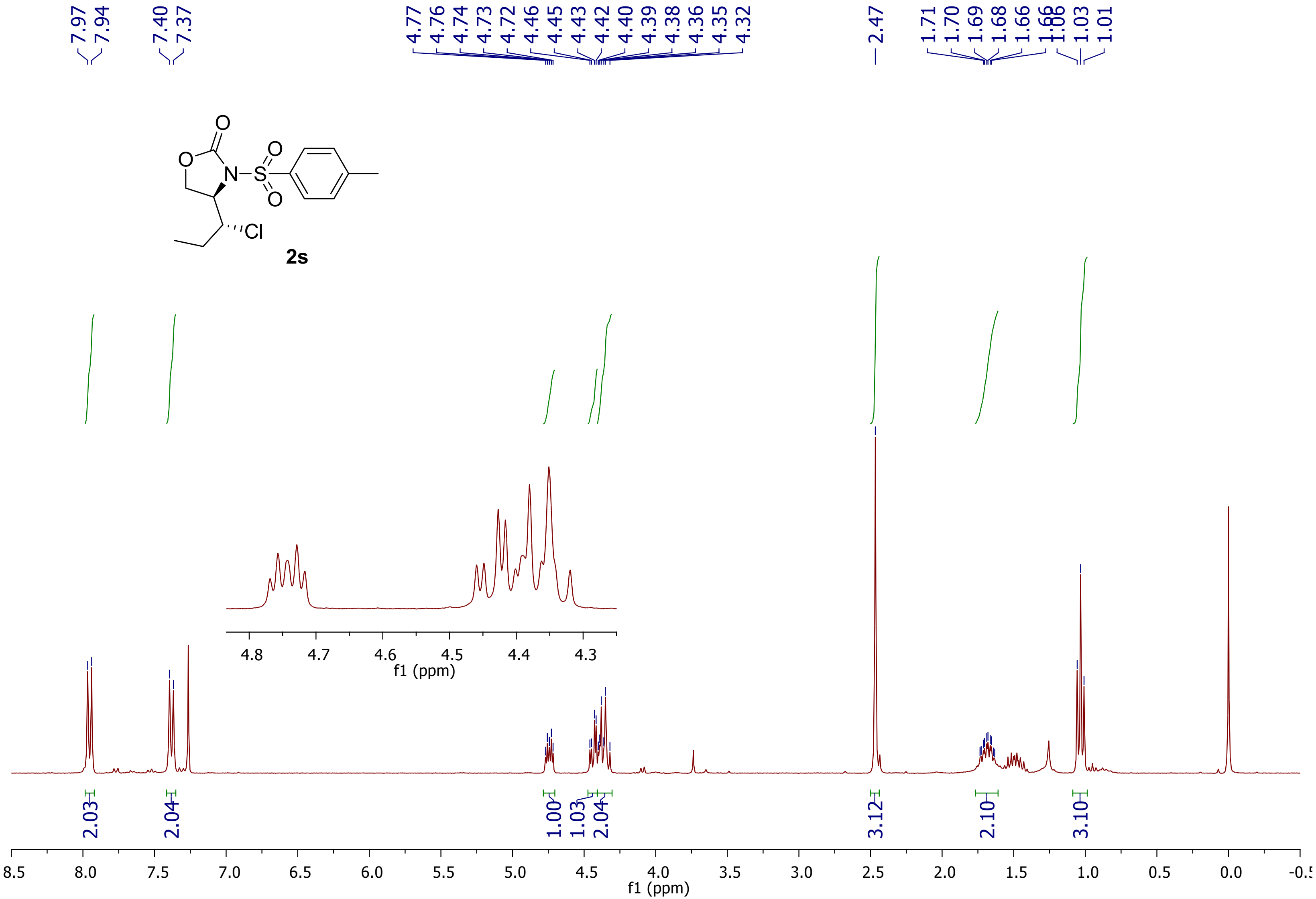
HSQC of substrate **2q**



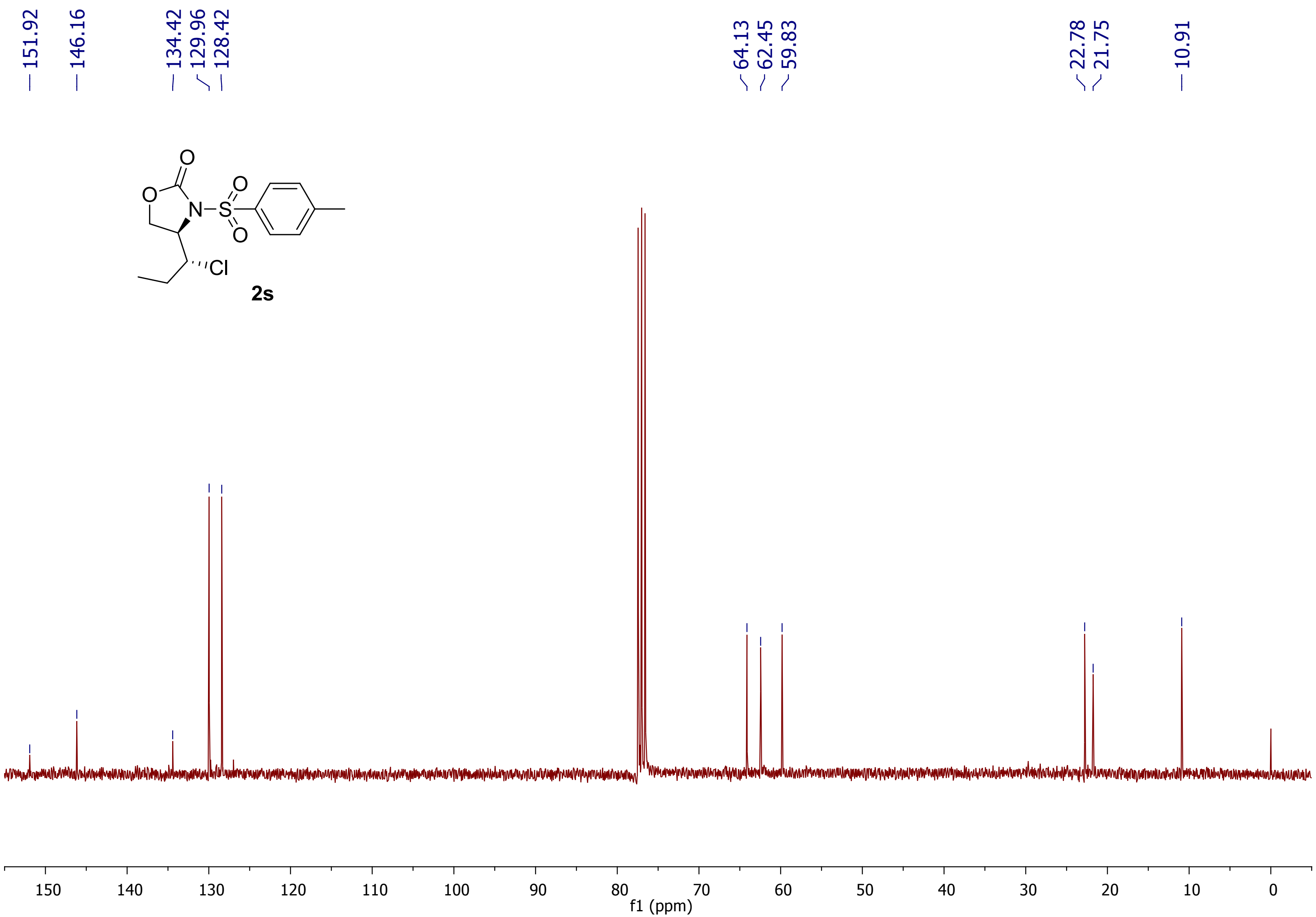
[1]H NMR (300 MHz, $CDCl_3$) of substrate **3r**



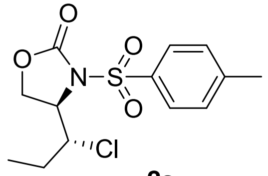
[1]H NMR (300 MHz, $CDCl_3$) of substrate **2s**

