Generating Fischer-type Rh-carbenes with Rh-carbynoids

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Supporting Information

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1. General information.

All reagents were used as purchased with no further purification. Rhodium(II) acetate dimer $Rh_2(OAc)_4$, and bis[rhodium(α,α,α′,α′-tetramethyl-1,3-benzenedipropionic acid)] $Rh_2(esp)_2$ were purchased from Sigma-Aldrich. Rhodium bis(1-adamantate) dimer $Rh_2(Adc)_4$ and rhodium(II) triphenylacetate dimer $Rh_2(TPA)_4$ were prepared according to reported procedures[1,2]. Ethyl diazoacetate, (≥13 wt. % dichloromethane) was purchased from Aldrich (Ref. E22201) and used without further purification. Anhydrous solvents were dried by passing through an activated alumina column on a PureSolvTM solvent purification system (Innovative Technologies, Inc., MA). Analytical thin layer chromatography (TLC) was carried out using aluminum sheets with 0.2 mm of silica gel (Merck GF234). Visualization of the developed chromatogram was performed by irradiation with UV light or treatment with a solution of potassium permanganate or vanillin stain followed by heating. Flash column chromatography was performed on silica gel (Aldrich, 230-400 mesh). Organic solutions were concentrated under reduced pressure on a Büchi rotatory evaporator. Unless otherwise stated, reactions were carried out under argon atmosphere. Yields refer to purified compounds unless otherwise noted. NMR spectra were recorded at 298 K on Bruker Avance 300, Bruker Avance 400 Ultrashield or Bruker Avance 500 Ultrashield apparatuses. Coupling constants (*J*) are quoted in hertz (Hz). Multiplicity is reported with the following abbreviations: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, dt = doublet of triplets, td = triplet of doublets, tt = triplet of triplets, sp = septet, m = multiplet, app = apparent. Melting points were measured using open glass capillaries in a Büchi B540 apparatus. Infrared spectra were recorded on a Bruker Tensor 27. Mass spectra were recorded on a Waters LCT Premier spectrometer. Gas chromatography-mass spectrometry (GC-MS) was carried out in Agilent 7890B - 5877A MSD.

2. Synthesis of diazo compounds 2

- Hypervalent iodine reagents **2a-e** are known compounds and were prepared following the reported literature protocols.[3,4]

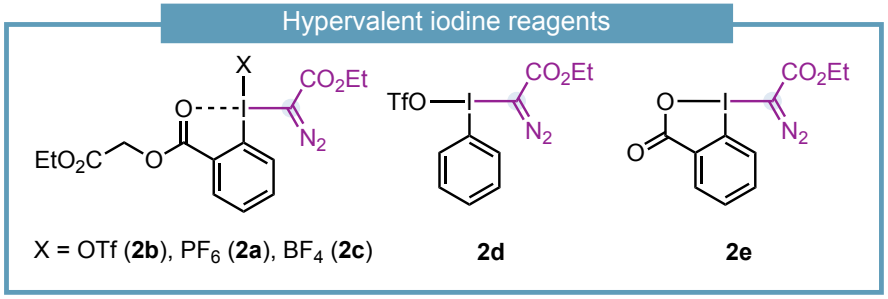
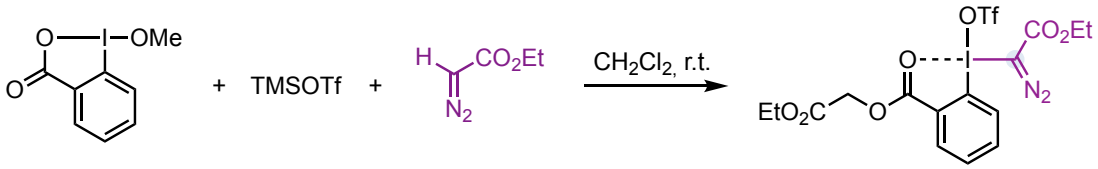


Figure S1. Pseudo-cyclic, linear, and cyclic hypervalent iodine reagents **2a-e**.

(1-Diazo-2-ethoxy-2-oxoethyl)(2-(2-ethoxy-2-oxoethoxy)carbonylphenyl)iodonium trifluoromethanesulfonate (2b)[3]

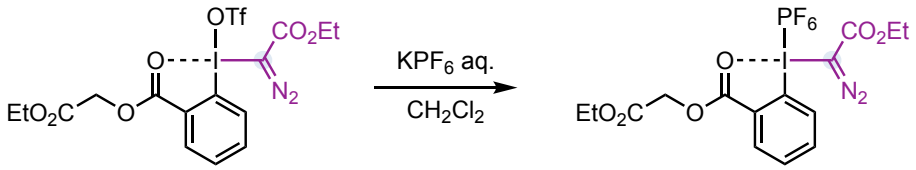


A solution of 1-methoxy-1,2-benziodoxol-3(1H)-one (4.0 g, 14.38 mmol, 1.0 equiv.) in dichloromethane (0.5 M) was treated with trimethylsilyl trifluoromethanesulfonate (2.6 mL, 14.38 mmol, 1.0 equiv.) at room temperature. After 30 minutes, a cloudy suspension was observed and then ethyl diazoacetate (3.3 mL, 31.64 mmol, 2.2 equiv.) was added dropwise for 15 minutes. Nitrogen evolution was observed, and the resulting reaction mixture was stirred at room temperature until a clear yellow solution was observed (usually 3 hours). Solvent was removed under vacuum and the crude was recrystallized from a mixture of diethyl ether/dichloromethane (5/1) during 12 hours at -30 °C (Note: the recrystallization process may be repeated if impurities are observed). The desired product was collected by filtration, washed with cold diethyl ether (500 mL), dried under high *vacuum*, and stored a -30 °C. The title compound was isolated as a yellow solid (8.2 g, 96 %).

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (dd, J = 7.5, 1.9 Hz, 1H), 8.32 (dd, J = 8.0, 1.2 Hz, 1H), 8.00 (td, J = 7.7, 1.9 Hz, 1H), 7.95 (td, J = 7.4, 1.3 Hz, 1H), 5.15 (s, 2H), 4.30 – 4.19 (m, 4H), 1.26 – 1.19 (m, 6H);

^{13}C NMR (101 MHz, DMSO-d_6) δ 167.4, 166.8, 161.6, 137.7, 133.4, 132.7, 132.7, 126.3, 120.7 (q, J = 324.2 Hz), 117.8, 63.7, 63.5, 61.5, 14.1, 14.0;
The data are consistent with that reported previously.

(1-Diazo-2-ethoxy-2-oxoethyl)(2-(2-ethoxy-2-oxoethoxy)carbonylphenyl)iodonium hexafluorophosphate (2a)[4]



To a 50 mL round bottom flask equipped with a stirring bar, 10.0 mL of saturated aqueous solution of sodium hexafluorophosphate and 10.0 mL of **2a** (2.98 g, 5 mmol) in dichloromethane (0.5 M) were added. The resulting biphasic mixture was stirred vigorously at room temperature for 10 minutes. The phases were separated, and the aqueous layer was extracted with dichloromethane (3 x 10 mL). The combined organic fractions were dried over anhydrous $MgSO_4$ and concentrated under *vacuum* to give the **2b** as a yellow solid (2.1 g, 70% yield).

IR (film, cm^{-1}): 2988, 2121, 1752, 1703, 1660, 1589, 1330, 1271, 1220, 1152, 1029, 837;
^{1}H NMR (400 MHz, CD_3CN) δ 8.45 – 8.40 (m, 1H), 8.06 – 8.01 (m, 2H), 7.93 (ddd, J = 7.6, 5.7, 2.6 Hz, 1H), 5.07 (s, 2H), 4.35 (q, J = 7.1 Hz, 2H), 4.26 (q, J = 7.1 Hz, 2H), 1.28 (t, J = 7.1 Hz, 7H);
^{13}C NMR (101 MHz, CD_3CN) δ 170.7, 167.2, 162.0, 139.5, 134.3, 133.5, 130.3, 126.1, 116.7, 65.4, 65.2, 62.9, 14.5, 14.4;
^{19}F NMR (376 MHz, CD_2Cl_2) δ -72.8 (d, J = 706.9 Hz);
^{31}P NMR (162 MHz, $CDCl_3$) δ -141.4 (sp, J = 714.4 Hz);
HRMS (MALDI) calculated for $C_{15}H_{16}IN_2O_6^+$ $[M\text{-}PF_6]^+$ m/z: 447.0053, found: 447.0036.

- *α*-onium diazoesters **2f,g** and bromo diazoacetate **2h** have been prepared according to the literature procedure by Weiss[4] and Bonge-Hansen.[5]

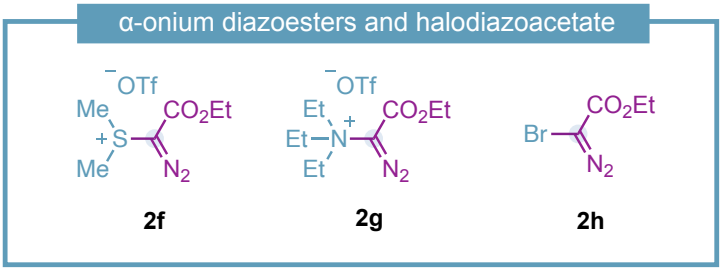
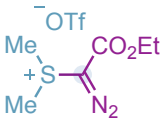


Figure S2. α-onium diazoesters and ethyl bromodiazoacetate

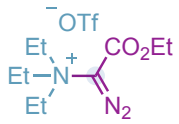
(1-Diazo-2-ethoxy-2-oxoethyl)dimethylsulfonium triflate (2f)[4]



2d (0.621 g, 1.17 mmol, 1.0 equiv.) was dissolved in dry dichloromethane (15 mL) at 0 °C. To this solution was added dimethyl sulfide (0.215 mL, 0.182 g, 2.93 mmol, 2.5 equiv.) with stirring. The mixture turned into a clear solution and was stirred at 0 °C for 1 h and then concentrated in vacuo at 20 °C. The title compound was isolated by recrystallization from diethyl ether at -30ºC overnight as a white solid (200.9 mg, 98% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.35 (q, J = 7.1 Hz, 2H), 3.32 (s, 6H), 1.34 (t, J = 7.1 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$): δ = 160.4, 120.3, 63.4, 26.6, 14.0;
The data are consistent with that reported previously.

1-Diazo-2-ethoxy-N,N,N-triethyl-2-oxoethanaminium triflate (2g)[4]



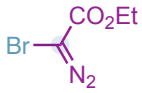
2d (0.487 g, 0.91 mmol, 1.0 equiv.) was dissolved in dry dichloromethane (15 mL) at 0 °C. To this solution was added triethylamine (0.134 mL, 0.097 g, 1.05 mmol, 1.05 equiv.). The mixture was stirred at 0 °C for 1 h and then concentrated in vacuo at 20 °C. The title compound was isolated by recrystallization from diethyl ether at -30ºC overnight as a sticky yellow solid (165.3 mg, 50% yield).

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.35 (q, J = 7.1 Hz, 2H), 3.86 (q, J = 7.1 Hz, 6H), 1.44 (t, J = 7.1 Hz, 9H), 1.34 (t, J = 7.1 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$): δ = 160.0, 120.9, 63.5, 56.4, 14.3, 8.5;

The data are consistent with that reported previously.

Ethyl 2-bromo-2-diazoacetate (2h)[5]



2d (46.6 mg, 0.1 mmol, 1.0 equiv.) was dissolved in dry dichloromethane (1 mL) at 0 °C. Tetrabutylammonium bromide (48.3 mg, 0.15 mmol, 1.5 equiv.) was added in one portion. The mixture was stirred at 0 °C for 1 h. The title compound was not isolated and was used directly in the reaction (***General procedure B***).

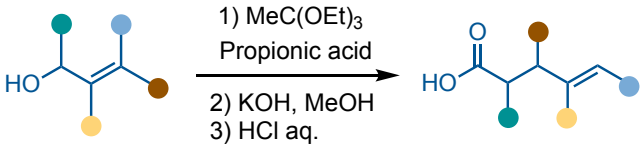
Notes:

(a) We have never observed any explosion during the preparation or manipulation of reagents **2a-h** at the scales indicated here in our laboratory. For safety precautions we always used an anti-blast shield.

(b) If impurities are observed after recrystallization, a subsequent recrystallization may be done.

(c) Reagents **2a-g** were kept at ≤ −20 ºC.

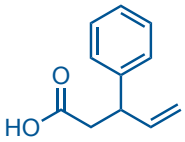
3. General procedure A for the synthesis of 4-pentenoic acids (1)[5-11]



1

A mixture of propionic acid (75 μL, 1 mmol, 0.1 equiv.), triethyl orthoacetate (18.0 mL, 100.0 mmol, 10 equiv.) and the corresponding allylic alcohol (10.0 mmol, 1 equiv.) was heated at 150 °C for 5 h in a Dean-Stark apparatus. After cooling to room temperature, a solution of KOH (800 mg, 14.3 mmol) in methanol (6.0 mL) was added and the resulting mixture was heated under reflux for 3 h. After this, the solvent was then evaporated under *vacuum* and the residue was dissolved in distilled water (6.0 mL). The solution was extracted with diethyl ether (10.0 mL), and the organic phase was discarded. Then the aqueous layer was acidified with 6 M HCl at 0 °C until pH = 1-2. The solution was extracted with Et_2O (3 x 15 mL). The combined organic phases were dried with Na_2SO_4, and the solvent was evaporated under *vacuum*. The product was purified by flash chromatography on silica gel (hexane/ethyl acetate, 10/1 to 5/1).

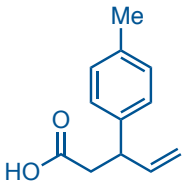
3-Phenylpent-4-enoic acid (1a)[6]



Prepared according to the general procedure A with cinnamyl alcohol (1.3 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (1.3 g, 75% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 2H), 7.26 – 7.20 (m, 3H), 6.04 – 5.94 (m, 1H), 5.14 – 5.05 (m, 2H), 3.91 – 3.82 (m, 1H), 2.85 – 2.72 (m, 2H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.0, 142.3, 140.1, 128.8, 127.7, 127.0, 115.2, 45.3, 40.0;
The data are consistent with that reported previously.

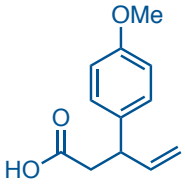
3-(*p*-Tolyl)pent-4-enoic acid (1b)[7]



Prepared according to the general procedure A with (*E*)-3-(*p*-tolyl)prop-2-en-1-ol (1.5 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (1.7 g, 88% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17 – 7.07 (m, 4H), 5.97 (ddd, *J* = 17.2, 10.1, 6.9 Hz, 1H), 5.10 – 5.05 (m, 2H), 3.83 (m, 1H), 2.84 – 2.67 (m, 2H), 2.32 (s, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 177.7, 140.3, 139.3, 136.5, 129.5, 127.5, 115.0, 44.9, 40.0, 21.2;
HRMS: (ESI) calculated for $C_{12}H_{13}O_2^-$ $[M-H]^-$ m/z: 189.0921, found: 189.0914;
The data are consistent with that reported previously.

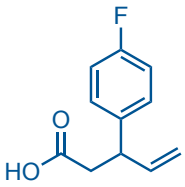
3-(4-Methoxyphenyl)pent-4-enoic acid (1c)[7]



Prepared according to the general procedure A with (*E*)-3-(4-methoxyphenyl)prop-2-en-1-ol (1.6 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (1.6 g, 75% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.07 (m, 2H), 6.90 – 6.79 (m, 2H), 5.96 (ddd, *J* = 17.0, 10.6, 6.8 Hz, 1H), 5.12 – 5.01 (m, 2H), 3.85 – 3.80 (m, 1H), 3.79 (s, 3H), 2.83 – 2.66 (m, 2H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 177.8, 158.5, 140.4, 134.3, 128.6, 114.8, 114.2, 55.4, 44.5, 40.2;
The data are consistent with that reported previously.

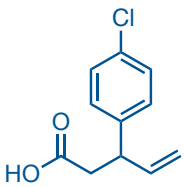
3-(4-Fluorophenyl)pent-4-enoic acid (1d)[8]



Prepared according to the general procedure A with (*E*)-3-(4-fluorophenyl)prop-2-en-1-ol (1.5 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (1.2 g, 60% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.21 – 7.15 (m, 2H), 7.04 – 6.96 (m, 2H), 6.01 – 5.90 (m, 1H), 5.13 – 5.04 (m, 2H), 3.85 (m, 1H), 2.84 – 2.67 (m, 2H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 177.5, 161.9 (d, *J* = 244.7 Hz), 139.9, 137.9 (d, *J* = 2.9 Hz), 129.2 (d, *J* = 8.1 Hz), 115.6 (d, *J* = 21.3 Hz), 115.3, 44.5, 40.0;
^{19}F NMR (471 MHz, $CDCl_3$) δ -116.5;
The data are consistent with that reported previously.

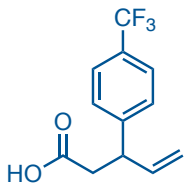
3-(4-Chlorophenyl)pent-4-enoic acid (1e)[8]



Prepared according to the general procedure A with (*E*)-3-(4-chlorophenyl)prop-2-en-1-ol (1.7 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (1.5 g, 72% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.26 (m, 2H), 7.17 – 7.12 (m, 2H), 5.94 (ddd, *J* = 17.1, 10.4, 6.7 Hz, 1H), 5.13 – 5.04 (m, 2H), 3.88 – 3.80 (m, 1H), 2.84 – 2.66 (m, 2H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.8, 140.7, 139.6, 132.8, 129.1, 128.9, 115.6, 44.6, 39.7;
The data are consistent with that reported previously.

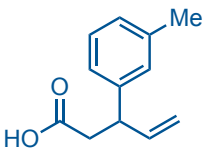
3-(4-(Trifluoromethyl)phenyl)pent-4-enoic acid (1f)[6]



Prepared according to the general procedure A with (*E*)-3-(4-(trifluoromethyl)phenyl)prop-2-en-1-ol (2.0 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (1.2 g, 50% yield).

IR (cm^{-1}): 3089, 3049, 2921, 1712, 1619, 1419, 1326, 1165, 1124, 1069, 1018, 925, 841;
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 8.7, 0.7 Hz, 2H), 7.33 (d, *J* = 8.6 Hz, 2H), 5.96 (ddd, *J* = 17.2, 10.4, 6.8 Hz, 1H), 5.17 – 5.06 (m, 2H), 3.97 – 3.87 (m, 1H), 2.87 – 2.71 (m, 2H);
^{13}C NMR (126 MHz, $CDCl_3$) δ 177.1, 146.2, 139.2, 129.3 (q, *J* = 32.6 Hz), 128.1, 125.8 (q, *J* = 3.7 Hz), 124.3 (q, *J* = 272.9 Hz), 116.0, 45.0, 39.6;
^{19}F NMR (282 MHz, $CDCl_3$) δ -62.5;
HRMS (ESI): calculated for $C_{12}H_{10}O_2F_3^-$ $[M-H]^-$ m/z: 243.0638, found: 243.0643.

3-(*m*-Tolyl)pent-4-enoic acid (1g)[6]



Prepared according to the general procedure A with (*E*)-3-(*m*-tolyl)prop-2-en-1-ol (1.5 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (1.3 g, 67% yield).

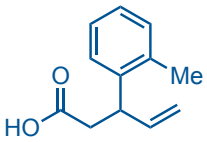
IR (cm^{-1}): 3021, 2916, 1708, 1638, 1490, 1415, 1293, 919, 754, 727;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.18 (m, 1H), 7.07 – 7.00 (m, 3H), 5.98 (ddd, *J* = 17.2, 10.0, 6.9 Hz, 1H), 5.13 – 5.06 (m, 2H), 3.83 (dt, *J* = 8.3, 6.9 Hz, 1H), 2.84 – 2.70 (m, 2H), 2.34 (s, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 178.0, 142.3, 140.2, 138.4, 128.7, 128.4, 127.7, 124.6, 115.1, 45.3, 40.0, 21.6;

HRMS (ESI): calculated for $C_{12}H_{13}O_2^-$ $[M-H]^-$ m/z: 189.0921, found: 189.0915.

3-(*o*-Tolyl)pent-4-enoic acid (1h)[6]



Prepared according to the general procedure A with (*E*)-3-(*o*-tolyl)prop-2-en-1-ol (1.5 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (1.2 g, 65% yield).

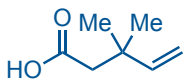
IR (cm^{-1}): 2920, 1705, 1606, 1413, 1291, 917, 785, 704;

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.23 – 7.07 (m, 4H), 5.93 (ddd, *J* = 17.1, 10.4, 6.6 Hz, 1H), 5.11 – 4.97 (m, 2H), 4.17 – 4.06 (m, 1H), 2.87 – 2.69 (m, 2H), 2.37 (s, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 178.3, 140.2, 139.7, 136.1, 130.8, 126.7, 126.4, 126.4, 115.1, 40.7, 39.4, 19.6;

HRMS (ESI): calculated for $C_{12}H_{13}O_2^-$ $[M-H]^-$ m/z: 189.0921, found: 189.0922.

3,3-Dimethylpent-4-enoic acid (1j)[8]



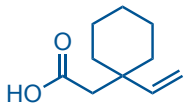
Prepared according to the general procedure A with (*E*)-4-methylpent-2-en-1-ol (1.0 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a colorless oil (1.2 g, 95% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 5.90 (dd, *J* = 17.6, 10.8 Hz, 1H), 5.02 – 4.93 (m, 2H), 2.33 (s, 2H), 1.15 (s, 6H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 178.2, 146.6, 111.3, 46.7, 36.1, 27.0;

The data are consistent with that reported previously.

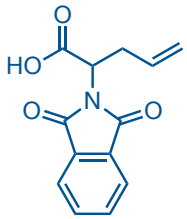
2-(1-Vinylcyclohexyl)acetic acid (1k)[8]



Prepared according to the general procedure A with 2-cyclohexylideneethan-1-ol (1.3 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a colorless oil (1.3 g, 80% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 5.79 (dd, *J* = 18.1, 11.0 Hz, 1H), 5.14 – 4.99 (m, 2H), 2.35 (s, 2H), 1.70 – 1.38 (m, 10H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 178.3, 144.7, 113.7, 45.8, 39.3, 35.7, 26.2, 22.2;
The data are consistent with that reported previously.

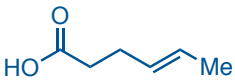
2-(1,3-Dioxo-1,3-dihydro-2*H*-isoindol-2-yl)pent-4-enoic acid (1m)[9]



Prepared according to the procedure reported in the literature with 2-aminopent-4-enoic acid (500 mg, 4.34 mmol). Flash column chromatography on silica gel provided the title compound as a white solid (533 mg, 50% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.83 (m, 2H), 7.76 – 7.70 (m, 2H), 5.71 (dddd, *J* = 17.0, 10.2, 8.5, 5.7 Hz, 1H), 5.11 – 5.04 (m, 1H), 5.05 – 4.96 (m, 2H), 3.11 – 2.91 (m, 2H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4, 167.6, 134.4, 133.0, 131.8, 123.8, 119.2, 51.5, 33.1;
The data are consistent with that reported previously.

(*E*)-Hex-4-enoic acid (1o)[6]



Prepared according to the general procedure A with 3-buten-2-ol (0.7 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a colorless oil (1.0 g, 95% yield).

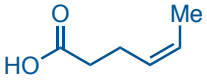
IR (cm^{-1}): 3027, 2920, 2858, 1706, 1436, 1412, 1279, 1248, 1211, 965, 935

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.56 – 5.38 (m, 2H), 2.44 – 2.38 (m, 2H), 2.37 – 2.24 (m, 2H), 1.67 – 1.63 (m, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 179.7, 129.0, 126.6, 34.2, 27.7, 18.0;

HRMS (ESI): calculated for $C_6H_9O_2^-$ $[M-H]^-$ m/z: 113.0608, found: 113.0612.

(*Z*)-Hex-4-enoic acid (1p)[10]



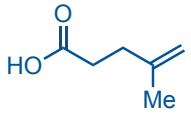
Prepared according to a literature procedure: To a solution of hex-4-ynoic acid (2.0 g, 17.8 mmol, 1.0 eq.) in ethyl acetate (20.0 mL), quinoline (4.2 mL, 35.7 mmol, 2.0 equiv.) and palladium on calcium carbonate (200 mg, Lindlar-catalyst) were added. The reaction flask was carefully evacuated and flushed with hydrogen gas. The procedure was repeated twice and the suspension was vigorously stirred at room temperature for six hours under hydrogen atmosphere. The suspension was filtered over a short pad of celite, washed with ethyl acetate (80.0 mL) and the solution was washed with 1 N NaOH solution (3 x 50.0 mL). The combined aqueous layers were acidified with concentrated HCl aq. solution (pH = 1) and extracted with dichloromethane (3 x 80 mL). The combined organic layers were dried over Na_2SO_4, filtered and the solvent was removed in *vacuo*. The residue was purified by column chromatography on silica gel (hexane/ ethyl acetate: 9/1) to afford the title compound as a yellow liquid in 99% yield (2.0 g, 17.6 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.57 – 5.47 (m, 1H), 5.42 – 5.33 (m, 1H), 2.45 – 2.34 (m, 4H), 1.63 (ddt, *J* = 6.8, 1.8, 0.8 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 180.0, 128.1, 125.9, 34.1, 22.3, 12.8;

The data are consistent with that reported previously.

4-Methylpent-4-enoic acid (1q)[8]



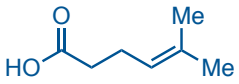
Prepared according to the general procedure A with methallyl alcohol (0.7 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a colorless oil (0.9 g, 85% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.77 (dt, *J* = 1.6, 0.7 Hz, 1H), 4.71 (dd, *J* = 1.6, 0.9 Hz, 1H), 2.54 – 2.49 (m, 2H), 2.35 (dd, *J* = 9.1, 6.1 Hz, 2H), 1.78 – 1.73 (m, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 180.1, 143.8, 110.6, 32.6, 32.3, 22.6;

The data are consistent with that reported previously.

5-Methylhex-4-enoic acid (1r)[11]



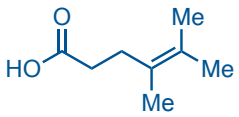
Prepared according to the general procedure A with 2-methylbut-3-en-2-ol (0.8 g, 10 mmol). Flash column chromatography on silica gel provided the title compound as a colorless oil (0.8 g, 60% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.13 – 5.07 (m, 1H), 2.40 – 2.35 (m, 2H), 2.35 – 2.28 (m, 2H), 1.69 (s, 3H), 1.62 (s, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 180.3, 133.5, 122.2, 34.4, 25.8, 23.5, 17.7;

The data are consistent with that reported previously.

4,5-Dimethylhex-4-enoic acid (1s)[12]



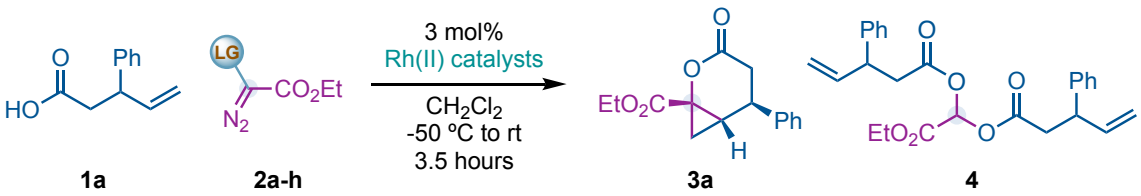
Prepared according to the general procedure A with 2,3-dimethylbut-3-en-2-ol (1.7 g, 14.8 mmol). Flash column chromatography on silica gel provided the title compound as a colorless oil (553 mg, 26% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 2.41 – 2.34 (m, 4H), 1.67 (s, 3H), 1.64 (s, 6H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 180.4, 126.1, 125.5, 33.0, 29.8, 20.8, 20.2;

The data are consistent with that reported previously.

4. General procedure B for reaction optimization



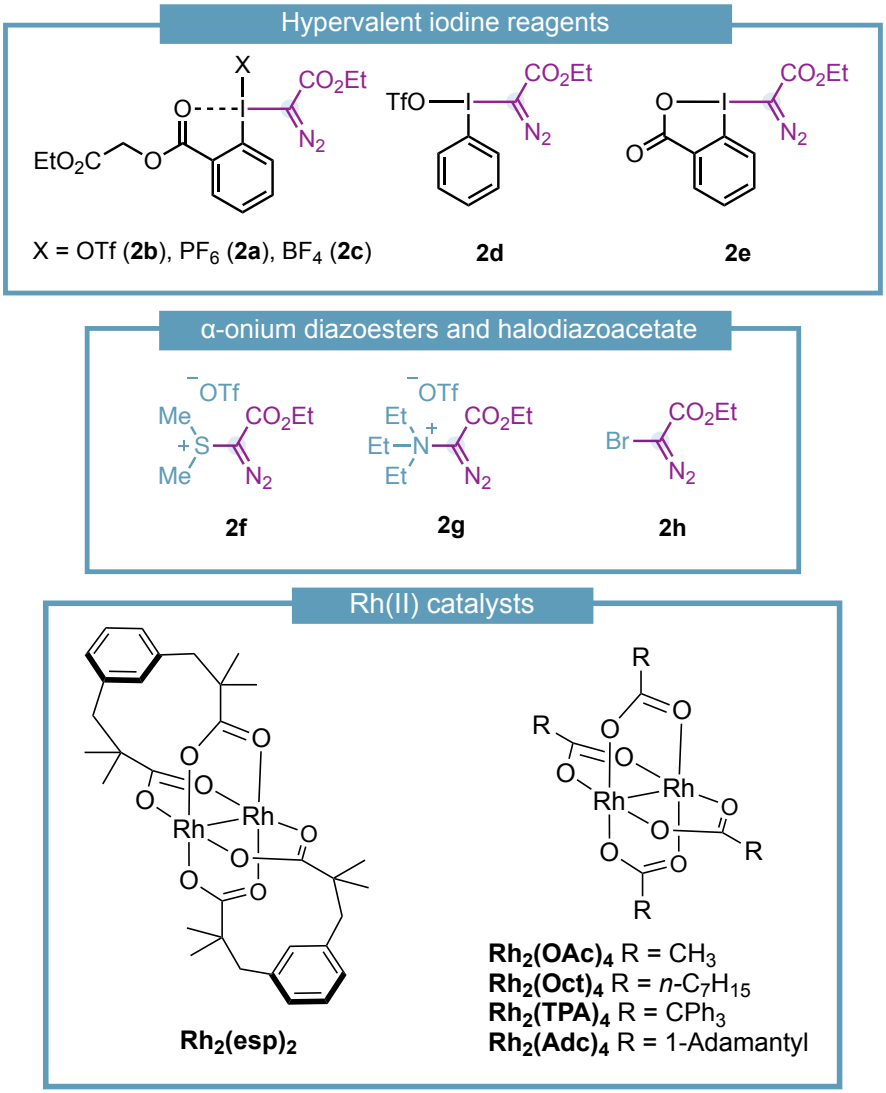
To a 10 mL oven-dried tube equipped with a stirring bar was added the corresponding Rh catalyst. The tube was sealed before being evacuated and backfilled with argon three times. 3-Phenylpent-4-enoic acid and degassed dichloromethane (0.5 mL) were added and the resulting mixture was placed into a cooling bath at -50 ºC. After this, a solution of the corresponding hypervalent iodine reagent (**2a-h**) in degassed dichloromethane (1.0 mL) was added dropwise to the reaction tube for 30 minutes using a syringe pump. Then the resulting mixture was allowed to warm to room temperature in 3 hours, filtered through a short plug of celite and washed with dichloromethane (3 x 1.0 mL). Solvent was removed under *vacuum* and ^{1}H NMR yield was measured using dibromomethane (7 μL, 0.1 mmol, 1.0 equiv.) as internal standard.

Table S1. Full optimization studies

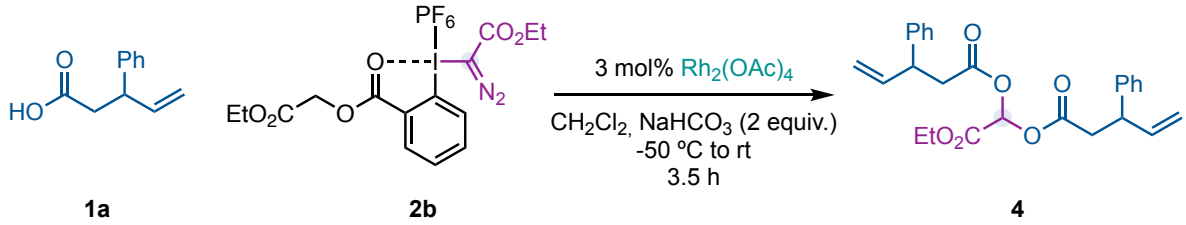
Entry	Reagent **2**	Stoichiometry(**2**:**1**)	Rh catalyst	Additive	Yield **3a** (**4**) [%]
1	**2b**	1: 1	$Rh_2(esp)_2$ (1 mol%)	/	26 (5)
2	**2b**	2: 1	$Rh_2(esp)_2$ (1 mol%)	/	41 (8)
3	**2b**	1: 2	$Rh_2(esp)_2$ (1 mol%)	/	27 (18)
4	**2b**	1.5: 1	$Rh_2(esp)_2$ (1 mol%)	/	42 (8)
5	**2b**	1.3: 1	$Rh_2(esp)_2$ (1 mol%)	/	43 (7)
6	**2b**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	/	45 (5)
7	**2b**	1.3: 1	$Rh_2(esp)_2$ (5 mol%)	/	45 (<5)
8	**2b**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	/	64 (<5)[a]
9	**2b**	1.3: 1	$Rh_2(OAc)_4$ (3 mol%)	/	30 (21)[a]
10	**2b**	1.3: 1	$Rh_2(TPA)_4$ (3 mol%)	/	0 (0)[a]
11	**2b**	1.3: 1	$Rh_2(Oct)_4$ (3 mol%)	/	31 (20)[a]
12	**2b**	1.3: 1	$Rh_2(Adc)_4$ (3 mol%)	/	40 (10)[a]
13	**2b**	1: 2	$Rh_2(OAc)_4$ (3 mol%)	/	0 (65)[a]
14	**2a**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	/	52 (5)[a]
15	**2c**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	/	43 (7)[a]
16	**2d**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	/	32 (12)[a]

17	**2e**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	/	0 (0)[a]
18	**2b**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	Na_2CO_3 (2 equiv)	60 (5)[a]
19	**2b**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	$NaHCO_3$ (2 equiv)	72 (<5)[a]
20	**2b**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	$KHCO_3$ (2 equiv)	61 (<5)[a]
21	**2b**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	NaOAc (2 equiv)	25 (5)[a]
22	**2b**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	Et_3N (2 equiv)	0 (0)[a]
23	**2b**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	DTBP (2 equiv)	10 (5)[a]
24	**2f**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	$NaHCO_3$ (2 equiv)	0 (0)[a]
25	**2g**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	$NaHCO_3$ (2 equiv)	0 (0)[a]
26	**2h**	1.3: 1	$Rh_2(esp)_2$ (3 mol%)	$NaHCO_3$ (2 equiv)	0 (0)

[a] Reagents **2a-g** and the carboxylic acid were dissolved in dichloromethane (1.0 mL) and added in the same syringe dropwise to the Rh catalyst dissolved in dichloromethane (0.5 mL).



- **Synthesis of 2-ethoxy-2-oxoethane-1,1-diyl bis(3-phenylpent-4-enoate) (4)**



1a **2b** **4**

To a 10 mL oven-dried flask equipped with a stirring bar was added $Rh_2(OAc)_4$ (2.6 mg, 0.006 mmol, 3 mol%) and $NaHCO_3$ (33.6 mg, 0.4 mmol, 2 equiv.). The flask was sealed before being evacuated and backfilled with argon three times. Degassed dichloromethane (0.5 mL) was added and the resulting mixture was cooled at -50 ºC. Then, a solution of hypervalent iodine reagent **2b** (118.4 mg, 0.2 mmol, 1.0 equiv.) and 3-phenylpent-4-enoic acid (**1a**) (70.4 mg, 0.4 mmol, 2.0 equiv.) in degassed dichloromethane (2.0 mL) was added dropwise to the reaction flask during 30 min using a syringe pump. The mixture was stirred at -50 ºC for 1 hour and then allowed to warm to room temperature in 3 hours, filtered through a short plug of celite and washed with dichloromethane (3 x 1.0 mL). Solvent was removed under *vacuum* and flash column chromatography on silica gel (hexane/ethyl acetate: 10/1) of the crude residue provided the title compound **4** as a mixture of 4 diastereoisomers (52.4 mg, 65% yield). Ratio of diastereoisomers was determined to be 1:1:1:1 using GC-MS.

IR (cm^{-1}): 3083, 3029, 2981, 2964, 2925, 2854, 1762, 1730, 1376, 1226, 1077, 1051, 921, 701;

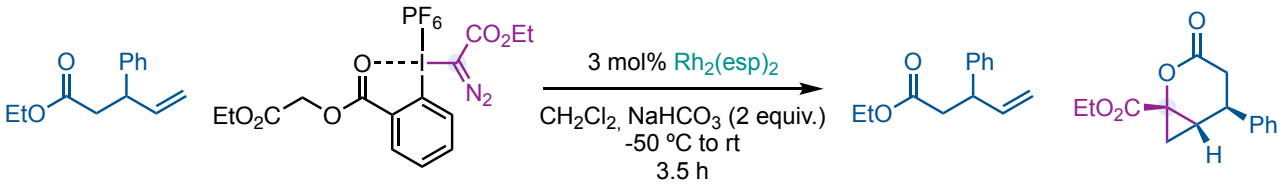
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 4H), 7.25 – 7.17 (m, 6H), 6.76 (t, J = 2.4 Hz, 1H), 6.03 – 5.89 (m, 1H), 5.14 – 5.01 (m, 4H), 4.26 – 4.16 (m, 2H), 3.91 – 3.82 (m, 2H), 2.89 – 2.73 (m, 4H), 1.27 – 1.20 (m, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.48, 169.46, 169.44, 169.42, 164.94, 164.91, 164.88, 141.98, 141.96, 128.80, 127.69, 127.67, 127.01, 115.35, 84.34, 62.67, 62.64, 62.62, 45.21, 45.20, 45.17, 39.66, 39.66, 39.62, 14.04;

HRMS (ESI): calculated for $C_{26}H_{28}O_6Na^+$ $[M+Na]^+$ m/z: 459.1778, found: 459.1780.

5. Control experiments

- **Reaction with ethyl 3-phenylpent-4-enoate (1a-ester)**

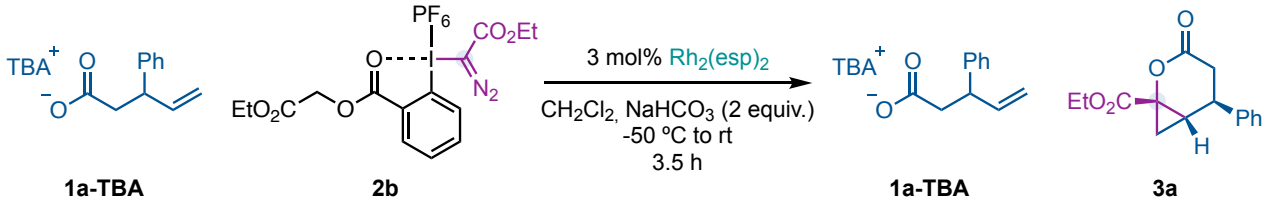


1a-ester **2b** **1a-ester** **3a**

99% **0%**

To a 10 mL oven-dried flask equipped with a stirring bar was added $Rh_2(esp)_2$ (4.6 mg, 0.006 mmol, 3 mol%) and $NaHCO_3$ (33.6 mg, 0.4 mmol, 2 equiv.). The flask was sealed before being evacuated and backfilled with argon three times. Degassed dichloromethane (0.5 mL) was added, and the resulting mixture was cooled at -50 ºC. Then, a solution of hypervalent iodine reagent (**2b**) (153.9 mg, 0.26 mmol, 1.3 equiv.) and ethyl 3-phenylpent-4-enoate (**1a-ester**) (40.8 mg, 0.2 mmol, 1.0 equiv.) in degassed dichloromethane (2.0 mL) was added dropwise to the reaction flask during 30 min using a syringe pump. Then the resulting reaction mixture was allowed to warm to room temperature for 3 hours, filtered through a short plug of Celite and washed with CH_2Cl_2 (3 x 1.0 mL). Solvent was removed under *vacuum* and ^{1}H-NMR yield was measured using dibromomethane (7 μL, 0.1 mmol, 1.0 equiv.) as internal standard. Analysis of the crude reaction by ^{1}H NMR showed no conversion to product **3a** and 99% NMR yield of **1a-ester**.

- **Reaction with tetrabutylammonium 3-phenylpent-4-en-1-carboxylate (1a-TBA)**



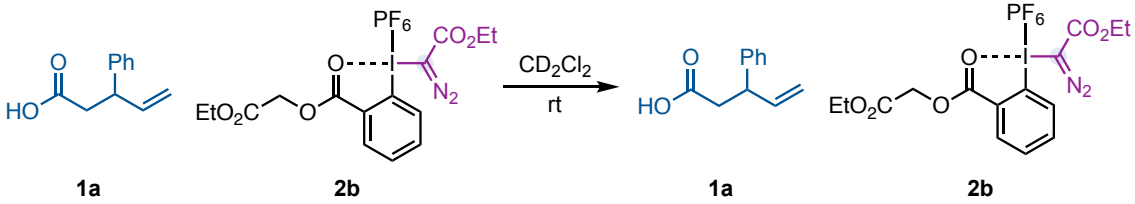
1a-TBA **2b** **1a-TBA** **3a**

99% **0%**

To a 10 mL oven-dried flask equipped with a stirring bar was added $Rh_2(esp)_2$ (4.6 mg, 0.006 mmol, 3 mol%) and $NaHCO_3$ (33.6 mg, 0.4 mmol, 2 equiv.). The flask was sealed before being evacuated and backfilled with argon three times. Degassed dichloromethane (0.5 mL) was added, and the resulting mixture was cooled at -50 ºC. Then, a solution of hypervalent iodine reagent (**2b**) (153.9 mg, 0.26 mmol, 1.3 equiv.) and tetrabutylammonium 3-phenylpent-4-en-1-carboxylate (**1a-TBA**) (40.8 mg, 0.2 mmol, 1.0

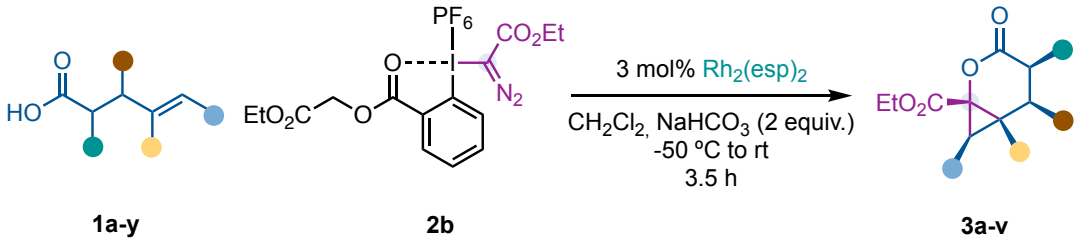
equiv.) in degassed dichloromethane (2.0 mL) was added dropwise to the reaction flask during 30 min using a syringe pump. Then the resulting reaction mixture was allowed to warm to room temperature for 3 hours, filtered through a short plug of celite and washed with dichloromethane (3 x 1.0 mL). Solvent was removed under *vacuum* and ^{1}H NMR yield was measured using dibromomethane (7 μL, 0.1 mmol, 1.0 equiv.) as internal standard. Analysis of the crude reaction by ^{1}H NMR showed no conversion to product **3a** and 99% NMR yield of **1a-TBA**.

- **Reaction without catalyst at room temperature**



To an NMR tube were added **1a** (3.5 mg, 0.02 mmol, 1 equiv.), **2b** (11.8 mg, 0.02 mmol, 1 equiv.) and CD_2Cl_2 (0.6 mL) at room temperature. A ^{1}H NMR experiment was measured every 30 minutes for 2 hours and not reaction was observed between **1a** and **2b**.

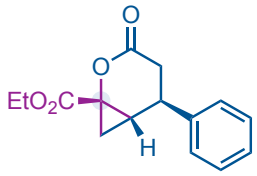
6. General procedure C for the synthesis of cyclopropyl-fused lactones 3



To a 10 mL oven-dried flask equipped with a stirring bar was added $Rh_2(esp)_2$ (4.6 mg, 0.006 mmol, 3 mol%) and $NaHCO_3$ (33.6 mg, 0.4 mmol, 2 equiv.). The flask was sealed before being evacuated and backfilled with argon three times. Degassed dichloromethane (0.5 mL) was added and the resulting mixture was cooled at -50 ºC. Then, a solution of hypervalent iodine reagent **2b** (153.9 mg, 0.26 mmol, 1.3 equiv.) and the corresponding acid (**1a-y)** (0.2 mmol, 1.0 equiv.) in degassed dichloromethane (2.0 mL) were added dropwise to the reaction flask during 30 min using a syringe pump. Then the resulting reaction mixture was allowed to warm to room temperature in 3 hours, filtered through a short plug of celite and washed with dichloromethane (3 x 1.0 mL). Solvent was removed under *vacuum* and the crude residue was purified by flash chromatography on silica gel to yield the corresponding cyclopropyl-fused lactones **3**. If

residual carboxylic acid was observed by ^{1}H NMR of the crude, the corresponding flash chromatography on silica gel was packed with hexane/ethyl acetate/Et_3N (10/1/0.1).

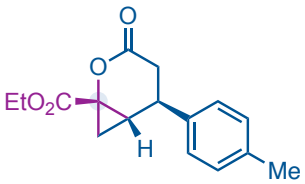
Ethyl (1*S,5*R**,6*S**)-3-oxo-5-phenyl-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3a)**



Prepared according to the general procedure C using 3-phenylpent-4-enoic acid (**1a**) (17.6 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (37.5 mg, 72% yield).

IR (cm^{-1}): 3081, 3048, 2974, 2956, 1760, 1725, 1454, 1376, 1284, 1218, 1194, 1148, 970, 845, 740;
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.25 (m, 5H), 4.27 (q, *J* = 7.1 Hz, 2H), 2.98 (ddd, *J* = 11.0, 6.5, 4.5 Hz, 1H), 2.73 – 2.60 (m, 2H), 2.06 (ddd, *J* = 9.7, 7.1, 6.5 Hz, 1H), 1.97 (dd, *J* = 9.7, 6.0 Hz, 1H), 1.47 – 1.42 (m, 1H), 1.31 (t, *J* = 7.1 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 170.3, 141.0, 129.3, 127.8, 126.9, 62.3, 61.7, 41.7, 35.8, 28.6, 24.3, 14.3;
HRMS (ESI): calculated for $C_{15}H_{16}O_4Na^+$ $[M+Na]^+$ m/z: 283.0941, found: 283.0951;
^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC, ^{1}H-^{13}C HMBC, ^{1}H-^{1}H NOESY spectra were measured.

Ethyl (1*S,5*R**,6*S**)-3-oxo-5-(*p*-tolyl)-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3b)**



Prepared according to the general procedure C using 3-(*p*-tolyl)pent-4-enoic acid (**1b**) (19.0 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (39.0 mg, 71% yield).

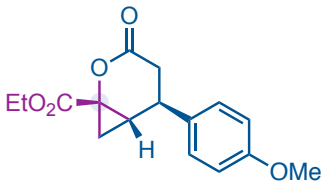
IR (cm^{-1}): 3082, 3039, 2980, 2965, 1765, 1724, 1452, 1380, 1289, 1246, 1172, 1131, 999, 823, 743;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 – 7.12 (m, 4H), 4.26 (q, *J* = 7.0 Hz, 2H), 2.94 (ddd, *J* = 11.0, 6.5, 4.6 Hz, 1H), 2.70 – 2.57 (m, 2H), 2.35 (s, 3H), 2.04 (ddd, *J* = 9.6, 7.1, 6.5 Hz, 1H), 1.96 (dd, *J* = 9.6, 5.9 Hz, 1H), 1.46 – 1.41 (m, 1H), 1.31 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.3, 138.1, 137.5, 129.9, 126.7, 62.3, 61.7, 41.4, 36.0, 28.7, 24.3, 21.1, 14.3.

HRMS (ESI): calculated for $C_{16}H_{18}O_4Na^+$ $[M+Na]^+$ m/z: 297.1097, found: 297.1095.

Ethyl (1*S,5*R**,6*S**)-5-(4-methoxyphenyl)-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3c)**



Prepared according to the general procedure C using 3-(4-methoxyphenyl)pent-4-enoic acid (**1c**) (41.2 mg, 1.0 equiv., 0.2 mmol). After dropwise addition of reagent **2b**, the resulting reaction mixture was stirred for an additional period of 30 minutes at –50 ºC. Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (29.0 mg, 50% yield).

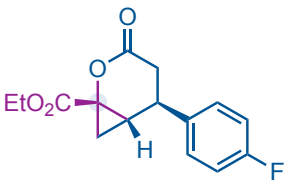
IR (cm^{-1}): 3049, 3003, 2923, 2900, 1763, 1730, 1493, 1339, 1239, 1269, 1103, 923, 834, 754;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 – 7.15 (m, 2H), 6.94 – 6.88 (m, 2H), 4.26 (q, *J* = 7.1 Hz, 2H), 3.81 (s, 3H), 2.93 (ddd, *J* = 10.8, 6.3, 4.3 Hz, 1H), 2.69 – 2.55 (m, 2H), 2.06 – 1.92 (m, 2H), 1.45 – 1.40 (m, 1H), 1.31 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.3, 159.2, 133.1, 127.9, 114.6, 62.3, 61.7, 55.5, 41.0, 36.1, 28.8, 24.3, 14.3;

HRMS (ESI): calculated for $C_{16}H_{18}O_5Na^+$ $[M+Na]^+$ m/z: 313.1046, found: 313.1035.

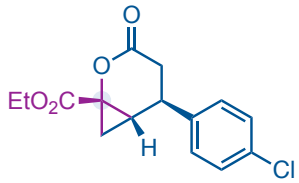
Ethyl (1*S,5*R**,6*S**)-5-(4-fluorophenyl)-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3d)**



Prepared according to the general procedure C using 3-(4-fluorophenyl)pent-4-enoic acid (**1d**) (38.8 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (36.7 mg, 66% yield).

IR (cm^{-1}): 3065, 3011, 2967, 2910, 1760, 1725, 1454, 1396, 1265, 1234, 1196, 900, 845, 705;
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 – 7.21 (m, 2H), 7.11 – 7.04 (m, 2H), 4.27 (qd, *J* = 7.2, 0.4 Hz, 2H), 2.98 (ddd, *J* = 11.0, 6.3, 4.3 Hz, 1H), 2.70 – 2.56 (m, 2H), 2.04 – 1.94 (m, 2H), 1.46 – 1.43 (m, 1H), 1.31 (t, *J* = 7.1 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 170.2, 162.3 (d, *J* = 246.9 Hz), 136.8 (d, *J* = 2.9 Hz), 128.4 (d, *J* = 8.1 Hz), 116.2 (d, *J* = 21.6 Hz), 62.4, 61.7, 41.0, 35.9, 28.6, 24.2, 14.3;
^{19}F NMR (376 MHz, $CDCl_3$) δ -114.3 (tt, *J* = 8.8, 5.3 Hz);
HRMS (ESI): calculated for $C_{15}H_{15}O_4FNa^+$ $[M+Na]^+$ m/z: 301.0847, found: 301.0850.

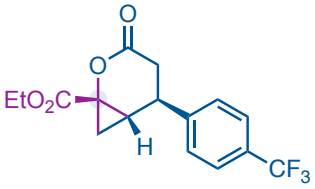
Ethyl (1*S,5*R**,6*S**)-5-(4-chlorophenyl)-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3e)**



Prepared according to the general procedure C using 3-(4-chlorophenyl)pent-4-enoic acid (**1e**) (42.1 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (33.0 mg, 56% yield).

IR (cm^{-1}): 3100, 3020, 2958, 2913, 1760, 1729, 1498, 1343, 1243, 1265, 990, 893, 714;
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.33 (m, 2H), 7.23 – 7.18 (m, 2H), 4.26 (qd, *J* = 7.2, 0.8 Hz, 2H), 3.00 – 2.94 (m, 1H), 2.69 – 2.57 (m, 2H), 2.03 – 1.94 (m, 2H), 1.48 – 1.41 (m, 1H), 1.31 (t, *J* = 7.1 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 170.1, 139.5, 133.7, 129.5, 128.2, 62.4, 61.7, 41.1, 35.7, 28.3, 24.2, 14.3;
HRMS (ESI): calculated for $C_{15}H_{15}O_4ClNa^+$ $[M+Na]^+$ m/z: 317.0551, found: 317.0549.

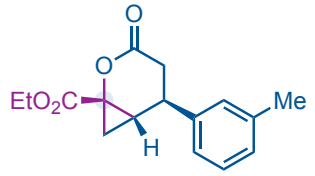
Ethyl (1*S,5*R**,6*S**)-3-oxo-5-(4-(trifluoromethyl)phenyl)-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3f)**



Prepared according to the general procedure C using 3-(4-(trifluoromethyl)phenyl)pent-4-enoic acid (**1f**) (48.8 mg, 1.0 equiv., 0.2 mmol). After dropwise addition of reagent **2b**, the resulting reaction mixture was stirred for an additional period of 1 hour at –50 ºC. Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (29.6 mg, 45% yield).

IR (cm^{-1}): 3087, 3008, 2945, 2900, 1770, 1724, 1458, 1328, 1257, 1222, 1187, 934, 870, 711;
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.61 (m, 2H), 7.43 – 7.37 (m, 2H), 4.27 (qd, *J* = 7.1, 0.5 Hz, 2H), 3.11 – 3.04 (m, 1H), 2.74 – 2.61 (m, 2H), 2.06 – 1.96 (m, 2H), 1.50 – 1.46 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 170.0, 144.9 (q, *J* = 1.5 Hz), 130.3 (q, *J* = 32.6 Hz), 127.4, 126.3 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 273.0 Hz), 62.5, 61.7, 41.4, 35.4, 28.1, 24.1, 14.3;
^{19}F NMR (376 MHz, $CDCl_3$) δ -62.8;
HRMS (ESI): calculated for $C_{16}H_{15}O_4F_3Na^+$ $[M+Na]^+$ m/z: 351.0815, found: 351.0804.

Ethyl (1*S,5*R**,6*S**)-3-oxo-5-(*m*-tolyl)-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3g)**



Prepared according to the general procedure C using 3-(*m*-tolyl)pent-4-enoic acid (**1g**) (19.0 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (35.7 mg, 65% yield).

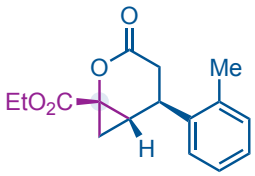
IR (cm^{-1}): 3067, 3023, 2956, 2876, 1754, 1702, 1465, 1343, 1245, 1190, 930, 875, 780;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.23 (m, 1H), 7.16 – 7.02 (m, 2H), 4.27 (q, *J* = 7.1 Hz, 2H), 2.94 (ddd, *J* = 11.1, 6.5, 5.1 Hz, 1H), 2.71 – 2.58 (m, 2H), 2.37 (s, 3H), 2.05 (ddd, *J* = 9.7, 7.1, 6.5 Hz, 1H), 1.96 (dd, *J* = 9.7, 5.9 Hz, 1H), 1.44 (ddd, *J* = 7.1, 5.9, 0.6 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 170.3, 141.0, 139.0, 129.2, 128.5, 127.6, 123.8, 62.3, 61.7, 41.7, 35.9, 28.7, 24.3, 21.6, 14.3;

HRMS (ESI): calculated for $C_{16}H_{18}O_4Na^+$ $[M+Na]^+$ m/z: 297.1097, found: 297.1095.

Ethyl (1*S,5*R**,6*S**)-3-oxo-5-(*o*-tolyl)-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3h)**



Prepared according to the general procedure C using 3-(*o*-tolyl)pent-4-enoic acid (**1h**) (19.0 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (32.4 mg, 59% yield).

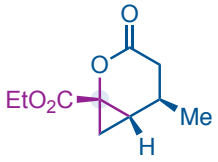
IR (cm^{-1}): 3087, 3065, 2943, 2907, 1763, 1720, 1460, 1330, 1250, 1243, 1200, 946, 870, 800;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.15 (m, 4H), 4.25 (q, *J* = 7.2 Hz, 2H), 3.12 (ddd, *J* = 12.3, 6.8, 3.6 Hz, 1H), 2.75 (dd, *J* = 15.6, 12.3 Hz, 1H), 2.64 (dd, *J* = 15.6, 3.6 Hz, 1H), 2.39 (s, 3H), 2.00 (dd, *J* = 9.6, 6.0 Hz, 1H), 1.88 (dt, *J* = 9.6, 7.2 Hz, 1H), 1.47 (ddd, *J* = 7.2, 6.0, 0.6 Hz, 1H), 1.30 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.4, 170.2, 139.2, 136.0, 131.0, 127.5, 126.9, 124.9, 62.3, 61.7, 37.9, 34.7, 28.6, 25.0, 20.0, 14.3;

HRMS (ESI): calculated for $C_{16}H_{18}O_4Na^+$ $[M+Na]^+$ m/z: 297.1097, found: 297.1097.

Ethyl (1*S,5*R**,6*S**)-5-methyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3i)**

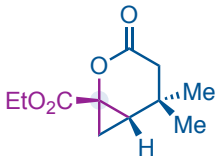


Prepared according to the general procedure C using 3-methylpent-4-enoic acid (22.8 mg, 1.0 equiv., 0.2 mmol). After dropwise addition of reagent **2b**, the resulting reaction mixture was stirred for an additional

period of 30 minutes at –50 ºC. Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (29.7 mg, 75% yield).

IR (cm^{-1}): 2970, 2900, 2864, 1754, 1723, 1454, 1319, 1289, 1245, 1215, 1201, 1167, 1100, 980;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.24 (qd, *J* = 7.1, 1.8 Hz, 2H), 2.41 (dd, *J* = 15.9, 3.6 Hz, 1H), 2.14 (dd, *J* = 15.9, 11.8 Hz, 1H), 1.91 – 1.81 (m, 2H), 1.62 (ddd, *J* = 9.7, 7.3, 6.1 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.27 (d, *J* = 6.8 Hz, 3H), 1.25 – 1.22 (m, 1H);
^{1}H NMR (500 MHz, CD_3OD) δ 4.15 (q, *J* = 7.1 Hz, 2H), 2.48 (dd, *J* = 15.6, 5.8 Hz, 1H), 2.27 (dd, *J* = 15.6, 8.1 Hz, 1H), 1.89 – 1.82 (m, 1H), 1.41 – 1.30 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.14 (d, *J* = 6.9 Hz, 3H), 0.77 (dd, *J* = 7.2, 4.6 Hz, 1H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 170.6, 62.2, 61.7, 36.9, 31.4, 28.6, 24.1, 21.1, 14.3;
^{13}C NMR (126 MHz, CD_3OD) δ 176.94, 176.42, 62.16, 57.98, 42.03, 34.94, 30.35, 22.03, 19.97, 14.50;
HRMS (ESI): calculated for $C_{10}H_{14}O_4Na^+$ $[M+Na]^+$ m/z: 221.0784, found: 221.0785;
^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC, ^{1}H-^{1}H NOESY spectra were measured in CD_3OD.

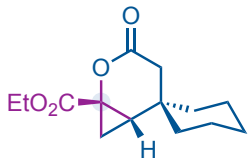
Ethyl (1*S,6*S**)-5,5-dimethyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3j)**



Prepared according to the general procedure C using 3,3-dimethylpent-4-enoic acid (**1j**) (25.6 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (36.1 mg, 85% yield).

IR (cm^{-1}): 2967, 2906, 2888, 1767, 1722, 1465, 1334, 1289, 1245, 1294, 1290, 1150, 992, 876, 812;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.25 (qd, *J* = 7.2, 1.4 Hz, 2H), 2.28 (dd, *J* = 16.3, 1.0 Hz, 1H), 2.15 (d, *J* = 16.3 Hz, 1H), 1.76 (ddd, *J* = 10.2, 7.7, 1.0 Hz, 1H), 1.66 (dd, *J* = 10.2, 6.5 Hz, 1H), 1.30 (t, *J* = 7.2 Hz, 3H), 1.29 (dd, *J* = 7.7, 6.5 Hz, 1H), 1.22 (s, 3H), 1.07 (s, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 168.6, 62.2, 62.0, 41.5, 31.5, 30.4, 30.1, 27.4, 18.6, 14.3;
HRMS (ESI): calculated for $C_{11}H_{16}O_4Na^+$ $[M+Na]^+$ m/z: 235.0941, found: 235.0942.

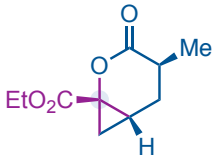
Ethyl (1*S,6*S**)-4-oxo-5-oxaspiro[bicyclo[4.1.0]heptane-2,1'-cyclohexane]-6-carboxylate (3k)**



Prepared according to the general procedure C using 2-(1-vinylcyclohexyl)acetic acid (**1k**) (33.6 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (40.9 mg, 81% yield).

IR (cm^{-1}): 2983, 2929, 2856, 1755, 1726, 1450, 1314, 1282, 1244, 1207, 1175, 1153, 1103, 1018;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.24 (qd, *J* = 7.1, 1.3 Hz, 2H), 2.30 (d, *J* = 15.8 Hz, 1H), 2.16 (d, *J* = 15.8 Hz, 1H), 1.82 – 1.70 (m, 2H), 1.68 – 1.11 (m, 11H), 1.30 (t, *J* = 7.2 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 170.0, 62.2, 62.0, 39.5, 34.5, 34.1, 25.5, 21.9, 21.7, 20.0, 14.3;
HRMS (ESI): calculated for $C_{14}H_{20}O_4Na^+$ $[M+Na]^+$ m/z: 275.1254, found: 275.1245.

Ethyl (1*S,4*S**,6*R**)-4-methyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3l)**

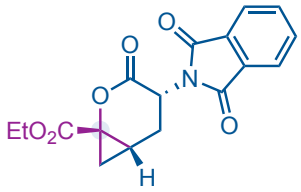


Prepared according to the general procedure C using 2-methylpent-4-enoic acid (22.8 mg, 1.0 equiv., 0.2 mmol). The reaction was stirred for an additional period of 1 hour at –50ºC. Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (27.0 mg, 68% yield).

IR (cm^{-1}): 2982, 2937, 2877, 1759, 1732, 1459, 1398, 1382, 1347, 1305, 1279, 1257, 1152, 1095, 1069, 1039, 1017;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.22 (qd, *J* = 7.1, 2.6 Hz, 2H), 2.55 – 2.48 (m, 1H), 2.48 – 2.40 (m, 1H), 2.05 – 1.95 (m, 1H), 1.84 (dd, *J* = 9.6, 5.8 Hz, 1H), 1.43 – 1.30 (m, 1H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.28 – 1.14 (m, 1H), 1.19 (d, *J* = 6.7 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 174.6, 170.8, 62.1, 60.9, 34.3, 32.0, 25.2, 22.7, 15.5, 14.3;

HRMS (ESI): calculated for $C_{10}H_{14}O_4Na^+$ $[M+Na]^+$ m/z: 221.0784, found: 221.0784;
^1H-^1H COSY, ^1H-^{13}C HSQC, ^1H-^1H NOESY spectra were measured.

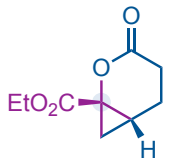
Ethyl (1*S,4*R**,6*R**)-4-(1,3-dioxoisoindolin-2-yl)-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3m)**



Prepared according to the general procedure C using 2-(1,3-dioxoisoindolin-2-yl)pent-4-enoic acid (**1m**) (49.0 mg, 1.0 equiv., 0.2 mmol). The reaction was stirred for an additional period of 1 hour at –50ºC. Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^1H NMR spectroscopy. Purification by flash chromatography on silica gel (dichloromethane/diethyl ether: 25/1) provided the title compound as a white solid (19.8 mg, 30% yield).

mp: 185-187ºC
IR (cm^{-1}): 3100, 3023, 2956, 1767, 1754, 1702, 1465, 1350, 1290, 1190, 998, 870, 765;
^1H NMR (400 MHz, $CDCl_3$) δ 7.92 – 7.82 (m, 2H), 7.80 – 7.71 (m, 2H), 5.02 – 4.90 (m, 1H), 4.37 – 4.20 (m, 2H), 2.70 – 2.56 (m, 2H), 2.19 – 2.06 (m, 1H), 1.96 (dd, *J* = 9.6, 6.1 Hz, 1H), 1.49 (dd, *J* = 7.3, 6.1 Hz, 1H), 1.33 (t, *J* = 7.2 Hz, 3H);
^1H NMR (500 MHz, MeOD) δ 7.93 – 7.83 (m, 5H), 5.11 (dd, *J* = 12.9, 5.4 Hz, 1H), 4.27 (qq, *J* = 7.2, 3.6 Hz, 2H), 2.70 (ddd, *J* = 13.3, 9.1, 5.4 Hz, 1H), 2.54 (td, *J* = 13.3, 7.4 Hz, 1H), 2.21 (tt, *J* = 9.1, 7.4 Hz, 1H), 1.92 (dd, *J* = 9.7, 6.2 Hz, 1H), 1.48 (dd, *J* = 8.0, 6.2 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 4H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 167.3, 167.2, 134.6, 131.9, 123.9, 62.6, 61.0, 47.1, 28.2, 25.4, 21.6, 14.3;
HRMS (ESI): calculated for $C_{17}H_{15}NO_6Na^+$ $[M+Na]^+$ m/z: 352.0792, found: 352.0787;
^1H-^1H COSY, ^1H-^1H NOESY spectra were measured in CD_3OD.

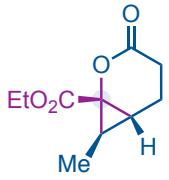
Ethyl (1*S,6*R**)-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3n)**



Prepared according to the general procedure C using pent-4-enoic acid (20.0 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (22.8 mg, 62% yield).

IR (cm^{-1}): 2984, 2937, 1760, 1726, 1307, 1244, 1207, 1152;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.23 (qd, *J* = 7.1, 1.8 Hz, 2H), 2.50 (dddd, *J* = 14.0, 8.0, 5.6, 4.5 Hz, 1H), 2.45 – 2.32 (m, 2H), 1.94 (dddd, *J* = 9.8, 8.0, 7.3, 6.3 Hz, 1H), 1.83 (dd, *J* = 9.8, 6.0 Hz, 1H), 1.71 – 1.61 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.27 – 1.23 (m, 1H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6, 170.6, 62.2, 61.9, 28.5, 23.8, 22.6, 21.4, 14.3;
HRMS (ESI): calculated for $C_9H_{13}O_4^+$ $[M+H]^+$ m/z: 185.0808, found: 185.0802.

Ethyl (1*S,6*R**,7*R**)-7-methyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3o)**

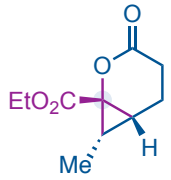


Prepared according to the general procedure C using (*E*)-hex-4-enoic acid (**1o**) (22.8 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (17.8 mg, 45% yield).

IR (cm^{-1}): 2981, 2937, 2878, 1763, 1727, 1455, 1372, 1283, 1246, 1151, 1115, 1037;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.25 (qq, *J* = 7.1, 3.7 Hz, 2H), 2.49 (dddd, *J* = 14.0, 8.3, 5.6, 4.1 Hz, 1H), 2.44 – 2.27 (m, 2H), 1.90 – 1.83 (m, 1H), 1.73 – 1.59 (m, 1H), 1.57 (dq, *J* = 8.0, 6.2 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.27 (d, *J* = 6.4 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 169.2, 65.7, 61.9, 33.4, 28.9, 27.6, 22.8, 14.4, 11.9;
HRMS (ESI): calculated for $C_{10}H_{14}O_4Na^+$ $[M+Na]^+$ m/z: 221.0784, found: 221.0782;

^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC, ^{1}H-^{1}H NOESY spectra were measured.

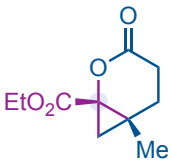
Ethyl (1*S,6*R**,7*R**)-7-methyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3p)**



Prepared according to the general procedure C using (*Z*)-hex-4-enoic acid (**1p**) (22.8 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (21.0 mg, 53% yield).

IR (cm^{-1}): 2980, 2939, 2870, 1762, 1724, 1454, 1378, 1288, 1240, 1151, 1115, 1041;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.22 (qd, *J* = 7.2, 1.8 Hz, 2H), 2.47 – 2.40 (m, 1H), 2.36 – 2.24 (m, 2H), 2.02 – 1.93 (m, 1H), 1.71 – 1.56 (m, 1H), 1.29 (t, *J* = 7.2 Hz, 3H), 1.09 (d, *J* = 6.3 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 171.3, 63.5, 62.0, 28.9, 25.2, 23.9, 16.4, 14.3, 6.3;
HRMS (ESI): calculated for $C_{10}H_{15}O_4^+$ $[M+H]^+$ m/z: 199.0965, found: 199.0962.

Ethyl (1*S,6*R**)-6-methyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3q)**

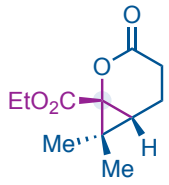


Prepared according to the general procedure C using 4-methylpent-4-enoic acid (**1q**) (22.8 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (19.8 mg, 50% yield).

IR (cm^{-1}): 2983, 2939, 2878, 1766, 1730, 1430, 1373, 1303, 1260, 1245, 1167, 1132, 1078, 1020;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.24 (qd, *J* = 7.2, 1.3 Hz, 2H), 2.48 – 2.33 (m, 2H), 2.21 (dt, *J* = 13.9, 4.7 Hz, 1H), 1.76 (m, 1H), 1.74 – 1.70 (m, 1H), 1.35 (m, 1H), 1.32 – 1.26 (m, 6H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 169.2, 65.7, 61.9, 33.4, 28.9, 27.6, 22.8, 14.4, 11.9;
HRMS (ESI): calculated for $C_{10}H_{14}O_4Na^+$ $[M+Na]^+$ m/z: 221.0784, found: 221.0782;

^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC, ^{1}H-^{1}H NOESY spectra were measured.

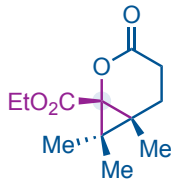
Ethyl (1*S,6*R**)-6-methyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3r)**



Prepared according to the general procedure C using 5-methylhex-4-enoic acid (**1r**) (26.6 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (25.9 mg, 61% yield).

IR (cm^{-1}): 2905, 1769, 1721, 1400, 1390, 1347, 1183, 1123, 1090, 1056, 734;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.32 – 4.15 (m, 2H), 2.45 – 2.38 (m, 1H), 2.37 – 2.31 (m, 1H), 2.30 – 2.24 (m, 1H), 1.94 (dd, *J* = 9.6, 6.8 Hz, 1H), 1.68 – 1.58 (m, 1H), 1.32 – 1.28 (m, 6H), 1.14 (s, 3H)**;**
^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 169.6, 67.8, 61.9, 31.7, 29.2, 28.9, 21.1, 17.8, 15.3, 14.4;
HRMS (ESI): calculated for $C_{11}H_{16}O_4Na^+$ $[M+Na]^+$ m/z: 235.2450, found: 235.2452.

Ethyl (1*S,6*R**)-6,7,7-trimethyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3s)**

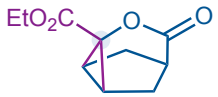


Prepared according to the general procedure C using 4,5-dimethylhex-4-enoic acid (**1s**) (28.4 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (19.0 mg, 42% yield).

IR (cm^{-1}): 2927, 1764, 1725, 1466, 1381, 1340, 1272, 1247, 1212, 1183, 1162, 1130, 1090, 1056;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.19 (qd, *J* = 7.2, 0.8 Hz, 2H), 2.43 (dt, *J* = 15.9, 3.1 Hz, 1H), 2.30 (ddd, *J* = 15.9, 11.2, 8.1 Hz, 1H), 1.91 – 1.85 (m, 2H), 1.40 (s, 3H), 1.30 (s, 3H), 1.27 (t, *J* = 7.1 Hz, 3H), 1.18 (s, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.0, 168.6, 69.4, 61.5, 33.7, 31.6, 28.5, 26.7, 17.8, 17.5, 16.1, 14.4;
HRMS (ESI): calculated for $C_{12}H_{19}O_4^+$ $[M+H]^+$ m/z: 227.1278, found: 227.1277.

Ethyl 4-oxo-3-oxatricyclo[3.2.1.0^{2,7}]octane-2-carboxylate (3t)

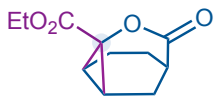


Prepared according to the general procedure C using cyclopent-3-ene-1-carboxylic acid (22.4 mg, 1.0 equiv., 0.2 mmol). Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a white solid (22.4 mg, 57% yield).

m.p.: 72-75 ºC
IR (cm^{-1}): 2982, 2941, 2876, 1764, 1747, 1466, 1448, 1380, 1335, 1310, 1268, 1200, 1128, 1100, 1051, 1021, 982, 731;
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.27 (q, J = 7.2 Hz, 2H), 2.90 (tt, J = 5.0, 0.8 Hz, 1H), 2.29 – 2.25 (m, 2H), 2.15 (ddd, J = 5.0, 1.5, 0.7 Hz, 1H), 2.11 (ddd, J = 5.0, 1.5, 0.7 Hz, 1H), 1.96 (d, J = 12.9 Hz, 2H), 1.32 (t, J = 7.2 Hz, 3H);
^{13}C NMR (101 MHz, $CDCl_3$) δ 169.2, 168.1, 63.1, 62.1, 38.5, 27.2, 25.2, 14.3;
HRMS (ESI): calculated for $C_{10}H_{12}O_4Na^+$ $[M+Na]^+$ m/z: 219.0628, found: 219.0635.

The crystal structure of **3t** has been deposited at the Cambridge Crystallographic Data Centre, CCDC 2238826.

Ethyl 4-oxo-3-oxatricyclo[3.3.1.0^{2,8}]nonane-2-carboxylate (3u)



Prepared according to the general procedure C using cyclohex-3-ene-1-carboxylic acid (25.2 mg, 1.0 equiv., 0.2 mmol). Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (25.2 mg, 60% yield).

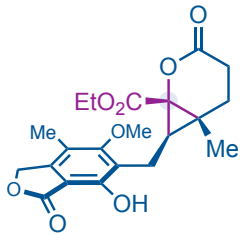
IR (cm^{-1}): 2940, 2872, 1753, 1721, 1450, 1370, 1360, 1348, 1297, 1265, 1212, 1184, 1159, 1124, 1093, 1061, 1047, 1021, 980;

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.25 (q, *J* = 7.1 Hz, 2H), 2.73 (tq, *J* = 3.1, 1.1 Hz, 1H), 2.31 – 2.22 (m, 1H), 2.15 – 2.08 (m, 1H), 2.08 – 2.00 (m, 2H), 1.94 – 1.81 (m, 3H), 1.62 – 1.54 (m, 1H), 1.31 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6, 169.6, 64.0, 62.1, 36.6, 24.6, 21.7, 21.5, 19.8, 15.5, 14.4;

HRMS (ESI): calculated for $C_{11}H_{14}O_4Na^+$ $[M+Na]^+$ m/z: 233.0784, found: 233.0785;

Ethyl (1*R,6*S**,7*S**)-7-((4-hydroxy-6-methoxy-7-methyl-3-oxo-1,3-dihydroisobenzofuran-5-yl)methyl)-6-methyl-3-oxo-2-oxabicyclo[4.1.0]heptane-1-carboxylate (3v)**



Prepared according to the general procedure C using mycophenolic acid (64.1 mg, 1.0 equiv., 0.2 mmol). The reaction was stirred for an additional period of 45 minutes at –50ºC. Ratio of diastereoisomers was determined to be 3:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (dichloromethane/diethyl ether: 20/1) provided the title compound as a colorless oil (28.3 mg, 35% yield).

Major isomer:

IR (cm^{-1}): 2928, 2900, 1760, 1728, 1723, 1504, 1500, 1495, 1269, 1035, 759, 704;

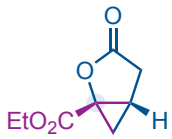
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (s, 1H), 5.21 (s, 2H), 4.28 (qd, *J* = 7.1, 1.6 Hz, 2H), 3.77 (s, 3H), 3.16 – 3.06 (m, 2H), 2.45 – 2.30 (m, 2H), 2.20 – 2.17 (m, 1H), 2.16 (s, 3H), 1.88 (dd, *J* = 7.5, 5.4 Hz, 1H), 1.64 (td, *J* = 13.6, 3.8 Hz, 1H), 1.38 (s, 3H), 1.33 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.0, 172.2, 168.4, 164.2, 153.9, 144.9, 121.4, 117.0, 106.7, 70.2, 67.6, 61.7, 61.2, 41.3, 33.2, 30.6, 28.5, 18.1, 14.4, 14.1, 11.8;

HRMS (ESI): calculated for $C_{21}H_{24}O_8Na^+$ $[M+Na]^+$ m/z: 427.4150, found: 427,4149;

^{1}H-^{13}C HSQC, ^{1}H-^{1}H NOESY spectra were measured.

Ethyl (1*S,5*S**)-3-oxo-2-oxabicyclo[3.1.0]hexane-1-carboxylate (3w)**



Prepared according to the general procedure C using but-3-enoic acid (17.2 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (30.9 mg, 91% yield).

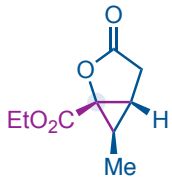
IR (cm^{-1}): 2984, 2941, 1789, 1726, 1468, 1447, 1404, 1380, 1309, 1277, 1248, 1176, 1130, 1063, 1017, 958, 860;

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.26 (qd, *J* = 7.2, 1.9 Hz, 2H), 2.99 (ddd, *J* = 18.9, 7.1, 1.1 Hz, 1H), 2.59 (dd, *J* = 18.9, 1.2 Hz, 1H), 2.24 (dddd, *J* = 9.1, 7.1, 6.1, 1.1 Hz, 1H), 1.87 (ddd, *J* = 9.1, 6.7, 1.1 Hz, 1H), 1.30 (t, *J* = 7.2 Hz, 3H), 1.07 – 1.03 (m, 1H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.0, 168.8, 63.7, 62.1, 33.1, 23.3, 20.7, 14.3;

HRMS (ESI): calculated for $C_8H_{10}O_4Na^+$ $[M+Na]^+$ m/z: 193.0471, found: 193.0466.

Ethyl (1*S,5*R**,6*R**)-6-methyl-3-oxo-2-oxabicyclo[3.1.0]hexane-1-carboxylate (3x)**



Prepared according to the general procedure C using (*E*)-pent-3-enoic acid (20.0 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a colorless oil (29.4 mg, 80% yield).

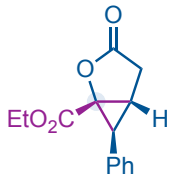
IR (cm^{-1}): 2984, 2938, 1791, 1728, 1463, 1414, 1373, 1341, 1290, 1265, 1225, 1135, 1110, 1094, 1023, 924, 719;

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.28 (q, *J* = 7.1 Hz, 2H), 2.94 (dd, *J* = 18.7, 7.3 Hz, 1H), 2.60 (dd, *J* = 18.7, 1.1 Hz, 1H), 2.03 (ddd, *J* = 6.9, 5.7, 1.0 Hz, 1H), 1.36 – 1.28 (m, 7H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.1, 167.8, 67.8, 61.9, 33.3, 32.9, 26.7, 14.3, 11.5;

HRMS (ESI): calculated for $C_9H_{12}O_4Na^+$ $[M+Na]^+$ m/z: 184.1910, found: 184.1912.

Ethyl (1*R,5*R**,6*S**)-3-oxo-6-phenyl-2-oxabicyclo[3.1.0]hexane-1-carboxylate (3y)**



Prepared according to the general procedure C using (*E*)-4-Phenylbut-3-enoic acid (32.4 mg, 1.0 equiv., 0.2 mmol). Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 10/1 to 10/3) provided the title compound as a white solid (36.9 mg, 75% yield).

mp: 94-98 ºC

IR (cm^{-1}): 2980, 1796, 1736, 1374, 1222, 1128, 1051, 824, 743;

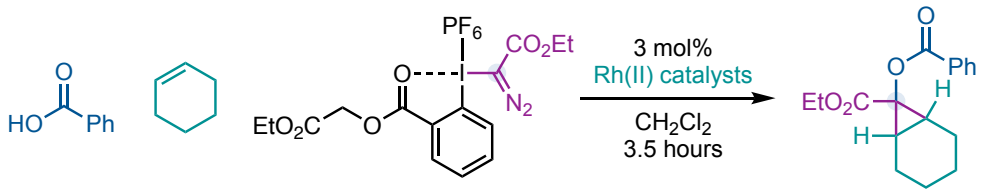
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 7.23 (m, 5H), 4.01 (qd, *J* = 7.1, 2.1 Hz, 2H), 3.15 (dd, *J* = 18.4, 6.8 Hz, 1H), 2.86 – 2.78 (m, 2H), 2.63 (d, *J* = 6.8 Hz, 1H), 0.98 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.6, 166.0, 132.5, 128.9, 128.5, 127.9, 68.8, 61.7, 41.7, 33.3, 23.5, 13.8;

HRMS (ESI): calculated for $C_{14}H_{14}O_4Na^+$ $[M+Na]^+$ m/z: 269.0784, found: 269.0781.

The crystal structure of **3y** has been deposited at the Cambridge Crystallographic Data Centre, CCDC 2192080.

7. General procedure D for intermolecular reaction optimization.



2b **5**

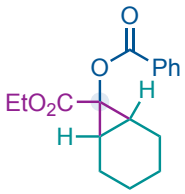
To a 10 mL oven-dried tube equipped with a stirring bar were added the corresponding Rh catalyst (3 mol%) and additive. The tube was sealed before being evacuated and backfilled with argon three times. Degassed dichloromethane (0.5 mL) and cyclohexene were added and the resulting mixture was cooled at the indicated temperature. Then, a solution of hypervalent iodine reagent **2b** and benzoic acid in degassed

dichloromethane (1 mL) were added dropwise to the reaction flask during 30 min using a syringe pump at the indicated temperature. Then the resulting reaction mixture was allowed to warm to room temperature in 3 hours. The solution was extracted with saturated aqueous solution of $NaHCO_3$ (3 mL) and dichloromethane (3 x 3 mL) following by filtering through a short plug of anhydrous Na_2SO_4. Solvent was removed under *vacuum* and ^1H NMR yield was measured using dibromomethane (7 μL, 0.1 mmol, 1.0 equiv.) as internal standard.

Table S2. Optimization studies for intramolecular reaction.

Entry	Stoichiometry (Acid **:** alkene : **2a**)	Rh catalyst	Additive (equiv.)	Temperature	Yield **5** [%]
1	1 : 1 : 1.3	$Rh_2(esp)_2$	$NaHCO_3$ (2)	-50 ºC	traces
2	1 : 5 : 1.3	$Rh_2(esp)_2$	$NaHCO_3$ (2)	-50 ºC	25
3	1 : 10 : 1.3	$Rh_2(esp)_2$	$NaHCO_3$ (2)	-50 ºC	23
4	1 : 5 : 1.3	$Rh_2(esp)_2$	$NaHCO_3$ (10)	-50 ºC	24
5	1 : 5 : 1.3	$Rh_2(esp)_2$	Na_2CO_3 (2)	-50 ºC	20
6	1 : 5 : 1.3	$Rh_2(esp)_2$	K_3PO_4 (2)	-50 ºC	21
7	1 : 5 : 1.3	$Rh_2(OAc)_2$	$NaHCO_3$ (2)	-50 ºC	0
8	1 : 5 : 1.3	$Rh_2(Oct)_2$	$NaHCO_3$ (2)	-50 ºC	0
9	1 : 5 : 1.3	$Rh_2(Adc)_2$	$NaHCO_3$ (2)	-50 ºC	20
10	2 : 5 : 1	$Rh_2(esp)_2$	$NaHCO_3$ (2)	-50 ºC	20
11	5 : 5 : 1	$Rh_2(esp)_2$	$NaHCO_3$ (2)	-50 ºC	22
12	5 : 2 : 1	$Rh_2(esp)_2$	$NaHCO_3$ (2)	-50 ºC	19
13	1 : 5 : 1.3	$Rh_2(esp)_2$	$NaHCO_3$ (2)	-78 ºC	15
14	1 : 5 : 1.3	$Rh_2(esp)_2$	$NaHCO_3$ (2)	-20 ºC	28
15	1 : 5 : 1.3	$Rh_2(esp)_2$	$NaHCO_3$ (2)	0 ºC	30

Ethyl-7-(benzoyloxy)bicyclo[4.1.0]heptane-7-carboxylate (5)



To a 10 mL oven-dried tube equipped with a stirring bar were added $Rh_2(esp)_2$ (3 mol%) and additive. The tube was sealed before being evacuated and backfilled with argon three times. Degassed dichloromethane (0.5 mL) and cyclohexene (51μL, 0.5 mmol, 5 equiv.) were added and the resulting mixture was cooled at 0ºC. Then, a solution of hypervalent iodine reagent **2b** (77 mg, 0.13 mmol, 1.3 equiv.) and benzoic acid (12.2 mg, 0.1 mmol, 1 equiv.) in degassed dichloromethane (1 mL) were added dropwise to the reaction flask during 30 min using a syringe pump. Then the resulting reaction mixture was allowed to warm to

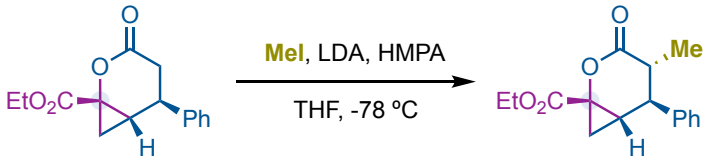
room temperature in 3 hours. The solution was extracted with saturated aqueous solution of $NaHCO_3$ (3 mL) and dichloromethane (3 x 3 mL) following by filtering through a short plug of anhydrous Na_2SO_4. Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^1H NMR spectroscopy. Purification by flash chromatography on silica gel (hexane/ethyl acetate: 40/1 to 10/1) provided the title compound as a colorless oil (5.6 mg, 30% yield).

