

Supporting Information for
**Palladium-Catalyzed Decarbonylative Dehydration of Fatty Acids
for the Production of Linear Alpha Olefins**

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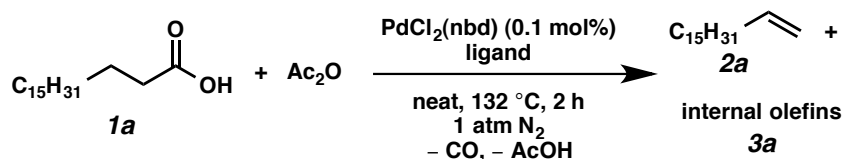
Table of Contents:

Materials and Methods	SI2
General Procedure for Optimization Reactions (Route A)	SI3
General Procedure for Optimization Reactions (Route B)	SI5
General Procedure for Preparative Pd-Catalyzed Decarbonylative Dehydration	SI6
Spectroscopic Data for Acid Substrates	SI8
Spectroscopic Data for Olefin Products	SI10
General Procedure for Pheromone Synthesis by Ru-Catalyzed Cross Metathesis	SI16
¹ H NMR and ¹³ C NMR Spectra	SI20

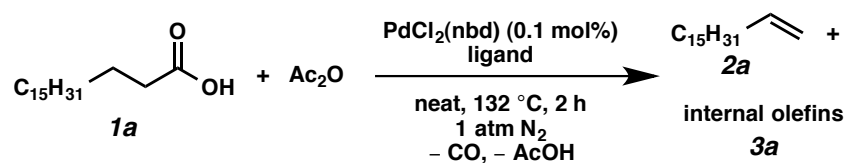
Materials and Methods.

Unless otherwise stated, reactions were performed in flame-dried glassware under a nitrogen atmosphere or under vacuum without the use of solvents. Reaction progress was monitored by ^1H NMR analysis of the crude reaction mixture. Silicycle SiliaFlash® P60 Academic Silica gel (particle size 40–63 nm) was used for flash chromatography. ^1H NMR spectra were recorded on a Varian Inova 500 MHz spectrometer and are reported relative to residual CHCl_3 (δ 7.26 ppm) or DMSO (δ 2.50 ppm). ^{13}C NMR spectra were recorded on a Varian Inova 500 MHz spectrometer (125 MHz) and are reported relative to CHCl_3 (δ 77.16 ppm) or DMSO (δ 39.52 ppm). Data for ^1H NMR are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sept = septuplet, m = multiplet, br s = broad singlet, br d = broad doublet, app = apparent. Data for ^{13}C NMR are reported in terms of chemical shifts (δ ppm). IR spectra were obtained by use of a Perkin Elmer Spectrum BXII spectrometer using thin films deposited on NaCl plates and reported in frequency of absorption (cm^{-1}). High resolution mass spectra (HRMS) were provided by the California Institute of Technology Mass Spectrometry Facility using a JEOL JMS-600H High Resolution Mass Spectrometer by positive-ion FAB, or obtained with an Agilent 6200 Series TOF using Agilent G1978A Multimode source in negative electrospray ionization (ESI $^-$), negative atmospheric pressure chemical ionization (APCI $^-$), or negative mixed ionization mode (NMM: ESI-APCI $^-$).

Reagents were purchased from Sigma-Aldrich, Acros Organics, Strem, or Alfa Aesar and used as received unless otherwise stated.

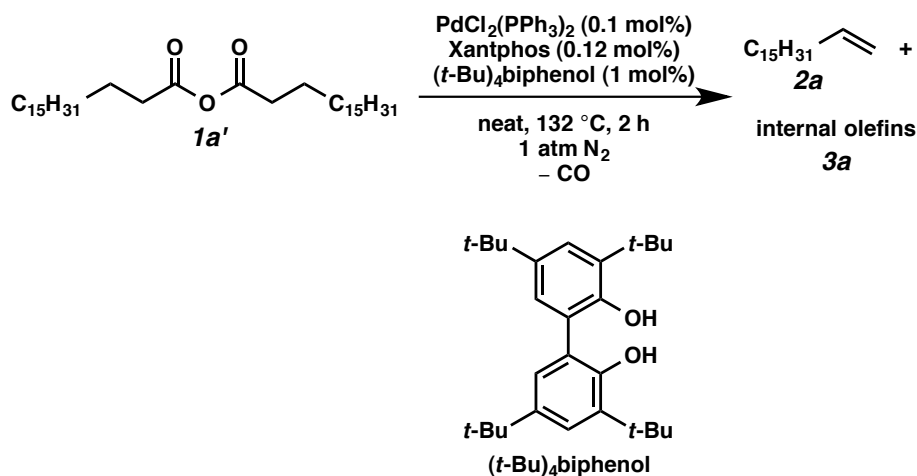
General Procedure for Optimization Reactions (Route A)

To a 20 x 150 mm Kimble glass tube equipped with a magnetic stir bar was added $\text{PdCl}_2(\text{nbd})$ (0.005 mmol, 0.1 mol%), ligand (monophosphine: 0.04 mmol, 0.8 mol%; diphosphine: 0.02 mmol, 0.4 mol%), and stearic acid **1a** (5 mmol, 1 equiv). The tube was sealed with a rubber septum, evacuated and refilled with N_2 (x 3), and acetic anhydride (10 mmol, 2 equiv) was added via syringe. The reaction tube placed in a preheated 132 °C oil bath (glass thermometer reading = 132 °C, IKA reading = 140 °C) and stirred for 2 h. The oil bath was removed, and methyl benzoate (internal standard, 5 mmol, 1 equiv) was added and the resulting mixture stirred for 1 min. An aliquot of the crude mixture was taken by pipette and analyzed by ^1H NMR. The results of additional ligand screen are listed below.

Table S1. Additional ligand screen.^[a]

Entry	Ligand (mol%)	Yield (%) ^[b]	Alpha (%) ^[b]	Y x A (%) ^[c]
1	PPh ₃ (0.8)	0	--	0
2	P(4-MeOC ₆ H ₄) ₃ (0.8)	0	--	0
3	P(4-CF ₃ C ₆ H ₄) ₃ (0.8)	0	--	0
4	P(2-furyl) ₃ (0.8)	0	--	0
5	P(<i>o</i> -tolyl) ₃ (0.8)	0	--	0
6	PCy ₃ (0.8)	0	--	0
7	RuPhos (0.8)	0	--	0
8	dppe (0.4)	0	--	0
9	dppp (0.4)	0	--	0
10	dppb (0.4)	0	--	0
11	dppf (0.4)	0	--	0
12	<i>rac</i> -BINAP (0.4)	0	--	0
13	DPEphos (0.4)	43	59	25
14	Xantphos (0.4)	60	55	33

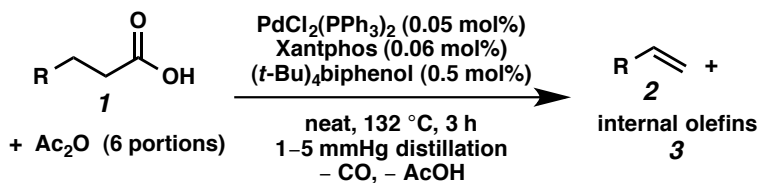
^[a] **1a** (5 mmol, 1 equiv), Ac₂O (2 equiv). ^[b] Determined by ¹H NMR with methyl benzoate as internal standard. ^[c] Y x A = Yield x Alpha.

General Procedure for Optimization Reactions (Route B)

The procedure for the representative reaction (Table 1, entry 12) is shown as follows. To a 20 x 150 mm Kimble glass tube equipped with a magnetic stir bar was added PdCl₂(PPh₃)₂ (0.005 mmol, 0.1 mol%), Xantphos (0.006 mmol, 0.12 mol%), (*t*-Bu)₄biphenol (0.05 mmol, 1 mol%), and stearic anhydride **1a'** (5 mmol, 1 equiv). The tube was sealed with a rubber septum, evacuated and refilled with N₂ (x 3), and placed in a preheated 132 °C oil bath and stirred for 2 h. The oil bath was removed, and methyl benzoate (internal standard, 5 mmol, 1 equiv) was added and the resulting mixture stirred for 1 min. An aliquot of the crude mixture was taken by pipette and analyzed by ¹H NMR.

General Procedure for Preparative Pd-Catalyzed Decarbonylative

Dehydration



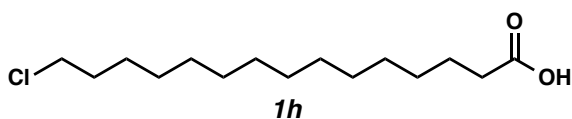
A 15 mL round-bottom flask was charged with $\text{PdCl}_2(\text{PPh}_3)_2$ (0.01 mmol, 0.05 mol%), Xantphos (0.012 mmol, 0.06 mol%), $(t\text{-Bu})_4\text{biphenol}$ (0.1 mmol, 0.5 mol%), and fatty acid substrate (20 mmol, 1 equiv). The flask was equipped with a distillation head and a 25 mL round-bottom receiving flask. The closed system was connected to a vacuum manifold, equipped with a needle valve and a digital vacuum gauge. The system was evacuated and refilled with N_2 (x 3), and the first portion of acetic anhydride (20 mmol, 1 equiv) was added via syringe through the septum that seals the top of the distillation head. The flask was lowered into a 20 °C oil bath and gradually heated to 132 °C in 23 min.[†] When oil bath temperature rose to 122 °C, the needle valve was closed, switched to vacuum, and the needle valve carefully and slowly opened to allow distillation of acetic acid into a receiving flask, which was cooled to -78 °C. When the oil bath temperature reached 130 °C, time was recorded as $t = 0$. After distillation ceased (about $t = 3$ min), the needle valve was opened fully and a vacuum of 1–5 mmHg was drawn. At $t = 30$ min, the system was refilled with N_2 , and the second portion of acetic anhydride (2.8 mmol, 0.14 equiv) was

[†] When the reaction was performed at 100 mmol scale with high-melting substrates such as stearic acid, the reaction flask was first heated to 85 °C until all solid melted, and then to 132 °C. Overall heating time from 20 to 132 °C was approximately 40 min.

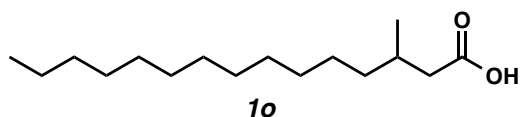
added via syringe. The system was then gradually ($t = 35$ min) resubjected to a vacuum of 1–5 mmHg. Acetic anhydride was added as follows (0.12, 0.10, 0.09, 0.08 equiv) in the same manner every 30 min. The reaction was stopped at $t = 3$ h and allowed to cool to ambient temperature. The residual reaction mixture was purified by flash chromatography. If it contained solids, it was suction-filtered first and the solids washed with hexanes, and the filtrate was concentrated and purified by chromatography. In cases where the product was distilled together with acetic acid, the distillate was added dropwise to a saturated NaHCO_3 solution, stirred for 30 min, and the resulting mixture was extracted with dichloromethane (30 mL x 3). The combined extracts were dried over Na_2SO_4 , filtered and concentrated. The crude product was then subjected to flash chromatography or distillation to afford the olefin in pure form.

Spectroscopic Data for Acid Substrates

Saturated fatty acids **1a–1d** and **1m** are commercially available. Carboxylic acids **1e**,^[1] **1f**,^[2] **1g**,^[3] **1i**,^[4] **1j**,^[5] **1k**,^[6] **1l**,^[7] and **1n**^[8] are known compounds and prepared according to literature methods.

15-Chloropentadecanoic acid (**1h**)

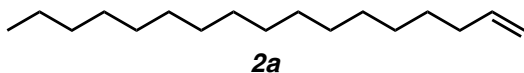
¹H NMR (500 MHz, CDCl₃) δ 3.52 (t, *J* = 6.8 Hz, 2H), 2.34 (t, *J* = 7.5 Hz, 2H), 1.79–1.73 (m, 2H), 1.62 (p, *J* = 7.5 Hz, 2H), 1.46–1.20 (m, 20H); ¹³C NMR (126 MHz, CDCl₃) δ 180.6, 45.3, 34.2, 32.8, 29.7, 29.7, 29.7, 29.7, 29.6, 29.6, 29.4, 29.2, 29.0, 27.0, 24.8; IR (Neat Film) 2916, 2848, 1701, 1462, 1410, 1302, 943, 721 cm⁻¹; HRMS (NMM: ESI-APCI-) *m/z* calc'd for C₁₅H₂₈O₂Cl [M-H]⁻: 275.1783, found 275.1794.

3-Methylpentadecanoic acid (**1o**)

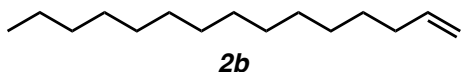
¹H NMR (500 MHz, CDCl₃) δ 2.35 (dd, *J* = 15.0, 5.9 Hz, 1H), 2.14 (dd, *J* = 15.0, 8.2 Hz, 1H), 2.01–1.90 (m, 1H), 1.38–1.15 (m, 22H), 0.96 (d, *J* = 6.7 Hz, 3H), 0.88 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 180.1, 41.8, 36.8, 32.1, 30.3, 29.9, 29.8, 29.8, 29.8, 29.8, 29.8, 29.5, 27.0, 22.9, 19.8, 14.3; IR (Neat Film) 2914, 2852, 1701, 1473, 1410,

1300, 1151, 1123, 954, 715; HRMS (NMM: ESI-APCI-) m/z calc'd for $C_{16}H_{31}O_2$ $[M-H]^-$:
255.2330, found 255.2328.

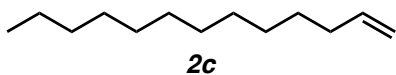
Spectroscopic Data for Olefin Products

1-Heptadecene (2a)^[9]

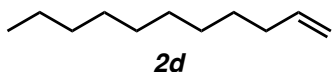
¹H NMR (500 MHz, CDCl₃) δ 5.82 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 5.07–4.86 (m, 2H), 2.11–1.98 (m, 2H), 1.49–1.08 (m, 26H), 0.88 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 139.4, 114.2, 34.0, 32.1, 29.9, 29.8, 29.8, 29.8, 29.7, 29.7, 29.5, 29.5, 29.4, 29.3, 29.1, 22.9, 14.3.

1-Pentadecene (2b)^[10]

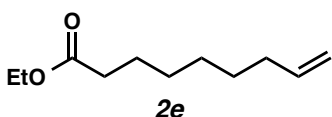
¹H NMR (500 MHz, CDCl₃) δ 5.82 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 5.07–4.85 (m, 2H), 2.11–1.97 (m, 2H), 1.46–1.08 (m, 22H), 0.88 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 139.4, 114.2, 34.0, 32.1, 29.9, 29.9, 29.8, 29.8, 29.8, 29.7, 29.6, 29.3, 29.1, 22.9, 14.3.

1-Tridecene (2c)^[11]

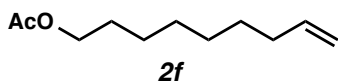
¹H NMR (500 MHz, CDCl₃) δ 5.82 (ddt, *J* = 17.0, 10.1, 6.7 Hz, 1H), 5.09–4.83 (m, 2H), 2.11–1.97 (m, 2H), 1.48–1.11 (m, 18H), 0.88 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 139.4, 114.2, 34.0, 32.1, 29.8, 29.8, 29.8, 29.7, 29.5, 29.3, 29.1, 22.9, 14.3.

1-Undecene (2d)^[12]

¹H NMR (500 MHz, CDCl₃) δ 5.82 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 5.08–4.84 (m, 2H), 2.11–1.98 (m, 2H), 1.47–1.09 (m, 14H), 0.88 (t, *J* = 6.9 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 139.4, 114.2, 34.0, 32.1, 29.8, 29.7, 29.5, 29.3, 29.1, 22.8, 14.3.

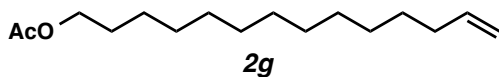
Ethyl non-8-enoate (2e)^[13]

¹H NMR (500 MHz, CDCl₃) δ 5.80 (ddt, *J* = 16.6, 9.9, 6.8 Hz, 1H), 5.07–4.87 (m, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 2.28 (t, *J* = 7.5 Hz, 2H), 2.10–1.98 (m, 2H), 1.69–1.54 (m, 2H), 1.46–1.28 (m, 6H), 1.25 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 174.0, 139.1, 114.4, 60.3, 34.5, 33.8, 29.1, 28.8, 28.8, 25.0, 14.4.

Non-8-en-1-yl acetate (2f)^[14]

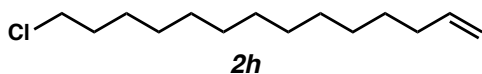
¹H NMR (500 MHz, CDCl₃) δ 5.80 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 5.07–4.87 (m, 2H), 4.05 (t, *J* = 6.8 Hz, 2H), 2.14–1.94 (m, 5H), 1.70–1.52 (m, 2H), 1.47–1.18 (m, 8H); ¹³C NMR (126 MHz, CDCl₃) δ 171.4, 139.2, 114.4, 64.8, 33.9, 29.2, 29.1, 29.0, 28.7, 26.0, 21.2.

Tetradec-13-en-1-yl acetate (2g)^[15]



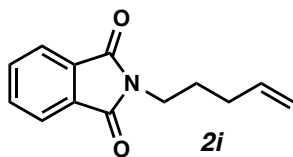
^1H NMR (500 MHz, CDCl_3) δ 5.81 (ddt, $J = 16.8, 10.1, 6.8$ Hz, 1H), 5.08–4.86 (m, 2H), 4.05 (t, $J = 6.8$ Hz, 2H), 2.11–1.98 (m, 5H), 1.69–1.53 (m, 2H), 1.45–1.09 (m, 18H); ^{13}C NMR (126 MHz, CDCl_3) δ 171.4, 139.4, 114.2, 64.8, 34.0, 29.8, 29.7, 29.7, 29.6, 29.6, 29.4, 29.3, 29.1, 28.7, 26.0, 21.2.

14-Chlorotetradec-1-ene (2h)



^1H NMR (500 MHz, CDCl_3) δ 5.81 (ddt, $J = 17.0, 10.2, 6.7$ Hz, 1H), 5.07–4.86 (m, 2H), 3.53 (t, $J = 6.8$ Hz, 2H), 2.11–1.98 (m, 2H), 1.77 (dt, $J = 14.5, 6.9$ Hz, 2H), 1.50–1.10 (m, 18H); ^{13}C NMR (126 MHz, CDCl_3) δ 139.4, 114.2, 45.3, 34.0, 32.8, 29.8, 29.7, 29.7, 29.6, 29.6, 29.3, 29.1, 29.0, 27.0; IR (Neat Film, NaCl) 3076, 2925, 2854, 1641, 1465, 1309, 993, 966, 909, 723 cm^{-1} ; HRMS (FAB+) m/z calc'd for $\text{C}_{14}\text{H}_{27}^{35}\text{Cl}$ $[\text{M}]^+$: 230.1801, found 230.1808.

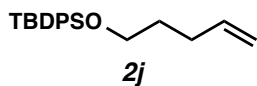
2-(Pent-4-en-1-yl)isoindoline-1,3-dione (2i)^[16]



^1H NMR (500 MHz, CDCl_3) δ 7.89–7.73 (m, 2H), 7.73–7.58 (m, 2H), 5.77 (ddt, $J = 16.9, 10.2, 6.6$ Hz, 1H), 5.10–4.87 (m, 2H), 3.74–3.57 (m, 2H), 2.17–2.00 (m, 2H), 1.74 (p, $J =$

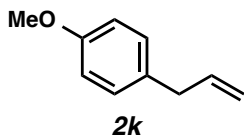
7.5 Hz, 2H); ^{13}C NMR (126 MHz, CDCl_3) δ 168.4, 137.3, 133.9, 132.2, 123.2, 115.3, 37.6, 31.0, 27.7.

***tert*-Butyl(pent-4-en-1-yloxy)diphenylsilane (**2j**)^[17]**



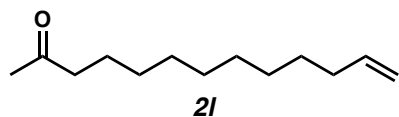
^1H NMR (500 MHz, CDCl_3) δ 7.67 (dt, $J = 6.5, 1.5$ Hz, 4H), 7.39 (dddd, $J = 14.4, 8.3, 6.0, 2.1$ Hz, 6H), 5.80 (ddt, $J = 16.9, 10.2, 6.6$ Hz, 1H), 5.09–4.87 (m, 2H), 3.68 (t, $J = 6.5$ Hz, 2H), 2.15 (tdd, $J = 8.1, 6.8, 1.4$ Hz, 2H), 1.73–1.60 (m, 2H), 1.05 (s, 9H); ^{13}C NMR (126 MHz, CDCl_3) δ 138.7, 135.7, 134.2, 129.7, 127.7, 114.7, 63.4, 32.0, 30.2, 27.0, 19.4.

1-Allyl-4-methoxybenzene (2k**)^[18]**



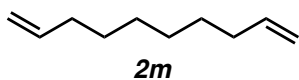
^1H NMR (500 MHz, CDCl_3) δ 7.17–7.06 (m, 2H), 6.91–6.78 (m, 2H), 5.96 (ddt, $J = 16.8, 10.1, 6.7$ Hz, 1H), 5.13–4.99 (m, 2H), 3.79 (s, 3H), 3.34 (d, $J = 6.7$ Hz, 2H); ^{13}C NMR (126 MHz, CDCl_3) δ 158.1, 138.0, 132.2, 129.6, 115.5, 113.9, 55.4, 39.5.

Tridec-12-en-2-one (2l**)^[19]**



^1H NMR (500 MHz, CDCl_3) δ 5.81 (ddt, $J = 16.9, 10.1, 6.7$ Hz, 1H), 5.06–4.87 (m, 2H), 2.41 (t, $J = 7.5$ Hz, 2H), 2.13 (s, 3H), 2.09–1.97 (m, 2H), 1.62–1.49 (m, 2H), 1.46–1.11 (m,

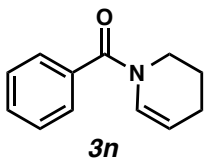
12H); ^{13}C NMR (126 MHz, CDCl_3) δ 209.5, 139.3, 114.2, 43.9, 33.9, 30.0, 29.5, 29.5, 29.5, 29.3, 29.2, 29.0, 24.0.