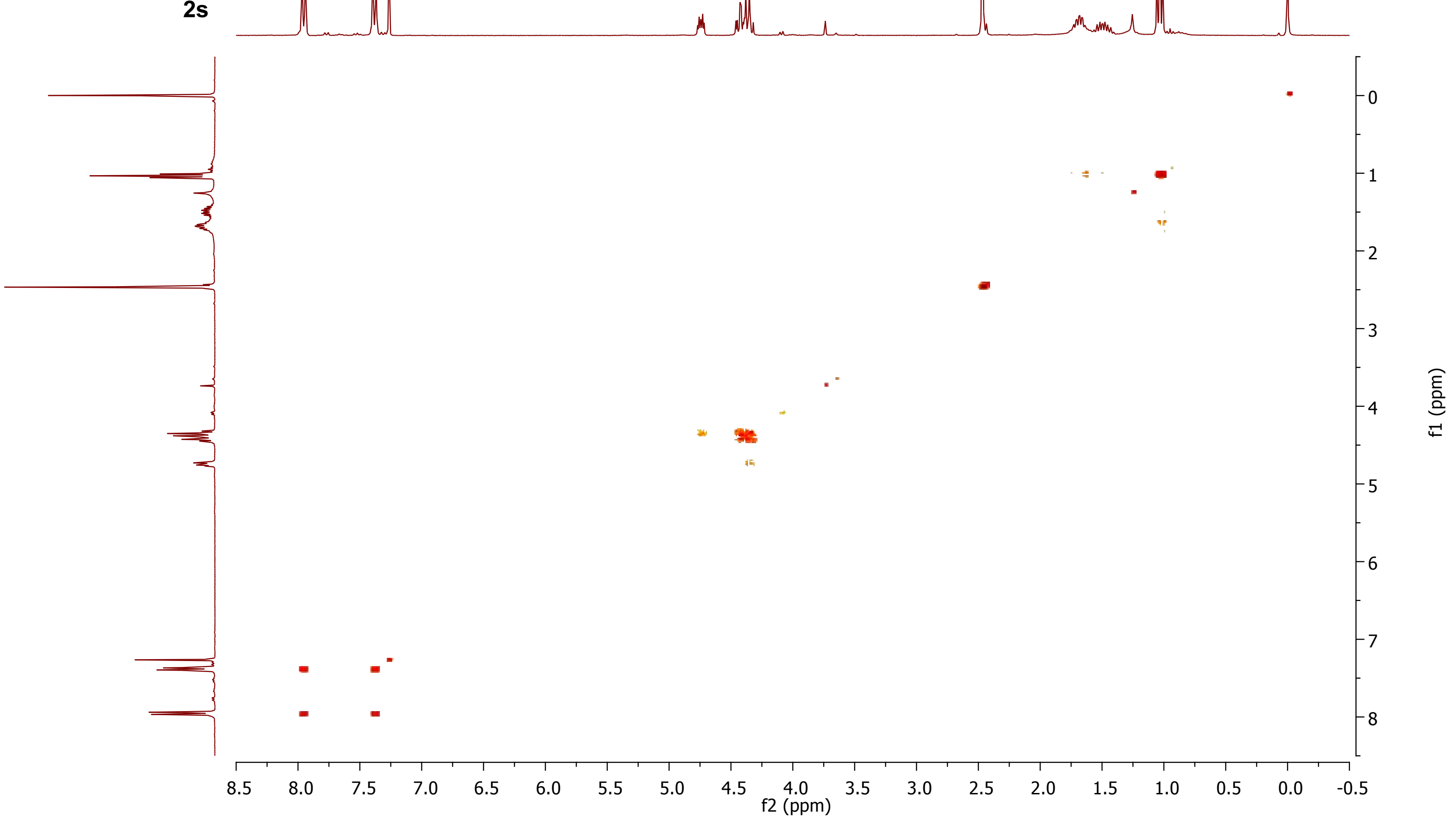


^{13}C NMR (75 MHz, $CDCl_3$) of substrate **2s**