^1H NMR (500 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 2H), 7.57 (ddt, J = 8.7, 7.2, 1.3 Hz, 1H), 7.44 (td, J = 7.5, 1.0 Hz, 2H), 4.21 (q, J = 7.1 Hz, 2H), 2.01 – 1.88 (m, 2H), 1.79 (m, J = 5.4 Hz, 2H), 1.79 – 1.74 (m, 2H), 1.58 (m, J = 4.6 Hz, 2H), 1.30 – 1.25 (m, 2H), 1.21 (t, J = 7.1 Hz, 3H);
^1H NMR (500 MHz, CD_3OD) δ 8.00 – 7.97 (m, 2H), 7.74 – 7.70 (m, 1H), 7.50 – 7.46 (m, 2H), 4.18 (q, J = 7.1 Hz, 2H), 2.01 – 1.93 (m, 2H), 1.80 – 1.77 (m, 2H), 1.76 – 1.70 (m, 2H), 1.62 – 1.55 (m, 2H), 1.34 – 1.25 (m, 2H), 1.18 (t, J = 7.1 Hz, 3H);
^{13}C NMR (126 MHz, $CDCl_3$) δ 168.8, 166.7, 133.3, 129.9, 129.8, 128.5, 63.5, 61.1, 25.7, 20.6, 17.4, 14.4;
HRMS (ESI): calculated for $C_{17}H_{20}O_4Na^+$ $[M+Na]^+$ m/z: 311.1254, found: 311.1259;
^1H-^1H COSY, ^1H-^{13}C HSQC, ^1H-^{13}C HMBC spectra were measured;

Note: We were unable to determine the relative configuration of **5** since NOESY and GOESY experiments were not conclusive.

8. Derivatizations of compound 3a.

- **Methylation with MeI[13]**



3a **6**

Ethyl (1*S,4*R**,5*S**,6*S**)-4-methyl-3-oxo-5-phenyl-2-oxabicyclo[4.1.0]heptane-1-carboxylate (6):** To a solution of LDA (420 μL, 0.42 mmol, 1M in THF) and HMPA (230 μL, 1.38 mmol) in THF (1.4 mL) at -78 ºC was added dropwise a solution of **3a** (90 mg, 0.35 mmol) in THF (0.5 mL). The mixture was stirred at -78 ºC for 50 min, then iodomethane (88 μL, 1.4 mmol) was added. The mixture was stirred for 30 min at -78 ºC and was allowed to warm up to – 20ºC over a period of 2 h. The reaction was quenched with

ammonium chloride and extracted with ethyl acetate. The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. Ratio of diastereoisomers was determined to be >20:1 from the crude reaction mixture using ^{1}H NMR spectroscopy. The crude product was purified by flash column chromatography to afford the title compound as a colorless oil (77.7 mg, 81%), R_f = 0.31 (30% ethyl acetate in hexane).

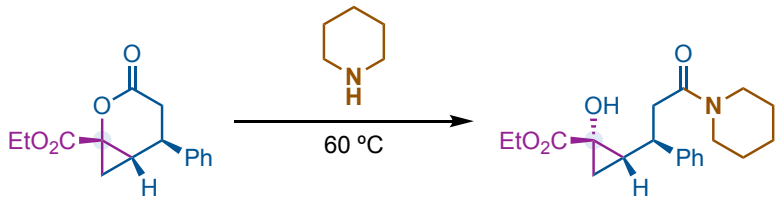
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.35 (m, 2H), 7.34 – 7.28 (m, 1H), 7.26 – 7.21 (m, 2H), 4.27 (qd, *J* = 7.1, 2.5 Hz, 2H), 2.71 (dq, *J* = 12.1, 6.8 Hz, 1H), 2.51 (dd, *J* = 12.2, 7.1 Hz, 1H), 2.12 (dt, *J* = 9.7, 7.2 Hz, 1H), 1.88 (dd, *J* = 9.7, 6.0 Hz, 1H), 1.37 (ddd, *J* = 7.3, 6.0, 0.6 Hz, 1H), 1.32 (t, *J* = 7.1 Hz, 3H), 0.92 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4, 170.6, 140.5, 129.3, 127.8, 127.8, 62.3, 60.0, 49.6, 40.2, 30.2, 24.9, 14.3, 13.2.

HRMS (ESI): calculated for $C_{16}H_{19}O_4^+$ $[M+H]^+$ m/z: 275.1278, found: 275.1291;

^{1}H-^{13}C HSQC, ^{1}H-^{1}H NOESY spectra were measured.

- **Ring opening with piperidine[14]**



3a **7**

Ethyl (1*R,2*S**)-2-((*S**)-3-ethoxy-3-oxo-1-phenylpropyl)-1-hydroxycyclopropane-1-carboxylate (7):** A 10 mL oven-dried tube equipped with a magnetic stirring bar was charged with **3a** (26.0 mg, 0.1 mmol) and piperidine (85 mg, 1.0 mmol). The mixture was stirred at 60 °C for 7 h until complete consumption of the starting material (monitored by TLC). The crude mixture was directly purified by column chromatography to afford the title compound as a colorless oil (31.0 mg, 90%); R_f = 0.55 (dichloromethane/diethyl ether: 2/1).

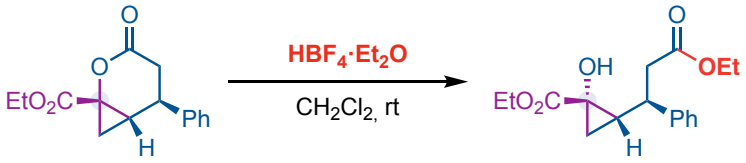
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.25 (m, 4H), 7.26 – 7.21 (m, 1H), 6.43 (s, 1H), 4.19 (qt, *J* = 7.2, 3.6 Hz, 2H), 3.63 (ddd, *J* = 13.2, 6.7, 4.3 Hz, 1H), 3.51 (ddd, *J* = 13.6, 7.2, 4.5 Hz, 1H), 3.39 (t, *J* = 5.6 Hz, 2H), 3.16 (td, *J* = 11.1, 3.0 Hz, 1H), 2.83 (dd, *J* = 16.3, 11.2 Hz, 1H), 2.58 (dd, *J* = 16.3, 3.1 Hz, 1H), 1.68 (dd, *J* = 10.0, 7.7 Hz, 1H), 1.65 – 1.45 (m, 6H), 1.40 (dd, *J* = 10.0, 5.2 Hz, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 0.76 (dd, *J* = 7.7, 5.2 Hz, 1H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.3, 170.5, 145.0, 128.8, 127.6, 126.7, 61.2, 57.6, 47.0, 43.4, 41.7, 38.9, 33.5, 26.6, 25.6, 24.5, 22.4, 14.5;

HRMS (ESI): calculated for $C_{20}H_{28}NO_4^+$ $[M+H]^+$ m/z: 346.2013, found: 346.2011;

^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC, ^{1}H-^{1}H NOESY spectra were measured.

- **Ring opening with $HBF_4{\cdot}Et_2O$**



3a **8**

Ethyl (1*S)-2-((*R**)-3-ethoxy-3-oxo-1-phenylpropyl)-1-hydroxycyclopropane-1-carboxylate (8):** A 10 mL oven-dried tube equipped with a magnetic stirring bar was charged with **3a** (13.0 mg, 0.05 mmol). The vial was sealed before being evacuated and backfilled with argon three times. Then degassed dichloromethane (0.5 mL) was added. Then tetrafluoroboric acid diethyl ether complex (75 μL, 0.5 mmol, 51-57% in Et_2O, 10 equiv.) was added to the solution. The mixture was stirred at room temperature for 48 h until complete consumption of the starting material (monitored by TLC). The crude mixture was directly purified by column chromatography to afford the title compound as a colorless oil (9.2 mg, 60%), R_f = 0.23 (dichloromethane/ethyl acetate: 25/1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.28 (m, 2H), 7.30 – 7.20 (m, 3H), 4.43 (s, 1H), 4.21 (qd, J = 7.1, 3.8 Hz, 2H), 4.13 (qd, J = 7.2, 1.0 Hz, 2H), 3.06 (td, J = 9.5, 6.3 Hz, 1H), 2.80 – 2.69 (m, 2H), 1.73 (td, J = 10.1, 7.7 Hz, 1H), 1.43 (dd, J = 10.0, 5.5 Hz, 1H), 1.29 (t, J = 7.2 Hz, 3H), 1.22 (t, J = 7.1 Hz, 3H), 0.81 (dd, J = 7.7, 5.5 Hz, 1H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.6, 173.7, 143.7, 128.8, 127.6, 126.9, 61.5, 61.3, 58.3, 42.5, 38.9, 33.0, 21.4, 14.4, 14.2;

HRMS (ESI): calculated for $C_{17}H_{22}O_5Na^+$ $[M+Na]^+$ m/z: 329.1359, found: 329.1355.

9. X-Ray crystal data of 3t and 3y.

Single-crystal X-Ray diffraction analysis of 3t: The crystal of **3t** used for the single-crystal X-ray diffraction experiment was grown by slow evaporation of a solution of **3t** in dichloromethane and hexane

at room temperature. An ORTEP diagram of the crystal structure of **3t** is shown below (CCDC No: 2238826):

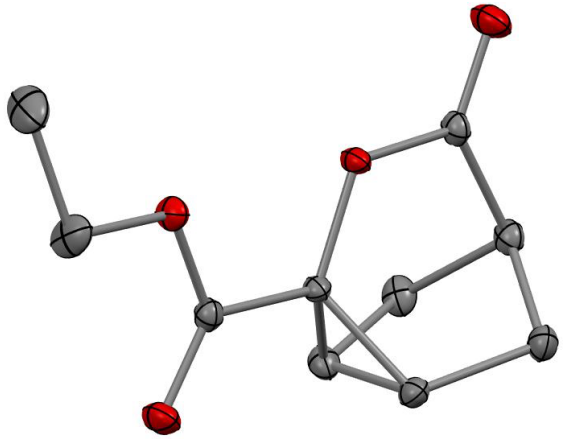


Table S3. Crystal data and structure refinement for **3t**.

Identification code	EPM454B_twin1_hklf5	
Empirical formula	C10 H12 O4	
Formula weight	196.20	
Temperature	100(2)K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 13.1462(5)Å	a= 90°.
	b = 9.0845(2)Å	b = 112.482(4)°.
	c = 16.6193(5)Å	g = 90°.
Volume	1833.95(11) $Å^3$	
Z	8	
Density (calculated)	1.421 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
F(000)	832	
Crystal size	0.700 x 0.400 x 0.300 mm^3	
Theta range for data collection	3.681 to 31.197°.	
Index ranges	-19<=h<=19,-13<=k<=13,-24<=l<=23	
Reflections collected	9762	
Independent reflections	9762[R(int) = ?]	
Completeness to theta =31.197°	94.3%	

Absorption correction	Multi-scan
Max. and min. transmission	1.00 and 0.82
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9762/ 0/ 256
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0640, wR2 = 0.1963
R indices (all data)	R1 = 0.0760, wR2 = 0.2209
Largest diff. peak and hole	0.989 and -1.125 e.Å^{-3}

Single-crystal X-Ray diffraction analysis of 3y: The crystal of **3y** used for the single-crystal X-ray diffraction experiment was grown by slow evaporation of a solution of **3y** in dichloromethane and hexane at room temperature. An ORTEP diagram of the crystal structure of **3y** is shown below (CCDC No: 2192080):

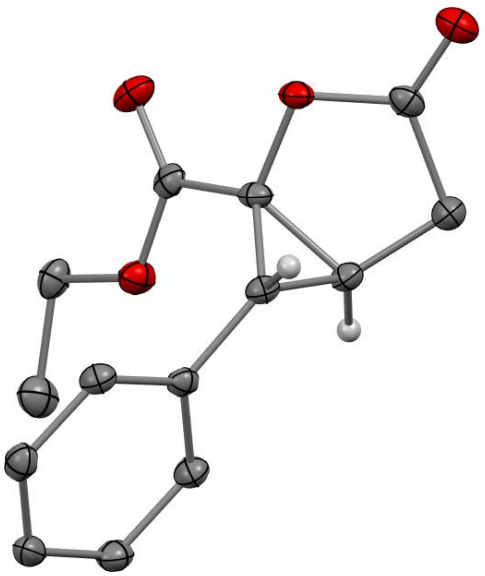


Table S4. Crystal data and structure refinement for **3y** .

Identification code	mo_EPM509I_0m
Empirical formula	C14 H14 O4
Formula weight	246.25
Temperature	100(2)K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P 21

Unit cell dimensions	a = 10.147(3)Å	a= 90°.
	b = 5.7189(19)Å	b = 115.309(7)°.
	c = 11.362(4)Å	g = 90°.
Volume	596.0(3) $Å^3$	
Z	2	
Density (calculated)	1.372 Mg/m^3	
Absorption coefficient	0.101 mm^{-1}	
F(000)	260	
Crystal size	0.400 x 0.250 x 0.150 mm^3	
Theta range for data collection	2.220 to 28.064°.	
Index ranges	-13<=h<=13,-7<=k<=7,-15<=l<=14	
Reflections collected	7235	
Independent reflections	2863[R(int) = 0.0281]	
Completeness to theta = 28.064°	99.1%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.74 and 0.64	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2863/ 1/ 164	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0781	
R indices (all data)	R1 = 0.0386, wR2 = 0.0804	
Flack parameter	x =0.1(5)	
Largest diff. peak and hole	0.185 and -0.178 $e.Å^{-3}$	

10. Computational details

The DFT calculations were performed with GAUSSIAN 16 Program.[15] For the geometry optimization, the B3LYP functional[16] with Grimme's third generation empirical dispersion correction including Becke-Johanson damping was used,[17] which is denoted as B3LYP-D3BJ. The SDD basis sets with associated effective core potential (ECP)[18] was used for Rh and Iodine, whereas the 6-31G* basis set were used for other atoms.[19] All geometry optimizations were performed with the IEFPCM implicit solvation method as implemented in GAUSSIAN 16 program with dichloromethane as solvent.[20] Hessian calculation were performed to confirm the stationary points; minima with no imaginary frequency and single imaginary frequency for the transition states (TSs). The TSs were further confirmed by intrinsic reaction coordinate (IRC) calculations.[21] The electronic energies of the stationary points were further computed using an improved basis set. The cc-PVTZ-PP[22] basis set was used for Rh and Iodine, where triple-zeta cc-PVTZ

basis set was used with effective core potentials (ECP28MDF). Both triple-zeta basis set (ECP28MDF_VTZ) and effective core potentials were downloaded from the Stuttgart/Cologne Group website.[23] For other atoms cc-PVTZ basis set was used.[24] The quasi-harmonic corrections proposed by Grimme with a cutoff of 100 cm^{-1} were employed to free energies, and correction for standard state of 1 M for all species were also applied using GoodVibes v3.0.1 program.[25]

The natural population analysis was used for computing charges on the atoms.[26] The charge decomposition analysis (CDA) proposed by Frenking[27] was used to analyze the Rh-carbene bonds using the MultiWFN-3.8 program.[28] For CDA $Rh_2(OAc)_4$ and carbene/Carbynoids were taken as two fragments. The electrophilicity was estimated using global electrophilicity Index (ω) = $\mu^2/2\eta$, where μ(electronegativity) = $(\varepsilon_{LUMO} + \varepsilon_{HOMO})/2$; η(hardness) = $\varepsilon_{LUMO} - \varepsilon_{HOMO}$.[29] For analysis was performed using the method used for energy calculation, i.e., PCM_{CH2Cl2}/B3LYP-D3BJ/cc-PVTZ-PP(Rh,I),cc-PVTZ(H,C,O,F,P). The crystal structure of the $Rh_2(esp)_2$ was used for the catalyst structure. To generate other stationary points, the crystal structure of $Rh_2(esp)_2$-carbene complex was used as template (that is, the conformation of ligands is kept like the crystal structure). The molecular geometries in the Figures were generated using open source Pymol program.[30]

- **Conversion from intermediate C to intermediate E**

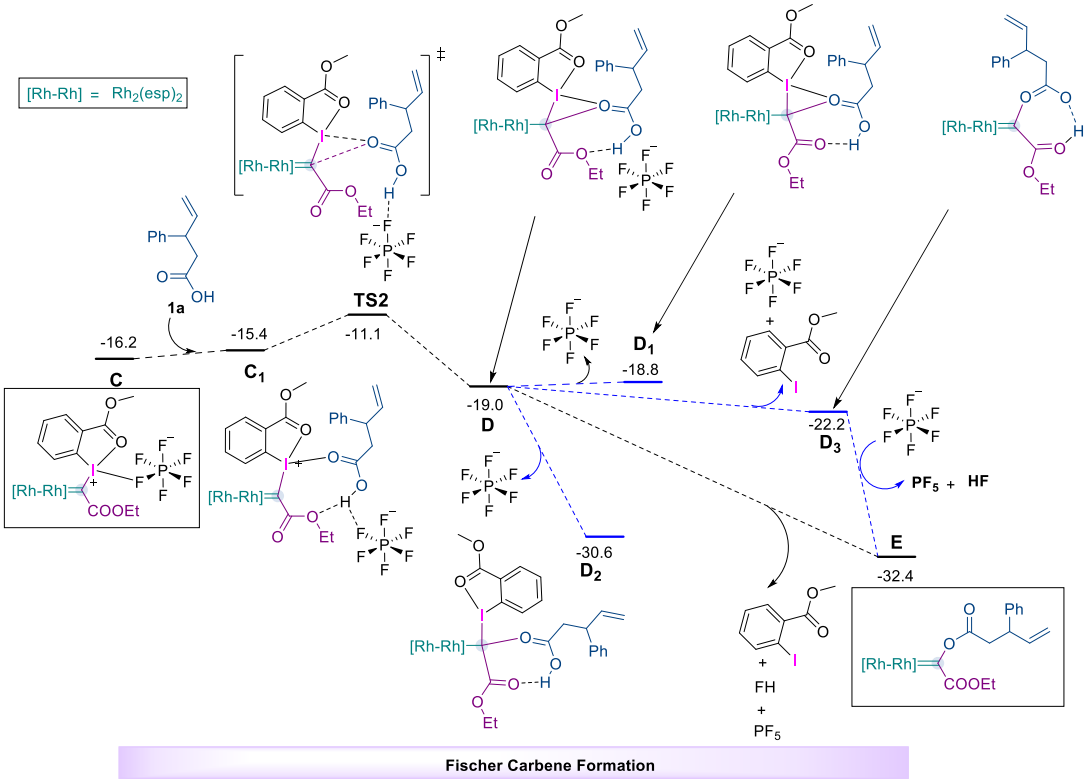
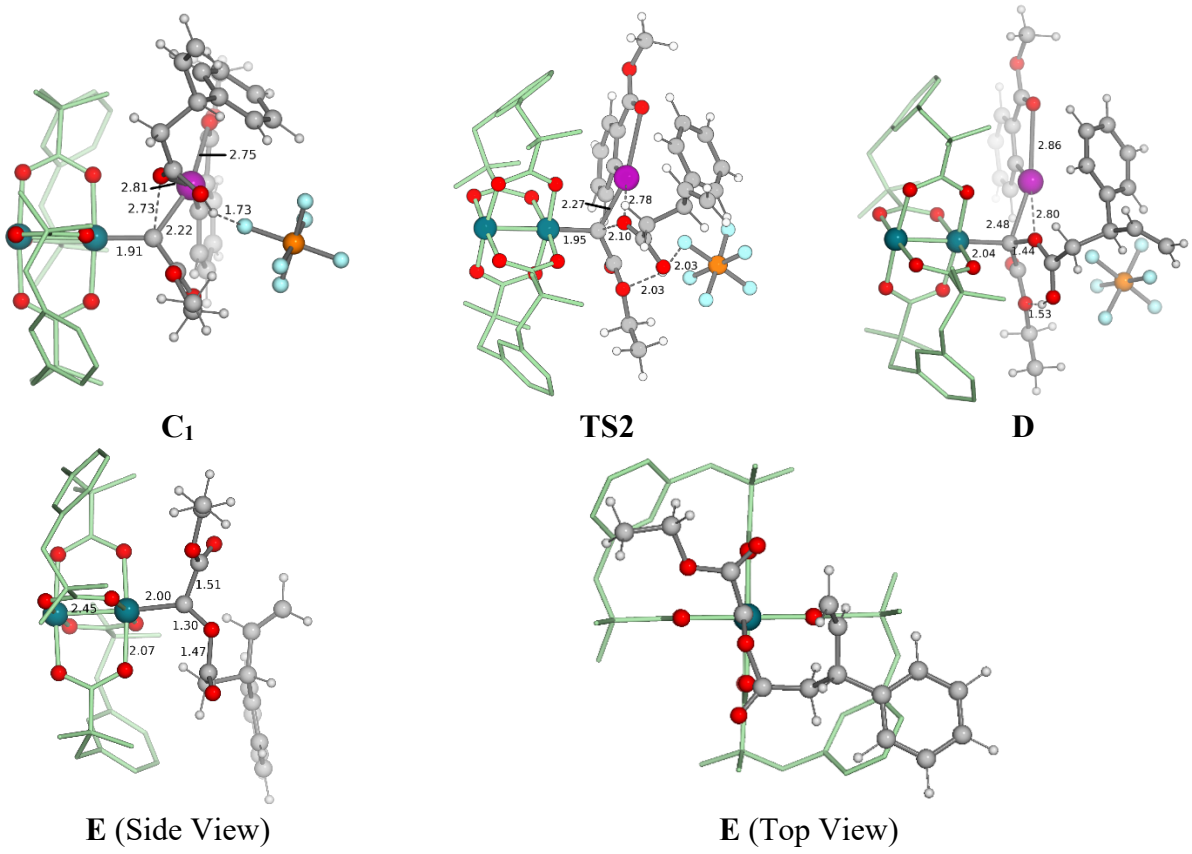


Figure S3. Free energy profile for Rh-carbynoid to Fischer-carbene conversion at PCM$_{CH2Cl2}$/B3LYP-D3BJ/cc-PVTZ-PP(Rh,I),cc-PVTZ(H,C,O,F,P)// PCM$_{CH2Cl2}$/B3LYP-D3BJ/SDD(Rh,I),6-31G*(H,C,O,F,P).



C$_1$ **TS2** **D**

E (Side View) **E** (Top View)

Figure S4. Optimized geometries of stationary points involved in conversion on intermediate **C** to **E**.

- **Competition between acid and olefin addition to C**

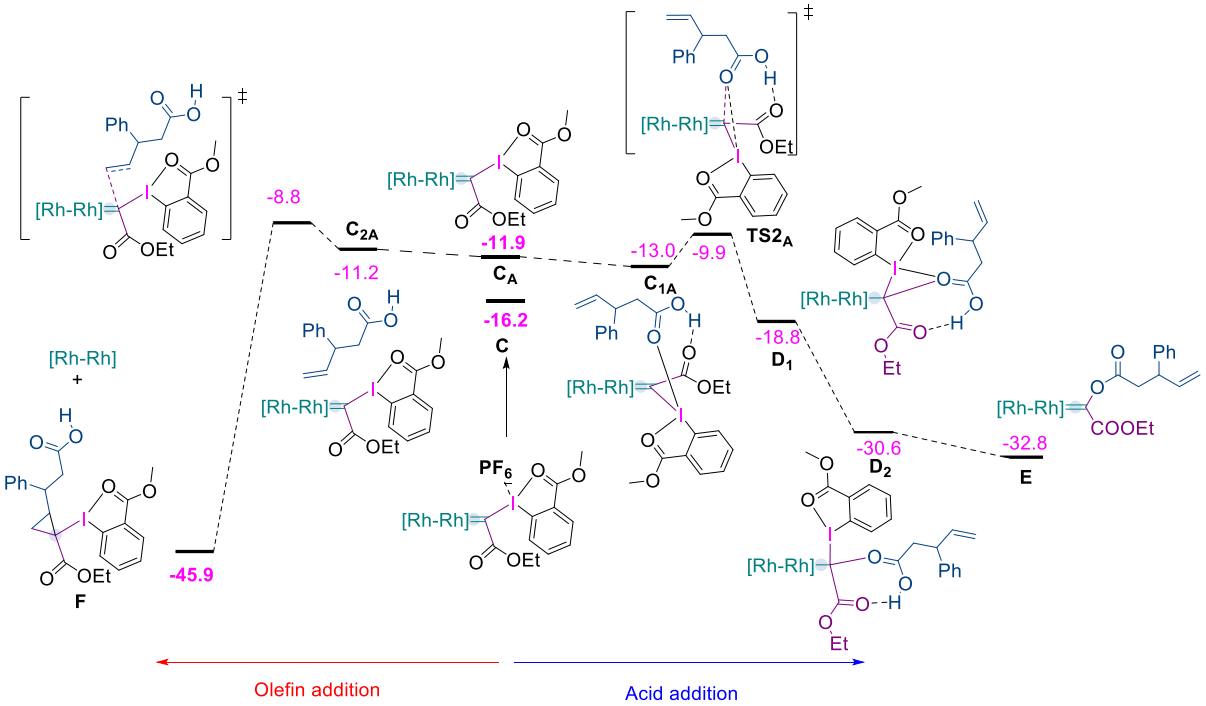


Figure S5. Comparison of potential energy surface for acid and olefin addition to Rh-carbynoid intermediate without PF_6^- at PCM$_{CH2Cl2}$/B3LYP-D3BJ/cc-PVTZ-PP(Rh,I),cc-PVTZ(H,C,O,F,P)// PCM$_{CH2Cl2}$/B3LYP-D3BJ/SDD(Rh,I),6-31G*(H,C,O,F,P).

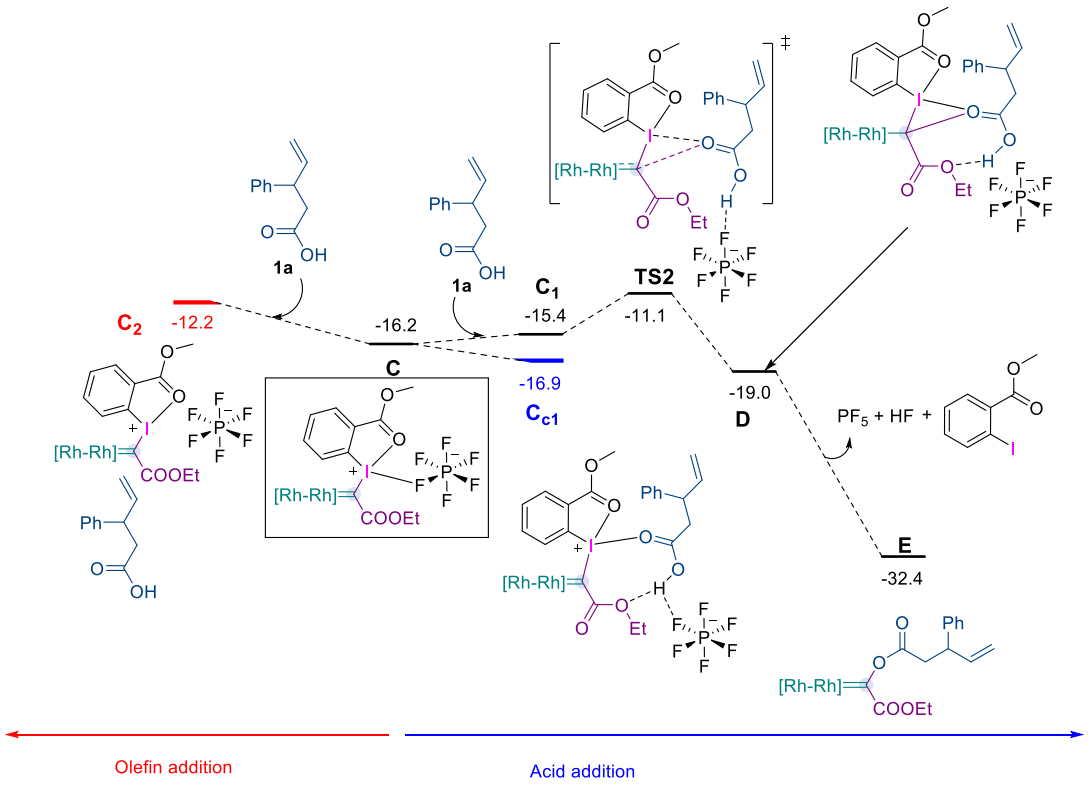


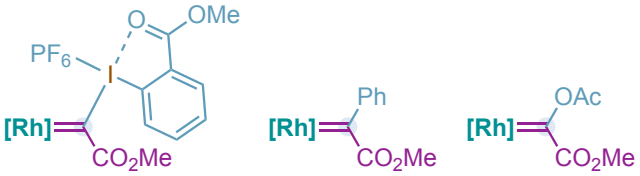
Figure S6. Comparison of potential energy surface for acid and olefin addition to Rh-carbynoid intermediate at PCM$_{CH2Cl2}$/B3LYP-D3BJ/cc-PVTZ-PP(Rh,I),cc-PVTZ(H,C,O,F,P)// PCM$_{CH2Cl2}$/B3LYP-D3BJ/SDD(Rh,I),6-

31G*(H,C,O,F,P). The TS corresponding to olefin addition could not be optimized even after repeated attempts, probably due to low barrier (as clear from previous Figure) and flat potential energy surface near the TS.

The carbynoid complex **C** reacts with the carboxylic group rather than with the olefin group present in the substrate (**1a**). To understand this, we explored the pathway for olefin addition to **C**. However, we could not locate the TS for the olefin addition. Hence, we explored the TSs in absence of PF_6^- (Figure S5). The transition state (TS) for alkenyl carboxylic acid (**1a**) addition through carboxylic acid (in absence of $PF6^-$) is lower in energy than in addition through olefin by 1.1 kcal/mol (Figure S5). It explains the experimental findings, however, the difference in energy of two TSs quantitatively cannot explain the exclusive carboxylic group addition to **C**. To further substantiate we explored energies of the pre-TS complexes ($\mathbf{C_2}$ and $\mathbf{C_{c1}}$) of both competing pathways (Figure S6). The adduct between **C** and **1a** for olefin addition ($\mathbf{C_2}$) is higher in energy than the adduct for acid addition ($\mathbf{C_{c1}}$) by 4.7 kcal/mol (Figure S6), whereas the difference is only 1.8 kcal/mol for adducts without $PF6^-$ (Figure 3, $\mathbf{C_{1A}}$ and $\mathbf{C_{2A}}$). Although, the corresponding TSs from the adducts ($\mathbf{C_2}$ and $\mathbf{C_{c1}}$) could not be optimized (probably due to the low barrier for TS and flat PES near the TS), but their energies explain the exclusive reaction of complex **C** with the carboxylic group.

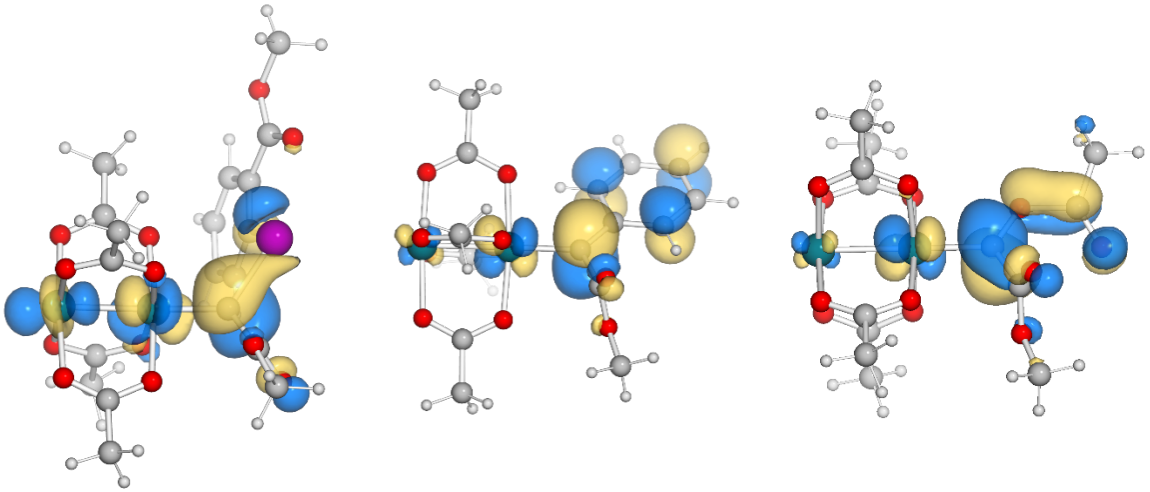
- **Comparison of Metallo-Carbenes/Carbynoids**

Table S5. Orbital energies and global electrophilicity index.



donation (d)	0.245	0.275	0.313
back donation (b)	0.123	0.037	0.066
d-b	0.122	0.238	0.247
ε_{LUMO} (eV)	-4.083	-3.496	-2.931
ω	5.78	4.68	3.30

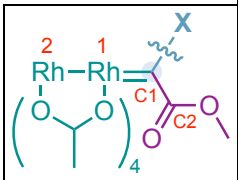
[a] Electrophilicity Index (ω) = $\mu^2/2\eta$; where, μ(electronegativity) = $(\varepsilon_{LUMO} + \varepsilon_{HOMO})/2$; η(hardness) = $\varepsilon_{LUMO} - \varepsilon_{HOMO}$.



IAr (LUMO) **Ph** (LUMO) **OCOMe** (LUMO)

Figure S7. LUMO of complexes for different substituent. For Rh-carbynoid, LUMO constitute mainly of carbene carbon *p*-orbital. For the metal-carbene with π-donor substituent (–Ph and –OCOMe), it is also distributed on substituent's pi-orbitals. For X = IAr metal-Carbene complex has lowest ε_{LUMO}.

Table S6. Bond order (Wiberg bond index (WBI) for selected bonds in complex.

	X	Wiberg bond index			
		Rh_1-Rh_2	Rh_1-C_1	C_1-C_2	C_1-X
	-IAr	0.66	1.02	1.00	0.96
	-Ph	0.63	0.81	1.01	**1.29**
	-OCOMe	0.64	0.84	0.96	**1.24**

The bond order (WBI) between carbene carbon and atom of X-substituent is >1 for Ph and OCOMe substituents. It is due to electron donation (π-donation) from Ph and OCOMe substituents to C_1.

Table S7. Computed total electronic energies (**E_{SPC}**), total electronic energy (**E**) at lower level of theory, zero-point energy correction (**ZPE**), enthalpy (**H**), temperature*entropy (**T.S**) term, **T.S** with quasiharmonic correction by Grimme (**T.qh-S**), free energy (with quasiharmonic corrections for entropy and correction for solution phase standard state of 1 mole/litre, **qh-G_{SPC}**) and relative energy w.r.t. substrates and catalyst (**ΔG_{SPC}(qh)**). The **E_{SPC}** is at PCM_{CH2Cl2}/B3LYP-D3BJ/cc-PVTZ-PP(Rh,I),cc-PVTZ(H,C,O,F,P) level of theory. The **E** and energy corrections are at PCM_{CH2Cl2}/B3LYP-D3BJ/SDD(Rh,I),6-31G*(H,C,O,F,P) level of theory.

	E_{SPC}	E	ZPE	H	T.S	T.qh-S	qh-G_{SPC}	ΔG_{SPC}(qh)
A	-2066.985979	-2066.961239	0.678074	-2066.266252	0.107008	0.102339	-2066.368591	0.0
$2b_A$	-1170.820538	-886.079766	0.229642	-1170.569974	0.070055	0.065753	-1170.635727	
2b*	-2111.899123	-1826.832843	0.249817	-2111.620212	0.090304	0.082464	-2111.702676	
IAr	-755.52921	-470.962475	0.133339	-755.384486	0.046861	0.04584	-755.430326	
HPF_6	-941.443347	-941.111235	0.027854	-941.406438	0.038711	0.038632	-941.445071	
PF_5	-840.95377	-840.675917	0.016419	-840.930864	0.033236	0.033225	-840.964089	
HF	-100.488223	-100.423111	0.008936	-100.475982	0.016723	0.016723	-100.492705	
PF_6-	-941.053874	-940.721133	0.018644	-941.02795	0.031678	0.03169	-941.05964	
N_2	-109.569019	-109.521835	0.005603	-109.560112	0.018735	0.018735	-109.578846	
1a	-577.107995	-576.878142	0.205915	-576.888936	0.050848	0.048196	-576.937132	
3a	-882.516159	-882.182064	0.285866	-882.212366	0.061914	0.058372	-882.270738	-60.8
B	-4178.91514	-3893.84611	0.929401	-4177.914594	0.172781	0.159362	-4178.073956	-1.7
TS1	-4178.897718	-3893.828126	0.926337	-4177.899821	0.174617	0.160472	-4178.060292	6.9
C_{N2}	-4178.923178	-3893.848223	0.925701	-4177.924094	0.182543	0.165343	-4178.089438	-11.4
C_A	-3128.272717	-2843.561664	0.899686	-3127.312105	0.149458	0.139638	-3127.451743	-11.9
C	-4069.353368	-3784.32631	0.920555	-4068.364084	0.165874	0.154196	-4068.51828	-16.2
C_1	-4646.483873	-4361.23774	1.128261	-4645.273069	0.198209	0.181099	-4645.454167	-15.4
TS2	-4646.478248	-4361.236496	1.128037	-4645.268584	0.19435	0.178664	-4645.447249	-11.1
D	-4646.492789	-4361.257137	1.129595	-4645.281666	0.193777	0.178239	-4645.459905	-19.0
C_{c1}	-4646.484584	-4361.236668	1.12781	-4645.274096	0.201364	0.182374	-4645.45647	-16.9
C_2	-4646.479122	-4361.231697	1.128589	-4645.267924	0.198544	0.181073	-4645.448997	-12.2
D_3	-2949.870117	-2949.515134	0.973858	-2948.834703	0.150306	0.140188	-2948.974892	-22.2
C_{1A}	-3705.408162	-3420.476486	1.108414	-3704.225599	0.178613	0.164981	-3704.39058	-13.0
$TS2_A$	-3705.40331	-3420.473732	1.1081	-3704.221735	0.177879	0.163927	-3704.385662	-9.9
D_1	-3705.418278	-3420.496708	1.10827	-3704.236493	0.176704	0.16337	-3704.399863	-18.8
C_{2A}	-3705.403443	-3420.469105	1.107684	-3704.220963	0.182467	0.166845	-3704.387809	-11.2
$TS4_A$	-3705.400509	-3420.468202	1.1074	-3704.219165	0.179329	0.164761	-3704.383925	-8.8
D_2	-3705.436957	-3420.511334	1.108333	-3704.25533	0.177104	0.163378	-3704.418708	-30.6
F	-1638.451569	-1353.539851	0.431584	-1637.988987	0.092755	0.085474	-1638.074461	-45.9
$TS3_{PRC}$	-2949.467799	-2949.115524	0.961342	-2948.444789	0.150891	0.140566	-2948.585355	-26.9
TS3	-2949.464313	-2949.113982	0.961568	-2948.442051	0.149127	0.138924	-2948.580975	-24.2
$TS3_{Prod}$	-2949.523312	-2949.174606	0.965874	-2948.497189	0.148421	0.137988	-2948.635177	-58.2

- ## Cartesian Coordinates

A

	Atom	X	Y	Z
1	Rh	-0.0405	0.0000	-1.1945
2	O	1.3924	1.4825	-1.1621

3	O	1.3921	-1.4830	-1.1624
4	O	1.4838	1.4584	1.0954
5	O	1.4831	-1.4589	1.0951
6	C	1.8482	1.8935	-0.0440
7	C	2.9014	3.0032	-0.0940
8	C	2.2549	4.2326	-0.7666
9	H	1.9077	3.9922	-1.7752
10	H	2.9876	5.0441	-0.8324
11	H	1.4006	4.5928	-0.1819
12	C	3.3773	3.3723	1.3165
13	H	2.5459	3.7371	1.9265
14	H	4.1293	4.1662	1.2492
15	H	3.8237	2.5160	1.8271
16	C	4.0946	2.5181	-0.9762
17	H	3.7335	2.4043	-2.0029
18	H	4.8382	3.3234	-0.9786
19	C	4.7254	1.2244	-0.5143
20	C	5.7927	1.2109	0.3931
21	H	6.2127	2.1501	0.7431
22	C	6.3260	0.0001	0.8380
23	H	7.1623	0.0001	1.5315
24	C	5.7927	-1.2107	0.3931
25	H	6.2126	-2.1499	0.7432
26	C	4.7255	-1.2242	-0.5143
27	C	4.2209	0.0001	-0.9689
28	H	3.4066	0.0001	-1.6849
29	C	4.0947	-2.5179	-0.9763
30	H	4.8382	-3.3233	-0.9787
31	H	3.7335	-2.4041	-2.0030
32	C	2.9015	-3.0031	-0.0939
33	C	3.3776	-3.3716	1.3167
34	H	3.8239	-2.5150	1.8269
35	H	4.1299	-4.1653	1.2496
36	H	2.5464	-3.7364	1.9268
37	C	2.2555	-4.2329	-0.7662
38	H	1.4013	-4.5932	-0.1814
39	H	2.9885	-5.0442	-0.8317
40	H	1.9083	-3.9930	-1.7749
41	C	1.8479	-1.8938	-0.0442
42	Rh	0.0405	-0.0000	1.1945
43	O	-1.3925	-1.4825	1.1621
44	O	-1.3921	1.4830	1.1624
45	O	-1.4838	-1.4584	-1.0954
46	O	-1.4831	1.4589	-1.0951
47	C	-1.8482	-1.8935	0.0440
48	C	-2.9014	-3.0032	0.0940
49	C	-2.2549	-4.2326	0.7667
50	H	-1.9077	-3.9922	1.7752
51	H	-2.9876	-5.0441	0.8324
52	H	-1.4006	-4.5928	0.1819
53	C	-3.3773	-3.3723	-1.3165
54	H	-2.5459	-3.7371	-1.9265
55	H	-4.1293	-4.1662	-1.2492

56	H	-3.8237	-2.5160	-1.8271
57	C	-4.0946	-2.5181	0.9762
58	H	-3.7335	-2.4043	2.0029
59	H	-4.8382	-3.3234	0.9786
60	C	-4.7254	-1.2244	0.5143
61	C	-5.7927	-1.2109	-0.3931
62	H	-6.2127	-2.1501	-0.7431
63	C	-6.3260	-0.0001	-0.8380
64	H	-7.1623	-0.0001	-1.5315
65	C	-5.7927	1.2107	-0.3931
66	H	-6.2126	2.1499	-0.7432
67	C	-4.7255	1.2242	0.5143
68	C	-4.2209	-0.0001	0.9689
69	H	-3.4066	-0.0001	1.6849
70	C	-4.0947	2.5179	0.9763
71	H	-4.8382	3.3233	0.9787
72	H	-3.7335	2.4041	2.0030
73	C	-2.9015	3.0031	0.0939
74	C	-3.3776	3.3716	-1.3167
75	H	-3.8239	2.5150	-1.8269
76	H	-4.1299	4.1653	-1.2496
77	H	-2.5464	3.7364	-1.9268
78	C	-2.2555	4.2329	0.7662
79	H	-1.4013	4.5932	0.1815
80	H	-2.9885	5.0442	0.8317
81	H	-1.9083	3.9930	1.7749
82	C	-1.8479	1.8938	0.0442

2b*

	Atom	X	Y	Z
1	I	0.6410	-0.3072	0.1219
2	O	2.7022	-1.8252	-0.3197
3	O	4.9351	-1.5950	-0.4703
4	O	-0.8018	1.9460	-1.7814
5	O	-2.2895	2.7556	-0.2614
6	C	2.4208	0.9402	0.2191
7	C	2.2897	2.2901	0.4793
8	H	1.3172	2.7385	0.6445
9	C	3.4522	3.0681	0.5258
10	H	3.3670	4.1305	0.7296
11	C	4.7040	2.4893	0.3126
12	H	5.5992	3.1002	0.3500
13	C	4.8073	1.1264	0.0502
14	H	5.7721	0.6632	-0.1176
15	C	3.6557	0.3267	-0.0011
16	C	3.7170	-1.1244	-0.2771
17	C	5.0475	-3.0129	-0.7476
18	H	4.4957	-3.2560	-1.6571
19	H	4.6543	-3.5860	0.0937
20	C	-0.6785	1.2764	0.4830
21	C	-1.2514	2.0118	-0.6554
22	C	-2.9473	3.5387	-1.2978
23	H	-3.2867	2.8524	-2.0776
24	H	-2.2106	4.2203	-1.7317
25	N	-1.2140	1.3553	1.6735
26	N	-1.6665	1.4408	2.7073
27	F	-2.0930	-1.2474	1.3143
28	F	-2.3807	-0.7010	-0.9141
29	P	-2.7662	-2.0071	0.0107
30	F	-4.2030	-1.3357	0.3632
31	F	-3.3912	-2.7486	-1.2921
32	F	-3.1036	-3.2946	0.9429
33	F	-1.2818	-2.6414	-0.3317
34	H	6.1129	-3.1907	-0.8775
35	C	-4.0948	4.2736	-0.6384
36	H	-4.6189	4.8748	-1.3882
37	H	-4.8077	3.5687	-0.2000
38	H	-3.7314	4.9418	0.1485

1a

	Atom	X	Y	Z
1	C	-1.8764	-1.3845	0.1174
2	O	-1.6817	-1.6132	1.2943
3	O	-2.2161	-2.3479	-0.7657
4	H	-2.2754	-3.1852	-0.2654
5	C	-1.8072	-0.0207	-0.5325
6	H	-1.5842	-0.1353	-1.5967
7	H	-2.8093	0.4229	-0.4664
8	C	-0.7901	0.9028	0.1699
9	C	-0.8704	2.3016	-0.3952
10	C	-1.2399	3.3746	0.3040
11	H	-1.2821	4.3630	-0.1458
12	H	-1.5124	3.3032	1.3551
13	H	-0.5996	2.4093	-1.4458
14	C	0.6253	0.3488	0.0672
15	C	1.3508	0.0472	1.2251
16	C	2.6505	-0.4562	1.1451
17	C	3.2452	-0.6654	-0.1005
18	C	2.5302	-0.3686	-1.2634
19	C	1.2312	0.1339	-1.1786
20	H	0.6885	0.3598	-2.0929
21	H	2.9835	-0.5285	-2.2377
22	H	4.2561	-1.0577	-0.1656
23	H	3.1963	-0.6869	2.0558
24	H	0.8884	0.2018	2.1961
25	H	-1.0637	0.9405	1.2289

3a

	Atom	X	Y	Z
1	O	1.4789	1.4917	0.5984
2	C	0.7663	2.0333	-0.4352
3	O	1.1547	3.0726	-0.9147
4	C	-0.4980	1.3097	-0.8451
5	H	-1.1227	2.0238	-1.3851
6	H	-0.2332	0.5058	-1.5432
7	C	-1.2271	0.7085	0.3792
8	C	-2.5415	0.0602	-0.0072
9	C	-2.5761	-1.0477	-0.8656
10	C	-3.7906	-1.6305	-1.2267
11	C	-4.9916	-1.1121	-0.7353
12	C	-4.9679	-0.0086	0.1186
13	C	-3.7496	0.5718	0.4784
14	H	-3.7357	1.4307	1.1445
15	H	-5.8958	0.4015	0.5069
16	H	-5.9375	-1.5662	-1.0161
17	H	-3.7991	-2.4893	-1.8918
18	H	-1.6501	-1.4617	-1.2565
19	C	-0.2590	-0.2663	1.0439
20	C	0.4367	0.0427	2.3337
21	H	0.7179	-0.7830	2.9783
22	H	0.1991	0.9789	2.8305
23	C	1.1939	0.1782	1.0352
24	C	2.2189	-0.8488	0.6825
25	O	2.1798	-1.9891	1.1101
26	O	3.1370	-0.3825	-0.1683
27	C	4.1529	-1.3297	-0.5922
28	C	5.0731	-0.6018	-1.5500
29	H	5.8571	-1.2843	-1.8939
30	H	4.5209	-0.2408	-2.4234
31	H	5.5488	0.2534	-1.0600
32	H	4.6801	-1.6906	0.2954
33	H	3.6554	-2.1827	-1.0626
34	H	-0.4051	-1.3169	0.8132
35	H	-1.4457	1.5269	1.0736

PF_6^-

	Atom	X	Y	Z
1	P	0.0000	0.0000	0.0000
2	F	-0.0000	-0.0000	1.6362
3	F	-0.0000	1.6362	-0.0000
4	F	-1.6362	-0.0000	-0.0000
5	F	-0.0000	-0.0000	-1.6362
6	F	-0.0000	-1.6362	0.0000
7	F	1.6362	-0.0000	0.0000

HPF_6

	Atom	X	Y	Z
1	P	0.2674	-0.0028	-0.0000
2	F	0.0239	0.0094	1.5756
3	F	-0.1807	-1.5417	-0.0039
4	F	1.8240	-0.1667	-0.0006
5	F	0.0236	0.0176	-1.5755
6	F	0.1316	1.5824	0.0041
7	F	-2.0082	0.1819	0.0005
8	H	-2.3389	-0.7048	-0.0016

PF_5

	Atom	X	Y	Z
1	P	0.0001	-0.0000	-0.0003
2	F	-1.6000	0.0016	0.0001
3	F	0.0004	-0.0089	1.5682
4	F	0.0016	1.3636	-0.7760
5	F	1.6001	-0.0017	-0.0006
6	F	-0.0023	-1.3547	-0.7913

HF

	Atom	X	Y	Z
1	F	0.0000	0.0000	0.0937
2	H	0.0000	0.0000	-0.8436

N_2

	Atom	X	Y	Z
1	N	-0.0000	-0.0000	0.5525
2	N	0.0000	-0.0000	-0.5525

IAr

	Atom	X	Y	Z
1	I	1.8354	-0.6788	-0.0612
2	O	-1.1084	-1.7229	0.7619
3	O	-2.8426	-0.8488	-0.3850
4	C	0.3246	0.8600	0.0373
5	C	0.7988	2.1704	-0.0159
6	H	1.8641	2.3621	-0.0671
7	C	-0.1007	3.2375	-0.0068
8	H	0.2792	4.2540	-0.0396
9	C	-1.4733	2.9950	0.0369
10	H	-2.1784	3.8198	0.0401
11	C	-1.9381	1.6849	0.0736
12	H	-3.0022	1.4839	0.1064
13	C	-1.0519	0.5924	0.0850
14	C	-1.6301	-0.7814	0.1987
15	C	-3.5200	-2.1128	-0.2595
16	H	-2.9342	-2.9050	-0.7311
17	H	-4.4727	-1.9827	-0.7713
18	H	-3.6777	-2.3567	0.7938

B

	Atom	X	Y	Z
1	C	4.5518	3.8940	2.5546
2	C	3.9069	4.3409	1.4052
3	C	3.2064	3.4547	0.5708
4	C	3.1771	2.1108	0.9548
5	C	3.7865	1.6440	2.1115
6	C	4.4910	2.5477	2.9096
7	I	2.1966	0.5329	-0.1579
8	C	0.1901	1.3816	-0.3497
9	Rh	-1.2031	-0.3115	0.0011
10	O	-2.5608	0.7117	1.1509
11	C	-3.5261	0.0778	1.6895
12	O	-3.7768	-1.1592	1.5239
13	Rh	-2.5138	-2.3025	0.3605
14	O	-1.3987	-2.6418	2.0673
15	C	-0.5030	-1.8003	2.3954
16	O	-0.1888	-0.7650	1.7228
17	C	2.5182	3.9743	-0.6427
18	O	2.3912	5.3022	-0.6268
19	C	1.6946	5.8771	-1.7540
20	C	-0.1500	2.4872	0.6102
21	O	0.2776	2.5391	1.7416
22	O	-0.9906	3.3426	0.0335
23	C	-1.4888	4.4394	0.8589
24	O	0.0976	-1.4194	-1.1299
25	C	-0.1524	-2.6579	-1.3401
26	O	-1.1325	-3.2876	-0.8392
27	C	0.8060	-3.4242	-2.2507
28	C	1.7950	-2.4747	-2.9382
29	C	1.5659	-4.4680	-1.3705
30	C	2.1826	-3.9075	-0.1086
31	C	3.4726	-3.3626	-0.0866
32	C	4.0093	-2.8726	1.1057
33	C	3.2548	-2.8884	2.2784
34	C	1.9510	-3.4021	2.2767
35	C	1.4425	-3.9217	1.0812
36	C	1.0829	-3.3754	3.5129
37	C	0.2691	-2.0538	3.6919
38	C	1.2012	-0.8761	4.0056
39	C	-0.0218	-4.1724	-3.3137
40	O	-2.3024	0.0267	-1.6972
41	C	-3.2194	-0.7956	-2.0296
42	O	-3.5446	-1.8303	-1.3665
43	C	-3.9925	-0.5126	-3.3196
44	C	-3.4081	0.6991	-4.0570
45	C	-5.4877	-0.2650	-2.9399
46	C	-5.6970	0.7850	-1.8732
47	C	-5.8150	2.1454	-2.1862
48	C	-5.9743	3.0913	-1.1718
49	C	-6.0128	2.6923	0.1657
50	C	-5.8955	1.3379	0.5040
51	C	-5.7510	0.4030	-0.5276

52	C	-5.8852	0.8721	1.9413
53	C	-4.4698	0.8648	2.6026
54	C	-3.9589	2.2956	2.8111
55	C	-3.9083	-1.7613	-4.2199
56	C	-0.7436	-2.2399	4.8381
57	C	-4.5556	0.1384	3.9590
58	O	2.0907	3.2721	-1.5450
59	N	-0.0320	1.6980	-1.6570
60	N	-0.3109	1.8453	-2.7316
61	F	4.8100	-0.2201	0.1194
62	H	-1.8116	4.0230	1.8139
63	H	-0.6532	5.1235	1.0317
64	H	0.8601	-5.2606	-1.1021
65	H	2.3367	-4.9188	-2.0058
66	H	4.0717	-3.3263	-0.9906
67	H	5.0147	-2.4716	1.1052
68	H	0.4431	-4.3458	1.0749
69	H	0.6459	-4.7686	-3.9445
70	H	-0.7526	-4.8384	-2.8483
71	H	-0.5576	-3.4663	-3.9587
72	H	2.4183	-3.0481	-3.6328
73	H	1.2686	-1.7032	-3.5092
74	H	2.4593	-1.9807	-2.2293
75	H	-6.0096	0.0155	-3.8620
76	H	-5.9124	-1.2148	-2.6005
77	H	-5.7981	2.4628	-3.2251
78	H	-6.0806	4.1425	-1.4250
79	H	-5.6713	-0.6498	-0.2764
80	H	-4.3111	-2.6412	-3.7119
81	H	-4.4820	-1.5924	-5.1375
82	H	-2.8699	-1.9696	-4.5020
83	H	-3.9875	0.8816	-4.9687
84	H	-3.4365	1.6001	-3.4408
85	H	-2.3678	0.5177	-4.3420
86	H	0.3733	-4.2081	3.4790
87	H	1.6929	-3.5014	4.4149
88	H	3.6835	-2.5123	3.2038
89	H	-0.2093	-2.4537	5.7701
90	H	-1.4277	-3.0663	4.6290
91	H	-1.3357	-1.3296	4.9869
92	H	1.7398	-1.0759	4.9384
93	H	0.6352	0.0524	4.1226
94	H	1.9316	-0.7230	3.2094
95	H	-6.5248	1.5138	2.5581
96	H	-6.2902	-0.1432	1.9968
97	H	-6.1499	3.4333	0.9485
98	H	-4.9029	-0.8902	3.8331
99	H	-5.2540	0.6674	4.6164
100	H	-3.5767	0.1154	4.4514
101	H	-4.6420	2.8329	3.4779
102	H	-3.8982	2.8388	1.8665
103	H	-2.9640	2.2910	3.2664
104	H	3.7336	0.5997	2.3909

105	H	3.9377	5.3879	1.1310
106	H	4.9810	2.1891	3.8087
107	H	5.0933	4.5994	3.1755
108	H	2.2270	5.6520	-2.6799
109	H	0.6799	5.4759	-1.8039
110	H	1.6802	6.9486	-1.5640
111	C	-2.6228	5.0849	0.0933
112	H	-3.0256	5.9177	0.6787
113	H	-2.2740	5.4750	-0.8681
114	H	-3.4276	4.3661	-0.0898
115	P	5.7651	-0.1681	-1.2546
116	F	4.4996	-0.7653	-2.1087
117	F	6.2575	-1.6900	-0.9348
118	F	6.6742	-0.1127	-2.5947
119	F	6.9769	0.4292	-0.3531
120	F	5.2118	1.3481	-1.5278

TS1

	Atom	X	Y	Z
1	C	4.2377	4.0382	2.6137
2	C	3.5883	4.4497	1.4531
3	C	2.9957	3.5199	0.5839
4	C	3.0697	2.1715	0.9464
5	C	3.6898	1.7374	2.1103
6	C	4.2897	2.6846	2.9429
7	I	2.1827	0.5710	-0.2007
8	C	0.0778	1.2153	-0.2071
9	Rh	-1.1518	-0.3622	-0.0102
10	O	-2.5215	0.7207	1.0681
11	C	-3.4886	0.1216	1.6463
12	O	-3.7524	-1.1174	1.5450
13	Rh	-2.4967	-2.3319	0.4378
14	O	-1.4132	-2.6265	2.1715
15	C	-0.5248	-1.7724	2.4761
16	O	-0.1889	-0.7750	1.7559
17	C	2.3297	3.9986	-0.6611
18	O	1.9532	5.2788	-0.5696
19	C	1.3081	5.8234	-1.7419
20	C	-0.1714	2.4421	0.6317
21	O	0.1520	2.4497	1.8014
22	O	-0.8500	3.3796	-0.0151
23	C	-1.3144	4.5264	0.7671
24	O	0.1486	-1.5312	-1.0654
25	C	-0.1157	-2.7762	-1.2245
26	O	-1.1061	-3.3727	-0.7068
27	C	0.8494	-3.5847	-2.0908
28	C	1.7999	-2.6611	-2.8639
29	C	1.6536	-4.5352	-1.1447
30	C	2.2417	-3.8704	0.0792
31	C	3.4948	-3.2451	0.0643
32	C	3.9994	-2.6532	1.2240
33	C	3.2509	-2.6549	2.4012
34	C	1.9843	-3.2535	2.4353
35	C	1.5071	-3.8666	1.2718
36	C	1.1173	-3.2248	3.6718
37	C	0.2243	-1.9480	3.7990
38	C	1.0801	-0.7108	4.1040
39	C	0.0323	-4.4376	-3.0797
40	O	-2.2267	-0.1118	-1.7364
41	C	-3.1639	-0.9319	-2.0282
42	O	-3.5106	-1.9187	-1.3102
43	C	-3.9326	-0.7064	-3.3322
44	C	-3.3242	0.4387	-4.1500
45	C	-5.4192	-0.3959	-2.9626
46	C	-5.5962	0.7163	-1.9550
47	C	-5.6560	2.0629	-2.3376
48	C	-5.7869	3.0649	-1.3742
49	C	-5.8554	2.7366	-0.0187
50	C	-5.7974	1.3973	0.3885
51	C	-5.6800	0.4062	-0.5927

52	C	-5.8199	1.0026	1.8466
53	C	-4.4114	0.9733	2.5223
54	C	-3.8532	2.3936	2.6793
55	C	-3.8869	-2.0120	-4.1514
56	C	-0.8025	-2.1647	4.9263
57	C	-4.5316	0.3037	3.9047
58	O	2.1326	3.3090	-1.6467
59	N	-0.0767	1.8404	-1.9088
60	N	-0.5159	1.7410	-2.9226
61	F	4.9362	-0.0142	0.0799
62	H	-1.6599	4.1577	1.7334
63	H	-0.4515	5.1798	0.9203
64	H	0.9826	-5.3394	-0.8255
65	H	2.4437	-4.9915	-1.7517
66	H	4.0911	-3.2233	-0.8414
67	H	4.9759	-2.1871	1.1944
68	H	0.5363	-4.3531	1.2940
69	H	0.7106	-5.0621	-3.6705
70	H	-0.6730	-5.0860	-2.5541
71	H	-0.5314	-3.8006	-3.7708
72	H	2.4348	-3.2681	-3.5182
73	H	1.2415	-1.9563	-3.4883
74	H	2.4518	-2.0893	-2.2040
75	H	-5.9352	-0.1525	-3.8984
76	H	-5.8694	-1.3130	-2.5705
77	H	-5.6176	2.3265	-3.3908
78	H	-5.8483	4.1051	-1.6818
79	H	-5.6464	-0.6350	-0.2875
80	H	-4.3063	-2.8474	-3.5852
81	H	-4.4649	-1.8866	-5.0732
82	H	-2.8566	-2.2632	-4.4282
83	H	-3.9085	0.5765	-5.0663
84	H	-3.3233	1.3784	-3.5943
85	H	-2.2926	0.2121	-4.4325
86	H	0.4590	-4.0995	3.6741
87	H	1.7326	-3.2759	4.5776
88	H	3.6573	-2.2041	3.3030
89	H	-0.2777	-2.3340	5.8726
90	H	-1.4392	-3.0285	4.7196
91	H	-1.4429	-1.2833	5.0457
92	H	1.5989	-0.8548	5.0579
93	H	0.4597	0.1871	4.1775
94	H	1.8247	-0.5370	3.3257
95	H	-6.4397	1.6972	2.4251
96	H	-6.2643	0.0073	1.9461
97	H	-5.9713	3.5214	0.7238
98	H	-4.9107	-0.7174	3.8164
99	H	-5.2180	0.8803	4.5340
100	H	-3.5580	0.2695	4.4070
101	H	-4.5216	2.9783	3.3206
102	H	-3.7689	2.8977	1.7150
103	H	-2.8612	2.3732	3.1404
104	H	3.7169	0.6866	2.3699

105	H	3.5381	5.5003	1.1948
106	H	4.7865	2.3544	3.8491
107	H	4.6973	4.7761	3.2623
108	H	1.9848	5.7807	-2.5973
109	H	0.4010	5.2564	-1.9603
110	H	1.0704	6.8538	-1.4841
111	C	-2.4172	5.1858	-0.0320
112	H	-2.7903	6.0550	0.5191
113	H	-2.0509	5.5262	-1.0055
114	H	-3.2480	4.4917	-0.1931
115	P	5.7695	-0.1580	-1.3562
116	F	4.4278	-0.8264	-2.0282
117	F	6.2650	-1.6431	-0.8935
118	F	6.5618	-0.2953	-2.7649
119	F	7.0673	0.5135	-0.6459
120	F	5.2183	1.3238	-1.7773

C_{N2}

	Atom	X	Y	Z
1	C	3.9711	4.1603	2.7998
2	C	3.3440	4.5385	1.6152
3	C	2.8422	3.5791	0.7221
4	C	2.9834	2.2368	1.0886
5	C	3.5872	1.8317	2.2699
6	C	4.0944	2.8112	3.1276
7	I	2.1652	0.6277	-0.0988
8	C	0.1045	1.1021	0.1744
9	Rh	-1.1089	-0.3704	0.0093
10	O	-2.4637	0.5745	1.2195
11	C	-3.4373	-0.0842	1.7196
12	O	-3.7143	-1.2954	1.4581
13	Rh	-2.4867	-2.3645	0.1780
14	O	-1.4324	-2.9567	1.8423
15	C	-0.5237	-2.1813	2.2646
16	O	-0.1671	-1.0958	1.6938
17	C	2.2124	4.0182	-0.5590
18	O	1.7559	5.2743	-0.4876
19	C	1.1479	5.7806	-1.6965
20	C	-0.1728	2.3075	1.0136
21	O	0.0110	2.2962	2.2146
22	O	-0.7063	3.2728	0.2827
23	C	-1.2246	4.4534	0.9822
24	O	0.1833	-1.3932	-1.1888
25	C	-0.1070	-2.5949	-1.5361
26	O	-1.1131	-3.2400	-1.1174
27	C	0.8450	-3.2774	-2.5167
28	C	1.8310	-2.2672	-3.1195
29	C	1.6063	-4.3969	-1.7345
30	C	2.2065	-3.9510	-0.4210
31	C	3.4703	-3.3526	-0.3414
32	C	3.9814	-2.9463	0.8924
33	C	3.2303	-3.1135	2.0558
34	C	1.9550	-3.6911	2.0004
35	C	1.4694	-4.1153	0.7585
36	C	1.0854	-3.8267	3.2278
37	C	0.2245	-2.5604	3.5436
38	C	1.1093	-1.4003	4.0210
39	C	0.0118	-3.9259	-3.6391
40	O	-2.2060	0.1195	-1.6540
41	C	-3.1582	-0.6366	-2.0482
42	O	-3.5121	-1.7125	-1.4751
43	C	-3.9313	-0.2177	-3.3004
44	C	-3.3261	1.0395	-3.9354
45	C	-5.4178	0.0268	-2.8867
46	C	-5.5956	0.9916	-1.7378
47	C	-5.6735	2.3760	-1.9377
48	C	-5.8018	3.2394	-0.8483
49	C	-5.8471	2.7332	0.4522
50	C	-5.7696	1.3528	0.6773
51	C	-5.6580	0.5019	-0.4283

52	C	-5.7610	0.7699	2.0710
53	C	-4.3380	0.6624	2.7065
54	C	-3.7708	2.0549	3.0149
55	C	-3.8803	-1.3858	-4.3065
56	C	-0.8095	-2.9122	4.6301
57	C	-4.4273	-0.1663	4.0030
58	O	2.1177	3.3207	-1.5514
59	N	-0.2500	2.2993	-3.0555
60	N	0.3107	1.3628	-3.2230
61	F	4.9341	-0.0714	0.3873
62	H	-1.5837	4.1348	1.9614
63	H	-0.3821	5.1371	1.1094
64	H	0.9050	-5.2168	-1.5486
65	H	2.3844	-4.7783	-2.4053
66	H	4.0673	-3.2056	-1.2350
67	H	4.9631	-2.4923	0.9329
68	H	0.4904	-4.5835	0.7075
69	H	0.6780	-4.4608	-4.3239
70	H	-0.7163	-4.6330	-3.2341
71	H	-0.5267	-3.1643	-4.2147
72	H	2.4593	-2.7793	-3.8561
73	H	1.3011	-1.4547	-3.6251
74	H	2.4869	-1.8269	-2.3684
75	H	-5.9390	0.3917	-3.7791
76	H	-5.8603	-0.9383	-2.6218
77	H	-5.6486	2.7771	-2.9470
78	H	-5.8768	4.3105	-1.0139
79	H	-5.6130	-0.5703	-0.2649
80	H	-4.3084	-2.2954	-3.8778
81	H	-4.4483	-1.1193	-5.2040
82	H	-2.8479	-1.5963	-4.6081
83	H	-3.9311	1.3324	-4.8002
84	H	-3.2936	1.8750	-3.2334
85	H	-2.3080	0.8471	-4.2818
86	H	0.4057	-4.6756	3.1017
87	H	1.6960	-4.0252	4.1161
88	H	3.6401	-2.8048	3.0138
89	H	-0.2887	-3.2267	5.5406
90	H	-1.4651	-3.7232	4.3036
91	H	-1.4294	-2.0425	4.8756
92	H	1.6182	-1.6926	4.9458
93	H	0.5094	-0.5079	4.2233
94	H	1.8645	-1.1370	3.2783
95	H	-6.3688	1.3803	2.7485
96	H	-6.2007	-0.2322	2.0499
97	H	-5.9569	3.4112	1.2941
98	H	-4.8119	-1.1697	3.8037
99	H	-5.0973	0.3328	4.7111
100	H	-3.4425	-0.2592	4.4749
101	H	-4.4217	2.5582	3.7381
102	H	-3.7110	2.6708	2.1153
103	H	-2.7664	1.9831	3.4417
104	H	3.6678	0.7833	2.5268

105	H	3.2448	5.5853	1.3554
106	H	4.5765	2.5084	4.0511
107	H	4.3600	4.9216	3.4674
108	H	1.8880	5.8219	-2.4982
109	H	0.3202	5.1340	-1.9931
110	H	0.7942	6.7782	-1.4424
111	C	-2.3262	5.0305	0.1199
112	H	-2.7256	5.9289	0.6019
113	H	-1.9493	5.3081	-0.8689
114	H	-3.1401	4.3098	-0.0048
115	P	5.7769	0.0243	-1.0416
116	F	4.4785	-0.6349	-1.8096
117	F	6.3690	-1.4720	-0.7755
118	F	6.5726	0.1264	-2.4510
119	F	7.0267	0.6861	-0.2425
120	F	5.1246	1.5115	-1.2759

C_A

	Atom	X	Y	Z
1	C	0.1881	0.3663	-1.7696
2	C	-0.4587	1.1415	-2.8700
3	C	-1.0811	3.2504	-3.7750
4	H	-0.4307	3.1970	-4.6517
5	H	-2.0407	2.7918	-4.0189
6	C	1.0554	-1.1718	2.0330
7	C	2.2477	-1.9464	2.5967
8	C	3.0997	-0.9470	3.4462
9	H	2.5628	-0.7494	4.3791
10	H	4.0301	-1.4636	3.7074
11	C	3.3882	0.3648	2.7543
12	C	4.4559	0.5241	1.8611
13	H	5.1427	-0.2994	1.6863
14	C	4.6582	1.7455	1.2156
15	H	5.4922	1.8598	0.5300
16	C	2.5421	1.4561	2.9824
17	H	1.7194	1.3453	3.6829
18	C	1.7193	-3.0666	3.5130
19	H	2.5649	-3.6005	3.9590
20	H	1.0971	-2.6625	4.3150
21	H	1.1242	-3.7886	2.9424
22	C	3.0911	-2.5519	1.4712
23	H	3.9186	-3.1226	1.9053
24	H	2.4973	-3.2256	0.8482
25	H	3.5074	-1.7801	0.8259
26	C	-2.1022	-2.3406	0.7521
27	C	-2.6594	-3.7531	0.5898
28	C	-4.2147	-3.6731	0.7180
29	H	-4.6000	-4.6821	0.5335
30	H	-4.4565	-3.4152	1.7537
31	C	-4.8650	-2.6783	-0.2153
32	C	-5.2641	-3.0348	-1.5098
33	H	-5.1496	-4.0620	-1.8448
34	C	-5.8238	-2.0821	-2.3627
35	H	-6.1439	-2.3711	-3.3598
36	C	-5.0511	-1.3544	0.2007
37	H	-4.7645	-1.0734	1.2090
38	C	-2.1058	-4.6179	1.7411
39	H	-2.3747	-4.1991	2.7142
40	H	-2.5196	-5.6289	1.6676
41	H	-1.0139	-4.6930	1.6843
42	C	-2.2449	-4.3537	-0.7600
43	H	-2.6588	-5.3636	-0.8474
44	H	-2.6077	-3.7555	-1.5985
45	H	-1.1554	-4.4221	-0.8358
46	O	1.0326	-0.9532	0.7710
47	O	0.1687	-0.7837	2.8529
48	O	-1.4508	-1.8471	-0.2344
49	O	-2.3109	-1.7368	1.8478
50	O	-0.4531	2.4527	-2.7160
51	Rh	-0.5910	-0.0168	-0.0652

52	Rh	-1.5358	0.1450	2.1673
53	O	-0.9118	0.5048	-3.8033
54	C	-0.0387	2.4746	1.4459
55	C	0.5597	3.8774	1.5674
56	C	1.7395	3.8032	2.5920
57	H	1.3126	3.6854	3.5931
58	H	2.2432	4.7759	2.5644
59	C	2.7221	2.6842	2.3368
60	C	3.7982	2.8199	1.4498
61	H	3.9751	3.7715	0.9565
62	C	-0.5205	4.8313	2.1107
63	H	-0.0924	5.8310	2.2377
64	H	-0.9023	4.4886	3.0754
65	H	-1.3614	4.9067	1.4123
66	C	1.0551	4.3742	0.2019
67	H	1.4426	5.3928	0.3097
68	H	0.2416	4.3871	-0.5282
69	H	1.8523	3.7418	-0.1938
70	O	0.2118	1.8430	0.3641
71	O	-0.7213	2.0168	2.4105
72	C	-3.2231	1.2349	0.0745
73	C	-4.4580	1.9321	-0.4985
74	C	-5.7045	1.0489	-0.1733
75	H	-6.5696	1.5391	-0.6337
76	H	-5.8581	1.0641	0.9100
77	C	-5.5910	-0.3811	-0.6482
78	C	-5.9828	-0.7622	-1.9380
79	H	-6.4248	-0.0276	-2.6055
80	C	-4.6070	3.2928	0.2126
81	H	-4.7060	3.1650	1.2935
82	H	-5.4982	3.8058	-0.1637
83	H	-3.7385	3.9322	0.0162
84	C	-4.3155	2.1500	-2.0096
85	H	-5.2227	2.6277	-2.3941
86	H	-4.1617	1.2110	-2.5448
87	H	-3.4687	2.8070	-2.2223
88	O	-2.3092	0.8836	-0.7484
89	O	-3.1842	1.0490	1.3291
90	I	2.3744	0.6167	-1.8938
91	C	2.7369	-1.5341	-1.9183
92	C	4.0538	-1.9805	-1.8029
93	C	1.6510	-2.3793	-2.0491
94	C	4.2656	-3.3688	-1.8161
95	C	1.8949	-3.7569	-2.0602
96	H	0.6395	-2.0000	-2.1242
97	C	3.1953	-4.2489	-1.9443
98	H	5.2797	-3.7380	-1.7252
99	H	1.0549	-4.4361	-2.1636
100	H	3.3765	-5.3180	-1.9558
101	C	5.1833	-1.0280	-1.6655
102	O	5.0458	0.1883	-1.7746
103	O	6.3424	-1.6146	-1.4085
104	C	7.4891	-0.7423	-1.2678

105	H	7.6429	-0.1792	-2.1899
106	H	7.3316	-0.0572	-0.4329
107	H	8.3276	-1.4073	-1.0724
108	C	-1.2248	4.6595	-3.2448
109	H	-1.6821	5.2883	-4.0152
110	H	-1.8648	4.6809	-2.3570
111	H	-0.2499	5.0829	-2.9859

C

	Atom	X	Y	Z
1	C	-0.3875	-0.3038	-1.2981
2	C	-0.3896	-1.4030	-2.2981
3	C	-0.3940	-3.6930	-2.8576
4	H	-1.3263	-3.5868	-3.4139
5	H	0.4534	-3.5321	-3.5281
6	C	0.0076	1.8186	2.2095
7	C	-0.8594	2.9492	2.7697
8	C	-1.8735	2.3153	3.7815
9	H	-1.3396	2.1193	4.7169
10	H	-2.6298	3.0800	3.9934
11	C	-2.5154	1.0324	3.3060
12	C	-3.6059	1.0106	2.4254
13	H	-4.0602	1.9414	2.0979
14	C	-4.1113	-0.2056	1.9628
15	H	-4.9369	-0.2223	1.2574
16	C	-1.9666	-0.1877	3.7151
17	H	-1.1209	-0.1808	4.3981
18	C	0.0341	3.9577	3.5123
19	H	-0.5900	4.7401	3.9571
20	H	0.6043	3.4708	4.3070
21	H	0.7396	4.4355	2.8231
22	C	-1.6096	3.6570	1.6356
23	H	-2.2039	4.4795	2.0475
24	H	-0.9138	4.0700	0.8997
25	H	-2.2805	2.9690	1.1224
26	C	3.0639	1.8675	0.2548
27	C	3.9491	3.0095	-0.2456
28	C	5.4241	2.4975	-0.2847
29	H	6.0330	3.3170	-0.6830
30	H	5.7491	2.3191	0.7448
31	C	5.6266	1.2436	-1.1031
32	C	5.8957	1.2970	-2.4769
33	H	6.0068	2.2606	-2.9667
34	C	6.0379	0.1203	-3.2140
35	H	6.2606	0.1712	-4.2762
36	C	5.5152	-0.0111	-0.4924
37	H	5.3252	-0.0624	0.5746
38	C	3.8490	4.1627	0.7752
39	H	4.1644	3.8373	1.7699
40	H	4.4922	4.9895	0.4556
41	H	2.8212	4.5379	0.8417
42	C	3.4972	3.5001	-1.6241
43	H	4.1684	4.2960	-1.9642
44	H	3.5072	2.6970	-2.3646
45	H	2.4839	3.9041	-1.5734
46	O	-0.2660	1.4149	1.0271
47	O	0.9213	1.3419	2.9487
48	O	2.1178	1.4575	-0.5035
49	O	3.3238	1.3950	1.4025
50	O	-0.3798	-2.6317	-1.8488
51	Rh	0.8687	-0.0411	0.1307

52	Rh	2.1736	-0.1128	2.1892
53	O	-0.3123	-1.0298	-3.4621
54	C	0.1041	-2.0656	2.1677
55	C	-0.7312	-3.2497	2.6620
56	C	-1.7729	-2.6890	3.6900
57	H	-1.2519	-2.5102	4.6364
58	H	-2.5024	-3.4879	3.8651
59	C	-2.4621	-1.4152	3.2617
60	C	-3.5476	-1.4121	2.3791
61	H	-3.9467	-2.3436	1.9966
62	C	0.1894	-4.2508	3.3836
63	H	-0.4132	-5.0745	3.7811
64	H	0.7248	-3.7785	4.2109
65	H	0.9257	-4.6728	2.6902
66	C	-1.4356	-3.9476	1.4915
67	H	-2.0102	-4.7968	1.8782
68	H	-0.7022	-4.3294	0.7754
69	H	-2.1046	-3.2843	0.9497
70	O	-0.1807	-1.5966	1.0165
71	O	1.0071	-1.6116	2.9367
72	C	3.0718	-1.9228	0.0812
73	C	3.9425	-3.0221	-0.5312
74	C	5.4239	-2.5286	-0.5273
75	H	6.0225	-3.3103	-1.0087
76	H	5.7558	-2.4561	0.5130
77	C	5.6318	-1.2016	-1.2198
78	C	5.9025	-1.1219	-2.5919
79	H	6.0177	-2.0338	-3.1713
80	C	3.8247	-4.2707	0.3670
81	H	4.1459	-4.0528	1.3890
82	H	4.4530	-5.0724	-0.0353
83	H	2.7905	-4.6326	0.3982
84	C	3.4799	-3.3590	-1.9545
85	H	4.1161	-4.1508	-2.3645
86	H	3.5360	-2.4909	-2.6146
87	H	2.4467	-3.7138	-1.9516
88	O	2.1475	-1.4357	-0.6536
89	O	3.3221	-1.5699	1.2751
90	I	-2.3121	0.7384	-1.2985
91	C	-1.4216	2.5839	-1.9615
92	C	-2.1031	3.7874	-1.7480
93	C	-0.2163	2.5258	-2.6438
94	C	-1.5133	4.9721	-2.2126
95	C	0.3383	3.7181	-3.1194
96	H	0.2862	1.5822	-2.8169
97	C	-0.3010	4.9375	-2.8960
98	H	-2.0297	5.9099	-2.0472
99	H	1.2716	3.6799	-3.6700
100	H	0.1362	5.8586	-3.2660
101	C	-3.4308	3.7990	-1.0887
102	O	-4.0857	2.7782	-0.8924
103	O	-3.8379	5.0106	-0.7310
104	C	-5.1304	5.0860	-0.0867

105	H	-5.9028	4.6946	-0.7511
106	H	-5.1141	4.5132	0.8425
107	H	-5.2869	6.1444	0.1122
108	P	-4.1129	-2.5957	-1.4669
109	F	-5.2804	-3.2736	-2.3641
110	F	-3.3096	-2.1339	-2.8255
111	F	-2.9155	-1.8759	-0.5692
112	F	-4.9149	-1.1629	-1.4665
113	F	-3.2716	-3.9909	-1.4459
114	F	-4.8724	-3.0220	-0.0892
115	C	-0.3132	-5.0105	-2.1206
116	H	-0.3106	-5.8281	-2.8490
117	H	0.6037	-5.0760	-1.5262
118	H	-1.1767	-5.1265	-1.4639

C_1

	Atom	X	Y	Z
1	C	-3.9449	-0.7754	-1.2049
2	C	-4.7844	-1.3703	-2.3384
3	C	-5.5342	-2.6193	-1.7756
4	H	-6.2990	-2.2688	-1.0755
5	H	-6.0529	-3.0888	-2.6192
6	C	-4.6391	-3.6175	-1.0796
7	C	-3.9894	-4.6446	-1.7765
8	H	-4.1601	-4.7646	-2.8427
9	C	-3.1417	-5.5262	-1.1032
10	H	-2.6530	-6.3287	-1.6485
11	C	-4.4204	-3.5034	0.2978
12	H	-4.9284	-2.7179	0.8484
13	C	-5.8224	-0.3189	-2.7771
14	H	-6.4589	-0.7379	-3.5638
15	H	-6.4545	-0.0154	-1.9388
16	H	-5.3283	0.5730	-3.1792
17	C	-3.8975	-1.7558	-3.5302
18	H	-4.5230	-2.1767	-4.3249
19	H	-3.3771	-0.8798	-3.9287
20	H	-3.1438	-2.4948	-3.2519
21	C	-2.7962	2.6260	-0.6039
22	C	-3.0040	3.9316	-1.3739
23	C	-2.9257	5.1090	-0.3524
24	H	-3.0209	6.0369	-0.9279
25	H	-3.7939	5.0442	0.3104
26	C	-1.6611	5.1273	0.4738
27	C	-0.5015	5.7771	0.0328
28	H	-0.5109	6.3182	-0.9093
29	C	0.6584	5.7510	0.8079
30	H	1.5404	6.2818	0.4661
31	C	-1.6248	4.4590	1.7033
32	H	-2.5238	3.9678	2.0614
33	C	-4.4163	3.8993	-1.9925
34	H	-5.1825	3.7775	-1.2225
35	H	-4.6016	4.8366	-2.5279
36	H	-4.5095	3.0750	-2.7086
37	C	-1.9560	4.0940	-2.4764
38	H	-2.1210	5.0411	-3.0017
39	H	-0.9428	4.0934	-2.0735
40	H	-2.0268	3.2821	-3.2037
41	O	-2.6762	-0.8070	-1.3527
42	O	-4.5541	-0.2971	-0.1995
43	O	-1.7977	1.8944	-0.9252
44	O	-3.6348	2.3540	0.3071
45	Rh	-3.4807	0.5849	1.3380
46	C	-2.2693	-1.9242	2.0224
47	C	-2.0963	-3.2402	2.7878
48	C	-3.3188	-4.1550	2.4620
49	H	-4.2087	-3.7079	2.9159
50	H	-3.1416	-5.1131	2.9640
51	C	-3.5611	-4.3667	0.9863

52	C	-2.9265	-5.3888	0.2693
53	H	-2.2752	-6.0867	0.7884
54	C	-2.0994	-2.9218	4.2963
55	H	-2.0009	-3.8514	4.8670
56	H	-3.0260	-2.4241	4.5932
57	H	-1.2570	-2.2713	4.5583
58	C	-0.7807	-3.9261	2.4071
59	H	-0.7005	-4.8830	2.9342
60	H	0.0662	-3.3032	2.6991
61	H	-0.7097	-4.1054	1.3342
62	O	-1.3960	-1.6433	1.1385
63	O	-3.2712	-1.2032	2.3192
64	C	-0.9910	1.4946	2.5389
65	C	-0.0751	2.1091	3.6005
66	C	-0.4664	3.6105	3.7709
67	H	0.2388	4.0454	4.4884
68	H	-1.4624	3.6547	4.2232
69	C	-0.4630	4.4000	2.4821
70	C	0.6829	5.0615	2.0215
71	H	1.5886	5.0504	2.6219
72	C	-0.3206	1.3684	4.9298
73	H	-1.3697	1.4319	5.2303
74	H	0.2981	1.8124	5.7170
75	H	-0.0488	0.3102	4.8401
76	C	1.3978	1.9694	3.1906
77	H	2.0348	2.3563	3.9940
78	H	1.6209	2.5242	2.2771
79	H	1.6586	0.9244	3.0084
80	O	-0.4196	1.0809	1.4765
81	O	-2.2380	1.4344	2.7692
82	Rh	-1.4716	0.1000	0.0335
83	C	0.1307	-0.4082	-0.8785
84	C	0.2429	-1.5850	-1.7759
85	O	0.2792	-2.7688	-1.2134
86	C	0.2222	-3.9179	-2.1306
87	O	0.1446	-1.3339	-2.9689
88	H	0.9471	-3.7415	-2.9232
89	H	-0.7888	-3.9427	-2.5446
90	C	0.5411	-5.1551	-1.3241
91	H	-0.1732	-5.2867	-0.5084
92	H	0.4769	-6.0281	-1.9823
93	H	1.5542	-5.1062	-0.9204
94	C	2.0268	3.5178	-2.1914
95	C	1.4879	2.2249	-2.2376
96	C	0.7156	1.7824	-3.3001
97	C	0.4606	2.6659	-4.3538
98	C	0.9650	3.9650	-4.3308
99	C	1.7404	4.3874	-3.2556
100	I	1.9604	0.8212	-0.6509
101	C	2.9427	3.9307	-1.1029
102	O	3.3018	5.2116	-1.1568
103	C	4.2587	5.6386	-0.1621
104	O	3.3588	3.1544	-0.2502