Deca-1,9-diene (2m)^[20]

^1H NMR (500 MHz, CDCl_3) δ 5.81 (ddt, $J = 17.0, 10.2, 6.7$ Hz, 2H), 5.08–4.86 (m, 4H), 2.11–1.98 (m, 4H), 1.48–1.21 (m, 8H); ^{13}C NMR (126 MHz, CDCl_3) δ 139.3, 114.3, 33.9, 29.1, 29.0.

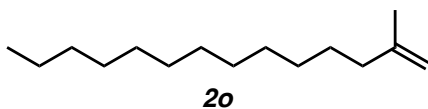
(3,6-Dihydropyridin-1(2H)-yl)(phenyl)methanone (2n)^[21]

^1H NMR (500 MHz, DMSO-d_6 , 130 °C) δ 7.41 (ddd, $J = 24.3, 6.8, 3.4$ Hz, 5H), 5.90–5.82 (m, 1H), 5.78–5.64 (m, 1H), 4.00 (p, $J = 2.8$ Hz, 2H), 3.56 (t, $J = 5.8$ Hz, 2H), 2.16 (dp, $J = 8.7, 3.2$ Hz, 2H); ^{13}C NMR (126 MHz, DMSO-d_6 , 130 °C) δ 168.8, 136.1, 128.5, 127.5, 125.9, 124.6, 123.7, 43.4, 41.1, 24.3.

(3,4-Dihydropyridin-1(2H)-yl)(phenyl)methanone (3n)^[22]

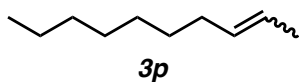
^1H NMR (500 MHz, DMSO- d_6 , 130 °C) δ 7.45 (tdd, J = 6.0, 3.9, 2.4 Hz, 5H), 6.78–6.61 (m, 1H), 4.97 (dt, J = 8.2, 3.9 Hz, 1H), 3.72–3.60 (m, 2H), 2.09 (tdd, J = 6.2, 3.8, 2.0 Hz, 2H), 1.85 (p, J = 6.1 Hz, 2H); ^{13}C NMR (126 MHz, DMSO- d_6 , 130 °C) δ 167.2, 135.0, 129.0, 127.5, 126.6, 125.6, 107.1, 42.0, 20.9, 20.8.

2-Methyltetradec-1-ene (2o)^[23]

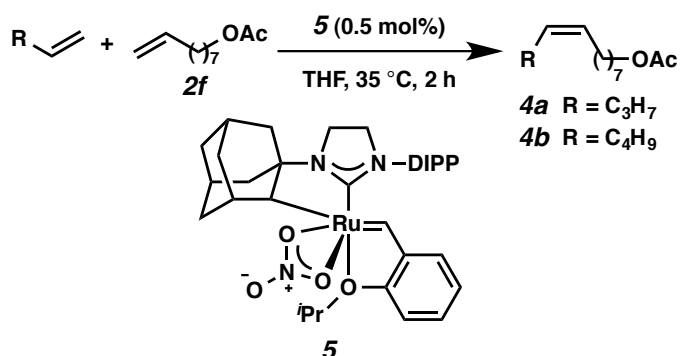


^1H NMR (500 MHz, CDCl_3) δ 4.72–4.63 (m, 2H), 2.00 (t, J = 7.7 Hz, 2H), 1.71 (s, 3H), 1.47–1.11 (m, 20H), 0.88 (t, J = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, CDCl_3) δ 146.5, 109.6, 38.0, 32.1, 29.9, 29.9, 29.8, 29.8, 29.7, 29.5, 29.5, 27.8, 22.9, 22.6, 14.3.

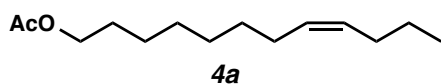
(E)- and (Z)-2-decene (3p)^[24]



^1H NMR (500 MHz, CDCl_3) δ 5.48–5.35 (m, 2H), 2.07–1.93 (m, 2H), 1.64 (d, J = 4.2 Hz, 3H, *E*-olefin), 1.60 (d, J = 6.1 Hz, 3H, *Z*-olefin), 1.43–1.20 (m, 10H), 0.88 (t, J = 6.6 Hz, 3H).

General Procedure for Pheromone Synthesis by Ru-Catalyzed Cross Metathesis^[25]

In a glovebox, a 20 mL vial was charged with 8-nonenyl acetate (**2f**,^{††} 1.0 mL, 4.8 mmol), 1-pentene or 1-hexene (48 mmol), and THF (2.6 mL). Ruthenium metathesis catalyst **5** (16 mg, 0.024 mmol, 0.5 mol%) was added and the reaction was stirred at 35 °C in an open vial for 2 hours. The vial was removed from the glovebox, quenched with ethyl vinyl ether (2.5 mL) and stirred for 30 minutes. The solvent was then removed *in vacuo*. The crude mixture was passed through a SiO₂ plug (hexane to 4% ethyl acetate in hexanes) to provide a mixture of unreacted 8-nonenyl acetate and pheromone **4**. Pheromone **4** was isolated by distillation using a Kugelrohr apparatus.

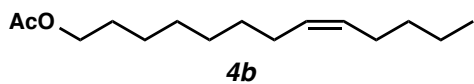
(Z)-dodec-8-en-1-yl acetate (4a)

¹H NMR (500 MHz, CDCl₃) δ 5.35 (2H, m), 4.04 (2H, t, *J* = 6.8 Hz), 2.04 (3H, s), 2.01 (4H, m), 1.61 (2H, m), 1.27–1.39 (10H, m), 0.89 (3H, t, *J* = 7.4 Hz); ¹³C NMR (CDCl₃): δ

^{††} An inseparable mixture of olefin isomers **2f** and **3f** was used for this reaction. For **4a**, the mixture was 98% alpha (**2f:3f** = 98:2); for **4b**, the mixture was 96% alpha (**2f:3f** = 96:4).

171.4, 130.1, 129.9, 64.8, 29.8, 29.4, 29.3 (2C), 28.7, 27.3, 26.0, 23.0, 21.2, 14.0; HRMS (EI+) m/z calc'd for $C_{14}H_{27}O_2$ $[M+H]^+$: 227.2011, found 227.2012.

(Z)-tridec-8-en-1-yl acetate (4b)

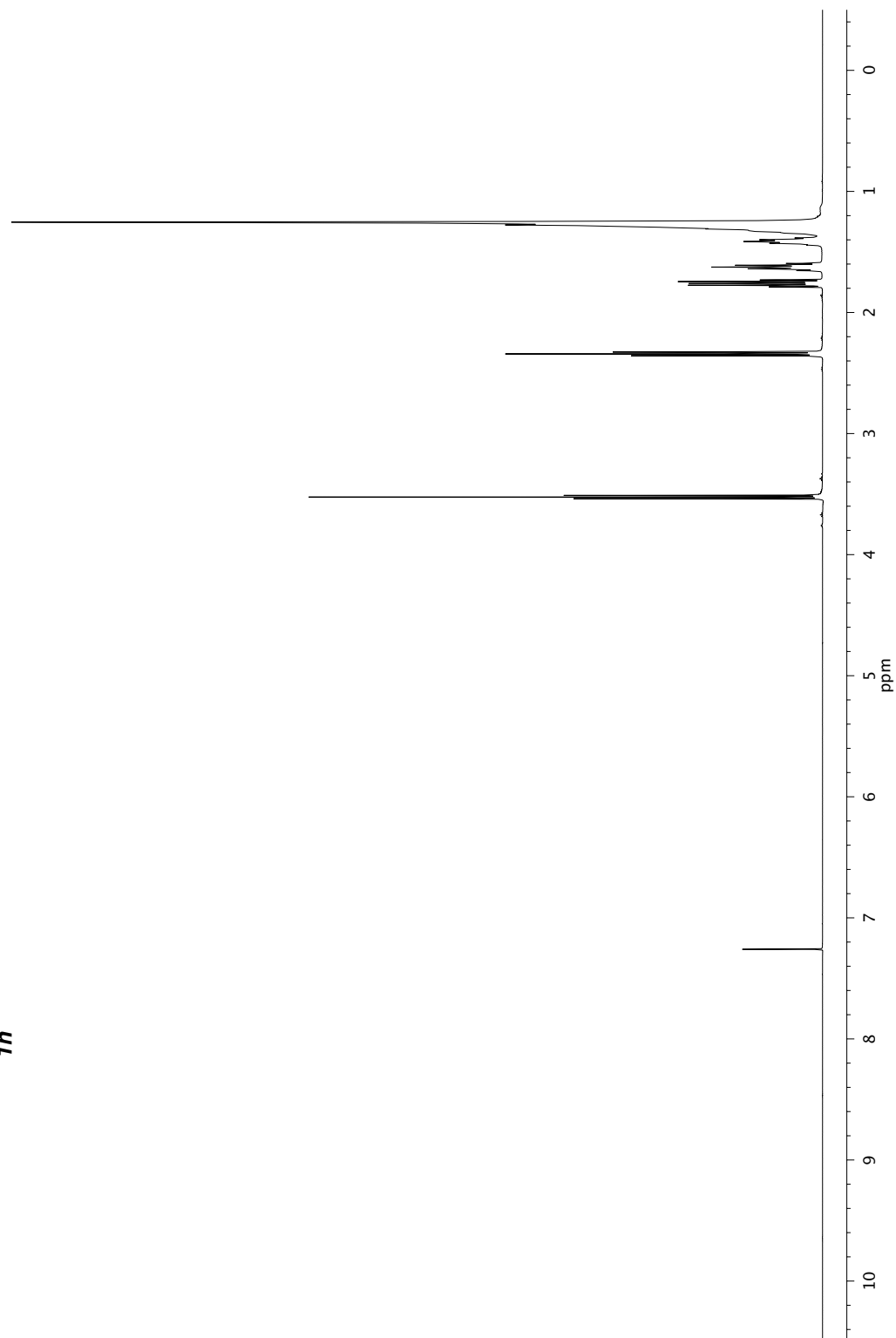
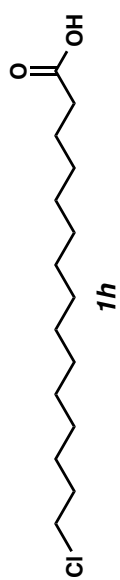


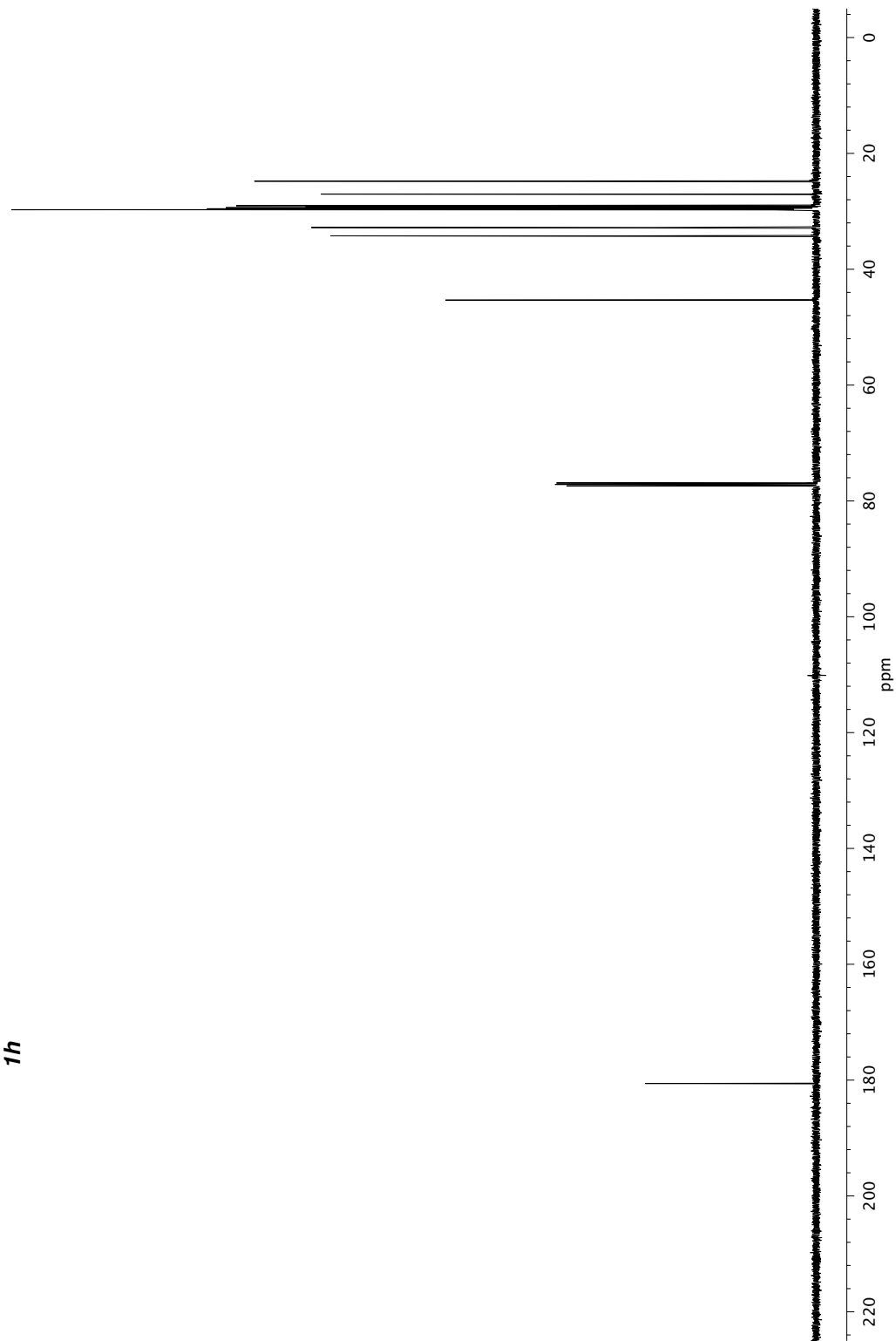
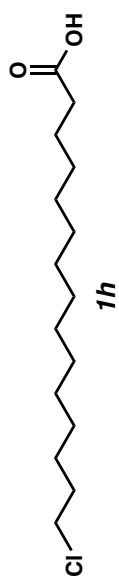
1H NMR (500 MHz, $CDCl_3$) δ 5.34 (m, 2H), 4.05 (t, $J = 6.8$ Hz, 2H), 2.00–2.04 (m, 7H), 1.60–1.63 (m, 2H), 1.29–1.36 (m, 12H), 0.88–0.91 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.4, 130.1, 129.9, 64.8, 32.1, 29.8, 29.3, 28.7, 27.3, 27.1, 26.0, 22.5, 21.2, 14.2; HRMS (EI+) m/z calc'd for $C_{15}H_{29}O_2$ $[M+H]^+$: 241.2168, found 241.2167.

References

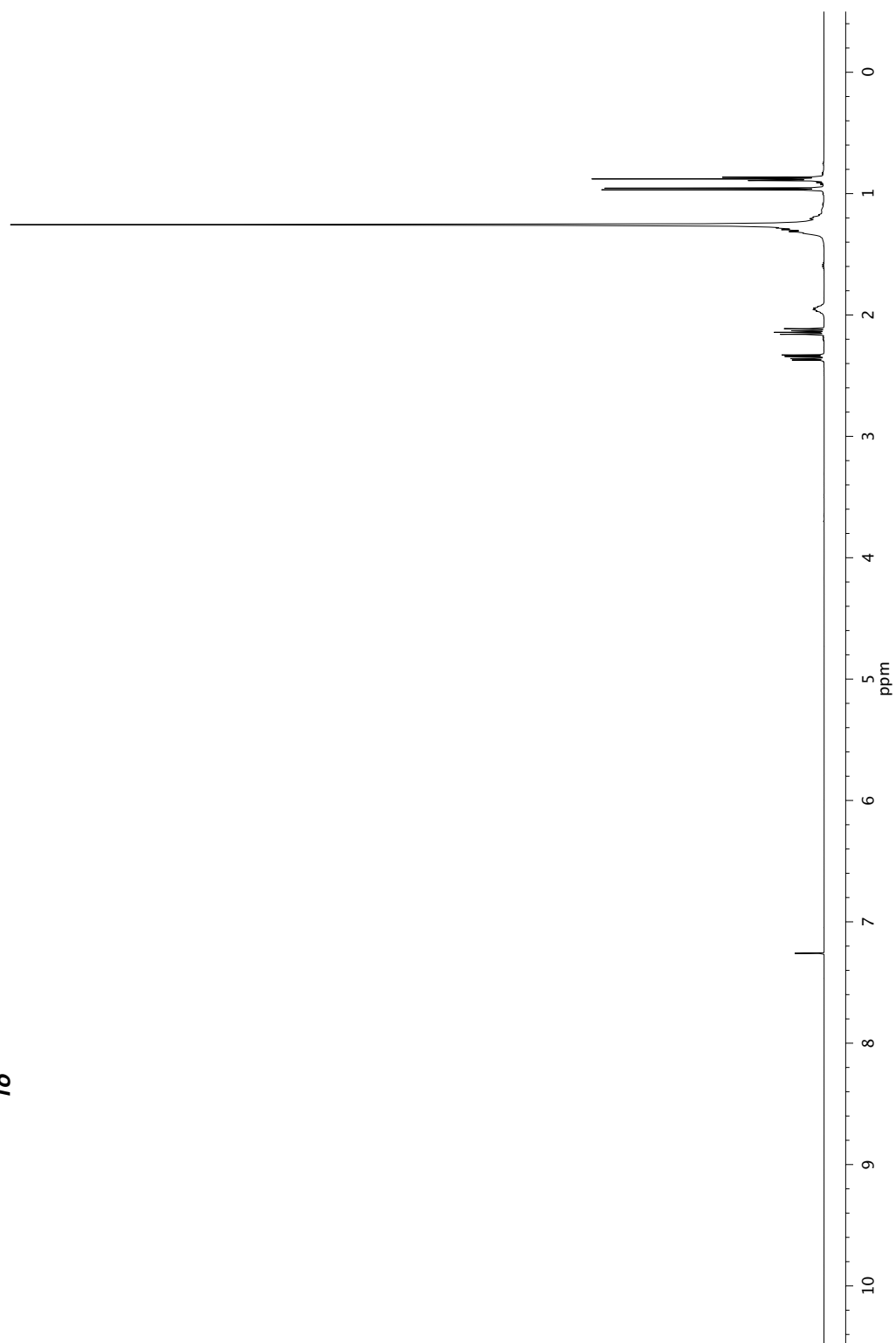
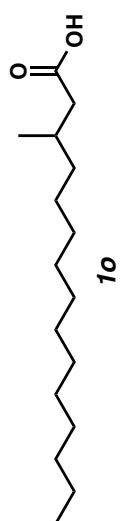
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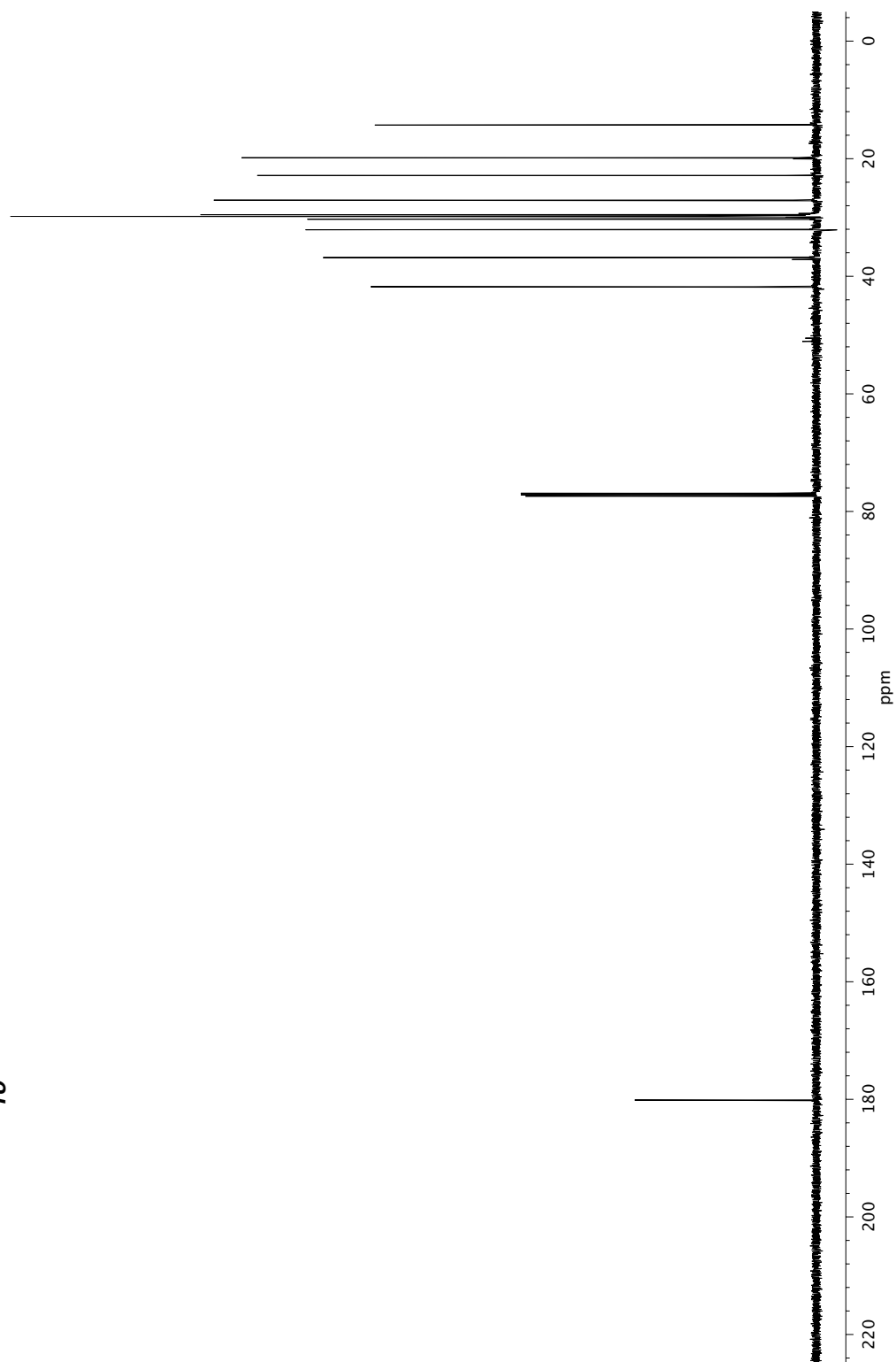
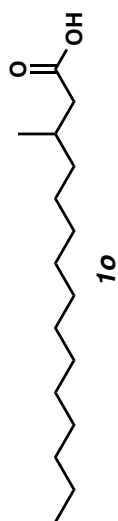
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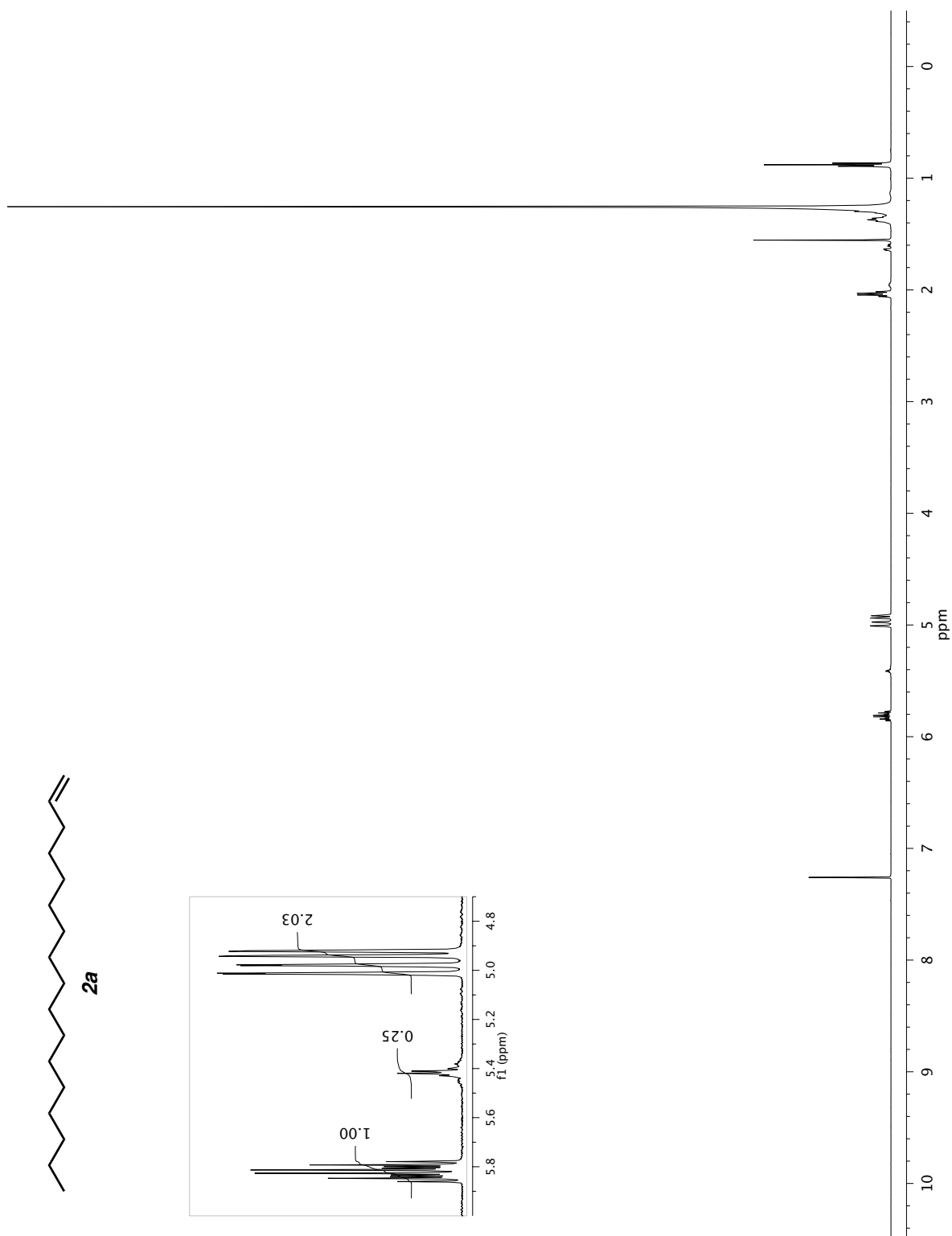


