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Part I Experimental Part

1. General information

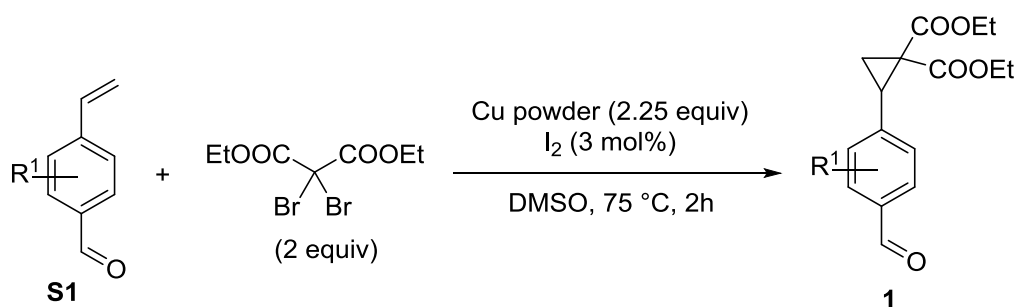
Unless otherwise indicated, all reactions were carried out under N₂ protection with magnetic stirring. Anhydrous THF, toluene and 1,4-dioxane were distilled from sodium and benzophenone. Anhydrous CH₃CN and CH₂Cl₂ were distilled from CaH₂. Analytical thin layer chromatography was carried out with silica gel pre-coated glass plates (TLC-Silica gel GF254, coating thickness: 0.25 mm) purchased from Xinnuo Chemical (Yantai, China). Visualization was accomplished with short wave UV light (254 nm, 365 nm) and/or 10% phosphomolybdic acid in ethanol or KMnO₄ staining solutions followed by heating. Column chromatograph was performed on silica gel (200~300 mesh). All ¹H NMR (400 MHz), ¹³C NMR (101 MHz); ¹H NMR (500 MHz), ¹³C NMR (126 MHz) spectra were recorded on a Bruker-DMX 400 and 500 spectrometers in CDCl₃, with tetramethylsilane as an internal standard and reported in parts per million (ppm, δ). ¹H NMR

spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br). High-resolution mass spectra (HRMS) were obtained with the mass analyzer of an orbitrap. Infrared spectra were recorded on a JASCO FT/IR-480 spectrophotometer and reported as wave number (cm⁻¹).

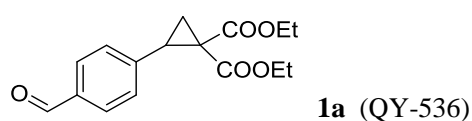
The amount of incorporated deuterium in a sample was quantified by the decrease of ¹H NMR integral intensities at the specified positions compared to the non-deuterated samples. Integral intensities were calibrated against hydrogen signals that do not undergo H/D-exchange.

2. Substrate Preparation.

General procedure A for synthesis of 1a-1i

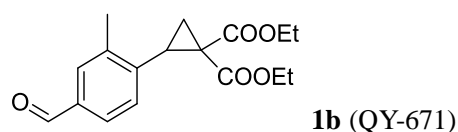


This procedure was performed according to known literature¹. To a 50 mL Schlenk tube were added Cu powder (2.25 equiv) and I₂ (3 mol%), the reaction tube was sealed with septum, and was evacuated and backfilled with nitrogen three times, vinyl substituted aryl aldehyde **S1** (1 equiv) and diethyl dibromomalonate (2 equiv) and DMSO (1 mL/mmol) were added with syringe. The reaction mixture was stirred at 75 °C under nitrogen atmosphere for 2h. After the reaction was complete, the reaction solution was then diluted with water, and extracted with EtOAc for three times. The combined organic extracts were washed with water, then with brine, dried over anhydrous MgSO₄ and concentrated under reduced pressure. The residual was purified by flash column chromatography and then recrystallization from petroleum ether/Et₂O afforded the desired product **1**.



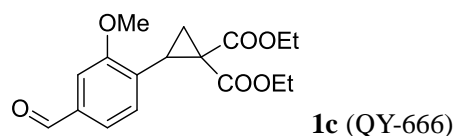
Diethyl 2-(4-formylphenyl)cyclopropane-1,1-dicarboxylate

2.05 g, 42% yield. White solid, m.p. 62-63 °C. $R_f = 0.21$ (petroleum ether/ethyl acetate, 7:1).
 $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.98 (s, 1H), 7.80 (d, $J = 8.1$ Hz, 2H), 7.38 (d, $J = 8.1$ Hz, 2H), 4.32 – 4.20 (m, 2H), 3.92 – 3.80 (m, 2H), 3.26 (t, $J = 8.5$ Hz, 1H), 2.21 (dd, $J = 7.9, 5.4$ Hz, 1H), 1.77 (dd, $J = 9.1, 5.3$ Hz, 1H), 1.31 (t, $J = 7.1$ Hz, 3H), 0.89 (t, $J = 7.1$ Hz, 3H).
 $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.8, 169.4, 166.3, 142.0, 135.5, 129.5, 129.2, 62.0, 61.4, 37.9, 31.8, 18.9, 14.1, 13.7.
IR (KBr) ν 2983, 1725, 1608, 1372, 1277, 1212, 1133, 1026, 836.
HRMS (APCI) m/z : Calcd for $\text{C}_{16}\text{H}_{17}\text{O}_5$ ($[\text{M}-\text{H}]^-$) 289.1082, found 289.1076.



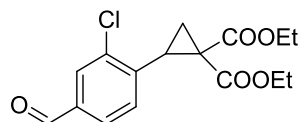
Diethyl 2-(4-formyl-2-methylphenyl)cyclopropane-1,1-dicarboxylate

1.09 g, 89% yield. Colorless oil. $R_f = 0.29$ (petroleum ether/ethyl acetate, 5:1).
 $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.95 (s, 1H), 7.67 (s, 1H), 7.63 (d, $J = 7.8$ Hz, 1H), 7.22 (d, $J = 7.8$ Hz, 1H), 4.34 – 4.23 (m, 2H), 3.80 (q, $J = 7.1$ Hz, 2H), 3.18 (t, $J = 8.6$ Hz, 1H), 2.46 (s, 3H), 2.31 (dd, $J = 8.1, 5.2$ Hz, 1H), 1.75 (dd, $J = 9.0, 5.2$ Hz, 1H), 1.31 (t, $J = 7.1$ Hz, 3H), 0.83 (t, $J = 7.1$ Hz, 3H).
 $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 192.1, 169.5, 166.3, 140.30, 140.26, 135.5, 130.3, 128.1, 127.5, 61.9, 61.3, 36.7, 30.8, 19.5, 18.3, 14.1, 13.6.
IR (KBr) ν 2983, 1725, 1696, 1374, 1321, 1281, 1210, 1132, 1027.
HRMS (APCI) m/z : Calcd for $\text{C}_{17}\text{H}_{19}\text{O}_5$ ($[\text{M}-\text{H}]^-$) 303.1238, found 303.1233.



Diethyl 2-(4-formyl-2-methoxyphenyl)cyclopropane-1,1-dicarboxylate

0.98 g, 78% yield. White solid, m.p. 52-54 °C. $R_f = 0.17$ (petroleum ether/ethyl acetate, 5:1).
 $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.94 (s, 1H), 7.37 – 7.34 (m, 2H), 7.17 (d, $J = 7.6$ Hz, 1H), 4.30 – 4.23 (m, 2H), 3.91 (s, 3H), 3.83 (q, $J = 7.1$ Hz, 2H), 3.33 (t, $J = 8.7$ Hz, 1H), 2.19 (dd, $J = 8.2, 5.2$ Hz, 1H), 1.75 (dd, $J = 9.0, 5.2$ Hz, 1H), 1.31 (t, $J = 7.0$ Hz, 3H), 0.85 (t, $J = 7.1$ Hz, 3H).
 $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.8, 169.6, 166.6, 159.8, 136.8, 131.2, 128.4, 123.9, 108.0, 61.7, 61.1, 55.8, 36.8, 27.8, 18.4, 14.1, 13.7.
IR (KBr) ν 2982, 1722, 1692, 1388, 1267, 1207, 1128, 1032.
HRMS (APCI) m/z : Calcd for $\text{C}_{17}\text{H}_{19}\text{O}_6$ ($[\text{M}-\text{H}]^-$) 319.1187, found 319.1181.



1d (QY-670)

Diethyl 2-(2-chloro-4-formylphenyl)cyclopropane-1,1-dicarboxylate

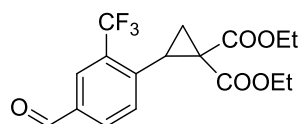
1.04 g, 76% yield. Yellow oil. $R_f = 0.26$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.95 (s, 1H), 7.88 (s, 1H), 7.70 (d, $J = 7.9$, 1H), 7.29 (d, $J = 7.9$ Hz, 1H), 4.33 – 4.25 (m, 2H), 3.86 (q, $J = 7.1$ Hz, 2H), 3.37 (t, $J = 8.6$ Hz, 1H), 2.25 (dd, $J = 8.1$, 5.5 Hz, 1H), 1.83 (dd, $J = 8.9$, 5.3 Hz, 1H), 1.32 (t, $J = 7.1$ Hz, 3H), 0.89 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 190.4, 169.0, 166.3, 139.8, 137.8, 136.6, 129.6, 127.7, 61.9, 61.4, 36.9, 30.7, 18.6, 14.1, 13.7.

IR (KBr) ν 2982, 1702, 1600, 1373, 1278, 1218, 1132, 835.

HRMS (APCI) m/z : Calcd for $\text{C}_{16}\text{H}_{16}\text{ClO}_5$ ($[\text{M}-\text{H}]^-$) 323.0692, found 323.0685.



1e (QY-713)

Diethyl 2-(4-formyl-2-(trifluoromethyl)phenyl)cyclopropane-1,1-dicarboxylate

1.93 g, 87% yield. Yellow oil. $R_f = 0.26$ (petroleum ether/ethyl acetate, 5:1).

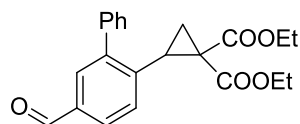
$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 10.03 (s, 1H), 8.16 (s, 1H), 7.97 (d, $J = 7.9$, 1H), 7.38 (d, $J = 8.0$ Hz, 1H), 4.32 – 4.23 (m, 2H), 3.88 – 3.81 (m, 2H), 3.48 (t, $J = 8.5$ Hz, 1H), 2.33 (dd, $J = 7.6$, 5.9 Hz, 1H), 1.87 (dd, $J = 8.9$, 5.5 Hz, 1H), 1.31 (t, $J = 7.1$ Hz, 3H), 0.86 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 190.3, 168.6, 166.2, 139.9, 135.2, 132.3, 131.9 (q, $^2J_{\text{CF}} = 30.9$ Hz), 129.5, 127.1 (q, $^3J_{\text{CF}} = 5.4$ Hz), 123.6 (q, $^1J_{\text{CF}} = 274.4$ Hz), 62.0, 61.4, 38.3, 29.3, 18.5, 14.1, 13.7.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -61.0 (s).

IR (KBr) ν 2921, 1708, 1319, 1289, 1222, 1191, 1167, 1132.

HRMS (APCI) m/z : Calcd for $\text{C}_{17}\text{H}_{16}\text{O}_5\text{F}_3$ ($[\text{M}-\text{H}]^-$) 357.0955, found 357.0947.



1f (QY-701)

Diethyl 2-(5-formyl-[1,1'-biphenyl]-2-yl)cyclopropane-1,1-dicarboxylate

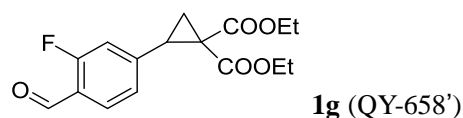
1.74 g, 90% yield. Yellow oil. $R_f = 0.31$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 10.02 (s, 1H), 7.77 – 7.79 (m, 2H), 7.47 – 7.38 (m, 5H), 7.22 (d, $J = 8.3$ Hz, 1H), 4.21 – 4.10 (m, 2H), 3.92 (q, $J = 7.1$ Hz, 2H), 3.03 (t, $J = 8.7$ Hz, 1H), 2.22 (dd, $J = 8.2$, 5.6 Hz, 1H), 1.72 (dd, $J = 9.1$, 5.5 Hz, 1H), 1.22 (t, $J = 7.1$ Hz, 3H), 0.90 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.8, 168.7, 166.3, 144.9, 139.6, 139.3, 135.3, 131.1, 129.3, 128.3, 128.0, 127.8, 126.9, 61.7, 61.4, 39.1, 31.7, 19.2, 14.1, 13.8.

IR (KBr) ν 2980, 1727, 1701, 1373, 1324, 1274, 1211, 1132, 1025, 703.

HRMS (APCI) m/z : Calcd for $C_{22}H_{21}O_6$ ($[M-H]^-$) 365.1395, found 365.1386.



Diethyl 2-(3-fluoro-4-formylphenyl)cyclopropane-1,1-dicarboxylate

2.34 g, 48% yield. White solid, m.p. 76-77 °C. R_f = 0.17 (petroleum ether/ethyl acetate, 10:1).

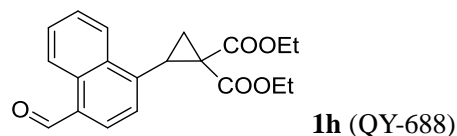
1H NMR (500 MHz, $CDCl_3$) δ 10.30 (s, 1H), 7.78 (t, J = 7.6 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 7.03 (d, J = 11.2 Hz, 1H), 4.32 – 4.20 (m, 2H), 3.98 – 3.87 (m, 2H), 3.21 (t, J = 8.5 Hz, 1H), 2.16 (dd, J = 7.6, 5.6 Hz, 1H), 1.78 (dd, J = 9.0, 5.5 Hz, 1H), 1.31 (t, J = 7.1 Hz, 3H), 0.96 (t, J = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 186.7 (d, $^3J_{CF}$ = 6.1 Hz), 169.1, 166.0, 164.3 (d, $^1J_{CF}$ = 258.9 Hz), 144.9 (d, $^3J_{CF}$ = 8.9 Hz), 128.4 (d, $^3J_{CF}$ = 2.0 Hz), 125.0 (d, $^4J_{CF}$ = 2.9 Hz), 123.1 (d, $^2J_{CF}$ = 8.2 Hz), 116.5 (d, $^2J_{CF}$ = 21.3 Hz), 62.1, 61.5, 38.0, 31.3, 19.0, 14.1, 13.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -122.1 (s)

IR (KBr) ν 2985, 1726, 1696, 1621, 1323, 1280, 1207, 1133.

HRMS (APCI) m/z : Calcd for $C_{16}H_{16}FO_5$ ($[M-H]^-$) 307.0987, found 307.0984.



Diethyl 2-(4-formylnaphthalen-1-yl)cyclopropane-1,1-dicarboxylate

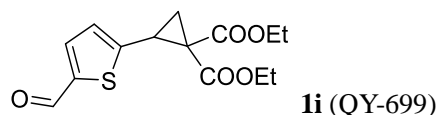
0.36 g, 26% yield. White solid, m.p. 82-84 °C. R_f = 0.19 (petroleum ether/ethyl acetate, 10:1).

1H NMR (500 MHz, $CDCl_3$) δ 10.35 (s, 1H), 9.27 (d, J = 8.2, 1H), 8.31 (dd, J = 8.4, 1H), 7.91 (d, J = 7.3 Hz, 1H), 7.71 – 7.64 (m, 2H), 7.48 (d, J = 7.3 Hz, 1H), 4.42 – 4.30 (m, 2H), 3.70 (t, J = 8.6 Hz, 1H), 3.62 – 3.51 (m, 2H), 2.44 (dd, J = 8.0, 5.2 Hz, 1H), 1.86 (dd, J = 8.9, 5.2 Hz, 1H), 1.36 (t, J = 7.1 Hz, 3H), 0.41 (t, J = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 193.3, 169.5, 166.4, 139.0, 136.0, 133.4, 131.1, 130.4, 128.9, 127.2, 125.2, 125.00, 124.96, 62.1, 61.1, 37.3, 30.0, 18.4, 14.1, 13.2.

IR (KBr) ν 2985, 1723, 1690, 1316, 1288, 1202, 1132, 760.

HRMS (APCI) m/z : Calcd for $C_{20}H_{19}O_5$ ($[M-H]^-$) 339.1238, found 339.1231.



Diethyl 2-(5-formylthiophen-2-yl)cyclopropane-1,1-dicarboxylate

0.74 g, 50% yield. Yellow oil. $R_f = 0.27$ (petroleum ether/ethyl acetate, 4:1).

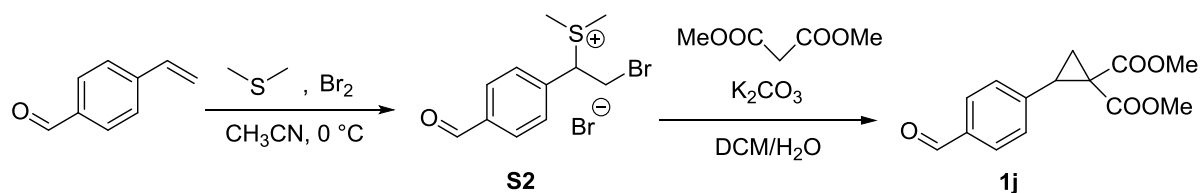
$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.81 (s, 1H), 7.59 (d, $J = 3.8$ Hz, 1H), 6.94 (d, $J = 3.8$ Hz, 1H), 4.32 – 4.19 (m, 2H), 4.04 – 3.93 (m, 2H), 3.29 (t, $J = 8.3$ Hz, 1H), 2.13 (dd, $J = 7.6, 5.4$ Hz, 1H), 1.86 (dd, $J = 9.1, 5.4$ Hz, 1H), 1.30 (t, $J = 7.1$ Hz, 3H), 1.02 (t, $J = 7.1$ Hz, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 182.5, 168.8, 165.9, 149.5, 142.9, 136.1, 127.3, 62.2, 61.7, 38.6, 26.9, 20.8, 14.1, 13.8.

IR (KBr) ν 2980, 2912, 1720, 1665, 1319, 1272, 1200, 1132, 670.

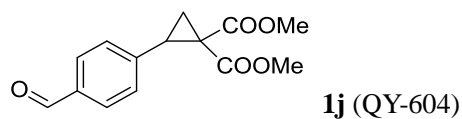
HRMS (APCI) m/z : Calcd for $\text{C}_{14}\text{H}_{15}\text{O}_5$ ($[\text{M}-\text{H}]^-$) 295.0646, found 295.0640.

Synthesis of 1j.



To a solution of dimethyl sulfide (3.4 mL, 46 mmol) in CH_3CN (20 mL) kept at 0 °C was added bromine (0.67 mL, 13 mmol) to give a yellow precipitate. 4-vinylbenzaldehyde (2.60 g, 19.7 mmol) was then added and stirring was continued for 30 min at the same temperature. The solution was then brought to room temperature and stirred further for 1 h, and diethyl ether (30 mL) was added to it to give a white precipitate that was then filtered and washed with diethyl ether to give the corresponding bromosulfonium bromide **S2** as a white solid (2.30 g, 50% yield), which was directly used in the next step.

Potassium carbonate (2.07 g, 15 mmol) was added to a solution containing **S2** (1.77 g, 5 mmol) in $\text{CH}_2\text{Cl}_2:\text{H}_2\text{O}$ (1:1) mixture (50 mL). Dimethyl malonate (0.63 mL, 5.5 mmol) was added to it and the reaction mixture was stirred for 48 h at room temperature. The CH_2Cl_2 layer was then separated and the aqueous layer was washed three times with dichloromethane (20 mL) and added to the organic layer. The combined organic layers were dried over anhydrous Na_2SO_4 and then evaporated. The residue was then purified by column chromatography on silica gel (petroleum ether/ethyl acetate, 5:1 - 3:1) to give product **1j**.



Dimethyl 2-(4-formylphenyl)cyclopropane-1,1-dicarboxylate

0.39 g, 30% yield. Colorless crystalline solid (0.39g, 30%), m.p. 44-46 °C. $R_f = 0.21$ (petroleum ether/ethyl acetate, 5:1).

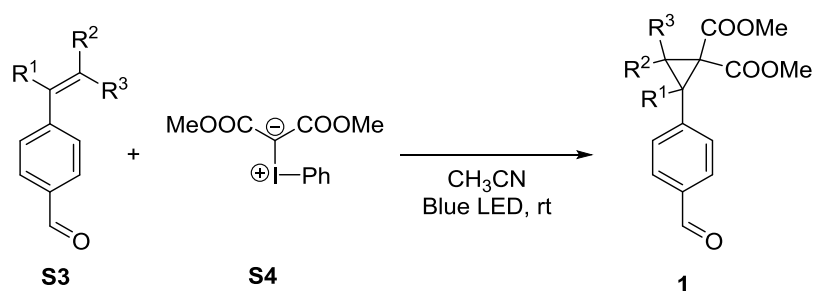
$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.98 (s, 1H), 7.80 (d, $J = 8.2$ Hz, 2H), 7.36 (d, $J = 8.1$ Hz, 2H), 3.81 (s, 3H), 3.39 (s, 3H), 3.27 (t, $J = 8.6$ Hz, 1H), 2.24 (dd, $J = 8.0, 5.4$ Hz, 1H), 1.81 (dd, $J = 9.1, 5.4$ Hz, 1H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.8, 169.8, 166.7, 141.9, 135.5, 129.6, 129.1, 53.1, 52.50, 37.7, 32.2, 19.3.

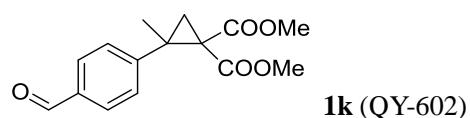
IR (KBr) ν 2955, 1730, 1702, 1608, 1439, 1334, 1280, 1175, 1132, 839.

HRMS (APCI) m/z : Calcd for $\text{C}_{14}\text{H}_{13}\text{O}_5$ ($[\text{M}-\text{H}]^-$) 261.0768, found 261.0763.

General procedure B for synthesis of 1k-1o



This procedure was performed according to the known literature². Into a suspension of iodonium ylide (1 equiv) in CH_3CN (10 mL/mmol) was added **S4** (2 equiv) in one portion under nitrogen atmosphere. The reaction mixture was irradiated with blue LED and stirred at room temperature for 24h. The mixture was then evaporated to dryness and diluted with EtOAc and washed with saturated aq. $\text{Na}_2\text{S}_2\text{O}_3$. The aqueous layer was washed with EtOAc once, and the combined organic layers were dried over anhydrous MgSO_4 and then evaporated. The residue was then purified by column chromatography on silica gel to afford the desired product **1**.



Dimethyl 2-(4-formylphenyl)-2-methylcyclopropane-1,1-dicarboxylate

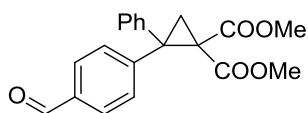
0.59 g, 27% yield. Yellow oil. $R_f = 0.19$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.98 (s, 1H), 7.83 (d, $J = 7.6$ Hz, 2H), 7.47 (d, $J = 7.6$ Hz, 2H), 3.86 (s, 3H), 3.39 (s, 3H), 2.21 (d, $J = 5.0$ Hz, 1H), 1.77 (d, $J = 4.9$ Hz, 1H), 1.51 (s, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.9, 168.3, 167.9, 148.2, 135.2, 129.8, 129.0, 52.9, 52.46, 40.4, 37.6, 25.0, 24.2.

IR (KBr) ν 2952, 1732, 1702, 1608, 1436, 1307, 1269, 1128, 1103, 835.

HRMS (APCI) m/z : Calcd for $\text{C}_{15}\text{H}_{15}\text{O}_5$ ($[\text{M}-\text{H}]^-$) 275.0925, found 275.0921.



1l (QY-633)

Dimethyl 2-(4-formylphenyl)-2-phenylcyclopropane-1,1-dicarboxylate

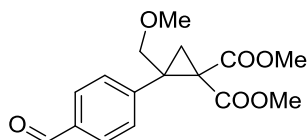
0.43 g, 18% yield. Yellow oil. $R_f = 0.16$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.94 (s, 1H), 7.78 (d, $J = 8.2$ Hz, 2H), 7.60 (d, $J = 8.1$ Hz, 2H), 7.42 (d, $J = 7.4$ Hz, 2H), 7.29 – 7.25 (m, 2H), 7.21 – 7.19 (m, 1H), 3.49 (s, 3H), 3.46 (s, 3H), 2.57 (d, $J = 5.4$ Hz, 1H), 2.48 (d, $J = 5.4$ Hz, 1H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.6, 167.5, 167.1, 147.2, 139.1, 135.2, 129.8, 129.5, 128.9, 128.6, 127.8, 52.6, 52.5, 46.9, 41.3, 23.8.

IR (KBr) ν 2954, 1734, 1701, 1605, 1436, 1338, 1248, 1118, 756, 701.

HRMS (APCI) m/z : Calcd for $\text{C}_{20}\text{H}_{17}\text{O}_5$ ($[\text{M}-\text{H}]^-$) 337.1081, found 337.1078.



1m (QY-611)

Dimethyl 2-(4-formylphenyl)-2-(methoxymethyl)cyclopropane-1,1-dicarboxylate

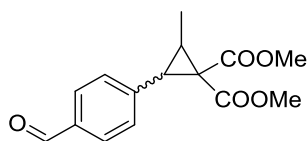
0.45 g, 24% yield. Yellow oil. $R_f = 0.19$ (petroleum ether/ethyl acetate, 3:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.99 (s, 1H), 7.83 (d, $J = 8.0$, 2H), 7.50 (d, $J = 8.0$, 2H), 3.82 (s, 3H), 3.73 (d, $J = 10.0$, 1H), 3.59 (d, $J = 10.0$, 1H), 3.41 (s, 3H), 3.23 (s, 3H), 2.16 (d, $J = 5.3$ Hz, 1H), 2.04 (d, $J = 5.2$, 1H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.8, 167.8, 167.7, 144.9, 135.6, 129.9, 129.6, 74.7, 58.8, 52.8, 52.6, 40.7, 38.4, 21.3.

IR (KBr) ν 2952, 1735, 1702, 1608, 1436, 1231, 1134, 1110, 837.

HRMS (APCI) m/z : Calcd for $\text{C}_{16}\text{H}_{19}\text{O}_6$ ($[\text{M}-\text{H}]^-$) 307.1176, found 307.1182.



1n (QY-617)

Dimethyl 2-(4-formylphenyl)-3-methylcyclopropane-1,1-dicarboxylate

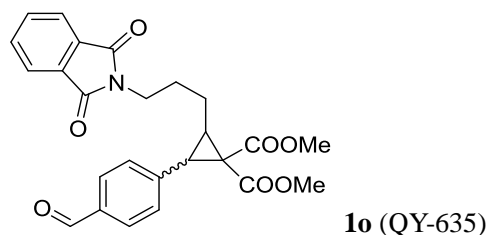
0.64 g, 29% yield. Colorless oil. $R_f = 0.26$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.97 (s, 1H), 7.79 (d, $J = 7.9$ Hz, 2H), 7.37 (d, $J = 7.9$ Hz, 2H), 3.82 (s, 3H), 3.41 (s, 3H), 3.10 (d, $J = 8.0$ Hz, 1H), 2.64 – 2.58 (m, 1H), 1.30 (d, $J = 6.3$ Hz, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.8, 167.9, 167.2, 142.4, 135.3, 129.5, 129.2, 52.8, 52.4, 43.6, 37.6, 25.5, 12.5.

IR (KBr) ν 2954, 1730, 1702, 1437, 1297, 1215, 1142, 841.

HRMS (APCI) m/z : Calcd for $\text{C}_{15}\text{H}_{17}\text{O}_5$ ($[\text{M}-\text{H}]^-$) 277.1071, found 277.1077.



dimethyl 2-(3-(1,3-dioxoisindolin-2-yl)propyl)-3-(4-formylphenyl)cyclopropane-1,1-dicarboxylate

0.60 g, 22% yield. Colorless wax. $R_f = 0.24$ (petroleum ether/dichloromethane/ethyl acetate/, 5:3:1).

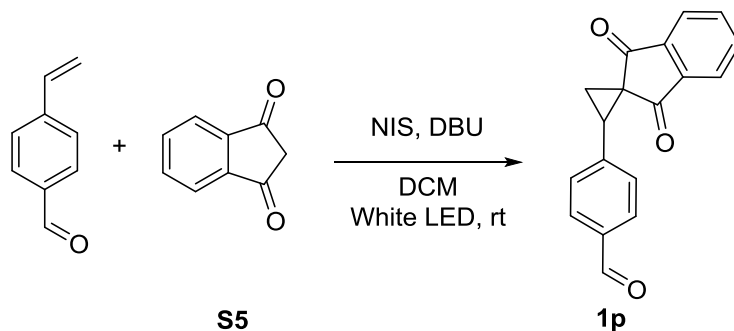
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.97 (s, 1H), 7.85 – 7.83 (m, 2H), 7.78 (d, $J = 8.0$ Hz, 2H), 7.73 – 7.71 (m, 2H), 7.37 (d, $J = 8.0$ Hz, 2H), 3.80 (s, 3H), 3.77 – 3.73 (m, 2H), 3.39 (s, 3H), 3.14 (d, $J = 8.1$ Hz, 1H), 2.63 (q, $J = 7.6$ Hz, 1H), 1.90 – 1.84 (m, 2H), 1.62 (q, $J = 7.5$ Hz, 2H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 191.8, 168.3, 167.9, 167.0, 142.1, 135.4, 134.0, 132.1, 129.6, 129.2, 123.2, 53.0, 52.5, 43.1, 37.4, 36.8, 30.5, 27.8, 24.8.

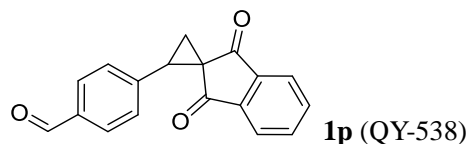
IR (KBr) ν 2946, 2845, 1711, 1608, 1437, 1397, 1297, 1211, 721.

HRMS (APCI) m/z : Calcd for $\text{C}_{25}\text{H}_{22}\text{O}_7\text{N}$ ($[\text{M}-\text{H}]^-$) 448.1402, found 448.1401.

Synthesis of 1p.



This procedure was performed according to the known literature³. Into an oven-dried reaction flask flushed with nitrogen was added **S5** (0.58g, 4 mmol), 4-vinylbenzaldehyde (1.0 mL, 8 mmol), NIS (1.80 g, 8 mmol), DBU (0.6 mL, 4 mmol), and DCM (40 mL). Then the reaction mixture was stirred for 2 h at room temperature under nitrogen atmosphere in the presence of white LED light. After the reaction was complete, the mixture was washed with aq. $\text{Na}_2\text{S}_2\text{O}_3$ (30 mL) and extracted with DCM three times. The combined organic layers were dried with anhydrous MgSO_4 and evaporated under vacuum. The crude mixture was purified by column chromatography on silica gel (petroleum ether/ethyl acetate, 5:1 – pure ethyl acetate) and then recrystallization from dichloromethane/petroleum ether to give product **1p**.



4-(1',3'-dioxo-1',3'-dihydrospiro[cyclopropane-1,2'-inden]-2-yl)benzaldehyde

0.81 g, 74% yield. White solid, m.p. 176-178 °C. $R_f = 0.17$ (petroleum ether/ethyl acetate, 5:1).

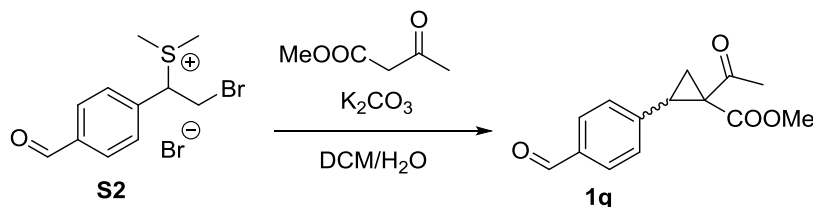
$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 9.99 (s, 1H), 8.00 (d, $J = 8.0$ Hz, 1H), 7.84 – 7.77 (m, 5H), 7.48 (d, $J = 7.9$ Hz, 2H), 3.47 (t, $J = 8.8$ Hz, 1H), 2.51 (dd, $J = 8.6, 4.4$ Hz, 1H), 2.35 (dd, $J = 8.9, 4.3$ Hz, 1H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 197.6, 195.6, 191.7, 142.5, 141.6, 140.7, 135.7, 135.1, 135.0, 129.9, 129.5, 122.7, 122.6, 42.5, 39.9, 22.2.

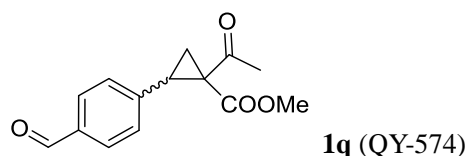
IR (KBr) ν 2923, 1702, 1605, 1334, 1313, 1221, 1039, 768.

HRMS (APCI) m/z : Calcd for $\text{C}_{18}\text{H}_{11}\text{O}_3$ ($[\text{M}-\text{H}]^-$) 275.0714, found 275.0711.

Synthesis of 1q.



Prepared from procedure similar with **1q**.



Methyl 1-acetyl-2-(4-formylphenyl)cyclopropane-1-carboxylate

0.53 g, 72% yield, 2:1 dr. Colorless oil. $R_f = 0.26$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ Major 9.99 (s, 1H), 7.81 – 7.79 (m, 2H), 7.36 (d, $J = 7.8$ Hz, 2H), 3.39 (d, $J = 19.3$ Hz, 3H), 3.36 (m, 1H), 2.46 (s, 3H), 2.28 (dd, $J = 7.7, 4.8$ Hz, 1H), 1.81 – 1.74 (m, 1H).

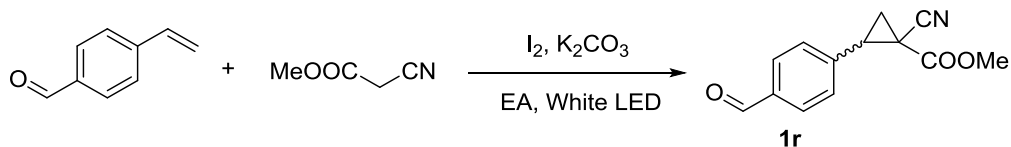
Minor δ 9.97 (s, 1H), 7.83 – 7.77 (m, 2H), 7.30 (d, $J = 7.8$ Hz, 2H), 3.83 (s, 3H), 3.35 (m, 1H), 2.38 (dd, $J = 7.7, 5.4$ Hz, 1H), 1.97 (s, 3H), 1.81 – 1.74 (m, 1H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 201.6, 199.3, 191.8, 191.7, 170.5, 168.3, 142.1, 141.0, 135.5, 135.4, 129.7, 129.5, 129.4, 129.1, 52.9, 52.2, 44.8, 44.6, 34.6, 34.3, 30.3, 29.6, 21.7, 18.3.

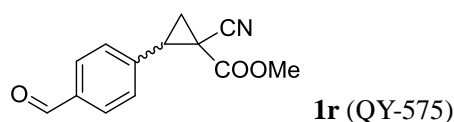
IR (KBr) ν 2954, 1701, 1608, 1437, 1324, 1210, 1170, 1119, 838.

HRMS (APCI) m/z : Calcd for $\text{C}_{14}\text{H}_{13}\text{O}_4$ ($[\text{M}-\text{H}]^-$) 245.0819, found 245.0813.

Synthesis of 1r.



This procedure was performed according to the known literature⁴. A solution of 4-vinylbenzaldehyde (0.51 mL, 4 mmol), methyl 2-cyanoacetate (0.35 mL, 4 mmol), I_2 (1.02 g, 4 mmol) and K_2CO_3 (0.55 g, 4 mmol) in EtOAc (40 mL) was irradiated with White LED under a nitrogen atmosphere and stirred for 20 h. The reaction mixture was washed with aq. $Na_2S_2O_3$, extracted with EtOAc, and then the organic layer was dried over $MgSO_4$ and concentrated in vacuo. Purification of the crude product by flash chromatography on silica gel (petroleum ether/acetone, 4:1) provided desired product **1r**.



Methyl 1-cyano-2-(4-formylphenyl)cyclopropane-1-carboxylate

0.49 g, 54% yield, 6:1 dr. White solid, m.p. 96-98 °C. R_f = 0.28 (petroleum ether/acetone, 4:1).

1H NMR (500 MHz, $CDCl_3$) Major δ 10.03 (s, 1H), 7.91 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 7.7 Hz, 2H), 3.89 (s, 3H), 3.24 (t, J = 8.7 Hz, 1H), 2.25 (dd, J = 9.0, 5.5 Hz, 1H), 2.17 (dd, J = 8.3, 5.5 Hz, 1H).

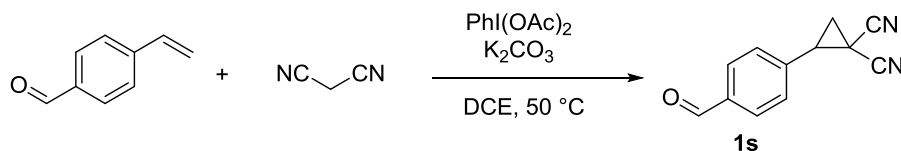
Minor δ 10.00 (s, 1H), 7.85 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 7.7 Hz, 2H), 3.59 (s, 3H), 3.34 (t, J = 9.1 Hz, 1H), 2.42 (dd, J = 8.8, 5.8 Hz, 1H), 2.17 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 191.5, 191.5, 167.4, 164.4, 139.5, 138.7, 136.4, 136.2, 130.1, 130.0, 129.7, 129.0, 118.4, 115.8, 53.9, 53.5, 36.1, 34.9, 23.0, 23.0, 21.0, 20.5.

IR (KBr) ν 2242, 1738, 1699, 1608, 1443, 1299, 1267, 1207, 1158.

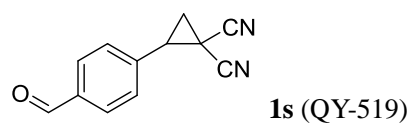
HRMS (APCI) m/z : Calcd for $C_{13}H_{10}O_3N$ ($[M-H]^+$) 228.0666, found 228.0660.

Synthesis of 1s.



This procedure was performed according to the known literature⁵. $PhI(OAc)_2$ (4.25 g, 13.2 mmol), K_2CO_3 (1.82 g, 13.2 mmol), malononitrile (0.48 g, 7.2 mmol) and 4-vinylbenzaldehyde (0.76 mL, 6 mmol) were dissolved in DCE (30 mL). The mixture was stirred at 50 °C for 2 h (monitored by TLC). Then the reaction mixture was cooled to room temperature. The undissolved solid was removed by filtration through a pad of Celite. The filtrate was concentrated under reduced pressure, and the residue was purified by flash silica gel column chromatography (petroleum

ether/acetone, 4:1) to give **1s**.



2-(4-formylphenyl)cyclopropane-1,1-dicarbonitrile

0.69 g, 58% yield. White solid, m.p. 82-84 °C. R_f = 0.31 (petroleum ether/acetone, 4:1).

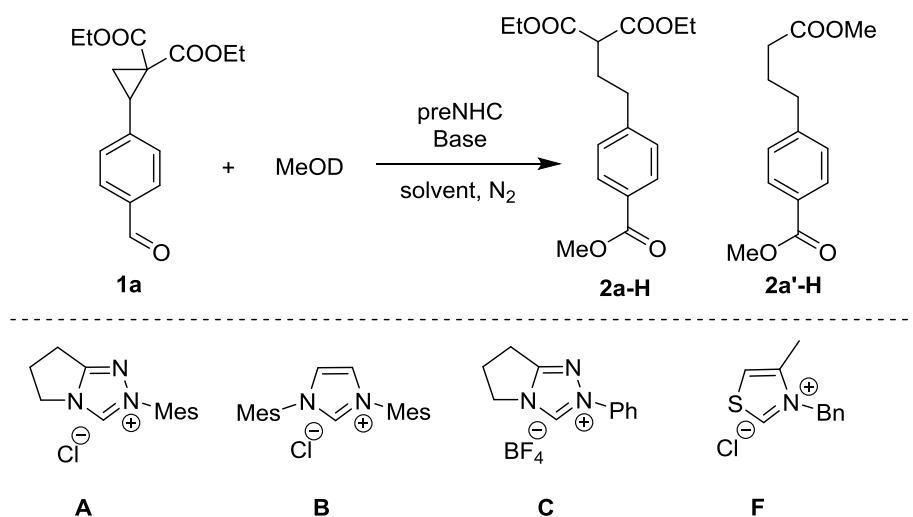
$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 10.05 (s, 1H), 7.95 (d, J = 8.0 Hz, 2H), 7.49 (d, J = 7.9 Hz, 2H), 3.36 (t, J = 9.0 Hz, 1H), 2.34 (d, J = 8.9 Hz, 2H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 191.2, 137.0, 136.9, 130.3, 129.1, 114.8, 112.6, 34.5, 22.5, 7.6.

IR (KBr) ν 2248, 1700, 1609, 1574, 1312, 1211, 1172, 987, 836.

HRMS (APCI) m/z : Calcd for $\text{C}_{12}\text{H}_7\text{ON}_2$ ($[\text{M}-\text{H}]^-$) 195.0564, found 195.0555.

3. Preliminary reaction optimization using MeOH.

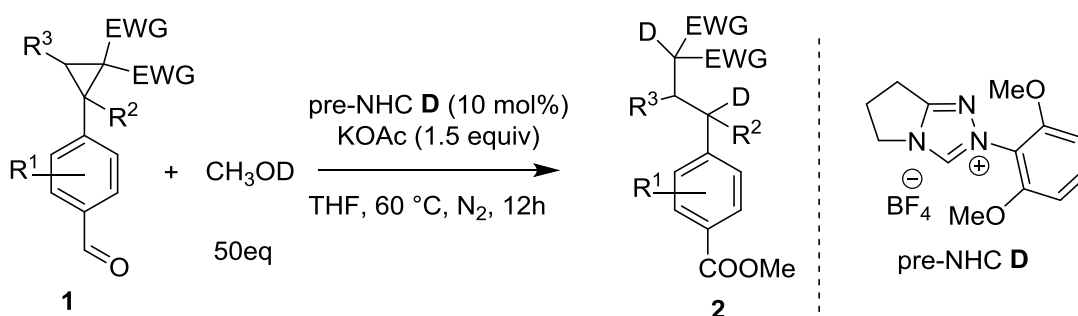


Entry	PreNHC (20 mol%)	Base (1.5 equiv)	T (°C)	Solvent	Yield/3a (%)	Yield/3a' (%)
1	A	Cs_2CO_3	rt	THF	0	0
2	A	Cs_2CO_3	70	THF	trace	0
3	A	Cs_2CO_3	100	THF	0	30
4	A	KOAc	100	THF	74	0
5	B	KOAc	100	THF	16	0
6	C	KOAc	100	THF	60	0
7	F	KOAc	100	THF	7	0
8	A	Cs_2CO_3 (0.2 eq)	100	THF	51	0

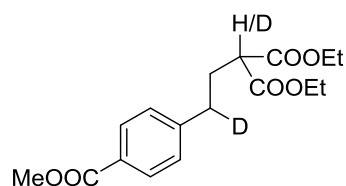
9	A	K ₃ PO ₄	100	THF	0	trace
10	A	DIPEA	100	THF	trace	0
11	A	KOAc	100	CH ₃ CN	66	0
12	A	KOAc	100	PhMe	28	0
13	A	KOAc	100	DCE	34	0

Reaction conditions: **1a** (0.3 mmol), **preNHC D** (20 mol%), Base (1.5 equiv), and MeOH (50 equiv) in solvent (4 mL) at indicated temperature for 12 h. Isolated yields reported.

4. General procedure for 1,3-deuteration via ring opening of DA cyclopropanes.



Typical procedure: To an oven-dried 25 mL Schlenk tube equipped with a stir bar was charged with donor-acceptor cyclopropane **1a** (R¹, R², R³ = H, EWG = COOEt, 58.0 mg, 0.2 mmol), pre-NHC **D** (6.7 mg, 0.02 mmol) and KOAc (29.4 mg, 0.3 mmol). This tube was closed with a septum, evacuated, backfilled with nitrogen three times. To this mixture was added CH₃OD (0.4 mL, 10 mmol) freshly distilled dry THF (4 mL). The reaction mixture was stirred at 60 °C until the full consumption of **1a** (Typically within 12 h). The reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel (petroleum ether/EtOAc, 5:1 as the eluent) to give the product **2a** (45.7 mg, 71% yield). The non-deuterated samples for NMR Spectroscopy analysis were prepared using MeOH under the same conditions.



2a (QY-565-1)

Diethyl 2-(2-(4-(methoxycarbonyl)phenyl)ethyl-2-*d*)malonate-*d*

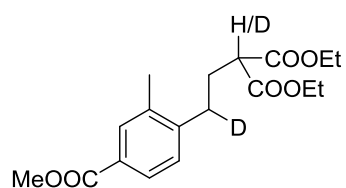
46 mg, 71% yield. Colorless oil. $R_f = 0.42$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.96 (d, $J = 8.2$ Hz, 2H), 7.26 (d, $J = 8.2$ Hz, 2H), 4.23 – 4.17 (m, 4H), 3.90 (s, 3H), 3.32 (t, $J = 7.4$ Hz, 0.91H, 9% D), 2.74 – 2.68 (m, 1.16H, 84% D), 2.22 (t, $J = 7.6$ Hz, 2H), 1.27 (t, $J = 7.1$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 169.1, 167.0, 146.1, 129.8, 128.6, 128.3, 61.4, 52.0, 51.2, 33.3, 33.2, 33.0, 32.8, 29.9, 14.1.

IR (KBr) ν 2983, 1725, 1612, 1436, 1279, 1179, 1108.

HRMS (ESI) m/z : Calcd for $\text{C}_{17}\text{H}_{21}\text{DNaO}_6$ ($[\text{M}+\text{Na}]^+$) 346.1377, found 346.1386.



2b (QY-697)

Diethyl 2-(2-(4-(methoxycarbonyl)-2-methylphenyl)ethyl-2-*d*)malonate-*d*

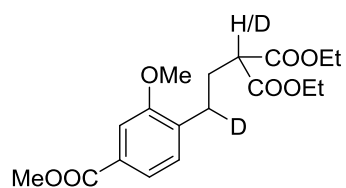
55 mg, 81% yield. Colorless oil. $R_f = 0.40$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.82 – 7.78 (m, 2H), 7.20 (d, $J = 7.9$ Hz, 1H), 4.24 – 4.18 (m, 4H), 3.89 (s, 3H), 3.38 (t, $J = 7.3$ Hz, 1H, <5% D), 2.72 – 2.66 (m, 1.22H, 78% D), 2.36 (s, 3H), 2.15 (t, $J = 7.8$ Hz, 2H), 1.28 (t, $J = 7.1$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 169.2, 167.2, 144.5, 136.3, 131.4, 129.1, 128.2, 127.3, 61.5, 52.0, 51.6, 31.0, 30.8, 30.6, 30.5, 28.8, 28.7, 19.1, 14.1.

IR (KBr) ν 2981, 1725, 1438, 1370, 1294, 1268, 1195, 1025.

HRMS (ESI) m/z : Calcd for $\text{C}_{18}\text{H}_{23}\text{DNaO}_6$ ($[\text{M}+\text{Na}]^+$) 360.1533, found 360.1525.



2c (QY-680)

Diethyl 2-(2-(2-methoxy-4-(methoxycarbonyl)phenyl)ethyl-2-*d*)malonate-*d*

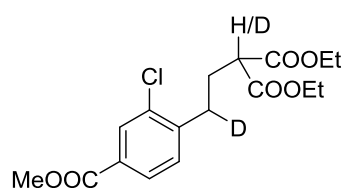
50 mg, 71% yield. Colorless oil. $R_f = 0.29$ (petroleum ether/ethyl acetate, 5:1).

¹H NMR (500 MHz, CDCl₃) δ 7.59 – 7.57 (m, 1H), 7.49 (s, 1H), 7.18 (d, *J* = 7.7 Hz, 1H), 4.22 – 4.17 (m, 4H), 3.91 (s, 3H), 3.87 (s, 3H), 3.32 (t, *J* = 7.5 Hz, 0.99H, <5% D), 2.73 – 2.68 (m, 1.20H, 80% D), 2.19 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.1 Hz, 6H).

¹³C NMR (126 MHz, CDCl₃) δ 169.4, 167.1, 157.4, 134.7, 129.9, 129.5, 122.0, 110.9, 61.3, 55.4, 52.1, 51.5, 28.4, 28.3, 28.0, 27.8, 27.7, 27.5, 14.1.

IR (KBr) ν 2982, 1722, 1436, 1410, 1289, 1272, 1036, 760.

HRMS (ESI) *m/z*: Calcd for C₁₈H₂₃DNaO₇ ([M+Na]⁺) 376.1482, found 376.1475.



2d (QY-690)

Diethyl 2-(2-(2-chloro-4-(methoxycarbonyl)phenyl)ethyl-2-*d*)malonate-*d*

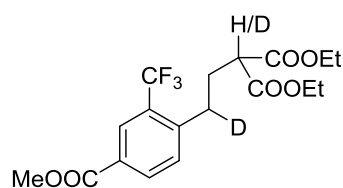
41 mg, 57% yield. Colorless oil. *R*_f = 0.39 (petroleum ether/ethyl acetate, 5:1).

¹H NMR (400 MHz, CDCl₃) δ 8.02 (d, *J* = 1.5 Hz, 1H), 7.86 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 4.24 – 4.18 (m, 4H), 3.91 (s, 3H), 3.36 (t, *J* = 7.4 Hz, 1H, <5% D), 2.86 – 2.80 (m, 1.17H, 83% D), 2.22 (q, *J* = 7.7 Hz, 2H), 1.28 (t, *J* = 7.1 Hz, 6H).

¹³C NMR (101 MHz, CDCl₃) δ 169.05, 165.9, 143.6, 134.2, 130.7, 130.5, 129.9, 128.0, 61.5, 52.3, 51.4, 31.2, 31.1, 30.9, 30.8, 28.1, 14.1.

IR (KBr) ν 2983, 1729, 1438, 1290, 1258, 1154, 1045, 763.

HRMS (ESI) *m/z*: Calcd for C₁₇H₂₀DClNaO₆ ([M+Na]⁺) 380.0987, found 380.0979.



2e (QY-717)

Diethyl 2-(2-(4-(methoxycarbonyl)-2-(trifluoromethyl)phenyl)ethyl-2-*d*)malonate-*d*

50 mg, 64% yield. Colorless oil. *R*_f = 0.35 (petroleum ether/ethyl acetate, 10:1).

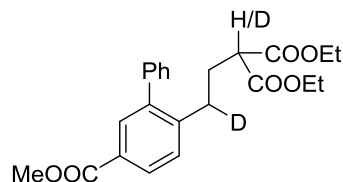
¹H NMR (500 MHz, CDCl₃) δ 8.30 (s, 1H), 8.14 (d, *J* = 8.0, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 4.24 – 4.20 (m, 4H), 3.94 (s, 3H), 3.42 (t, *J* = 7.3 Hz, 0.97H, <5% D), 2.91 – 2.85 (m, 1.17H, 83% D), 2.21 (t, *J* = 7.8 Hz, 2H), 1.29 (t, *J* = 7.1 Hz, 6H).

¹³C NMR (126 MHz, CDCl₃) δ 169.0, 165.8, 144.9, 132.8, 131.5, 128.9 (q, ²*J*_{CF} = 30.6 Hz), 128.6, 127.5 (q, ³*J*_{CF} = 5.6 Hz), 124.0 (q, ¹*J*_{CF} = 274.2 Hz), 61.6, 52.4, 51.6, 30.2, 30.1, 30.0, 29.9, 29.8, 14.1.

¹⁹F NMR (376 MHz, CDCl₃) δ -60.0 (s)

IR (KBr) ν 2985, 1731, 1620, 1442, 1327, 1257, 1123, 1054, 761.

HRMS (ESI) m/z : Calcd for $C_{18}H_{20}DF_3NaO_6$ ($[M+Na]^+$) 414.1251, found 414.1248.



2f (QY-705)

Diethyl 2-(2-(5-(methoxycarbonyl)-[1,1'-biphenyl]-2-yl)ethyl-2-*d*)malonate-*d*

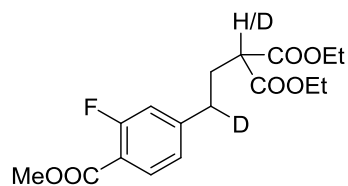
64 mg (0.2mmol scale), 80% yield. Colorless oil. R_f = 0.33 (petroleum ether/ethyl acetate, 5:1).

1H NMR (500 MHz, $CDCl_3$) δ 7.96 (dd, J = 7.9, 1.6 Hz, 1H), 7.89 (d, J = 1.5 Hz, 1H), 7.44 – 7.35 (m, 4H), 7.29 – 7.26 (m, 2H), 4.10 (q, J = 7.1 Hz, 4H), 3.90 (s, 3H), 3.18 (t, J = 7.4 Hz, 0.94H, 6% D), 2.70 – 2.65 (m, 1.18H, 82% D), 2.05 (t, J = 7.8 Hz, 2H), 1.20 (t, J = 7.1 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 169.0, 167.0, 143.6, 142.2, 140.5, 131.4, 129.5, 129.1, 128.6, 128.3, 128.1, 127.3, 61.4, 52.1, 51.5, 30.7, 30.5, 30.4, 30.2, 29.7, 29.6, 14.0.

IR (KBr) ν 2924, 1724, 1439, 1306, 1240, 1153, 1109, 1025.

HRMS (ESI) m/z : Calcd for $C_{23}H_{25}DNaO_6$ ($[M+Na]^+$) 422.1690, found 422.1686.



2g (QY-661)

Diethyl 2-(2-(3-fluoro-4-(methoxycarbonyl)phenyl)ethyl-2-*d*)malonate-*d*

27 mg, 39% yield. Colorless oil. R_f = 0.34 (petroleum ether/ethyl acetate, 10:1).

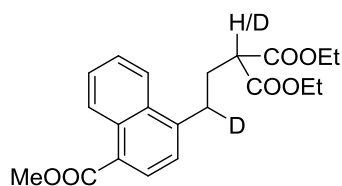
1H NMR (500 MHz, $CDCl_3$) δ 7.86 (t, J = 7.8 Hz, 1H), 7.04 – 7.02 (m, 1H), 6.98 (d, J = 11.5 Hz, 1H), 4.23 – 4.18 (m, 4H), 3.92 (s, 3H), 3.31 (t, J = 7.4 Hz, 0.90H, 10% D), 2.72 – 2.67 (m, 1.15H, 85% D), 2.24 – 2.20 (m, 2H), 1.28 (t, J = 7.1 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 169.0, 164.8 (d, $^3J_{CF}$ = 3.6 Hz), 162.0 (d, $^1J_{CF}$ = 206.2 Hz), 148.6, 132.3, 124.2 (d, $^4J_{CF}$ = 3.0 Hz), 116.9 (d, $^2J_{CF}$ = 22.4 Hz), 116.5 (d, $^2J_{CF}$ = 10.0 Hz), 61.6, 52.2, 51.1, 33.0, 29.7, 29.6, 29.5, 14.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -109.6 (s)

IR (KBr) ν 2921, 1730, 1623, 1432, 1296, 1152, 1021.

HRMS (ESI) m/z : Calcd for $C_{17}H_{20}DFNaO_6$ ($[M+Na]^+$) 364.1283, found 364.1278.



2h (QY-696)

Diethyl 2-(2-(4-(methoxycarbonyl)naphthalen-1-yl)ethyl-2-*d*)malonate-*d*

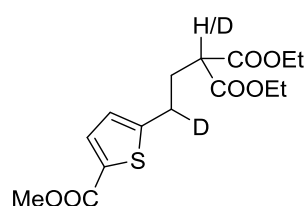
51 mg, 68% yield. Colorless oil. $R_f = 0.33$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.96 – 8.94 (m, 1H), 8.15 – 8.13 (m, 1H), 8.09 (d, $J = 7.4$ Hz, 1H), 7.62 – 7.57 (m, 2H), 7.36 (d, $J = 7.4$ Hz, 1H), 4.25 – 4.19 (m, 4H), 3.99 (s, 3H), 3.45 (t, $J = 7.3$ Hz, 0.82H, 18% D), 3.19 – 3.13 (m, 1.17H, 83% D), 2.34 (t, $J = 7.7$ Hz, 2H), 1.28 (t, $J = 7.1$ Hz, 6H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 169.2, 168.0, 142.7, 132.1, 131.7, 129.9, 127.4, 126.5, 126.4, 126.1, 125.2, 124.1, 61.5, 52.1, 51.6, 31.2, 31.0, 30.9, 30.7, 29.6, 29.5, 29.4, 14.1.

IR (KBr) ν 2983, 1725, 1588, 1516, 1437, 1250, 1129, 1037, 777.

HRMS (ESI) m/z : Calcd for $\text{C}_{21}\text{H}_{23}\text{DNaO}_6$ ($[\text{M}+\text{Na}]^+$) 396.1533, found 396.1528.



2i (QY-704)

Diethyl 2-(2-(5-(methoxycarbonyl)thiophen-2-yl)ethyl-2-*d*)malonate-*d*

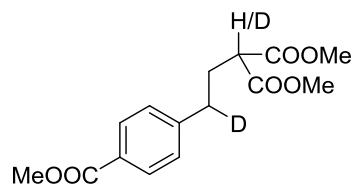
28 mg, 42% yield. Yellow oil. $R_f = 0.31$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.64 (d, $J = 3.6$ Hz, 1H), 6.82 (d, $J = 3.6$ Hz, 1H), 4.23 – 4.19 (m, 4H), 3.86 (s, 3H), 3.38 (t, $J = 7.4$ Hz, 0.99H, <5% D), 2.92 – 2.87 (m, 1.21H, 79% D), 2.27 (t, $J = 7.6$ Hz, 2H), 1.28 (t, $J = 7.1$ Hz, 6H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 168.9, 162.6, 151.2, 133.7, 131.4, 125.9, 61.6, 52.0, 50.83, 50.81, 30.14, 30.06, 27.9, 27.7, 27.5, 27.4, 14.1.

IR (KBr) ν 2982, 1715, 1460, 1290, 1260, 1154, 1094, 1025, 750.

HRMS (ESI) m/z : Calcd for $\text{C}_{15}\text{H}_{19}\text{DNaO}_6\text{S}$ ($[\text{M}+\text{Na}]^+$) 352.0941, found 352.0937.



2j (QY-614)

Dimethyl 2-(2-(4-(methoxycarbonyl)phenyl)ethyl-2-*d*)malonate-*d*

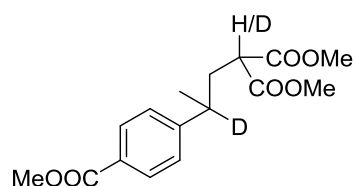
36 mg, 60% yield. Colorless oil. $R_f = 0.29$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.97 (d, $J = 7.9$ Hz, 2H), 7.26 (d, $J = 7.9$ Hz, 2H), 3.91 (s, 3H), 3.74 (s, 6H), 3.37 (t, $J = 7.4$ Hz, 0.99H, <5% D), 2.73 – 2.68 (m, 1.16H, 84% D), 2.24 (t, $J = 7.5$ Hz, 2H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 169.5, 167.0, 145.9, 129.8, 128.6, 128.3, 52.6, 52.1, 50.8, 33.3, 33.1, 33.0, 32.8, 30.0, 29.9.

IR (KBr) ν 2955, 1732, 1649, 1613, 1435, 1280, 1108, 760.

HRMS (APCI) m/z : Calcd for $\text{C}_{15}\text{H}_{18}\text{DO}_6$ ($[\text{M}+\text{H}]^+$) 296.1239, found 296.1236.



2k (QY-615)

Dimethyl 2-(2-(4-(methoxycarbonyl)phenyl)propyl-2-*d*)malonate-*d*

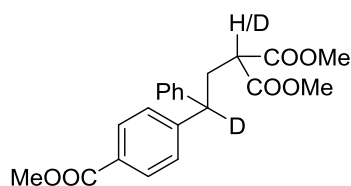
32 mg, 52% yield. Colorless oil. $R_f = 0.33$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.98 (d, $J = 8.0$ Hz, 2H), 7.24 (d, $J = 8.0$ Hz, 2H), 3.91 (d, $J = 1.8$ Hz, 3H), 3.74 (s, 3H), 3.64 (s, 3H), 3.18 (dd, $J = 8.7, 6.4$ Hz, 0.99H, <5% D), 2.81 – 2.77 (m, 0.32H, 68% D), 2.27 – 2.15 (m, 2H), 1.29 (s, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 169.73, 169.64, 167.0, 150.72, 150.68, 130.0, 128.5, 127.18, 127.16, 52.59, 52.57, 52.1, 49.9, 49.8, 37.9, 37.6, 37.5, 37.3, 36.7, 36.6, 22.2, 22.1.

IR (KBr) ν 2956, 1731, 1611, 1436, 1281, 1155, 1113, 776, 709.

HRMS (ESI) m/z : Calcd for $\text{C}_{16}\text{H}_{20}\text{DO}_6$ ($[\text{M}+\text{H}]^+$) 310.1395, found 310.1400.



2l (QY-645)

Dimethyl 2-(2-(4-(methoxycarbonyl)phenyl)-2-phenylethyl-2-*d*)malonate-*d*

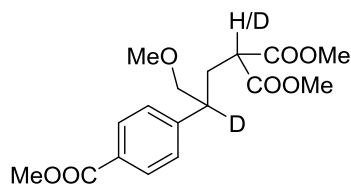
58 mg, 78% yield. Yellow oil. $R_f = 0.31$ (petroleum ether/ethyl acetate, 5:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.96 (d, $J = 8.0$ Hz, 2H), 7.32 – 7.21 (m, 7H), 4.03 – 4.00 (m, 0.17H, 83% D), 3.88 (s, 3H), 3.70 (s, 3H), 3.69 (s, 3H), 3.26 (t, $J = 7.3$ Hz, 0.73H, 27% D), 2.68 (d, $J = 7.2$ Hz, 2H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 169.5, 166.9, 148.6, 142.3, 130.0, 128.8, 128.6, 127.89, 127.86, 126.9, 52.6, 52.1, 49.8, 48.7, 48.2, 48.1, 34.1.

IR (KBr) ν 2954, 1725, 1611, 1435, 1280, 1155, 1110, 707.

HRMS (ESI) m/z : Calcd for $\text{C}_{21}\text{H}_{21}\text{DNaO}_6$ ($[\text{M}+\text{Na}]^+$) 394.1377, found 394.1372.



2m (QY-622)

Dimethyl 2-(3-methoxy-2-(4-(methoxycarbonyl)phenyl)propyl-2-*d*)malonate-*d*

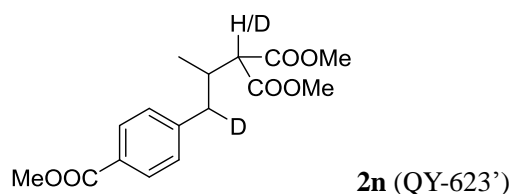
35 mg, 52% yield. Colorless oil. $R_f = 0.30$ (petroleum ether/ethyl acetate, 3:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.99 (d, $J = 8.2$ Hz, 2H), 7.27 – 7.26 (m, 2H), 3.91 (s, 3H), 3.73 (s, 3H), 3.61 (s, 3H), 3.53 – 3.52 (m, 2H), 3.29 (s, 3H), 3.23 (dd, $J = 9.2, 5.6$ Hz, 1H, <5% D), 2.99 – 2.93 (m, 0.19H, 81% D), 2.45 (dd, $J = 14.1, 9.4$ Hz, 1H), 2.17 (dd, $J = 14.1, 5.6$ Hz, 1H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 169.6, 169.5, 166.9, 146.6, 129.9, 129.0, 128.0, 58.9, 52.6, 52.5, 52.1, 49.6, 31.6.

IR (KBr) ν 2921, 2850, 1731, 1718, 1435, 1279, 1106, 1018.

HRMS (ESI) m/z : Calcd for $\text{C}_{17}\text{H}_{22}\text{DO}_7$ ($[\text{M}+\text{H}]^+$) 340.1501, found 340.1502.



Dimethyl 2-(1-(4-(methoxycarbonyl)phenyl)propan-2-yl-1-*d*)malonate-*d*

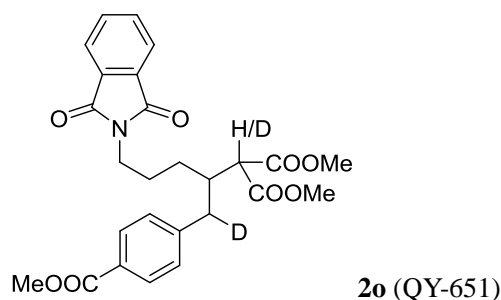
44 mg, 72% yield. Temperature: 100 °C. Reaction time: 60 h. Colorless oil. $R_f = 0.23$ (petroleum ether/ethyl acetate, 7:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.96 (d, $J = 8.1$ Hz, 2H), 7.26 (d, $J = 8.0$ Hz, 2H), 3.91 (s, 3H), 3.75 (s, 3H), 3.74 (s, 3H), 3.32 (d, $J = 7.4, 0.81\text{H}$, 19% D), 2.90 – 2.86 (m, 0.72H, 28% D), 2.60 – 2.55 (m, 1H), 2.50 – 2.45 (m, 0.43H, 57% D), 0.94 – 0.93 (m, 3H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 169.2, 168.9, 167.1, 145.3, 129.7, 129.3, 128.3, 56.5, 52.45, 52.38, 52.0, 40.6, 40.4, 40.2, 40.1, 35.3, 35.2, 35.1, 16.8.

IR (KBr) ν 2954, 1722, 1645, 1435, 1384, 1279, 688, 560.

HRMS (ESI) m/z : Calcd for $\text{C}_{16}\text{H}_{18}\text{D}_2\text{NaO}_6$ ($[\text{M}+\text{Na}]^+$) 333.1278, found 333.1276.



Dimethyl 2-(1-(4-(methoxycarbonyl)phenyl)propan-2-yl-1-*d*)malonate-*d*

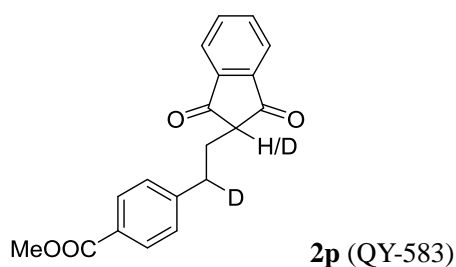
25 mg (0.1 mmol scale), 52% yield. Temperature: 100 °C. Reaction time: 24 h. Colorless wax. $R_f = 0.19$ (petroleum ether/ethyl acetate, 3:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.88 (d, $J = 8.1$ Hz, 2H), 7.82 (dd, $J = 5.4, 3.0$ Hz, 2H), 7.71 (dd, $J = 5.5, 3.0$ Hz, 2H), 7.23 (d, $J = 8.1$ Hz, 2H), 3.89 (s, 3H), 3.72 (s, 3H), 3.68 (s, 3H), 3.61 (t, $J = 7.1$ Hz, 2H), 3.43 – 3.41 (m, 0.93H, 7% D), 2.82 – 2.78 (m, 0.63H, 37% D), 2.67 – 2.63 (m, 0.55H, 45% D), 2.52 – 2.48 (m, 1H), 1.76 – 1.66 (m, 2H), 1.47 – 1.36 (m, 2H).

^{13}C NMR (126 MHz, CDCl_3) δ 169.0, 168.9, 168.3, 166.9, 145.1, 133.9, 132.0, 129.7, 129.2, 128.3, 123.2, 53.8, 52.44, 52.40, 52.0, 39.7, 37.7, 37.5, 37.0, 29.7, 27.8, 25.5.

IR (KBr) ν 2953, 2924, 1711, 1436, 1397, 1280, 1108, 1021, 721.

HRMS (ESI) m/z : Calcd for $\text{C}_{26}\text{H}_{26}\text{DNNaO}_8$ ($[\text{M}+\text{Na}]^+$) 505.1697, found 505.1691.



Methyl 4-(2-(1,3-dioxo-2,3-dihydro-1H-inden-2-yl-2-*d*)ethyl-1-*d*)benzoate

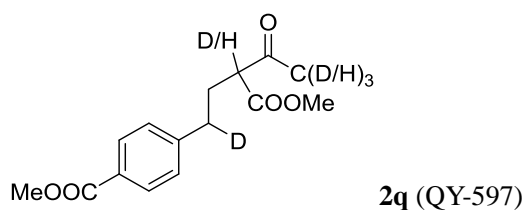
29 mg (0.2 mmol scale), 47% yield. White solid, m.p. 114-116 °C. R_f = 0.33 (petroleum ether/dichloromethane/ethyl acetate, 9:3:1).

^1H NMR (500 MHz, CDCl_3) δ 7.98 – 7.92 (m, 4H), 7.86 – 7.84 (m, 2H), 7.29 (d, J = 8.1 Hz, 2H), 3.89 (s, 3H), 3.00 (t, J = 6.4 Hz, 0.95 H, <5% D), 2.88 (t, J = 7.9 Hz, 1.06H, 94% D), 2.24 (t, J = 6.9 Hz, 2H).

^{13}C NMR (126 MHz, CDCl_3) δ 199.5, 166.0, 145.2, 141.2, 134.7, 128.8, 127.7, 127.2, 122.2, 51.2, 51.0, 31.4, 31.2, 31.0, 30.9, 27.2.

IR (KBr) ν 1702, 1593, 1281, 1179, 1110, 753, 709.

HRMS (ESI) m/z : Calcd for $\text{C}_{19}\text{H}_{14}\text{DO}_4$ ($[\text{M}-\text{H}]^-$) 308.1039, found 308.1047.



Methyl 4-(3-(methoxycarbonyl)-4-oxopentyl-1,3,5,5,5-*d*5)benzoate

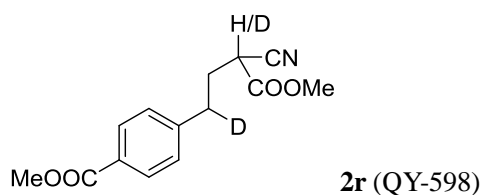
39 mg, 70% yield. Colorless oil. R_f = 0.22 (petroleum ether/ethyl acetate, 5:1).

^1H NMR (500 MHz, CDCl_3) δ 7.96 (d, J = 7.5 Hz, 2H), 7.24 (d, J = 7.7 Hz, 2H), 3.90 (s, 3H), 3.74 (s, 3H), 3.43 (t, J = 7.1 Hz, 0.92H, 8% D), 2.69 – 2.62 (m, 1.07H, 93% D), 2.21 – 2.16 (m, 3.71H, 43% D(C(D/H)₃)).

^{13}C NMR (126 MHz, CDCl_3) δ 202.59, 202.54, 202.49, 170.0, 167.0, 146.0, 129.9, 128.5, 128.3, 58.5, 52.5, 52.0, 33.3, 33.1, 33.0, 32.8, 29.1, 29.0, 28.9, 28.8, 28.6.

IR (KBr) ν 2954, 1717, 1612, 1436, 1281, 1179, 1109.

HRMS (ESI) m/z : Calcd for $\text{C}_{15}\text{H}_{15}\text{D}_2\text{O}_5$ ($[\text{M}-\text{H}]^-$) 279.1207, found 279.1214.



Methyl 4-(3-cyano-4-methoxy-4-oxobutyl-1,3-*d*2)benzoate

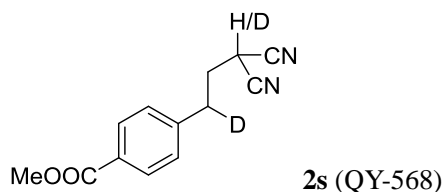
20 mg, 38% yield. Colorless oil. $R_f = 0.26$ (petroleum ether/ethyl acetate, 4:1).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.99 (d, $J = 7.9$ Hz, 2H), 7.29 (d, $J = 7.7$ Hz, 2H), 3.91 (s, 3H), 3.80 (s, 3H), 3.47 (t, $J = 7.1$ Hz, 0.98H, <5% D), 2.94 – 2.84 (m, 1.16H, 84% D), 2.28 (t, $J = 6.8$ Hz, 2H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.8, 166.2, 144.3, 130.1, 128.8, 128.6, 116.0, 53.6, 52.1, 36.5, 32.6, 32.5, 32.3, 32.1, 30.9, 30.8.

IR (KBr) ν 2955, 1747, 1716, 1612, 1436, 1279, 1108, 758, 706.

HRMS (ESI) m/z : Calcd for $\text{C}_{14}\text{H}_{13}\text{DNO}_4$ ($[\text{M}-\text{H}]^-$) 261.0991, found 261.0997.



Methyl 4-(3,3-dicyanopropyl-1,3-*d*2)benzoate

17 mg, 25% yield. Colorless oil. $R_f = 0.26$ (petroleum ether/acetone, 4:1).

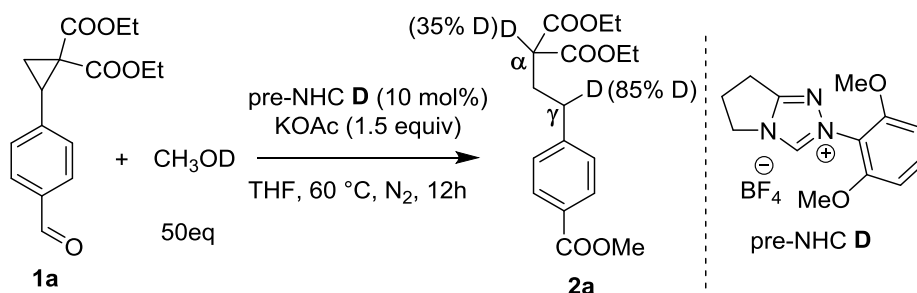
$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.02 (d, $J = 7.9$ Hz, 2H), 7.29 (d, $J = 7.9$ Hz, 2H), 3.92 (s, 3H), 3.63 (t, $J = 7.0$ Hz, 0.95H, 5% D), 3.02 – 2.98 (m, 1.10H, 90% D), 2.38 (t, $J = 7.2$ Hz, 2H).

$^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 166.6, 142.5, 130.4, 129.4, 128.5, 112.2, 52.2, 32.2, 32.1, 32.03, 31.96, 31.9, 31.8, 21.7.

IR (KBr) ν 2953, 2919, 1715, 1648, 1613, 1435, 1280, 1108, 757.

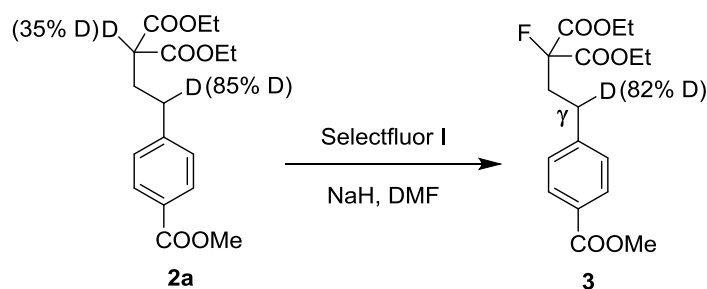
HRMS (ESI) m/z : Calcd for $\text{C}_{13}\text{H}_{10}\text{DN}_2\text{O}_2$ ($[\text{M}-\text{H}]^-$) 228.0889, found 228.0892.

5. Gram-scale synthesis.

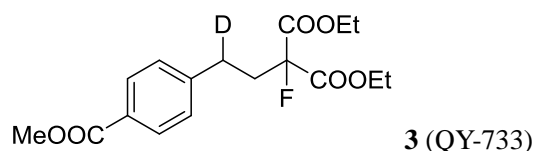


To an oven-dried 250 mL flask equipped with a stir bar was charged with pre-NHC **D** (0.17 g, 0.5 mmol) and KOAc (0.77 g, 7.8 mmol). This tube was closed with a septum, evacuated, backfilled with nitrogen three times. To this mixture was added **1a** (1.51 g, 5.2 mmol), MeOD (10.4 mL, 260 mmol), freshly distilled dry THF (100 mL). The reaction was complete after stirring at 60°C for 12 h, as indicated by TLC. The reaction mixture was concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate, 5:1) to give the product **2a** (1.03 g, 61% yield, α : 35% D , γ : 85% D).

6. Chemical transformations of **2a**.



To a 10 mL Schlenk tube was added NaH (60% w/w in mineral oil) (14.4 mg, 0.36 mmol), 0.5 mL dry DMF and then **2a** (87 μL , 0.3 mmol) under N_2 atmosphere. The reaction mixture was stirred at room temperature for 1 h, then Selectfluor I (127.5 mg, 0.36 mmol) was added, and 1 mL dry DMF was added to rinse the tube. The mixture was stirred at room temperature overnight, then diluted with water (15 mL), and extracted with EtOAc for three times (3×10 mL). The combined organic extracts were washed with water, then with brine, dried over anhydrous MgSO_4 and concentrated under reduced pressure. The residual was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate, 5:1) to give the product **3** colorless oil (92 mg, 90% yield, γ : 82% D).



Diethyl 2-fluoro-2-(2-(4-(methoxycarbonyl)phenyl)ethyl-2-*d*)malonate

92 mg, 90% yield. Colorless oil. $R_f = 0.35$ (petroleum ether/ethyl acetate, 5:1).

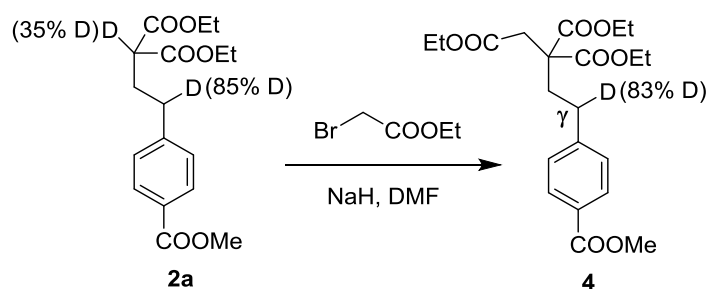
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.97 (d, $J = 8.2$ Hz, 2H), 7.27 (d, $J = 8.2$ Hz, 2H), 4.28 (q, $J = 7.1$ Hz, 4H), 3.90 (s, 3H), 2.81 – 2.75 (m, 1.18H, 82% D), 2.53 – 2.44 (m, 2H), 2.48 – 2.42 (m, 1H), 1.31 (t, $J = 7.1$ Hz, 6H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 166.9, 166.1, 165.8, 145.5, 129.9, 128.49, 128.43, 94.2 (d, $^1J_{\text{CF}} = 199.4$ Hz), 62.7, 52.0, 35.5 (d, $^2J_{\text{CF}} = 21.2$ Hz), 14.0.

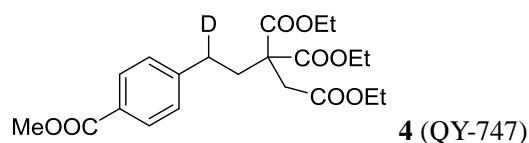
$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -167.4 (s)

IR (KBr) ν 2982, 1749, 1720, 1279, 1195, 1097, 1063, 1020.

HRMS (ESI) m/z : Calcd for $\text{C}_{17}\text{H}_{21}\text{FNaO}_6$ ($[\text{M}+\text{Na}]^+$) 364.1283, found 364.1293.



To a 10 mL Schlenk tube was added NaH (60% w/w in mineral oil) (9.6 mg, 0.24 mmol), 0.5 mL dry DMF and then **2a** (58 μL , 0.2 mmol) under N_2 atmosphere. The reaction mixture was stirred at room temperature for 1 h, then ethyl 2-bromoacetate (27 μL , 0.24 mmol) was added, and 1 mL dry DMF was added to rinse the tube. The mixture was stirred at room temperature overnight, then diluted with water (15 mL), and extracted with EtOAc for three times (3×10 mL). The combined organic extracts were washed with water, then with brine, dried over anhydrous MgSO_4 and concentrated under reduced pressure. The residual was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate, 5:1) to give the product **4** colorless oil (73 mg, 89% yield, γ : 83% D).



Triethyl 4-(4-(methoxycarbonyl)phenyl)butane-1,2,2-tricarboxylate-4-*d*

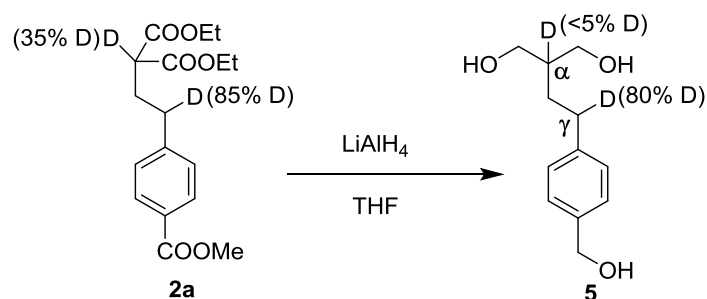
73 mg, 89% yield. Colorless oil. $R_f = 0.31$ (petroleum ether/acetone, 5:1).

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.95 (d, $J = 8.2$ Hz, 2H), 7.24 (d, $J = 8.1$ Hz, 2H), 4.22 (q, $J = 7.1$ Hz, 4H), 4.13 (q, $J = 7.1$ Hz, 1H), 3.90 (s, 3H), 3.04 (s, 2H), 2.66 – 2.58 (m, 1.16H, 84% D), 2.33 – 2.28 (m, 2H), 1.30 – 1.23 (m, 9H).