105	H	0.3282	0.7717	-3.3311
106	H	-0.1384	2.3233	-5.1915
107	H	0.7624	4.6461	-5.1503
108	H	2.1539	5.3882	-3.2307
109	H	5.1890	5.0788	-0.2770
110	H	3.8547	5.4796	0.8395
111	H	4.4163	6.6981	-0.3546
112	C	2.2255	-2.2523	1.6421
113	O	1.6561	-1.2517	1.2208
114	O	2.6083	-3.2680	0.8739
115	H	2.5331	-2.9999	-0.0727
116	C	2.6418	-2.4114	3.0823
117	H	2.1486	-1.6299	3.6649
118	H	2.3369	-3.3900	3.4651
119	C	4.1959	-2.2840	3.1976
120	C	4.5934	-2.2181	4.6496
121	C	5.3226	-3.1468	5.2680
122	H	5.5820	-3.0620	6.3198
123	H	5.6899	-4.0260	4.7427
124	H	4.2380	-1.3541	5.2105
125	C	4.6844	-1.1028	2.3694
126	C	5.1864	-1.3397	1.0848
127	C	5.5384	-0.2823	0.2449
128	C	5.4018	1.0331	0.6889
129	C	4.9015	1.2819	1.9707
130	C	4.5443	0.2222	2.8043
131	H	4.1391	0.4344	3.7891
132	H	4.7726	2.3046	2.3122
133	H	5.6579	1.8626	0.0384
134	H	5.8832	-0.4976	-0.7606
135	H	5.2685	-2.3559	0.7175
136	H	4.6225	-3.1937	2.7635
137	F	2.9752	-2.1403	-1.5072
138	P	3.9987	-2.7332	-2.6988
139	F	4.9796	-3.3109	-3.8518
140	F	2.8087	-2.4885	-3.7872
141	F	4.5355	-1.2115	-2.9400
142	F	5.1469	-2.9622	-1.5632
143	F	3.4100	-4.2276	-2.3937

TS2

	Atom	X	Y	Z
1	C	3.6649	-0.7709	-1.5003
2	C	4.5284	-0.5262	-2.7418
3	C	5.8688	0.1277	-2.2816
4	H	6.4289	-0.6149	-1.7049
5	H	6.4479	0.3455	-3.1862
6	C	5.6915	1.3798	-1.4545
7	C	5.6227	2.6492	-2.0429
8	H	5.7421	2.7514	-3.1181
9	C	5.4201	3.7823	-1.2533
10	H	5.3818	4.7641	-1.7165
11	C	5.5576	1.2798	-0.0646
12	H	5.6238	0.3028	0.4019
13	C	4.8335	-1.8945	-3.3841
14	H	5.4789	-1.7549	-4.2580
15	H	5.3386	-2.5574	-2.6768
16	H	3.9106	-2.3823	-3.7184
17	C	3.8032	0.3710	-3.7521
18	H	4.4354	0.5053	-4.6367
19	H	2.8553	-0.0748	-4.0656
20	H	3.5880	1.3546	-3.3304
21	C	1.2663	-3.3874	-0.7683
22	C	0.8239	-4.5997	-1.5938
23	C	0.3101	-5.6903	-0.6020
24	H	-0.0953	-6.5094	-1.2070
25	H	1.1706	-6.0840	-0.0523
26	C	-0.7234	-5.1922	0.3800
27	C	-2.0904	-5.1724	0.0753
28	H	-2.4387	-5.5615	-0.8774
29	C	-3.0087	-4.6757	1.0011
30	H	-4.0673	-4.6957	0.7663
31	C	-0.3106	-4.7059	1.6256
32	H	0.7457	-4.7284	1.8743
33	C	2.0538	-5.1473	-2.3447
34	H	2.8531	-5.4173	-1.6503
35	H	1.7676	-6.0374	-2.9156
36	H	2.4435	-4.4033	-3.0487
37	C	-0.2657	-4.2208	-2.5972
38	H	-0.5594	-5.1069	-3.1706
39	H	-1.1501	-3.8193	-2.1024
40	H	0.0978	-3.4655	-3.2971
41	O	2.5281	-0.1924	-1.4562
42	O	4.1362	-1.5356	-0.6034
43	O	0.6268	-2.2906	-0.9165
44	O	2.2460	-3.5646	0.0176
45	Rh	3.0037	-1.9747	1.0715
46	C	3.0875	0.7977	1.8988
47	C	3.6368	2.0174	2.6476
48	C	5.1244	2.2281	2.2269
49	H	5.7027	1.3686	2.5792
50	H	5.4862	3.1104	2.7673
51	C	5.3301	2.4017	0.7403

52	C	5.2704	3.6610	0.1293
53	H	5.1163	4.5481	0.7377
54	C	3.5861	1.7034	4.1570
55	H	3.9847	2.5520	4.7233
56	H	4.1774	0.8148	4.3936
57	H	2.5545	1.5305	4.4849
58	C	2.8059	3.2699	2.3502
59	H	3.2457	4.1316	2.8639
60	H	1.7839	3.1456	2.7118
61	H	2.7620	3.4849	1.2816
62	O	2.0553	0.9710	1.1700
63	O	3.6932	-0.3052	2.0637
64	C	0.5547	-1.8283	2.6390
65	C	-0.3792	-2.0960	3.8239
66	C	-0.6971	-3.6238	3.8612
67	H	-1.4276	-3.7793	4.6635
68	H	0.2173	-4.1545	4.1451
69	C	-1.2151	-4.1839	2.5571
70	C	-2.5776	-4.1787	2.2323
71	H	-3.3027	-3.8015	2.9482
72	C	0.3551	-1.7055	5.1209
73	H	1.2880	-2.2647	5.2292
74	H	-0.2842	-1.9181	5.9846
75	H	0.5910	-0.6350	5.1281
76	C	-1.6685	-1.2758	3.6880
77	H	-2.3124	-1.4606	4.5552
78	H	-2.2212	-1.5308	2.7819
79	H	-1.4441	-0.2077	3.6445
80	O	0.0803	-1.1137	1.6959
81	O	1.7216	-2.3280	2.6660
82	Rh	1.2378	-0.5905	0.0973
83	C	-0.1498	0.5581	-0.6528
84	C	0.1621	1.5468	-1.7265
85	O	0.6974	2.6788	-1.3023
86	C	1.3379	3.5190	-2.3264
87	O	0.1024	1.1699	-2.8828
88	H	0.5759	3.7686	-3.0619
89	H	2.1193	2.9140	-2.7893
90	C	1.8943	4.7326	-1.6186
91	H	2.6282	4.4425	-0.8626
92	H	2.3967	5.3693	-2.3543
93	H	1.0937	5.3123	-1.1537
94	C	-3.6513	-2.3274	-2.1701
95	C	-2.6066	-1.3913	-2.2000
96	C	-1.7976	-1.2183	-3.3097
97	C	-2.0251	-2.0212	-4.4325
98	C	-3.0341	-2.9822	-4.4283
99	C	-3.8409	-3.1318	-3.3048
100	I	-2.3029	-0.1256	-0.4620
101	C	-4.5861	-2.4078	-1.0247
102	O	-5.4684	-3.4009	-1.1192
103	C	-6.4876	-3.4435	-0.0955
104	O	-4.5705	-1.6115	-0.0924

105	H	-1.0069	-0.4801	-3.3159
106	H	-1.3963	-1.8876	-5.3069
107	H	-3.2015	-3.6061	-5.2997
108	H	-4.6449	-3.8575	-3.2931
109	H	-7.0765	-2.5245	-0.1210
110	H	-6.0306	-3.5601	0.8889
111	H	-7.1025	-4.3067	-0.3422
112	C	-0.7475	2.7687	1.5334
113	O	-0.7603	1.6263	1.0511
114	O	-0.6009	3.8792	0.8501
115	H	-0.6038	3.6864	-0.1146
116	C	-0.9749	2.9719	3.0071
117	H	-0.8515	2.0076	3.5034
118	H	-0.2323	3.6732	3.3982
119	C	-2.3991	3.5515	3.2762
120	C	-2.6312	3.6235	4.7642
121	C	-2.7933	4.7610	5.4395
122	H	-2.9560	4.7682	6.5137
123	H	-2.7732	5.7278	4.9406
124	H	-2.6524	2.6733	5.2970
125	C	-3.4571	2.7497	2.5311
126	C	-3.9577	3.2530	1.3269
127	C	-4.8716	2.5218	0.5675
128	C	-5.3068	1.2747	1.0150
129	C	-4.8113	0.7599	2.2177
130	C	-3.8913	1.4906	2.9698
131	H	-3.5118	1.0719	3.8965
132	H	-5.1321	-0.2191	2.5607
133	H	-6.0056	0.6908	0.4248
134	H	-5.2055	2.9209	-0.3845
135	H	-3.6085	4.2085	0.9557
136	H	-2.4090	4.5705	2.8761
137	F	-2.1806	3.0388	-1.2114
138	P	-2.6040	4.2035	-2.3155
139	F	-2.9872	5.3520	-3.3952
140	F	-1.7179	3.4194	-3.4425
141	F	-3.9132	3.3200	-2.7180
142	F	-3.4673	4.9749	-1.1653
143	F	-1.2646	5.0449	-1.8551

D

	Atom	X	Y	Z
1	C	3.2239	-1.8723	-1.5157
2	C	4.2234	-1.8322	-2.6769
3	C	5.6632	-1.7765	-2.0737
4	H	5.8728	-2.7436	-1.6066
5	H	6.3595	-1.6598	-2.9122
6	C	5.8679	-0.6756	-1.0590
7	C	6.2679	0.6136	-1.4341
8	H	6.4867	0.8279	-2.4767
9	C	6.4036	1.6183	-0.4738
10	H	6.7262	2.6116	-0.7733
11	C	5.6258	-0.9297	0.2960
12	H	5.3298	-1.9285	0.5989
13	C	4.0715	-3.1346	-3.4874
14	H	4.8032	-3.1489	-4.3025
15	H	4.2324	-4.0118	-2.8556
16	H	3.0705	-3.2044	-3.9282
17	C	3.9709	-0.6248	-3.5841
18	H	4.6844	-0.6353	-4.4153
19	H	2.9585	-0.6521	-3.9976
20	H	4.0926	0.3108	-3.0373
21	C	-0.0825	-3.3282	-1.2484
22	C	-0.9234	-4.1089	-2.2630
23	C	-1.7255	-5.2023	-1.4922
24	H	-2.3386	-5.7318	-2.2306
25	H	-1.0122	-5.9226	-1.0805
26	C	-2.5953	-4.6583	-0.3829
27	C	-3.9297	-4.2986	-0.6070
28	H	-4.3696	-4.4437	-1.5900
29	C	-4.7008	-3.7708	0.4292
30	H	-5.7400	-3.5201	0.2466
31	C	-2.0617	-4.4775	0.8991
32	H	-1.0361	-4.7732	1.0882
33	C	0.0472	-4.7982	-3.2441
34	H	0.7398	-5.4587	-2.7160
35	H	-0.5218	-5.3914	-3.9683
36	H	0.6315	-4.0551	-3.7987
37	C	-1.8677	-3.1835	-3.0320
38	H	-2.4447	-3.7681	-3.7572
39	H	-2.5660	-2.6769	-2.3652
40	H	-1.3085	-2.4177	-3.5745
41	O	2.3845	-0.9163	-1.4158
42	O	3.3098	-2.8644	-0.7276
43	O	-0.2411	-2.0628	-1.1790
44	O	0.7271	-4.0080	-0.5445
45	Rh	1.9556	-3.0647	0.8096
46	C	3.0303	-0.7107	2.1396
47	C	3.9465	0.0192	3.1290
48	C	5.4252	-0.2589	2.7117
49	H	5.6355	-1.3166	2.8971
50	H	6.0625	0.3245	3.3863
51	C	5.7439	0.0672	1.2712

52	C	6.1393	1.3502	0.8705
53	H	6.2584	2.1346	1.6130
54	C	3.7085	-0.5748	4.5320
55	H	4.3752	-0.0913	5.2543
56	H	3.9012	-1.6504	4.5417
57	H	2.6754	-0.4054	4.8571
58	C	3.6646	1.5237	3.1561
59	H	4.3571	2.0120	3.8501
60	H	2.6481	1.7135	3.5092
61	H	3.7817	1.9802	2.1720
62	O	2.2333	-0.0134	1.4223
63	O	3.1353	-1.9736	2.1002
64	C	-0.3624	-2.2093	2.3572
65	C	-1.4370	-2.3201	3.4441
66	C	-2.1666	-3.6902	3.2916
67	H	-2.9249	-3.7364	4.0818
68	H	-1.4410	-4.4852	3.4888
69	C	-2.8088	-3.9164	1.9416
70	C	-4.1430	-3.5689	1.6927
71	H	-4.7481	-3.1542	2.4945
72	C	-0.7196	-2.2890	4.8099
73	H	0.0027	-3.1056	4.8938
74	H	-1.4549	-2.3866	5.6160
75	H	-0.1880	-1.3403	4.9486
76	C	-2.4345	-1.1593	3.3520
77	H	-3.1775	-1.2548	4.1522
78	H	-2.9582	-1.1440	2.3943
79	H	-1.9263	-0.1992	3.4675
80	O	-0.4001	-1.1796	1.6048
81	O	0.4991	-3.1391	2.2838
82	Rh	0.9562	-0.9577	0.0830
83	C	0.1549	0.8472	-0.4363
84	C	0.5350	1.3924	-1.7908
85	O	1.6926	2.0839	-1.7519
86	C	2.2649	2.5390	-3.0344
87	O	-0.0069	1.0765	-2.8235
88	H	1.5400	3.2228	-3.4688
89	H	2.3695	1.6527	-3.6573
90	C	3.5871	3.1980	-2.7168
91	H	4.2566	2.5153	-2.1850
92	H	4.0684	3.4889	-3.6563
93	H	3.4348	4.0994	-2.1182
94	C	-4.6932	-0.6242	-1.6970
95	C	-3.4297	-0.0471	-1.9182
96	C	-2.8717	0.0339	-3.1859
97	C	-3.5697	-0.5042	-4.2704
98	C	-4.8058	-1.1183	-4.0805
99	C	-5.3612	-1.1692	-2.8063
100	I	-2.3184	0.7869	-0.2594
101	C	-5.3639	-0.6048	-0.3707
102	O	-6.5646	-1.1991	-0.3841
103	C	-7.2913	-1.1604	0.8601
104	O	-4.9006	-0.0745	0.6266

105	H	-1.8985	0.4812	-3.3266
106	H	-3.1298	-0.4453	-5.2609
107	H	-5.3437	-1.5442	-4.9209
108	H	-6.3339	-1.6180	-2.6490
109	H	-7.4872	-0.1253	1.1480
110	H	-6.7192	-1.6559	1.6473
111	H	-8.2218	-1.6909	0.6655
112	C	0.9368	2.6331	1.1587
113	O	0.1355	1.7301	0.6975
114	O	1.9657	3.0766	0.5512
115	H	2.0218	2.7368	-0.4048
116	C	0.5953	3.2064	2.4843
117	H	0.3006	2.4000	3.1584
118	H	1.4973	3.6833	2.8689
119	C	-0.5343	4.2844	2.3729
120	C	-0.4865	5.1590	3.6048
121	C	-0.2530	6.4705	3.5600
122	H	-0.2427	7.0801	4.4592
123	H	-0.0730	6.9795	2.6156
124	H	-0.6768	4.6622	4.5563
125	C	-1.9298	3.7041	2.1990
126	C	-2.7941	4.2837	1.2623
127	C	-4.1109	3.8393	1.1423
128	C	-4.5837	2.8090	1.9572
129	C	-3.7290	2.2247	2.8936
130	C	-2.4130	2.6723	3.0157
131	H	-1.7669	2.2115	3.7583
132	H	-4.0822	1.4132	3.5221
133	H	-5.6021	2.4495	1.8531
134	H	-4.7649	4.2951	0.4041
135	H	-2.4253	5.0667	0.6124
136	H	-0.3120	4.9097	1.5079
137	F	-0.5426	3.8312	-0.7909
138	P	-0.3698	5.2008	-1.7083
139	F	-0.1825	6.5376	-2.6084
140	F	-0.3754	4.2675	-3.0522
141	F	-1.9922	5.3315	-1.7890
142	F	-0.3647	6.1014	-0.3370
143	F	1.2558	5.0292	-1.5882

C_{c1}

	Atom	X	Y	Z
1	C	3.9481	0.2467	1.3475
2	C	4.8139	-0.0214	2.5815
3	C	5.9423	-1.0195	2.1676
4	H	6.6304	-0.4942	1.4978
5	H	6.4987	-1.2692	3.0783
6	C	5.4411	-2.2733	1.4900
7	C	5.0522	-3.4043	2.2194
8	H	5.1570	-3.4102	3.3008
9	C	4.5472	-4.5279	1.5628
10	H	4.2583	-5.4044	2.1360
11	C	5.3234	-2.3054	0.0958
12	H	5.6351	-1.4390	-0.4791
13	C	5.4577	1.3080	3.0215
14	H	6.1102	1.1318	3.8833
15	H	6.0525	1.7442	2.2150
16	H	4.6915	2.0333	3.3186
17	C	3.9694	-0.5953	3.7271
18	H	4.6108	-0.7708	4.5976
19	H	3.1777	0.1021	4.0164
20	H	3.4996	-1.5391	3.4448
21	C	1.9296	3.1296	0.3720
22	C	1.6673	4.4780	1.0474
23	C	1.2588	5.4947	-0.0648
24	H	0.9916	6.4298	0.4407
25	H	2.1394	5.6967	-0.6823
26	C	0.1263	5.0254	-0.9472
27	C	-1.2163	5.2263	-0.6017
28	H	-1.4666	5.7678	0.3062
29	C	-2.2333	4.7538	-1.4319
30	H	-3.2685	4.9425	-1.1681
31	C	0.4147	4.3466	-2.1365
32	H	1.4525	4.1989	-2.4187
33	C	2.9792	4.9534	1.7025
34	H	3.7821	5.0354	0.9658
35	H	2.8226	5.9348	2.1628
36	H	3.2980	4.2574	2.4869
37	C	0.5698	4.3615	2.1076
38	H	0.4016	5.3415	2.5672
39	H	-0.3708	4.0121	1.6810
40	H	0.8609	3.6606	2.8936
41	O	2.7333	-0.1451	1.4015
42	O	4.4871	0.8316	0.3590
43	O	1.1552	2.1561	0.6670
44	O	2.8981	3.0679	-0.4433
45	Rh	3.3574	1.2695	-1.3222
46	C	2.9692	-1.5324	-1.8835
47	C	3.2493	-2.8752	-2.5633
48	C	4.6484	-3.3730	-2.0801
49	H	5.4096	-2.7121	-2.5062
50	H	4.7994	-4.3684	-2.5131
51	C	4.8072	-3.4178	-0.5786

52	C	4.4212	-4.5352	0.1727
53	H	4.0351	-5.4166	-0.3317
54	C	3.3017	-2.6407	-4.0864
55	H	3.5238	-3.5854	-4.5942
56	H	4.0730	-1.9120	-4.3480
57	H	2.3379	-2.2737	-4.4576
58	C	2.1569	-3.8987	-2.2357
59	H	2.4054	-4.8571	-2.7043
60	H	1.1932	-3.5678	-2.6299
61	H	2.0469	-4.0522	-1.1613
62	O	1.9764	-1.4742	-1.0839
63	O	3.7440	-0.5654	-2.1577
64	C	0.8538	1.3026	-2.8024
65	C	-0.0845	1.5312	-3.9900
66	C	-0.2146	3.0718	-4.2116
67	H	-0.9621	3.2195	-4.9995
68	H	0.7414	3.4438	-4.5941
69	C	-0.5924	3.8467	-2.9703
70	C	-1.9273	4.0631	-2.6058
71	H	-2.7272	3.7053	-3.2480
72	C	0.5509	0.8934	-5.2403
73	H	1.5430	1.3084	-5.4357
74	H	-0.0862	1.0804	-6.1113
75	H	0.6472	-0.1915	-5.1166
76	C	-1.4590	0.9006	-3.7230
77	H	-2.0903	1.0197	-4.6104
78	H	-1.9640	1.3706	-2.8770
79	H	-1.3702	-0.1643	-3.4956
80	O	0.3236	0.7957	-1.7596
81	O	2.0759	1.6282	-2.9155
82	Rh	1.4578	0.2823	-0.1484
83	C	-0.0216	-0.5061	0.7621
84	C	0.1206	-1.5898	1.7828
85	O	0.2657	-1.0836	2.9880
86	C	0.3725	-2.0241	4.1115
87	O	0.2265	-2.7741	1.5039
88	H	1.3672	-2.4718	4.0626
89	H	-0.3901	-2.7883	3.9679
90	C	0.1501	-1.2137	5.3682
91	H	-0.8568	-0.7873	5.3656
92	H	0.2493	-1.8675	6.2405
93	H	0.8858	-0.4074	5.4547
94	C	-3.1057	2.7576	1.8444
95	C	-2.1644	1.7234	1.9365
96	C	-1.3396	1.5787	3.0388
97	C	-1.4470	2.5014	4.0832
98	C	-2.3564	3.5554	4.0124
99	C	-3.1798	3.6816	2.8983
100	I	-2.0480	0.2820	0.3202
101	C	-4.0469	2.8239	0.7069
102	O	-4.8388	3.8926	0.7147
103	C	-5.8471	3.9413	-0.3202
104	O	-4.1072	1.9511	-0.1538

105	H	-0.6275	0.7718	3.1084
106	H	-0.8053	2.3854	4.9509
107	H	-2.4316	4.2709	4.8241
108	H	-3.9066	4.4821	2.8334
109	H	-6.5166	3.0843	-0.2244
110	H	-5.3770	3.9334	-1.3053
111	H	-6.3822	4.8738	-0.1523
112	C	-1.1938	-3.0116	-1.4886
113	O	-1.0627	-1.8042	-1.2861
114	O	-0.8555	-3.9438	-0.6167
115	H	-0.4904	-3.5001	0.1974
116	C	-1.8016	-3.5778	-2.7450
117	H	-1.6463	-2.8750	-3.5666
118	H	-1.3124	-4.5262	-2.9829
119	C	-3.3253	-3.8287	-2.5299
120	C	-3.8778	-4.6318	-3.6828
121	C	-4.3986	-5.8526	-3.5616
122	H	-4.7862	-6.3954	-4.4194
123	H	-4.4593	-6.3526	-2.5971
124	H	-3.8325	-4.1591	-4.6637
125	C	-4.0738	-2.5186	-2.3370
126	C	-4.6415	-2.2050	-1.0976
127	C	-5.3290	-1.0027	-0.9180
128	C	-5.4617	-0.1028	-1.9758
129	C	-4.8858	-0.4017	-3.2126
130	C	-4.1960	-1.6004	-3.3895
131	H	-3.7475	-1.8170	-4.3554
132	H	-4.9713	0.2983	-4.0392
133	H	-5.9875	0.8347	-1.8302
134	H	-5.7408	-0.7717	0.0582
135	H	-4.5279	-2.8835	-0.2594
136	H	-3.4327	-4.4255	-1.6176
137	F	-2.6407	-2.7206	1.3840
138	P	-3.4990	-2.5865	2.7786
139	F	-4.3370	-2.4465	4.1670
140	F	-2.4858	-1.3798	3.2663
141	F	-4.4628	-1.4617	2.0772
142	F	-4.4938	-3.7722	2.2665
143	F	-2.5082	-3.6870	3.4758

C₂

	Atom	X	Y	Z
1	C	3.4120	-1.6457	0.8033
2	C	4.9118	-1.3390	0.8392
3	C	5.3570	-1.2523	2.3322
4	H	5.2472	-2.2445	2.7806
5	H	6.4255	-1.0087	2.3321
6	C	4.5836	-0.2387	3.1430
7	C	5.0001	1.0943	3.2502
8	H	5.9280	1.4076	2.7796
9	C	4.2351	2.0167	3.9656
10	H	4.5711	3.0464	4.0511
11	C	3.3961	-0.6197	3.7780
12	H	3.0753	-1.6542	3.7192
13	C	5.6435	-2.5150	0.1603
14	H	6.7240	-2.3389	0.1885
15	H	5.4287	-3.4593	0.6675
16	H	5.3417	-2.6083	-0.8895
17	C	5.2267	-0.0317	0.1022
18	H	6.3071	0.1477	0.1327
19	H	4.9148	-0.0893	-0.9419
20	H	4.7198	0.8209	0.5571
21	C	1.3153	-3.4999	-1.5595
22	C	1.6245	-4.2667	-2.8467
23	C	0.5644	-5.4041	-2.9925
24	H	0.7502	-5.8916	-3.9563
25	H	0.7538	-6.1453	-2.2099
26	C	-0.8704	-4.9374	-2.9032
27	C	-1.5786	-4.5055	-4.0318
28	H	-1.1063	-4.5376	-5.0098
29	C	-2.8956	-4.0584	-3.9079
30	H	-3.4456	-3.7478	-4.7924
31	C	-1.5142	-4.9108	-1.6600
32	H	-0.9783	-5.2579	-0.7826
33	C	3.0228	-4.9005	-2.7024
34	H	3.0677	-5.5612	-1.8329
35	H	3.2548	-5.4842	-3.5996
36	H	3.7921	-4.1278	-2.5908
37	C	1.6005	-3.3329	-4.0634
38	H	1.8108	-3.9116	-4.9691
39	H	0.6323	-2.8416	-4.1802
40	H	2.3661	-2.5577	-3.9679
41	O	2.6627	-0.8125	0.1918
42	O	3.0084	-2.7042	1.3735
43	O	1.0182	-2.2615	-1.6788
44	O	1.3655	-4.1352	-0.4648
45	Rh	0.9962	-3.1396	1.3124
46	C	0.3372	-0.7873	2.8788
47	C	0.0554	-0.0223	4.1755
48	C	1.3061	-0.1618	5.1009
49	H	1.3945	-1.2109	5.3992
50	H	1.0905	0.4183	6.0053
51	C	2.6058	0.2952	4.4834

52	C	3.0432	1.6228	4.5754
53	H	2.4540	2.3453	5.1333
54	C	-1.1423	-0.7019	4.8728
55	H	-1.3313	-0.2013	5.8288
56	H	-0.9334	-1.7577	5.0662
57	H	-2.0411	-0.6141	4.2621
58	C	-0.2619	1.4525	3.9068
59	H	-0.4311	1.9579	4.8644
60	H	-1.1616	1.5568	3.3045
61	H	0.5626	1.9543	3.3977
62	O	0.2941	-0.1472	1.7725
63	O	0.6138	-2.0225	2.9897
64	C	-1.7709	-2.6805	0.5865
65	C	-3.2692	-2.9953	0.5797
66	C	-3.4463	-4.3745	-0.1364
67	H	-4.5244	-4.5625	-0.1927
68	H	-3.0105	-5.1507	0.5002
69	C	-2.8259	-4.4448	-1.5124
70	C	-3.5155	-4.0244	-2.6576
71	H	-4.5426	-3.6814	-2.5714
72	C	-3.7423	-3.1223	2.0425
73	H	-3.1475	-3.8584	2.5896
74	H	-4.7904	-3.4415	2.0527
75	H	-3.6785	-2.1552	2.5466
76	C	-4.0829	-1.9106	-0.1296
77	H	-5.1421	-2.1917	-0.1050
78	H	-3.7835	-1.8011	-1.1704
79	H	-3.9742	-0.9470	0.3644
80	O	-1.3572	-1.6530	-0.0526
81	O	-1.0180	-3.4893	1.2126
82	Rh	0.6386	-1.1285	-0.0097
83	C	0.4495	0.4180	-1.1098
84	C	1.0320	0.5818	-2.4763
85	O	2.3518	0.4844	-2.5198
86	C	2.9439	0.4909	-3.8578
87	O	0.2977	0.6914	-3.4440
88	H	2.6619	1.4249	-4.3501
89	H	2.5070	-0.3384	-4.4175
90	C	4.4403	0.3553	-3.6934
91	H	4.6968	-0.5904	-3.2069
92	H	4.9119	0.3748	-4.6810
93	H	4.8467	1.1802	-3.1004
94	C	-3.7931	2.0031	-1.7614
95	C	-2.6064	1.2698	-1.7835
96	C	-2.4536	0.1040	-2.5110
97	C	-3.5252	-0.3216	-3.3022
98	C	-4.7190	0.3980	-3.3291
99	C	-4.8576	1.5428	-2.5500
100	I	-0.9448	2.0240	-0.5787
101	C	-3.9328	3.1936	-0.8898
102	O	-5.1781	3.6267	-0.7720
103	C	-5.4039	4.6361	0.2408
104	O	-2.9734	3.7179	-0.3304

105	H	-1.5498	-0.4830	-2.4736
106	H	-3.4157	-1.2379	-3.8724
107	H	-5.5478	0.0582	-3.9410
108	H	-5.7885	2.0968	-2.5353
109	H	-4.7831	5.5127	0.0485
110	H	-5.1742	4.2062	1.2168
111	H	-6.4609	4.8839	0.1616
112	C	4.2409	5.9356	-1.5152
113	O	3.6251	6.8641	-1.0334
114	O	5.2070	6.1014	-2.4441
115	H	5.2902	7.0621	-2.6020
116	C	4.0636	4.4800	-1.1475
117	H	4.2547	3.8594	-2.0282
118	H	4.8464	4.2272	-0.4203
119	C	2.6807	4.1961	-0.5371
120	C	2.6123	2.7626	-0.0587
121	C	2.2025	2.3959	1.1607
122	H	1.8897	3.1328	1.8965
123	H	2.1825	1.3583	1.4667
124	H	2.9321	1.9979	-0.7632
125	C	1.5448	4.4807	-1.5103
126	C	0.4789	5.3016	-1.1245
127	C	-0.6158	5.4942	-1.9687
128	C	-0.6606	4.8637	-3.2141
129	C	0.4056	4.0560	-3.6161
130	C	1.5012	3.8731	-2.7713
131	H	2.3248	3.2443	-3.0946
132	H	0.3825	3.5609	-4.5820
133	H	-1.5157	5.0052	-3.8686
134	H	-1.4381	6.1263	-1.6480
135	H	0.5043	5.7843	-0.1515
136	H	2.5527	4.8572	0.3254
137	F	-3.0354	2.5051	2.2606
138	P	-4.0702	1.2600	2.5103
139	F	-2.8590	0.1992	2.1744
140	F	-3.6664	1.2351	4.0905
141	F	-5.2738	2.3257	2.8183
142	F	-4.4705	1.2843	0.9145
143	F	-5.0946	0.0104	2.7386

D_3

	Atom	X	Y	Z
1	C	-1.5139	-0.9405	2.1846
2	C	-2.6015	-0.6950	3.2331
3	C	-3.7599	-1.7101	2.9561
4	H	-3.4337	-2.6967	3.3000
5	H	-4.6065	-1.4095	3.5837
6	C	-4.1728	-1.8058	1.5064
7	C	-5.1015	-0.9299	0.9302
8	H	-5.5927	-0.1803	1.5441
9	C	-5.4233	-1.0375	-0.4248
10	H	-6.1667	-0.3721	-0.8559
11	C	-3.5879	-2.7847	0.6953
12	H	-2.8747	-3.4750	1.1368
13	C	-2.0234	-0.9638	4.6343
14	H	-2.8099	-0.8328	5.3851
15	H	-1.6316	-1.9807	4.7111
16	H	-1.2131	-0.2630	4.8640
17	C	-3.1171	0.7472	3.1516
18	H	-3.8856	0.9036	3.9158
19	H	-2.3094	1.4649	3.3269
20	H	-3.5514	0.9599	2.1744
21	C	1.9309	0.1384	2.0889
22	C	2.7746	0.9401	3.0830
23	C	4.2335	0.3866	3.0532
24	H	4.8164	0.9863	3.7611
25	H	4.2148	-0.6396	3.4322
26	C	4.8828	0.4114	1.6884
27	C	5.6557	1.4990	1.2624
28	H	5.8278	2.3337	1.9366
29	C	6.2156	1.5090	-0.0167
30	H	6.8247	2.3511	-0.3331
31	C	4.6987	-0.6621	0.8080
32	H	4.1273	-1.5218	1.1393
33	C	2.1806	0.7042	4.4881
34	H	2.1865	-0.3584	4.7448
35	H	2.7719	1.2485	5.2321
36	H	1.1485	1.0693	4.5415
37	C	2.7486	2.4370	2.7539
38	H	3.3732	2.9777	3.4729
39	H	3.1247	2.6365	1.7490
40	H	1.7306	2.8304	2.8220
41	O	-1.4109	-0.0804	1.2439
42	O	-0.8011	-1.9837	2.2990
43	O	1.2977	0.7844	1.1870
44	O	1.9065	-1.1224	2.2380
45	Rh	0.7627	-2.2865	0.9869
46	C	-1.0515	-2.6967	-1.2334
47	C	-1.9100	-3.4699	-2.2367
48	C	-3.1908	-3.9623	-1.4852
49	H	-2.9004	-4.7876	-0.8274
50	H	-3.8658	-4.3735	-2.2444
51	C	-3.8907	-2.9034	-0.6652

52	C	-4.8229	-2.0164	-1.2201
53	H	-5.0977	-2.1065	-2.2671
54	C	-1.1208	-4.6938	-2.7359
55	H	-1.7463	-5.2799	-3.4174
56	H	-0.8157	-5.3331	-1.9040
57	H	-0.2223	-4.3826	-3.2809
58	C	-2.2910	-2.5742	-3.4248
59	H	-2.8987	-3.1502	-4.1308
60	H	-1.3972	-2.2225	-3.9502
61	H	-2.8618	-1.6998	-3.1060
62	O	-1.0309	-1.4265	-1.3673
63	O	-0.4370	-3.3397	-0.3304
64	C	2.4562	-1.5220	-1.2579
65	C	3.6219	-1.6710	-2.2383
66	C	4.9442	-1.8117	-1.4216
67	H	5.7568	-1.9200	-2.1488
68	H	4.8922	-2.7428	-0.8492
69	C	5.2277	-0.6568	-0.4881
70	C	5.9957	0.4436	-0.8914
71	H	6.4331	0.4591	-1.8859
72	C	3.3887	-2.9696	-3.0393
73	H	3.3326	-3.8360	-2.3750
74	H	4.2146	-3.1193	-3.7427
75	H	2.4577	-2.9118	-3.6147
76	C	3.6966	-0.4737	-3.1944
77	H	4.5296	-0.6176	-3.8908
78	H	3.8622	0.4595	-2.6513
79	H	2.7752	-0.3759	-3.7754
80	O	1.7066	-0.4938	-1.3894
81	O	2.2983	-2.4302	-0.3873
82	Rh	0.0949	-0.2382	-0.1363
83	C	-0.5942	1.2464	-1.2104
84	C	0.3407	2.0822	-2.0287
85	O	1.3629	2.4948	-1.3945
86	C	2.4218	3.2619	-2.1027
87	O	0.2707	2.2548	-3.3041
88	H	1.9257	4.1175	-2.5634
89	H	2.8153	2.5993	-2.8748
90	C	3.4417	3.6422	-1.0610
91	H	3.8935	2.7567	-0.6094
92	H	4.2323	4.2220	-1.5476
93	H	2.9896	4.2588	-0.2796
94	C	-2.6627	1.9599	-2.3846
95	O	-1.8900	1.2223	-1.4658
96	O	-2.2710	2.1608	-3.5099
97	H	-0.6582	2.0494	-3.6434
98	C	-3.9440	2.3678	-1.7452
99	H	-4.4306	3.0862	-2.4079
100	H	-4.5876	1.4830	-1.6649
101	C	-3.6902	2.9399	-0.3154
102	C	-4.9169	3.6855	0.1520
103	C	-5.6685	3.3087	1.1856
104	H	-6.5415	3.8787	1.4900

105	H	-5.4354	2.4222	1.7697
106	H	-5.1705	4.5829	-0.4115
107	C	-2.4388	3.8100	-0.2755
108	C	-1.4139	3.5146	0.6378
109	C	-0.2475	4.2826	0.6699
110	C	-0.0843	5.3479	-0.2177
111	C	-1.0937	5.6416	-1.1379
112	C	-2.2641	4.8784	-1.1655
113	H	-3.0405	5.1210	-1.8858
114	H	-0.9742	6.4664	-1.8338
115	H	0.8226	5.9450	-0.1950
116	H	0.5382	4.0326	1.3745
117	H	-1.5295	2.6754	1.3172
118	H	-3.5253	2.0871	0.3464

C1A

	Atom	X	Y	Z
1	C	-3.6927	-0.2568	-1.3291
2	C	-4.5708	-0.7406	-2.4844
3	C	-5.4610	-1.9070	-1.9445
4	H	-6.2187	-1.4761	-1.2827
5	H	-5.9851	-2.3336	-2.8072
6	C	-4.6990	-2.9764	-1.1978
7	C	-4.0740	-4.0438	-1.8563
8	H	-4.1752	-4.1476	-2.9330
9	C	-3.3463	-4.9894	-1.1316
10	H	-2.8793	-5.8233	-1.6482
11	C	-4.5811	-2.8901	0.1939
12	H	-5.0734	-2.0735	0.7138
13	C	-5.4816	0.4177	-2.9338
14	H	-6.1479	0.0699	-3.7301
15	H	-6.0898	0.7860	-2.1041
16	H	-4.8889	1.2517	-3.3264
17	C	-3.7069	-1.2127	-3.6619
18	H	-4.3571	-1.5516	-4.4754
19	H	-3.0807	-0.3978	-4.0380
20	H	-3.0515	-2.0360	-3.3737
21	C	-2.0007	2.8962	-0.7560
22	C	-1.9306	4.1793	-1.5833
23	C	-1.5685	5.3492	-0.6122
24	H	-1.4208	6.2409	-1.2317
25	H	-2.4334	5.5377	0.0313
26	C	-0.3532	5.0885	0.2462
27	C	0.9460	5.3561	-0.2035
28	H	1.0980	5.8047	-1.1810
29	C	2.0455	5.0666	0.6058
30	H	3.0470	5.2904	0.2530
31	C	-0.5166	4.5344	1.5212
32	H	-1.5210	4.3388	1.8847
33	C	-3.3222	4.4425	-2.1910
34	H	-4.0861	4.5182	-1.4133
35	H	-3.3011	5.3807	-2.7553
36	H	-3.6055	3.6382	-2.8793
37	C	-0.8863	4.0565	-2.6970
38	H	-0.8632	4.9858	-3.2764
39	H	0.1095	3.8728	-2.2951
40	H	-1.1310	3.2340	-3.3755
41	O	-2.4388	-0.4931	-1.4217
42	O	-4.2546	0.3314	-0.3558
43	O	-1.1273	1.9902	-0.9904
44	O	-2.9141	2.8053	0.1187
45	Rh	-3.1188	1.0755	1.2043
46	C	-2.3877	-1.5604	2.0440
47	C	-2.4342	-2.8494	2.8669
48	C	-3.7096	-3.6408	2.4296
49	H	-4.5871	-3.1092	2.8111
50	H	-3.6699	-4.6121	2.9356
51	C	-3.8459	-3.8218	0.9358

52	C	-3.2312	-4.8806	0.2555
53	H	-2.6759	-5.6299	0.8126
54	C	-2.5570	-2.4771	4.3566
55	H	-2.6333	-3.3910	4.9550
56	H	-3.4425	-1.8635	4.5398
57	H	-1.6741	-1.9223	4.6937
58	C	-1.1681	-3.6844	2.6381
59	H	-1.2156	-4.5896	3.2526
60	H	-0.2737	-3.1211	2.9183
61	H	-1.0724	-3.9780	1.5918
62	O	-1.4599	-1.4710	1.1729
63	O	-3.2689	-0.6748	2.2622
64	C	-0.5892	1.5531	2.5465
65	C	0.3478	2.0147	3.6642
66	C	0.3301	3.5776	3.6856
67	H	1.0897	3.8942	4.4092
68	H	-0.6423	3.9013	4.0701
69	C	0.5739	4.2221	2.3408
70	C	1.8639	4.4988	1.8684
71	H	2.7248	4.2899	2.4976
72	C	-0.1956	1.4865	5.0059
73	H	-1.2172	1.8321	5.1821
74	H	0.4413	1.8416	5.8228
75	H	-0.1919	0.3907	5.0235
76	C	1.7728	1.4909	3.4353
77	H	2.4074	1.8060	4.2707
78	H	2.2043	1.8775	2.5103
79	H	1.7884	0.3983	3.3819
80	O	-0.0406	0.9958	1.5349
81	O	-1.8344	1.7552	2.6773
82	Rh	-1.1722	0.2135	0.0219
83	C	0.3373	-0.6869	-0.7137
84	C	0.2438	-2.0401	-1.3348
85	O	0.1260	-1.9321	-2.6465
86	C	-0.1416	-3.1652	-3.3984
87	O	0.1991	-3.0801	-0.6985
88	H	-1.0685	-3.5890	-3.0044
89	H	0.6783	-3.8600	-3.2037
90	C	-0.2445	-2.7756	-4.8553
91	H	0.6907	-2.3296	-5.2076
92	H	-0.4472	-3.6704	-5.4520
93	H	-1.0590	-2.0625	-5.0118
94	C	3.3415	2.4394	-1.5464
95	C	2.4414	1.3760	-1.6717
96	C	1.6279	1.2162	-2.7836
97	C	1.7050	2.1656	-3.8065
98	C	2.5772	3.2492	-3.7041
99	C	3.3883	3.3860	-2.5813
100	I	2.3748	-0.1167	-0.1172
101	C	4.2641	2.5226	-0.3886
102	O	4.9522	3.6560	-0.3316
103	C	5.8856	3.7853	0.7664
104	O	4.3915	1.6138	0.4289

105	H	0.9492	0.3768	-2.8739
106	H	1.0720	2.0503	-4.6802
107	H	2.6301	3.9837	-4.5001
108	H	4.0803	4.2150	-2.4963
109	H	6.6392	2.9978	0.7081
110	H	5.3515	3.7203	1.7159
111	H	6.3369	4.7671	0.6399
112	C	2.6045	-3.2374	1.6810
113	O	2.1841	-2.0990	1.8661
114	O	1.8640	-4.1926	1.1215
115	H	1.0511	-3.7746	0.7501
116	C	4.0053	-3.6909	1.9985
117	H	4.5450	-2.8499	2.4395
118	H	3.9655	-4.5035	2.7321
119	C	4.7234	-4.2120	0.7196
120	C	6.1230	-4.6599	1.0654
121	C	6.5568	-5.9134	0.9363
122	H	7.5719	-6.1953	1.2016
123	H	5.9119	-6.7041	0.5586
124	H	6.7955	-3.8943	1.4509
125	C	4.7103	-3.1765	-0.4013
126	C	3.8767	-3.3624	-1.5132
127	C	3.8771	-2.4506	-2.5727
128	C	4.7152	-1.3346	-2.5363
129	C	5.5351	-1.1275	-1.4237
130	C	5.5269	-2.0368	-0.3633
131	H	6.1738	-1.8588	0.4908
132	H	6.1819	-0.2566	-1.3782
133	H	4.7241	-0.6281	-3.3609
134	H	3.2304	-2.6195	-3.4290
135	H	3.2310	-4.2351	-1.5528
136	H	4.1627	-5.0842	0.3713

TS2$_A$

	Atom	X	Y	Z
1	C	-3.4967	-1.5767	0.6964
2	C	-4.5229	-2.0637	1.7233
3	C	-5.8884	-1.3753	1.4052
4	H	-6.2668	-1.7900	0.4657
5	H	-6.5867	-1.6684	2.1974
6	C	-5.8090	0.1292	1.2953
7	C	-5.9398	0.9615	2.4144
8	H	-6.1563	0.5271	3.3865
9	C	-5.8116	2.3454	2.2828
10	H	-5.9290	2.9842	3.1537
11	C	-5.5612	0.7184	0.0504
12	H	-5.4749	0.0830	-0.8252
13	C	-4.6801	-3.5886	1.5613
14	H	-5.4360	-3.9557	2.2636
15	H	-4.9898	-3.8470	0.5457
16	H	-3.7369	-4.1032	1.7777
17	C	-4.0659	-1.7370	3.1506
18	H	-4.8114	-2.1035	3.8642
19	H	-3.1101	-2.2205	3.3722
20	H	-3.9452	-0.6618	3.2966
21	C	-0.5357	-3.1814	-0.7034
22	C	0.0861	-4.5614	-0.4753
23	C	0.9053	-4.9313	-1.7522
24	H	1.4107	-5.8808	-1.5422
25	H	0.2005	-5.1096	-2.5700
26	C	1.9049	-3.8801	-2.1724
27	C	3.2028	-3.8394	-1.6471
28	H	3.5269	-4.6027	-0.9453
29	C	4.0889	-2.8360	-2.0405
30	H	5.1011	-2.8357	-1.6505
31	C	1.5275	-2.8976	-3.0947
32	H	0.5293	-2.9317	-3.5197
33	C	-1.0577	-5.5808	-0.3027
34	H	-1.7175	-5.5859	-1.1737
35	H	-0.6361	-6.5835	-0.1750
36	H	-1.6569	-5.3487	0.5850
37	C	0.9804	-4.5695	0.7651
38	H	1.4075	-5.5689	0.9015
39	H	1.7975	-3.8533	0.6780
40	H	0.4060	-4.3181	1.6600
41	O	-2.5047	-0.9034	1.1406
42	O	-3.6963	-1.8711	-0.5214
43	O	-0.1737	-2.2215	0.0618
44	O	-1.3736	-3.0807	-1.6486
45	Rh	-2.3273	-1.2952	-1.9610
46	C	-2.8842	1.4902	-1.4821
47	C	-3.5605	2.8403	-1.7378
48	C	-5.0879	2.6752	-1.4570
49	H	-5.5086	2.0295	-2.2339
50	H	-5.5405	3.6663	-1.5747
51	C	-5.4134	2.1021	-0.0980

52	C	-5.5461	2.9140	1.0358
53	H	-5.4576	3.9925	0.9396
54	C	-3.3650	3.1975	-3.2255
55	H	-3.8652	4.1476	-3.4413
56	H	-3.7835	2.4251	-3.8753
57	H	-2.3012	3.3121	-3.4634
58	C	-2.9580	3.9409	-0.8605
59	H	-3.4909	4.8808	-1.0400
60	H	-1.9068	4.0964	-1.1127
61	H	-3.0208	3.7005	0.2016
62	O	-2.0072	1.4243	-0.5553
63	O	-3.2432	0.5190	-2.2144
64	C	0.1808	-0.0689	-2.7859
65	C	1.2619	0.4330	-3.7461
66	C	1.9080	-0.8074	-4.4409
67	H	2.7349	-0.4352	-5.0563
68	H	1.1665	-1.2422	-5.1188
69	C	2.3955	-1.8705	-3.4837
70	C	3.6894	-1.8525	-2.9473
71	H	4.3903	-1.0801	-3.2518
72	C	0.5877	1.3162	-4.8137
73	H	-0.1901	0.7648	-5.3481
74	H	1.3372	1.6556	-5.5365
75	H	0.1320	2.2013	-4.3551
76	C	2.3218	1.2452	-2.9868
77	H	3.0479	1.6494	-3.7005
78	H	2.8563	0.6312	-2.2593
79	H	1.8630	2.0751	-2.4430
80	O	0.3984	0.1286	-1.5442
81	O	-0.8453	-0.6424	-3.2629
82	Rh	-1.0072	-0.3368	-0.1478
83	C	0.0331	0.4441	1.2612
84	C	-0.5023	0.9171	2.5788
85	O	-0.5099	-0.0816	3.4422
86	C	-1.1507	0.1426	4.7456
87	O	-0.9741	2.0231	2.7983
88	H	-2.2032	0.3585	4.5543
89	H	-0.6806	1.0173	5.1989
90	C	-0.9479	-1.1183	5.5549
91	H	0.1159	-1.3119	5.7222
92	H	-1.4334	-0.9988	6.5284
93	H	-1.3924	-1.9819	5.0515
94	C	4.0252	-2.0192	1.7245
95	C	2.7796	-1.4392	2.0038
96	C	1.8804	-2.0121	2.8866
97	C	2.2323	-3.2083	3.5204
98	C	3.4544	-3.8213	3.2528
99	C	4.3415	-3.2311	2.3578
100	I	2.2799	0.4506	1.0472
101	C	5.0080	-1.3443	0.8464
102	O	6.1123	-2.0500	0.6286
103	C	7.1373	-1.4007	-0.1594
104	O	4.8255	-0.2216	0.3857

105	H	0.9214	-1.5602	3.0874
106	H	1.5307	-3.6573	4.2160
107	H	3.7196	-4.7526	3.7410
108	H	5.3013	-3.6869	2.1476
109	H	7.4622	-0.4851	0.3380
110	H	6.7524	-1.1653	-1.1533
111	H	7.9494	-2.1224	-0.2181
112	C	0.3326	3.6987	0.3405
113	O	0.6364	2.5090	0.2096
114	O	-0.4432	4.1493	1.3044
115	H	-0.7220	3.3715	1.8648
116	C	0.8746	4.7680	-0.5679
117	H	1.2107	4.2985	-1.4948
118	H	0.0853	5.4887	-0.7979
119	C	2.0523	5.5163	0.1252
120	C	2.5959	6.5742	-0.8052
121	C	2.5375	7.8834	-0.5638
122	H	2.9431	8.6100	-1.2623
123	H	2.0834	8.2764	0.3434
124	H	3.0586	6.2107	-1.7225
125	C	3.1370	4.5495	0.5761
126	C	3.4633	4.4433	1.9324
127	C	4.4623	3.5648	2.3616
128	C	5.1457	2.7782	1.4343
129	C	4.8230	2.8725	0.0767
130	C	3.8264	3.7495	-0.3474
131	H	3.5835	3.8056	-1.4045
132	H	5.3392	2.2495	-0.6458
133	H	5.9168	2.0877	1.7608
134	H	4.7060	3.5006	3.4183
135	H	2.9362	5.0585	2.6570
136	H	1.6447	6.0130	1.0119

D_1

	Atom	X	Y	Z
1	C	3.1032	-2.0895	-0.8880
2	C	4.0664	-2.6402	-1.9450
3	C	5.5241	-2.3500	-1.4670
4	H	5.7274	-2.9803	-0.5960
5	H	6.1956	-2.6749	-2.2699
6	C	5.7837	-0.9057	-1.1088
7	C	6.1628	0.0426	-2.0679
8	H	6.3225	-0.2657	-3.0974
9	C	6.3569	1.3761	-1.7023
10	H	6.6667	2.1014	-2.4496
11	C	5.6147	-0.4848	0.2147
12	H	5.3317	-1.2143	0.9665
13	C	3.8655	-4.1664	-2.0320
14	H	4.5621	-4.5880	-2.7646
15	H	4.0439	-4.6422	-1.0644
16	H	2.8460	-4.4088	-2.3537
17	C	3.8088	-2.0070	-3.3173
18	H	4.5511	-2.3755	-4.0334
19	H	2.8189	-2.2852	-3.6866
20	H	3.8673	-0.9174	-3.2818
21	C	-0.2926	-3.0171	0.1364
22	C	-1.2548	-4.1108	-0.3360
23	C	-2.0348	-4.6459	0.9039
24	H	-2.7141	-5.4268	0.5435
25	H	-1.3179	-5.1210	1.5802
26	C	-2.8092	-3.5814	1.6457
27	C	-4.1464	-3.3016	1.3387
28	H	-4.6581	-3.8845	0.5775
29	C	-4.8293	-2.2922	2.0179
30	H	-5.8723	-2.1053	1.7876
31	C	-2.1823	-2.8285	2.6460
32	H	-1.1557	-3.0556	2.9094
33	C	-0.4031	-5.2544	-0.9256
34	H	0.2953	-5.6487	-0.1828
35	H	-1.0581	-6.0665	-1.2587
36	H	0.1724	-4.9063	-1.7912
37	C	-2.2221	-3.5806	-1.3975
38	H	-2.8883	-4.3876	-1.7214
39	H	-2.8341	-2.7636	-1.0130
40	H	-1.6800	-3.2119	-2.2697
41	O	2.2979	-1.1642	-1.2447
42	O	3.1757	-2.5887	0.2763
43	O	-0.3743	-1.8679	-0.4158
44	O	0.5337	-3.3348	1.0459
45	Rh	1.8778	-1.9392	1.7451
46	C	3.1079	0.6971	1.7725
47	C	4.0817	1.7545	2.3060
48	C	5.5339	1.2490	2.0309
49	H	5.7238	0.3922	2.6841
50	H	6.2150	2.0514	2.3367
51	C	5.7903	0.8496	0.5972

52	C	6.1706	1.7800	-0.3788
53	H	6.3372	2.8169	-0.1003
54	C	3.8772	1.8724	3.8299
55	H	4.5834	2.6028	4.2391
56	H	4.0401	0.9117	4.3240
57	H	2.8619	2.2135	4.0631
58	C	3.8522	3.1193	1.6532
59	H	4.5948	3.8318	2.0276
60	H	2.8623	3.5030	1.9107
61	H	3.9400	3.0698	0.5664
62	O	2.3198	1.0128	0.8131
63	O	3.1604	-0.4408	2.3280
64	C	-0.3040	-0.2724	2.7325
65	C	-1.3088	0.2462	3.7651
66	C	-2.1010	-0.9657	4.3451
67	H	-2.8064	-0.5625	5.0806
68	H	-1.3960	-1.6047	4.8855
69	C	-2.8399	-1.7873	3.3127
70	C	-4.1786	-1.5303	2.9899
71	H	-4.7151	-0.7443	3.5150
72	C	-0.5009	0.9050	4.9031
73	H	0.1931	0.1926	5.3574
74	H	-1.1847	1.2709	5.6765
75	H	0.0746	1.7589	4.5270
76	C	-2.2620	1.2738	3.1409
77	H	-2.9541	1.6374	3.9086
78	H	-2.8470	0.8464	2.3244
79	H	-1.7081	2.1293	2.7448
80	O	-0.3319	0.2616	1.5729
81	O	0.4987	-1.1860	3.0948
82	Rh	0.9492	-0.3866	0.1144
83	C	0.2045	0.9108	-1.2511
84	C	0.5586	0.6324	-2.6744
85	O	-0.0793	-0.3804	-3.1985
86	C	0.3950	-0.9140	-4.4834
87	O	1.5010	1.2157	-3.2328
88	H	1.4681	-0.7408	-4.5409
89	H	-0.1049	-0.3382	-5.2661
90	C	0.0391	-2.3837	-4.5189
91	H	-1.0416	-2.5396	-4.4633
92	H	0.3999	-2.8127	-5.4590
93	H	0.5126	-2.9153	-3.6885
94	C	-4.8671	-0.5381	-1.3837
95	C	-3.6145	-0.2263	-1.9393
96	C	-3.1928	-0.7703	-3.1443
97	C	-4.0076	-1.6989	-3.7963
98	C	-5.2296	-2.0733	-3.2409
99	C	-5.6573	-1.4860	-2.0542
100	I	-2.2882	1.1370	-0.9165
101	C	-5.4083	0.1685	-0.1911
102	O	-6.6093	-0.2844	0.1816
103	C	-7.2192	0.4017	1.2947
104	O	-4.8441	1.0970	0.3675

105	H	-2.2368	-0.4958	-3.5618
106	H	-3.6757	-2.1273	-4.7366
107	H	-5.8589	-2.8027	-3.7395
108	H	-6.6239	-1.7366	-1.6353
109	H	-7.3857	1.4507	1.0413
110	H	-6.5769	0.3348	2.1747
111	H	-8.1642	-0.1111	1.4638
112	C	1.3220	3.1083	-0.9157
113	O	0.3088	2.2923	-0.8735
114	O	2.3344	2.9358	-1.6624
115	H	2.1580	2.1572	-2.3485
116	C	1.1951	4.3417	-0.1008
117	H	0.8958	4.0649	0.9118
118	H	2.1750	4.8169	-0.0681
119	C	0.1635	5.3461	-0.7138
120	C	0.3553	6.6865	-0.0398
121	C	0.7496	7.7891	-0.6754
122	H	0.8621	8.7351	-0.1537
123	H	0.9690	7.7869	-1.7407
124	H	0.1351	6.7145	1.0269
125	C	-1.2850	4.8978	-0.5857
126	C	-2.1366	4.9907	-1.6926
127	C	-3.4947	4.6869	-1.5767
128	C	-4.0194	4.2831	-0.3481
129	C	-3.1771	4.1826	0.7622
130	C	-1.8218	4.4894	0.6445
131	H	-1.1862	4.4135	1.5224
132	H	-3.5735	3.8558	1.7183
133	H	-5.0714	4.0341	-0.2553
134	H	-4.1406	4.7672	-2.4462
135	H	-1.7347	5.3160	-2.6487
136	H	0.4018	5.4641	-1.7765

C_{2A}

	Atom	X	Y	Z
1	C	3.4048	-0.4208	-1.7503
2	C	4.1365	-0.0564	-3.0434
3	C	5.5015	0.5981	-2.6590
4	H	6.1284	-0.1692	-2.1946
5	H	5.9872	0.8962	-3.5949
6	C	5.3750	1.7819	-1.7281
7	C	5.2072	3.0853	-2.2128
8	H	5.2160	3.2666	-3.2840
9	C	5.0457	4.1524	-1.3272
10	H	4.9323	5.1618	-1.7124
11	C	5.3877	1.5814	-0.3423
12	H	5.5391	0.5785	0.0432
13	C	4.4033	-1.3636	-3.8177
14	H	4.9510	-1.1376	-4.7385
15	H	4.9945	-2.0621	-3.2201
16	H	3.4618	-1.8521	-4.0936
17	C	3.2966	0.8970	-3.9021
18	H	3.8333	1.1138	-4.8318
19	H	2.3296	0.4529	-4.1539
20	H	3.1133	1.8399	-3.3832
21	C	1.1155	-3.1209	-0.9808
22	C	0.5304	-4.2119	-1.8801
23	C	-0.1090	-5.2965	-0.9516
24	H	-0.6687	-5.9801	-1.5997
25	H	0.7017	-5.8718	-0.4933
26	C	-0.9965	-4.7394	0.1360
27	C	-2.3524	-4.4548	-0.0718
28	H	-2.8126	-4.6808	-1.0296
29	C	-3.1203	-3.9054	0.9565
30	H	-4.1753	-3.7059	0.7954
31	C	-0.4427	-4.4662	1.3914
32	H	0.6043	-4.6978	1.5659
33	C	1.6661	-4.8531	-2.6974
34	H	2.4442	-5.2566	-2.0451
35	H	1.2611	-5.6682	-3.3061
36	H	2.1244	-4.1201	-3.3707
37	C	-0.5261	-3.6204	-2.8241
38	H	-0.9086	-4.4112	-3.4780
39	H	-1.3643	-3.1907	-2.2739
40	H	-0.0946	-2.8338	-3.4511
41	O	2.2652	0.1227	-1.5485
42	O	3.9735	-1.2403	-0.9653
43	O	0.4551	-2.0290	-0.9124
44	O	2.1882	-3.3586	-0.3495
45	Rh	3.0051	-1.8236	0.7546
46	C	3.1358	0.8984	1.7949
47	C	3.7233	2.0621	2.5931
48	C	5.1558	2.3538	2.0440
49	H	5.7912	1.4935	2.2754
50	H	5.5435	3.2088	2.6091
51	C	5.2044	2.6356	0.5601

52	C	5.0381	3.9301	0.0508
53	H	4.9160	4.7659	0.7341
54	C	3.8312	1.6136	4.0652
55	H	4.2685	2.4212	4.6615
56	H	4.4613	0.7256	4.1622
57	H	2.8414	1.3850	4.4764
58	C	2.8319	3.3073	2.4890
59	H	3.2857	4.1221	3.0632
60	H	1.8350	3.1152	2.8943
61	H	2.7168	3.6357	1.4538
62	O	2.0435	1.1164	1.1650
63	O	3.7508	-0.2108	1.8066
64	C	0.7671	-1.7780	2.6308
65	C	-0.0053	-2.1368	3.9016
66	C	-0.5158	-3.6071	3.7475
67	H	-1.1961	-3.7956	4.5857
68	H	0.3412	-4.2773	3.8670
69	C	-1.1937	-3.9065	2.4307
70	C	-2.5475	-3.6293	2.1997
71	H	-3.1601	-3.2169	2.9961
72	C	0.9533	-2.0629	5.1048
73	H	1.8136	-2.7218	4.9650
74	H	0.4230	-2.3663	6.0134
75	H	1.3193	-1.0402	5.2499
76	C	-1.1826	-1.1756	4.1161
77	H	-1.7166	-1.4600	5.0287
78	H	-1.8873	-1.2000	3.2826
79	H	-0.8303	-0.1476	4.2324
80	O	0.2075	-0.9473	1.8325
81	O	1.8927	-2.3232	2.4306
82	Rh	1.1579	-0.3810	0.1111
83	C	-0.3485	0.5146	-0.6562
84	C	-0.2497	1.3168	-1.9151
85	O	0.2212	2.5191	-1.6274
86	C	0.5240	3.4142	-2.7459
87	O	-0.4649	0.8667	-3.0248
88	H	-0.4257	3.7051	-3.2035
89	H	1.1078	2.8507	-3.4746
90	C	1.2838	4.5884	-2.1702
91	H	2.2203	4.2568	-1.7122
92	H	1.5205	5.2921	-2.9747
93	H	0.6869	5.1133	-1.4176
94	C	-4.8430	-1.0900	-1.3996
95	C	-3.4948	-0.8135	-1.6537
96	C	-2.9230	-0.9203	-2.9071
97	C	-3.7456	-1.3065	-3.9726
98	C	-5.0972	-1.5765	-3.7667
99	C	-5.6401	-1.4721	-2.4888
100	I	-2.2491	-0.2268	0.0477
101	C	-5.4065	-1.0068	-0.0322
102	O	-6.7260	-1.1261	0.0095
103	C	-7.3349	-1.0777	1.3219
104	O	-4.7076	-0.8457	0.9656

105	H	-1.8810	-0.6901	-3.0768
106	H	-3.3114	-1.3923	-4.9634
107	H	-5.7282	-1.8737	-4.5971
108	H	-6.6863	-1.6895	-2.3110
109	H	-7.1265	-0.1145	1.7910
110	H	-6.9459	-1.8875	1.9416
111	H	-8.4010	-1.2009	1.1434
112	C	-3.4910	6.1423	1.3887
113	O	-4.5442	5.7821	1.8742
114	O	-3.3138	7.3675	0.8514
115	H	-4.1557	7.8520	0.9581
116	C	-2.2240	5.3182	1.3332
117	H	-1.6615	5.5804	0.4322
118	H	-1.5999	5.6190	2.1850
119	C	-2.5110	3.8078	1.4094
120	C	-1.2201	3.0288	1.5280
121	C	-0.9612	2.1507	2.5004
122	H	-1.6821	1.9518	3.2907
123	H	-0.0288	1.5985	2.5278
124	H	-0.4777	3.1950	0.7484
125	C	-3.3169	3.3231	0.2103
126	C	-4.5537	2.6945	0.3926
127	C	-5.2725	2.2024	-0.6991
128	C	-4.7555	2.3157	-1.9911
129	C	-3.5263	2.9499	-2.1859
130	C	-2.8212	3.4580	-1.0933
131	H	-1.8737	3.9592	-1.2564
132	H	-3.1194	3.0535	-3.1877
133	H	-5.3041	1.9131	-2.8371
134	H	-6.2358	1.7262	-0.5407
135	H	-4.9557	2.5917	1.3962
136	H	-3.1084	3.6288	2.3085

TS4$_A$

	Atom	X	Y	Z
1	C	3.4375	-0.2054	-1.7983
2	C	4.1215	0.2198	-3.0992
3	C	5.4984	0.8612	-2.7364
4	H	6.1422	0.0765	-2.3273
5	H	5.9504	1.1999	-3.6754
6	C	5.4044	2.0043	-1.7524
7	C	5.2243	3.3275	-2.1752
8	H	5.1992	3.5543	-3.2375
9	C	5.0938	4.3557	-1.2399
10	H	4.9701	5.3807	-1.5777
11	C	5.4619	1.7448	-0.3778
12	H	5.6241	0.7264	-0.0406
13	C	4.3634	-1.0504	-3.9403
14	H	4.8743	-0.7813	-4.8708
15	H	4.9800	-1.7710	-3.3971
16	H	3.4141	-1.5323	-4.2007
17	C	3.2492	1.2081	-3.8828
18	H	3.7507	1.4682	-4.8211
19	H	2.2738	0.7736	-4.1182
20	H	3.0844	2.1260	-3.3154
21	C	1.1981	-2.9626	-1.0539
22	C	0.5903	-4.0382	-1.9562
23	C	0.0474	-5.1763	-1.0314
24	H	-0.5118	-5.8678	-1.6717
25	H	0.9052	-5.7250	-0.6299
26	C	-0.8116	-4.6918	0.1129
27	C	-2.1881	-4.4702	-0.0251
28	H	-2.6798	-4.6923	-0.9682
29	C	-2.9348	-3.9906	1.0523
30	H	-4.0030	-3.8333	0.9432
31	C	-0.2144	-4.4272	1.3504
32	H	0.8493	-4.6113	1.4711
33	C	1.6943	-4.6100	-2.8646
34	H	2.5210	-5.0146	-2.2758
35	H	1.2781	-5.4123	-3.4829
36	H	2.0904	-3.8364	-3.5320
37	C	-0.5404	-3.4521	-2.8124
38	H	-0.9425	-4.2341	-3.4651
39	H	-1.3535	-3.0638	-2.1978
40	H	-0.1731	-2.6350	-3.4410
41	O	2.3034	0.3208	-1.5324
42	O	4.0386	-1.0554	-1.0717
43	O	0.5408	-1.8722	-0.9429
44	O	2.2895	-3.2133	-0.4610
45	Rh	3.1434	-1.7117	0.6617
46	C	3.2933	0.9585	1.8080
47	C	3.9071	2.0886	2.6355
48	C	5.3158	2.4136	2.0456
49	H	5.9634	1.5481	2.2156
50	H	5.7209	3.2456	2.6325
51	C	5.3101	2.7593	0.5745

52	C	5.1292	4.0745	0.1270
53	H	5.0309	4.8804	0.8489
54	C	4.0768	1.5732	4.0799
55	H	4.5334	2.3553	4.6955
56	H	4.7153	0.6865	4.1096
57	H	3.1060	1.3177	4.5196
58	C	3.0093	3.3327	2.6275
59	H	3.4920	4.1286	3.2045
60	H	2.0403	3.1200	3.0878
61	H	2.8322	3.6985	1.6137
62	O	2.1731	1.1889	1.2343
63	O	3.9227	-0.1404	1.7440
64	C	0.9664	-1.7551	2.6137
65	C	0.2405	-2.1554	3.8984
66	C	-0.2272	-3.6390	3.7352
67	H	-0.8697	-3.8656	4.5935
68	H	0.6557	-4.2814	3.8109
69	C	-0.9445	-3.9361	2.4387
70	C	-2.3192	-3.7214	2.2764
71	H	-2.9136	-3.3634	3.1121
72	C	1.2285	-2.0681	5.0767
73	H	2.1048	-2.6975	4.9037
74	H	0.7330	-2.4011	5.9946
75	H	1.5665	-1.0367	5.2276
76	C	-0.9599	-1.2327	4.1546
77	H	-1.4508	-1.5302	5.0871
78	H	-1.6937	-1.2860	3.3476
79	H	-0.6384	-0.1914	4.2544
80	O	0.3626	-0.9188	1.8542
81	O	2.0960	-2.2713	2.3644
82	Rh	1.2555	-0.2703	0.1377
83	C	-0.2924	0.6804	-0.4966
84	C	-0.2442	1.6112	-1.6676
85	O	0.2685	2.7778	-1.3178
86	C	0.5666	3.7251	-2.3930
87	O	-0.5141	1.2516	-2.7994
88	H	-0.3847	4.0496	-2.8238
89	H	1.1352	3.1941	-3.1575
90	C	1.3463	4.8610	-1.7696
91	H	2.2838	4.4968	-1.3396
92	H	1.5834	5.6000	-2.5417
93	H	0.7623	5.3554	-0.9869
94	C	-4.7103	-1.1075	-1.5495
95	C	-3.3687	-0.7621	-1.7462
96	C	-2.7743	-0.7179	-2.9934
97	C	-3.5634	-1.0202	-4.1090
98	C	-4.9063	-1.3611	-3.9585
99	C	-5.4730	-1.4070	-2.6884
100	I	-2.1599	-0.3346	0.0274
101	C	-5.3091	-1.1684	-0.1960
102	O	-6.6311	-1.2825	-0.2051
103	C	-7.2763	-1.3539	1.0879
104	O	-4.6394	-1.1167	0.8317

105	H	-1.7400	-0.4329	-3.1152
106	H	-3.1105	-0.9861	-5.0946
107	H	-5.5119	-1.5956	-4.8272
108	H	-6.5139	-1.6752	-2.5547
109	H	-7.0719	-0.4431	1.6535
110	H	-6.9128	-2.2240	1.6377
111	H	-8.3382	-1.4465	0.8698
112	C	-4.8594	4.8820	2.1703
113	O	-5.5133	4.0118	2.7107
114	O	-5.3579	6.1020	1.8893
115	H	-6.2800	6.1182	2.2131
116	C	-3.4055	4.7613	1.7703
117	H	-3.1805	5.4759	0.9739
118	H	-2.8102	5.0549	2.6451
119	C	-3.0271	3.3235	1.3472
120	C	-1.5269	3.2043	1.2638
121	C	-0.7944	2.2846	1.9060
122	H	-1.2537	1.5415	2.5547
123	H	0.2861	2.2617	1.8288
124	H	-1.0133	3.9297	0.6374
125	C	-3.7159	2.9509	0.0360
126	C	-4.9474	2.2810	0.0580
127	C	-5.6017	1.9527	-1.1303
128	C	-5.0250	2.2672	-2.3628
129	C	-3.8000	2.9339	-2.3964
130	C	-3.1589	3.2841	-1.2059
131	H	-2.2168	3.8195	-1.2498
132	H	-3.3395	3.1842	-3.3475
133	H	-5.5215	1.9862	-3.2863
134	H	-6.5548	1.4335	-1.0922
135	H	-5.3943	2.0269	1.0134
136	H	-3.3906	2.6443	2.1251

D_2

	Atom	X	Y	Z
1	C	3.4843	-0.8383	-1.5478
2	C	4.3450	-0.7991	-2.8146
3	C	5.6482	-0.0043	-2.4830
4	H	6.2607	-0.6214	-1.8184
5	H	6.2016	0.1135	-3.4218
6	C	5.4090	1.3384	-1.8337
7	C	5.1798	2.4985	-2.5846
8	H	5.2163	2.4545	-3.6696
9	C	4.9259	3.7133	-1.9446
10	H	4.7651	4.6112	-2.5349
11	C	5.3841	1.4316	-0.4377
12	H	5.5682	0.5395	0.1523
13	C	4.7259	-2.2426	-3.1967
14	H	5.3663	-2.2320	-4.0853
15	H	5.2632	-2.7361	-2.3832
16	H	3.8325	-2.8341	-3.4288
17	C	3.5859	-0.1422	-3.9735
18	H	4.2362	-0.0895	-4.8534
19	H	2.7066	-0.7365	-4.2374
20	H	3.2532	0.8665	-3.7213
21	C	0.9339	-3.1707	-0.4201
22	C	0.3311	-4.4294	-1.0496
23	C	-0.2441	-5.3116	0.1040
24	H	-0.7555	-6.1605	-0.3643
25	H	0.5981	-5.7126	0.6764
26	C	-1.1786	-4.5788	1.0381
27	C	-2.5460	-4.4435	0.7648
28	H	-2.9681	-4.9134	-0.1192
29	C	-3.3720	-3.7260	1.6316
30	H	-4.4291	-3.6264	1.4094
31	C	-0.6697	-3.9866	2.1996
32	H	0.3866	-4.0941	2.4255
33	C	1.4557	-5.2061	-1.7612
34	H	2.2578	-5.4634	-1.0649
35	H	1.0524	-6.1298	-2.1900
36	H	1.8836	-4.6113	-2.5766
37	C	-0.7674	-4.0680	-2.0579
38	H	-1.1771	-4.9864	-2.4925
39	H	-1.5820	-3.5130	-1.5890
40	H	-0.3659	-3.4534	-2.8674
41	O	2.3743	-0.2101	-1.5690
42	O	3.9448	-1.4853	-0.5556
43	O	0.3771	-2.0560	-0.7009
44	O	1.9364	-3.3138	0.3434
45	Rh	2.8251	-1.6358	1.1726
46	C	3.0076	1.2285	1.6763
47	C	3.6248	2.4740	2.3224
48	C	5.0587	2.6594	1.7306
49	H	5.6943	1.8622	2.1276
50	H	5.4448	3.6091	2.1186
51	C	5.1199	2.6373	0.2213

52	C	4.8944	3.7845	-0.5506
53	H	4.7117	4.7371	-0.0611
54	C	3.7431	2.2284	3.8397
55	H	4.2176	3.0931	4.3162
56	H	4.3425	1.3392	4.0490
57	H	2.7535	2.0928	4.2913
58	C	2.7704	3.7191	2.0714
59	H	3.2568	4.5917	2.5204
60	H	1.7876	3.6070	2.5361
61	H	2.6326	3.9090	1.0058
62	O	1.9726	1.3719	0.9391
63	O	3.5875	0.1252	1.9176
64	C	0.4523	-1.0924	2.7817
65	C	-0.4089	-1.1180	4.0473
66	C	-0.8617	-2.5940	4.2844
67	H	-1.5679	-2.5840	5.1225
68	H	0.0138	-3.1691	4.6016
69	C	-1.4800	-3.2542	3.0749
70	C	-2.8436	-3.1315	2.7785
71	H	-3.4957	-2.5853	3.4548
72	C	0.4504	-0.6618	5.2418
73	H	1.3312	-1.2978	5.3584
74	H	-0.1424	-0.7100	6.1616
75	H	0.7870	0.3728	5.1081
76	C	-1.6216	-0.1912	3.8987
77	H	-2.2302	-0.2346	4.8084
78	H	-2.2445	-0.4722	3.0477
79	H	-1.2973	0.8434	3.7531
80	O	-0.0232	-0.4848	1.7626
81	O	1.5730	-1.6844	2.8223
82	Rh	1.1221	-0.3033	0.0640
83	C	-0.4724	0.8109	-0.8678
84	C	-0.1649	0.9952	-2.3038
85	O	-0.5191	-0.0111	-3.0676
86	C	-0.1496	0.0359	-4.4852
87	O	0.4546	1.9859	-2.7353
88	H	0.8375	0.4888	-4.5645
89	H	-0.8830	0.6800	-4.9773
90	C	-0.1845	-1.3837	-5.0036
91	H	-1.1714	-1.8330	-4.8588
92	H	0.0412	-1.3784	-6.0747
93	H	0.5623	-2.0008	-4.4953
94	C	-5.0033	0.2857	-1.7741
95	C	-3.6750	0.7188	-1.7077
96	C	-3.2362	1.8387	-2.3939
97	C	-4.1429	2.5353	-3.1986
98	C	-5.4675	2.1145	-3.3015
99	C	-5.8956	1.0006	-2.5868
100	I	-2.2657	-0.4064	-0.4899
101	C	-5.4584	-0.8725	-0.9725
102	O	-6.7568	-1.1197	-1.0694
103	C	-7.2553	-2.2363	-0.2956
104	O	-4.6951	-1.5312	-0.2695

105	H	-2.2243	2.2065	-2.3142
106	H	-3.8005	3.4135	-3.7359
107	H	-6.1670	2.6574	-3.9275
108	H	-6.9259	0.6707	-2.6396
109	H	-7.0644	-2.0662	0.7655
110	H	-6.7685	-3.1584	-0.6184
111	H	-8.3236	-2.2679	-0.4994
112	C	-0.1137	3.1321	-0.0238
113	O	-0.7726	2.0189	-0.1281
114	O	0.7733	3.5190	-0.8450
115	H	0.8040	2.8755	-1.6928
116	C	-0.5426	4.0198	1.0907
117	H	-0.5126	3.4500	2.0226
118	H	0.1781	4.8343	1.1568
119	C	-1.9634	4.6284	0.8697
120	C	-2.1708	5.7128	1.9047
121	C	-2.3210	7.0045	1.6145
122	H	-2.4807	7.7464	2.3916
123	H	-2.2945	7.3662	0.5889
124	H	-2.2078	5.3713	2.9391
125	C	-3.1173	3.6352	0.9399
126	C	-4.2402	3.8535	0.1303
127	C	-5.3668	3.0395	0.2334
128	C	-5.3849	1.9815	1.1452
129	C	-4.2712	1.7526	1.9546
130	C	-3.1494	2.5779	1.8560
131	H	-2.2968	2.3791	2.4957
132	H	-4.2717	0.9319	2.6656
133	H	-6.2599	1.3426	1.2238
134	H	-6.2238	3.2229	-0.4067
135	H	-4.2322	4.6748	-0.5812
136	H	-1.9719	5.1000	-0.1197

F

	Atom	X	Y	Z
1	C	-1.9438	-0.2973	-0.8201
2	C	-2.7989	-1.4319	-0.3317
3	O	-3.9467	-0.9673	0.1545
4	C	-4.8984	-1.9604	0.6484
5	O	-2.4862	-2.6055	-0.3895
6	H	-4.4059	-2.5330	1.4383
7	H	-5.1363	-2.6369	-0.1758
8	C	-6.1092	-1.2033	1.1478
9	H	-6.5699	-0.6258	0.3406
10	H	-6.8479	-1.9158	1.5280
11	H	-5.8374	-0.5213	1.9592
12	C	2.3287	-1.6076	0.3498
13	C	0.9393	-1.7041	0.2554
14	C	0.1485	-2.2764	1.2344
15	C	0.7818	-2.7686	2.3810
16	C	2.1650	-2.6816	2.5226
17	C	2.9310	-2.1041	1.5156
18	I	-0.0073	-0.9365	-1.5702
19	C	3.1470	-1.0528	-0.7551
20	O	4.3850	-0.7468	-0.3929
21	C	5.2464	-0.2229	-1.4308
22	O	2.7102	-0.9069	-1.8928
23	H	-0.9202	-2.3729	1.1224
24	H	0.1756	-3.2244	3.1569
25	H	2.6487	-3.0674	3.4132
26	H	4.0078	-2.0322	1.6075
27	H	4.8276	0.7048	-1.8246
28	H	5.3511	-0.9558	-2.2329
29	H	6.2012	-0.0418	-0.9416
30	C	-0.4596	4.5709	-0.1274
31	O	0.3890	4.5422	-0.9964
32	O	-0.6244	5.6161	0.7045
33	H	0.0340	6.2937	0.4540
34	C	-1.4751	3.4795	0.1317
35	H	-1.8290	3.5389	1.1641
36	H	-2.3355	3.6852	-0.5194
37	C	-0.9075	2.0800	-0.1837
38	C	-2.0812	1.1101	-0.2743
39	C	-2.6291	0.7966	-1.6310
40	H	-2.0989	1.2100	-2.4846
41	H	-3.6937	0.6528	-1.7797
42	H	-2.7935	1.1589	0.5448
43	C	0.1666	1.6775	0.8109
44	C	1.5148	1.8942	0.4919
45	C	2.5222	1.5663	1.3982
46	C	2.1945	1.0069	2.6351
47	C	0.8561	0.7832	2.9592
48	C	-0.1518	1.1200	2.0537
49	H	-1.1889	0.9345	2.3188
50	H	0.5943	0.3381	3.9142
51	H	2.9775	0.7360	3.3365

52	H	3.5620	1.7315	1.1327
53	H	1.7681	2.3293	-0.4696
54	H	-0.4404	2.1503	-1.1707

TS3PRC

	Atom	X	Y	Z
1	C	0.1107	3.0056	-0.9953
2	C	-0.3543	4.1562	-1.8952
3	C	-1.2397	5.1165	-1.0405
4	H	-0.5982	5.5909	-0.2914
5	H	-1.5983	5.9055	-1.7118
6	C	-2.4041	4.4436	-0.3512
7	C	-3.6517	4.3091	-0.9743
8	H	-3.8078	4.7330	-1.9626
9	C	-4.6966	3.6473	-0.3271
10	H	-5.6644	3.5596	-0.8133
11	C	-2.2383	3.9094	0.9321
12	H	-1.2790	4.0172	1.4270
13	C	0.8951	4.9247	-2.3705
14	H	0.5921	5.7737	-2.9932
15	H	1.4715	5.3007	-1.5212
16	H	1.5455	4.2782	-2.9707
17	C	-1.1321	3.6290	-3.1077
18	H	-1.4523	4.4730	-3.7291
19	H	-0.5048	2.9715	-3.7168
20	H	-2.0167	3.0644	-2.8058
21	C	3.1115	0.8654	-0.9778
22	C	4.3714	0.8042	-1.8504
23	C	5.5881	0.4370	-0.9458
24	H	6.4708	0.4000	-1.5948
25	H	5.7396	1.2553	-0.2352
26	C	5.4415	-0.8656	-0.1924
27	C	5.9330	-2.0721	-0.7071
28	H	6.4619	-2.0758	-1.6566
29	C	5.7580	-3.2639	-0.0012
30	H	6.1519	-4.1931	-0.4038
31	C	4.7857	-0.8862	1.0444
32	H	4.4218	0.0453	1.4617
33	C	4.5985	2.2126	-2.4382
34	H	4.7185	2.9547	-1.6442
35	H	5.5014	2.2134	-3.0588
36	H	3.7530	2.5130	-3.0679
37	C	4.2103	-0.2130	-2.9865
38	H	5.1267	-0.2378	-3.5867
39	H	4.0226	-1.2169	-2.6003
40	H	3.3767	0.0590	-3.6402
41	O	-0.2333	1.8264	-1.3380
42	O	0.8030	3.3053	0.0254
43	O	2.1225	0.1410	-1.3273
44	O	3.1436	1.6427	0.0263
45	Rh	0.3693	0.1944	-0.2403
46	Rh	1.4887	1.7895	1.2565
47	C	-1.2433	1.1091	2.0147
48	C	-2.4962	1.1430	2.8979
49	C	-3.0154	2.6141	2.9472
50	H	-2.2776	3.2154	3.4874
51	H	-3.9355	2.6113	3.5432

52	C	-3.2687	3.2273	1.5895
53	C	-4.5072	3.1066	0.9459
54	H	-5.3270	2.5988	1.4471
55	C	-2.0913	0.7083	4.3204
56	H	-2.9629	0.7519	4.9826
57	H	-1.3119	1.3606	4.7227
58	H	-1.7151	-0.3212	4.3212
59	C	-3.5804	0.2026	2.3574
60	H	-4.4668	0.2602	2.9992
61	H	-3.2342	-0.8347	2.3480
62	H	-3.8713	0.4724	1.3398
63	O	-1.2858	0.3742	0.9718
64	O	-0.2534	1.8125	2.3804
65	C	1.7815	-1.0052	2.0177
66	C	2.2685	-2.1550	2.9092
67	C	3.8172	-2.0486	3.0601
68	H	4.1354	-2.8806	3.6990
69	H	4.0418	-1.1212	3.5957
70	C	4.5795	-2.0747	1.7547
71	C	5.0781	-3.2683	1.2177
72	H	4.9439	-4.1999	1.7612
73	C	1.6221	-1.9715	4.2982
74	H	1.8949	-1.0065	4.7335
75	H	1.9578	-2.7682	4.9712
76	H	0.5293	-2.0235	4.2290
77	C	1.8717	-3.5176	2.3308
78	H	2.2612	-4.3150	2.9735
79	H	2.2714	-3.6564	1.3245
80	H	0.7845	-3.6178	2.2813
81	O	1.0897	-1.3050	0.9904
82	O	2.0976	0.1702	2.3823
83	O	-1.7736	-0.5314	-1.9236
84	C	-2.6513	-1.1097	-2.9629
85	O	-2.6074	-0.6133	-4.0428
86	C	-3.6959	-2.0390	-2.4035
87	H	-4.6564	-1.5856	-2.6744
88	H	-3.6228	-2.9694	-2.9758
89	C	-3.6636	-2.3147	-0.8817
90	C	-4.9891	-2.9318	-0.4491
91	C	-5.8055	-2.2617	0.4687
92	C	-7.0203	-2.8145	0.8788
93	C	-7.4340	-4.0486	0.3746
94	C	-6.6256	-4.7249	-0.5426
95	C	-5.4122	-4.1704	-0.9506
96	H	-4.7933	-4.7097	-1.6627
97	H	-6.9393	-5.6856	-0.9409
98	H	-8.3782	-4.4808	0.6928
99	H	-7.6417	-2.2798	1.5917
100	H	-5.4886	-1.3004	0.8626
101	C	-2.5172	-3.2112	-0.4817
102	C	-1.6190	-2.9135	0.4623
103	H	-0.8182	-3.6004	0.7148
104	H	-1.6421	-1.9706	0.9987

105	C	-0.6255	-0.9649	-1.5139
106	C	-0.1721	-2.2336	-2.2372
107	O	-0.8446	-2.7582	-3.1110
108	O	1.0012	-2.6490	-1.8109
109	C	1.5232	-3.8583	-2.4355
110	C	2.8395	-4.1810	-1.7664
111	H	3.2722	-5.0734	-2.2302
112	H	3.5491	-3.3569	-1.8695
113	H	2.7011	-4.3774	-0.7001
114	H	0.7794	-4.6493	-2.3056
115	H	1.6344	-3.6597	-3.5050
116	H	-2.4498	-4.1610	-1.0115
117	H	-3.5532	-1.3599	-0.3602

TS3

	Atom	X	Y	Z
1	C	0.4601	2.8191	-1.4388
2	C	0.0838	3.8470	-2.5115
3	C	-0.4079	5.1427	-1.7928
4	H	0.4495	5.5929	-1.2826
5	H	-0.7280	5.8422	-2.5739
6	C	-1.5228	4.9197	-0.7976
7	C	-2.8704	4.9582	-1.1786
8	H	-3.1321	5.1938	-2.2066
9	C	-3.8760	4.7097	-0.2429
10	H	-4.9186	4.7546	-0.5455
11	C	-1.2154	4.6371	0.5386
12	H	-0.1751	4.6147	0.8457
13	C	1.3507	4.1816	-3.3237
14	H	1.1153	4.9370	-4.0815
15	H	2.1419	4.5690	-2.6764
16	H	1.7299	3.2912	-3.8382
17	C	-1.0004	3.2912	-3.4441
18	H	-1.2589	4.0479	-4.1935
19	H	-0.6434	2.3978	-3.9649
20	H	-1.9042	3.0169	-2.8968
21	C	2.8429	0.0150	-1.3828
22	C	3.8455	-0.5379	-2.4031
23	C	5.1359	-0.9857	-1.6500
24	H	5.8356	-1.3604	-2.4061
25	H	5.5885	-0.0986	-1.1968
26	C	4.9070	-2.0382	-0.5887
27	C	5.0487	-3.4038	-0.8671
28	H	5.3635	-3.7205	-1.8580
29	C	4.7977	-4.3560	0.1226
30	H	4.9200	-5.4124	-0.1003
31	C	4.5213	-1.6574	0.7024
32	H	4.4311	-0.6028	0.9343
33	C	4.2057	0.6133	-3.3654
34	H	4.6363	1.4583	-2.8214
35	H	4.9345	0.2636	-4.1049
36	H	3.3170	0.9635	-3.9029
37	C	3.2452	-1.7073	-3.1922
38	H	3.9774	-2.0687	-3.9228
39	H	2.9818	-2.5360	-2.5317
40	H	2.3436	-1.3985	-3.7282
41	O	-0.1969	1.7284	-1.4291
42	O	1.3942	3.1261	-0.6341
43	O	1.6689	-0.4811	-1.3849
44	O	3.2543	0.9410	-0.6160
45	Rh	0.2438	0.2445	-0.0767
46	Rh	1.9737	1.7479	0.7949
47	C	-0.6202	1.9545	2.1166
48	C	-1.6222	2.4817	3.1501
49	C	-1.8166	4.0108	2.9019
50	H	-0.8799	4.5159	3.1577
51	H	-2.5790	4.3576	3.6095