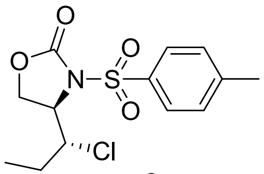


COSY of substrate **2s**

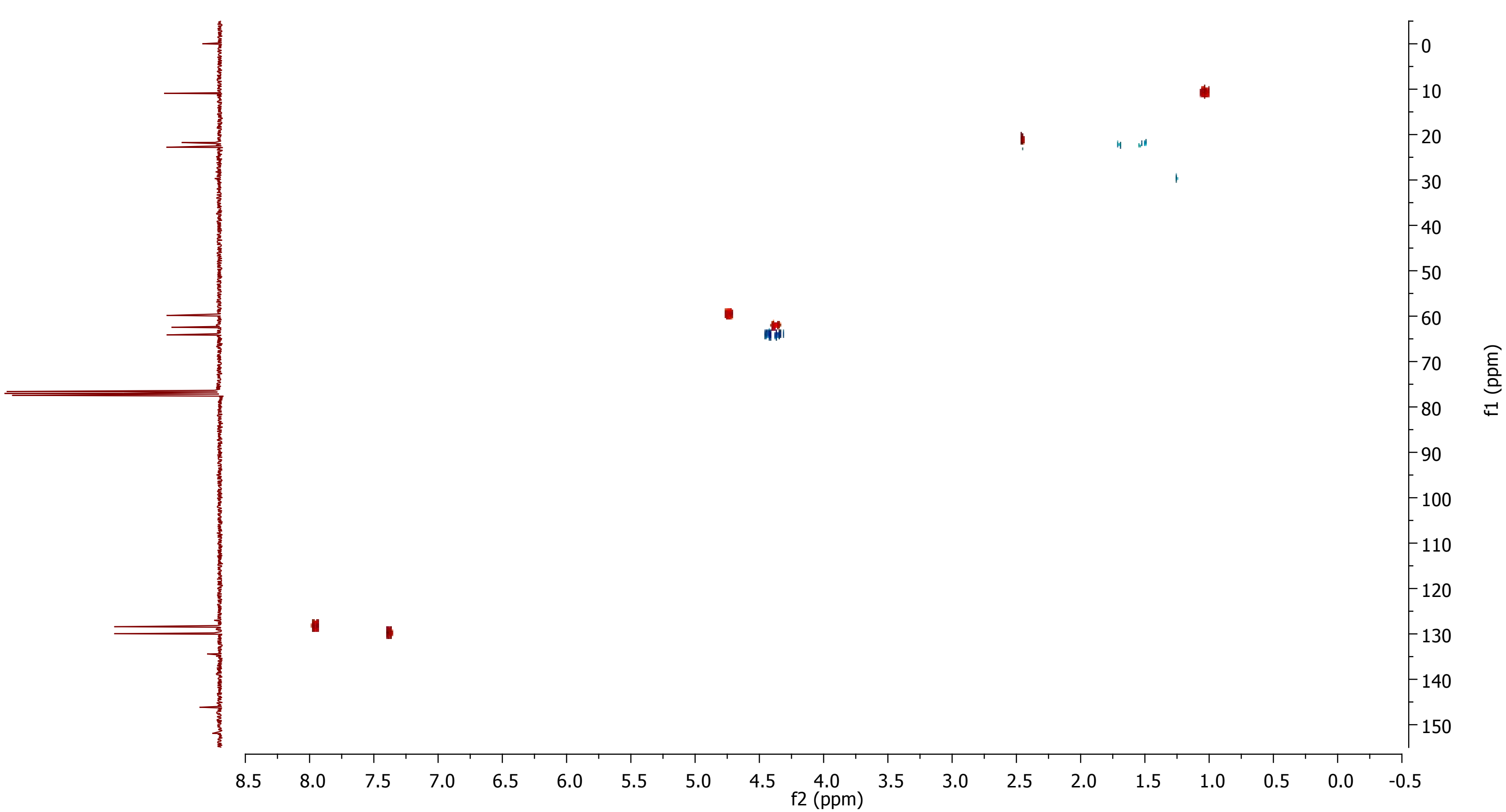

2s