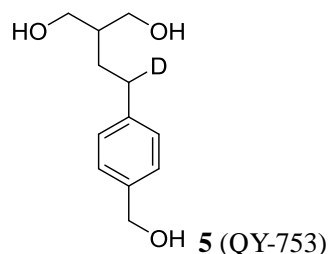
$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 170.17, 170.14, 167.0, 146.5, 129.8, 128.4, 128.2, 61.7, 60.8, 55.5, 52.0, 37.8, 34.6, 31.0, 30.9, 30.7, 30.5, 14.1, 14.0.

IR (KBr) ν 2982, 1725, 1612, 1438, 1370, 1280, 1181, 1106, 760.

HRMS (ESI) m/z : Calcd for $\text{C}_{21}\text{H}_{27}\text{DNaO}_8$ ($[\text{M}+\text{Na}]^+$) 432.1739, found 432.1752.



To a solution of **2a** (58 μL , 0.2 mmol) in dry THF (0.1 M) was added LiAlH_4 (0.6 mL, 1 M solution in THF) dropwise under N_2 atmosphere at 0 $^\circ\text{C}$. Then, the reaction mixture was stirred at room temperature for 5 h. TLC showed that the reduction reaction was complete. The reaction mixture was quenched with water, and the 0.5 M HCl was added to adjust the pH to 5~7. The solvents were evaporated under reduced pressure, then diluted with EtOAc, dried over anhydrous Na_2SO_4 , filtered, and concentrated under reduced pressure. The residue was purified by column chromatography (dichloromethane/methanol, 15:1 – 10:1) to give **5** as white solid (35 mg, 83% yield, γ : 80% D).

**2-(2-(4-(hydroxymethyl)phenyl)ethyl-2-*d*)propane-1,3-diol**

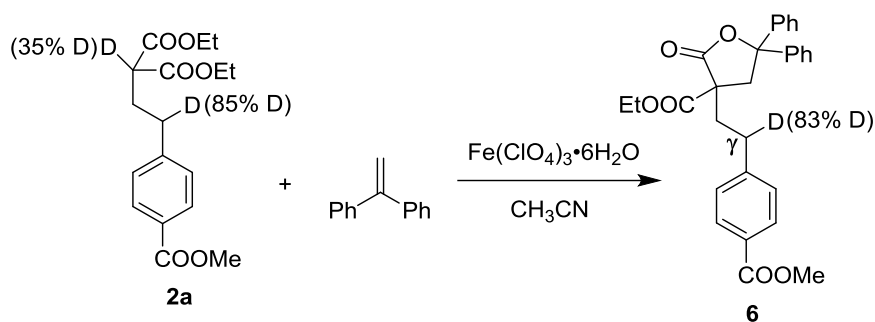
35 mg, 83% yield. White solid, m.p. 67-68 $^\circ\text{C}$. $R_f = 0.11$ (dichloromethane/methanol, 20:1).

¹H NMR (400 MHz, Acetone-*d*₆) δ 7.25 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 4.58 (d, *J* = 3.5 Hz, 2H), 4.24 – 4.21 (m, 1H), 3.78 (br, 2H), 3.63 (br, 4H), 2.68 – 2.62 (m, 1.20H, 80% D), 1.68 – 1.60 (m, 3H).

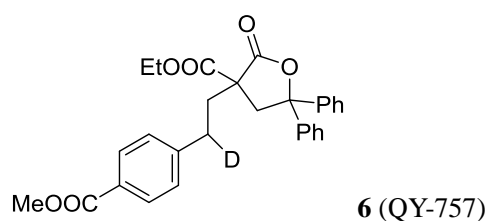
¹³C NMR (101 MHz, Acetone-*d*₆) δ 141.4, 139.7, 128.1, 126.7, 63.7, 63.4, 63.3, 42.6, 32.9, 32.7, 32.5, 32.3.

IR (KBr) ν 3356, 2920, 2852, 1657, 1632, 1468, 1420, 1033.

HRMS (APCI) *m/z*: Calcd for C₁₂H₁₇DNaO₃ ([M+Na]⁺) 234.1211, found 234.1222.



To a 10 mL Schlenk tube was added Fe(ClO₄)₃·6H₂O (192.0 mg, 0.4 mmol), **2a** (58 μL, 0.2 mmol) and ethene-1,1-diyldibenzene (192.0 mg, 0.22 mmol), 3mL dry CH₃CN under N₂ atmosphere. The reaction mixture was stirred at room temperature for 6 h. The solvent was evaporated under reduced pressure, the residual was then diluted with water, and extracted with DCM for three times. The combined organic extracts were dried over anhydrous MgSO₄ and concentrated under reduced pressure. The residual was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate, 5:1) to give the product **6** colorless oil (72 mg, 76% yield, γ: 83% D).



2-(2-(4-(hydroxymethyl)phenyl)ethyl-2-*d*)propane-1,3-diol

72 mg, 76% yield. Colorless wax. R_f = 0.26 (petroleum ether/acetone, 5:1).

¹H NMR (400 MHz, CDCl₃) δ 7.91 (d, *J* = 8.2 Hz, 2H), 7.48 – 7.46 (m, 2H), 7.42 – 7.40 (m, 2H), 7.36 – 7.31 (m, 4H), 7.28 – 7.25 (m, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 3.91 – 3.83 (m, 4H), 3.77 – 3.68 (m, 2H), 2.91 – 2.85 (m, 1.59H, 41% D), 2.64 – 2.57 (m, 0.60H, 40% D), 2.24 – 2.17 (m, 1H), 2.10 – 2.04 (m, 1H), 1.00 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (101 MHz, CDCl₃) δ 173.2, 169.5, 167.0, 146.0, 143.9, 142.3, 129.8, 128.7, 128.46, 128.41, 128.3, 128.0, 127.9, 125.6, 124.9, 87.2, 62.2, 55.5, 52.0, 45.0, 36.5, 36.4, 31.0, 30.8, 30.6, 30.4, 13.6.

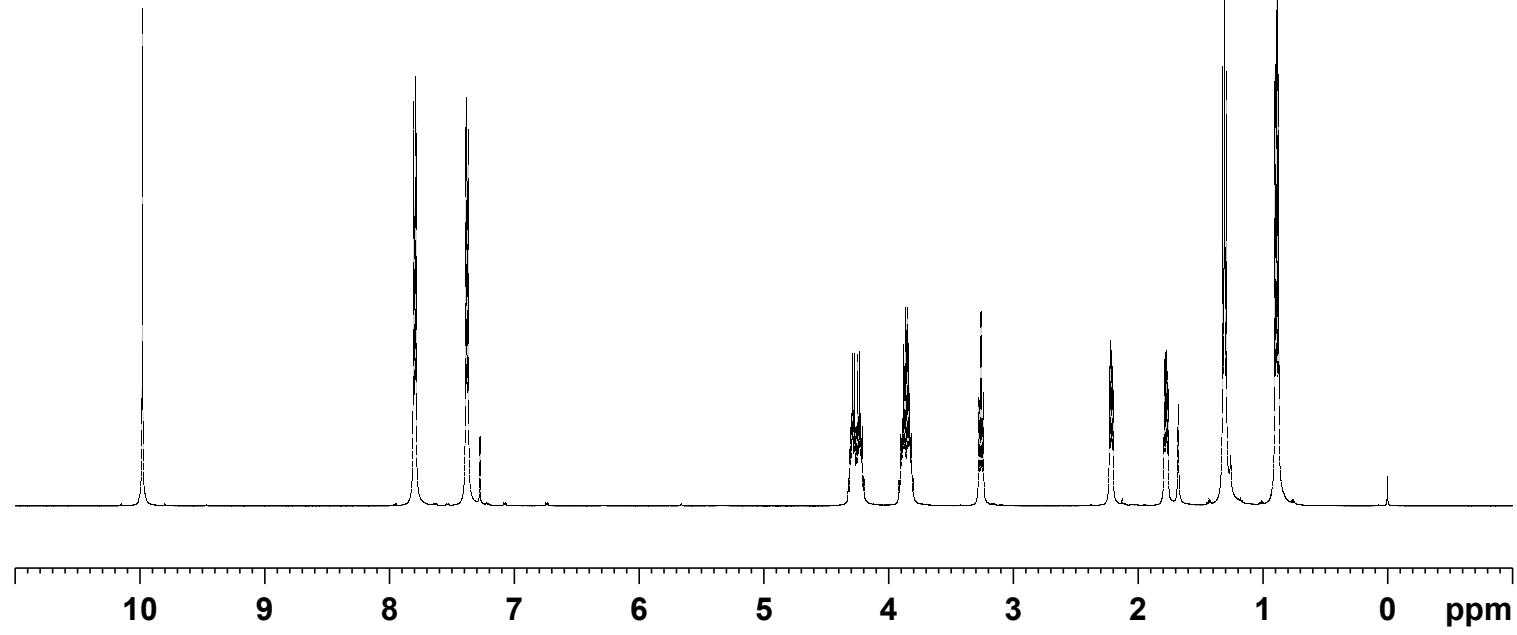
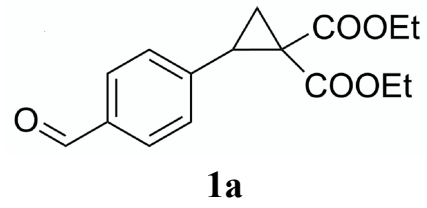
IR (KBr) ν 2954, 1781, 1718, 1612, 1450, 1281, 1110, 1022 974, 757, 702.

HRMS (APCI) m/z : Calcd for $C_{29}H_{27}DNaO_6$ ($[M+Na]^+$) 496.1846, found 496.1856.

7. References

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- 2 T. Chidley, I. Jameel, S. Rizwan, P. A. Peixoto, L. Pouysegou, S. Quideau, W. S. Hopkins and G. K. Murphy, *Angew. Chem. Int. Ed.*, 2019, **58**, 16959.
- 3 P. Qian, B. Du, R. Song, X. Wu, H. Mei, J. Han and Y. Pan, *J. Org. Chem.*, 2016, **81**, 6546.
- 4 K. Usami, Y. Nagasawa, E. Yamaguchi, N. Tada and A. Itoh, *Org. Lett.*, 2016, **18**, 8.
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9.978
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7.385
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4.257
4.246
4.231
4.224
4.210
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3.887
3.880
3.865
3.850
3.836
3.829
3.822
3.814
3.274
3.257
3.240
2.228
2.217
2.212
2.201
1.789
1.778
1.770
1.760
1.320
1.306
1.291
0.901
0.886
0.872



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2.00
2.00
2.06
2.04
1.01
1.05
1.02
3.47
3.27

Current Data Parameters
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 EXPNO 97
 PROCNO 1

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 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

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 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
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 PCPD2 0 usec
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 PLW13 0 W

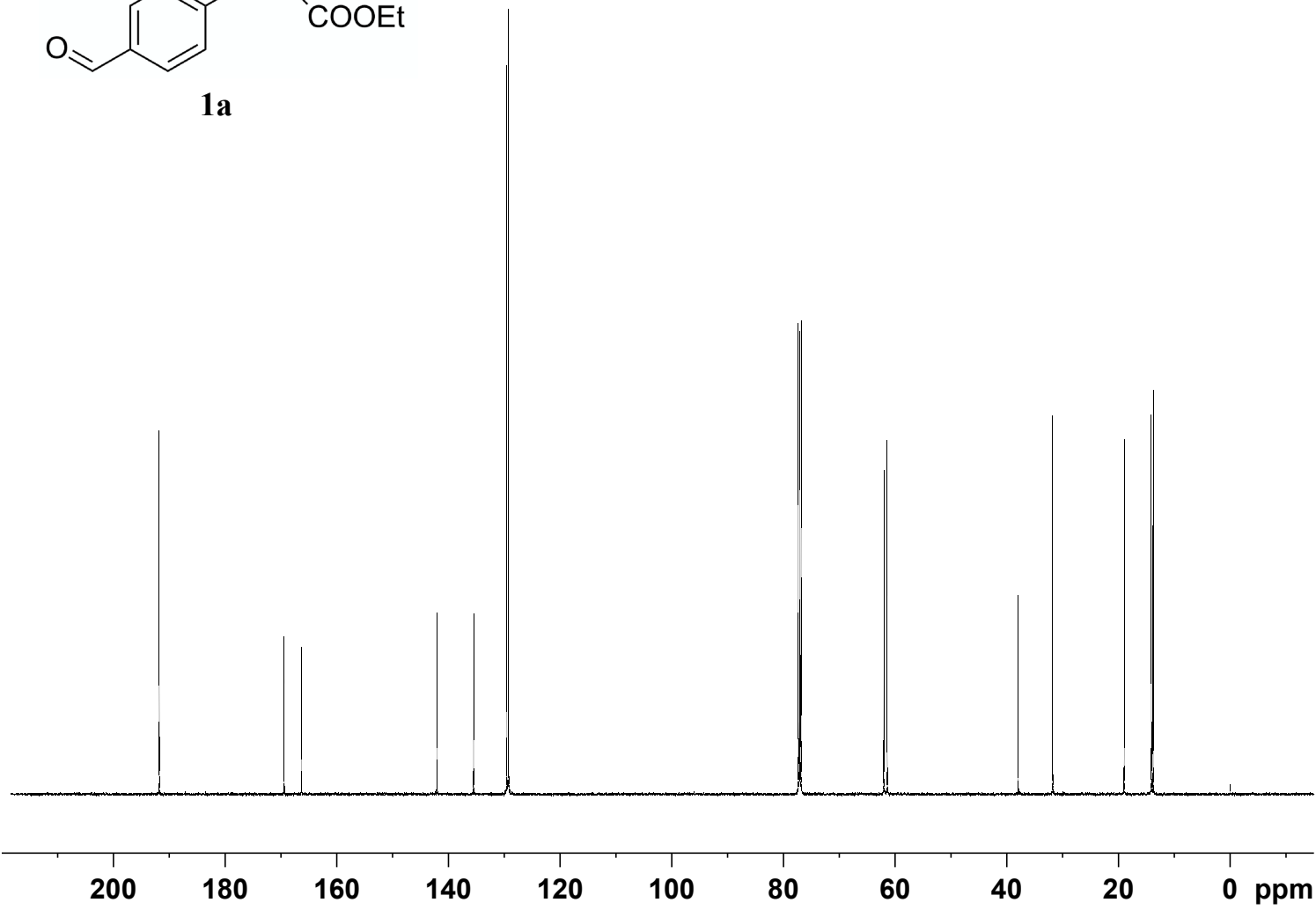
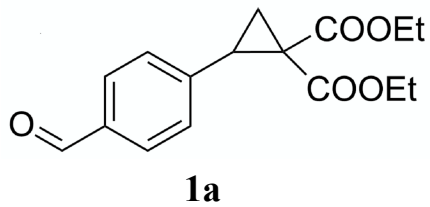
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 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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 — 166.27
 — 142.04
 — 135.46
 — 129.52
 — 129.20

— 61.97
 — 61.38

— 37.91
 — 31.76

— 18.91
 — 14.08
 — 13.74



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 134
 PROCNO 1

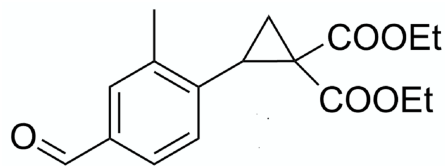
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 Time 9.24
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 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
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 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

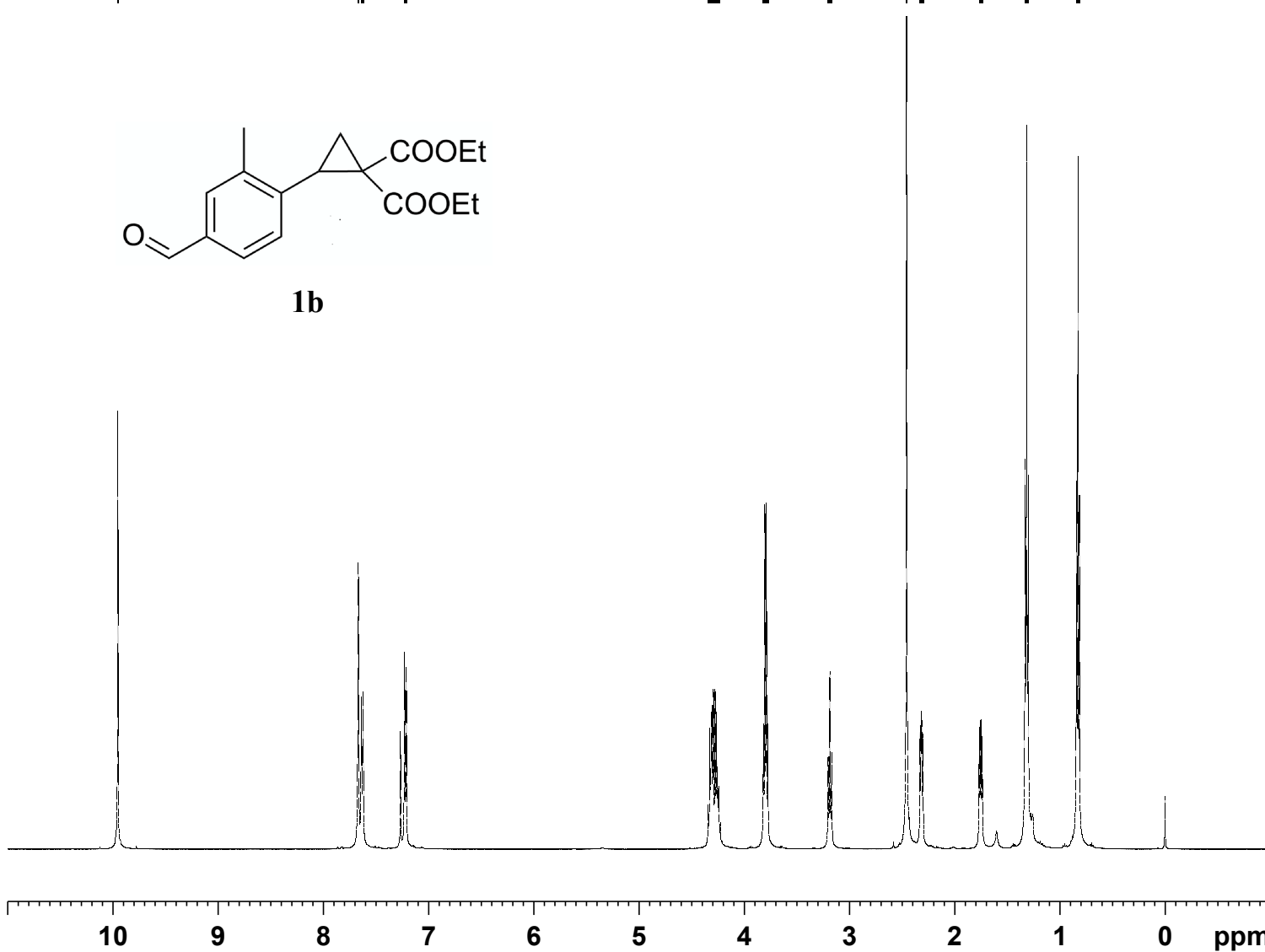
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 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
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 SF 125.7577869 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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3.168
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2.328
2.317
2.312
2.301
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1.755
1.747
1.737
1.329
1.314
1.300
0.842
0.828
0.814



1b



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0.99
3.06
1.12
1.02
3.68
3.14

Current Data Parameters
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 EXPNO 17
 PROCNO 1

F2 - Acquisition Parameters
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 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 55.37
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
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 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

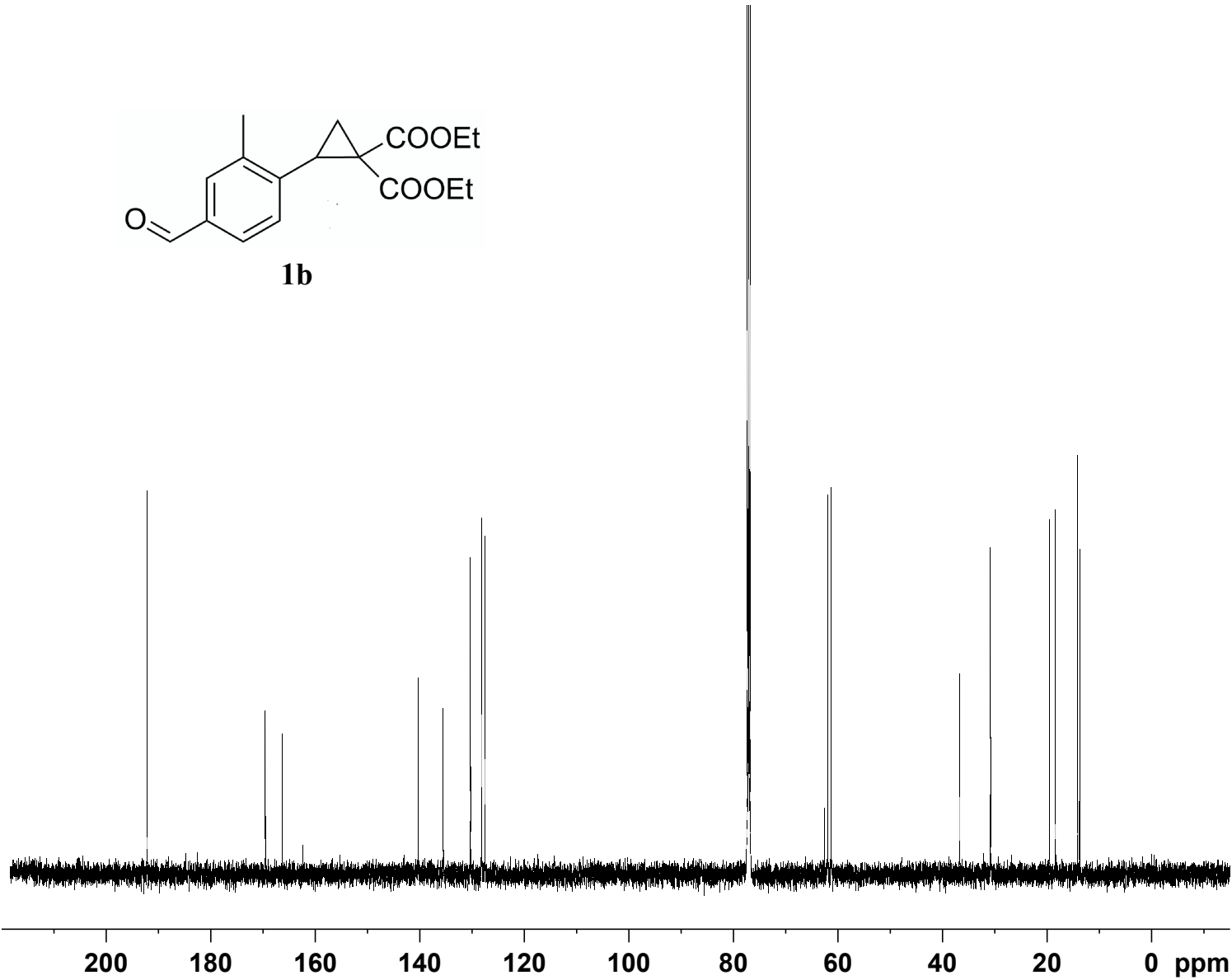
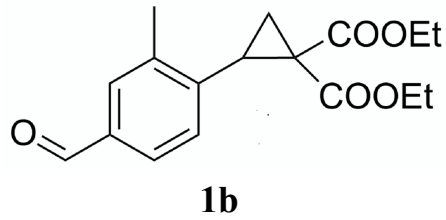
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 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 192.10
 — 169.50
 — 166.31
 — 140.29
 — 140.26
 — 135.55
 — 130.26
 — 128.09
 — 127.49

— 61.91
 — 61.27

— 36.67
 — 30.75
 — 19.46
 — 18.33
 — 14.12
 — 13.64



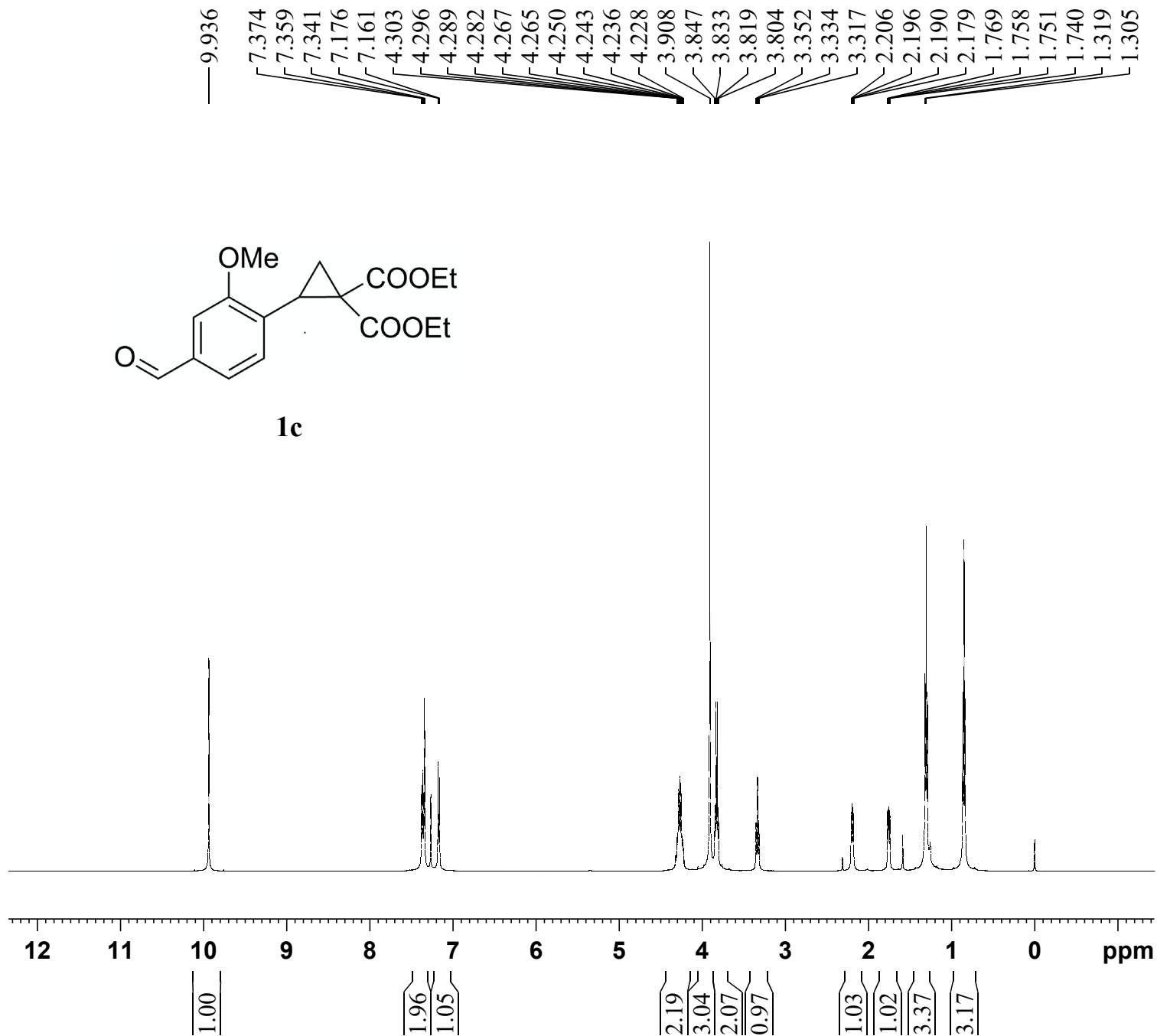
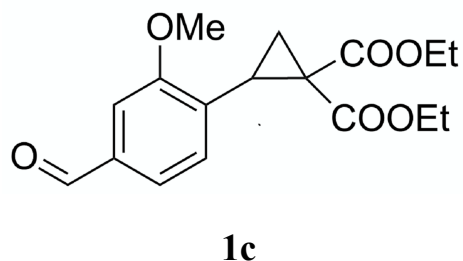
Current Data Parameters
 NAME 500M-2022
 EXPNO 18
 PROCNO 1

F2 - Acquisition Parameters
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 Time 6.22
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 50
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 243
 PROCNO 1

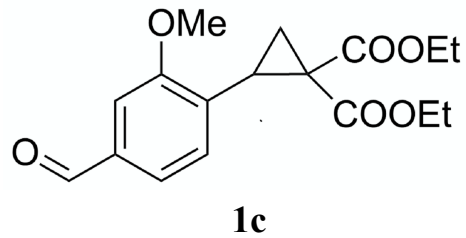
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 Date_ 20220208
 Time 23.27
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

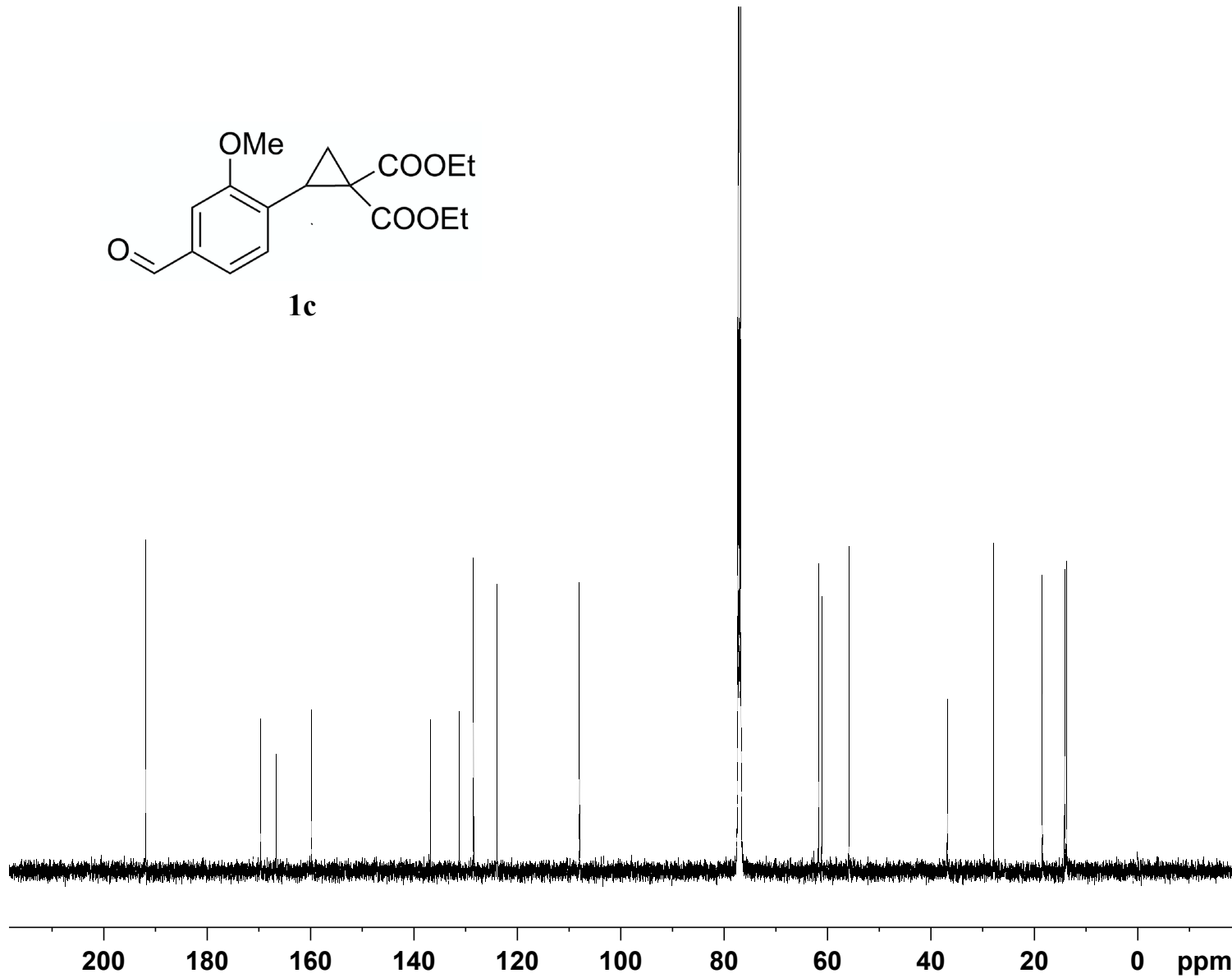
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 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 191.83
 \ 169.62
 \ 166.64
 — 159.77
 \ 136.82
 \ 131.17
 \ 128.43
 \ 123.87
 — 107.95



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 \ 55.84
 — 36.80
 — 27.85
 \ 18.42
 \ 14.11
 \ 13.75



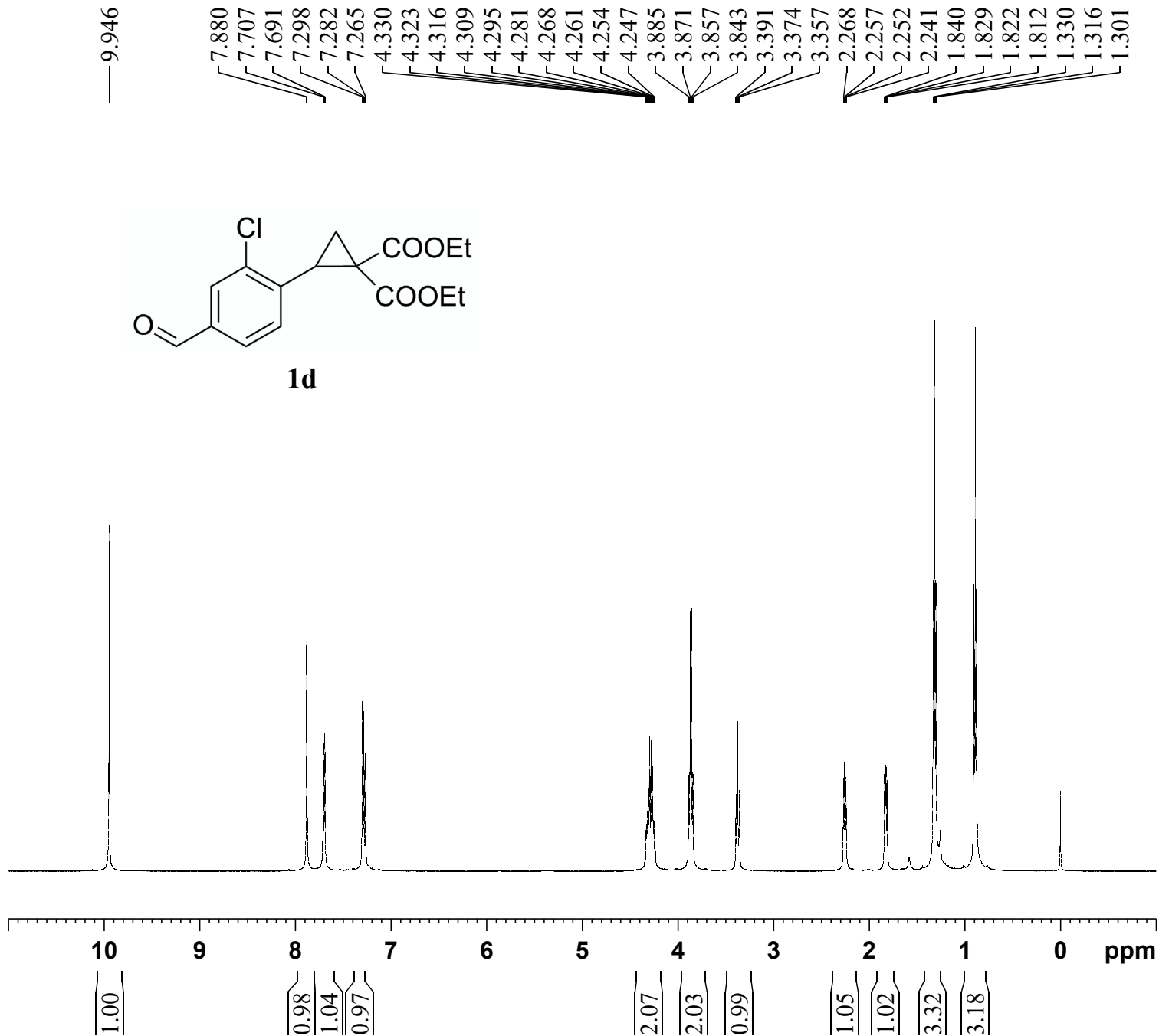
Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
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 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



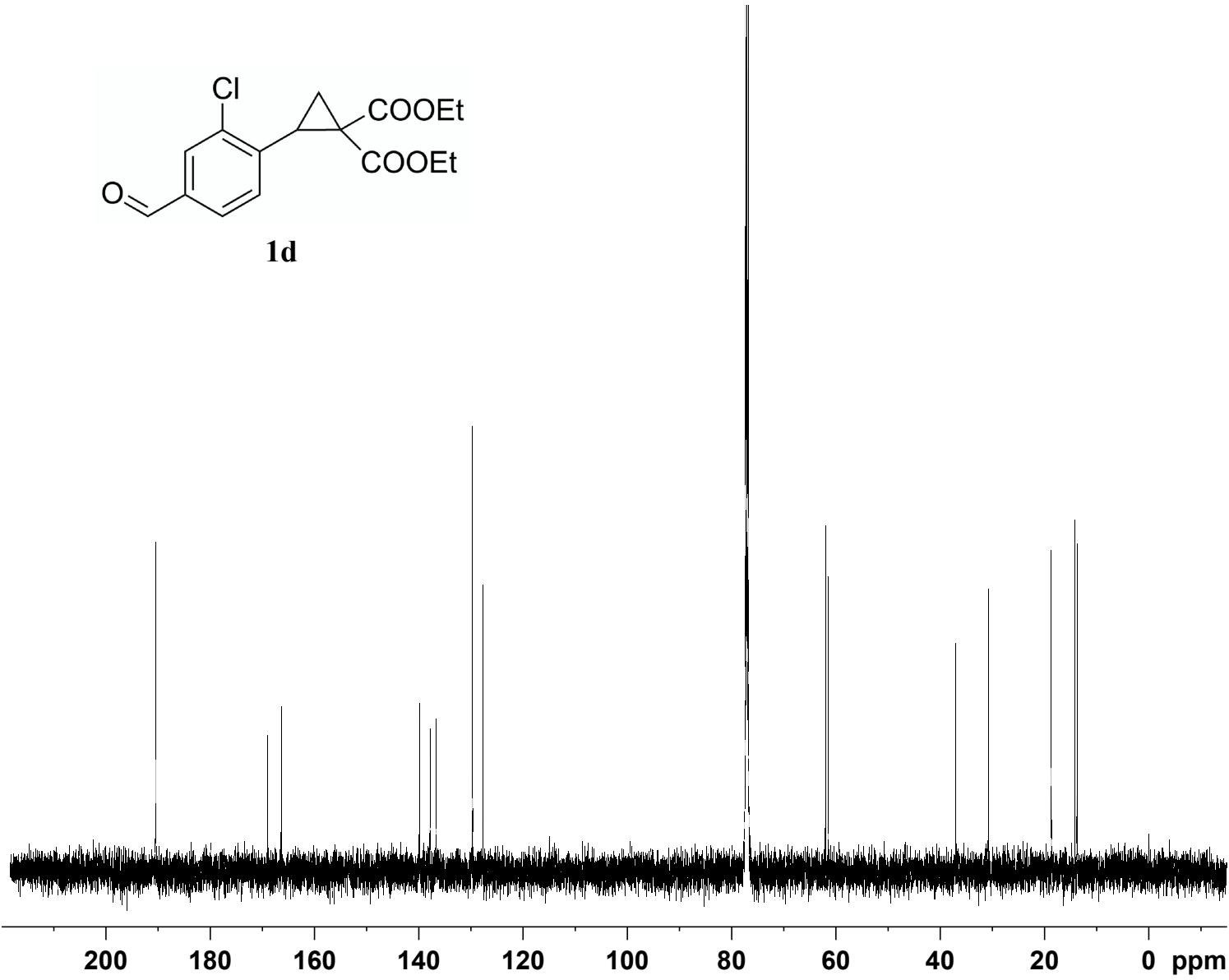
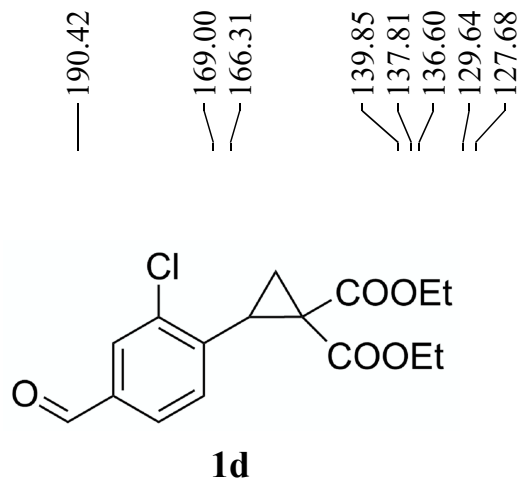
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 PROCNO 1

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 INSTRUM spect
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300100 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



$\text{---} 61.94$
 $\text{---} 61.41$
 $\text{---} 36.92$
 $\text{---} 30.71$
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Current Data Parameters
 NAME 500M-2020xia
 EXPNO 237
 PROCNO 1

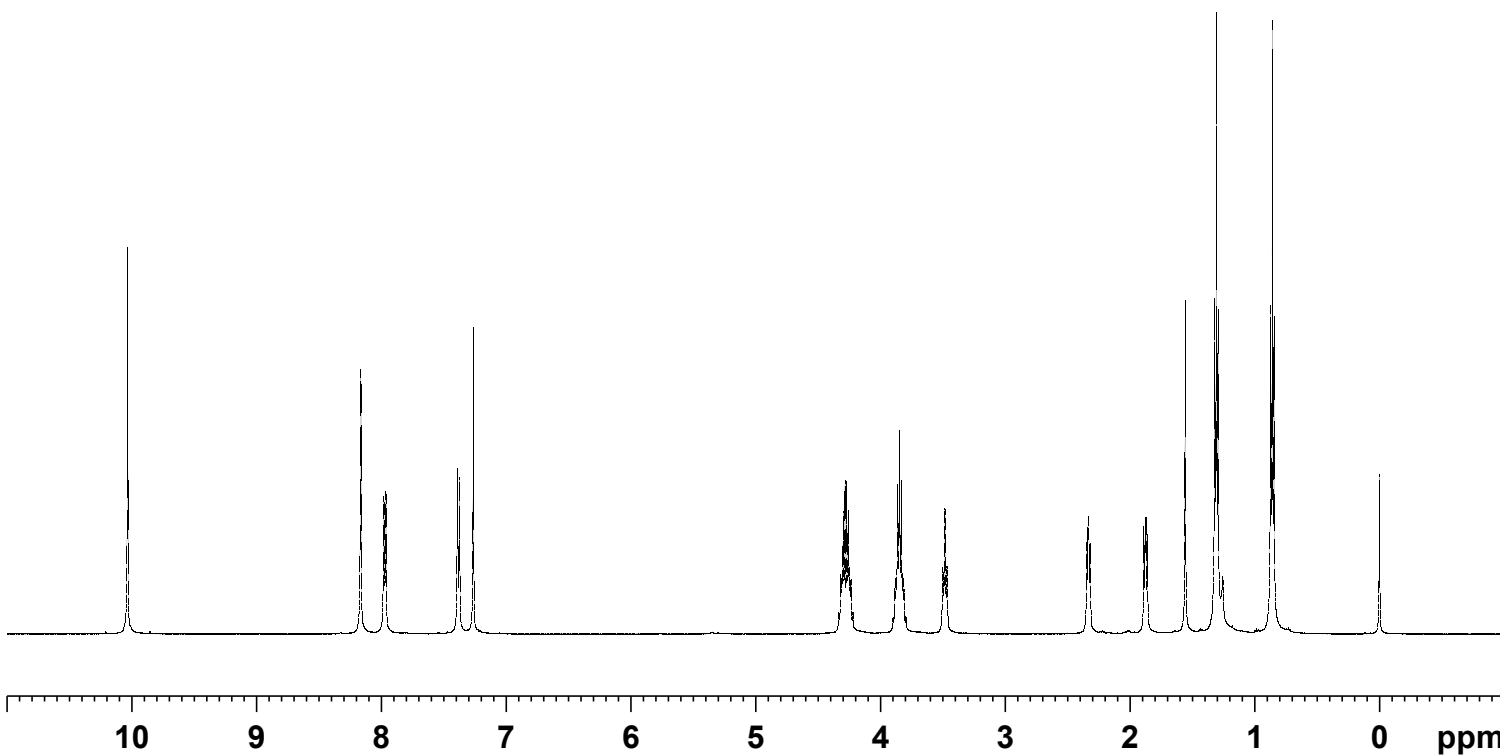
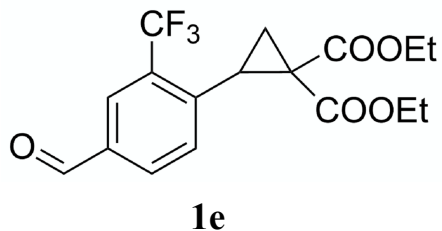
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 SOLVENT CDCl3
 NS 100
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
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 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

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4.241
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3.884
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3.862
3.846
3.832
3.824
3.817
3.499
3.482
3.465
2.345
2.333
2.330
2.318
1.888
1.877
1.870
1.859
1.321
1.307
1.292
0.872
0.858
0.844



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1.01
1.01
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1.00
1.03
1.03
3.31
3.26

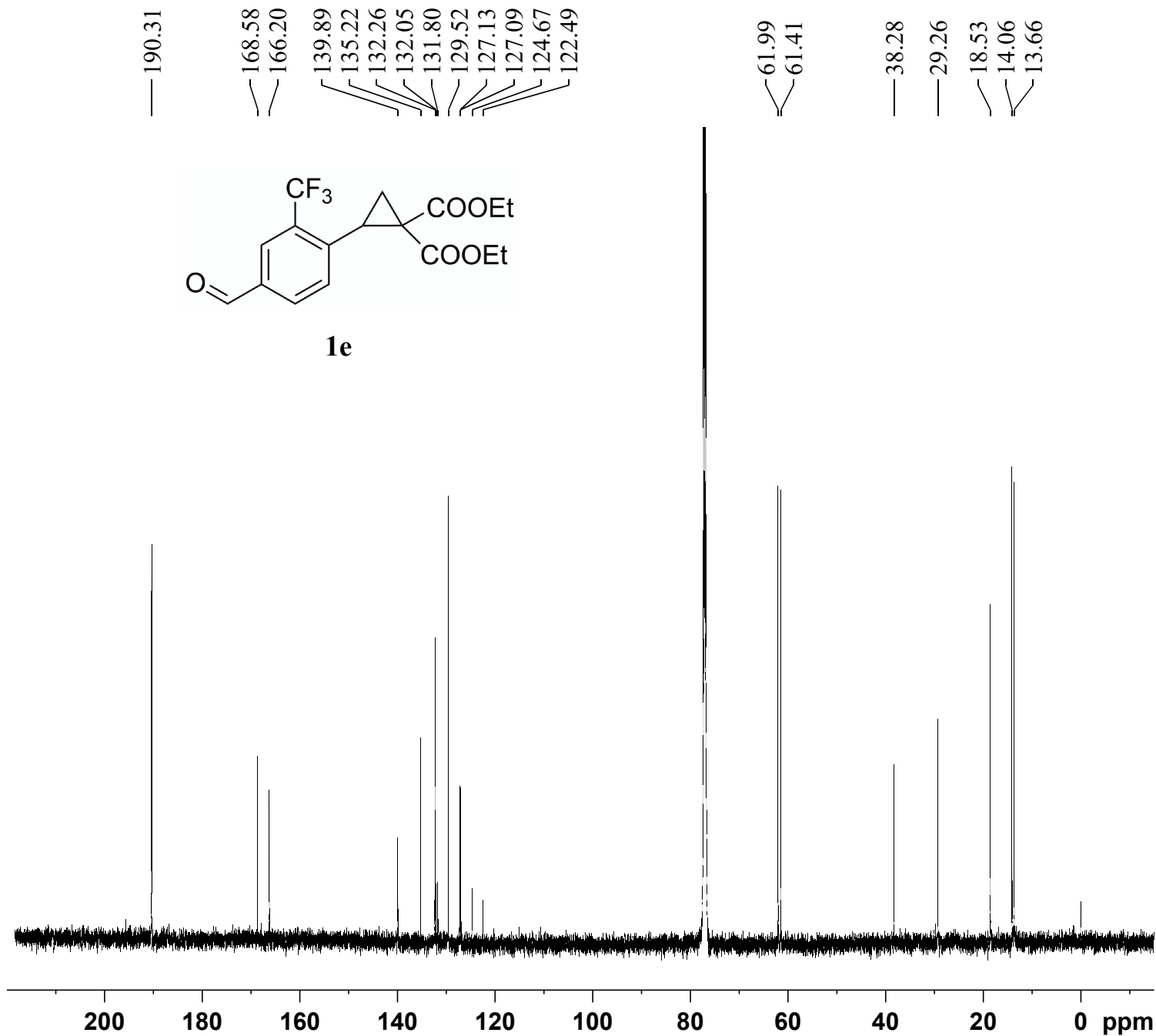
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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 62.06
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

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NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
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NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



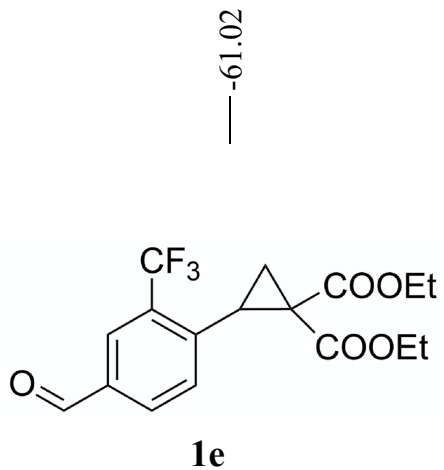
Current Data Parameters
 NAME 500M-2022
 EXPNO 56
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220321
 Time 5.30
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



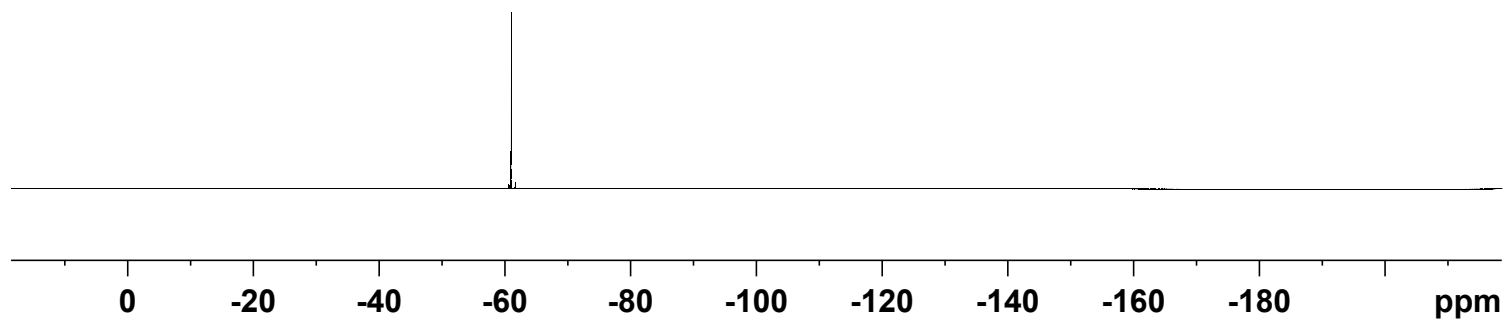
Current Data Parameters
 NAME 400M-2023-F
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230506
 Time 19.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 206.33
 DW 5.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

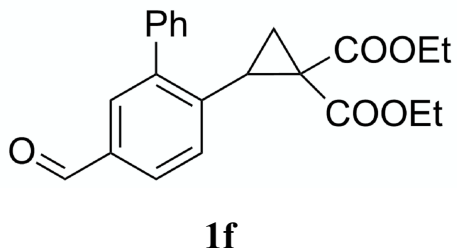
==== CHANNEL f1 =====
 SFO1 376.5642094 MHz
 NUC1 19F
 P1 14.50 usec
 PLW1 17.98900032 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 65536
 SF 376.6018696 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



10.017
7.792
7.778
7.466
7.451
7.435
7.422
7.406
7.396
7.382
7.228
7.212
4.198
4.184
4.177
4.162
4.147
4.133
4.126
4.112
3.942
3.928
3.913
3.899
3.047
3.030
3.013
2.237
2.226
2.220
2.209
1.732
1.721
1.714
1.702
1.235
1.221
1.207
0.914
0.900
0.885



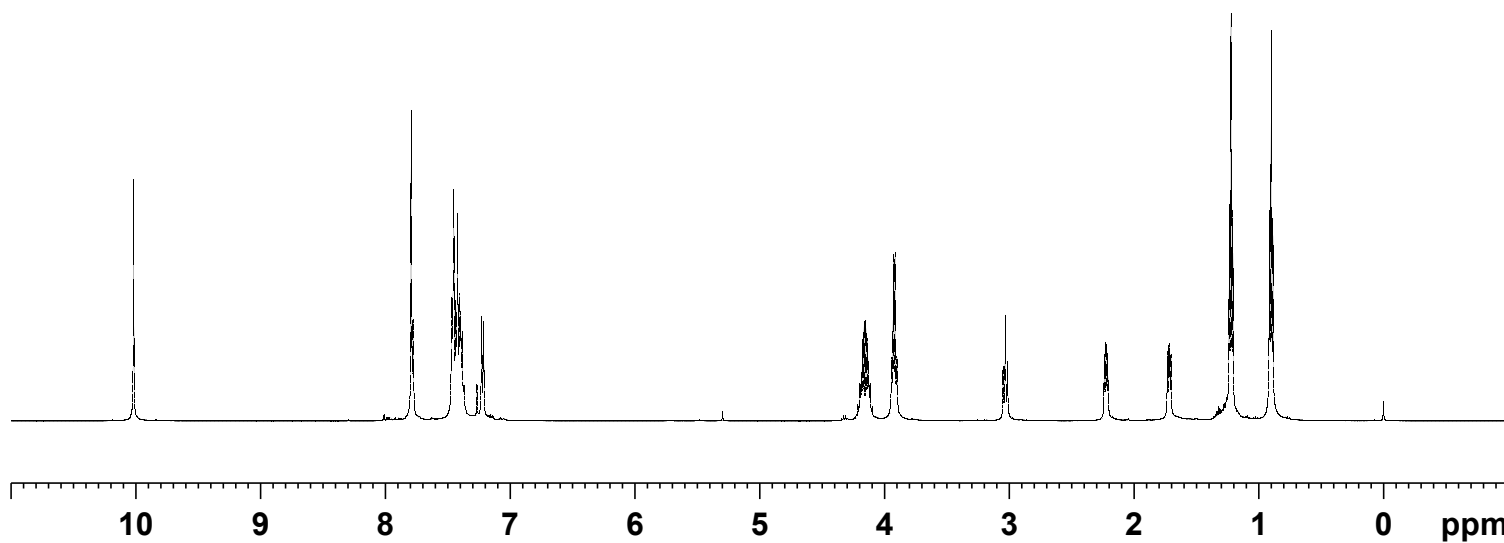
Current Data Parameters
NAME 500M-2022
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220315
Time 10.29
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



0.94

1.91
5.03
1.04

2.07
2.13

1.00

1.05

1.16

3.54

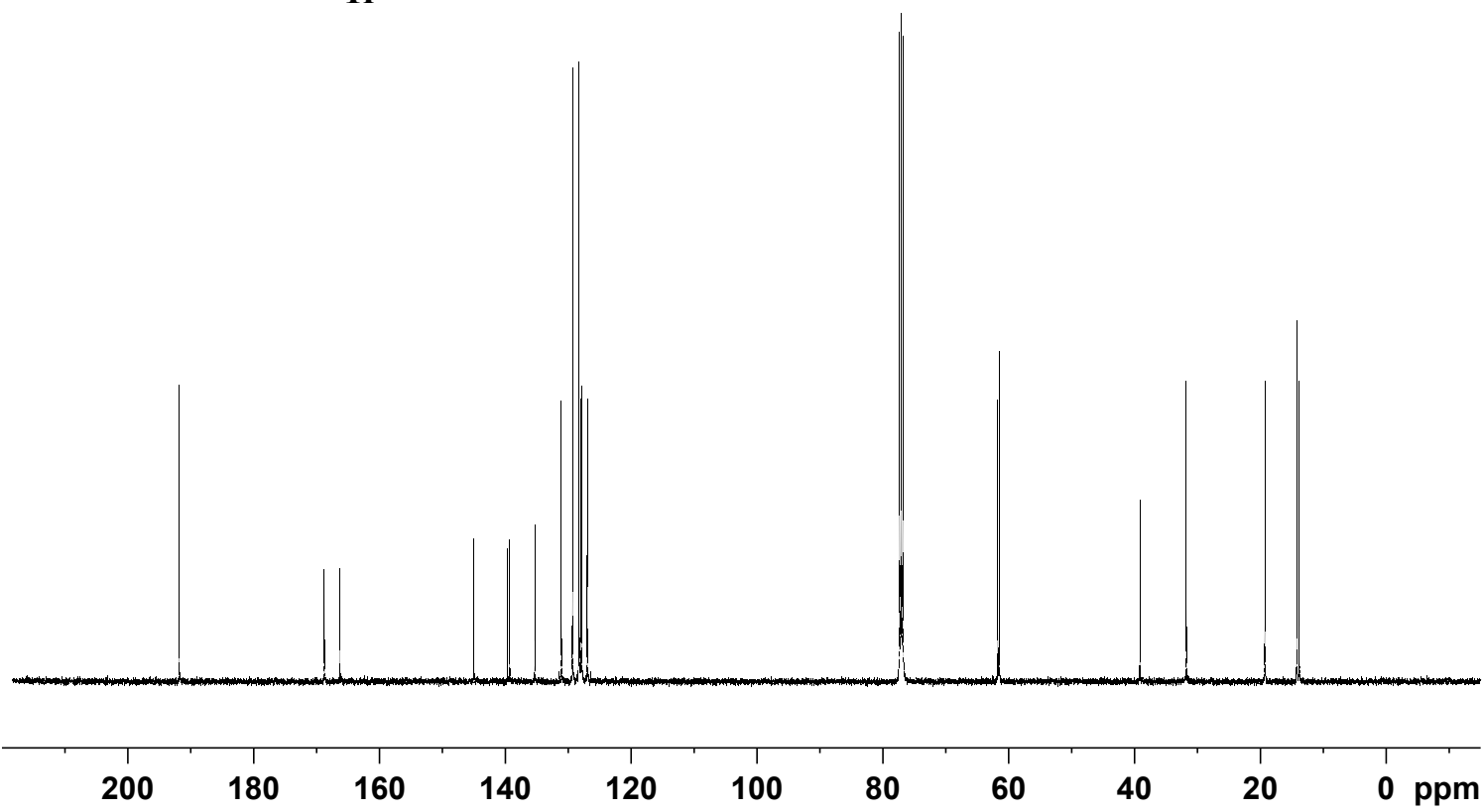
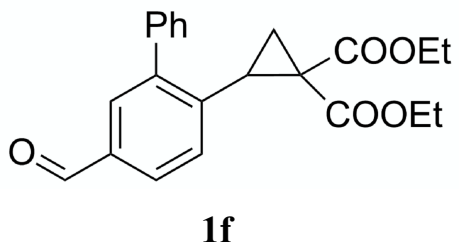
3.20

— 191.80
 { 168.71
 { 166.25
 { 144.94
 { 139.59
 { 139.27
 { 135.27
 { 131.06
 { 129.27
 { 128.29
 { 128.01
 { 127.80
 { 126.91

{ 61.68
 { 61.44

— 39.07
 — 31.73

{ 19.22
 { 14.14
 { 13.75



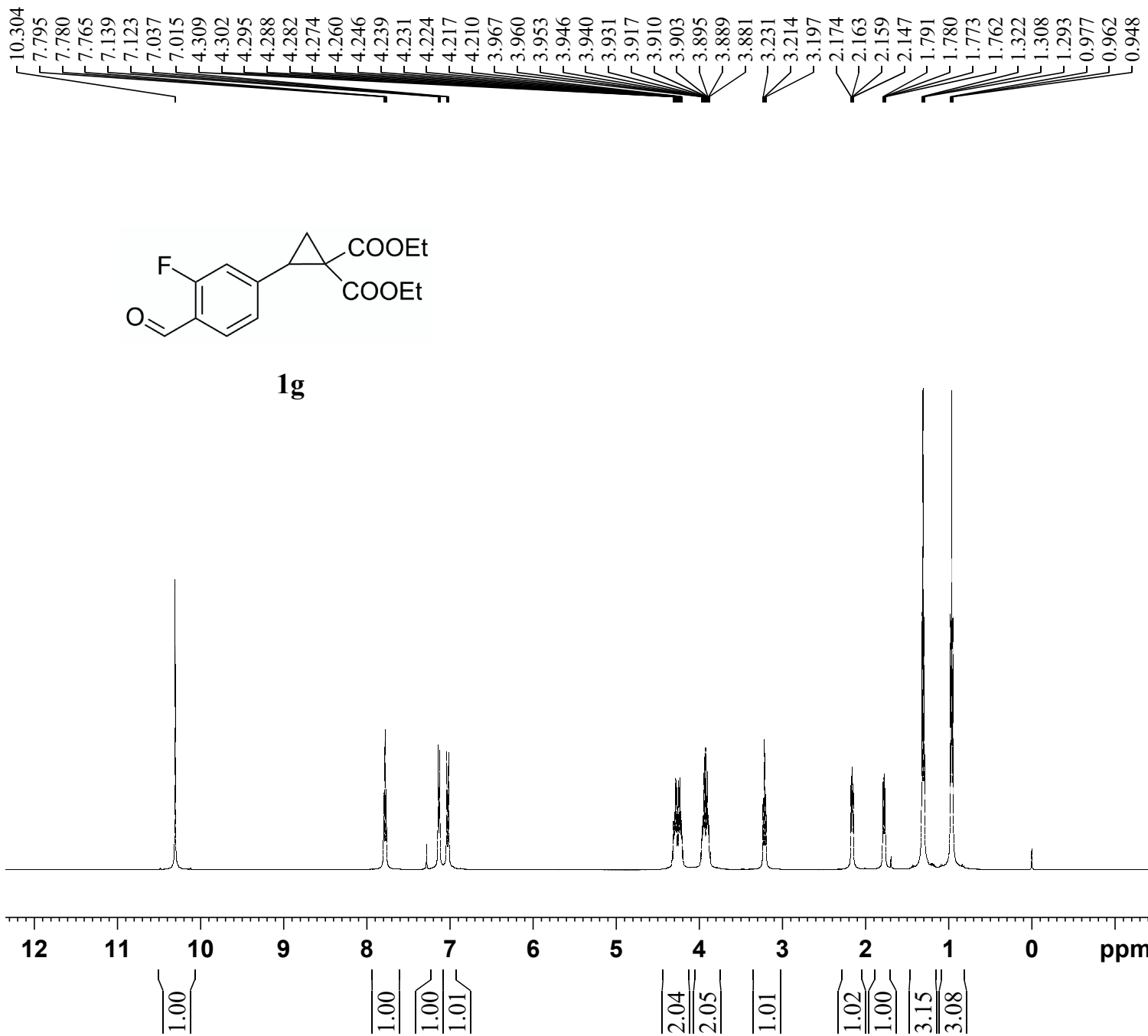
Current Data Parameters
 NAME 500M-2022
 EXPNO 37
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220315
 Time 5.50
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



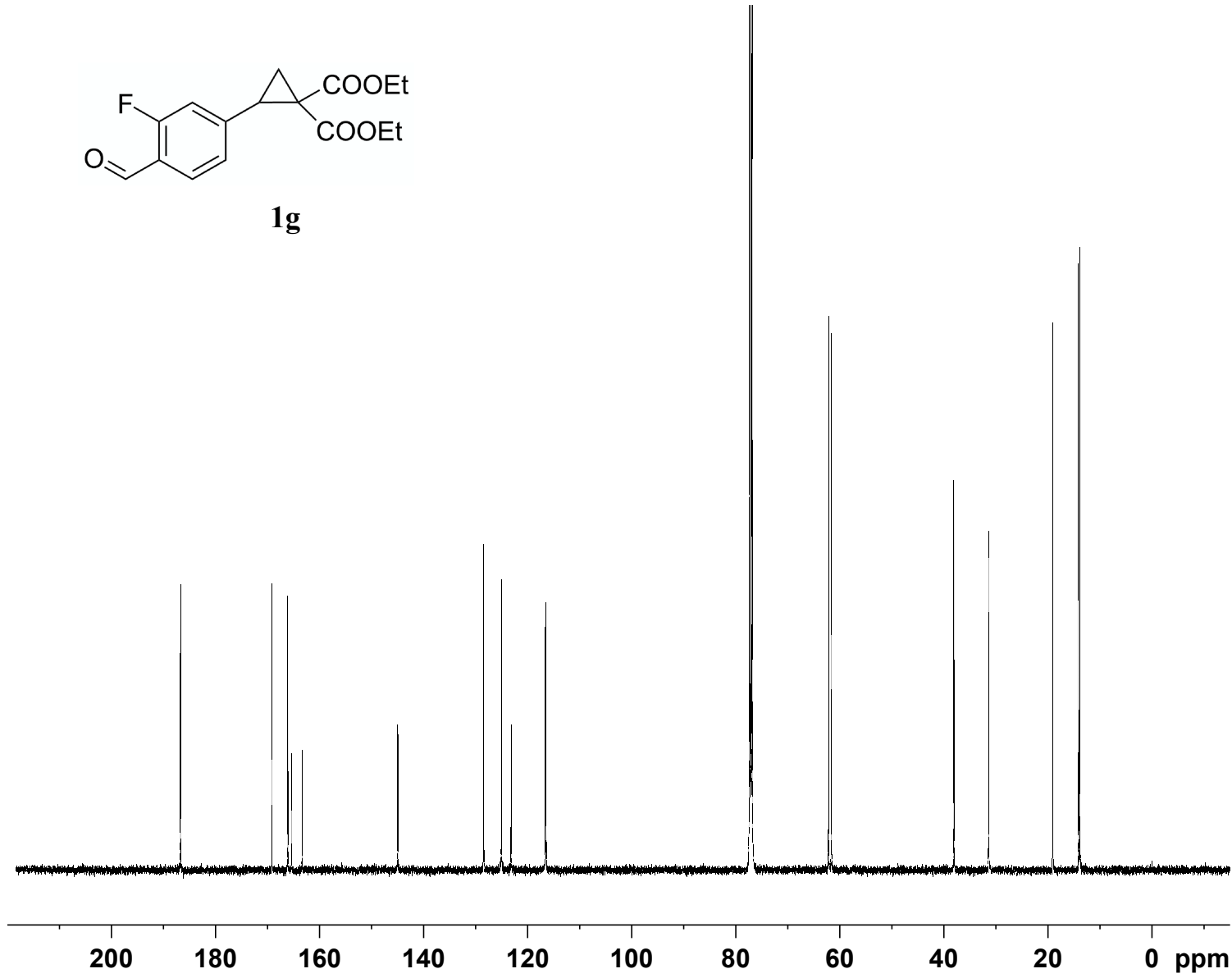
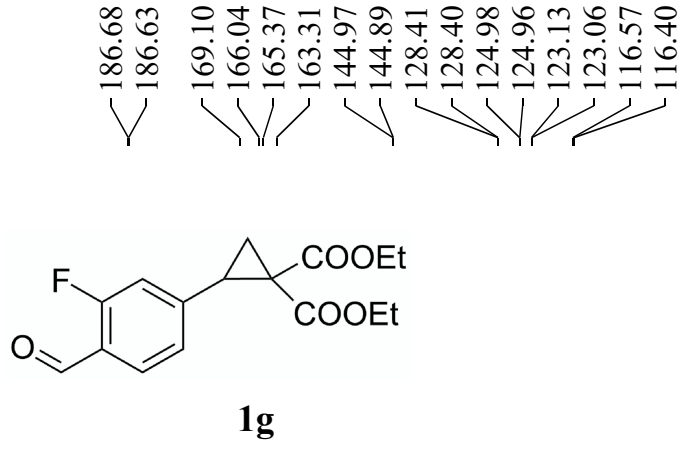
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 239
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220208
 Time 22.23
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300022 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



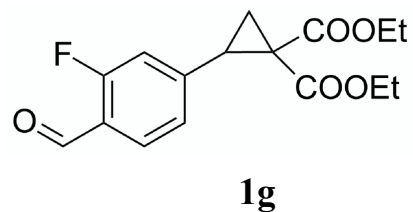
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 240
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220208
 Time 22.51
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

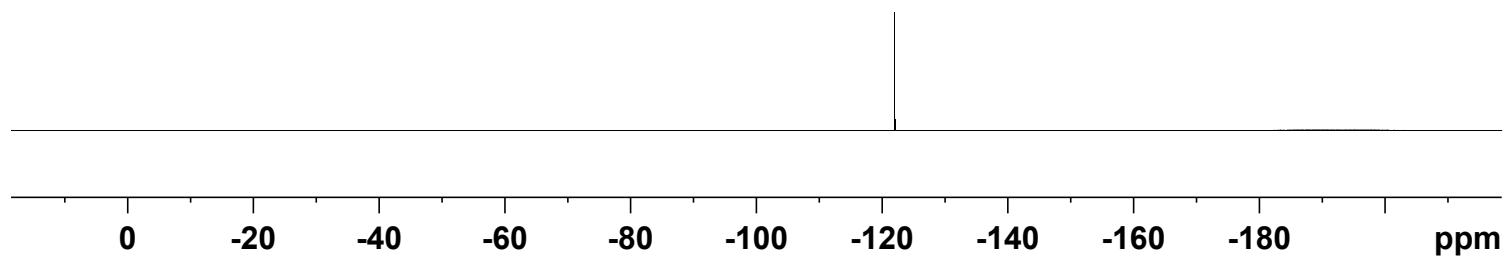
==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



— -122.06



Current Data Parameters
 NAME 400M-2023-F
 EXPNO 9
 PROCNO 1

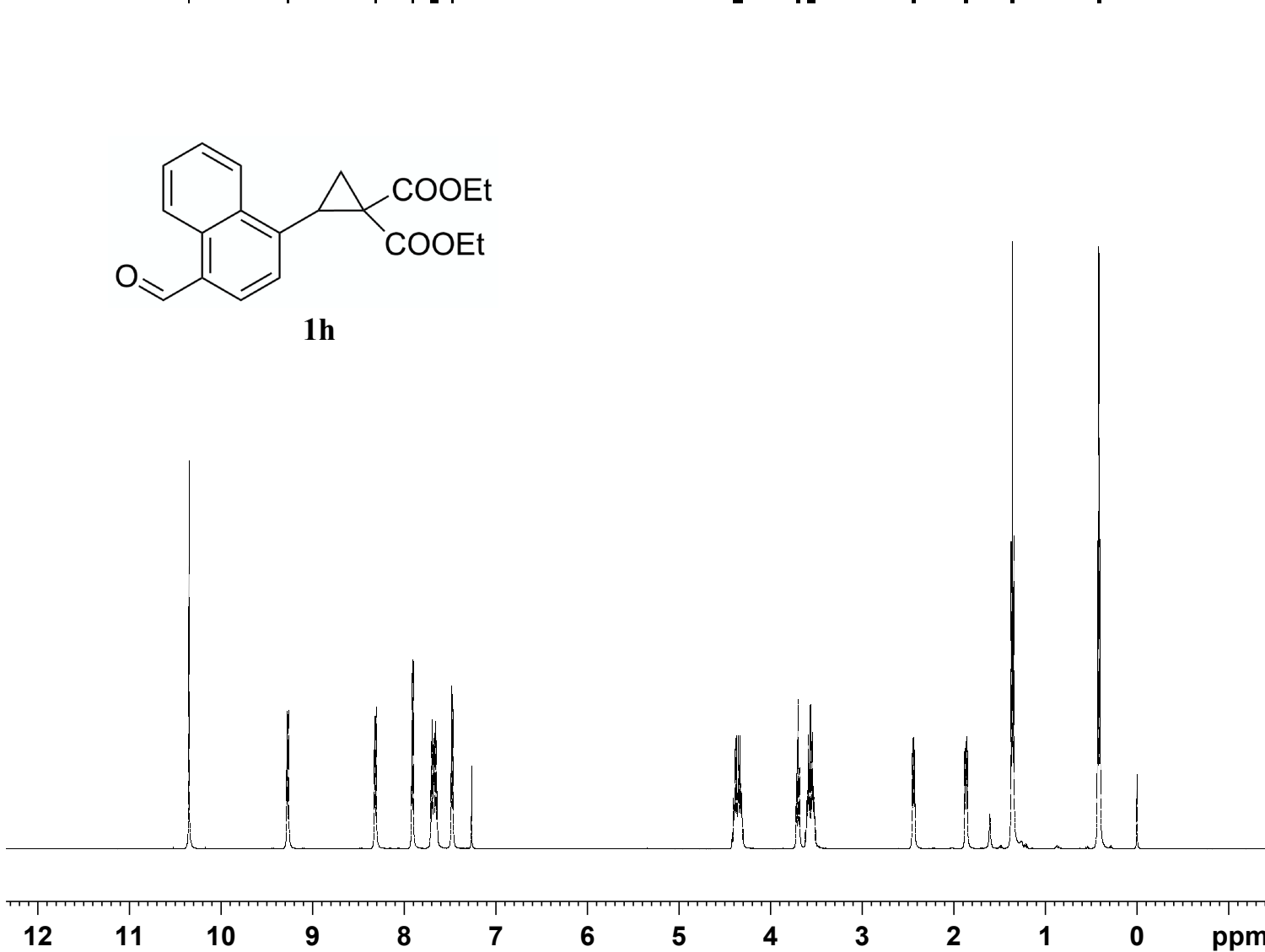
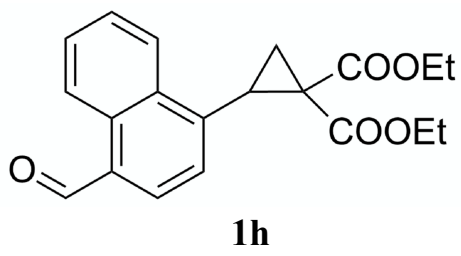
F2 - Acquisition Parameters
 Date_ 20230506
 Time 19.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT CDC13
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 206.33
 DW 5.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 376.5642094 MHz
 NUC1 19F
 P1 14.50 usec
 PLW1 17.98900032 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 65536
 SF 376.6018696 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10.348
9.277
9.261
8.321
8.304
7.915
7.901
7.712
7.709
7.695
7.681
7.679
7.671
7.668
7.654
7.653
7.641
7.639
7.483
7.469
4.404
4.390
4.383
4.368
4.362
4.354
4.348
4.333
4.326
4.312
3.717
3.700
3.683
3.593
3.585
3.571
3.556
3.542
3.535
3.528
3.520
2.452
2.441
2.436
2.425
1.878
1.868
1.860
1.850
1.373
1.358
1.344
0.429
0.415
0.401



1.00
0.98
1.00
1.01
2.01
1.02
2.02
0.99
2.04
1.01
1.01
3.19
3.03

Current Data Parameters
NAME 500M-2022
EXPNO 101
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220608
Time 20.47
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

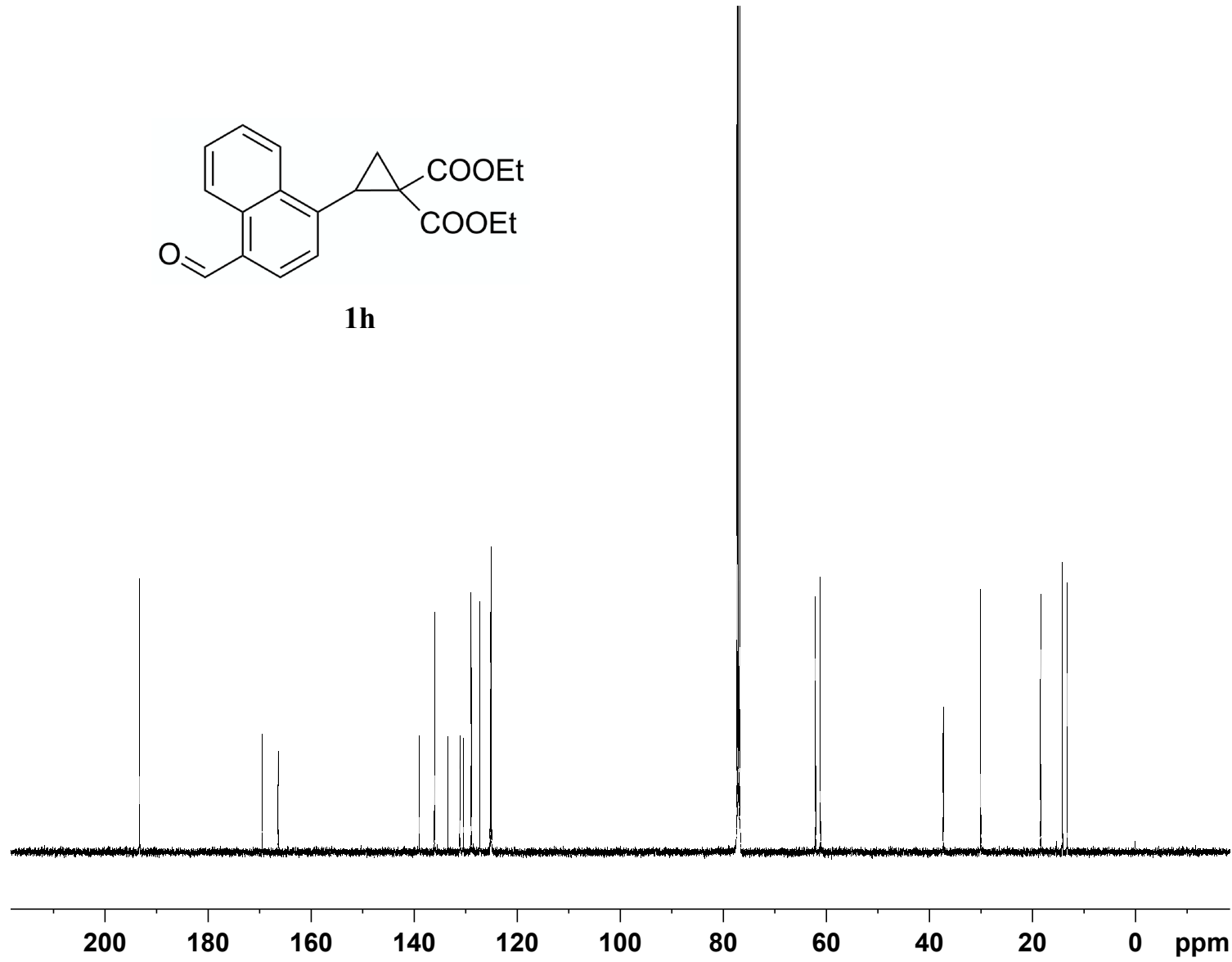
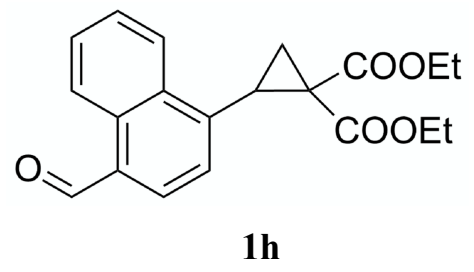
==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

— 193.28
 — 169.49
 — 166.37
 — 138.98
 — 136.00
 — 133.42
 — 131.10
 — 130.38
 — 128.90
 — 127.22
 — 125.20
 — 125.00
 — 124.96

— 62.08
 — 61.12
 — 37.29
 — 30.01
 — 18.37
 — 14.14
 — 13.21



Current Data Parameters
 NAME 500M-2022
 EXPNO 20
 PROCNO 1

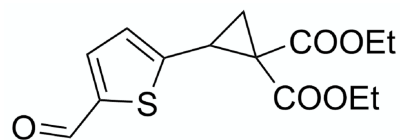
 F2 - Acquisition Parameters
 Date_ 20220226
 Time 6.41
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