^{13}C NMR (126 MHz, CDCl_3) of compound **1h**.

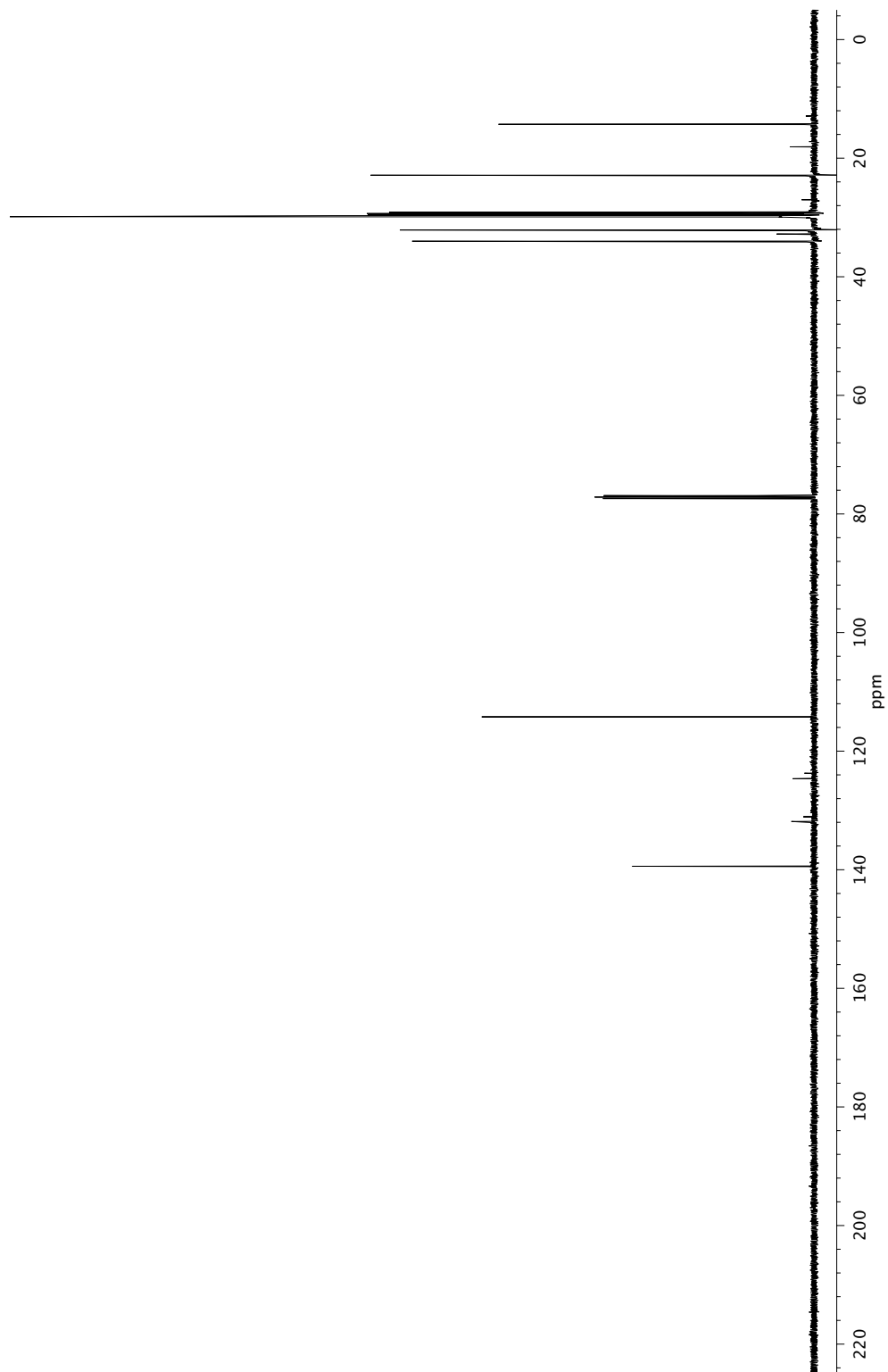
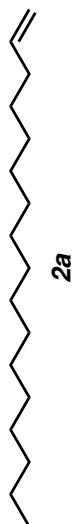


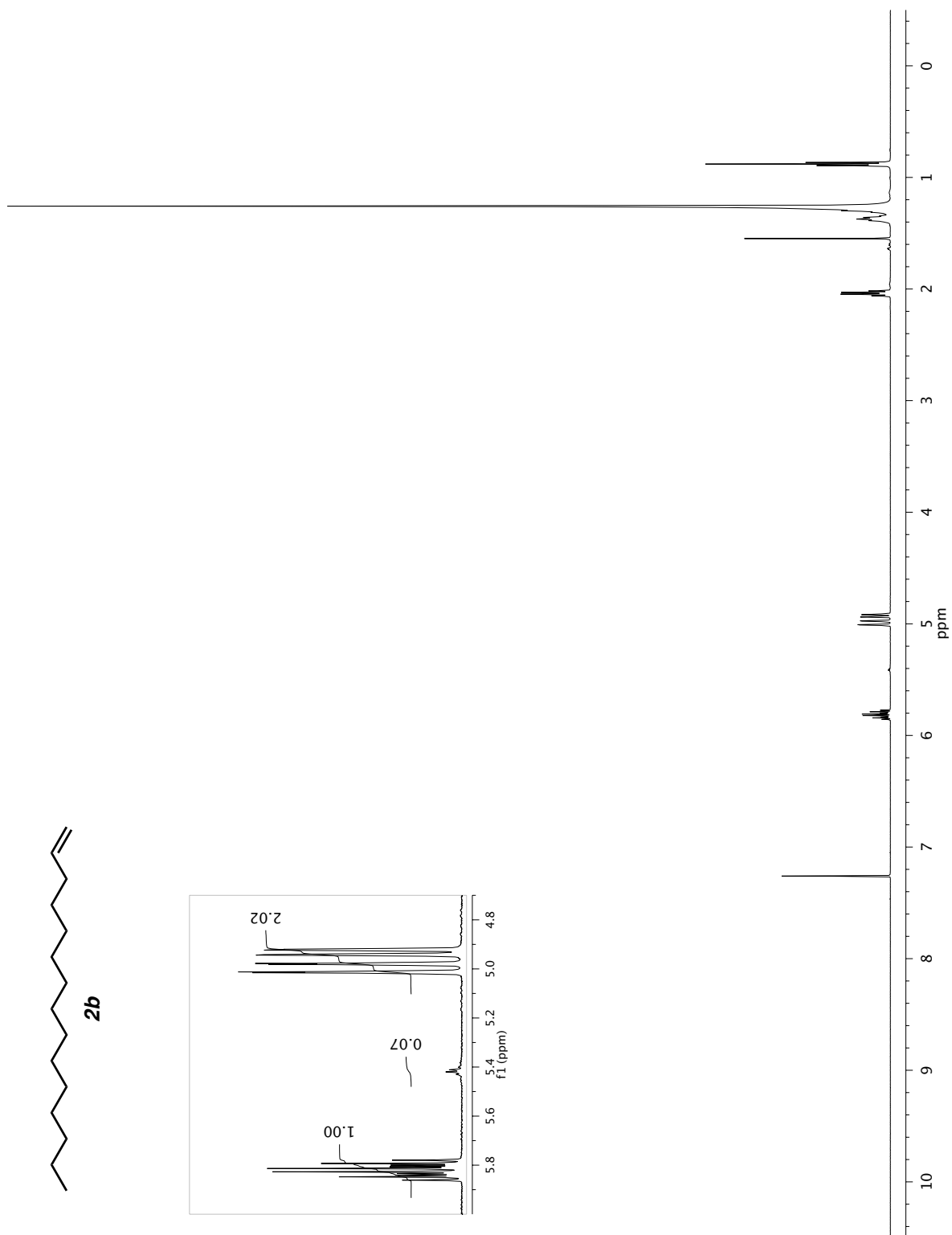


^{13}C NMR (126 MHz, CDCl_3) of compound **10**.

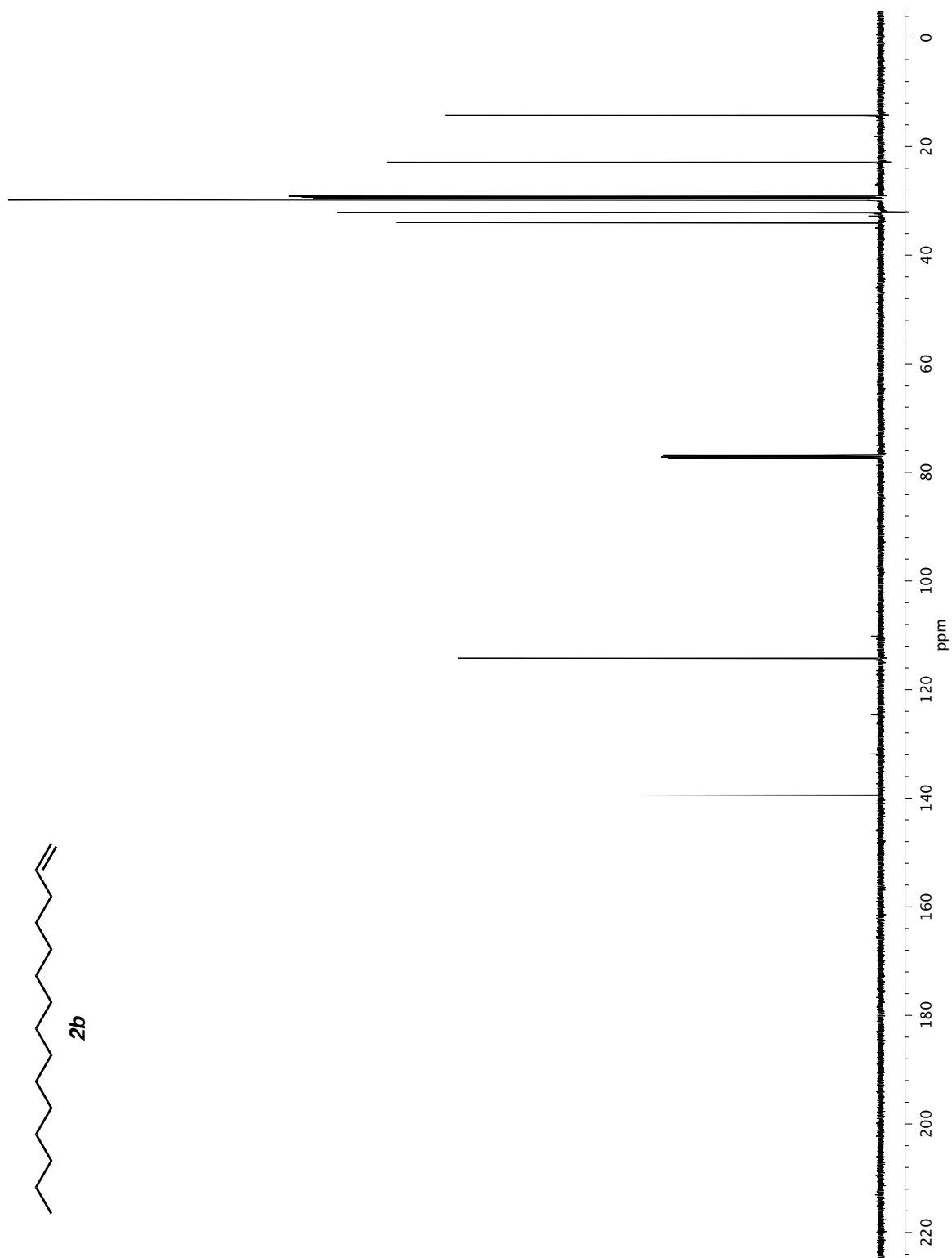


¹H NMR (500 MHz, CDCl₃) of compound **2a**.

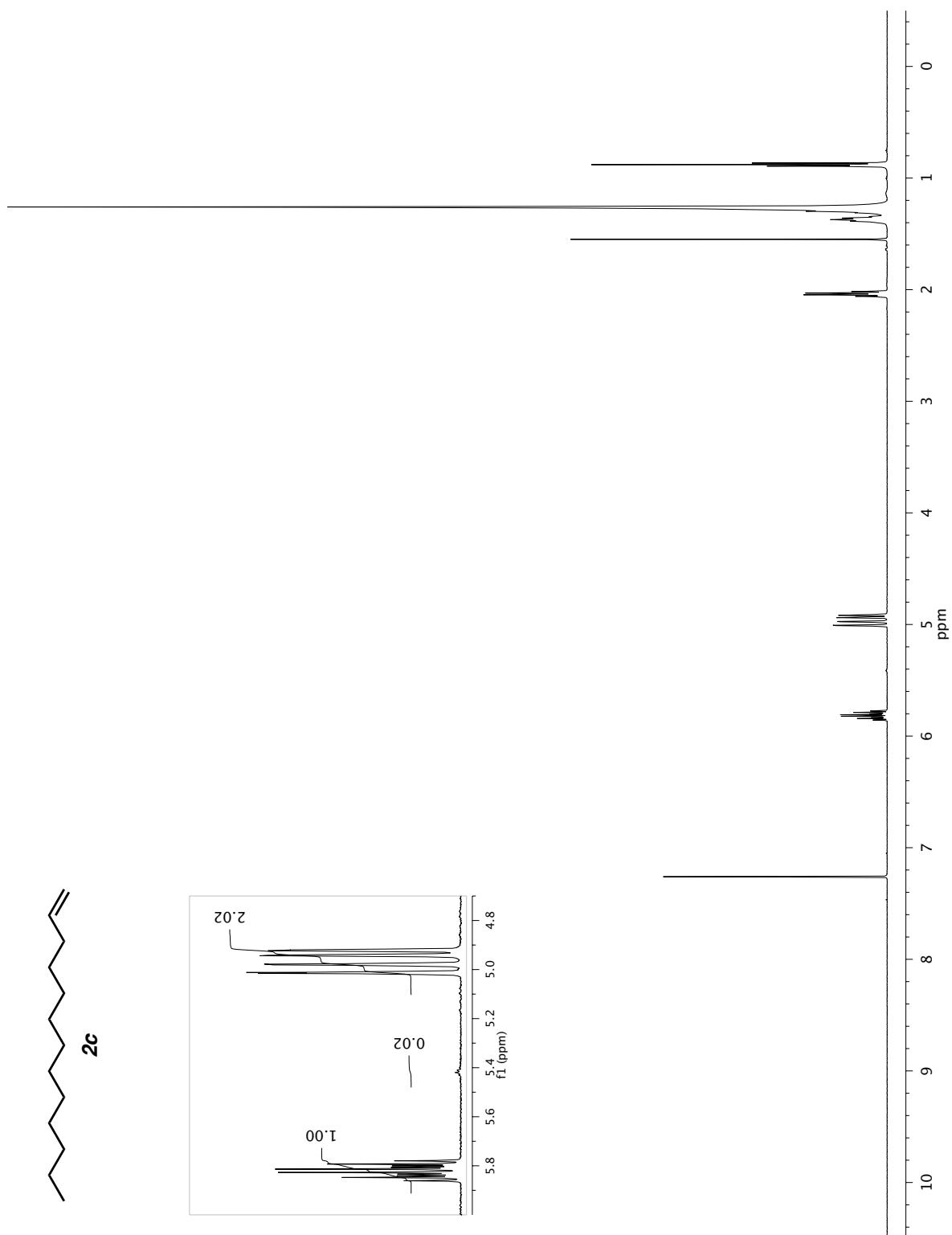




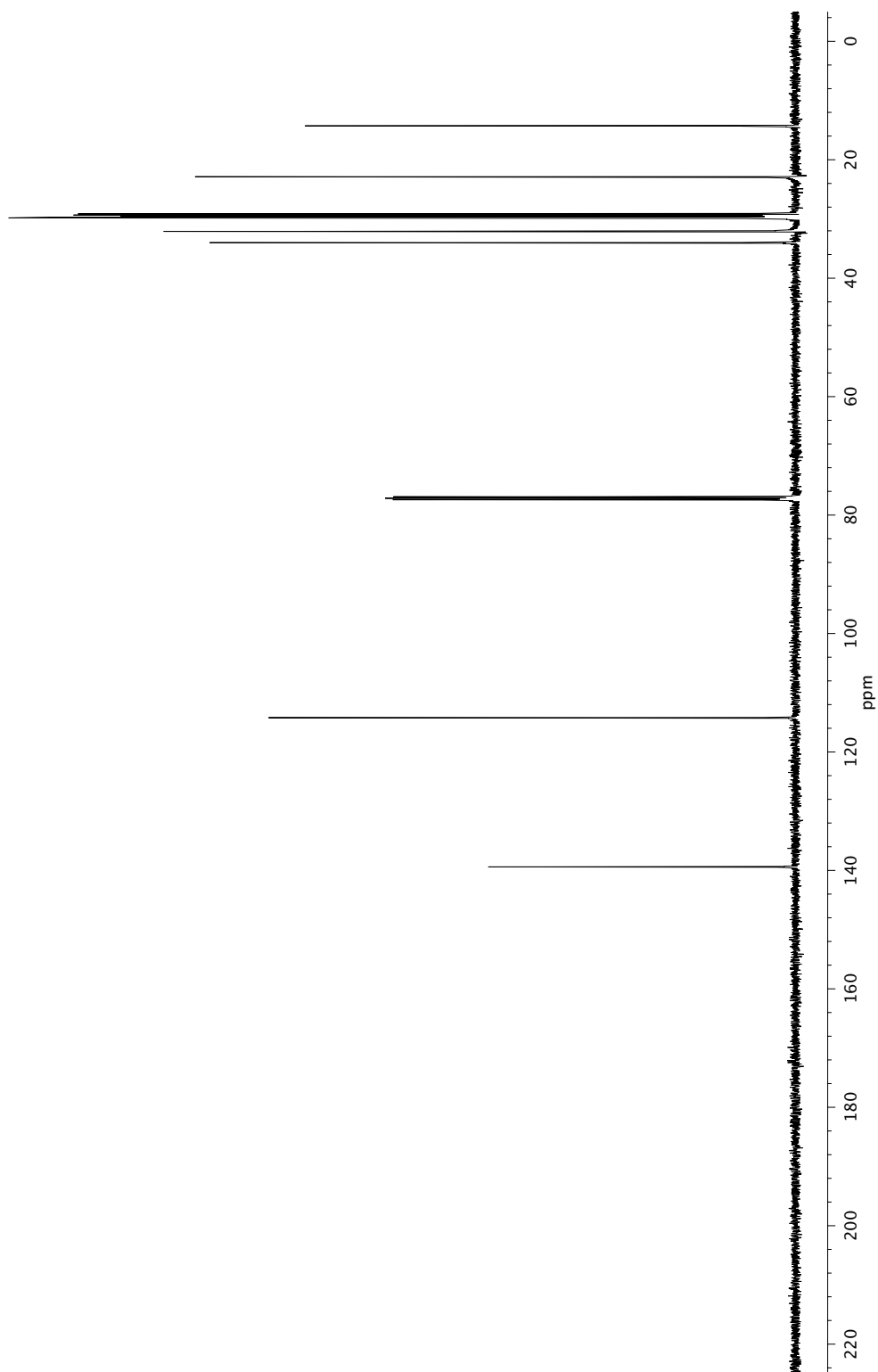
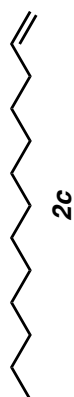
¹H NMR (500 MHz, CDCl₃) of compound **2b**.



