Electronic Supporting Information

Nils Tenhumberg[a], *Hendrik Büttner*[a], *Benjamin Schäffner*[b], *Daniela Kruse*[b], *Michael Blumenstein*[c], *Thomas Werner*[a]*

[a] Leibniz-Institut für Katalyse e. V. an der Universität Rostock, Albert-Einstein-Strasse 29a, 18059 Rostock, Germany.

[b] Evonik Industries AG, Paul-Baumann-Str. 1, 45772 Marl, Germany.

[c] HOBUM Oleochemicals, Seehafenstraße 20, 21079 Hamburg, Germany.

1. General

All reagents were purchased from commercial sources and used as received without further purification. Epoxidized high-oleic sunflower oil (techn. methyl oleate, 86% purity, prepared by Hobum, oxirane number= 4.87 mmol·g^{-1}), epoxidized sunflower oil (techn. grade, prepared by Hobum, oxirane number= 7.02 mmol·g^{-1}), *iso*-octyl oletae (techn. grade , prepared by Hobum; oxirane number= 2.46 mmol·g^{-1}) and epoxidized linseed oil (techn. grade, prepared by Hobum, oxirane number= 8.62 mmol·g^{-1}) were provided by HOBUM Oleochemicals. Epoxidized soybean oil (EPOXOL D65, oxirane number= 4.81 mmol·g^{-1}) and epoxidized methyl soyate (NEXO E1, oxirane numer= 4.36 mmol·g^{-1}) were provided by Evonik Industries AG. Thin layer chromatography was performed on Merck TLC plates with fluorescence indication (silica type 60, F_{254}), spots were visualized using UV-light, vanillin or iodine stains. Flash chromatography was performed using silica gel with a grain size of 40–63 µm from Macherey-Nagel. Deuterated solvents were purchased from Deutero. NMR spectra were recorded on Bruker 300 Fourier, Bruker AV 300 and Bruker AV 400 spectrometers. The chemical shifts (δ) for ^{1}H and ^{13}C in $CDCl_3$ are given in parts per million (ppm) and referenced to 7.27 and 77.00 ppm, respectively. Coupling constants are expressed in Hertz (Hz). The following abbreviations are used: s= singlet, d= doublet, t= triplet, q= quadruplet, m= multiplet. Infrared spectra were recorded on a Nicolet iS10 MIR FT-IR-spectrometer from Thermo Fisher Scientific. Gas chromatography was performed on Agilent 7890A GC system and mass spectra were measured on downstream 5975C inert XL MSD mass detector also from Agilent. The reported GC yields are based on a calibrated area of *n*-hexadecane as internal standard. Elemental analysis was performed on a TruSpec CHNS Micro from Leco and halogenes were determined with TitraLab 870 from Radiometer Analytical SAS. High resolution mass spectra (HRMS) were obtained either from a MAT 95 XP from Thermo (EI) or from an HPLC system 1200 and downstream ESI-TOF-MS 6210 from Agilent (ESI). The yield, conversion and selectivity of cyclic carbonates produced from epoxidized vegetable oils were determined via ^{1}H NMR spectroscopy. In general, *cis*:*trans*-stereoselectivity is referred to epoxide and carbonate diastereoisomers, respectively

2. Synthesis and NMR Spectra of epoxidized fatty acid esters

Epoxidation of fatty acid esters 2 (**GP2**): The fatty acid ester 1 (1.0 equiv) was added to a solution of $Ru(acac)_3$ (0.005–0.010 equiv) and dipicolinic acid (0.1–0.2 equiv) in acetonitrile (0.25 M in respect to **1**). The resulting suspension was sonicated to obtain a homogeneous mixture. Subsequently, aqueous hydrogen peroxide (35%, 3.3 equiv) was added in portions and the reaction mixture was allowed to stir for 4–24 h at 25 °C. The resulting mixture was extracted with cyclohexane (cHex) and the combined organic layers were concentrated to approximately 1/4 of the initial volume and subsequently washed with water. The organic phase was dried over $MgSO_4$ and all volatiles were removed in vacuum to yield product **2**. If necessary the crude product was purified by flash chromatography on silica (SiO2) employing cyclohexane (cHex)/ ethyl acetate (EtOAc) as eluent.

***cis*-Methyl 8-(3-octyloxiran-2-yl)octanoate** (*cis*-**2a**)[1]: According to **GP2**, methyl oleate (*cis*-**1a**, 11.84 g, 39.93 mmol), $Ru(acac)_3$ (80 mg, 0.20 mmol), dipicolinic acid (668 mg, 4.00 mmol) and hydrogen peroxide (35%, 12.8 g, 132 mmol) in acetonitrile (160 mL) were stirred for 4 h at 25 °C. Subsequently, the reaction mixture was extracted with cyclohexane (4×200 mL), the combined organic layers were concentrated to 100 mL and washed with H_2O (100 mL). After removal of all volatiles in vacuum *cis*-**2a** (12.08 g, 38.66 mmol, 97%) was obtained as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ= 0.88 (t, $^3J_{H,H}$= 6.7 Hz, 3H), 1.23–1.54 (m, 24H), 1.57–1.67 (m, 2H), 2.30 (t, $^3J_{H,H}$= 7.5 Hz, 2H), 2.86–2.92 (m, 2H), 3.66 (s, 3H) ppm; $^{13}C\{^1H\}$l NMR (75 MHz, $CDCl_3$, 22 °C): δ= 14.07 (CH_3), 22.63 (CH_2), 24.86 (CH_2), 26.52 (CH_2), 26.57 (CH_2), 27.76 (CH_2), 27.80 (CH_2), 29.00 (CH_2), 29.15 (CH_2), 29.19 (CH_2), 29.30 (CH_2), 29.50 (CH_2), 29.52 (CH_2), 31.82 (CH_2), 34.02 (CH_2), 51.42 (OCH_3), 57.15 (CH), 57.20 (CH), 174.23 (C=O) ppm; MS (EI): *m/z* (%): 281 (1) [M^+–OCH_3], 264 (1), 199 (14) , 171 (17), 155 (100), 153 (20), 139 (19), 127 (23), 121 (10), 109 (26), 97 (34), 87 (32), 83 (32), 74 (54), 69 (46), 55 (63), 43 (29), 41 (35); elemental analysis calcd. (%) for $C_{19}H_{36}O_3$ (312.49): C 73.03, H 11.61, found: C 73.01, H 11.73.

***trans*-Methyl 8-(3-octyloxiran-2-yl)octanoate** (*trans*-**2a**):[2] According to **GP2**, methyl elaidate (*trans*-**1a**, 498 mg 1.68 mmol), $Ru(acac)_3$ (7.0 mg, 0.018 mmol), dipicolinic acid (59 mg, 0.35 mmol) and hydrogen peroxide (35%, 655 mg, 5.78 mmol) in acetonitrile (7 mL) were stirred for 24 h at 25 °C. Subsequently, the reaction mixture was extracted with cyclohexane (4×10 mL), the combined organic layers were concentrated to 10 mL and washed with H_2O (10 mL). The crude product was purified by flash chromatography (SiO_2, *c*Hex:EtOAc= 10:1). After removal of all volatiles in vacuum the product *trans*-**2a** (364 mg, 1.16 mmol, 69%) was obtained as a colorless solid. R_f= 0.45 (*c*Hex:EtOAc= 5:1) ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.88 (t, $^3J_{H,H}$= 6.7 Hz, 3H), 1.22–1.56 (m, 24H), 1.57–1.67 (m, 2H), 2.30 (t, $^3J_{H,H}$= 7.5 Hz, 2H), 2.63–2.67 (m, 2H), 3.66 (s, 3H) ppm; $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 22 °C): δ = 14.08 (CH_3), 22.64 (CH_2), 24.87 (CH_2), 25.96 (CH_2), 26.03 (CH_2),

29.00 (CH_2), 29.14 (CH_2), 29.21 (2×CH_2), 29.43 (CH_2), 29.50 (CH_2), 31.83 (CH_2), 32.08 (CH_2), 32.11 (CH_2), 34.04 (CH_2), 51.43 (OCH_3), 58.84 (CH), 58.89 (CH), 174.25 (C=O) ppm; MS (EI): *m/z* (%): 281 (1) [M^+–OCH_3], 264 (1), 199 (16), 171 (17), 155 (100), 153 (21), 139 (20), 127 (23), 121 (10), 109 (26), 97 (34), 87 (32), 83 (32), 74 (54), 69 (45), 55 (60), 43 (28), 41 (34); elemental analysis calcd. (%) for $C_{19}H_{36}O_3$ (312.49): C 73.03, H 11.61; found: C 72.92, H 11.59.

***cis*-Ethyl 8-(3-octyloxiran-2-yl)octanoate** (*cis*-**2b**):[3] According to **GP2**, ethyl oleate (*cis*-**1b**, 4.97 g, 16.0 mmol), $Ru(acac)_3$ (32 mg, 0.080 mmol), dipicolinic acid (267 mg, 1.60 mmol) and hydrogen peroxide (30%, 5.98 g, 52.7 mmol) in acetonitrile (64 mL) were stirred for 24 h at 25 °C. Subsequently, the resulting mixture was extracted with cyclohexane (4×70 mL), concentrated to 100 mL and treated with H_2O (100 mL). The product *cis*-**2b** (4.63 g, 1.42 mmol, 89%) was obtained as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.87 (t, $^3J_{H,H}$= 6.7 Hz, 3H), 1.22–1.54 (m, 24H), 1.25 (t, $^3J_{H,H}$= 7.2 Hz, 3H), 1.57–1.67 (m, 2H), 2.28 (t, $^3J_{H,H}$= 7.5 Hz, 2H), 2.86–2.92 (m, 2H), 4.12 (q, $^3J_{H,H}$= 7.2 Hz, 2H) ppm; $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 22 °C): δ = 14.06 (CH_3), 14.21 (CH_3), 22.62 (CH_2), 24.88 (CH_2), 26.52 (CH_2), 26.56 (CH_2), 27.75 (CH_2), 27.78 (CH_2), 28.98 (CH_2), 29.15 (CH_2), 29.18 (CH_2), 29.30 (CH_2), 29.49 (CH_2), 29.51 (CH_2), 31.81 (CH_2), 34.29 (CH_2), 57.14 (CH), 57.18 (CH), 60.11 (OCH_2), 173.79 (C=O) ppm; MS (EI): *m/z* (%): 308 (5), 281 (7), 213 (14), 185 (17), 171 (14), 167 (10), 155 (100), 153 (33), 141 (28), 139 (24), 125 (21), 121 (17), 111 (20), 109 (34), 101 (45), 97 (37), 88 (56), 83 (41),69 (50), 55 (68), 43 (31), 41 (38); elemental analysis calcd. (%) for $C_{20}H_{38}O_3$ (326.52): C 73.57, H 11.73; found C 73.72, H 11.67.

***cis*-Methyl 10-(3-octyloxiran-2-yl)decanoate** (*cis*-**2d**): According to **GP2**, methyl eicosenoate (*cis*-**1d**, 3.25 g, 10.0 mmol), $Ru(acac)_3$ (20 mg, 0.050 mmol), dipicolinic acid (167 mg, 1.00 mmol) and hydrogen peroxide (30%, 3.74 g, 33.0 mmol) in acetonitrile (40 mL) were stirred for 24 h at 25 °C. Subsequently, the resulting mixture was extracted with cyclohexane (4×50 mL), concentrated to 50 mL and treated with H_2O (50 mL). The product *cis*-**2d** (3.09 g, 9.07 mmol, 91%) was obtained as a colorless solid. ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.88 (t, $^3J_{H,H}$= 6.7 Hz, 3H), 1.18–1.55 (m, 28H), 1.57–1.66 (m, 2H), 2.30 (t, $^3J_{H,H}$= 7.5 Hz, 2H), 2.87–2.93 (m, 2H), 3.66 (s, 3H) ppm; $^{13}C\{^1H\}$ NMR (75 MHz, C_6D_6, 22 °C): δ = 14.06 (CH_3), 22.62 (CH_2), 24.89 (CH_2), 26.56 (2×CH_2), 27.78 (2×CH_2), 29.08 (CH_2), 29.18 (2×CH_2), 29.29 (CH_2), 29.45 (CH_2), 29.48 (CH_2), 29.49 (CH_2), 29.52 (CH_2), 31.82 (CH_2), 34.05 (CH_2), 51.39 (OCH_3), 57.19 (2×CH_2), 174.27 (C=O) ppm; MS (EI): *m/z* (%): 340 (1) [M^+], 322 (1), 227 (5), 199 (36), 198 (13), 183 (65), 167 (17), 164 (18), 155 (65), 149 (23), 141 (13), 135 (14), 129 (16), 124 (25), 111 (16), 97 (40), 95 (54), 87 (72), 83 (64), 74 (88), 69 (88), 55 (100), 43 (48), 41 (53); elemental analysis calcd. (%) for $C_{21}H_{40}O_3$ (340.54): C 74.07, H 11.84; found: C 74.01, H 11.68.

***cis*-Methyl 12-(3-octyloxiran-2-yl)dodecanoate** (*cis*-**2e**):[4] According to **GP2**, methyl erucate (*cis*-**1e**, 10.58 g, 30.00 mmol), $Ru(acac)_3$ (60 mg, 0.15 mmol), dipicolinic acid (502 mg, 3.00 mmol) and hydrogen peroxide (30%, 11.22 g, 98.97 mmol) in acetonitrile (120 mL) were stirred for 24 h at 25 °C. Subsequently the resulting

mixture was extracted with cyclohexane (4×150 mL), concentrated to 100 mL and treated with H_2O (100 mL). The crude product was purified by flash chromatography (SiO_2, *c*Hex:EtOAC= 10:1). After removal of all volatiles in vacuum the product *cis*-**2e** (4.01 g, 10.9 mmol, 36%) was obtained as a colorless solid as. R_f= 0.50 (*c*Hex:EtOAc= 5:1); ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.88 (t, $^3J_{H,H}$= 6.6 Hz, 3H), 1.20–1.55 (m, 32H), 1.57–1.66 (m, 2H), 2.30 (t, $^3J_{H,H}$= 7.5 Hz, 2H), 2.86–2.93 (m, 2H) 3.66 (s, 3H) ppm; $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 22 °C): δ = 14.06 (CH_3), 22.63 (CH_2), 24.92 (CH_2), 26.57 (2×CH_2), 26.80 (2×CH_2), 29.12 (CH_2), 29.19 (CH_2), 29.22 (CH_2), 29.40 (CH_2), 29.52 (br., 6×CH_2), 31.83 (CH_2), 34.08 (CH_2), 51.39 (OCH_3), 57.20 (2×CH), 174.28 (C=O) ppm; MS (EI): *m/z* (%): 368 (1) [M^+], 350 (2), 255 (27), 227 (30), 211 (28), 193 (13), 183 (14), 175 (14), 155 (40), 143 (37), 124 (19), 109 (31), 95 (58), 83 (66), 74 (76), 69 (81), 55 (100), 41 (51); elemental analysis calcd. (%) $C_{23}H_{44}O_3$ (368.59): C 74.95, H 12.03; found: C 74.60, H 12.08.

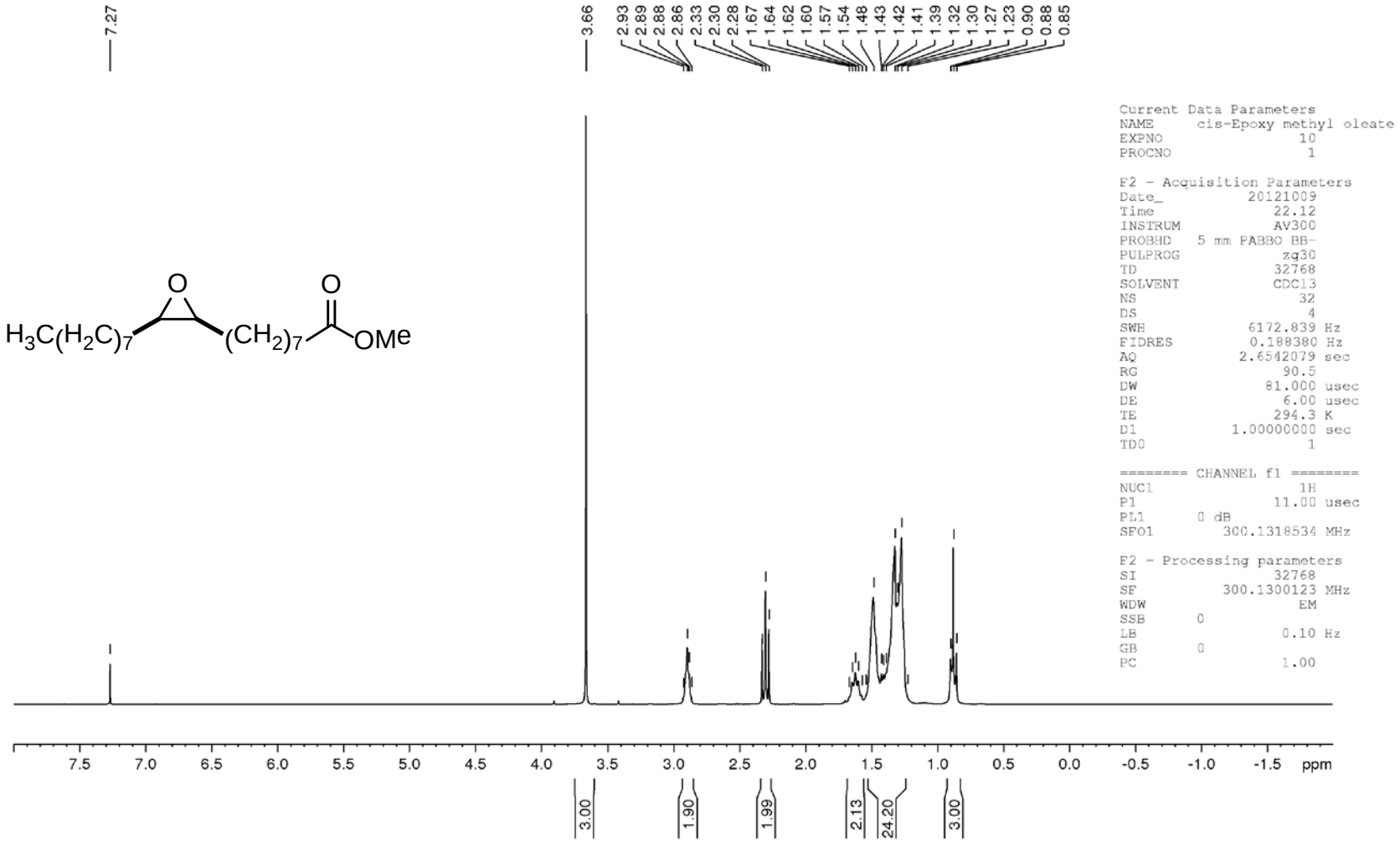
Methyl 8-(3-((2*R*)-hydroxyoctyl)oxiran-2-yl)octanoate (**2f**):[5] According to **GP2**, methyl ricinoleate (*cis*-**1f**, 9.37 g, 30.0 mmol), $Ru(acac)_3$ (60 mg, 0.15 mmol), dipicolinic acid (502 mg, 3.00 mmol) and hydrogen peroxide (30%, 11.22 g, 98.97 mmol) in acetonitrile (120 mL) were stirred for 24 h at 25 °C. Subsequently, the resulting mixture was extracted with cyclohexane (6×150 mL), concentrated to 100 mL and treated with H_2O (100 mL). The crude product was purified by flash chromatography (SiO_2, *c*Hex:EtOAc= 5:1). After removal of all volatiles in vacuum the product *cis*-**2f** (3.96 g, 12.1 mmol, 40%) was obtained as a colorless oil as a mixture of two diastereoisomers *(dr*= 50:50). R_f= 0.13 (*c*Hex:EtOAc= 5:1); ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.87 (t, $^3J_{H,H}$= 6.8 Hz, 3H), 1.21–1.83 (m, 25H), 2.29 (t, $^3J_{H,H}$= 7.5 Hz, 2H), 2.88–2.97 (m, 1H), 3.09–3.16 (m, 1H), 3.65 (s, 3H) 3.79–3.93 (m, 1H) ppm; $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 22 °C) δ= 14.02 (CH_3), 22.55 (CH_2), 24.81 (CH_2), 25.45 (CH_2), 25.54 (CH_2), 26.32 (CH_2), 26.36 (CH_2), 27.83 (CH_2), 27.95 (CH_2), 28.94 (CH_2), 29.09 (CH_2), 29.20 (2×CH_2), 31.75 (CH_2), 33.98 (CH_2), 34.66 (CH_2), 35.07 (CH_2), 37.38 (CH_2), 37.71 (CH_2), 51.41 (OCH_3), 54.41 (CH), 55.39 (CH), 56.26 (CH_2), 57.07 (CH), 70.05 (CH_2) 70.83 (CH_2), 174.23 (C=O) ppm; MS (EI): *m/z* (%): 310 (2) [M^+–H_2O], 225 (18), 193 (12) 187 (14), 155 (100) 139 (11), 127 (11), 121 (10), 115 (16), 109 (22), 97 (34), 87 (30), 74 (33), 69 (29), 55 (68), 43 (28), 41 (27); elemental analysis calcd. (%) for $C_{19}H_{36}O_4$ (328.49): C 69.47, H 11.05; found: C 69.45, H 11.00.