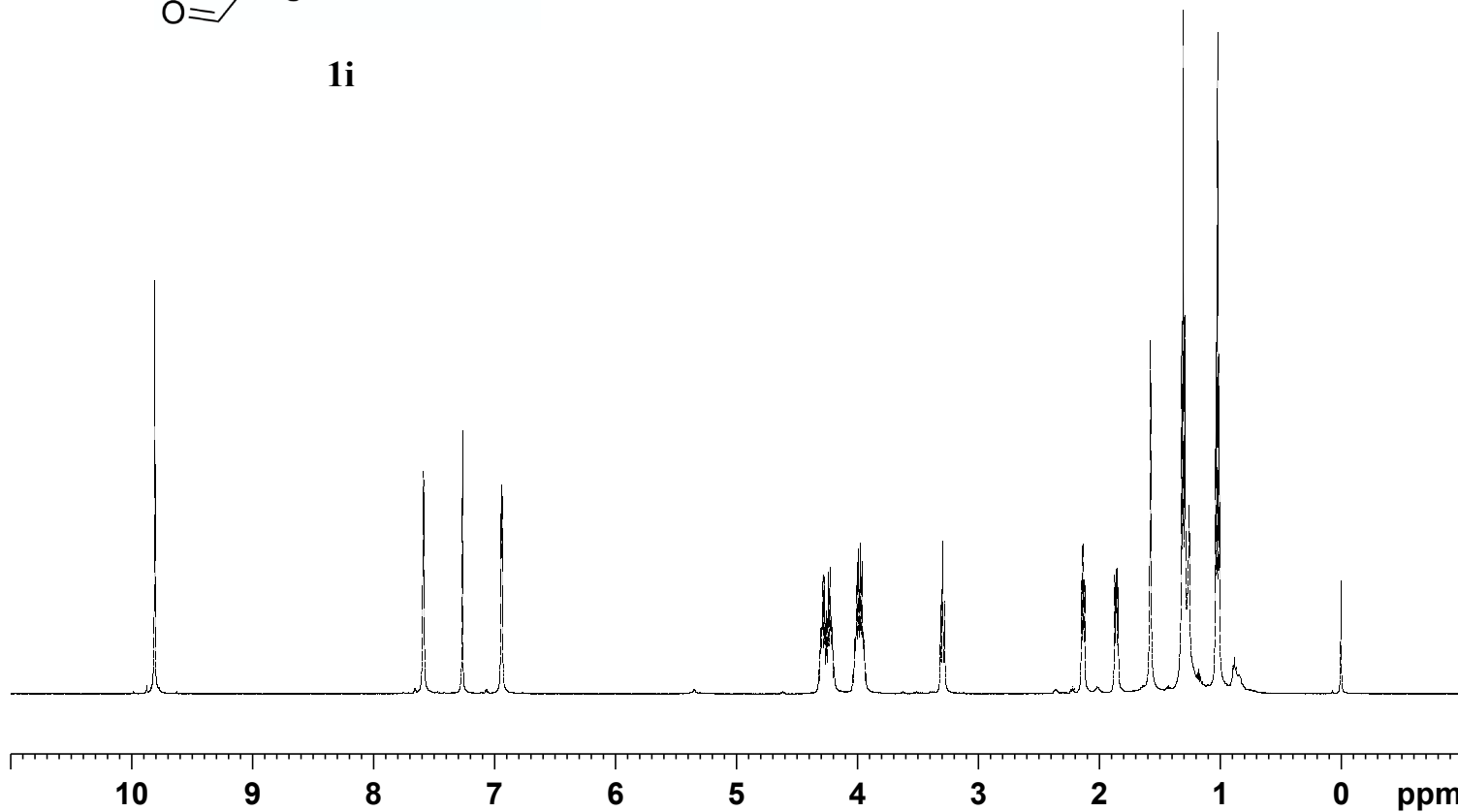
===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

9.808
7.590
7.582
6.943
6.935
4.304
4.297
4.290
4.283
4.276
4.269
4.254
4.240
4.226
4.218
4.211
4.204
4.190
4.023
4.016
4.009
4.001
3.987
3.976
3.962
3.955
3.948
3.940
3.311
3.294
3.277
2.146
2.135
2.131
2.120
1.871
1.861
1.853
1.842
1.317
1.303
1.289
1.035
1.021
1.007



1i



0.97
1.00
0.99
2.12
2.02
0.98
1.03
1.03
3.70
3.21

Current Data Parameters
 NAME 500M-2022
 EXPNO 102
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220608
 Time 20.52
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

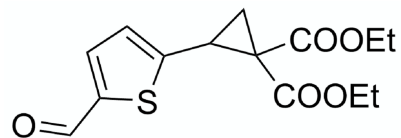
==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

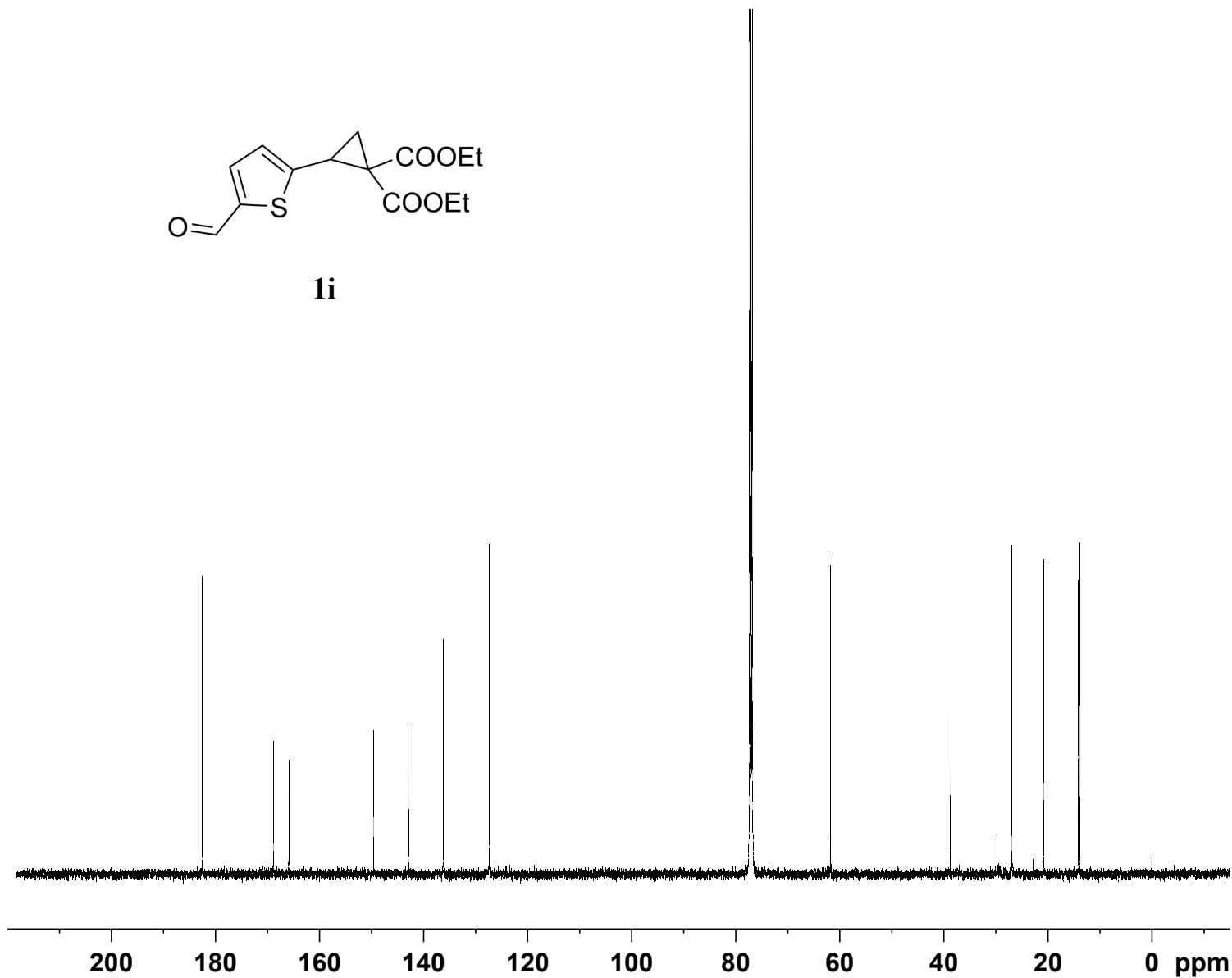
F2 - Processing parameters
 SI 65536
 SF 500.1300113 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 182.50
 \ 168.82
 / 165.86
 — 149.54
 — 142.87
 — 136.15
 — 127.33

< 62.17
 > 61.71
 — 38.62
 — 26.89
 — 20.76
 < 14.06
 > 13.80



1i



Current Data Parameters
 NAME 500M-2022
 EXPNO 103
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220608
 Time 21.46
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

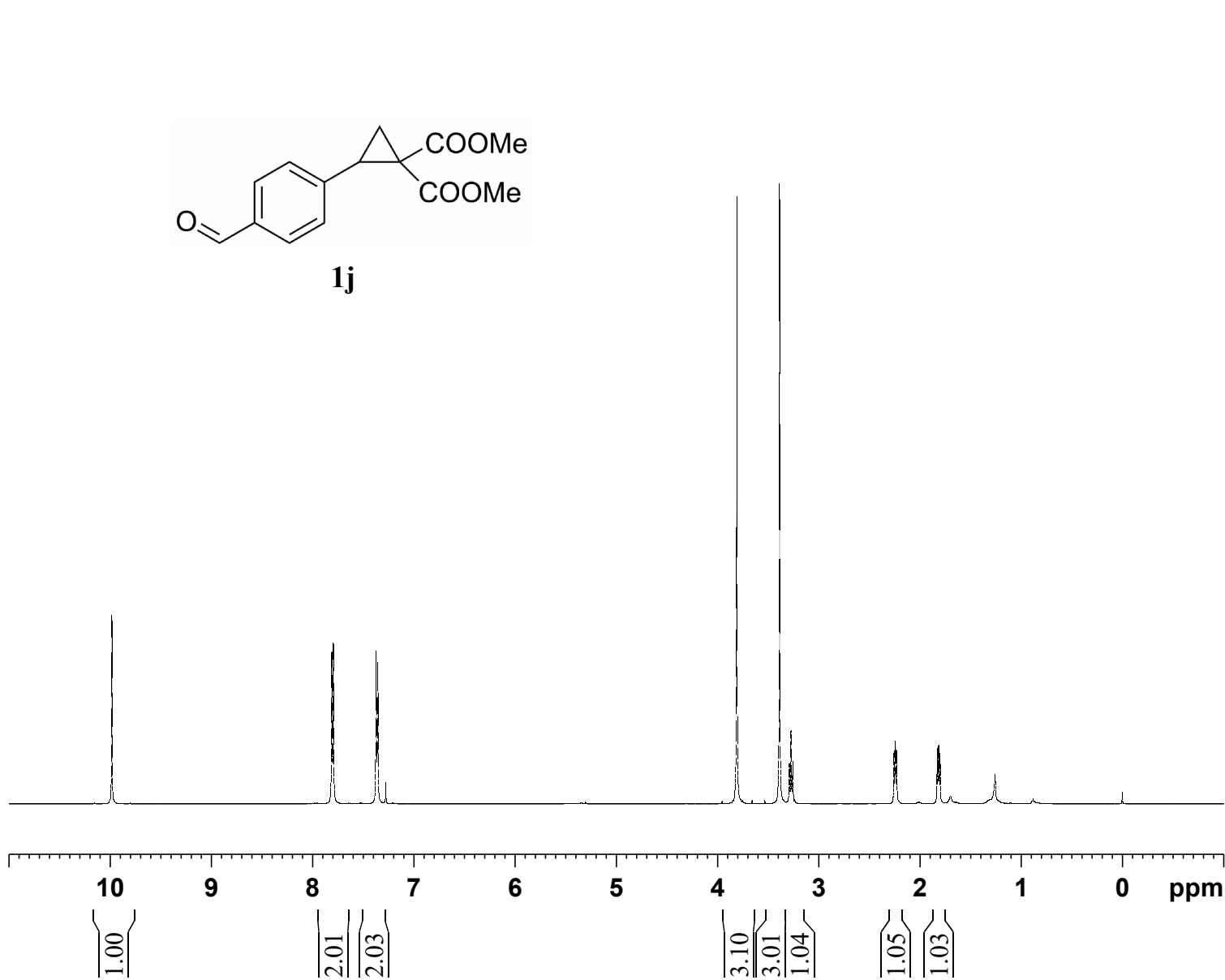
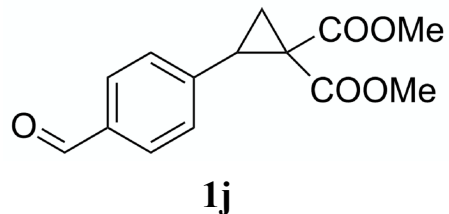
==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

— 9.982

7.810
7.793
7.371
7.355

3.808
3.386
3.289
3.272
3.255
2.255
2.244
2.239
2.229
1.829
1.818
1.810
1.800



Current Data Parameters
NAME 500M-2022
EXPNO 98
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220608
Time 20.25
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

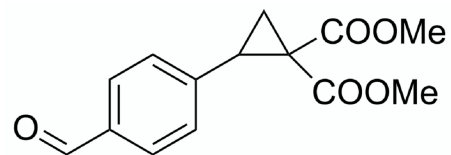
==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

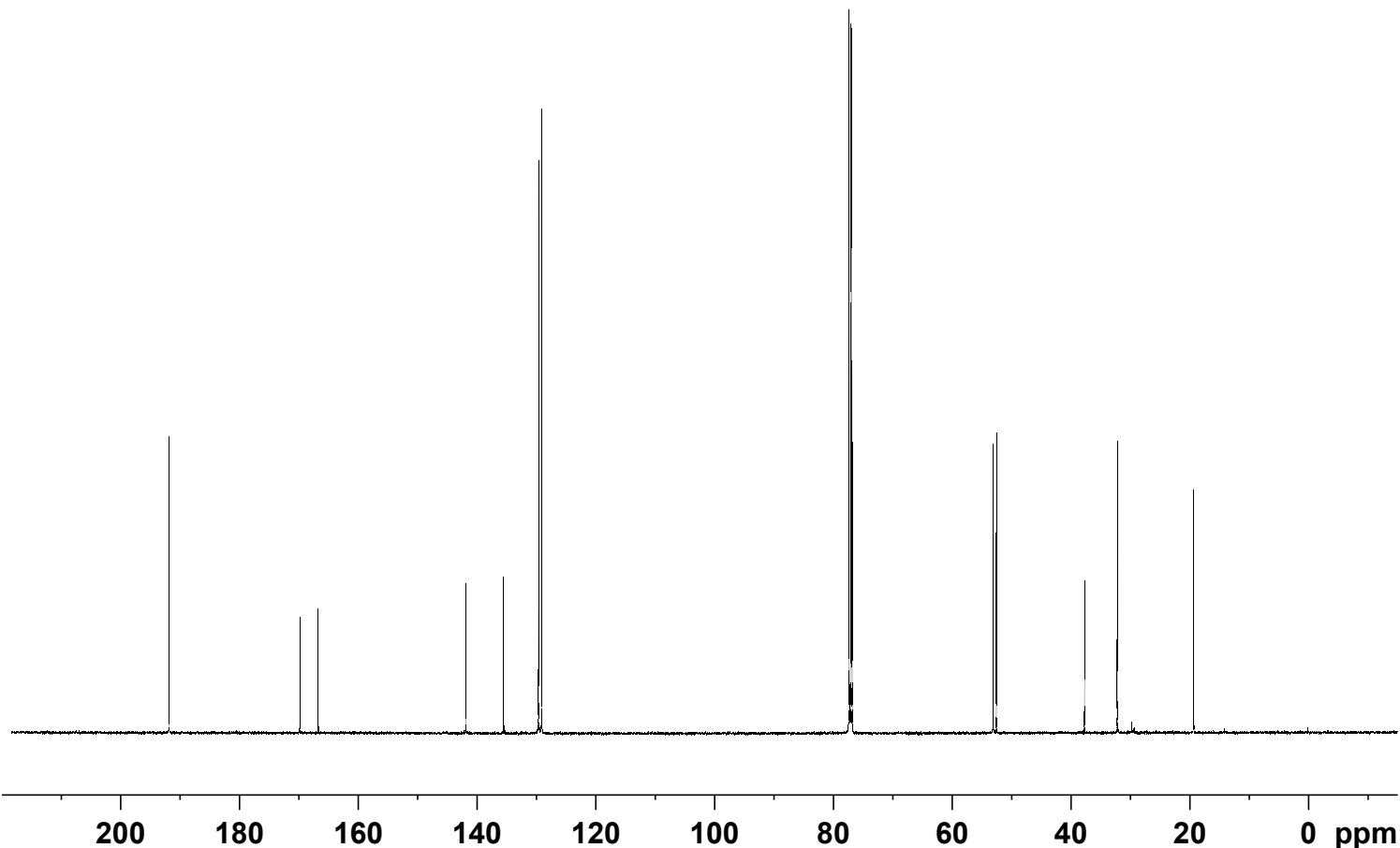
F2 - Processing parameters
SI 65536
SF 500.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

— 191.81
 — 169.79
 — 166.70
 — 141.86
 — 135.48
 — 129.60
 — 129.08

— 53.06
 — 52.50
 — 37.67
 — 32.15
 — 19.29



1j



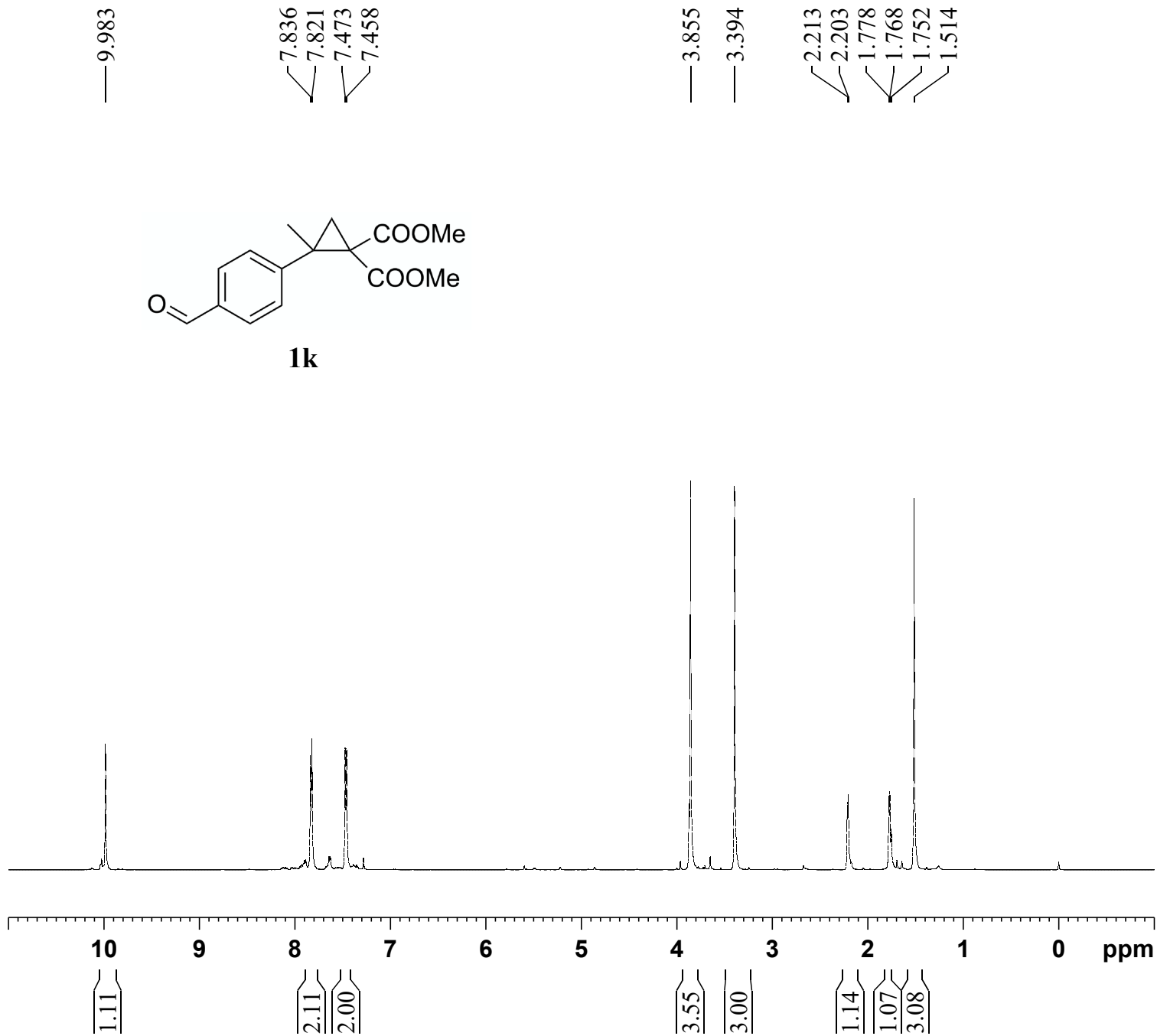
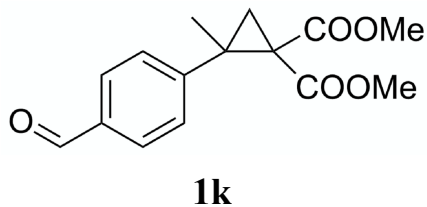
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 174
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211121
 Time 21.32
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 171
 PROCNO 1

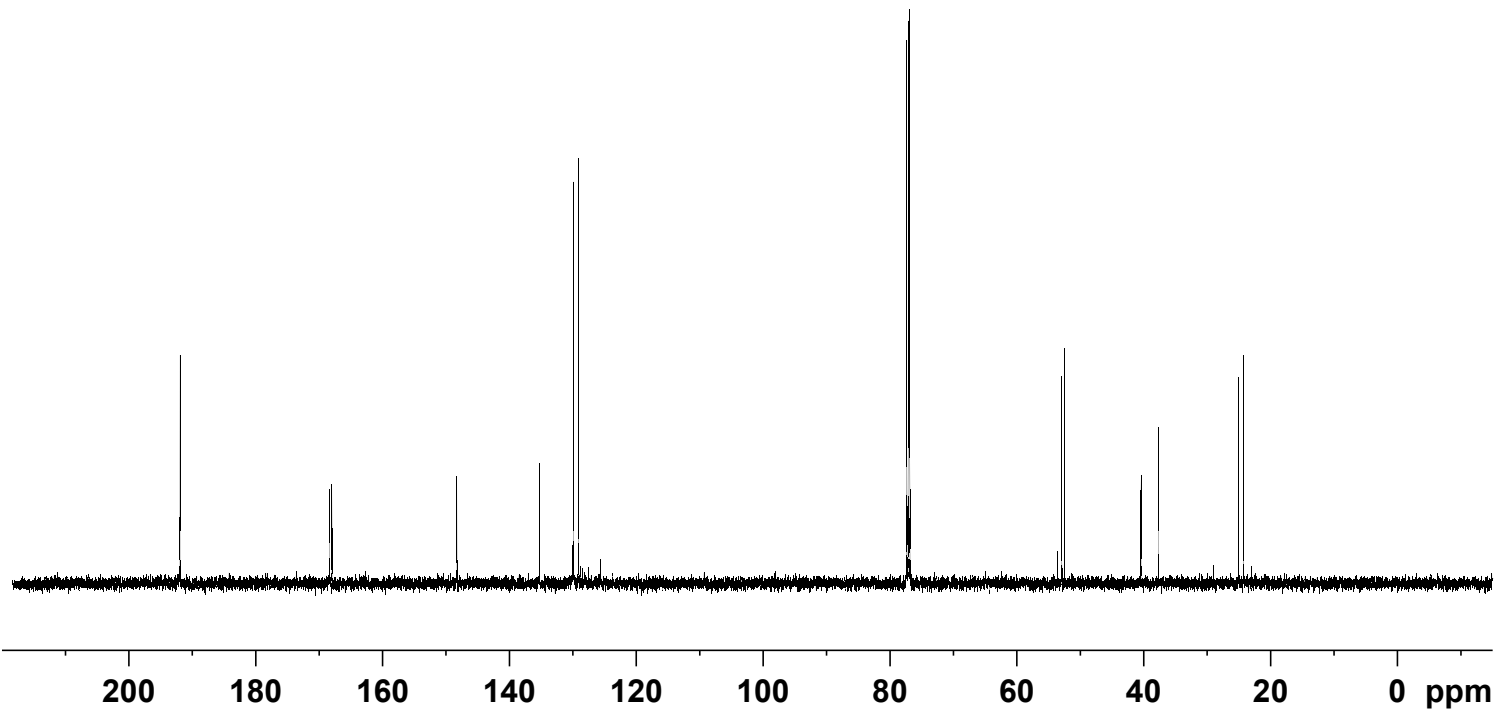
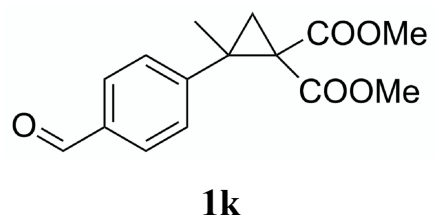
F2 - Acquisition Parameters
 Date_ 20211121
 Time 20.33
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300006 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 191.90
 — 168.32
 — 167.93
 — 148.23
 — 135.22
 — 129.84
 — 129.03
 — 52.86
 — 52.45
 — 40.36
 — 37.63
 — 25.02
 — 24.24



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 182
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211122
 Time 9.58
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 9
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.0000000 W

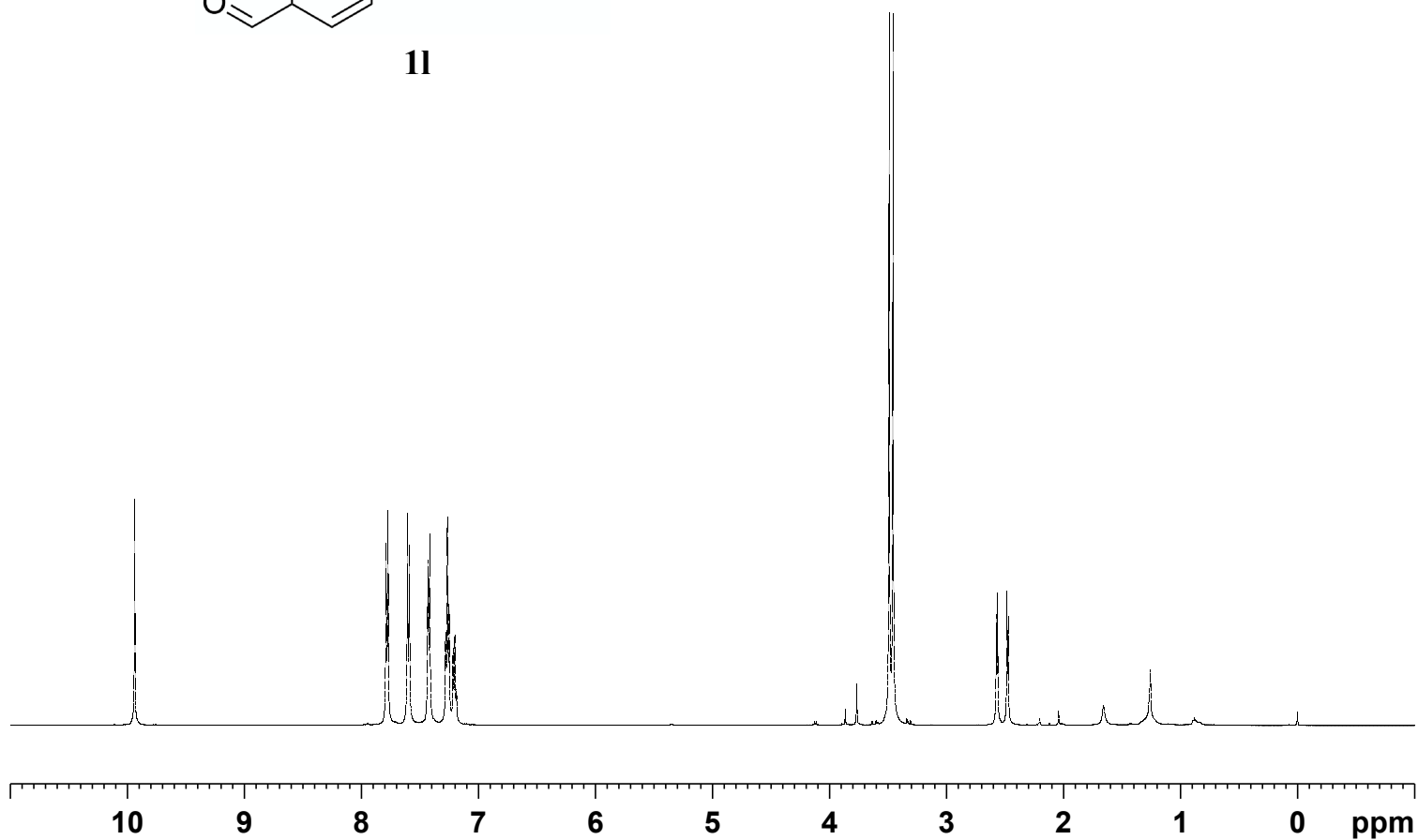
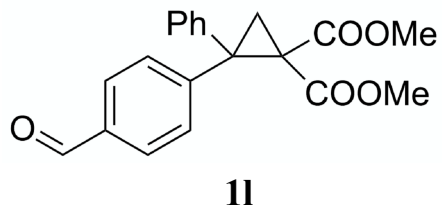
===== CHANNEL f2 =====
 SFO2 500.132005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.0000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

— 9.937

7.788
7.772
7.605
7.589
7.429
7.415
7.279
7.264
7.249
7.215
7.200
7.186

3.488
3.455
2.573
2.562
2.482
2.471



Current Data Parameters
NAME 500M-2022
EXPNO 99
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220608
Time 20.29
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

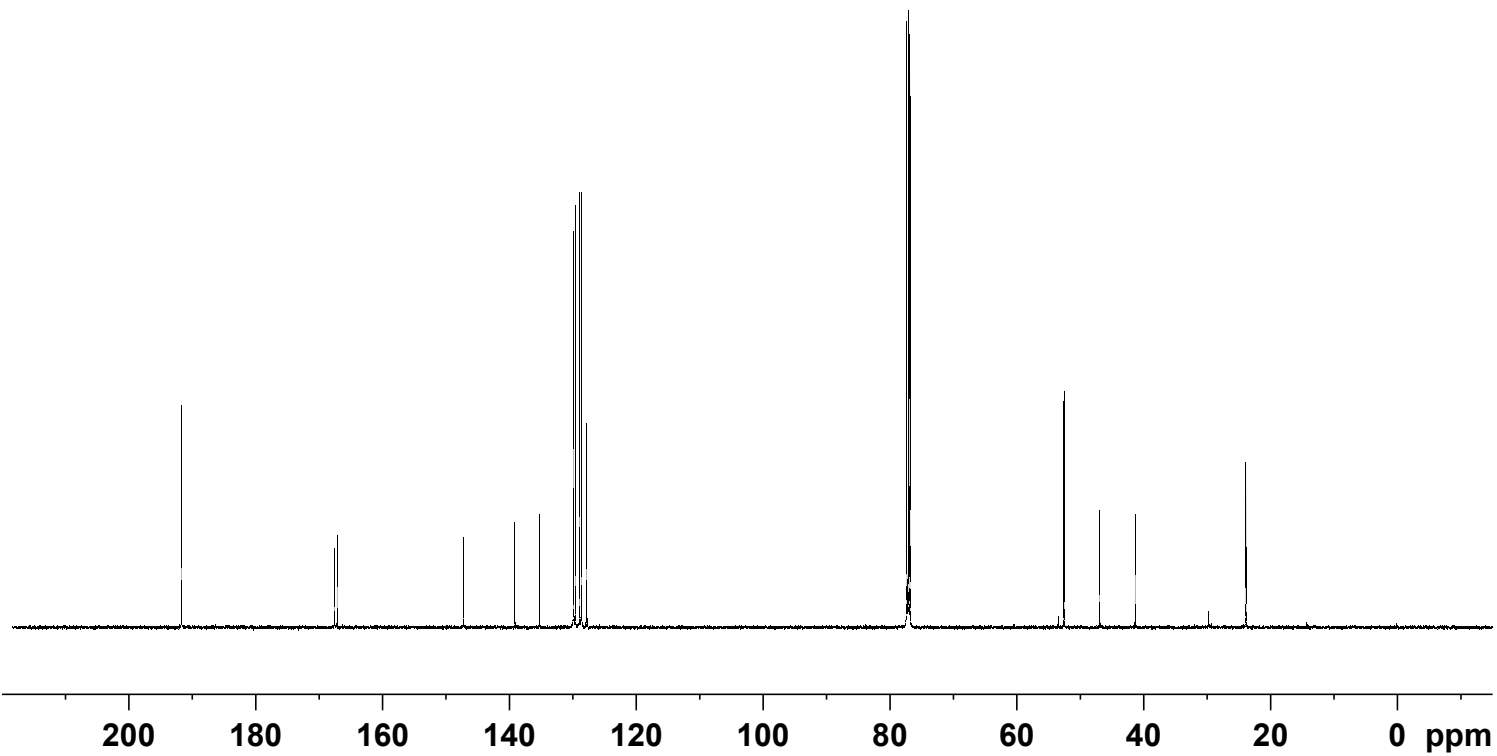
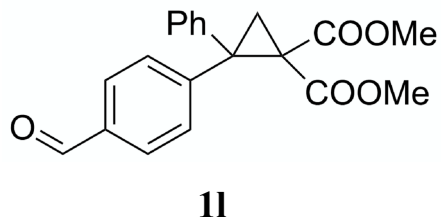
==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

— 191.64
 < 167.54
 < 167.11
 < 147.18
 < 139.12
 < 135.24
 < 129.84
 < 129.55
 < 128.88
 < 128.59
 < 127.77

< 52.59
 < 52.50
 < 46.86
 < 41.28
 — 23.81



Current Data Parameters
 NAME 500M-2022
 EXPNO 100
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220608
 Time 20.43
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

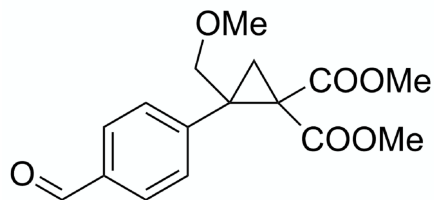
==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

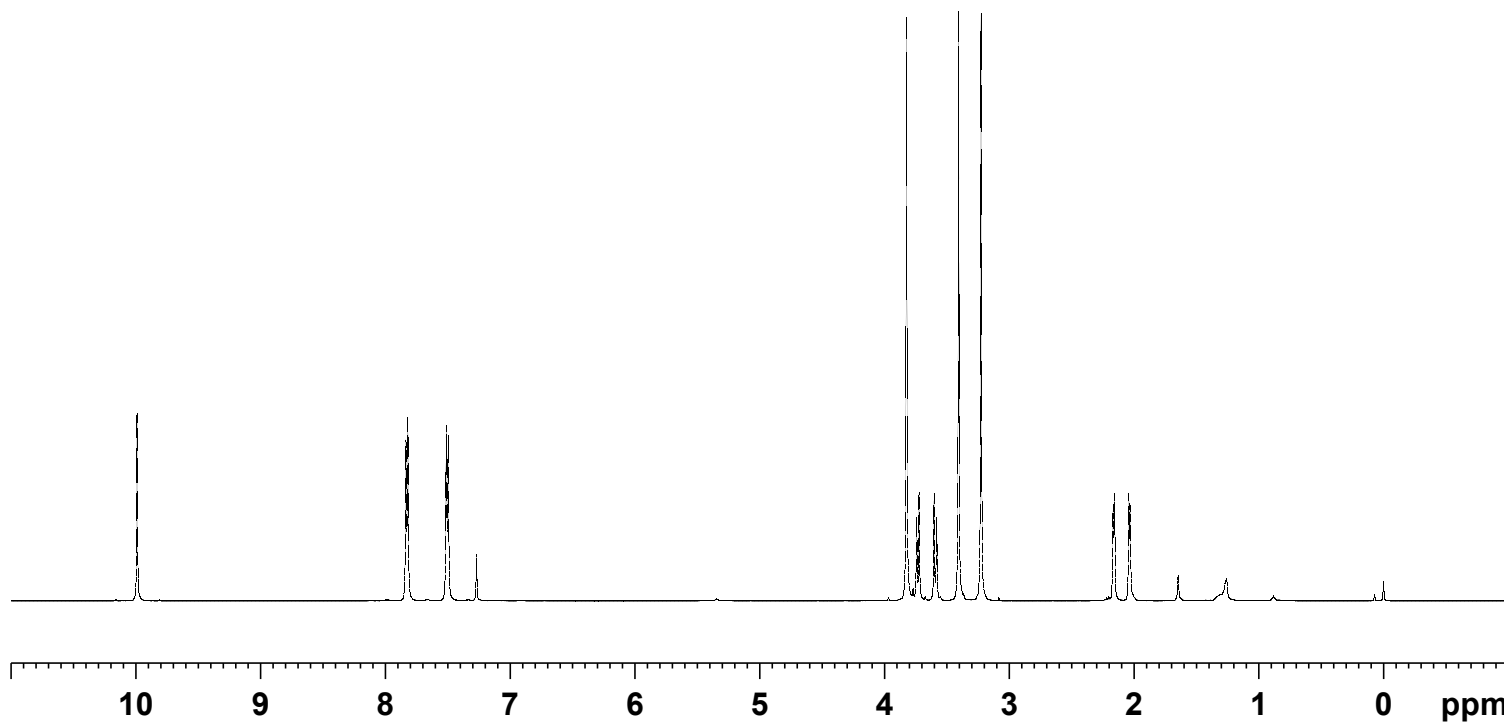
—9.989

7.835
7.819
7.511
7.496

3.823
3.741
3.721
3.602
3.582
3.405
3.225
2.166
2.156
2.040
2.030



1m



1.00

2.00
2.00

3.06
1.13
1.06
3.03
3.06

1.11
1.09

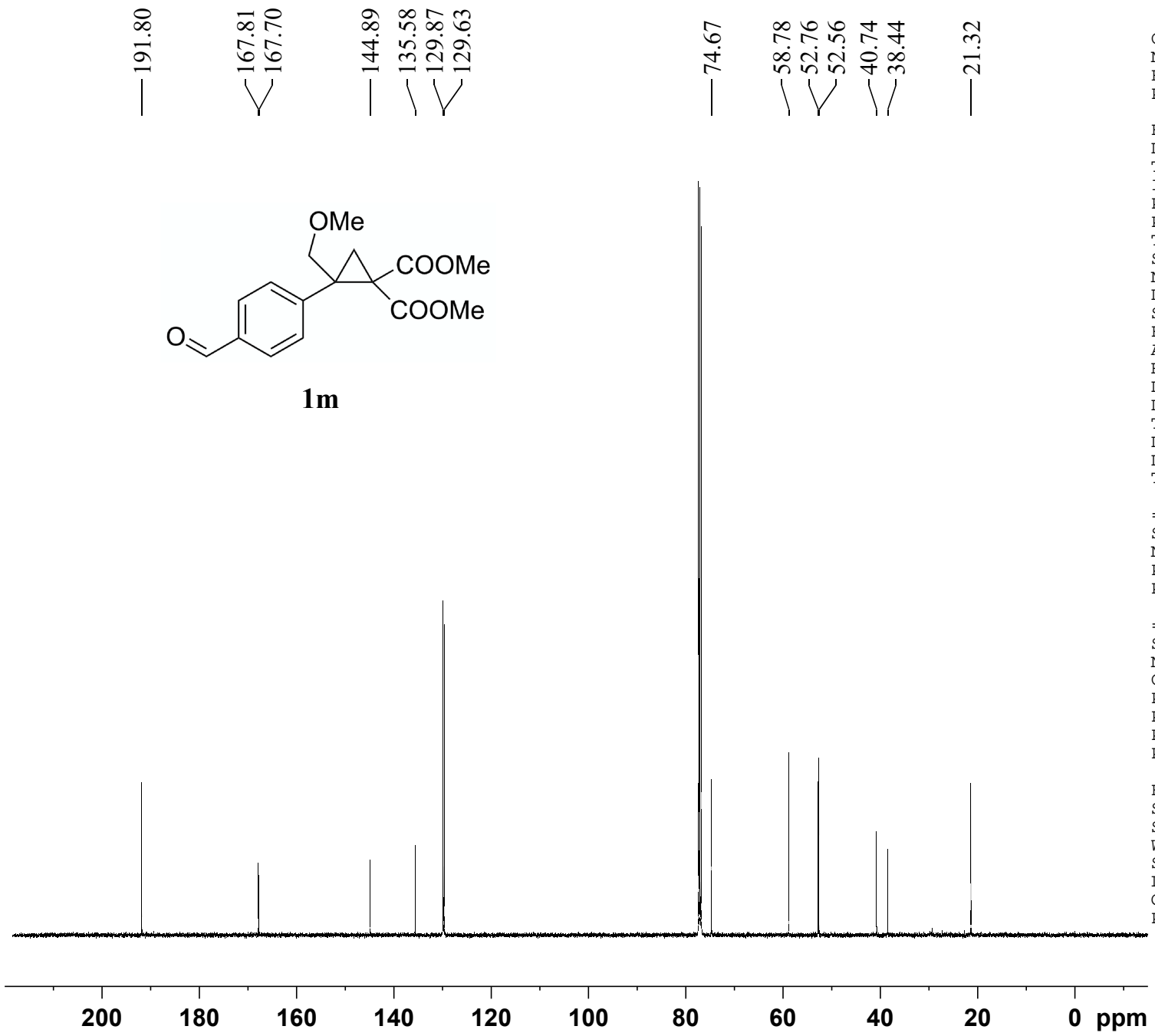
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 206
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211214
 Time 9.23
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300049 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 207
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211214
 Time 9.30
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 133
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

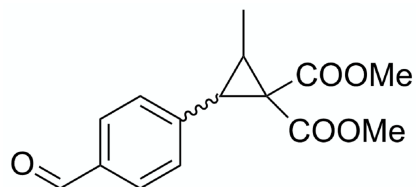
==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

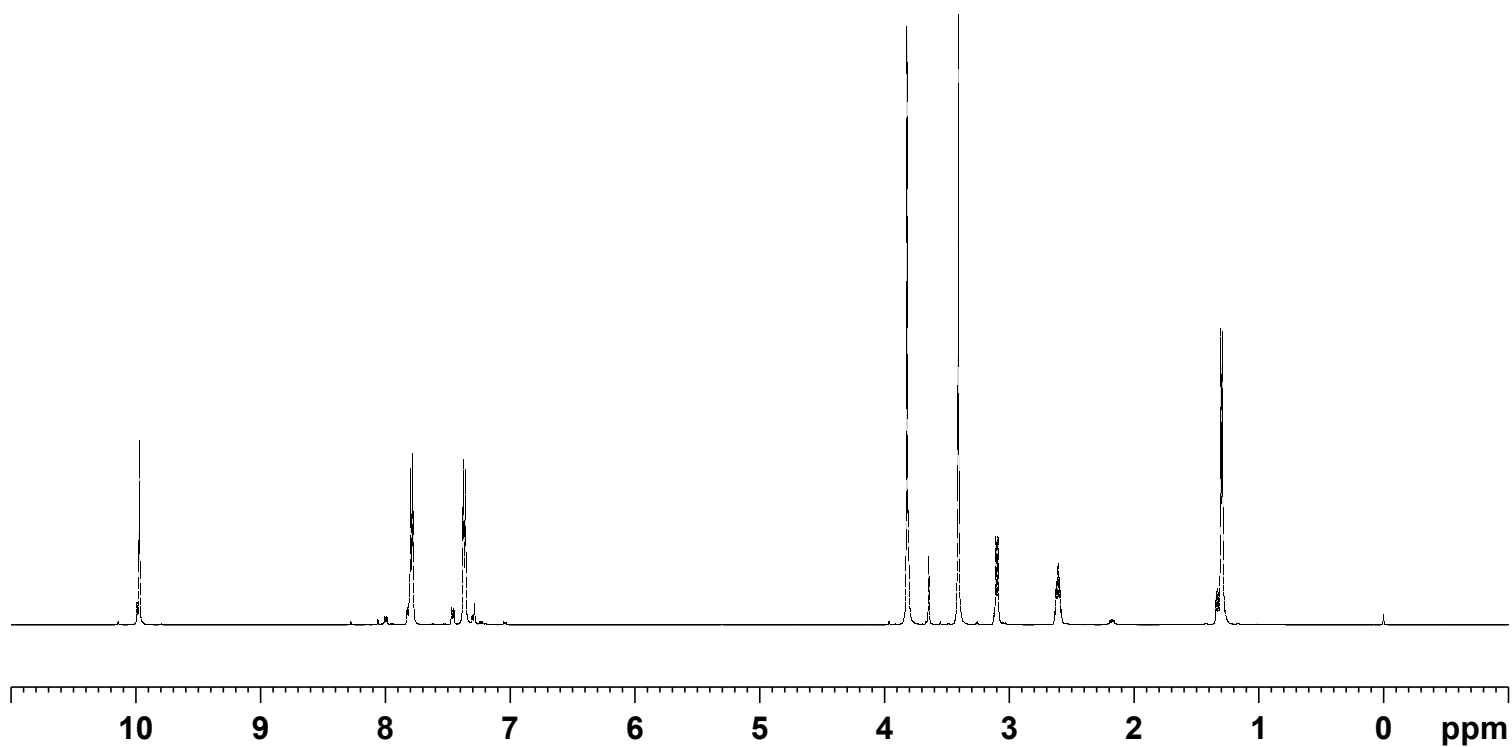
— 9.971

7.797
7.781
7.374
7.358

3.818
3.807
3.407
3.106
3.090
2.635
2.622
2.607
2.594
2.581
1.303
1.291



1n



1.07

2.17
0.23
2.00

3.58
3.16
1.16
1.08

3.66

Current Data Parameters
 NAME 500M-2020xia
 EXPNO 202
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211214
 Time 4.33
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1299981 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 191.79

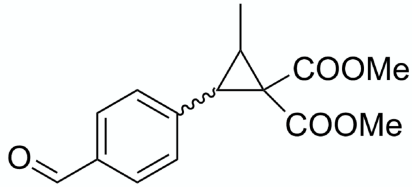
— 167.95
— 167.18

— 142.42
— 135.34
— 129.54
— 129.17

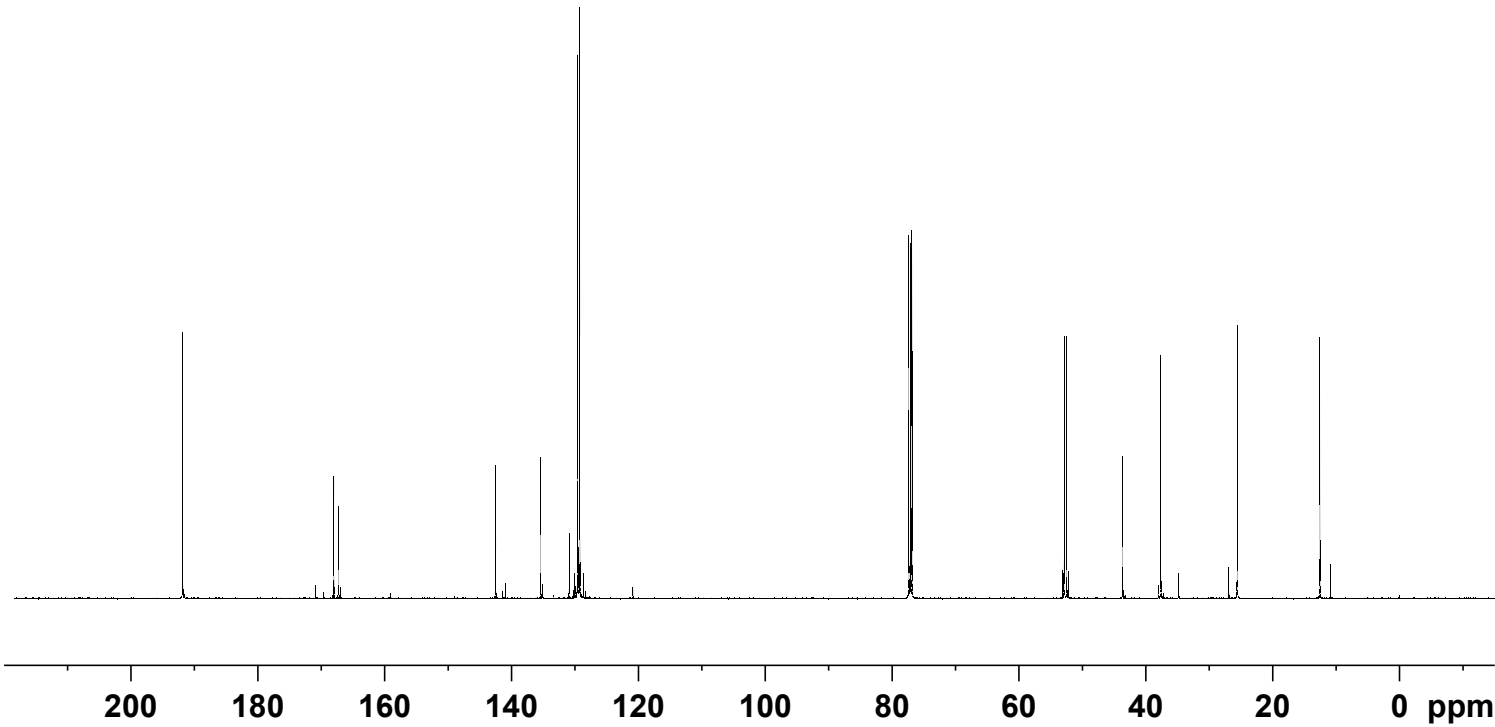
— 52.81
— 52.43
— 43.63
— 37.59

— 25.52

— 12.49



1n



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 203
 PROCNO 1

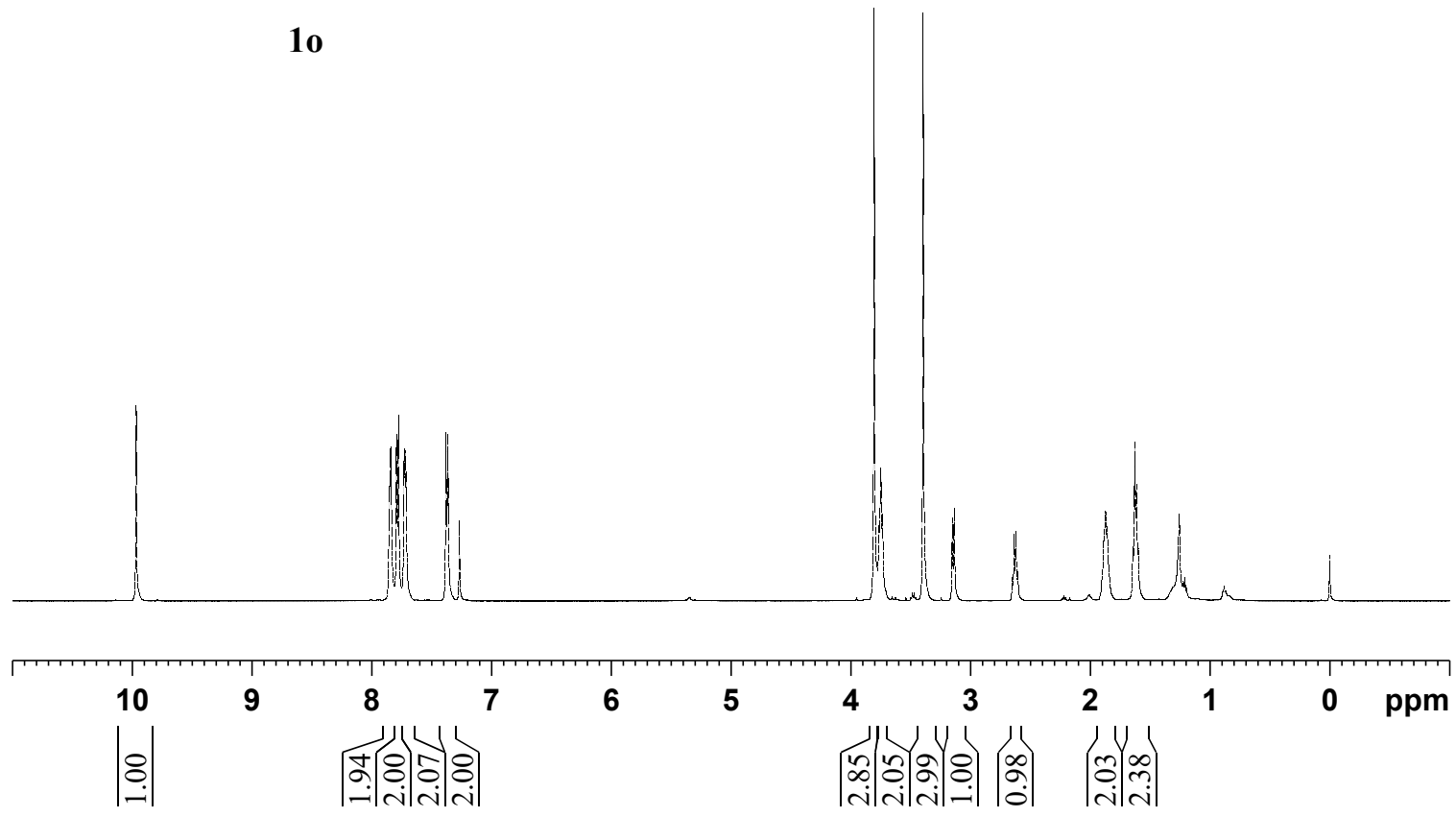
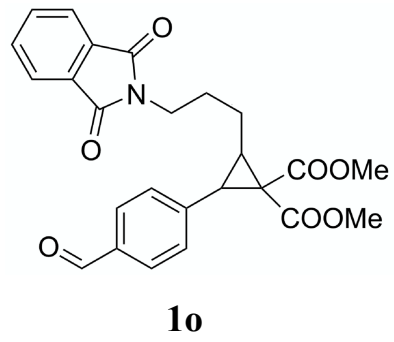
F2 - Acquisition Parameters
 Date_ 20211214
 Time 5.27
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.0000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.0000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

9.967
 7.854
 7.848
 7.843
 7.837
 7.792
 7.776
 7.729
 7.723
 7.718
 7.712
 7.379
 7.363
 3.804
 3.779
 3.765
 3.761
 3.750
 3.736
 3.734
 3.394
 3.151
 3.135
 2.650
 2.635
 2.620
 2.605
 1.903
 1.885
 1.871
 1.858
 1.846
 1.643
 1.627
 1.613
 1.598



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 214
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211228
 Time 15.25
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 69.95
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

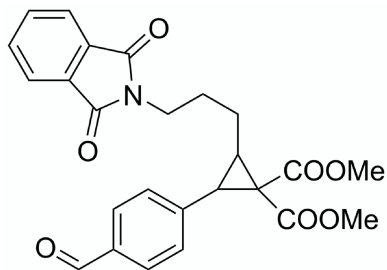
==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

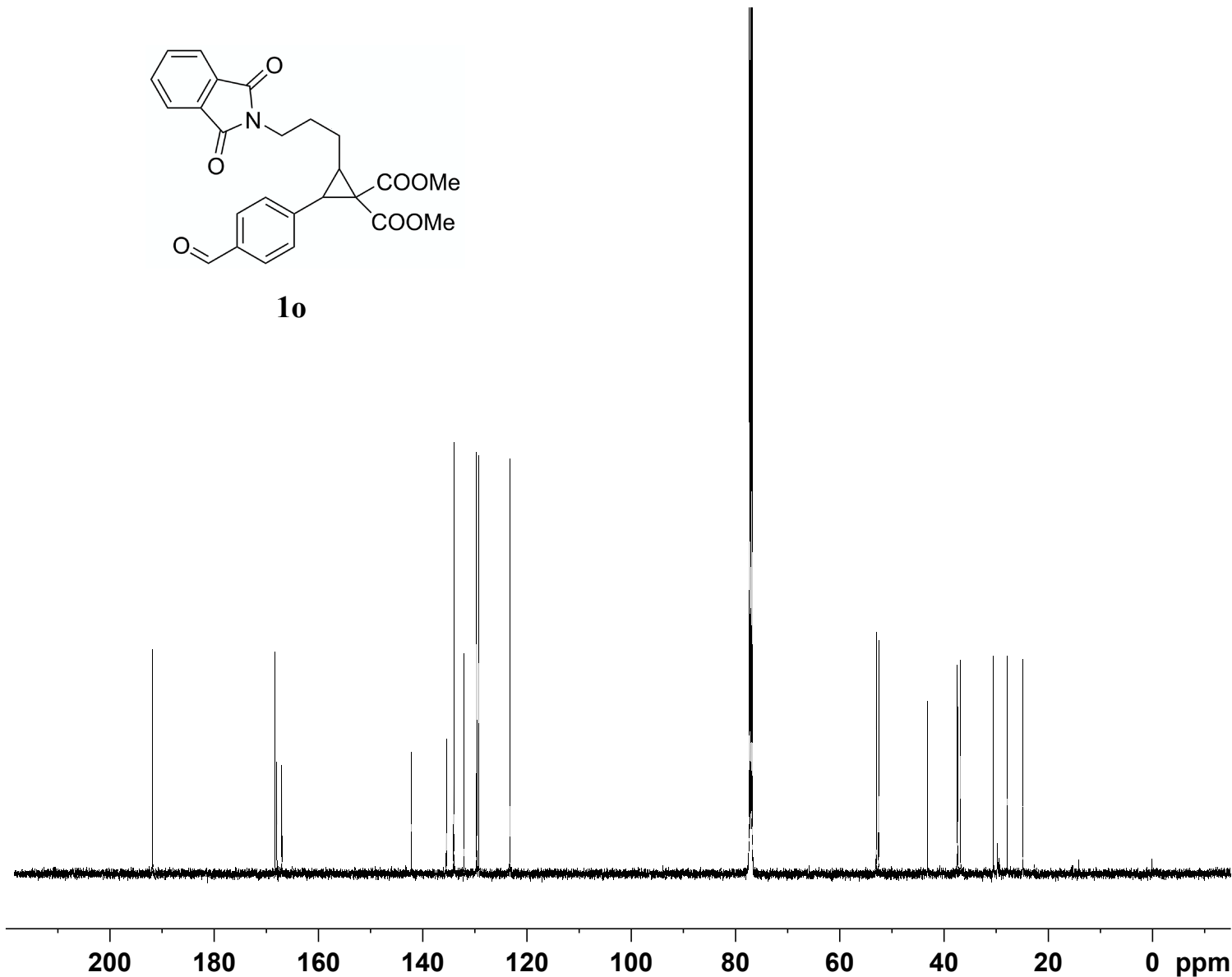
F2 - Processing parameters
 SI 65536
 SF 500.1300037 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

191.77
 168.33
 167.93
 166.98
 142.13
 135.42
 133.99
 132.07
 129.61
 129.21
 123.24

52.95
 52.49
 43.12
 37.36
 36.77
 30.49
 27.81
 24.81



10



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 215
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211228
 Time 15.52
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

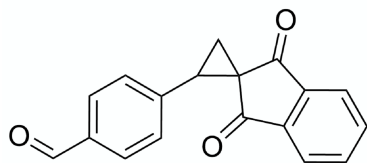
==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

9.986
 8.006
 7.990
 7.836
 7.820
 7.795
 7.781
 7.766
 7.489
 7.473

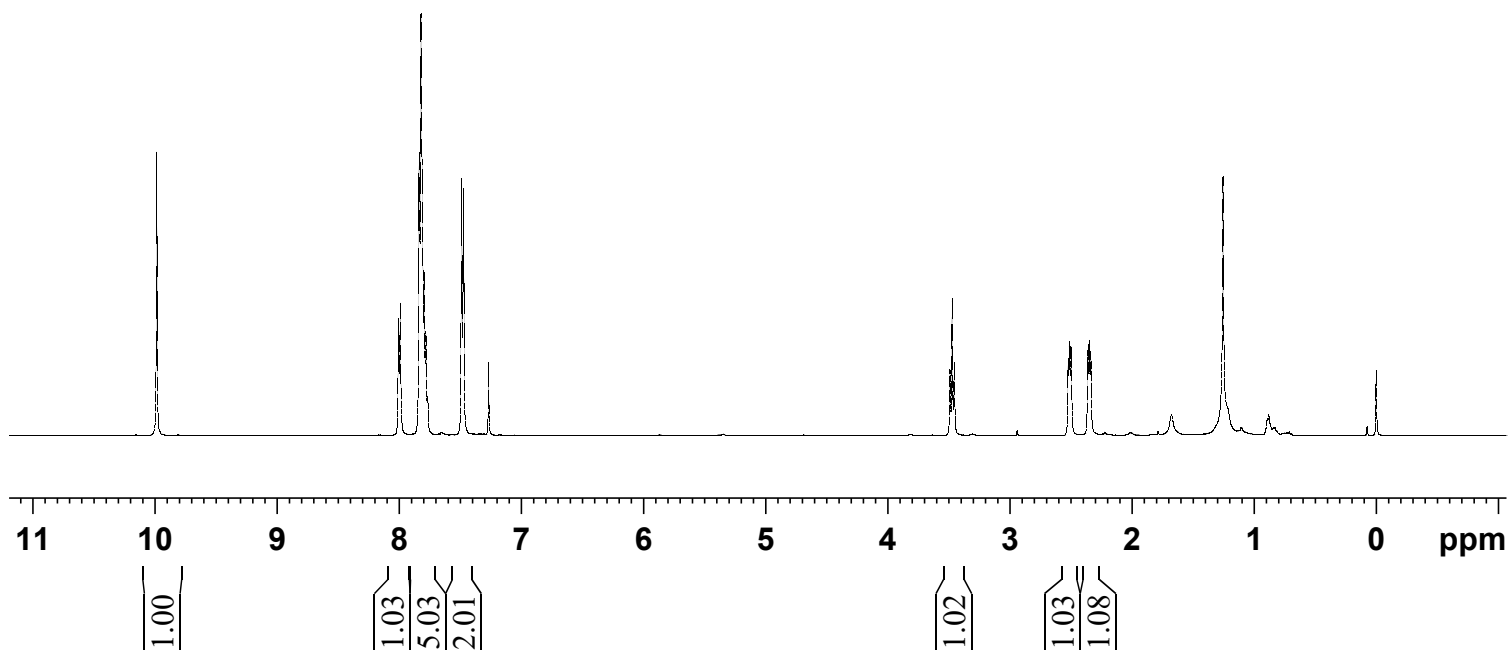
3.489
 3.472
 3.454
 2.522
 2.514
 2.505
 2.496
 2.363
 2.354
 2.345
 2.336



1p

Current Data Parameters
 NAME qy-538-new
 EXPNO 1
 PROCNO 1

F2 - Processing parameters
 SI 65536
 SF 500.1300063 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

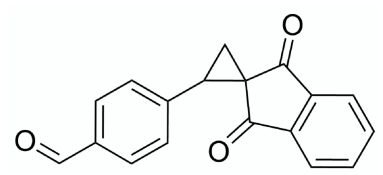


197.57
195.62
191.72

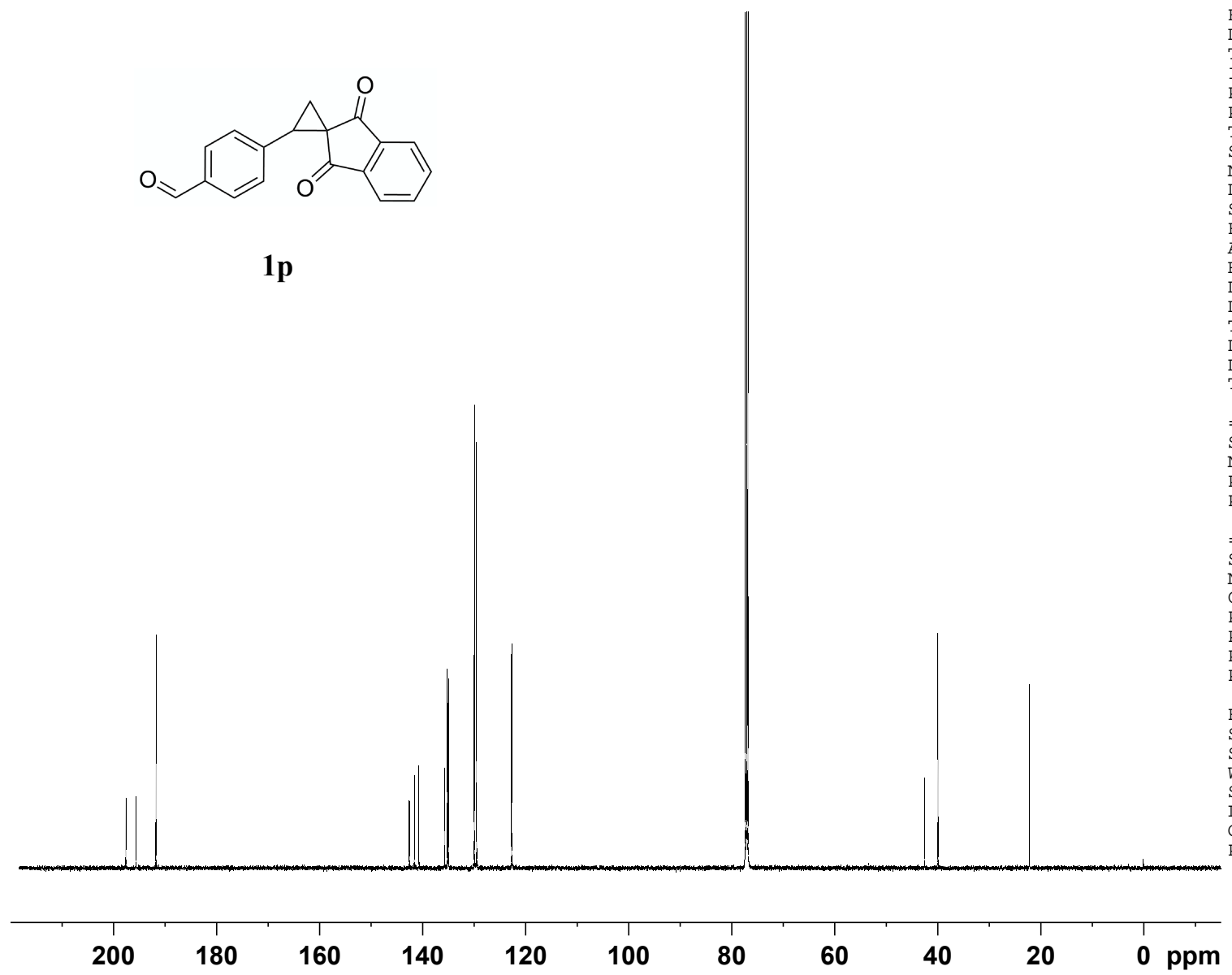
142.54
141.58
140.68
135.69
135.14
134.97
129.92
129.49
122.68
122.65

42.48
39.89

22.16



1p



Current Data Parameters
NAME 500M-2022
EXPNO 105
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220613
Time 22.40
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 10.50 usec
PLW1 57.00000000 W

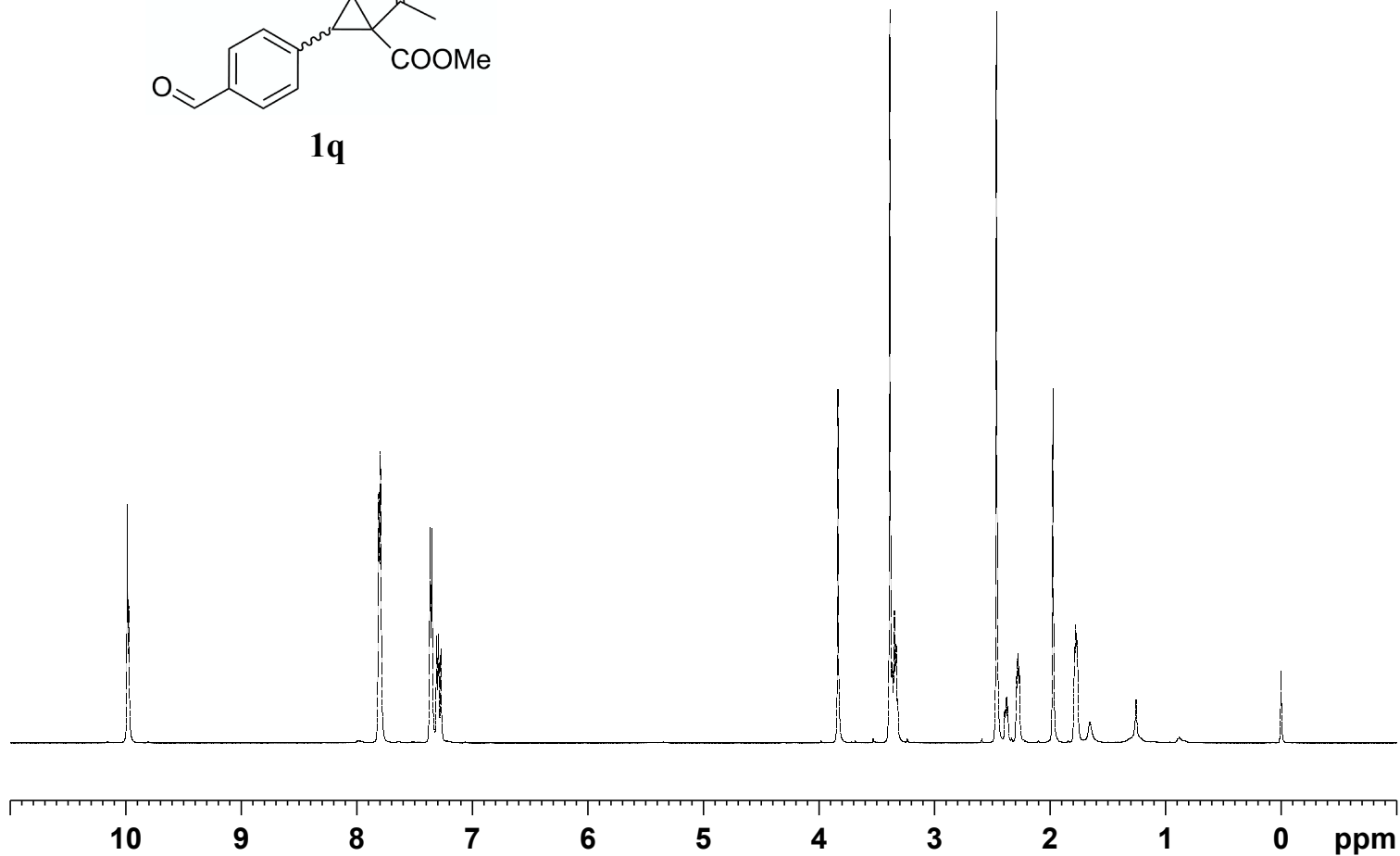
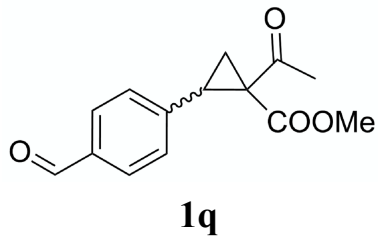
==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.39550999 W
PLW13 0.25312999 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

9.986
9.973

7.811
7.809
7.795
7.793
7.365
7.349
7.308
7.292
7.272

3.835
3.385
3.363
3.346
3.330
3.318
2.463
2.391
2.380
2.375
2.365
2.290
2.281
2.275
2.265
1.973
1.786
1.784
1.777
1.769
1.760



Current Data Parameters
NAME 500M-2020xia
EXPNO 169
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211120
Time 10.58
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
D11 0 sec
TD0 1

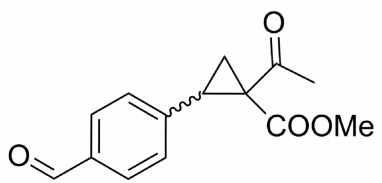
==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 10.59 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

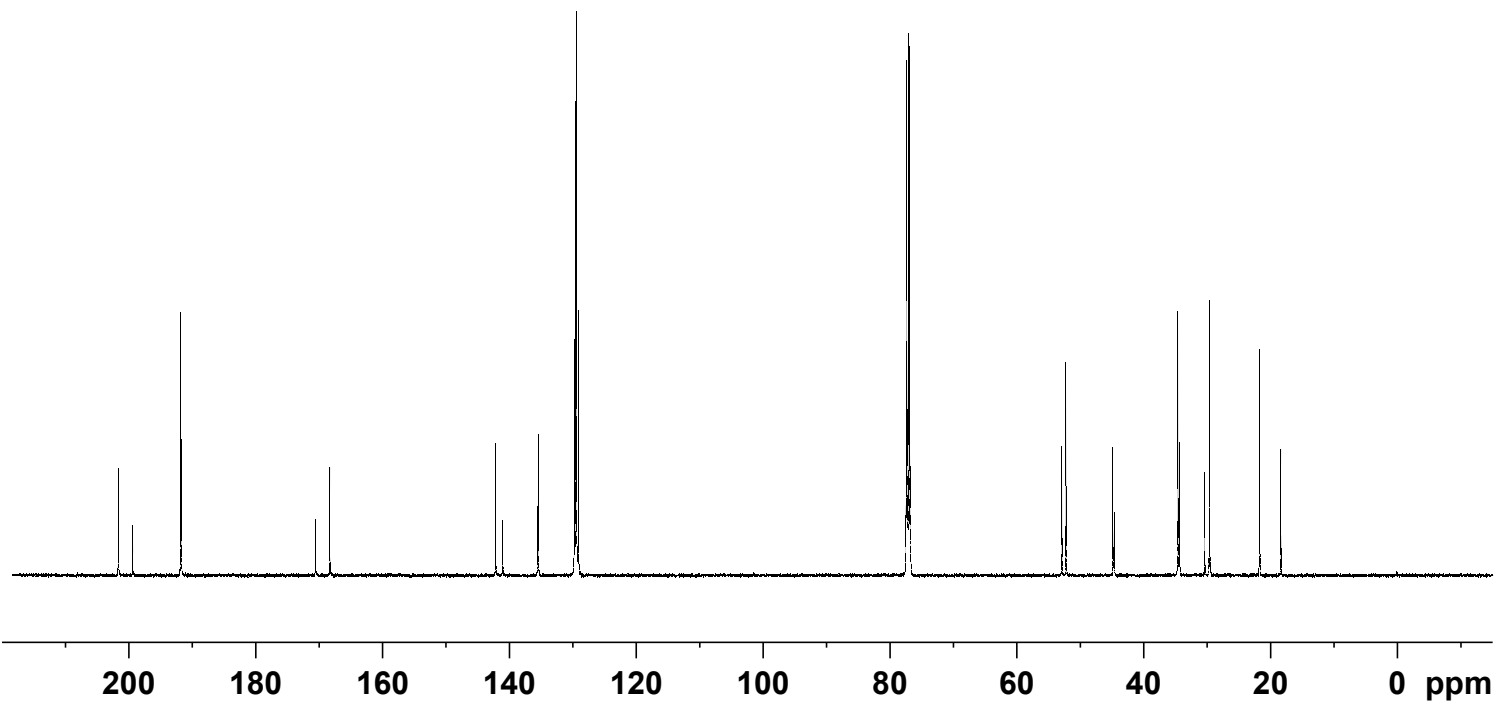
F2 - Processing parameters
SI 65536
SF 500.1300044 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

201.61
199.33
191.80
191.69
170.52
168.26
142.12
141.00
135.49
135.42
129.70
129.53
129.38
129.10

77.34
77.09
76.84
52.84
52.21
44.80
44.60
34.54
34.31
30.31
29.70
29.55
21.67
18.30
0.01



1q



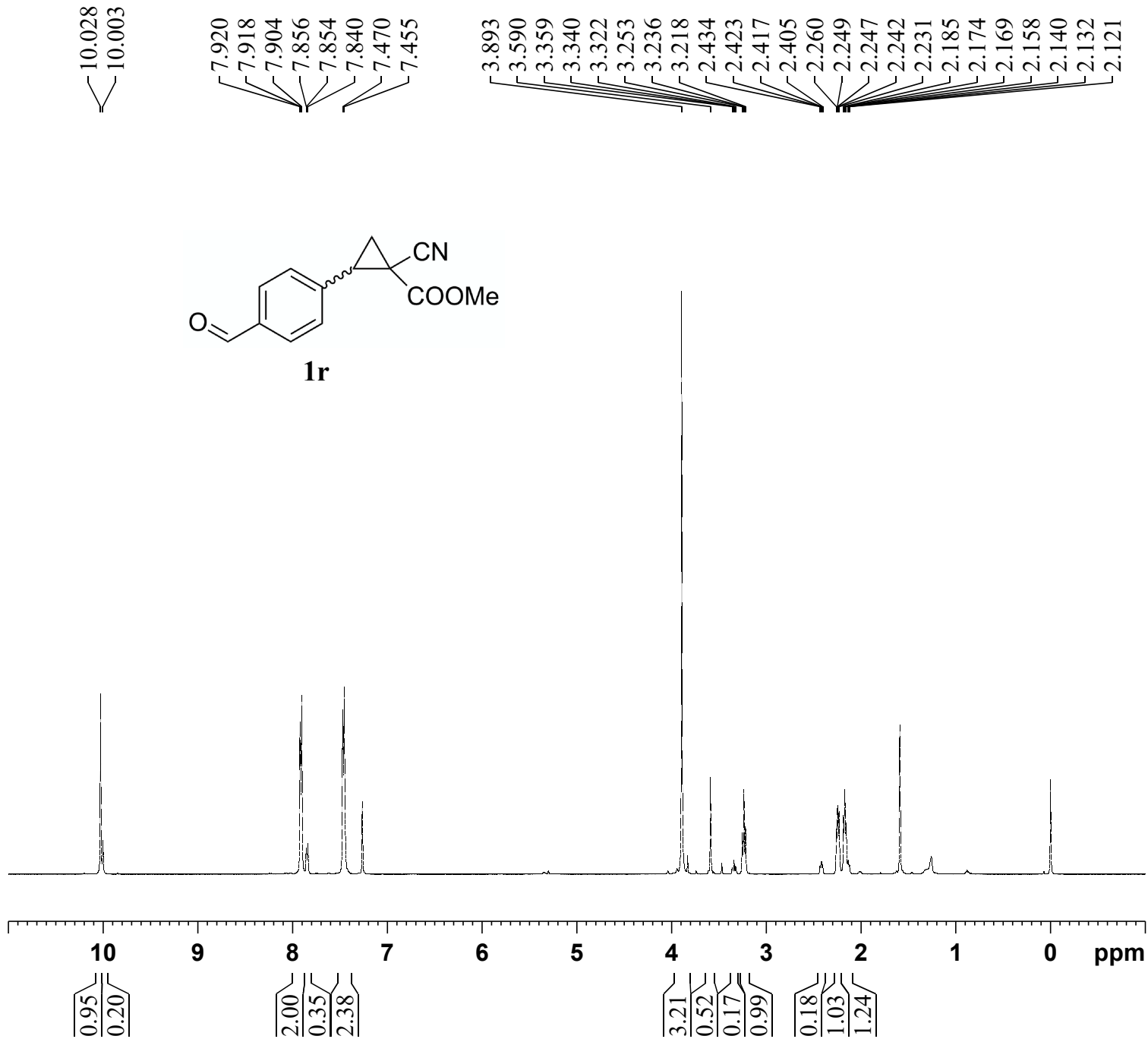
Current Data Parameters
NAME 500M-2020xia
EXPNO 150
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211120
Time 5.25
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.0000000 W

==== CHANNEL f2 =====
SFO2 500.132005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.0000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 131
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211101
 Time 9.53
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 55.37
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

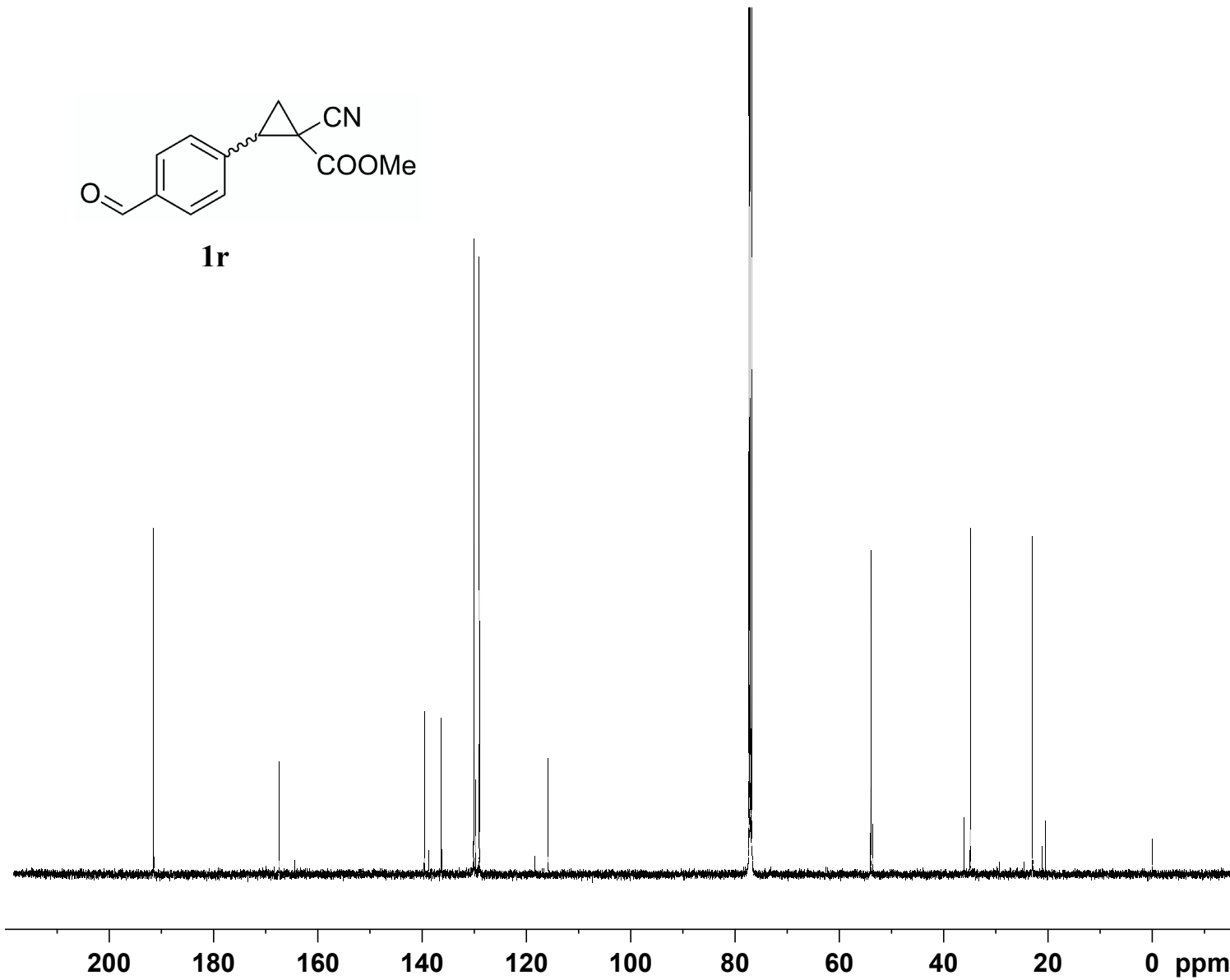
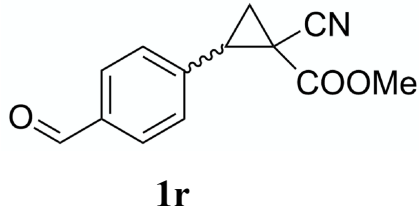
==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