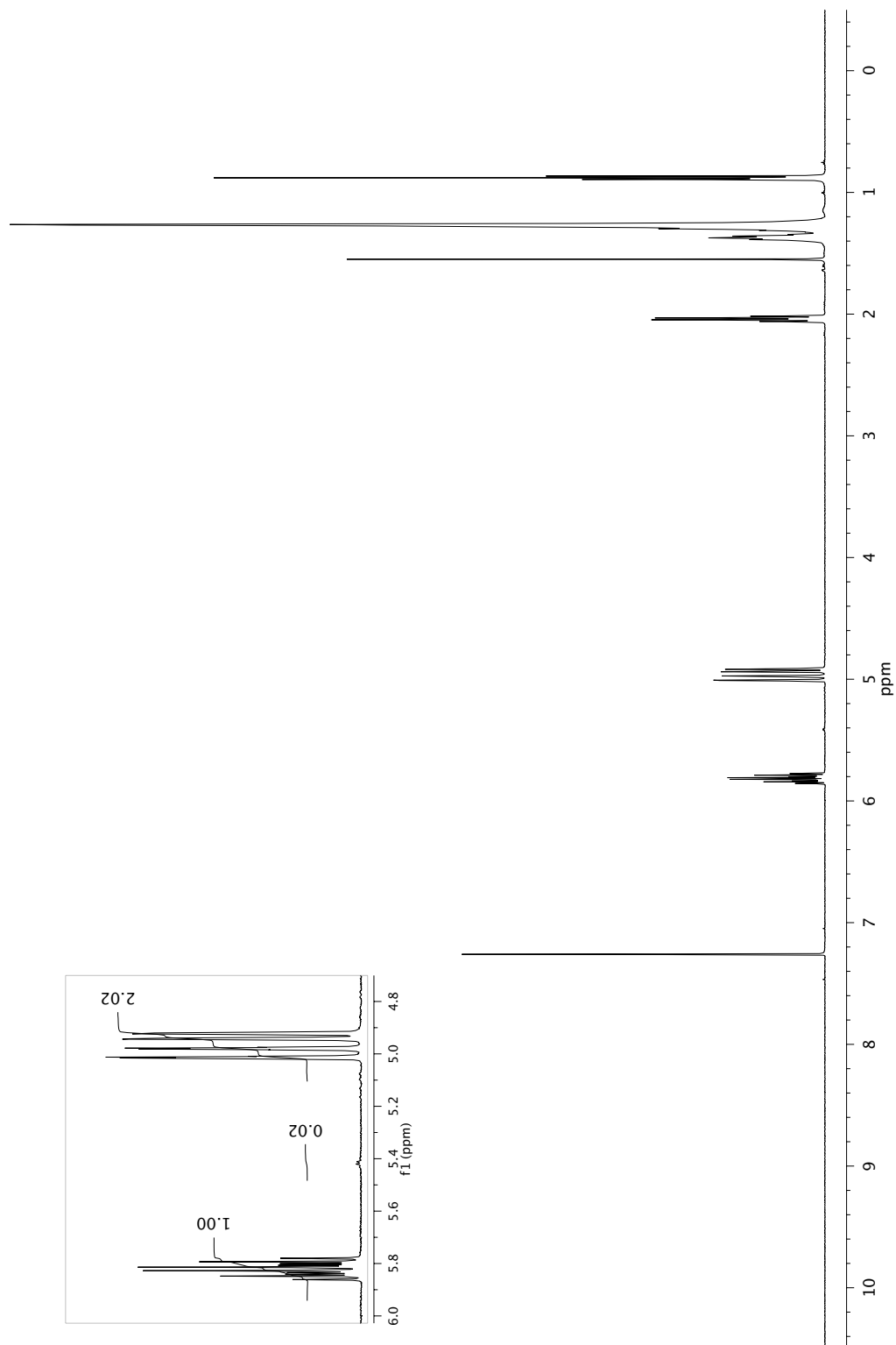
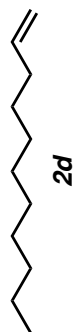
^{13}C NMR (126 MHz, CDCl_3) of compound **2b**.



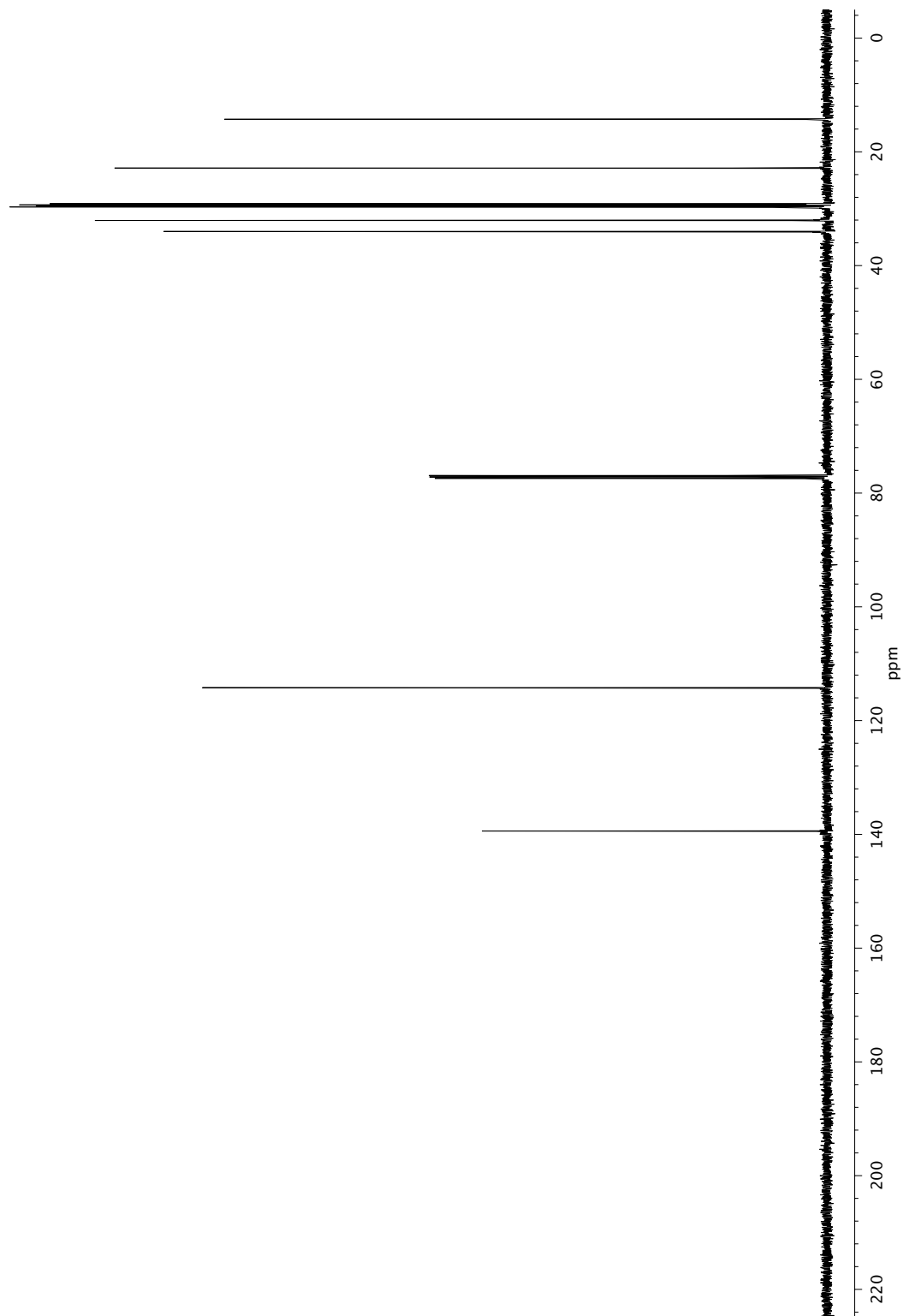
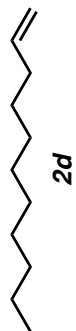
^1H NMR (500 MHz, CDCl_3) of compound **2c**.