Methyl 8-(3-((2*R*)-acetoxyoctyl)oxiran-2-yl)octanoate (**2g**):[6] According to **GP2**, *O*-acetylricinoleic acid methyl ester (*cis*-**1g**, 10.64 g, 30.03 mmol), $Ru(acac)_3$ (60 mg, 0.15 mmol), dipicolinic acid (502 mg, 3.00 mmol) and hydrogen peroxide (30%, 11.22 g, 98.97 mmol) in acetonitrile (120 mL) were stirred for 24 h at 25 °C. Subsequently, the resulting mixture was extracted with cyclohexane (6×150 mL), concentrated to 50 mL and treated with H_2O (50 mL). The crude product was purified by flash chromatography (SiO_2, *c*Hex:EtOAc= 5:1) to yield **2g** (3.83 g, 10.3 mmol, 35%) as a colorless oil as a mixture of two diastereoisomers (*dr*= 50:50). R_f= 0.32 (*c*Hex:EtOAc= 5:1); ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ= 0.87 (t, $^3J_{H,H}$= 6.8 Hz, 3H), 1.21–1.41 (m, 15H), 1.42–1.55 (m, 4H), 1.56–1.68 (m, 4H), 1.69–1.87 (m, 2H),

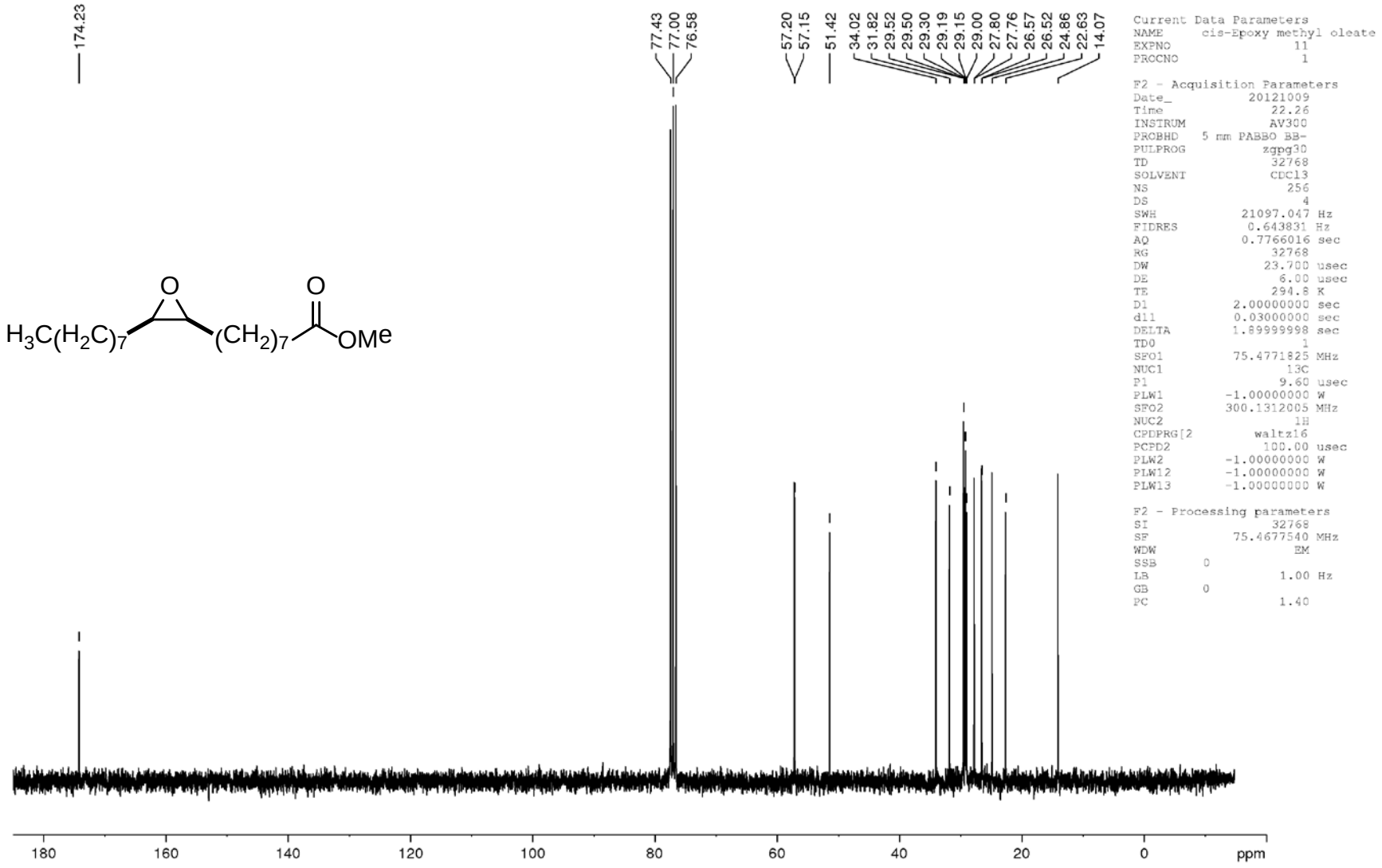
2.05 (s, 3H, isomer 1), 2.06 (s, 3H, isomer 2), 2.30 (t, $^{3}J_{H,H}$= 7.5 Hz, 2H), 2.84–3.14 (m, 2H), 3.66 (s, 3H), 4.99–5.10 (m, 1H) ppm; $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 22 °C): as a mixture of two diastereoisomers δ = 14.01 (2×CH_3), 21.19 (CH_3), 21.22 (CH_3), 22.52 (2×CH_2), 22.84 (2×CH_2), 25.17 (CH_2), 25.32 (CH_2), 26.44 (CH_2), 26.48 (CH_2), 27.84 (CH_2), 27.91 (CH_2), 28.97 (2×CH_2), 29.02 (CH_2), 29.04 (CH_2), 29.12 (2×CH_2), 29.25 (2×CH_2), 31.65 (2×CH_2), 32.58 (CH_2), 32.73 (CH_2), 34.01 (CH_2), 34.04 (CH_2), 34.30 (2×CH_2), 51.41 (2×OCH_3), 53.64 (CH), 53.86 (CH), 56.11 (CH), 56.75 (CH), 72.38 (CH), 72.40 (CH), 170.61 (C=O), 170.77 (C=O) 174.23 (2×C=O) ppm; MS (EI): *m/z* (%): 339 (4) [M^+–OMe], 310 (9), 225 (100), 213 (39), 193 (53), 187 (22), 181 (29), 168 (16), 155 (33), 135 (14), 113 (22), 109 (16), 97 (20), 95 (24), 81 (42), 67 (26), 55 (46), 43 (86), 41 (20); HRMS (ESI–TOF): *m/z* found for $C_{21}H_{43}O_5$ [M^++H]: 371.2792; found: 371.2788.

Methyl 8-(3-((3-pentyloxiran-2-yl)methyl)oxiran-2-yl)octanoate (**2h**):[3] According to **GP2**, methyl linoleate (**1h**, 8.83 g, 30.0 mmol), $Ru(acac)_3$ (120 mg, 0.301 mmol), dipicolinic acid (1.00 g, 5.98 mmol) and hydrogen peroxide (30%, 11.2 g, 99.0 mmol) in acetonitrile (120 mL) were stirred for 8 h at 25 °C. A second portion of hydrogen peroxide (30%, 11.2 g, 99.0 mmol) was added and the reaction mixture was allowed to stir for 16 h at 25 °C. Subsequently, the resulting mixture was extracted with cyclohexane (4×150 mL), concentrated to 100 mL and treated with H_2O (100 mL). The product **2h** (6.65 g, 20.4 mmol, 68%) was obtained as a colorless solid as a mixture of two diastereoisomers (*dr*= 50:50). ^{1}H NMR (400 MHz, $CDCl_3$, 22 °C): δ = 0.90 (t, $^{3}J_{H,H}$= 6.7 Hz, 3H), 1.25-1.41 (m, 10H), 1.41-1.57 (m, 8H), 1.58-1.66 (m, 2H), 1.70-1.83 (m, 2H), 2.30 (t, $^{3}J_{H,H}$= 7.5 Hz, 2H), 2.94–2.99 (m, 2H), 3.04–3.14 (m, 2H), 3.66 (s, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$, 22 °C): δ = 13.93 (CH_3), 22.52 (CH_2), 24.85 (CH_2), 26.10 (CH_2), 26.20 (CH_2), 26.38 (CH_2), 26.49 (CH_2), 26.89 (CH_2), 27.18 (CH_2), 27.78 (CH_2), 27.85 (CH_2), 28.98 (CH_2), 29.11 (CH_2), 29.25 (CH_2), 31.63 (CH_2), 34.01 (CH_2), 51.40 (OCH_3), 54.14 (CH_2), 54.14 (CH), 54.30 (CH), 54.31 (CH), 56.63 (CH), 56.69 (CH), 56.92 (CH), 56.97 (CH), 174.18 (C=O) ppm;[7] MS (EI): *m/z* (%): 326 (1) [M^+], 187 (8), 165 (8), 155 (100), 123 (13), 109 (33), 95 (25), 83 (42), 69 (44), 55 (69), 41 (39); elemental analysis calcd. (%) for $C_{19}H_{34}O_4$ (326.48): C 69.90, H 10.50; found: C 69.87, H 10.59.

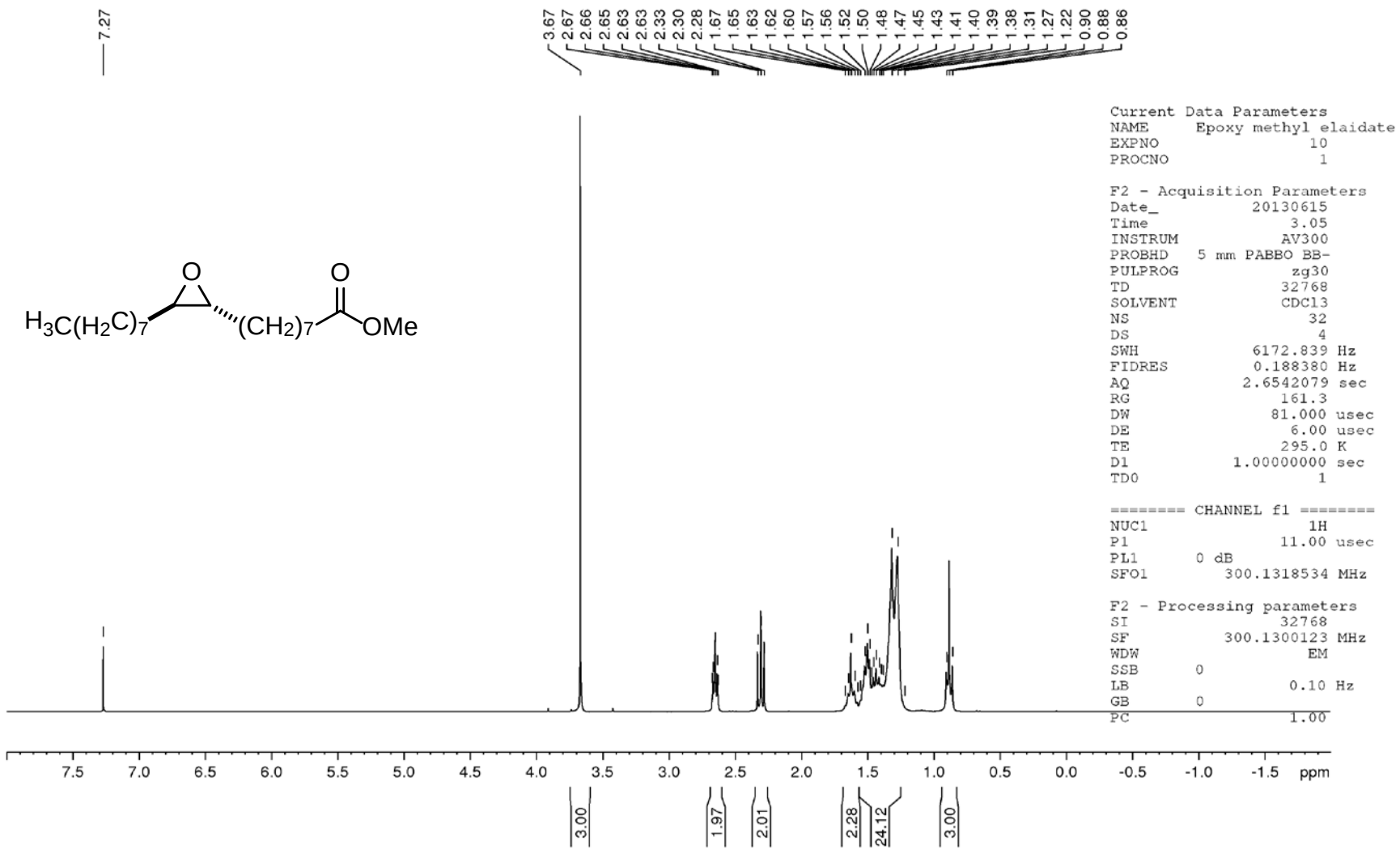
^{1}H NMR *cis*-Methyl 8-(3-octyloxiran-2-yl)octanoate (*cis*-**2a**)[1]



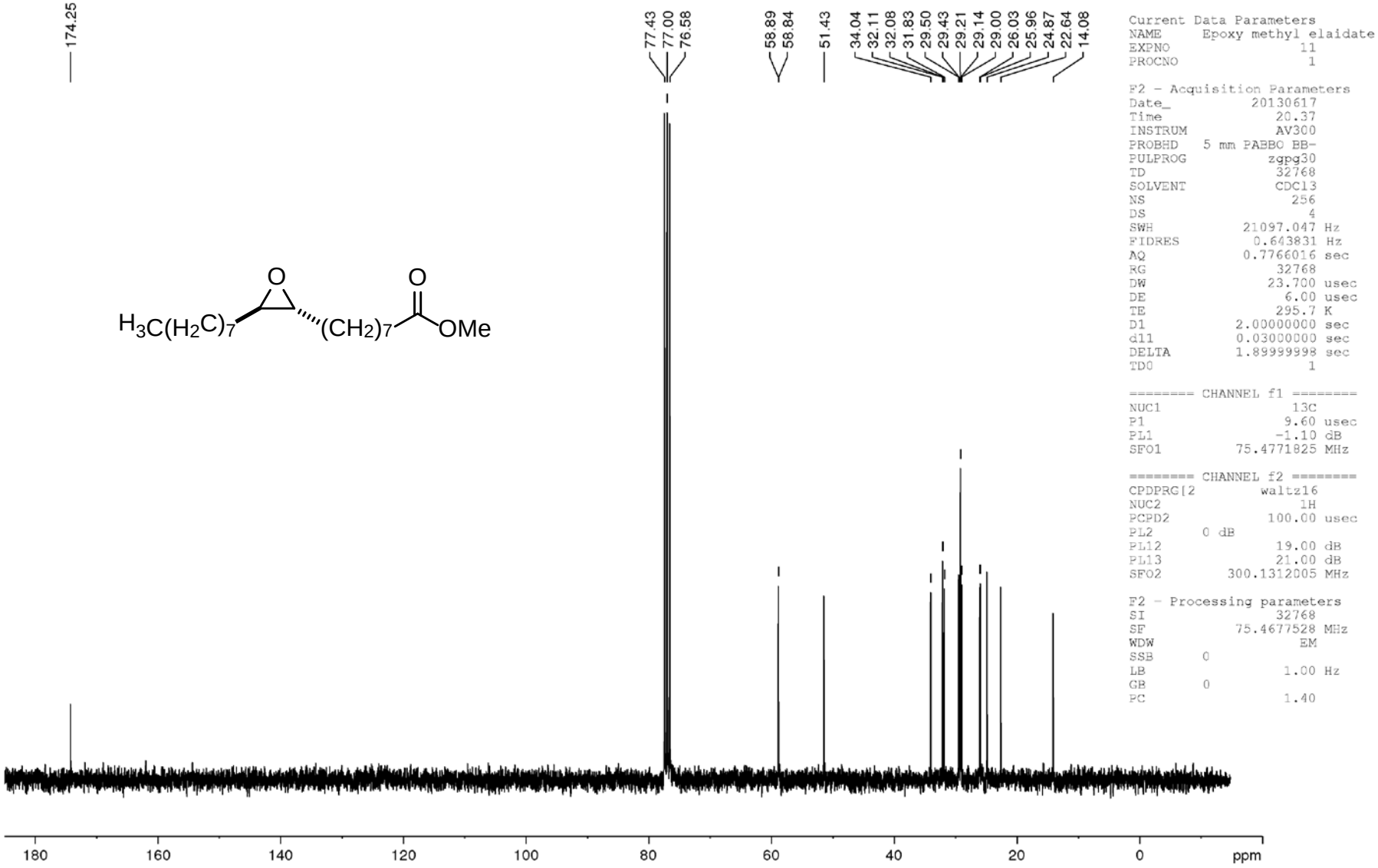
^{13}C NMR *cis*-Methyl 8-(3-octyloxiran-2-yl)octanoate (*cis*-**2a**)


174.23
77.43
77.00
76.58
57.20
57.15
51.42
34.02
31.82
29.52
29.50
29.30
29.19
29.15
29.00
27.80
27.76
26.57
26.52
24.86
22.63
14.07
O
O
H3C(H2C)7
(CH2)7
OMe
Current Data Parameters
NAME cis-Epoxy methyl oleate
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121009
Time 22.26
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 256
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766016 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 75.4771825 MHz
NUC1 13C
P1 9.60 usec
PLW1 -1.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 100.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
F2 - Processing parameters
SI 32768
SF 75.4677540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
160
140
120
100
80
60
40
20
0
ppm

^{1}H NMR *trans*-Methyl 8-(3-octyloxiran-2-yl)octanoate (*trans*-**2a**)[2]

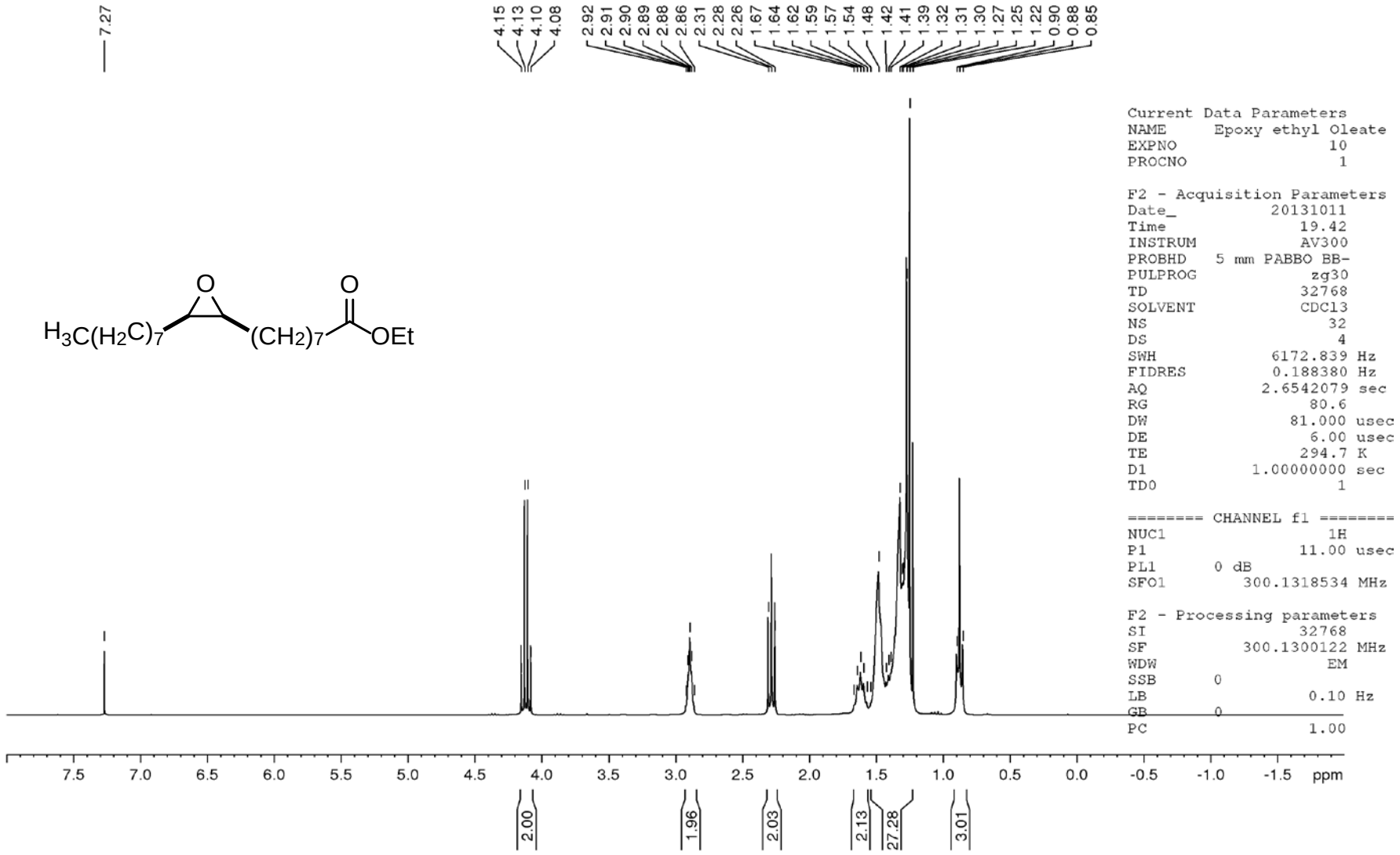


^{13}C NMR *trans*-Methyl 8-(3-octyloxiran-2-yl)octanoate (*trans*-**2a**)