191.52
191.48
167.37
164.44
139.54
138.67
136.36
136.17
130.03
129.68
118.41
115.82

53.95
53.52
36.09
34.86
23.01
22.95
21.03
20.50



Current Data Parameters
NAME 500M-2020xia
EXPNO 135
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211102
Time 9.54
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

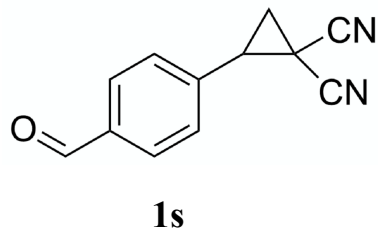
==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

— 10.047

7.962
7.946
7.497
7.481

3.380
3.363
3.345
2.348
2.330



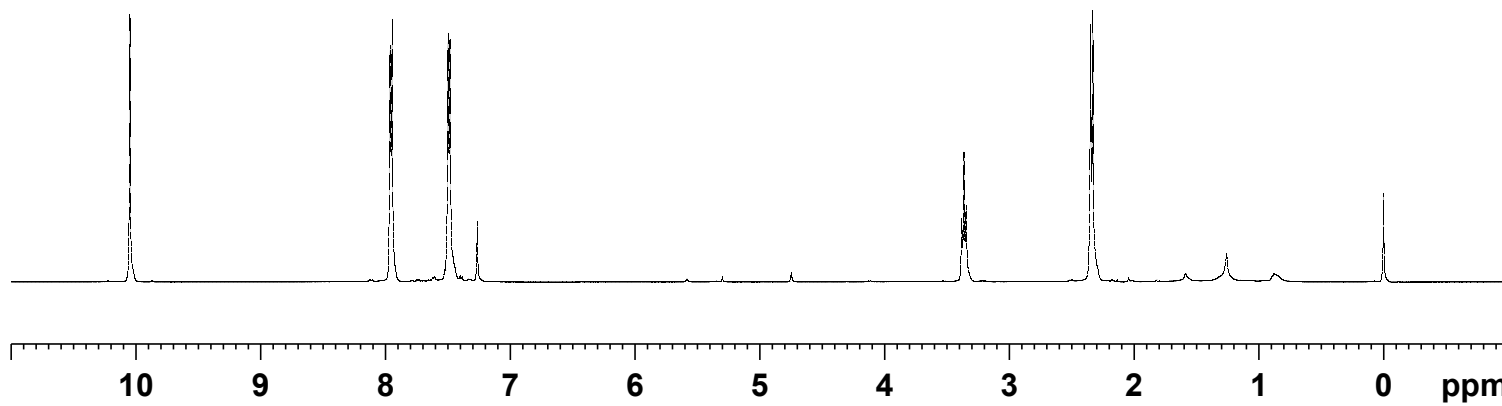
Current Data Parameters
NAME 500M-2020xia
EXPNO 137
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211113
Time 0.57
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 62.06
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 10.59 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



0.98

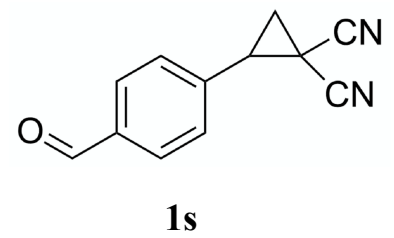
2.00

2.25

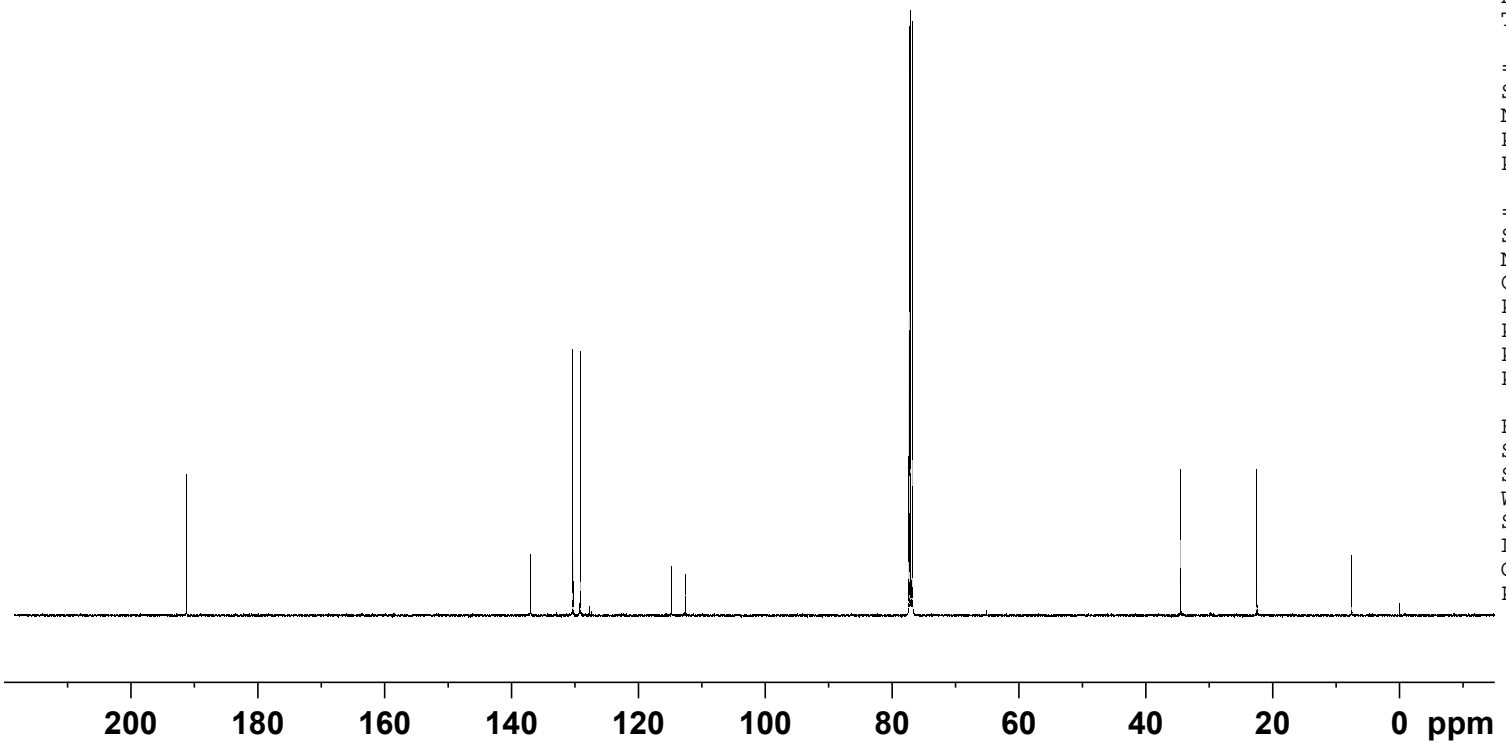
1.07

2.24

—191.21
 —136.99
 —136.95
 —130.29
 —129.11
 —114.76
 —112.57



—34.55
 —22.46
 —7.57



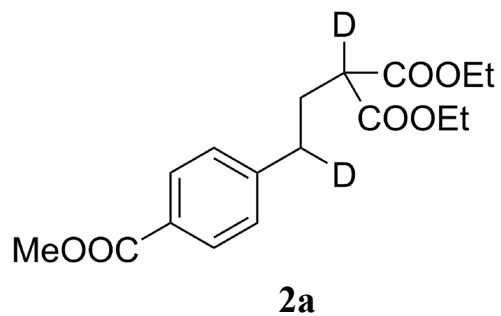
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 138
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 1.24
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577898 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.974
7.953
7.270
7.249

4.231
4.227
4.213
4.209
4.195
4.192
4.177
4.174
3.903
3.342
3.323
3.304
2.740
2.722
2.702
2.684
2.242
2.224
2.205
1.291
1.273
1.255

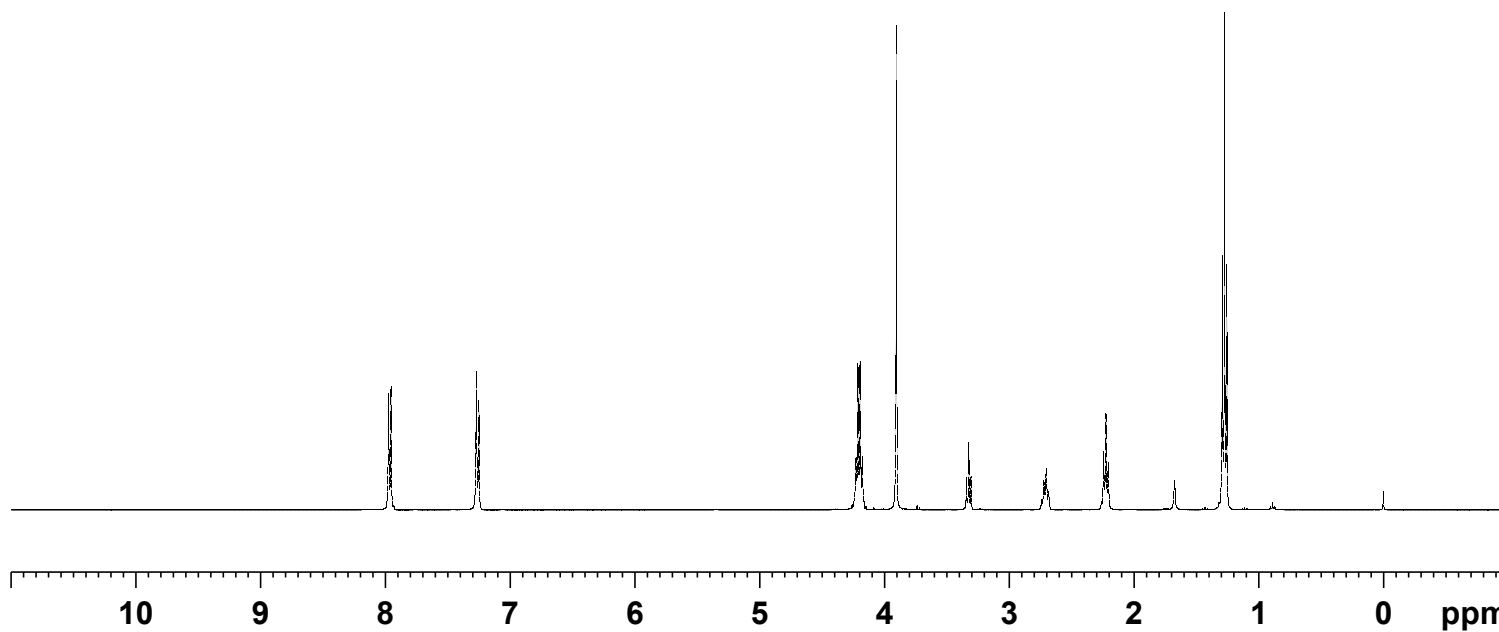
Current Data Parameters
 NAME 400M-2022
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 3.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 92.09
 DW 62.400 usec
 DE 6.50 usec
 TE 300.7 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

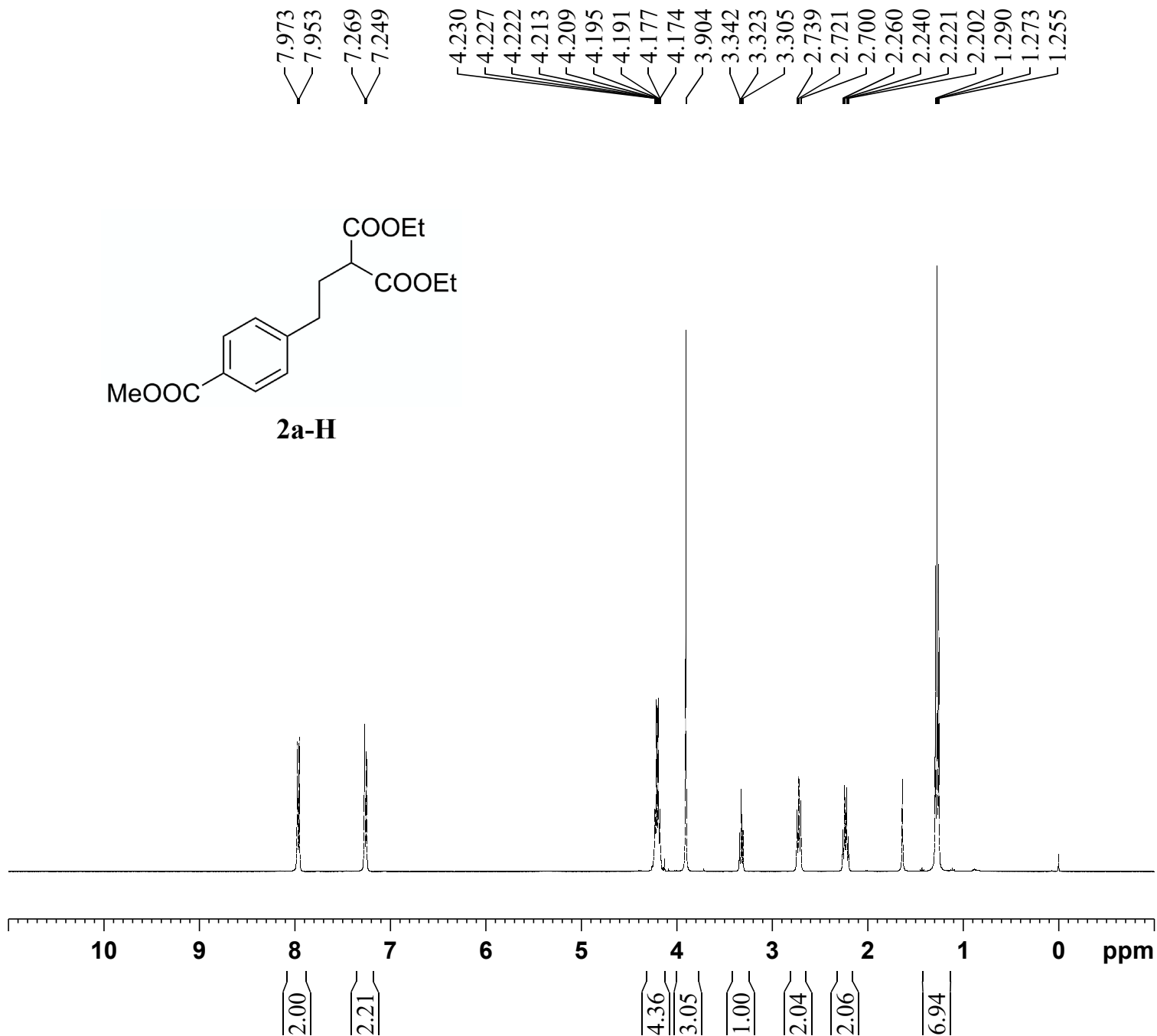
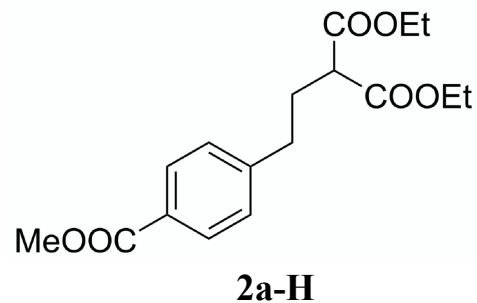
==== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2.00
2.15

3.98
3.10
0.91
1.16
2.03
6.07



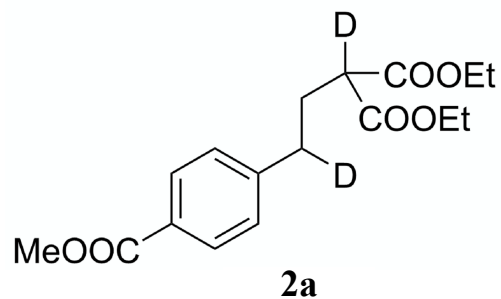
Current Data Parameters
 NAME 400M-2022
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 4.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 206.33
 DW 62.400 usec
 DE 6.50 usec
 TE 300.9 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

==== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400066 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



169.14
167.01

146.11

129.83
128.55
128.28

61.45
51.98
51.17
33.32
33.17
32.97
32.78
29.92
29.85
14.07

Current Data Parameters
NAME 400M-2022
EXPNO 4
PROCNO 1

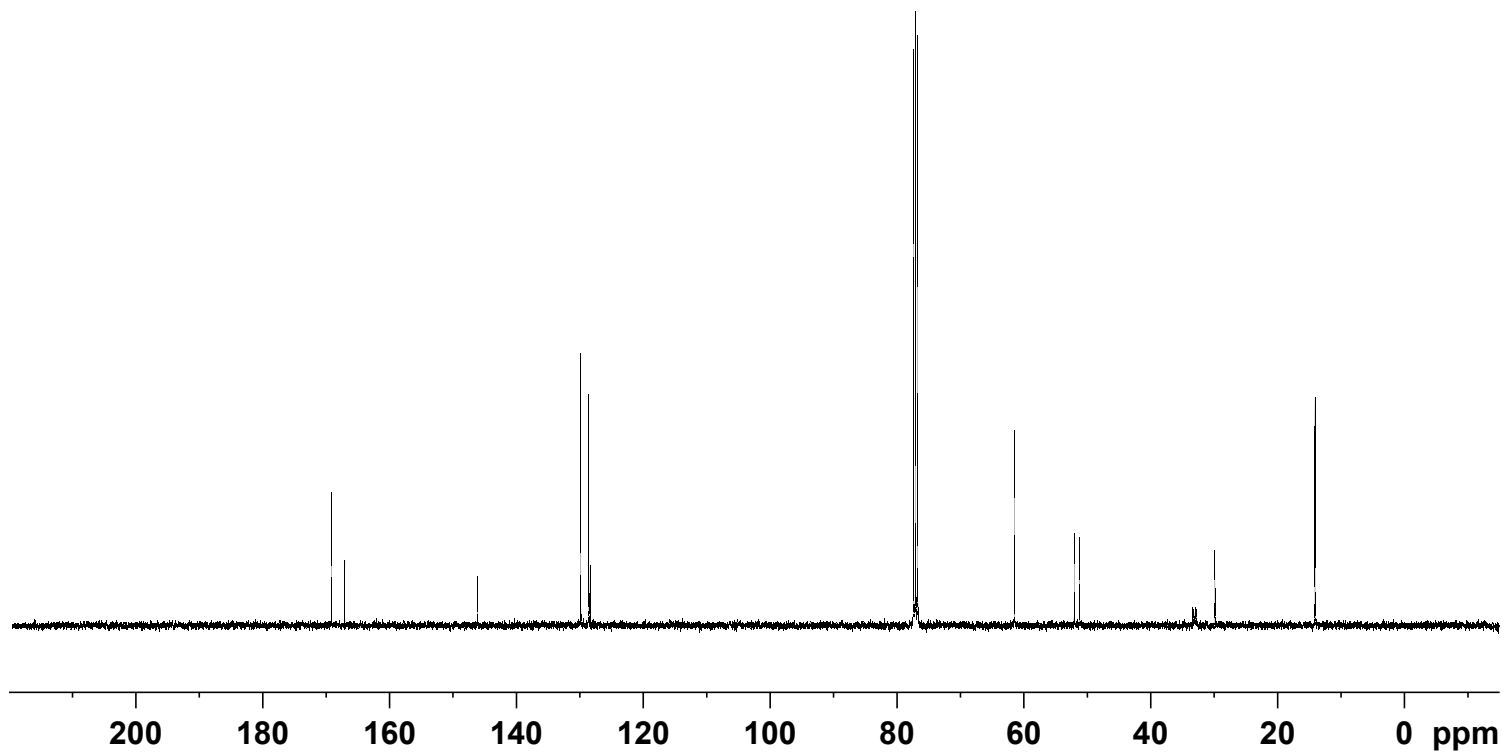
F2 - Acquisition Parameters

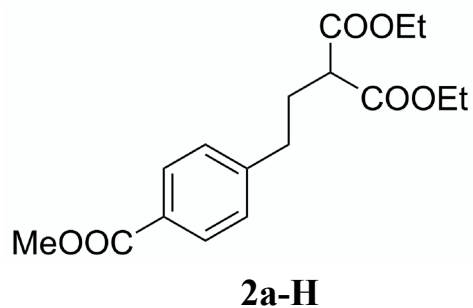
Date_ 20220701
Time 4.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 301.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.0000000 W

==== CHANNEL f2 =====
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 12.0000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





169.15
167.02

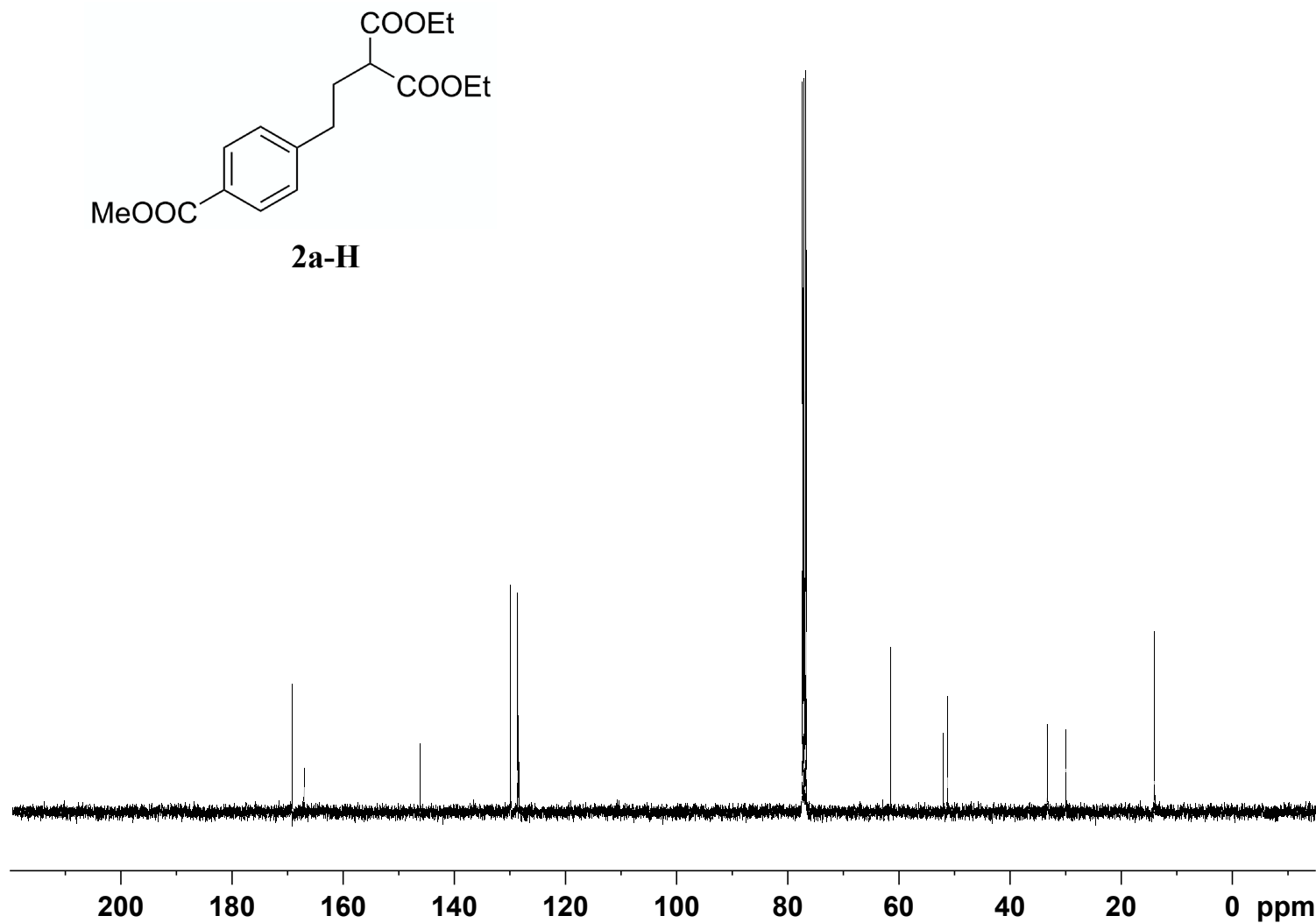
146.14

129.83
128.56
128.28

61.46
51.99
51.20

33.33
29.92

14.07



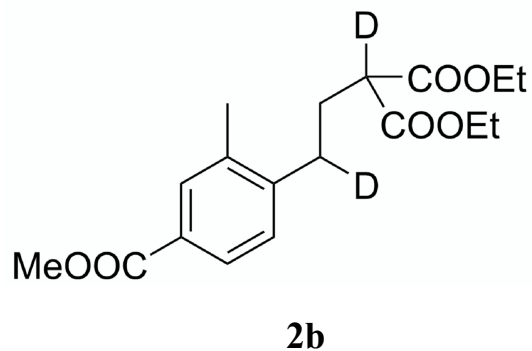
Current Data Parameters
 NAME 400M-2022
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 4.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

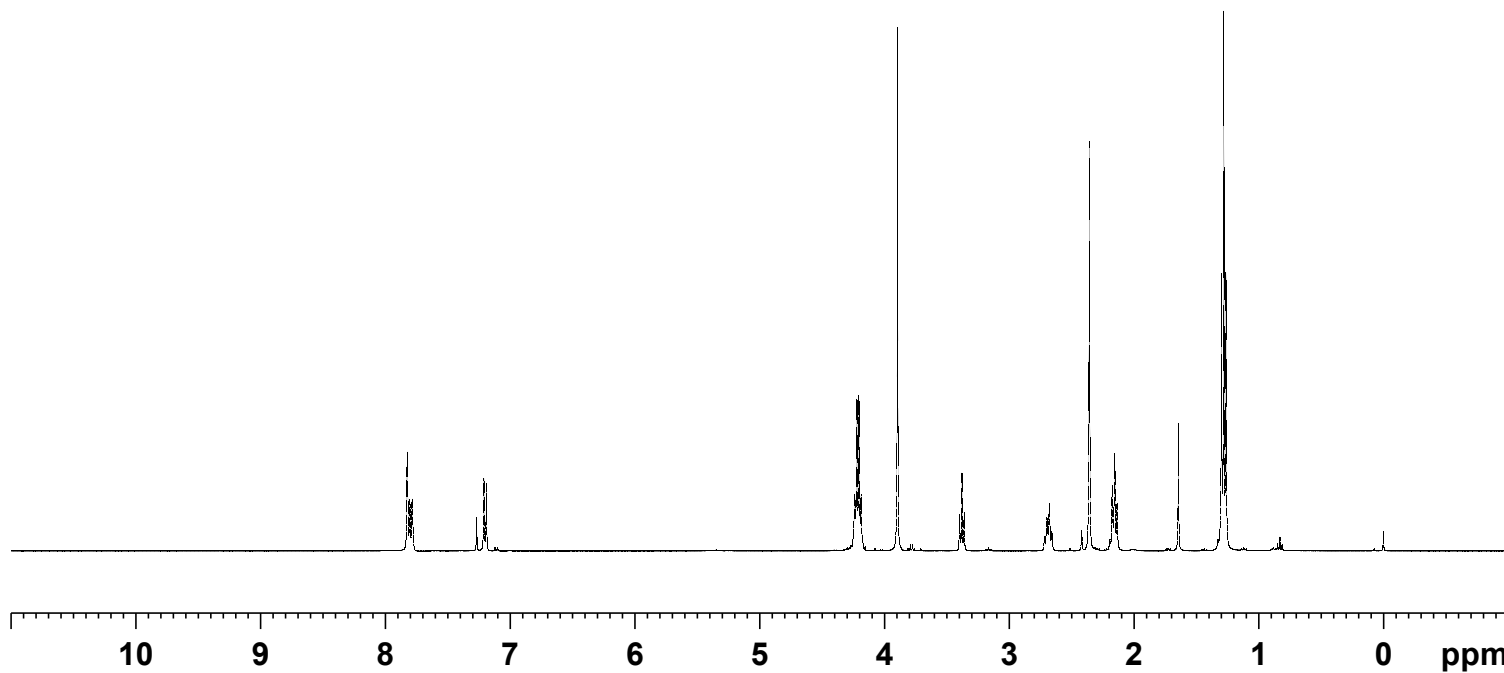
==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Chemical shift values (ppm) for the peaks in the spectrum:

- 7.822, 7.804, 7.784, 7.209, 7.189
- 4.240, 4.236, 4.222, 4.218, 4.204, 4.200, 4.187, 4.183, 3.894, 3.396, 3.378, 3.360, 2.716, 2.697, 2.677, 2.658, 2.356, 2.173, 2.154, 2.134, 1.297, 1.279, 1.261



Integration values for the peaks in the spectrum:

- 2.07
- 1.00
- 4.13
- 3.16
- 0.99
- 1.22
- 3.09
- 2.09
- 6.74

Current Data Parameters

NAME 400M-2022
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20220701
 Time 5.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 102.73
 DW 62.400 usec
 DE 6.50 usec
 TE 300.9 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====

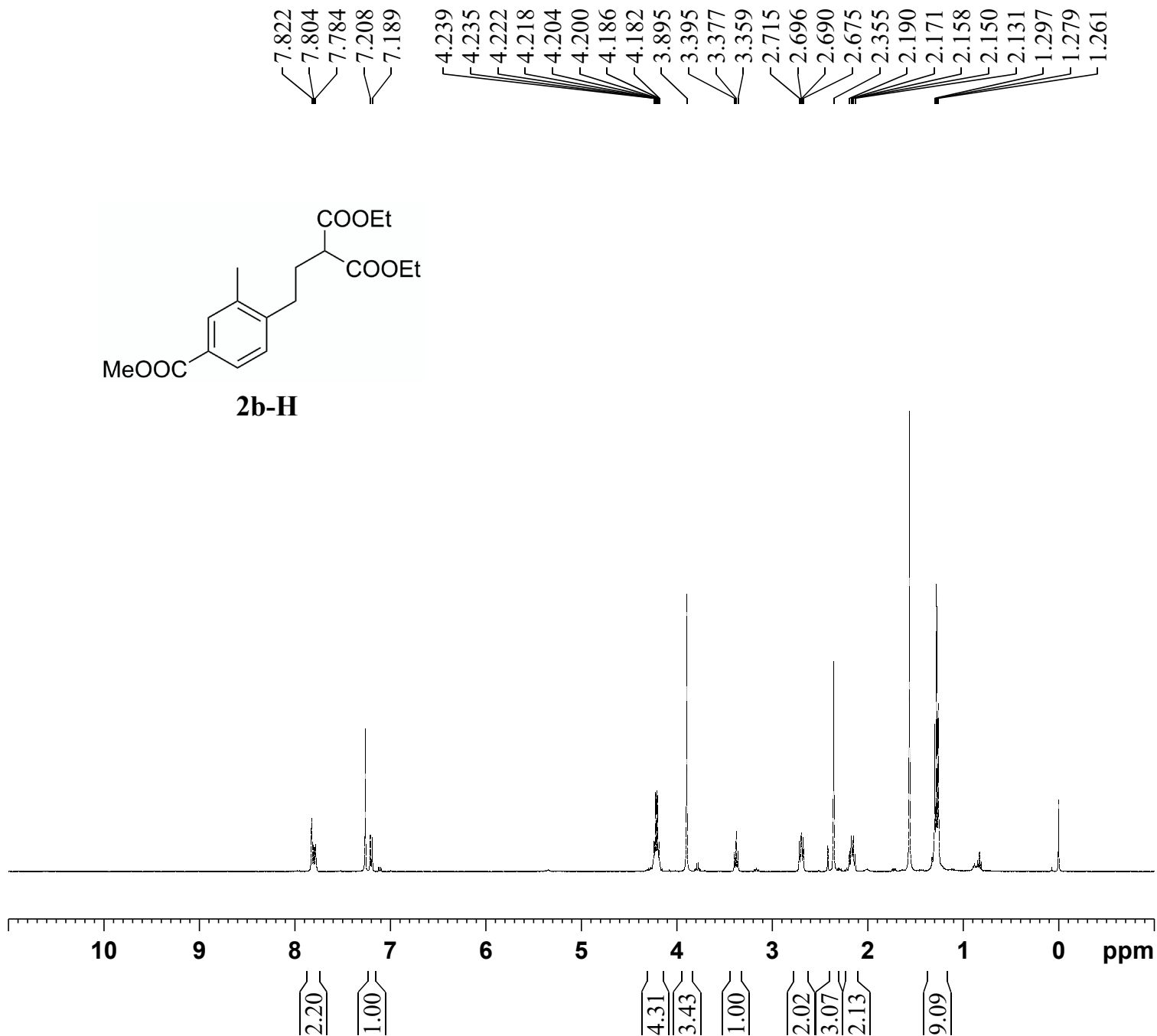
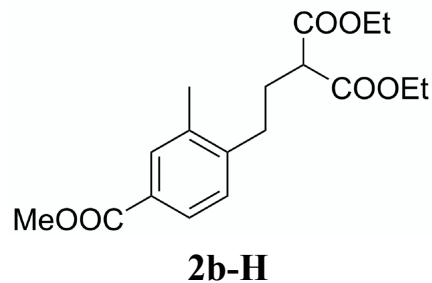
SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

==== CHANNEL f2 =====

SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters

SI 65536
 SF 400.2400067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



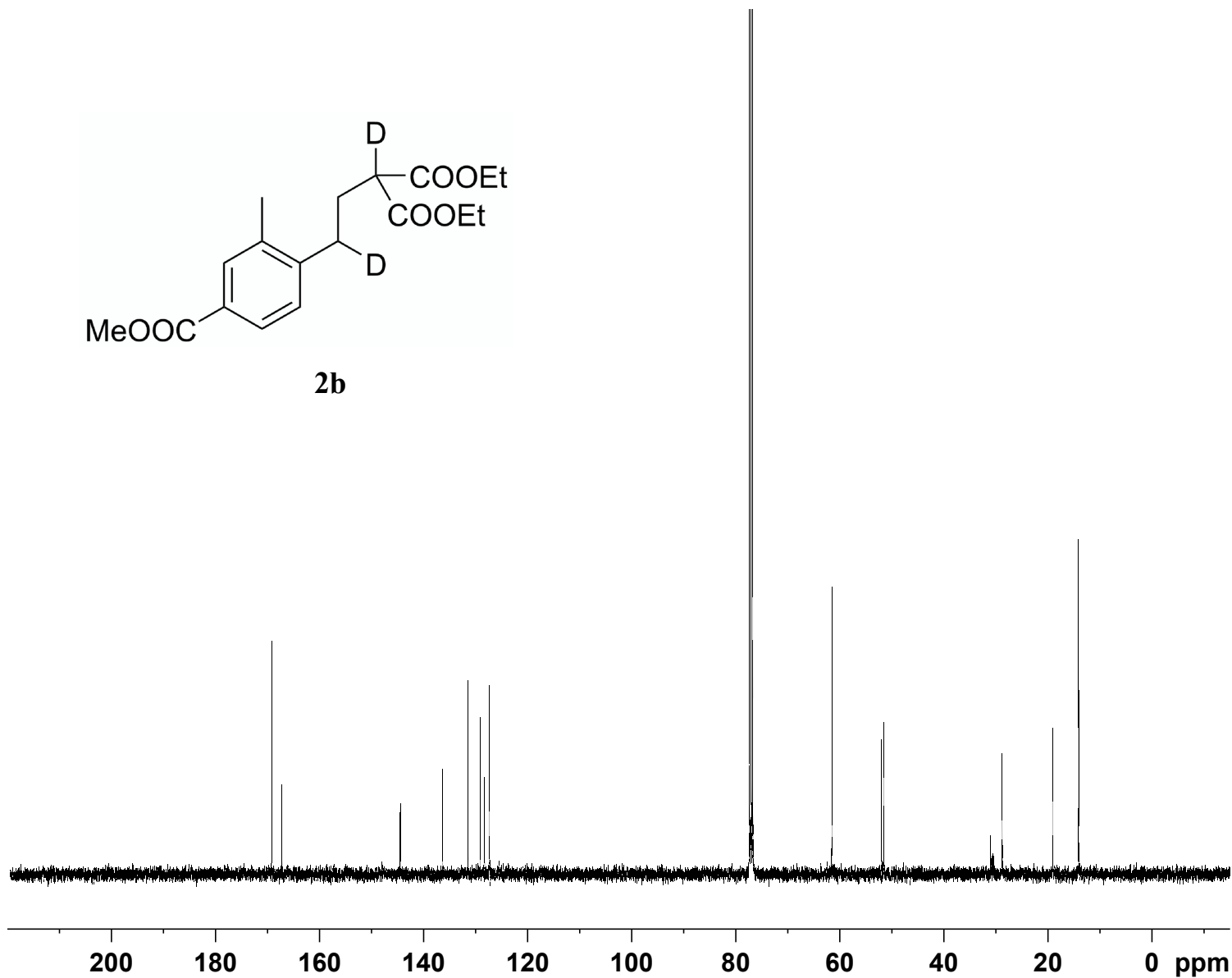
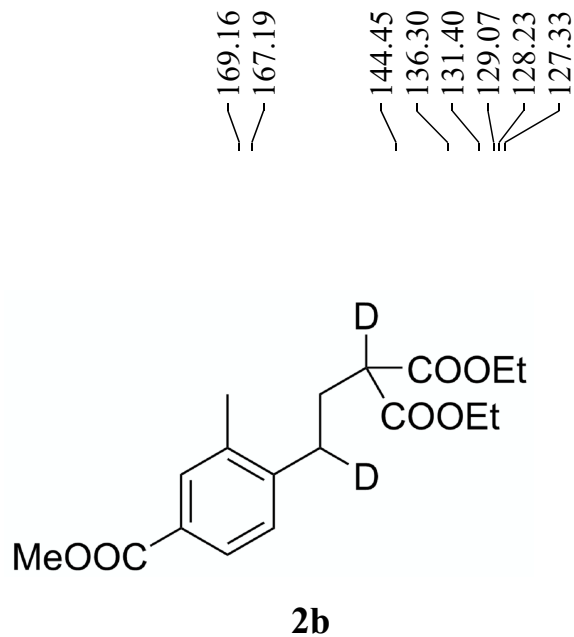
Current Data Parameters
 NAME 400M-2022
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 6.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 206.33
 DW 62.400 usec
 DE 6.50 usec
 TE 300.9 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



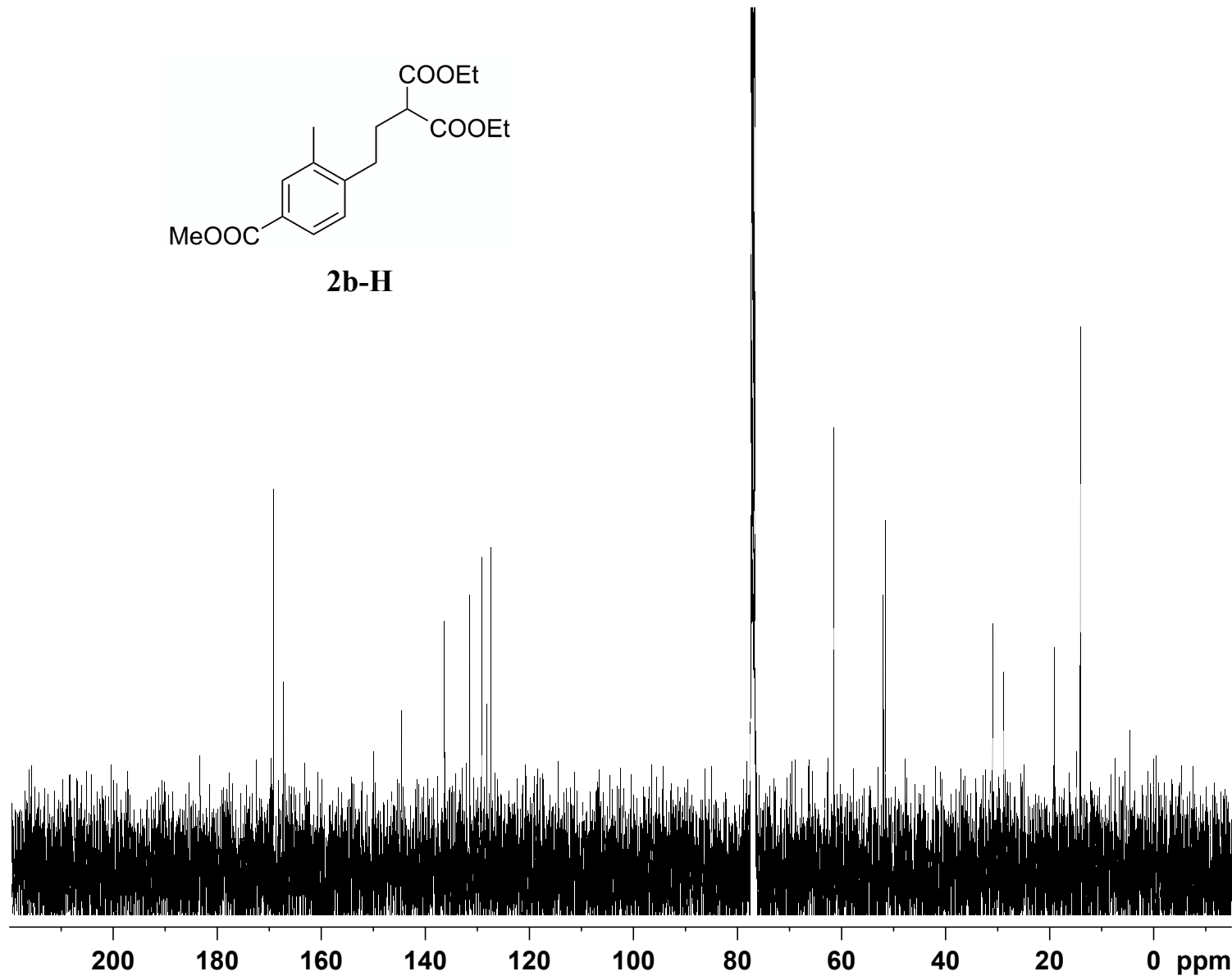
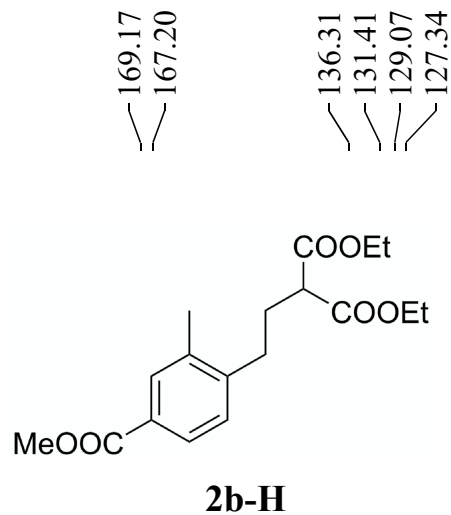
Current Data Parameters
 NAME 400M-2022
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 6.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



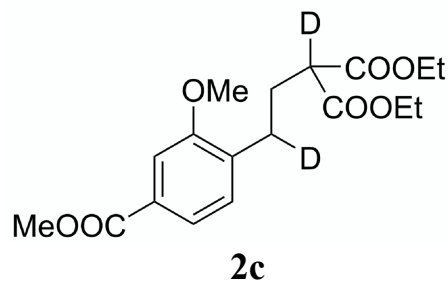
Current Data Parameters
 NAME 400M-2022
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 7.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.6 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.0000000 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.0000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.588
7.572
7.570
7.495
7.188
7.173

4.219
4.205
4.196
4.191
4.182
4.168
3.907
3.866
3.331
3.316
3.301
2.729
2.711
2.679
2.201
2.186
2.171
1.284
1.270
1.255

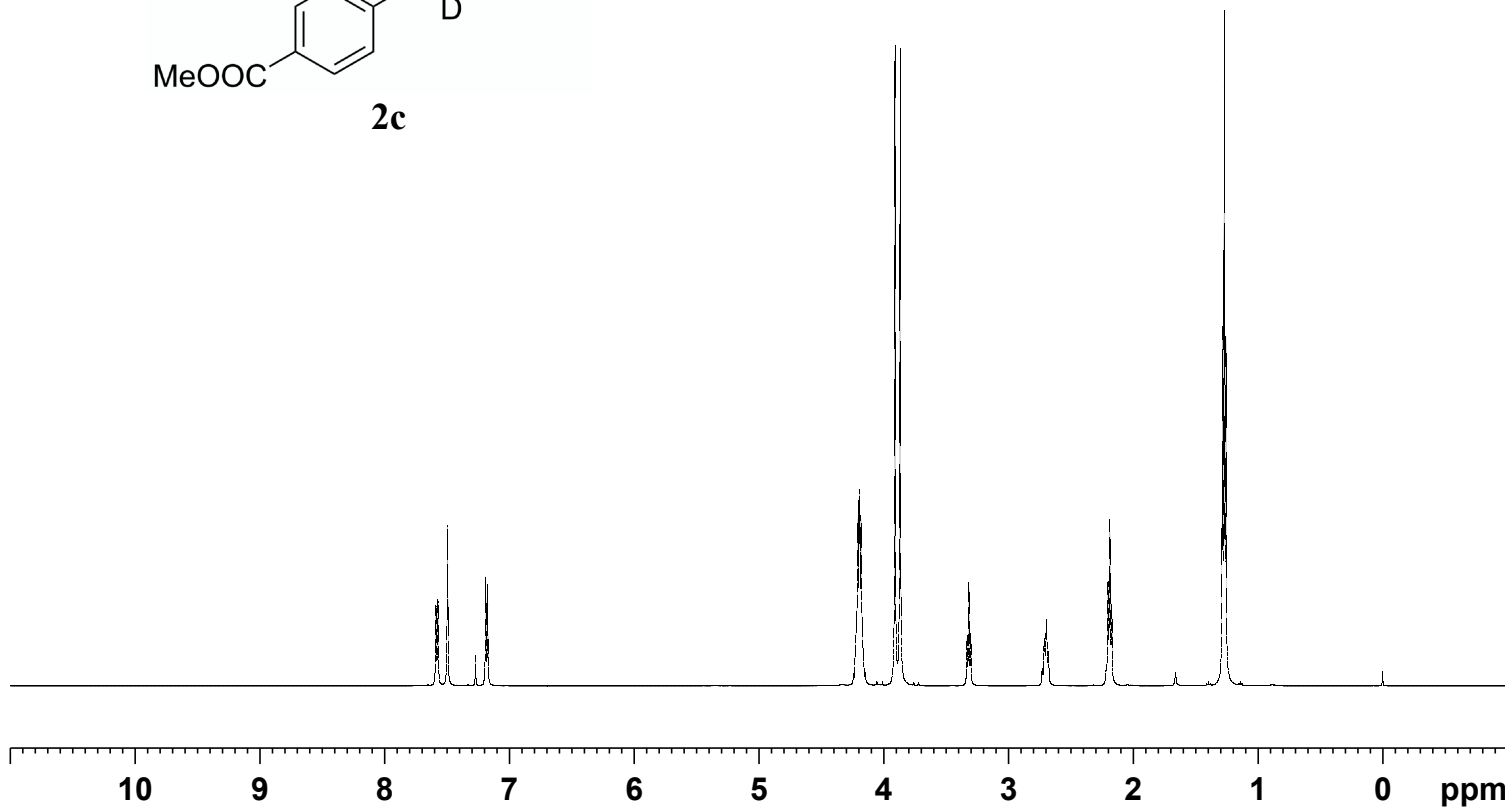
Current Data Parameters
NAME 500M-2022
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220218
Time 21.46
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

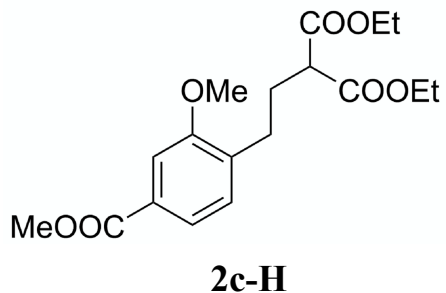
==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

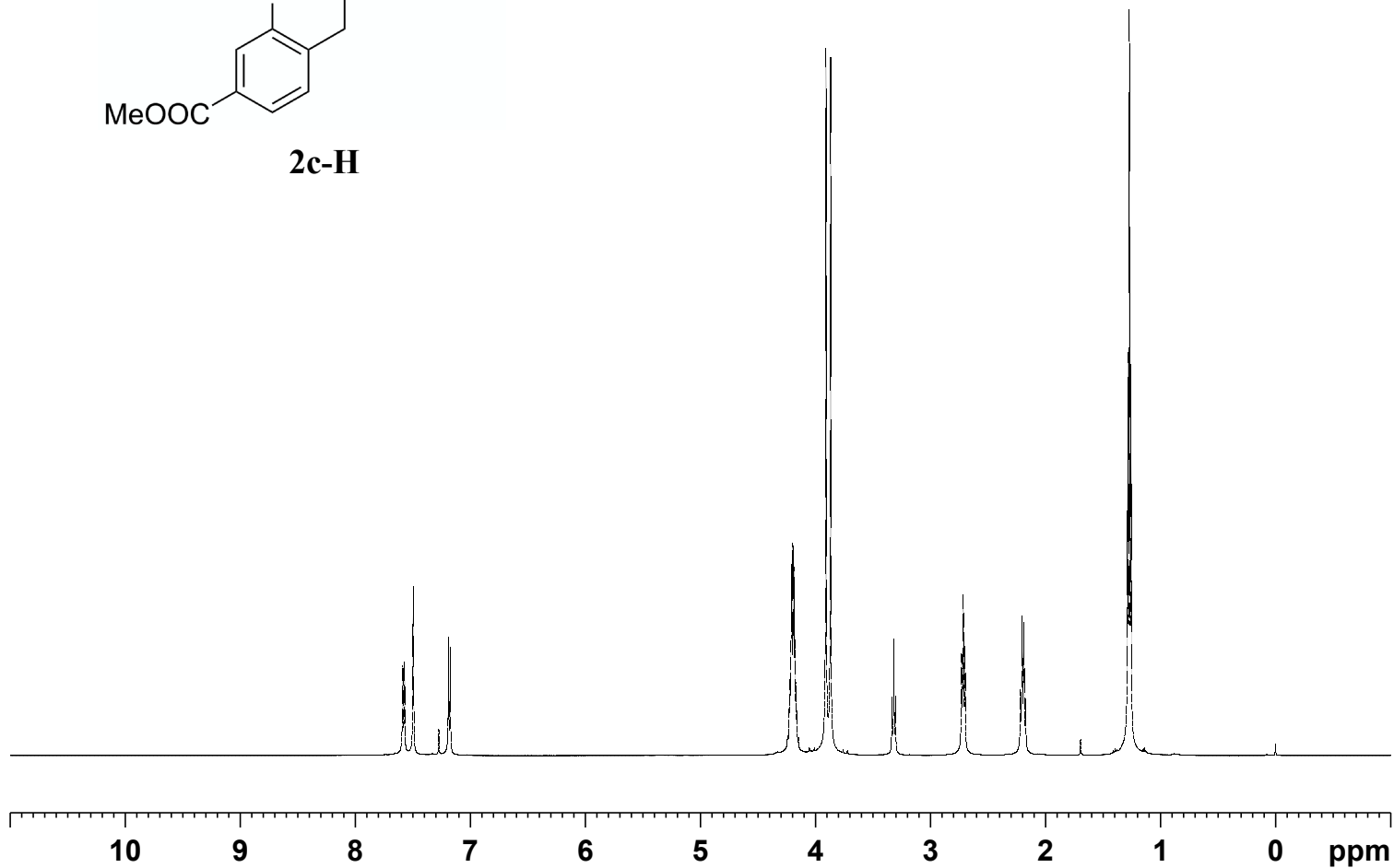


1.00
1.01
1.01

4.05
6.11
0.99
1.20
2.06
6.38



7.586
 7.571
 7.495
 7.189
 7.173
 4.226
 4.219
 4.209
 4.205
 4.196
 4.191
 4.182
 4.168
 4.160
 3.907
 3.867
 3.332
 3.318
 3.303
 2.729
 2.714
 2.699
 2.217
 2.202
 2.187
 2.172
 1.284
 1.270
 1.255



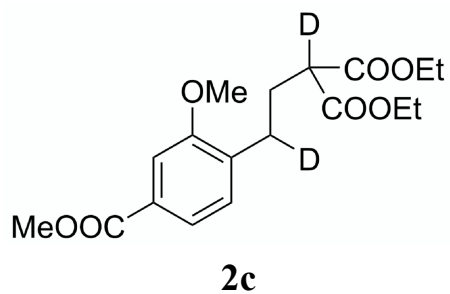
Current Data Parameters
 NAME 500M-2022
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220218
 Time 21.28
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

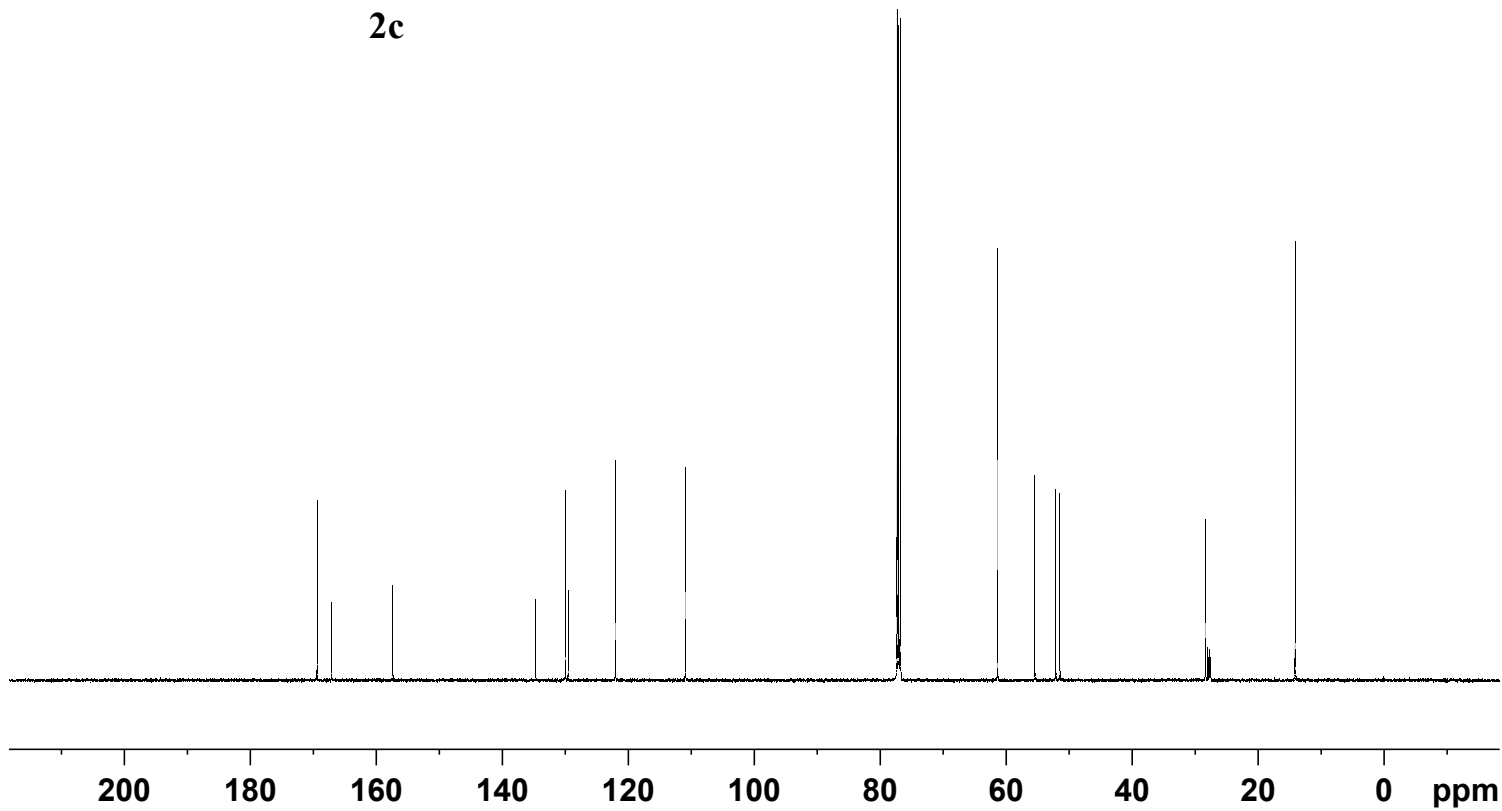
===== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300056 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



169.35
167.07
157.37
134.70
134.67
129.94
129.51
122.00
110.90

61.35
55.43
52.09
51.45
28.37
28.30
28.00
27.82
27.67
27.51
14.09
-0.01



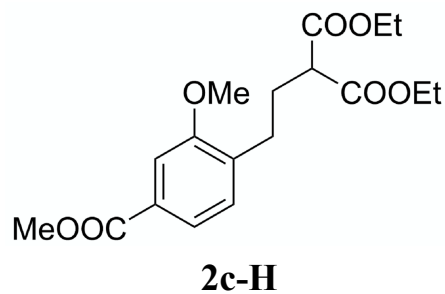
Current Data Parameters
NAME 500M-2022
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220218
Time 22.01
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 10.50 usec
PLW1 57.00000000 W

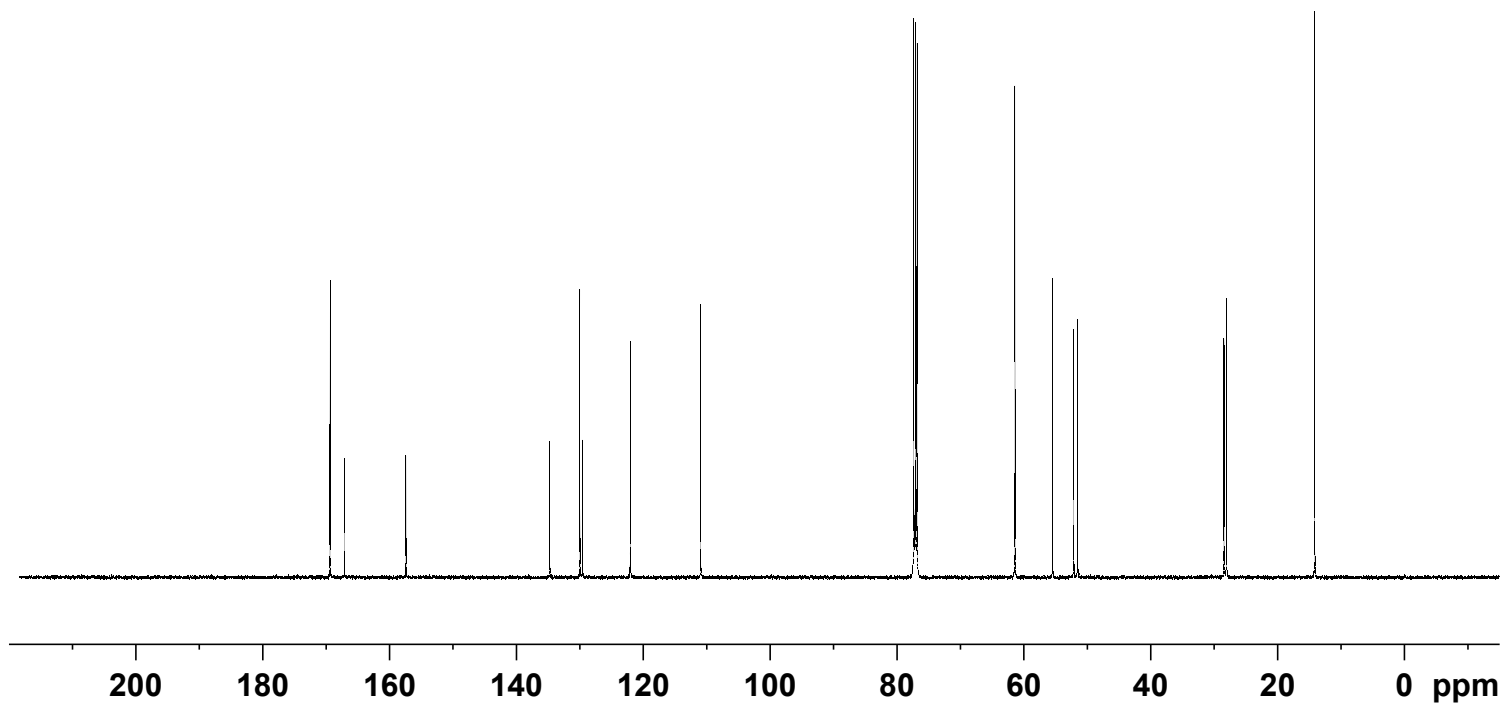
==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.39550999 W
PLW13 0.25312999 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



169.34
 167.06
 157.36
 134.70
 129.94
 129.50
 121.99
 110.90

77.31
 77.05
 76.80
 61.34
 55.42
 52.08
 51.47
 28.37
 27.99
 14.08



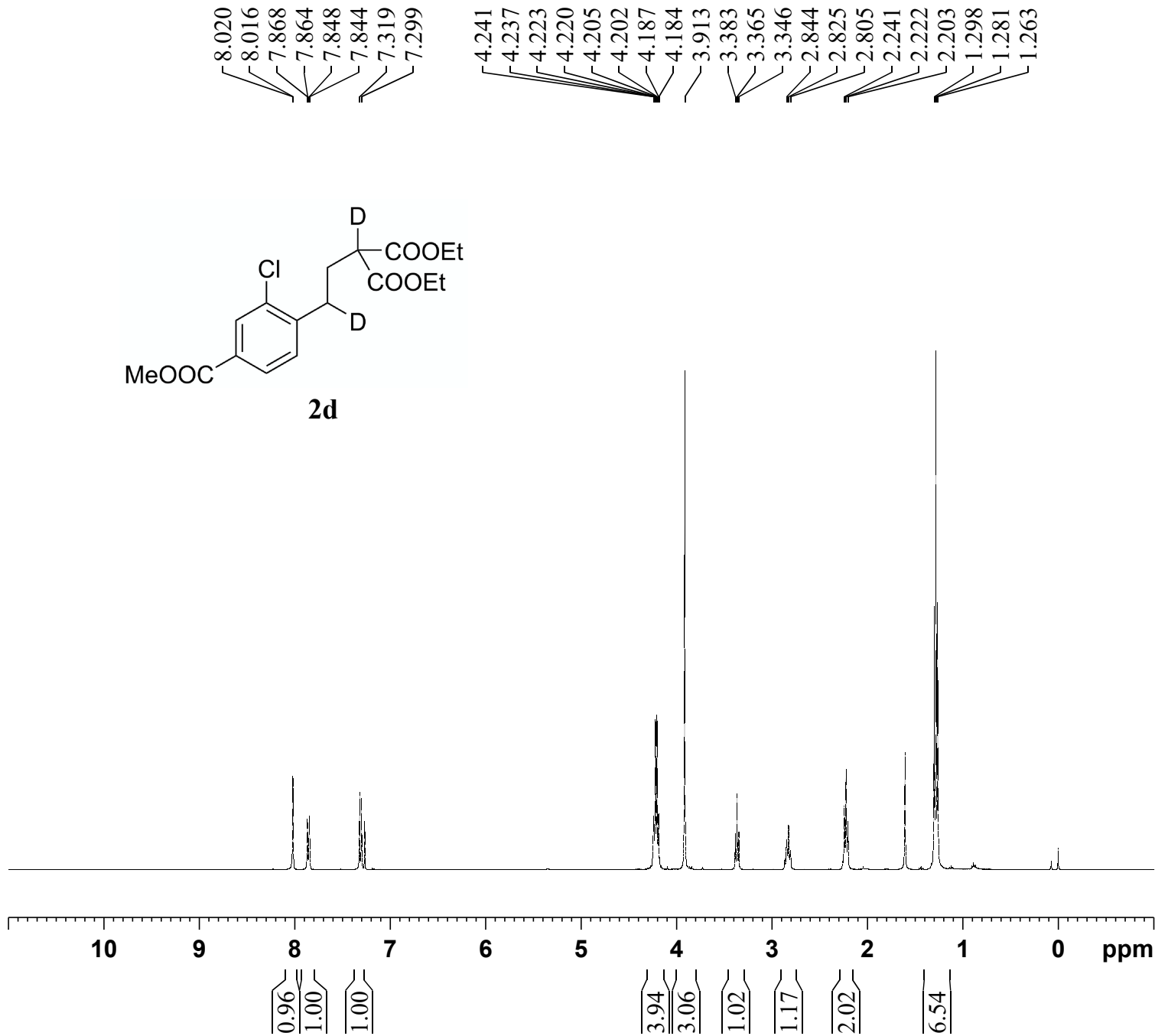
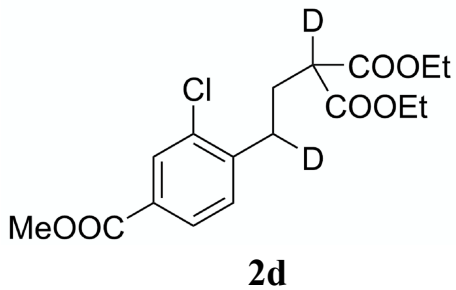
Current Data Parameters
 NAME 500M-2022
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220218
 Time 21.43
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



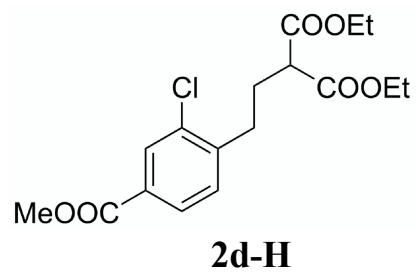
Current Data Parameters
 NAME 400M-2022
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 4.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 206.33
 DW 62.400 usec
 DE 6.50 usec
 TE 300.9 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

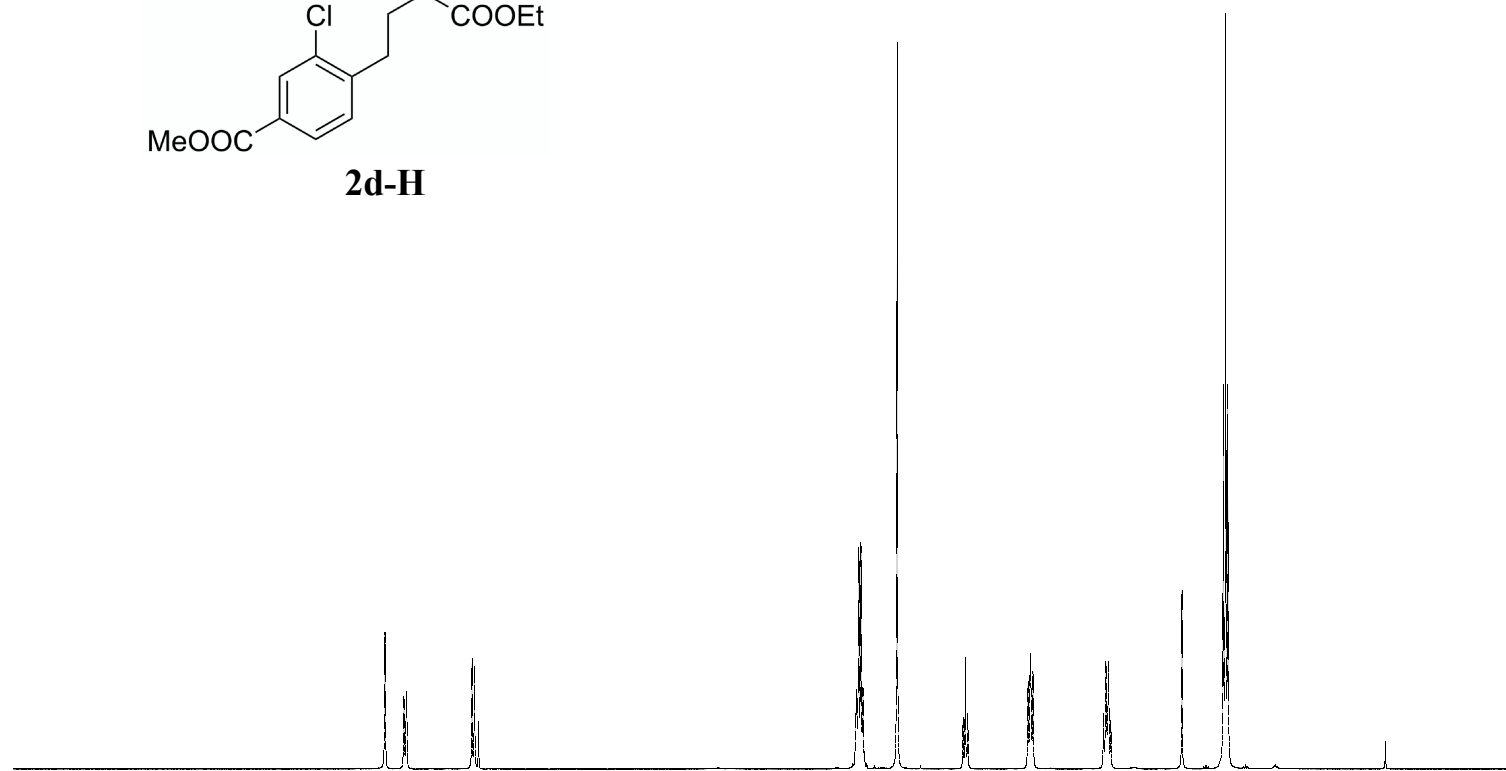
==== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400072 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8.020
8.016
7.868
7.864
7.848
7.844
7.320
7.300

4.241
4.238
4.223
4.220
4.205
4.202
4.188
4.184
3.913
3.385
3.366
3.348
2.864
2.845
2.824
2.259
2.240
2.220
2.201
1.299
1.281
1.263



1.00
1.04
1.06

4.21
3.20
1.04
2.13
2.15
6.77

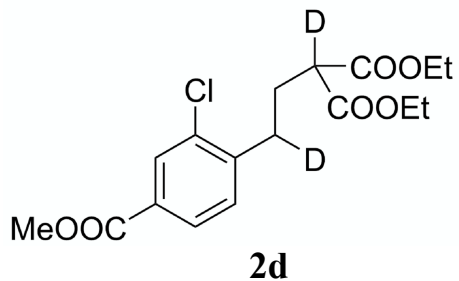
Current Data Parameters
NAME 400M-2022
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220701
Time 5.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 206.33
DW 62.400 usec
DE 6.50 usec
TE 300.9 K
D1 2.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

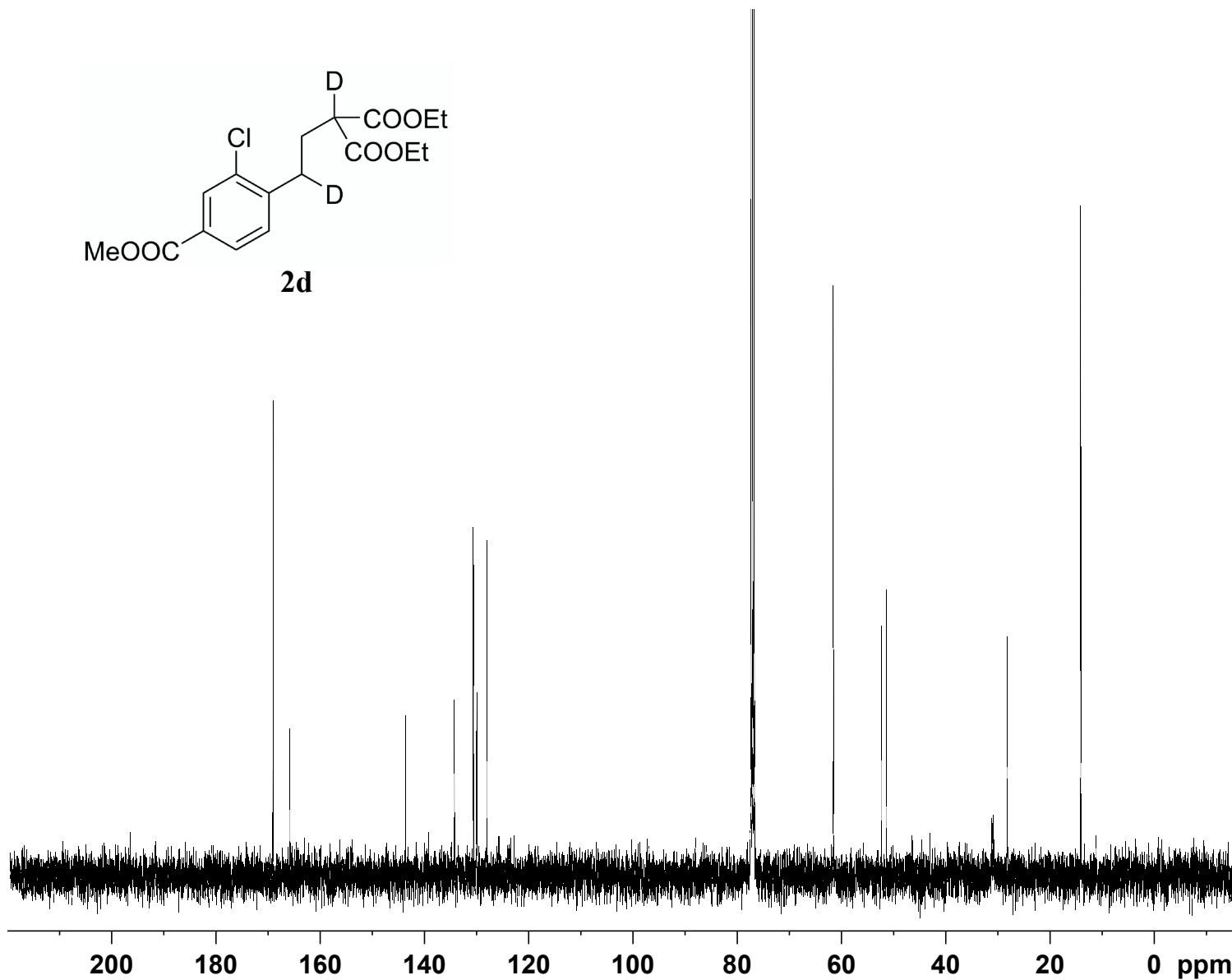
==== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



169.04
 165.86
 143.59
 134.22
 130.70
 130.46
 129.95
 127.98

61.52
 52.29
 51.36
 31.23
 30.90
 28.13
 14.07



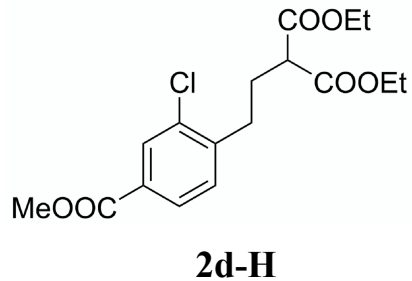
Current Data Parameters
 NAME 400M-2022
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 5.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

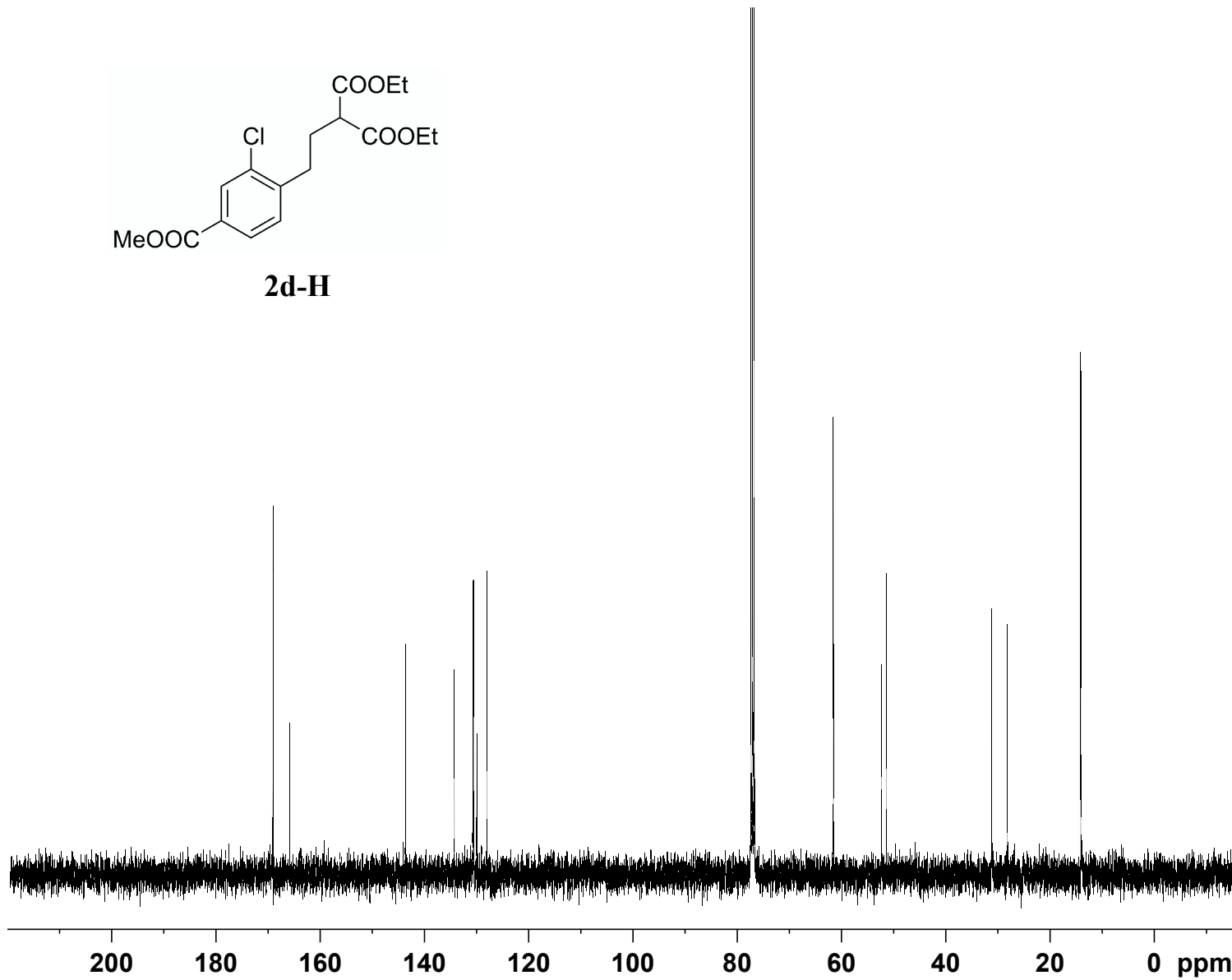
===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



169.03
 165.86
 143.62
 134.22
 130.70
 130.46
 129.94
 127.98

61.52
 52.28
 51.38
 31.22
 28.20
 14.07



Current Data Parameters
 NAME 400M-2022
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 5.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

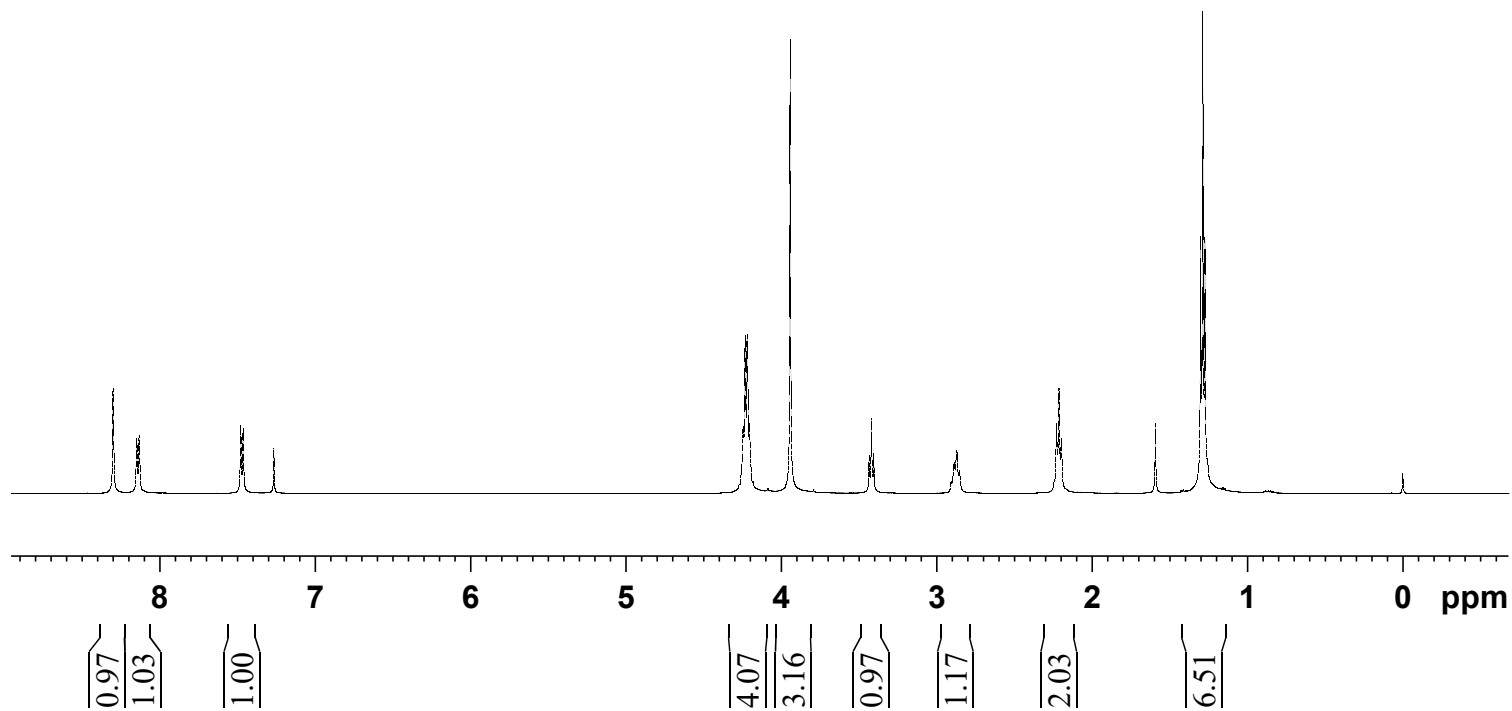
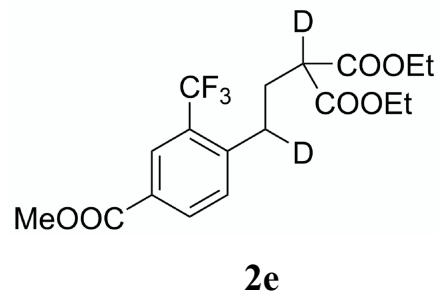
===== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