52	C	-2.2091	4.3687	1.4871
53	C	-3.5492	4.4138	1.0817
54	H	-4.3374	4.2291	1.8068
55	C	-1.0188	2.2790	4.5540
56	H	-1.7044	2.6734	5.3121
57	H	-0.0594	2.7942	4.6470
58	H	-0.8604	1.2140	4.7602
59	C	-2.9603	1.7378	3.0492
60	H	-3.6587	2.1422	3.7904
61	H	-2.8283	0.6705	3.2517
62	H	-3.4065	1.8424	2.0580
63	O	-1.0395	1.0679	1.3013
64	O	0.5539	2.4369	2.1419
65	C	1.8198	-0.8343	2.1359
66	C	2.2276	-1.8964	3.1644
67	C	3.7644	-2.1382	3.0595
68	H	4.0245	-2.8841	3.8195
69	H	4.2722	-1.2070	3.3287
70	C	4.2373	-2.5986	1.6992
71	C	4.3853	-3.9581	1.3954
72	H	4.1856	-4.7045	2.1598
73	C	1.9106	-1.3290	4.5640
74	H	2.4559	-0.3981	4.7421
75	H	2.1963	-2.0556	5.3325
76	H	0.8382	-1.1273	4.6687
77	C	1.4549	-3.2034	2.9457
78	H	1.7869	-3.9497	3.6762
79	H	1.6172	-3.6040	1.9426
80	H	0.3803	-3.0494	3.0804
81	O	0.8694	-1.1261	1.3397
82	O	2.4491	0.2693	2.1614
83	O	-2.2460	-0.1800	-1.4351
84	C	-3.2322	-0.6300	-2.3782
85	O	-3.4502	0.0900	-3.3055
86	C	-4.0207	-1.8502	-1.9787
87	H	-5.0132	-1.7187	-2.4167
88	H	-3.5702	-2.7201	-2.4671
89	C	-4.1419	-2.0846	-0.4483
90	C	-5.2560	-3.0765	-0.1427
91	C	-6.2647	-2.7332	0.7640
92	C	-7.2855	-3.6358	1.0668
93	C	-7.3059	-4.8964	0.4674
94	C	-6.3001	-5.2487	-0.4357
95	C	-5.2811	-4.3451	-0.7375
96	H	-4.5060	-4.6340	-1.4423
97	H	-6.3082	-6.2274	-0.9066
98	H	-8.0996	-5.5997	0.7013
99	H	-8.0638	-3.3526	1.7695
100	H	-6.2510	-1.7528	1.2328
101	C	-2.8426	-2.5796	0.1217
102	C	-2.0590	-1.8697	0.9630
103	H	-1.1283	-2.2692	1.3470
104	H	-2.3711	-0.9055	1.3517

105	C	-1.2158	-0.8685	-0.9764
106	C	-0.8179	-2.0602	-1.8297
107	O	-1.1022	-2.1238	-3.0154
108	O	-0.0682	-2.9252	-1.1674
109	C	0.4491	-4.0558	-1.9196
110	C	1.3482	-4.8305	-0.9815
111	H	1.7696	-5.6936	-1.5071
112	H	2.1726	-4.2057	-0.6289
113	H	0.7868	-5.1931	-0.1145
114	H	-0.4008	-4.6482	-2.2719
115	H	0.9868	-3.6697	-2.7880
116	H	-2.5183	-3.5640	-0.2111
117	H	-4.3930	-1.1308	0.0263

TS3$_{Prod}$

	Atom	X	Y	Z
1	C	-0.2505	-2.3597	-1.4463
2	C	0.4451	-3.2720	-2.4586
3	C	1.1616	-4.4097	-1.6583
4	H	0.3958	-5.1081	-1.3054
5	H	1.7919	-4.9520	-2.3726
6	C	1.9806	-3.9450	-0.4754
7	C	3.3108	-3.5275	-0.6025
8	H	3.7918	-3.5296	-1.5755
9	C	4.0218	-3.0958	0.5183
10	H	5.0567	-2.7824	0.4097
11	C	1.3897	-3.9115	0.7935
12	H	0.3589	-4.2357	0.9014
13	C	-0.6205	-3.9072	-3.3725
14	H	-0.1378	-4.5989	-4.0715
15	H	-1.3650	-4.4582	-2.7925
16	H	-1.1376	-3.1391	-3.9589
17	C	1.4525	-2.4872	-3.3071
18	H	1.9140	-3.1661	-4.0332
19	H	0.9517	-1.6855	-3.8599
20	H	2.2359	-2.0354	-2.7011
21	C	-2.9651	0.0140	-1.8001
22	C	-3.7852	0.4622	-3.0115
23	C	-5.1719	0.9644	-2.4958
24	H	-5.7095	1.3670	-3.3620
25	H	-5.7344	0.0966	-2.1371
26	C	-5.0918	1.9971	-1.3954
27	C	-4.9830	3.3664	-1.6710
28	H	-4.9983	3.7113	-2.7013
29	C	-4.8744	4.2892	-0.6293
30	H	-4.8039	5.3502	-0.8526
31	C	-5.0981	1.5848	-0.0579
32	H	-5.1919	0.5270	0.1661
33	C	-4.0060	-0.7545	-3.9314
34	H	-4.5122	-1.5639	-3.3992
35	H	-4.6201	-0.4608	-4.7896
36	H	-3.0505	-1.1340	-4.3112
37	C	-3.0558	1.5707	-3.7818
38	H	-3.6577	1.8673	-4.6479
39	H	-2.8895	2.4520	-3.1587
40	H	-2.0835	1.2212	-4.1417
41	O	0.2219	-1.1924	-1.2628
42	O	-1.2597	-2.8421	-0.8325
43	O	-1.9058	0.6651	-1.5311
44	O	-3.4007	-0.9785	-1.1303
45	Rh	-0.7218	0.0852	0.0376
46	Rh	-2.3062	-1.6572	0.4820
47	C	-0.0912	-1.5797	2.3433
48	C	0.7091	-2.0142	3.5742
49	C	1.3626	-3.3991	3.2539
50	H	0.5724	-4.1565	3.2712
51	H	2.0500	-3.6269	4.0771

52	C	2.0801	-3.4645	1.9253
53	C	3.4153	-3.0659	1.7755
54	H	3.9828	-2.7429	2.6443
55	C	-0.2552	-2.1817	4.7637
56	H	0.2989	-2.5350	5.6401
57	H	-1.0439	-2.9023	4.5344
58	H	-0.7253	-1.2257	5.0218
59	C	1.7817	-0.9750	3.9241
60	H	2.3161	-1.2960	4.8250
61	H	1.3298	0.0020	4.1220
62	H	2.5057	-0.8533	3.1181
63	O	0.3427	-0.5951	1.6666
64	O	-1.1396	-2.2507	2.0674
65	C	-2.7846	0.7954	1.9586
66	C	-3.4993	1.7015	2.9644
67	C	-4.9368	1.9837	2.4216
68	H	-5.4011	2.7065	3.1025
69	H	-5.5126	1.0553	2.4891
70	C	-4.9778	2.4938	0.9997
71	C	-4.8705	3.8577	0.6983
72	H	-4.7981	4.5833	1.5039
73	C	-3.6121	0.9510	4.3058
74	H	-4.1489	0.0068	4.1848
75	H	-4.1510	1.5706	5.0308
76	H	-2.6190	0.7344	4.7164
77	C	-2.7255	3.0110	3.1655
78	H	-3.2554	3.6371	3.8918
79	H	-2.6269	3.5700	2.2330
80	H	-1.7199	2.8149	3.5496
81	O	-1.7639	1.2639	1.3606
82	O	-3.2668	-0.3706	1.7784
83	O	3.4024	-0.3931	-1.5024
84	C	4.6209	-0.2871	-2.1008
85	O	4.9860	-1.1906	-2.8185
86	C	5.4476	0.9282	-1.7471
87	H	6.4852	0.7093	-2.0058
88	H	5.1176	1.7719	-2.3653
89	C	5.2834	1.2860	-0.2518
90	C	6.1816	2.4338	0.1620
91	C	7.1664	2.2428	1.1371
92	C	8.0061	3.2911	1.5198
93	C	7.8697	4.5478	0.9284
94	C	6.8892	4.7491	-0.0468
95	C	6.0528	3.6997	-0.4265
96	H	5.2959	3.8706	-1.1880
97	H	6.7763	5.7237	-0.5131
98	H	8.5214	5.3649	1.2239
99	H	8.7647	3.1244	2.2792
100	H	7.2757	1.2656	1.6004
101	C	3.8040	1.5799	-0.0123
102	C	2.8965	0.6235	0.6978
103	H	2.0561	1.0099	1.2569
104	H	3.3216	-0.2992	1.0789

105	C	2.8430	0.6944	-0.7998
106	C	1.7728	1.3625	-1.5913
107	O	1.7760	1.4248	-2.8011
108	O	0.8457	1.9754	-0.8055
109	C	0.0456	3.0018	-1.4916
110	C	-0.7076	3.7923	-0.4452
111	H	-1.2887	4.5730	-0.9484
112	H	-1.3964	3.1557	0.1121
113	H	-0.0185	4.2731	0.2574
114	H	0.7444	3.6226	-2.0566
115	H	-0.6253	2.4930	-2.1811
116	H	3.5345	2.6313	0.0280
117	H	5.5683	0.4051	0.3342

$Rh(oac)_4C(COOMe)(Ph)$

	Atom	X	Y	Z
1	C	1.9351	0.5756	-0.2147
2	C	3.0762	-0.2745	-0.1444
3	C	2.9337	-1.6557	0.1665
4	C	4.0494	-2.4746	0.2552
5	C	5.3252	-1.9484	0.0219
6	C	5.4936	-0.5922	-0.2919
7	C	4.3881	0.2376	-0.3656
8	H	1.9444	-2.0493	0.3451
9	H	3.9331	-3.5249	0.5022
10	H	6.1946	-2.5959	0.0862
11	H	6.4869	-0.1945	-0.4714
12	H	4.5185	1.2861	-0.6115
13	C	2.1735	2.0235	-0.4194
14	O	2.1602	2.5484	-1.5192
15	O	2.3607	2.6686	0.7382
16	C	2.4194	4.1089	0.6556
17	H	1.4796	4.4955	0.2553
18	H	3.2499	4.4201	0.0186
19	H	2.5701	4.4496	1.6785
20	Rh	-0.0056	0.0751	-0.0779
21	O	-0.5389	1.0307	-1.8255
22	C	-1.7565	1.0345	-2.2130
23	C	-2.0466	1.8078	-3.4760
24	O	-0.4601	1.7967	0.9660
25	C	-1.6578	2.0084	1.3594
26	O	-2.6502	1.2396	1.1773
27	Rh	-2.3818	-0.5295	0.1454
28	O	-1.8962	-1.4936	1.9057
29	C	-0.6896	-1.5008	2.2939
30	C	-0.3551	-2.2348	3.5693
31	O	0.2266	-1.6802	-1.1403
32	C	-0.7763	-2.4524	-1.3277
33	C	-0.5077	-3.6978	-2.1362
34	O	0.2946	-0.9424	1.6964
35	C	-1.8824	3.2852	2.1323
36	O	-1.9568	-2.2538	-0.9101
37	O	-2.7289	0.4695	-1.6245
38	H	-2.0195	2.8796	-3.2493
39	H	-3.0329	1.5508	-3.8652
40	H	-1.2771	1.6064	-4.2254
41	H	-2.9474	3.5119	2.1989
42	H	-1.3467	4.1104	1.6563
43	H	-1.4789	3.1637	3.1439
44	H	0.3911	-4.1971	-1.7638
45	H	-1.3611	-4.3758	-2.0944
46	H	-0.3221	-3.4140	-3.1779
47	H	-1.2605	-2.6149	4.0438
48	H	0.3173	-3.0684	3.3408
49	H	0.1722	-1.5632	4.2532

$Rh(oac)_4C(COOMe)(OCOMe)$

	Atom	X	Y	Z
1	C	0.8637	2.3377	1.1923
2	C	0.6905	3.6931	1.8322
3	C	1.1321	1.2058	-2.3358
4	C	1.1005	1.9329	-3.6576
5	H	1.6467	4.0741	2.1928
6	H	-0.0246	3.6256	2.6568
7	H	0.2791	4.3877	1.0916
8	H	0.4359	1.4156	-4.3543
9	H	2.1044	2.0090	-4.0775
10	H	0.6999	2.9405	-3.4998
11	O	-0.2160	1.7198	0.8930
12	O	2.0427	1.9189	0.9862
13	O	0.0001	0.8314	-1.8739
14	O	0.0114	-1.0614	1.7902
15	Rh	-0.1126	-0.1173	-0.0403
16	Rh	2.3300	0.0935	0.0553
17	O	0.1657	-1.9354	-0.9730
18	O	2.2576	1.0359	-1.7759
19	C	1.1496	-1.2317	2.3498
20	O	2.4276	-1.7420	-0.8893
21	O	2.2684	-0.8584	1.8851
22	C	1.3561	-2.3533	-1.1866
23	C	1.1343	-1.9598	3.6709
24	C	1.4758	-3.7144	-1.8278
25	H	2.1110	-1.8997	4.1530
26	H	0.3647	-1.5358	4.3215
27	H	0.8812	-3.0114	3.4969
28	H	0.7273	-3.8279	-2.6157
29	H	2.4785	-3.8608	-2.2321
30	H	1.2835	-4.4813	-1.0687
31	C	-2.0867	-0.2715	-0.0633
32	C	-2.9093	0.9290	0.3328
33	O	-3.2991	1.0285	1.4801
34	O	-2.9644	1.8541	-0.6136
35	C	-3.5492	3.1189	-0.2230
36	H	-2.9534	3.5651	0.5756
37	H	-4.5771	2.9693	0.1125
38	H	-3.5204	3.7352	-1.1194
39	O	-2.6803	-1.4243	-0.2096
40	C	-4.1345	-1.5568	-0.2915
41	O	-4.8105	-0.6091	-0.5443
42	C	-4.4956	-2.9802	-0.0543
43	H	-5.5734	-3.1054	-0.1536
44	H	-3.9674	-3.6169	-0.7710
45	H	-4.1681	-3.2728	0.9492

$[Rh(oac)_4C(COOMe)(IAr)]^+$

	Atom	X	Y	Z
1	Rh	0.9969	0.0698	-0.1772
2	O	-0.5649	-1.0344	0.5598
3	C	-0.3349	-2.1357	1.1749
4	C	-1.5511	-2.9072	1.6119
5	O	2.6716	1.0657	-0.8345
6	C	3.8341	0.6239	-0.5219
7	O	4.0659	-0.4237	0.1539
8	Rh	2.4916	-1.5710	0.8218
9	O	2.4584	-2.5721	-0.9718
10	C	1.7547	-2.1261	-1.9257
11	C	1.7626	-2.8600	-3.2377
12	O	1.1086	1.0146	1.6664
13	C	1.7988	0.5331	2.6318
14	C	1.7798	1.3228	3.9130
15	O	1.0332	-1.0666	-1.8713
16	C	5.0022	1.4330	-1.0183
17	O	2.4838	-0.5312	2.5853
18	O	0.8135	-2.6108	1.4232
19	H	2.2208	2.3087	3.7346
20	H	2.1717	-3.8629	-3.1099
21	H	2.3852	-2.3055	-3.9485
22	H	0.7503	-2.9091	-3.6457
23	H	-2.1942	-2.2645	2.2204
24	H	-1.2624	-3.7926	2.1787
25	H	-2.1227	-3.2018	0.7260
26	H	5.9402	1.0197	-0.6469
27	H	5.0040	1.4282	-2.1131
28	H	4.8923	2.4713	-0.6912
29	H	0.7452	1.4738	4.2346
30	H	2.3416	0.8023	4.6891
31	C	-3.4621	-2.4066	-2.2739
32	C	-4.2053	-1.9416	-1.1914
33	C	-3.8735	-0.7302	-0.5644
34	C	-2.7720	-0.0387	-1.0656
35	C	-2.0268	-0.4531	-2.1520
36	C	-2.3856	-1.6628	-2.7570
37	C	-4.6830	-0.1856	0.5539
38	O	-5.5761	-1.0426	1.0249
39	C	-6.4241	-0.5662	2.0972
40	I	-2.1506	1.7945	-0.0607
41	C	-0.0753	1.5850	-0.6828
42	C	0.4984	2.8895	-1.1180
43	O	0.4479	3.1383	-2.3087
44	O	1.0492	3.6145	-0.1644
45	C	1.7576	4.8100	-0.5941
46	O	-4.5348	0.9549	0.9851
47	H	-1.1754	0.1087	-2.5130
48	H	-1.8137	-2.0115	-3.6102
49	H	-3.7330	-3.3432	-2.7487
50	H	-5.0573	-2.4992	-0.8218
51	H	-6.9998	0.2972	1.7592

52	H	-5.8126	-0.2936	2.9591
53	H	1.0742	5.4769	-1.1216
54	H	2.5873	4.5236	-1.2425
55	H	2.1191	5.2665	0.3244
56	H	-7.0785	-1.4028	2.3329

$Rh(oac)_4C(COOMe)(IAr.PF_6)$

	Atom	X	Y	Z
1	C	-0.4478	-0.4369	-1.1884
2	C	-1.0953	-1.5421	-1.9464
3	C	-1.8884	-3.7450	-2.0294
4	H	-2.8764	-3.4094	-2.3434
5	H	-1.2803	-4.0308	-2.8893
6	O	-1.2361	-2.6752	-1.3005
7	O	-1.3423	-1.3159	-3.1212
8	I	-1.8569	1.1509	-0.7515
9	C	-0.4172	2.6684	-1.2663
10	C	-0.3609	3.8530	-0.5266
11	C	0.4423	2.4011	-2.3181
12	C	0.6383	4.7804	-0.8518
13	C	1.4232	3.3485	-2.6313
14	H	0.3816	1.4743	-2.8746
15	C	1.5265	4.5280	-1.8963
16	H	0.6960	5.7032	-0.2870
17	H	2.1036	3.1490	-3.4522
18	H	2.2893	5.2590	-2.1420
19	C	-1.3552	4.1312	0.5393
20	O	-2.4080	3.5133	0.6461
21	O	-0.9860	5.1125	1.3581
22	C	-1.9184	5.4491	2.4112
23	H	-2.8676	5.7720	1.9799
24	H	-2.0788	4.5822	3.0549
25	H	-1.4448	6.2598	2.9613
26	P	-4.2648	-1.5414	0.4406
27	F	-5.7235	-1.7395	-0.2455
28	F	-3.6370	-1.1503	-1.0545
29	F	-2.7733	-1.3100	1.0896
30	F	-4.5805	0.0528	0.6718
31	F	-3.9012	-3.1047	0.1669
32	F	-4.8623	-1.8984	1.9063
33	H	-1.9704	-4.5594	-1.3142
34	C	1.6204	1.4019	1.8761
35	C	1.2398	2.6329	2.6550
36	C	3.7682	0.6277	-1.0833
37	C	4.6269	1.4896	-1.9684
38	O	0.8778	1.1255	0.8694
39	O	2.6241	0.7273	2.2555
40	O	2.5458	0.4897	-1.4408
41	O	4.2853	0.1162	-0.0453
42	Rh	1.2397	-0.5528	-0.2635
43	Rh	3.1168	-0.9934	1.2339
44	C	0.6797	-2.1618	2.1490
45	C	-0.2576	-2.9520	3.0229
46	O	0.1580	-1.6469	1.1047
47	O	1.9014	-2.0726	2.4842
48	C	2.7402	-2.9647	-0.8710
49	C	3.0097	-4.2349	-1.6336
50	O	1.7540	-2.2594	-1.2841
51	O	3.4799	-2.6913	0.1229
52	H	2.2414	-4.9711	-1.3722
53	H	2.9424	-4.0483	-2.7082
54	H	-0.1030	-4.0193	2.8273
55	H	-1.2906	-2.6927	2.7877
56	H	1.2278	3.5006	1.9897
57	H	1.9394	2.8011	3.4741
58	H	4.4396	1.2530	-3.0186

59	H	4.3534	2.5382	-1.8064
60	H	-0.0355	-2.7642	4.0761
61	H	0.2276	2.5061	3.0525
62	H	3.9914	-4.6349	-1.3769
63	H	5.6819	1.3521	-1.7288

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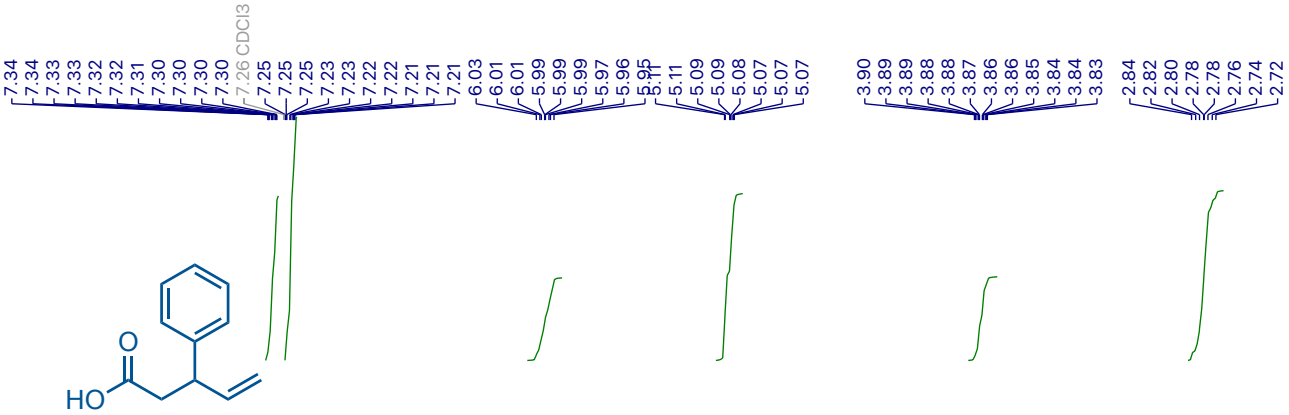
12. NMR Spectra



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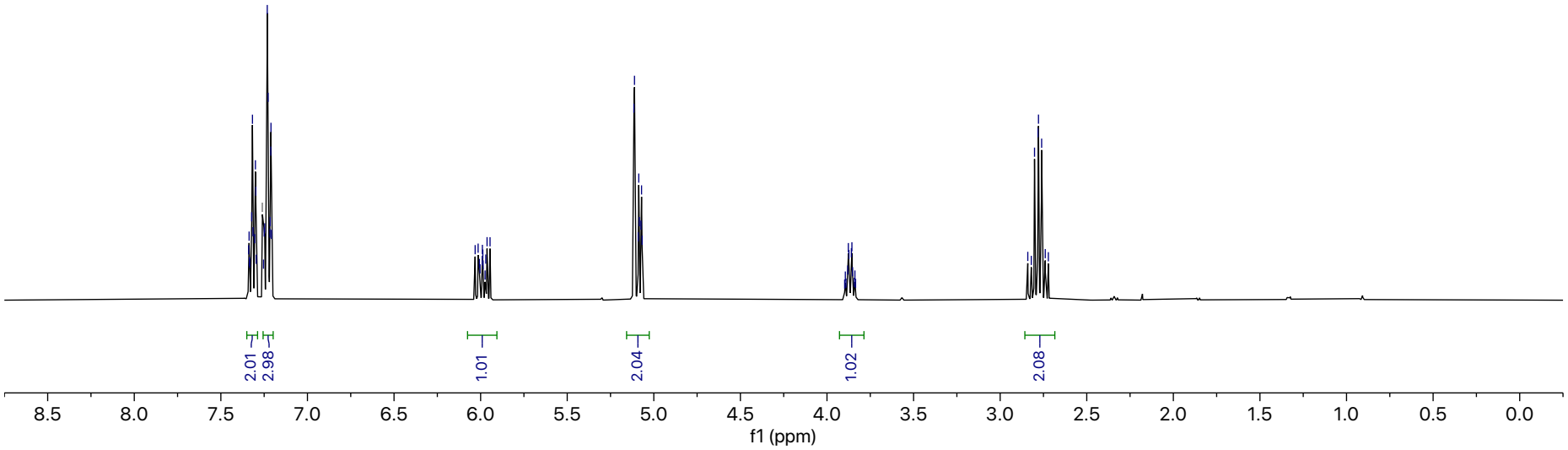

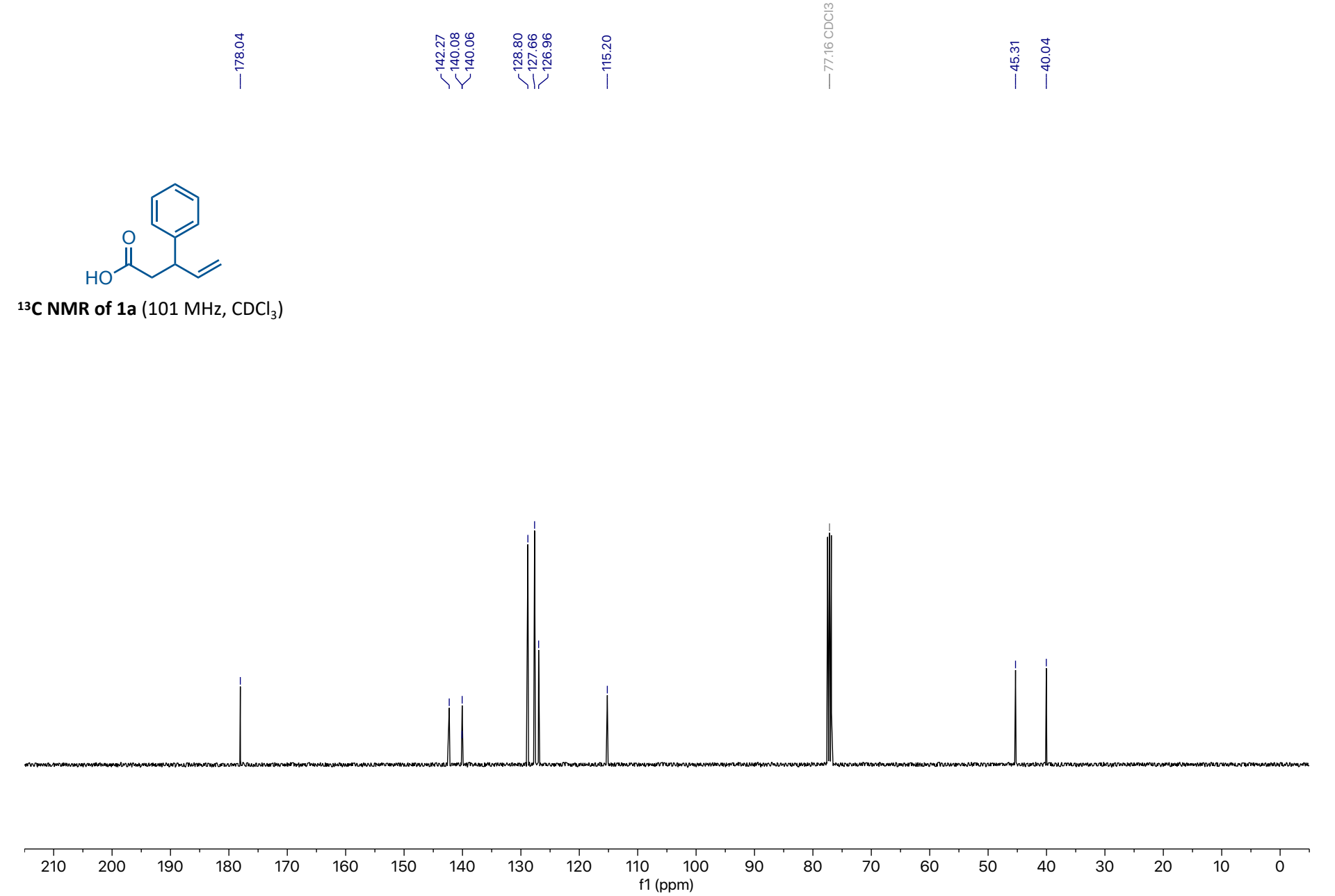

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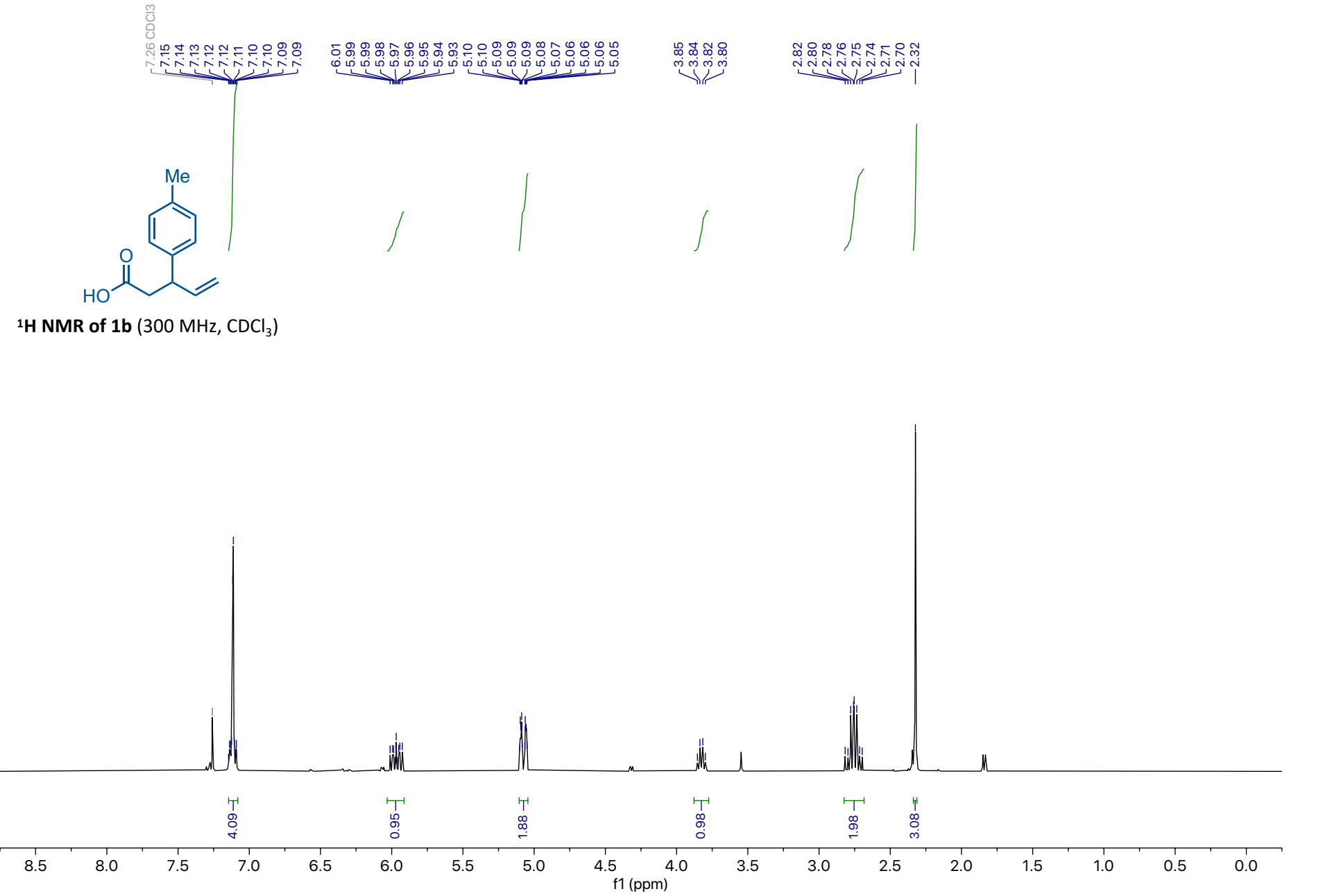

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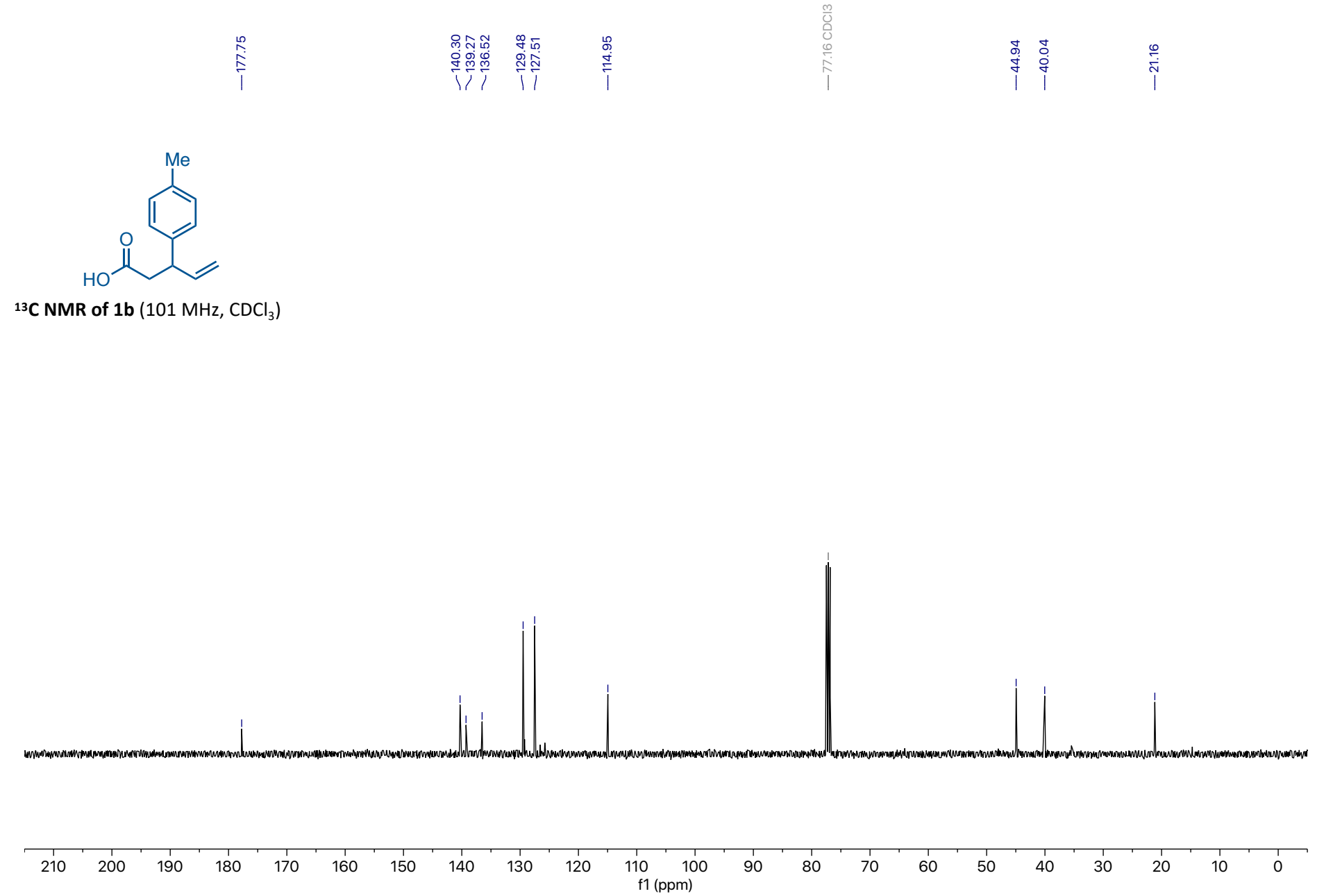

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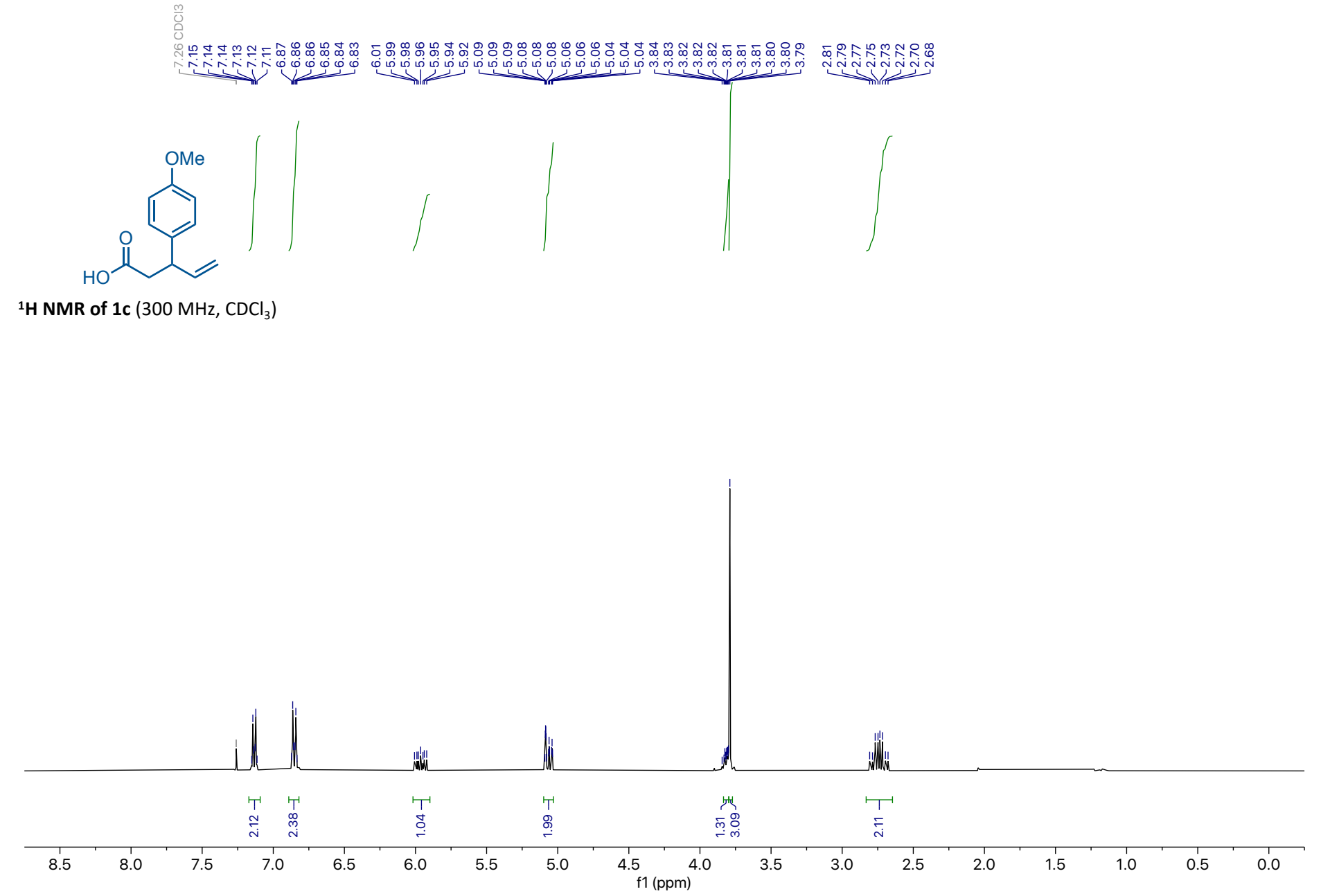

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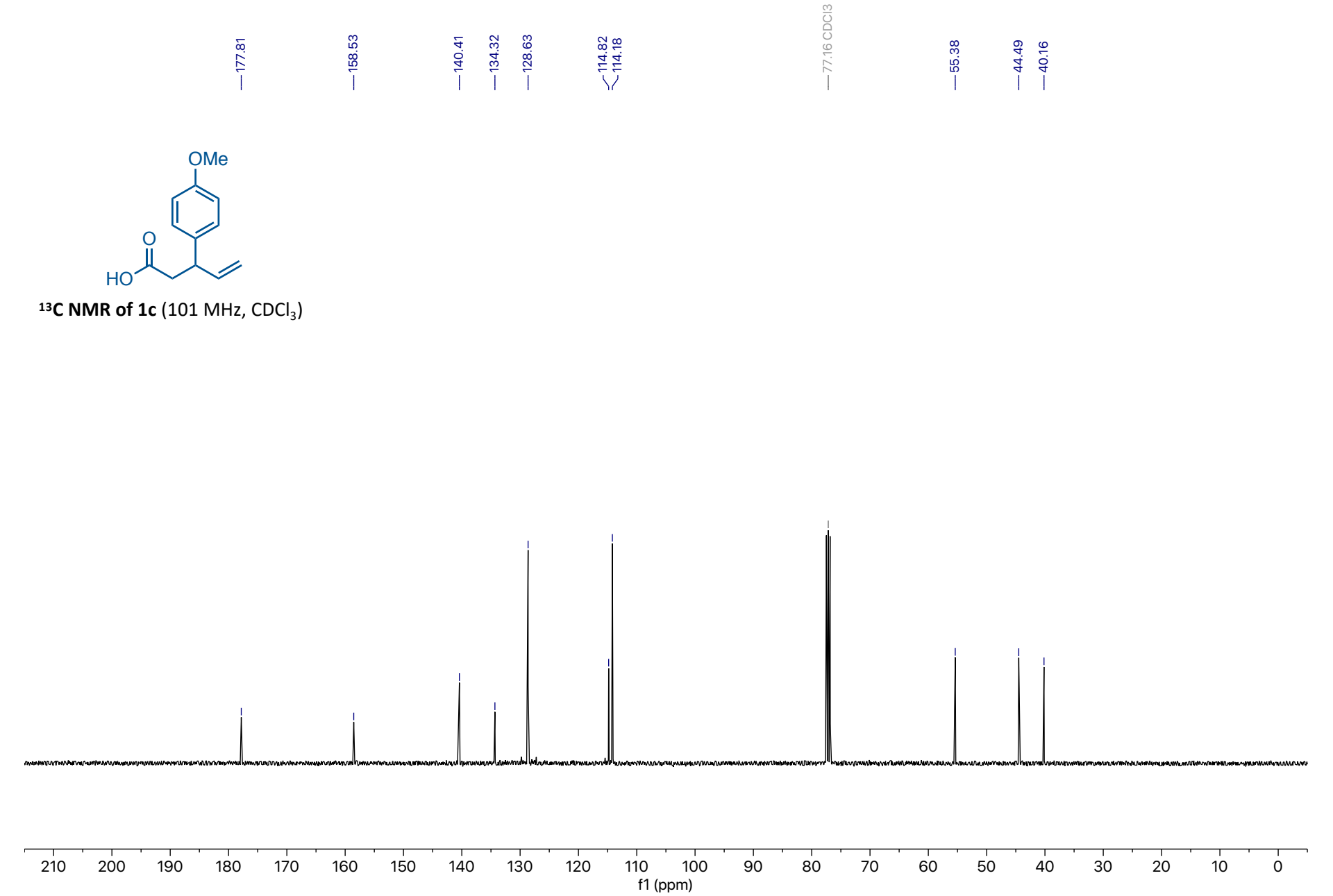

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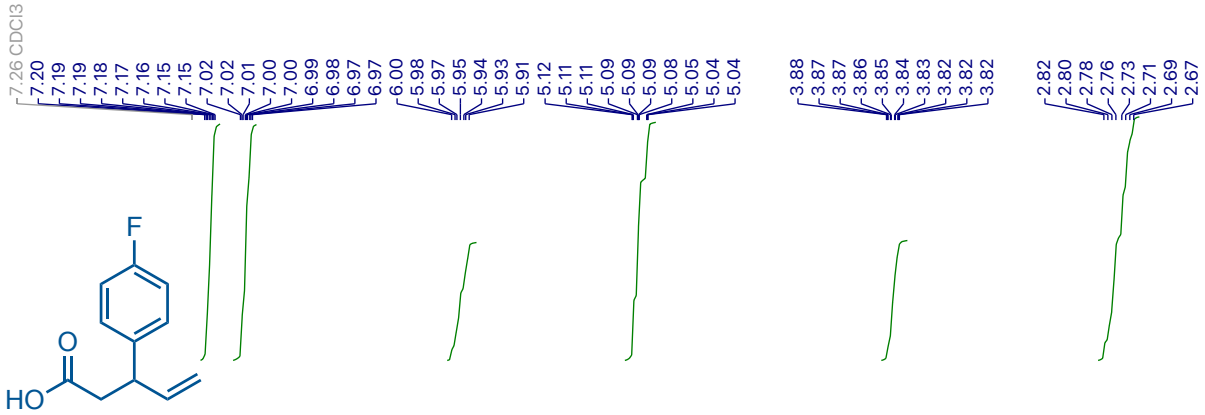

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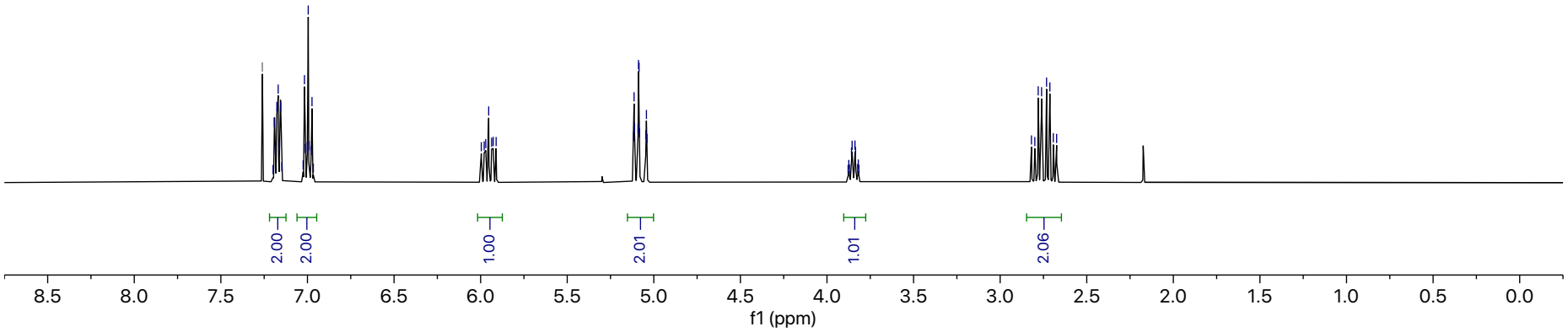

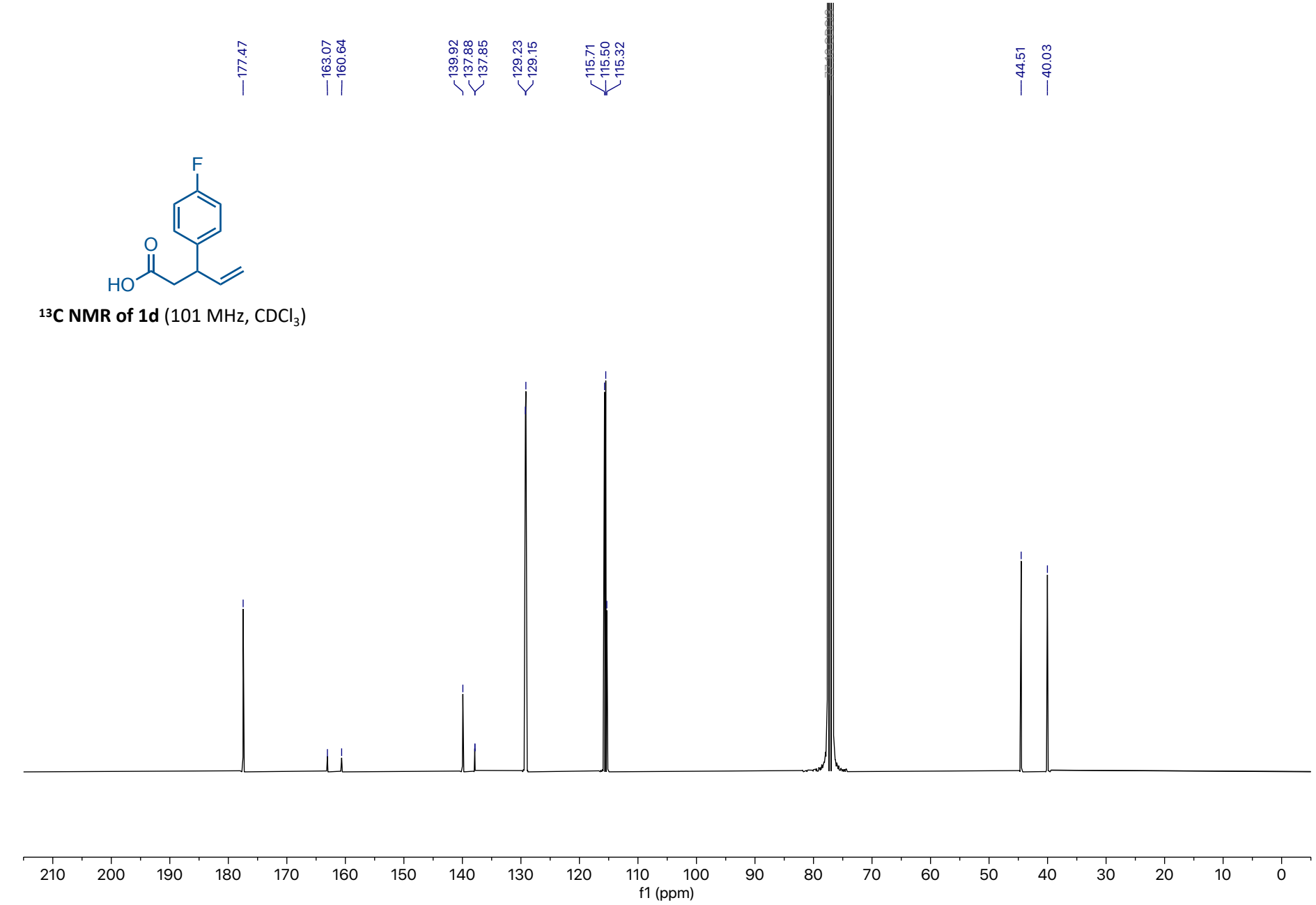

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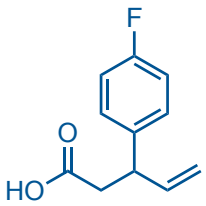

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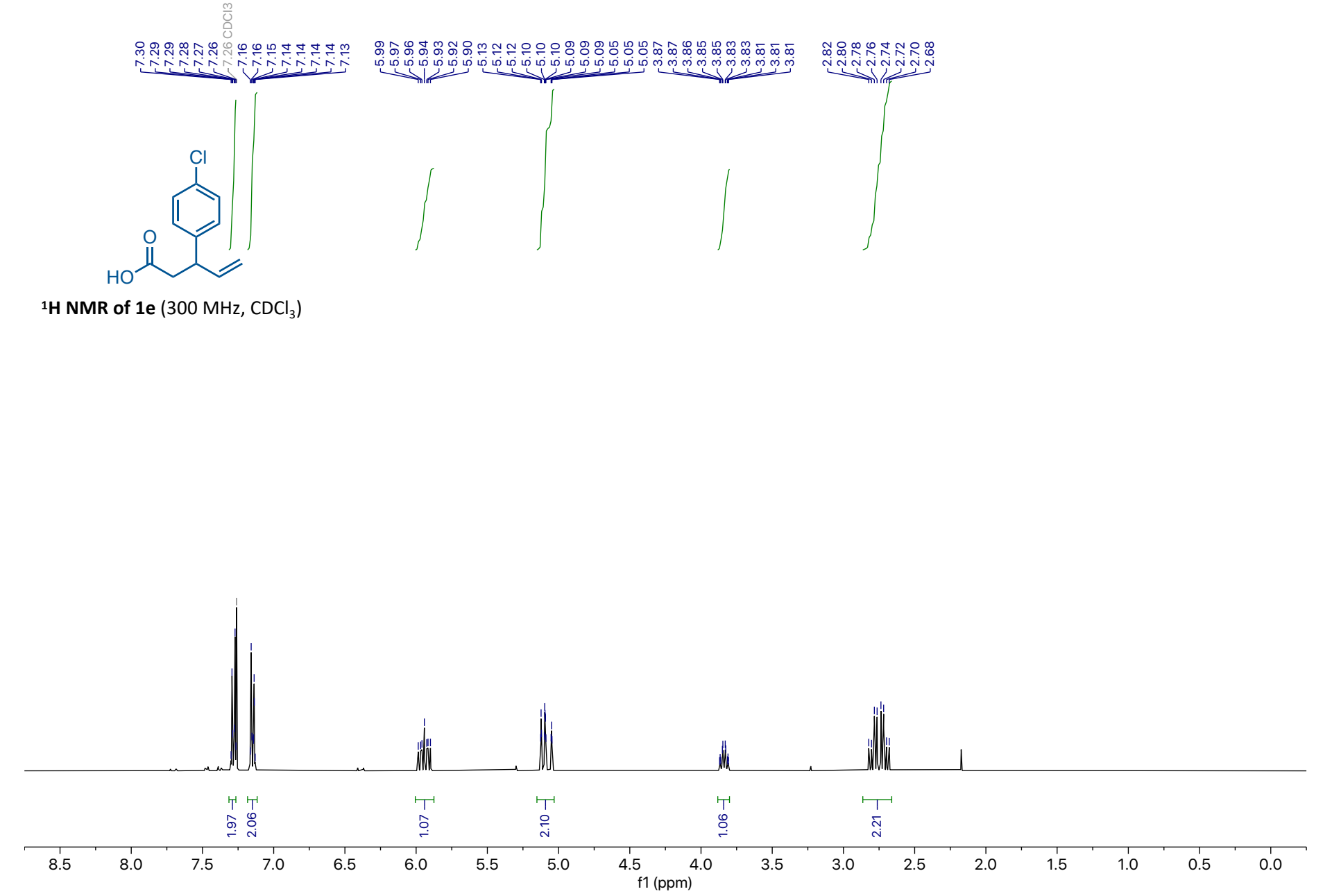
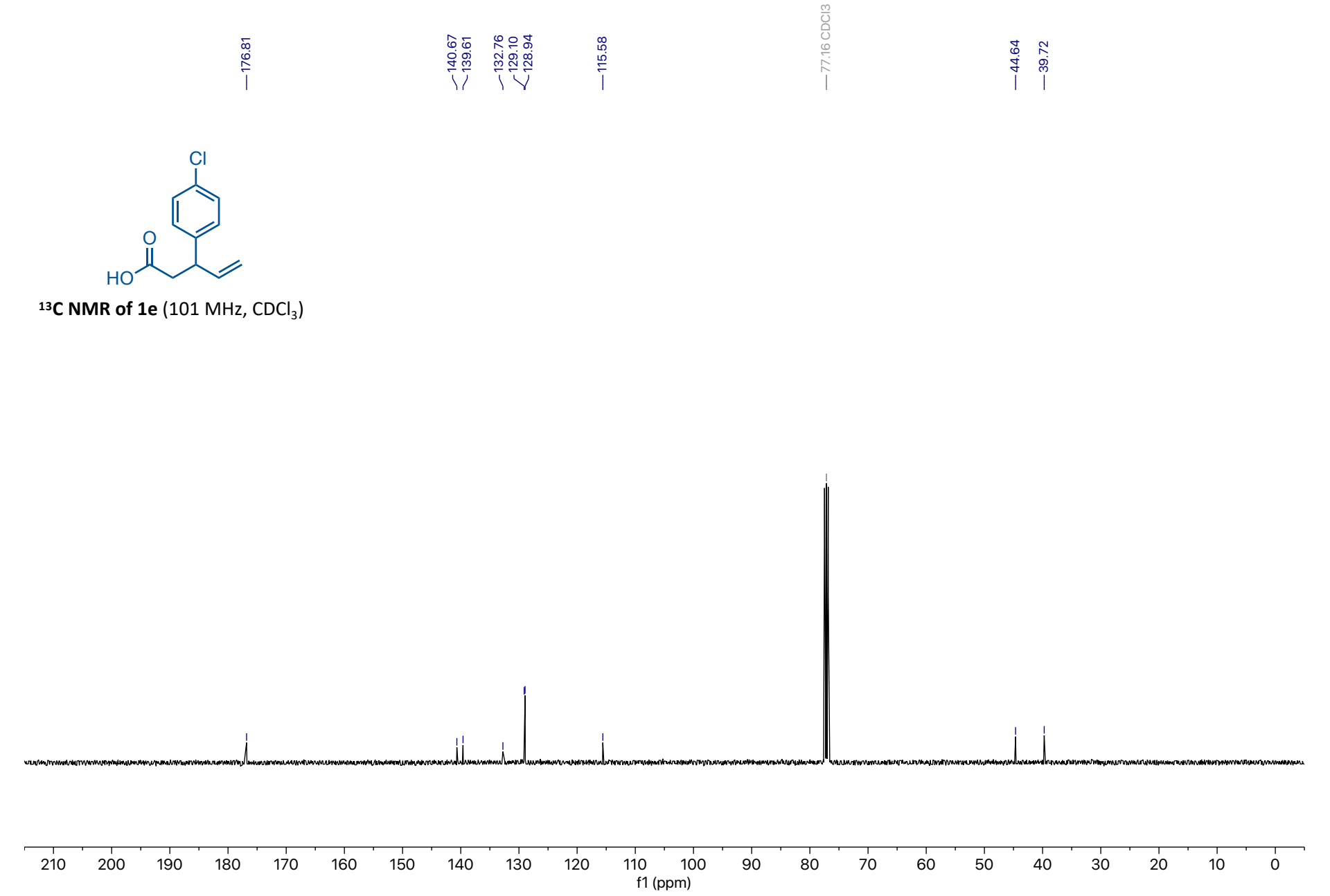
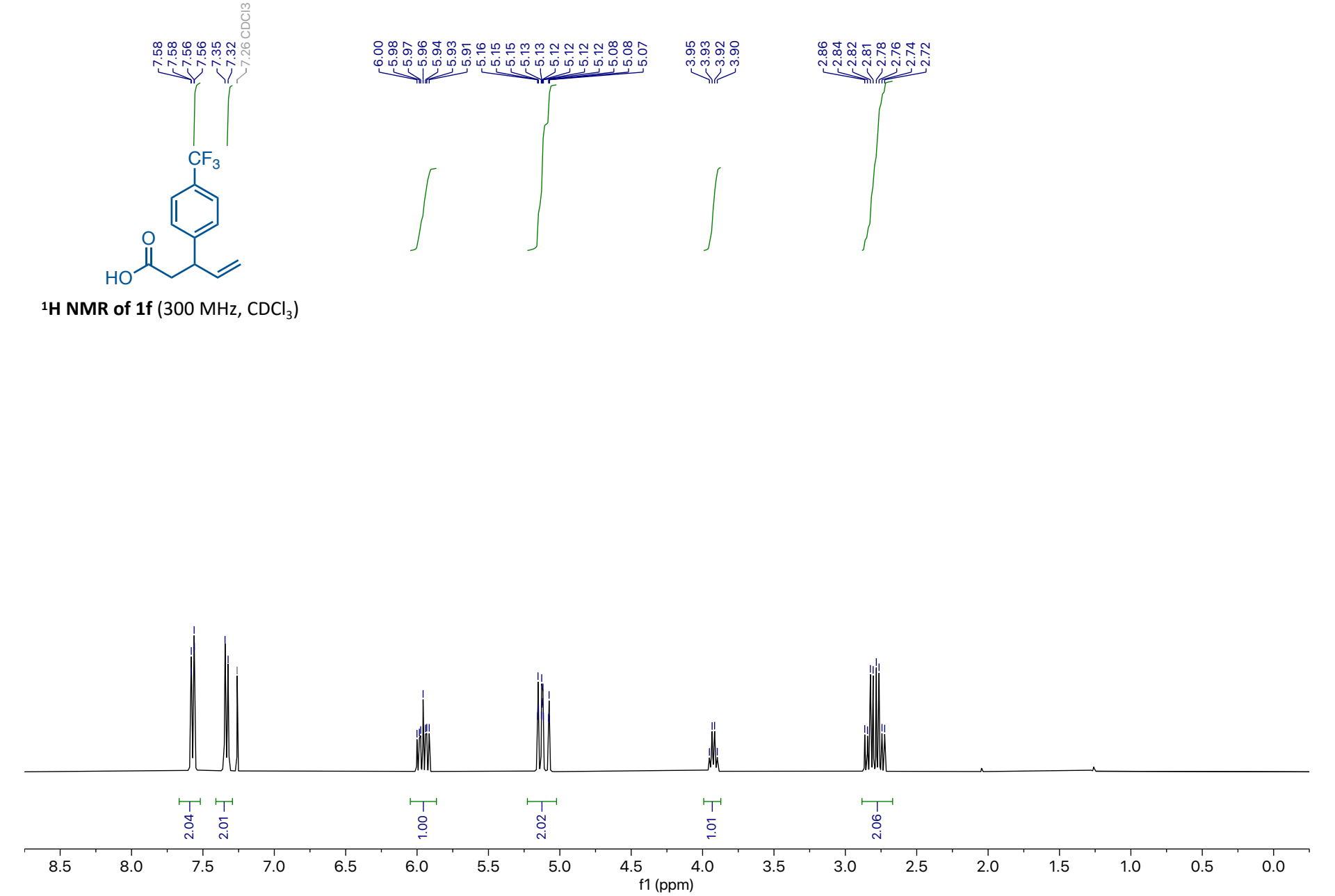


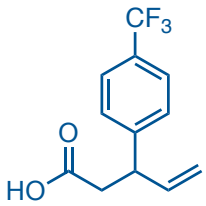
^{1}H NMR of 1e (300 MHz, $CDCl_3$)



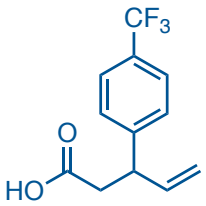
^{13}C NMR of 1e (101 MHz, $CDCl_3$)



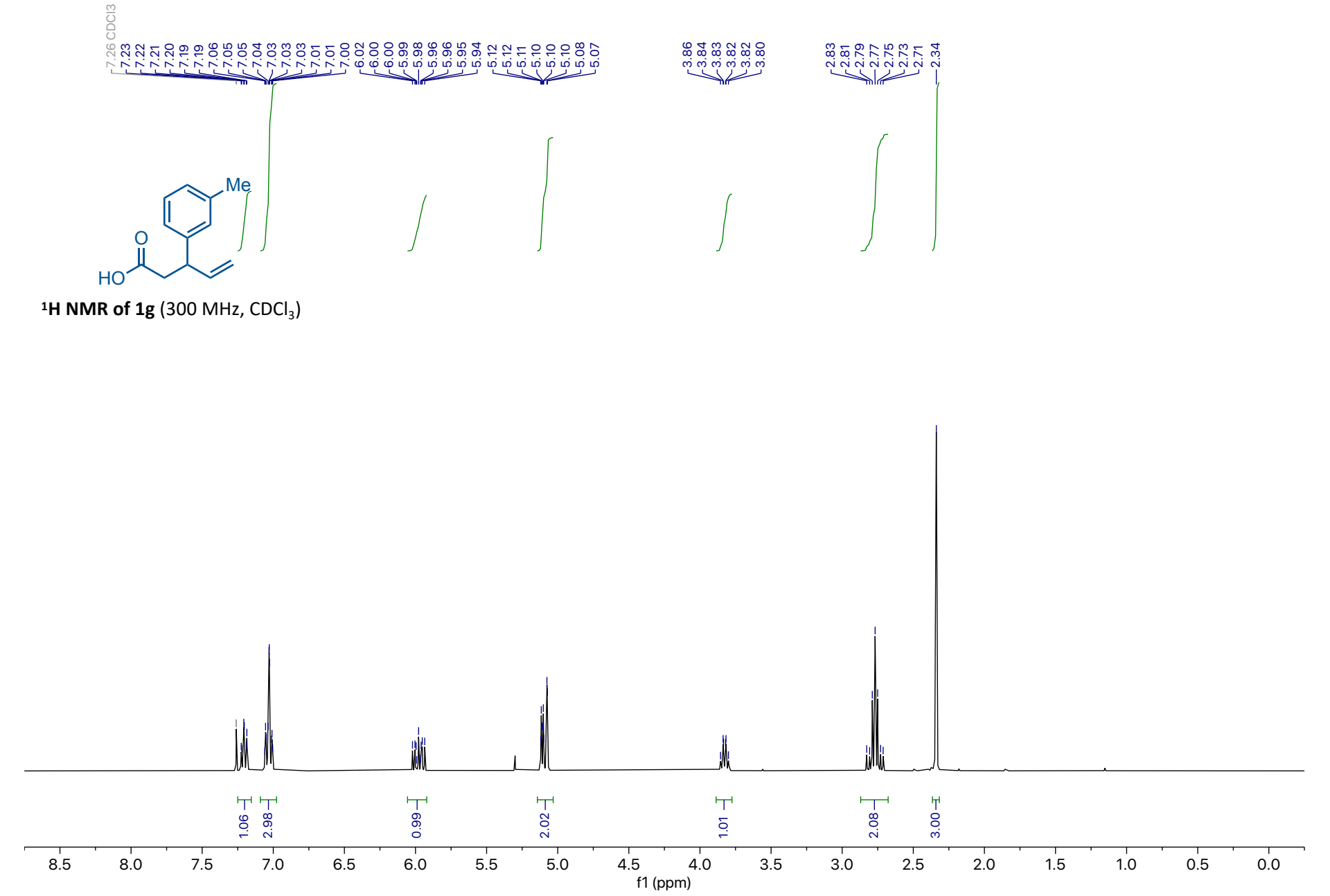
^{1}H NMR of 1f (300 MHz, $CDCl_3$)



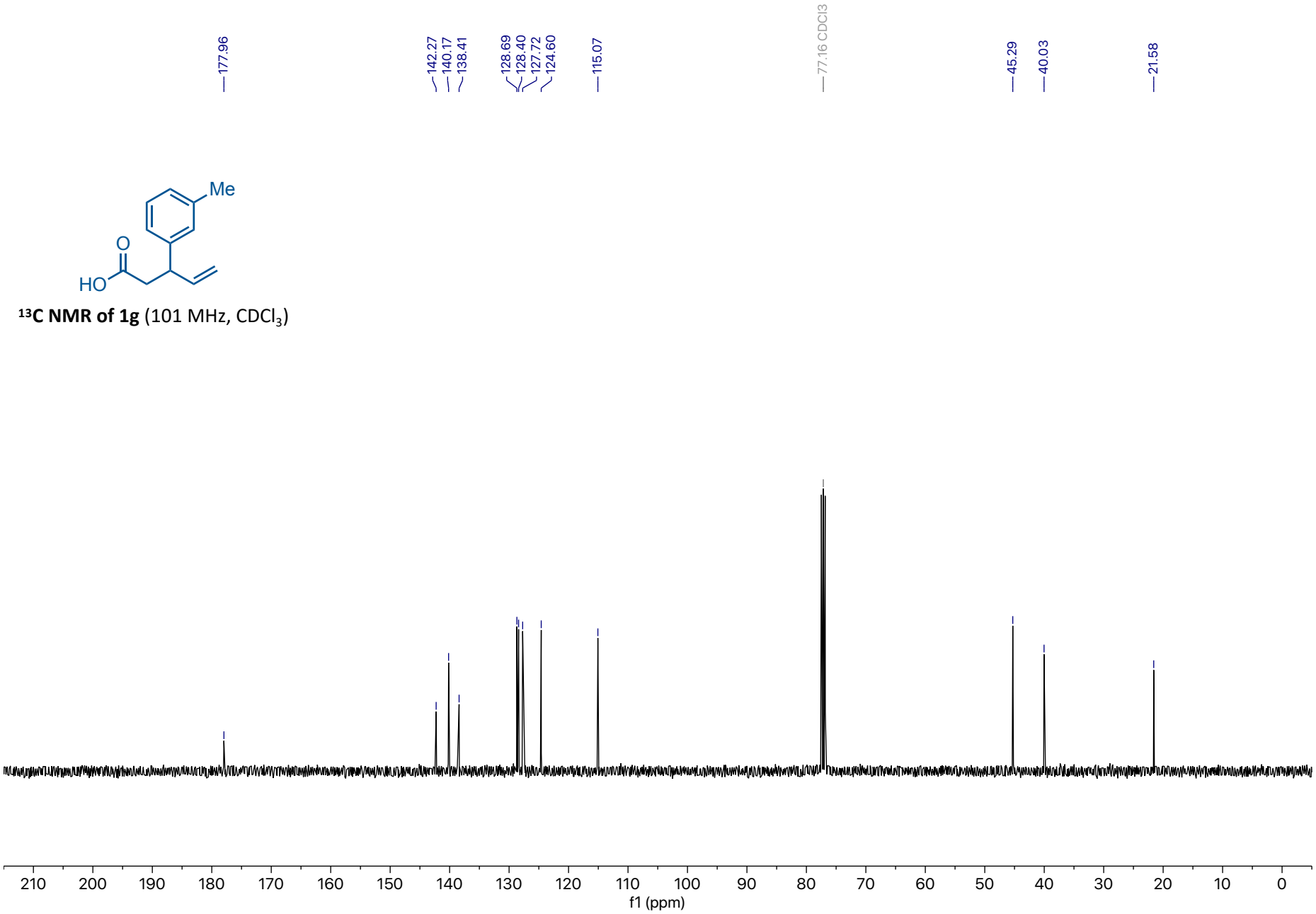
^{13}C NMR of 1f ($CDCl_3$)



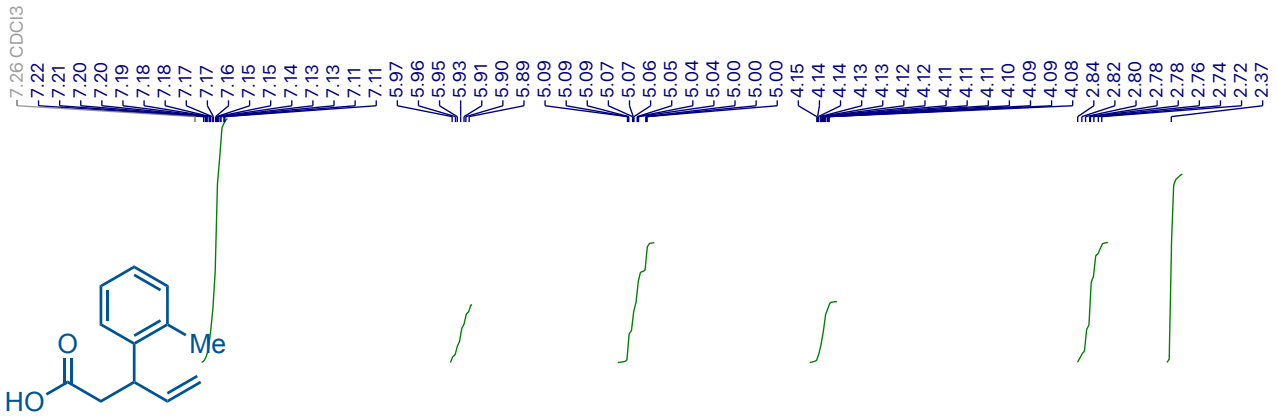
^{19}F NMR of 1f (282 MHz, $CDCl_3$)



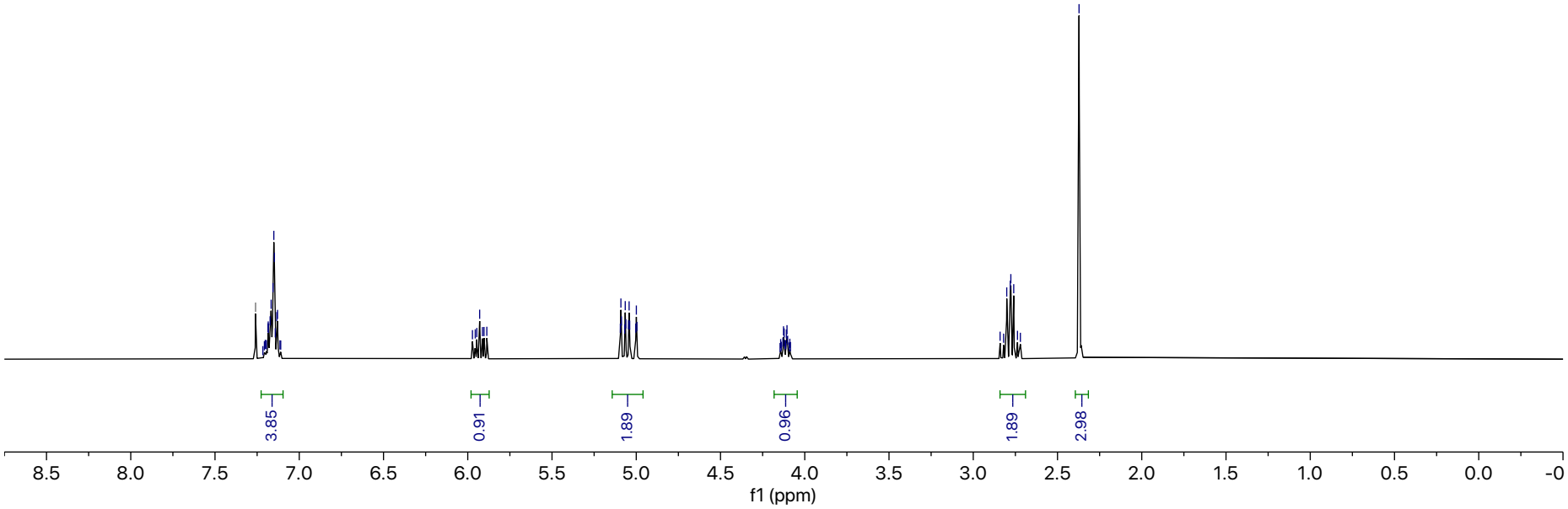
^{1}H NMR of 1g (300 MHz, $CDCl_3$)

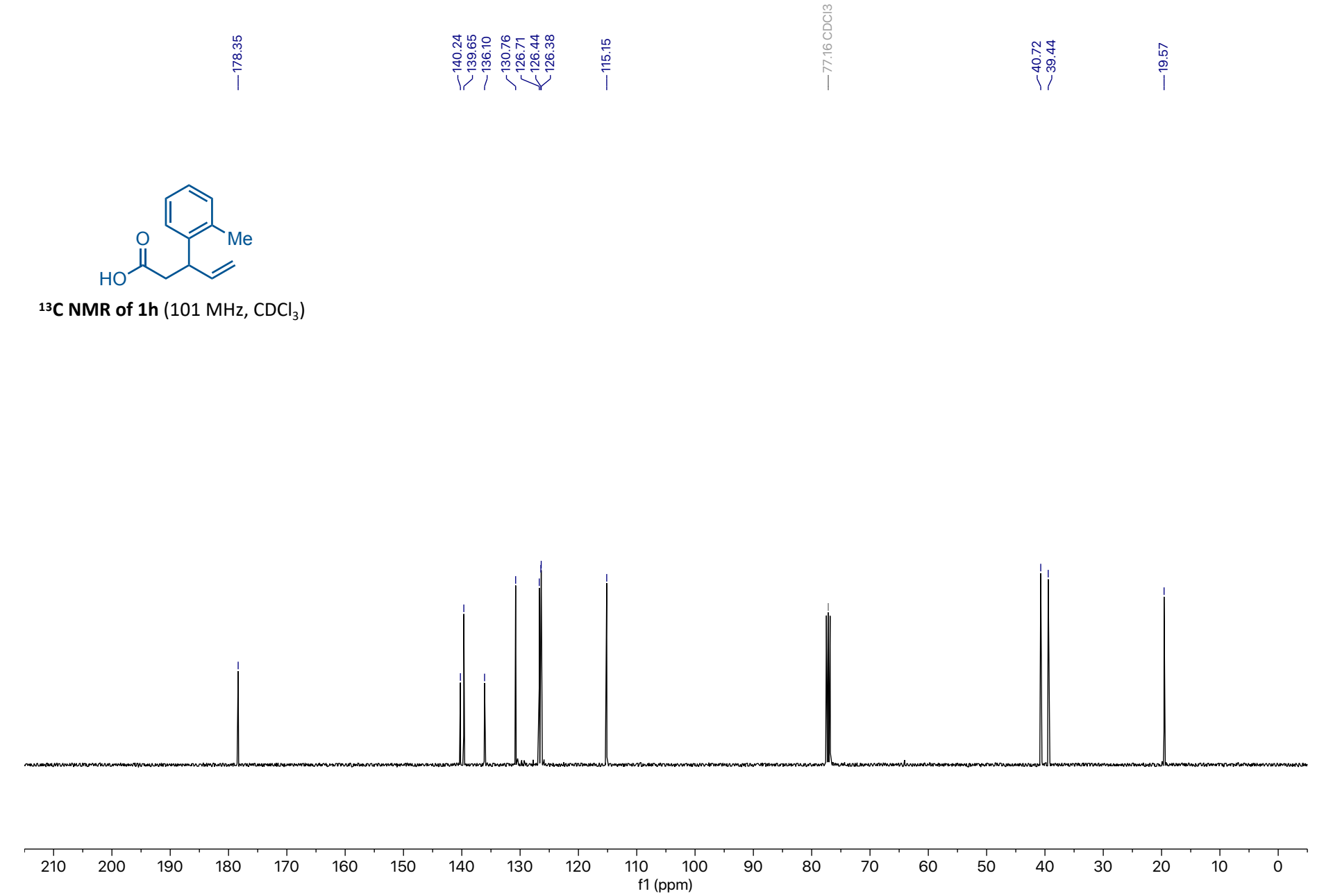


^{13}C NMR of 1g (101 MHz, $CDCl_3$)

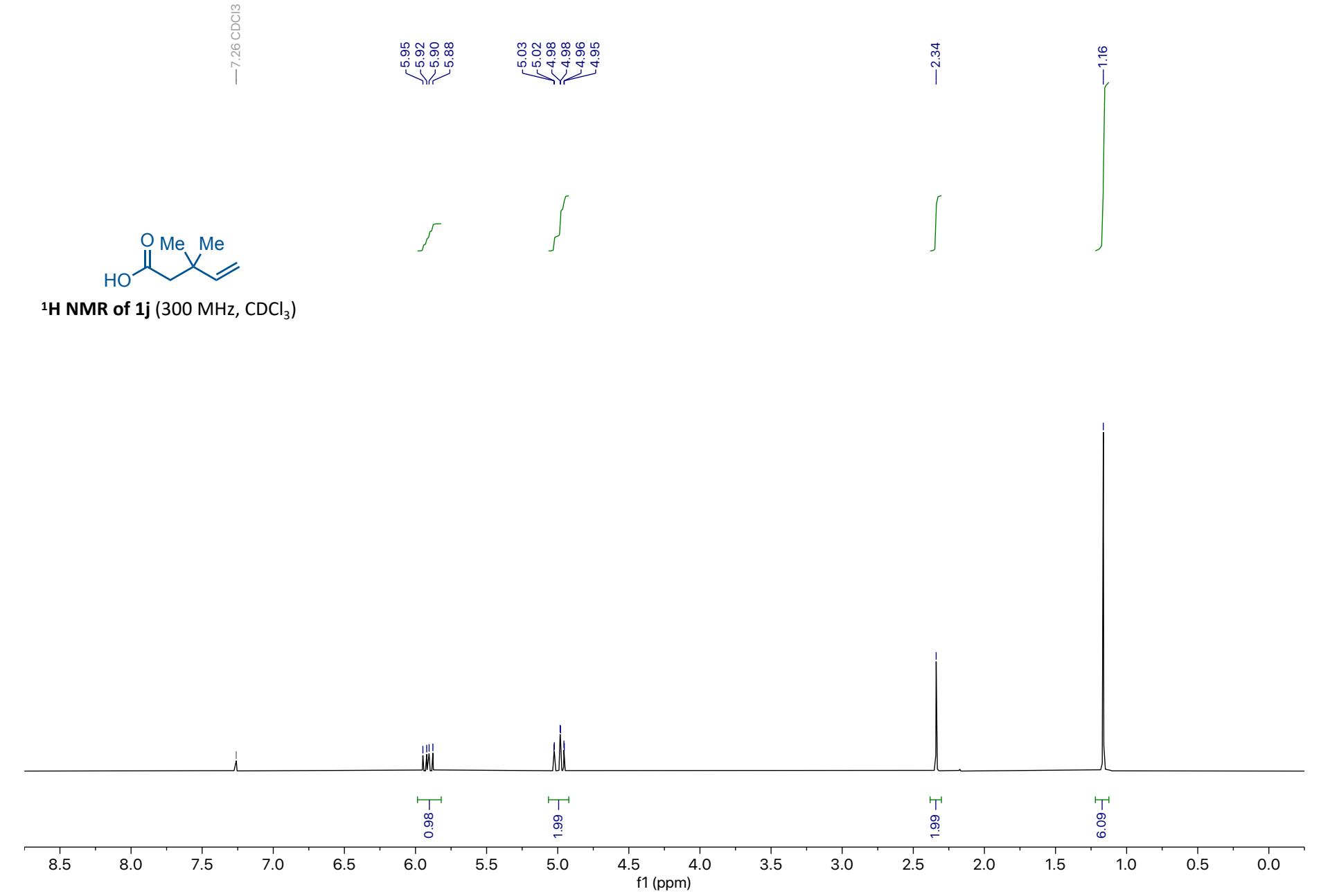


^{1}H NMR of 1h (300 MHz, $CDCl_3$)

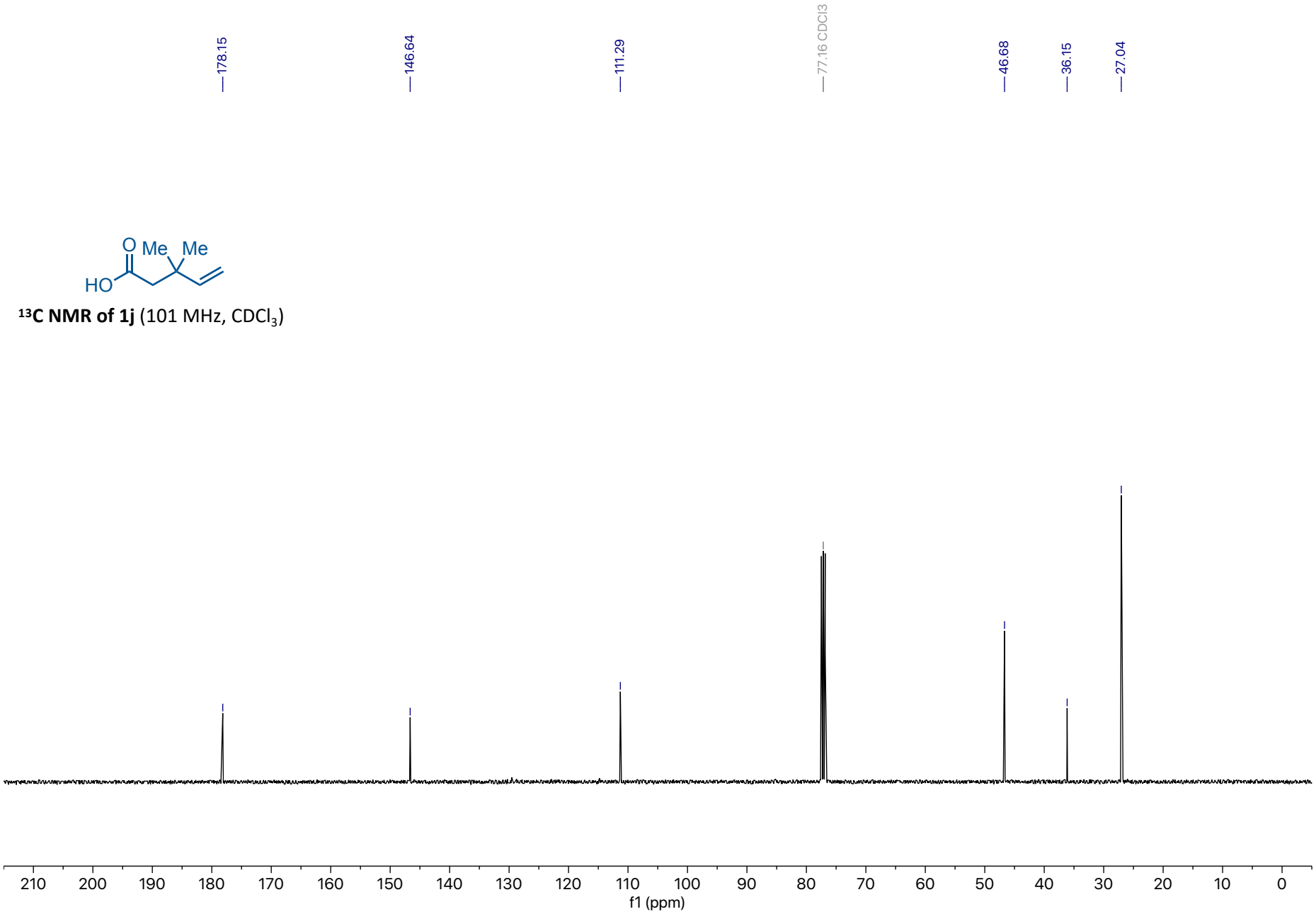




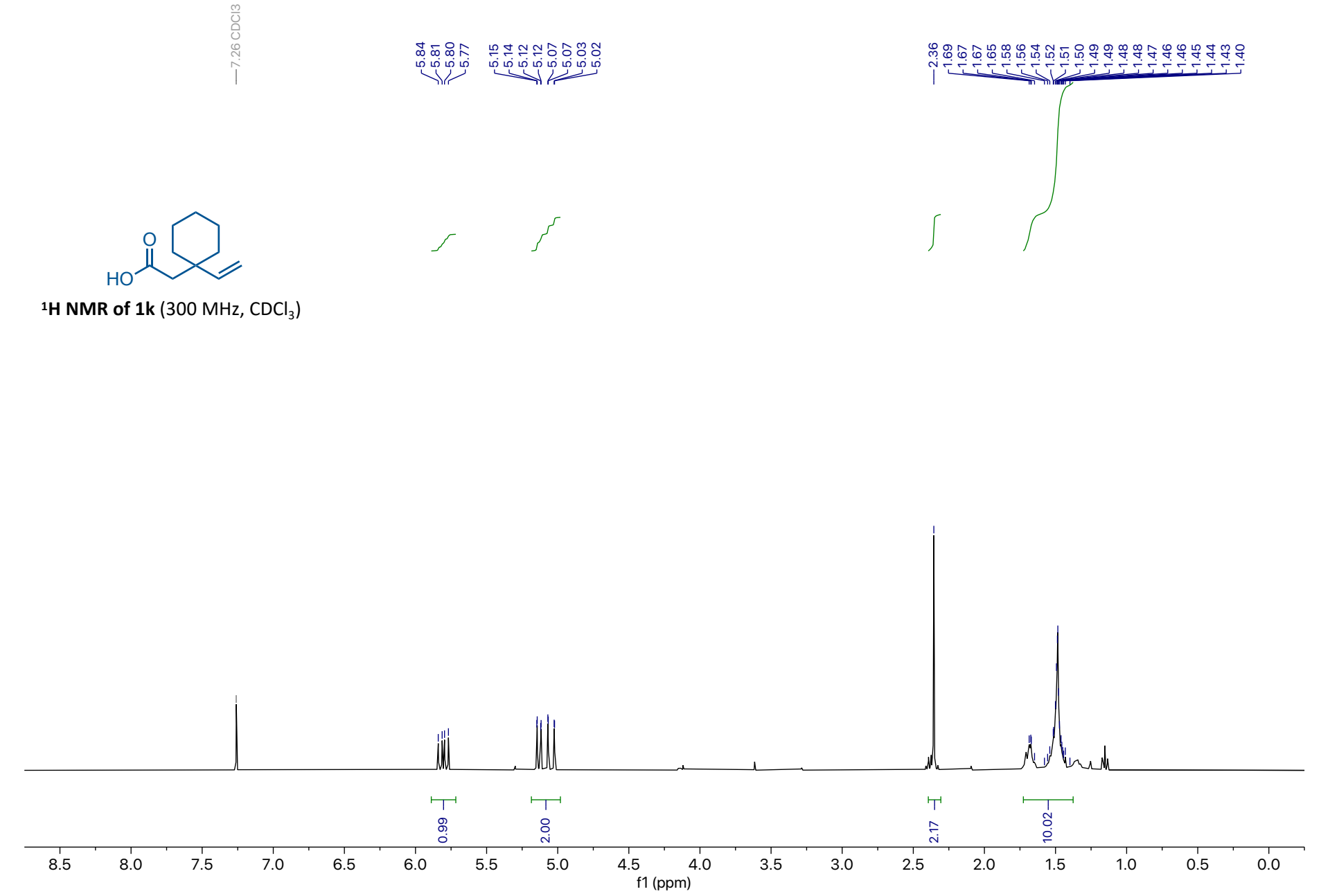
^{13}C NMR of 1h (101 MHz, $CDCl_3$)