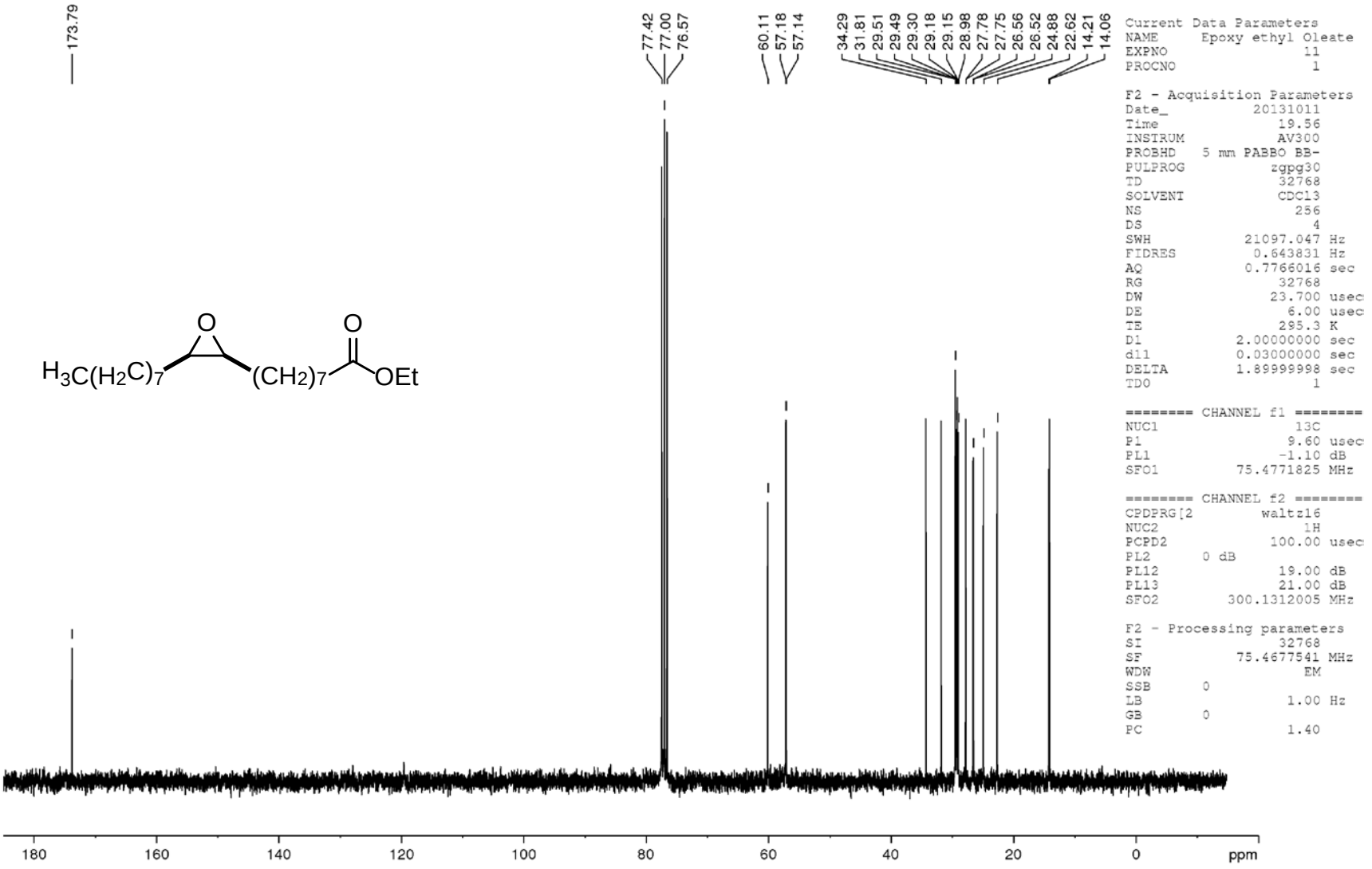



```
Current Data Parameters
NAME      Epoxy methyl elaidate
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20130617
Time                      20.37
INSTRUM                  AV300
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                        32768
SOLVENT                  CDCl3
NS                          256
DS                            4
SWH                  21097.047 Hz
FIDRES                0.643831 Hz
AQ                    0.7766016 sec
RG                        32768
DW                       23.700 usec
DE                        6.00 usec
TE                       295.7 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                         9.60 usec
PL1                       -1.10 dB
SFO1                 75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                    100.00 usec
PL2       0 dB
PL12                      19.00 dB
PL13                      21.00 dB
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                   75.4677528 MHz
WDW                          EM
SSB       0
LB                        1.00 Hz
GB        0
PC                        1.40
```

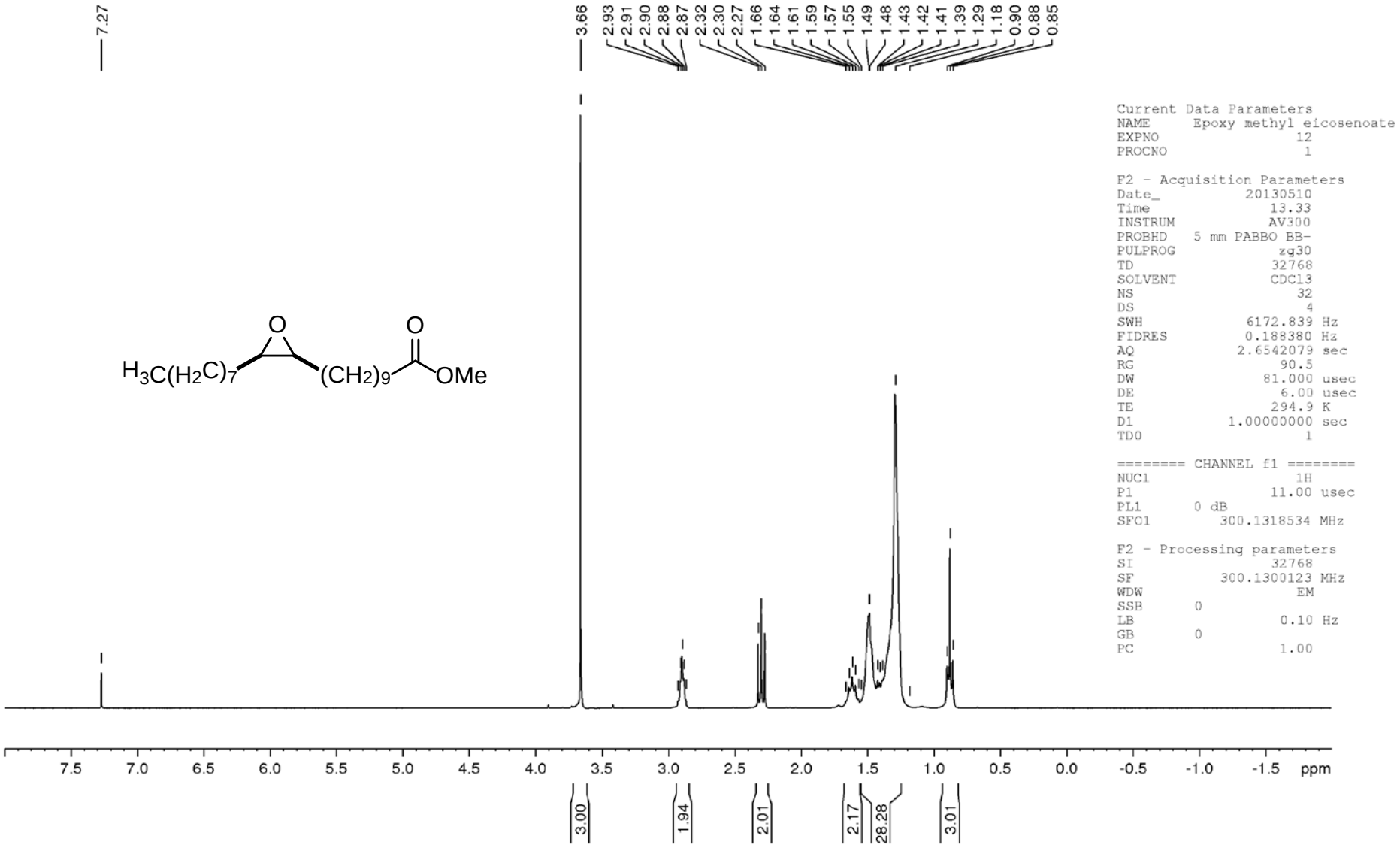
^{1}H NMR *cis*-Ethyl 8-(3-octyloxiran-2-yl)octanoate (*cis*-**2b**)[3]



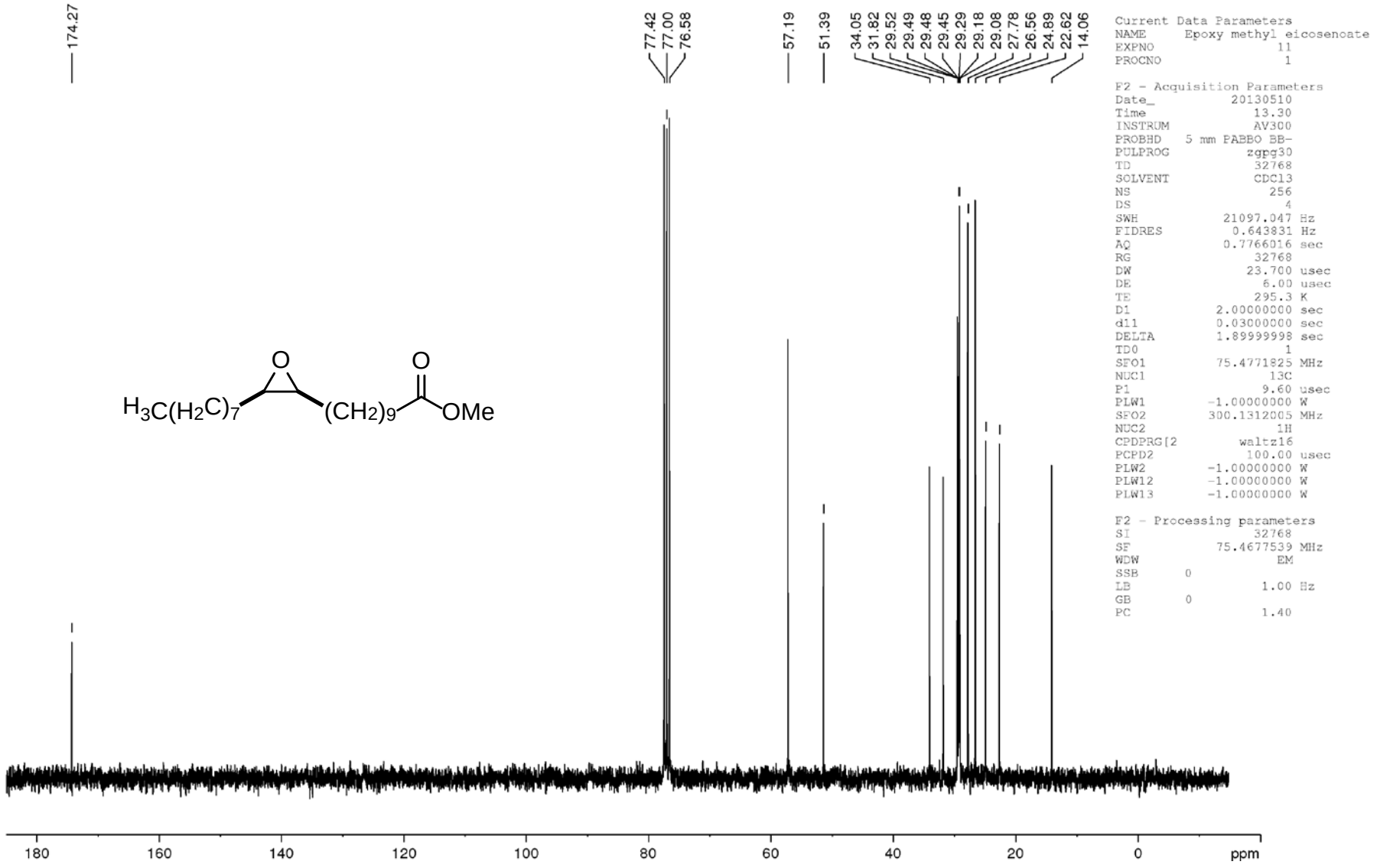
^{13}C NMR *cis*-Ethyl 8-(3-octyloxiran-2-yl)octanoate (*cis*-**2b**)



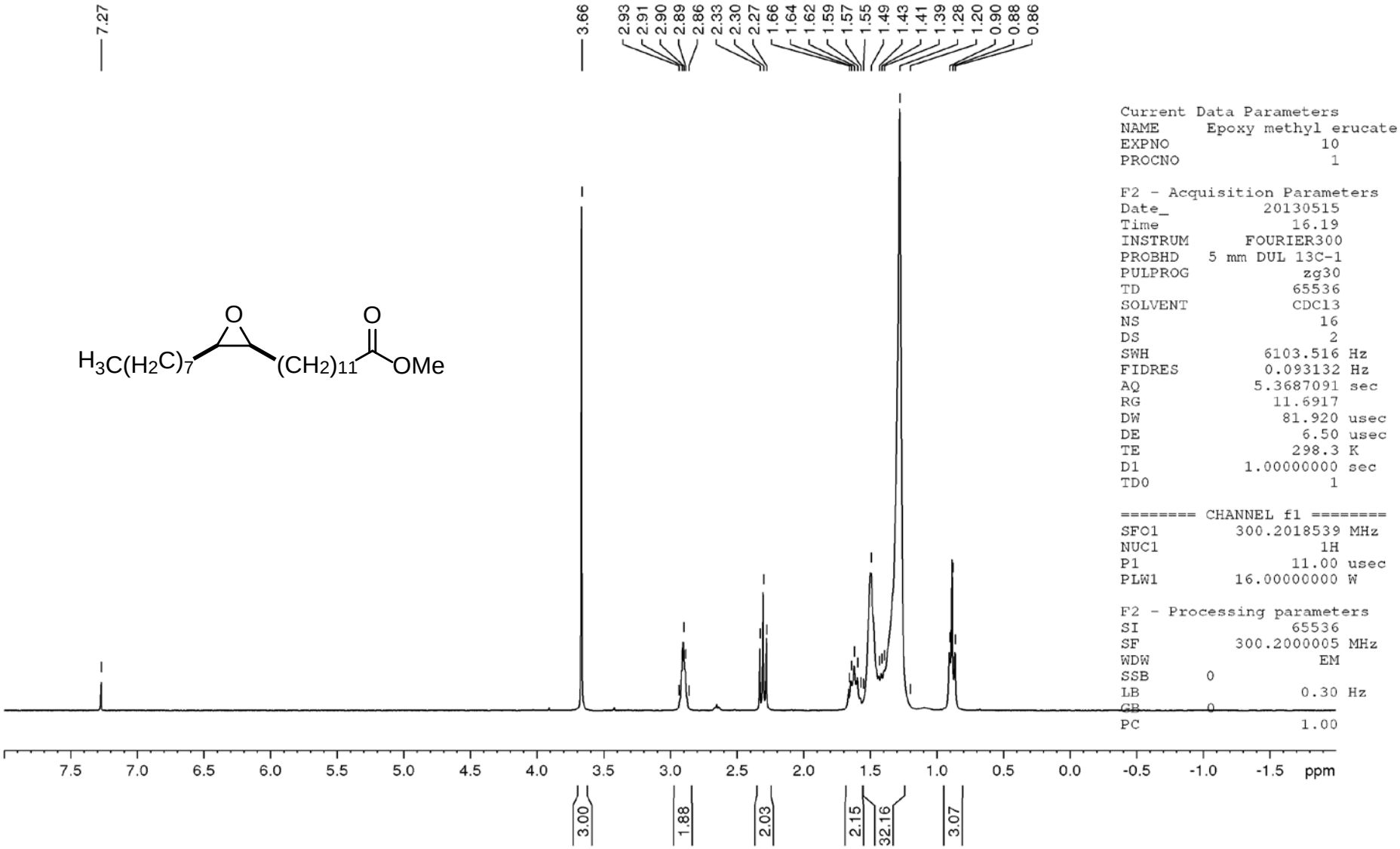
^{1}H NMR *cis*-Methyl 10-(3-octyloxiran-2-yl)decanoate (*cis*-**2d**)



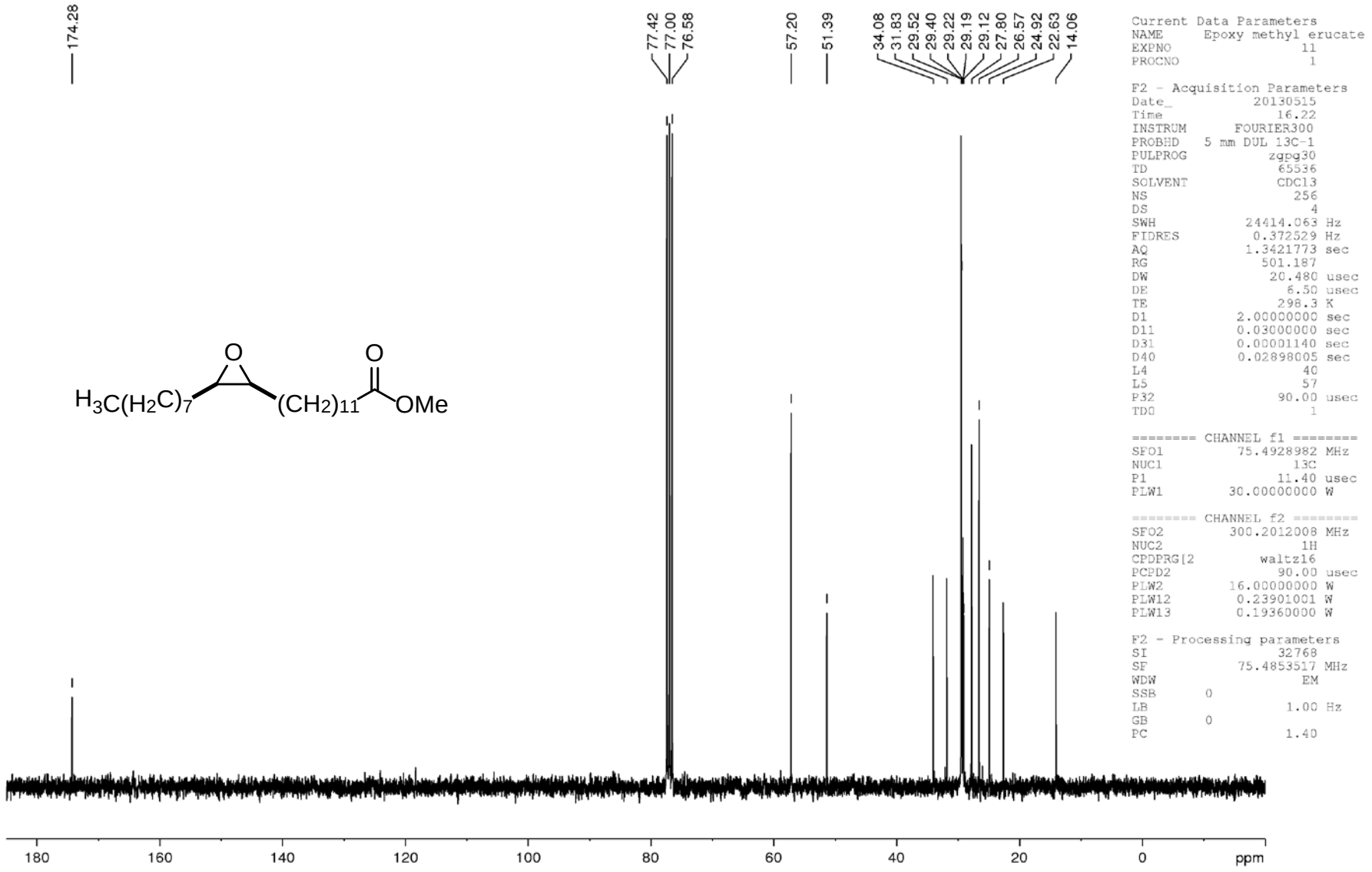
^{13}C NMR *cis*-Methyl 10-(3-octyloxiran-2-yl)decanoate (*cis*-**2d**)