8.300
8.148
8.132
7.479
7.463

4.245
4.234
4.231
4.220
4.217
4.207
4.203
3.942
3.434
3.420
3.405
2.907
2.886
2.871
2.854
2.228
2.213
2.197
1.301
1.287
1.273



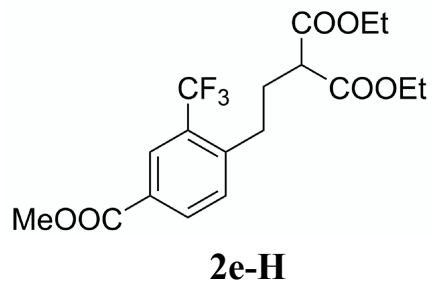
Current Data Parameters
NAME 500M-2022
EXPNO 59
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220324
Time 22.19
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

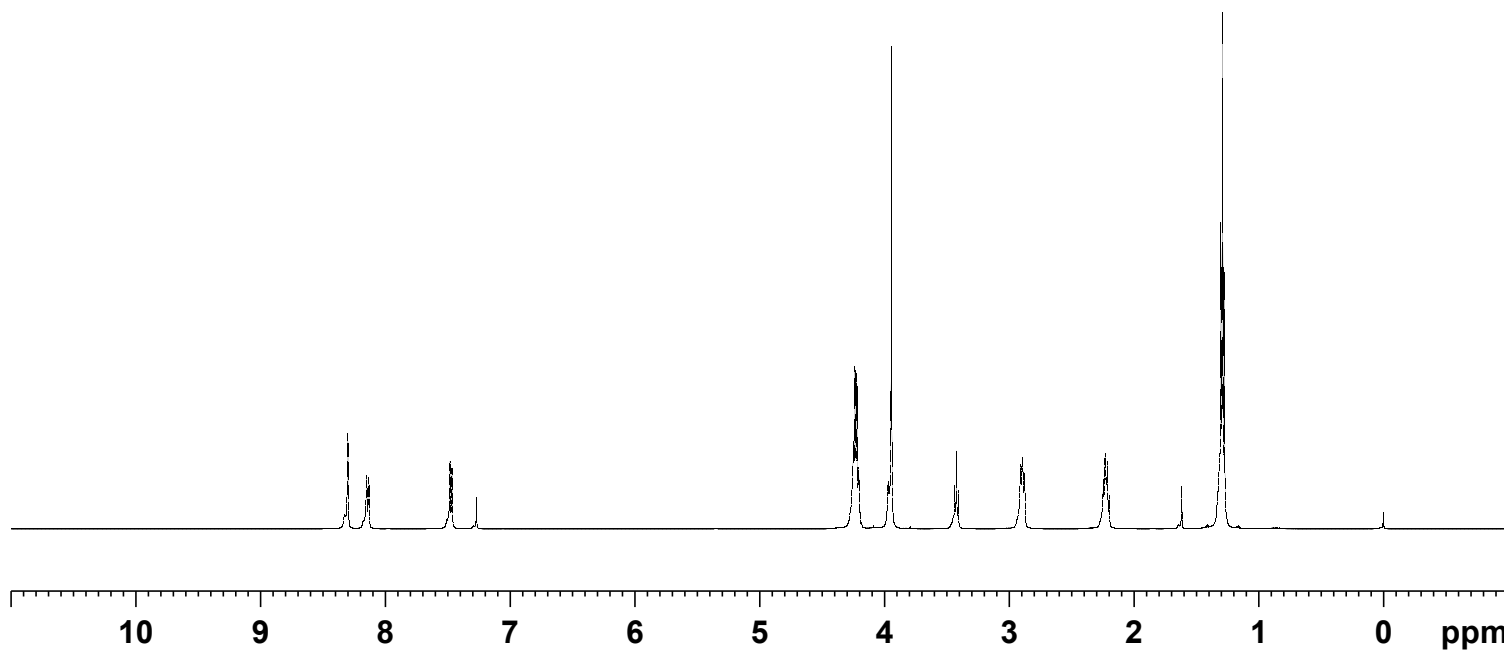
==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



8.301
8.150
8.134
7.481
7.465

4.257
4.250
4.245
4.236
4.231
4.221
4.217
4.207
4.203
3.943
3.436
3.421
3.407
2.908
2.893
2.876
2.245
2.230
2.223
2.213
2.198
1.302
1.288
1.273



1.01
1.00
1.02

4.04
3.05
1.01
2.03
2.05
6.22

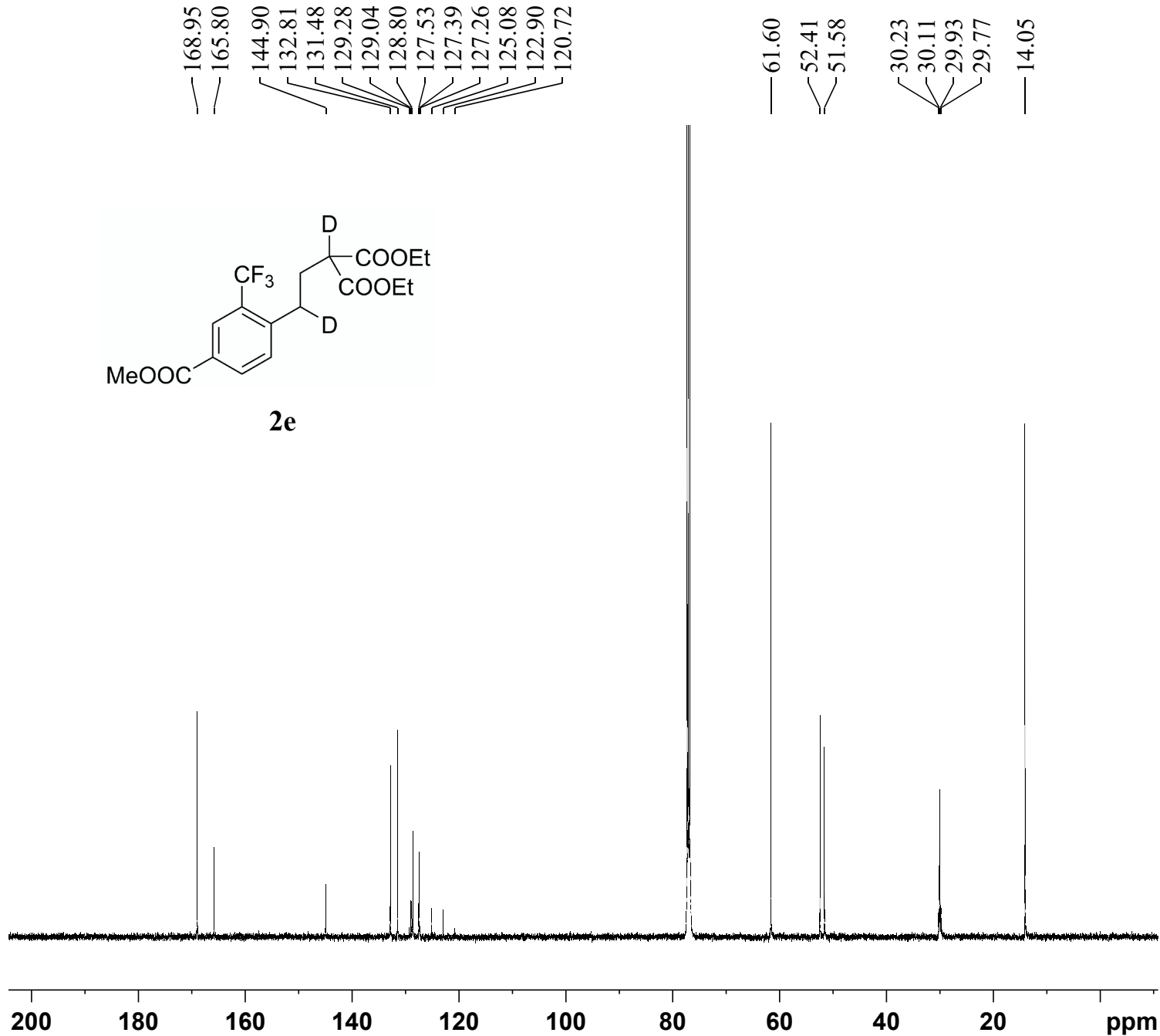
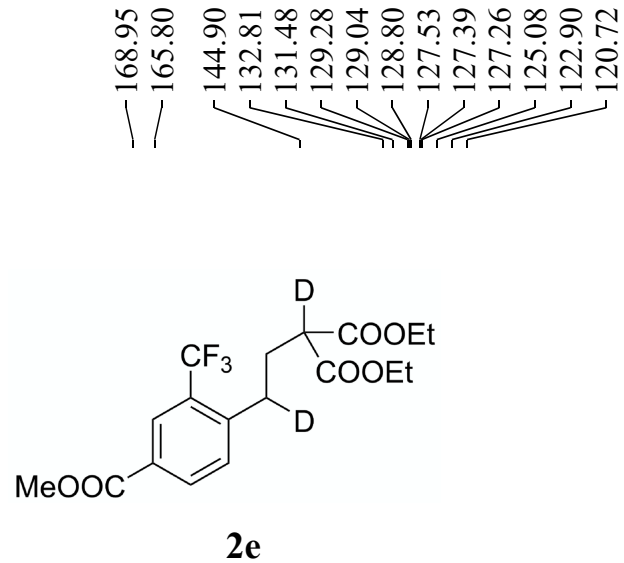
Current Data Parameters
NAME 500M-2022
EXPNO 57
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220324
Time 21.47
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



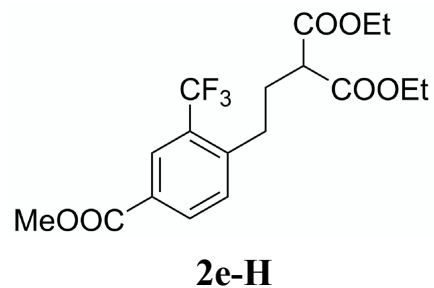
Current Data Parameters
 NAME 500M-2022
 EXPNO 60
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220324
 Time 22.46
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 500
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

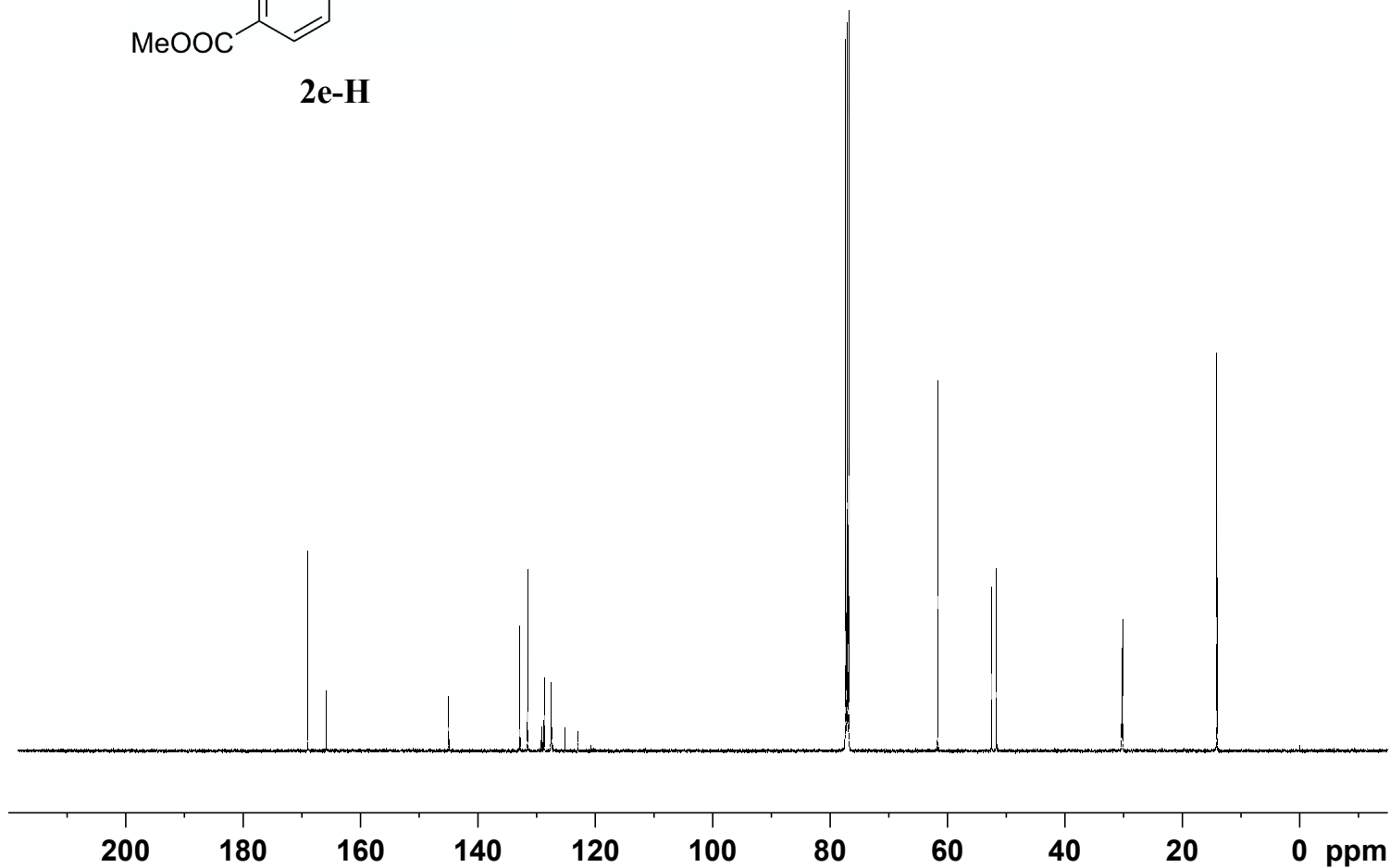
==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



168.94
 165.79
 144.93
 132.80
 131.48
 129.04
 128.79
 128.60
 127.48
 127.43
 127.39
 125.08
 122.90

61.60
 52.41
 51.60
 30.24
 30.11
 14.05



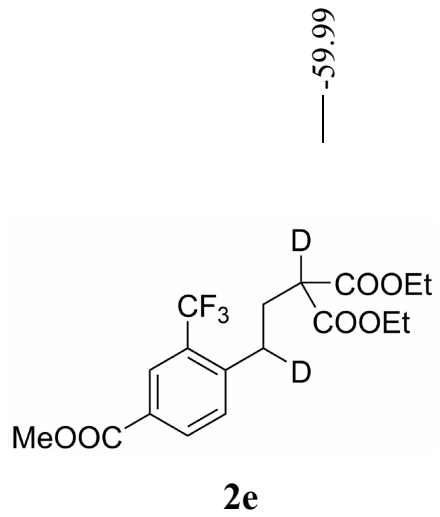
Current Data Parameters
 NAME 500M-2022
 EXPNO 58
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220324
 Time 22.14
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 500
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



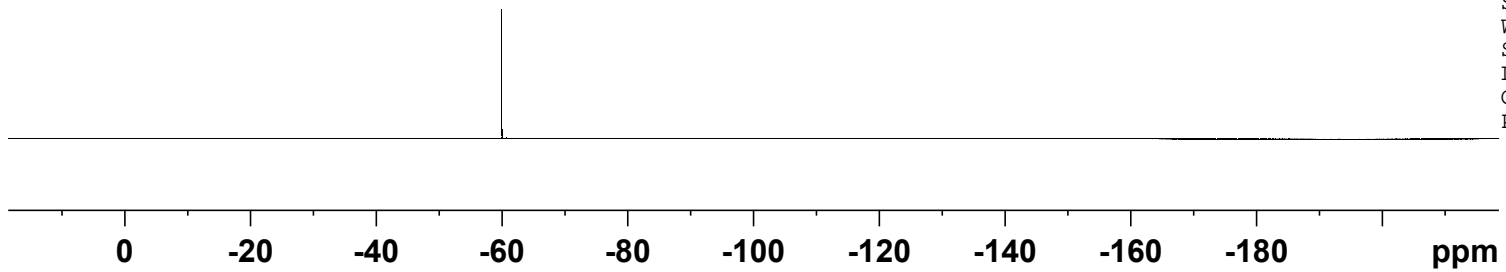
Current Data Parameters
 NAME 400M-2023-F
 EXPNO 5
 PROCNO 1

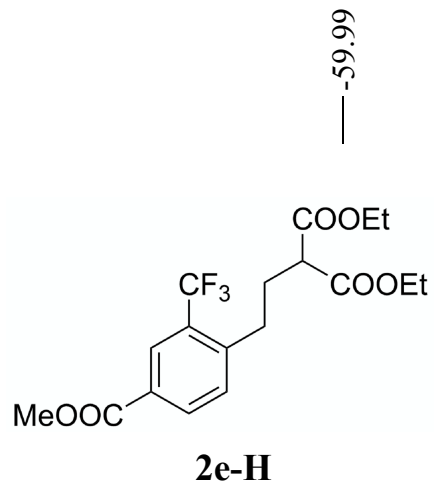
F2 - Acquisition Parameters
 Date_ 20230506
 Time 19.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT CDC13
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 206.33
 DW 5.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 376.5642094 MHz
 NUC1 19F
 P1 14.50 usec
 PLW1 17.98900032 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 65536
 SF 376.6018696 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





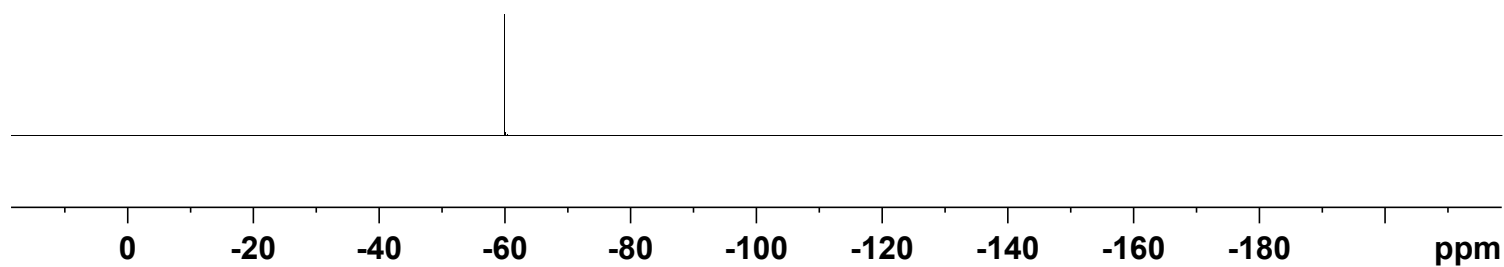
Current Data Parameters
 NAME 400M-2023-F
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230506
 Time 18.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT CDC13
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 206.33
 DW 5.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

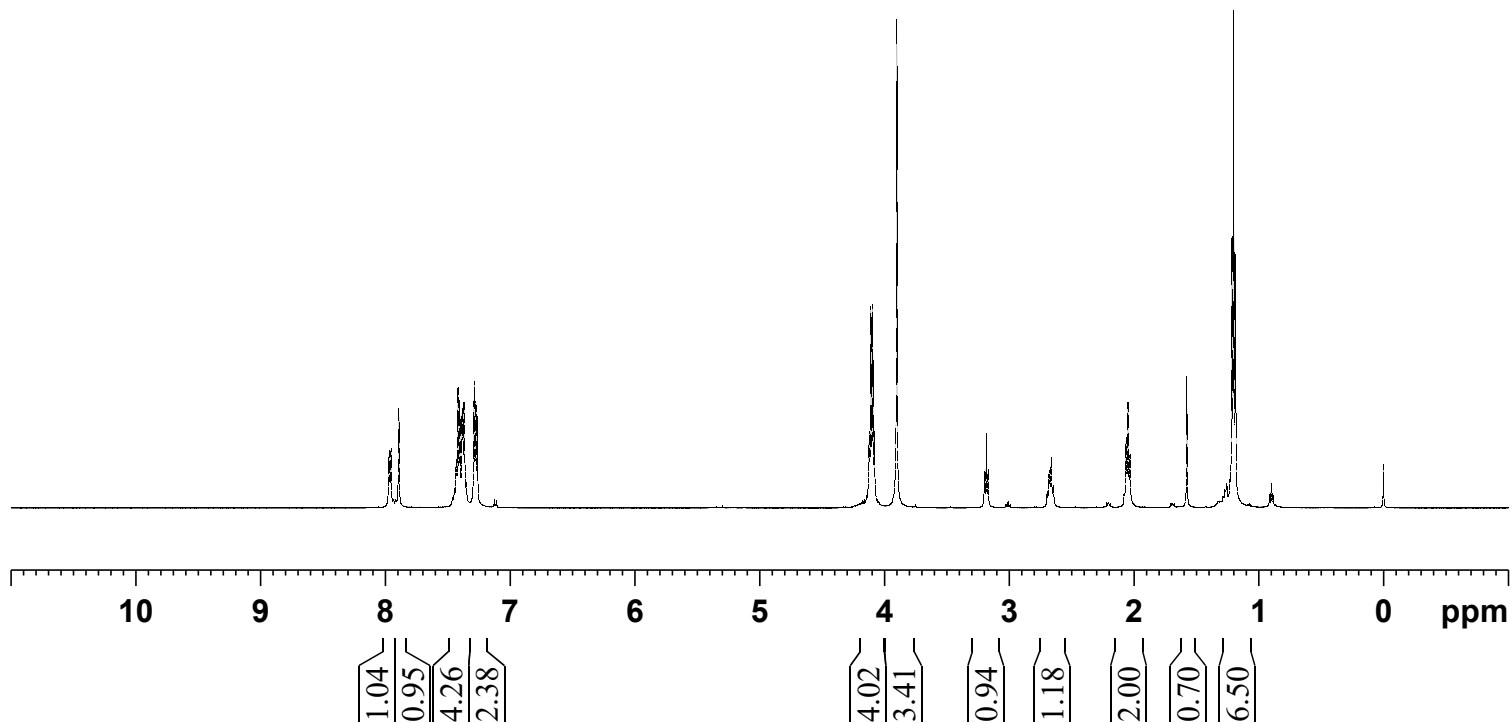
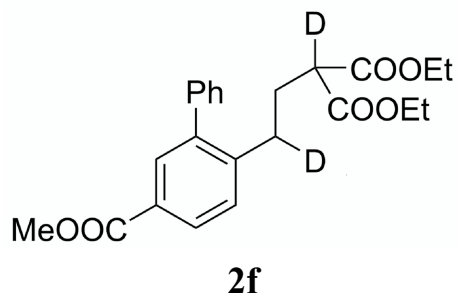
==== CHANNEL f1 =====
 SFO1 376.5642094 MHz
 NUC1 19F
 P1 14.50 usec
 PLW1 17.98900032 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 65536
 SF 376.6018696 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



7.972
7.969
7.957
7.953
7.893
7.891
7.444
7.431
7.417
7.402
7.385
7.379
7.369
7.350
7.287
7.273
7.261
4.121
4.107
4.093
4.079
3.899
3.198
3.183
3.168
2.695
2.679
2.662
2.646
2.062
2.047
2.031
1.214
1.200
1.185



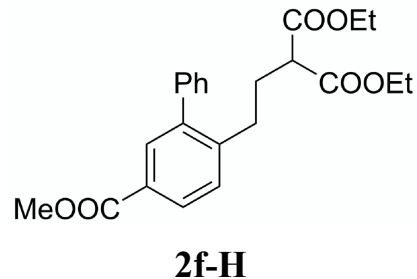
Current Data Parameters
NAME 500M-2022
EXPNO 51
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220315
Time 10.33
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.970
7.954
7.891
7.431
7.417
7.402
7.386
7.379
7.370
7.350
7.288
7.273
7.262

4.122
4.108
4.094
4.080
3.899
3.199
3.184
3.170
2.696
2.680
2.664
2.079
2.063
2.047
2.032
1.214
1.200
1.186

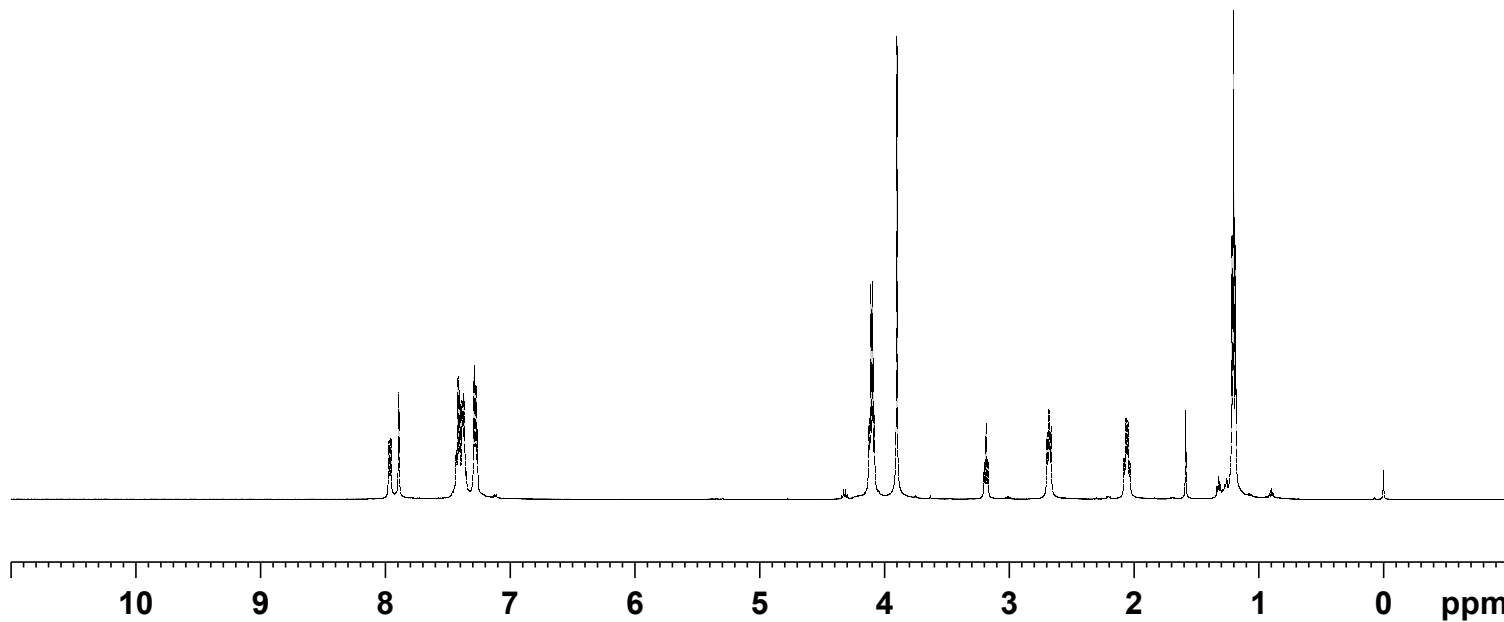
Current Data Parameters
 NAME 500M-2022
 EXPNO 44
 PROCNO 1

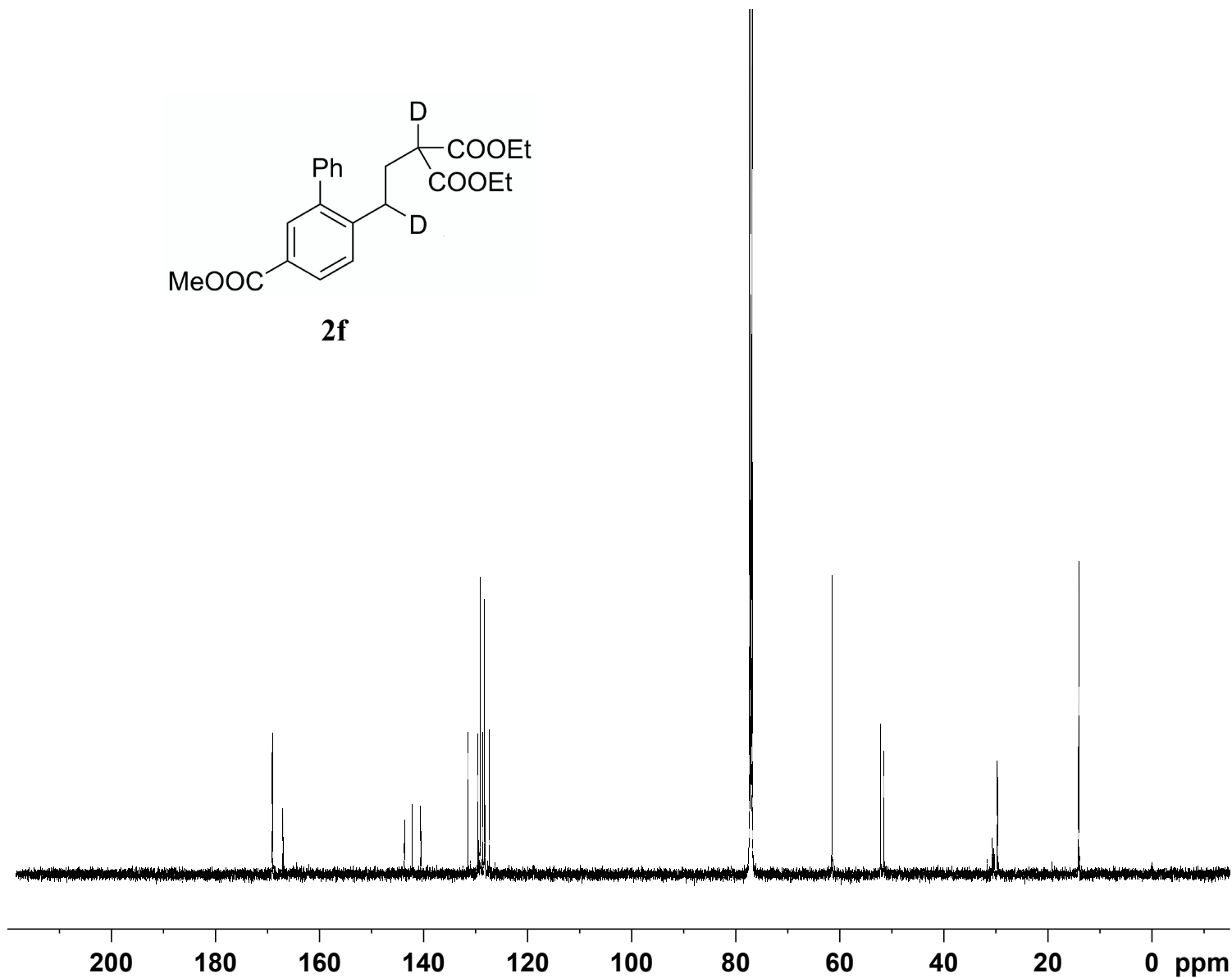
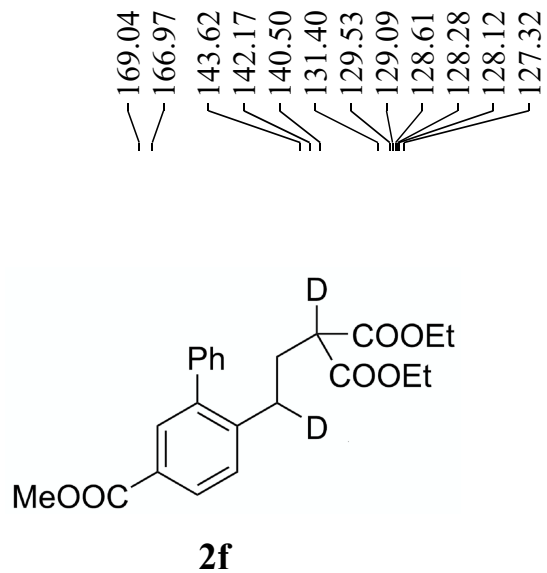
F2 - Acquisition Parameters
 Date_ 20220315
 Time 6.46
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300115 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





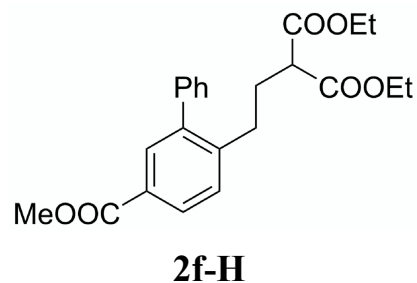
Current Data Parameters
 NAME 500M-2022
 EXPNO 49
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220315
 Time 7.33
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

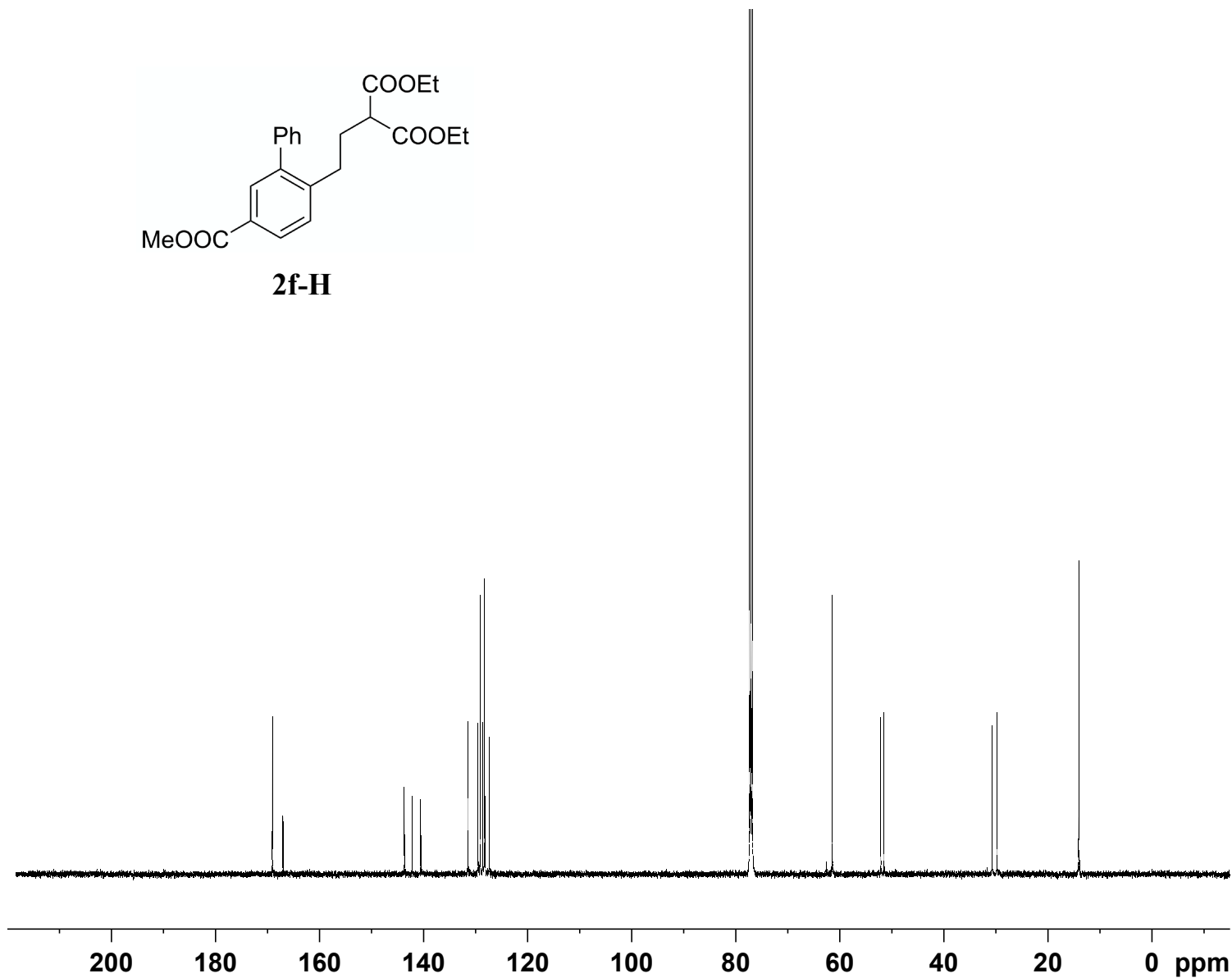
==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



169.03
 166.97
 143.66
 142.17
 140.50
 131.40
 129.53
 129.09
 128.61
 128.28
 128.12
 127.32

61.38
 52.07
 51.47
 30.68
 29.71
 14.02



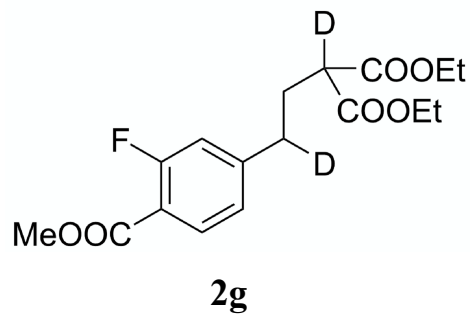
Current Data Parameters
 NAME 500M-2022
 EXPNO 46
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220315
 Time 7.07
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 300
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.880
7.865
7.849
7.041
7.039
7.023
6.987
6.964
4.231
4.226
4.218
4.213
4.203
4.199
4.190
4.185
4.178
3.919
3.329
3.314
3.299
2.718
2.702
2.686
2.670
2.242
2.226
2.211
2.196
1.292
1.277
1.263

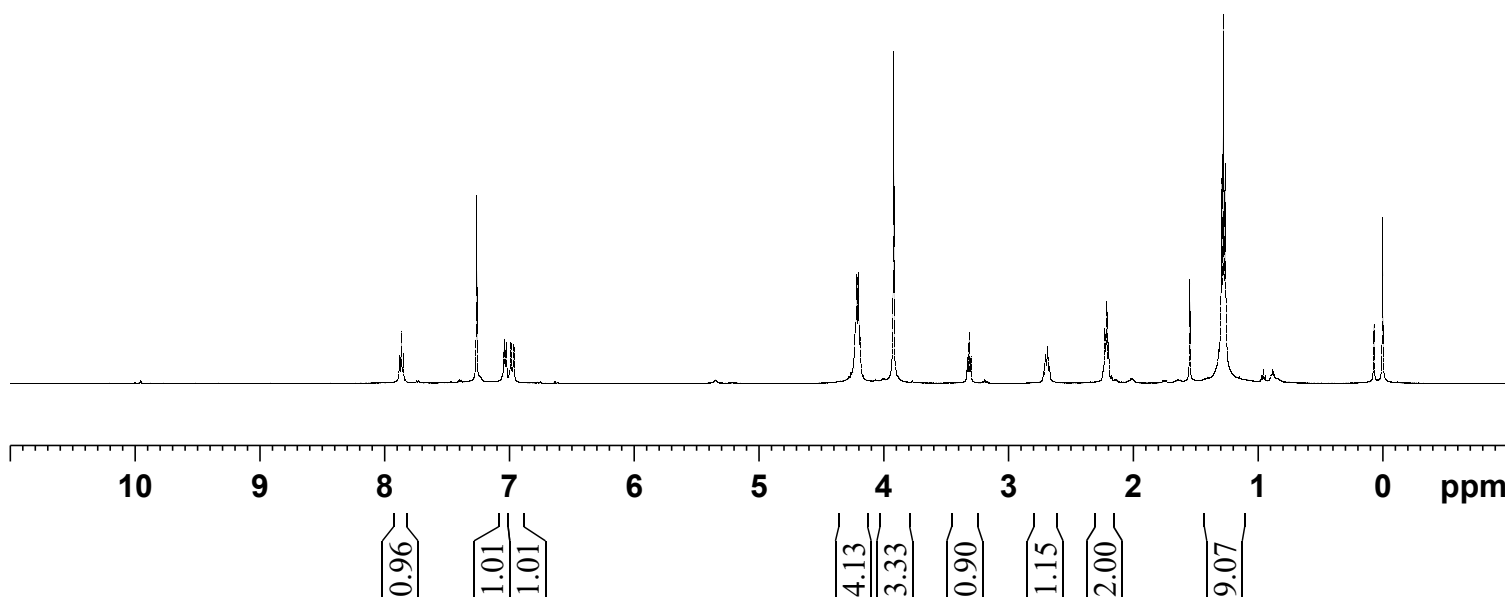
Current Data Parameters
NAME 500M-2022
EXPNO 5
PROCNO 1

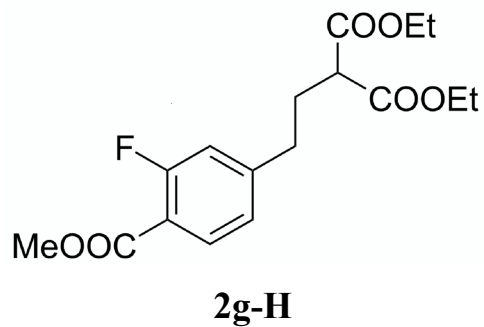
F2 - Acquisition Parameters
Date_ 20220216
Time 23.37
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 62.06
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

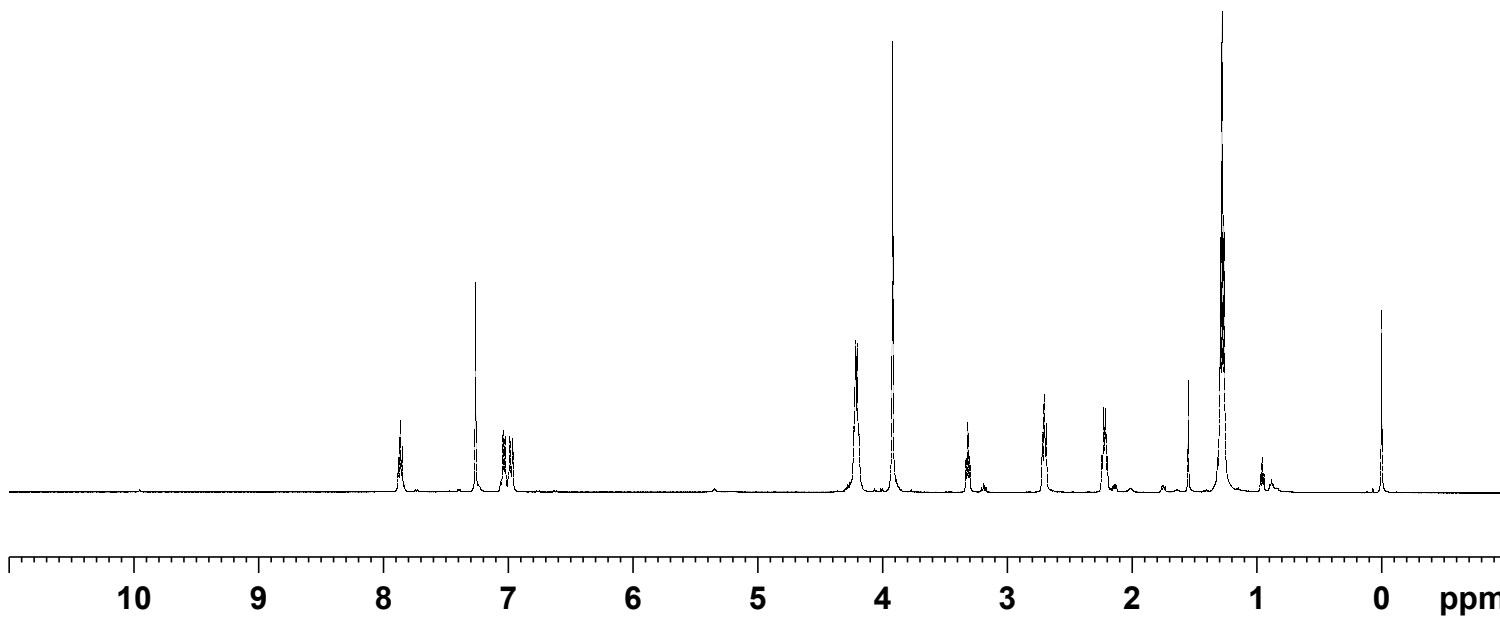
F2 - Processing parameters
SI 65536
SF 500.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





7.880
7.865
7.849
7.039
7.023
6.987
6.964

4.227
4.218
4.214
4.204
4.199
4.190
3.919
3.330
3.315
3.300
2.718
2.703
2.687
2.242
2.227
2.211
2.196
1.292
1.278
1.263



1.54
1.45
1.47

5.10
4.47
1.36
2.42
2.42
9.22

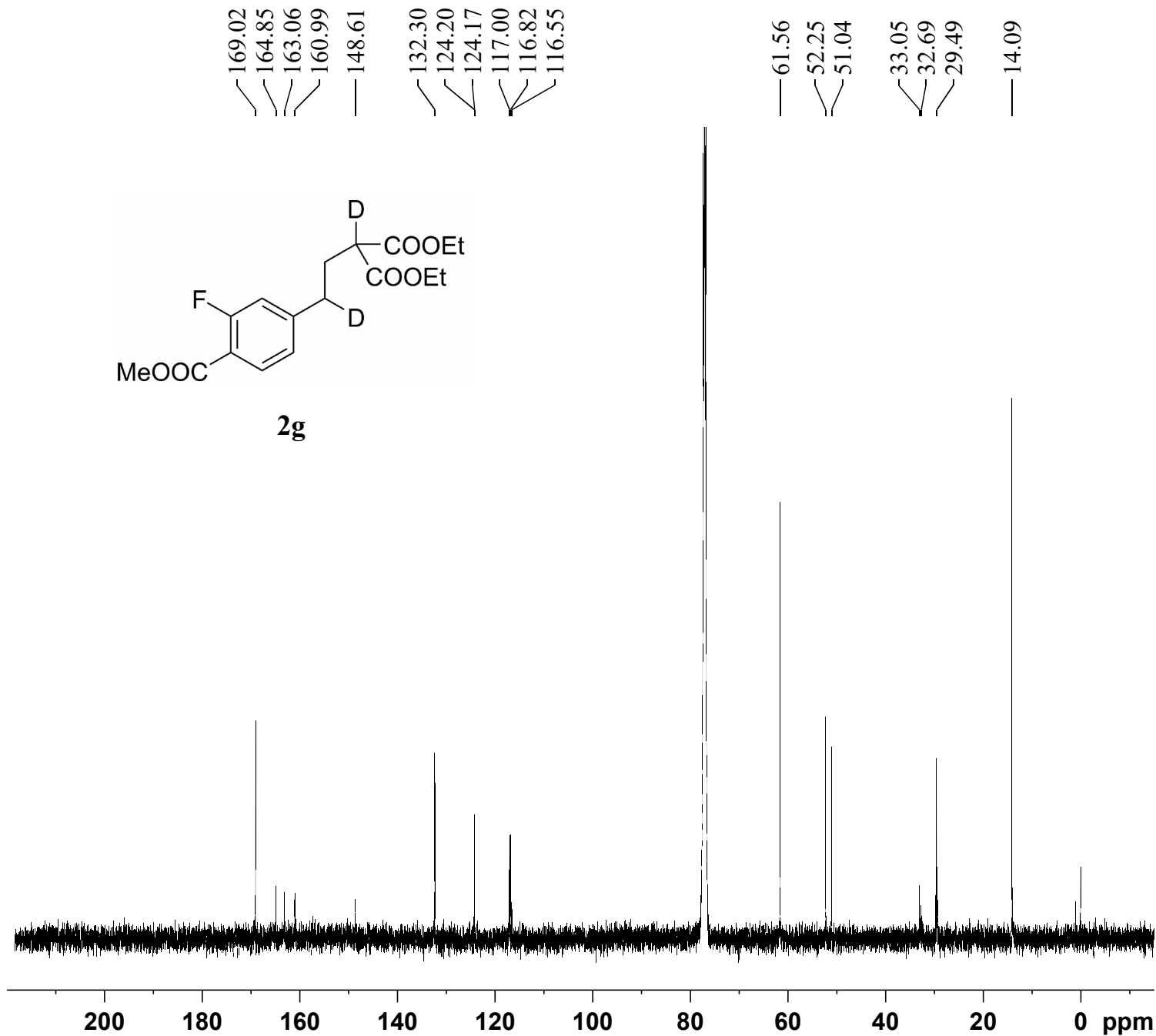
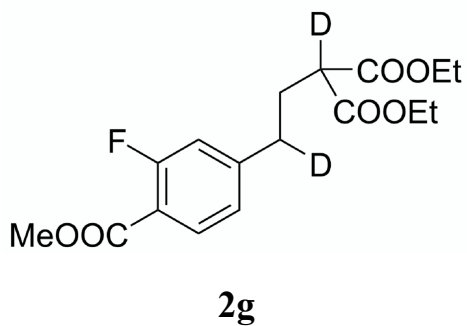
Current Data Parameters
NAME 500M-2022
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220216
Time 22.38
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 62.06
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



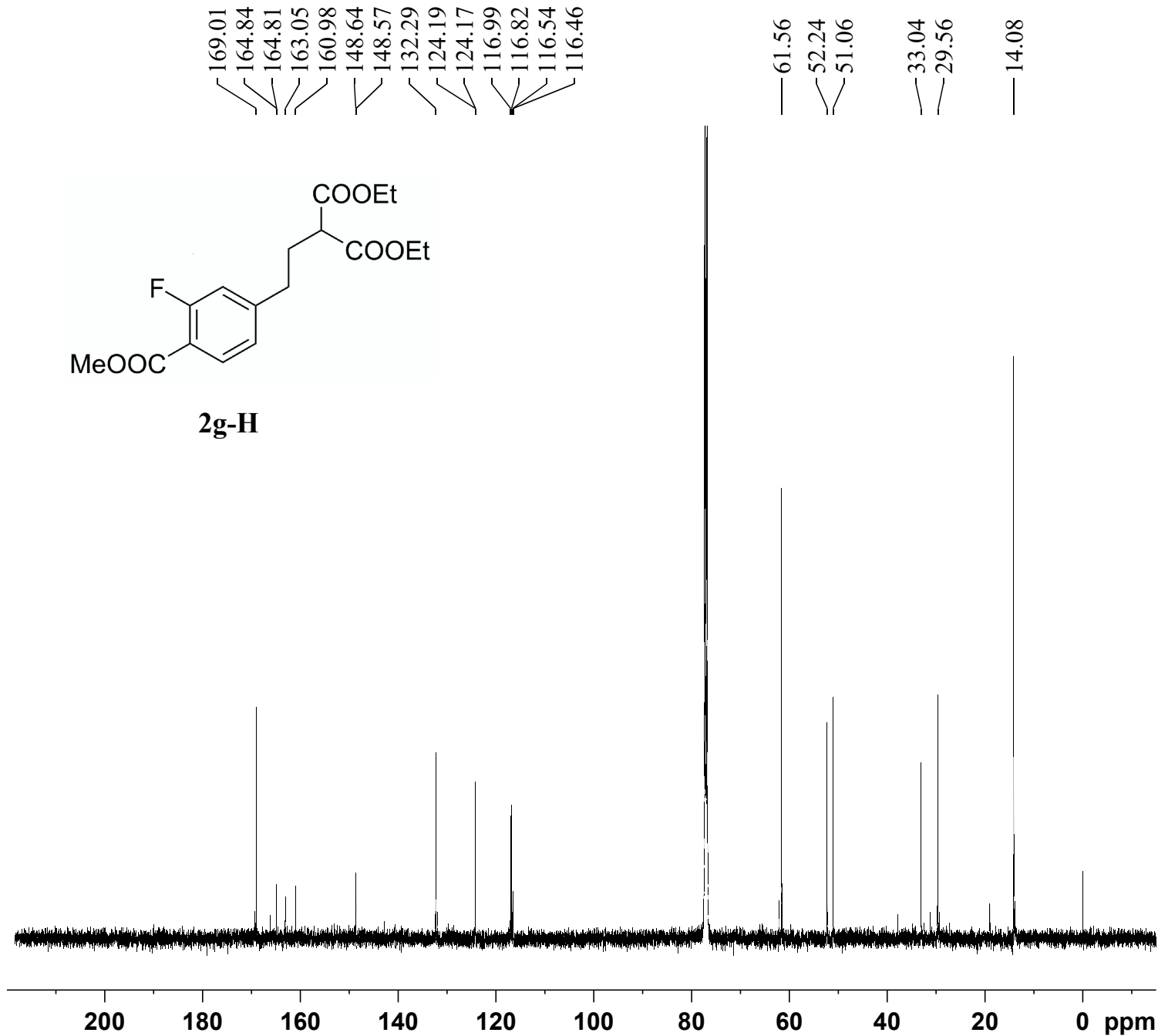
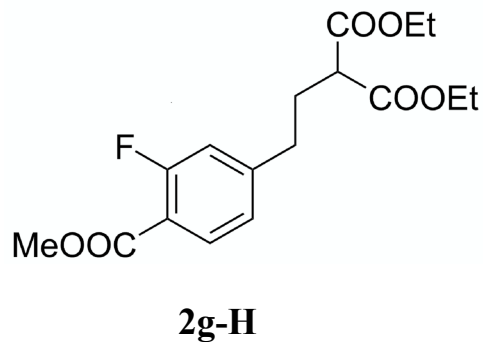
Current Data Parameters
 NAME 500M-2022
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220217
 Time 0.32
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.0000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.0000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



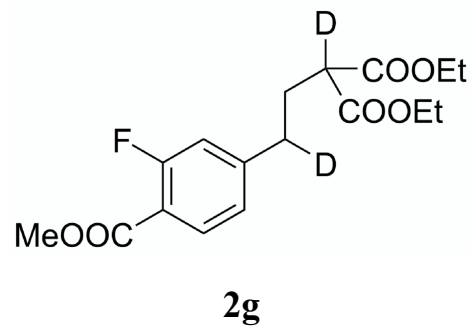
Current Data Parameters
 NAME 500M-2022
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220216
 Time 23.32
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

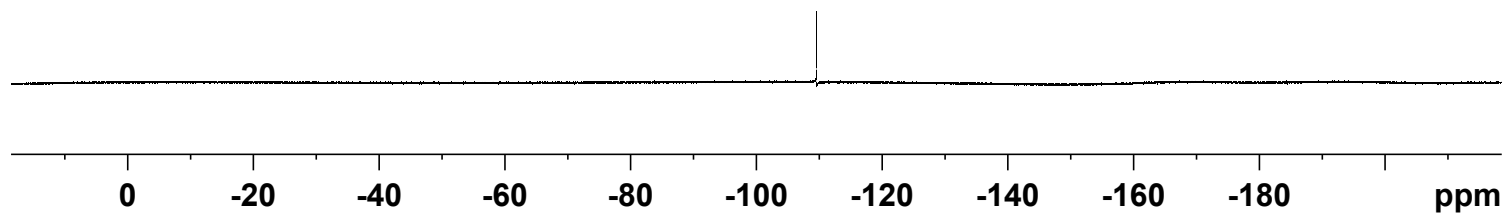
==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577891 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



— -109.60



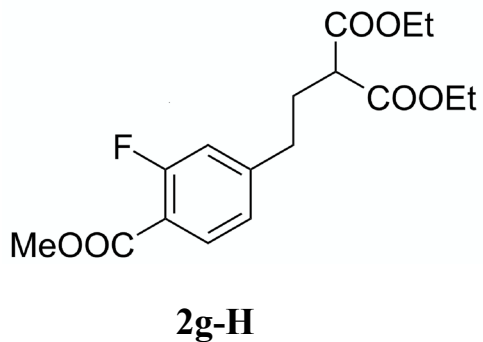
Current Data Parameters
 NAME 400M-2023-F
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230506
 Time 18.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT CDC13
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 206.33
 DW 5.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 376.5642094 MHz
 NUC1 19F
 P1 14.50 usec
 PLW1 17.98900032 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 65536
 SF 376.6018696 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



— -109.60

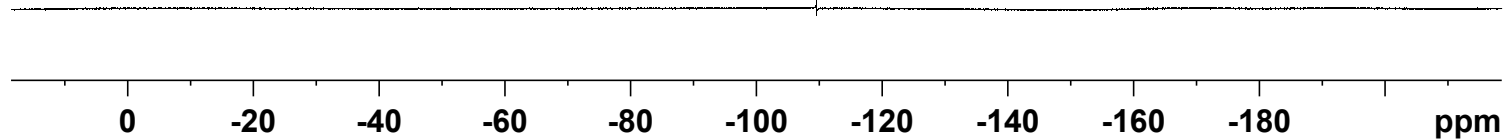
Current Data Parameters
 NAME 400M-2023-F
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230506
 Time 18.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT CDC13
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 206.33
 DW 5.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

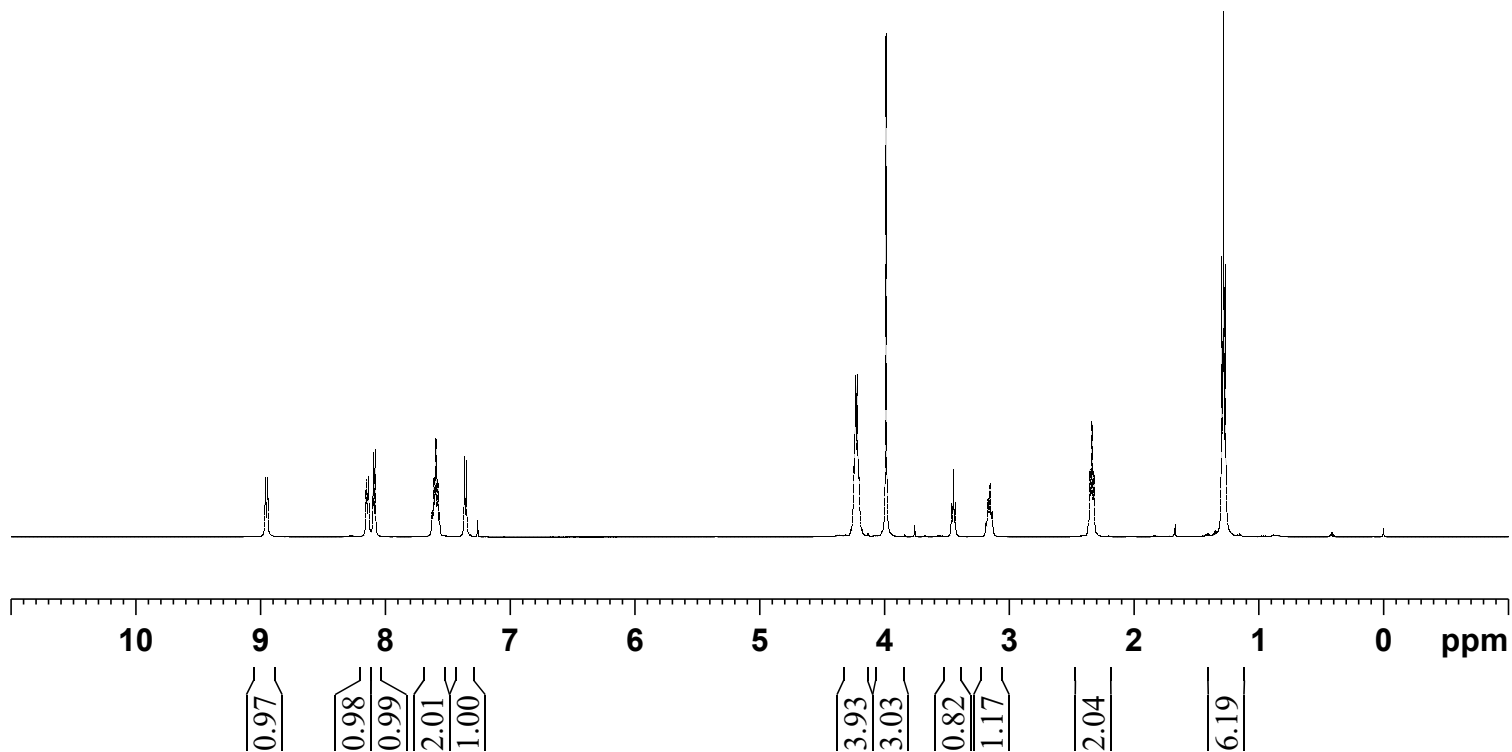
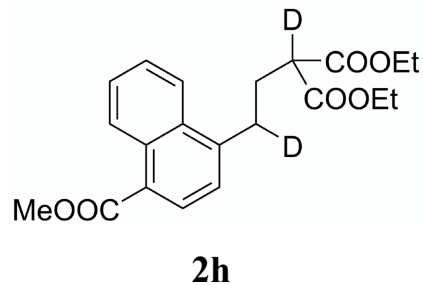
==== CHANNEL f1 =====
 SFO1 376.5642094 MHz
 NUC1 19F
 P1 14.50 usec
 PLW1 17.98900032 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 65536
 SF 376.6018696 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8.959
8.943
8.151
8.136
8.134
8.095
8.081
7.623
7.612
7.610
7.596
7.593
7.580
7.566
7.365
7.350
4.254
4.247
4.242
4.233
4.228
4.218
4.214
4.204
4.200
4.192
3.986
3.461
3.446
3.432
3.186
3.168
3.152
3.136
2.351
2.336
2.321
1.295
1.281
1.267



Current Data Parameters
NAME 500M-2022
EXPNO 31
PROCNO 1

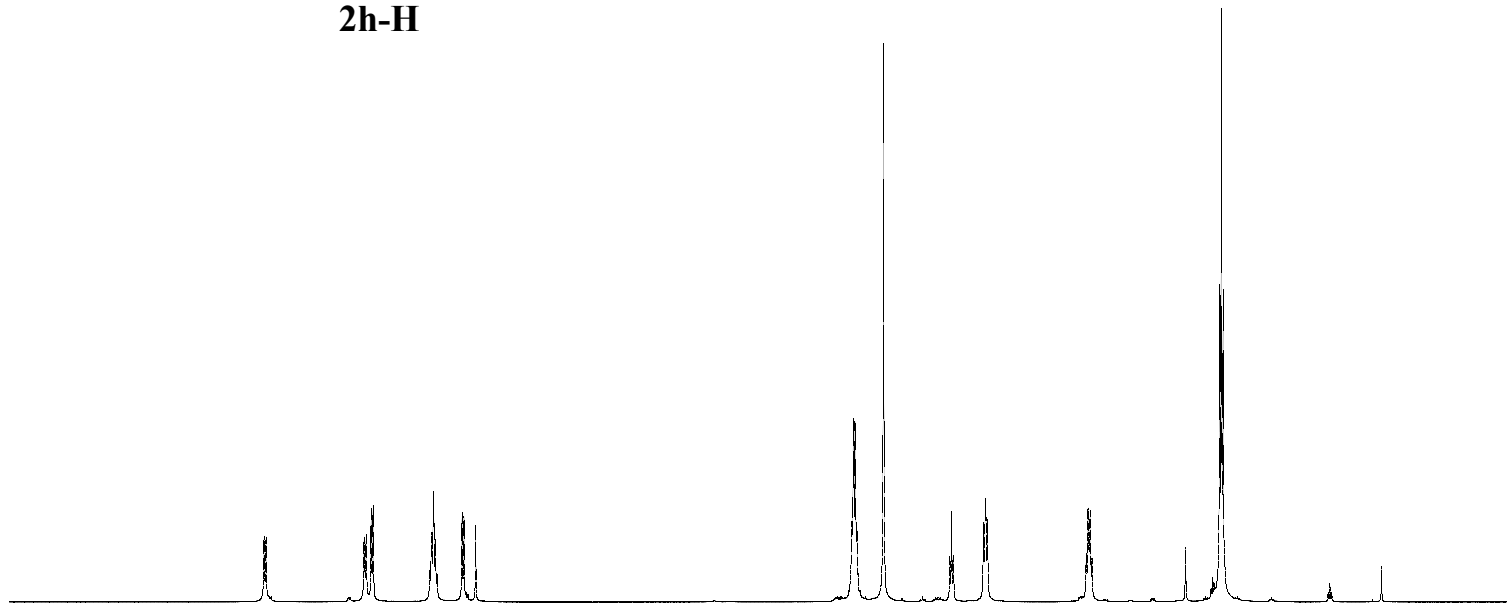
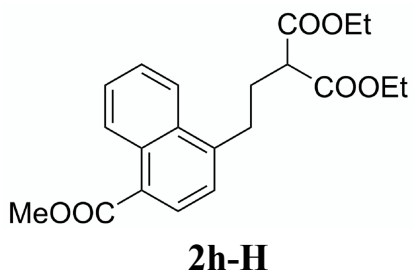
F2 - Acquisition Parameters
Date_ 20220304
Time 2.40
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.955
8.939
8.153
8.137
8.097
8.082
7.627
7.613
7.600
7.597
7.582
7.369
7.354
4.255
4.248
4.244
4.234
4.230
4.220
4.216
4.206
4.202
4.194
3.991
3.460
3.445
3.431
3.189
3.174
3.157
2.367
2.351
2.335
2.320
1.298
1.284
1.269



0.99
2.00
2.09
1.08
3.99
3.22
0.97
2.00
2.00
6.67

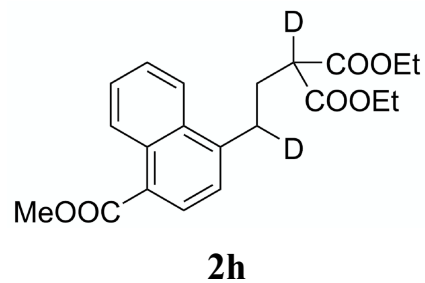
Current Data Parameters
NAME 500M-2022
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220304
Time 2.09
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 55.37
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

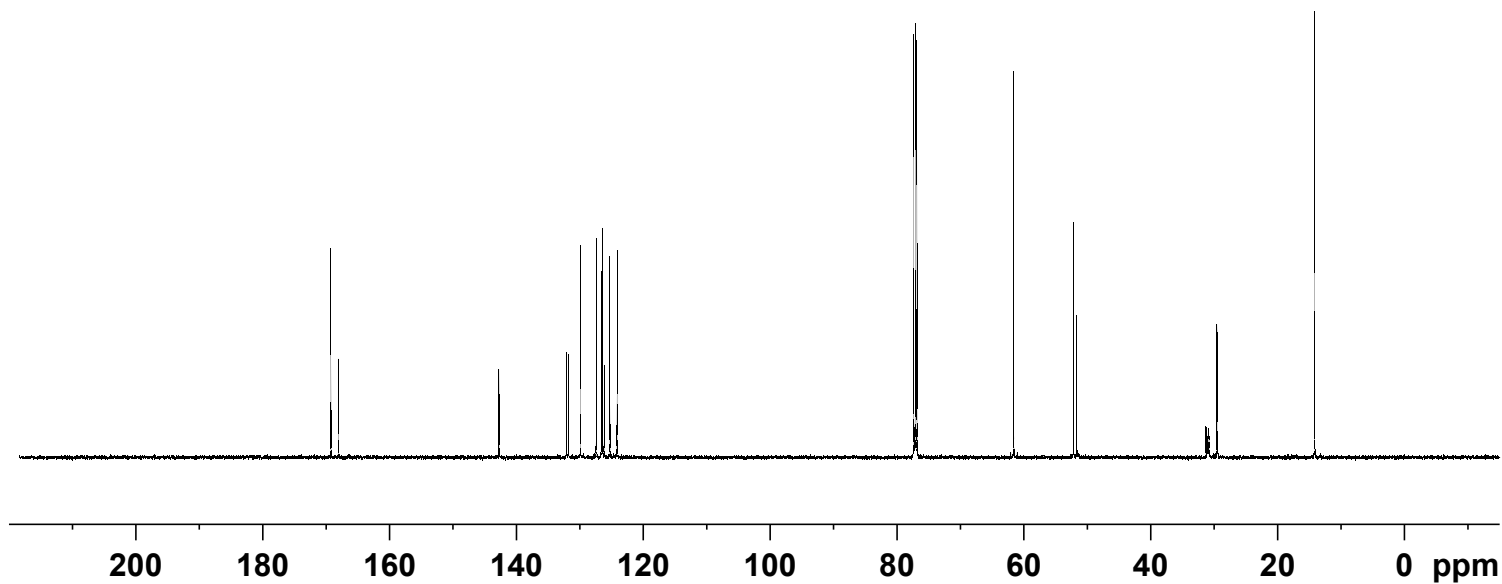
==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



169.20
168.05
142.70
132.07
131.75
129.86
127.37
126.54
126.38
126.12
125.23
124.08

61.54
52.12
51.62
31.22
31.04
30.89
30.73
29.55
29.48
29.39
14.11



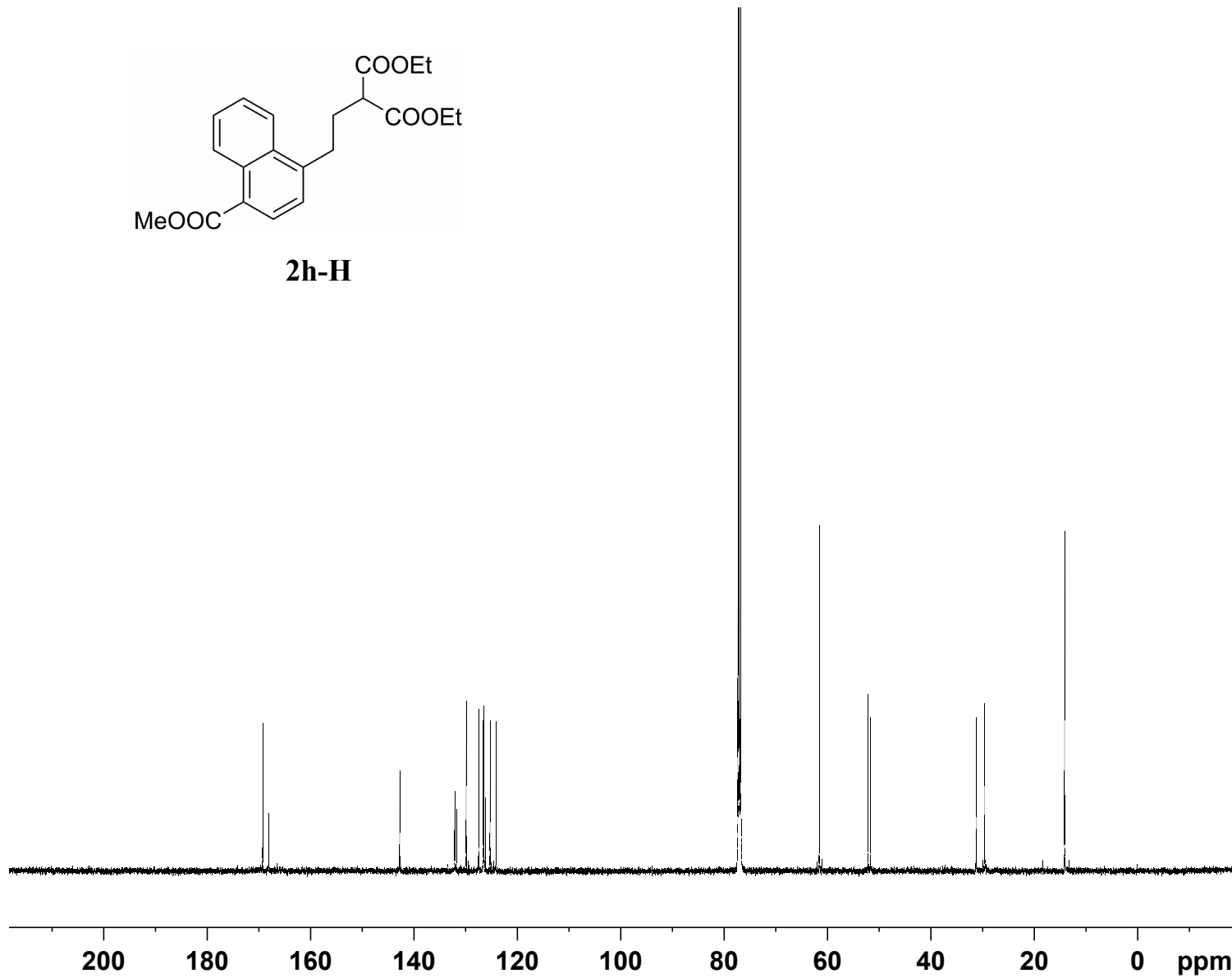
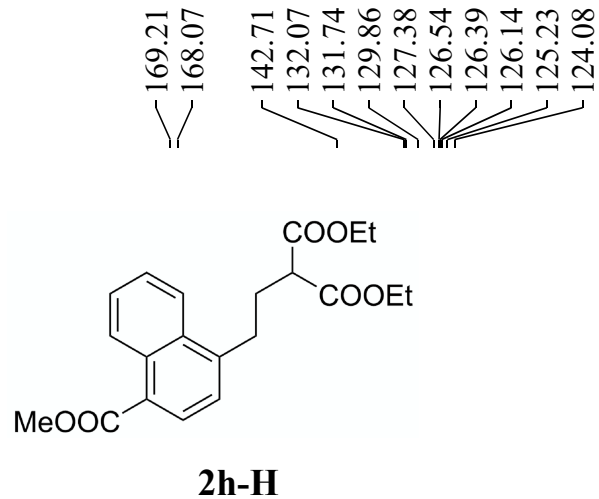
Current Data Parameters
NAME 500M-2022
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220304
Time 2.46
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 10.50 usec
PLW1 57.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.39550999 W
PLW13 0.25312999 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



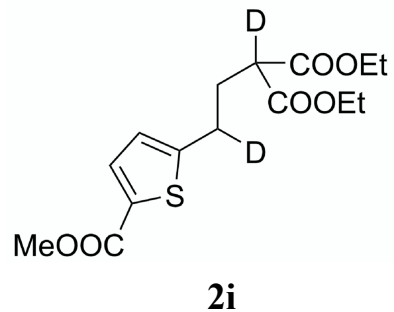
Current Data Parameters
 NAME 500M-2022
 EXPNO 30
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220304
 Time 2.36
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 400
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Chemical shift values (ppm) for the peaks in the spectrum:

- 7.640, 7.633
- 6.826, 6.819
- 4.233, 4.230, 4.219, 4.216, 4.205, 4.202, 4.191, 4.188
- 3.862, 3.391, 3.376, 3.361
- 2.922, 2.906, 2.890, 2.874, 2.287, 2.272, 2.257, 1.291, 1.277, 1.263

Current Data Parameters

NAME	500M-2022
EXPNO	41
PROCNO	1

F2 - Acquisition Parameters

Date_	20220315
Time	6.20
INSTRUM	spect
PROBHD	5 mm CPPBBO BB
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2767999 sec
RG	31.72
DW	50.000 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
D11	0 sec
TD0	1

==== CHANNEL f1 =====

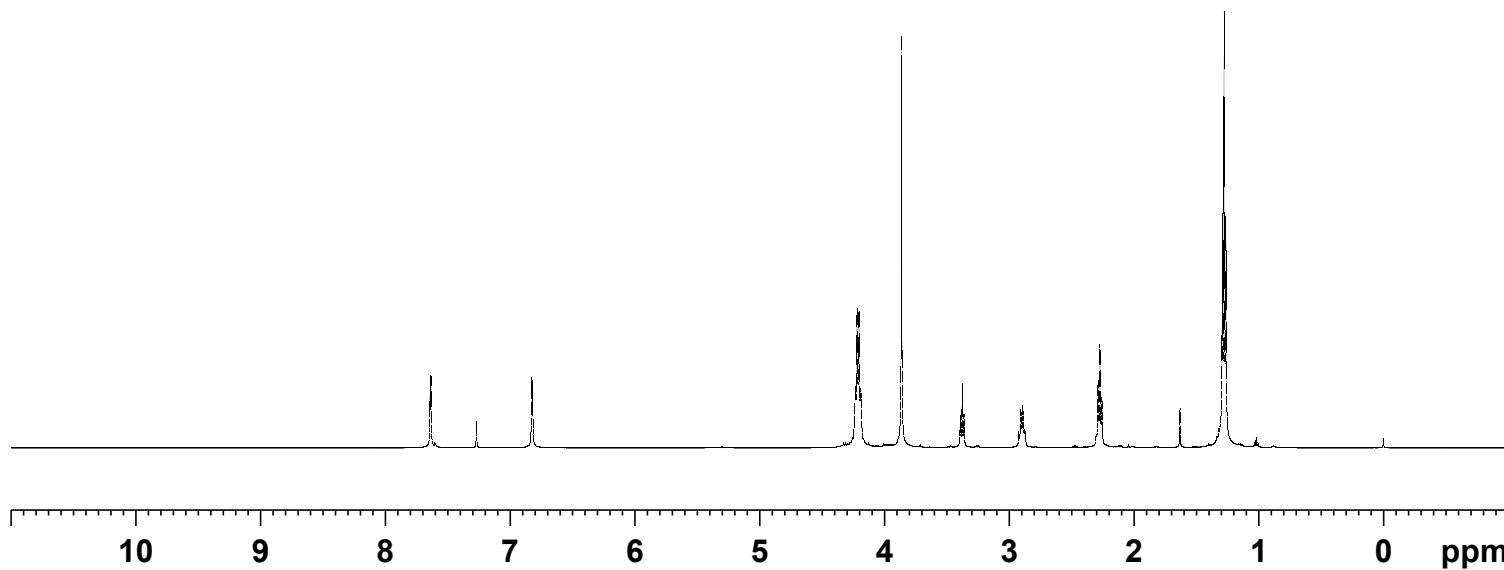
SFO1	500.1330885 MHz
NUC1	1H
P1	11.25 usec
PLW1	20.00000000 W

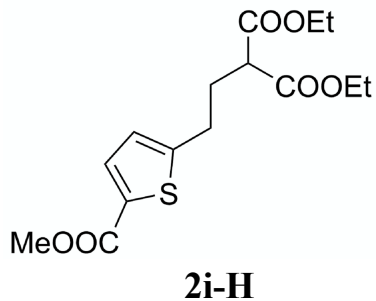
==== CHANNEL f2 =====

SFO2	500.1330885 MHz
NUC2	off
CPDPRG[2]	
PCPD2	0 usec
PLW2	0 W
PLW12	0 W
PLW13	0 W

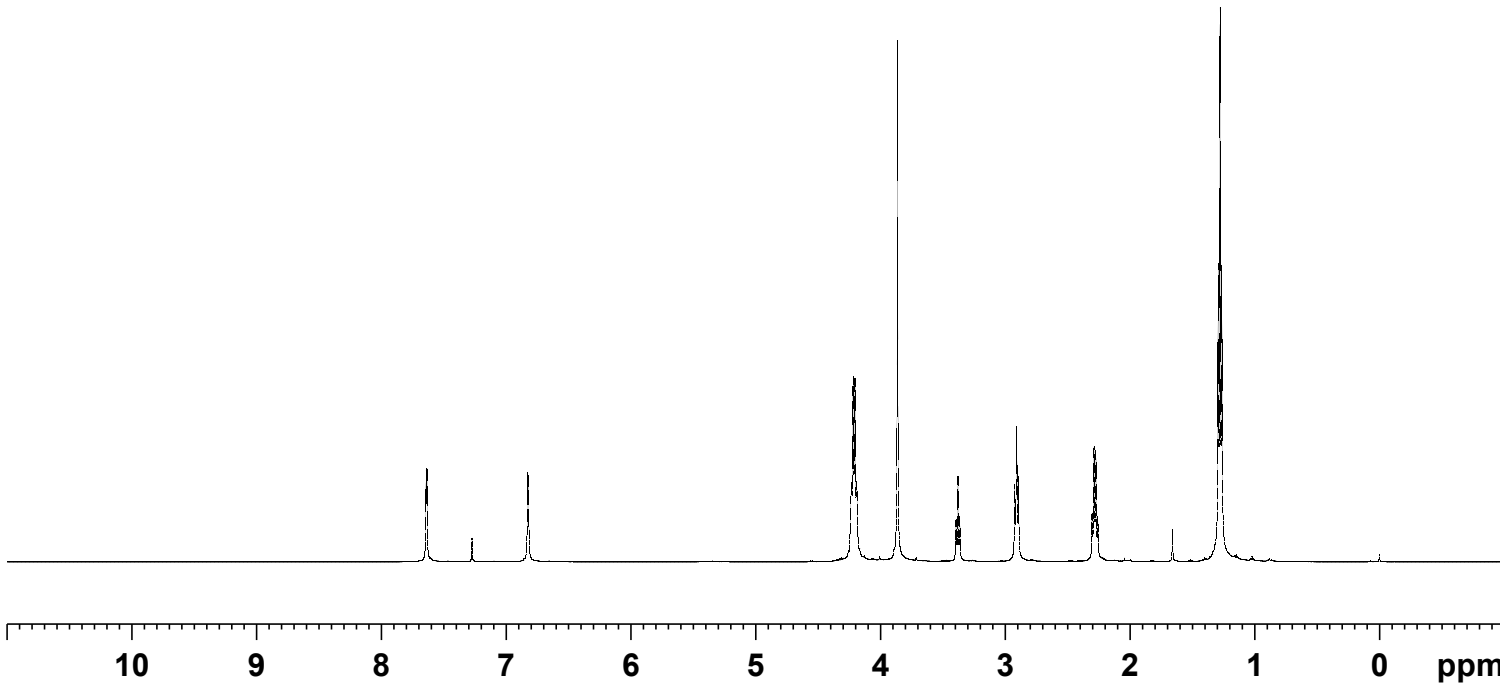
F2 - Processing parameters

SI	65536
SF	500.1300078 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





7.640
 7.633
 6.827
 6.820
 4.230
 4.219
 4.217
 4.205
 4.203
 4.192
 4.189
 3.862
 3.393
 3.378
 3.363
 2.923
 2.908
 2.892
 2.302
 2.287
 2.272
 2.257
 1.291
 1.277
 1.263