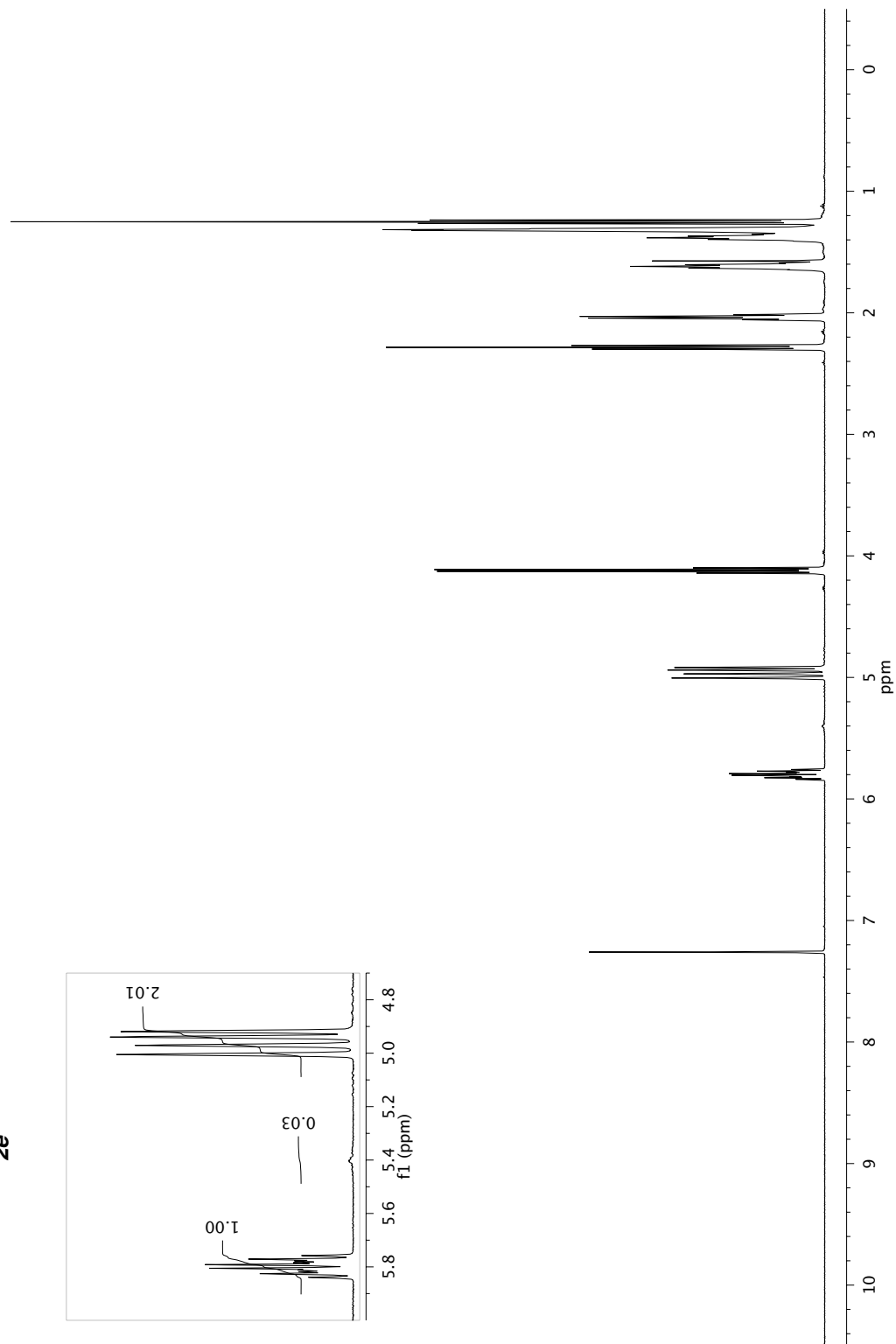
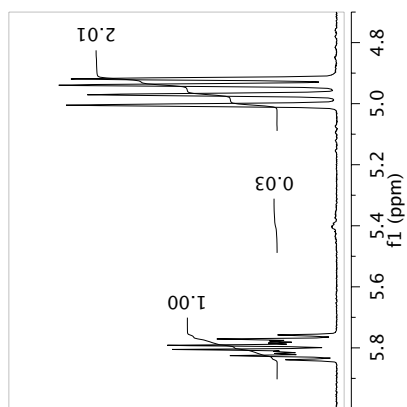
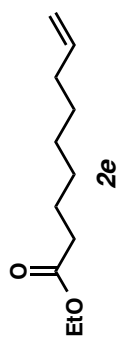
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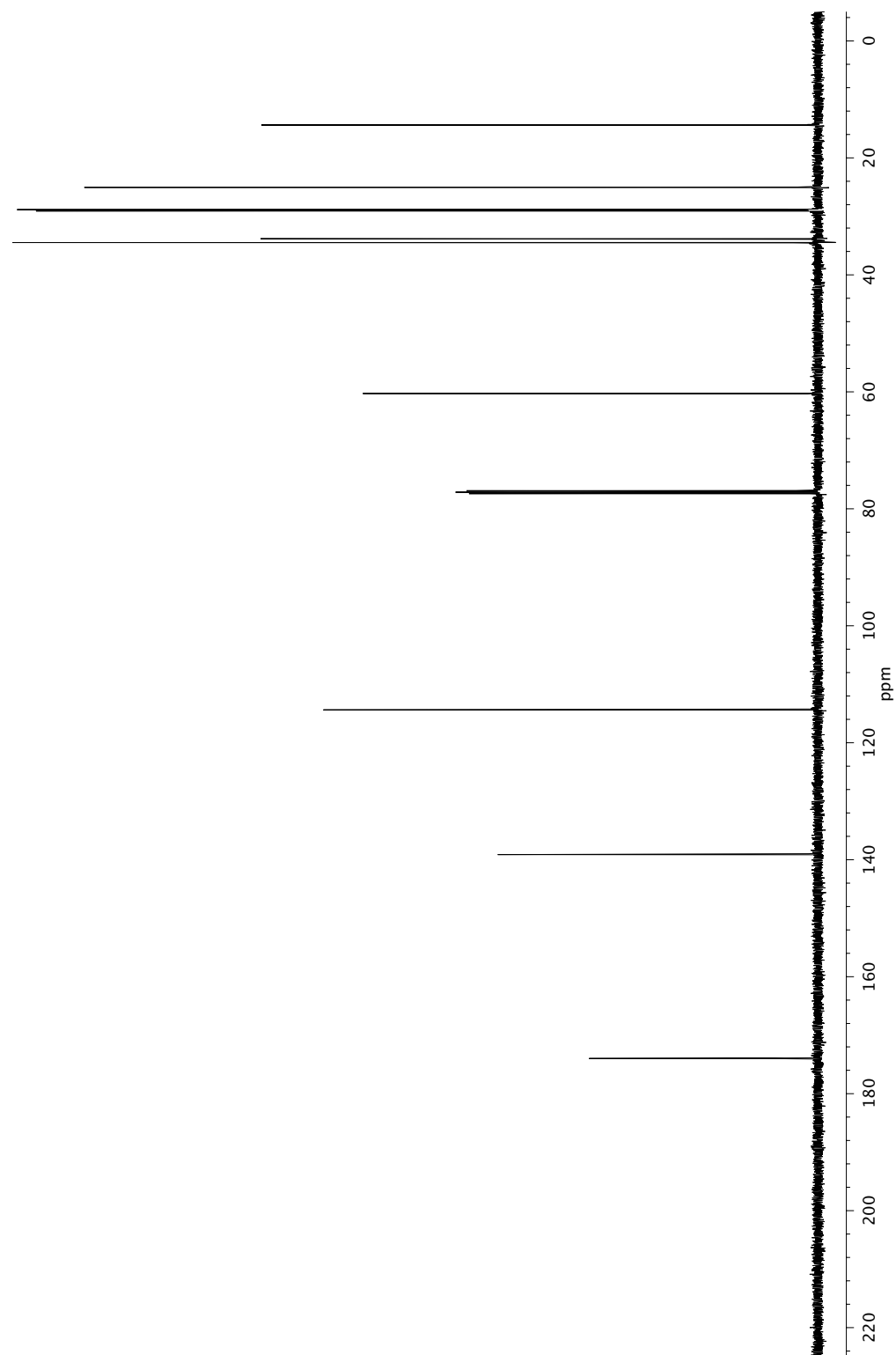
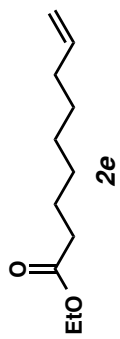
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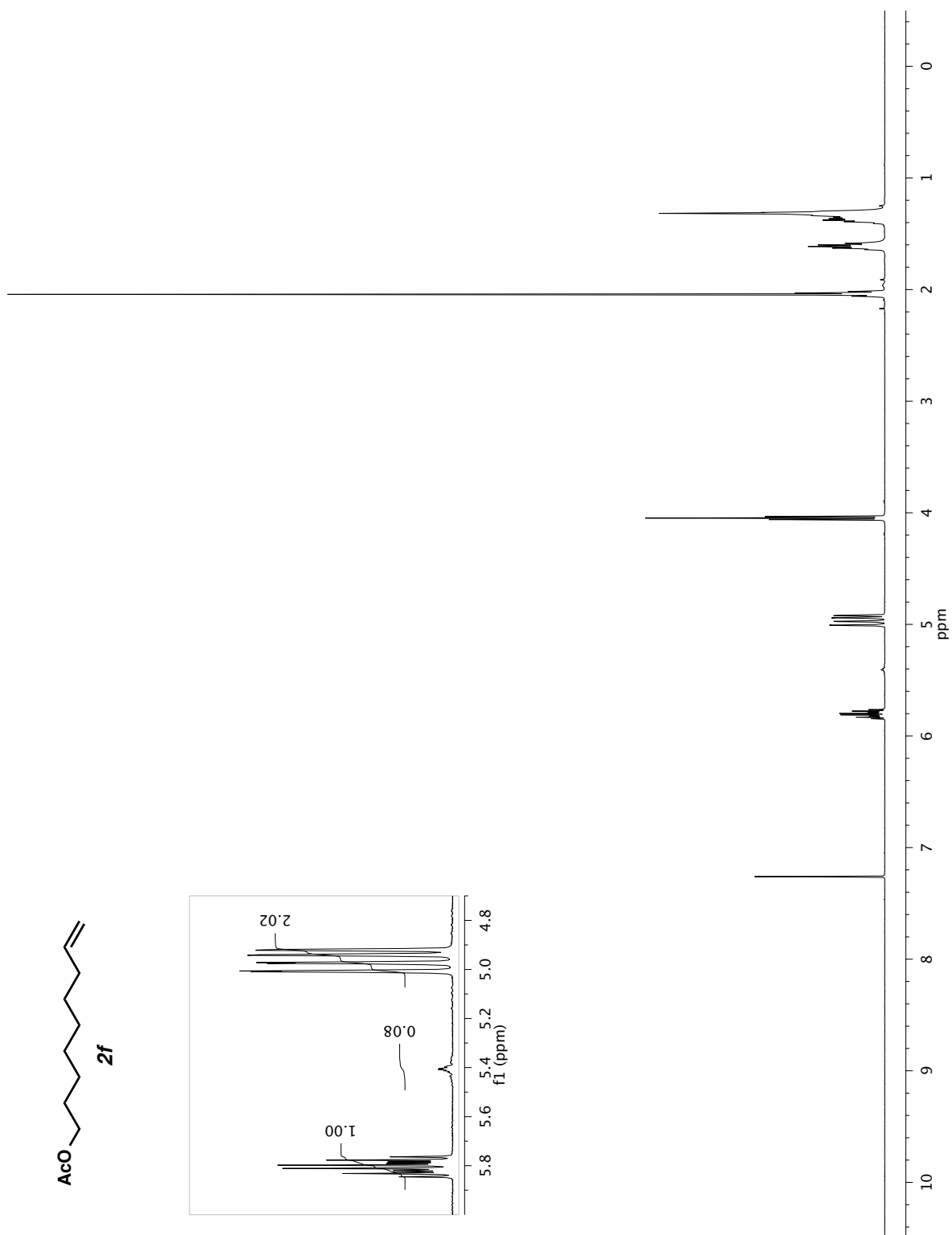
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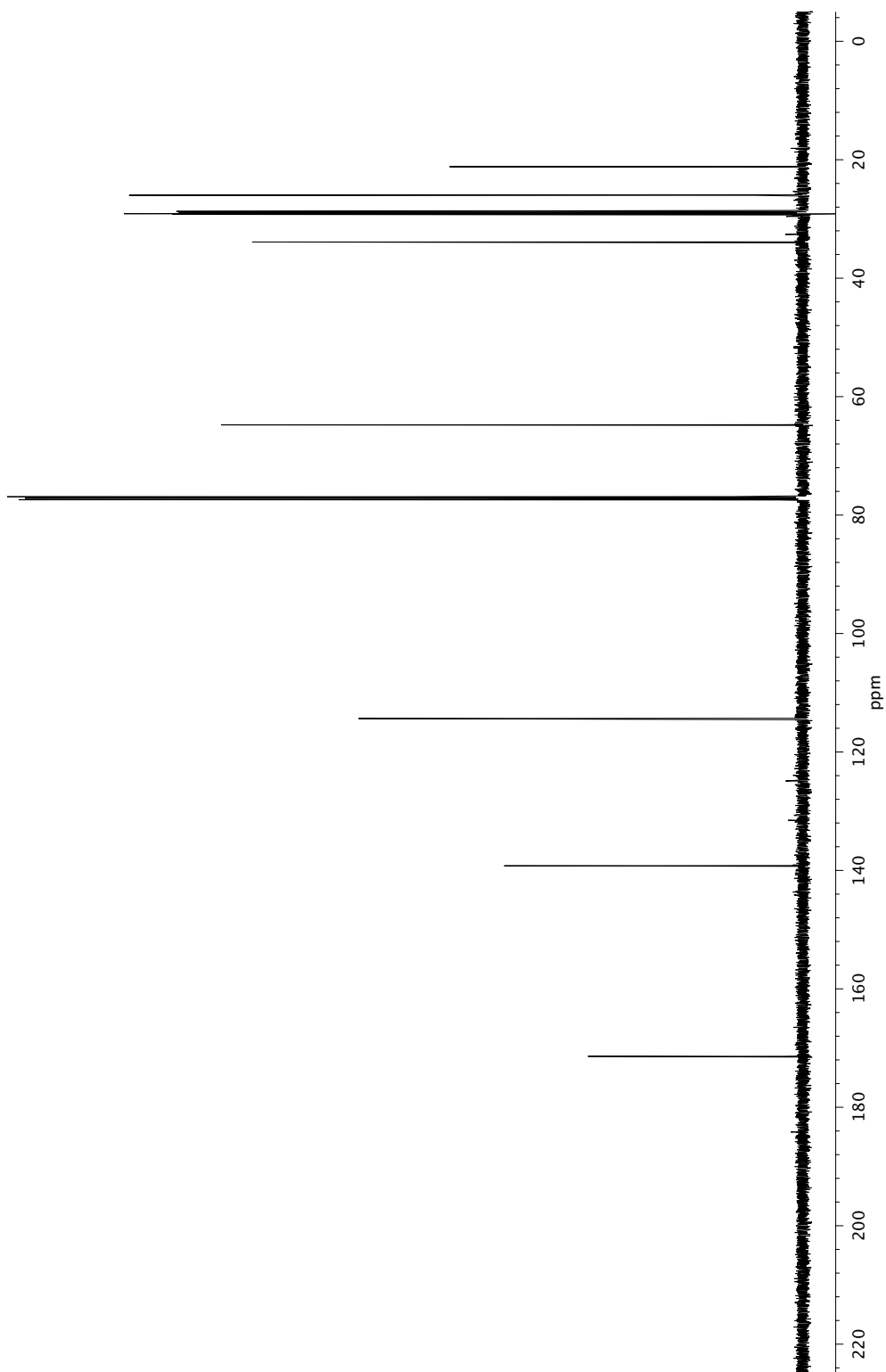
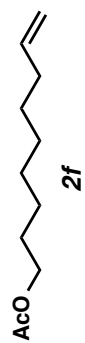
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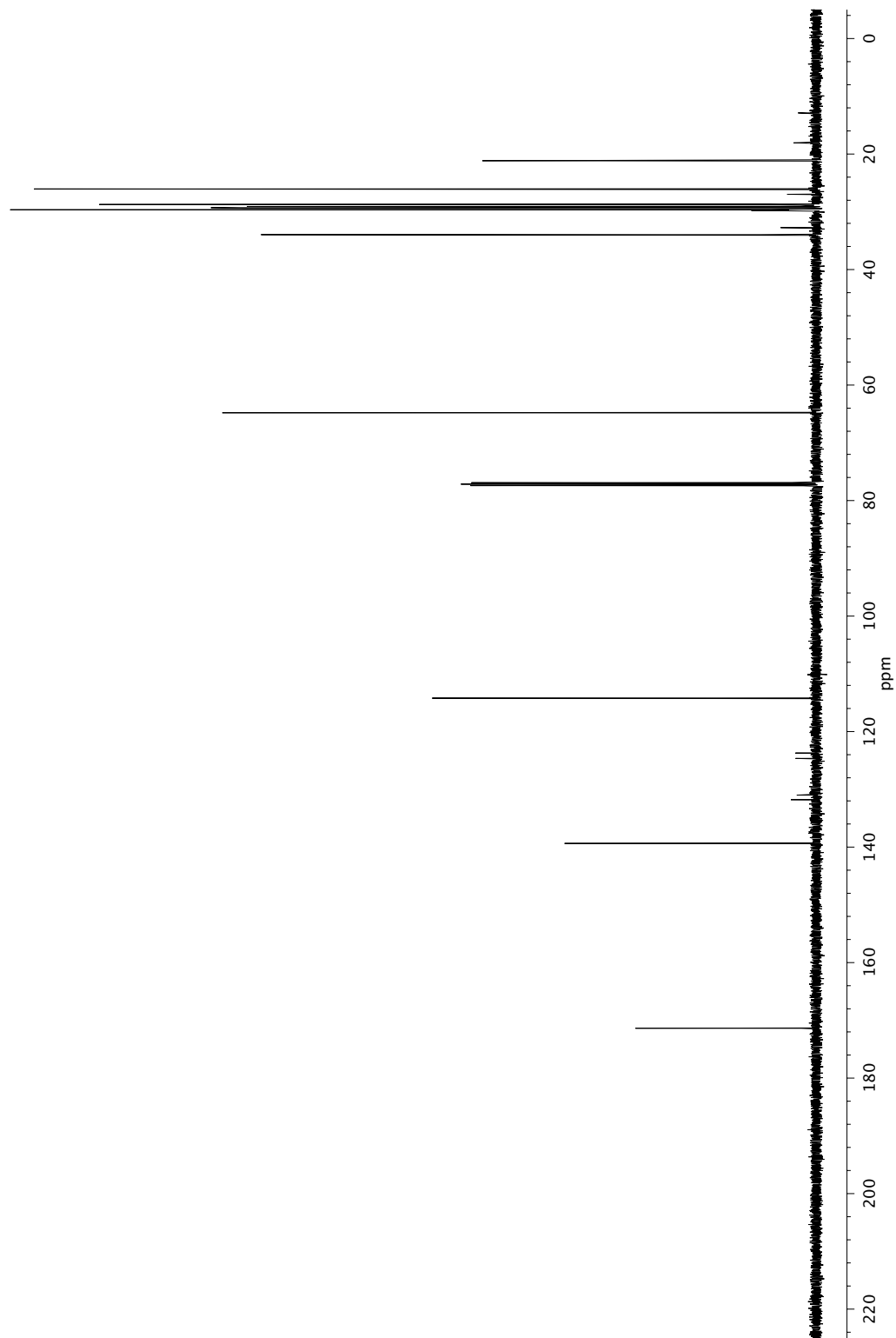
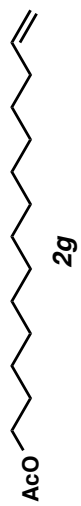
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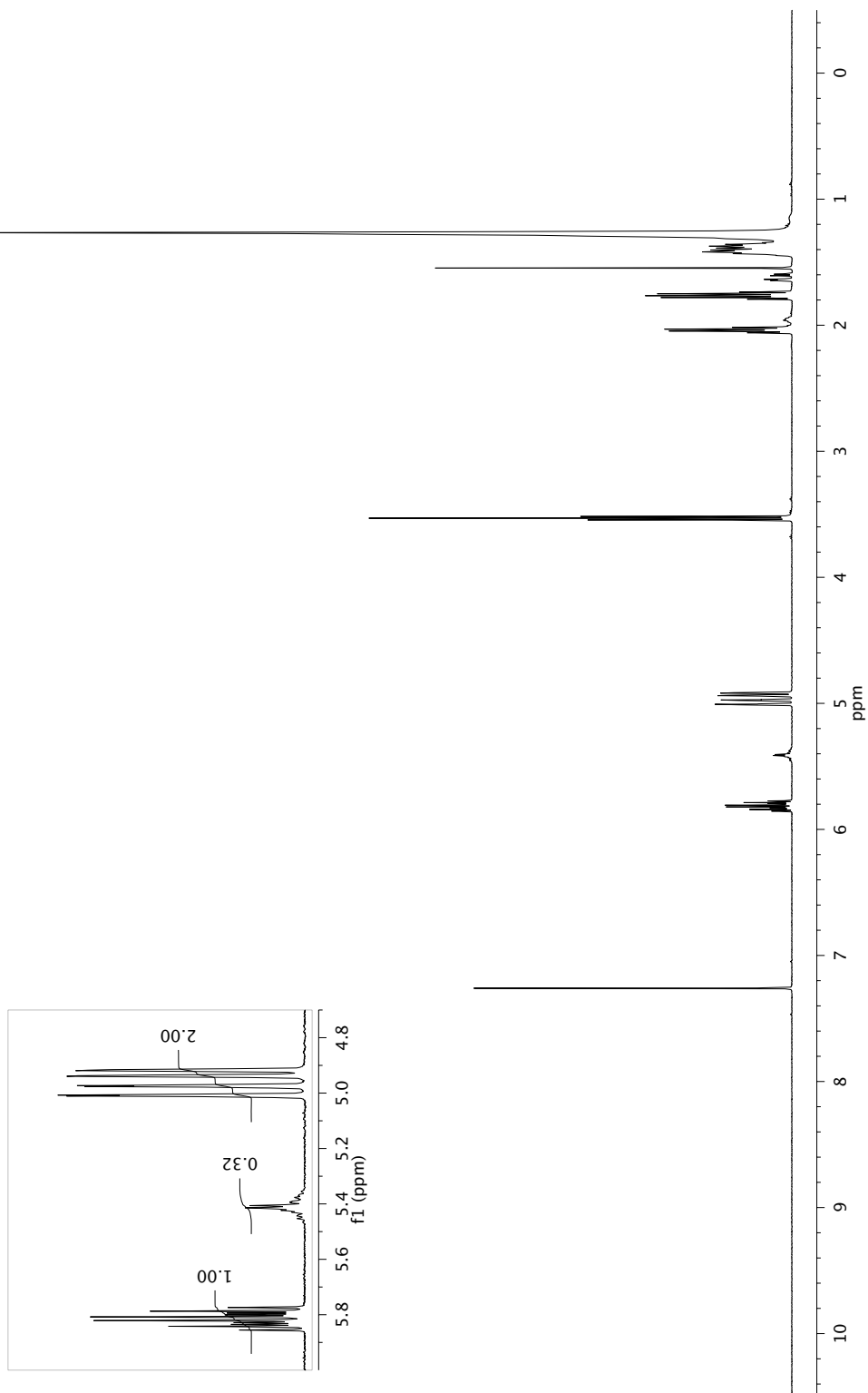
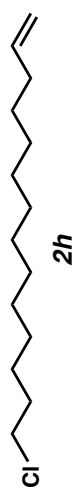
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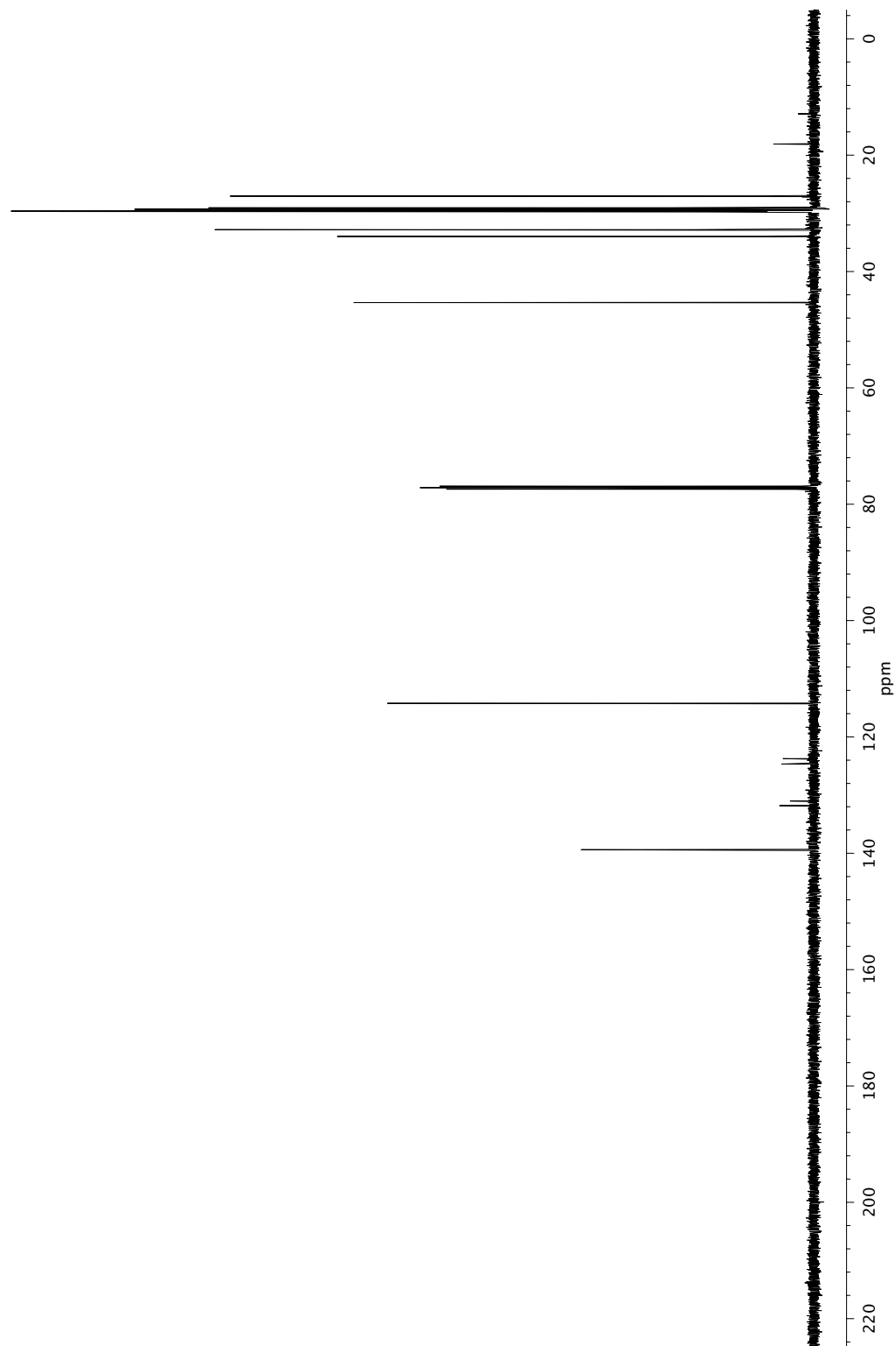
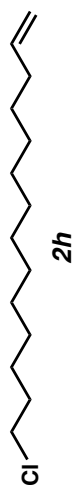


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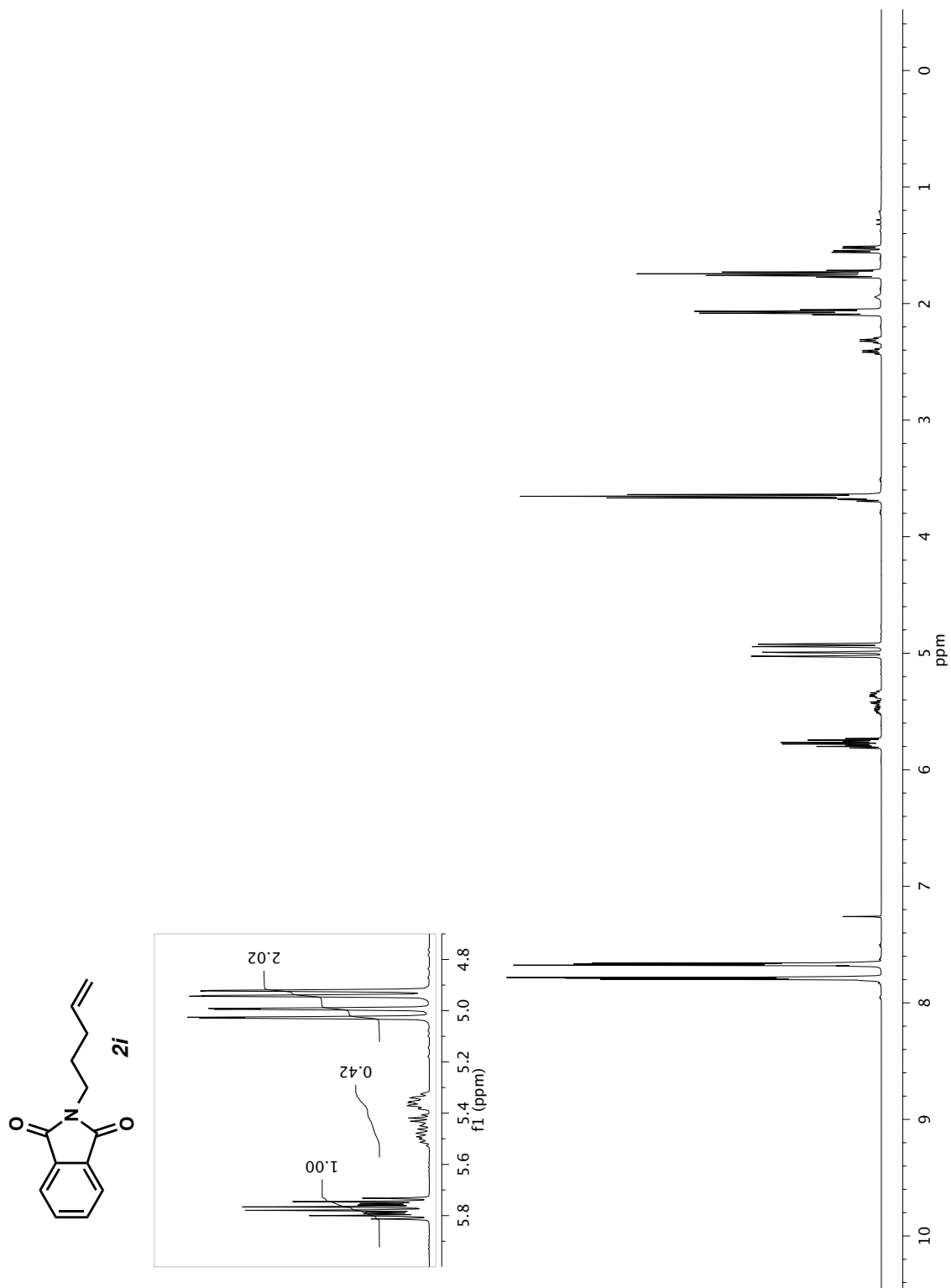


¹³C NMR (126 MHz, CDCl₃) of compound **2g**.

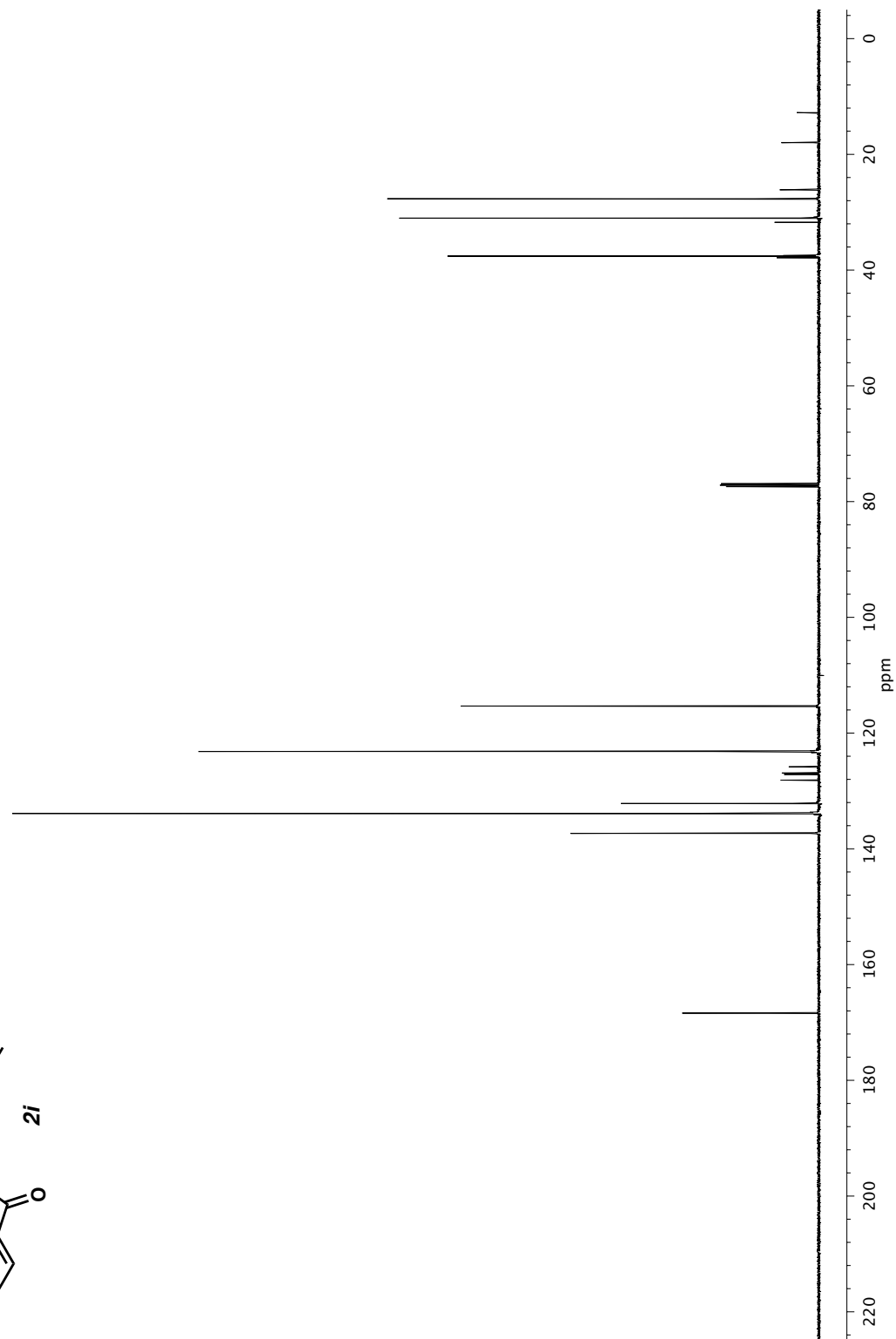
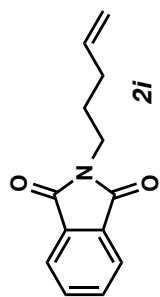