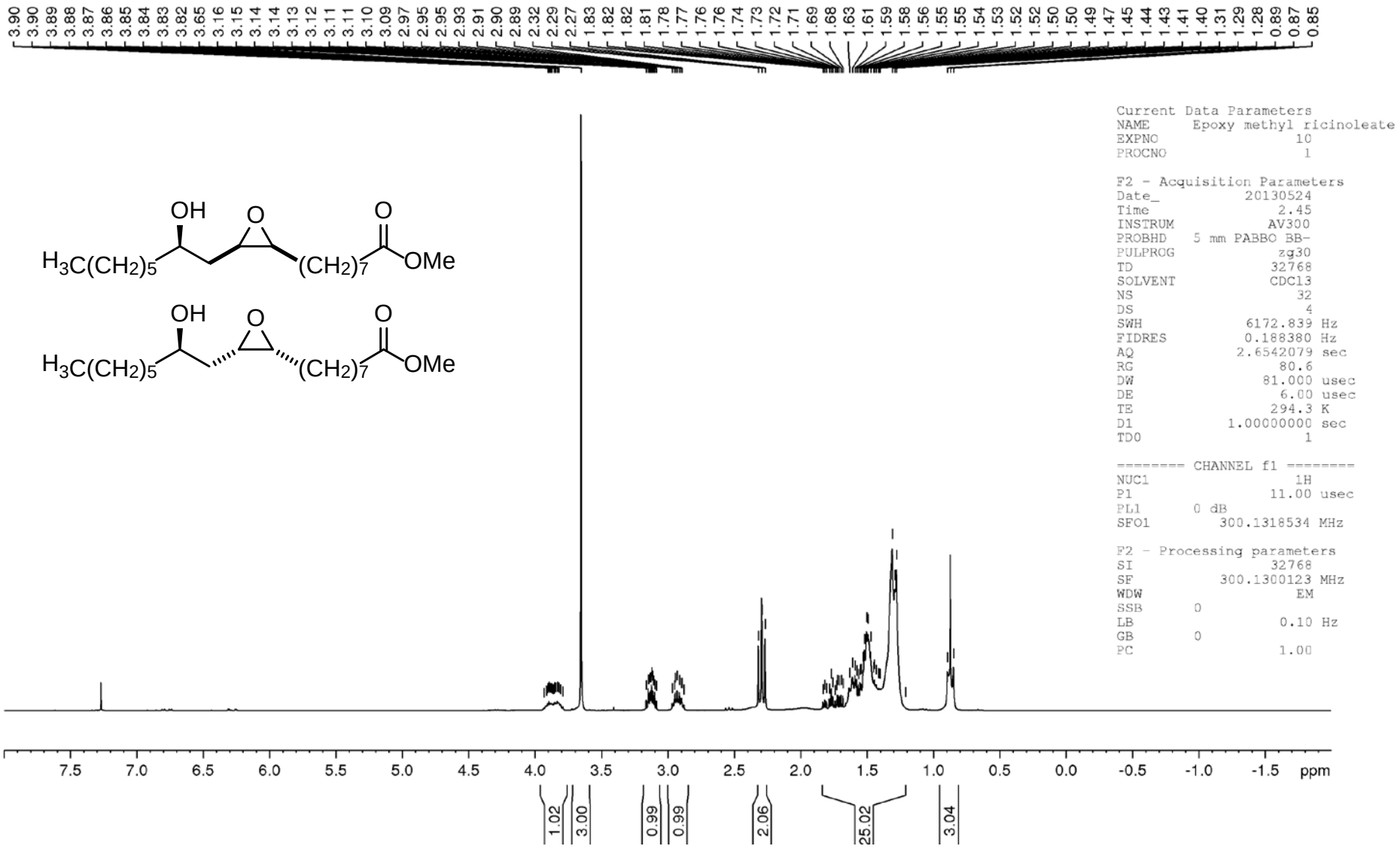
^{1}H NMR *cis*-Methyl 12-(3-octyloxiran-2-yl)dodecanoate (*cis*-**2e**)[4]



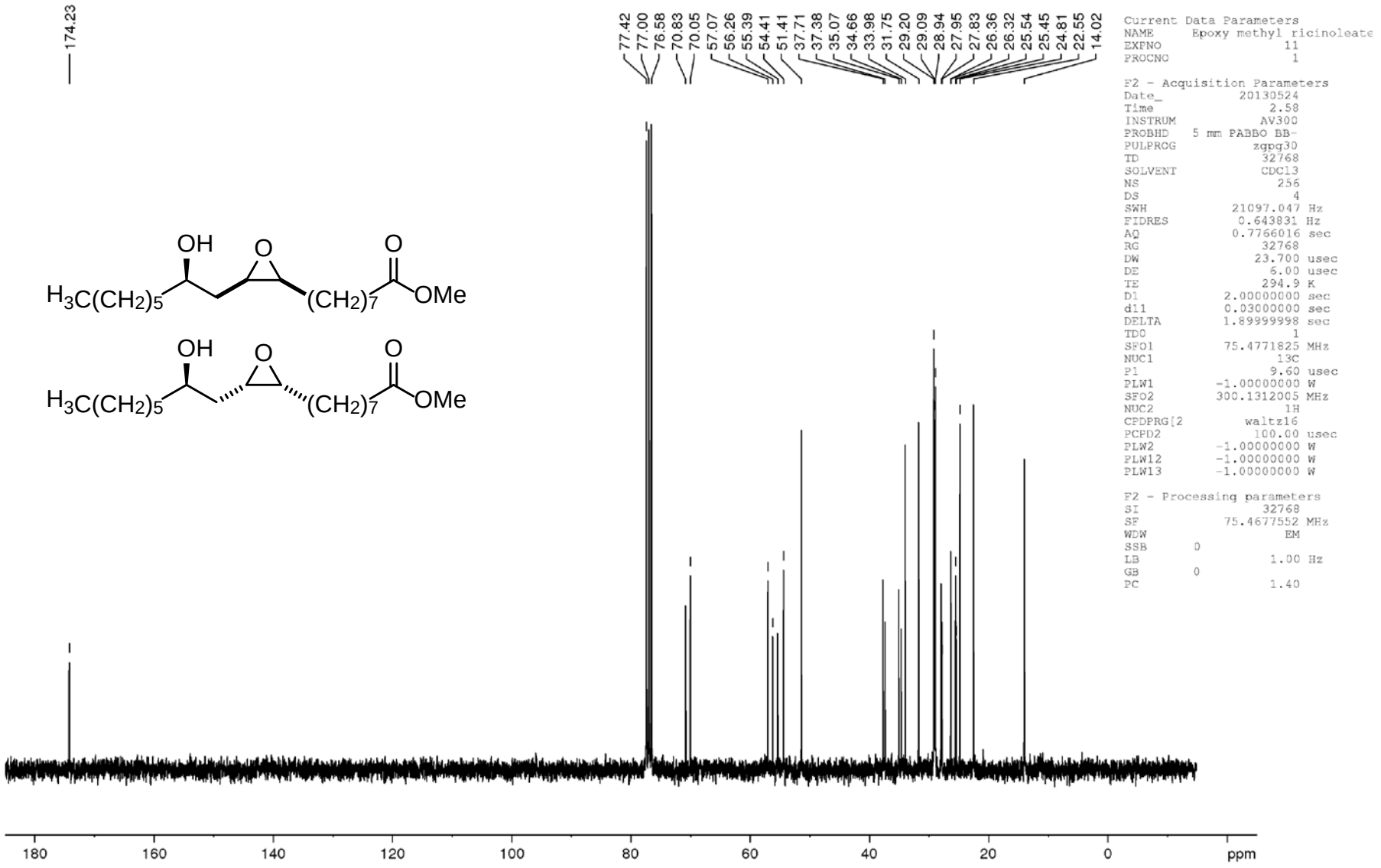
^{13}C NMR *cis*-Methyl 12-(3-octyloxiran-2-yl)dodecanoate (*cis*-**2e**)



^{1}H NMR Methyl 8-(3-((2*R*)-hydroxyoctyl)oxiran-2-yl)octanoate (**2f**)[5]



^{13}C NMR Methyl 8-(3-((2*R*)-hydroxyoctyl)oxiran-2-yl)octanoate (**2f**)

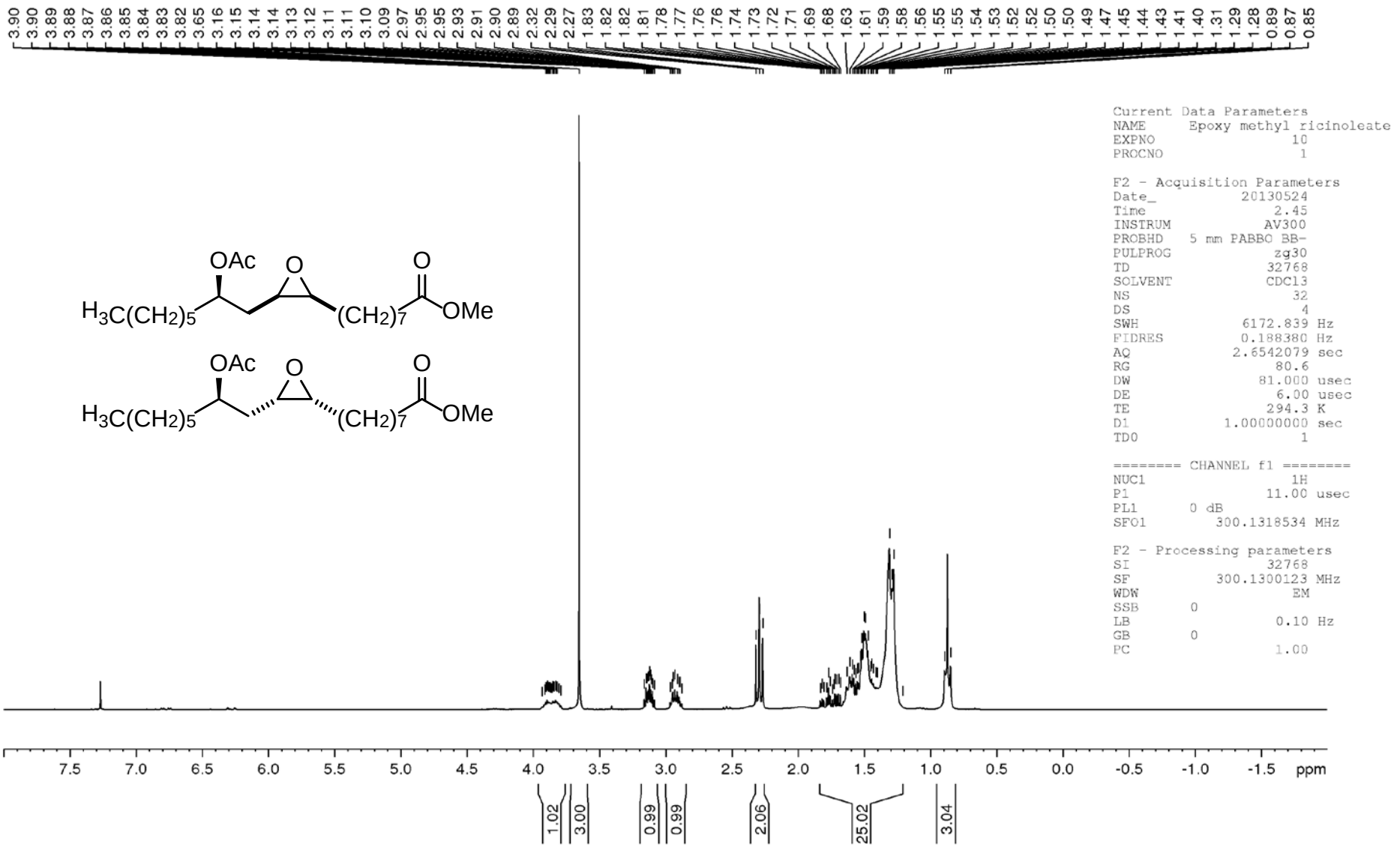


Current Data Parameters
NAME Epoxy methyl ricinoleate
EXPNO 11
PROCNO 1

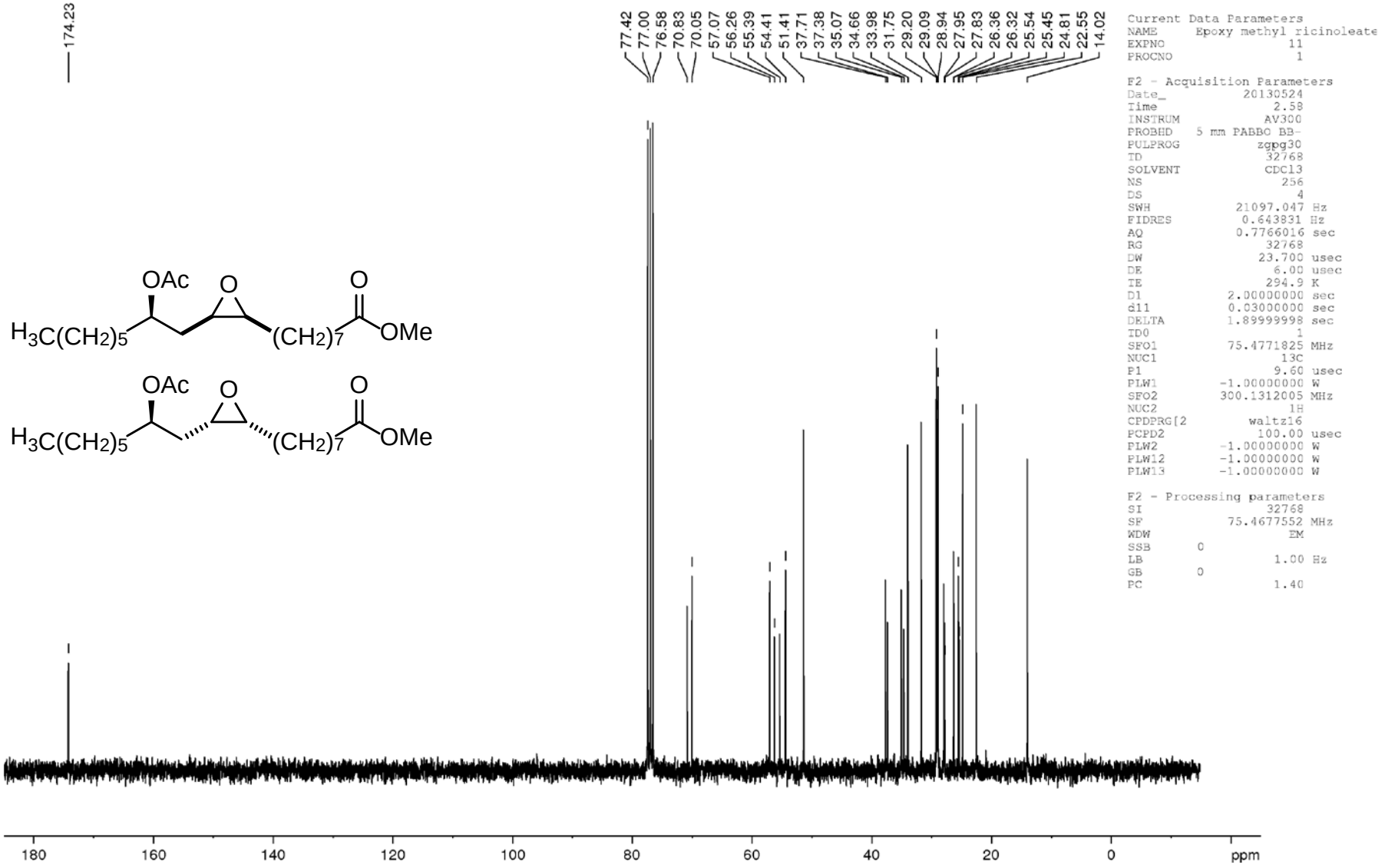
F2 - Acquisition Parameters
Date_ 20130524
Time 2.58
INSTRUM AV300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 256
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766016 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
SFO1 75.4771825 MHz
NUC1 13C
P1 9.60 usec
PLW1 -1.00000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 100.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W

F2 - Processing parameters
SI 32768
SF 75.4677552 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H NMR Methyl 8-(3-((2*R*)-acetoxyoctyl)oxiran-2-yl)octanoate (**2g**)[6]

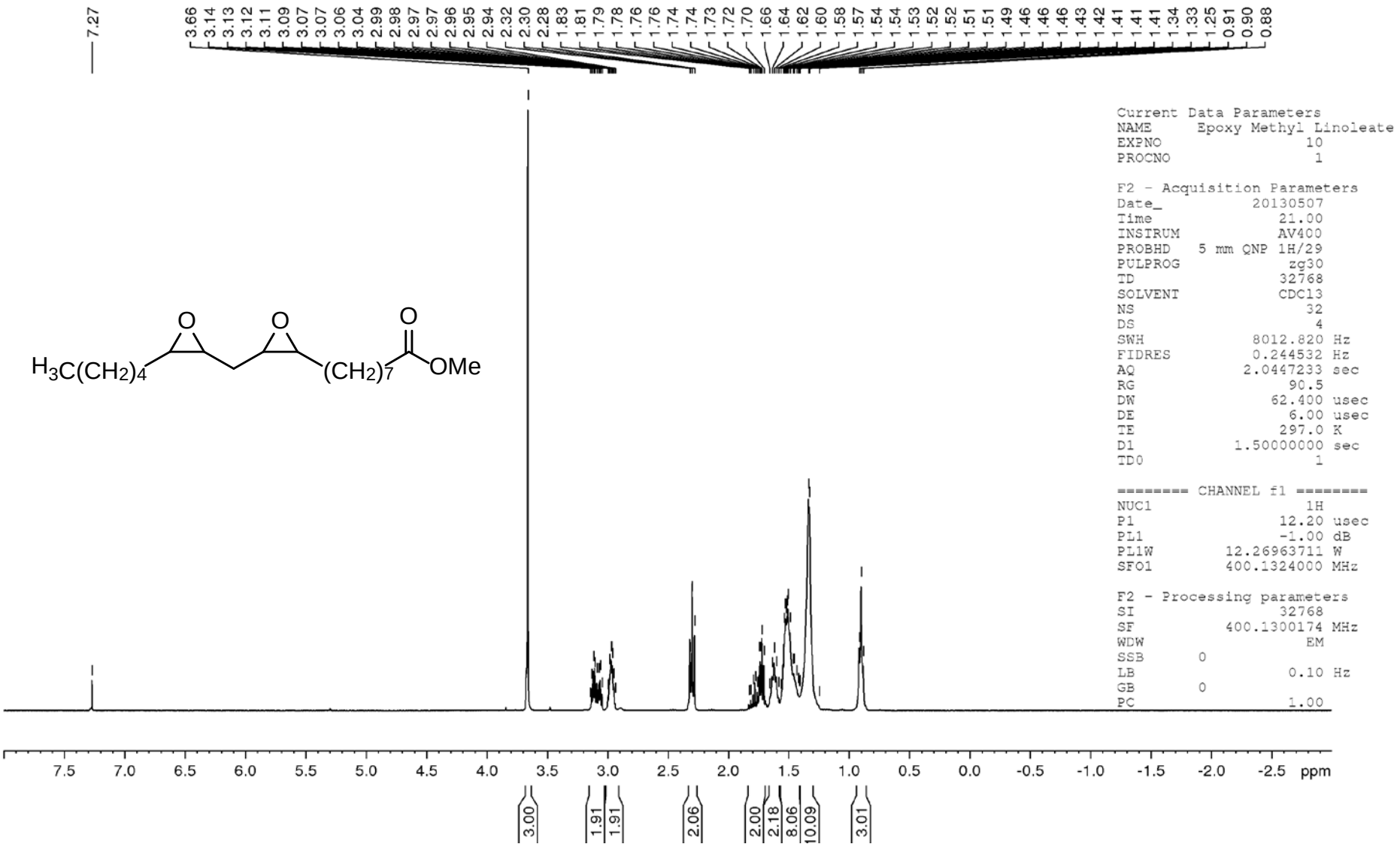


^{13}C NMR Methyl 8-(3-((2*R*)-acetoxyoctyl)oxiran-2-yl)octanoate (**2g**)