1.00
 1.02
 4.36
 3.18
 1.00
 2.03
 2.07
 7.01

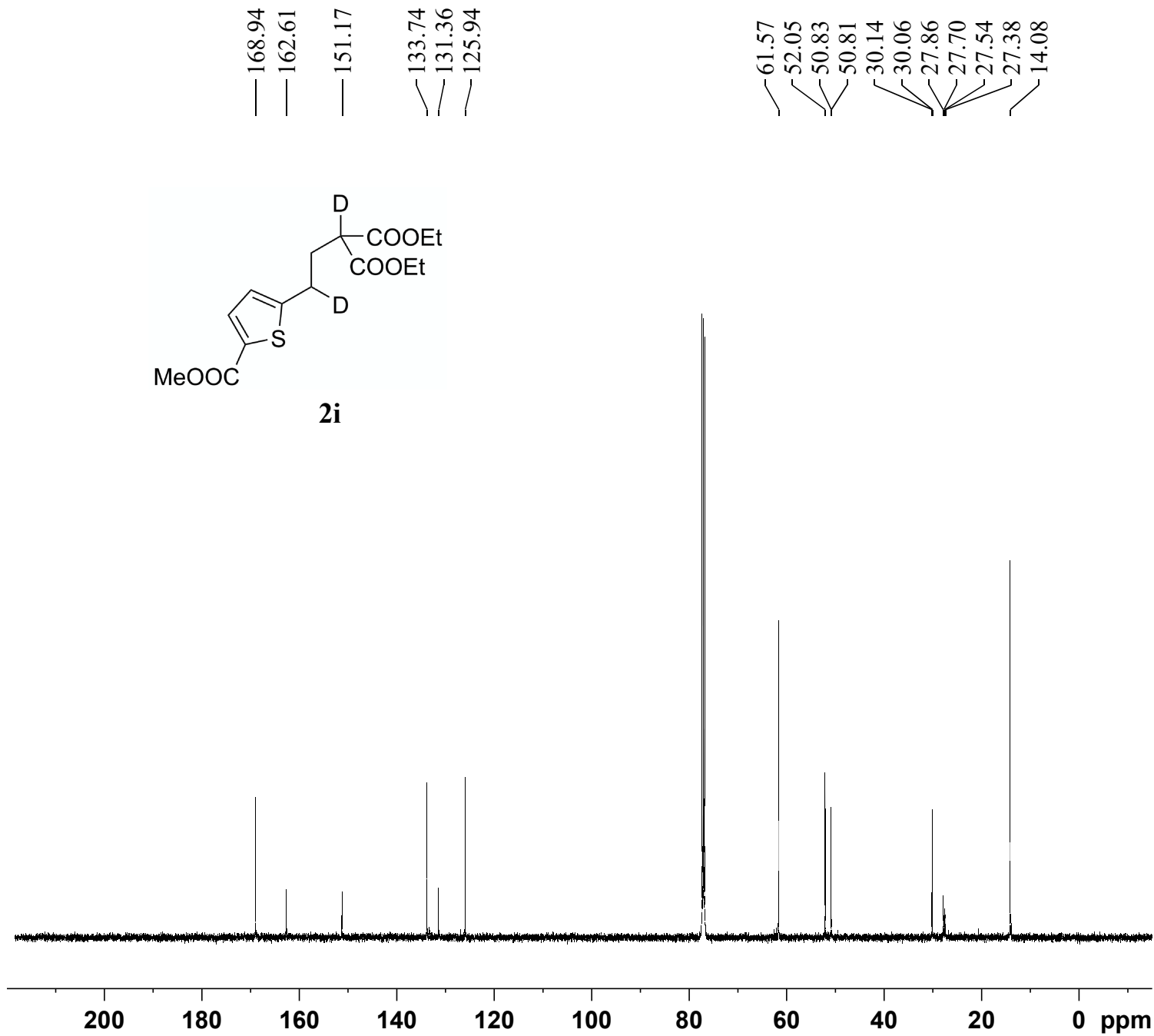
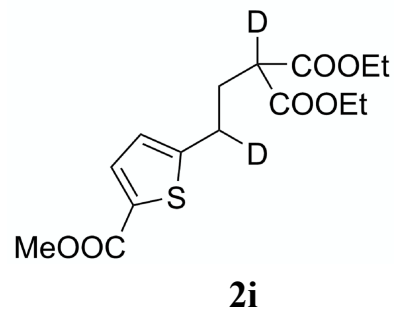
Current Data Parameters
 NAME 500M-2022
 EXPNO 38
 PROCNO 1

 F2 - Acquisition Parameters
 Date_ 20220315
 Time 5.54
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

 ===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

 ===== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

 F2 - Processing parameters
 SI 65536
 SF 500.1300060 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



S105

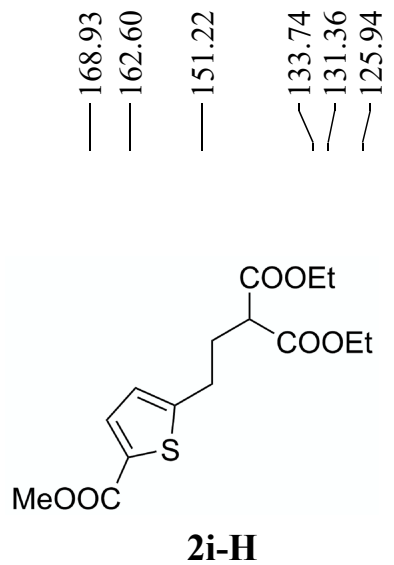
Current Data Parameters
 NAME 500M-2022
 EXPNO 42
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220315
 Time 6.24
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 80
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

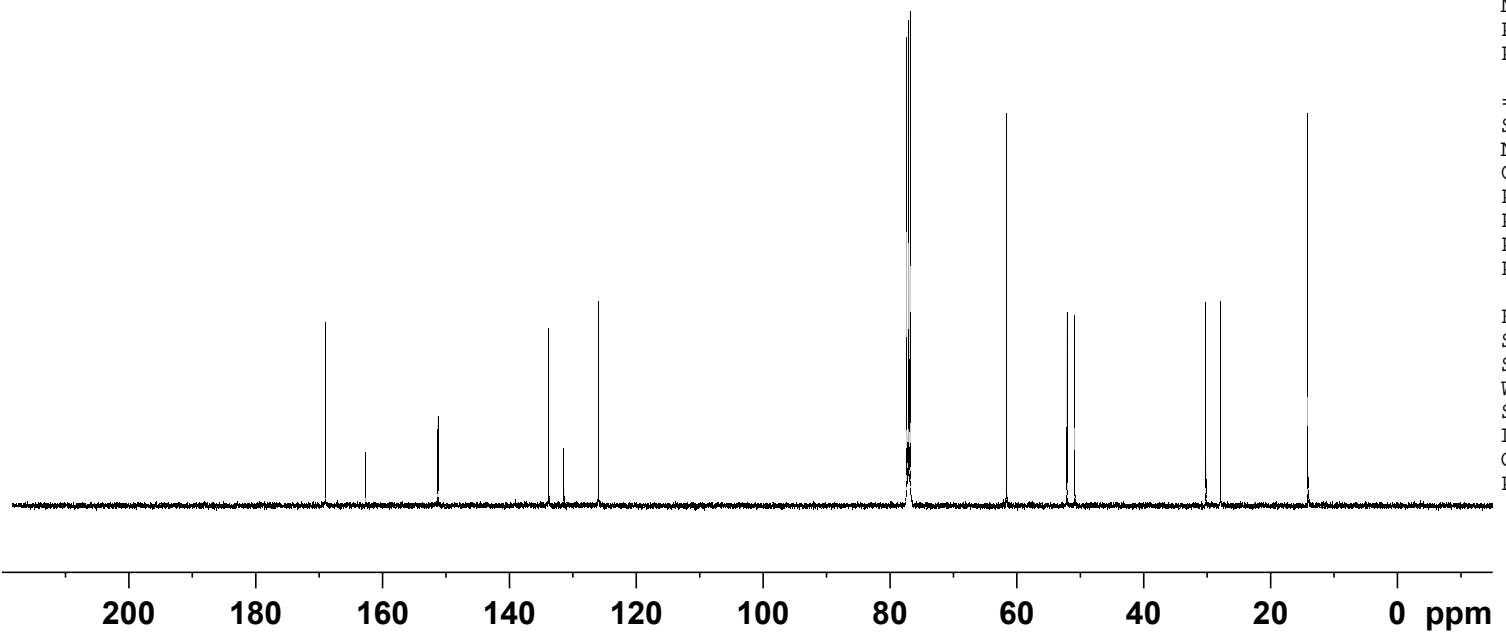


— 168.93
 — 162.60
 — 151.22
 — 133.74
 — 131.36
 — 125.94

 — 61.57
 — 52.04
 — 50.82

 — 30.14
 — 27.86

 — 14.08



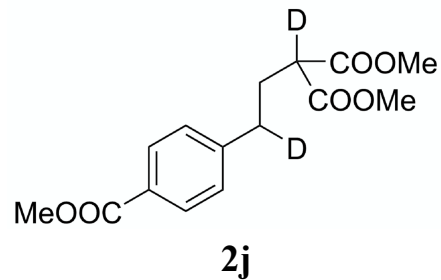
Current Data Parameters
 NAME 500M-2022
 EXPNO 39
 PROCNO 1

 F2 - Acquisition Parameters
 Date_ 20220315
 Time 5.59
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 80
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

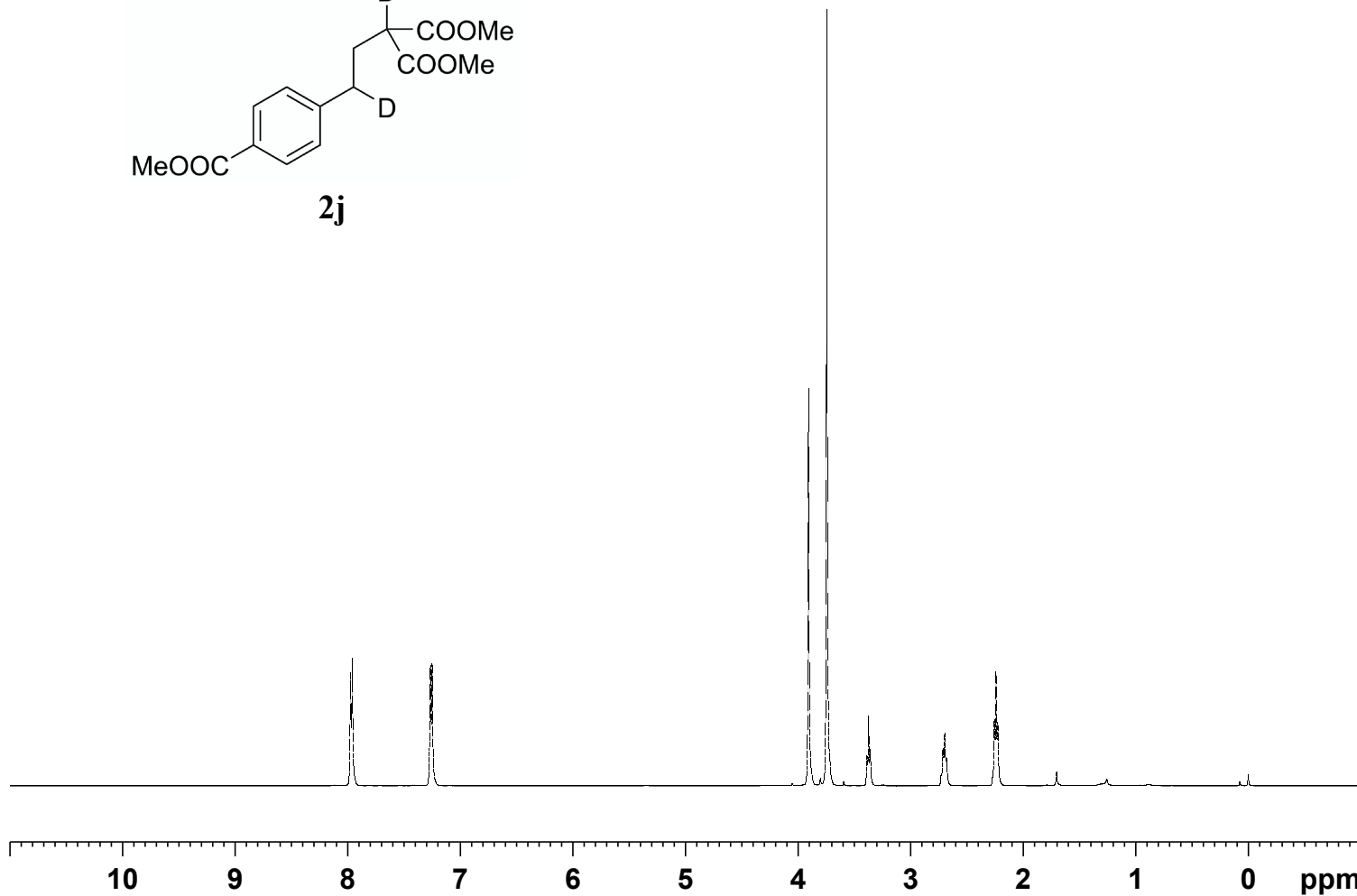
 ===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.974
7.958
7.264
7.248

3.905
3.743
3.387
3.372
3.357
2.711
2.695
2.680
2.255
2.240
2.225



2.00

2.15

3.11

6.04

0.99

1.18

2.05

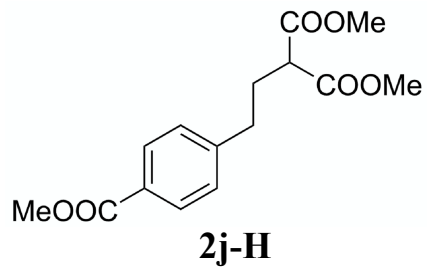
Current Data Parameters
NAME 500M-2020xia
EXPNO 187
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211124
Time 18.45
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 10.59 usec
PLW1 20.00000000 W

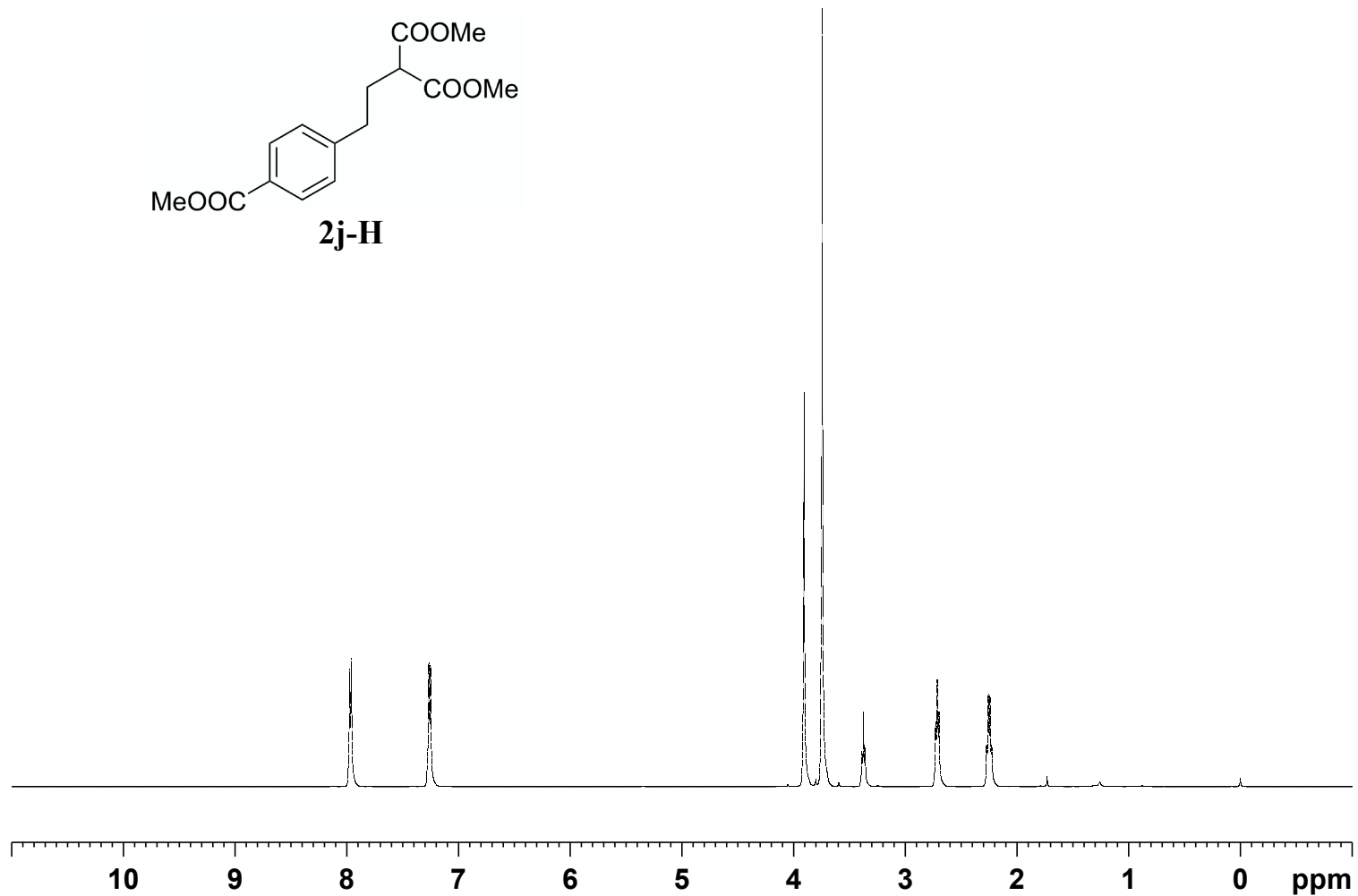
==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300028 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.974
 7.958
 7.264
 7.249

3.905
 3.743
 3.388
 3.373
 3.359
 2.727
 2.712
 2.697
 2.270
 2.255
 2.240
 2.225



2.00

2.14

3.15

5.99

1.04

2.02

2.05

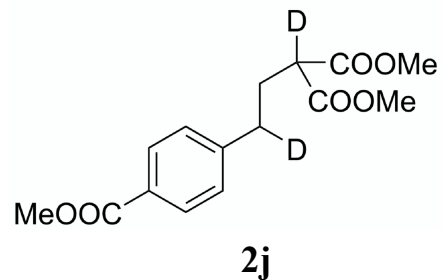
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 185
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211124
 Time 18.26
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300013 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

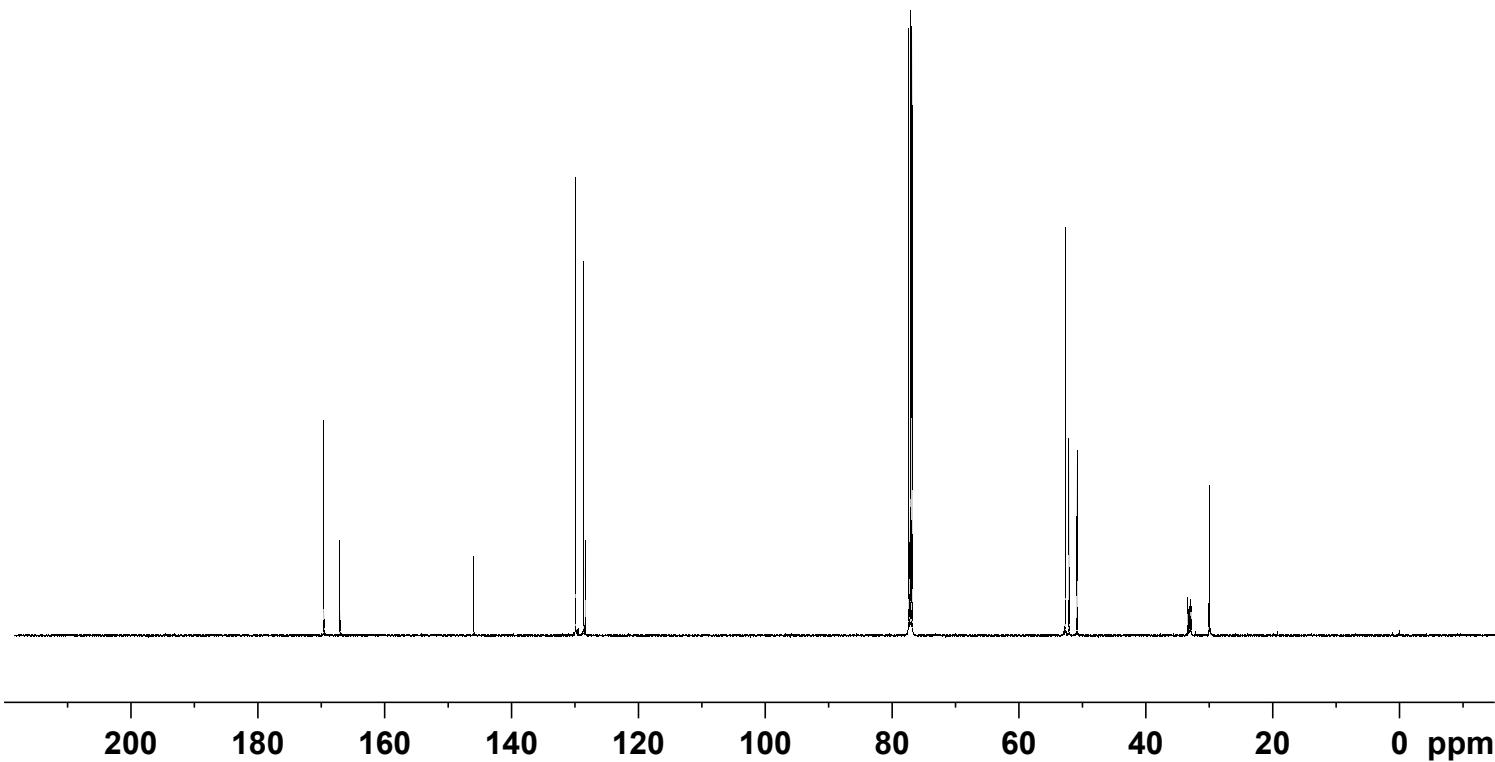


169.55
167.01

145.92

129.85
128.56
128.27

52.63
52.05
50.78
33.31
33.11
32.96
32.80
29.97
29.90



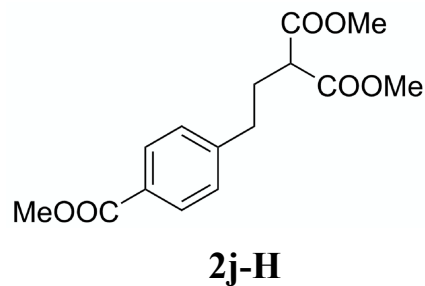
Current Data Parameters
NAME 500M-2020xia
EXPNO 188
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211124
Time 19.13
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.0000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.0000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



169.54
 167.00
 145.95
 129.84
 128.56
 128.27

52.62
 52.05
 50.80
 33.30
 29.97

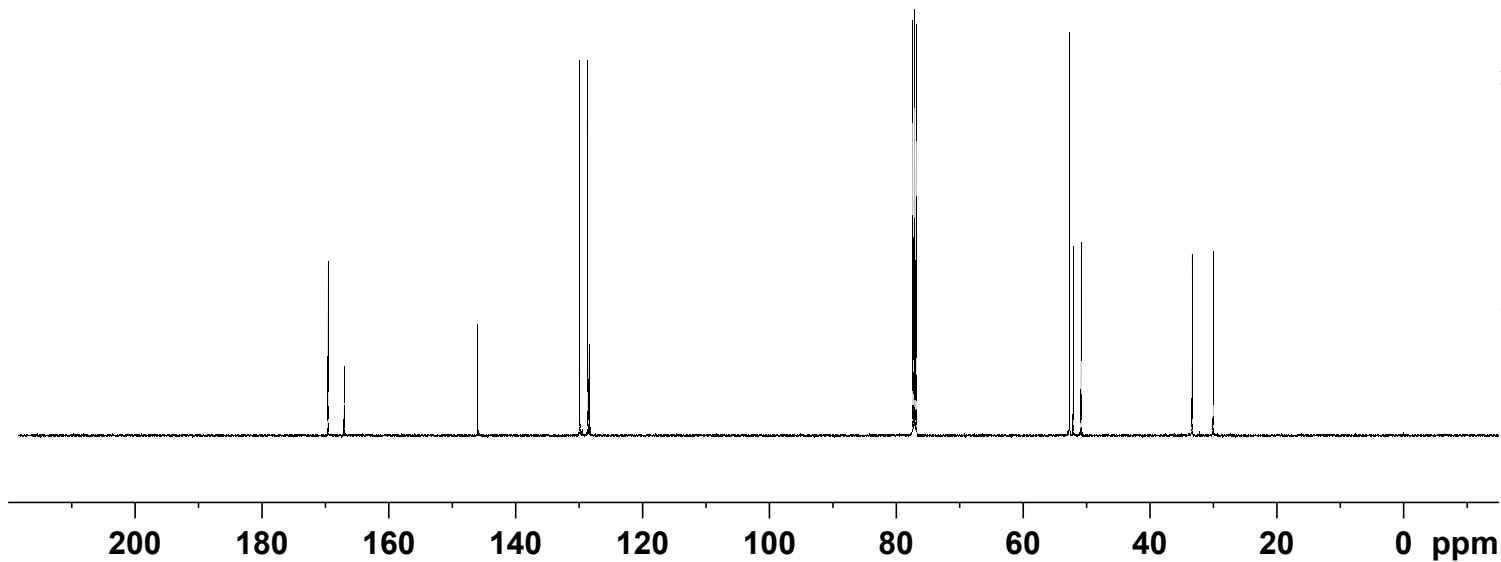
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 186
 PROCNO 1

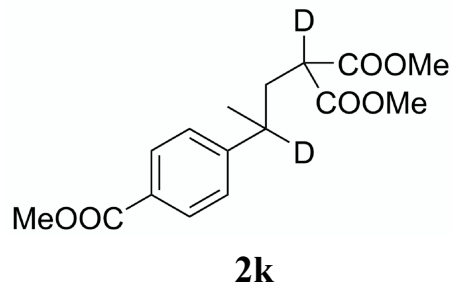
F2 - Acquisition Parameters
 Date_ 20211124
 Time 18.41
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 293
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

===== CHANNEL f2 =====
 SFO2 500.132005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

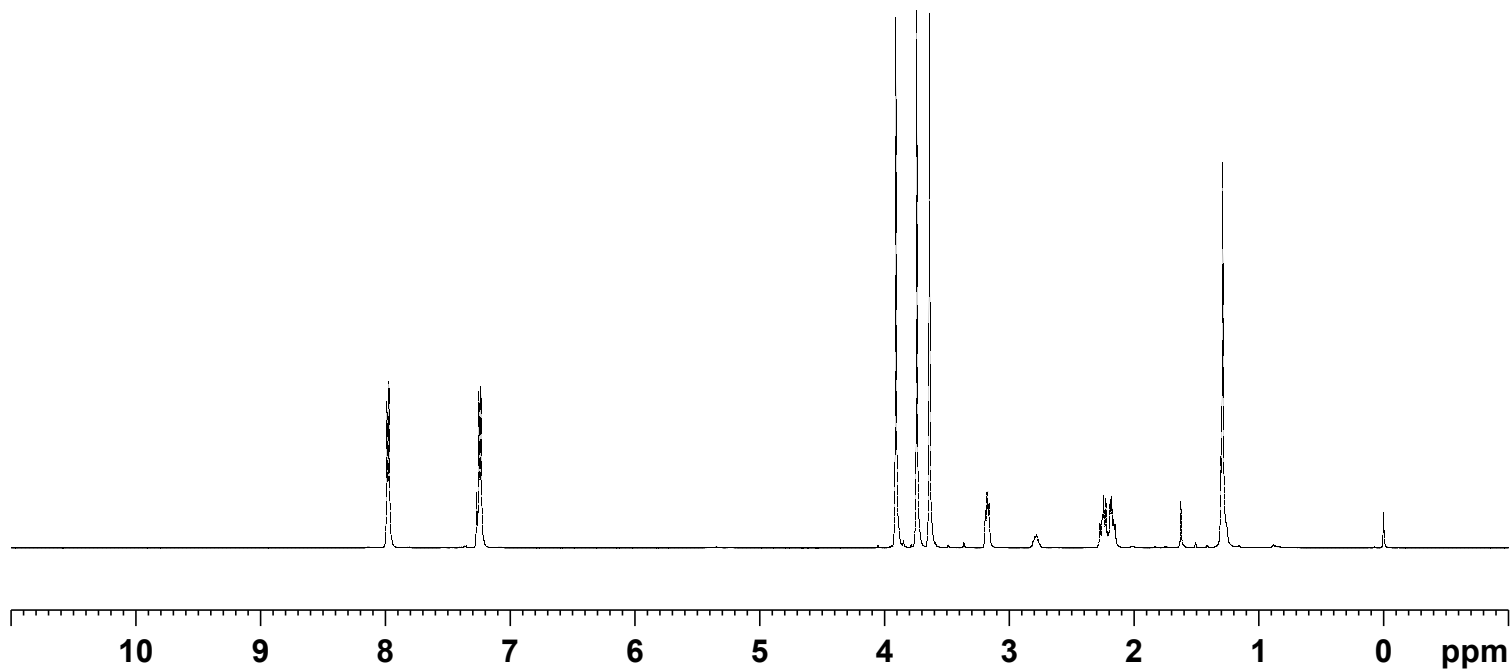
F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40





7.987
7.971
7.250
7.234

3.908
3.741
3.639
3.190
3.177
3.173
3.161
2.792
2.779
2.271
2.253
2.243
2.225
2.190
2.178
2.162
2.150
1.303
1.289



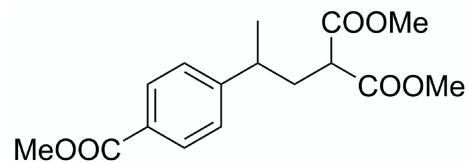
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 193
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211125
 Time 9.08
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

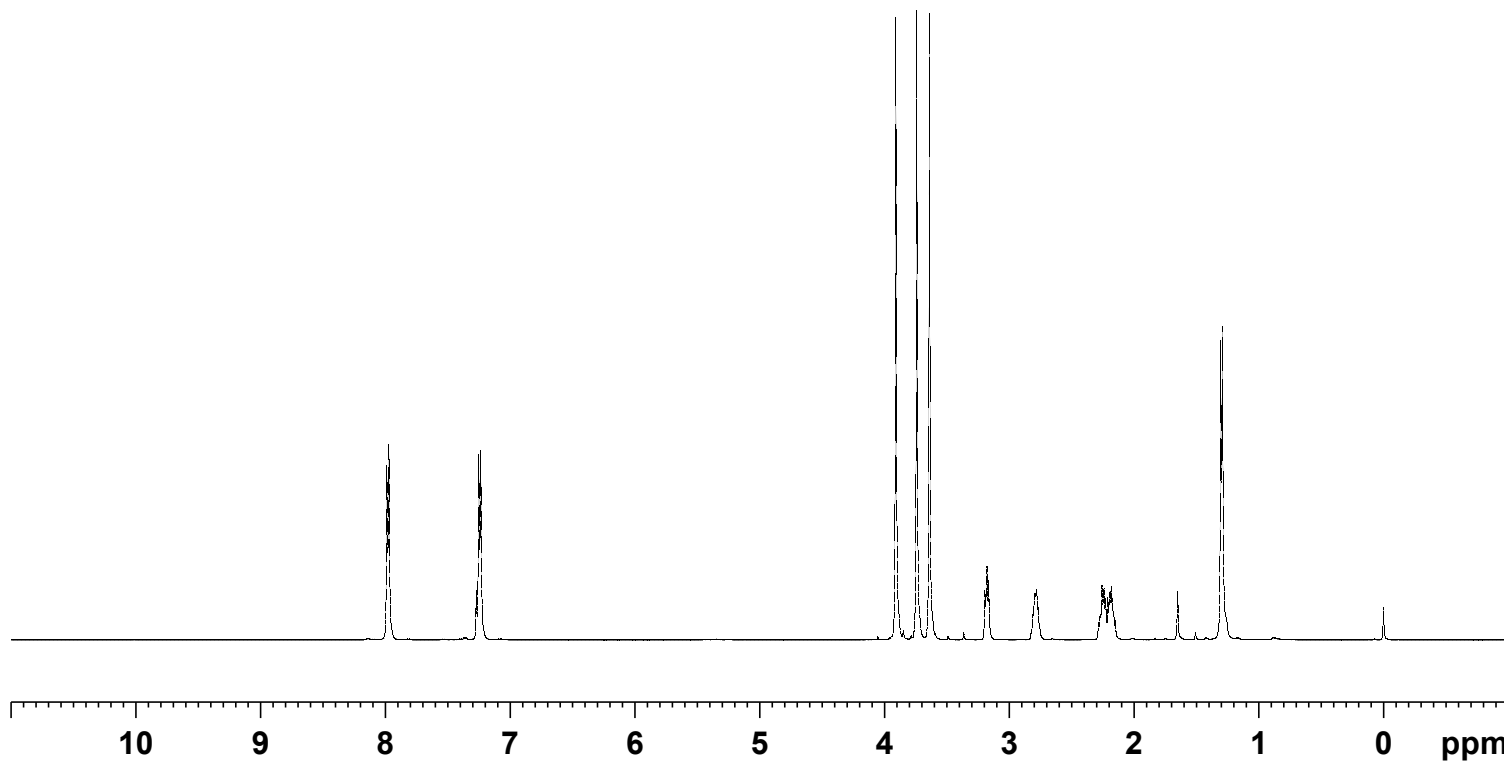
F2 - Processing parameters
 SI 65536
 SF 500.1300067 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2k-H

7.988
7.971
7.251
7.235

3.908
3.741
3.639
3.194
3.182
3.177
3.164
2.810
2.793
2.780
2.767
2.284
2.273
2.266
2.256
2.245
2.238
2.227
2.208
2.196
2.190
2.177
2.169
2.162
2.149



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 194
 PROCNO 1

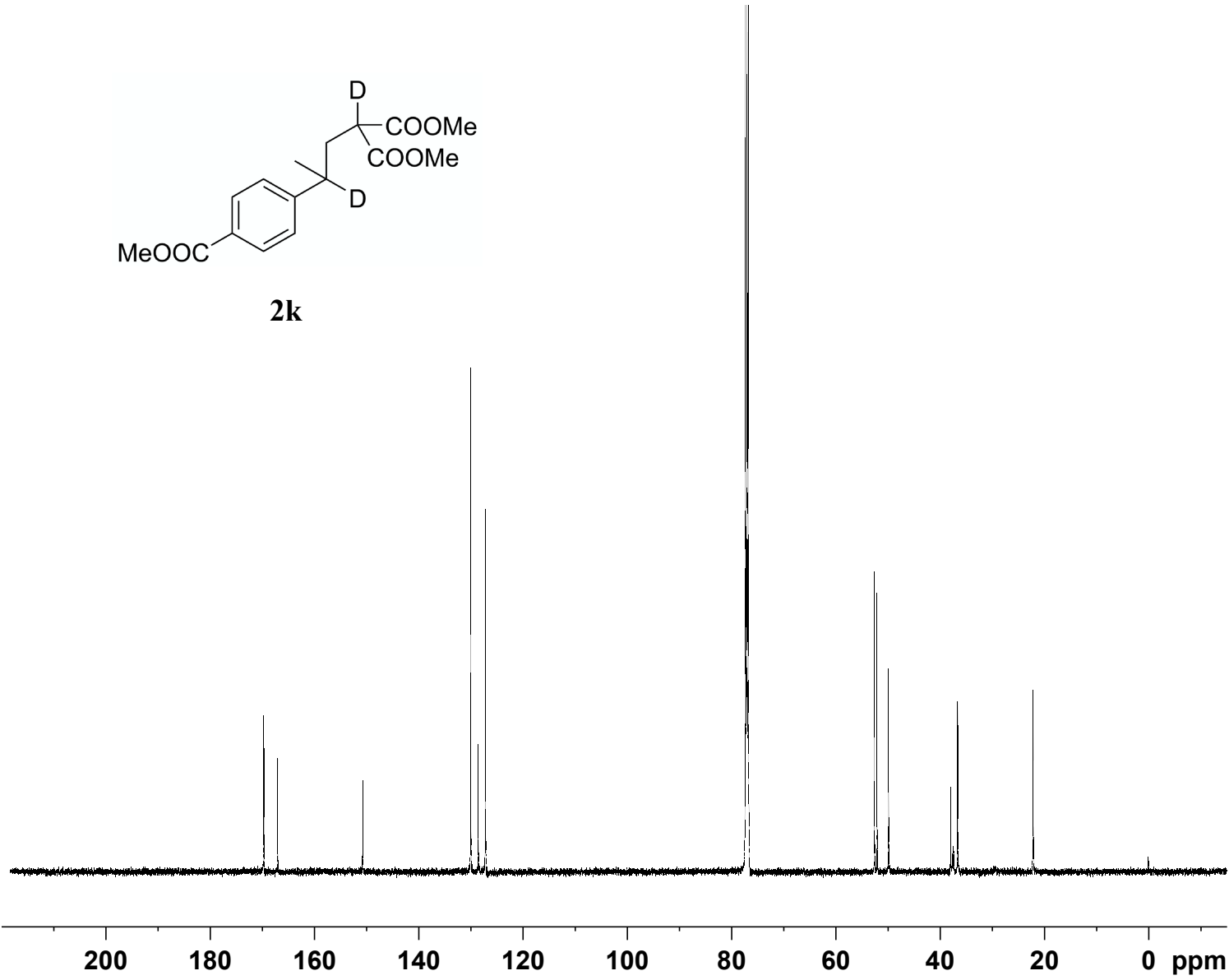
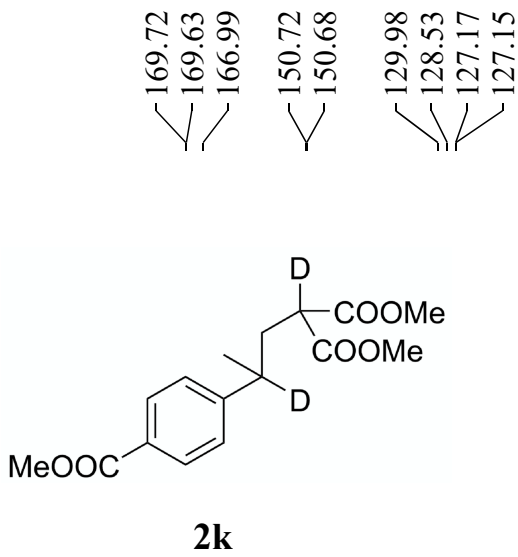
F2 - Acquisition Parameters
 Date_ 20211125
 Time 10.39
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 49.27
 DW 50.000 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