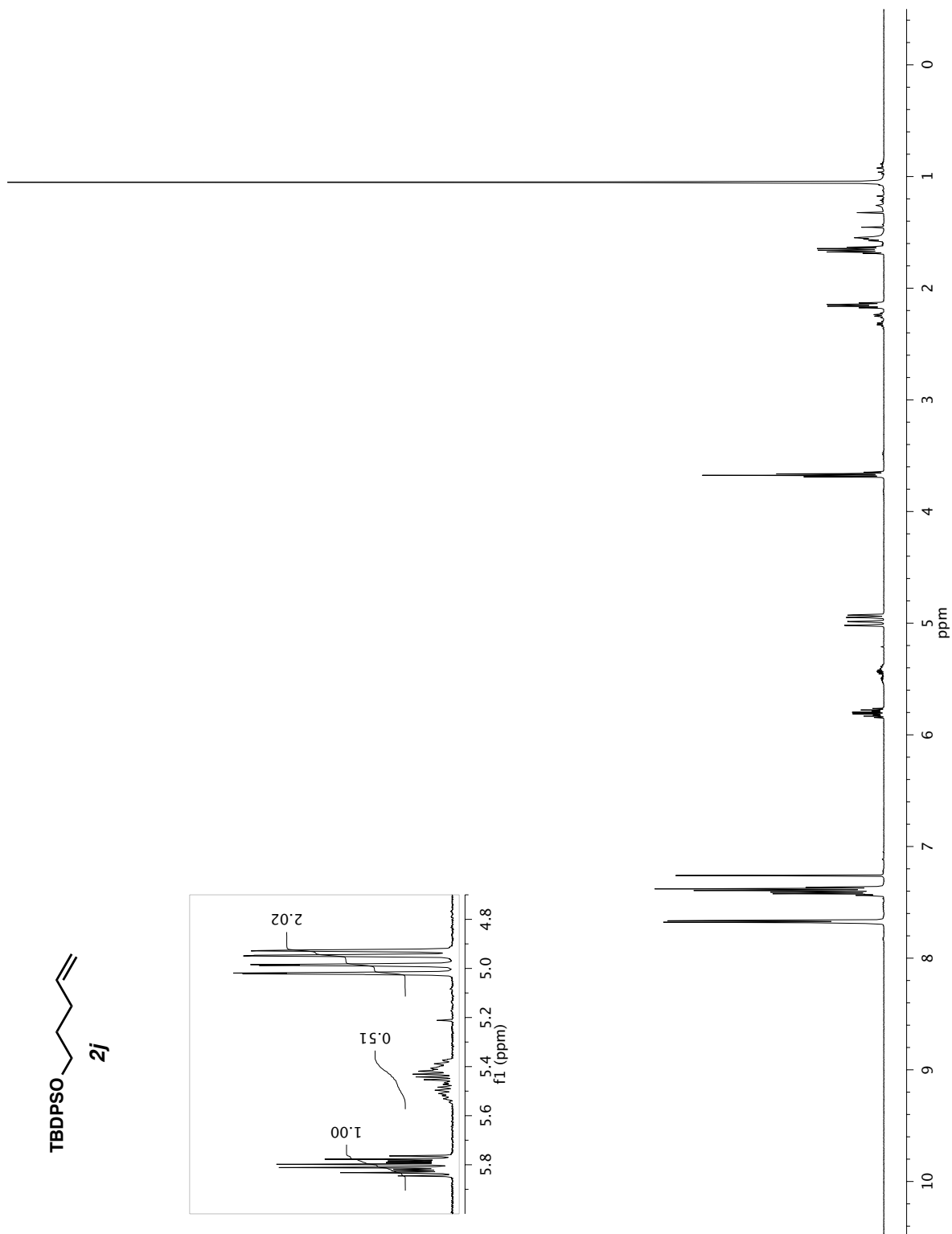
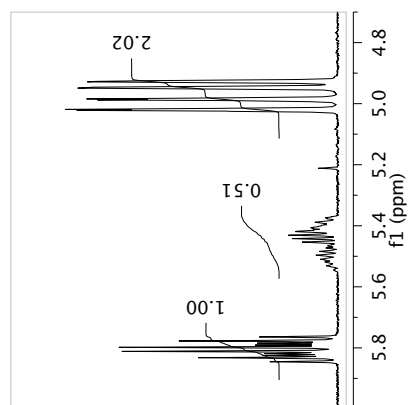
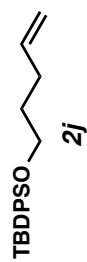


^{13}C NMR (126 MHz, CDCl_3) of compound **2h**.

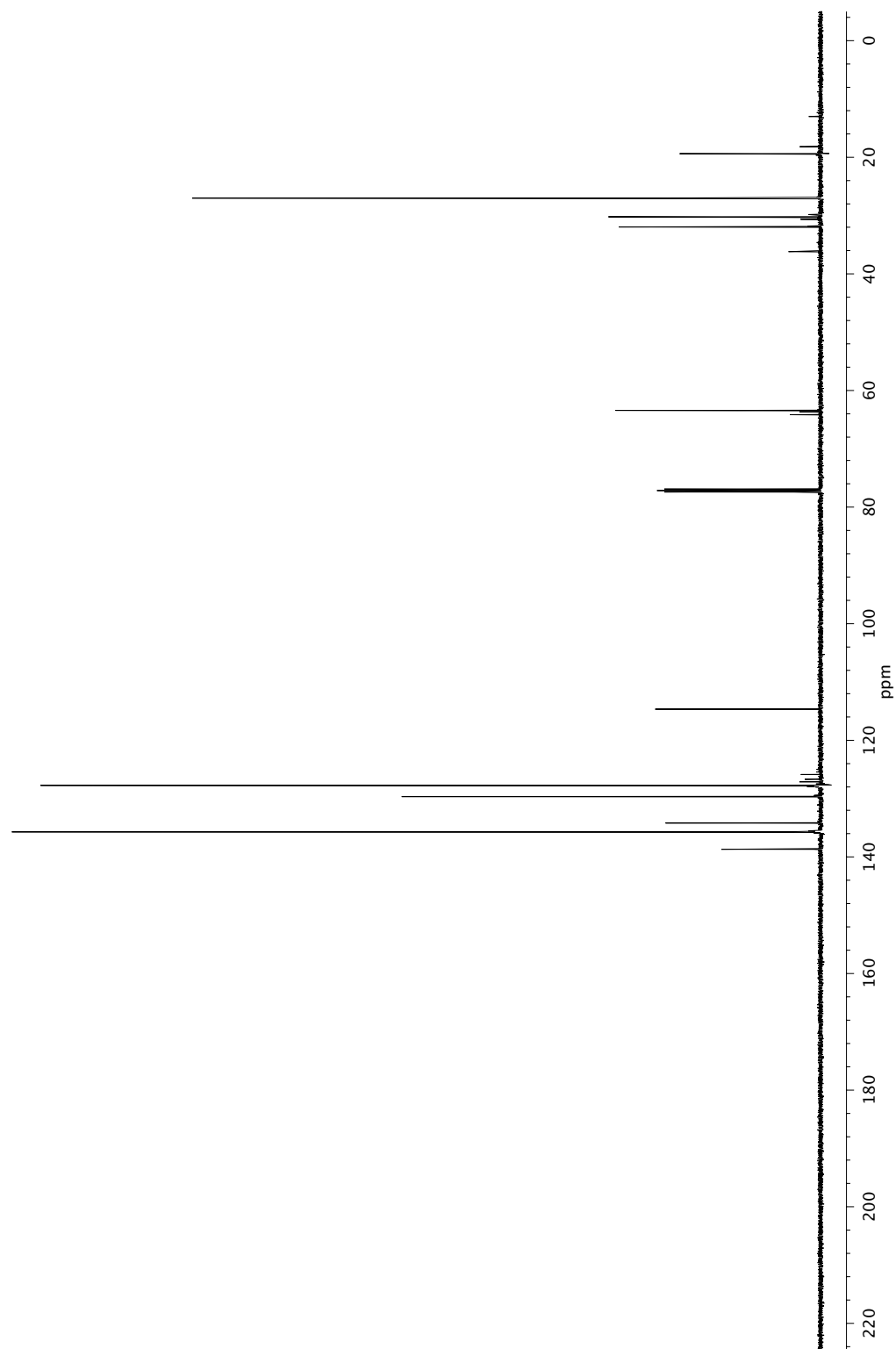
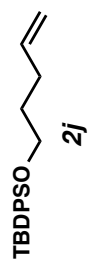


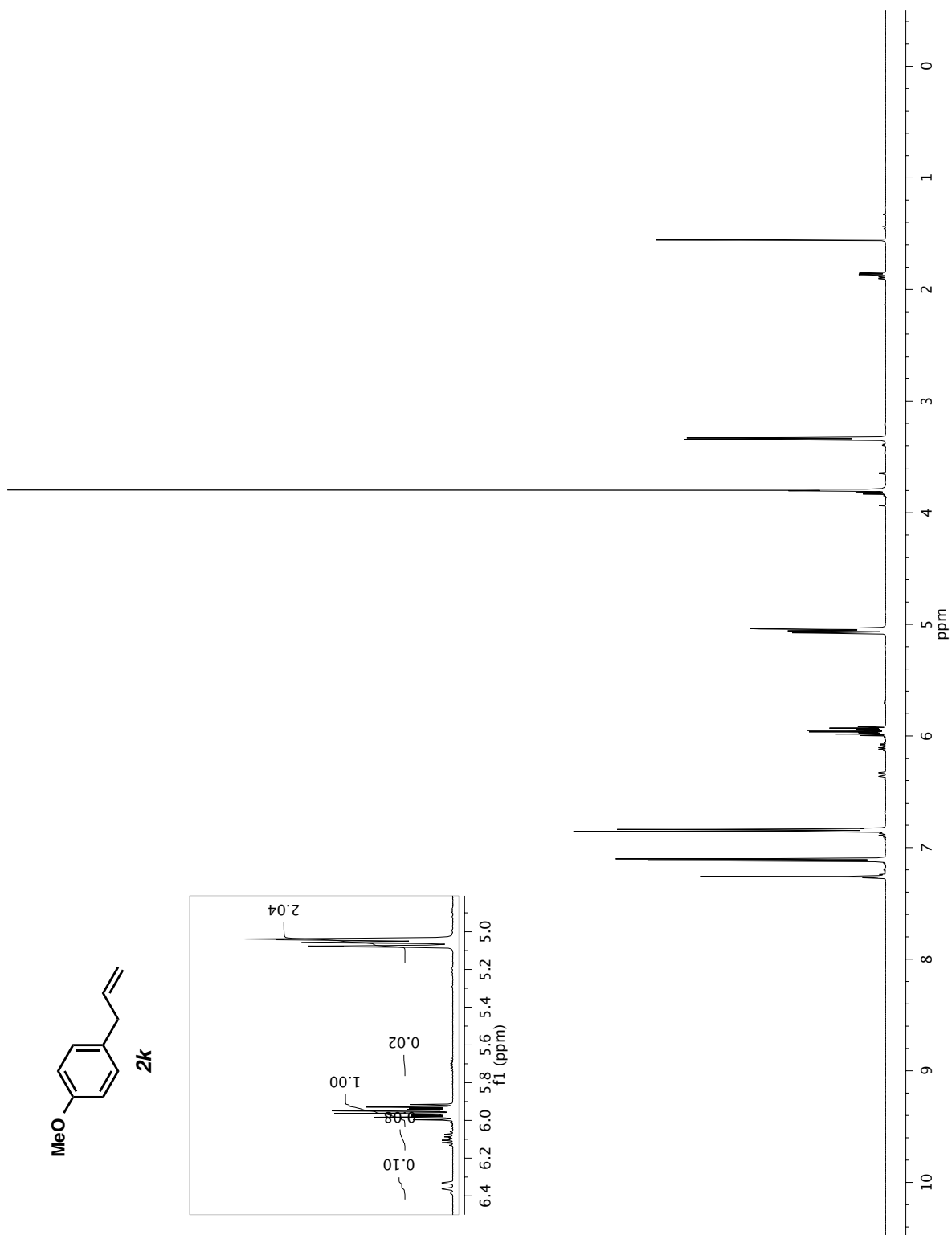
¹H NMR (500 MHz, CDCl₃) of compound **2i**.

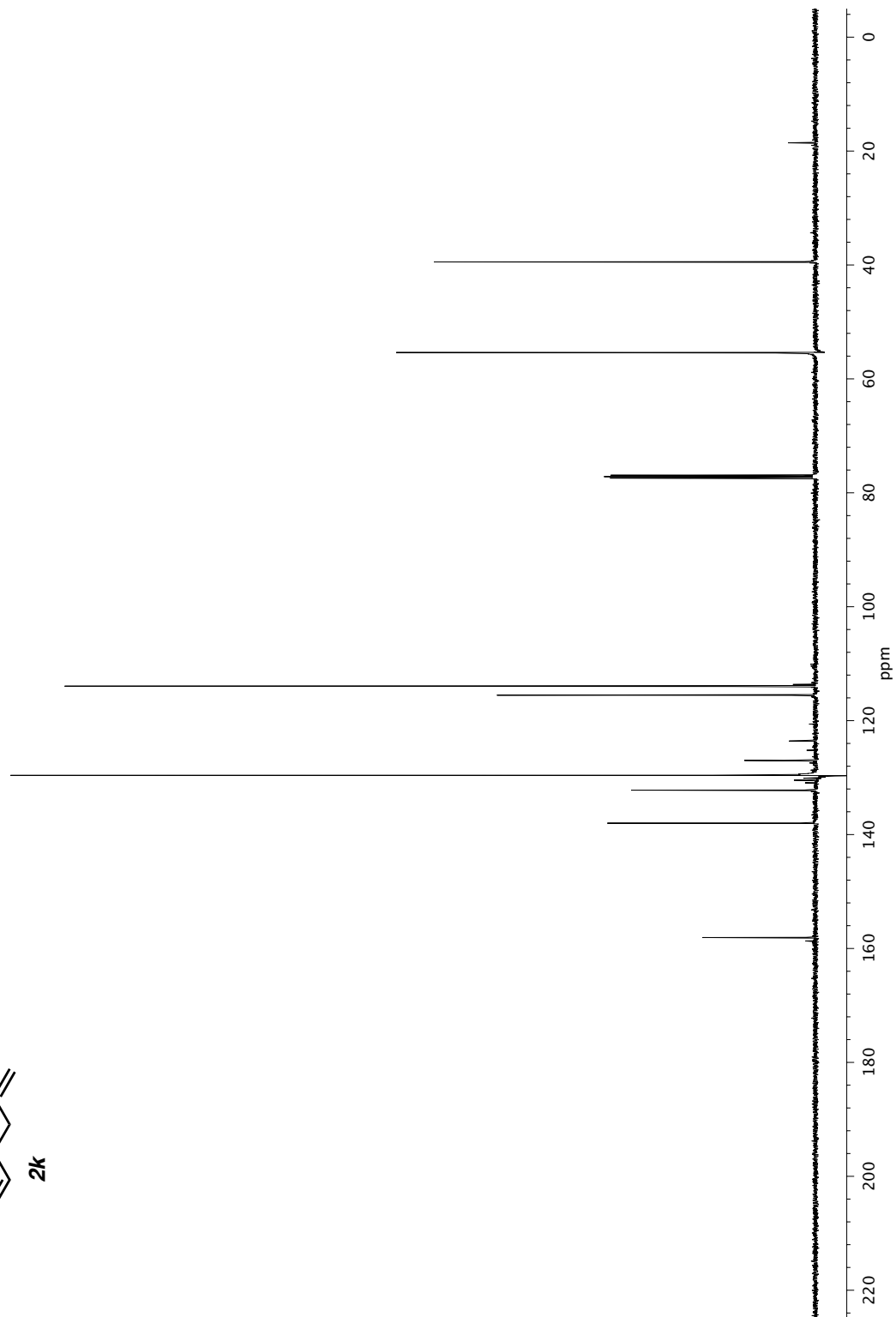
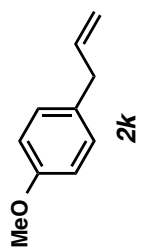




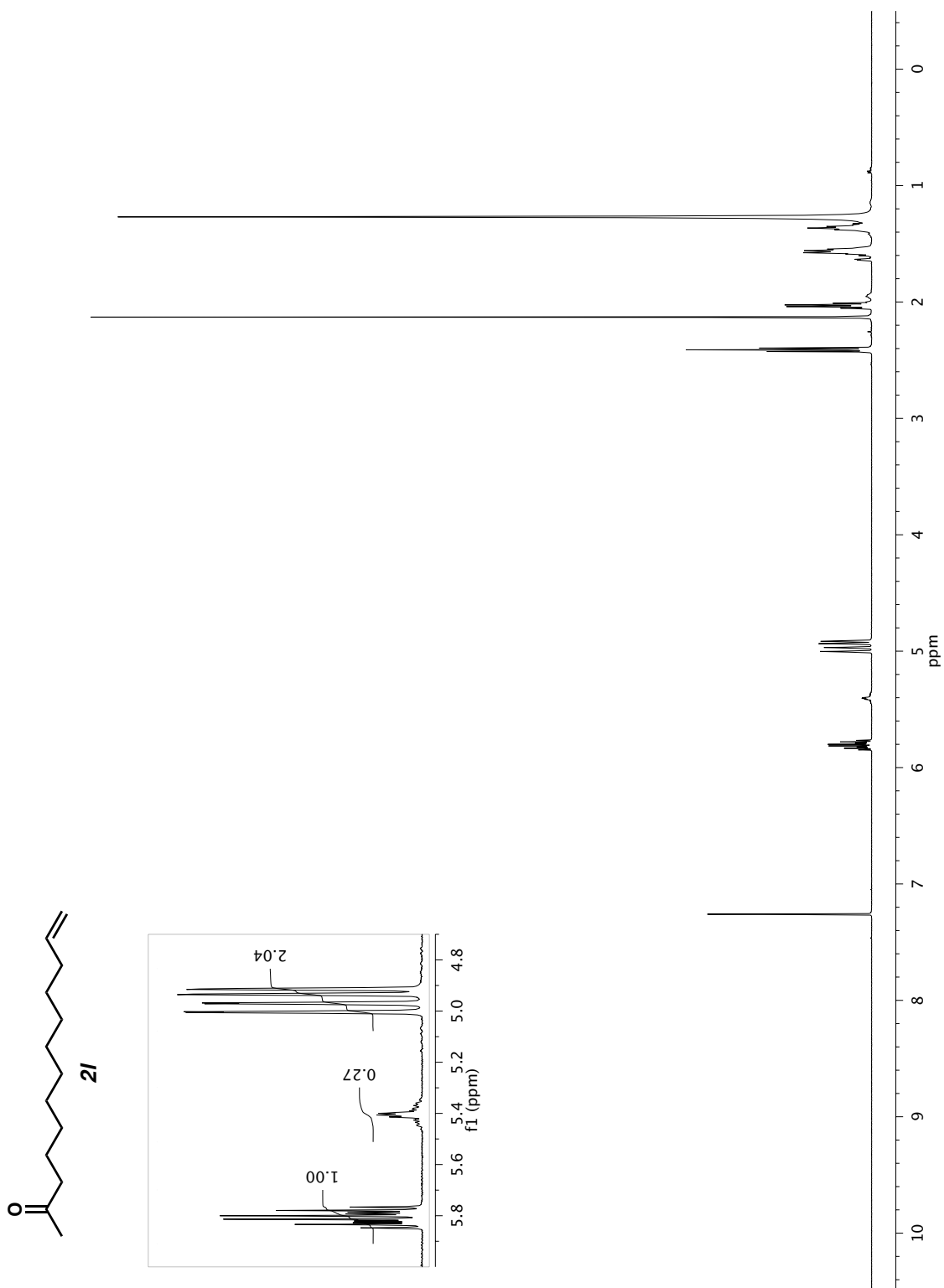
¹H NMR (500 MHz, CDCl₃) of compound **2j**.