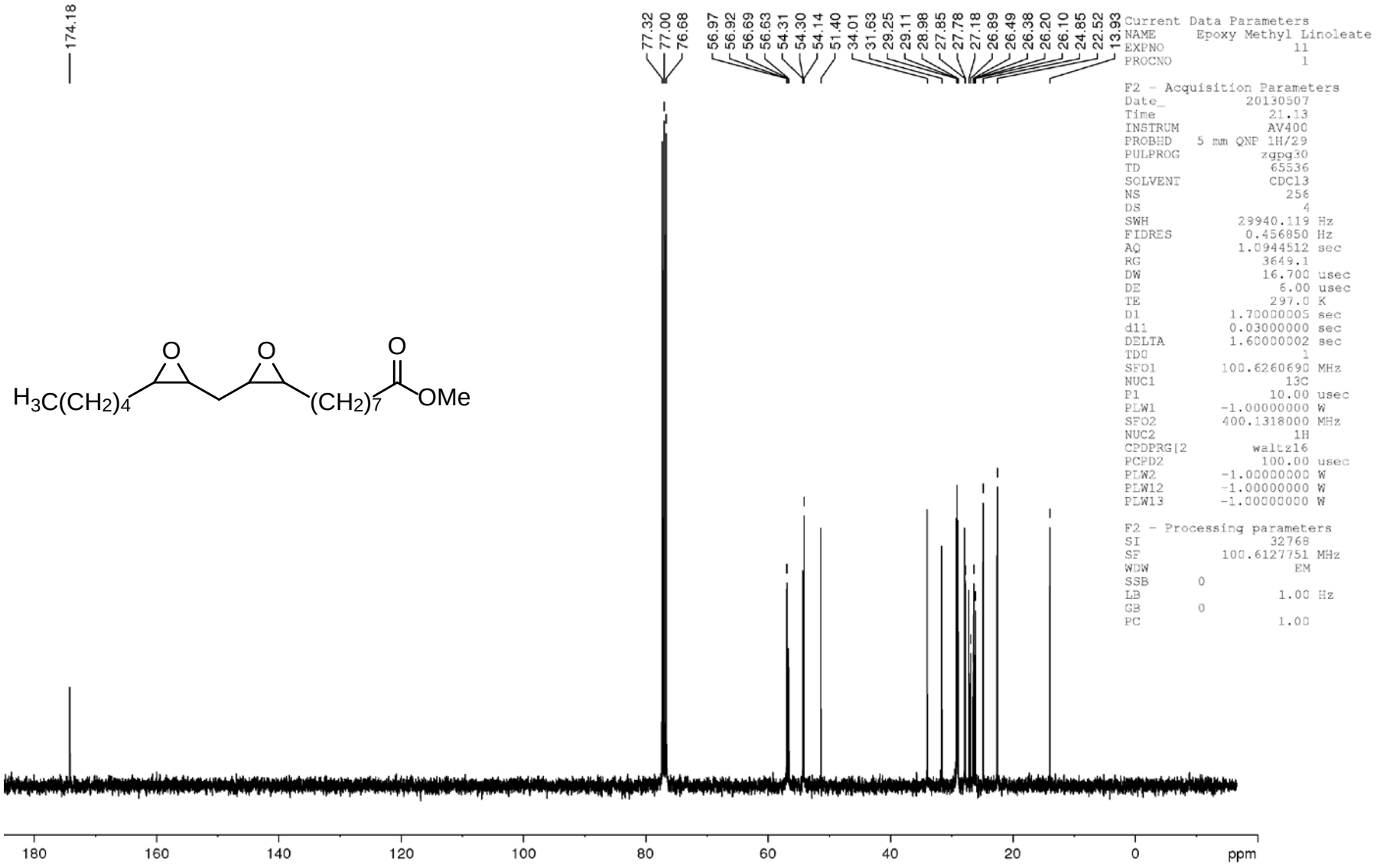



```
Current Data Parameters
NAME      Epoxy methyl ricinoleate
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130524
Time                2.58
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           21097.047 Hz
FIDRES         0.643831 Hz
AQ             0.7766016 sec
RG                32768
DW               23.700 usec
DE                6.00 usec
TE               294.9 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1
SFO1          75.4771825 MHz
NUC1                 13C
P1                9.60 usec
PLW1         -1.00000000 W
SFO2         300.1312005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2           100.00 usec
PLW2         -1.00000000 W
PLW12        -1.00000000 W
PLW13        -1.00000000 W

F2 - Processing parameters
SI                32768
SF           75.4677552 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{1}H NMR Methyl 8-(3-((3-pentyloxiran-2-yl)methyl)oxiran-2-yl)octanoate (**2h**)[3]

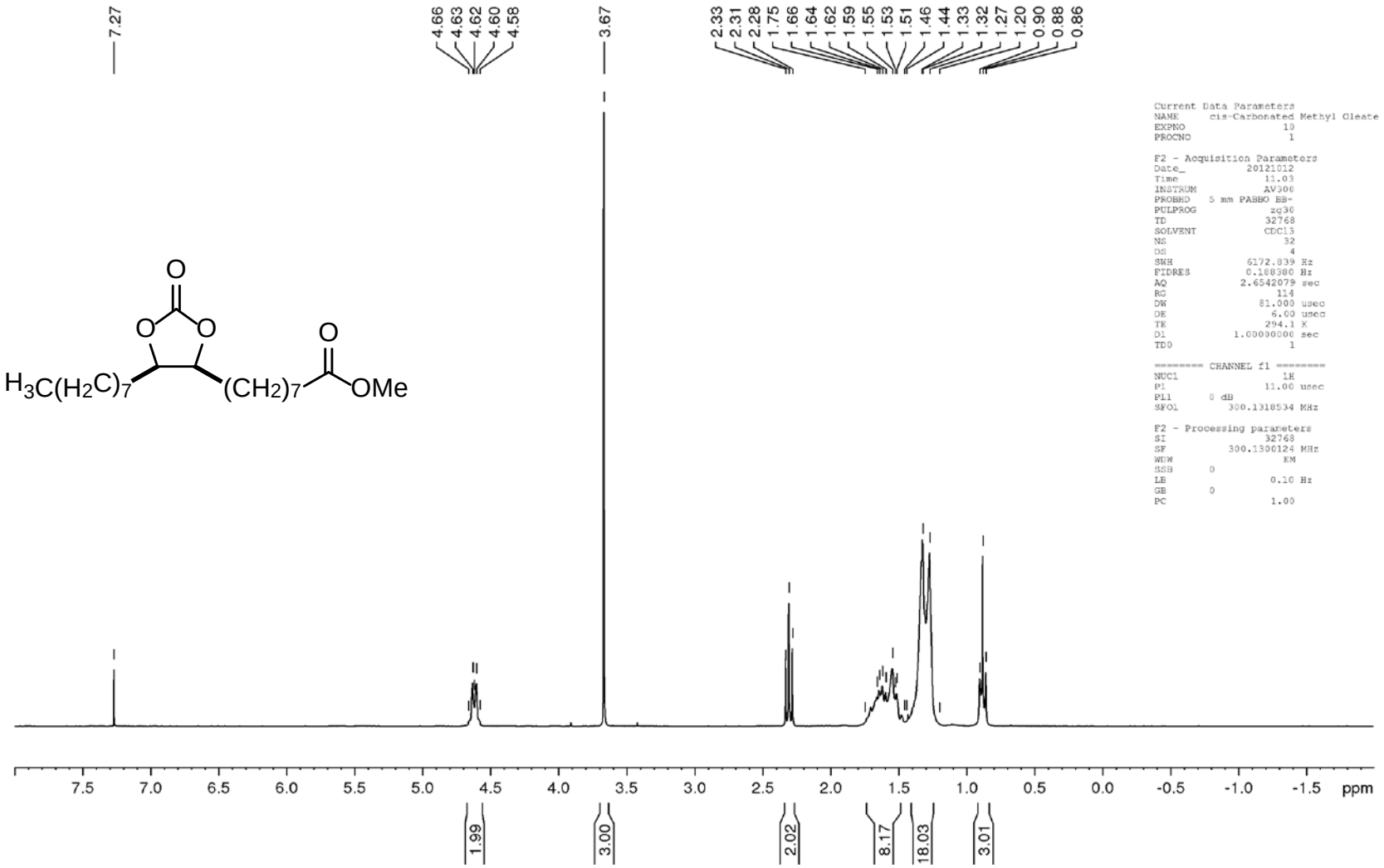


^{13}C NMR Methyl 8-(3-((3-pentyloxiran-2-yl)methyl)oxiran-2-yl)octanoate (**2h**)

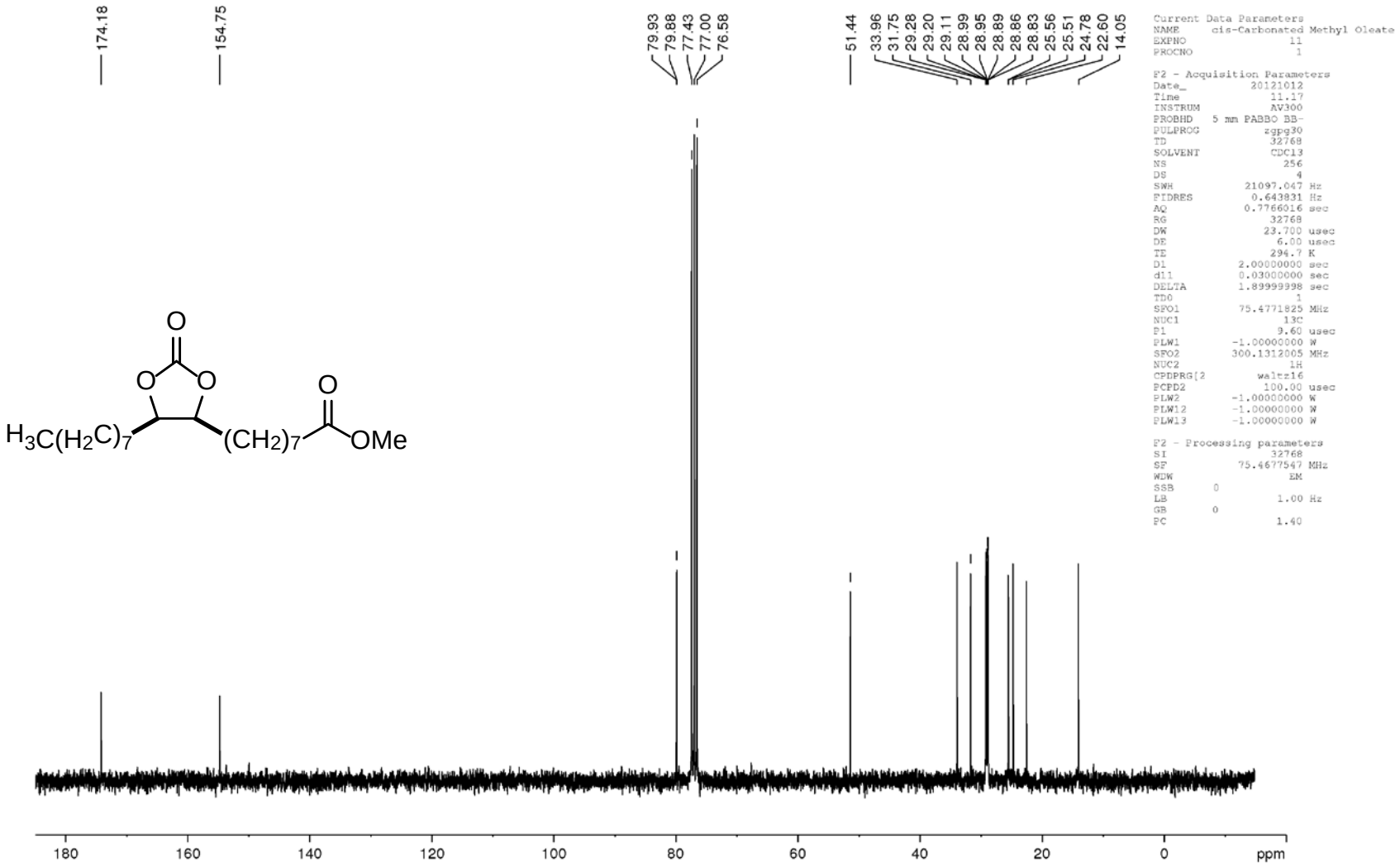


3. NMR Spectra of carbonated fatty acid esters

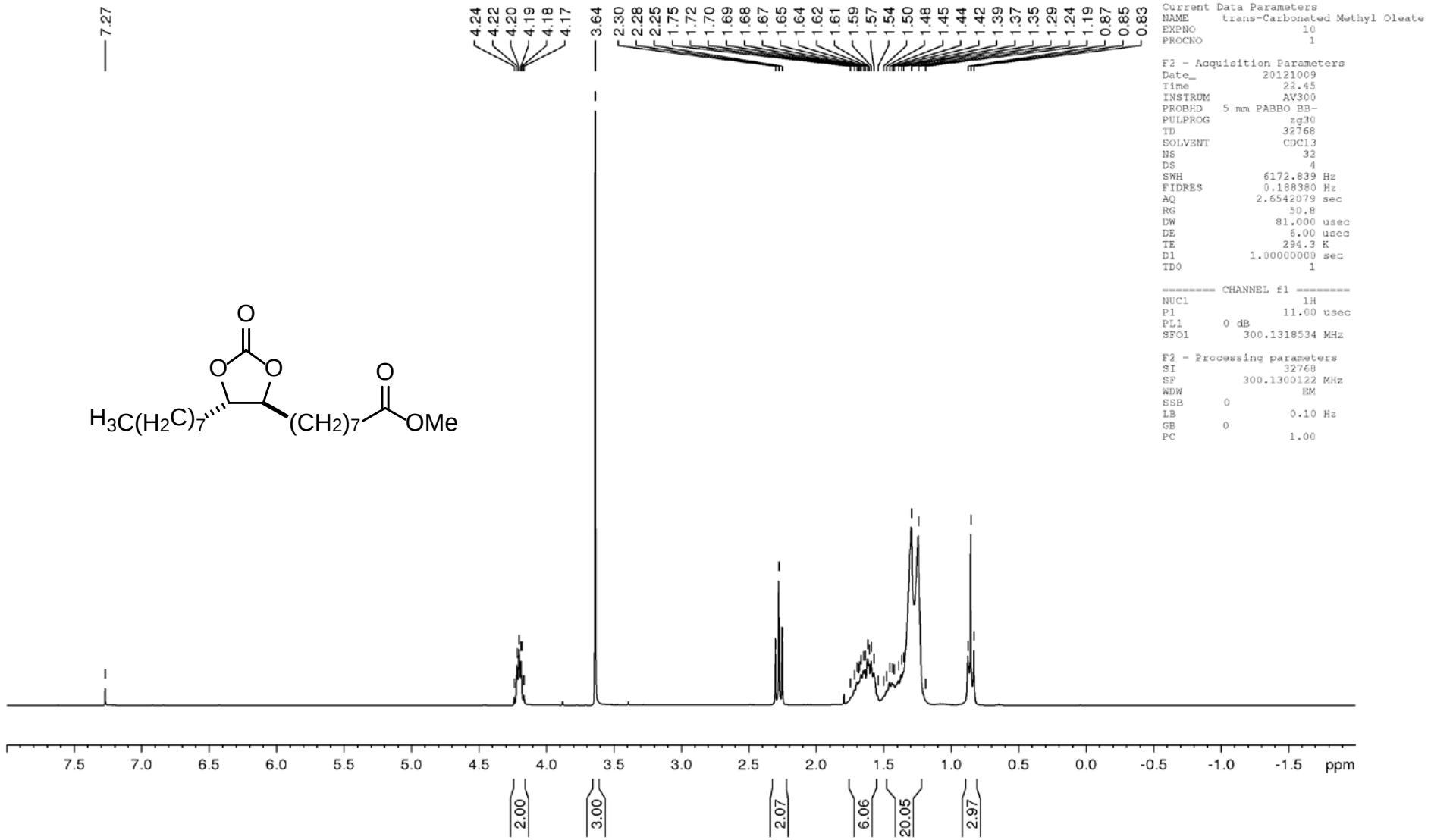