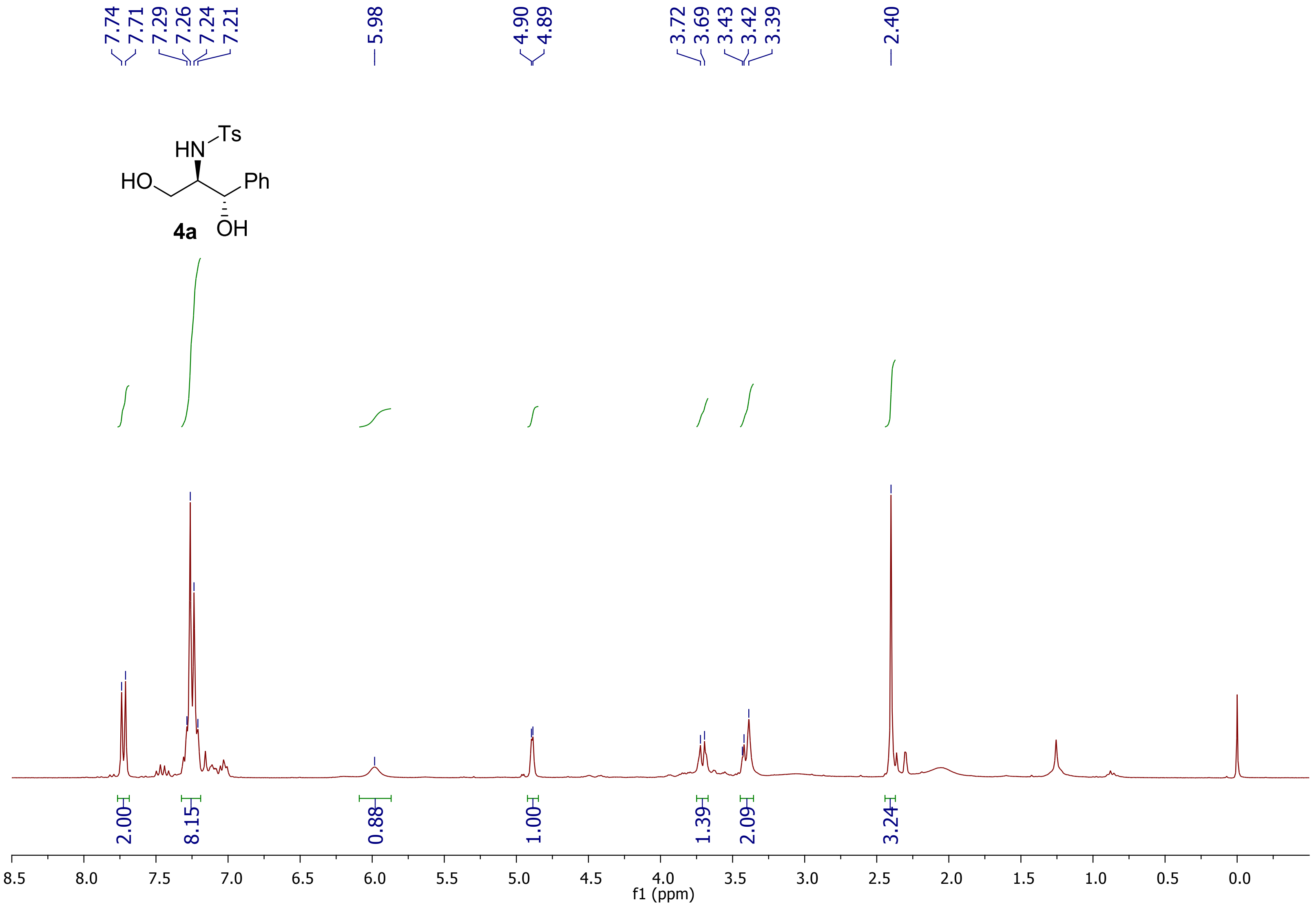
HSQC of substrate **2s**



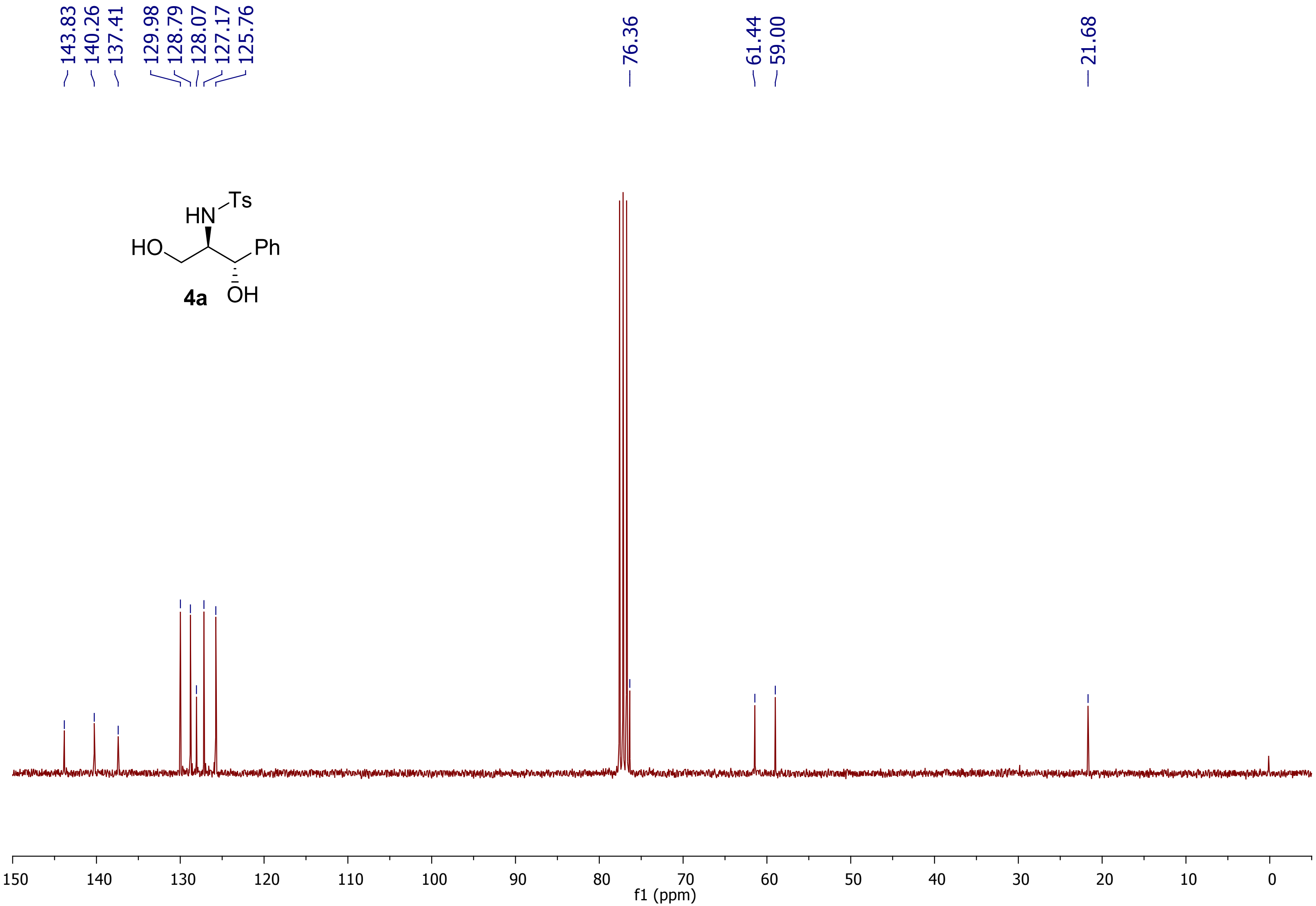