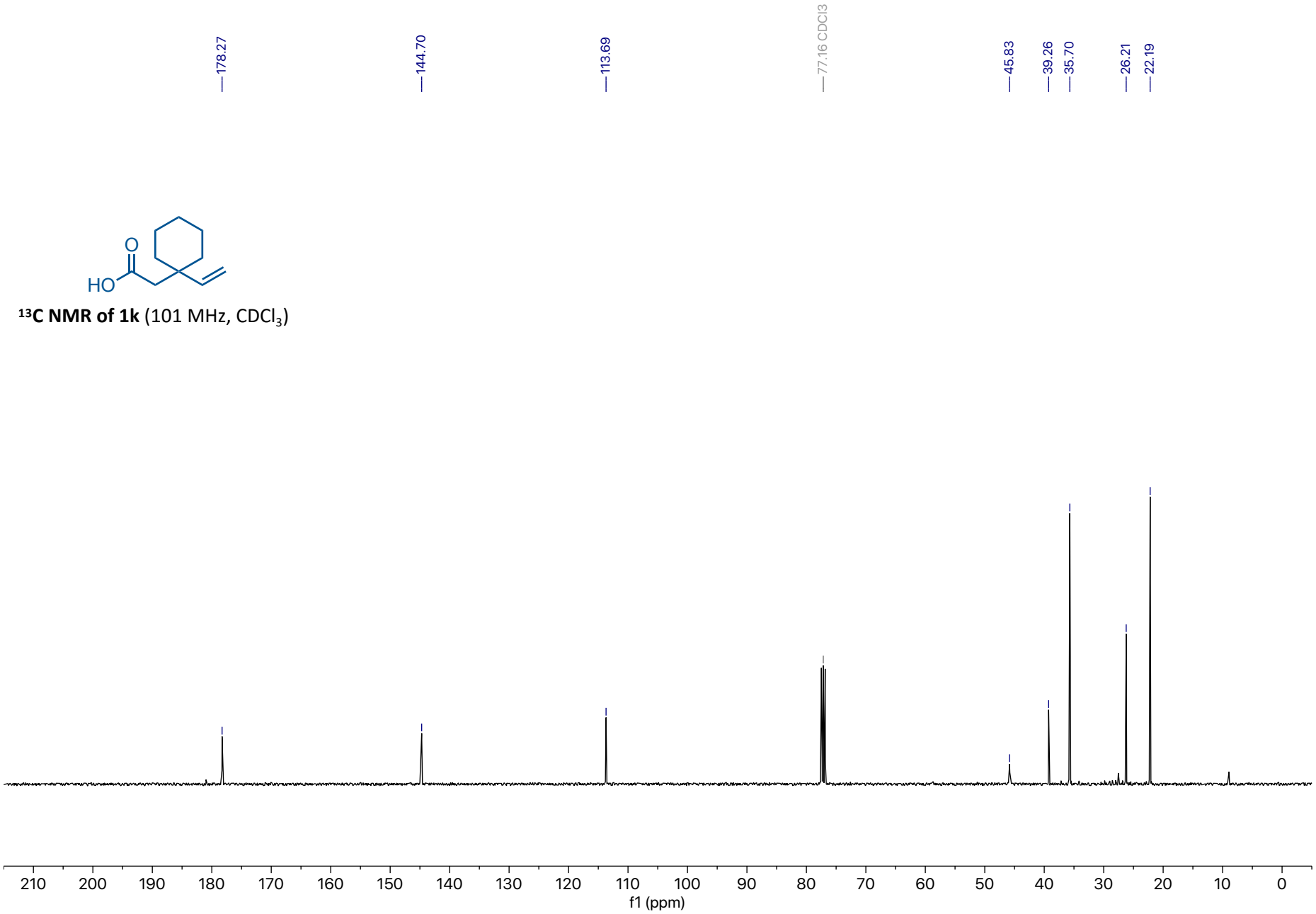
^{1}H NMR of 1j (300 MHz, $CDCl_3$)



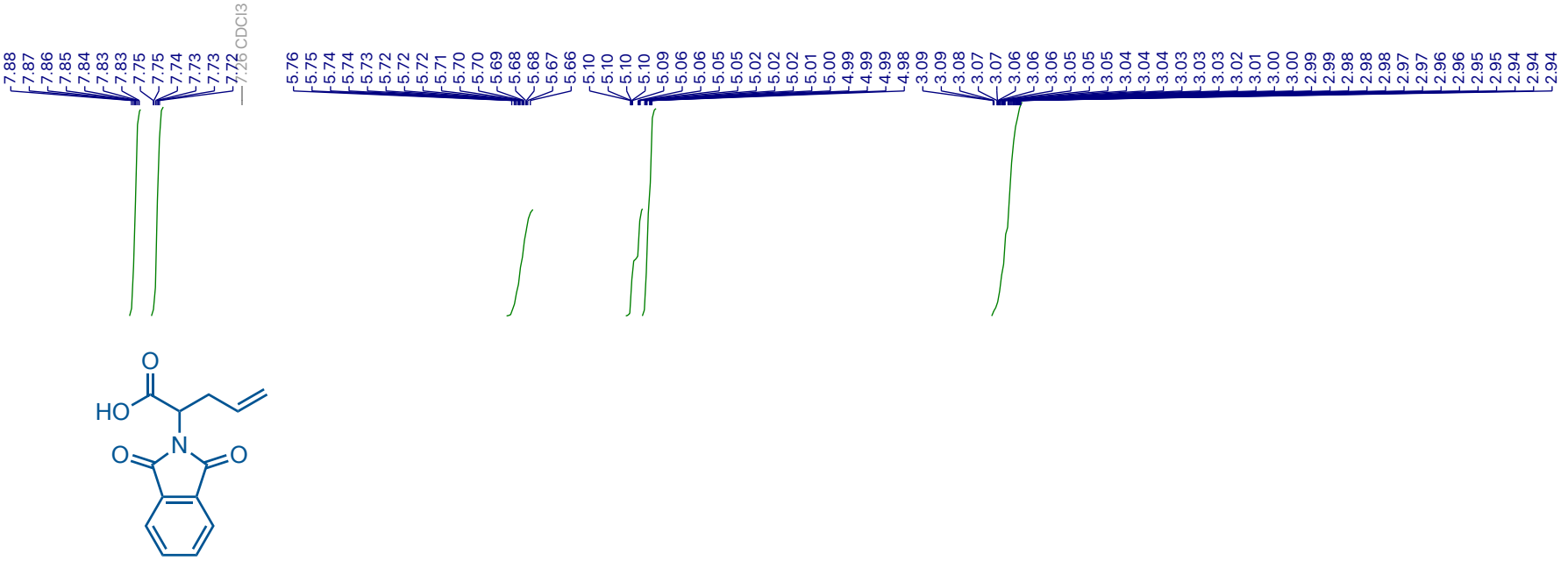
^{13}C NMR of 1j (101 MHz, $CDCl_3$)



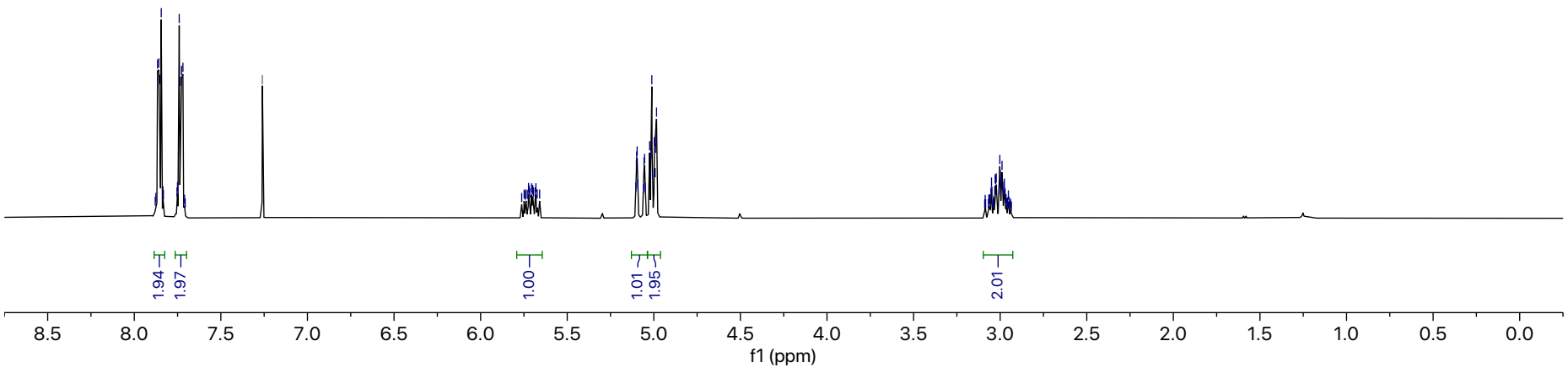
^{1}H NMR of 1k (300 MHz, $CDCl_3$)

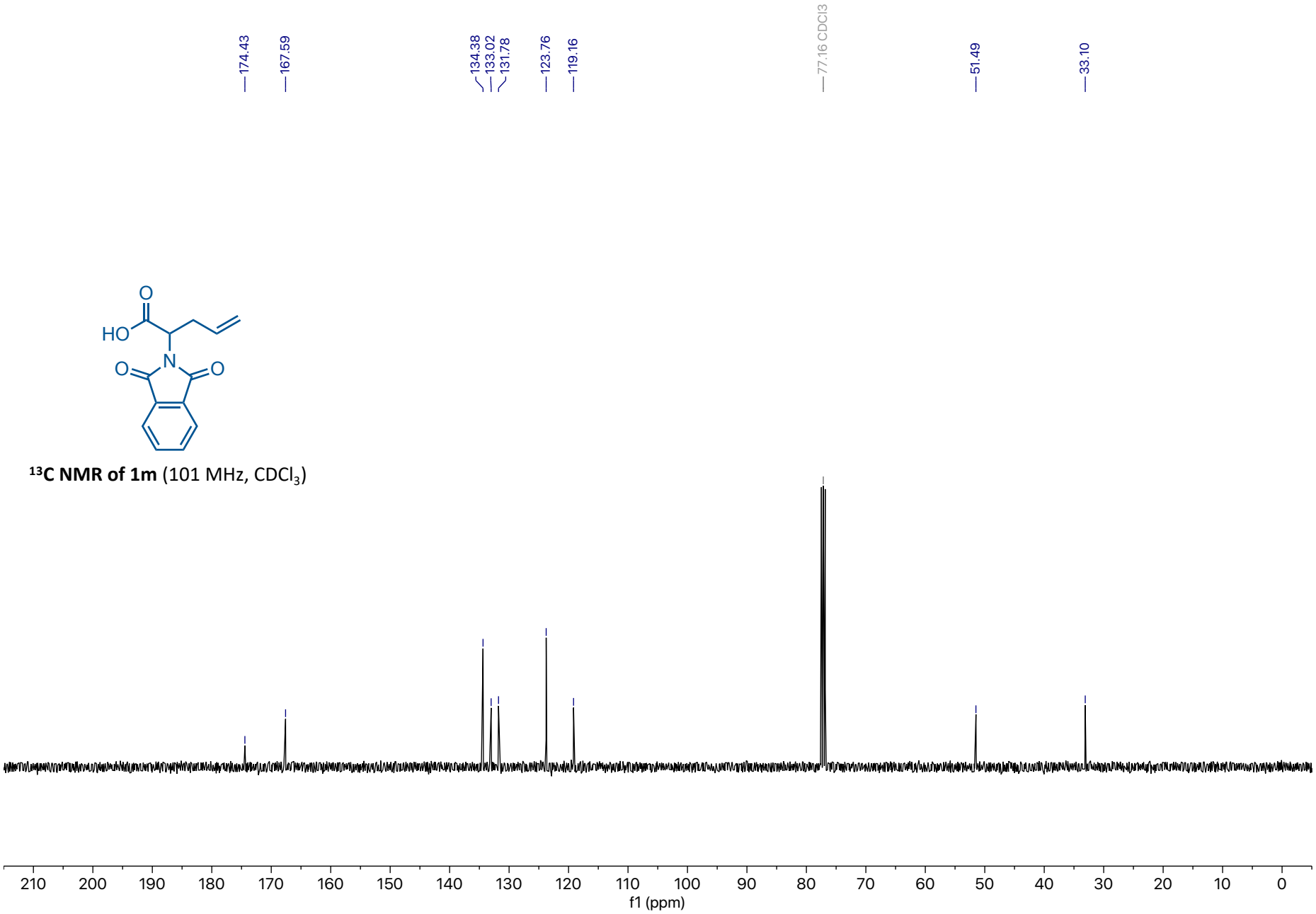


^{13}C NMR of 1k (101 MHz, $CDCl_3$)

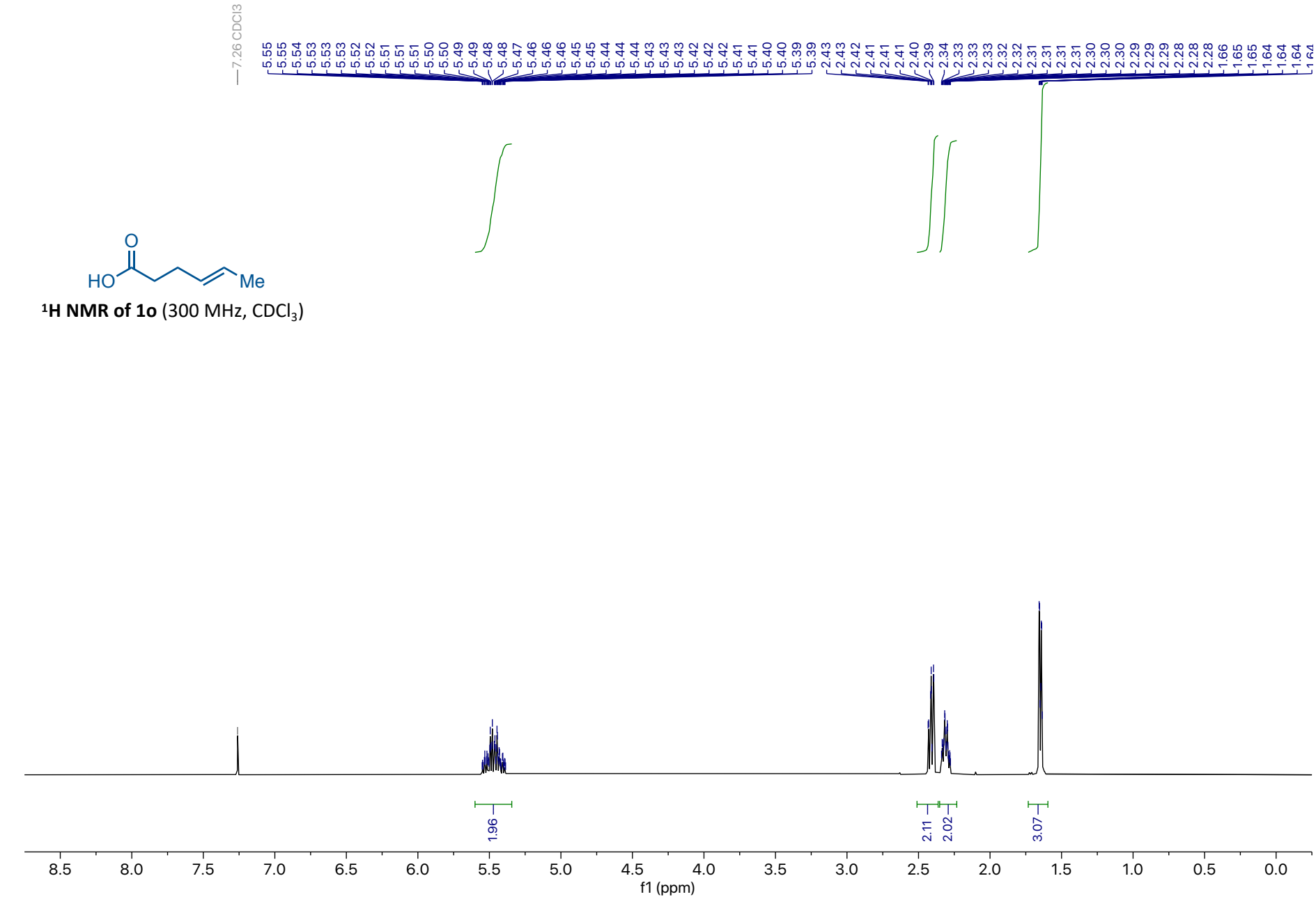


^{1}H NMR of 1m (300 MHz, $CDCl_3$)

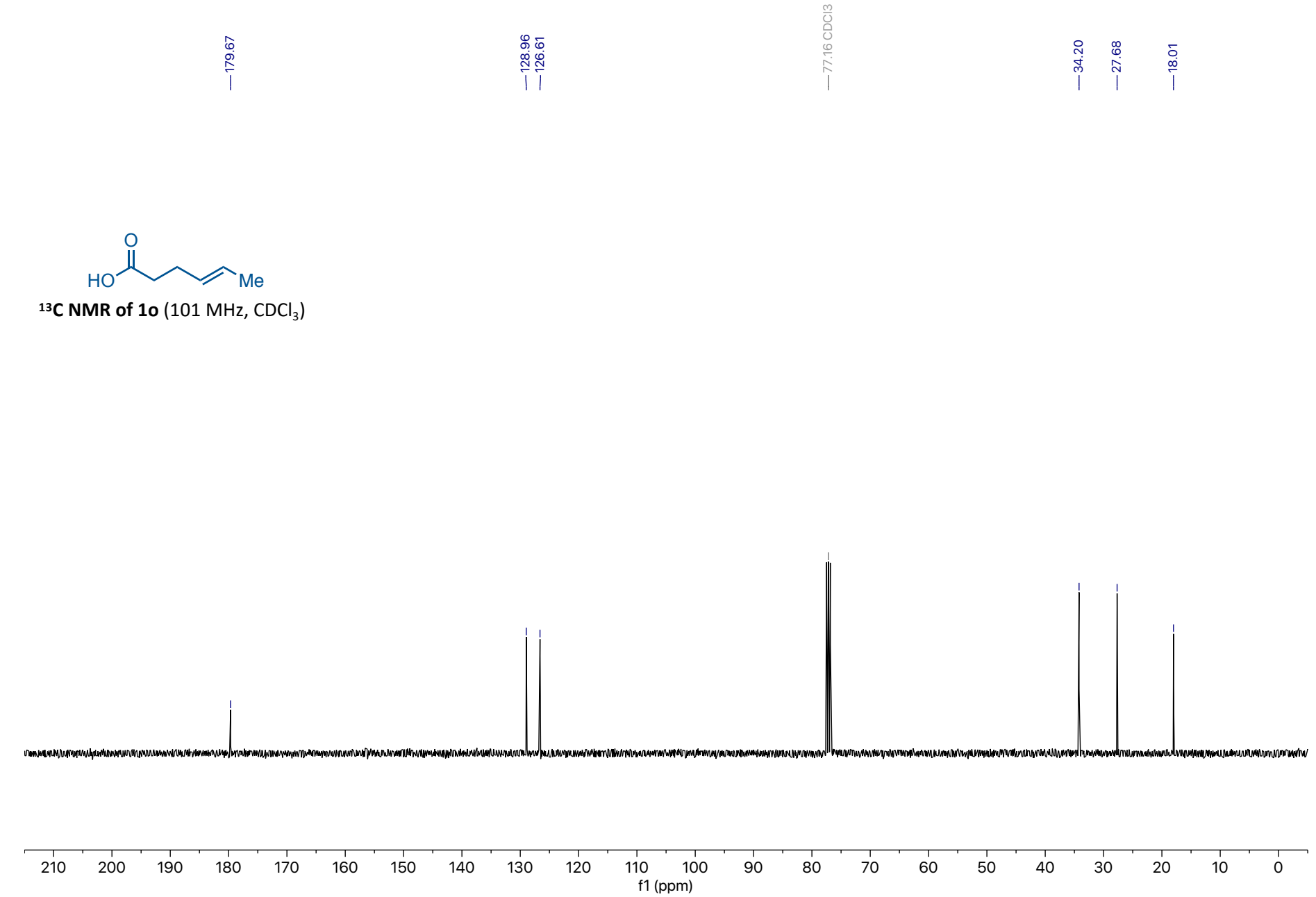




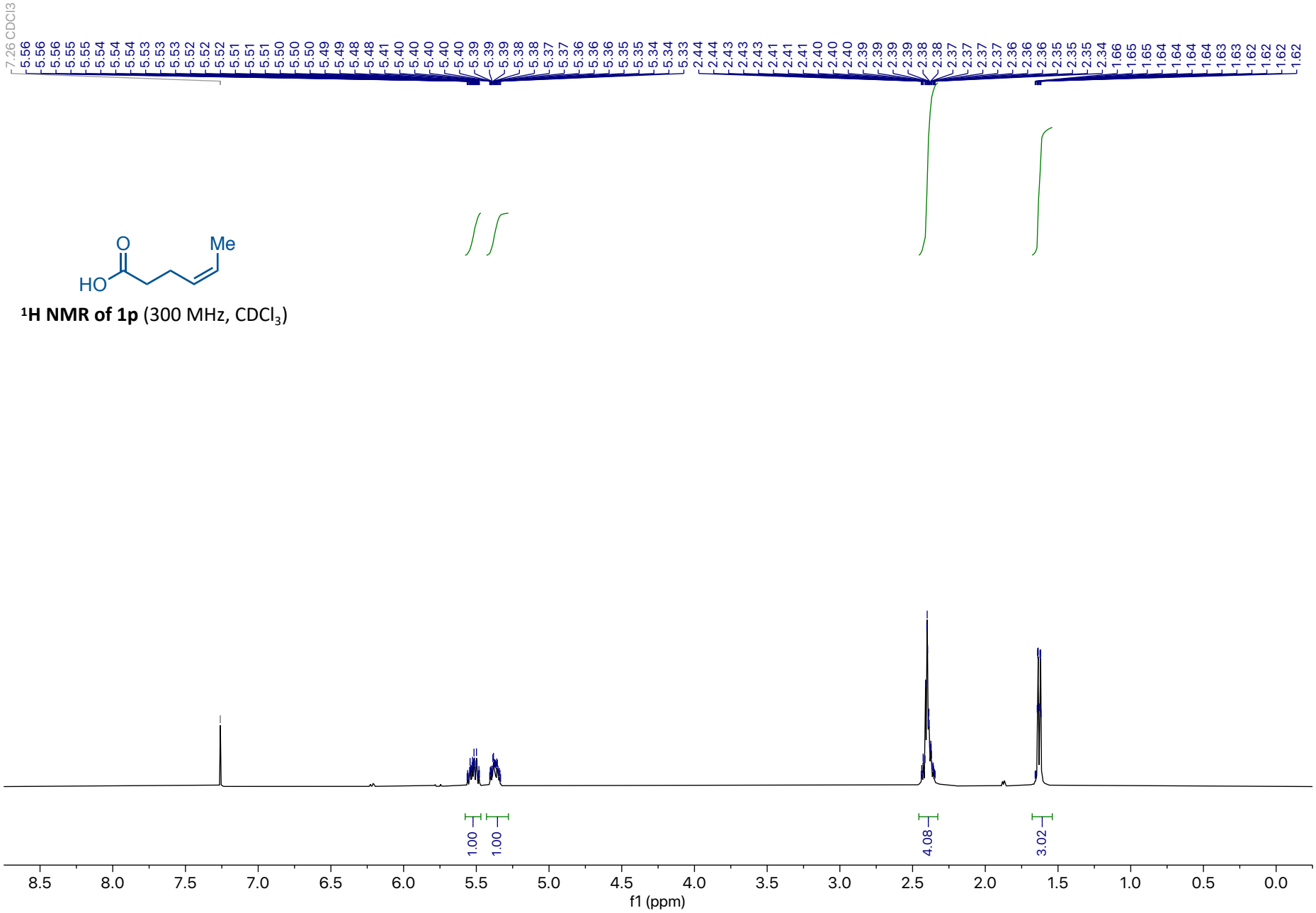
^{13}C NMR of 1m (101 MHz, $CDCl_3$)



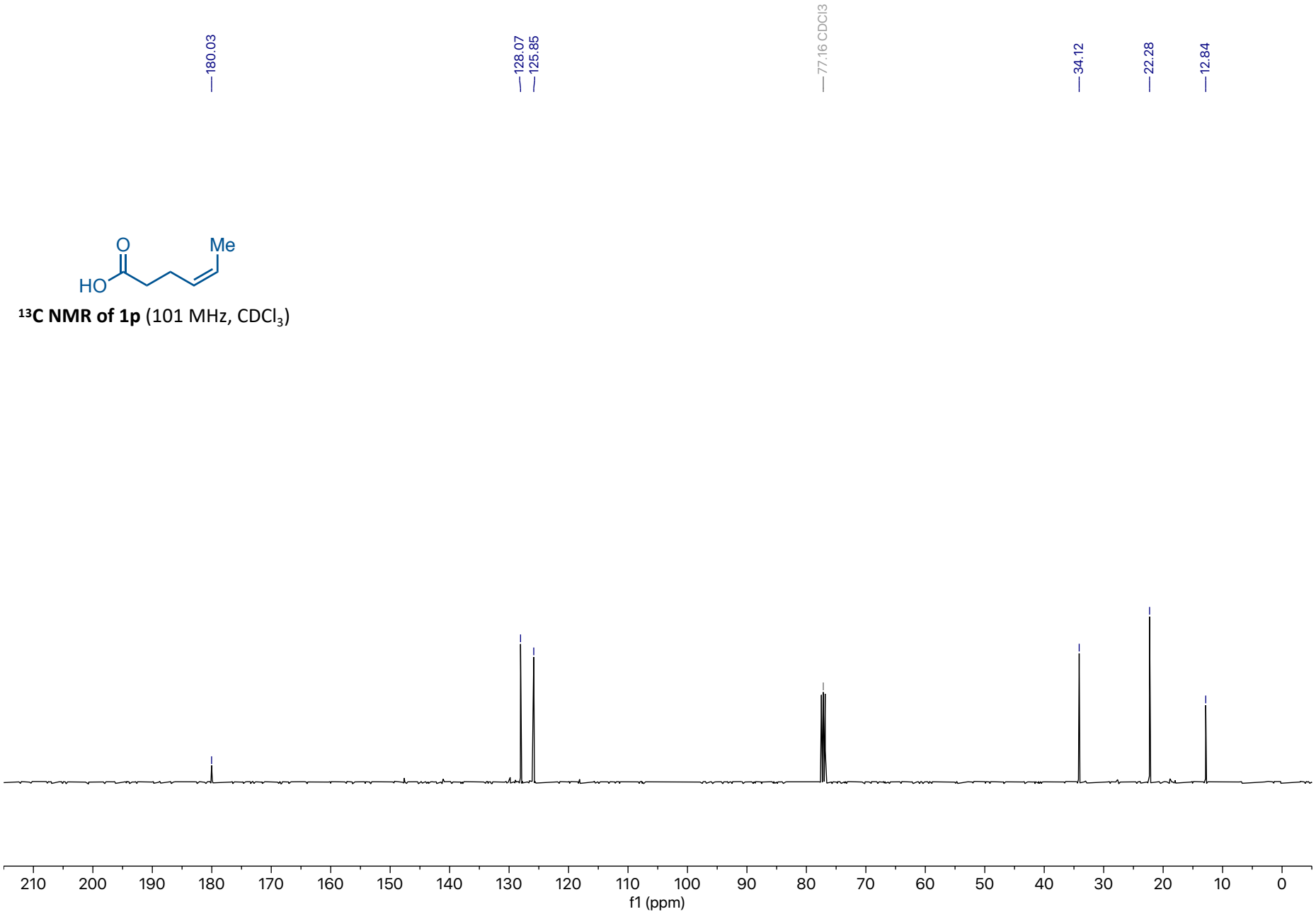
^{1}H NMR of 1o (300 MHz, $CDCl_3$)



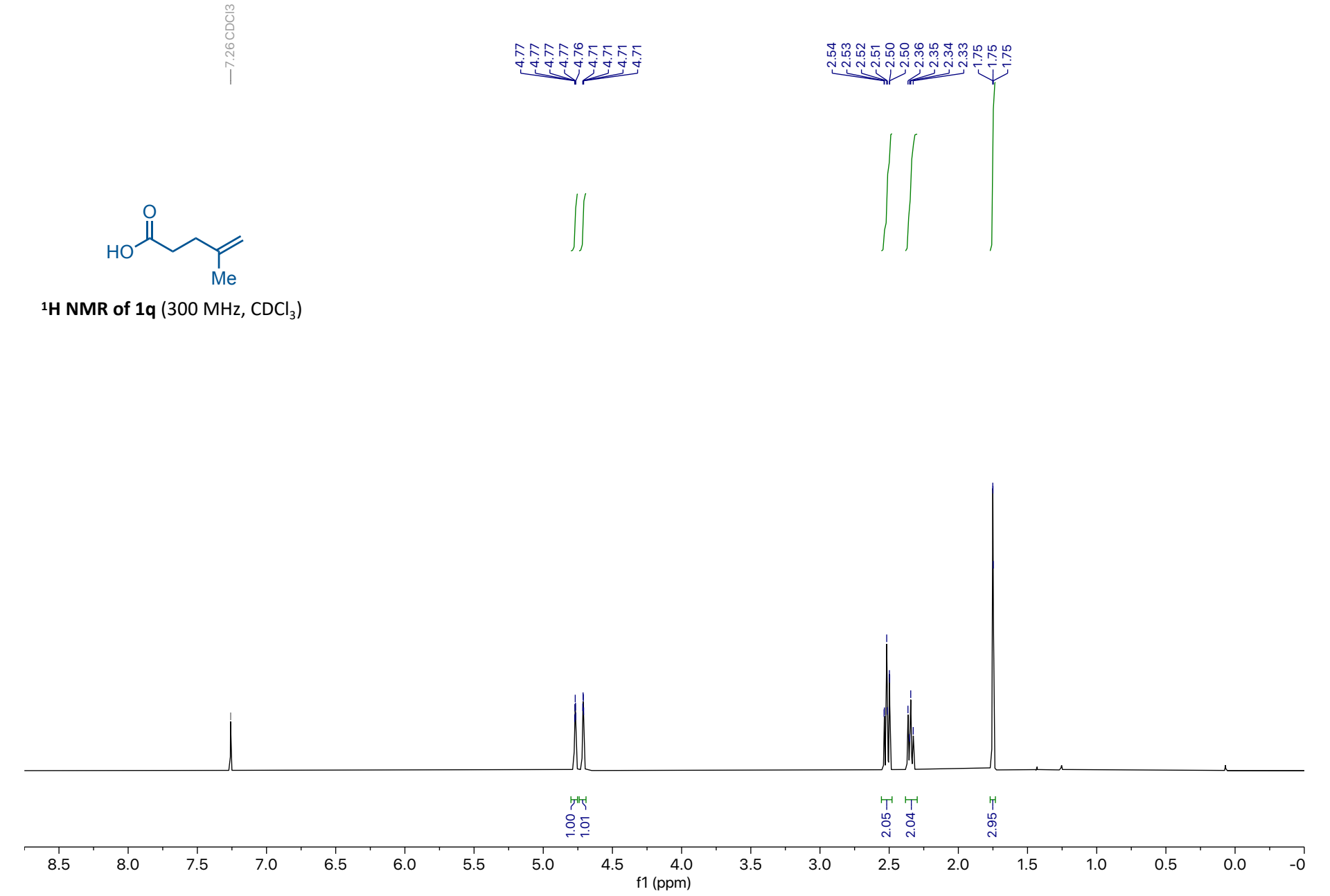
^{13}C NMR of 1o (101 MHz, $CDCl_3$)



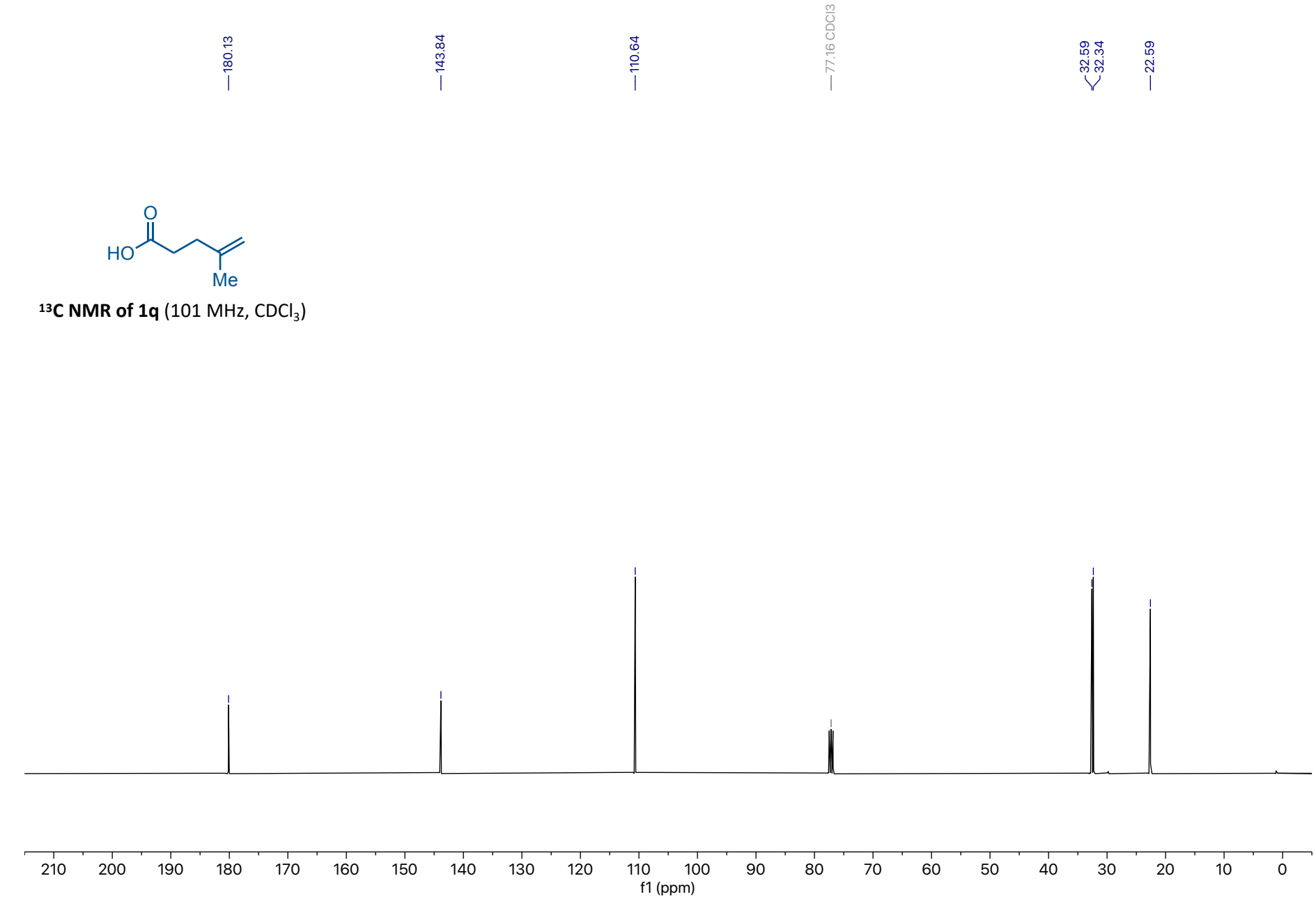
^{1}H NMR of 1p (300 MHz, $CDCl_3$)



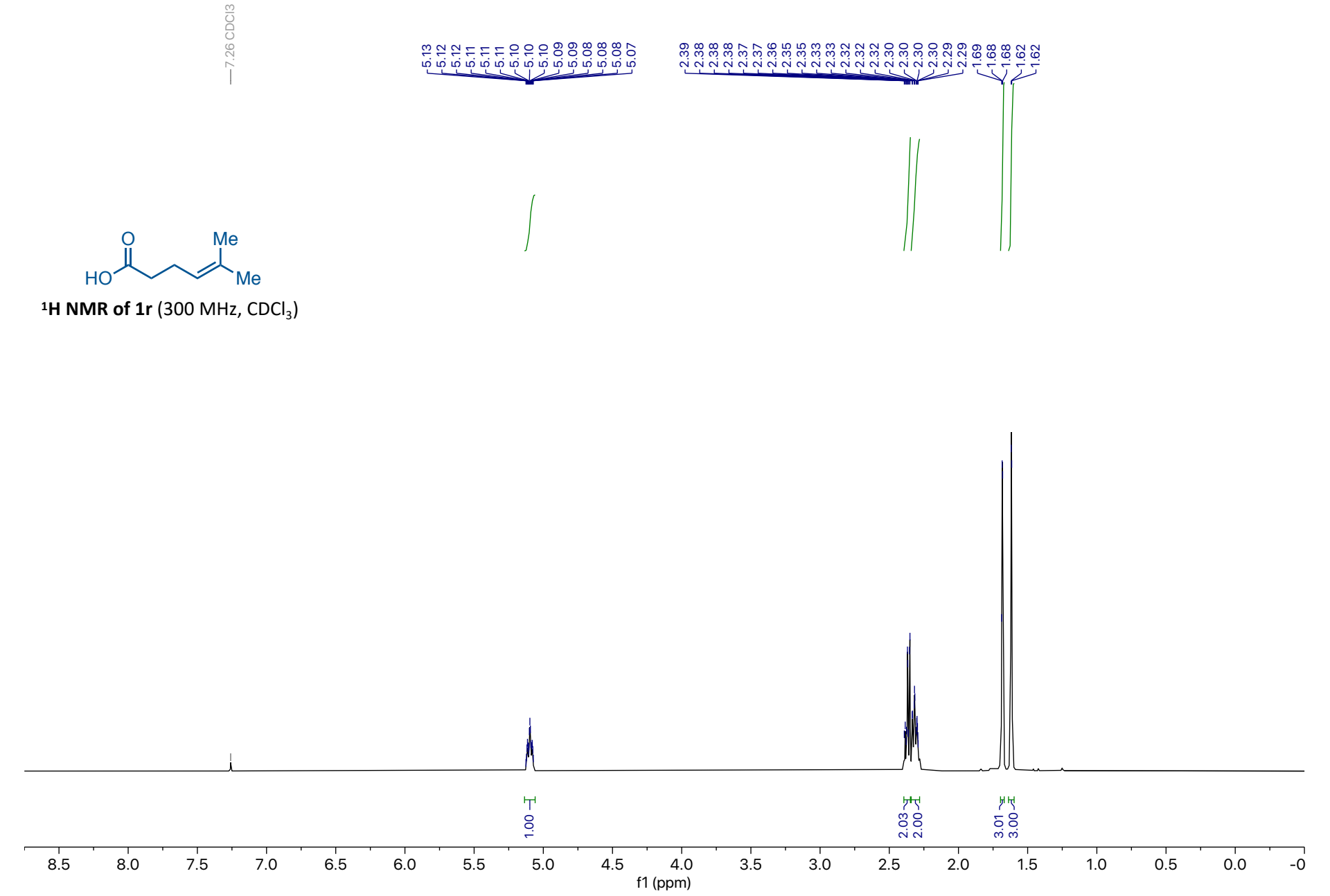
^{13}C NMR of 1p (101 MHz, $CDCl_3$)



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

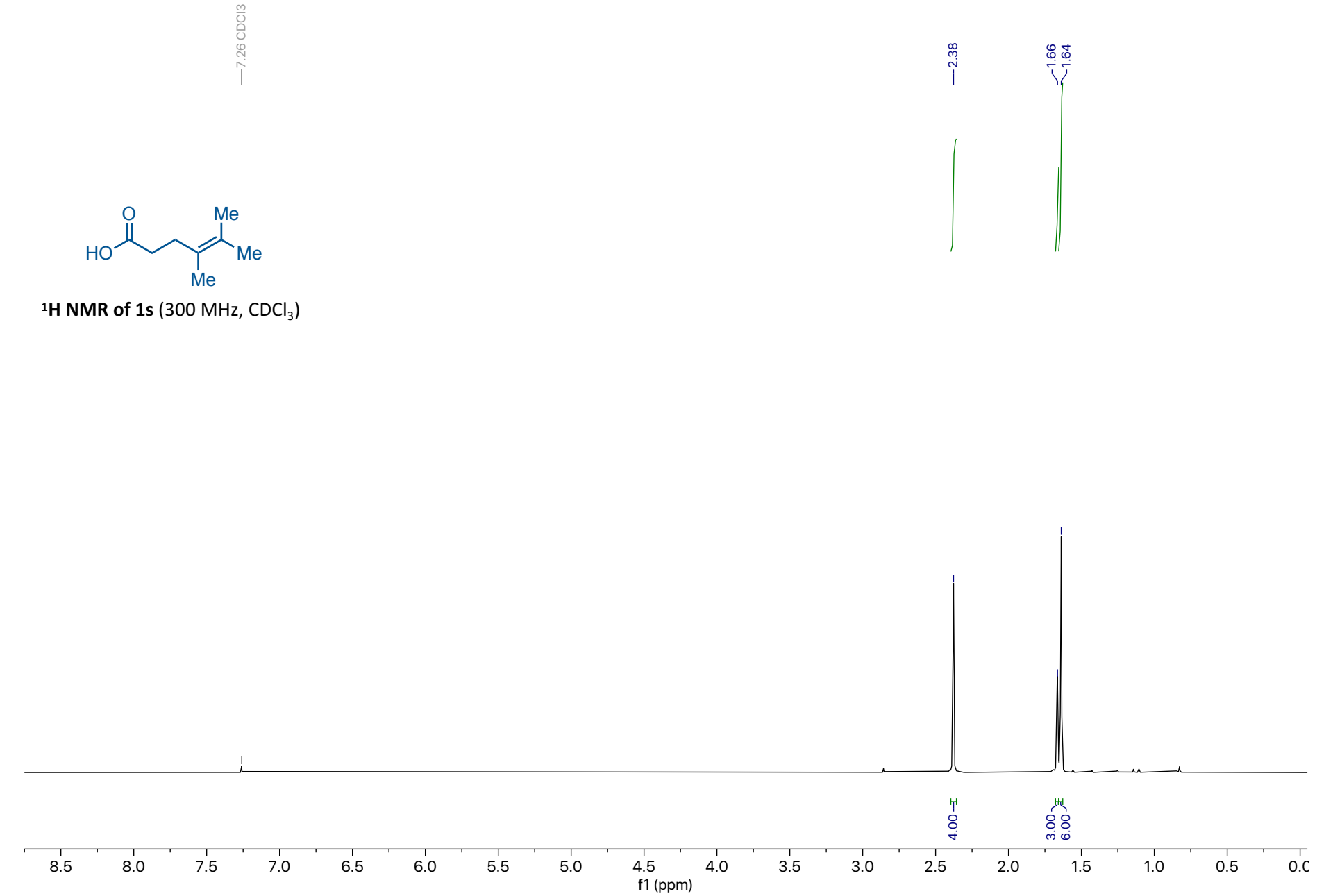


^{13}C NMR of 1q (101 MHz, $CDCl_3$)

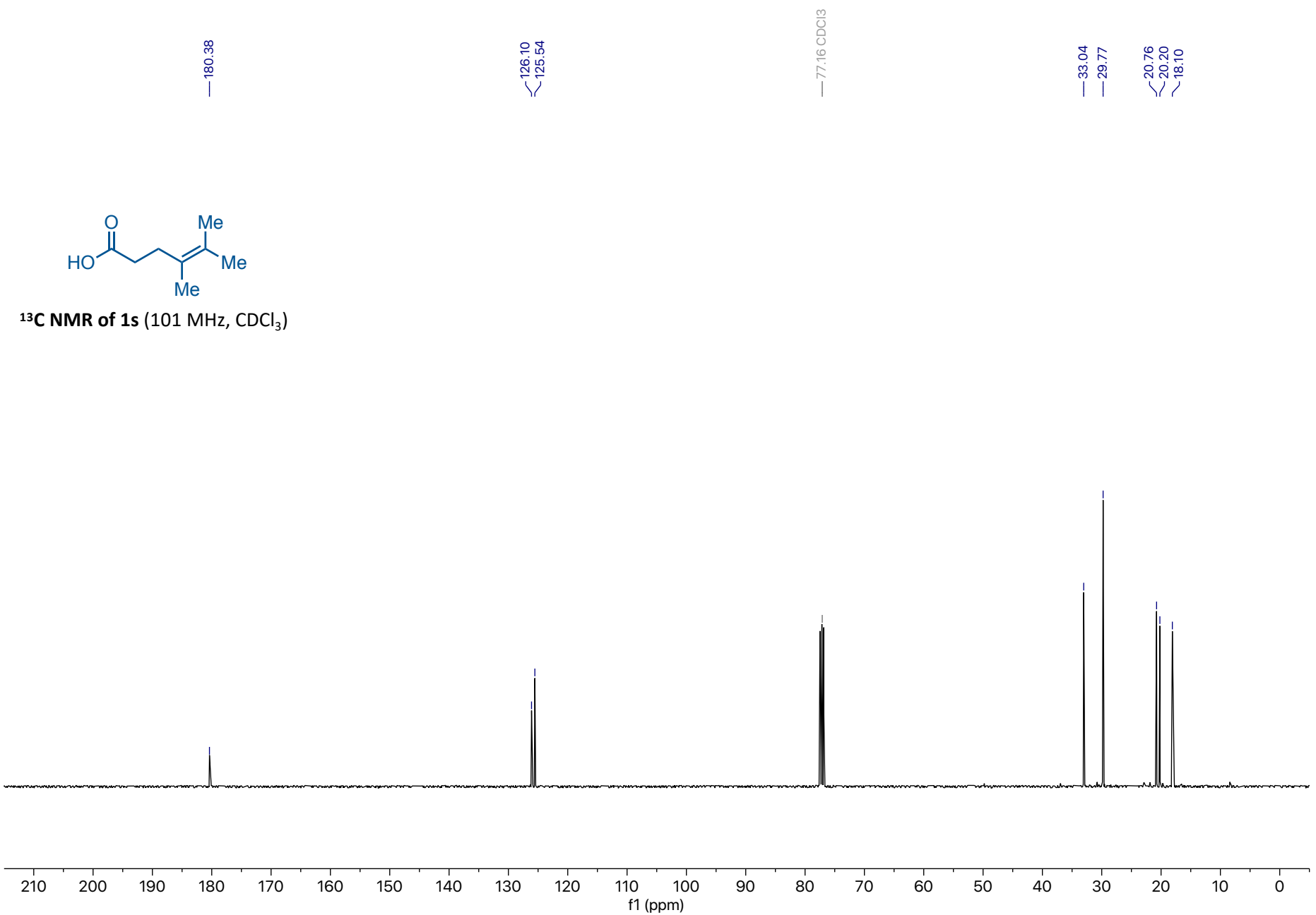


^{1}H NMR of 1r (300 MHz, $CDCl_3$)

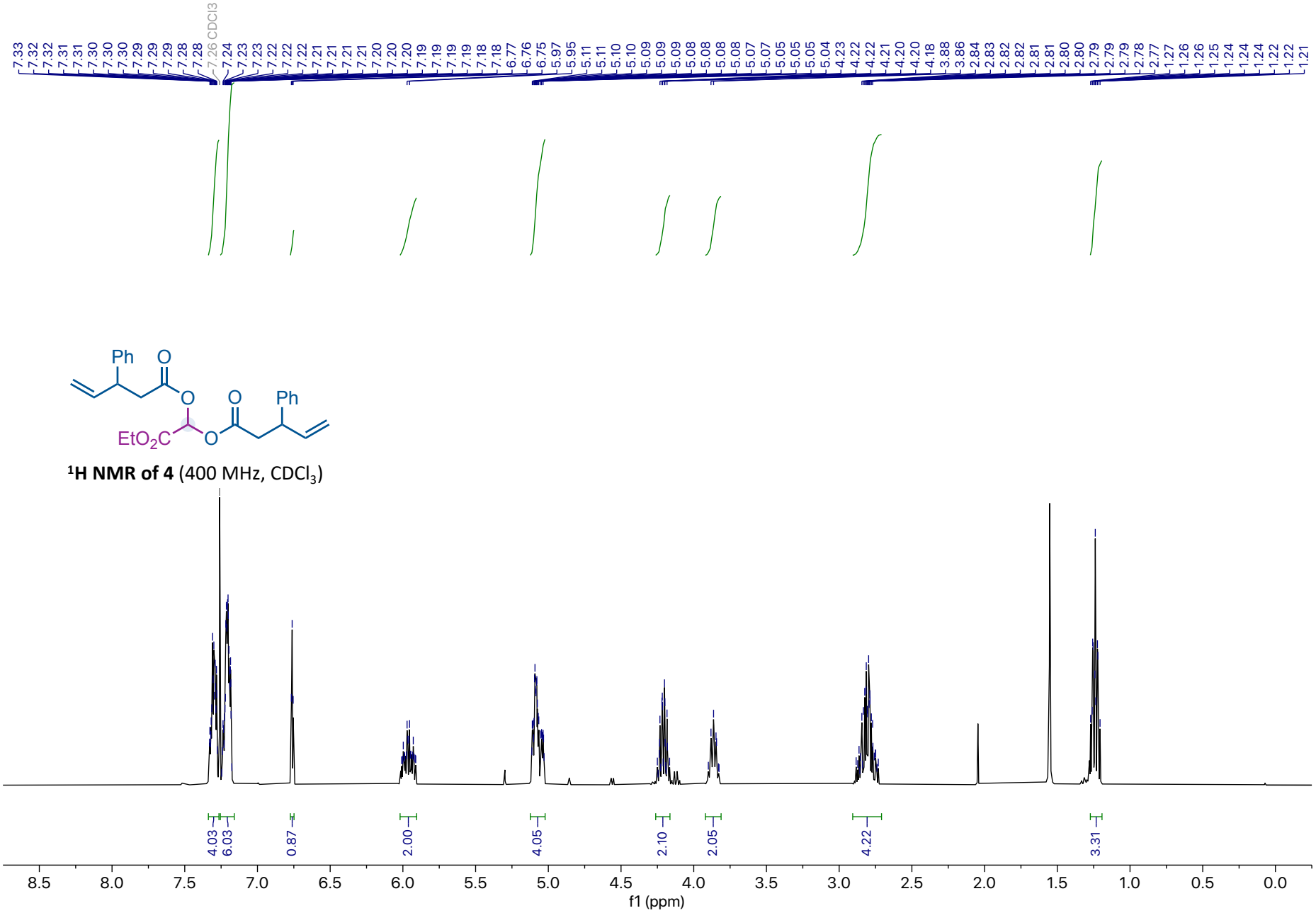
^{13}C NMR of 1r ($CDCl_3$)



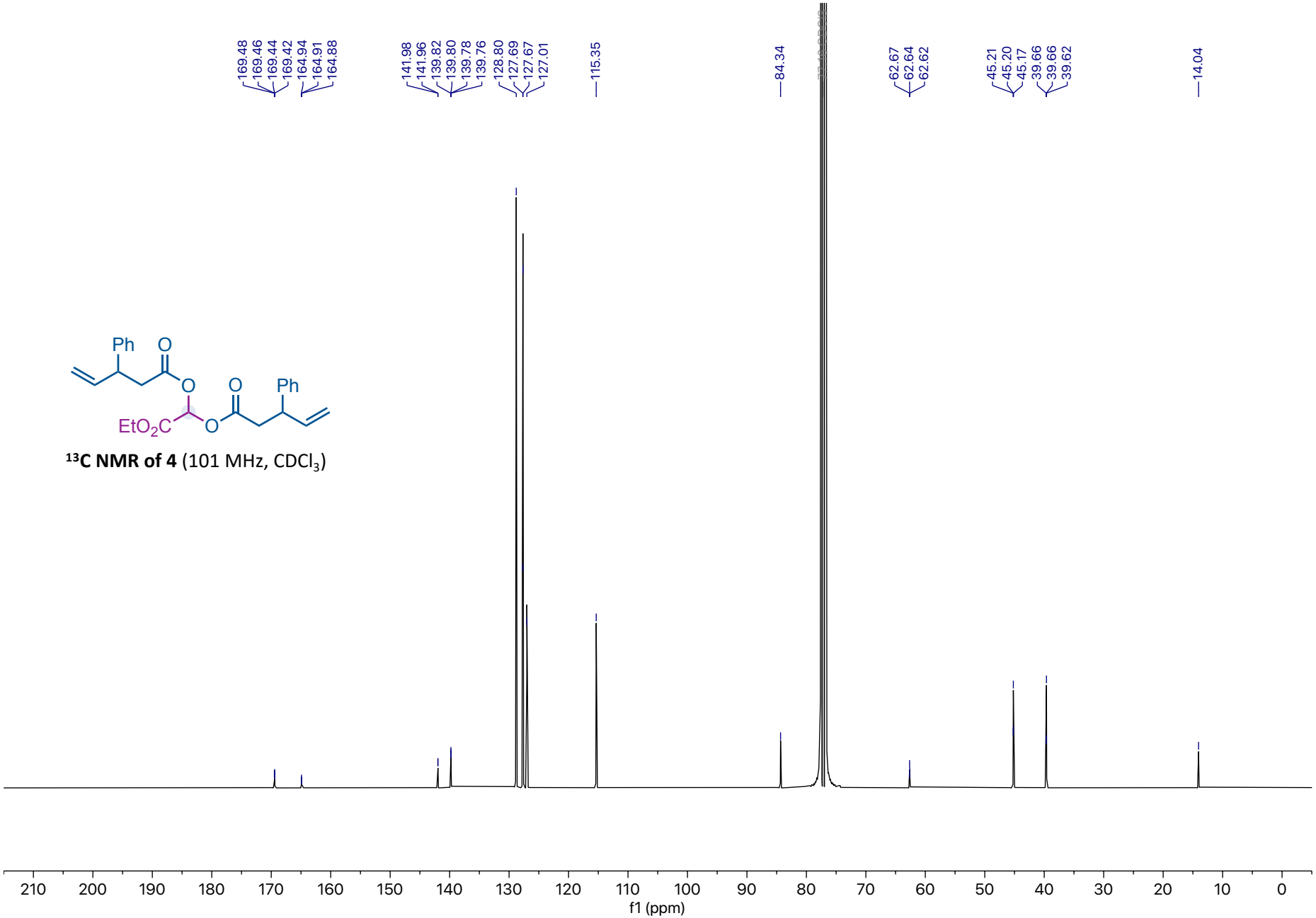
^{1}H NMR of 1s (300 MHz, $CDCl_3$)



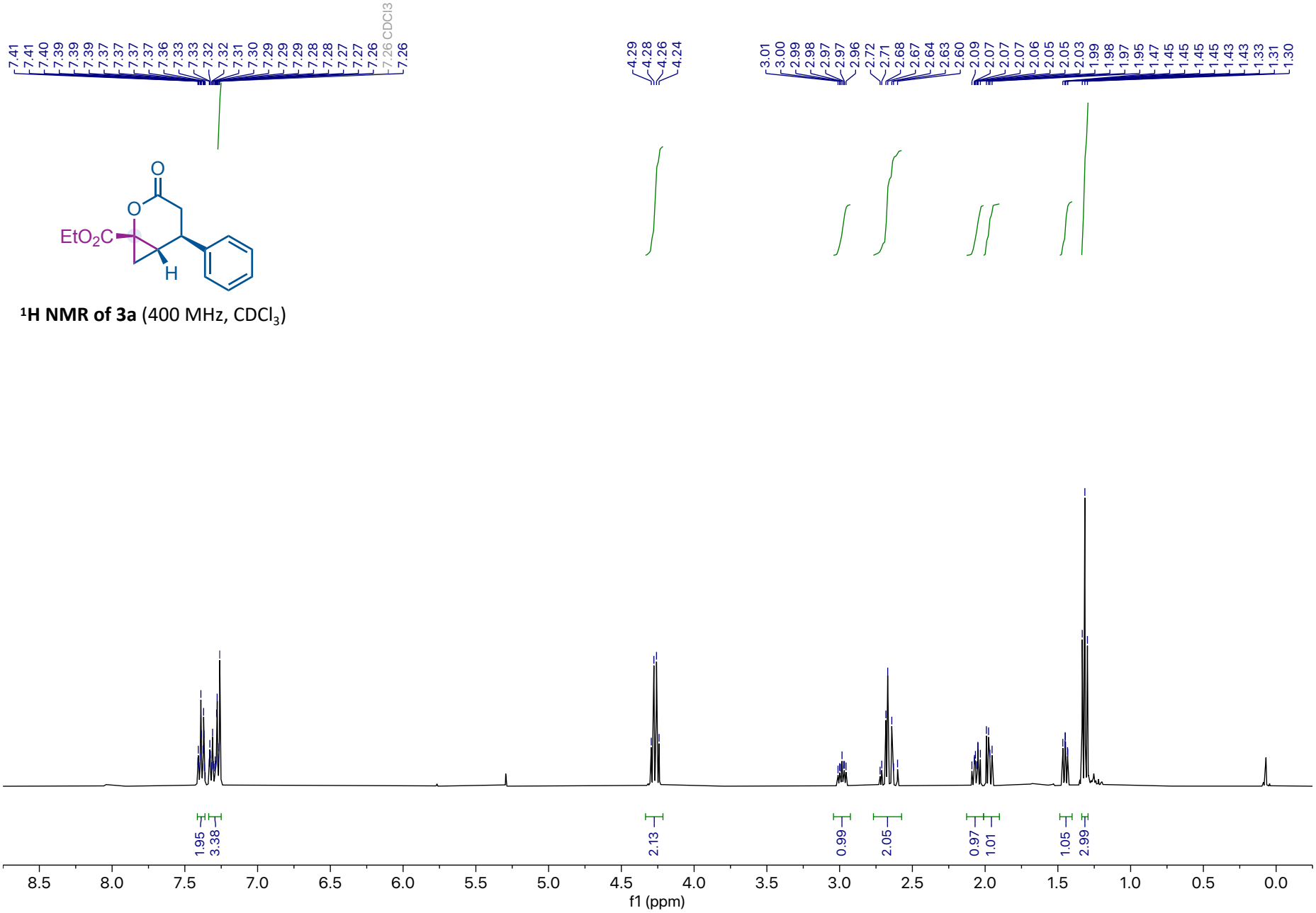
^{13}C NMR of 1s (101 MHz, $CDCl_3$)



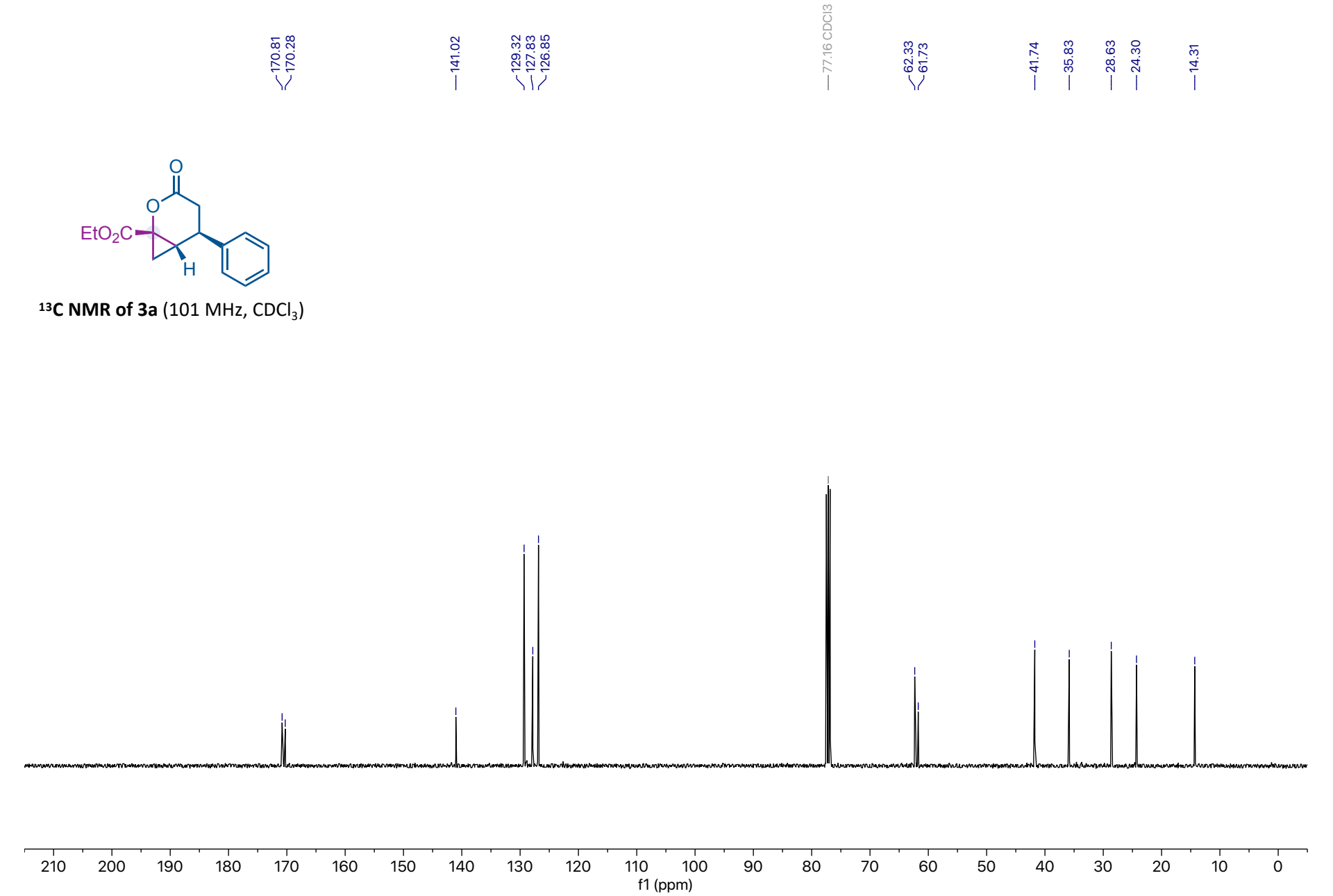
^{1}H NMR of 4 (400 MHz, $CDCl_3$)



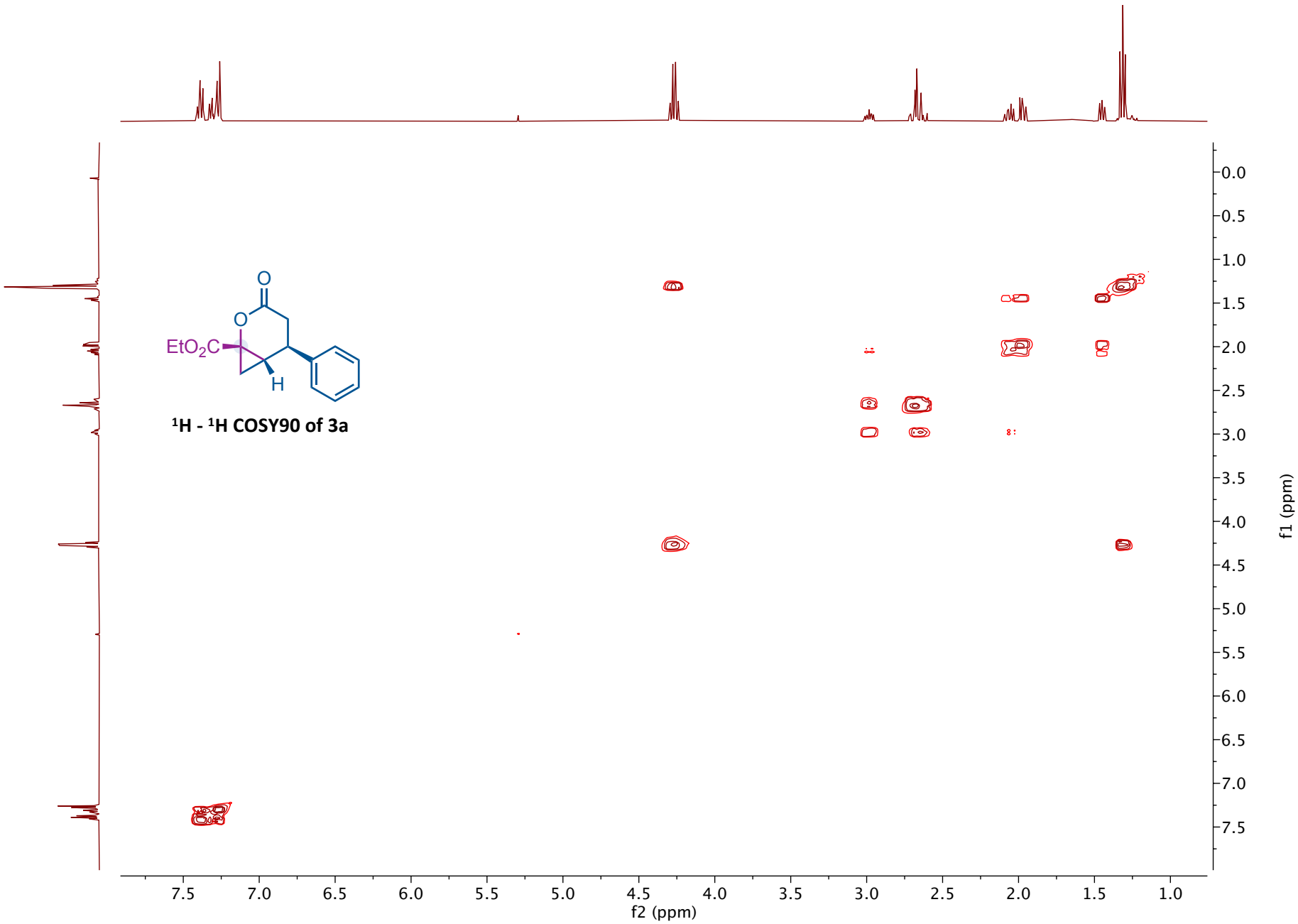
^{13}C NMR of 4 (101 MHz, $CDCl_3$)



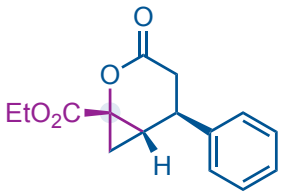
^{1}H NMR of 3a (400 MHz, $CDCl_3$)



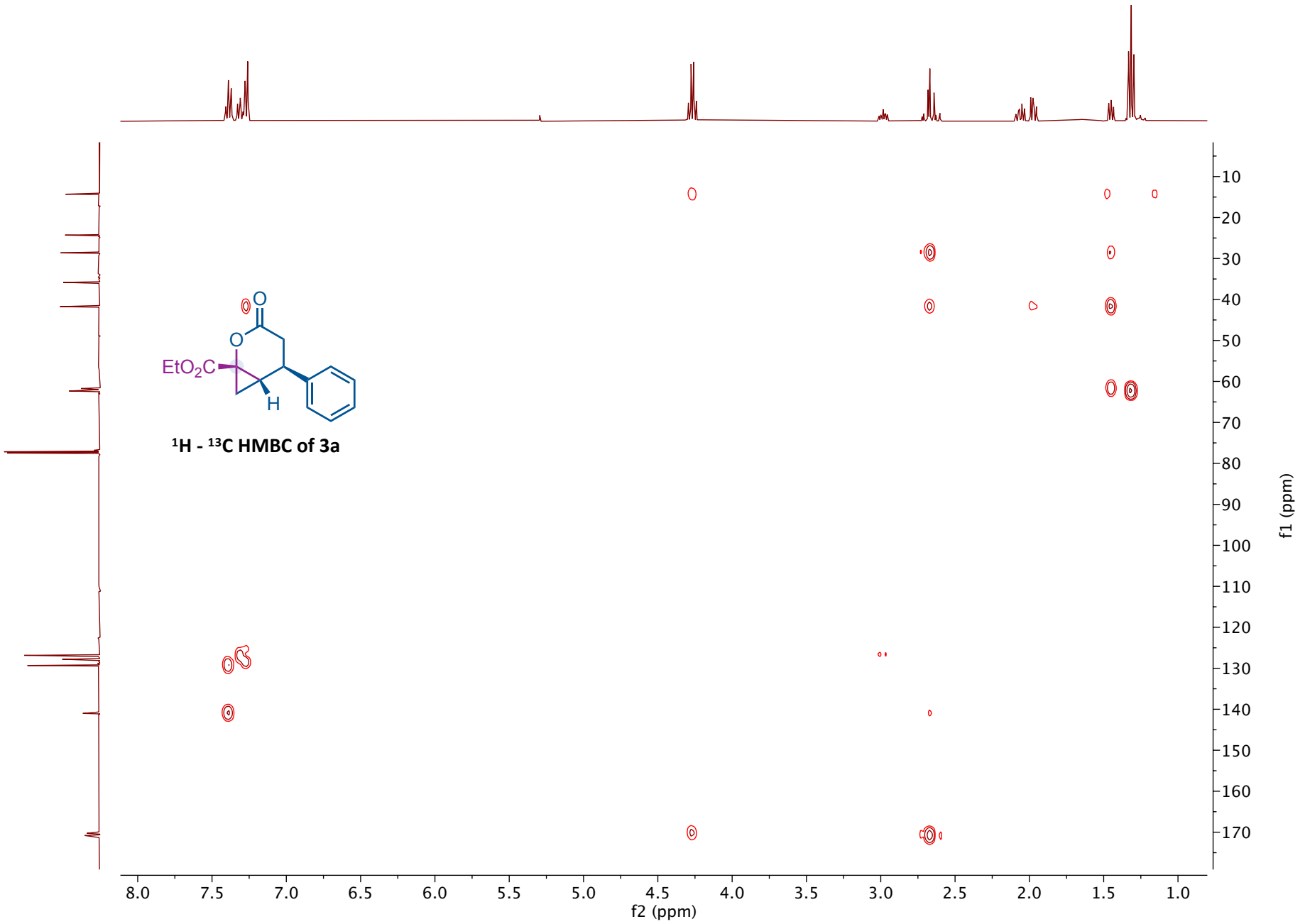
^{13}C NMR of 3a (101 MHz, $CDCl_3$)



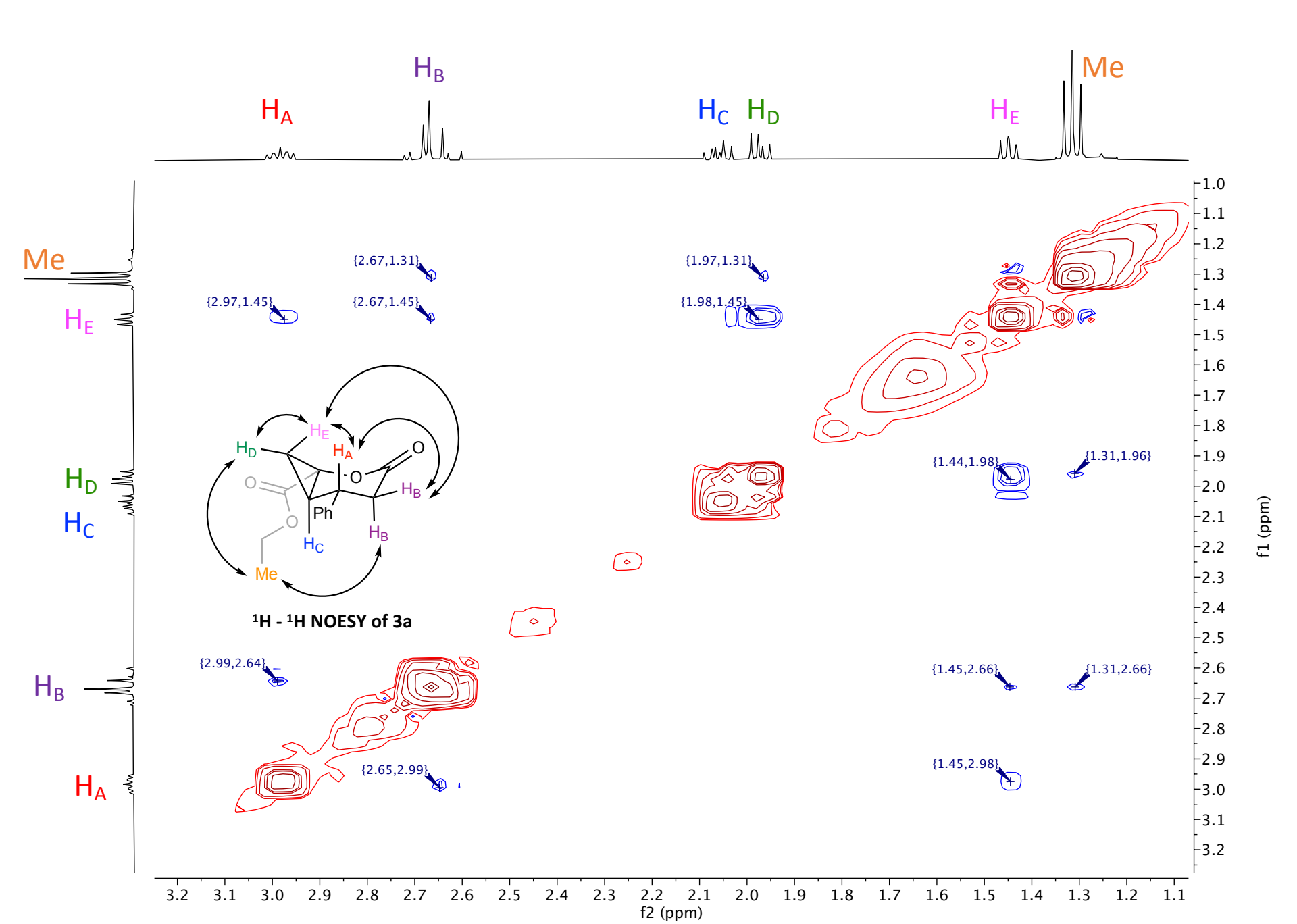
^{1}H - ^{1}H COSY90 of 3a



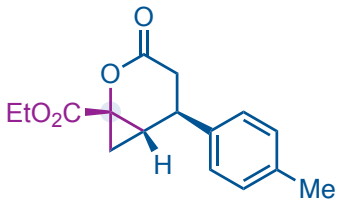
^{1}H - ^{13}C HSQC of 3a



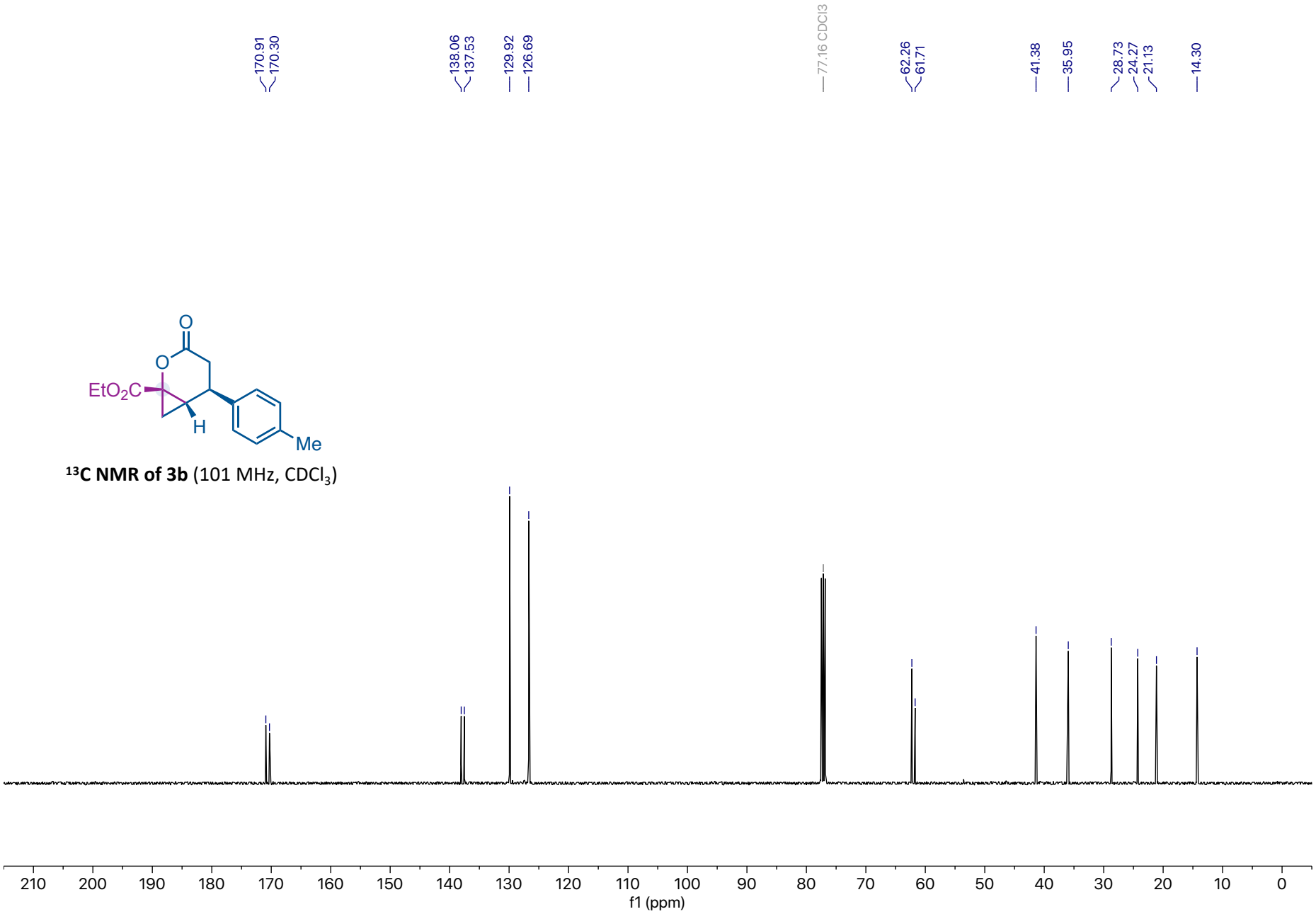
^{1}H - ^{13}C HMBC of 3a



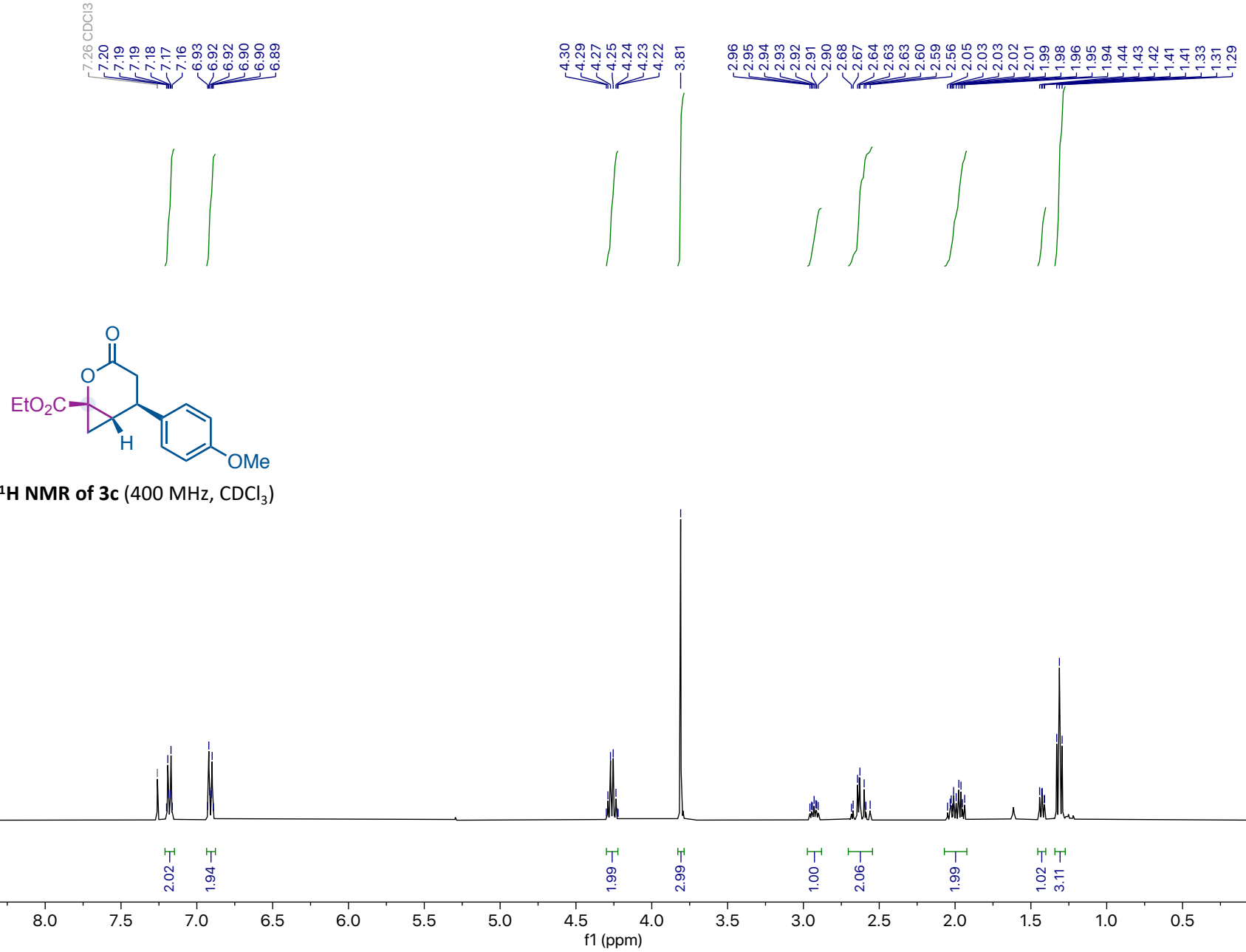
^{1}H - ^{1}H NOESY of 3a



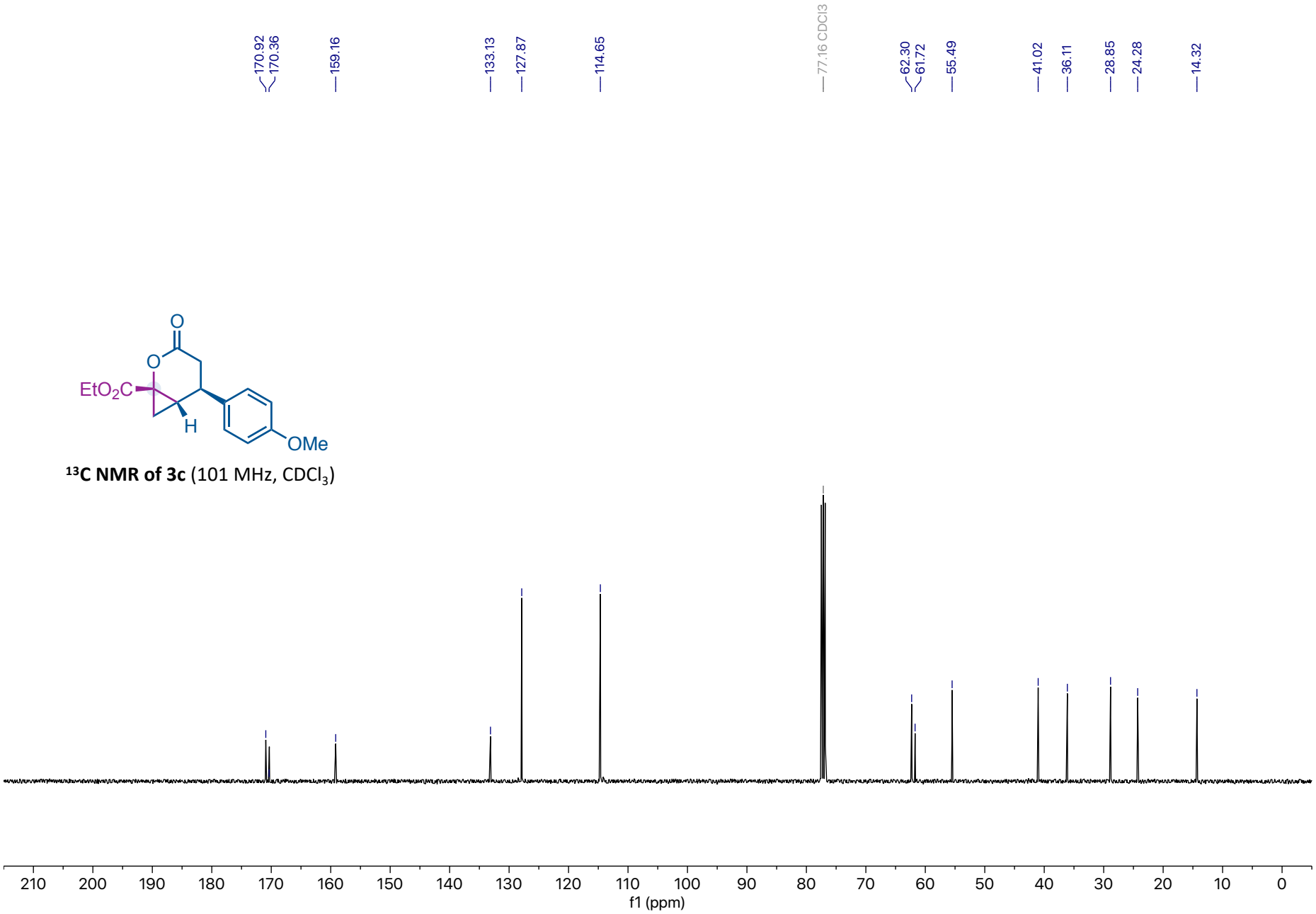
^{1}H NMR of 3b (400 MHz, $CDCl_3$)