^{1}H NMR *cis*-Methyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3a**)[8]



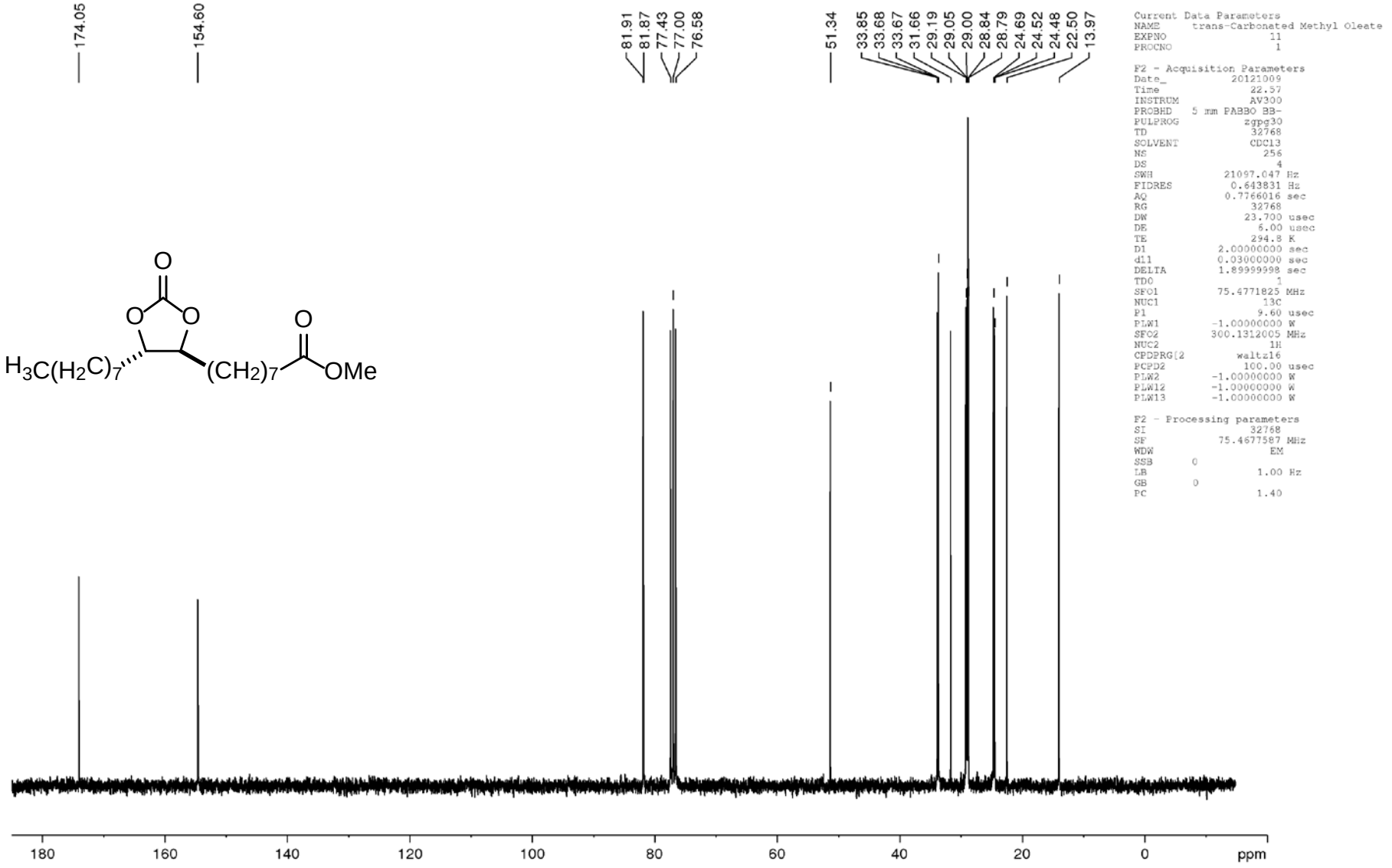
^{13}C NMR *cis*-Methyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3a**)



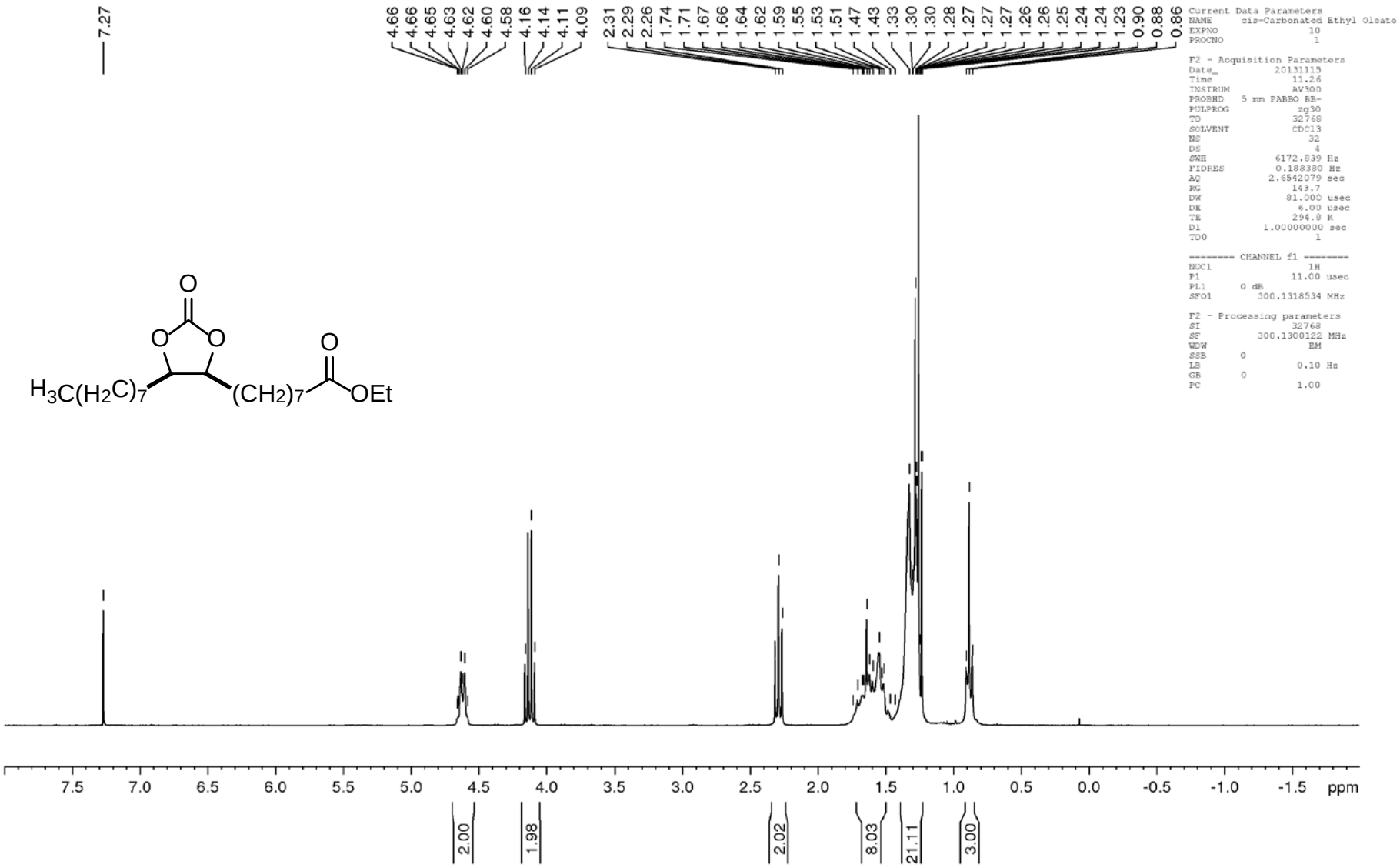
^{1}H NMR *trans*-Methyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*trans*-**3a**)



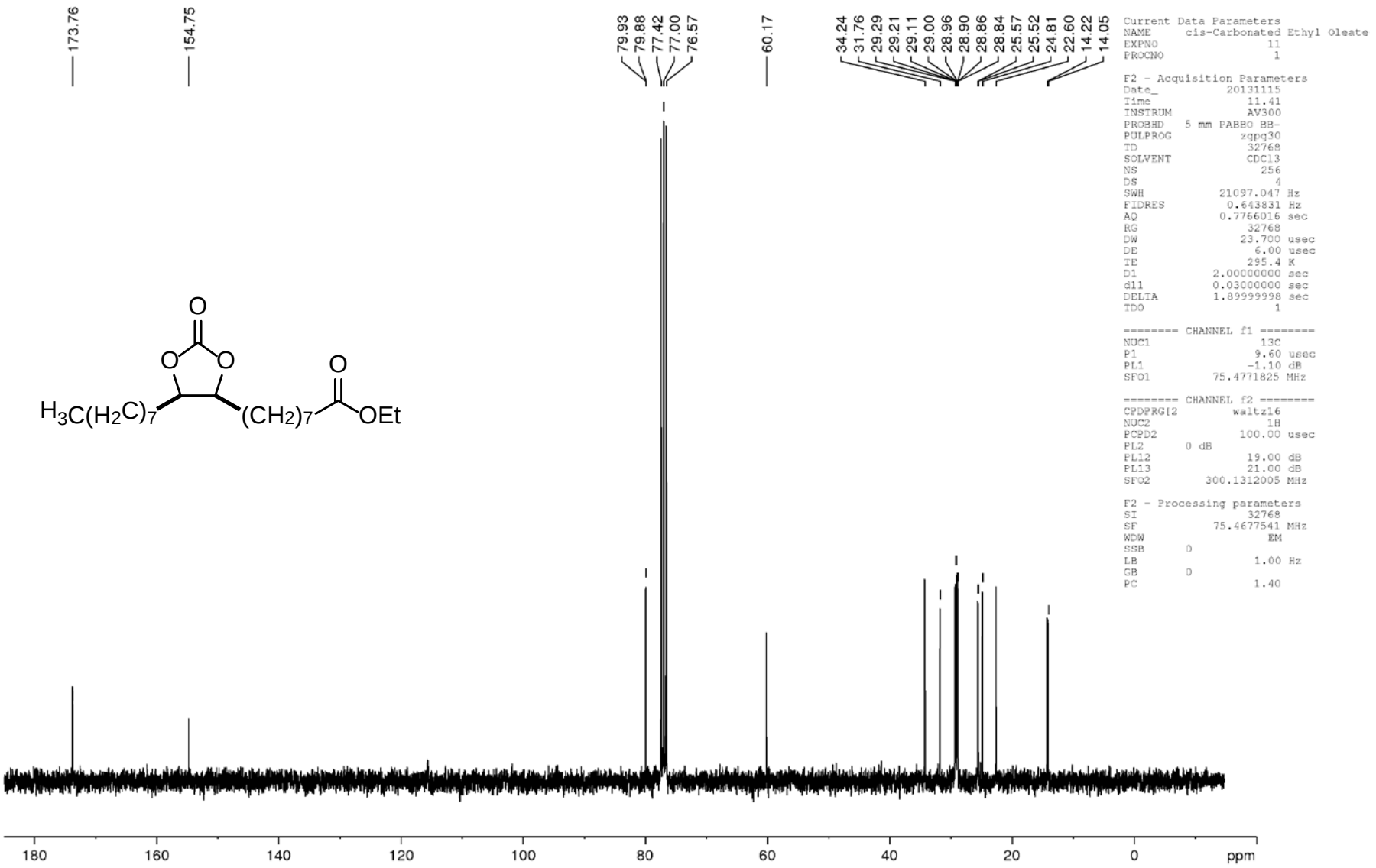
^{13}C NMR *trans*-Methyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*trans*-**3a**)



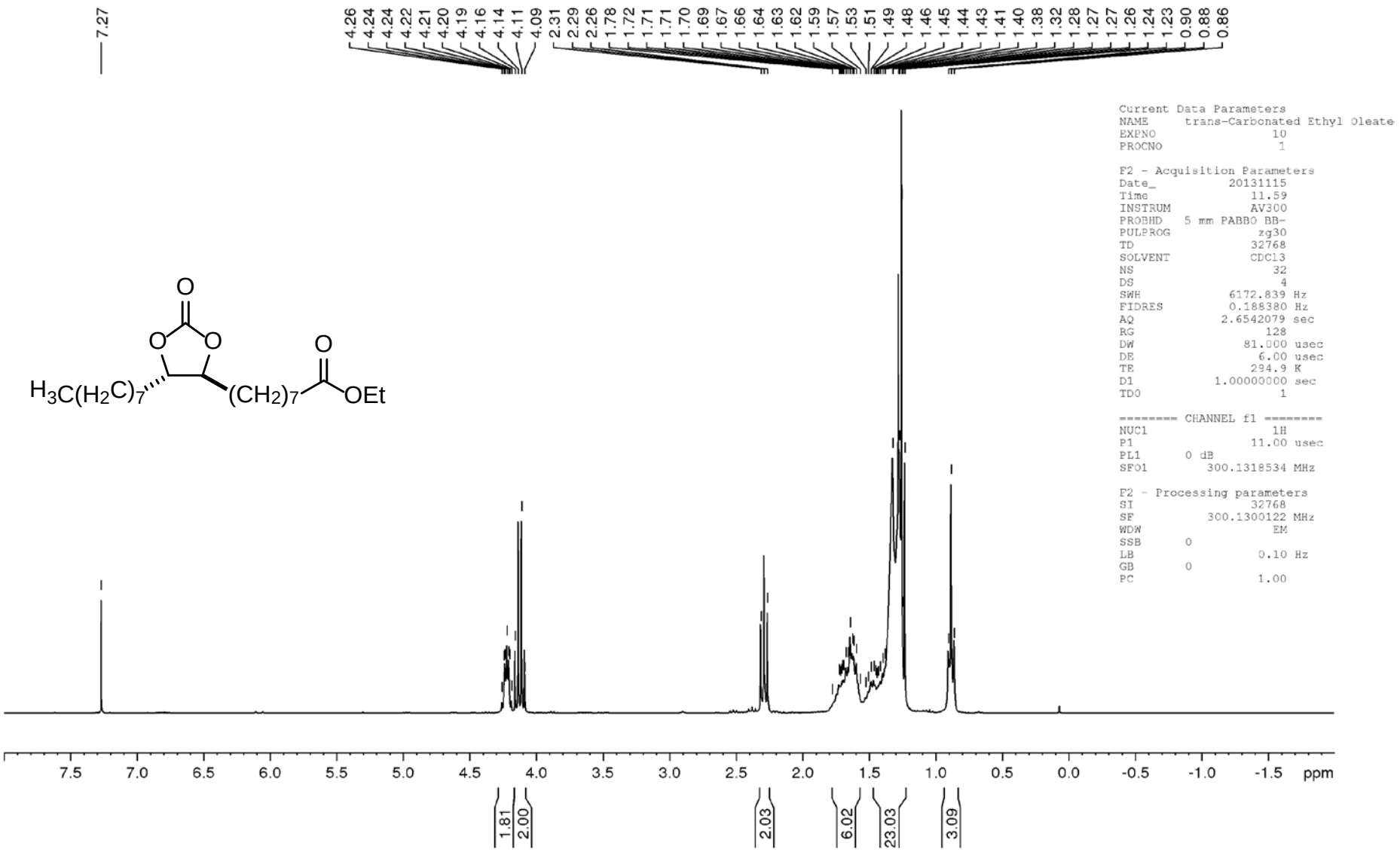
^{1}H NMR *cis*-Ethyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3b**)



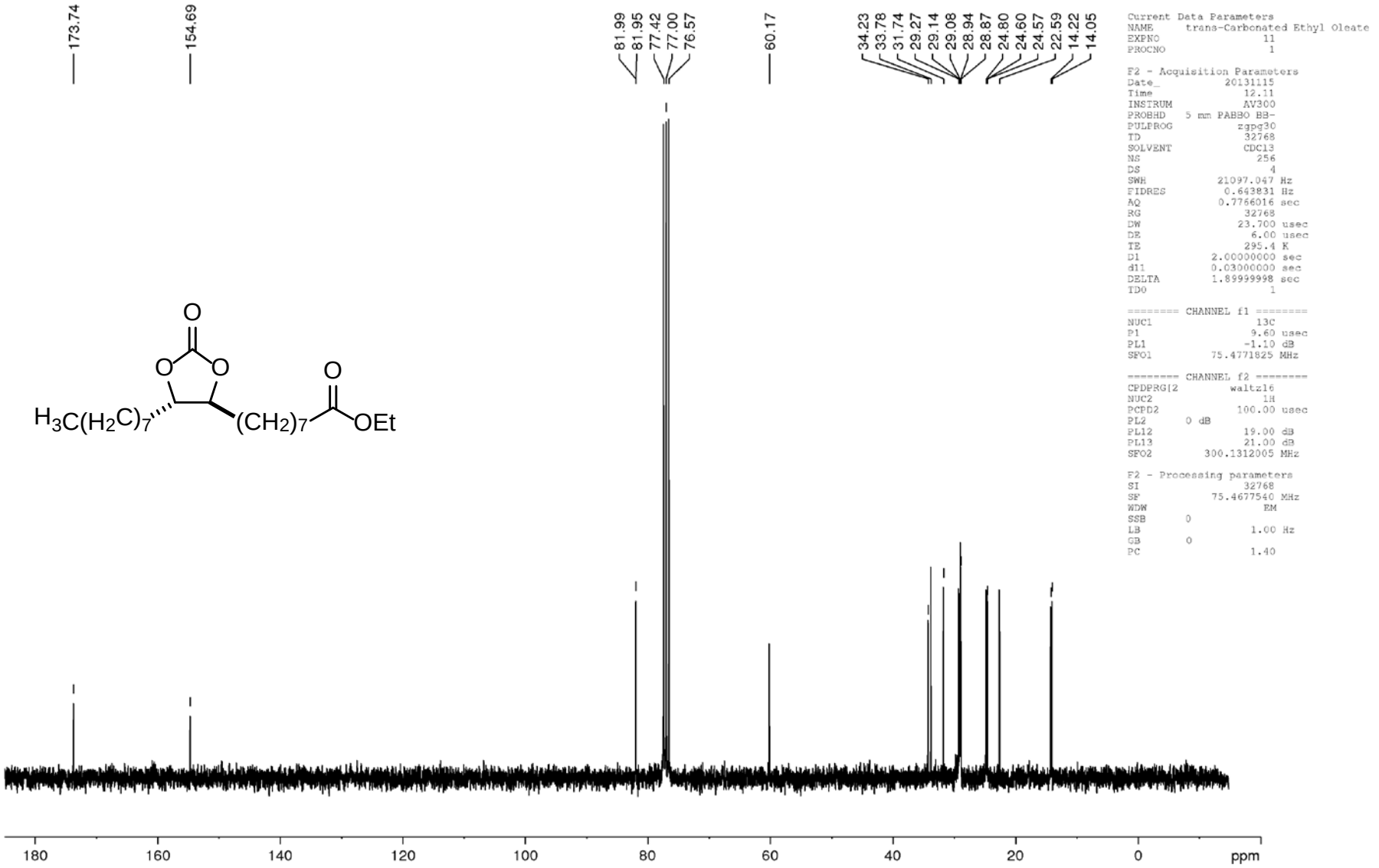
^{13}C NMR *cis*-Ethyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3b**)



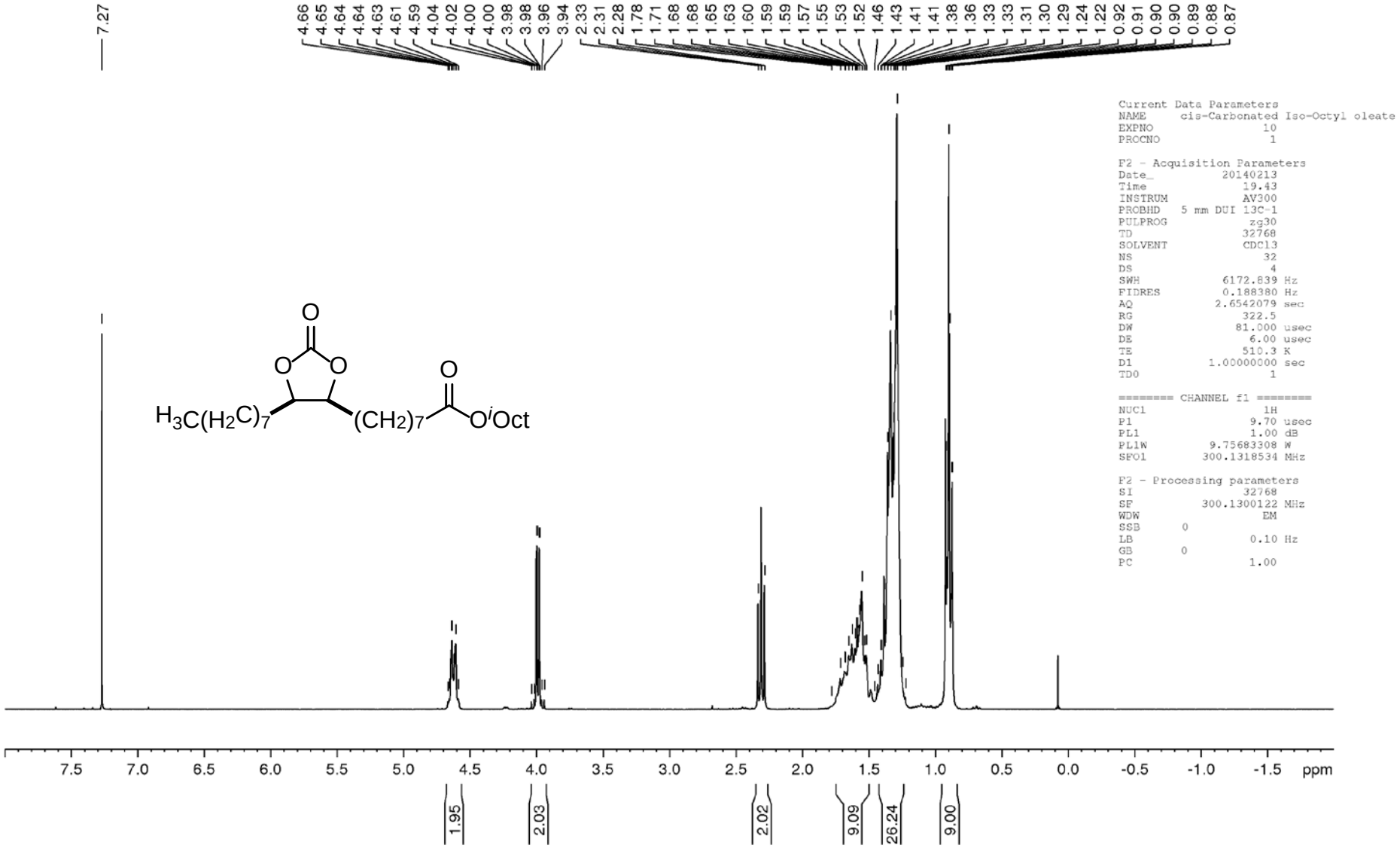
^{1}H NMR *trans*-Ethyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*trans*-**3b**)



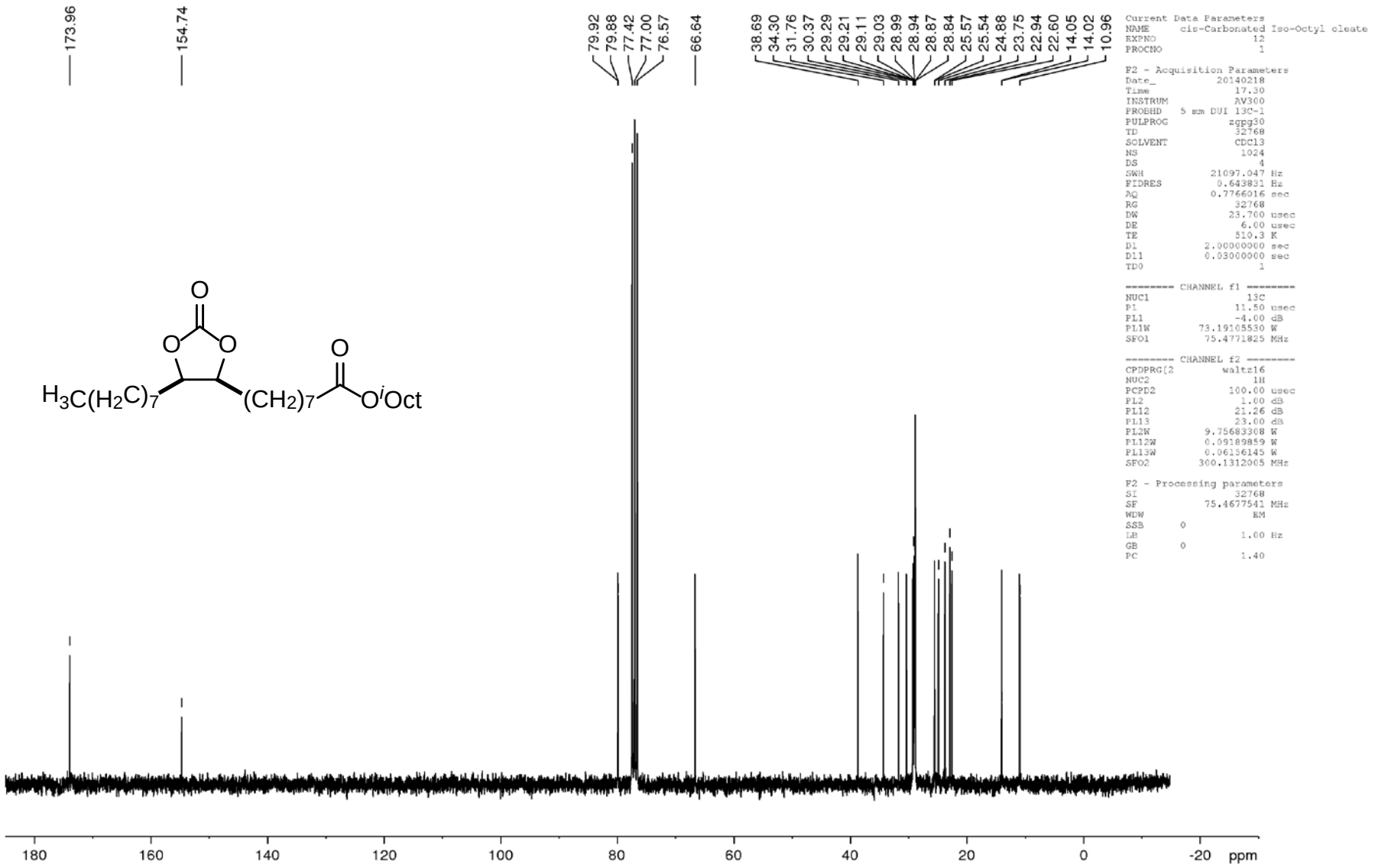
^{13}C NMR *trans*-Ethyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*trans*-**3b**)



^{1}H NMR *cis-iso*-Octyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3c**)

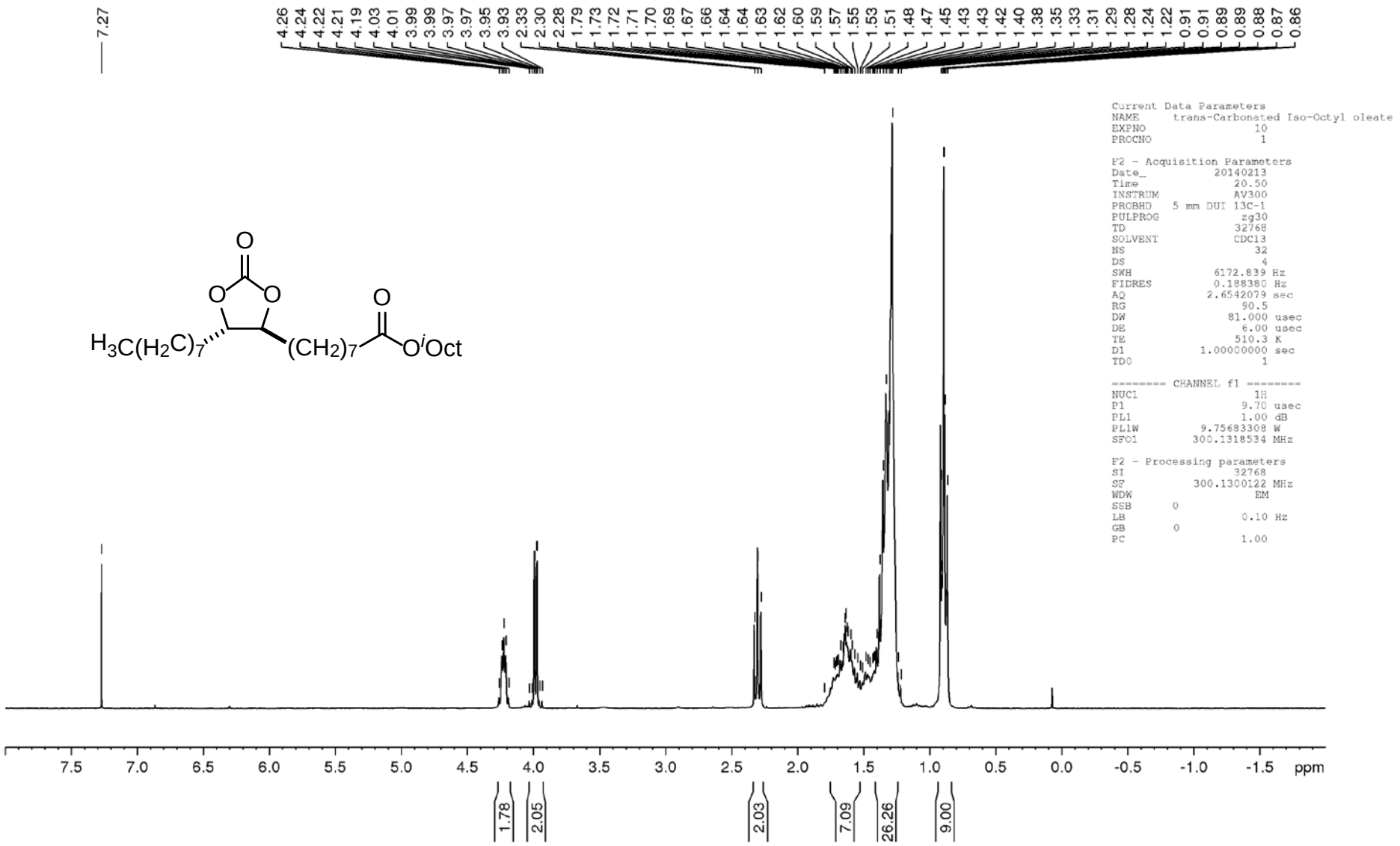


^{13}C NMR *cis-iso*-Octyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3c**)

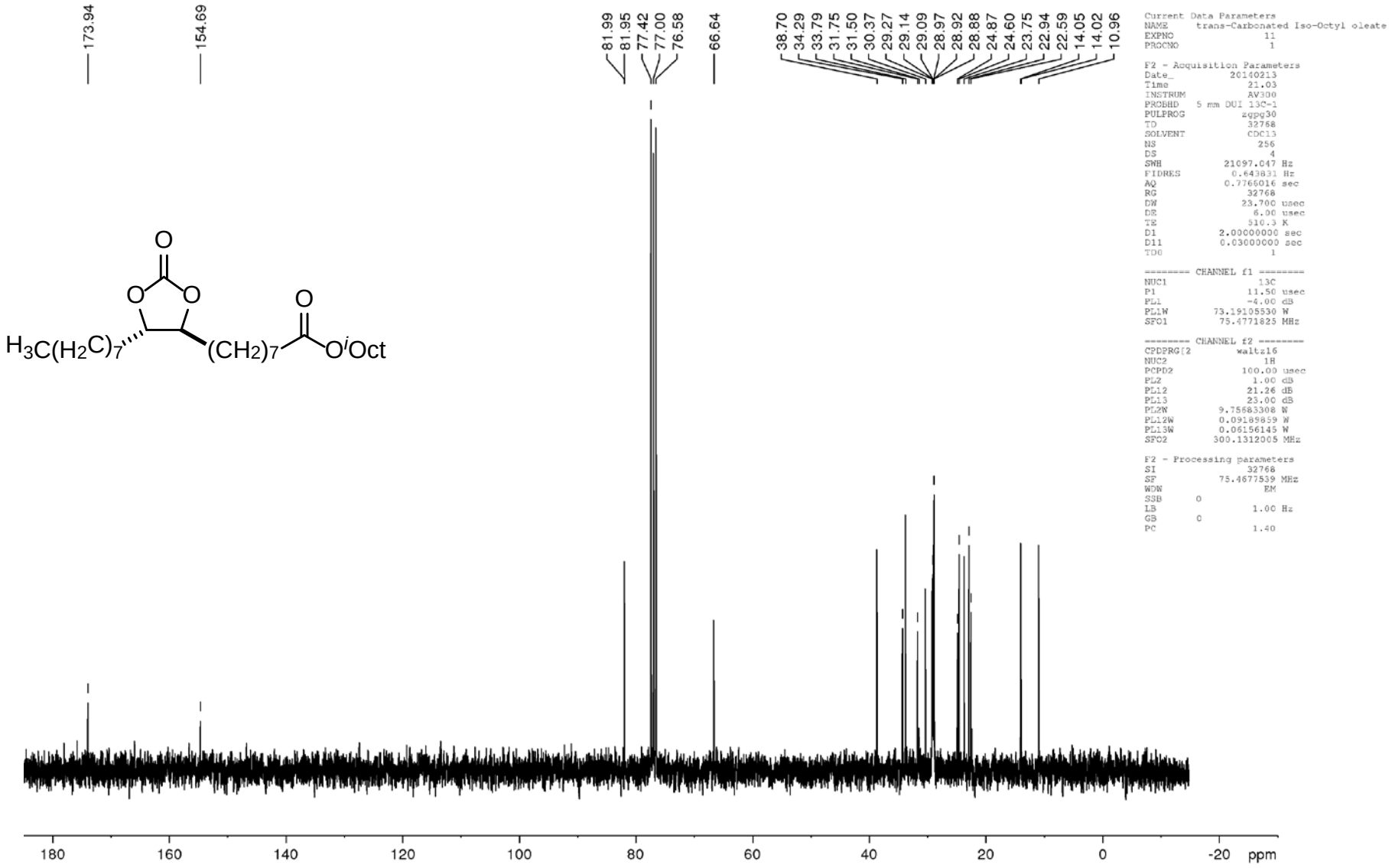