2s



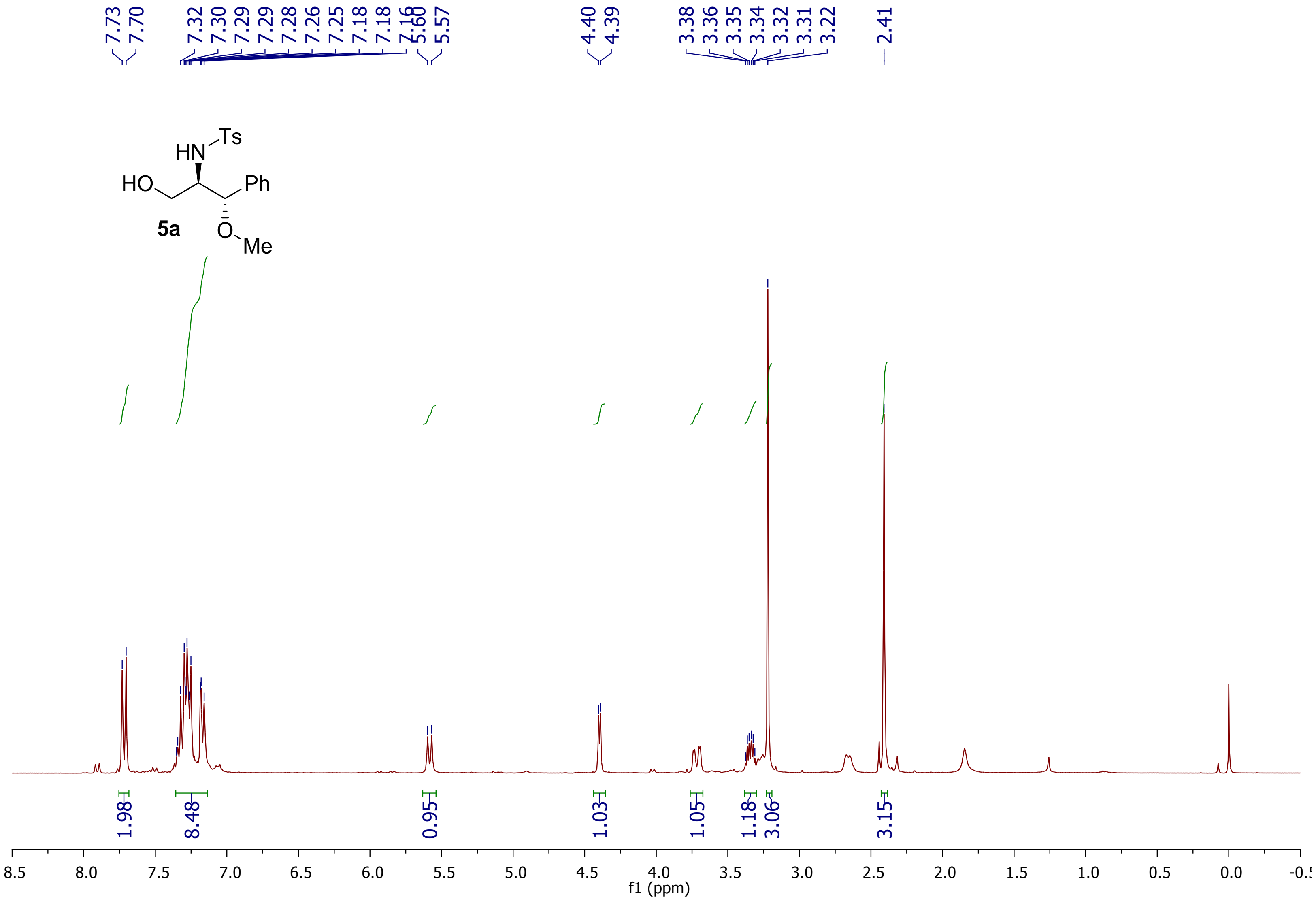
^{1}H NMR (300 MHz, $CDCl_3$) of compound **4a**