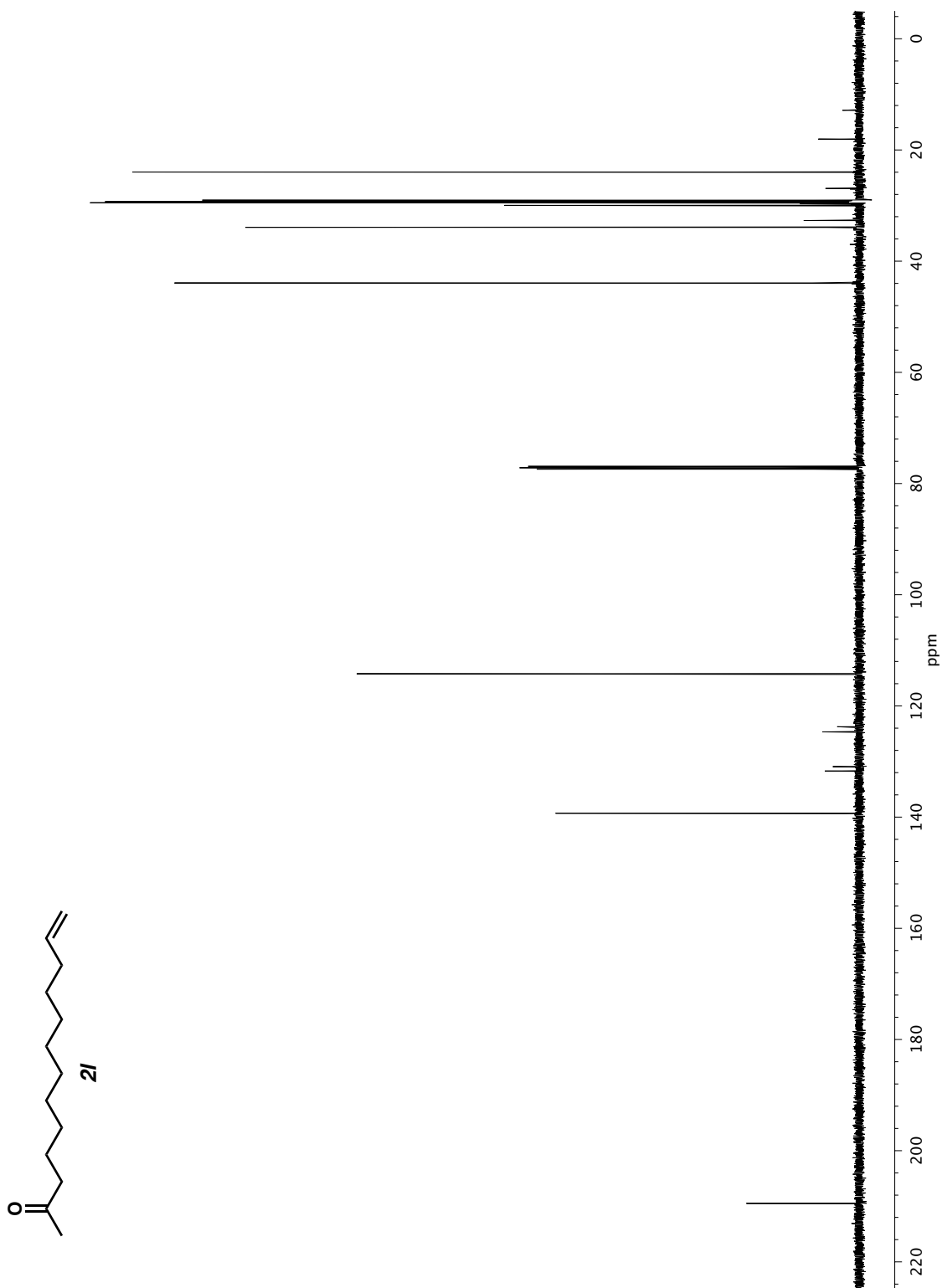


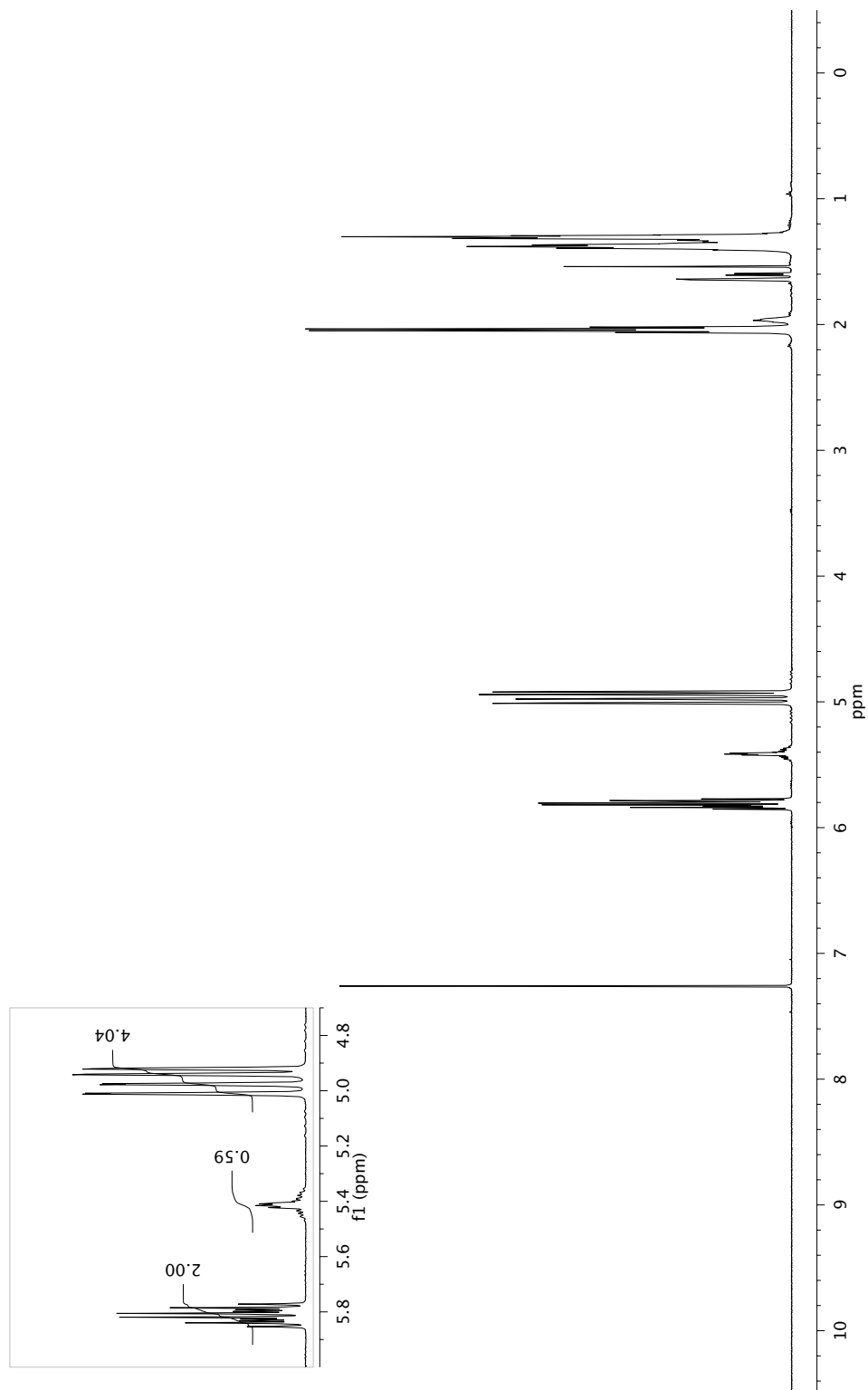
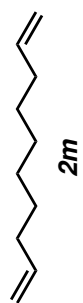


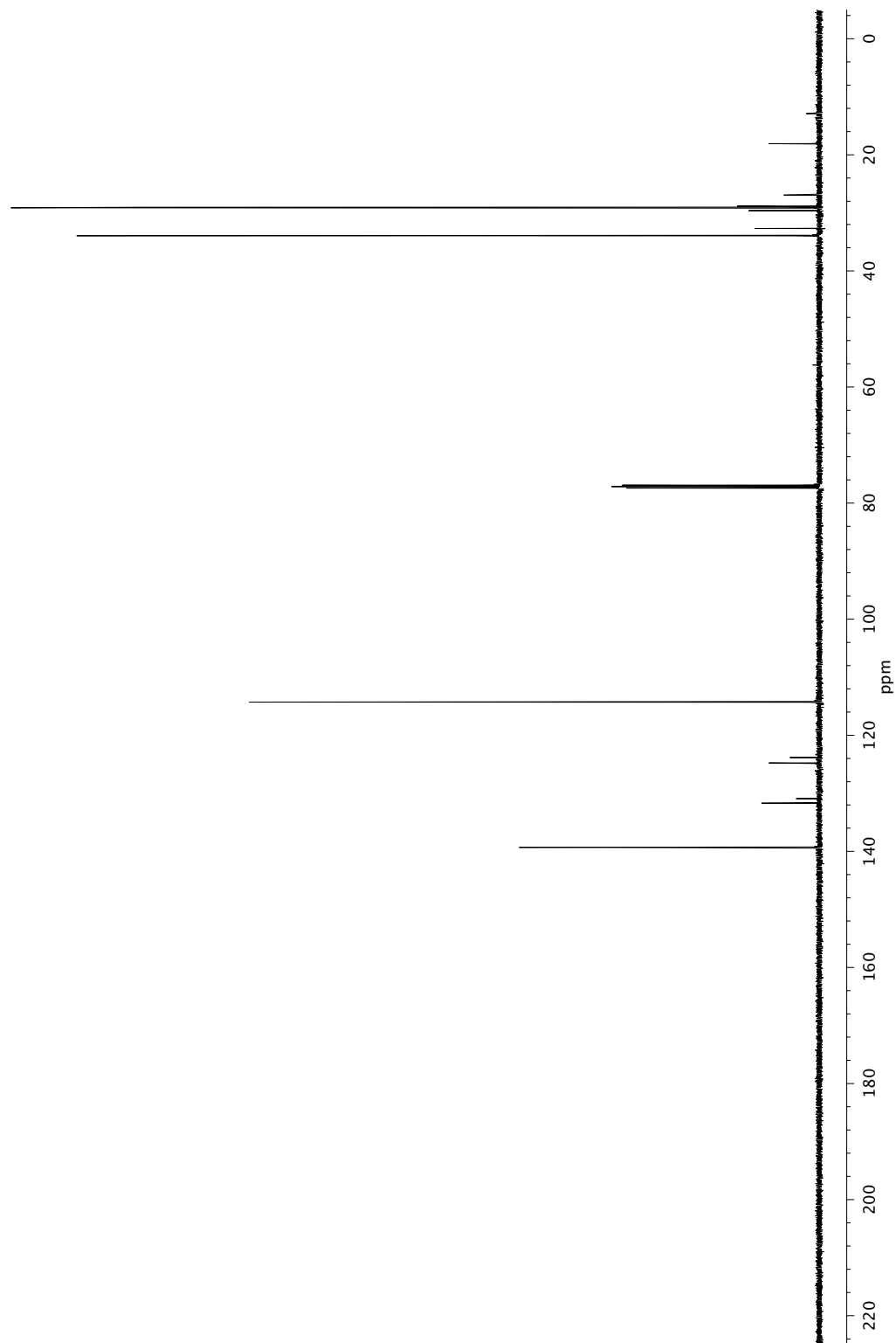
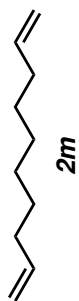


^{13}C NMR (126 MHz, CDCl_3) of compound **2k**.

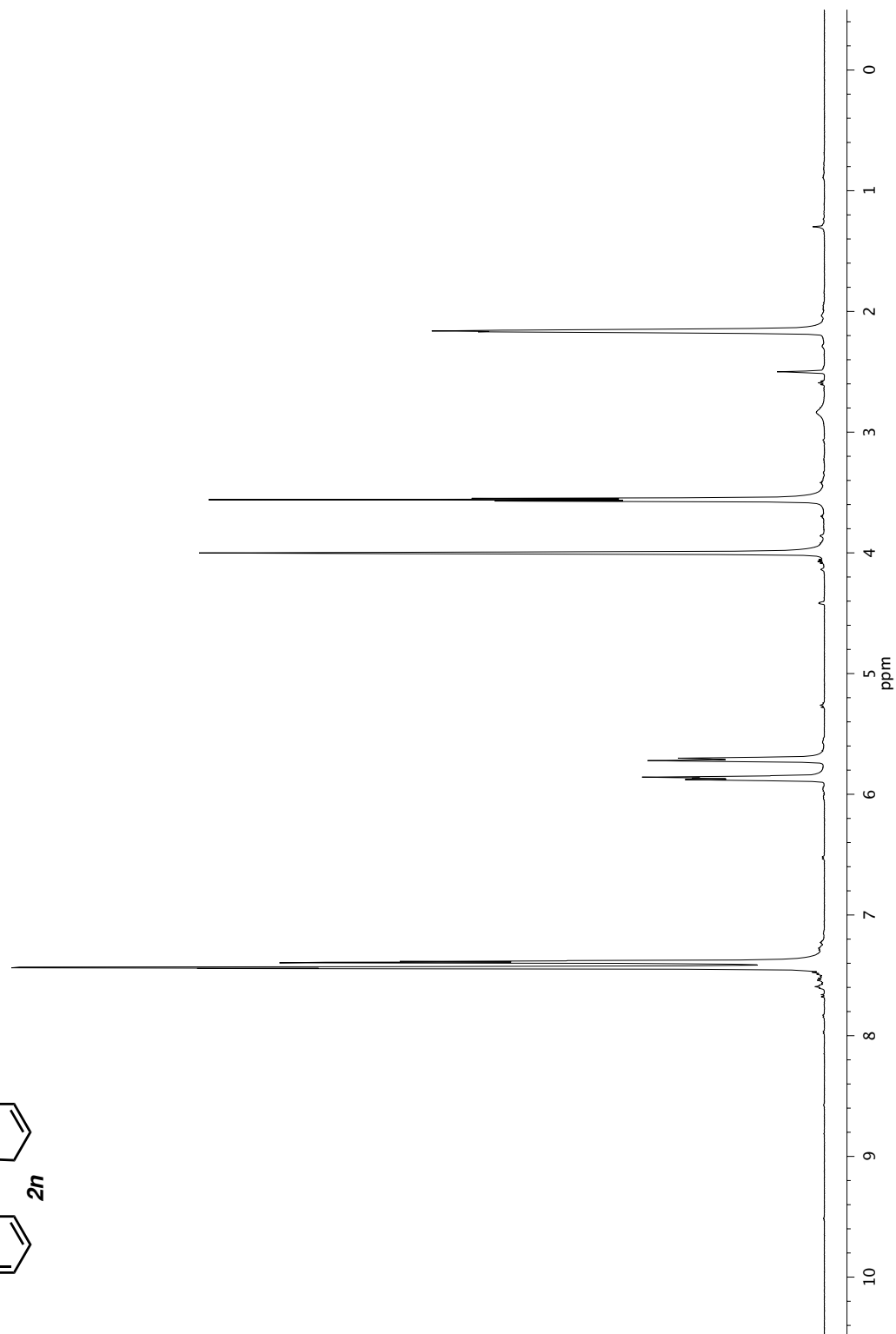
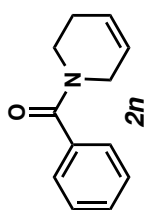




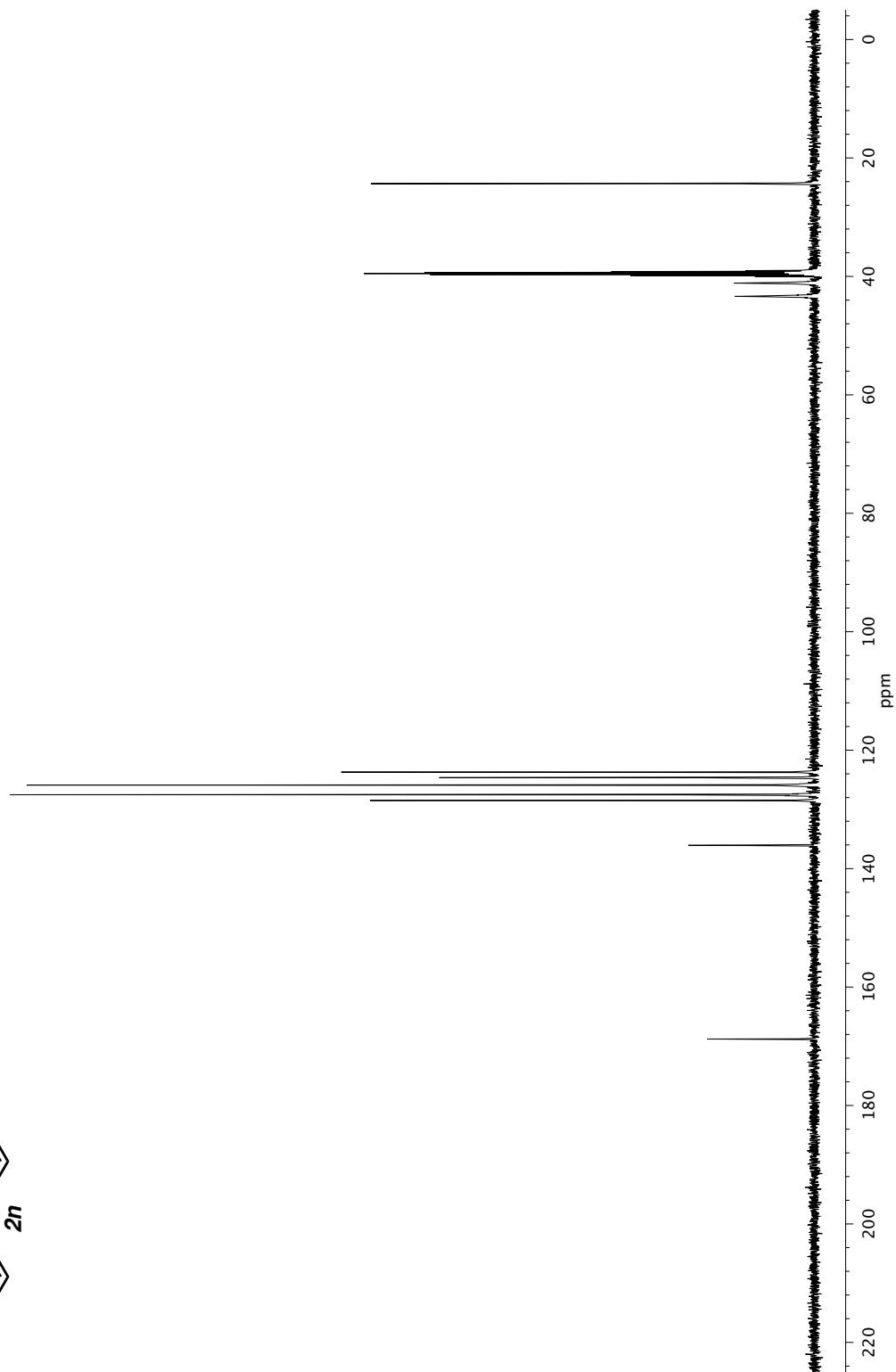
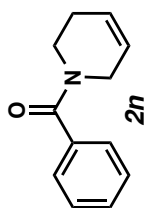


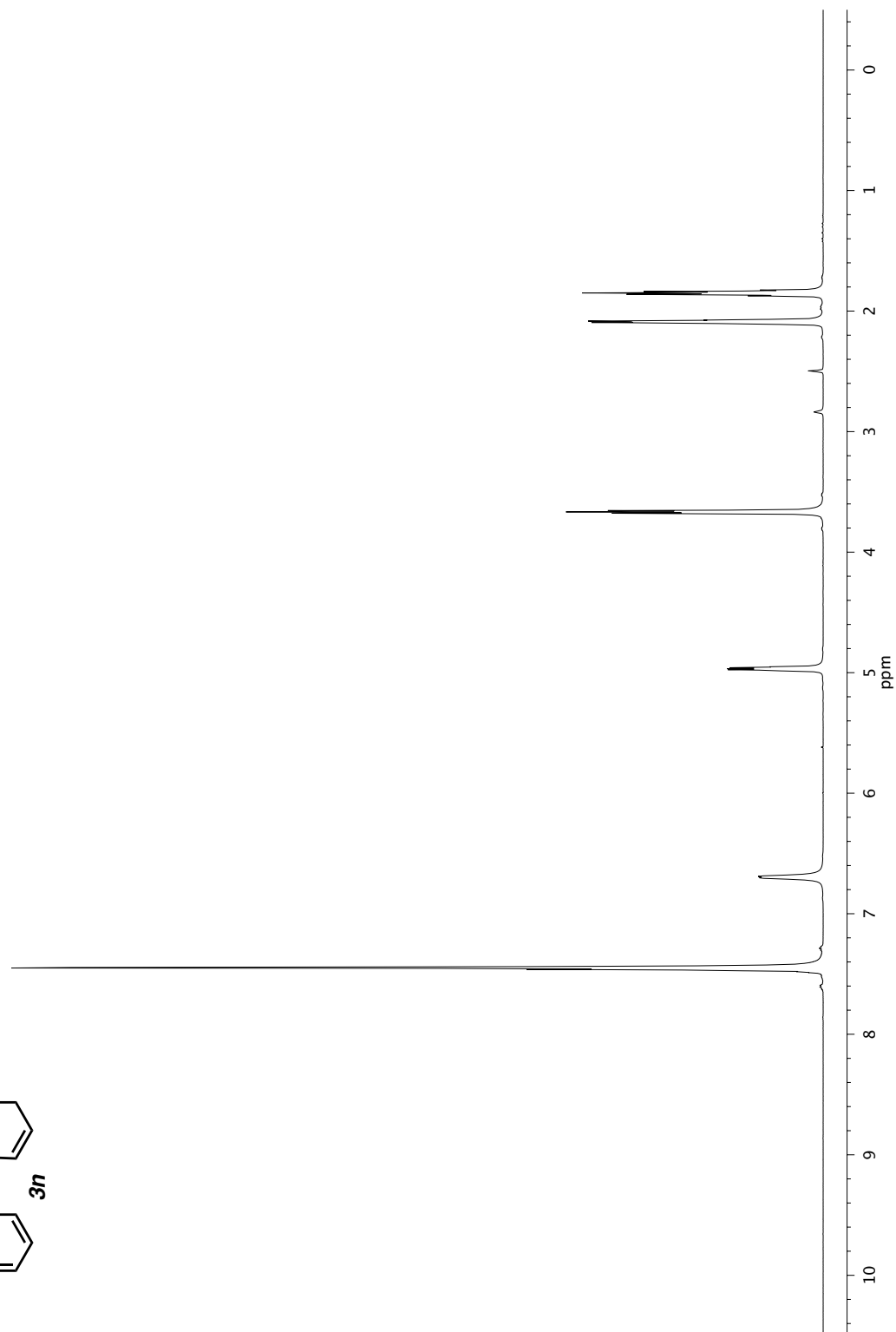
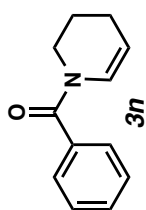


¹³C NMR (126 MHz, CDCl₃) of compound **2m**.