2.00
2.23
3.12
3.03
3.02
0.99
1.01
2.07
3.33



```

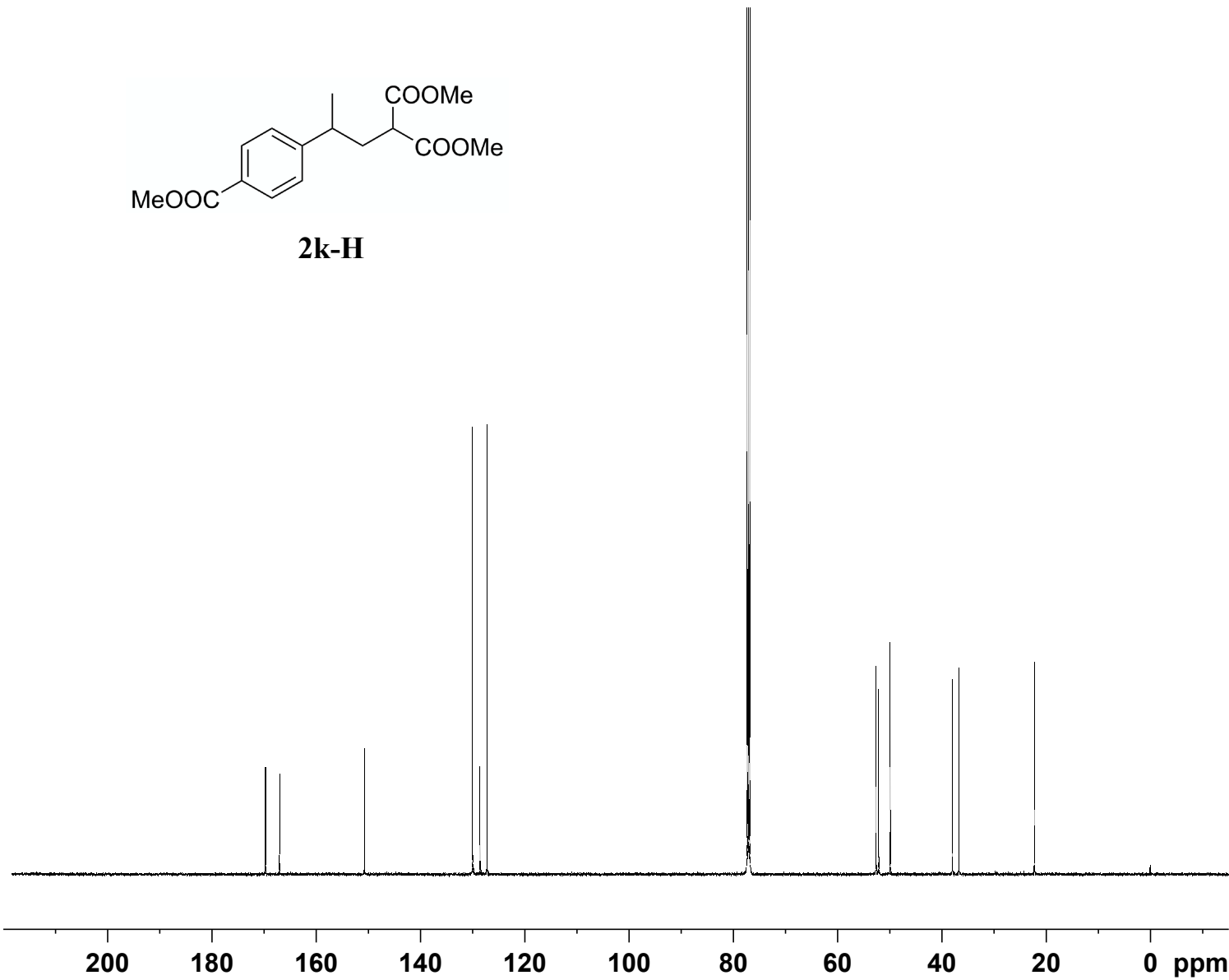
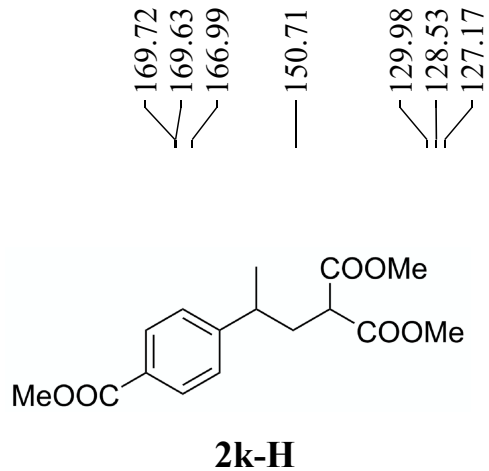
Current Data Parameters
NAME      500M-2020xia
EXPNO     192
PROCNO    1

F2 - Acquisition Parameters
Date_     20211124
Time      21.11
INSTRUM   spect
PROBHD    5 mm CPPBBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010048 sec
RG         192.89
DW         16.800 usec
DE         18.00 usec
TE         0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      125.7703637 MHz
NUC1       13C
P1         9.80 usec
PLW1       57.00000000 W

===== CHANNEL f2 =====
SFO2      500.1320005 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2     80.00 usec
PLW2      20.00000000 W
PLW12     0.35778001 W
PLW13     0.22898000 W

F2 - Processing parameters
SI         32768
SF         125.7577885 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



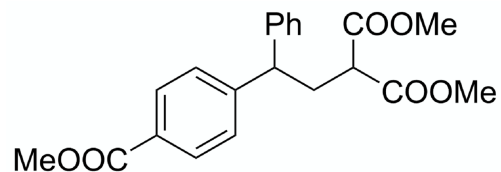
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 190
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211124
 Time 20.12
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.0000000 W

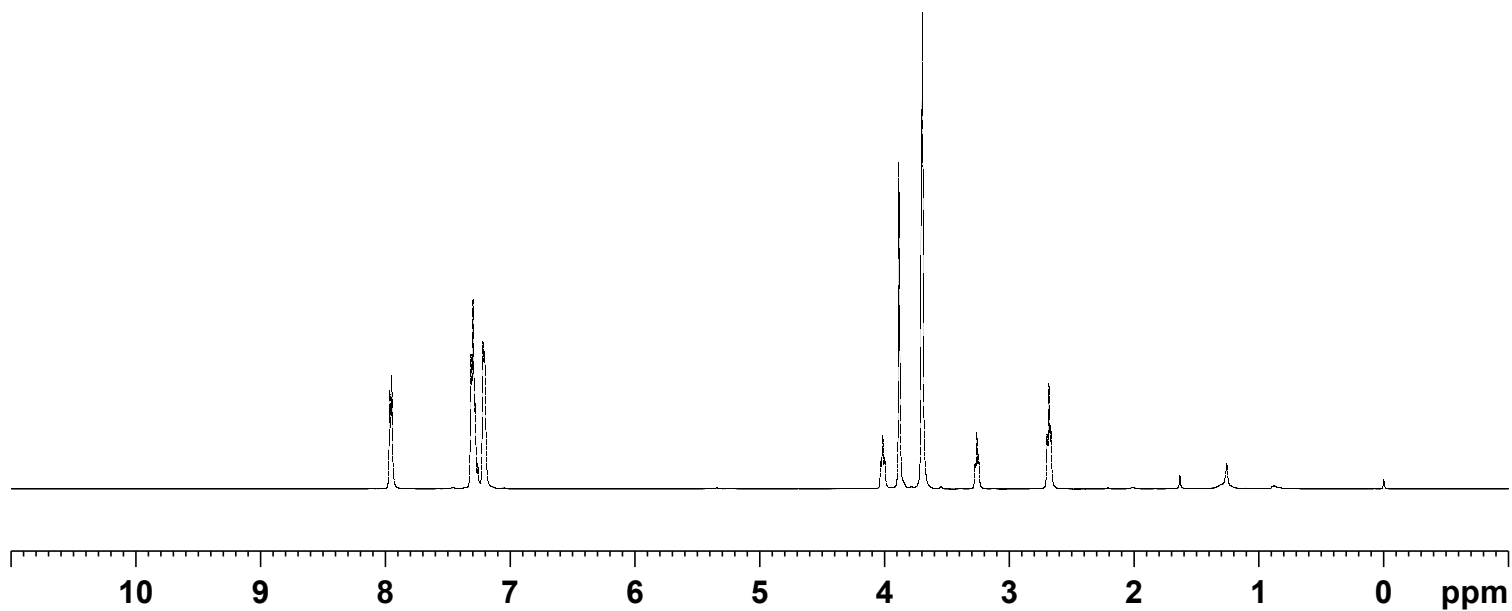
==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.0000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



21-H

7.964
7.951
7.948
7.312
7.296
7.282
7.217
7.209
7.203
4.028
4.014
3.999
3.884
3.881
3.878
3.705
3.702
3.696
3.690
3.276
3.273
3.270
3.261
3.247
2.698
2.695
2.692
2.682
2.667



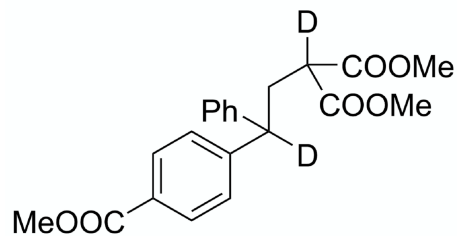
Current Data Parameters
NAME 500M-2020xia
EXPNO 210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211221
Time 2.36
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

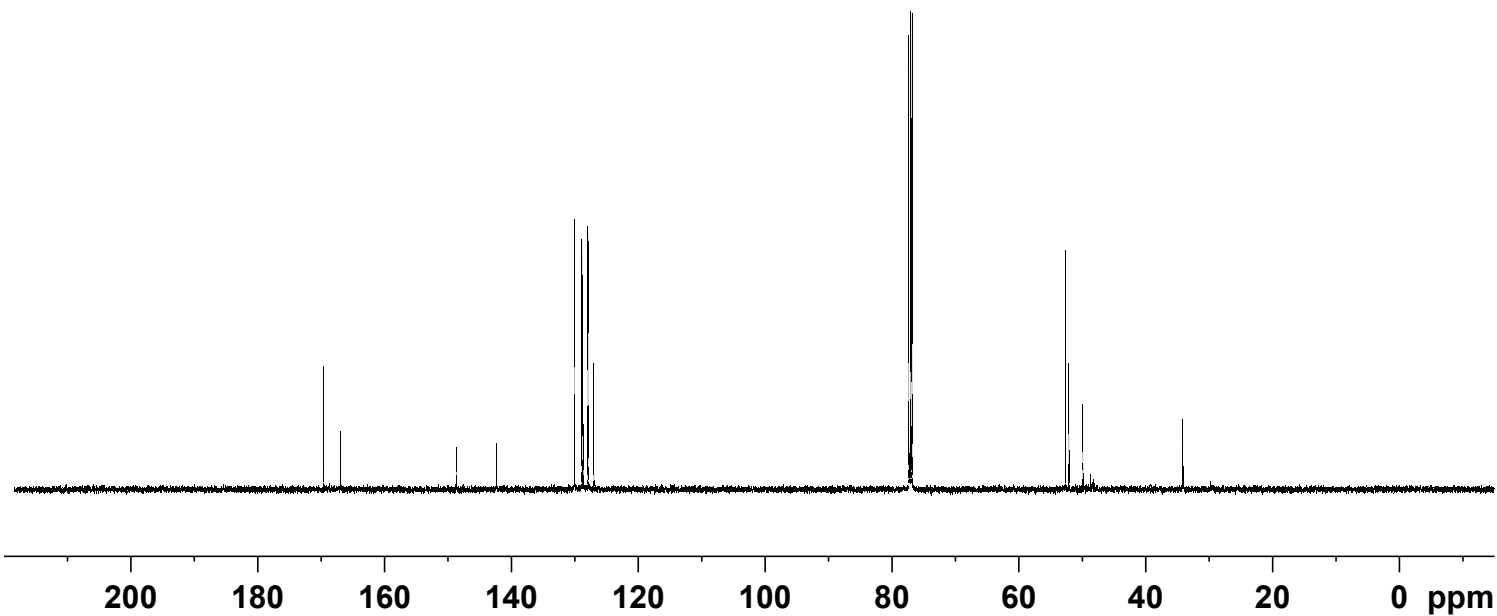
F2 - Processing parameters
SI 65536
SF 500.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



21

169.54
166.86
148.64
142.31
129.98
128.81
128.58
127.89
127.86
126.95

52.63
52.06
49.84
34.08



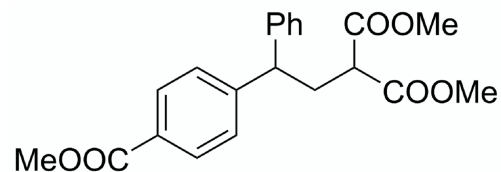
Current Data Parameters
NAME 500M-2020xia
EXPNO 213
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211221
Time 3.10
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 20
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 10.50 usec
PLW1 57.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.39550999 W
PLW13 0.25312999 W

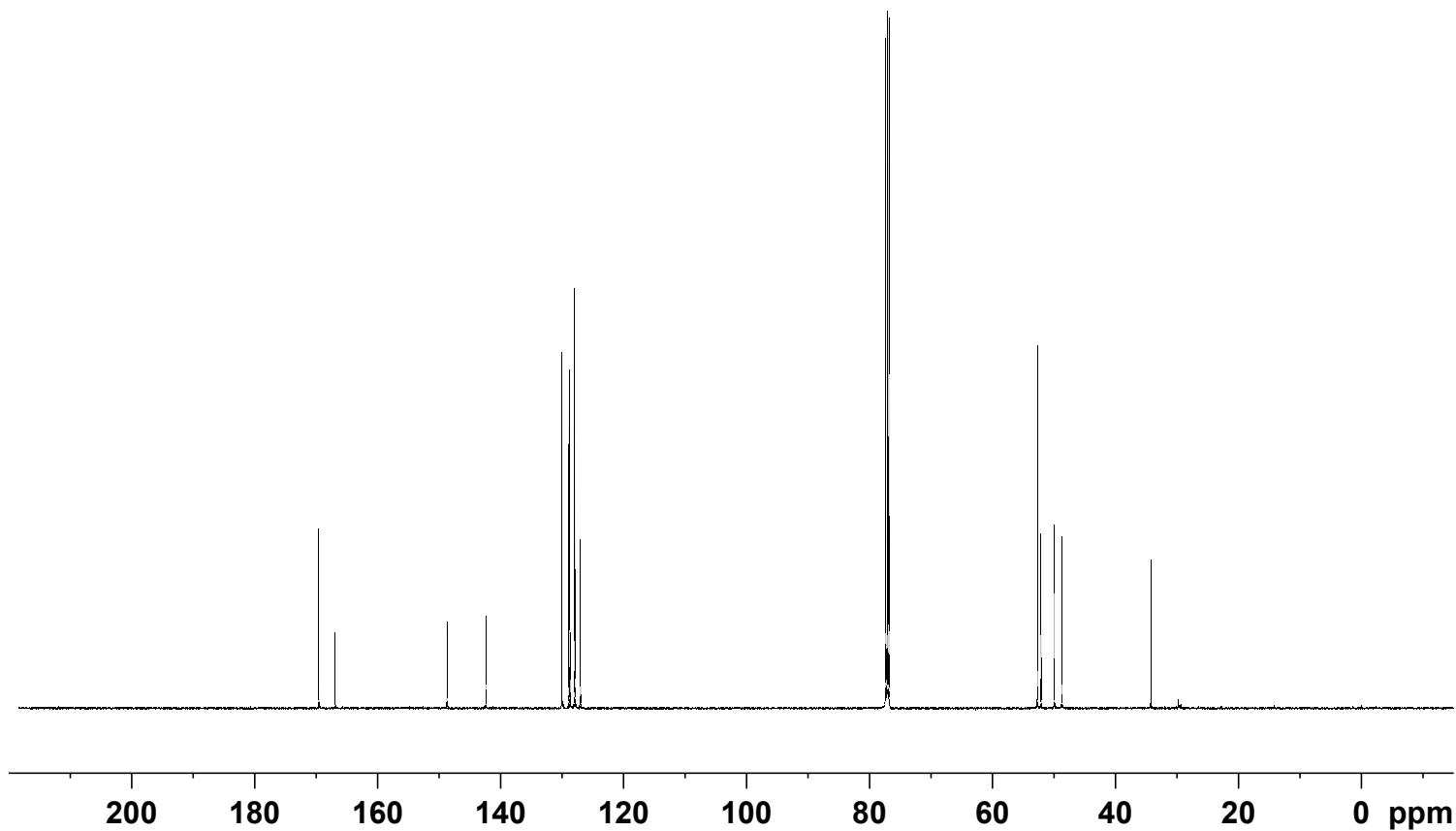
F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2I-H

169.54
166.86
148.68
142.36
129.98
128.81
128.57
127.91
127.89
126.95

52.63
52.06
49.86
48.66
34.17



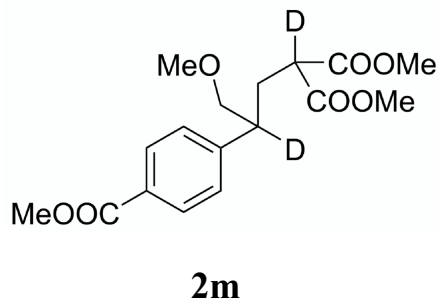
Current Data Parameters
NAME 500M-2020xia
EXPNO 211
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211221
Time 3.04
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 10.50 usec
PLW1 57.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.39550999 W
PLW13 0.25312999 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.994
7.978
7.274
7.261

3.906
3.732
3.612
3.518
3.294
3.246
3.234
3.227
3.216
2.978
2.968
2.958
2.947
2.472
2.453
2.444
2.425
2.193
2.182
2.171
2.165
2.154

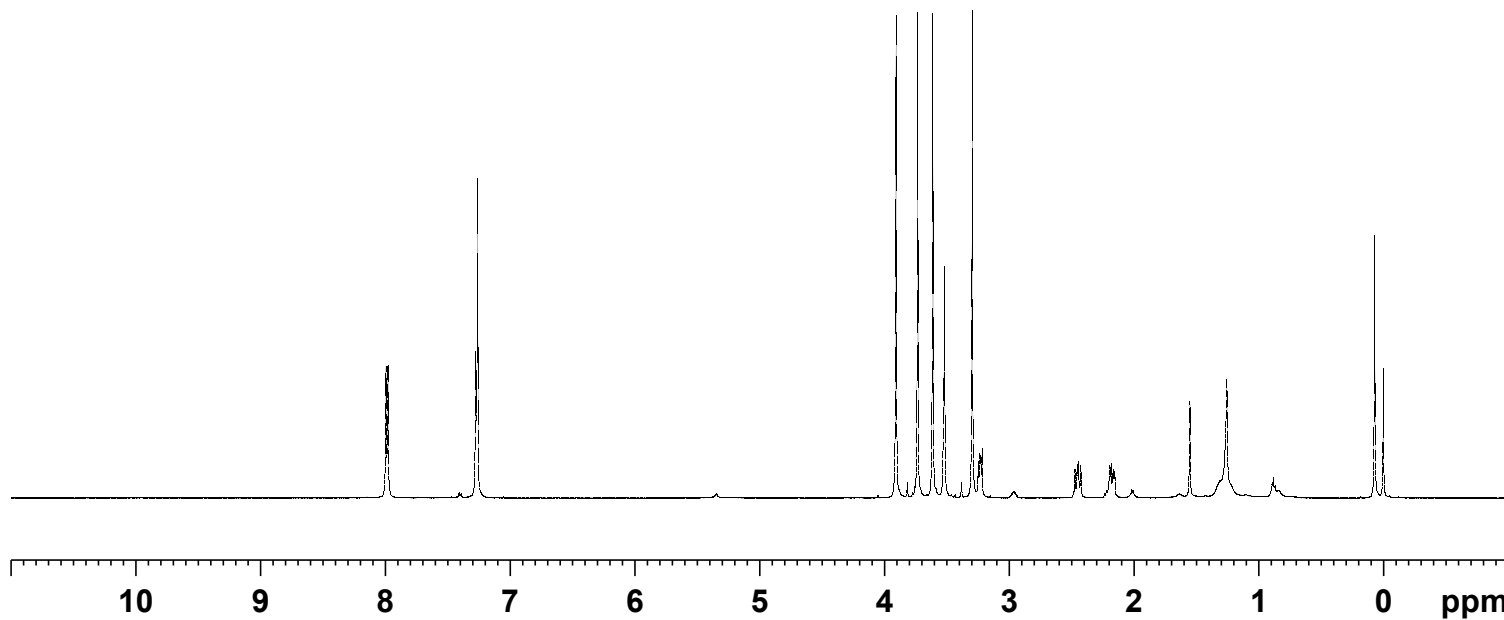
Current Data Parameters
NAME 500M-2020xia
EXPNO 230
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220207
Time 21.08
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

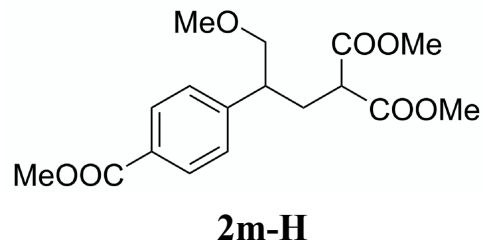
==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.00
3.30

3.03
3.01
3.01
2.01
2.87
1.11
0.19
0.99
1.16



7.994
7.978
7.274
7.260

3.906
3.733
3.611
3.529
3.516
3.295
3.249
3.237
3.230
3.217
2.978
2.968
2.958
2.947
2.465
2.455
2.446
2.437
2.211
2.200
2.191
2.181
2.172

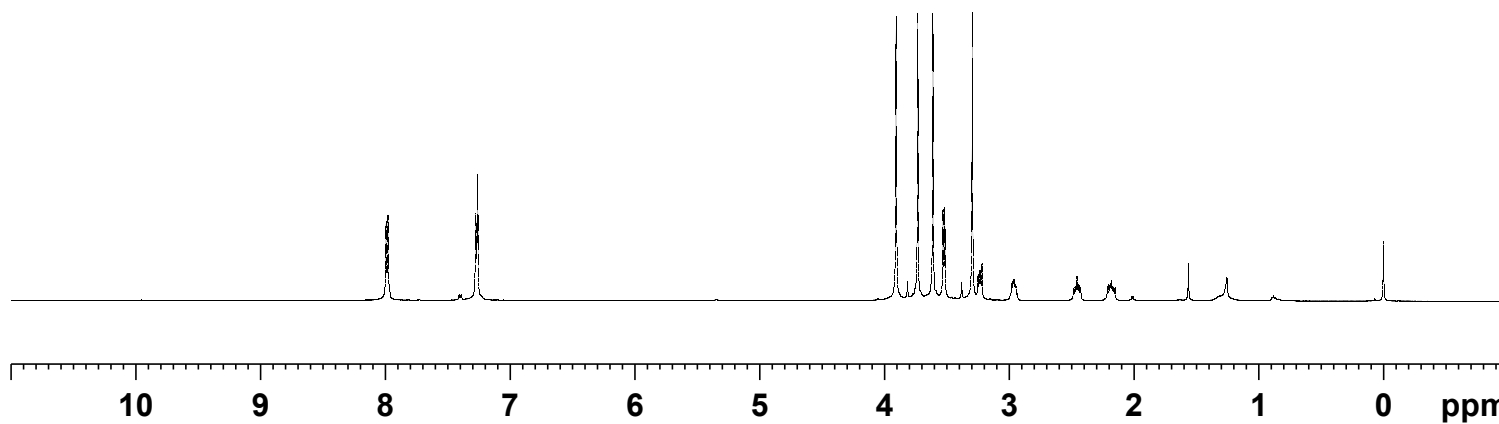
Current Data Parameters
NAME 500M-2022
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220216
Time 21.39
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 55.37
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.13

2.60

3.04

2.95

2.84

1.94

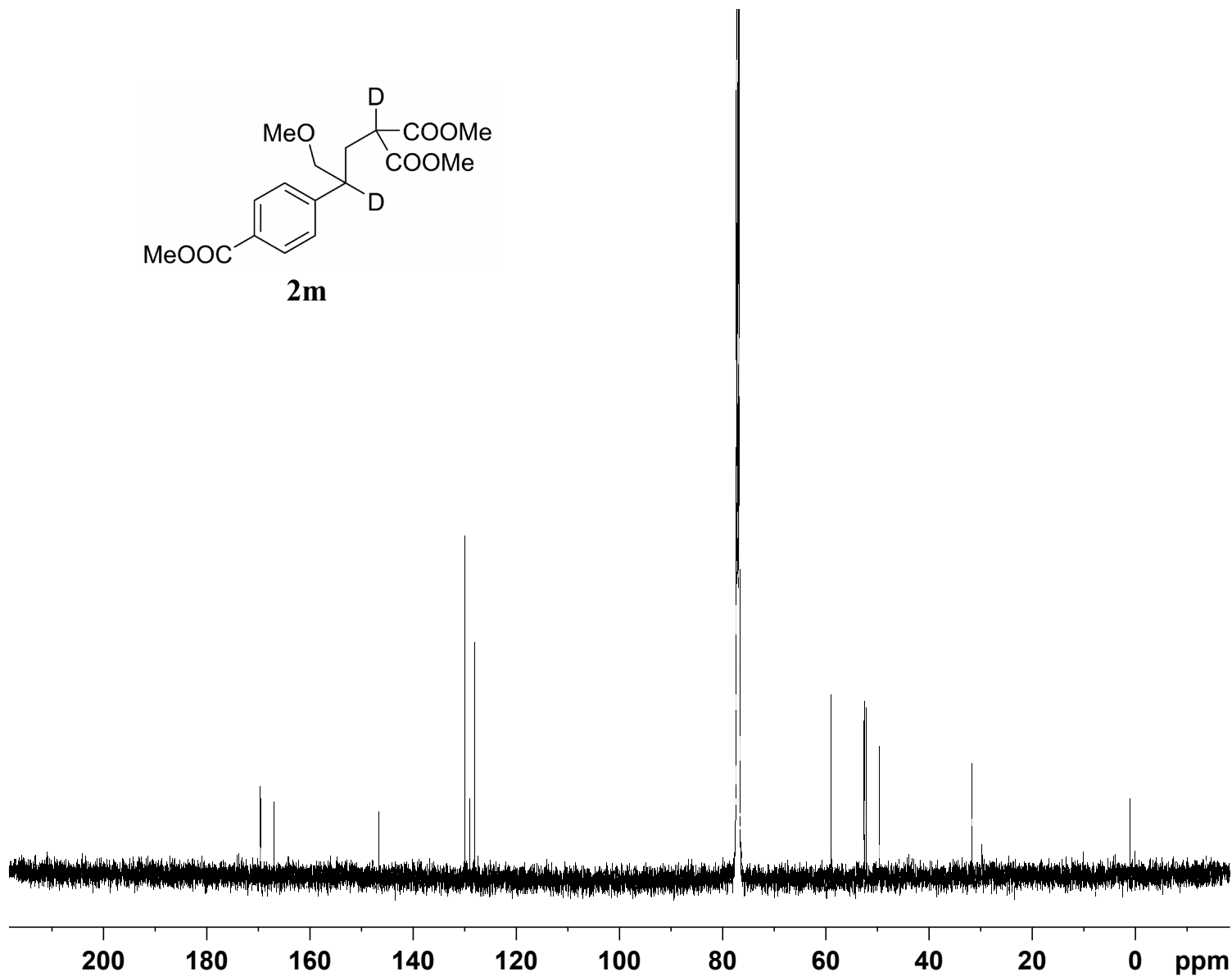
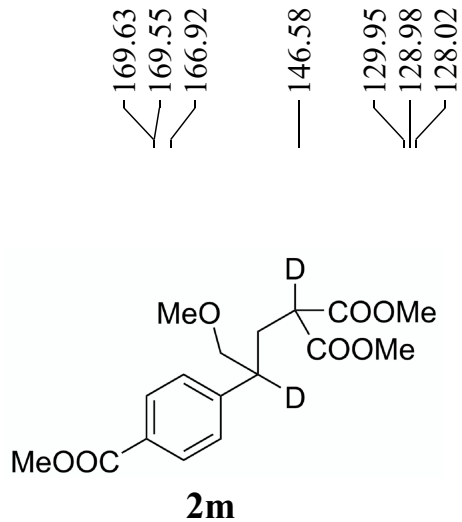
2.96

1.09

1.04

1.00

1.09



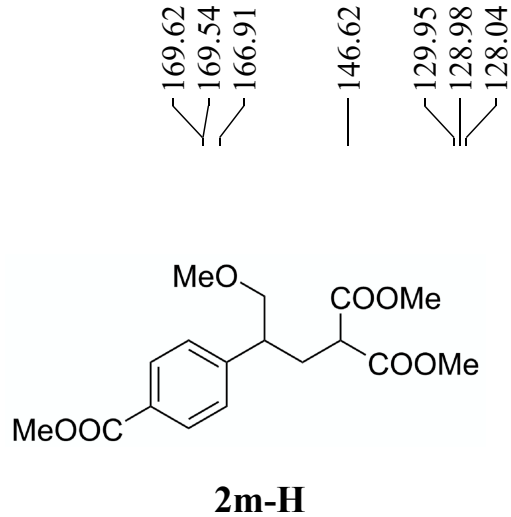
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 238
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220208
 Time 14.51
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

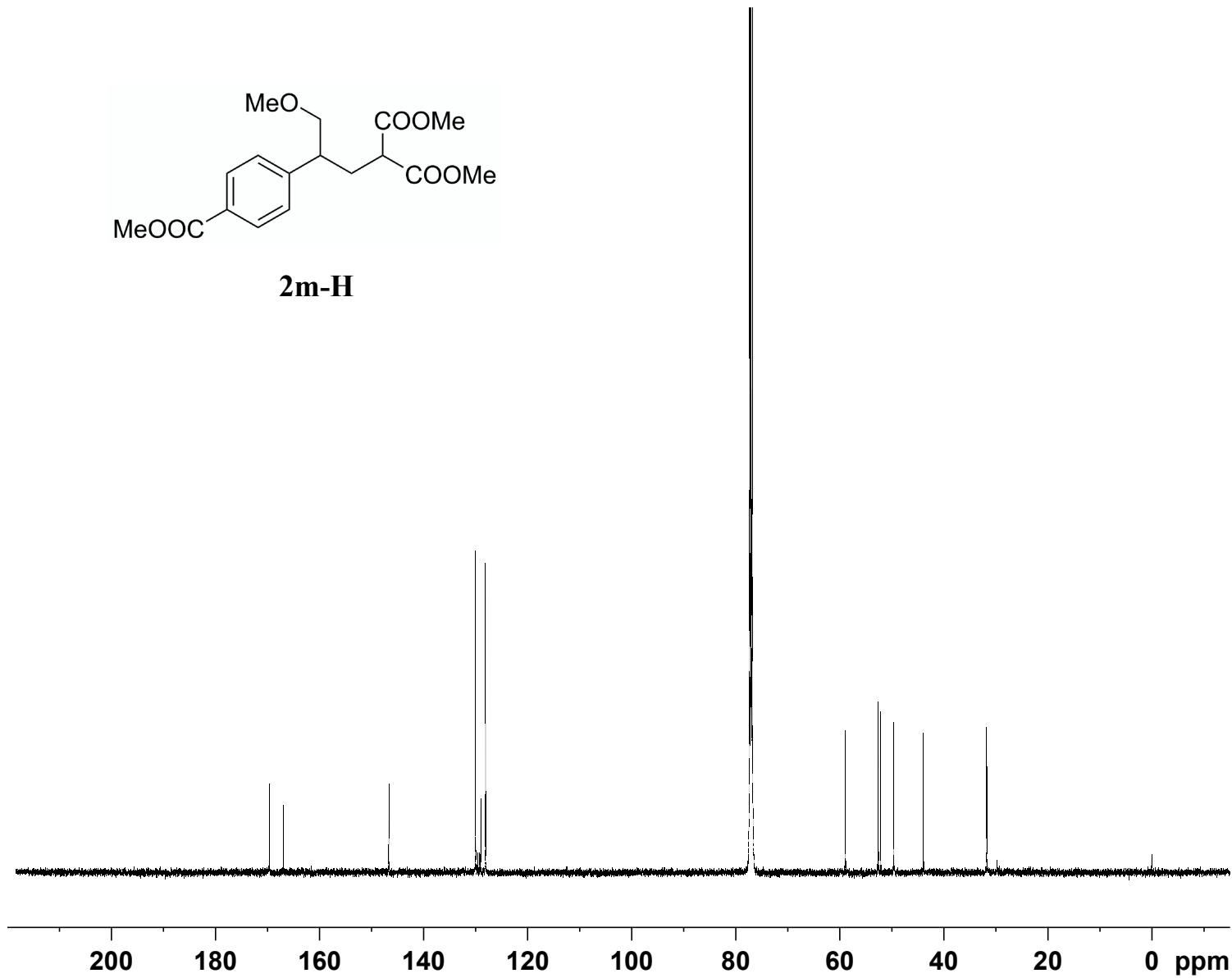
==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



58.91
 52.57
 52.53
 52.08
 49.61
 43.88
 31.71



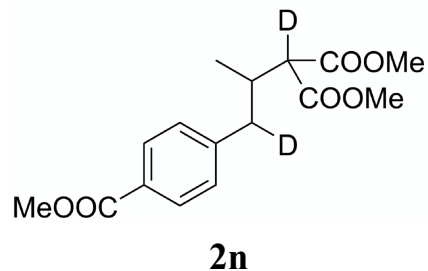
Current Data Parameters
 NAME 500M-2022
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220216
 Time 22.33
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.972
7.955
7.269
7.265
7.253

3.906
3.750
3.741
3.328
3.313
2.898
2.889
2.865
2.857
2.602
2.588
2.575
2.562
2.549
2.502
2.483
2.471
2.452
0.942
0.929

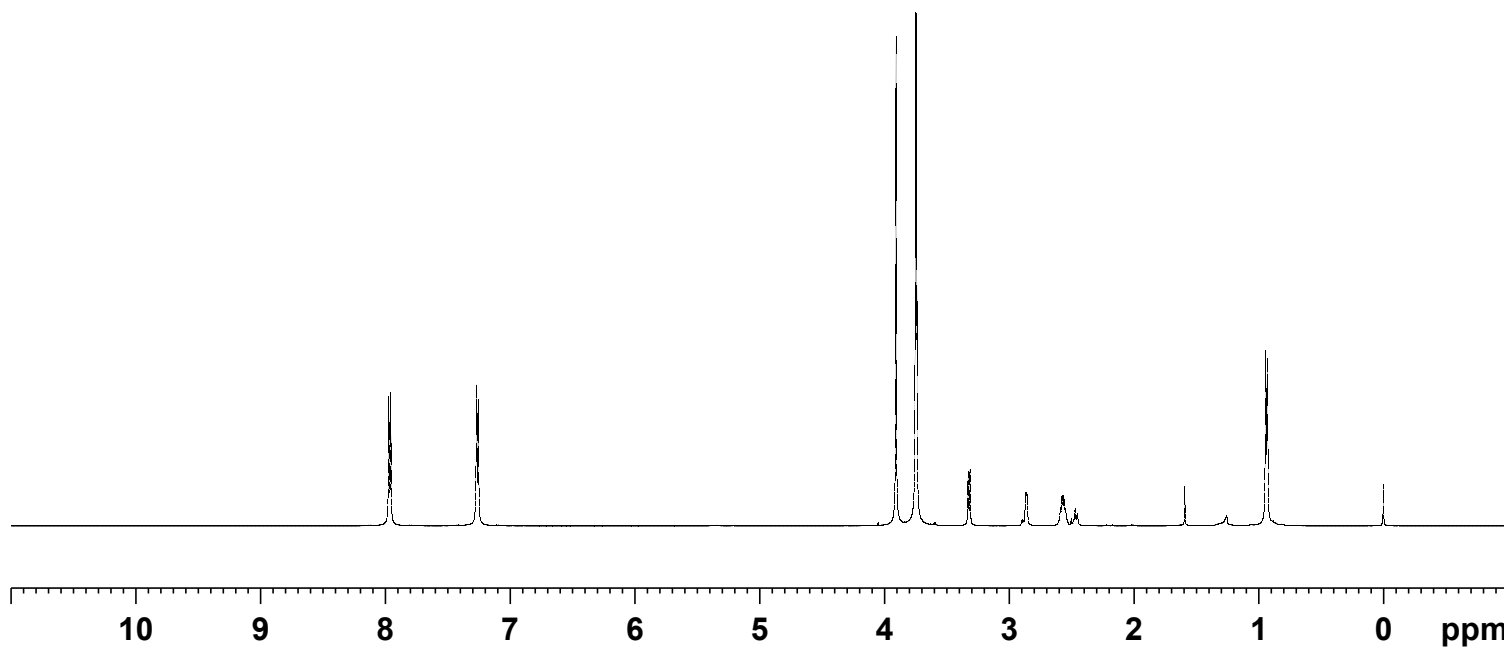
Current Data Parameters
NAME 500M-2020xia
EXPNO 220
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220105
Time 17.04
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

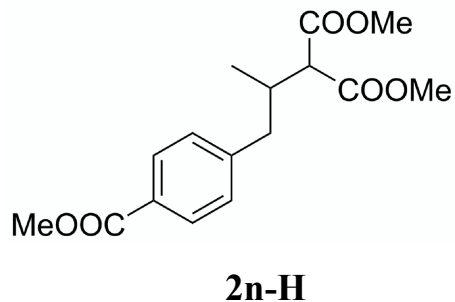
F2 - Processing parameters
SI 65536
SF 500.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.00
2.33

3.05
6.08
0.81
0.72
0.98
0.43

3.10



7.972
 7.955
 7.269
 7.265
 7.253

3.906
 3.750
 3.740
 3.327
 3.313
 2.899
 2.889
 2.872
 2.863
 2.604
 2.590
 2.575
 2.562
 2.548
 2.502
 2.484
 2.476
 2.458
 0.945
 0.932

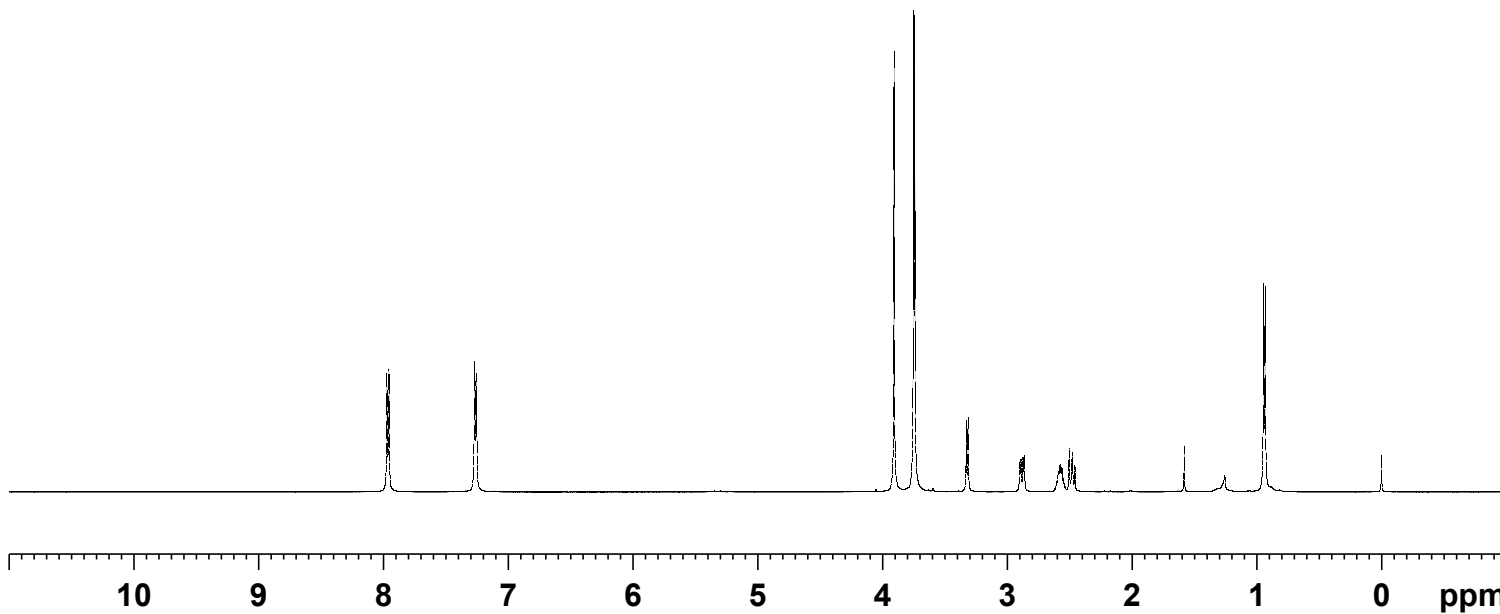
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 218
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220105
 Time 16.32
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 11.25 usec
 PLW1 20.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300103 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2.00

2.39

3.08

6.06

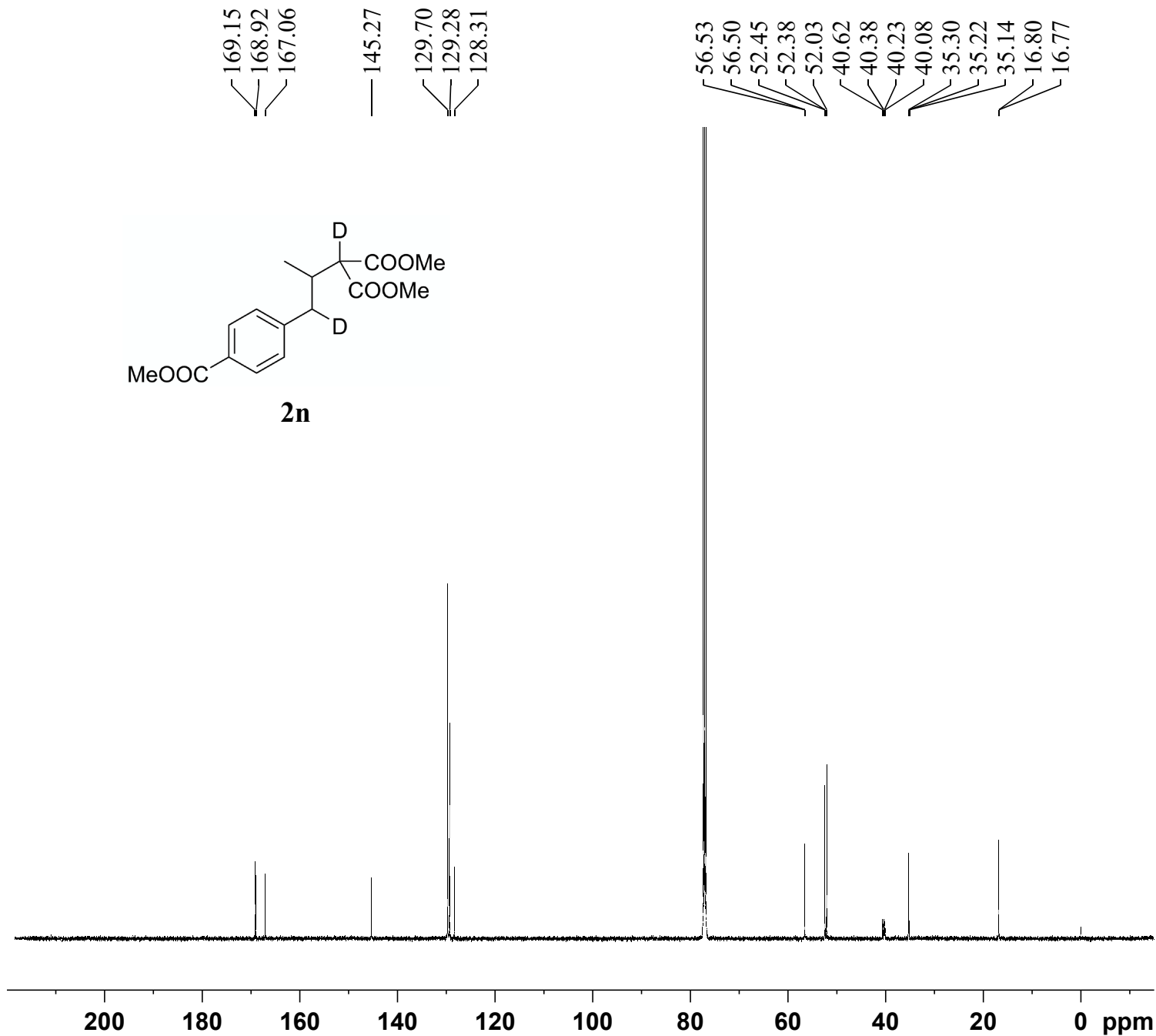
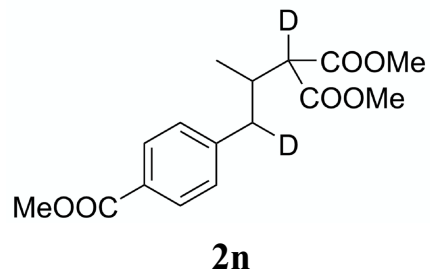
0.98

0.99

1.00

1.03

3.19



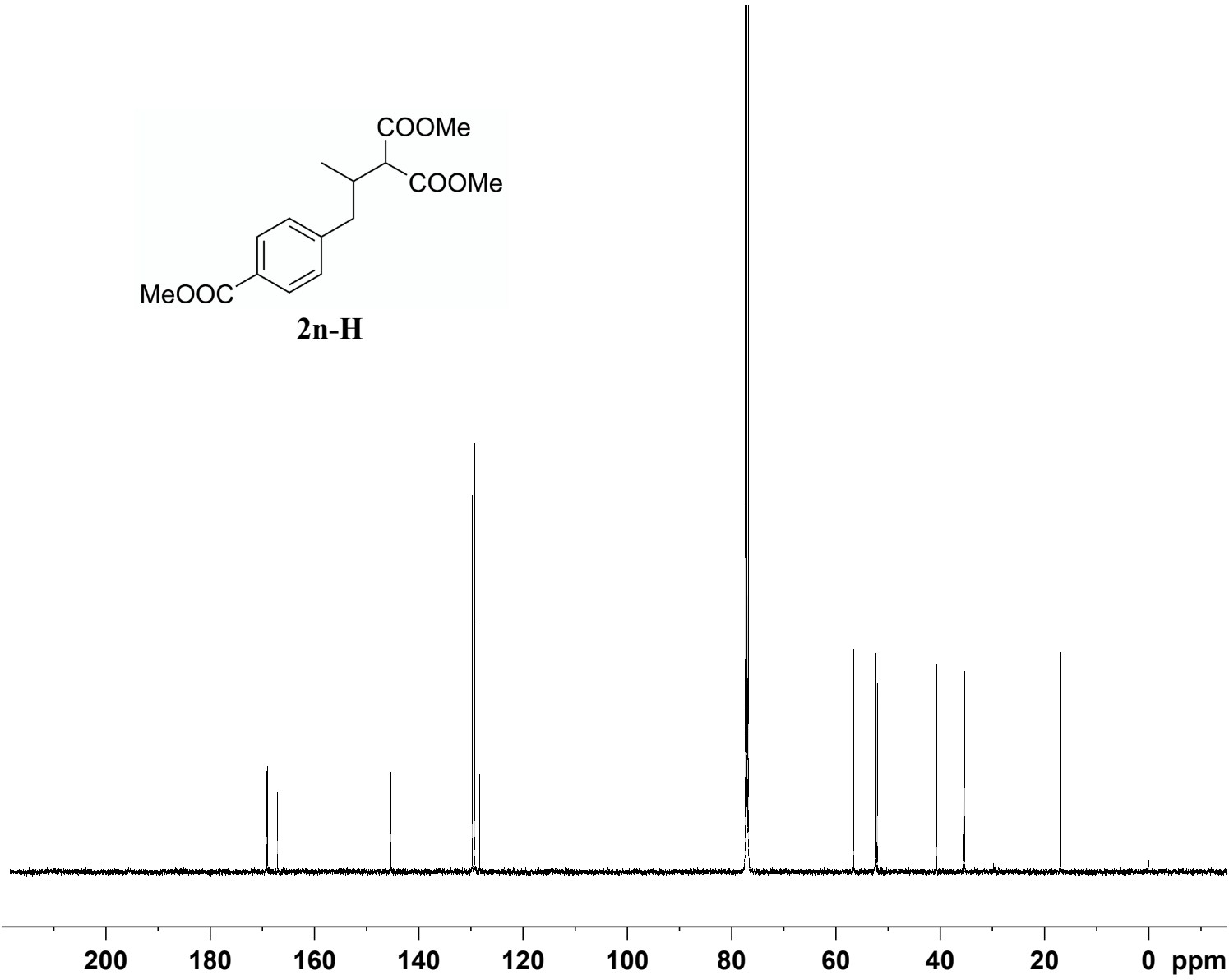
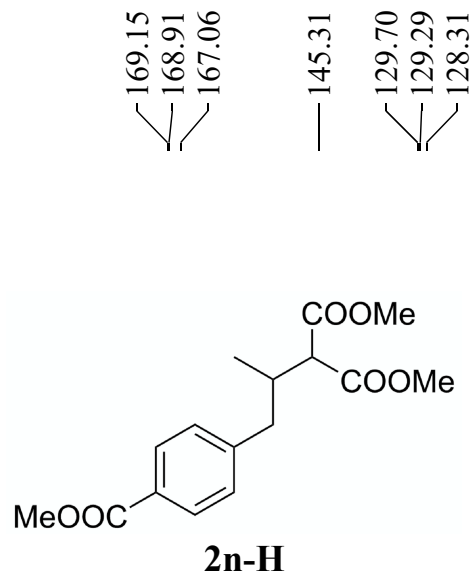
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 221
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220105
 Time 17.32
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 219
 PROCNO 1

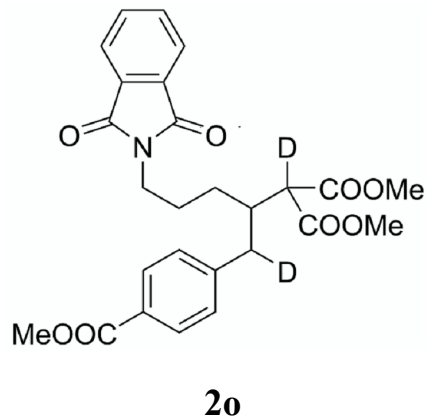
F2 - Acquisition Parameters
 Date_ 20220105
 Time 17.00
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

7.884
7.867
7.829
7.823
7.818
7.812
7.717
7.711
7.706
7.700
7.242
7.226
3.892
3.716
3.678
3.624
3.610
3.596
3.426
3.414
2.790
2.777
2.644
2.628
2.504
2.491
2.479
1.756
1.743
1.734
1.722
1.708
1.690
1.681
1.670
1.657
1.428
1.420
1.408
1.397
1.387



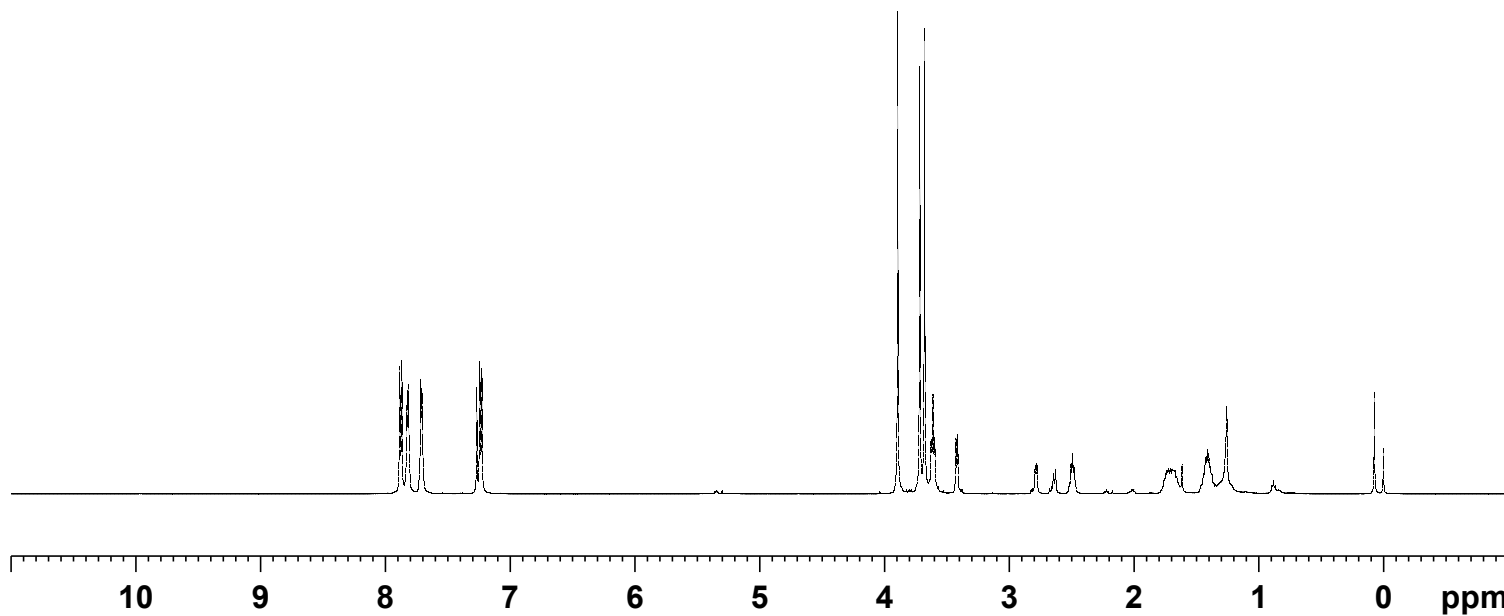
Current Data Parameters
NAME 500M-2020xia
EXPNO 229
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220112
Time 13.30
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

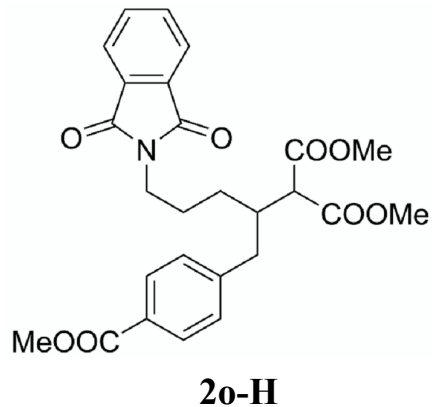
==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.96
2.02
2.08
2.00
3.00
2.92
3.00
2.19
0.93
0.63
0.55
1.01
2.29
2.22

7.883
7.869
7.825
7.821
7.814
7.713
7.709
7.703
7.242
7.227
3.894
3.892
3.718
3.716
3.679
3.677
3.625
3.611
3.597
3.426
3.415
2.810
2.796
2.783
2.675
2.659
2.649
2.632
2.505
2.493
1.723
1.708
1.693
1.681
1.672
1.626
1.432
1.423
1.411
1.400
1.390



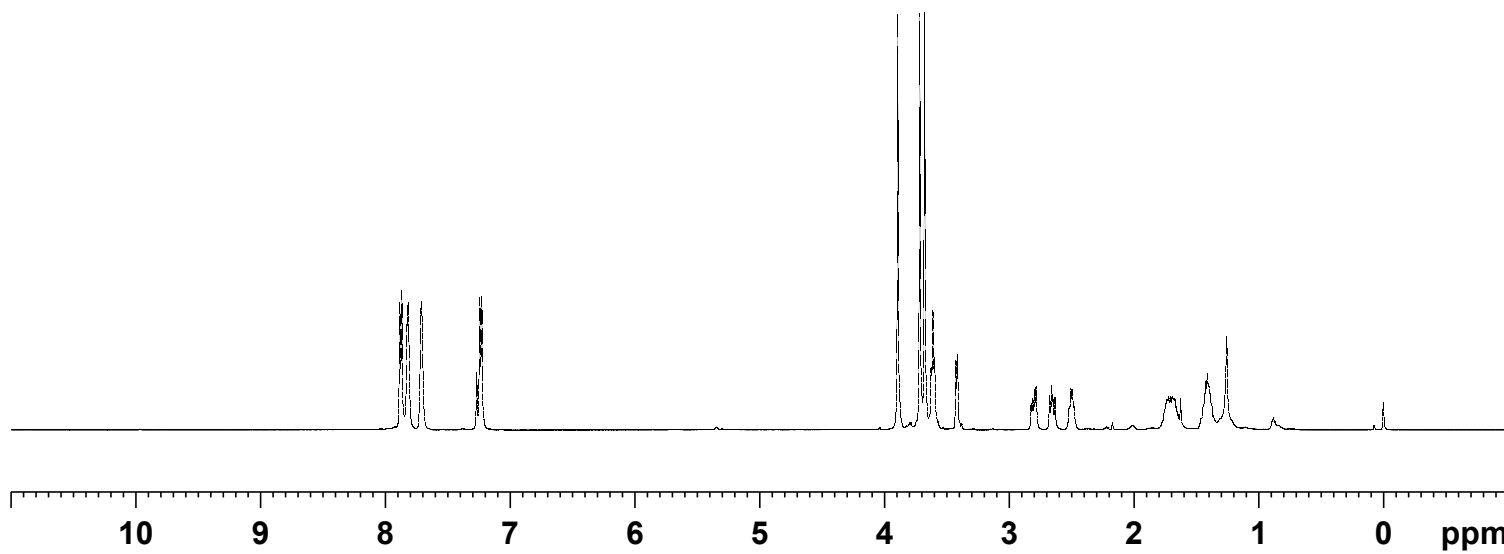
Current Data Parameters
NAME 500M-2020xia
EXPNO 216
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211228
Time 15.56
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 49.27
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

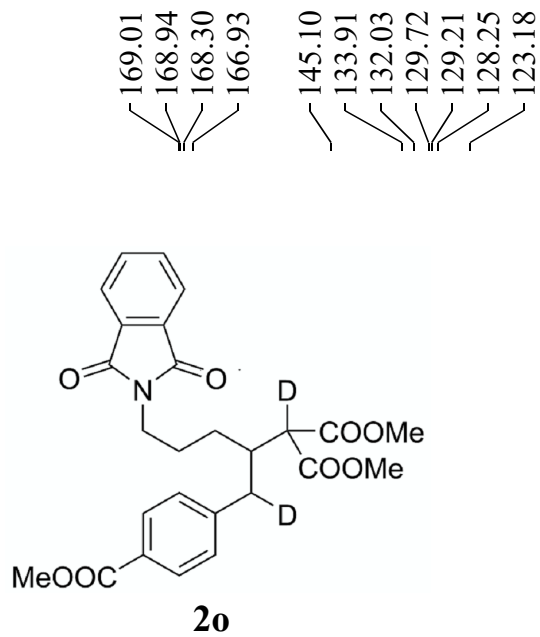
==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 11.25 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

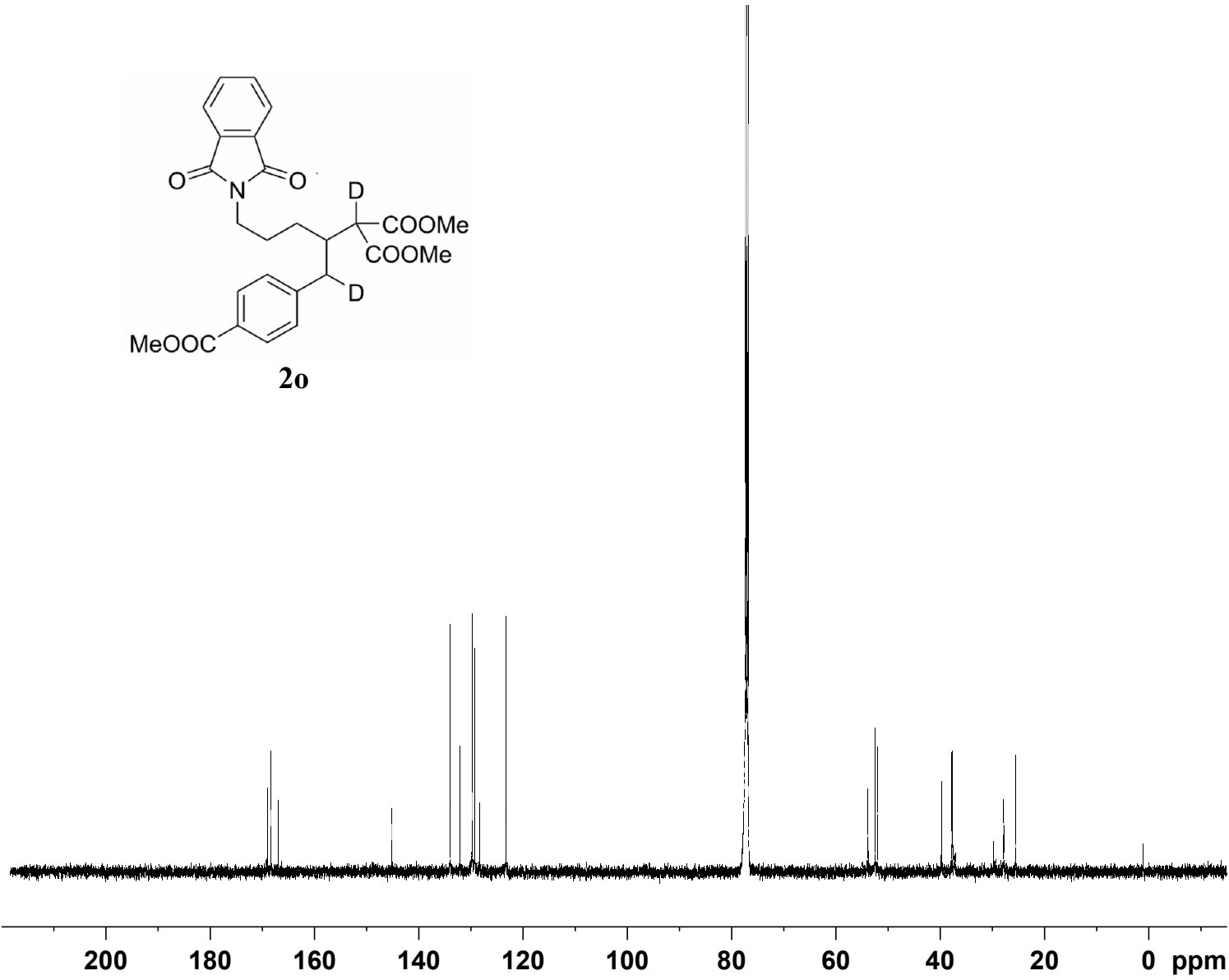
F2 - Processing parameters
SI 65536
SF 500.1300046 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



3.96
2.00
2.34
3.03
5.83
2.06
1.04
0.98
1.00
0.99
2.34
2.09



53.80
52.44
52.40
51.98
39.65
37.52
37.15
37.01
29.71
27.75
25.47



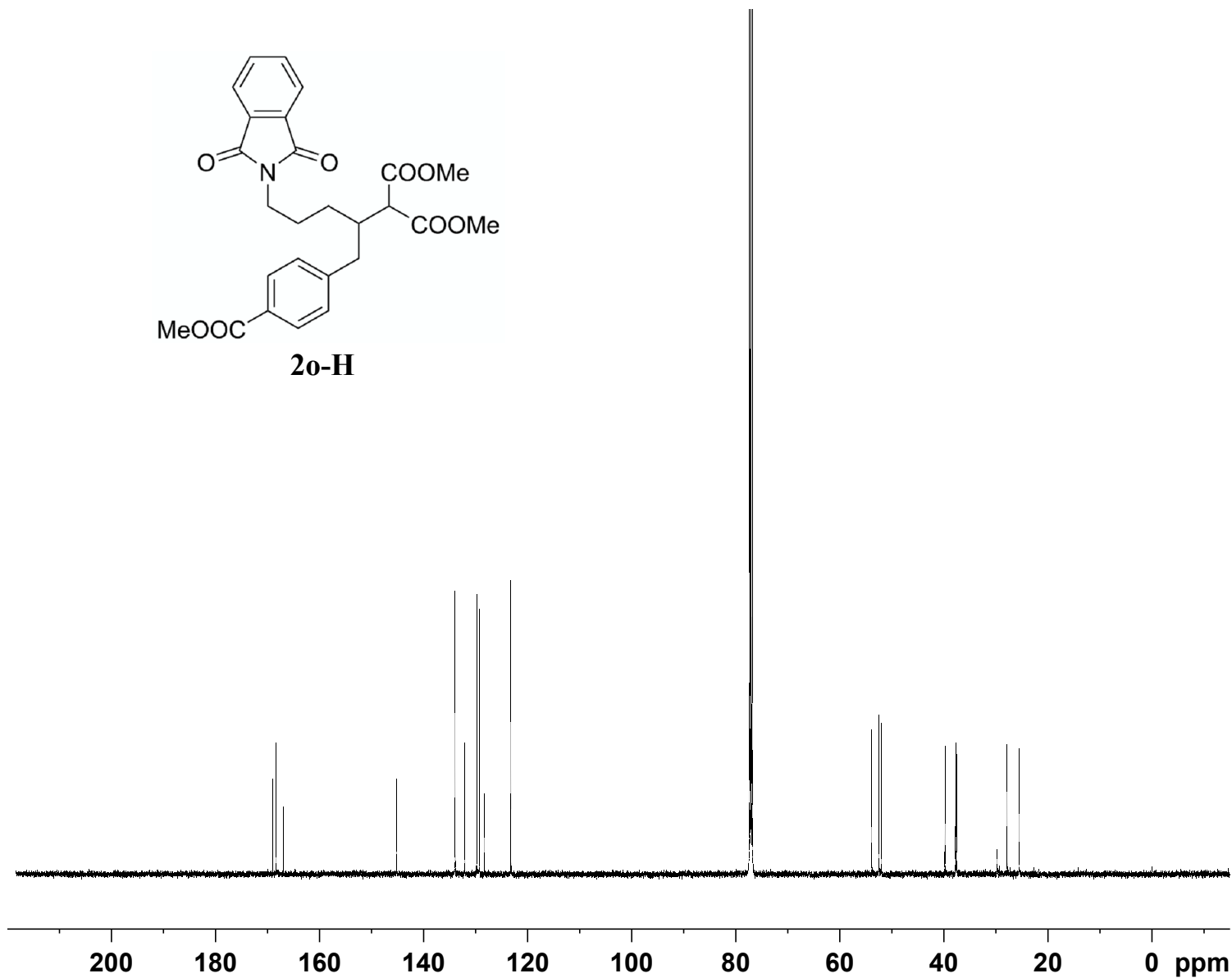
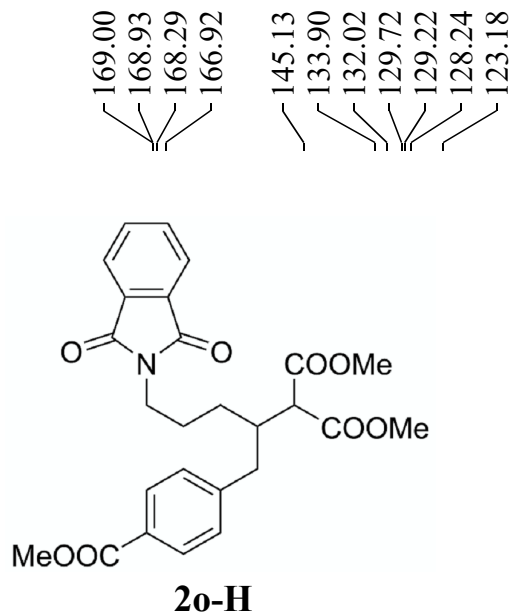
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 226
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220111
 Time 12.31
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.0000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.0000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 217
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211228
 Time 16.24
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.39550999 W
 PLW13 0.25312999 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

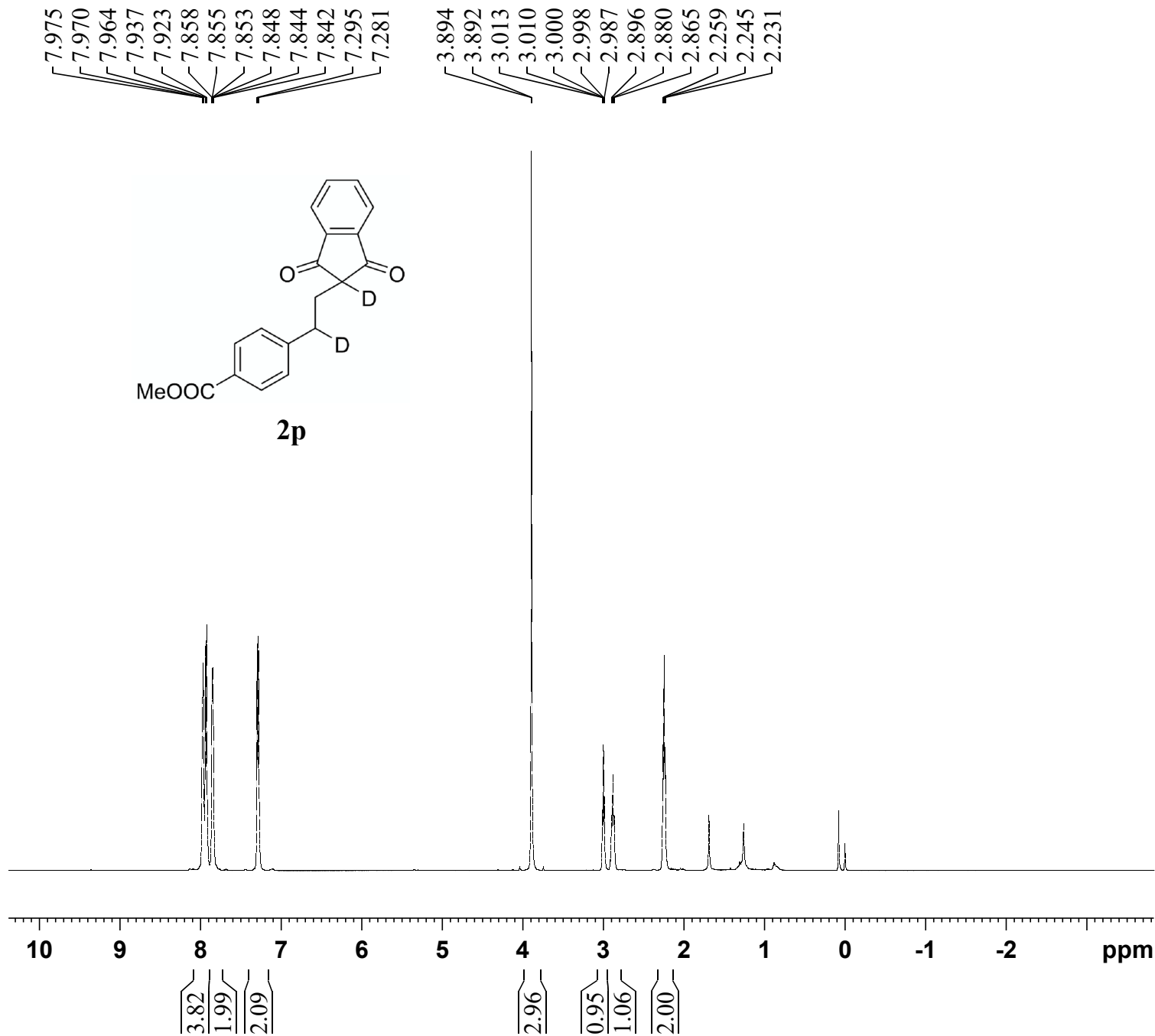
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 133
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211101
 Time 10.00
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

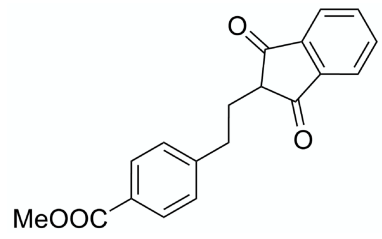
==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300046 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

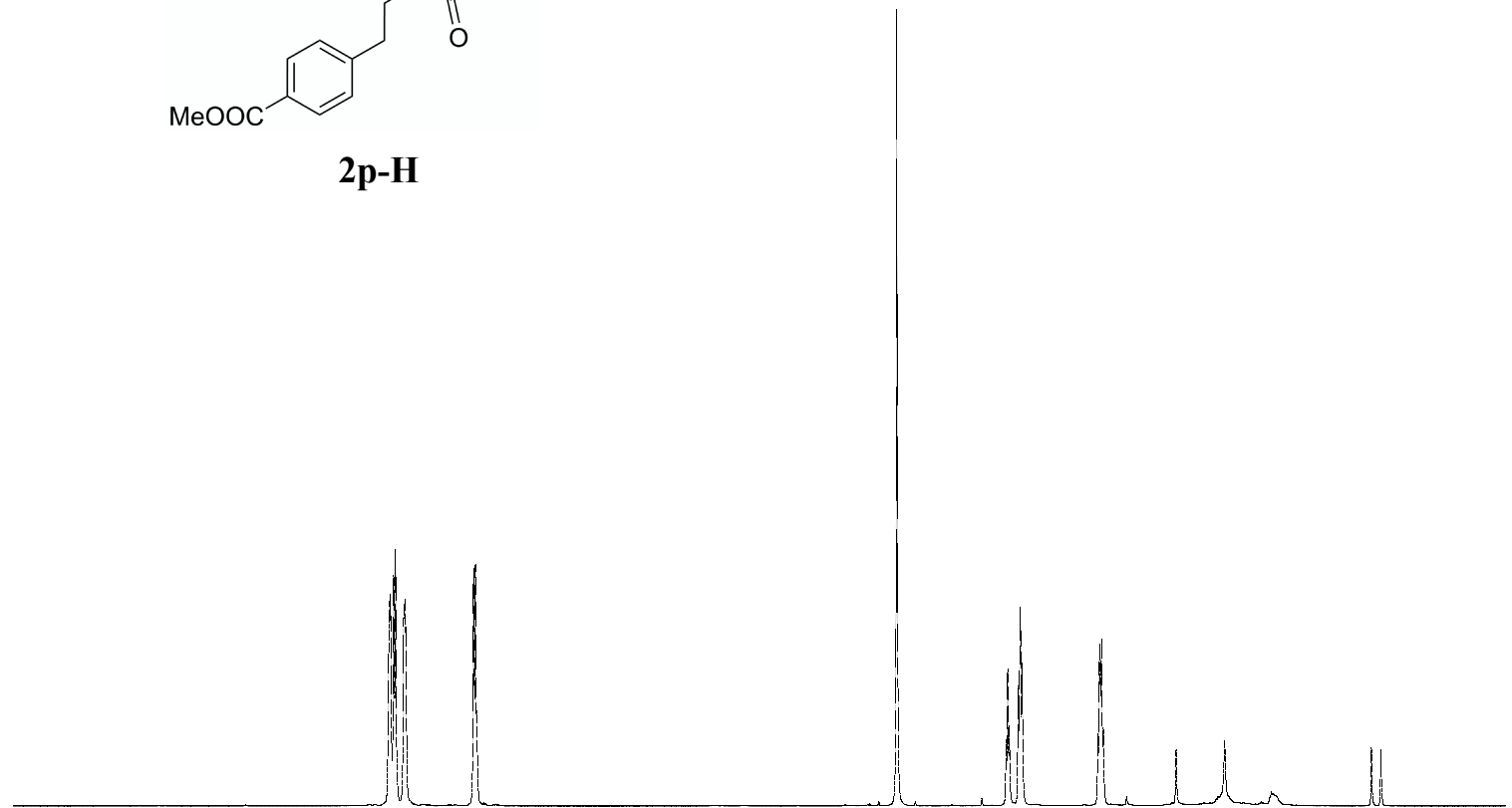


7.975
7.970
7.964
7.939
7.923
7.858
7.856
7.852
7.847
7.841
7.295
7.280

3.894
3.013
3.000
2.988
2.916
2.900
2.884
2.276
2.261
2.245
2.232



2p-H



3.90
2.01
2.21

3.06
1.00
2.01
2.04

Current Data Parameters
 NAME 500M-2020xia
 EXPNO 163
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 15.47
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 49.27
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300064 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

— 199.52

— 166.00

— 145.22

— 141.22

— 134.71

— 128.76

— 127.71

— 127.19

— 122.17

— 51.21

— 50.97

— 31.39

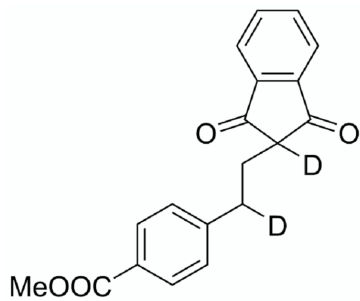
— 31.20

— 31.05

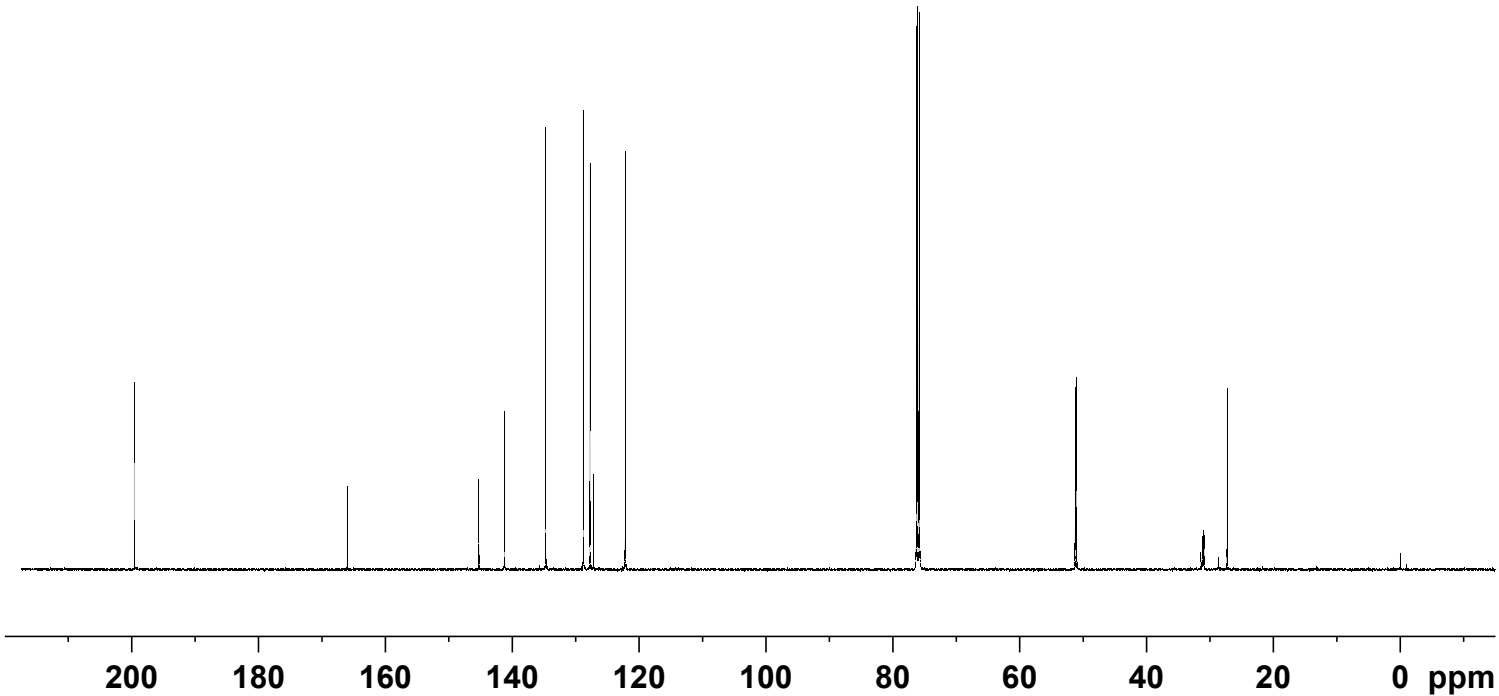
— 30.89

— 27.30

— 27.23



2p



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 136
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211102
 Time 10.24
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

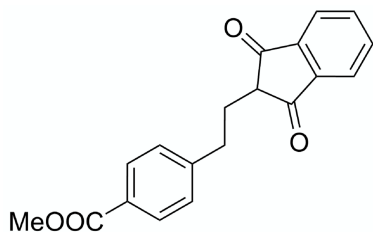
==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

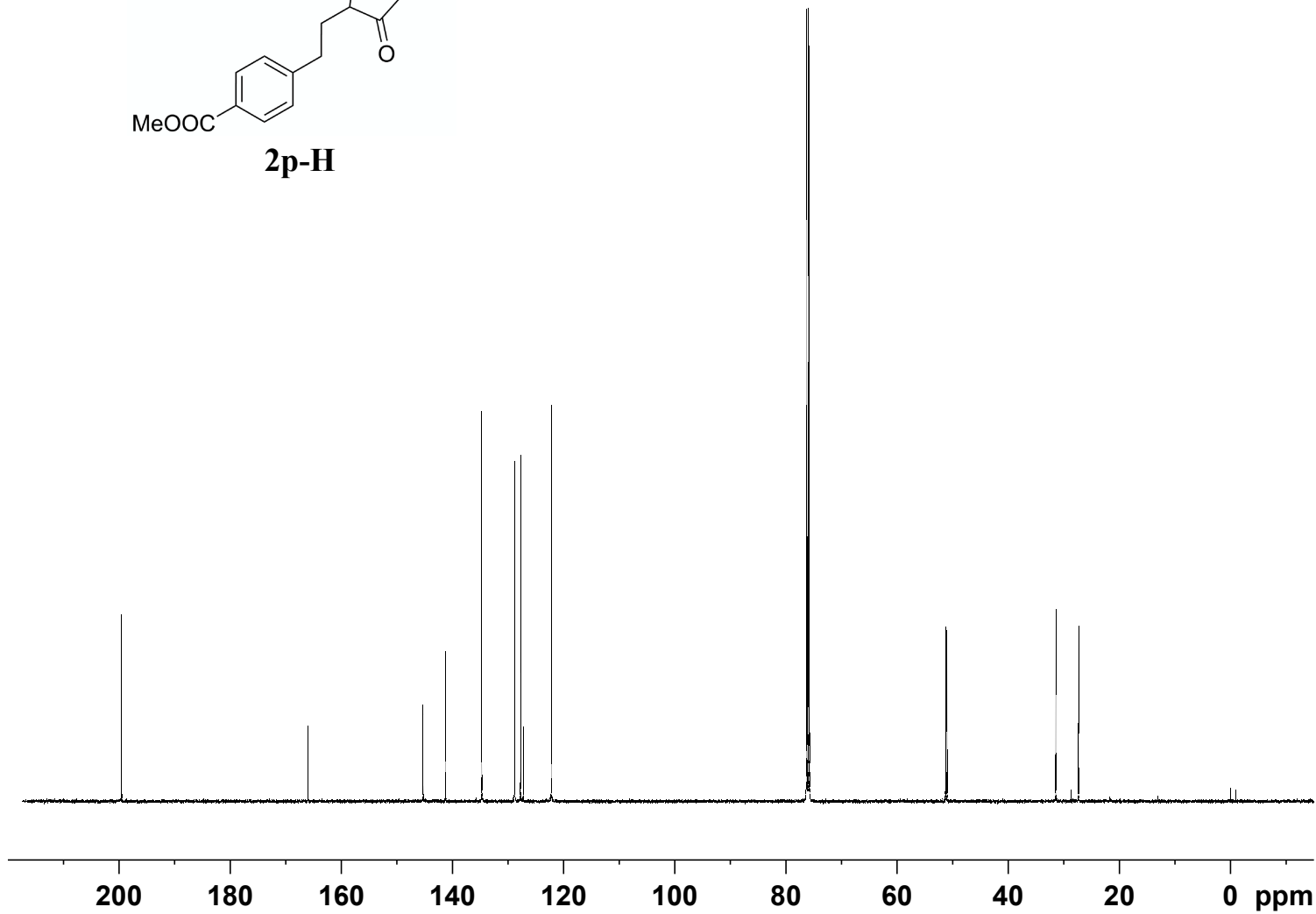
F2 - Processing parameters
 SI 32768
 SF 125.7579178 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

— 199.51
 — 166.00
 / 145.26
 / 141.23
 / 134.71
 / 128.76
 / 127.71
 / 127.19
 / 122.17

< 51.24
 < 50.97
 < 31.39
 < 27.31



2p-H



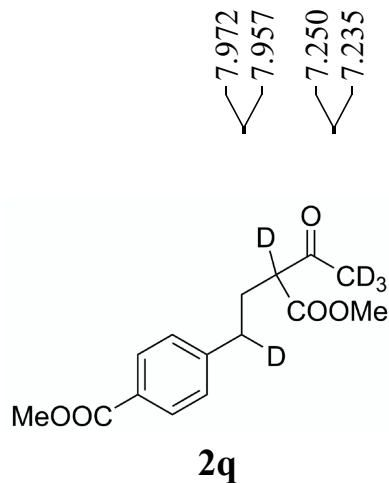
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 164
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 16.14
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7579178 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



$\begin{matrix} \text{3.904} \\ \text{3.743} \\ \text{3.714} \\ \text{3.443} \\ \text{3.429} \\ \text{3.415} \\ \text{2.672} \\ \text{2.655} \\ \text{2.637} \\ \text{2.622} \\ \text{2.215} \\ \text{2.200} \\ \text{2.186} \\ \text{2.172} \\ \text{2.158} \end{matrix}$

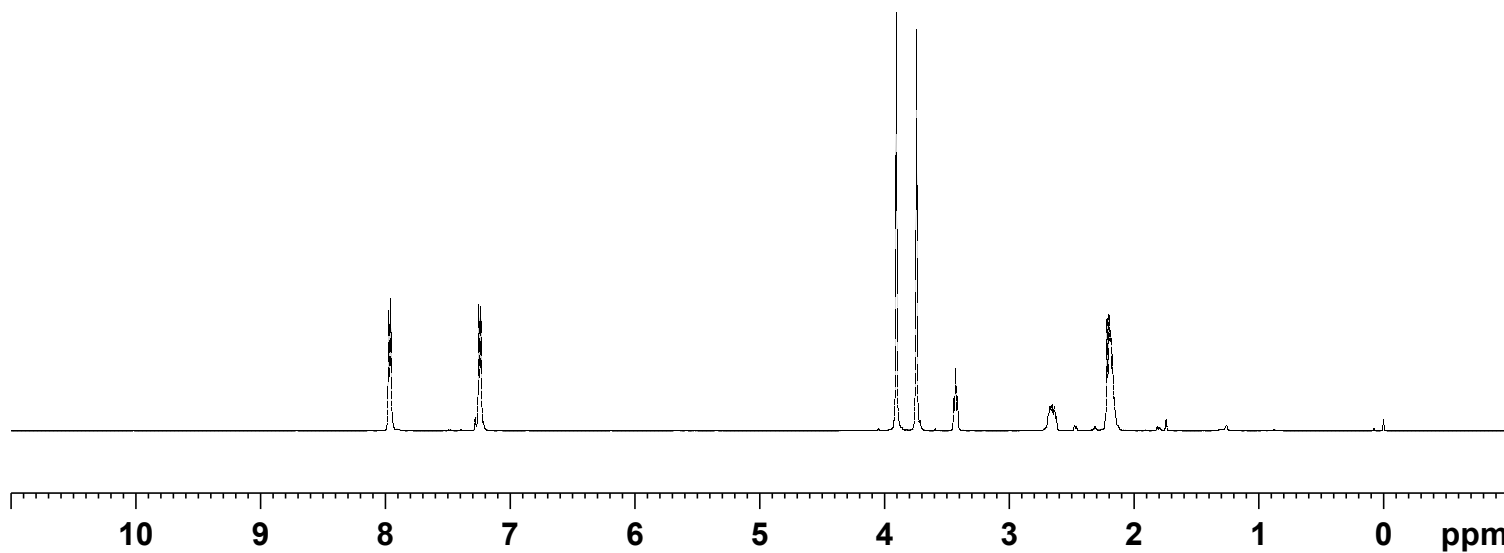
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 157
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 7.02
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

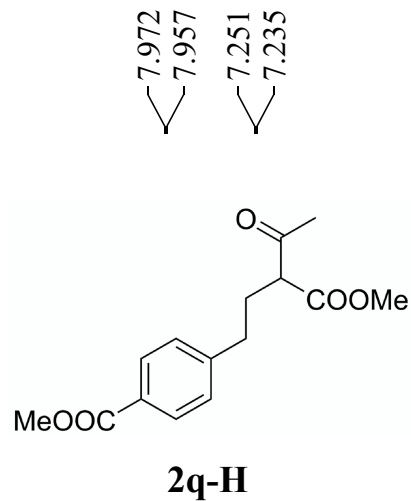
==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300012 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



$\begin{matrix} \text{2.00} \\ \text{2.09} \\ \text{3.12} \\ \text{3.00} \\ \text{0.92} \\ \text{1.07} \\ \text{3.71} \end{matrix}$



3.904
 3.742
 3.446
 3.431
 3.417
 2.707
 2.695
 2.679
 2.664
 2.649
 2.638
 2.216
 2.186
 2.172
 2.158

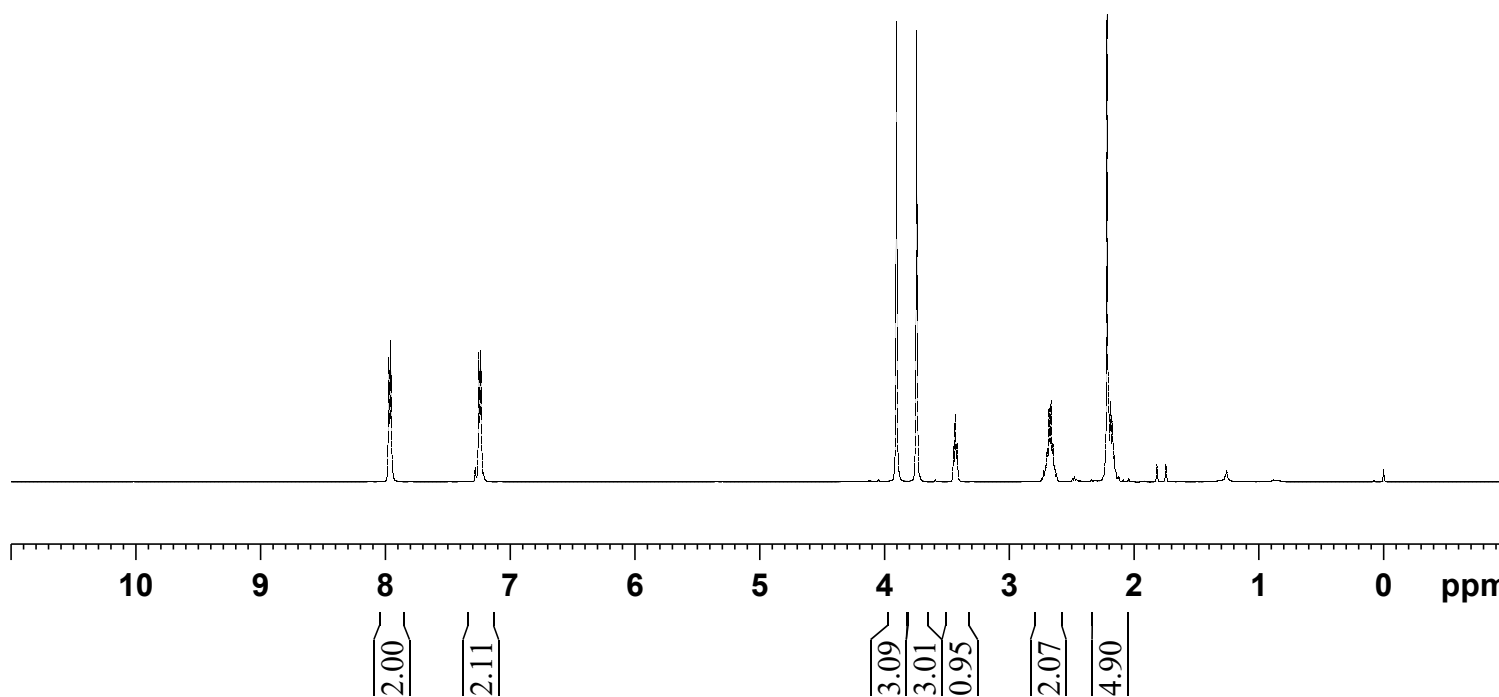
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 153
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 5.32
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300010 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

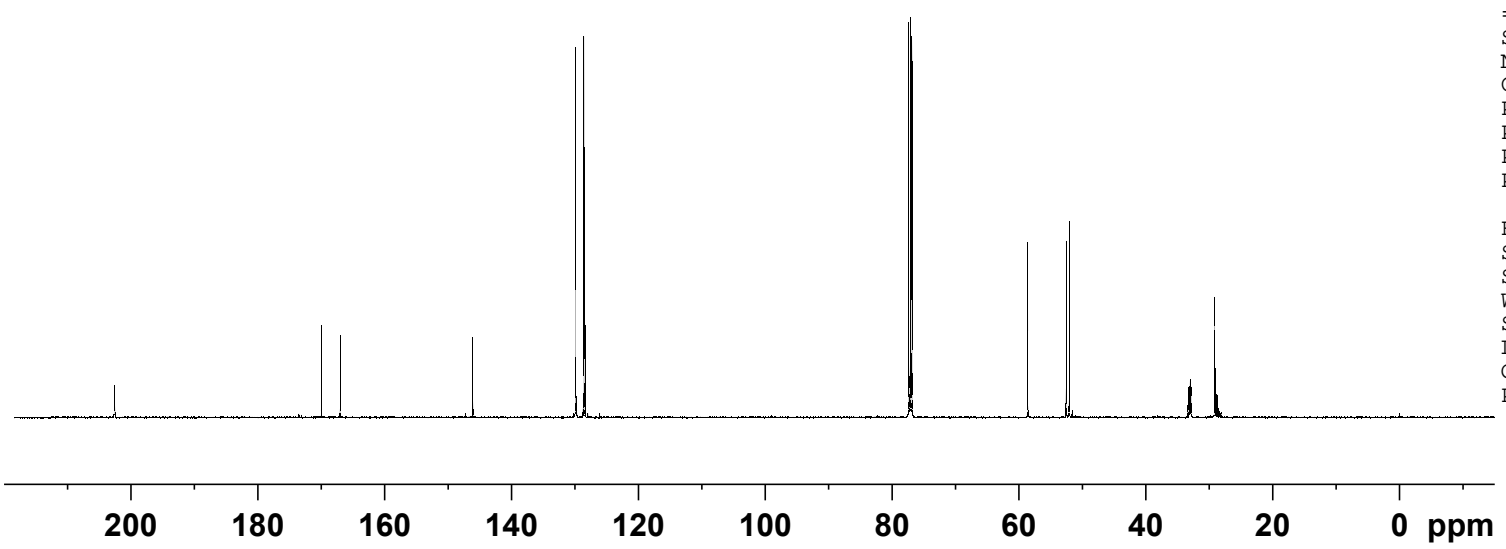
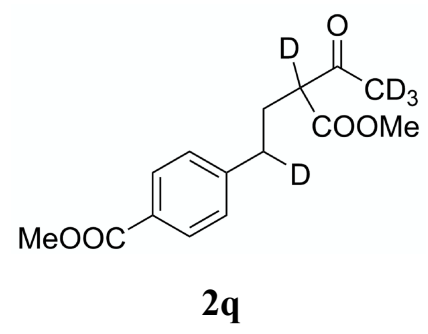


202.58
202.54
202.49

169.95
166.97

146.04
129.86
129.64
128.51
128.30

58.54
52.50
52.02
33.12
32.96
32.81
29.07
29.03
28.93
28.78
28.62



Current Data Parameters
NAME 500M-2020xia
EXPNO 158
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211113
Time 7.29
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

— 202.48

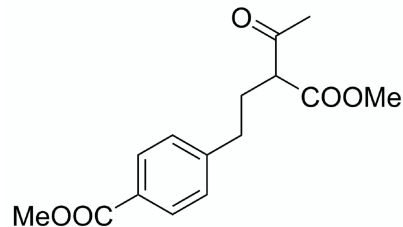
— 169.95
— 166.97

— 146.08

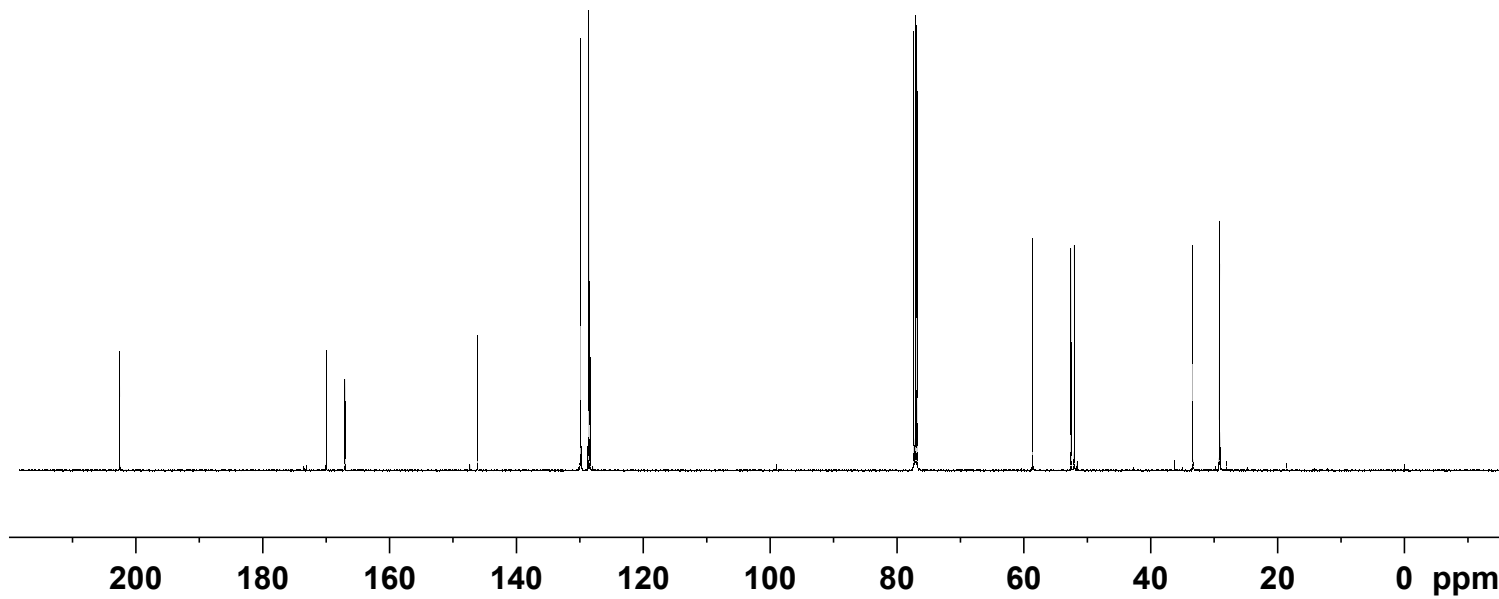
— 129.86
— 128.51
— 128.30

— 58.56
— 52.50
— 52.02

— 33.31
— 29.15
— 29.03



2q-H



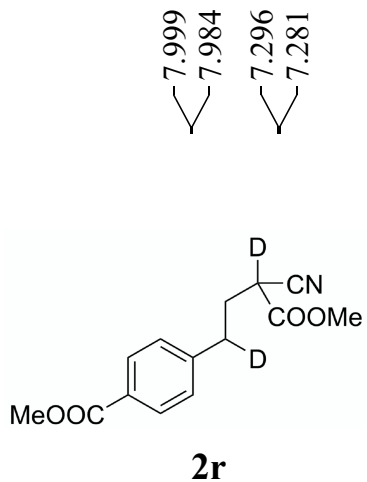
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 154
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 5.59
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

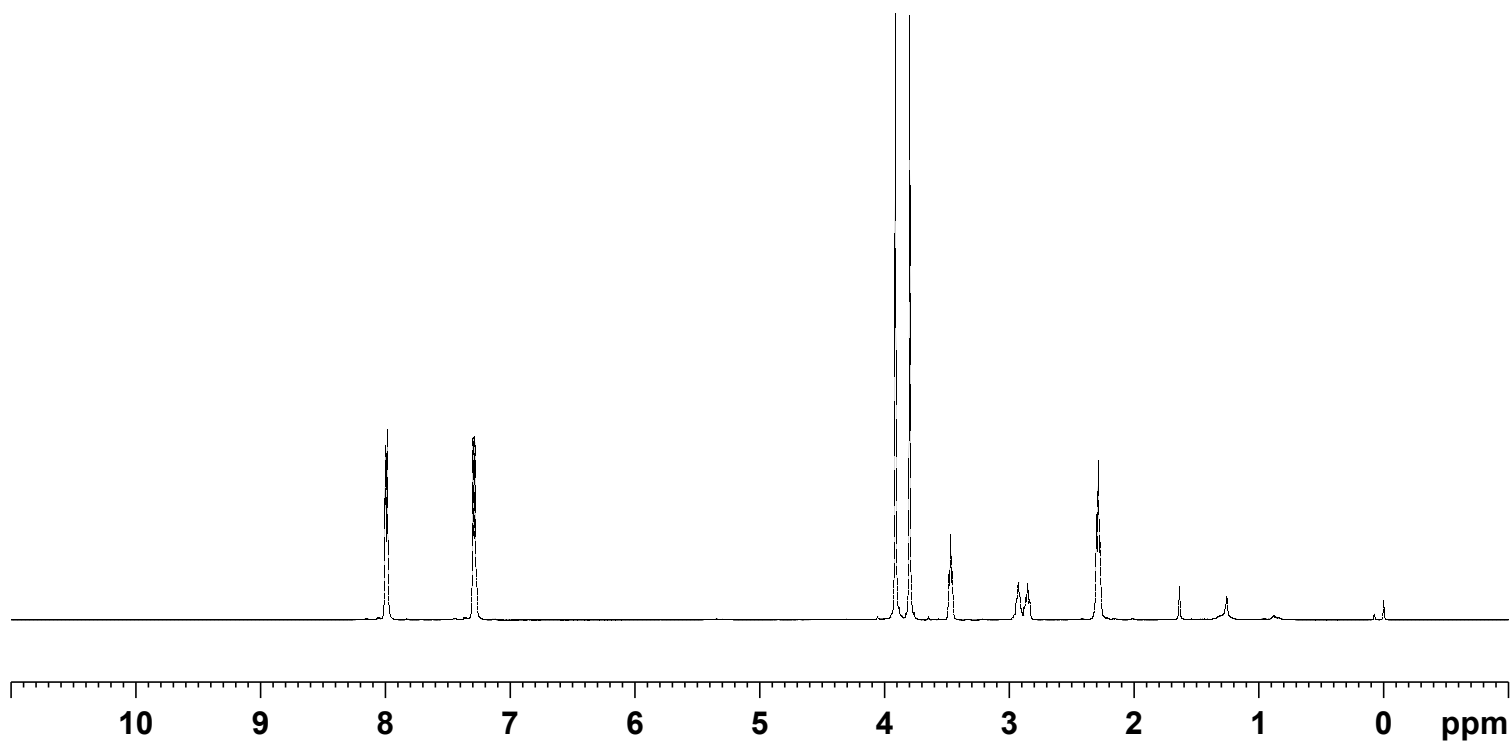
==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



$\begin{matrix} \text{3.912} \\ \text{3.799} \\ \text{3.483} \\ \text{3.469} \\ \text{3.455} \\ \text{2.939} \\ \text{2.926} \\ \text{2.880} \\ \text{2.866} \\ \text{2.852} \\ \text{2.836} \\ \text{2.300} \\ \text{2.285} \\ \text{2.271} \end{matrix}$



Current Data Parameters
 NAME 500M-2020xia
 EXPNO 161
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 8.04
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 49.27
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

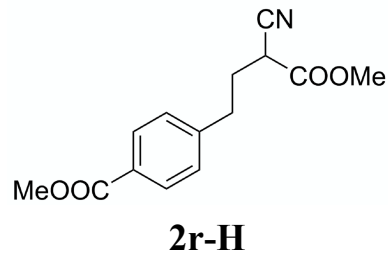
==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300065 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

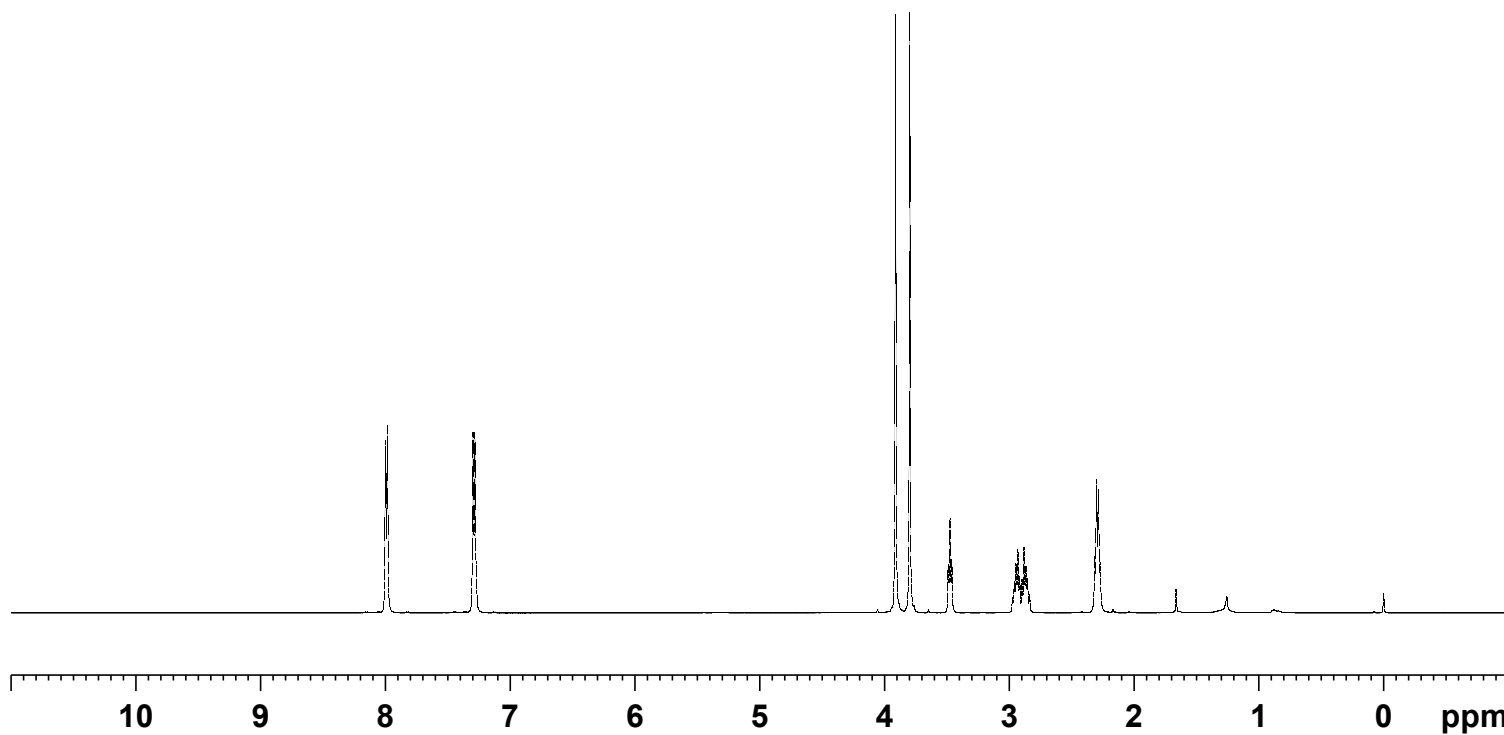
2.00
2.18

3.17
3.01
0.98
1.16
2.08



7.998
7.983
7.297
7.282

3.912
3.798
3.488
3.474
3.460
2.958
2.944
2.930
2.916
2.896
2.880
2.865
2.852
2.315
2.299
2.285
2.270



2.00
2.14

3.11
3.03
0.99
2.05
2.06

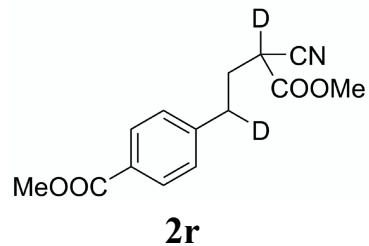
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 159
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 7.33