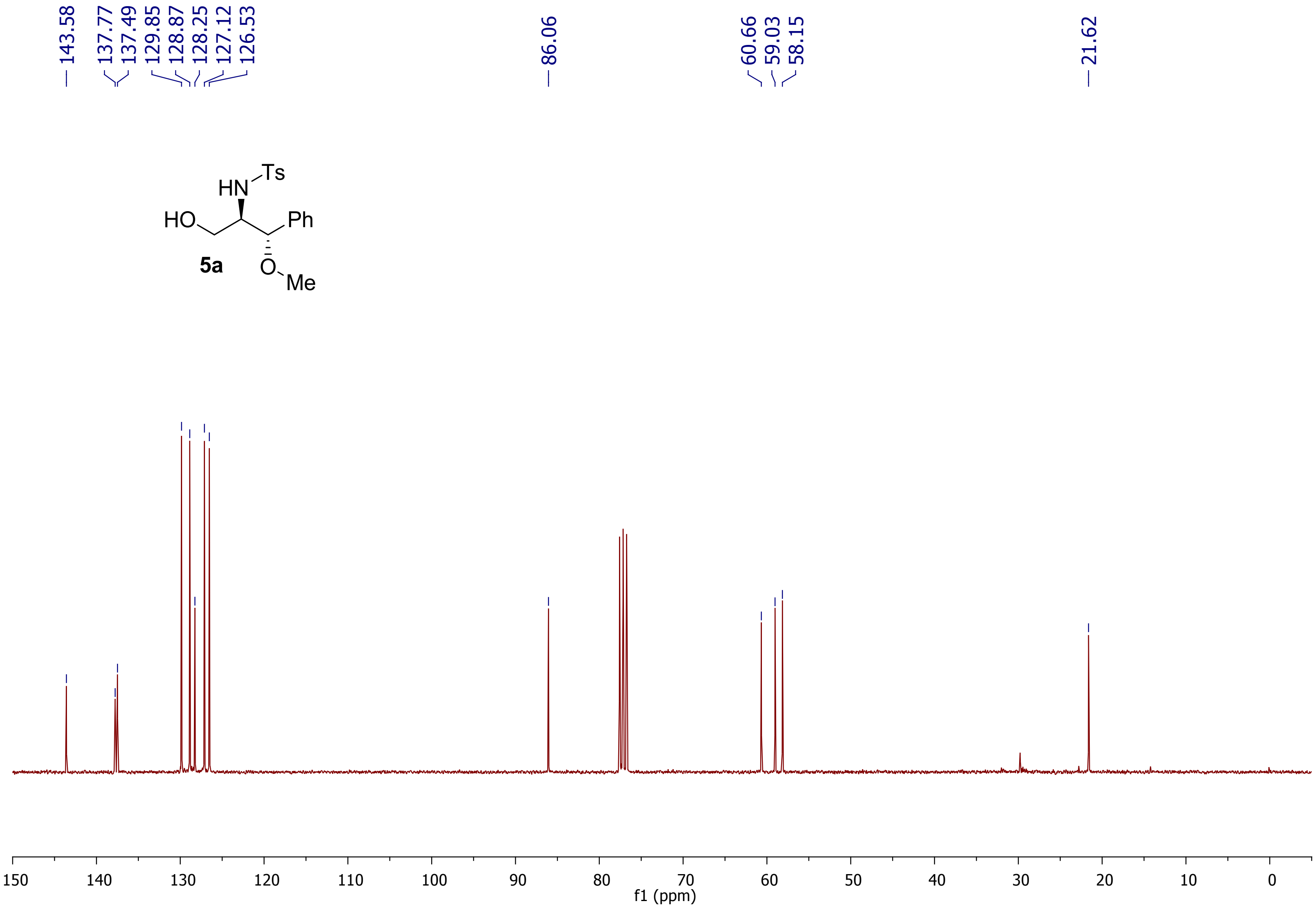
^{13}C NMR (75 MHz, $CDCl_3$) of compound **4a**