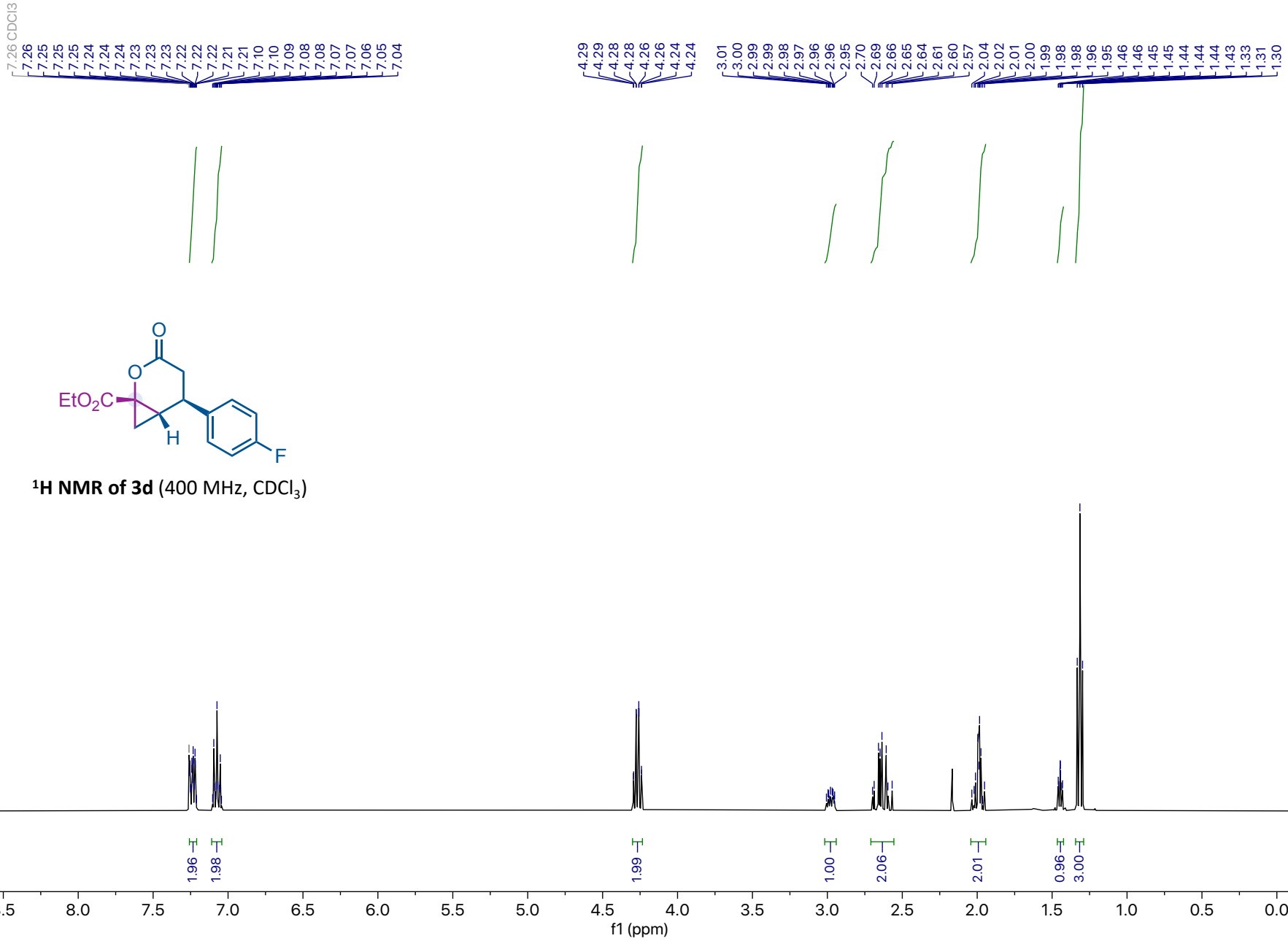
^{13}C NMR of 3b (101 MHz, $CDCl_3$)



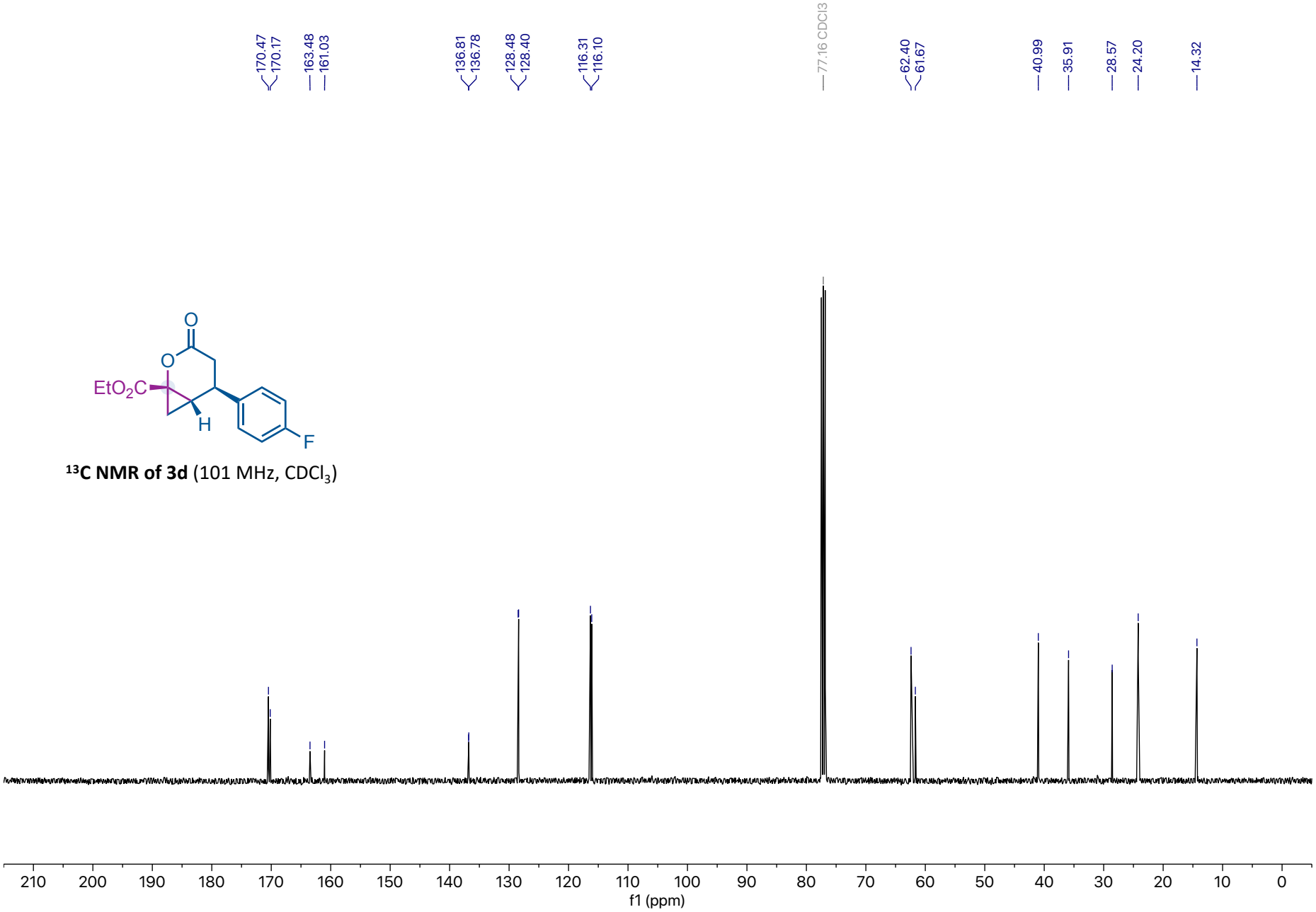
^{1}H NMR of 3c (400 MHz, $CDCl_3$)



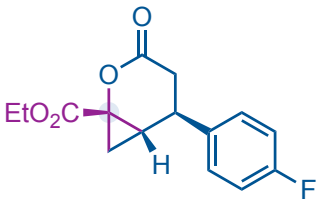
^{13}C NMR of 3c (101 MHz, $CDCl_3$)



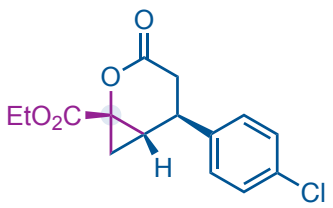
^{1}H NMR of 3d (400 MHz, $CDCl_3$)



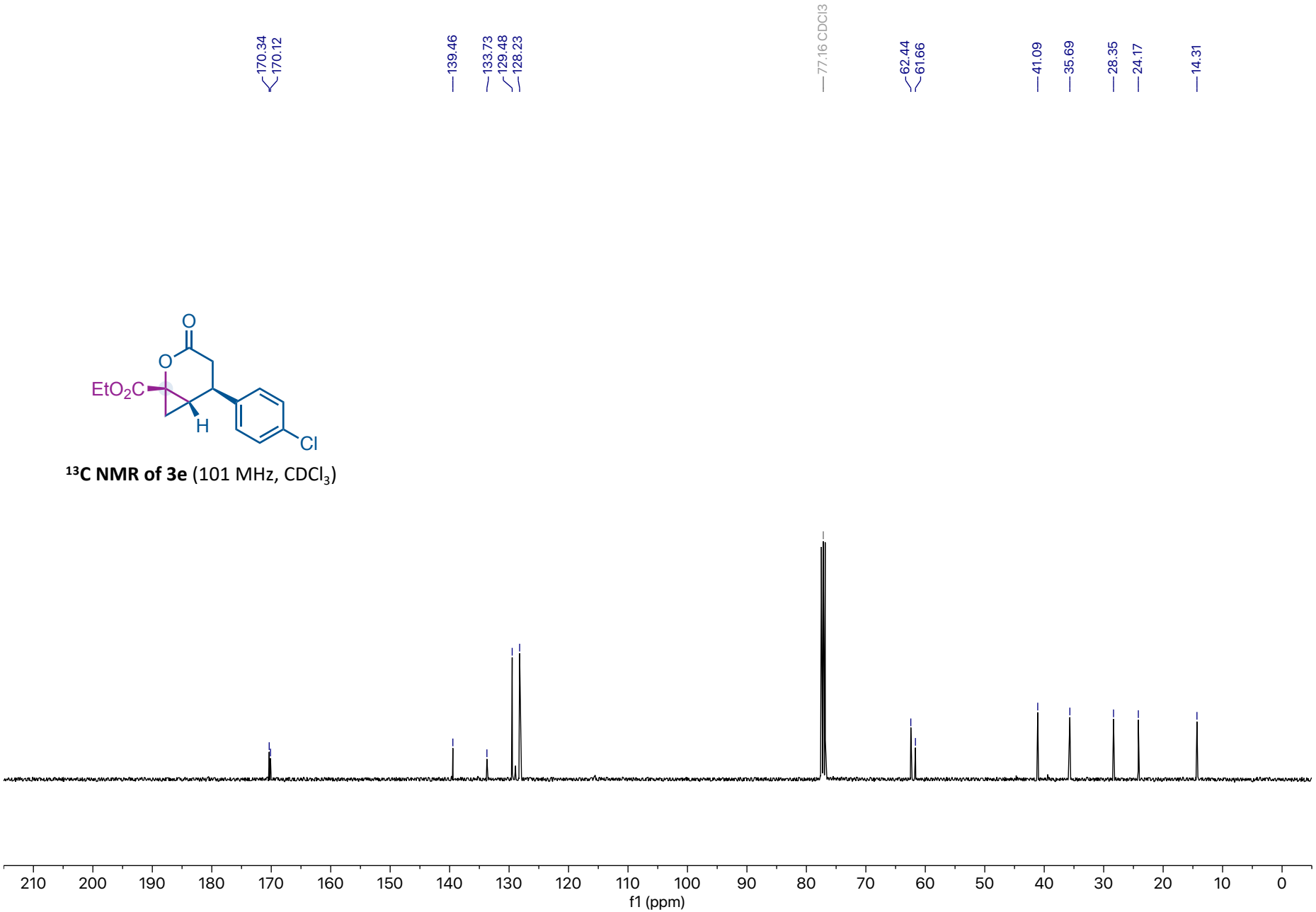
^{13}C NMR of 3d (101 MHz, $CDCl_3$)



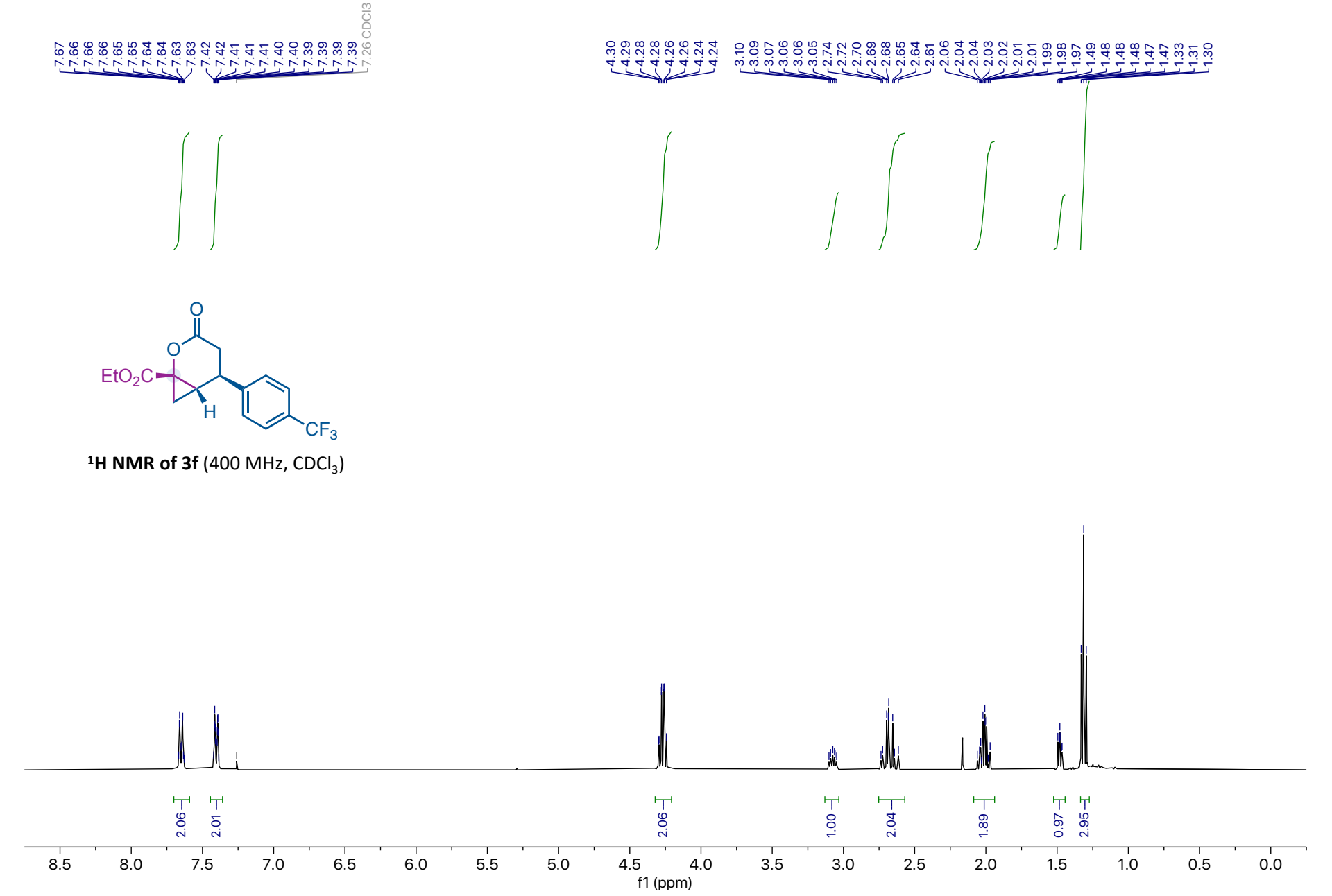
^{19}F NMR of 3d (376 MHz, $CDCl_3$)



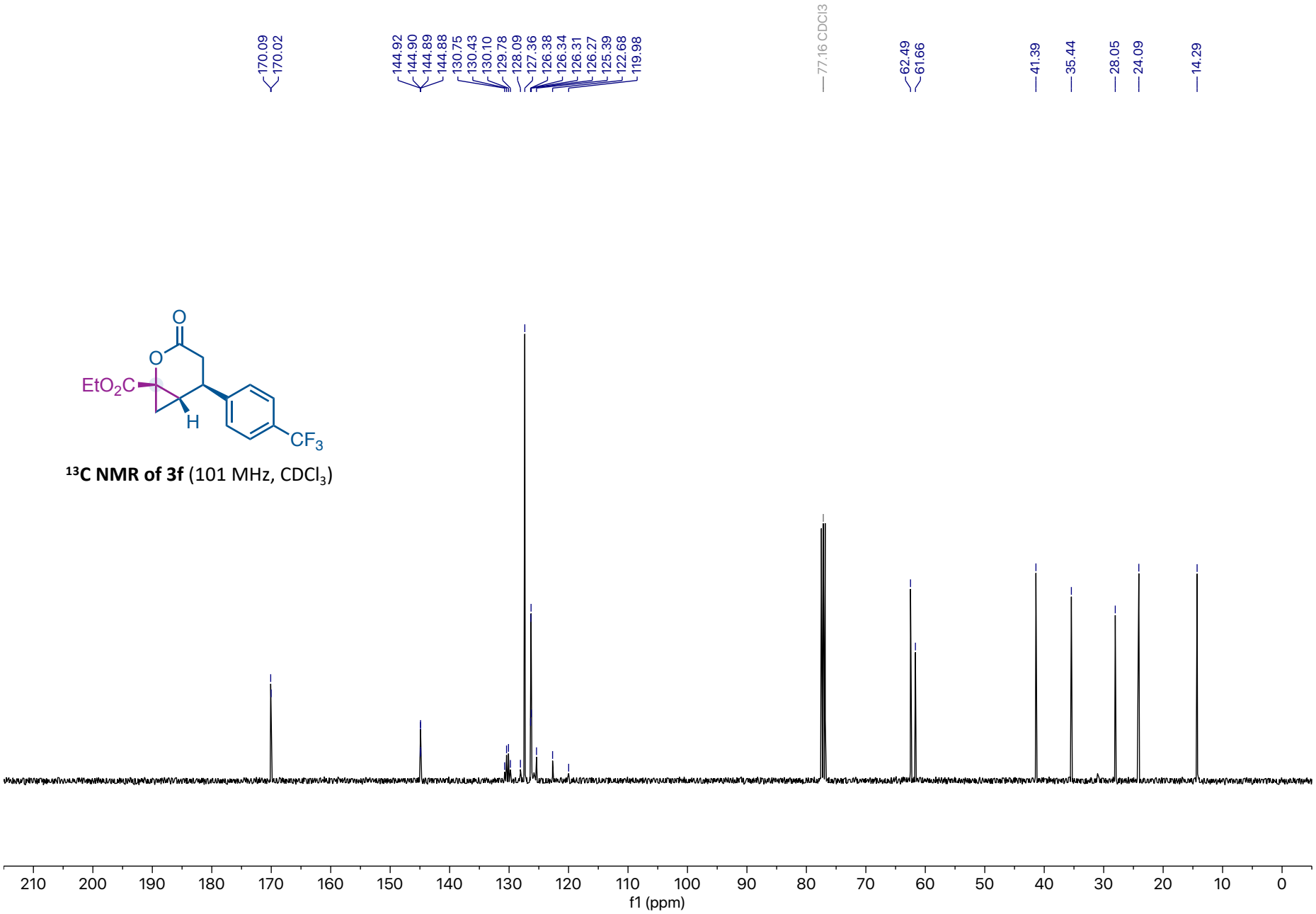
^{1}H NMR of 3e (400 MHz, $CDCl_3$)



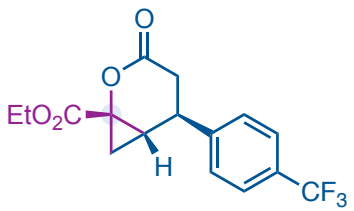
^{13}C NMR of 3e (101 MHz, $CDCl_3$)



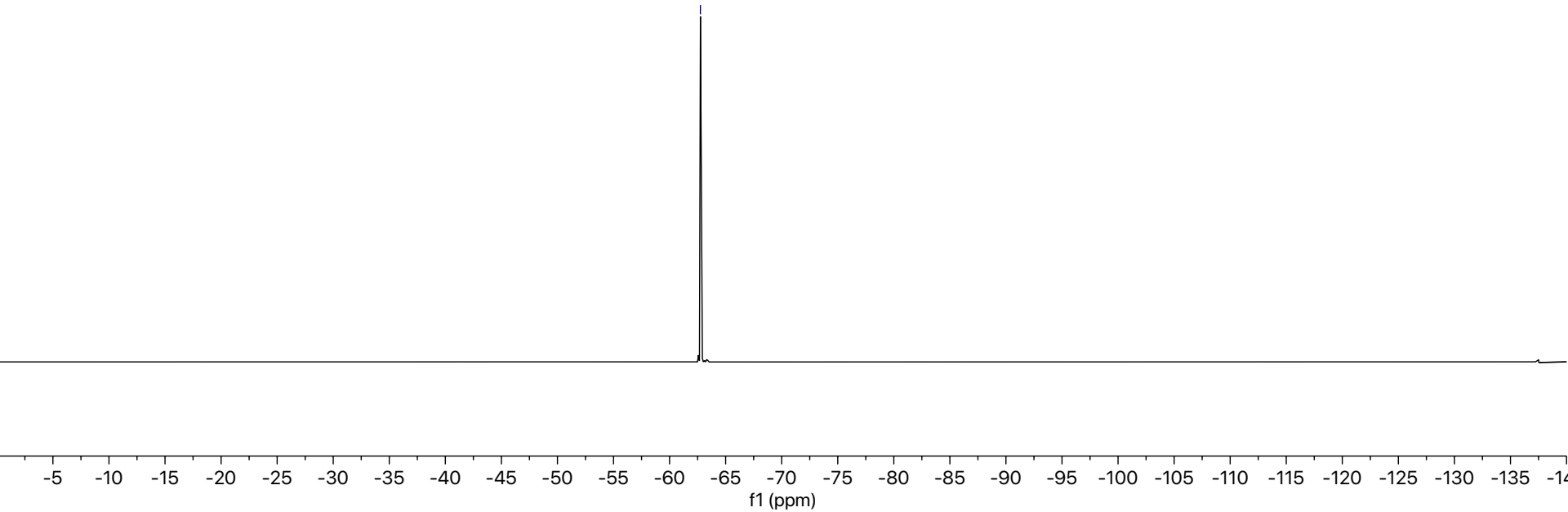
^{1}H NMR of 3f (400 MHz, $CDCl_3$)

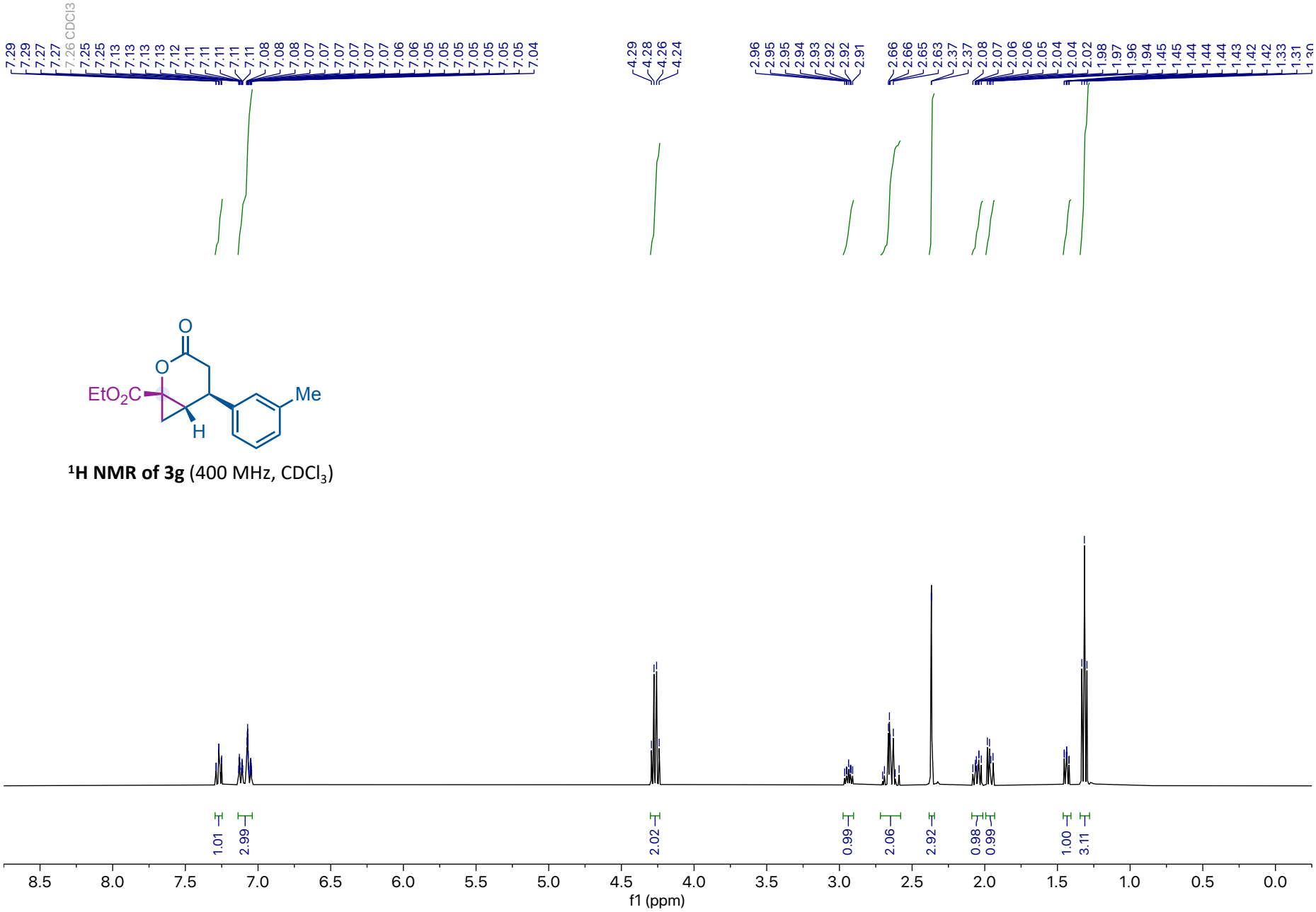


^{13}C NMR of 3f (101 MHz, $CDCl_3$)

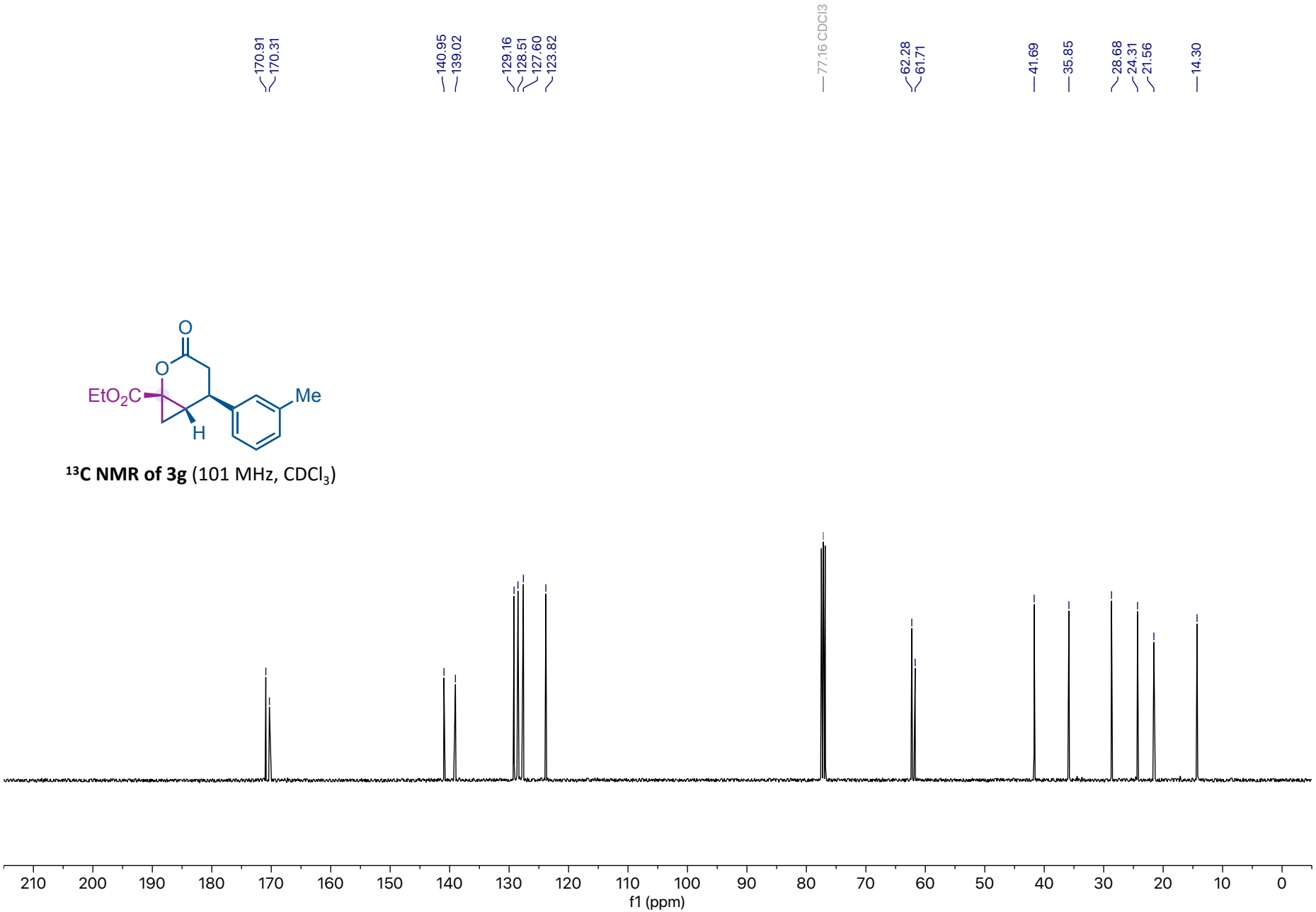


^{19}F NMR of 3f (376 MHz, $CDCl_3$)

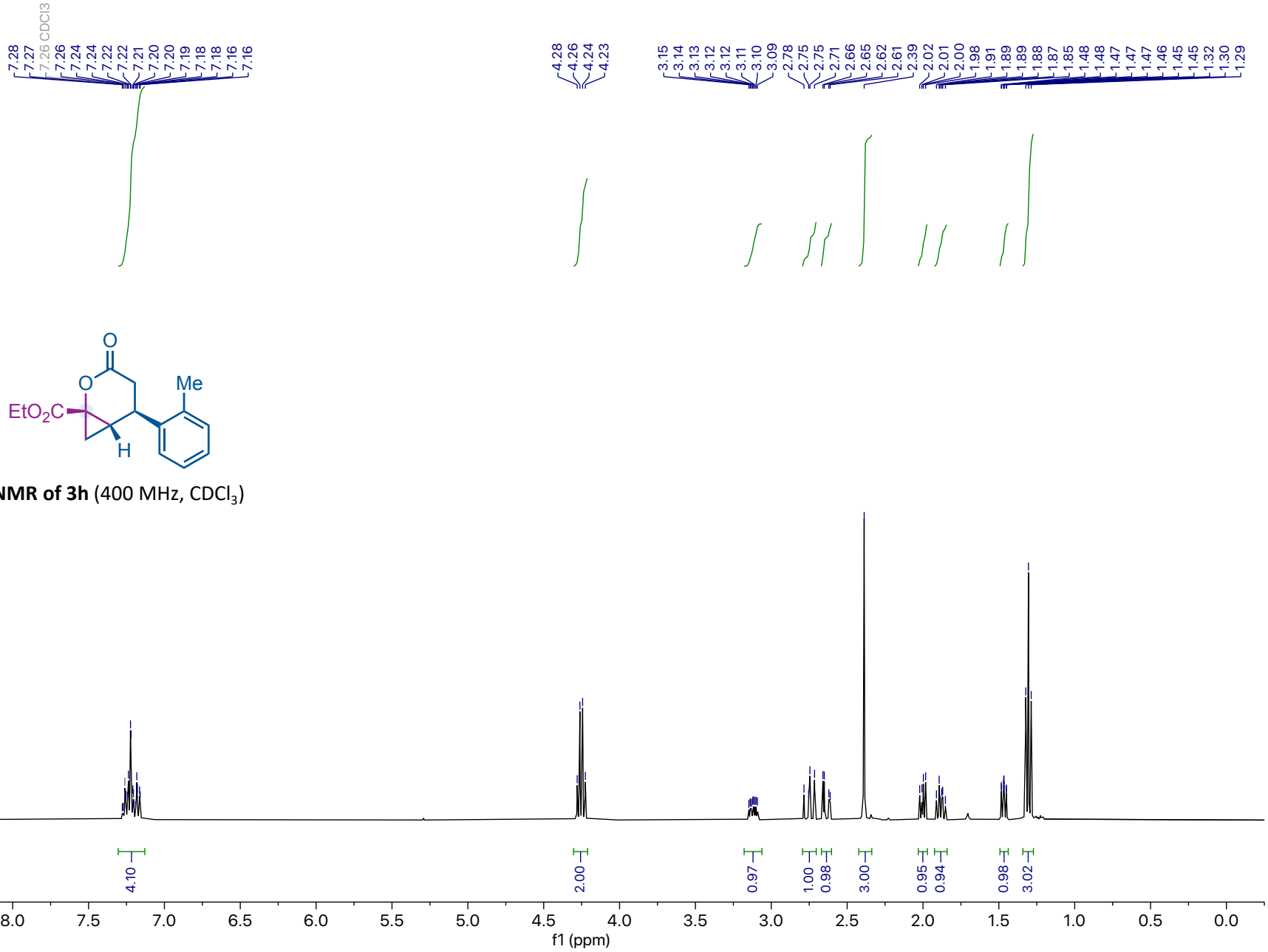




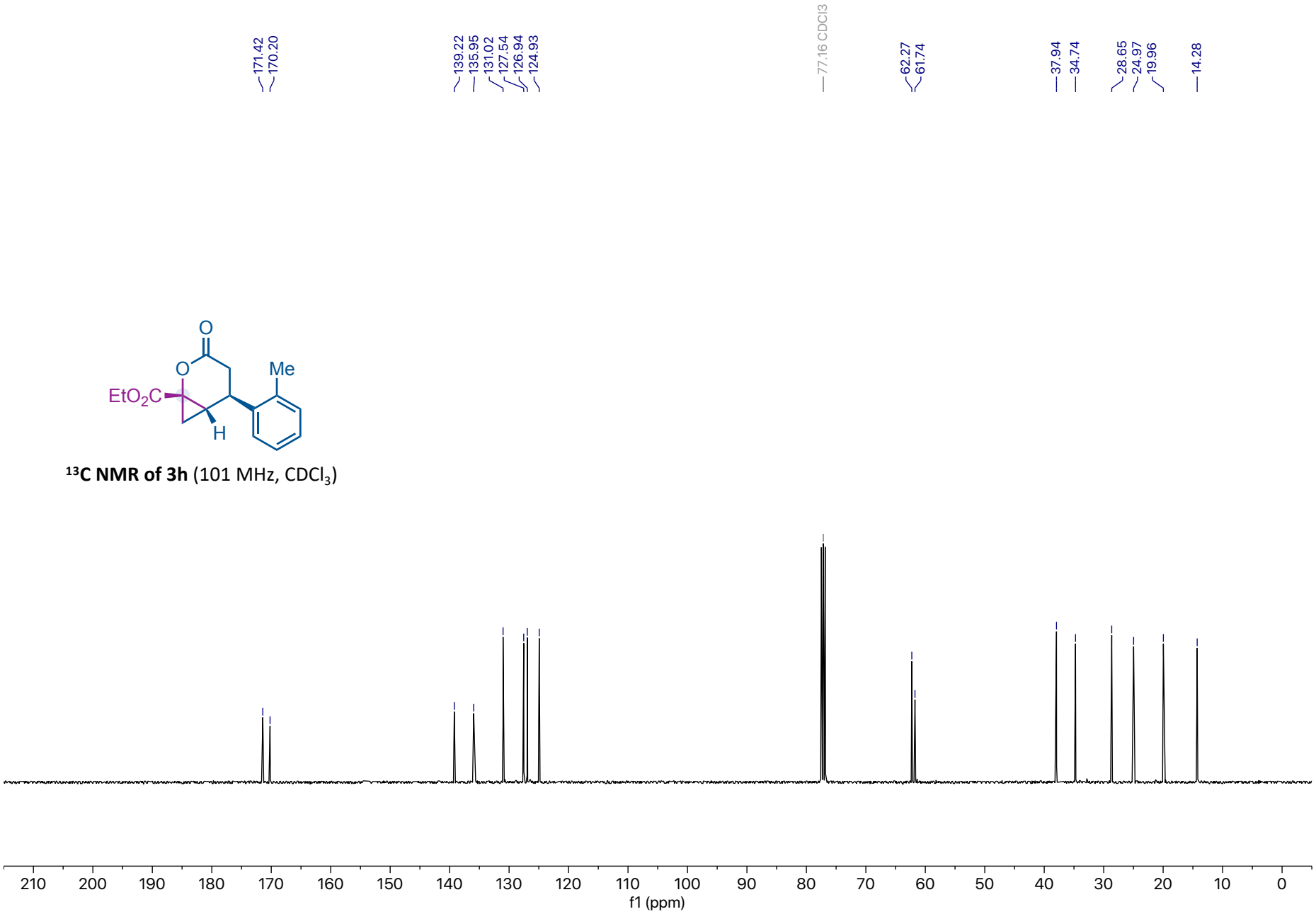
^{1}H NMR of 3g (400 MHz, $CDCl_3$)



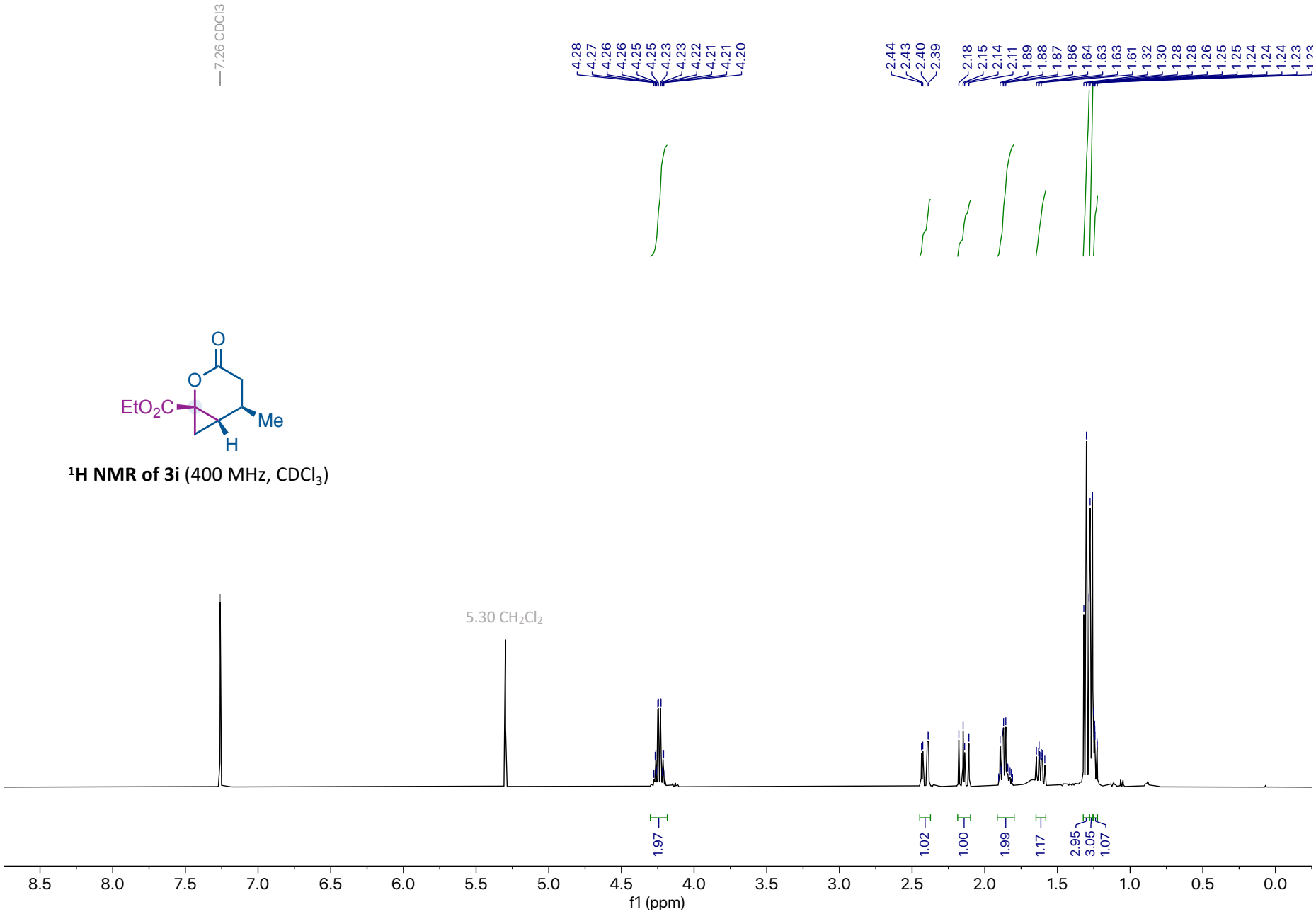
^{13}C NMR of 3g (101 MHz, $CDCl_3$)



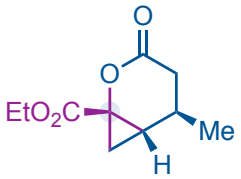
^{1}H NMR of 3h (400 MHz, $CDCl_3$)



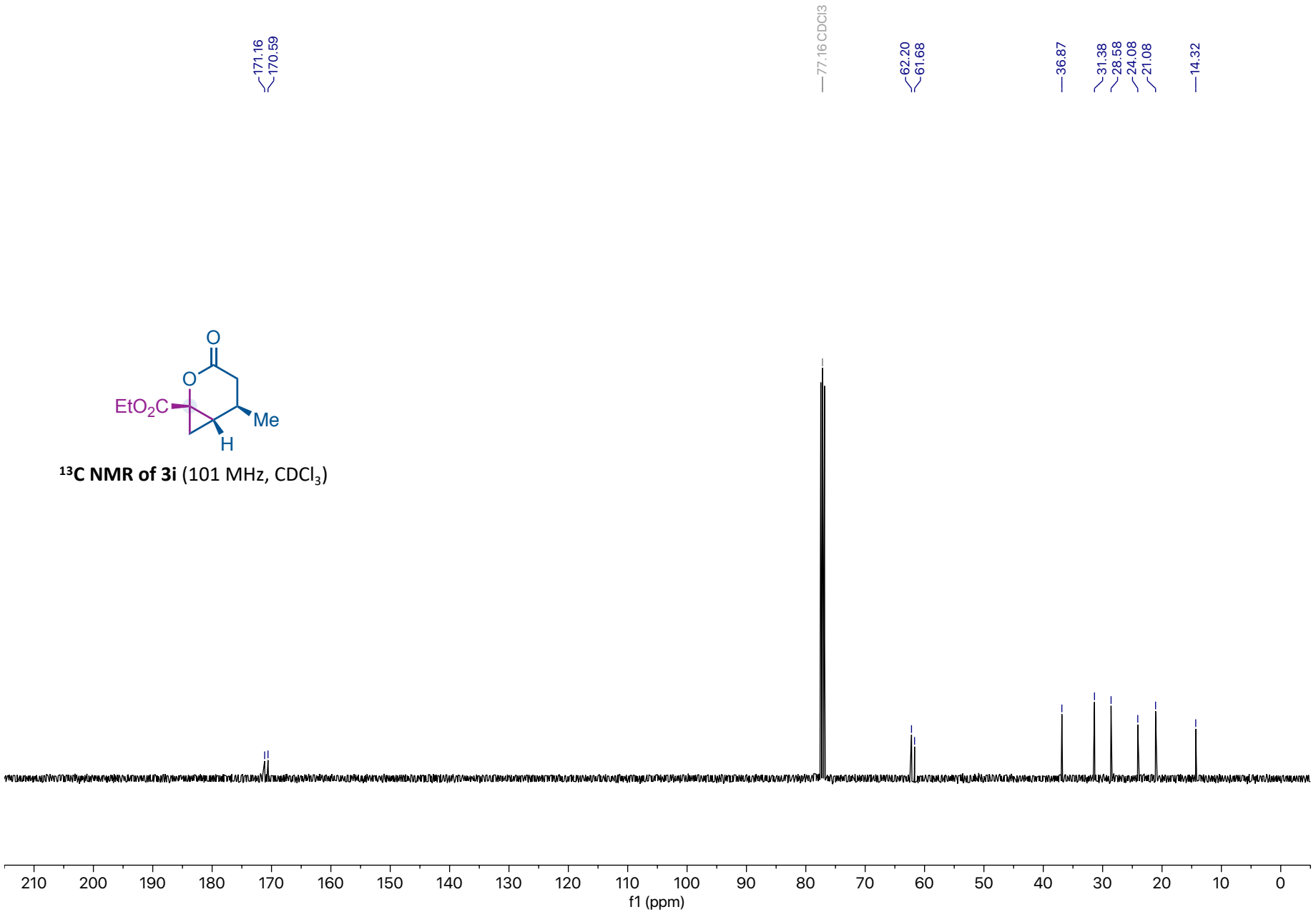
^{13}C NMR of 3h (101 MHz, $CDCl_3$)



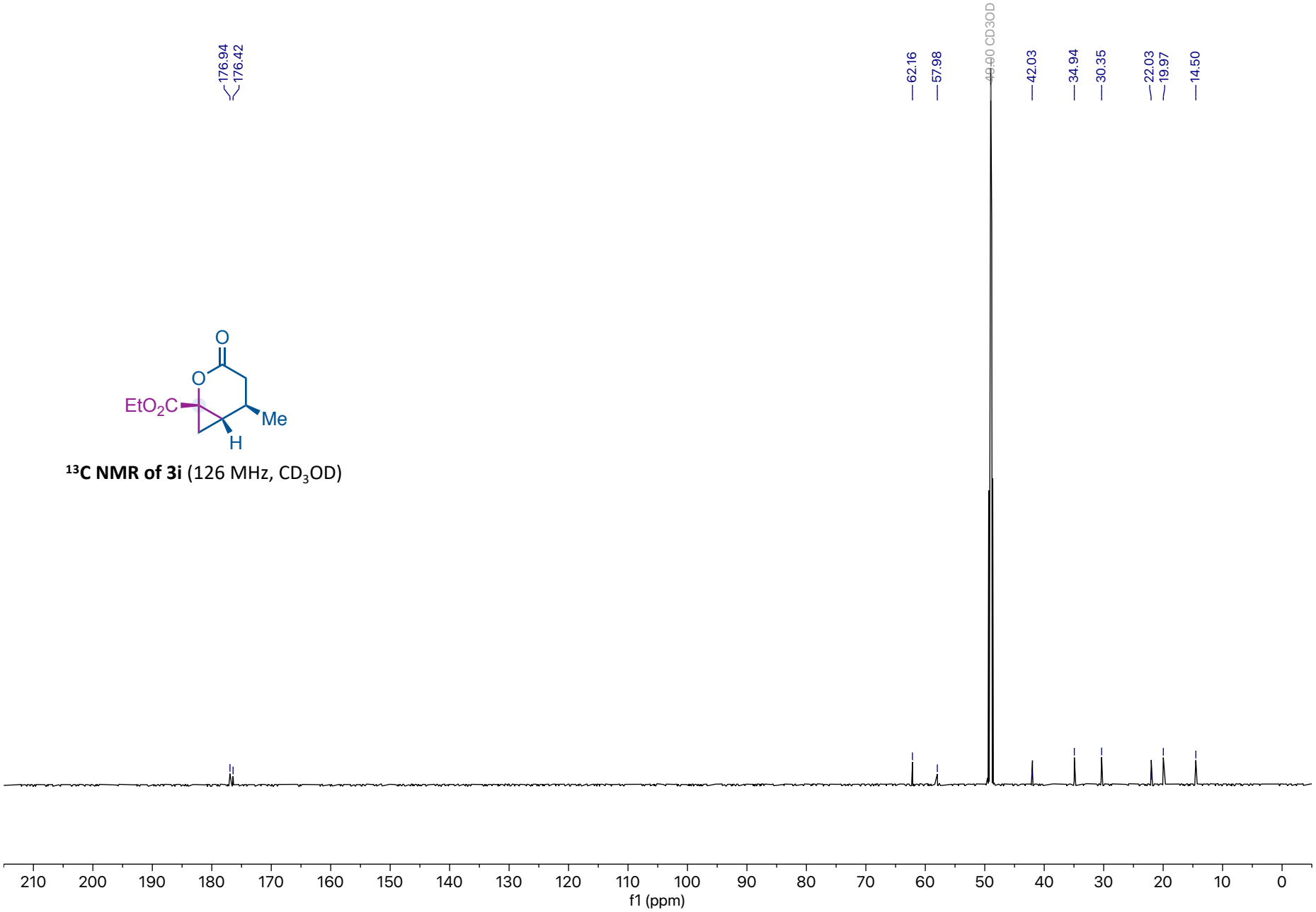
^{1}H NMR of 3i (400 MHz, $CDCl_3$)



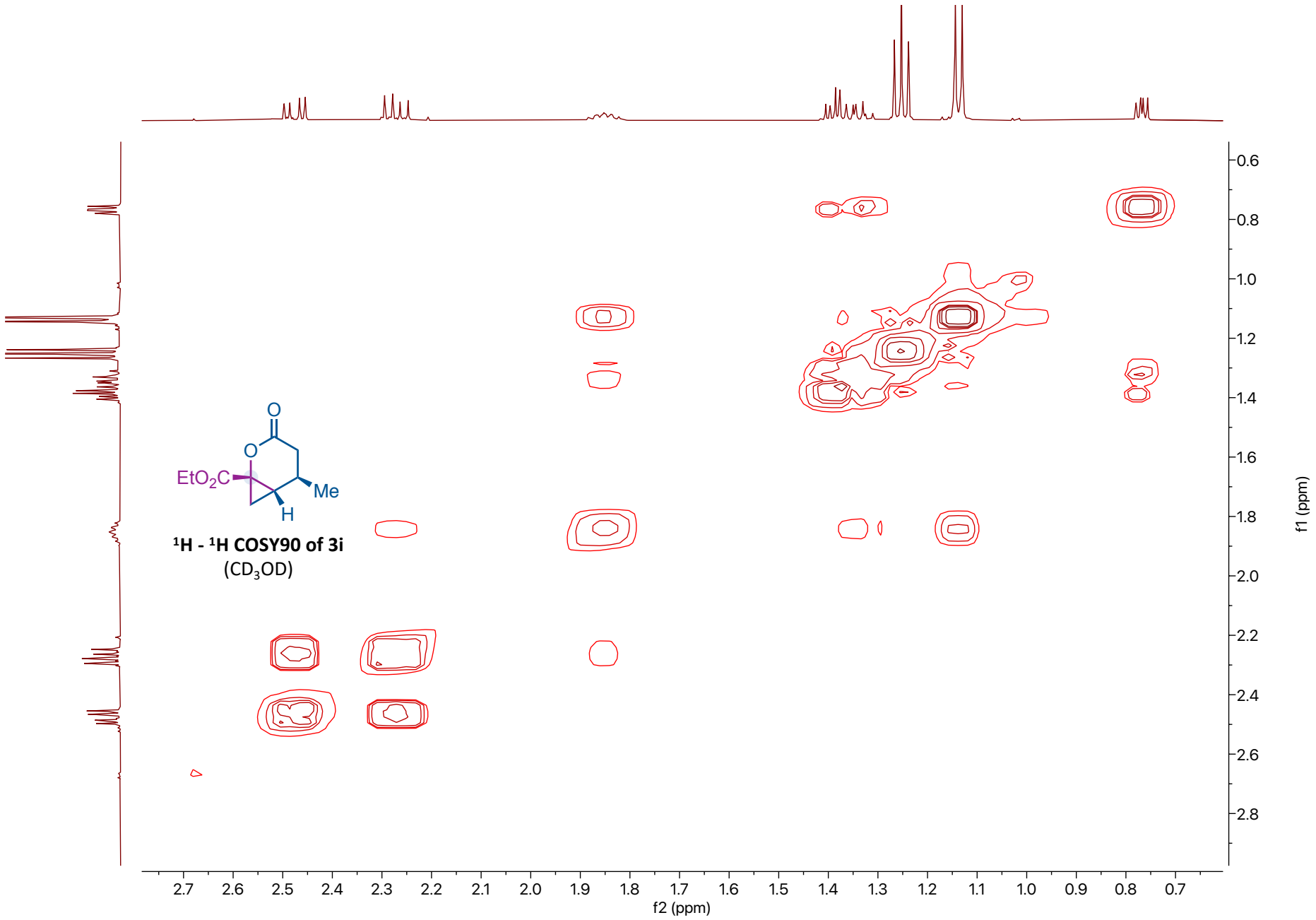
^{1}H NMR of 3i (500 MHz, CD_3OD)

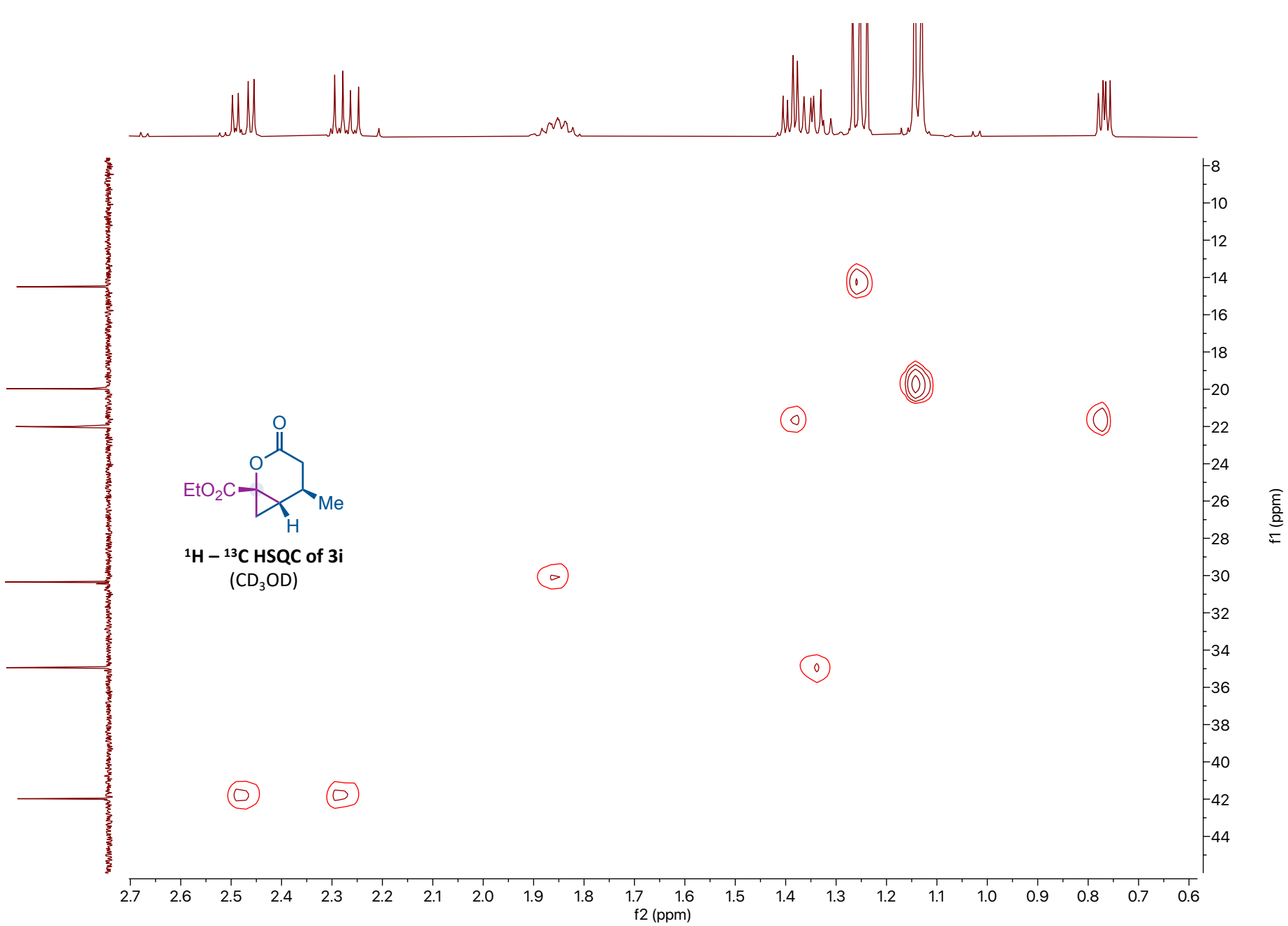


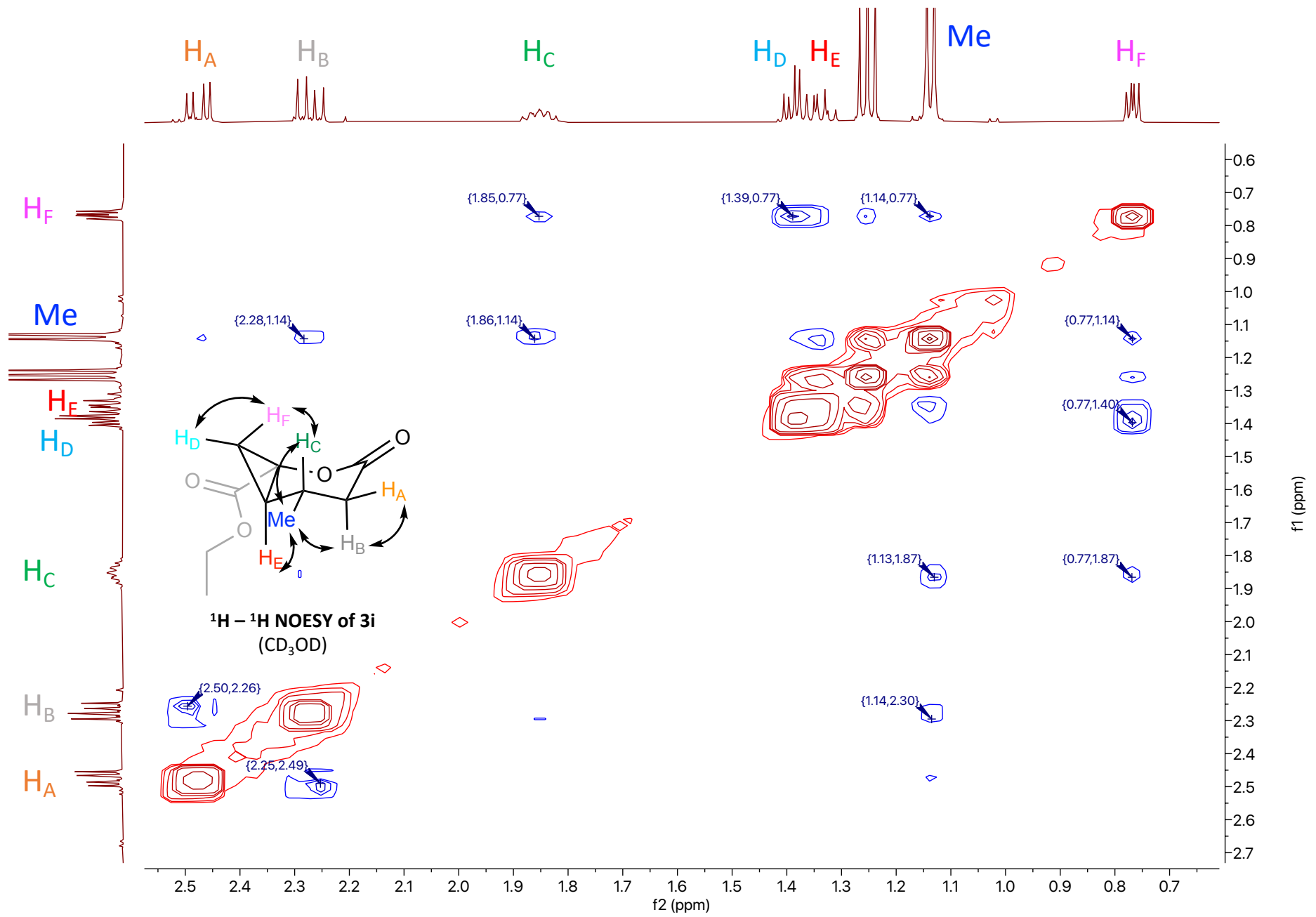
^{13}C NMR of 3i (101 MHz, $CDCl_3$)

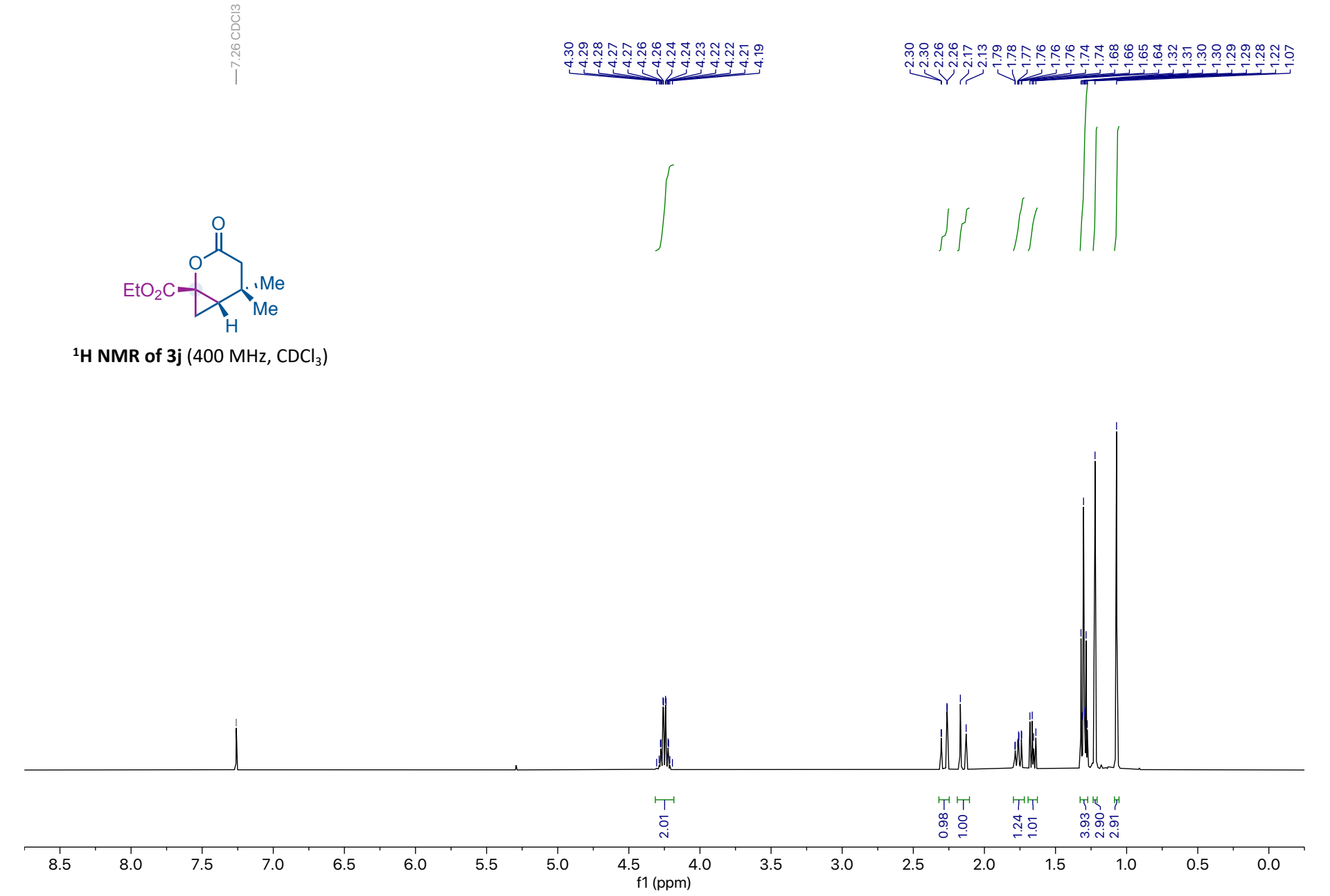


^{13}C NMR of 3i (126 MHz, CD_3OD)

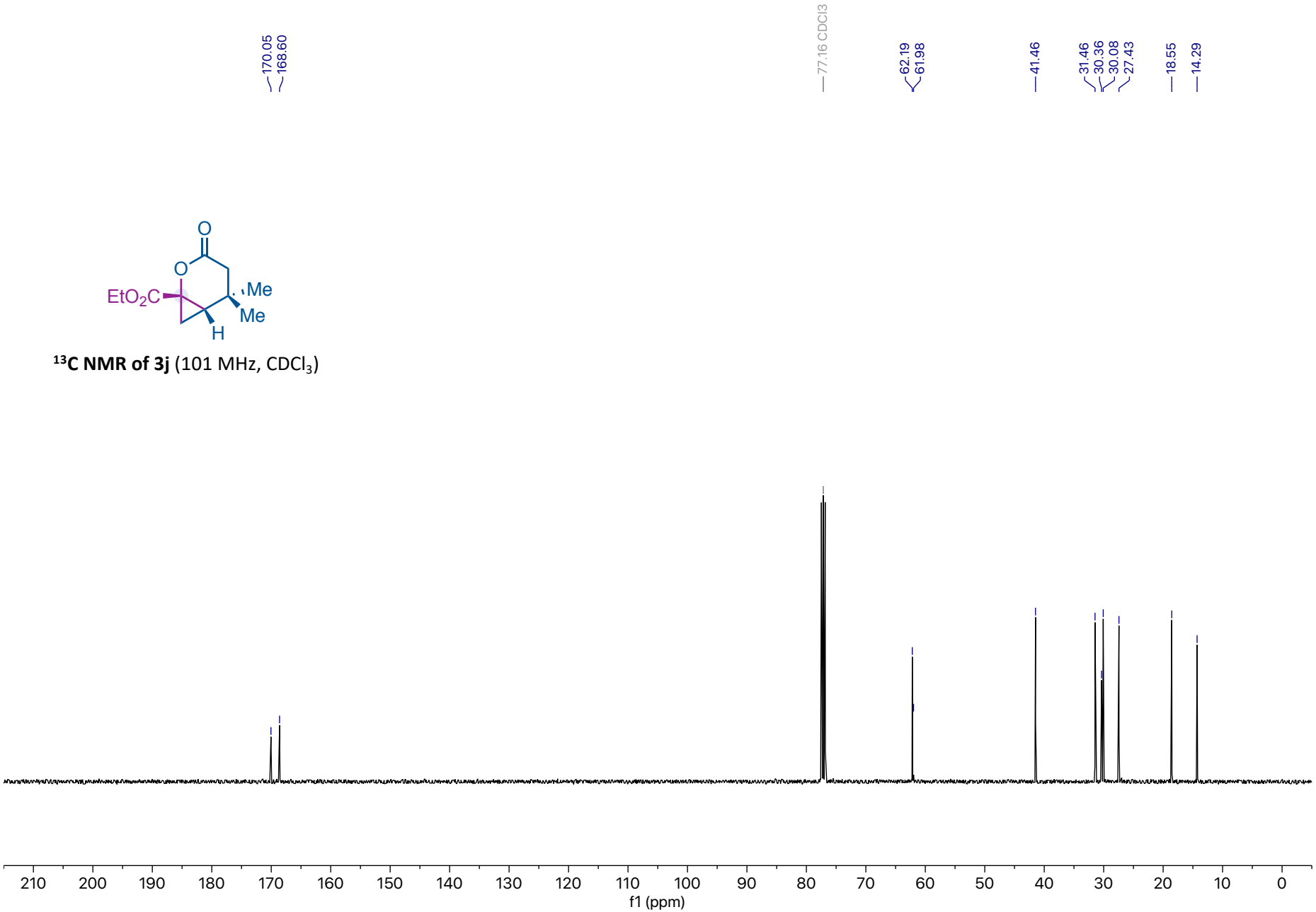

O
O
EtO2C
Me
H
¹H - ¹H COSY90 of 3i
(CD3OD)
f2 (ppm)
f1 (ppm)


O
O
EtO2C
Me
H
1H – 13C HSQC of 3i
(CD3OD)
f2 (ppm)
f1 (ppm)

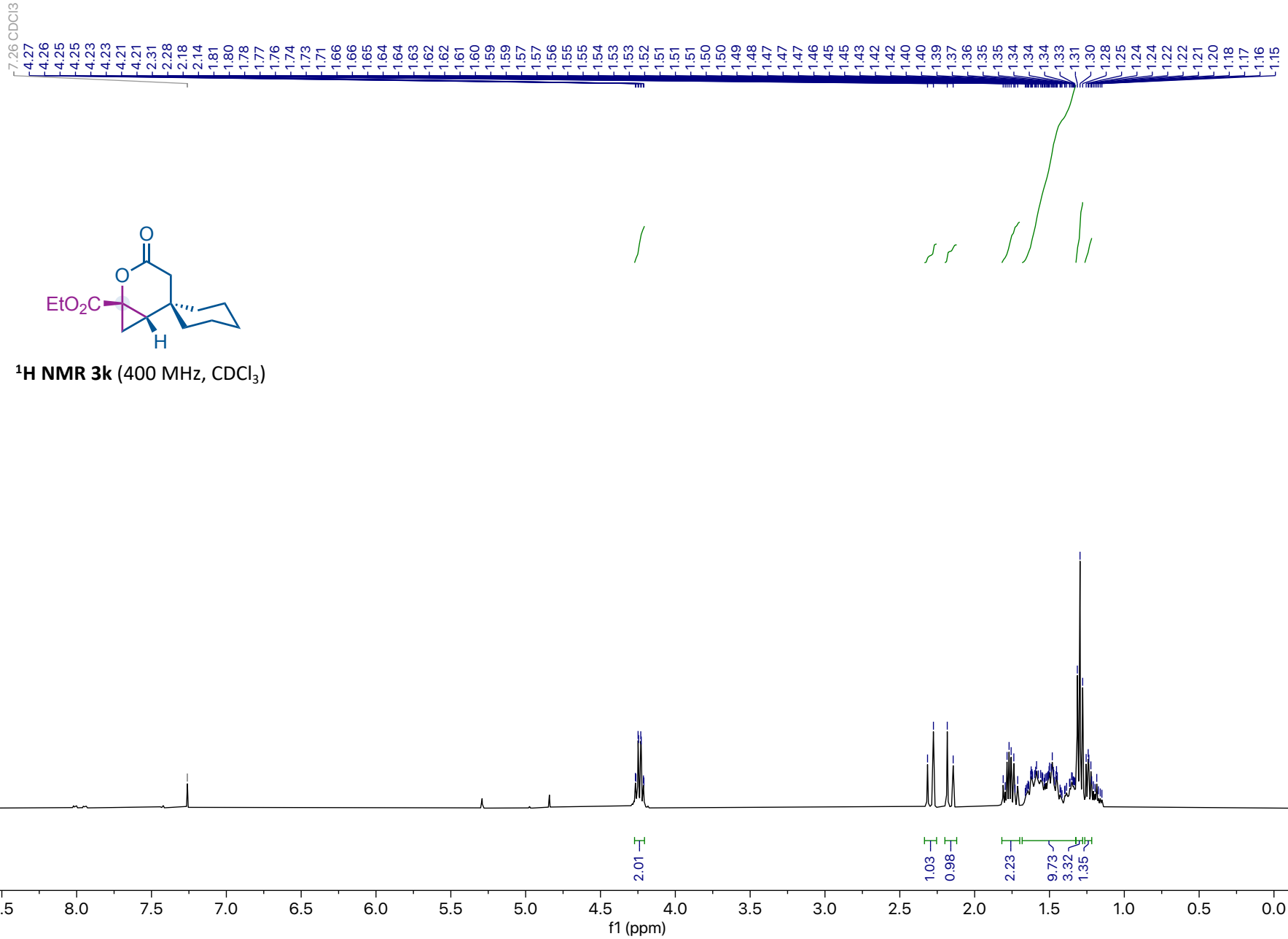

HA
HB
HC
HD
HE
Me
HF
{1.85,0.77}
{1.39,0.77}
{1.14,0.77}
{2.28,1.14}
{1.86,1.14}
{0.77,1.14}
{0.77,1.40}
{1.13,1.87}
{0.77,1.87}
{1.14,2.30}
{2.50,2.26}
{2.25,2.49}
1H – 1H NOESY of 3i
(CD3OD)
f2 (ppm)
f1 (ppm)



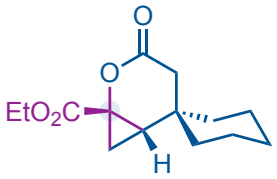
^{1}H NMR of 3j (400 MHz, $CDCl_3$)



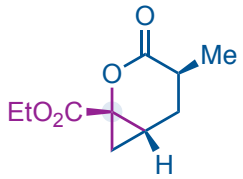
^{13}C NMR of 3j (101 MHz, $CDCl_3$)



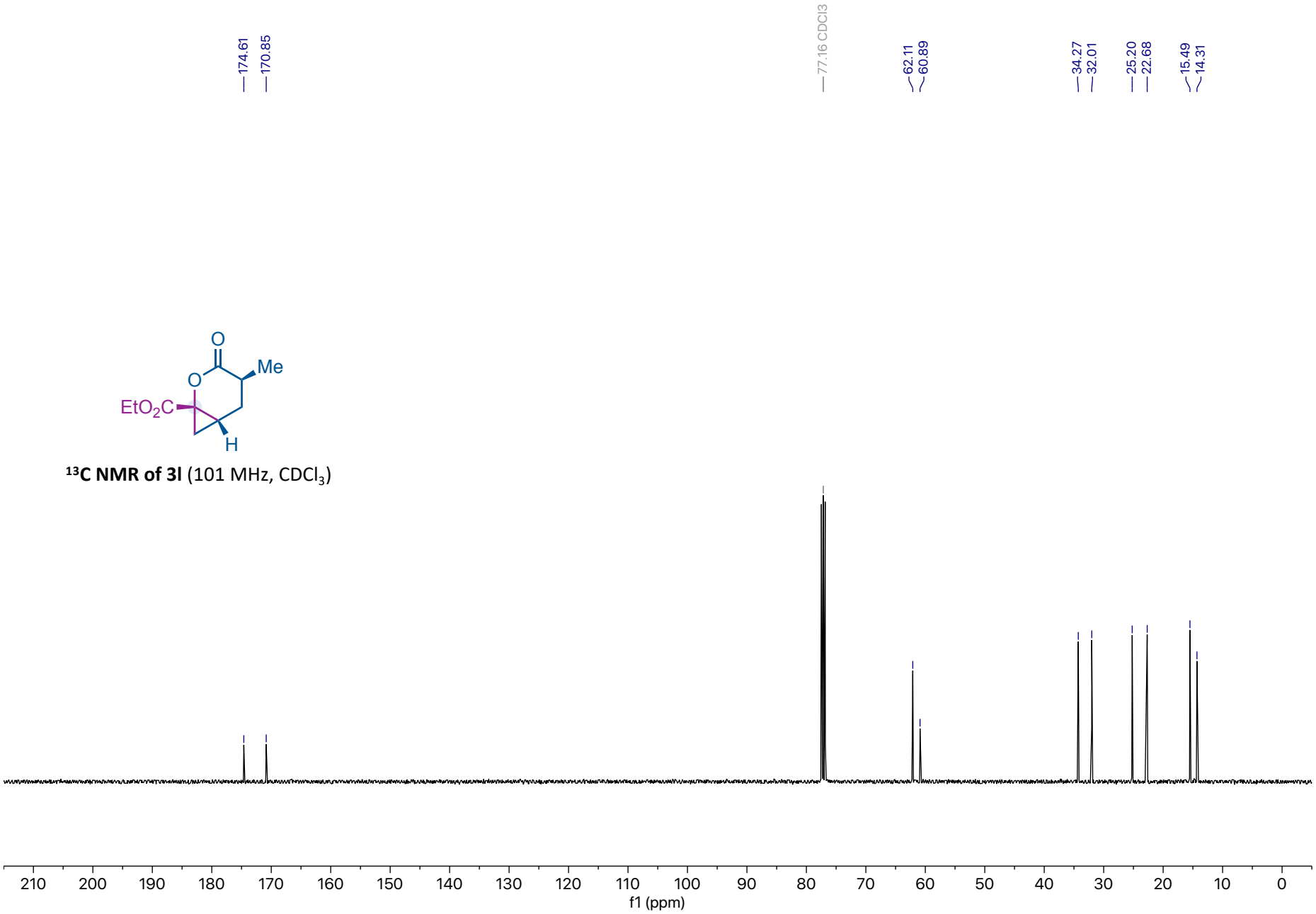
^{1}H NMR 3k (400 MHz, $CDCl_3$)



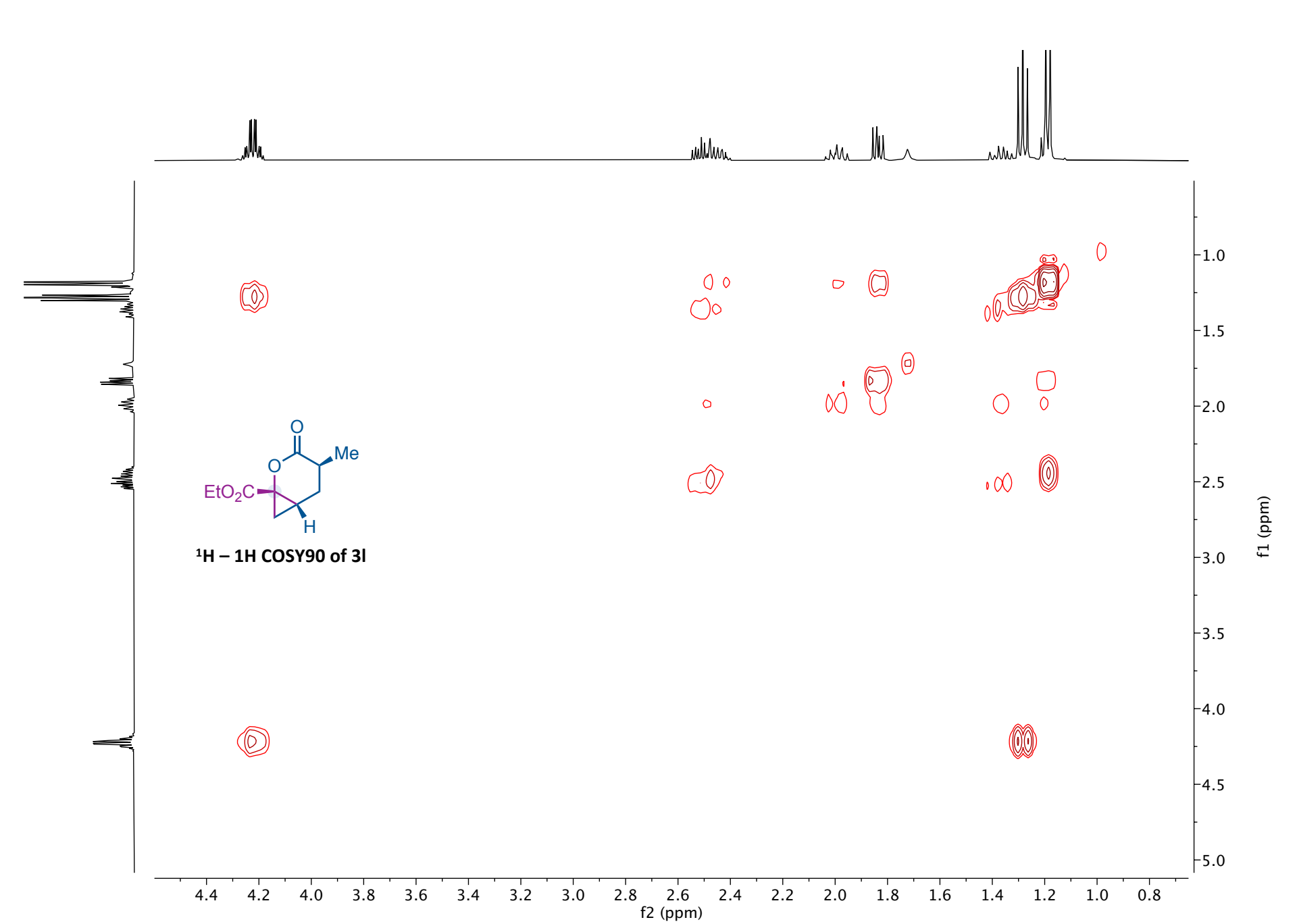
^{13}C NMR of 3k (101 MHz, $CDCl_3$)



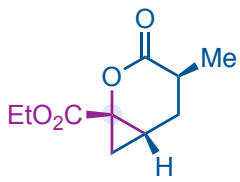
^{1}H NMR of 3l (400 MHz, $CDCl_3$)



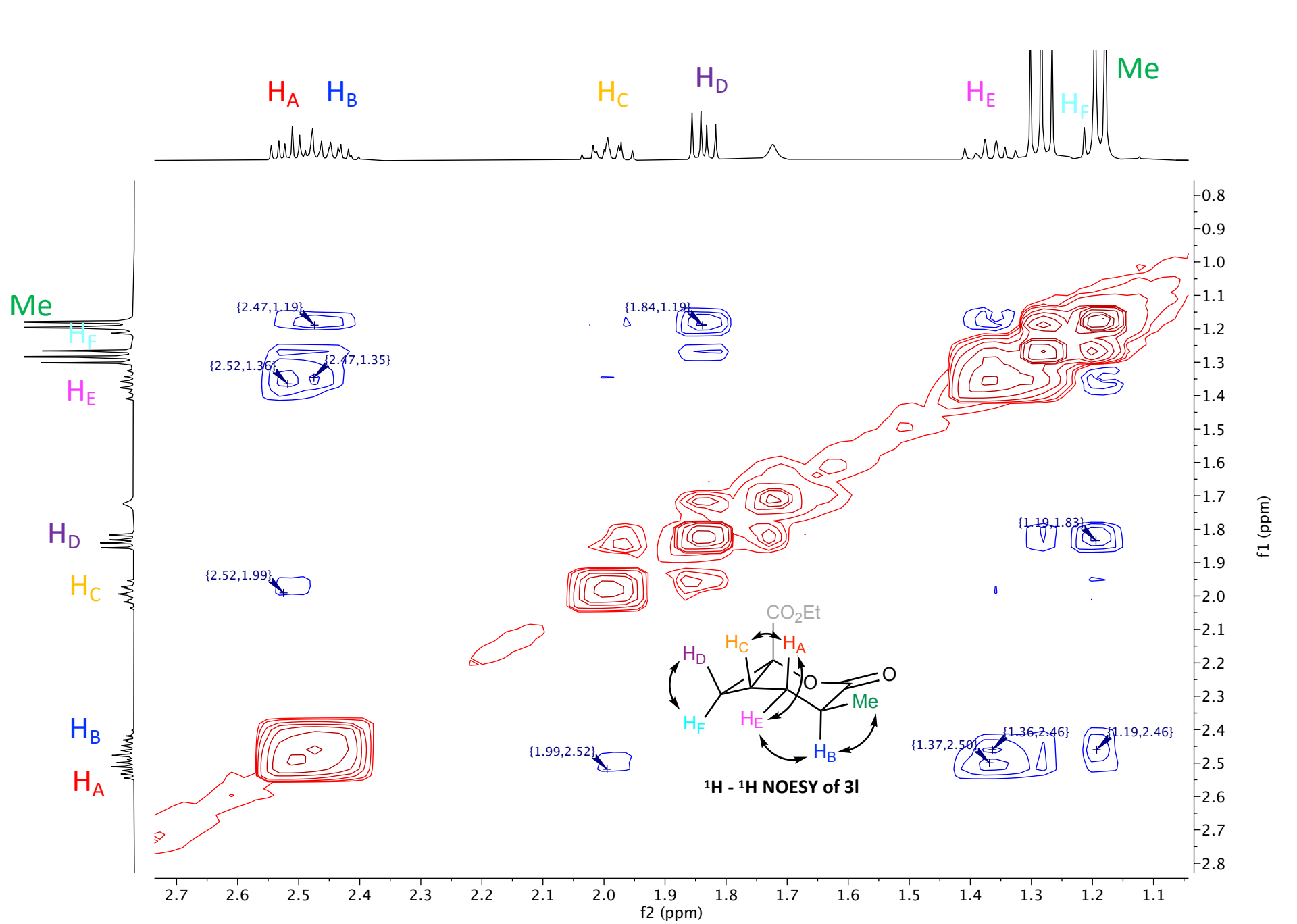
^{13}C NMR of 3l (101 MHz, $CDCl_3$)