```
Current Data Parameters
NAME      cis-Carbonated Iso-Octyl cleate
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140218
Time              17.30
INSTRUM           AV300
PROBHD   5 mm DUI 13C-1
PULPROG           zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           21097.047 Hz
FIDRES         0.643831 Hz
AQ             0.7766016 sec
RG                32768
DW               23.700 usec
DE                6.00 usec
TE                310.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 11.50 usec
PL1                -4.00 dB
PL1W         73.19105530 W
SFO1          75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.00 dB
PL12              21.26 dB
PL13              23.00 dB
PL2W          9.75683308 W
PL12W         0.09189859 W
PL13W         0.06156145 W
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677541 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

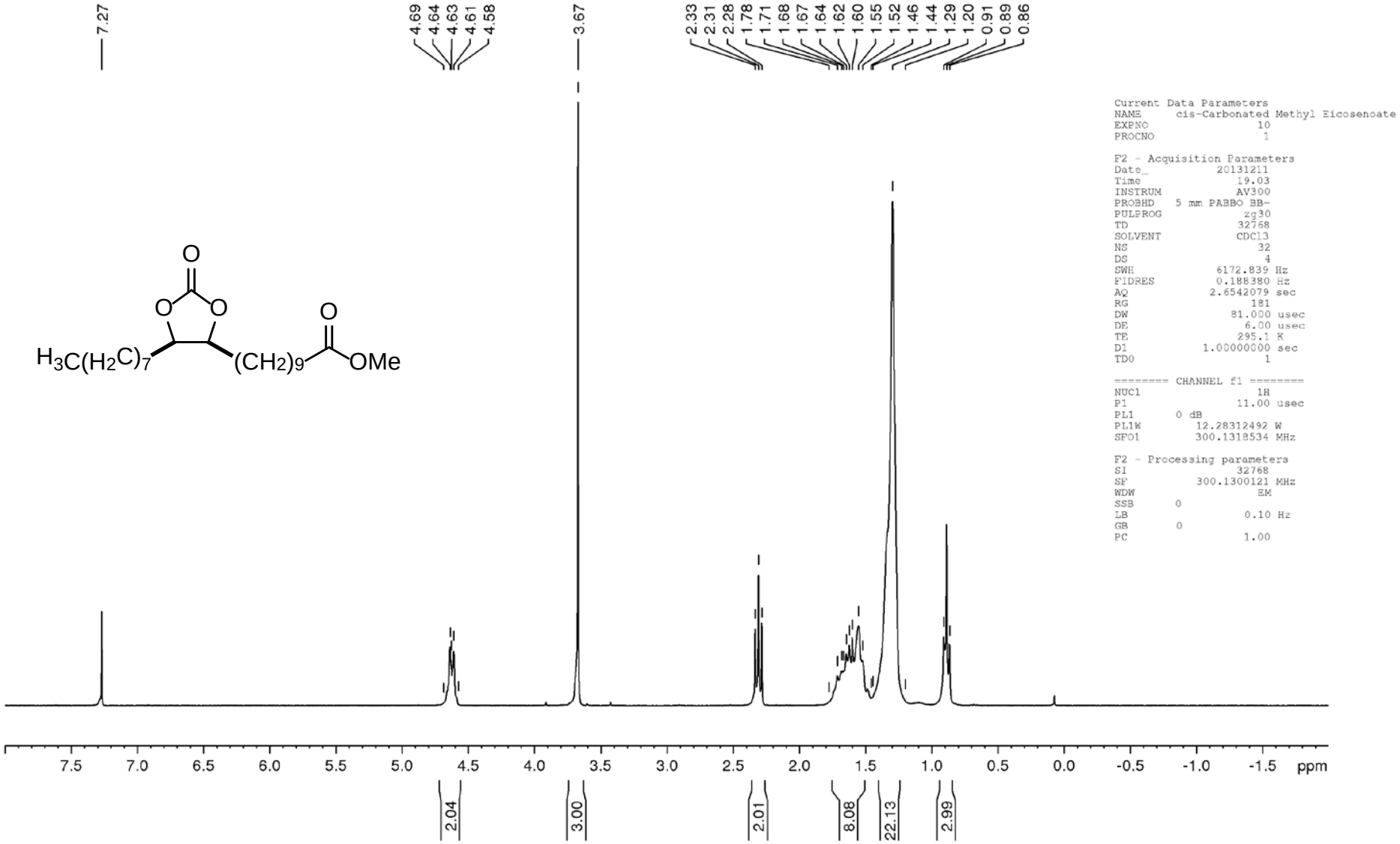
^{1}H NMR *trans-iso*-Octyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3c**)



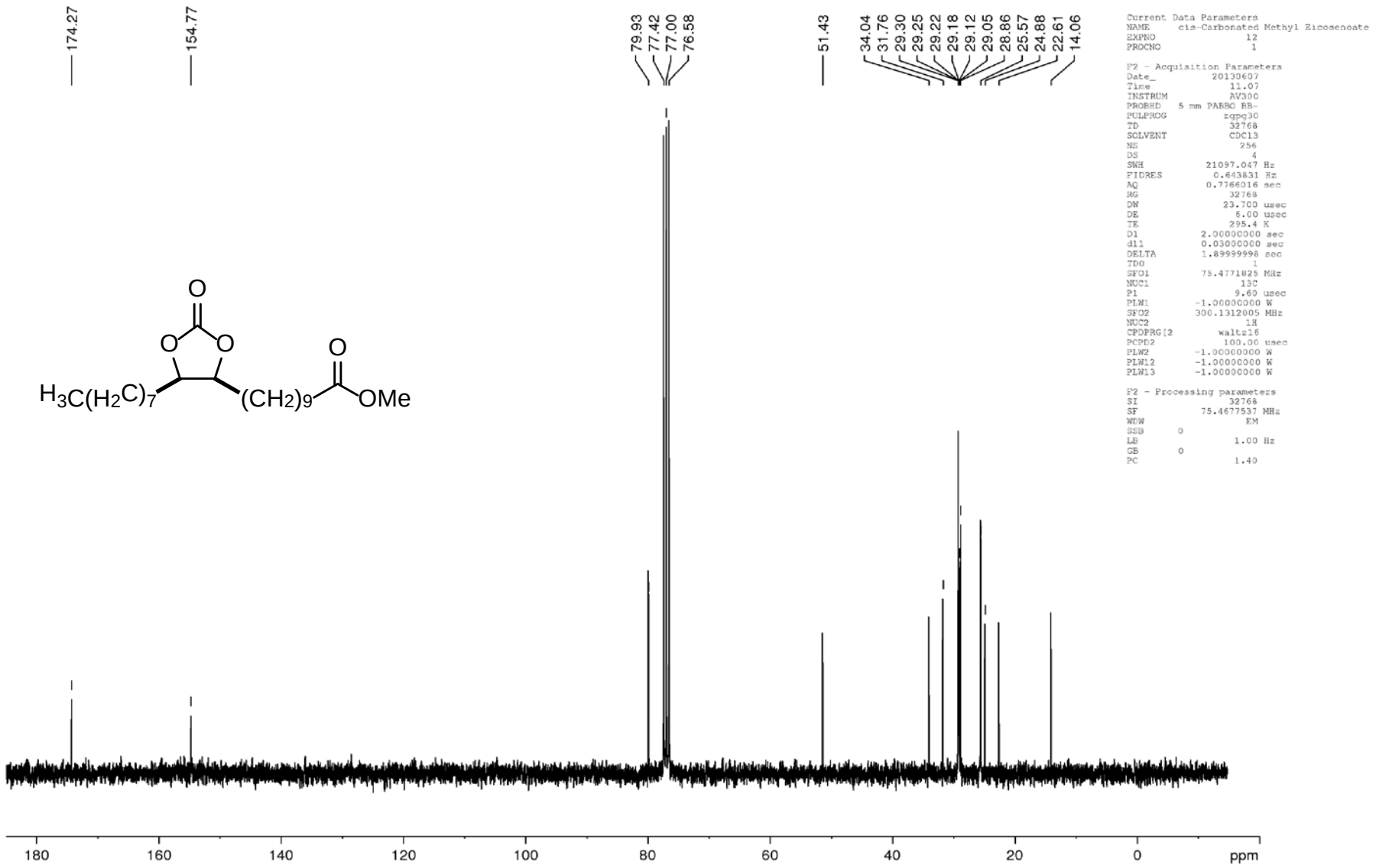
^{13}C NMR *trans-iso*-Octyl 8-(5-octyl-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3c**)



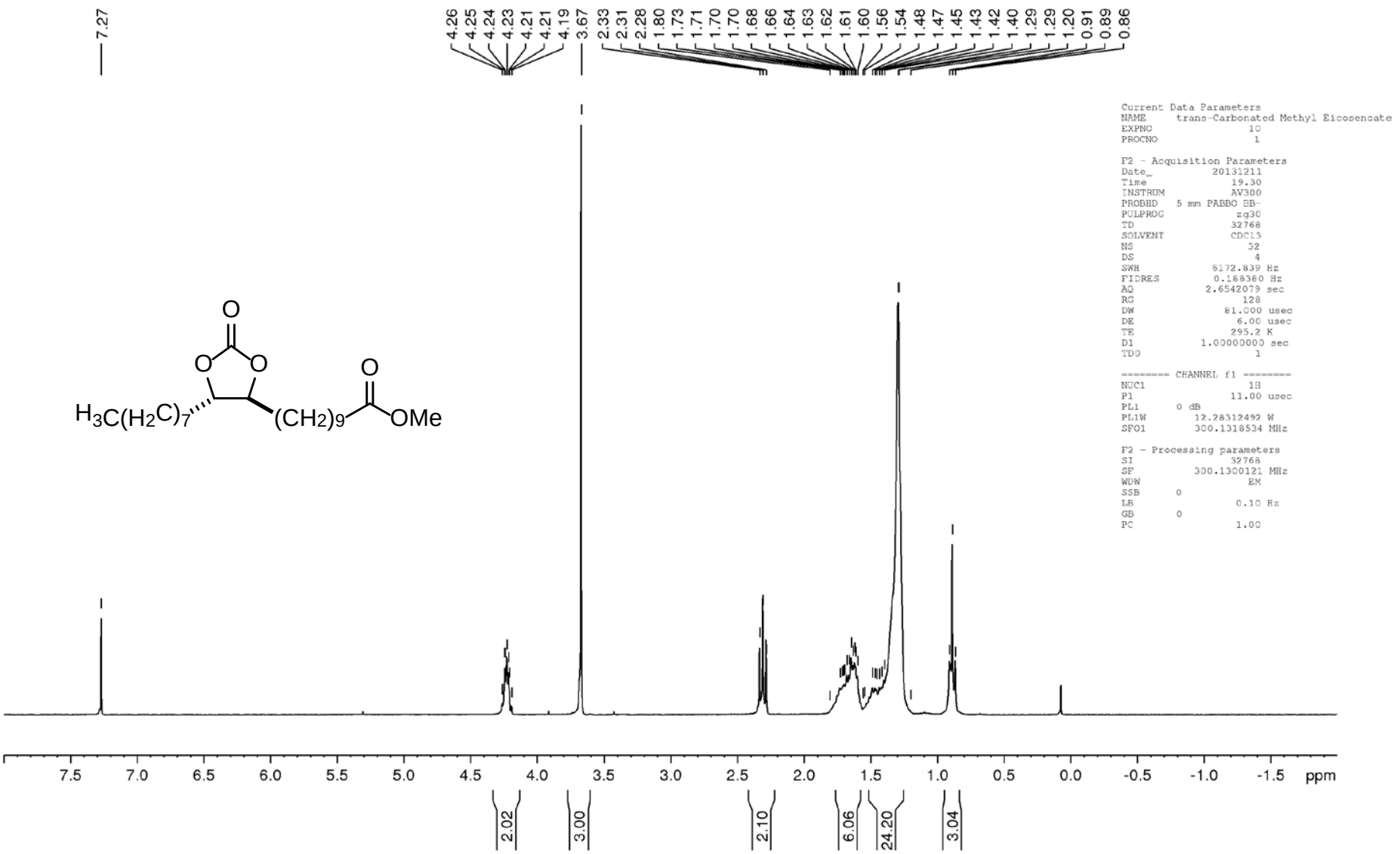
^{1}H NMR *cis*-Methyl 10-(5-octyl-2-oxo-1,3-dioxolan-4-yl)decanoate (*cis*-**3d**)