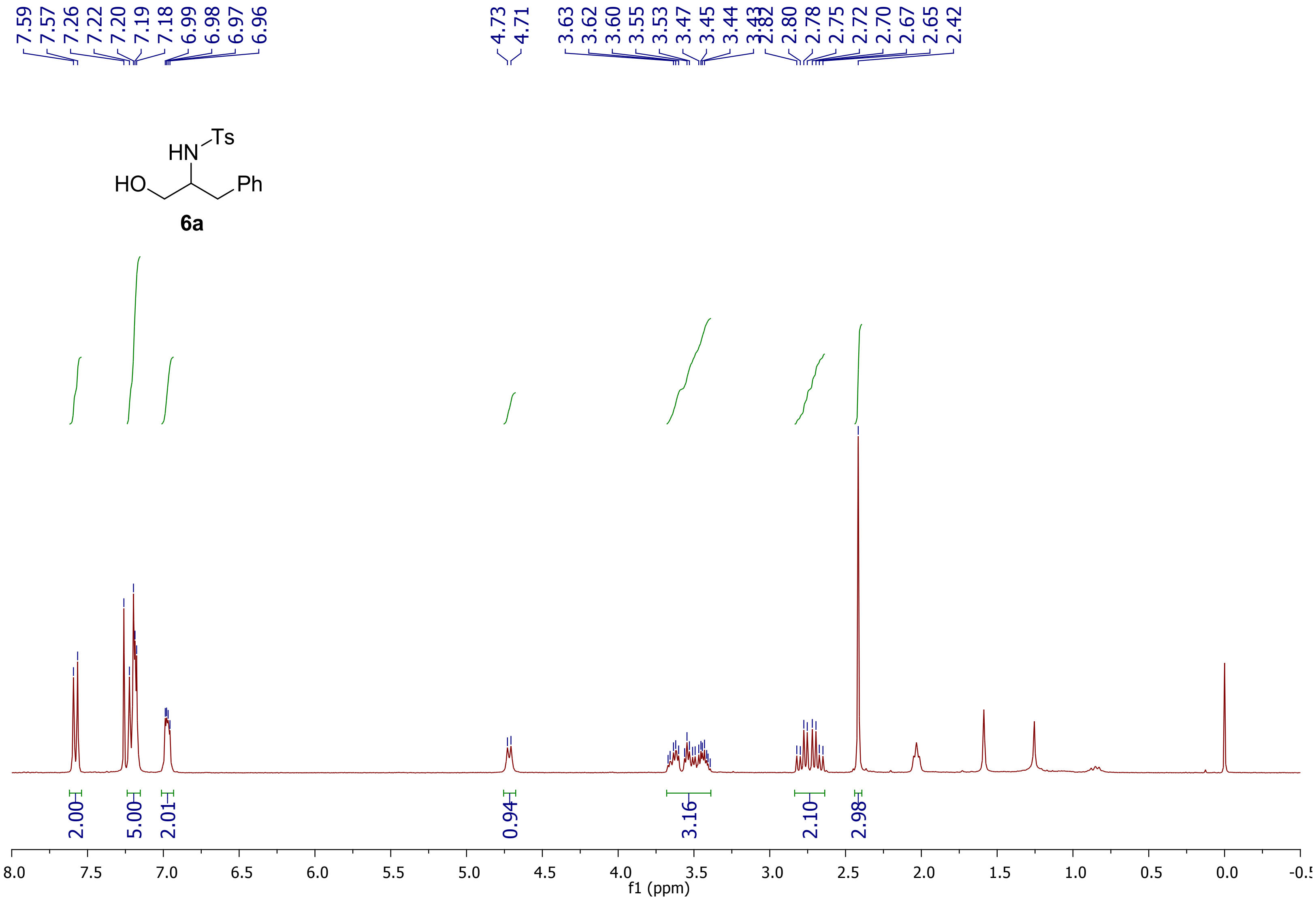
^{1}H NMR (300 MHz, $CDCl_3$) of compound **5a**



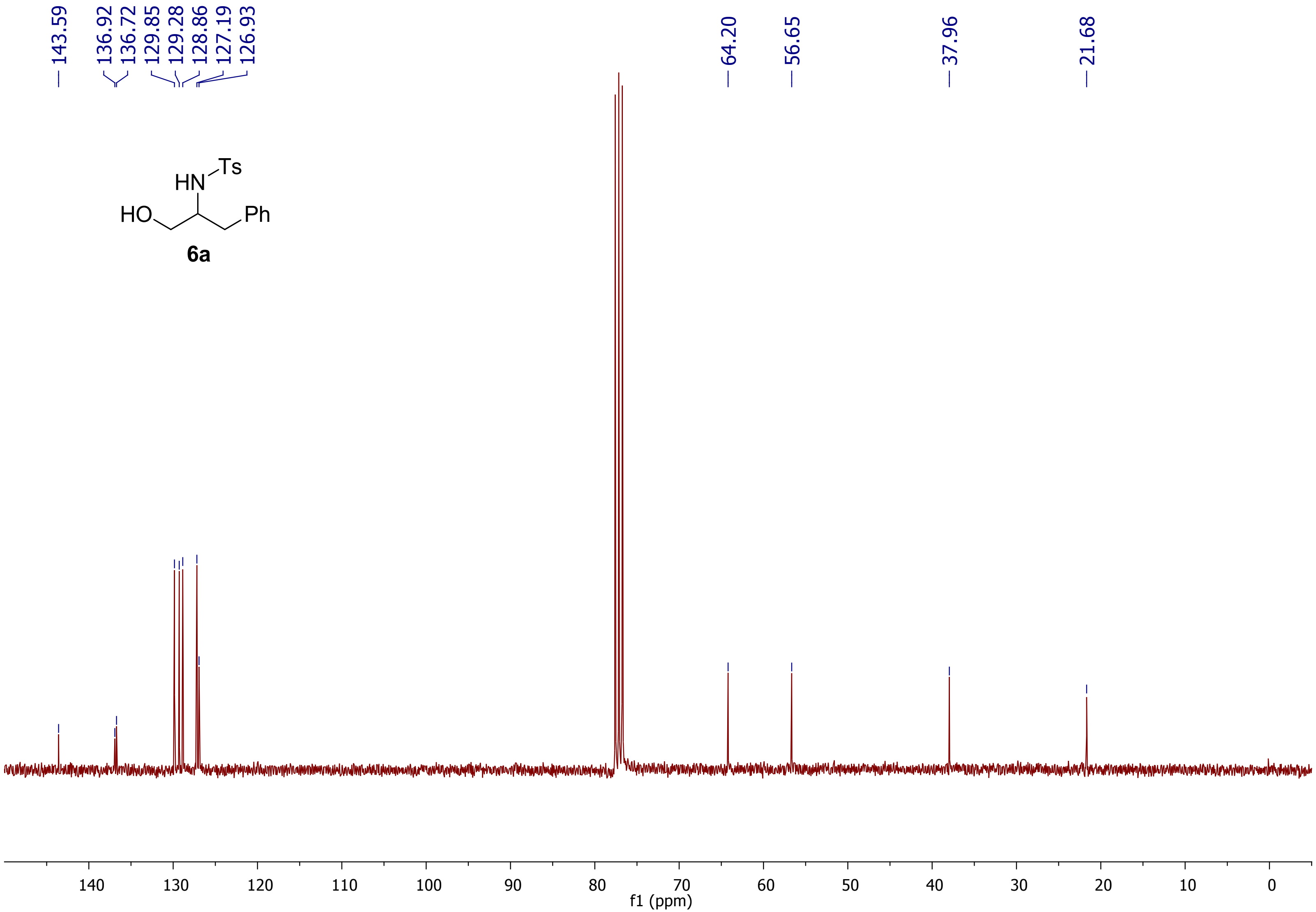
^{13}C NMR (75 MHz, $CDCl_3$) of compound **5a**