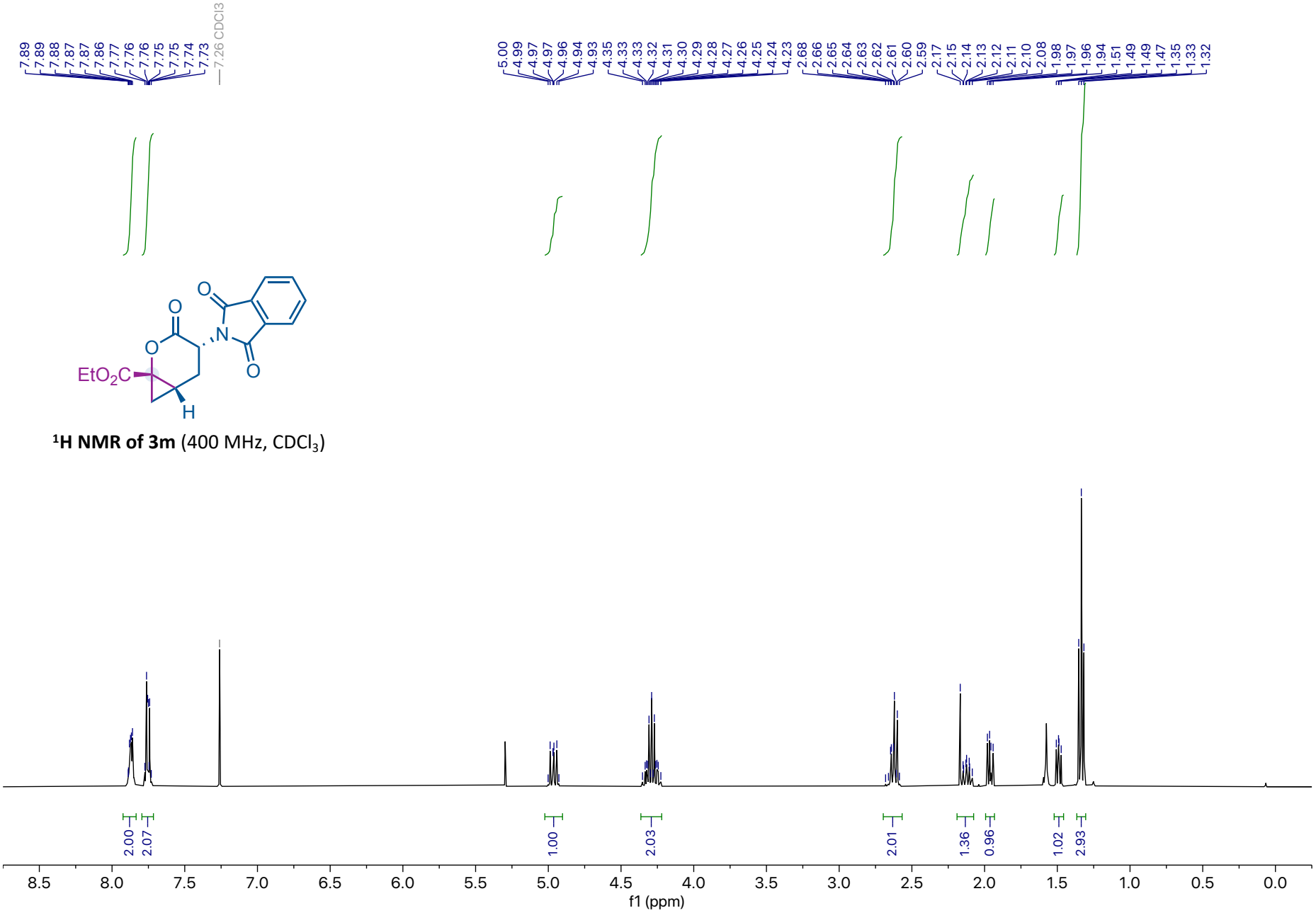
^{1}H – 1H COSY90 of 3l



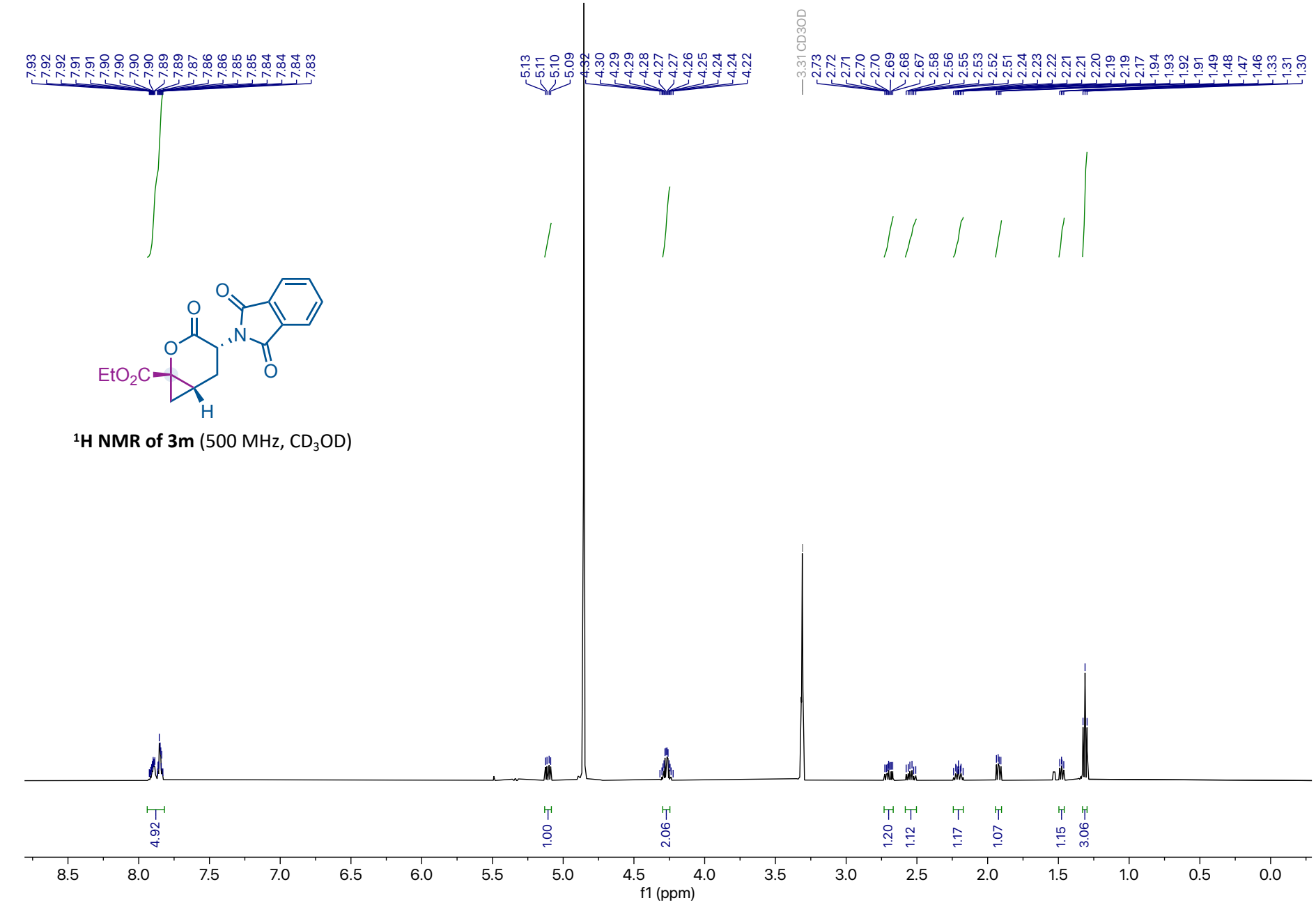
^{1}H – ^{13}C HSQC of 3l



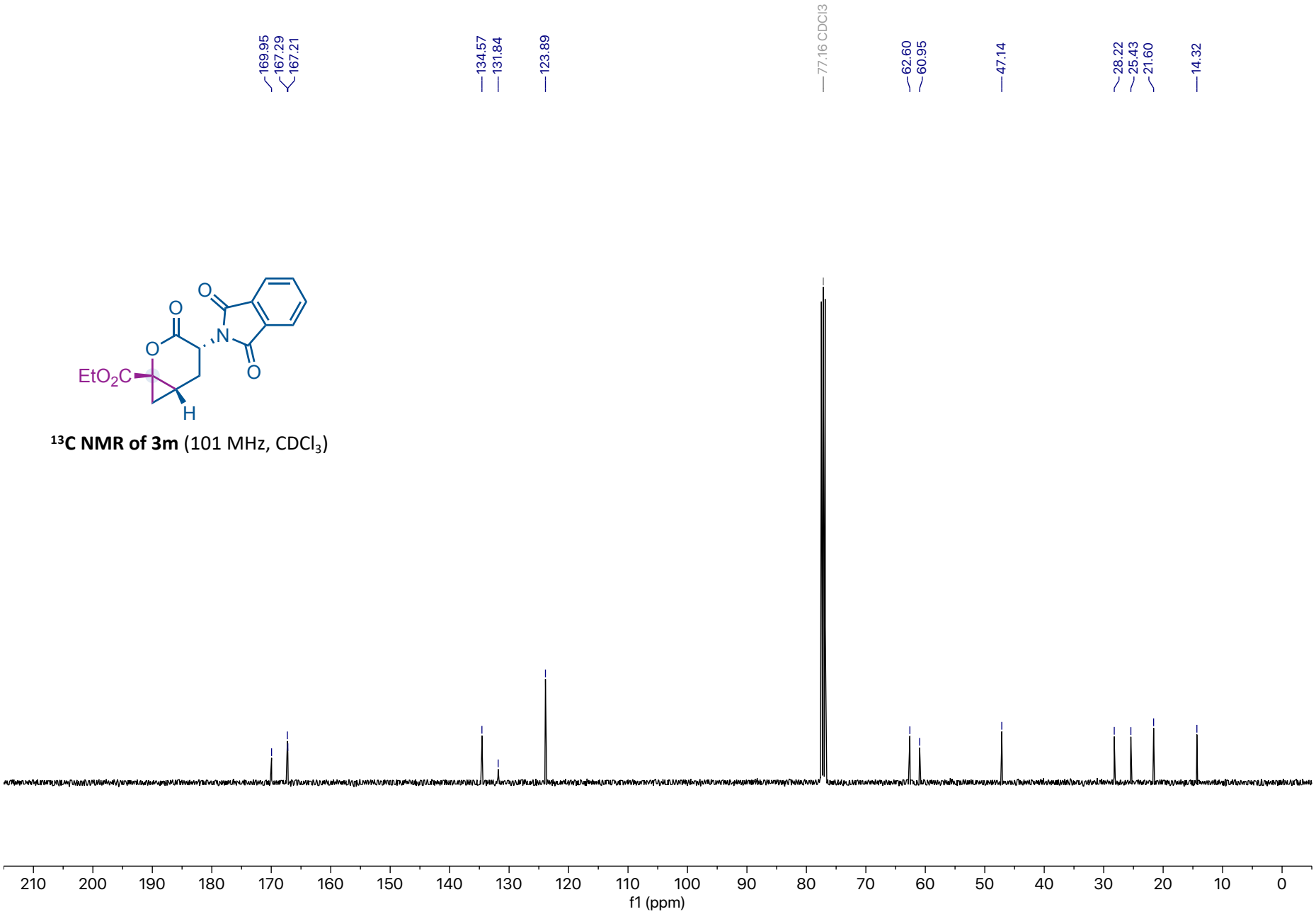
^{1}H - ^{1}H NOESY of 3l



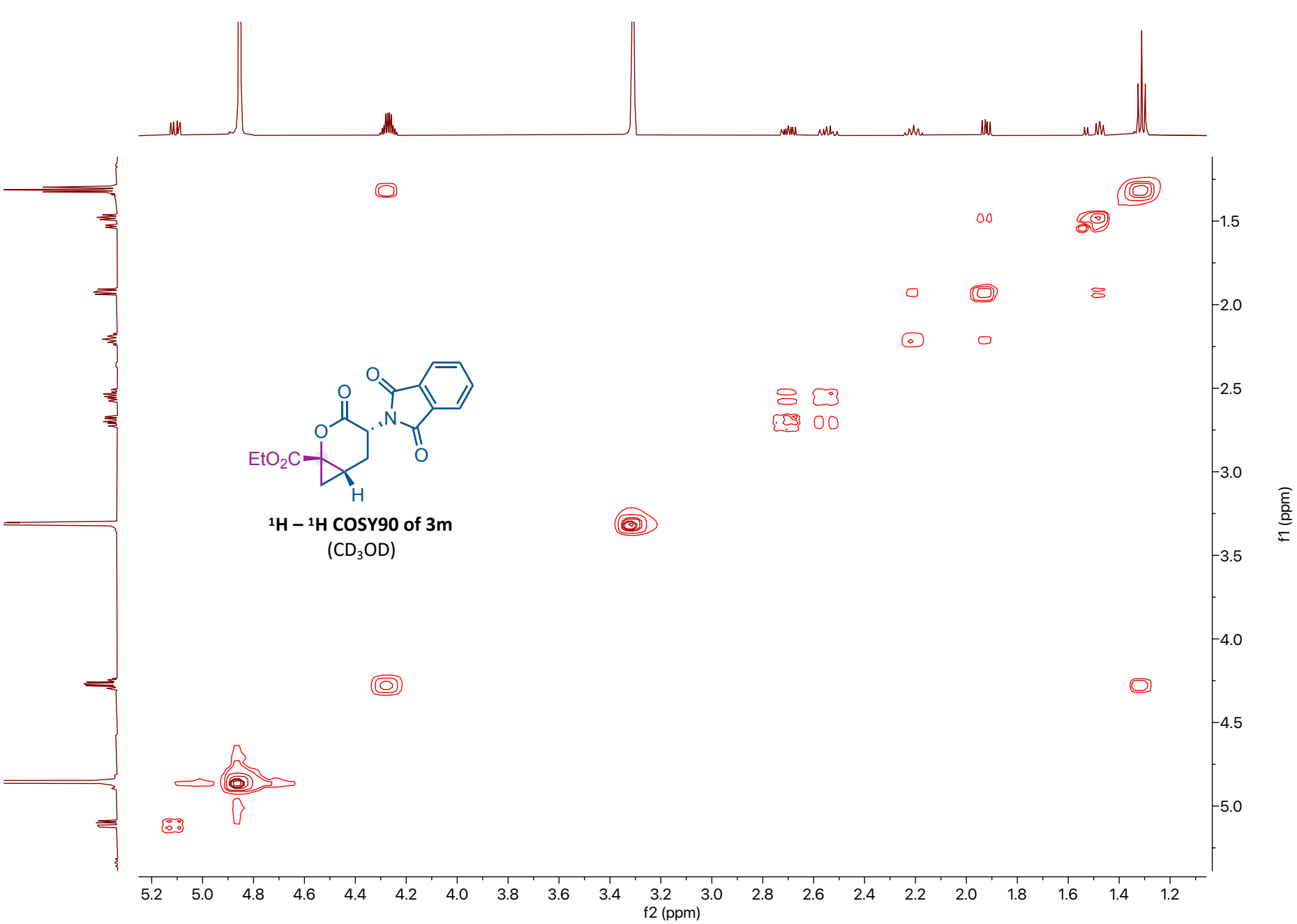
^{1}H NMR of 3m (400 MHz, $CDCl_3$)

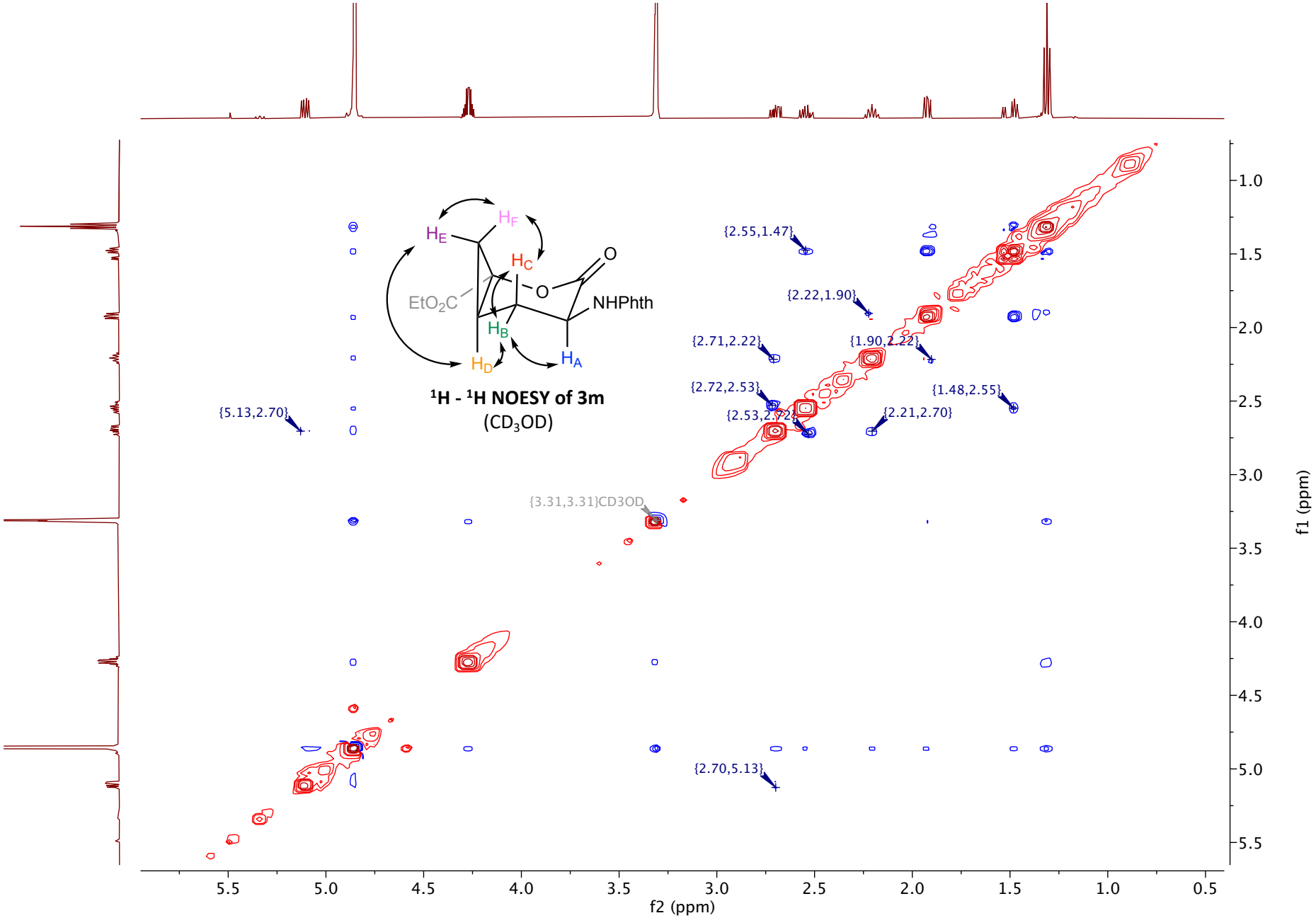


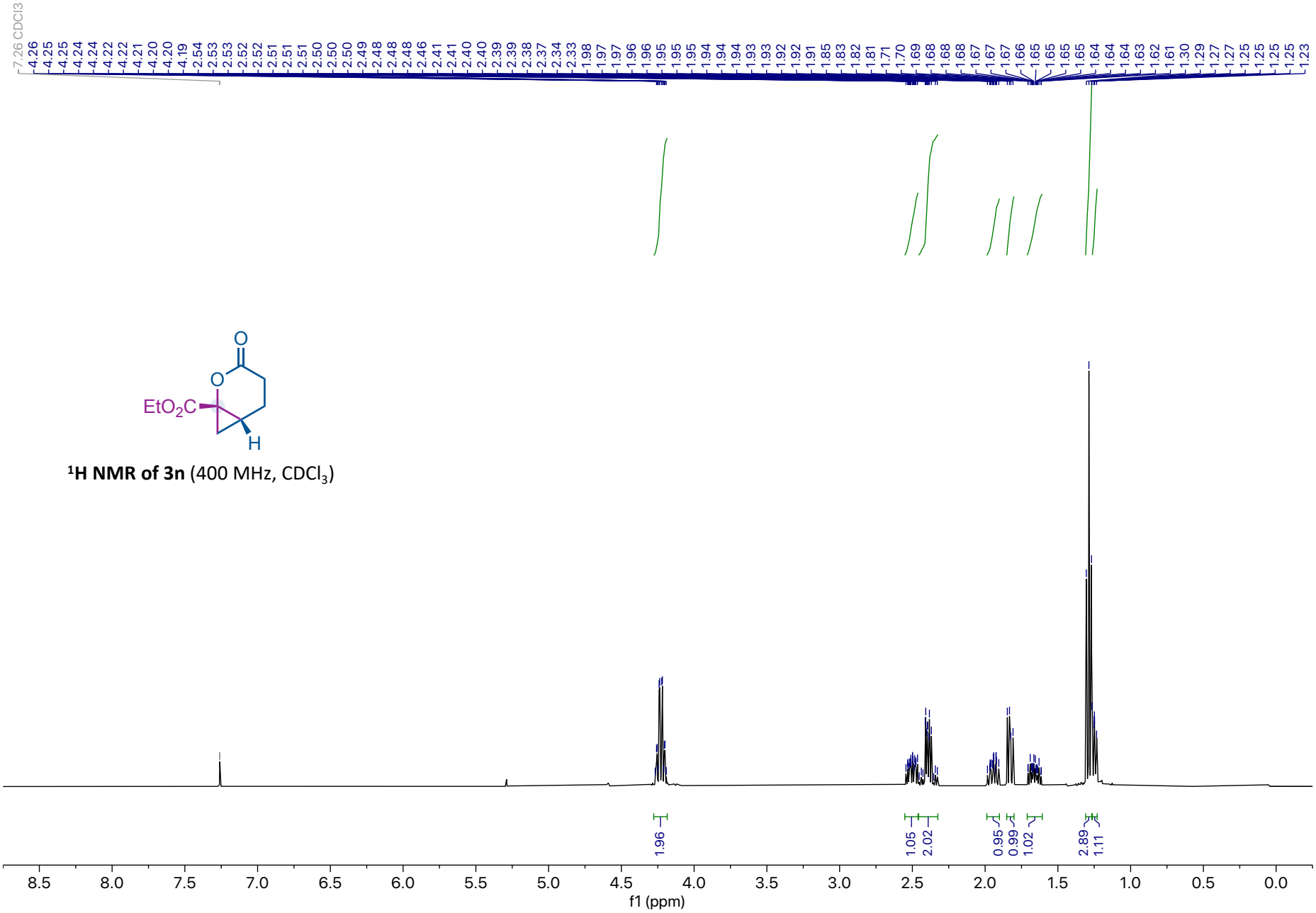
^{1}H NMR of 3m (500 MHz, CD_3OD)



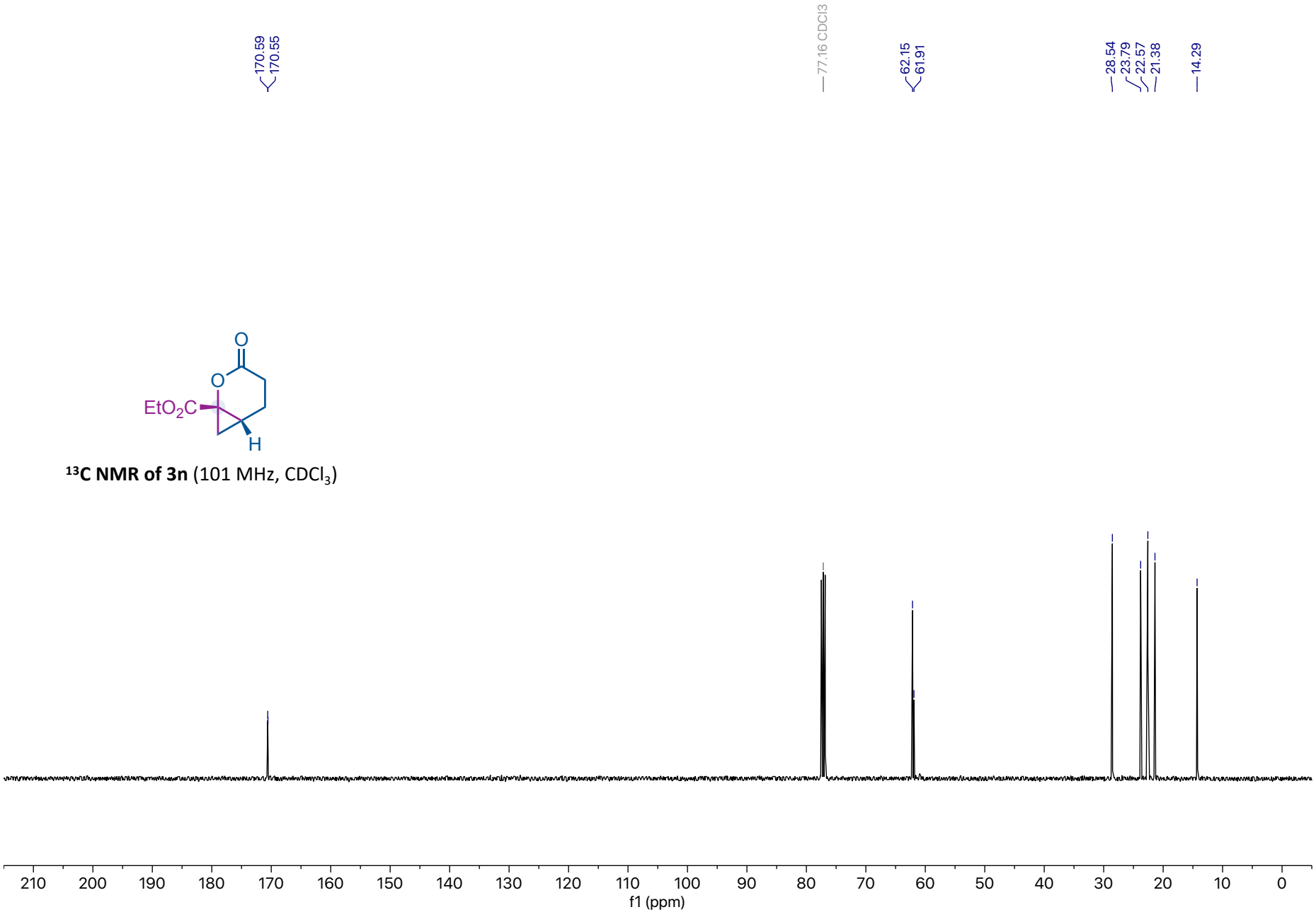
^{13}C NMR of 3m (101 MHz, $CDCl_3$)


EtO2C
H
O
O
O
N
O
1H – 1H COSY90 of 3m
(CD3OD)
f2 (ppm)
f1 (ppm)
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0

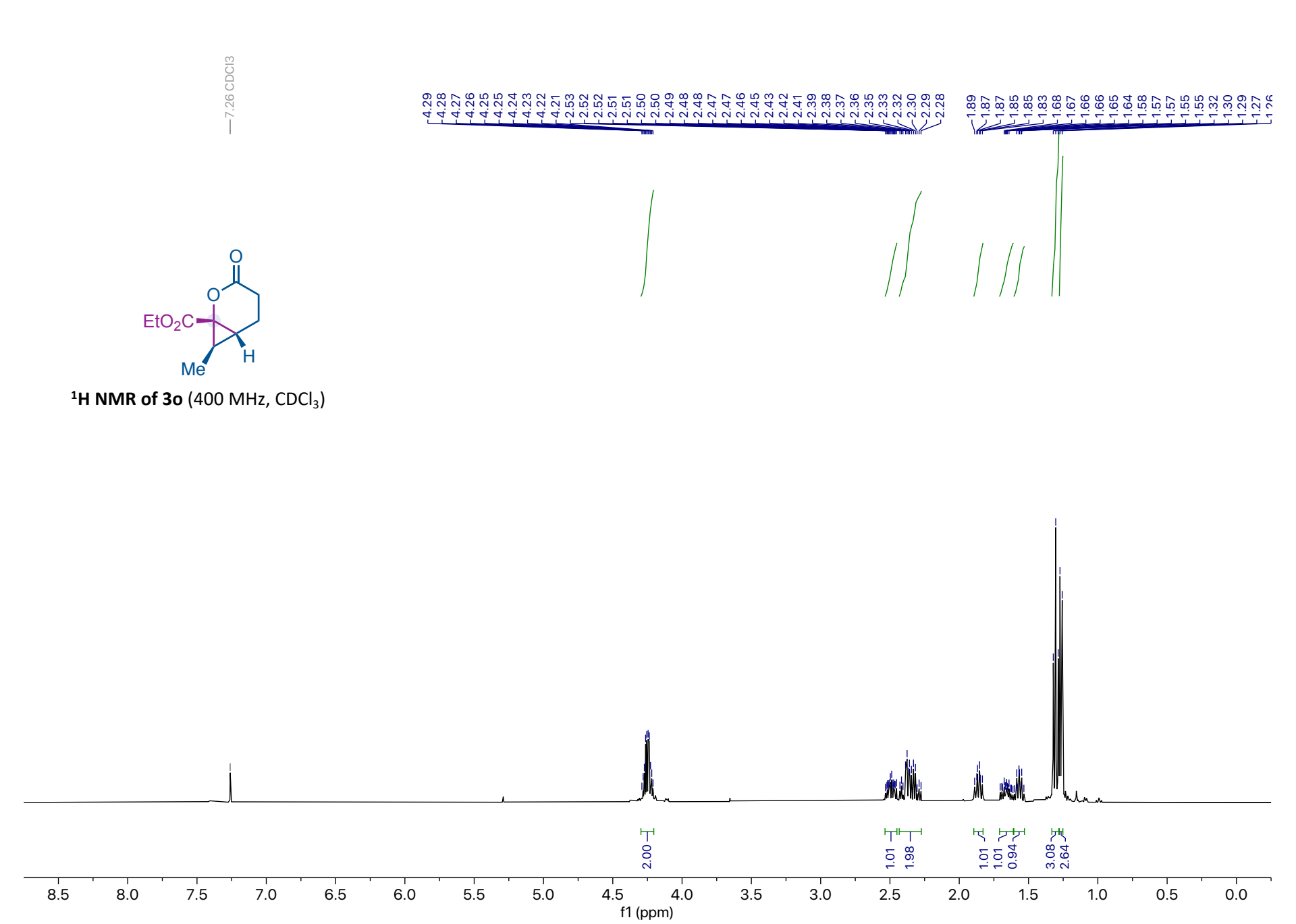

H_F
H_E
H_C
O
O
EtO2C
NHPhth
H_B
H_D
H_A
1H - 1H NOESY of 3m
(CD3OD)
{2.55,1.47}
{2.22,1.90}
{2.71,2.22}
{1.90,2.22}
{2.72,2.53}
{1.48,2.55}
{2.53,2.72}
{2.21,2.70}
{5.13,2.70}
{3.31,3.31}CD3OD
{2.70,5.13}
f2 (ppm)
f1 (ppm)



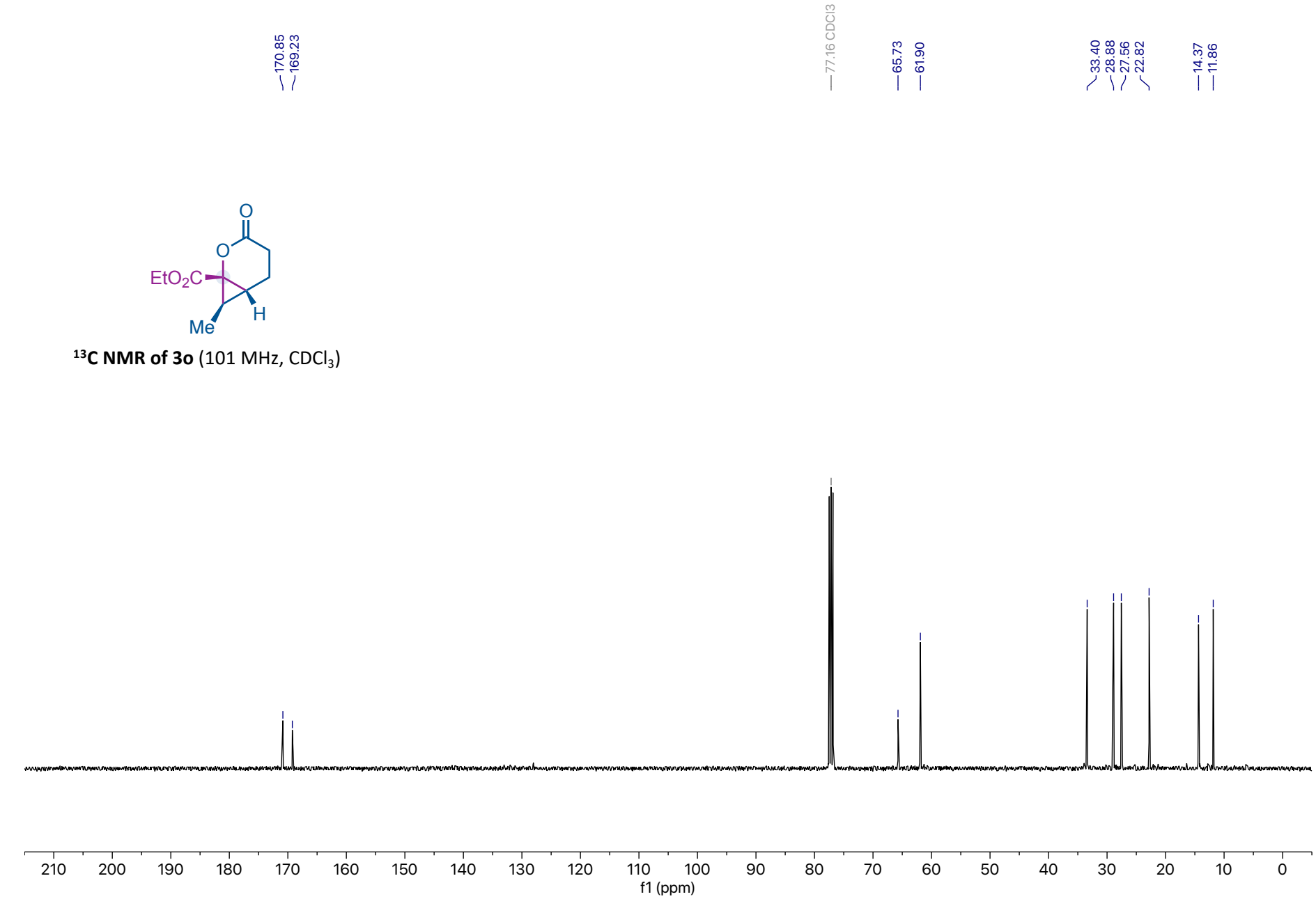
^{1}H NMR of 3n (400 MHz, $CDCl_3$)



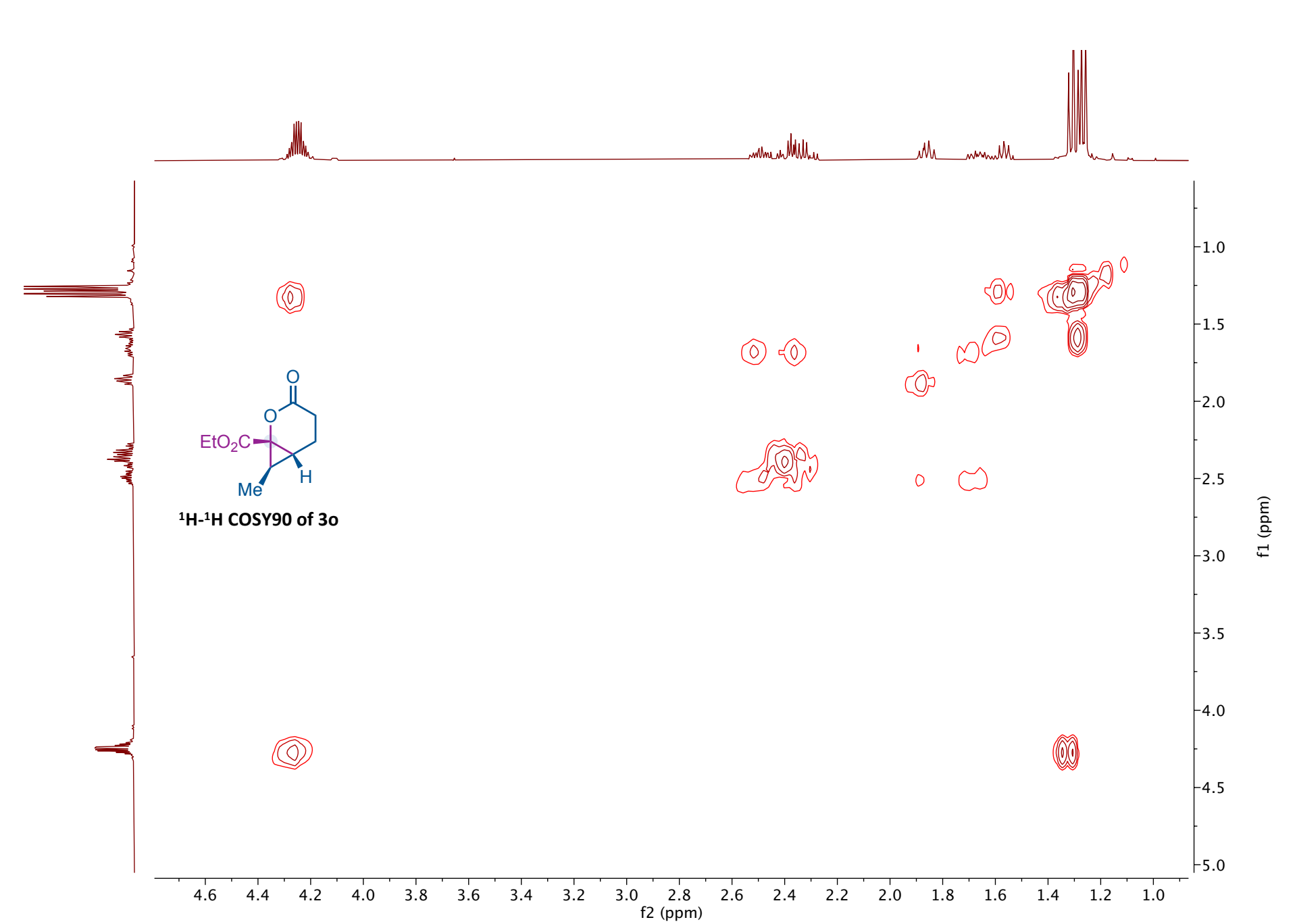
^{13}C NMR of 3n (101 MHz, $CDCl_3$)



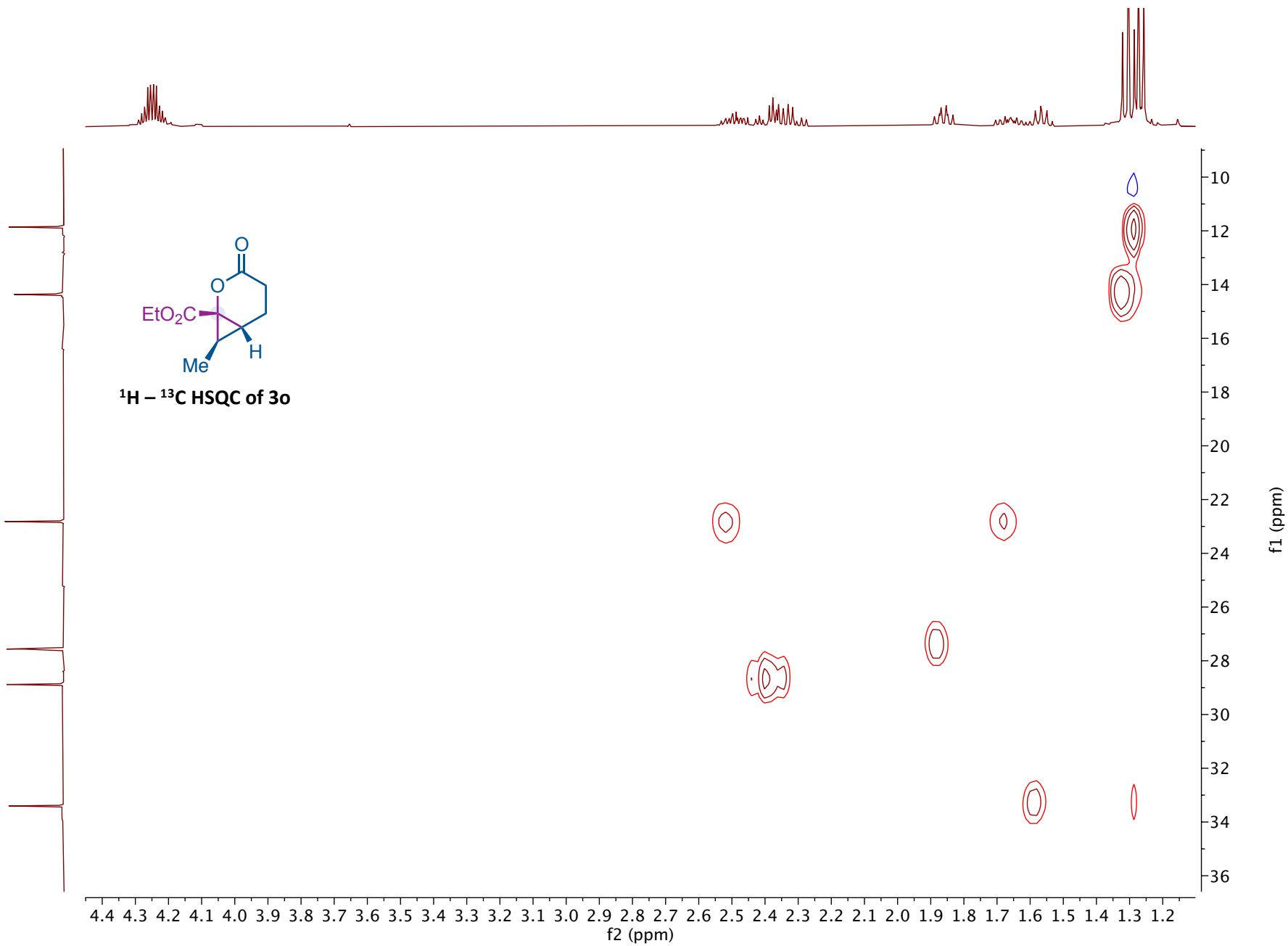
^{1}H NMR of 3o (400 MHz, $CDCl_3$)



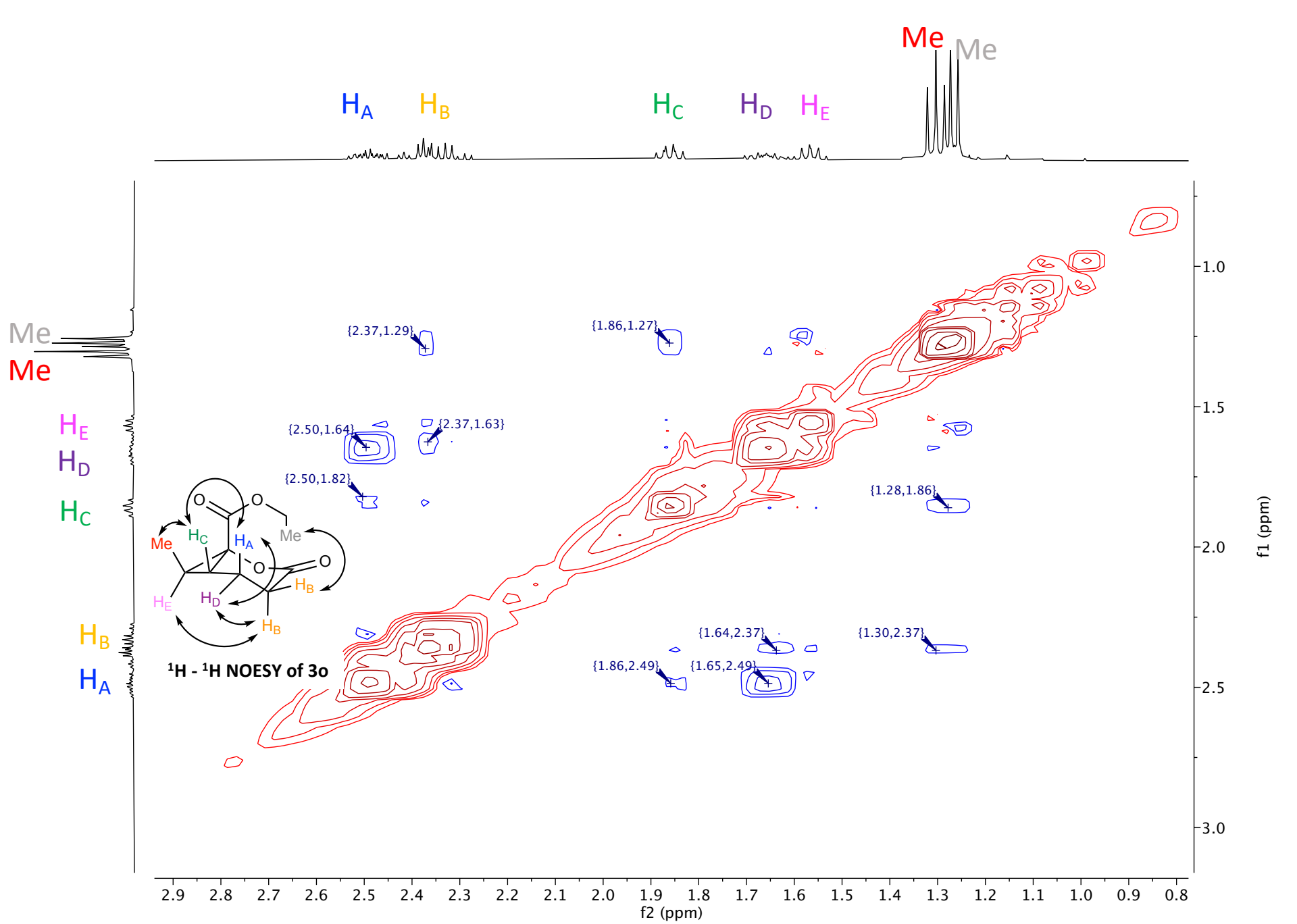
^{13}C NMR of 3o (101 MHz, $CDCl_3$)

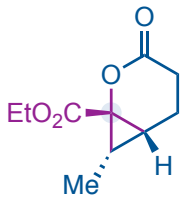


^{1}H-^{1}H COSY90 of 3o

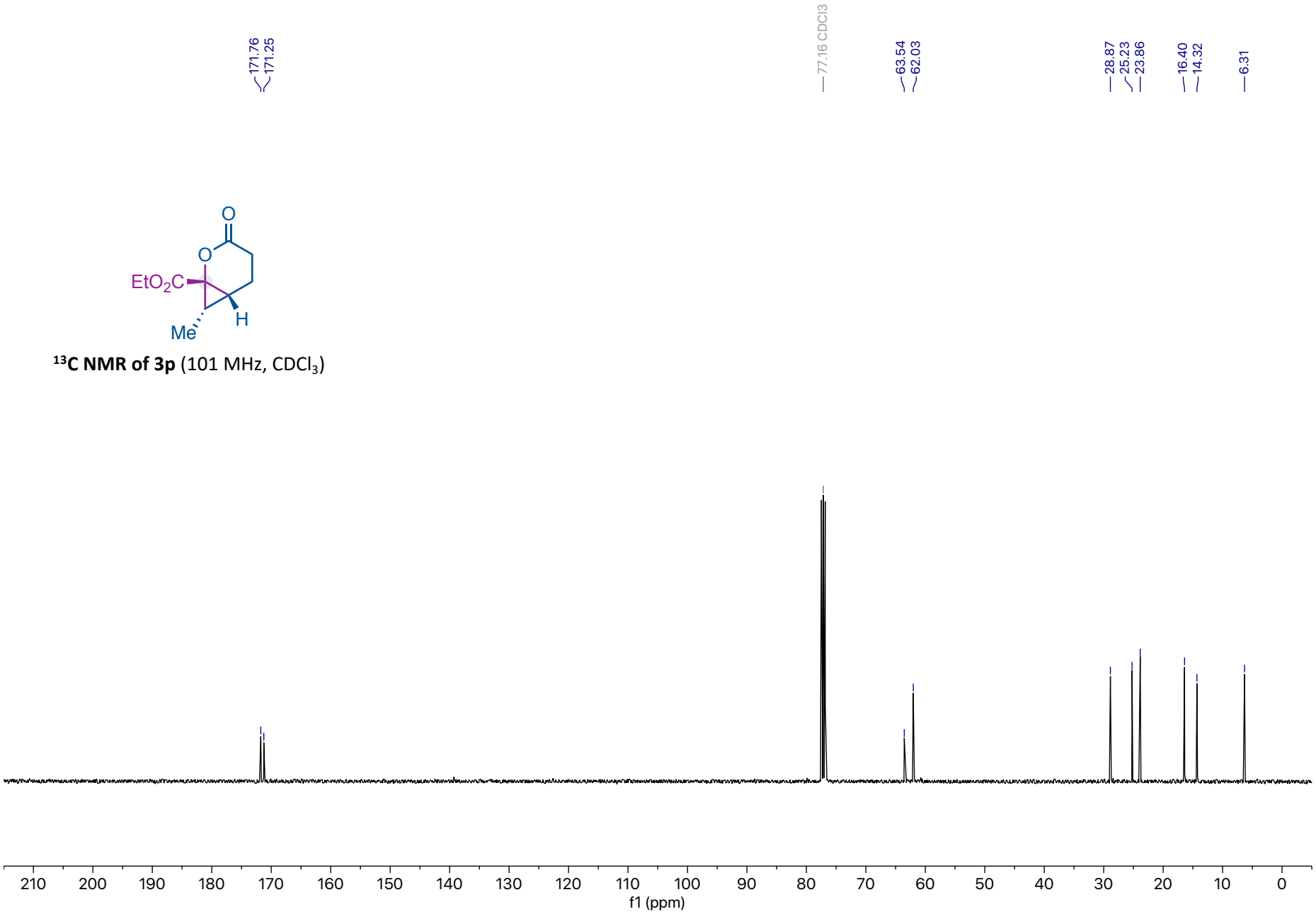


^{1}H – ^{13}C HSQC of 3o

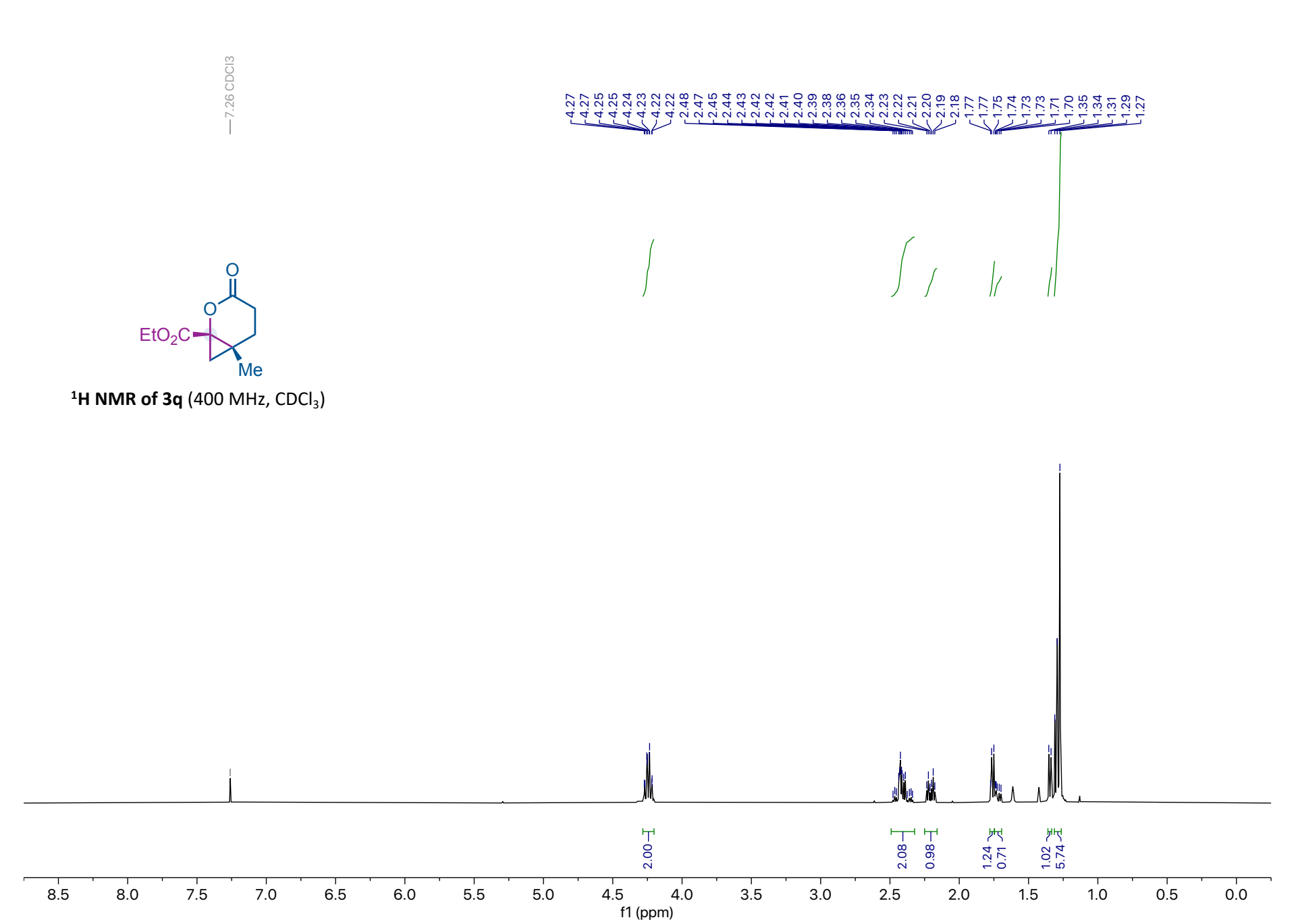

Me
Me
H_A
H_B
H_C
H_D
H_E
{2.37,1.29}
{1.86,1.27}
{2.50,1.64}
{2.37,1.63}
{2.50,1.82}
{1.28,1.86}
{1.64,2.37}
{1.30,2.37}
{1.86,2.49}
{1.65,2.49}
¹H - ¹H NOESY of 3o
f2 (ppm)
f1 (ppm)



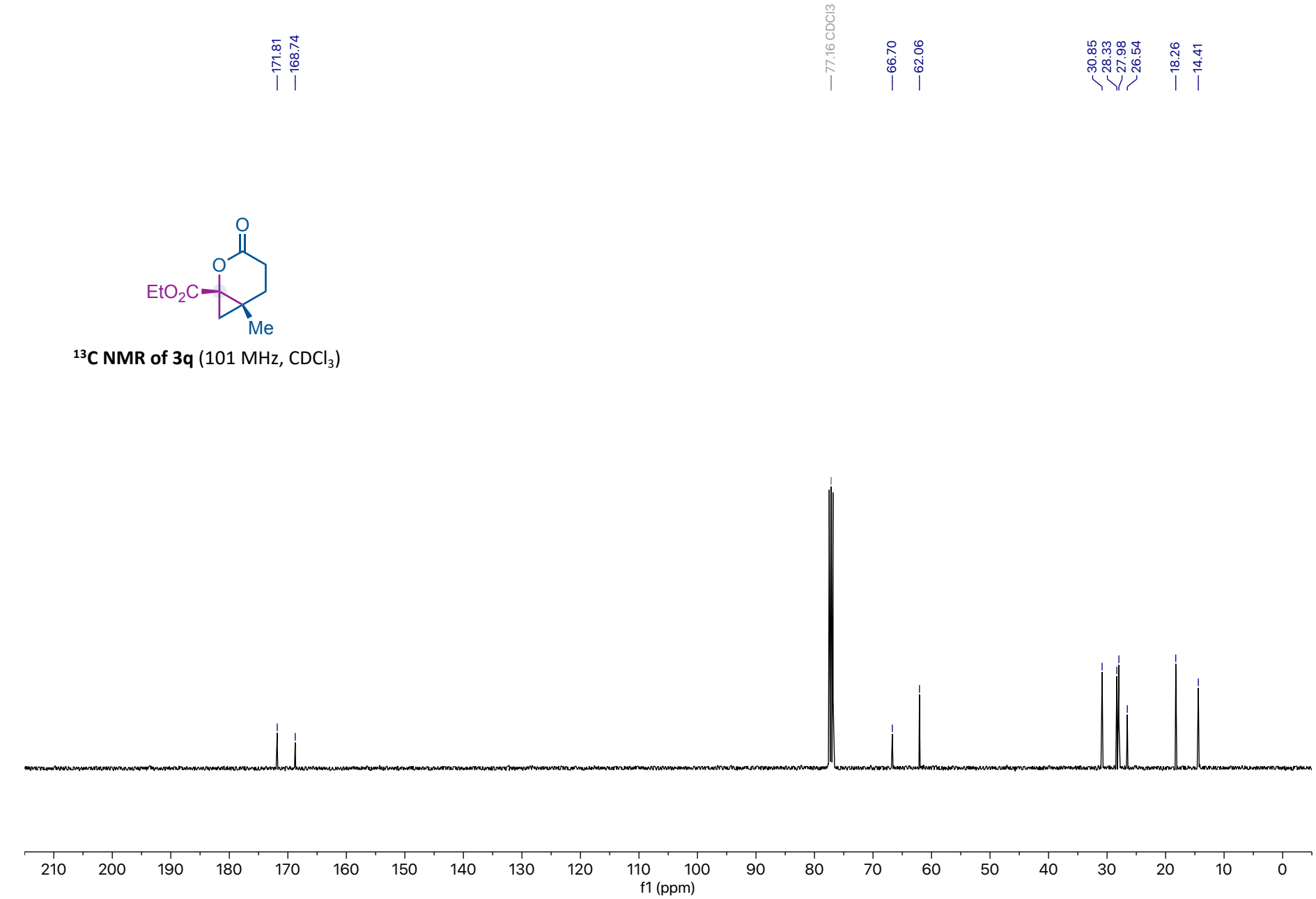
^{1}H NMR of 3p (400 MHz, $CDCl_3$)



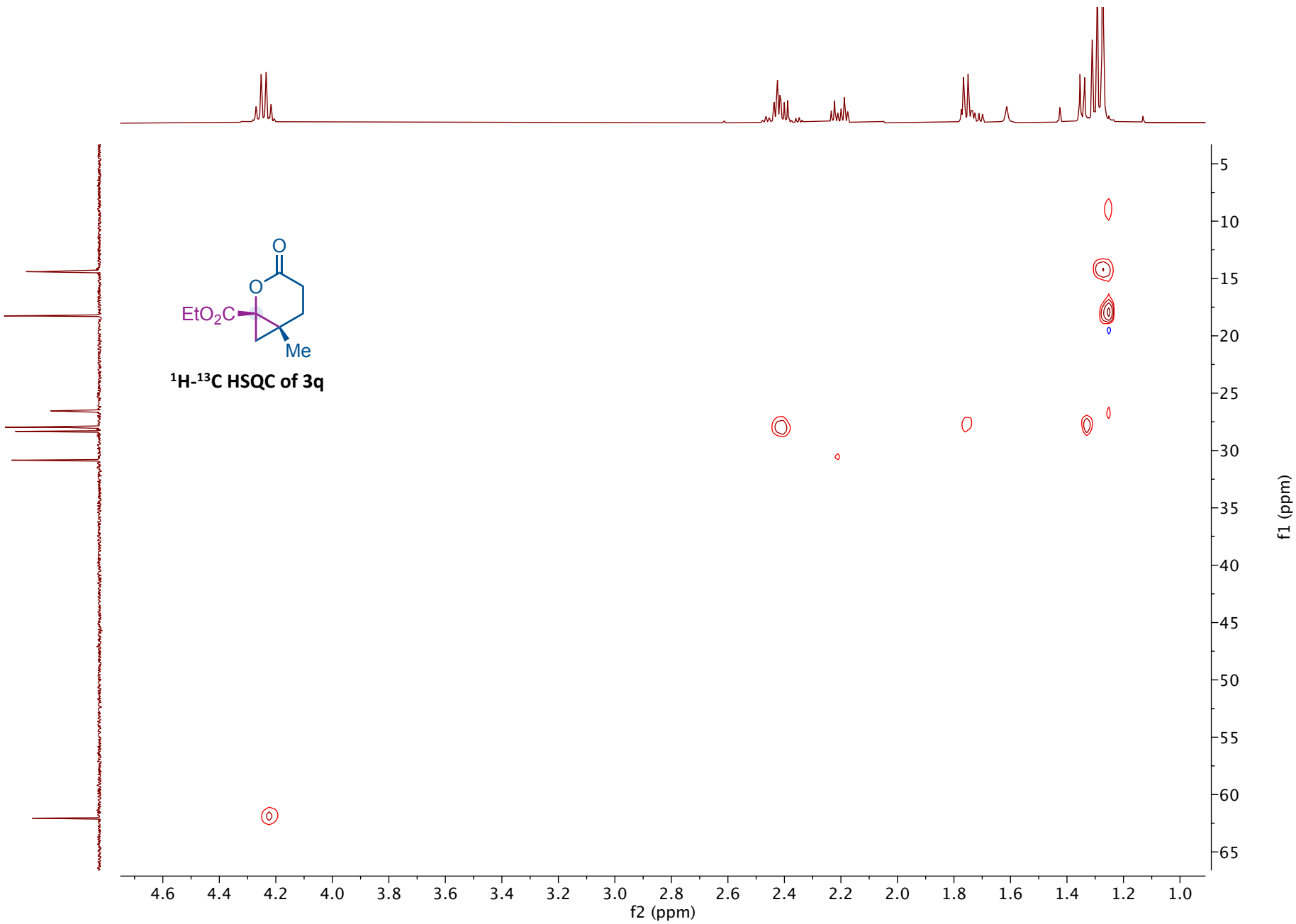
^{13}C NMR of 3p (101 MHz, $CDCl_3$)



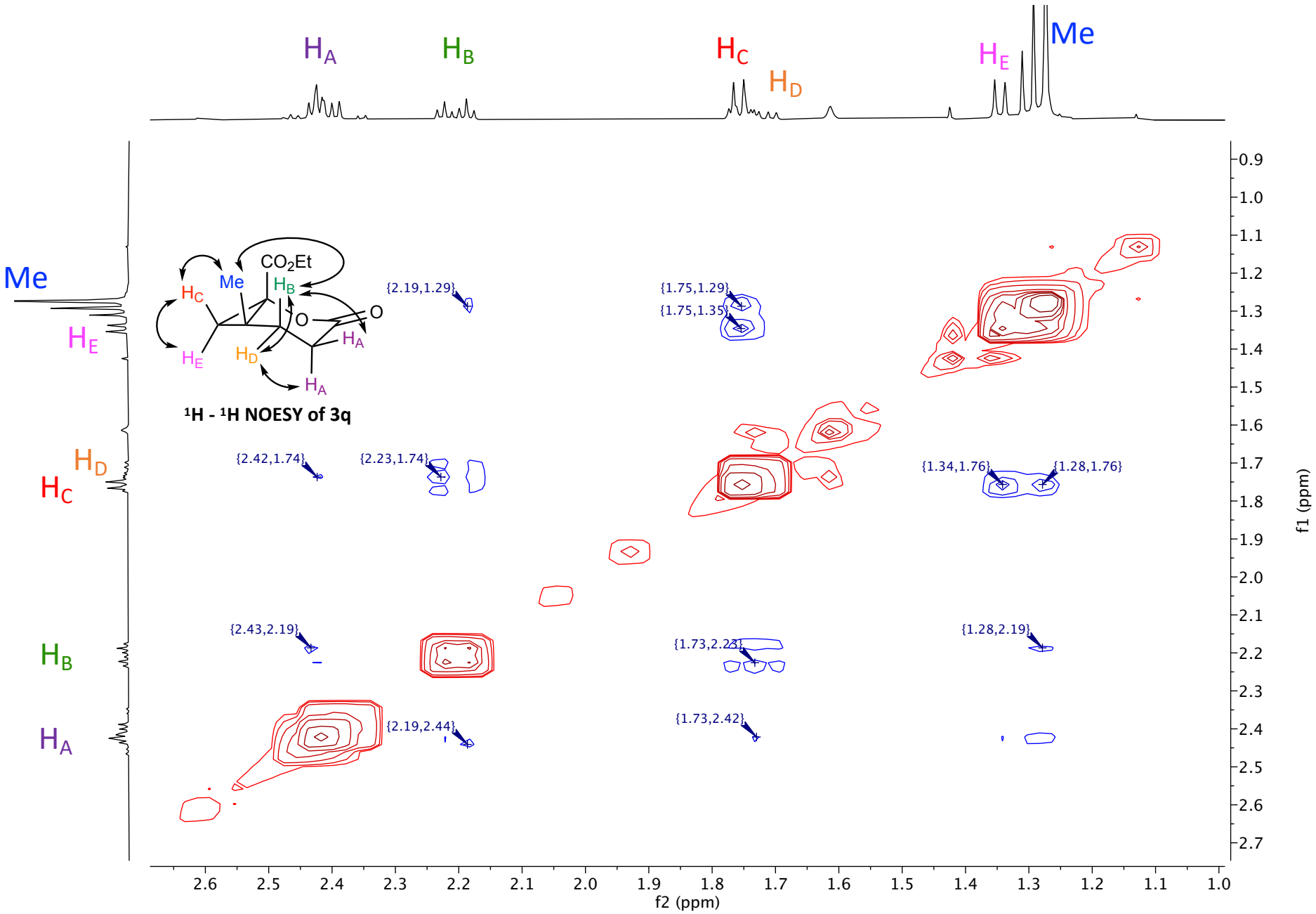
^{1}H NMR of 3q (400 MHz, $CDCl_3$)

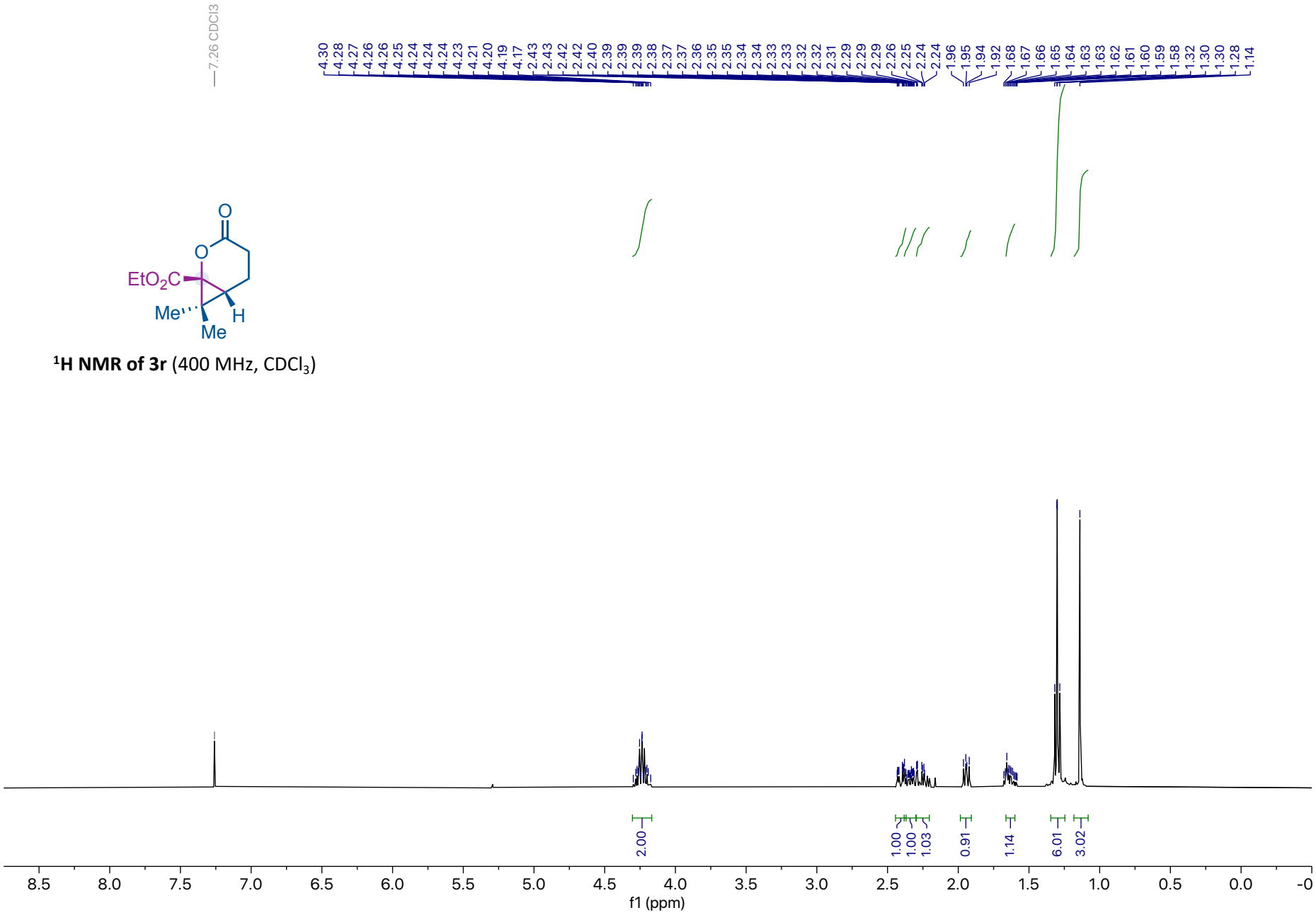


^{13}C NMR of 3q (101 MHz, $CDCl_3$)

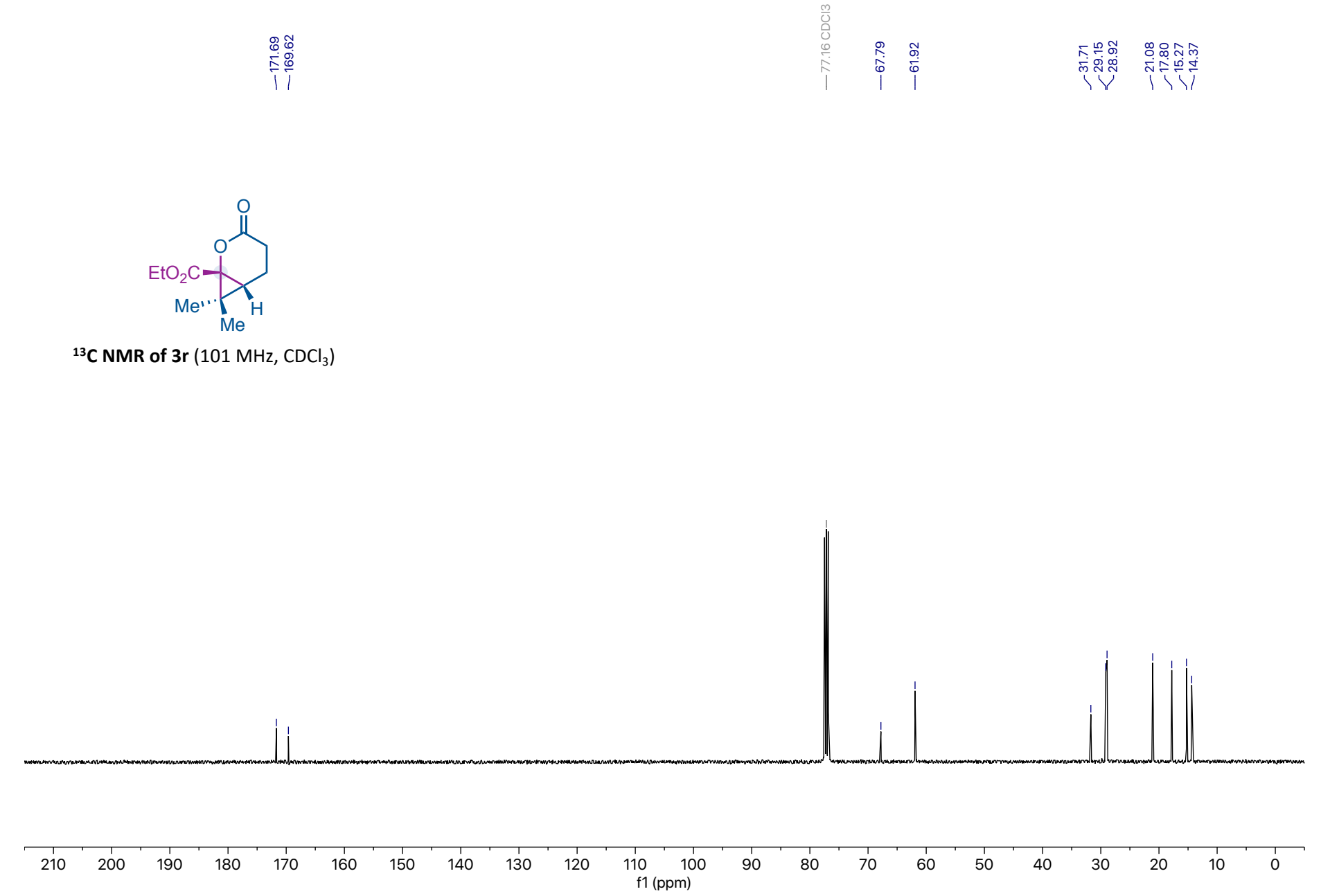


^{1}H-^{13}C HSQC of 3q

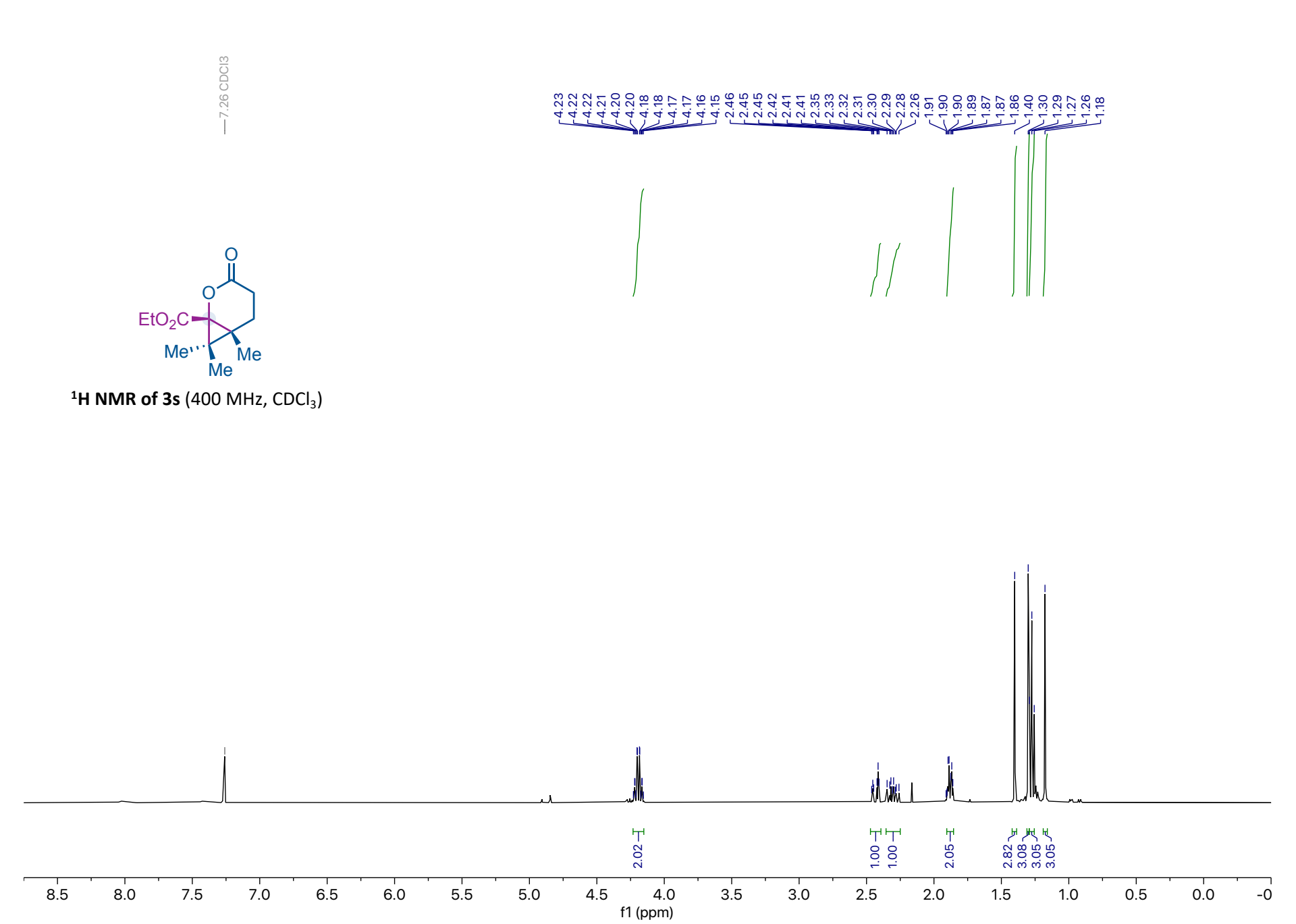

H_A
H_B
H_C
H_D
H_E
Me
CO2Et
{2.19,1.29}
{1.75,1.29}
{1.75,1.35}
{2.42,1.74}
{2.23,1.74}
{1.34,1.76}
{1.28,1.76}
{2.43,2.19}
{1.73,2.23}
{1.28,2.19}
{2.19,2.44}
{1.73,2.42}
¹H - ¹H NOESY of 3q
f2 (ppm)
f1 (ppm)



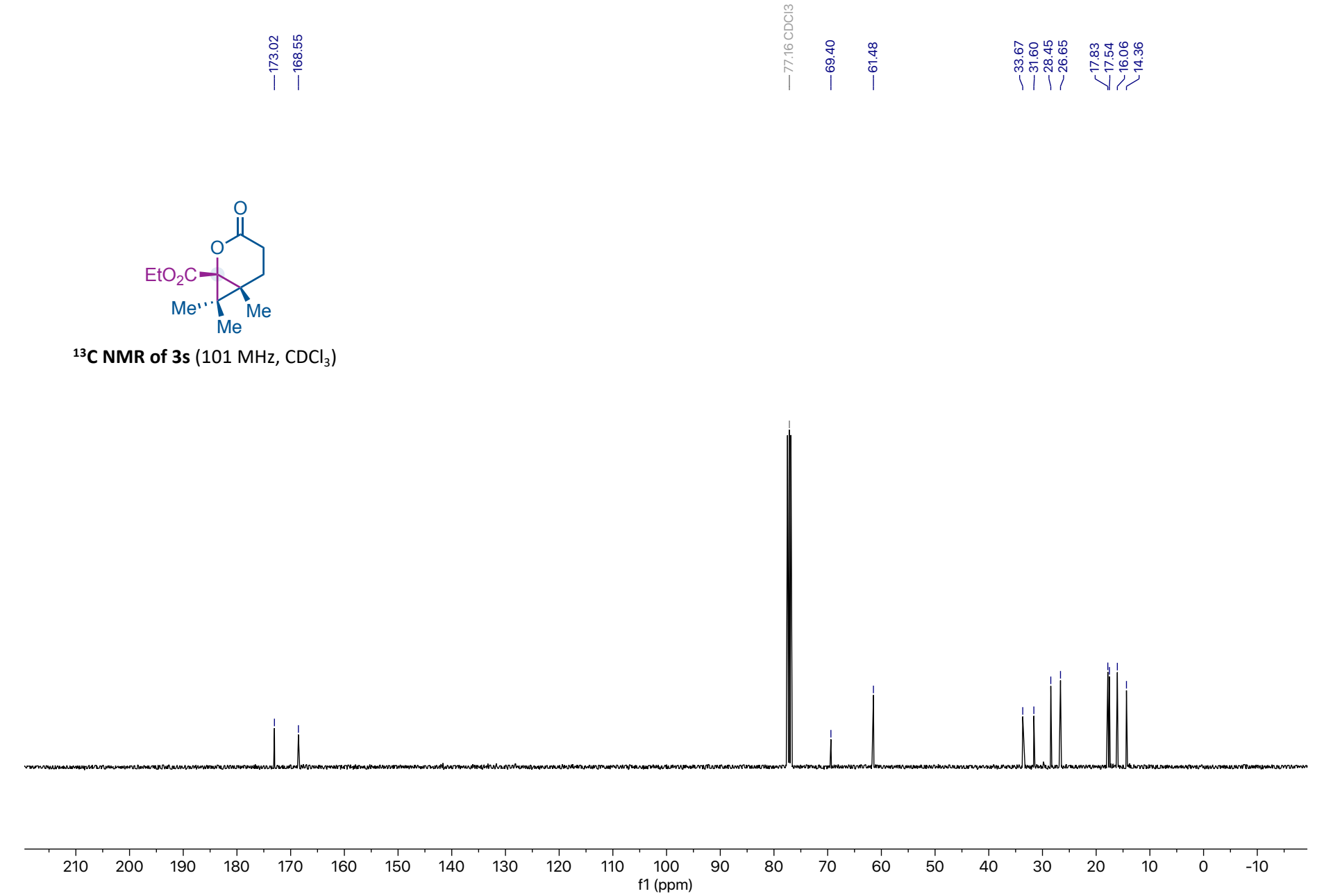
^{1}H NMR of 3r (400 MHz, $CDCl_3$)



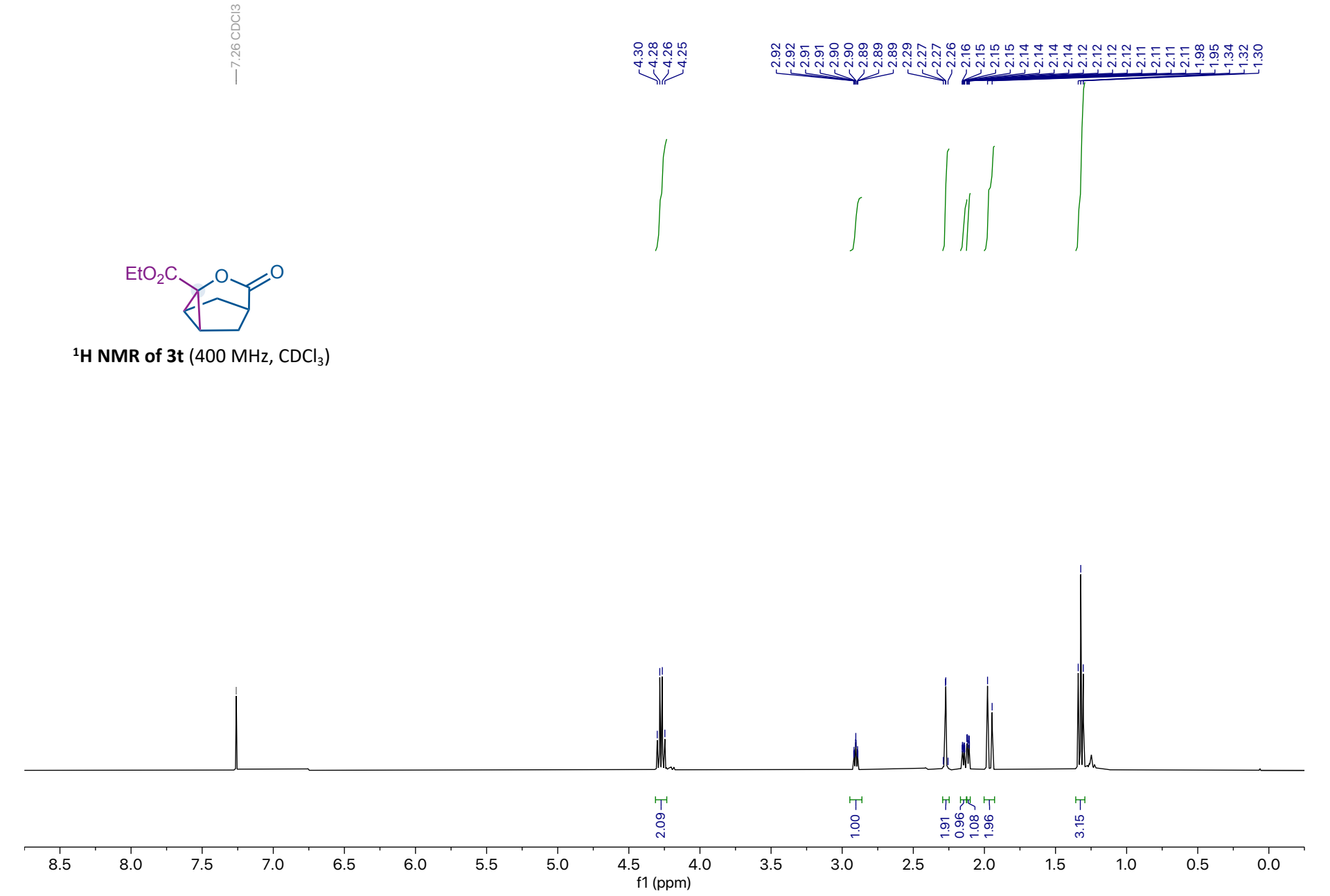
^{13}C NMR of 3r (101 MHz, $CDCl_3$)