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 31.72
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

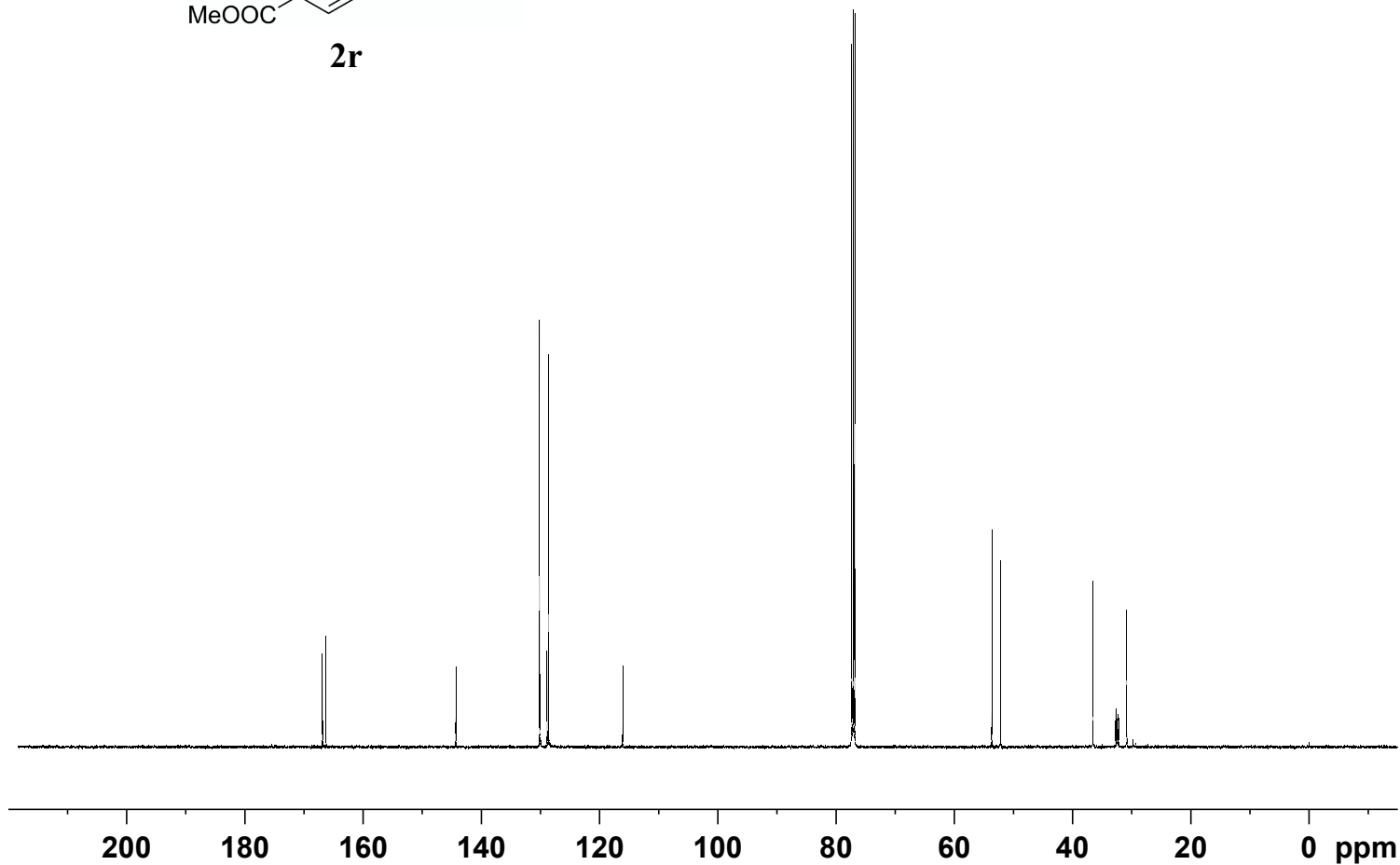
==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300054 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



166.83
 166.23
 144.27
 130.09
 128.83
 128.57
 116.03

53.60
 52.11
 36.50
 32.64
 32.46
 32.30
 32.15
 30.85
 30.78



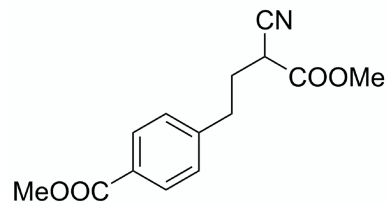
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 162
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 8.32
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

===== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

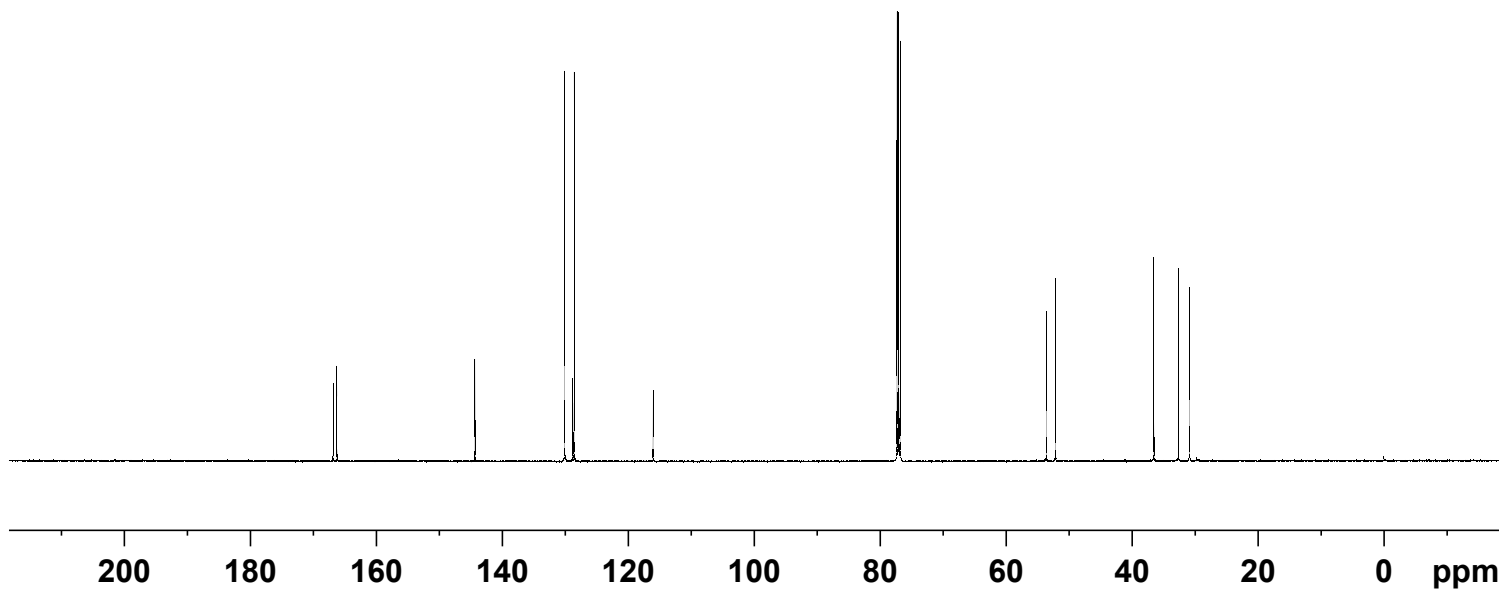
F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



2r-H

166.82
166.24
— 144.31
130.09
128.82
128.58
— 116.03

53.59
52.11
36.52
32.64
30.85



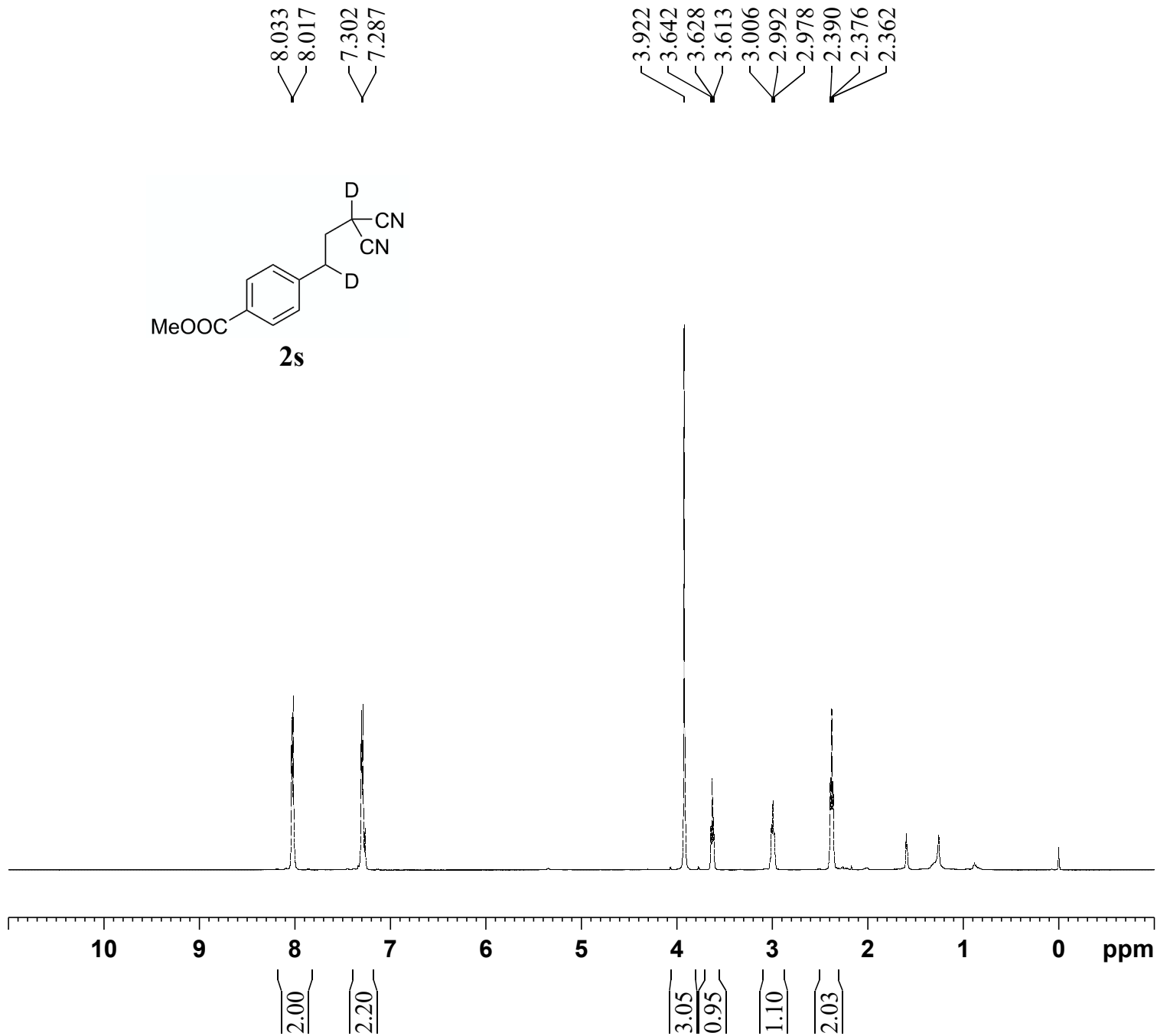
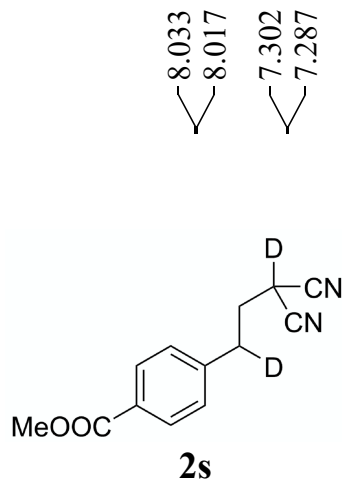
Current Data Parameters
NAME 500M-2020xia
EXPNO 160
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211113
Time 8.01
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W

==== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 20.00000000 W
PLW12 0.35778001 W
PLW13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



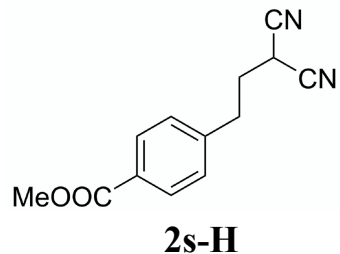
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 145
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 3.30
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 62.06
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.59 usec
 PLW1 20.00000000 W

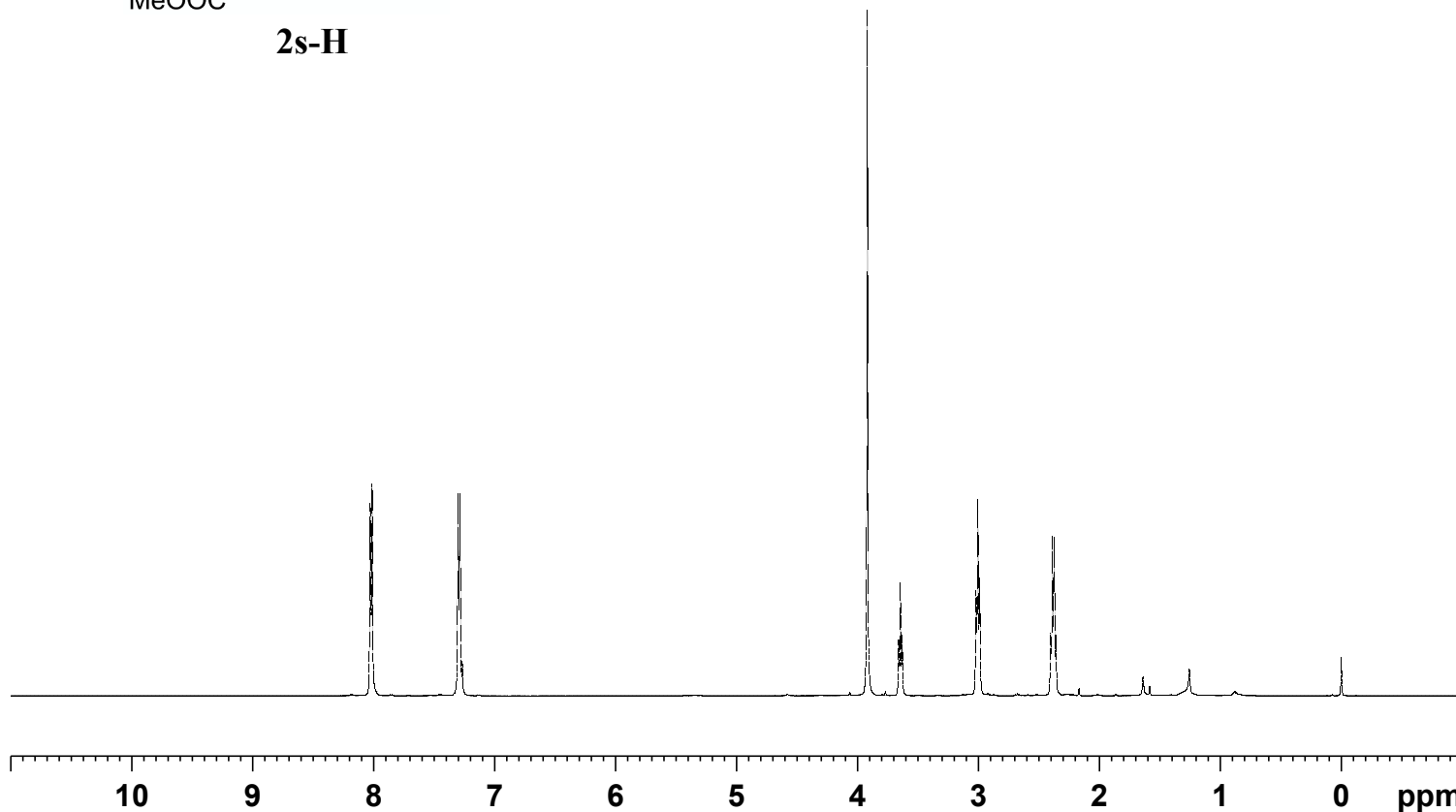
==== CHANNEL f2 =====
 SFO2 500.1330885 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 500.1300088 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



8.028
8.012
7.301
7.286

3.919
3.659
3.645
3.631
3.019
3.004
2.989
2.403
2.387
2.373
2.358



2.07

2.20

3.18

1.00

2.11

2.09

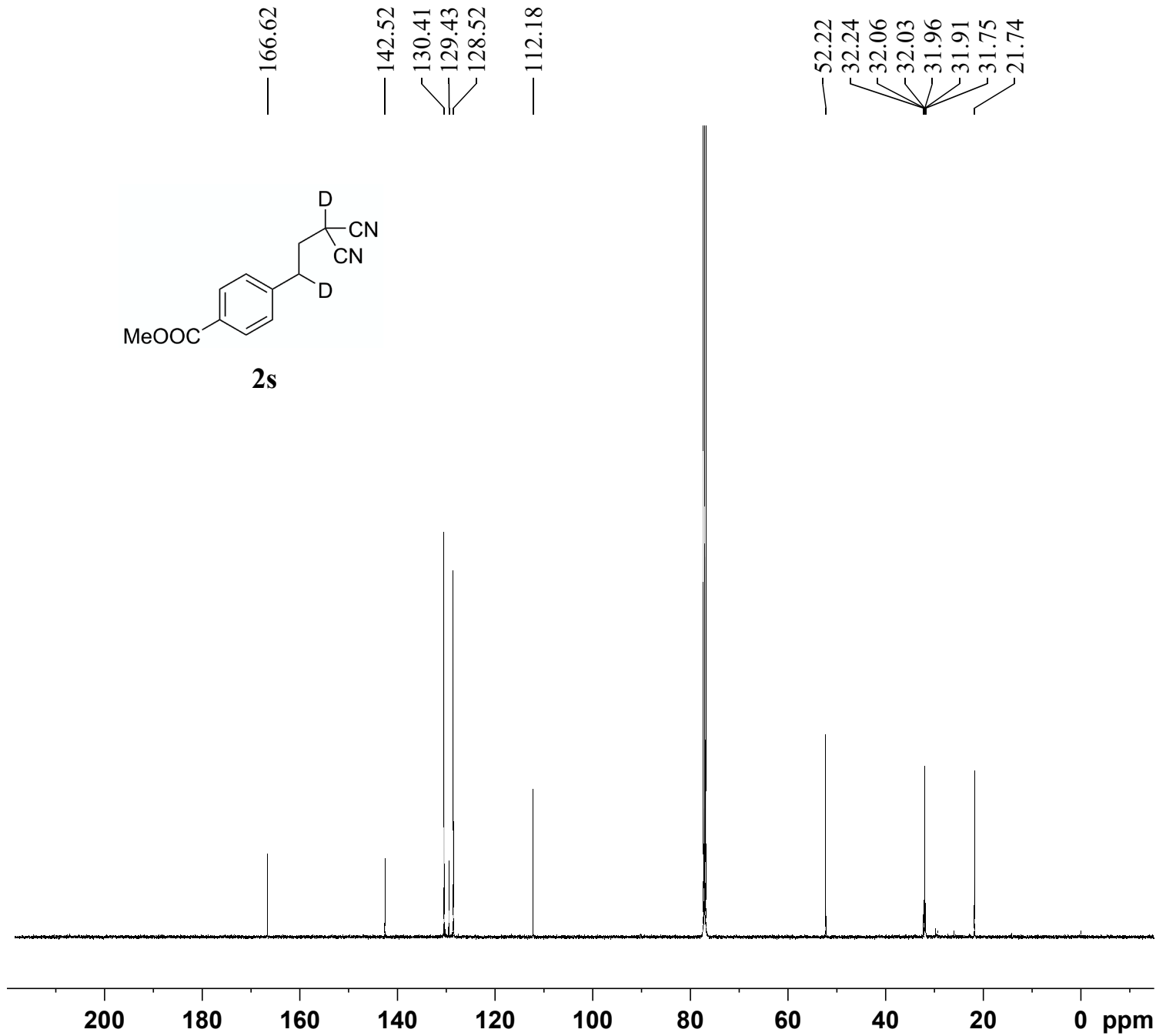
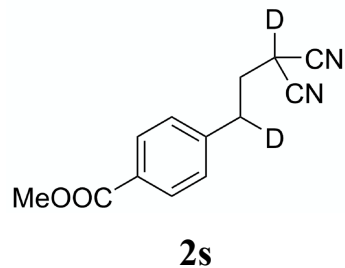
Current Data Parameters
NAME 500M-2020xia
EXPNO 143
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211113
Time 2.59
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 31.72
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 10.59 usec
PLW1 20.00000000 W

==== CHANNEL f2 =====
SFO2 500.1330885 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 500.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



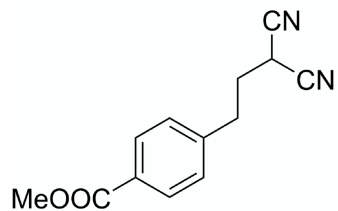
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 146
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 3.58
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

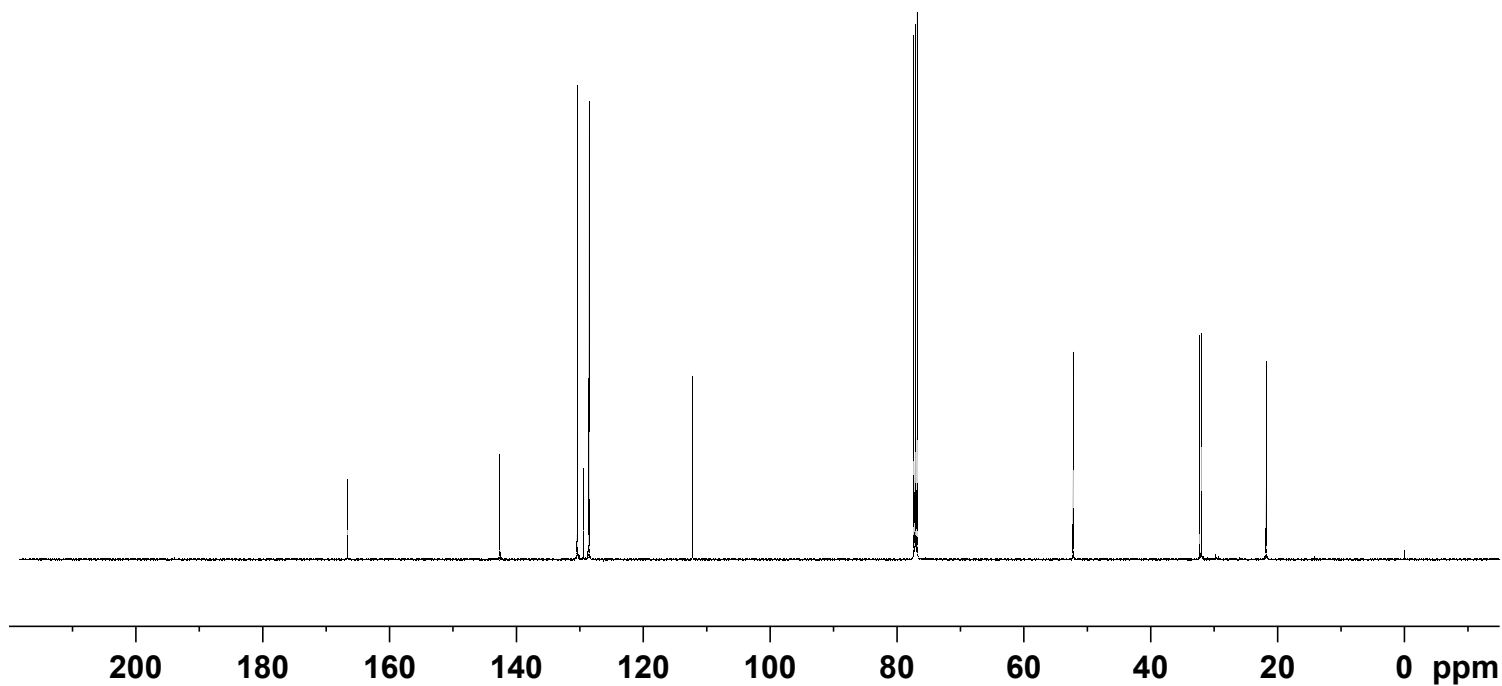
F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



2s-H

— 166.63
 — 142.60
 130.39
 129.40
 128.53
 — 112.21

— 52.21
 32.24
 32.00
 — 21.77



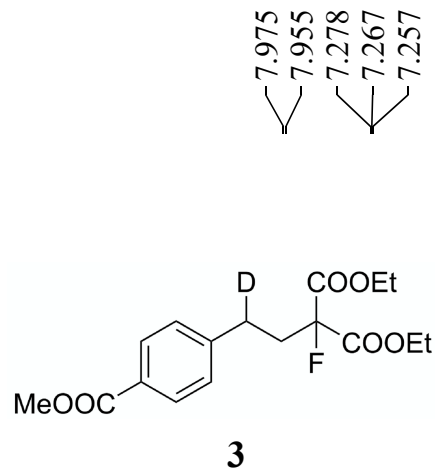
Current Data Parameters
 NAME 500M-2020xia
 EXPNO 144
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211113
 Time 3.27
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W

==== CHANNEL f2 =====
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 20.00000000 W
 PLW12 0.35778001 W
 PLW13 0.22898000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.975
7.955
7.278
7.267
7.257

4.311
4.293
4.276
4.258
3.905
2.813
2.794
2.773
2.754
2.516
2.494
2.460
2.438
1.330
1.312
1.294

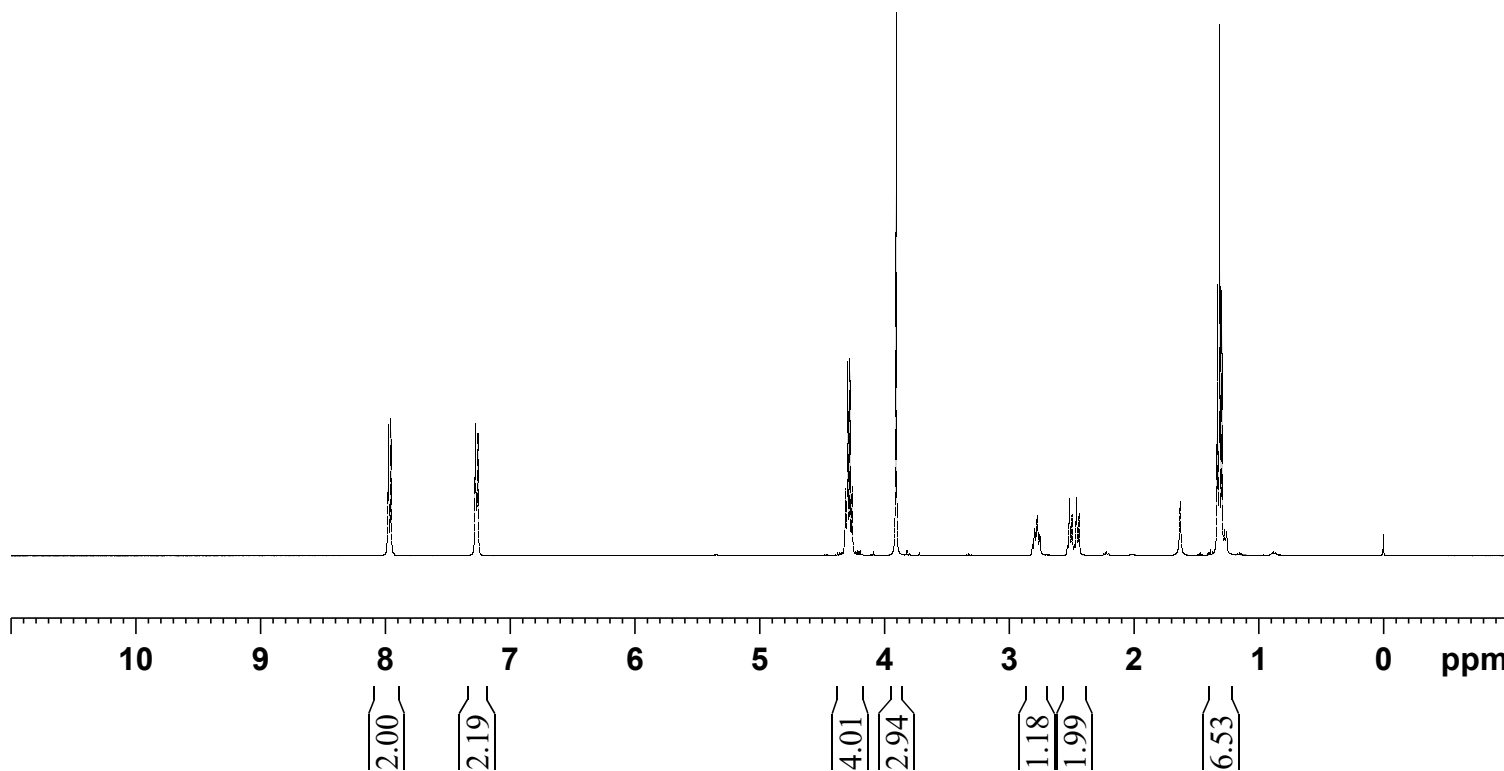
Current Data Parameters
NAME 400M-2022
EXPNO 15
PROCNO 1

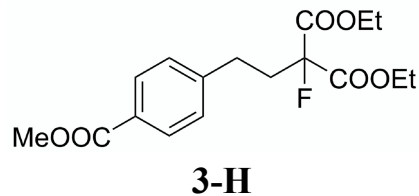
F2 - Acquisition Parameters
Date_ 20220701
Time 7.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 116.67
DW 62.400 usec
DE 6.50 usec
TE 300.9 K
D1 2.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

==== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

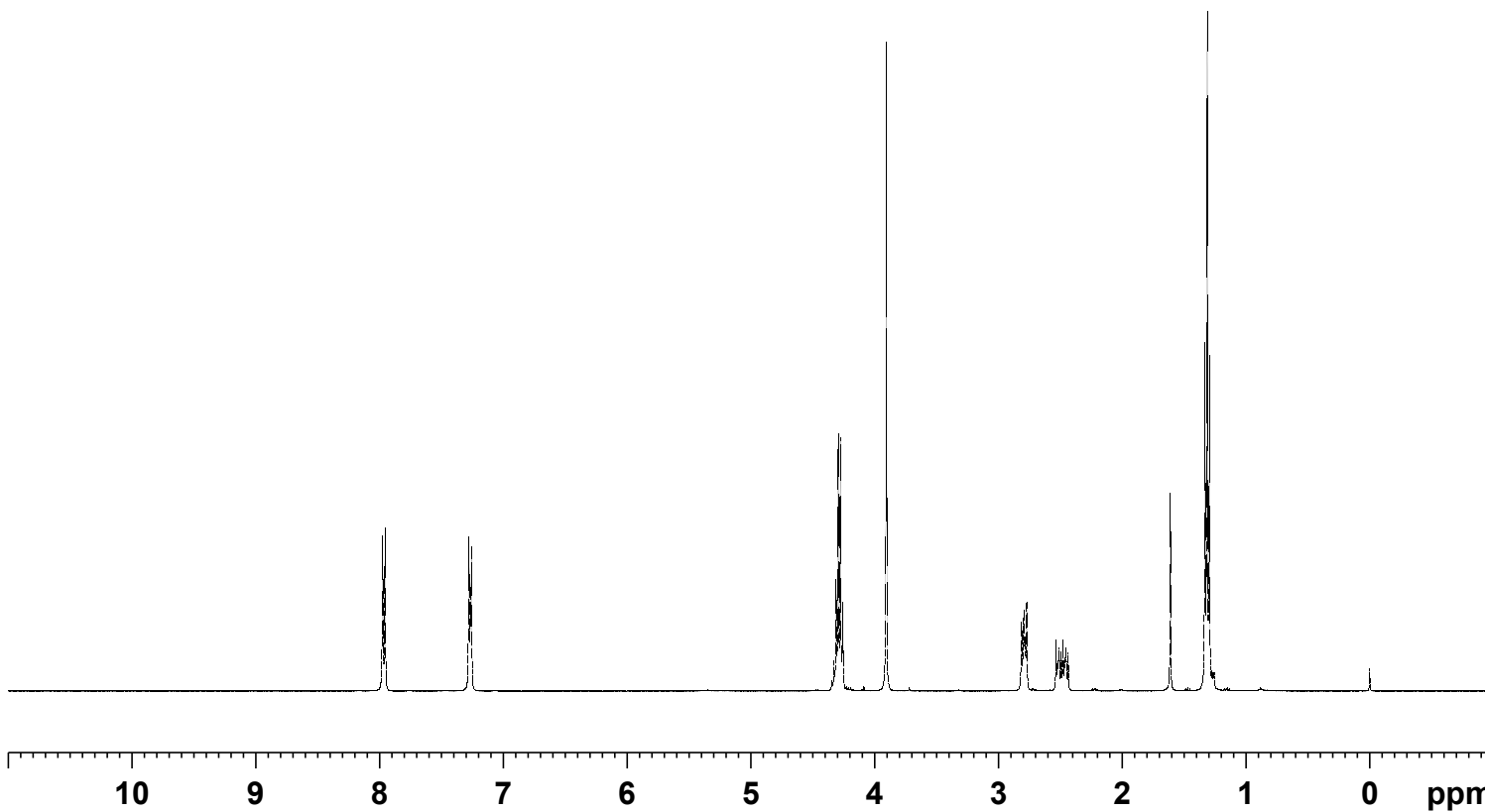
F2 - Processing parameters
SI 65536
SF 400.2400066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





7.975
 7.954
 7.277
 7.266
 7.257

4.329
 4.311
 4.293
 4.275
 4.258
 3.905
 2.813
 2.793
 2.783
 2.771
 2.534
 2.521
 2.512
 2.507
 2.492
 2.477
 2.465
 2.456
 2.450
 2.436
 1.330
 1.312
 1.294



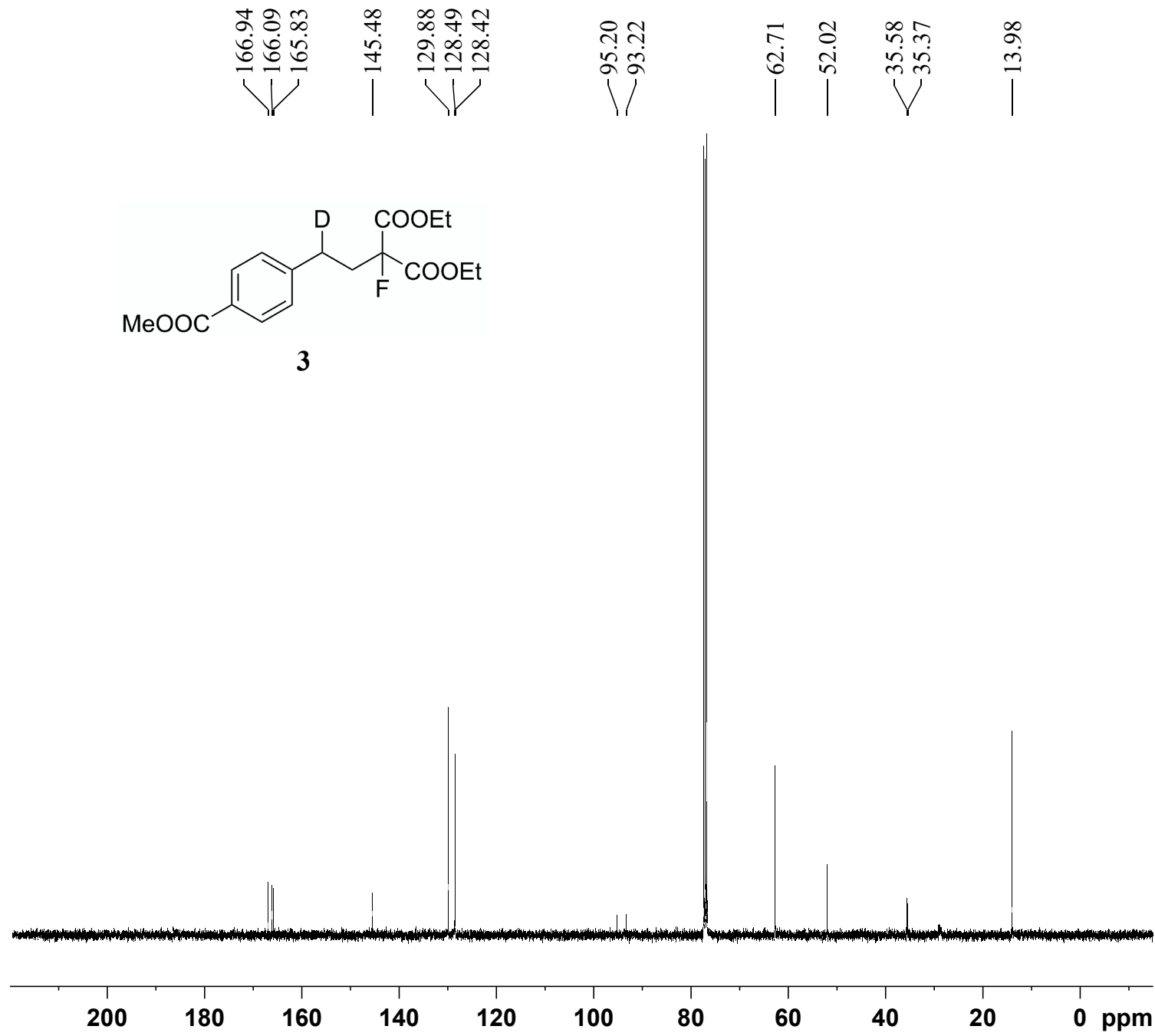
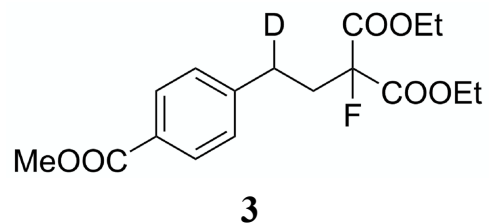
Current Data Parameters
 NAME 400M-2022
 EXPNO 17
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 7.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 206.33
 DW 62.400 usec
 DE 6.50 usec
 TE 301.0 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400072 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



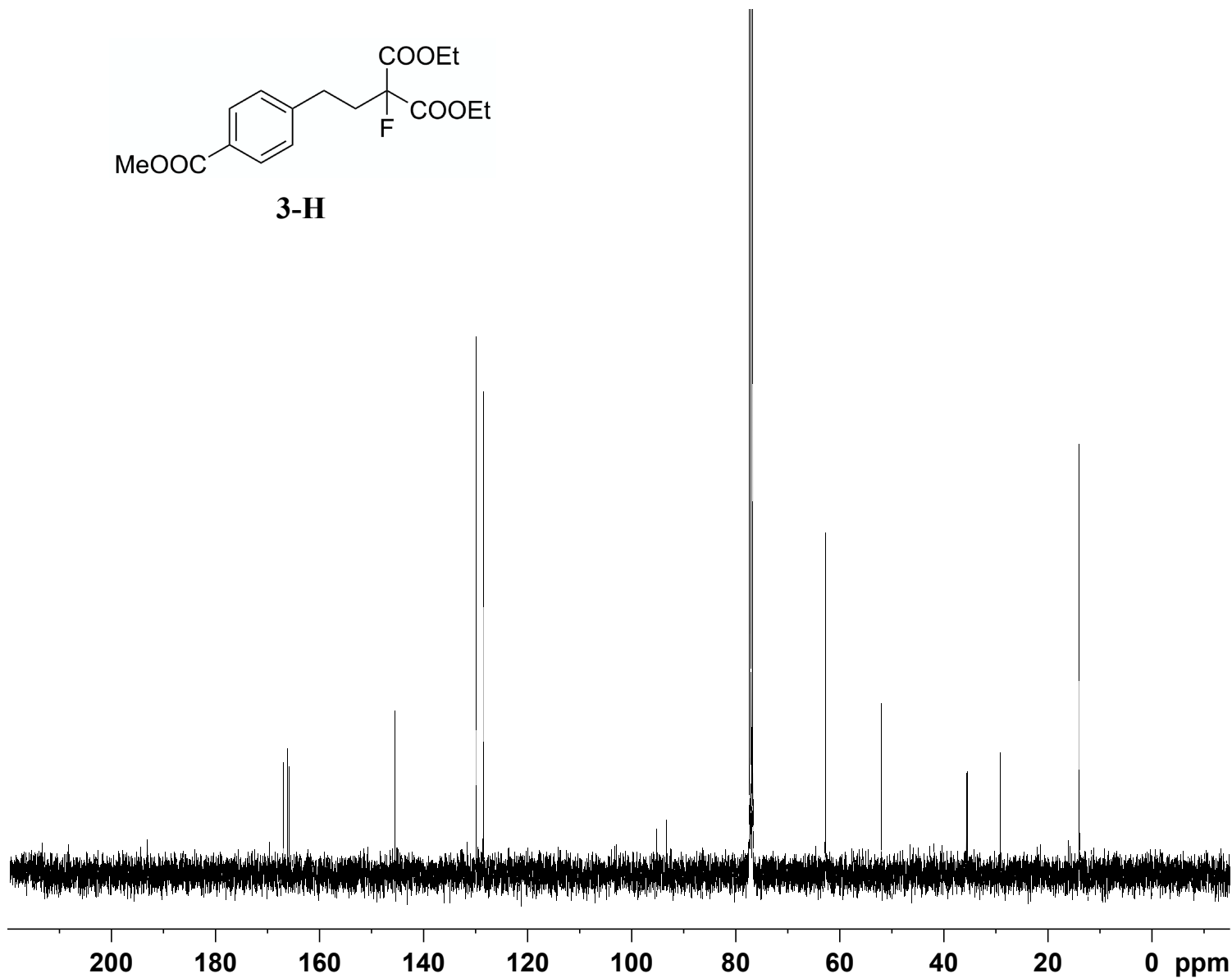
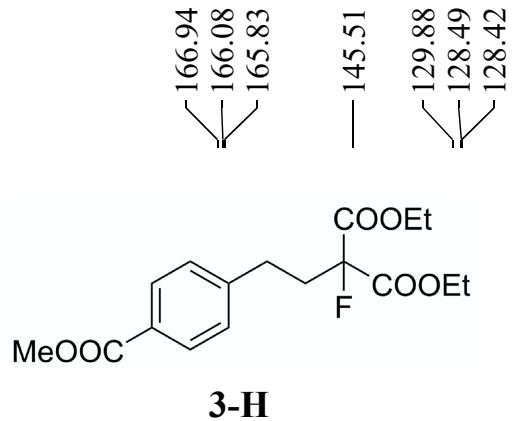
Current Data Parameters
 NAME 400M-2022
 EXPNO 16
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 7.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.7 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.0000000 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.0000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



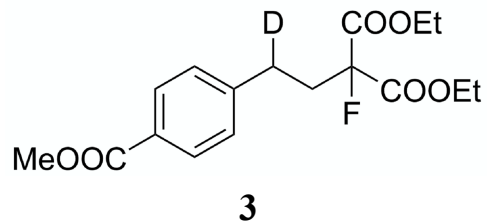
Current Data Parameters
 NAME 400M-2022
 EXPNO 18
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 8.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.8 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.0000000 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.0000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



— -167.44

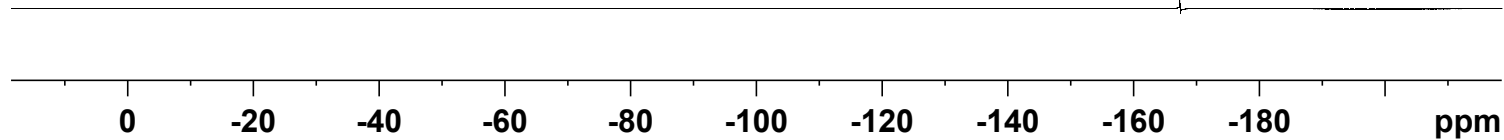
Current Data Parameters
 NAME 400M-2023-F
 EXPNO 7
 PROCNO 1

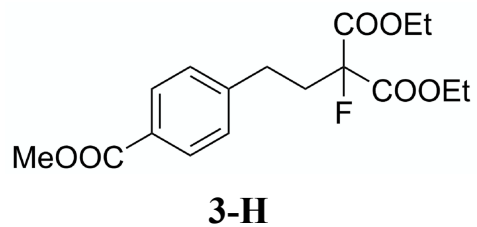
F2 - Acquisition Parameters
 Date_ 20230506
 Time 19.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT CDC13
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 206.33
 DW 5.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 376.5642094 MHz
 NUC1 19F
 P1 14.50 usec
 PLW1 17.98900032 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 65536
 SF 376.6018696 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





— -167.46

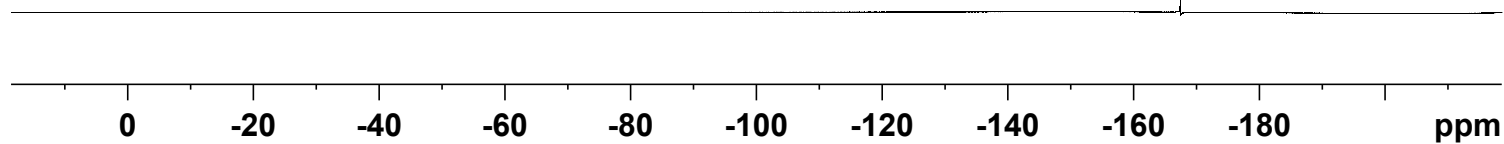
Current Data Parameters
 NAME 400M-2023-F
 EXPNO 6
 PROCNO 1

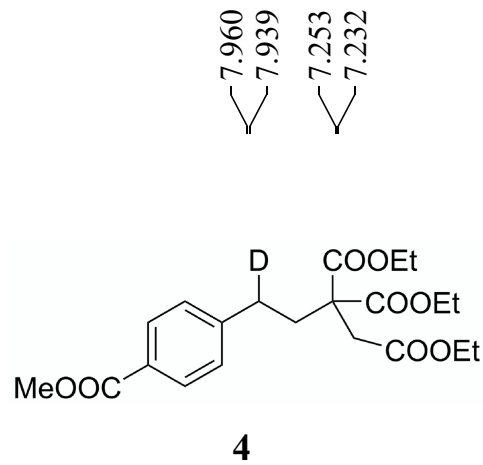
F2 - Acquisition Parameters
 Date_ 20230506
 Time 19.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfhigqn.2
 TD 131072
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 206.33
 DW 5.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 376.5642094 MHz
 NUC1 19F
 P1 14.50 usec
 PLW1 17.98900032 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 65536
 SF 376.6018696 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





7.960
7.939
7.253
7.232

4.251
4.233
4.216
4.198
4.160
4.142
4.125
4.107
3.899
3.040
2.646
2.625
2.604
2.326
2.307
2.285
1.295
1.278
1.260
1.243
1.226

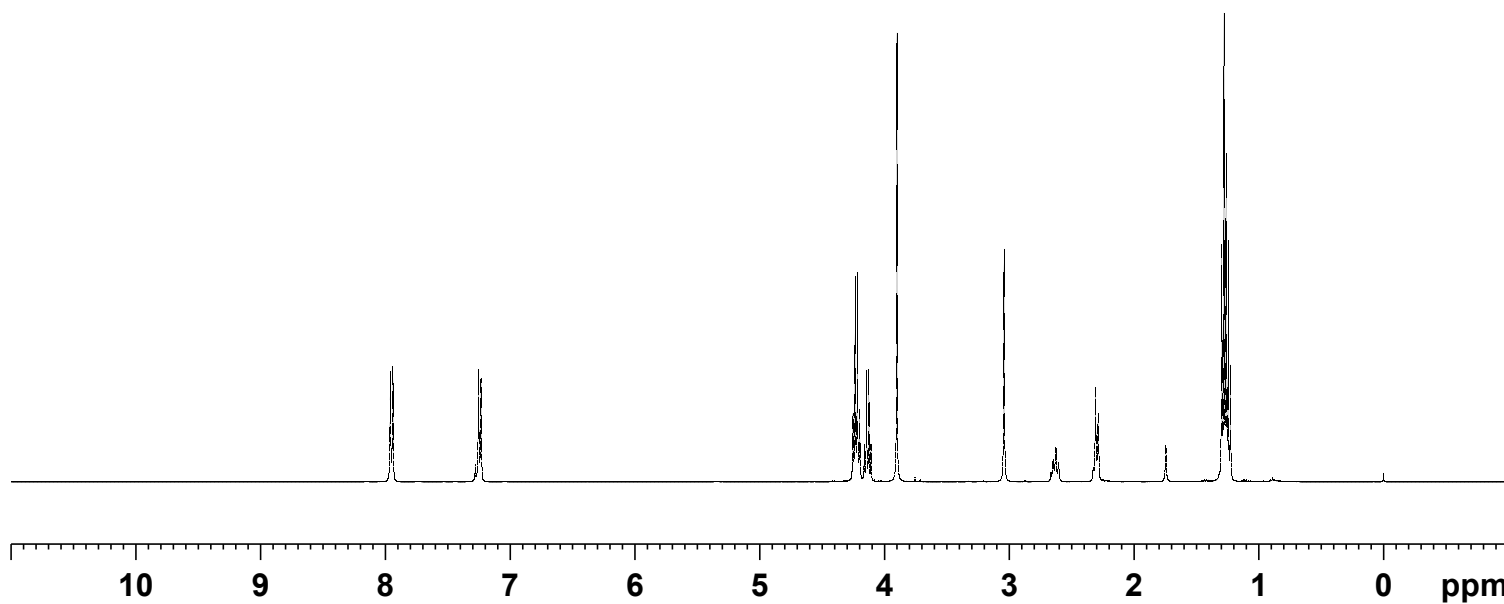
Current Data Parameters
NAME 400M-2022
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220701
Time 8.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 73.9
DW 62.400 usec
DE 6.50 usec
TE 301.2 K
D1 2.00000000 sec
D11 0 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

==== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400021 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

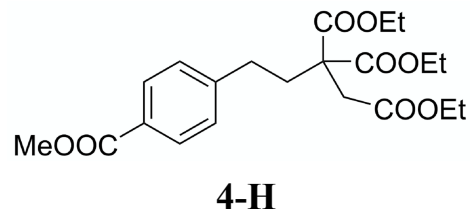


2.00
2.10

3.98
2.00
3.05

1.97
1.16
1.97

9.31



7.959 7.939 7.252 7.231
 4.250 4.232 4.215 4.197 4.160 4.142 4.124 4.106 3.899 3.040 2.664 2.650 2.643 2.633 2.621 2.325 2.313 2.303 2.295 2.282 1.295 1.277 1.259 1.243 1.225

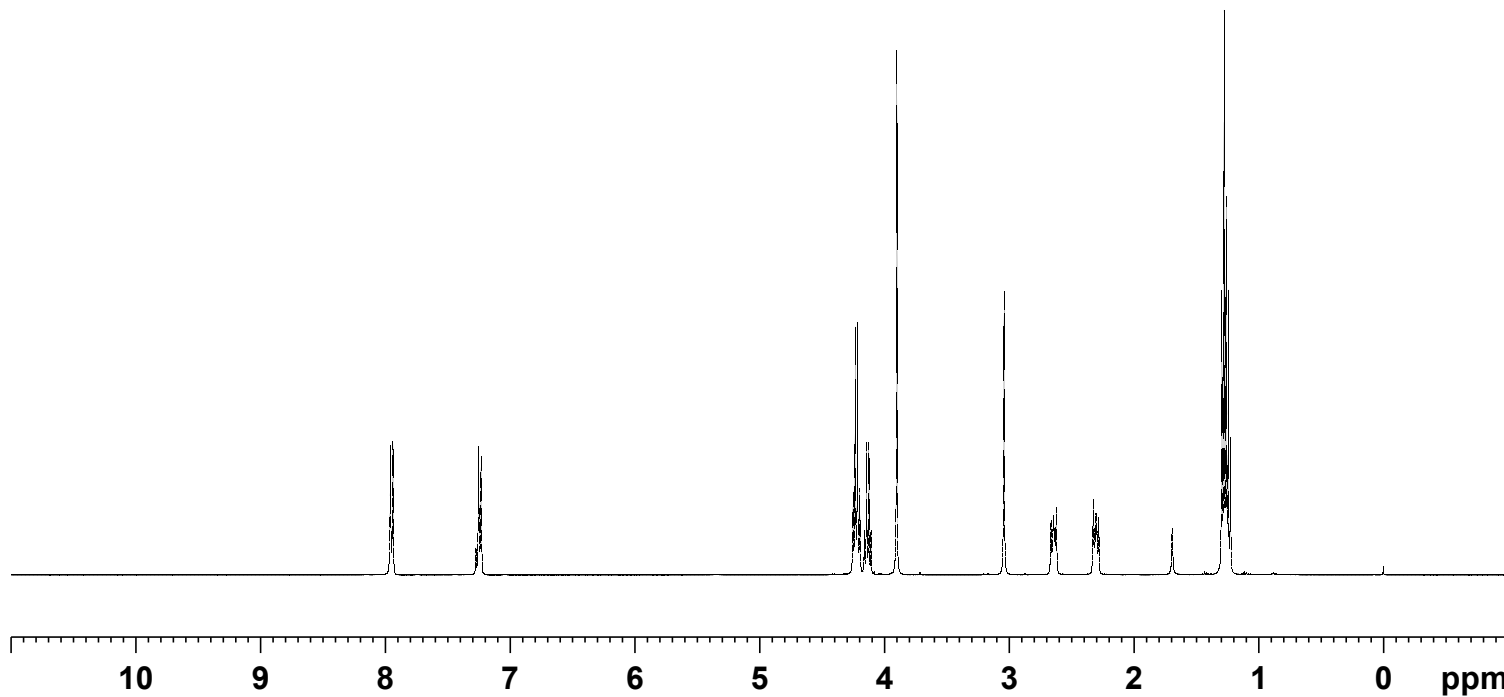
Current Data Parameters
 NAME 400M-2022
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 8.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 80.72
 DW 62.400 usec
 DE 6.50 usec
 TE 301.2 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

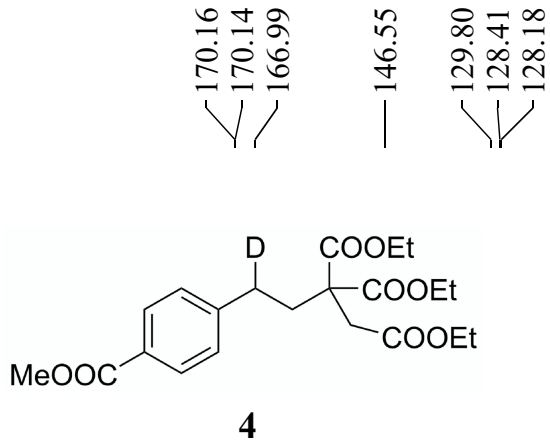
===== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400042 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



2.00 2.14 4.07 2.04 3.02 2.02 2.02 2.02 9.44



61.73
60.79
55.47
51.96
37.82
34.61
30.99
30.85
30.66
30.46
14.09
14.00

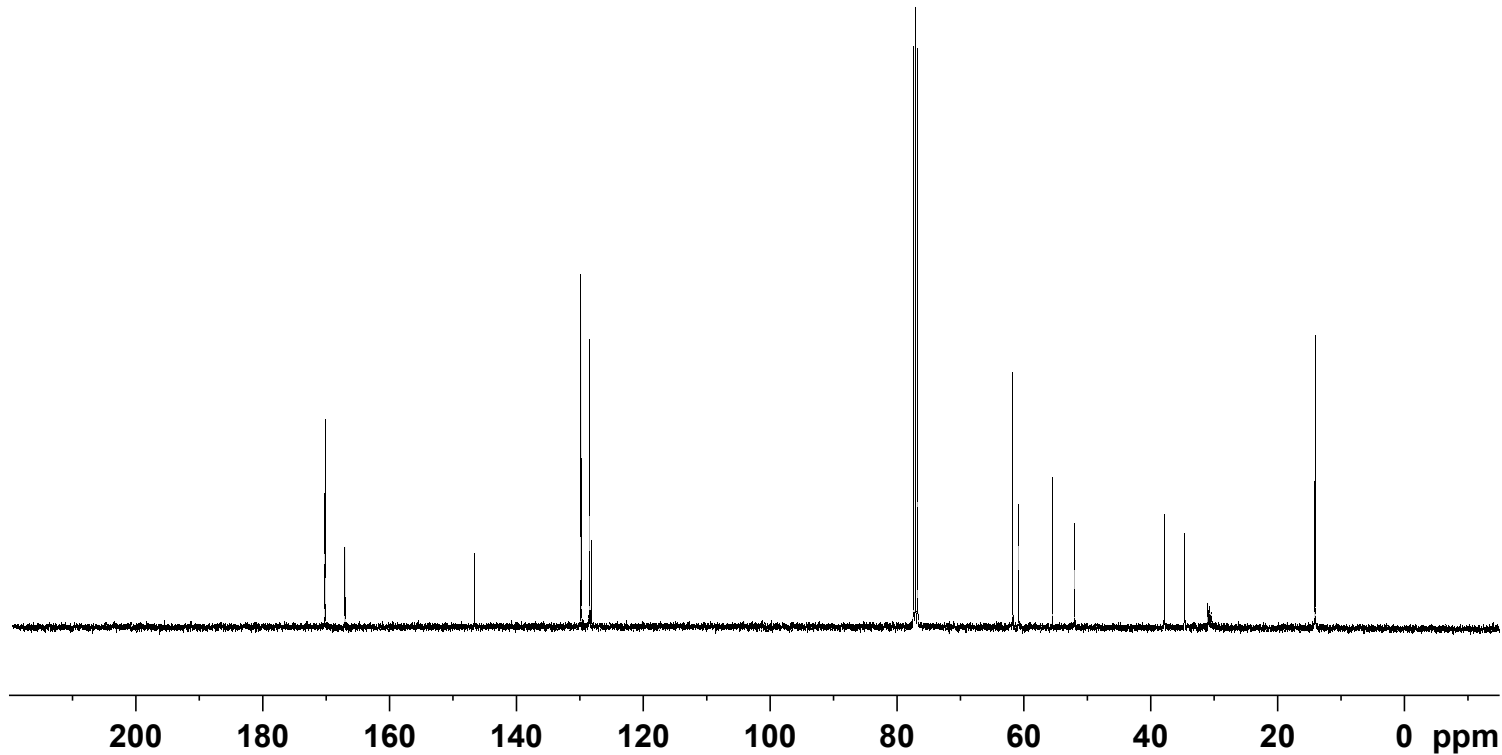
Current Data Parameters
NAME 400M-2022
EXPNO 20
PROCNO 1

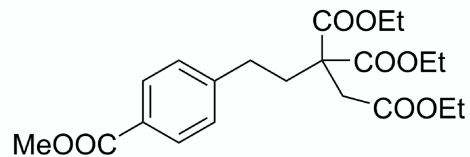
F2 - Acquisition Parameters
Date_ 20220701
Time 8.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 302.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

==== CHANNEL f2 =====
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





4-H

170.17
170.14
167.00
146.58
129.81
128.43
128.18

61.74
60.80
55.48
51.97
37.82
34.67
30.99
14.10
14.01

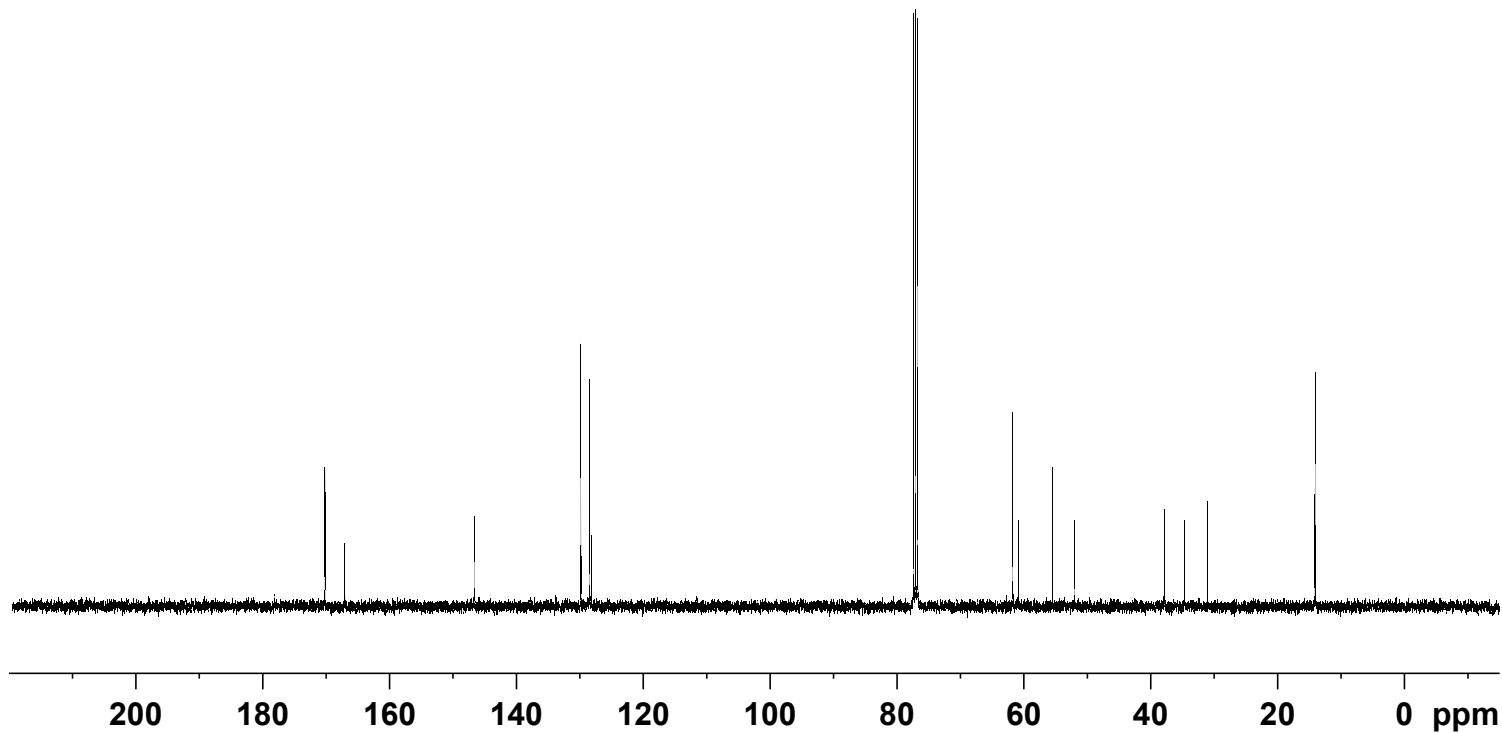
Current Data Parameters
NAME 400M-2022
EXPNO 22
PROCNO 1

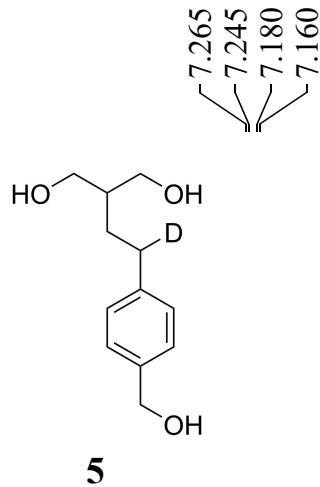
F2 - Acquisition Parameters
Date_ 20220701
Time 8.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 201
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 301.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.00000000 W

==== CHANNEL f2 =====
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





7.265
7.245
7.180
7.160

4.581
4.573
4.239
4.226
4.213
3.775
3.641
2.676
2.656
2.636
2.617
1.682
1.666
1.653
1.638
1.620
1.604

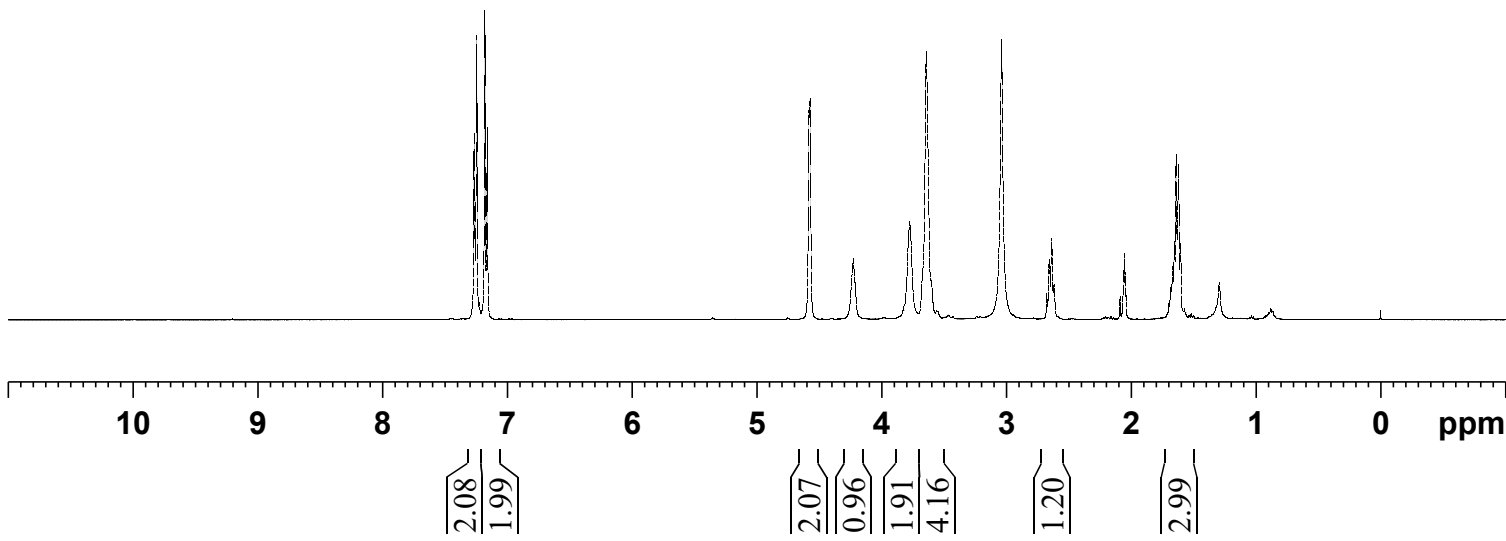
Current Data Parameters
 NAME 400M-2022
 EXPNO 23
 PROCNO 1

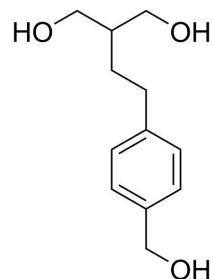
F2 - Acquisition Parameters
 Date_ 20220701
 Time 8.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT Acetone
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 73.9
 DW 62.400 usec
 DE 6.50 usec
 TE 301.0 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

==== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400058 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





5-H

7.267
7.248
7.183
7.163
4.587
4.573
4.135
4.121
4.106
3.666
3.648
3.635
3.620
2.898
2.866
2.681
2.662
2.642
2.077
2.071
2.066
2.060
2.055
2.049
2.044
1.656
1.639
1.620

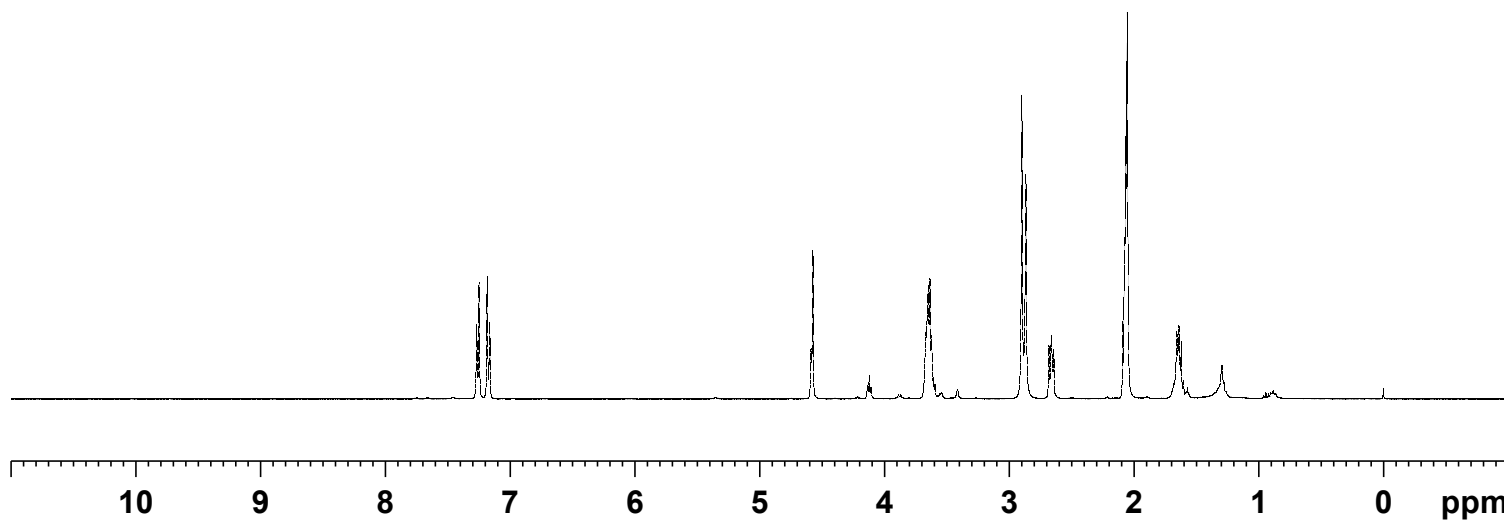
Current Data Parameters
NAME 400M-2022
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220702
Time 23.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 206.33
DW 62.400 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
D11 0 sec
TD0 1

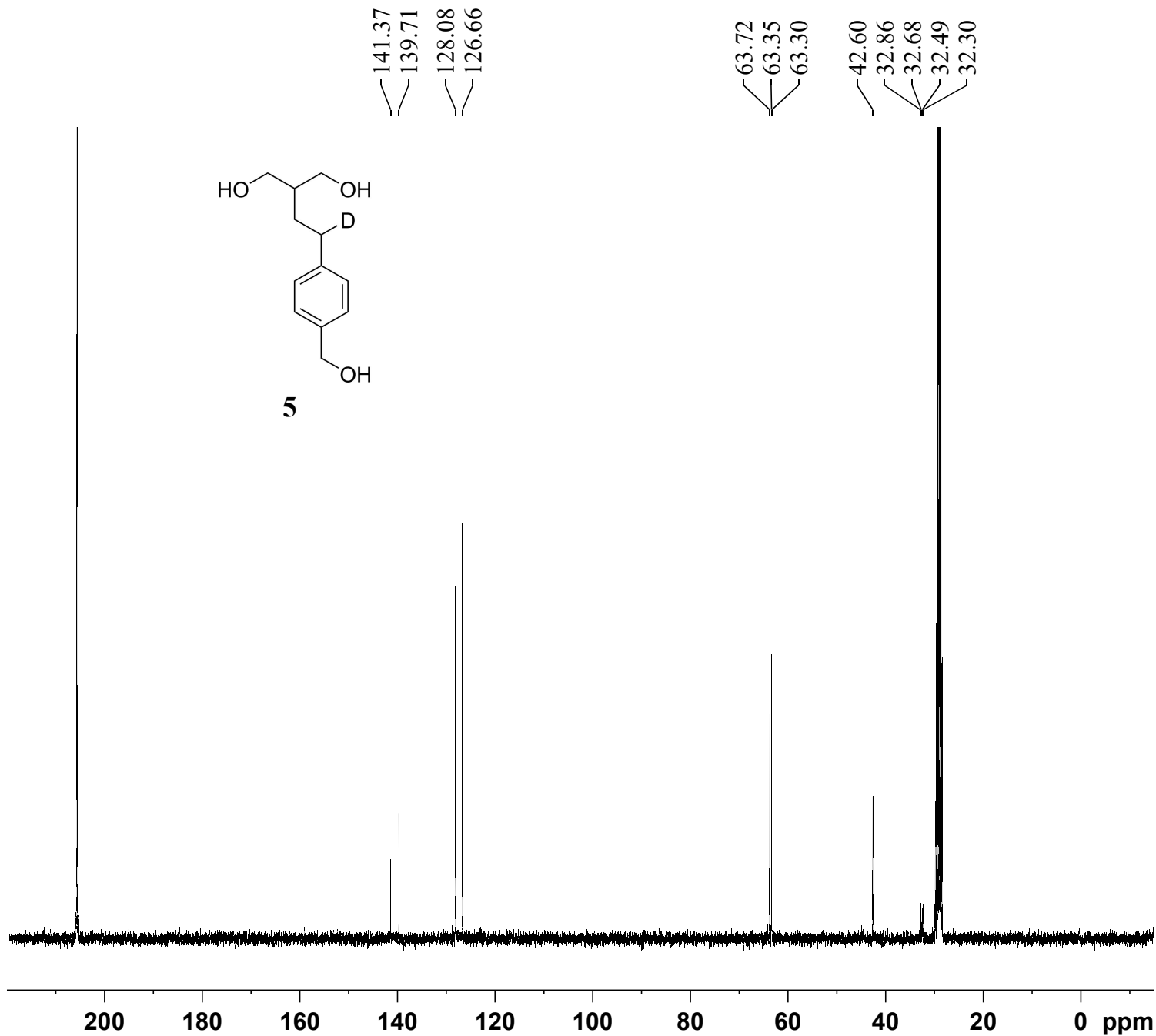
==== CHANNEL f1 =====
SFO1 400.2424716 MHz
NUC1 1H
P1 14.30 usec
PLW1 12.00000000 W

==== CHANNEL f2 =====
SFO2 400.2424716 MHz
NUC2 off
CPDPRG[2]
PCPD2 0 usec
PLW2 0 W
PLW12 0 W
PLW13 0 W

F2 - Processing parameters
SI 65536
SF 400.2400050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.00
2.03
2.05
0.52
5.18
7.35
2.14
9.28
3.50



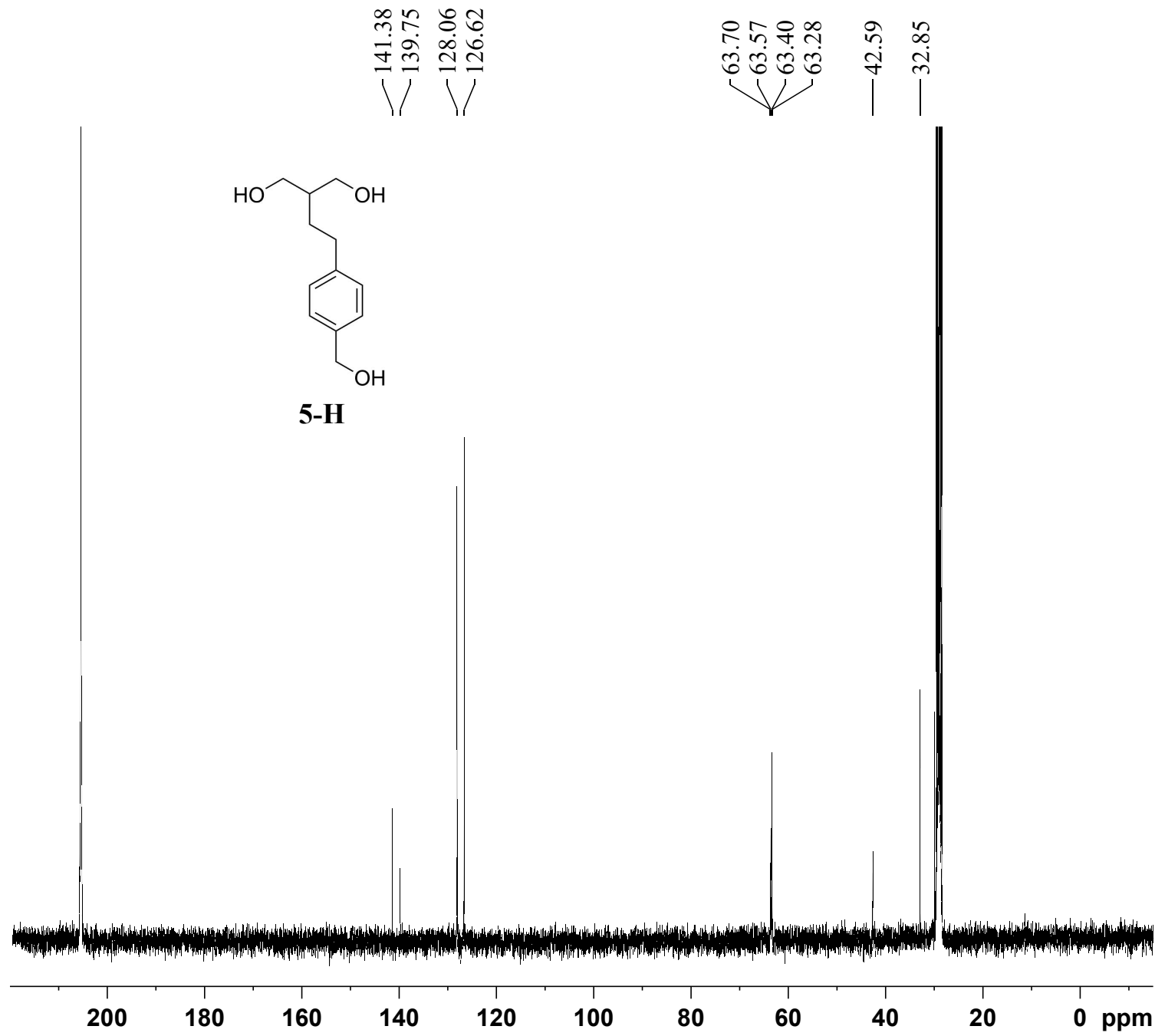
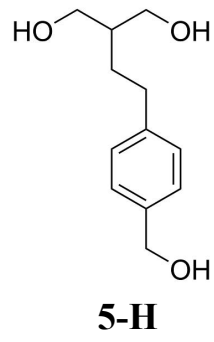
Current Data Parameters
 NAME 400M-2022
 EXPNO 24
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 9.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME 400M-2022
 EXPNO 34
 PROCNO 1

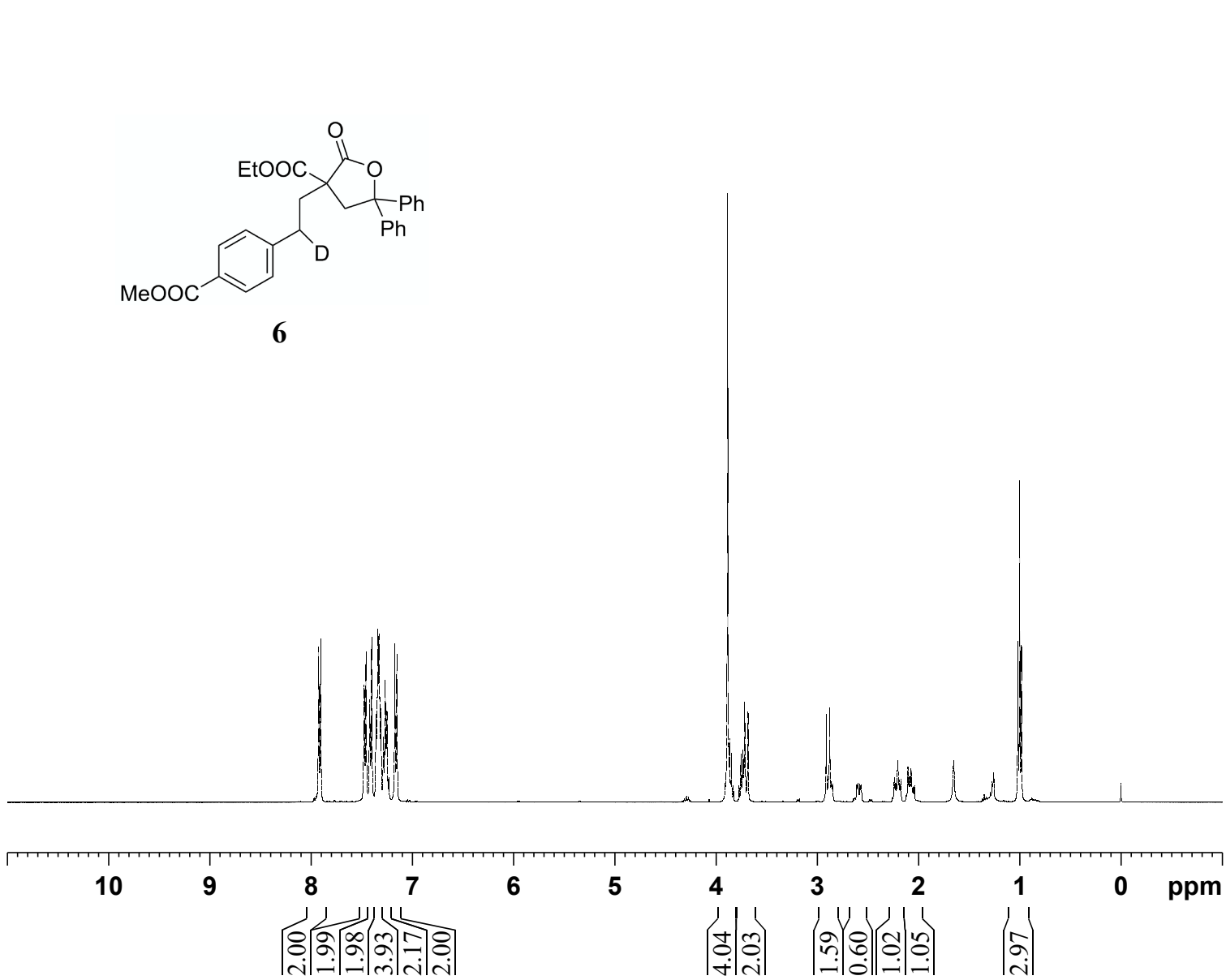
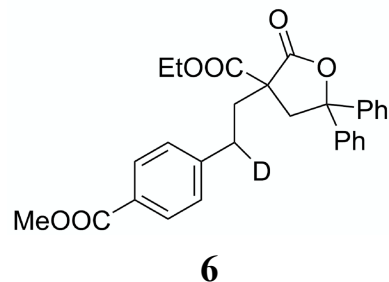
F2 - Acquisition Parameters
 Date_ 20220706
 Time 13.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.0000000 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.0000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

7.925
7.904
7.475
7.456
7.419
7.400
7.357
7.346
7.339
7.329
7.320
7.309
7.284
7.267
7.258
7.250
7.172
7.152
3.885
3.874
3.865
3.847
3.754
3.736
3.727
3.717
3.709
3.683
2.909
2.876
2.860
2.238
2.204
2.190
2.174
2.104
2.088
2.074
1.018
1.000
0.982



Current Data Parameters
 NAME 400M-2022
 EXPNO 27
 PROCNO 1

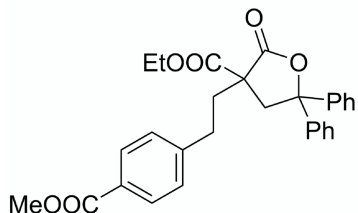
F2 - Acquisition Parameters
 Date_ 20220701
 Time 11.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 92.09
 DW 62.400 usec
 DE 6.50 usec
 TE 300.5 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

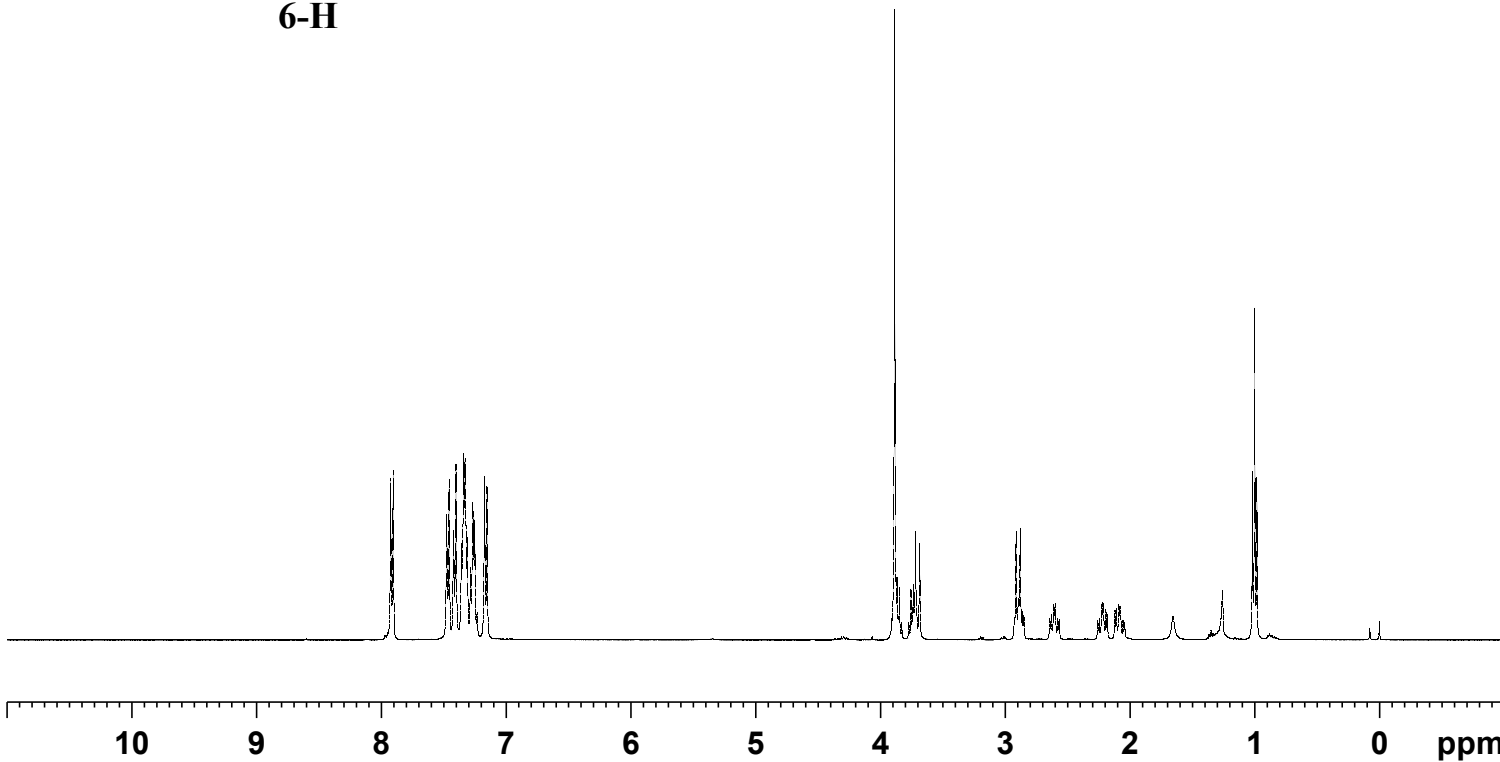
==== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

7.925
7.904
7.475
7.456
7.420
7.401
7.357
7.346
7.339
7.329
7.320
7.309
7.284
7.266
7.258
7.250
7.172
7.152
3.885
3.874
3.864
3.846
3.754
3.736
3.727
3.718
3.710
3.684
2.911
2.893
2.878
2.611
2.598
2.223
2.210
2.107
2.089
2.077
1.017
1.000
0.982



6-H



1.99
1.98
1.99
4.04
2.44
2.00

3.98
2.02
1.95
1.00
1.01
1.06

2.93

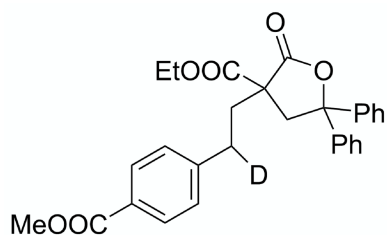
Current Data Parameters
 NAME 400M-2022
 EXPNO 29
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 13.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0447233 sec
 RG 80.72
 DW 62.400 usec
 DE 6.50 usec
 TE 300.4 K
 D1 2.00000000 sec
 D11 0 sec
 TD0 1

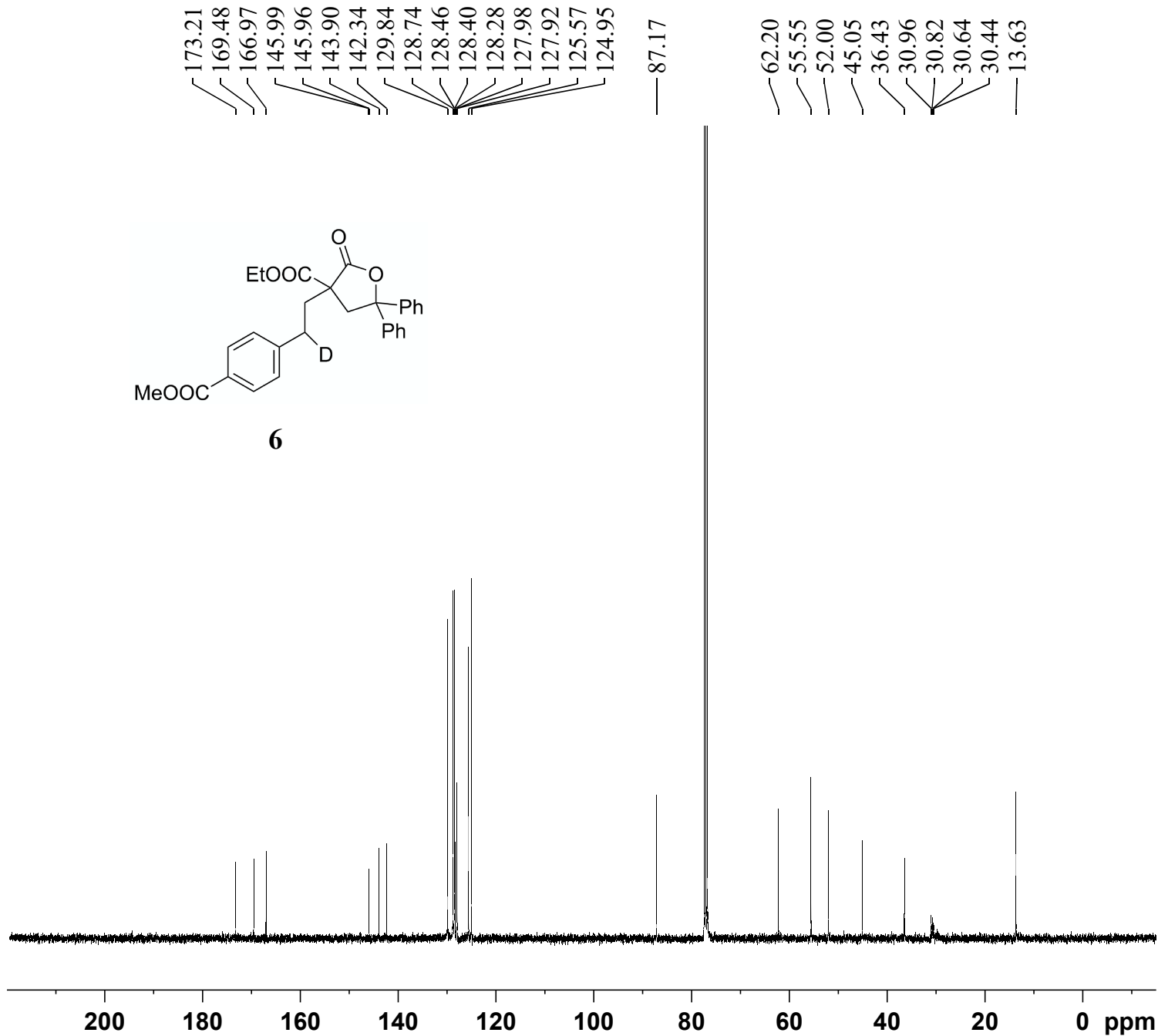
==== CHANNEL f1 =====
 SFO1 400.2424716 MHz
 NUC1 1H
 P1 14.30 usec
 PLW1 12.00000000 W

==== CHANNEL f2 =====
 SFO2 400.2424716 MHz
 NUC2 off
 CPDPRG[2]
 PCPD2 0 usec
 PLW2 0 W
 PLW12 0 W
 PLW13 0 W

F2 - Processing parameters
 SI 65536
 SF 400.2400102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



6



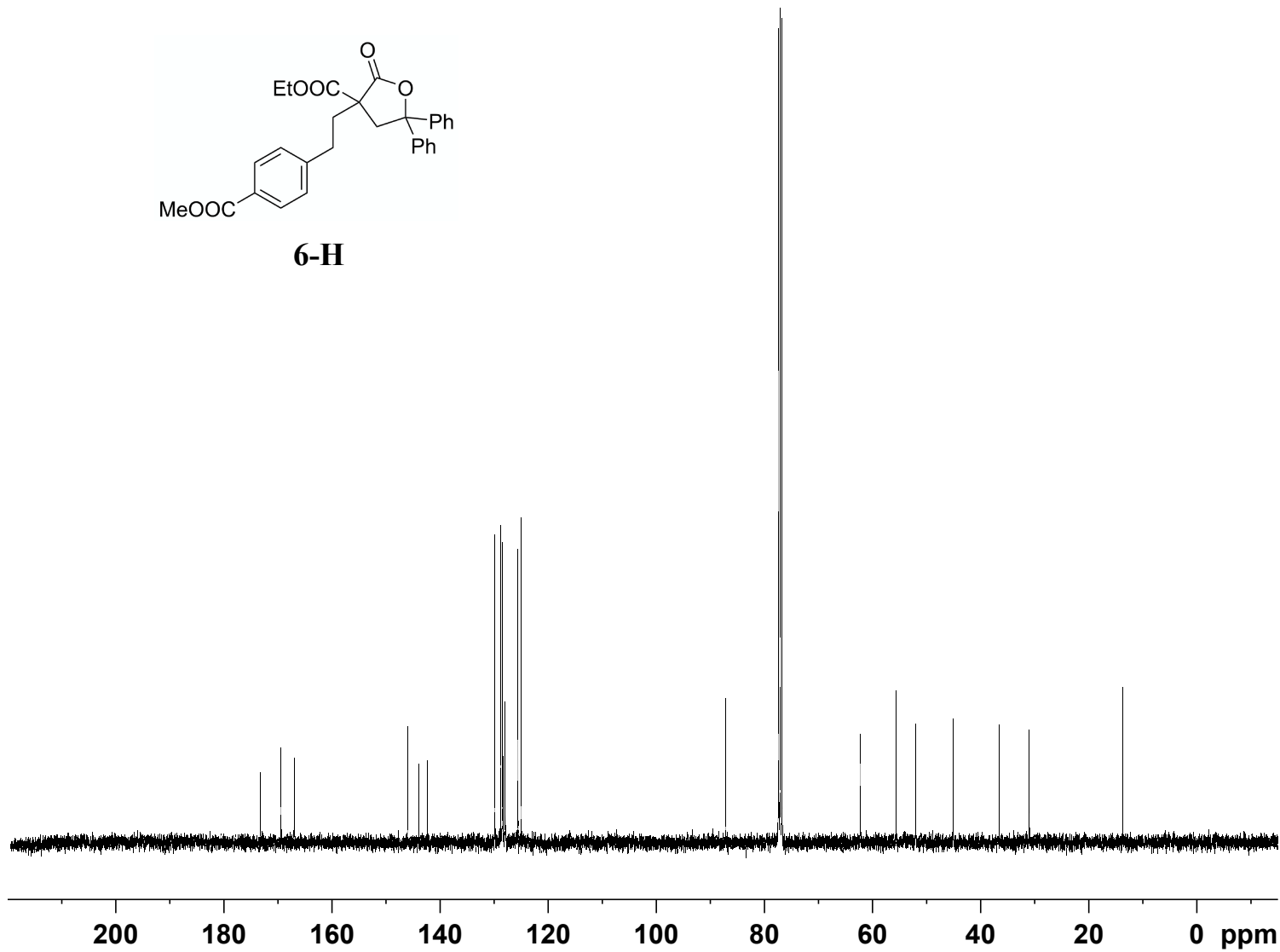
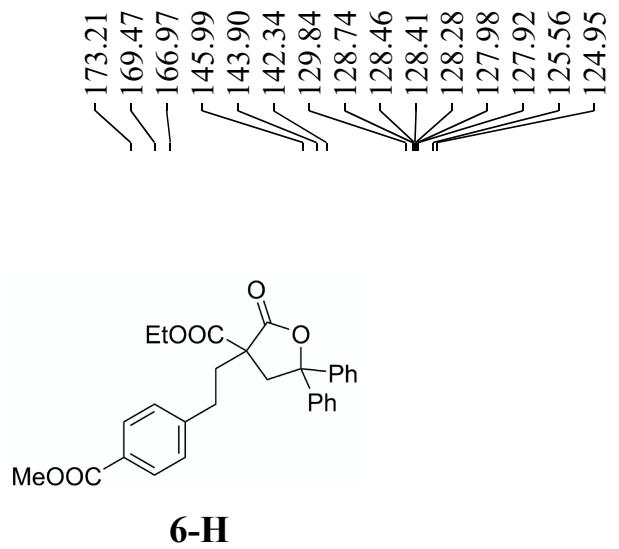
Current Data Parameters
 NAME 400M-2022
 EXPNO 28
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220701
 Time 12.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 301.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.00000000 W

==== CHANNEL f2 =====
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.30294999 W
 PLW13 0.24539000 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
NAME 400M-2022
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220701
Time 13.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 301.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6504916 MHz
NUC1 13C
P1 10.00 usec
PLW1 54.0000000 W

==== CHANNEL f2 =====
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 12.0000000 W
PLW12 0.30294999 W
PLW13 0.24539000 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40