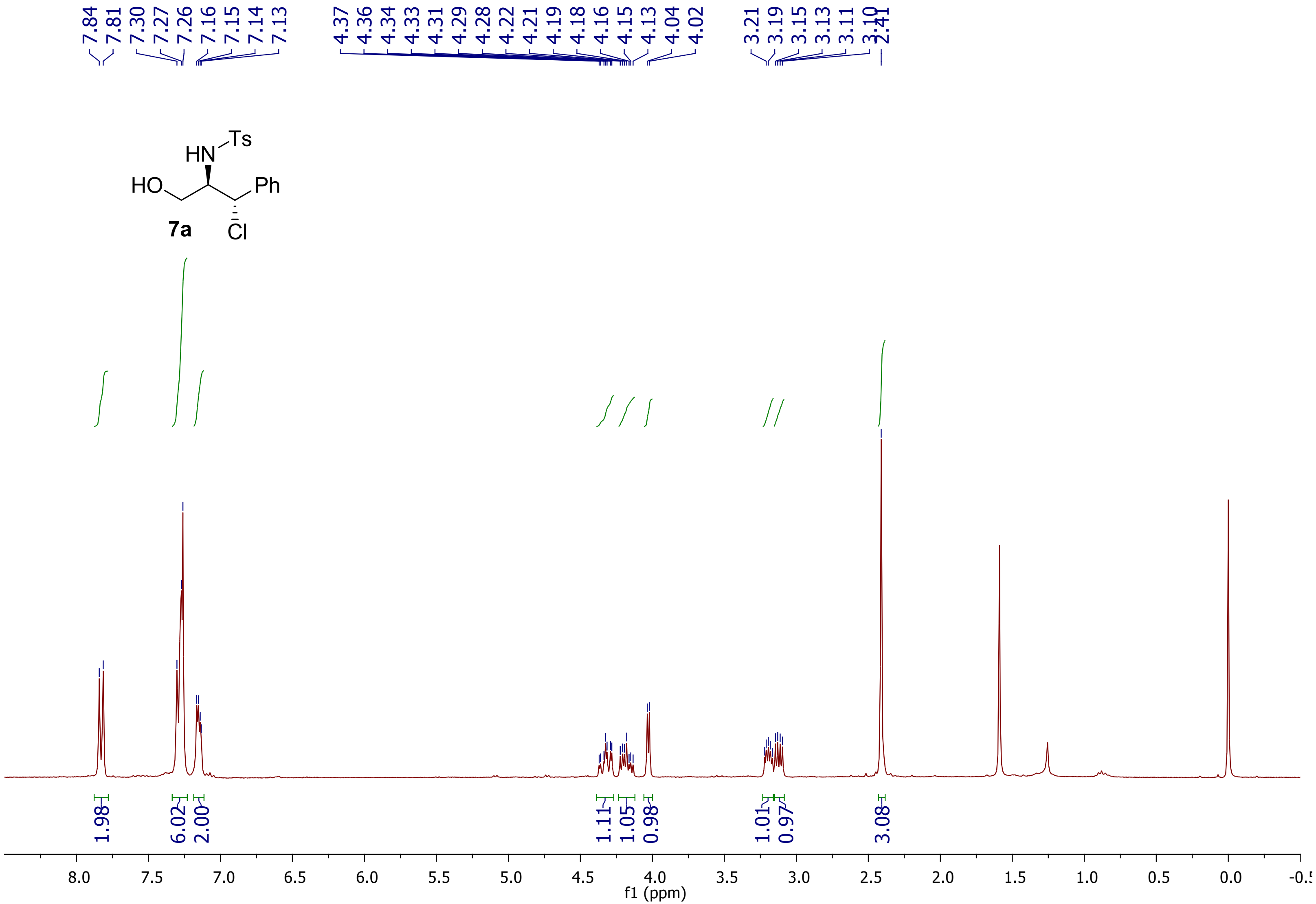
[1]H NMR (300 MHz, $CDCl_3$) of compound **6a**



^{13}C NMR (75 MHz, $CDCl_3$) of compound **6a**



[1]H NMR (300 MHz, $CDCl_3$) of compound **7a**



^{13}C NMR (75 MHz, $CDCl_3$) of compound **7a**