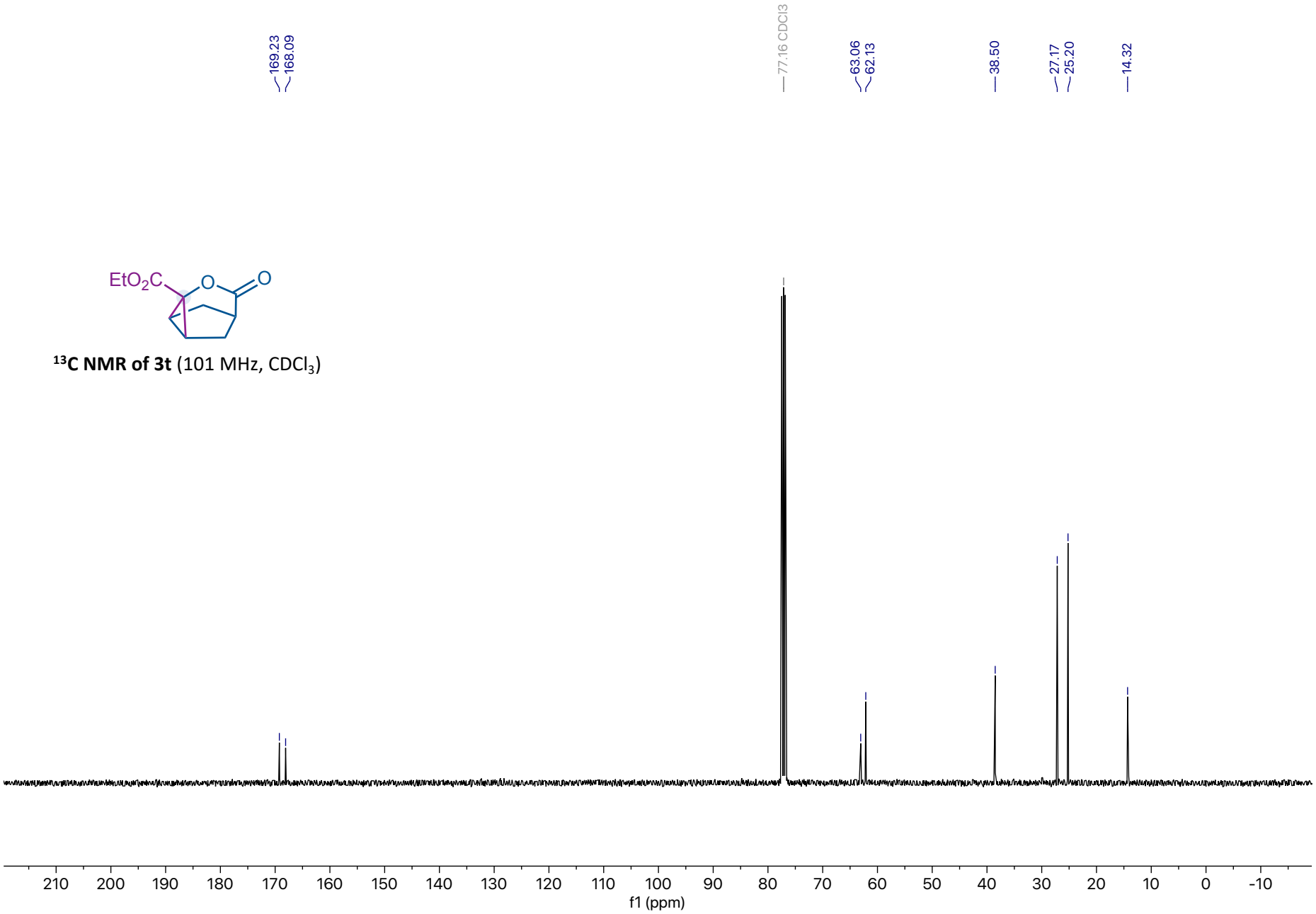
^{1}H NMR of 3s (400 MHz, $CDCl_3$)



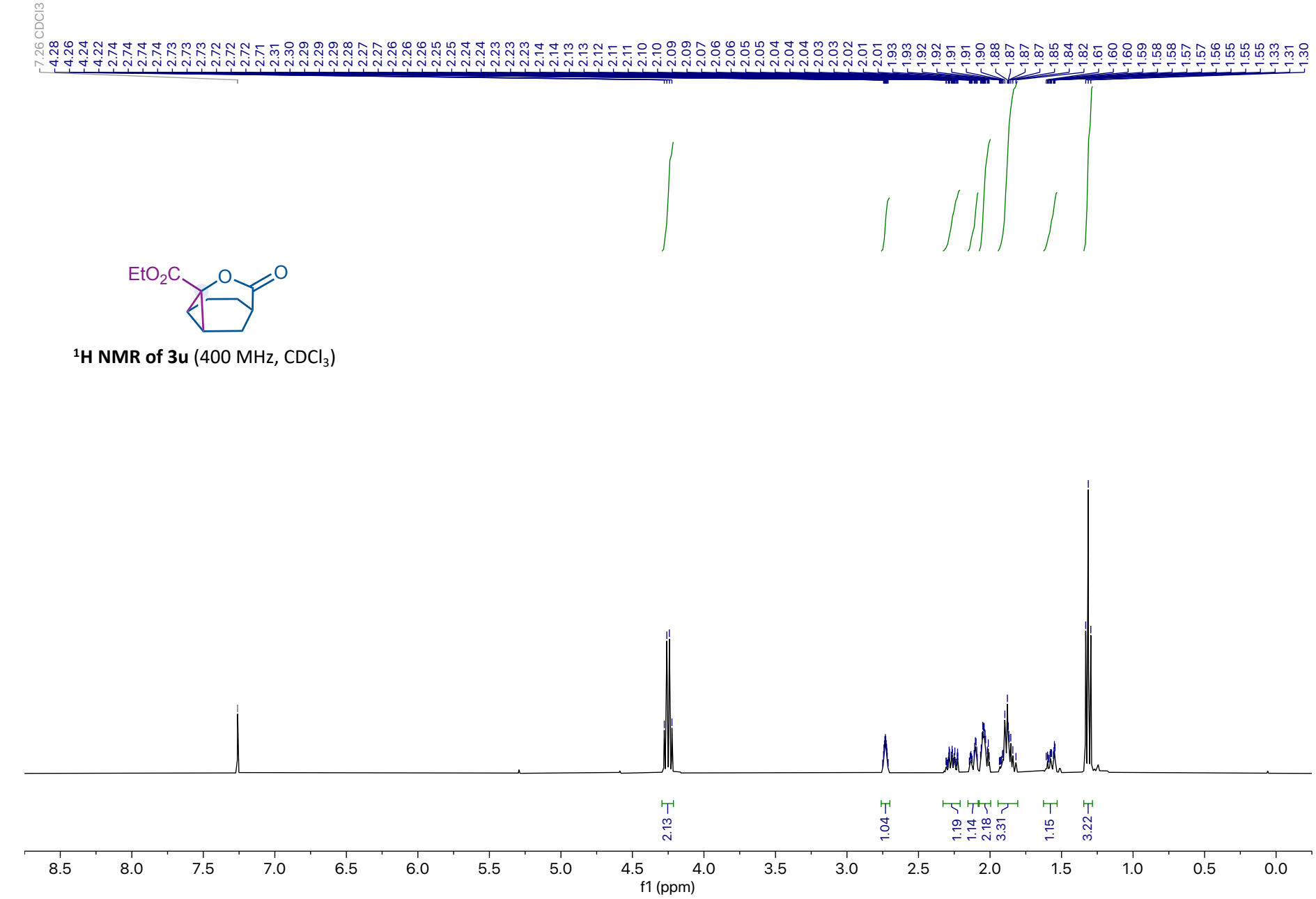
^{13}C NMR of 3s (101 MHz, $CDCl_3$)



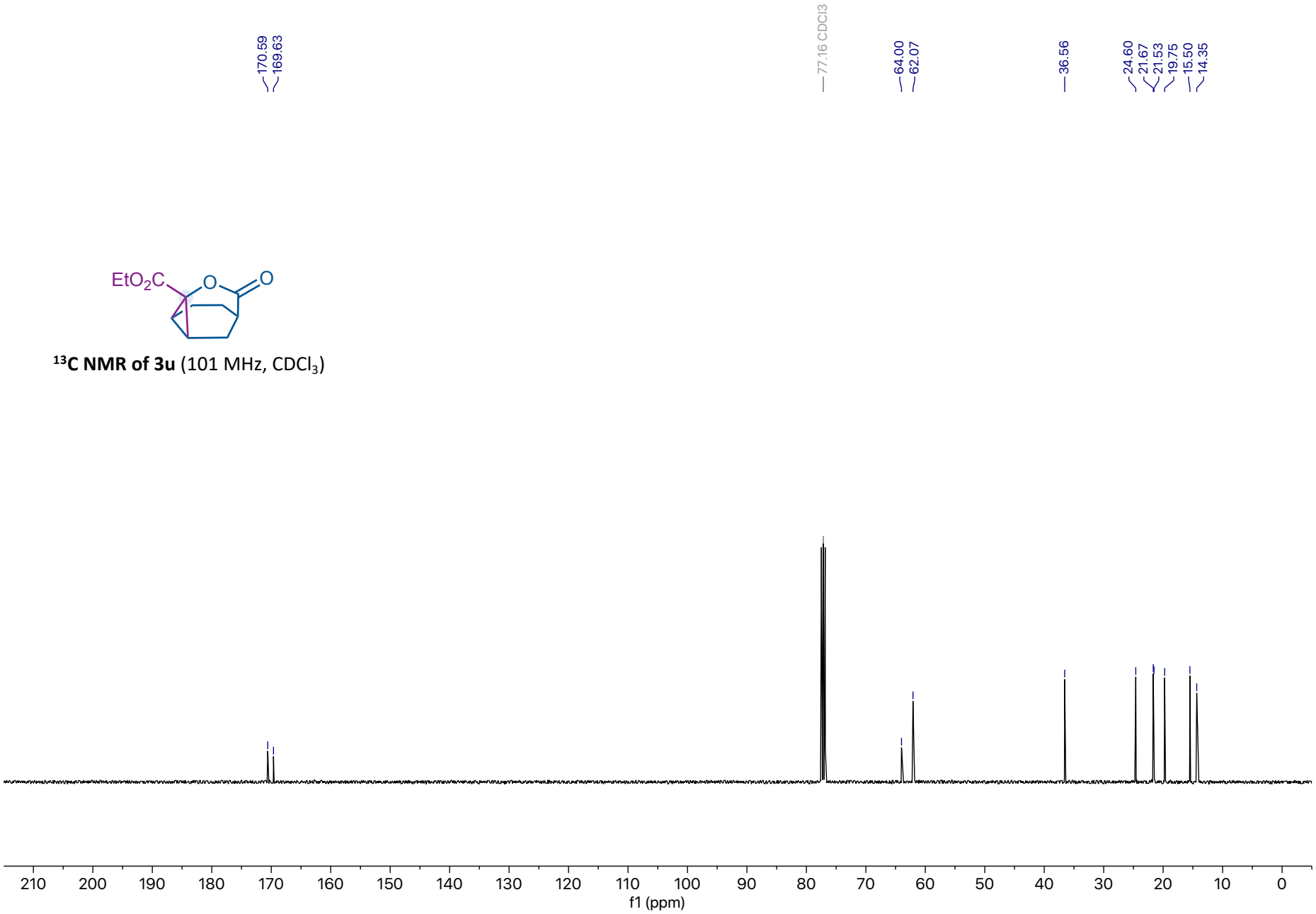
^{1}H NMR of 3t (400 MHz, $CDCl_3$)



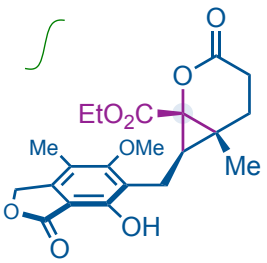
^{13}C NMR of 3t (101 MHz, $CDCl_3$)



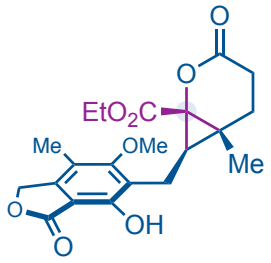
^{1}H NMR of 3u (400 MHz, $CDCl_3$)



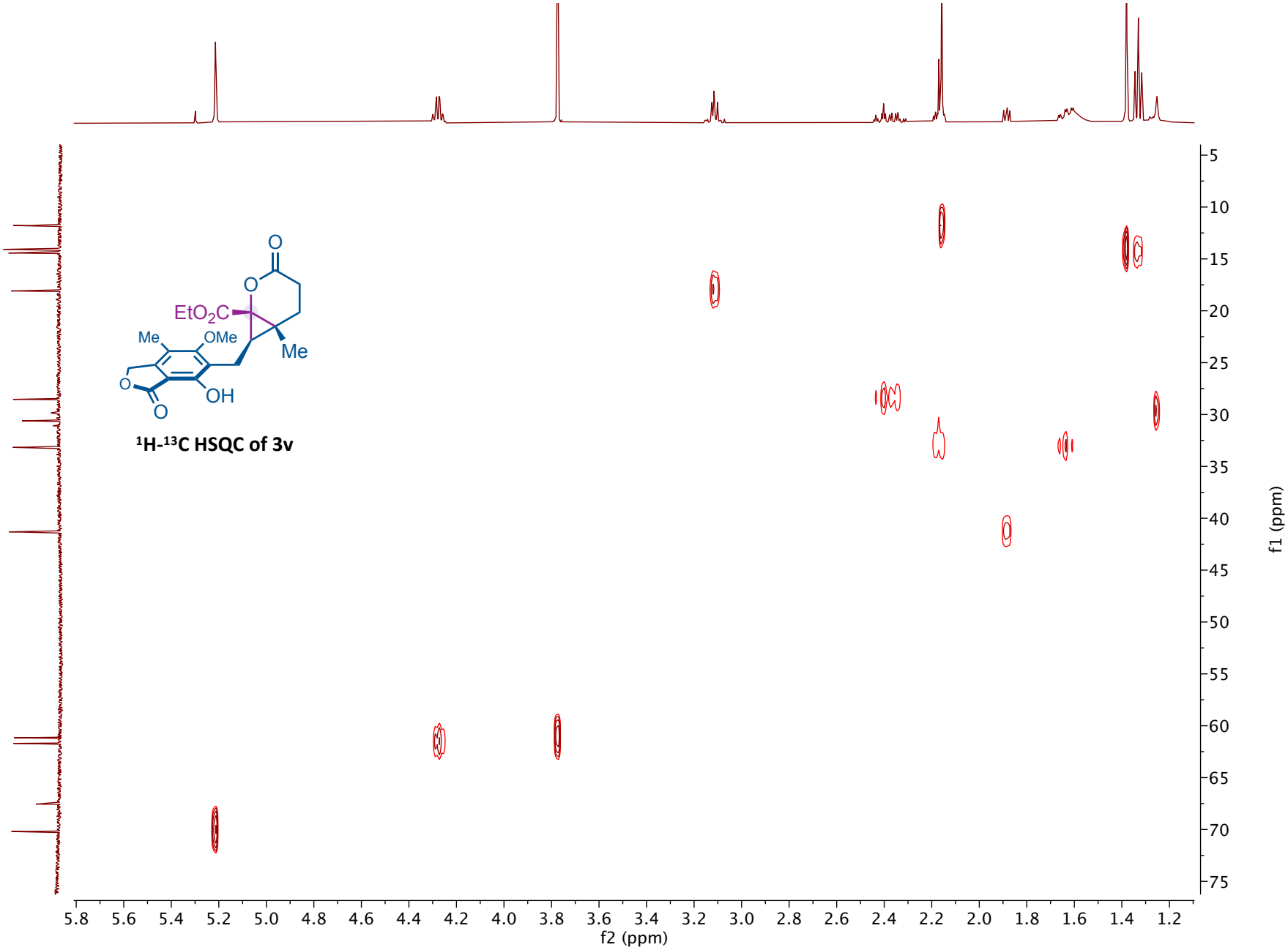
^{13}C NMR of 3u (101 MHz, $CDCl_3$)

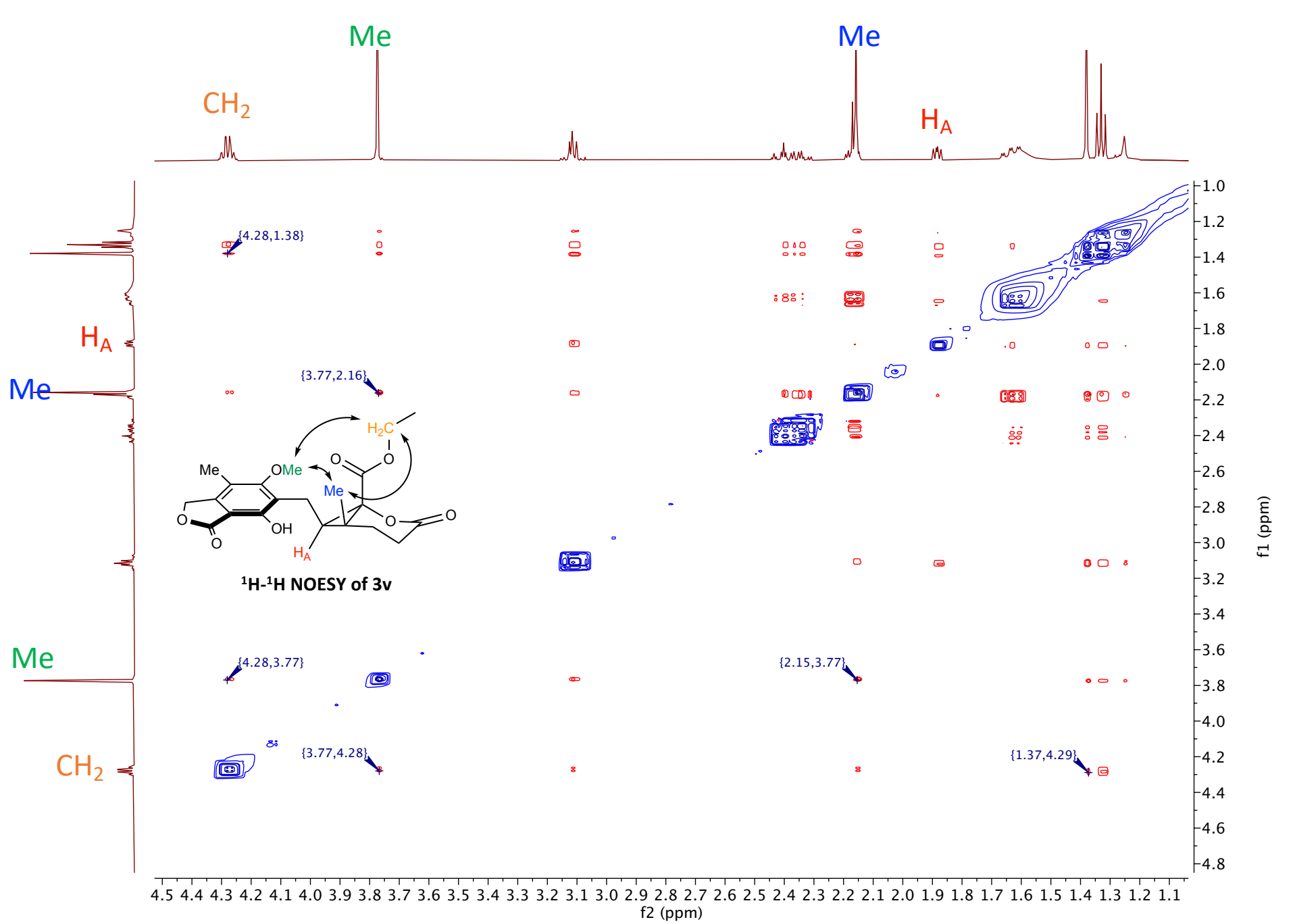


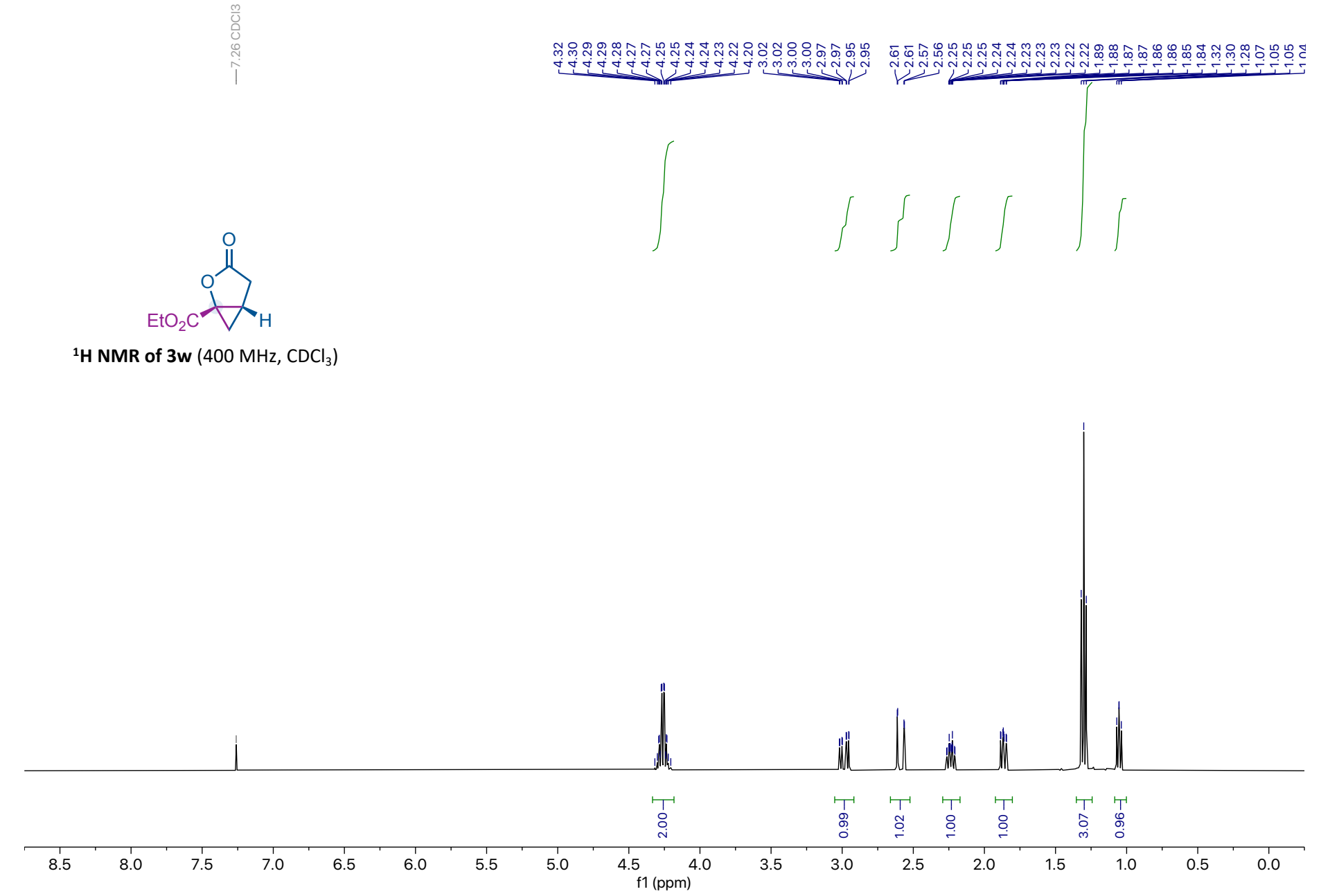
^{1}H NMR of 3v (500 MHz, $CDCl_3$)



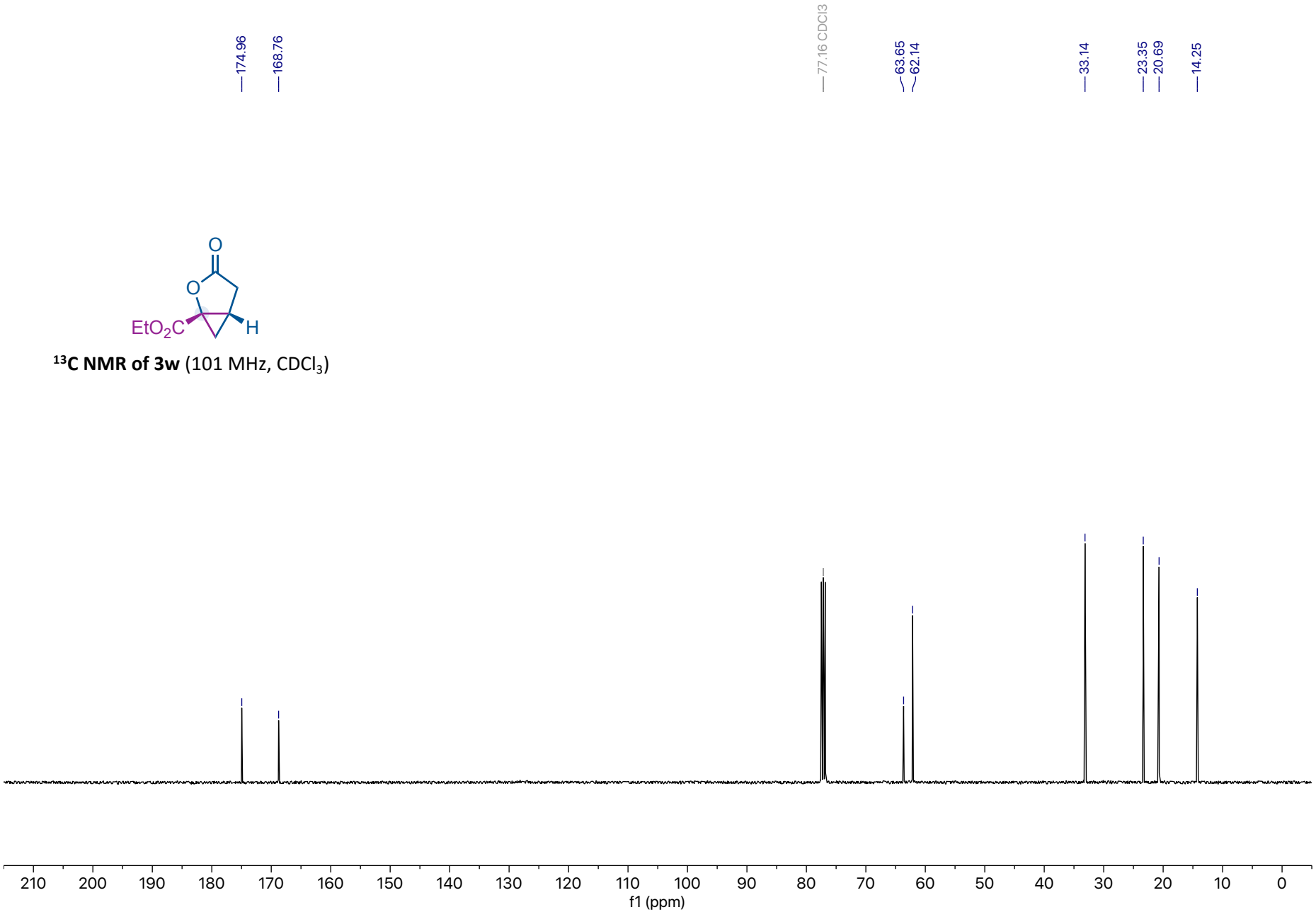
^{13}C NMR of 3v (126 MHz, $CDCl_3$)


O
O
EtO2C
Me
OMe
Me
O
OH
O
1H-13C HSQC of 3v
5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2
f2 (ppm)
5 10 15 20 25 30 35 40 45 50 55 60 65 70 75
f1 (ppm)

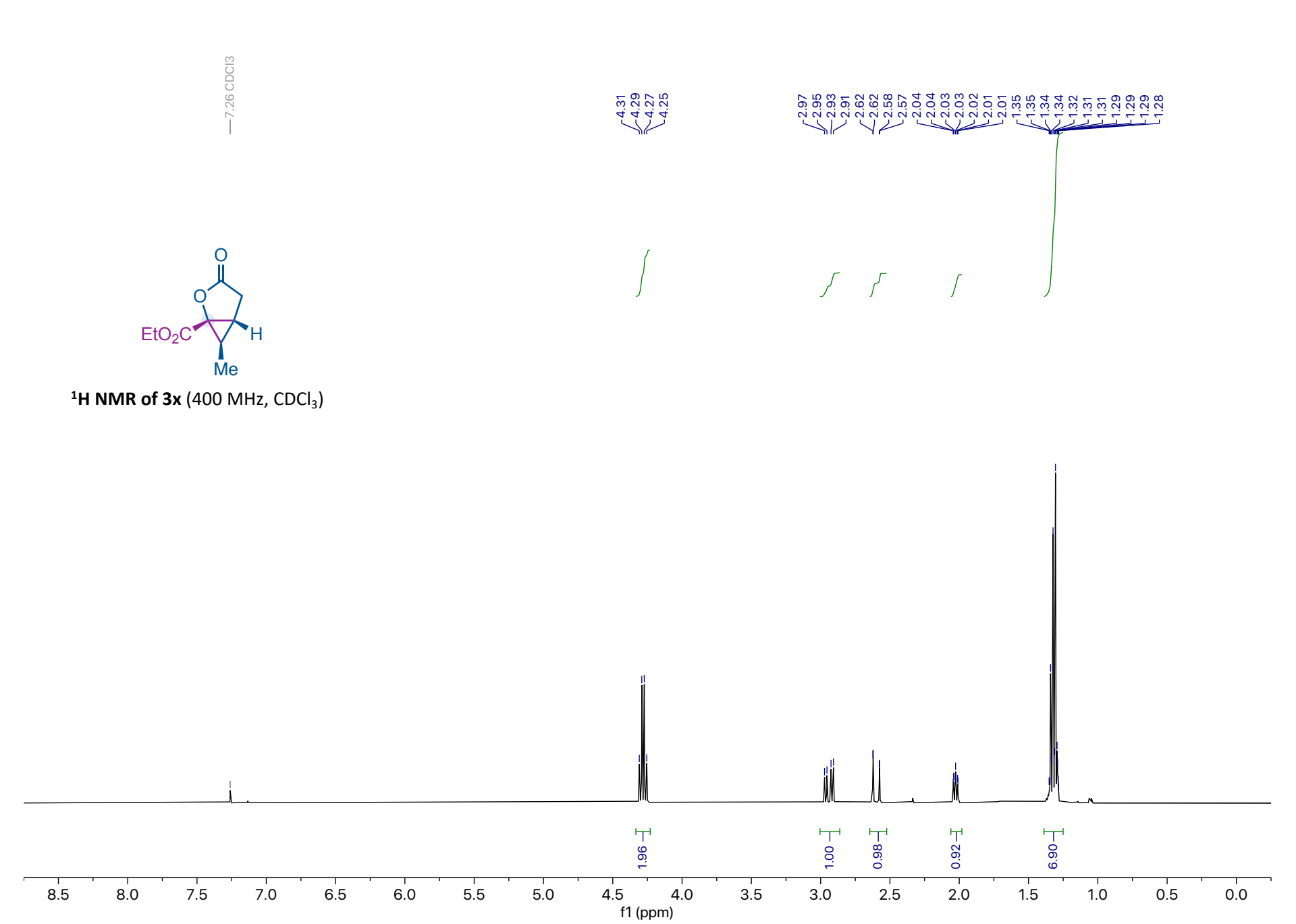

Me
Me
CH2
HA
HA
Me
Me
CH2
{4.28,1.38}
{3.77,2.16}
{4.28,3.77}
{2.15,3.77}
{3.77,4.28}
{1.37,4.29}
H2C
Me
OMe
Me
OH
HA
O
O
O
O
O
O
1H-1H NOESY of 3v
f1 (ppm)
f2 (ppm)
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
3.2
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1



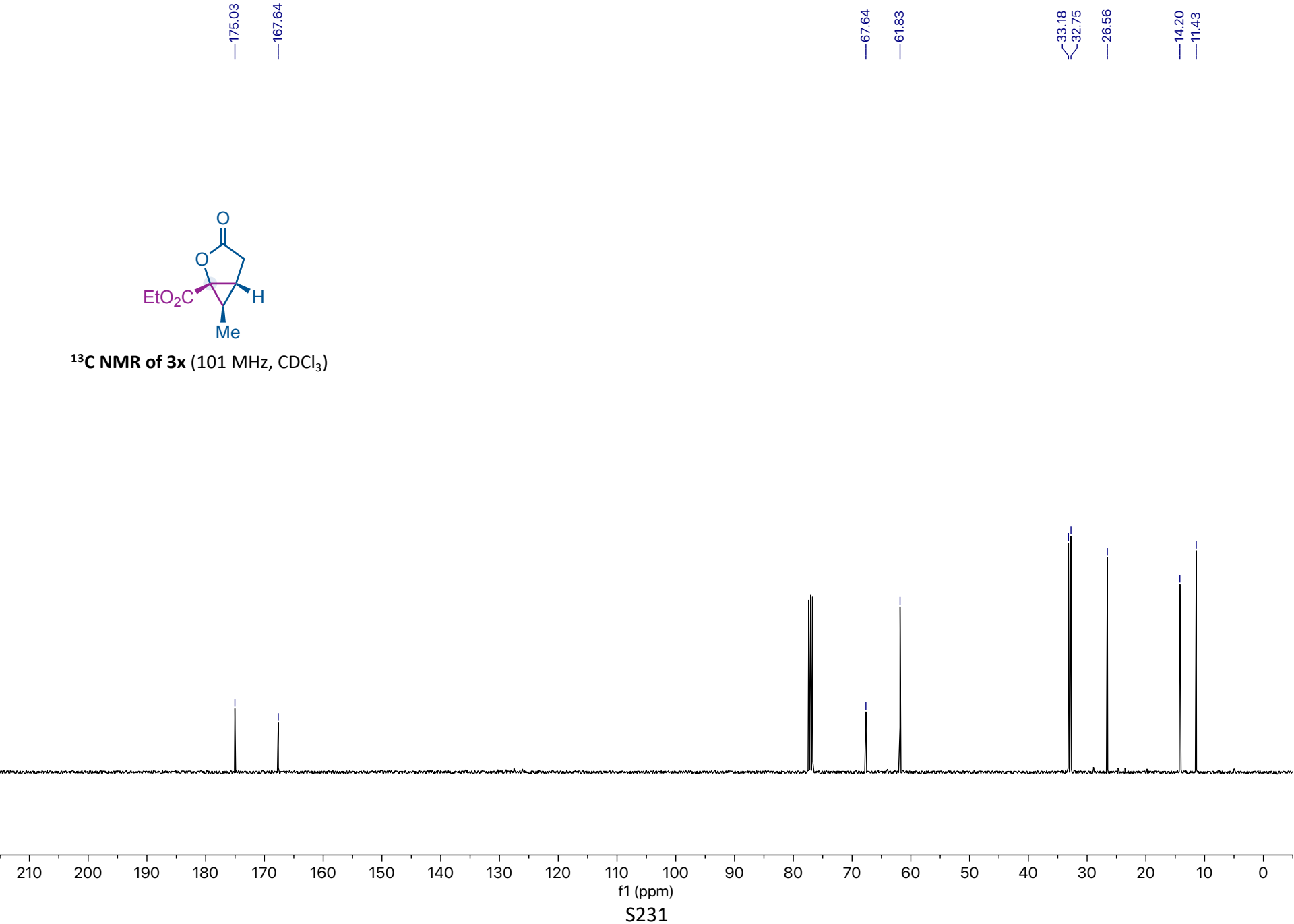
^{1}H NMR of 3w (400 MHz, $CDCl_3$)



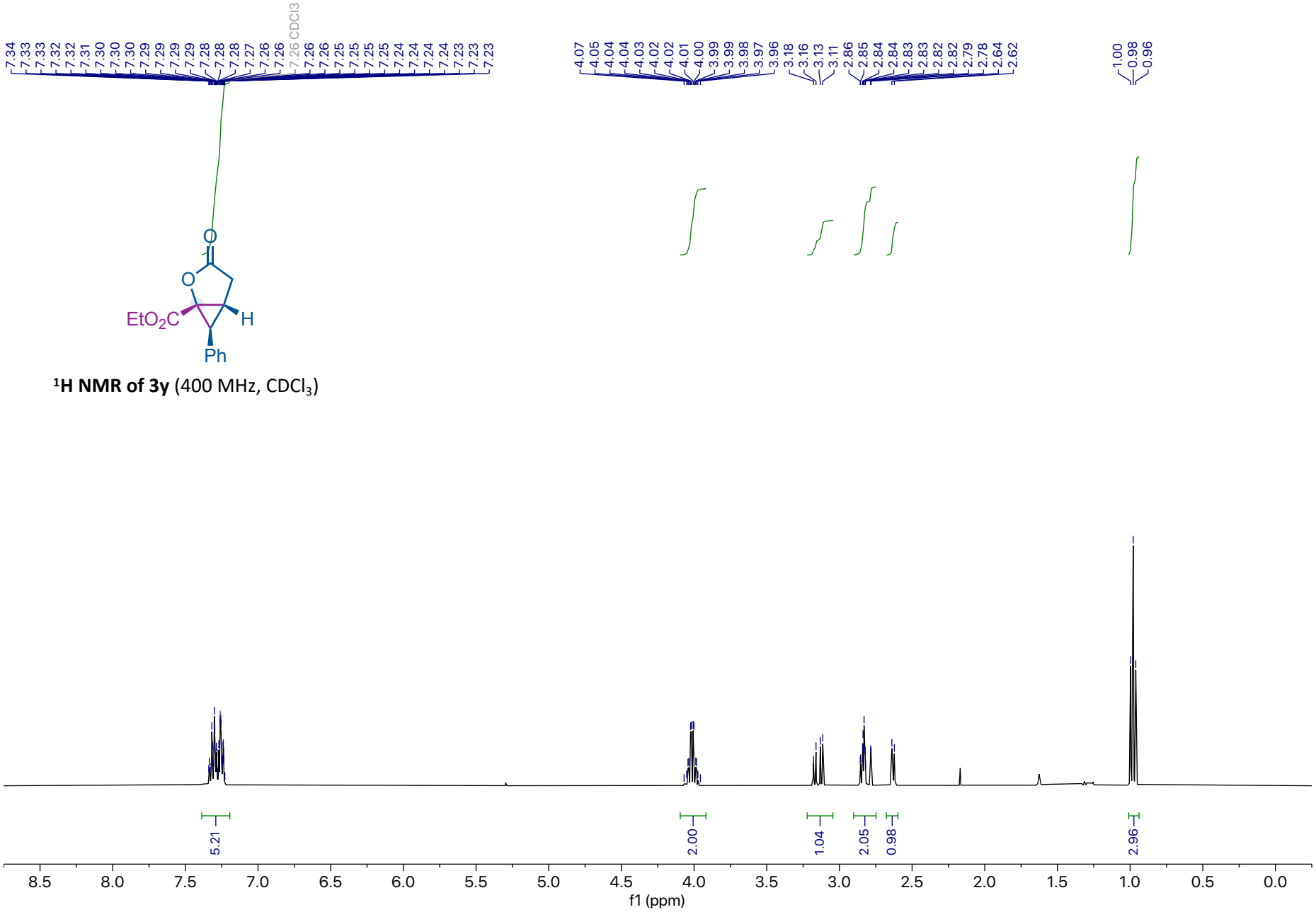
^{13}C NMR of 3w (101 MHz, $CDCl_3$)



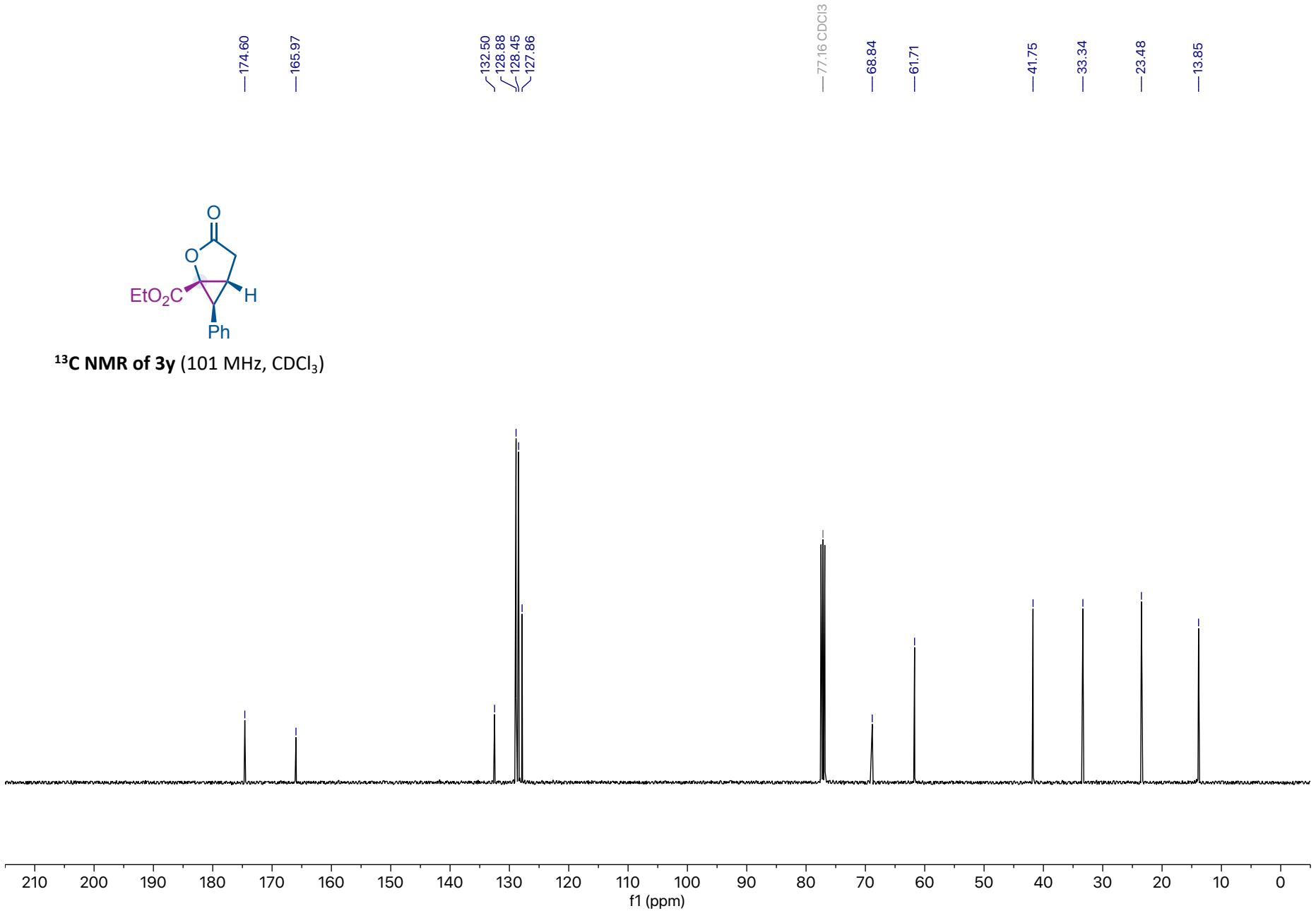
^{1}H NMR of 3x (400 MHz, $CDCl_3$)



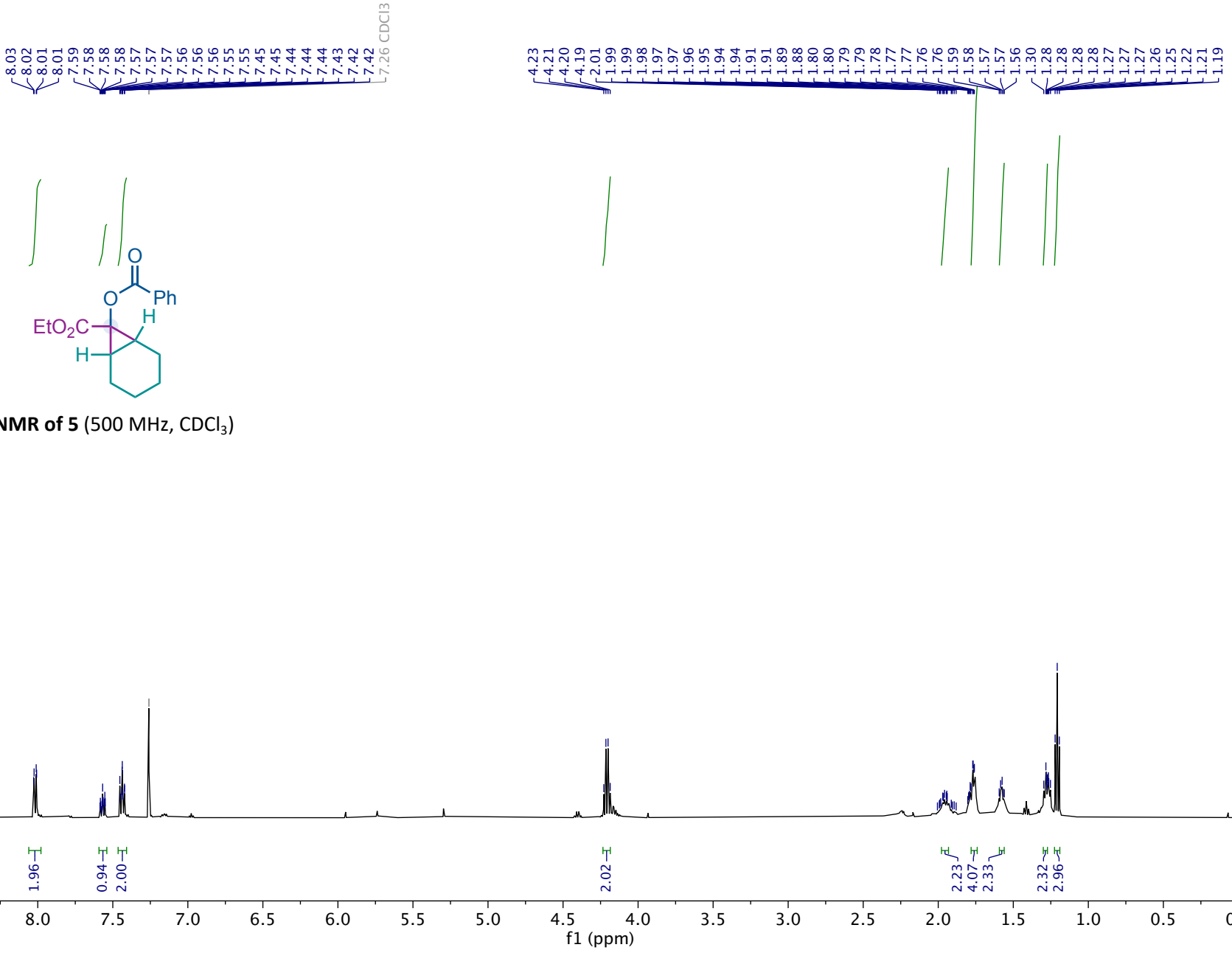
^{13}C NMR of 3x (101 MHz, $CDCl_3$)



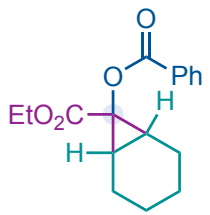
^{1}H NMR of 3y (400 MHz, $CDCl_3$)



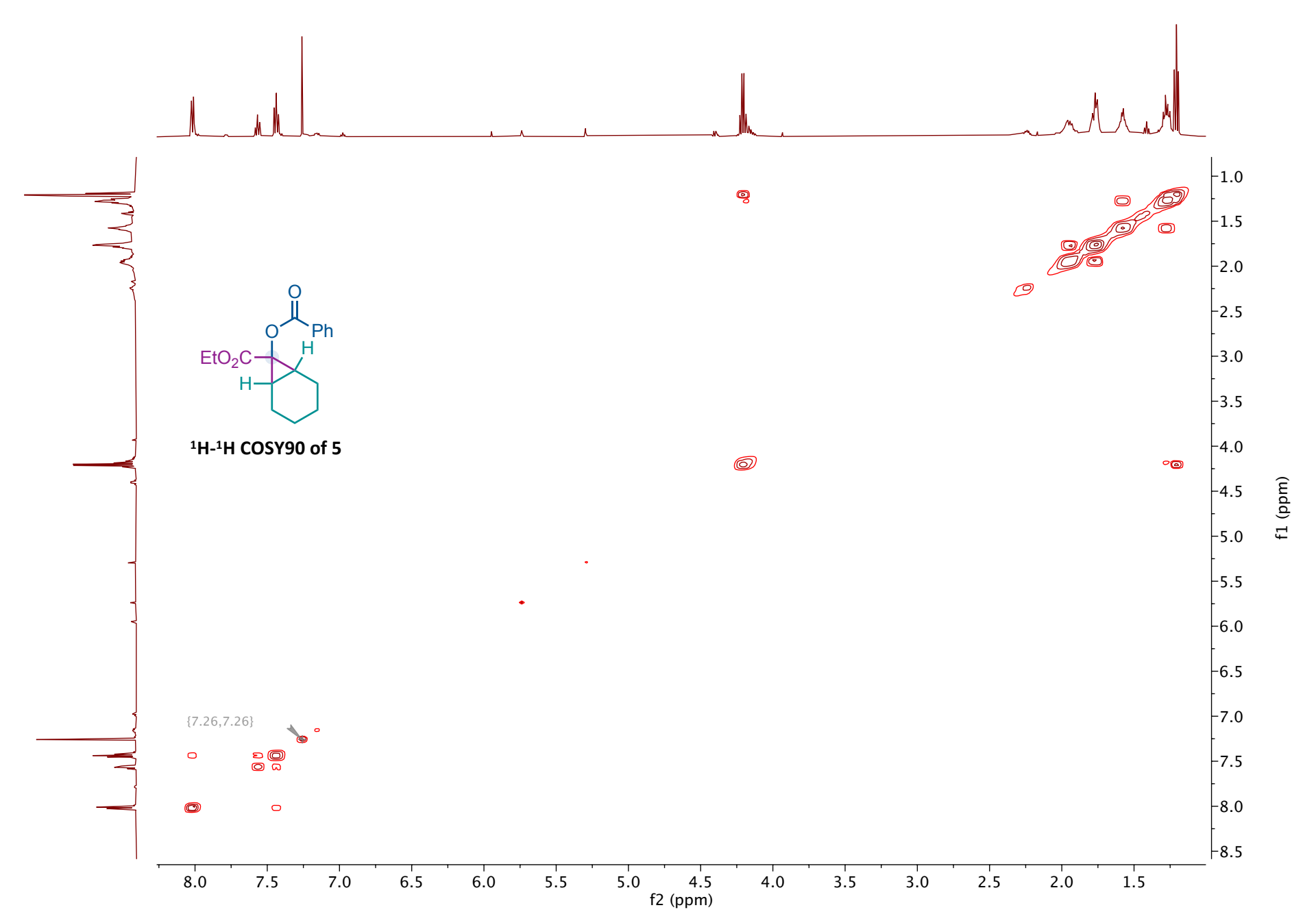
^{13}C NMR of 3y (101 MHz, $CDCl_3$)

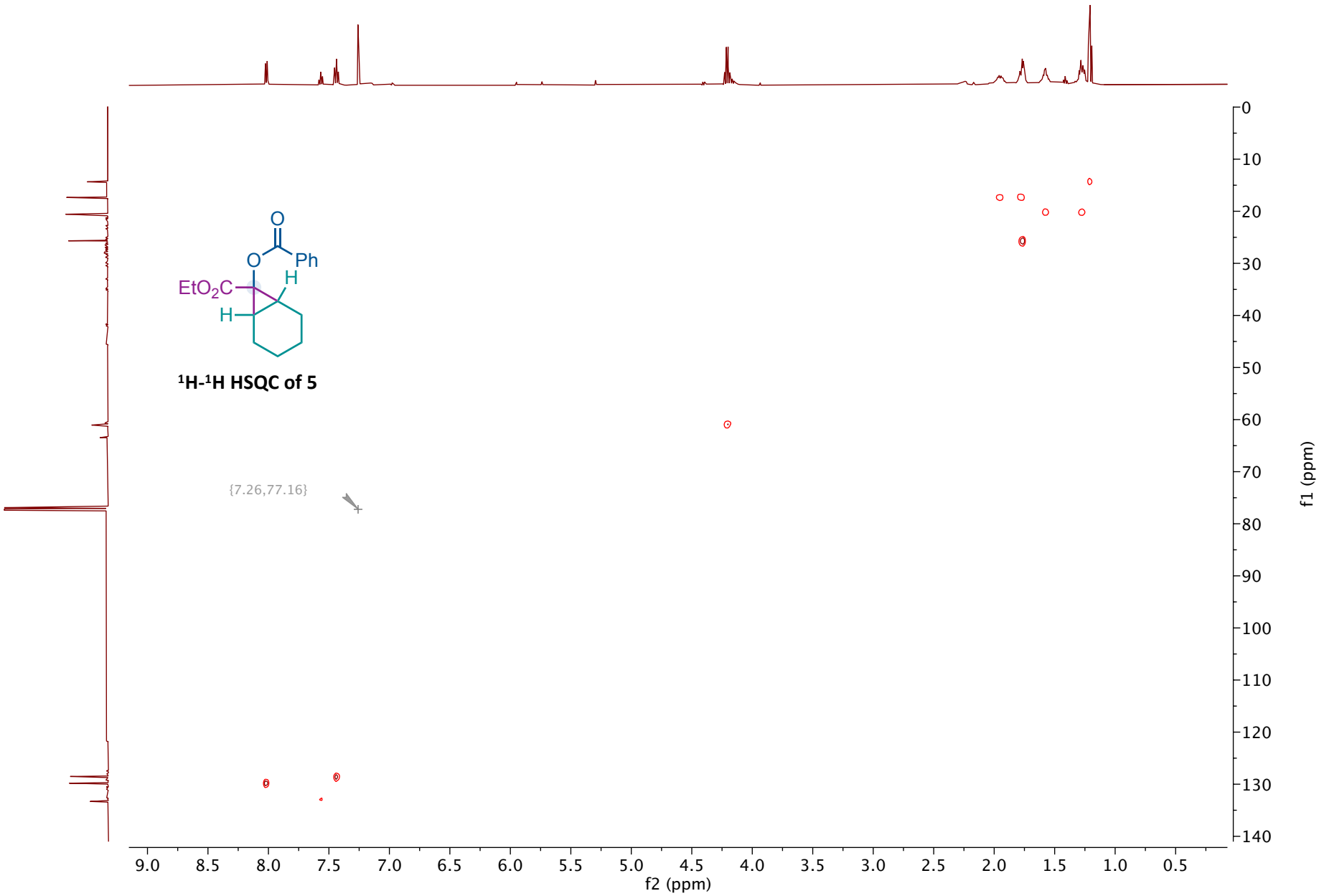


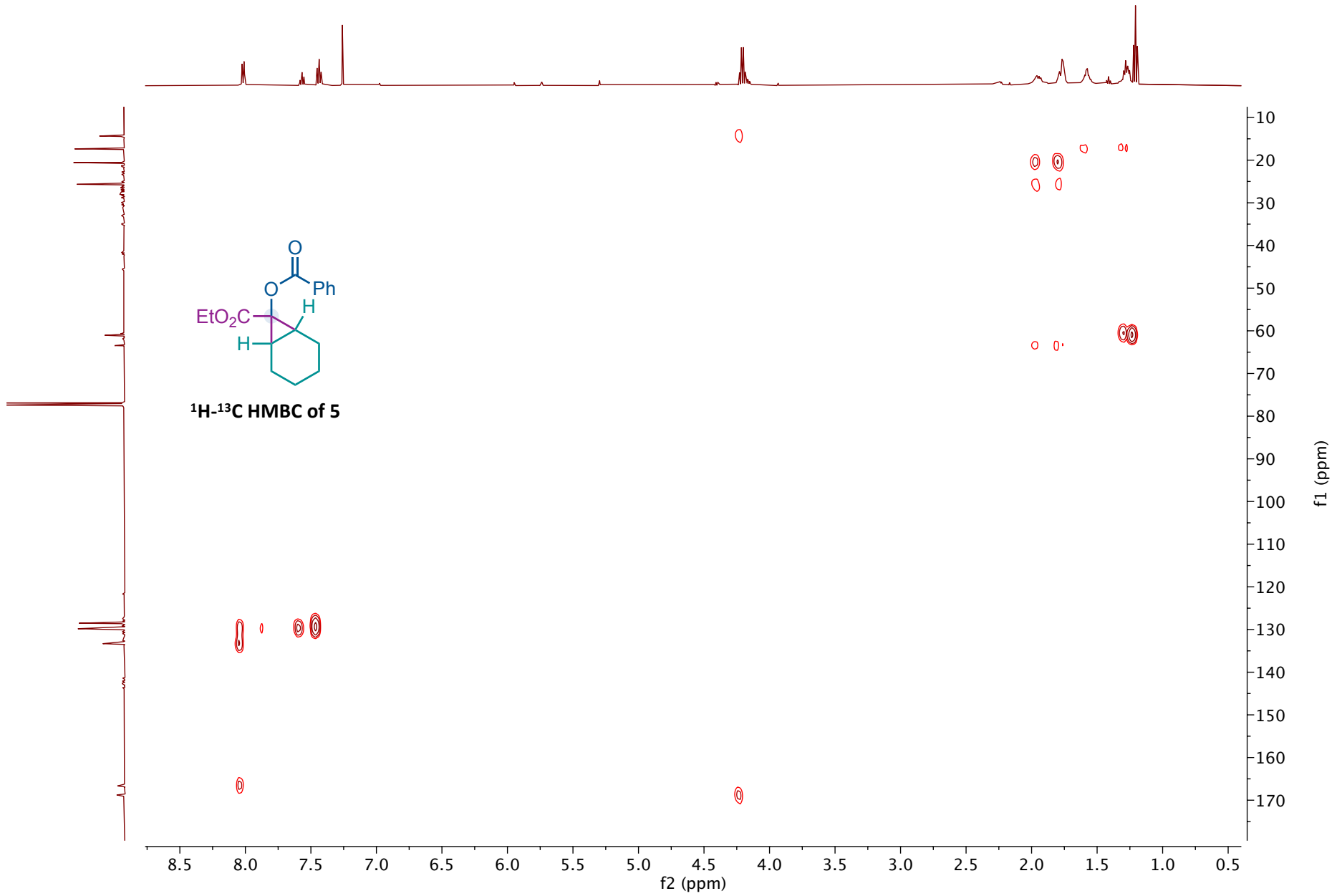
^{1}H NMR of 5 (500 MHz, $CDCl_3$)

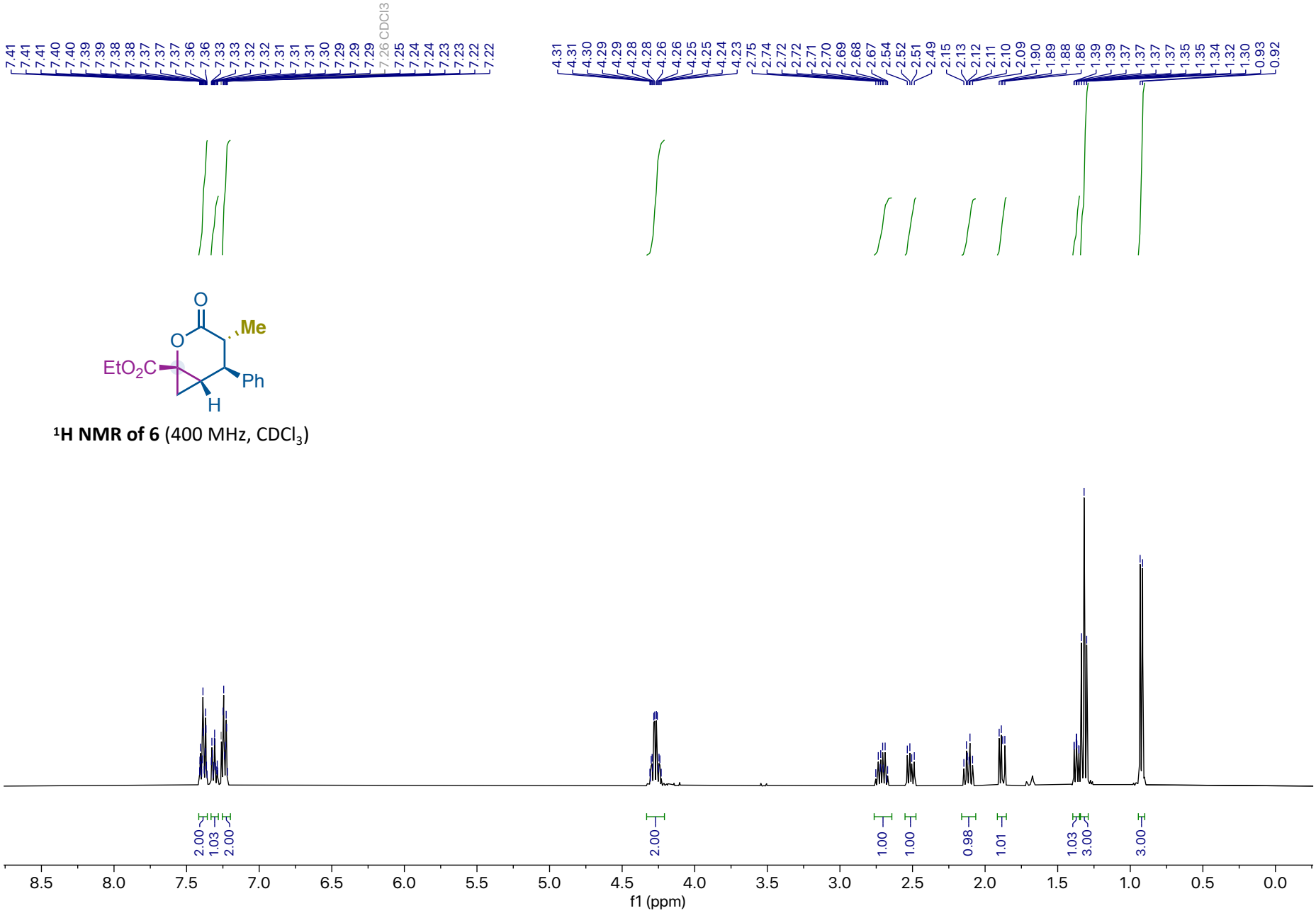


^{13}C NMR of 5 (126 MHz, $CDCl_3$)

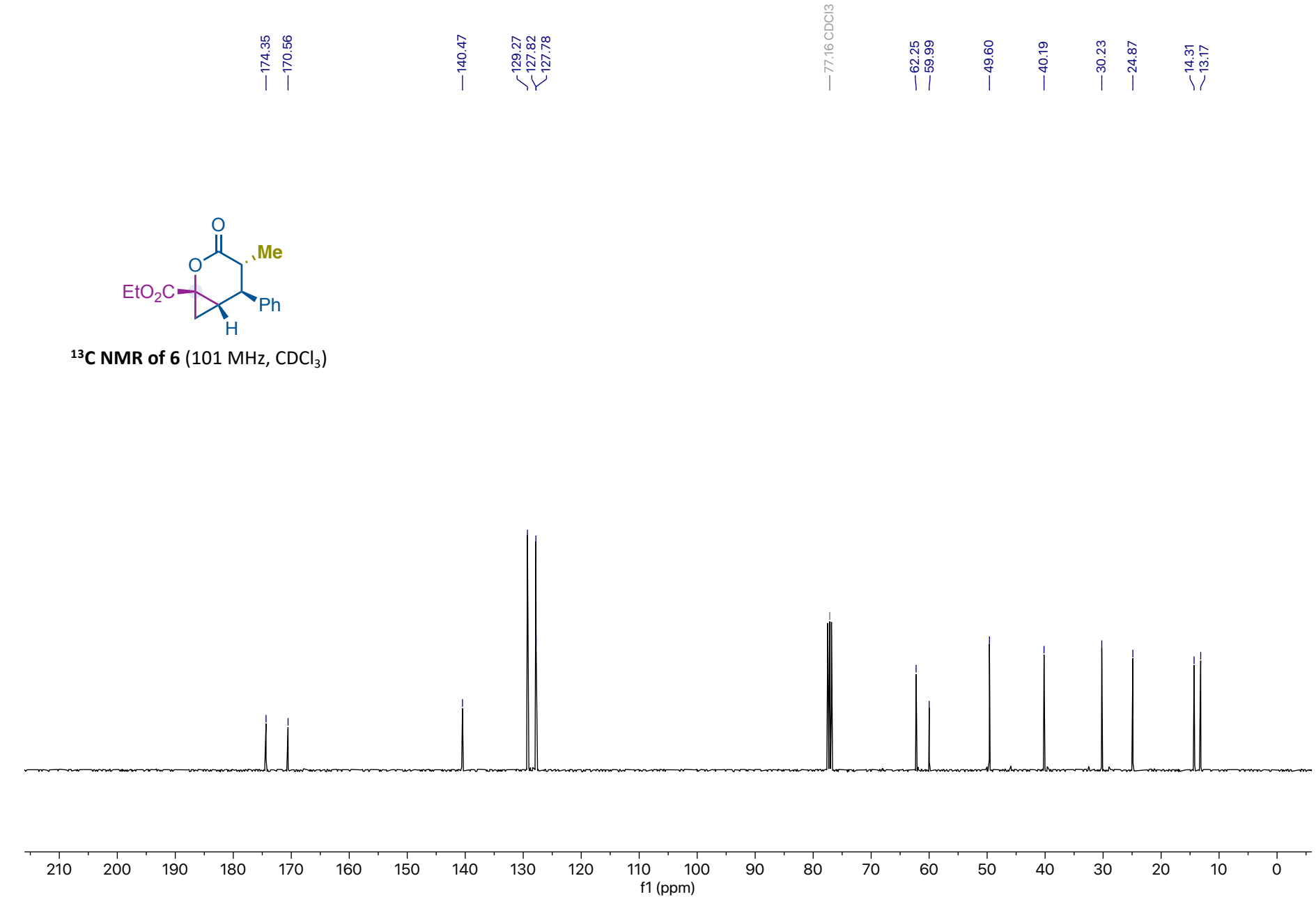

O
O
Ph
EtO2C
H
H
1H-1H COSY90 of 5
{7.26,7.26}
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f2 (ppm)
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
f1 (ppm)


O
O
Ph
H
EtO2C
H
1H-1H HSQC of 5
{7.26,77.16}
f2 (ppm)
f1 (ppm)

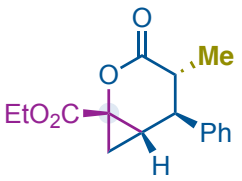

O
O
Ph
H
EtO2C
H
1H-13C HMBC of 5
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
f1 (ppm)



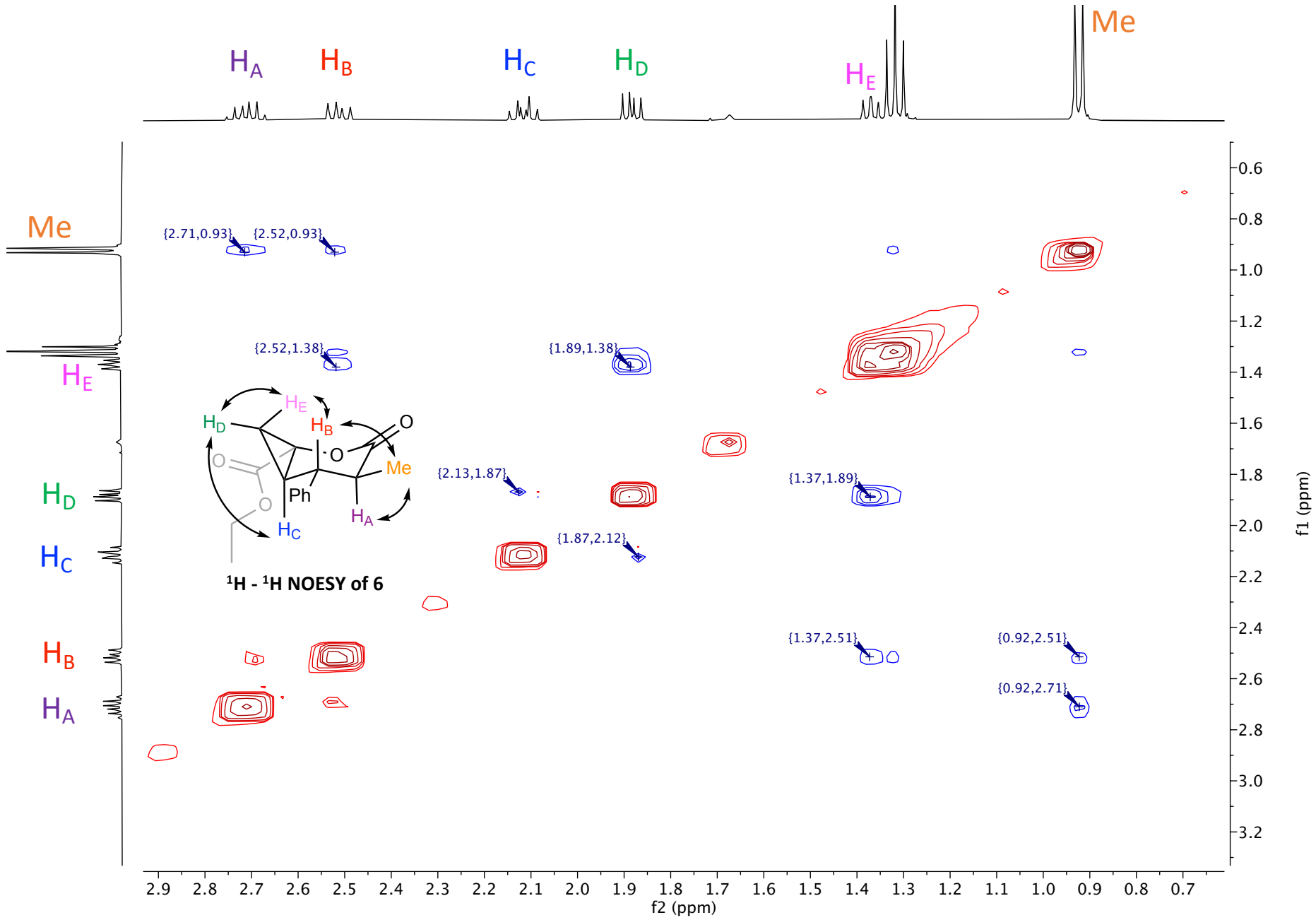
^{1}H NMR of 6 (400 MHz, $CDCl_3$)



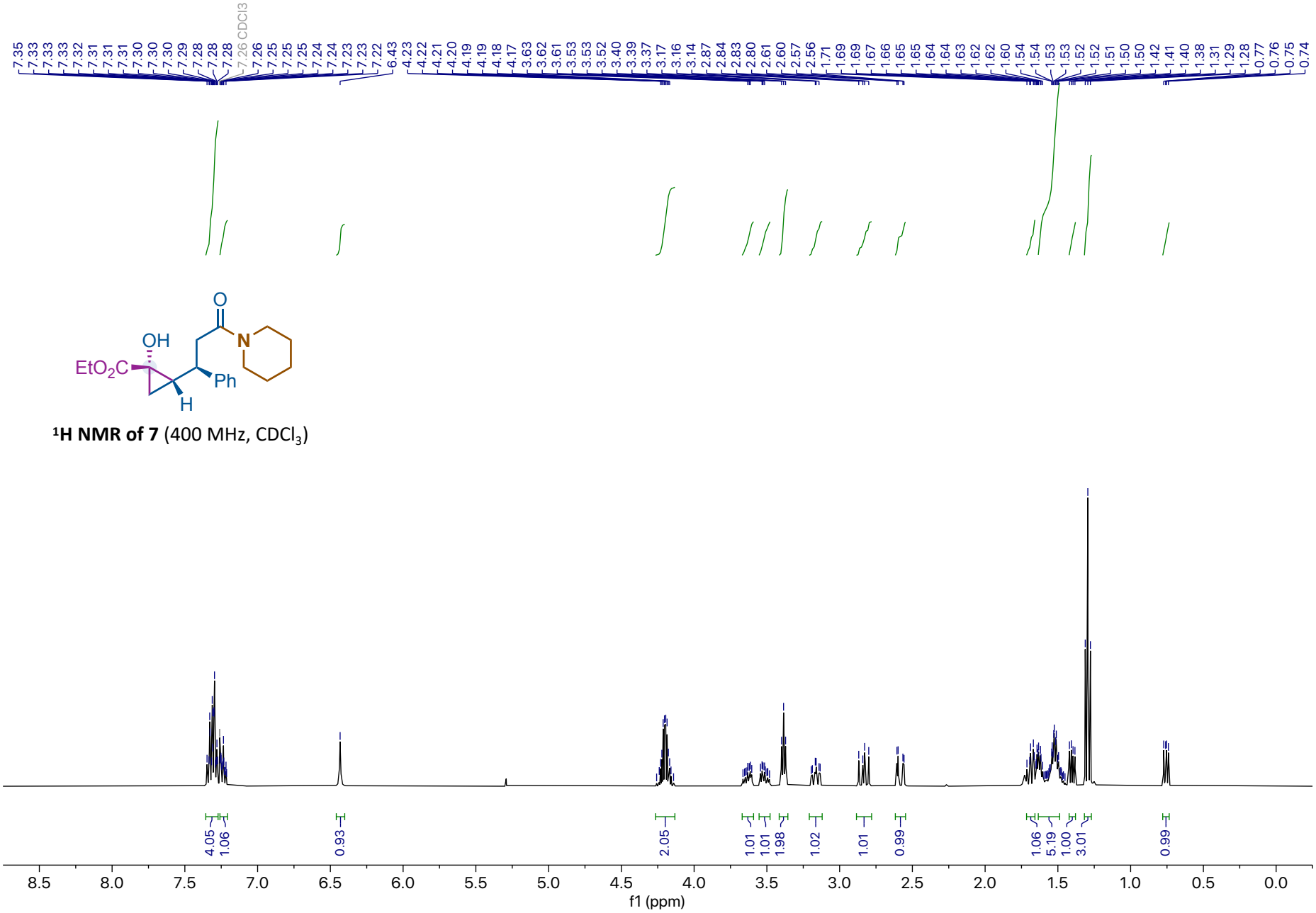
^{13}C NMR of 6 (101 MHz, $CDCl_3$)



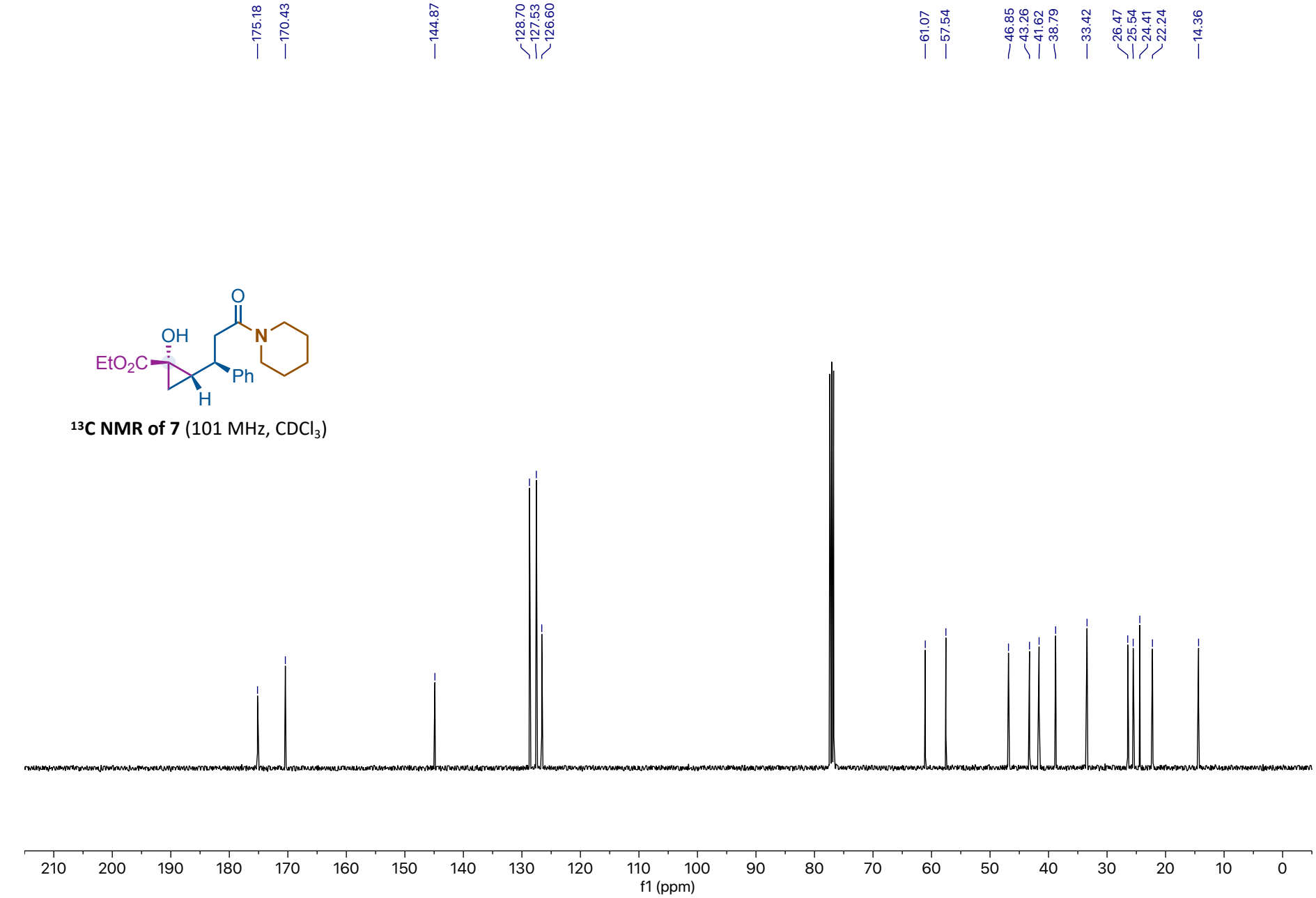
^{1}H-^{13}C HSQC of 6



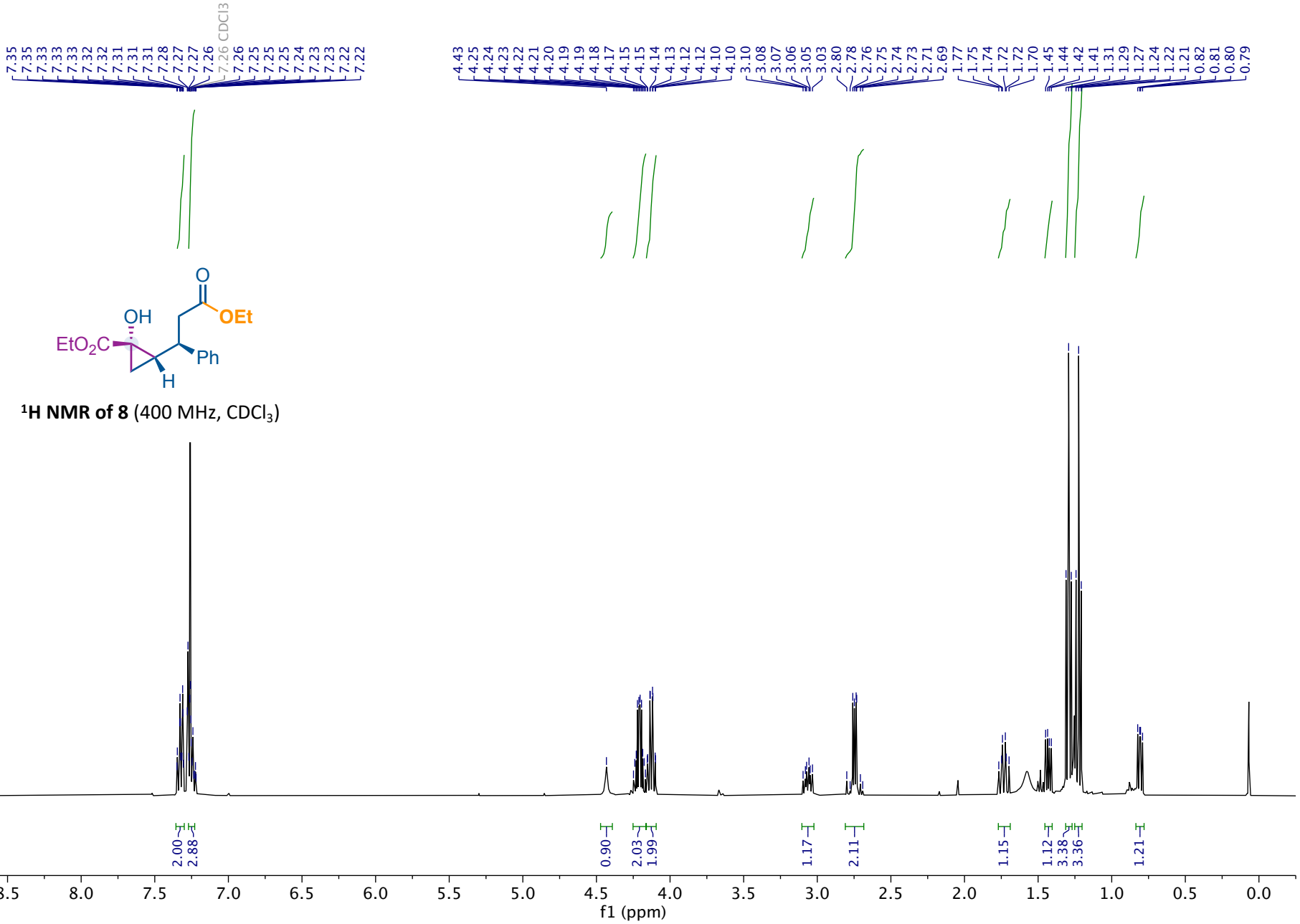
^{1}H - ^{1}H NOESY of 6



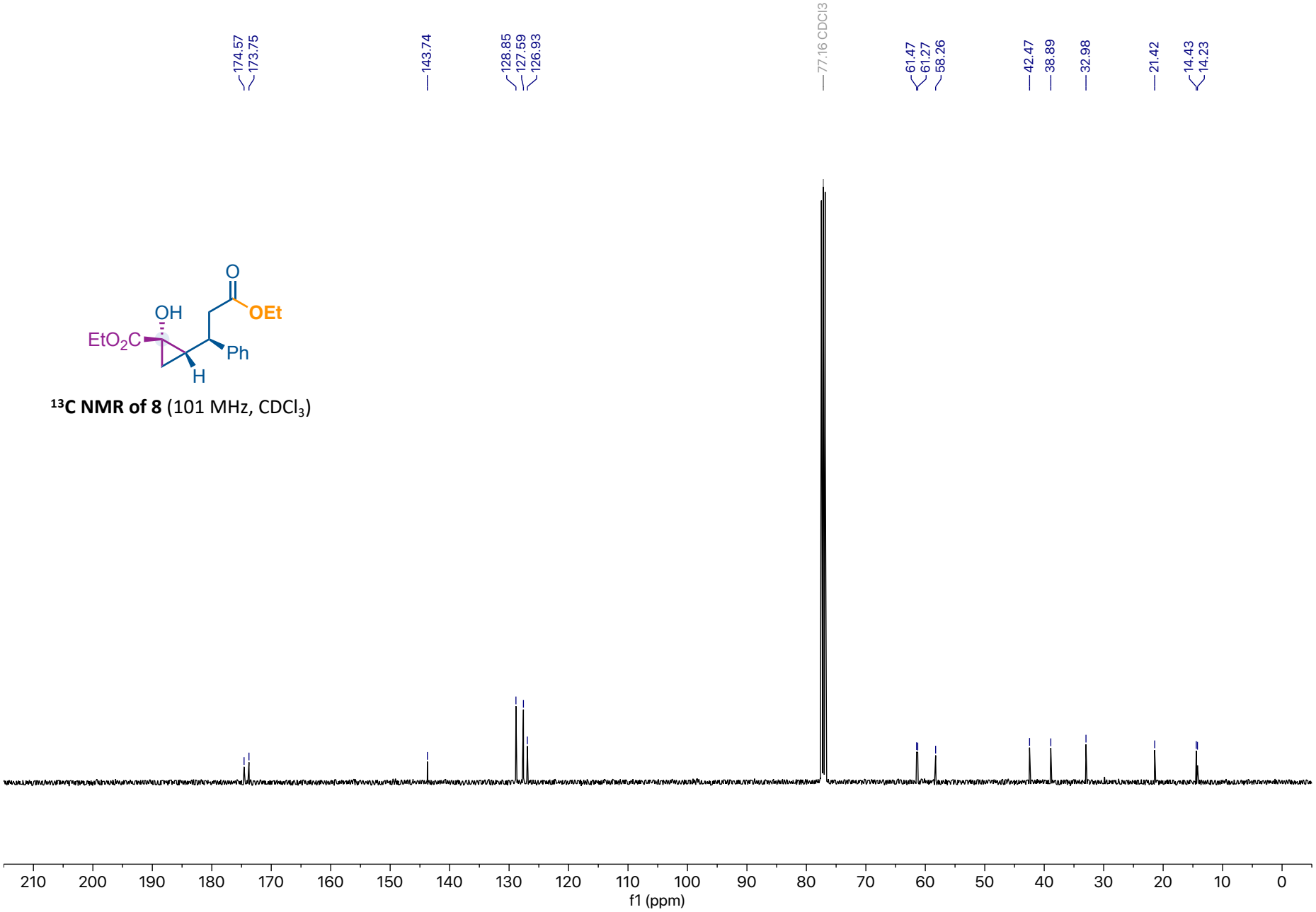
^{1}H NMR of 7 (400 MHz, $CDCl_3$)



^{13}C NMR of 7 (101 MHz, $CDCl_3$)



^{1}H NMR of 8 (400 MHz, $CDCl_3$)



^{13}C NMR of 8 (101 MHz, $CDCl_3$)