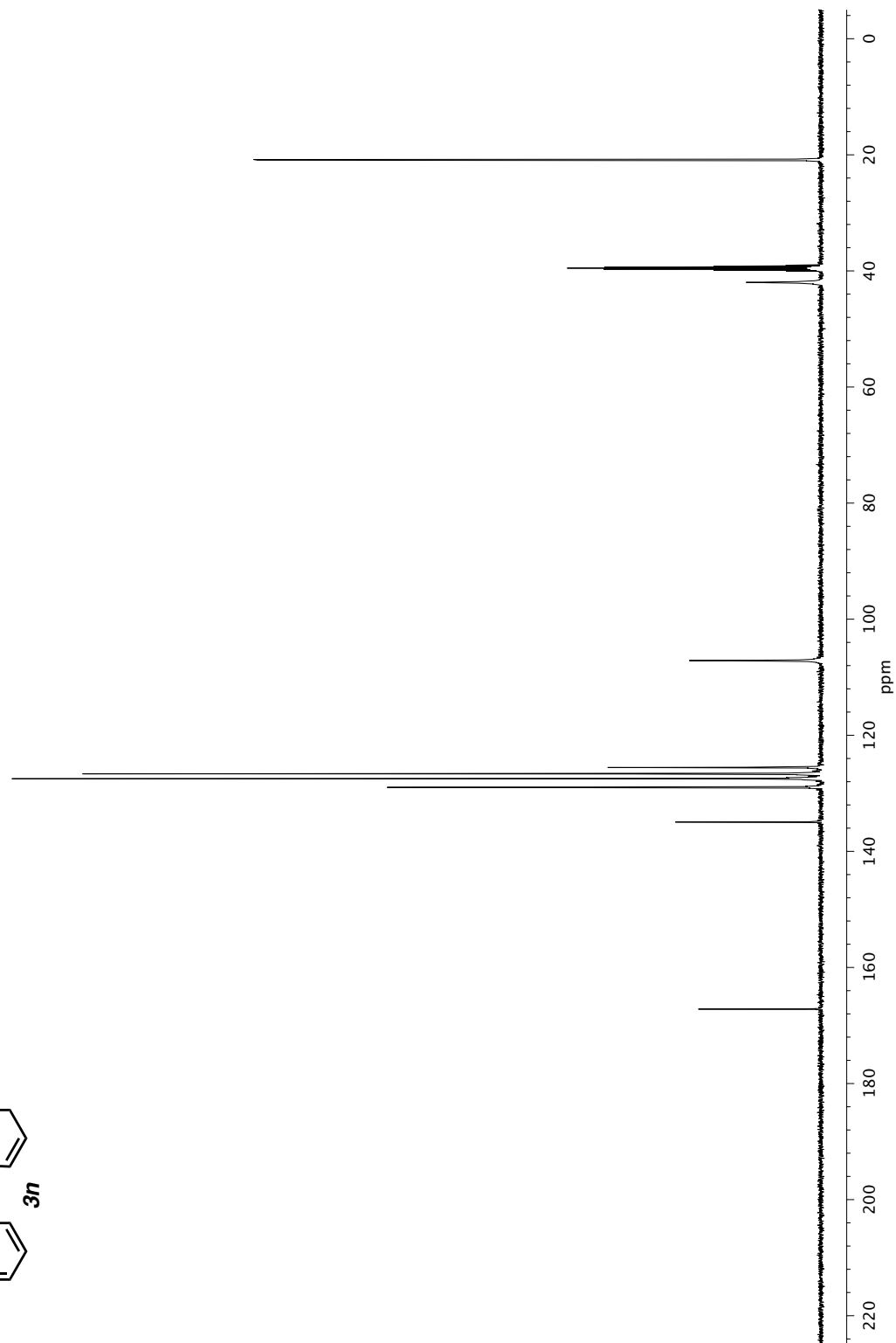
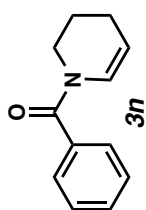


¹H NMR (500 MHz, DMSO-d₆, 130 °C) of compound **2n**.

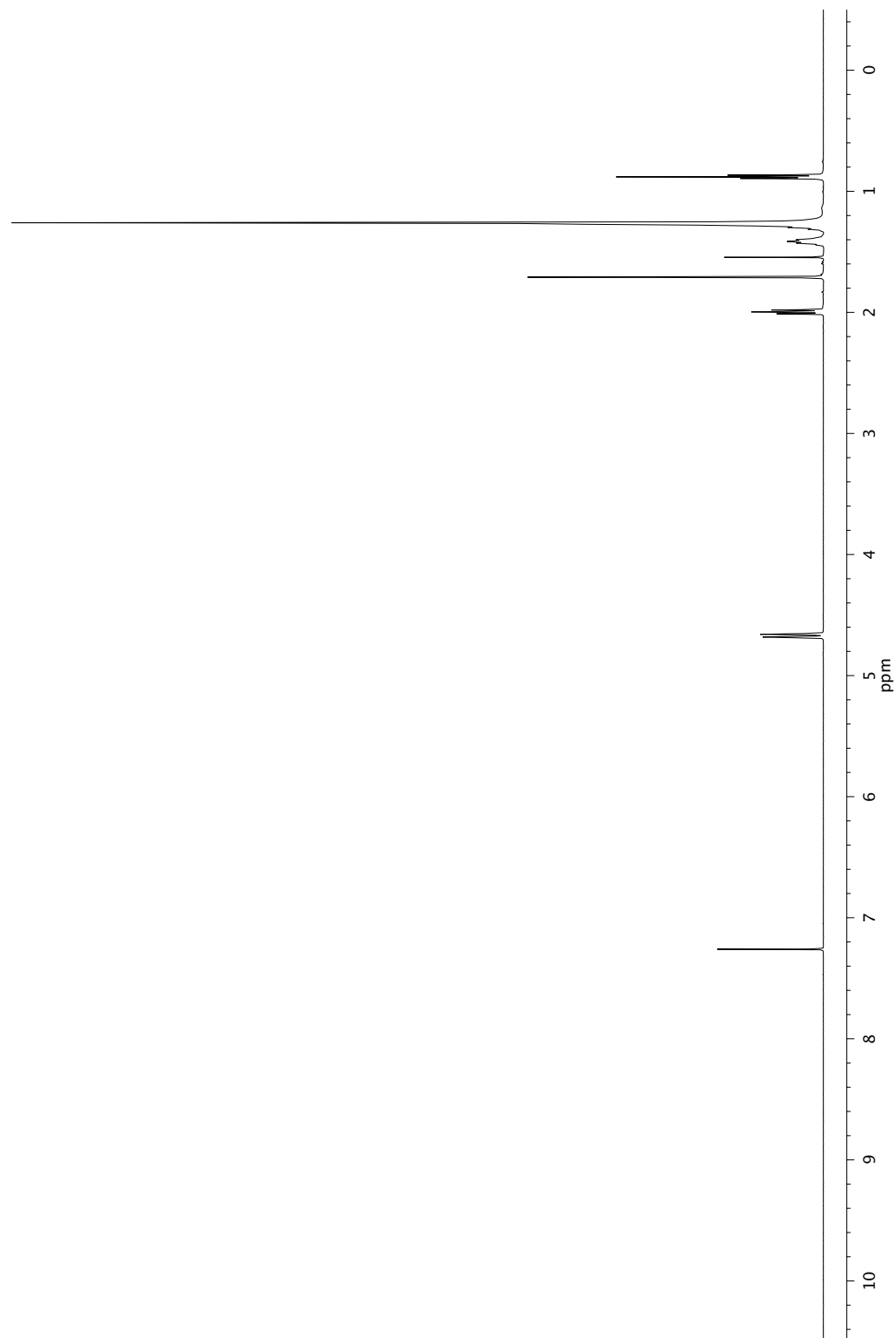
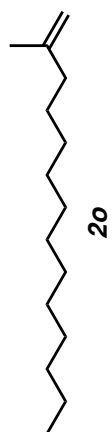




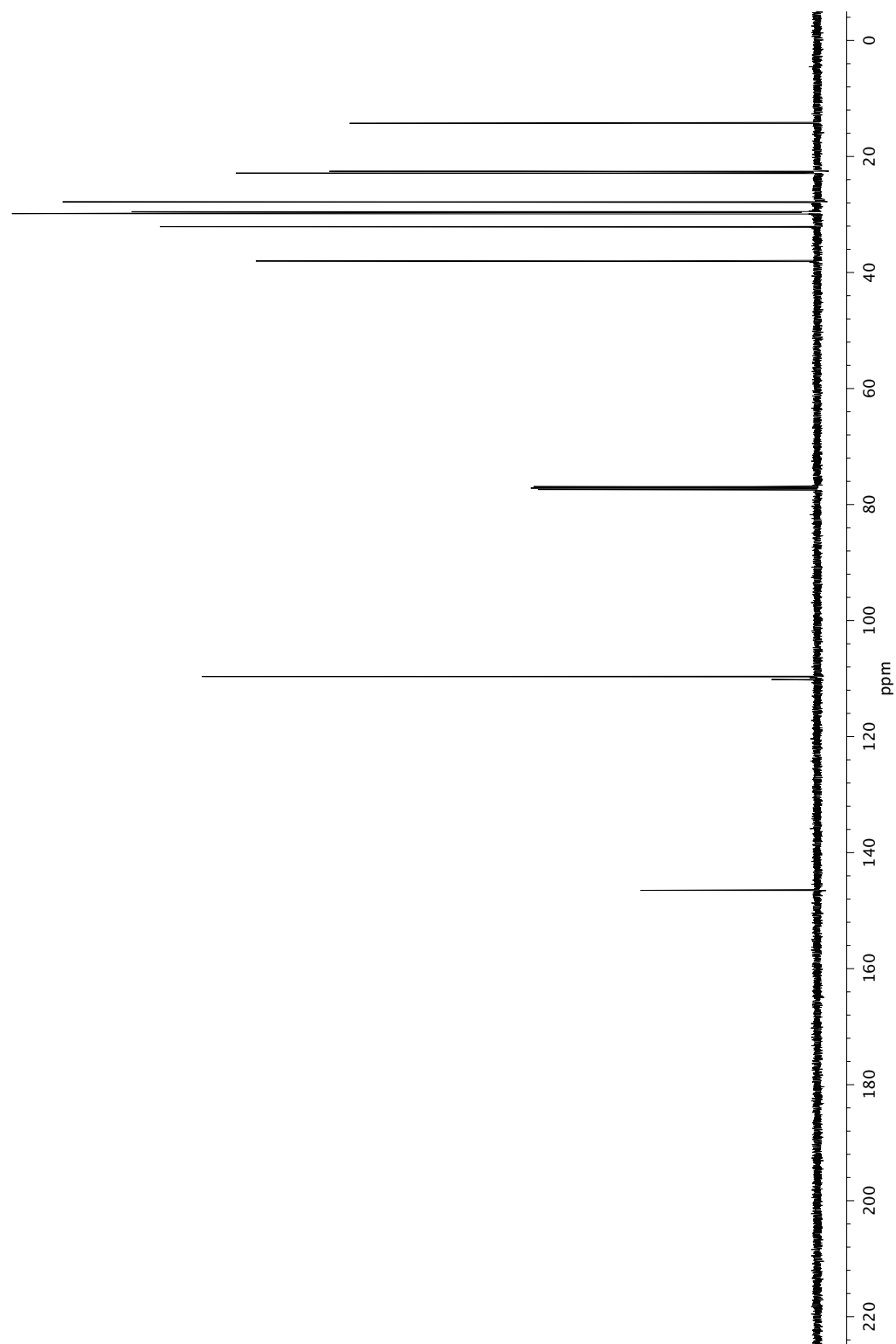
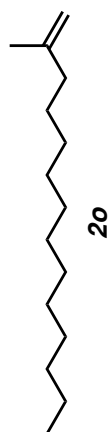
¹H NMR (500 MHz, DMSO-d₆, 130 °C) of compound **3n**.



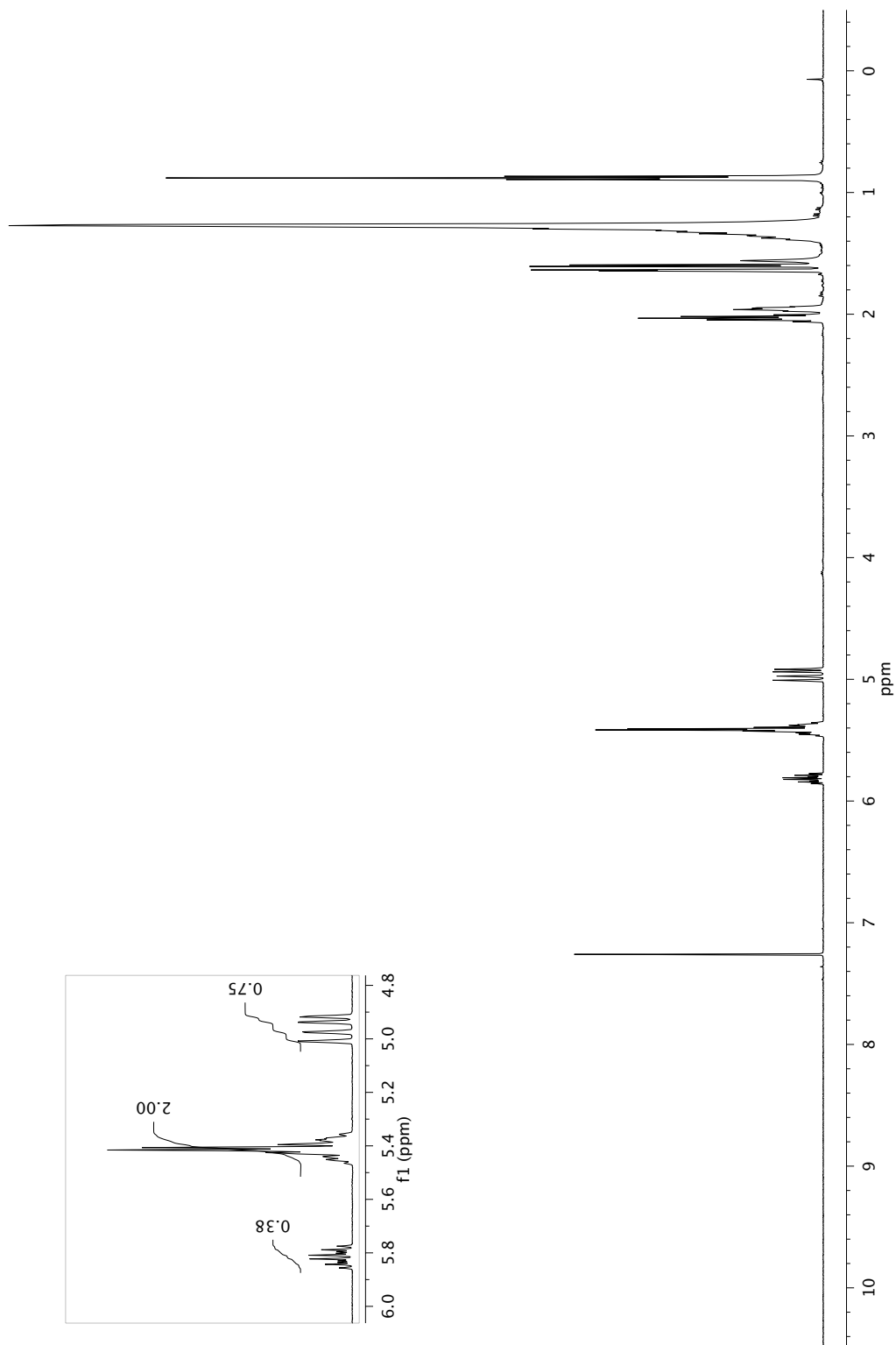
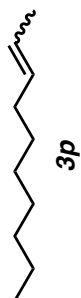
^{13}C NMR (126 MHz, DMSO- d_6 , 130 °C) of compound **3n**.

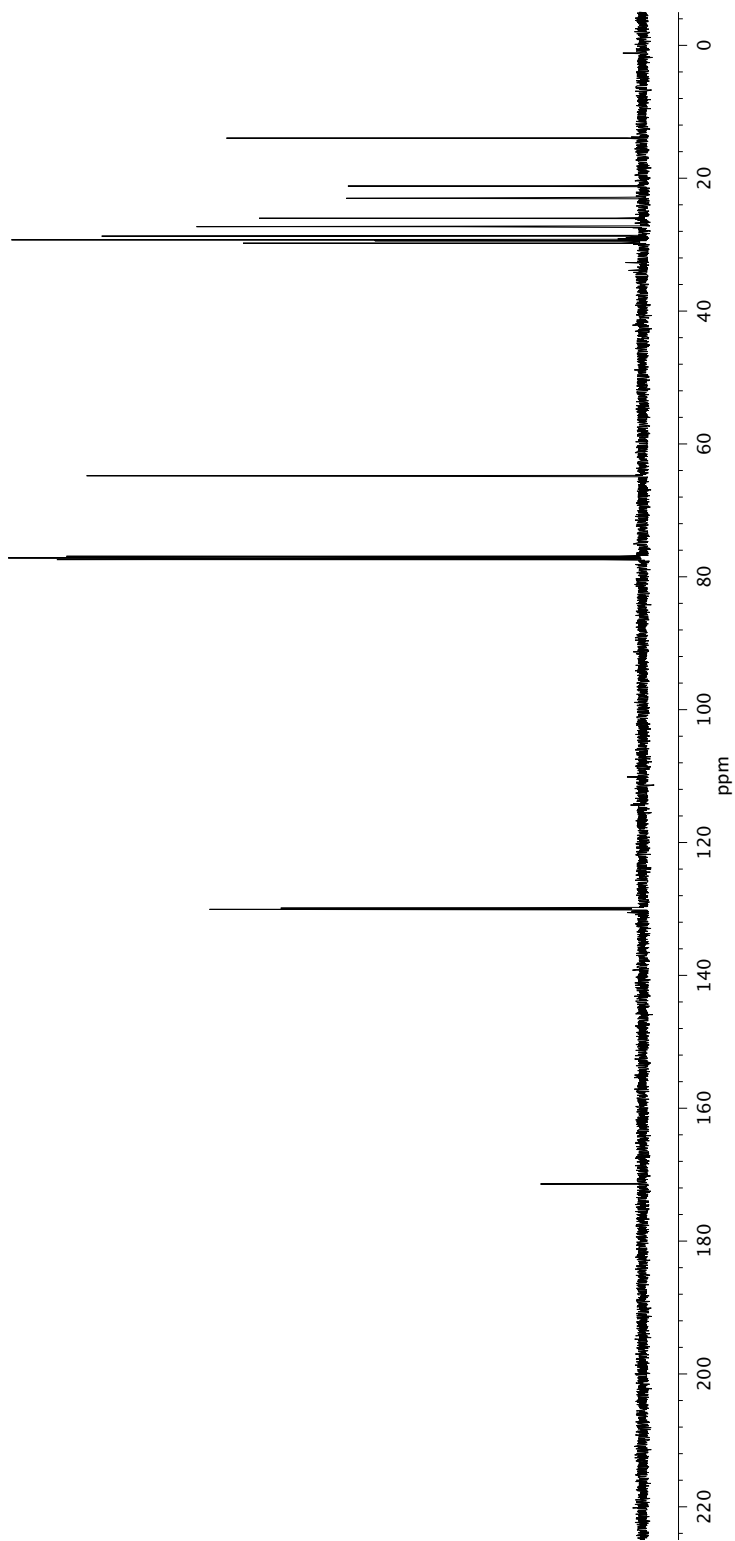


¹H NMR (500 MHz, CDCl₃) of compound **20**.

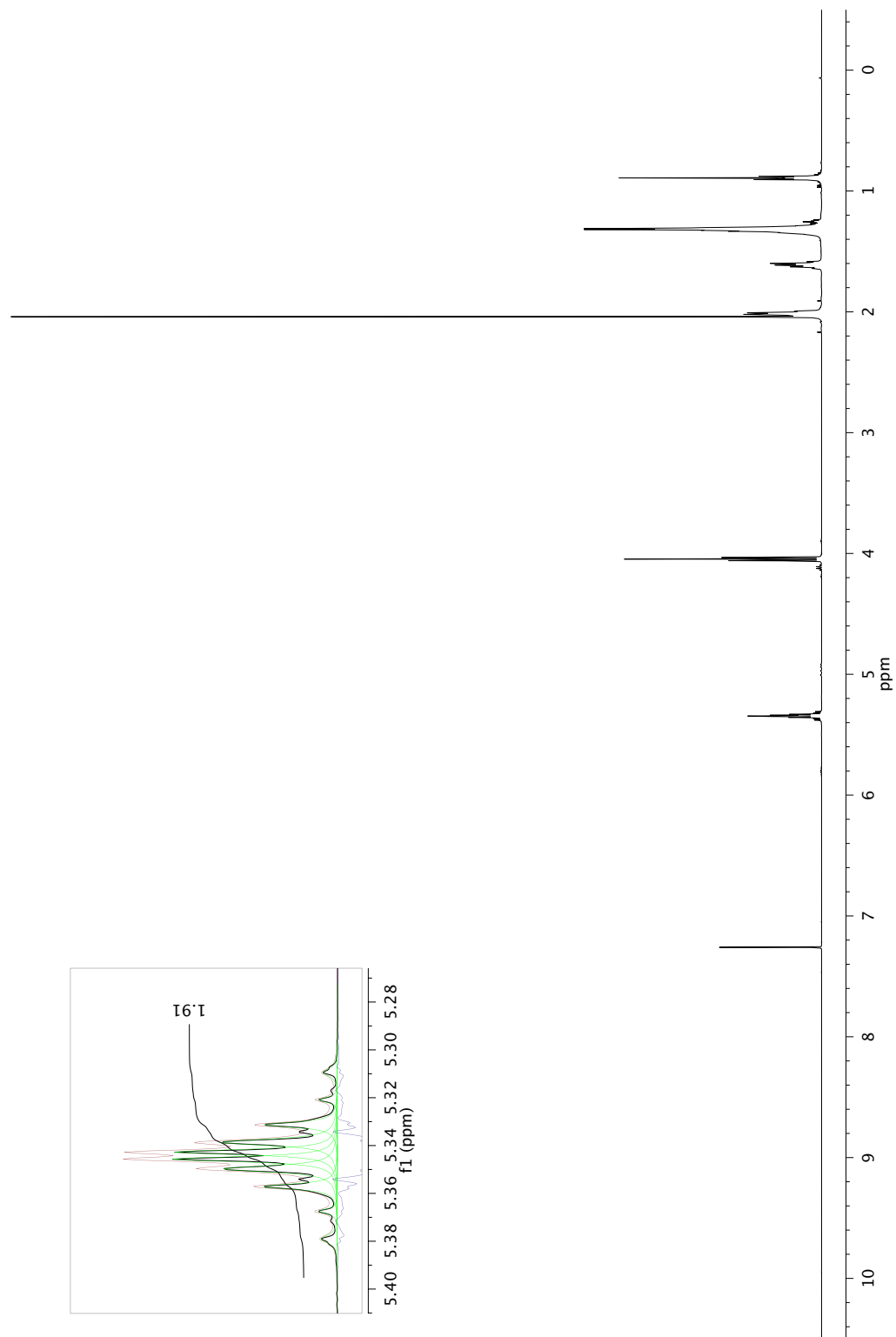
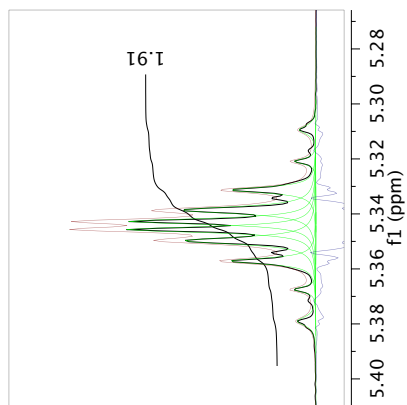
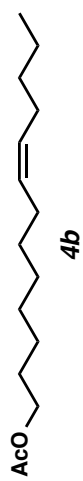


^{13}C NMR (126 MHz, CDCl_3) of compound **20**.





¹³C NMR (126 MHz, CDCl₃) of compound **4a**.



¹H NMR (500 MHz, CDCl₃) of compound **4b**.