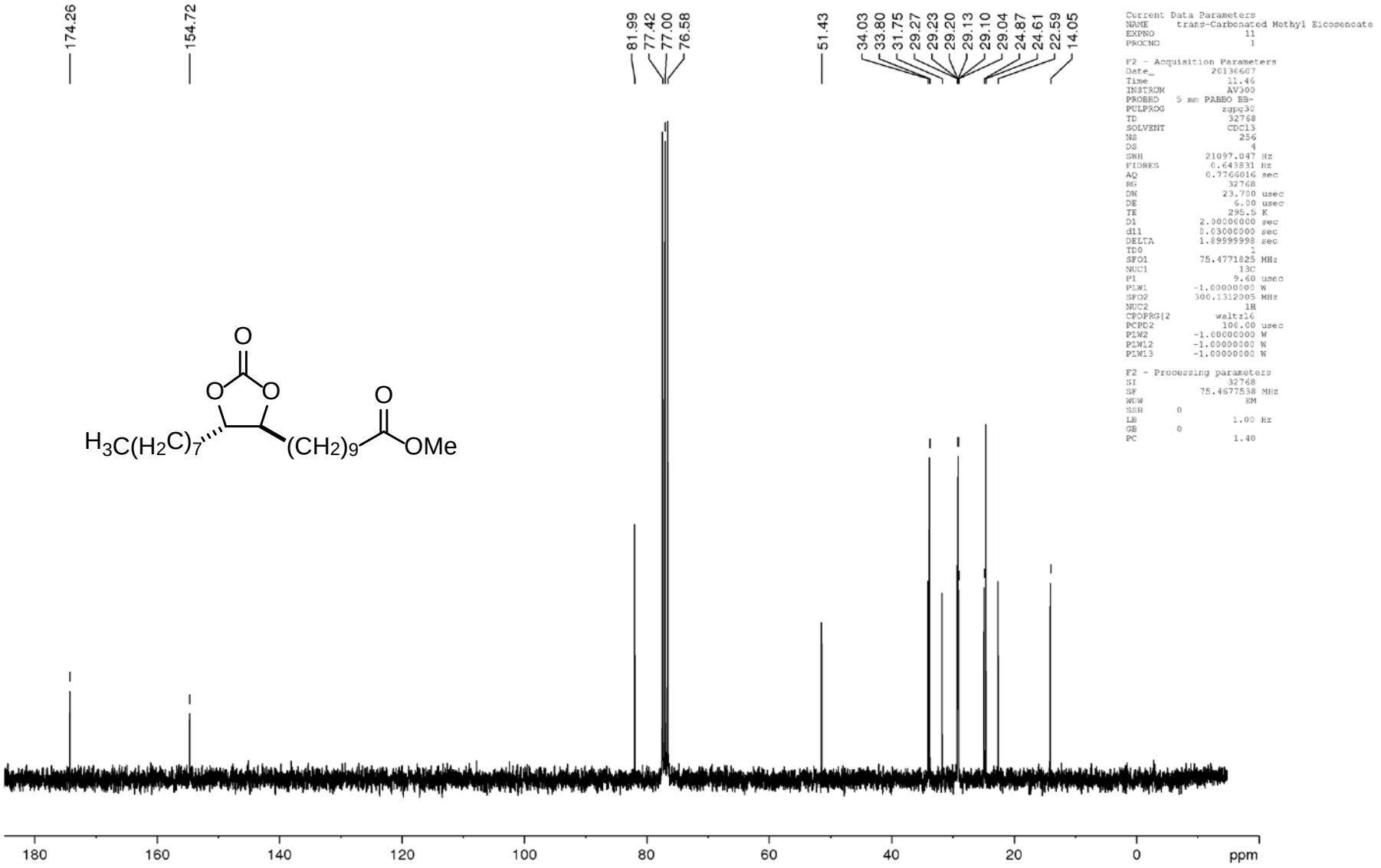
^{13}C NMR *cis*-Methyl 10-(5-octyl-2-oxo-1,3-dioxolan-4-yl)decanoate (*cis*-**3d**)



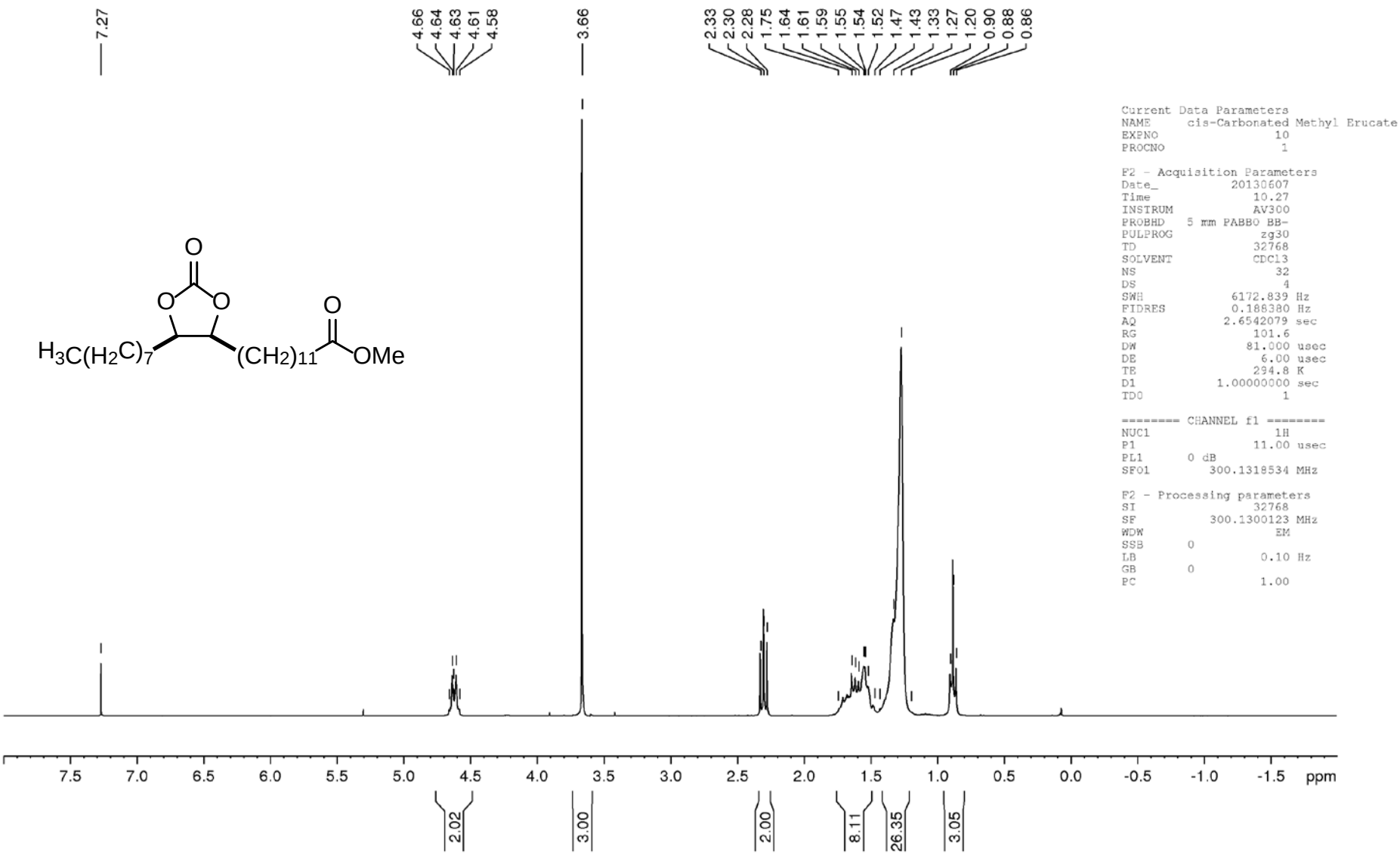
^{1}H NMR *trans*-Methyl 10-(5-octyl-2-oxo-1,3-dioxolan-4-yl)decanoate (*trans*-**3d**)



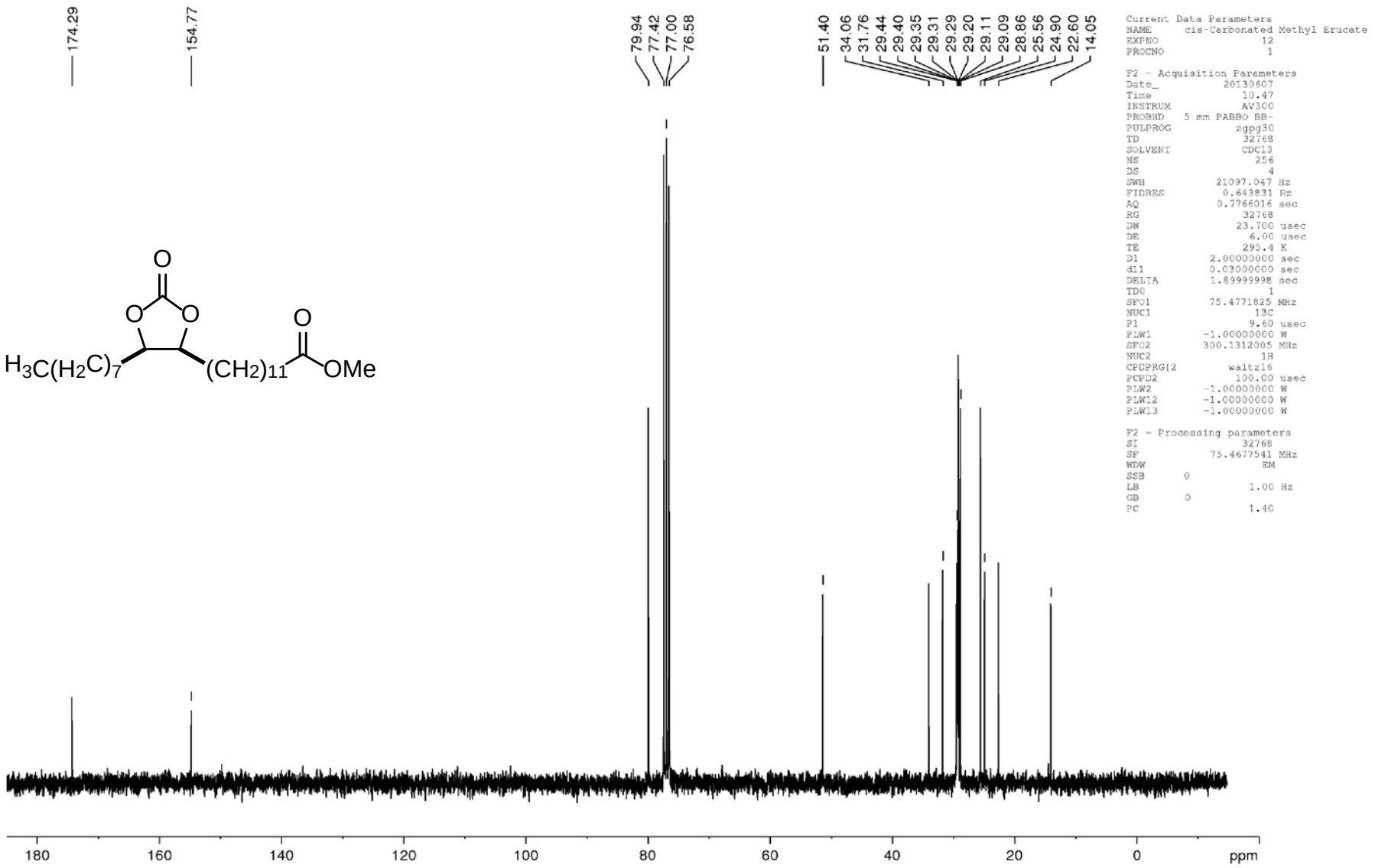
^{13}C NMR *trans*-Methyl 10-(5-octyl-2-oxo-1,3-dioxolan-4-yl)decanoate (*trans*-**3d**)



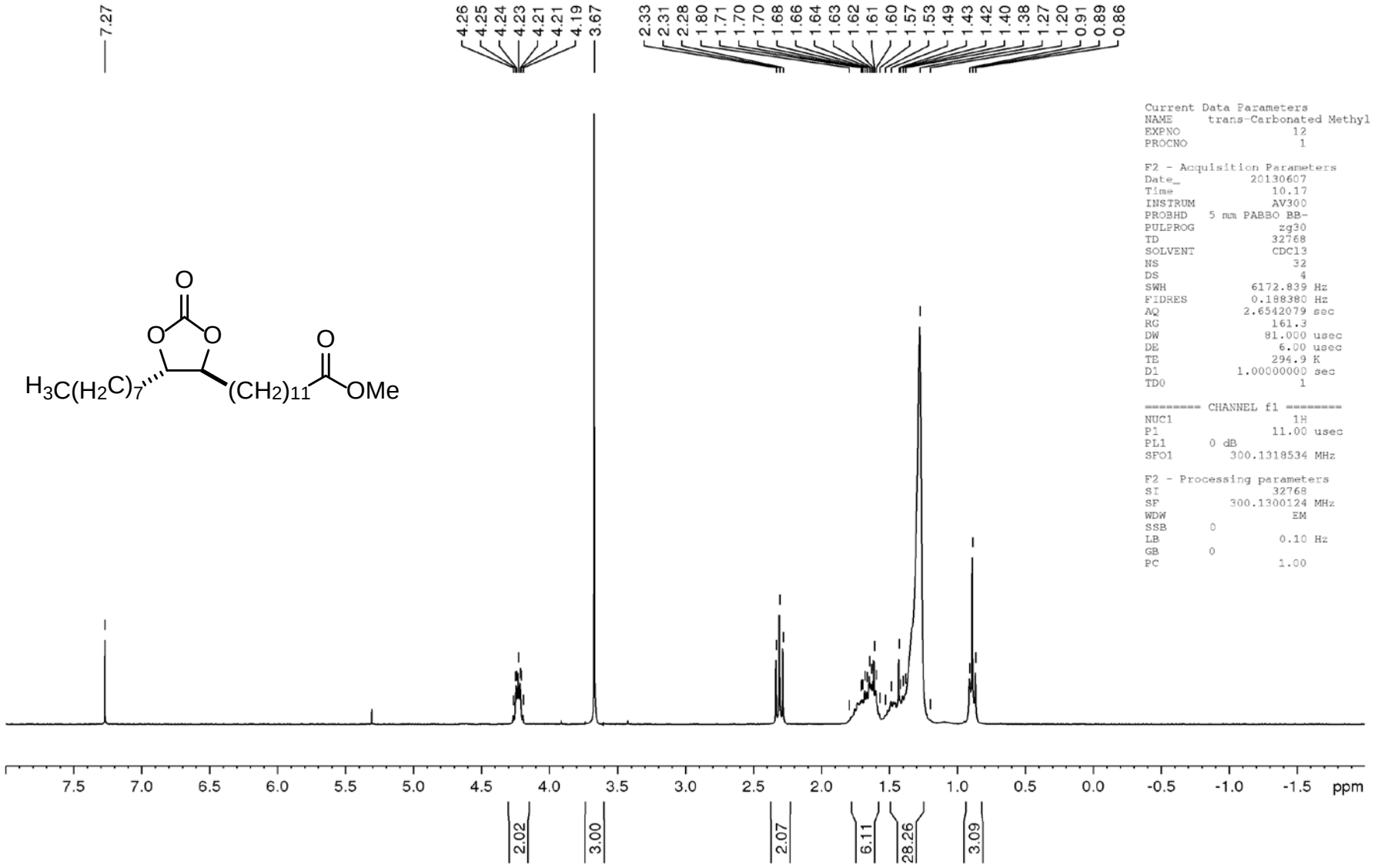
^{1}H NMR *cis*-Methyl 12-(5-octyl-2-oxo-1,3-dioxolan-4-yl)dodecanoate (*cis*-**3e**)



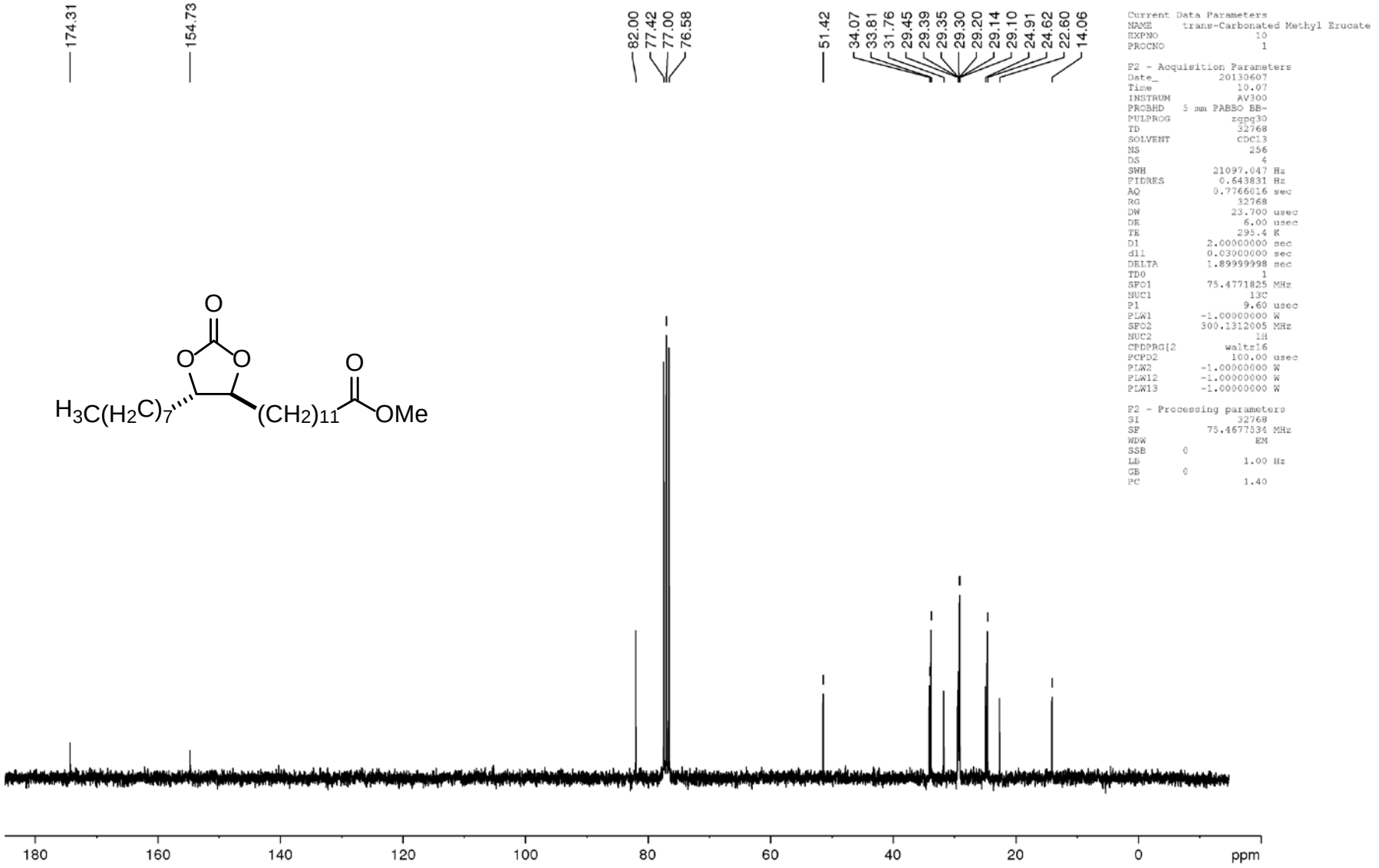
^{13}C NMR *cis*-Methyl 12-(5-octyl-2-oxo-1,3-dioxolan-4-yl)dodecanoate (*cis*-**3e**)



^{1}H NMR *trans*-Methyl 12-(5-octyl-2-oxo-1,3-dioxolan-4-yl)dodecanoate (*trans*-**3e**)

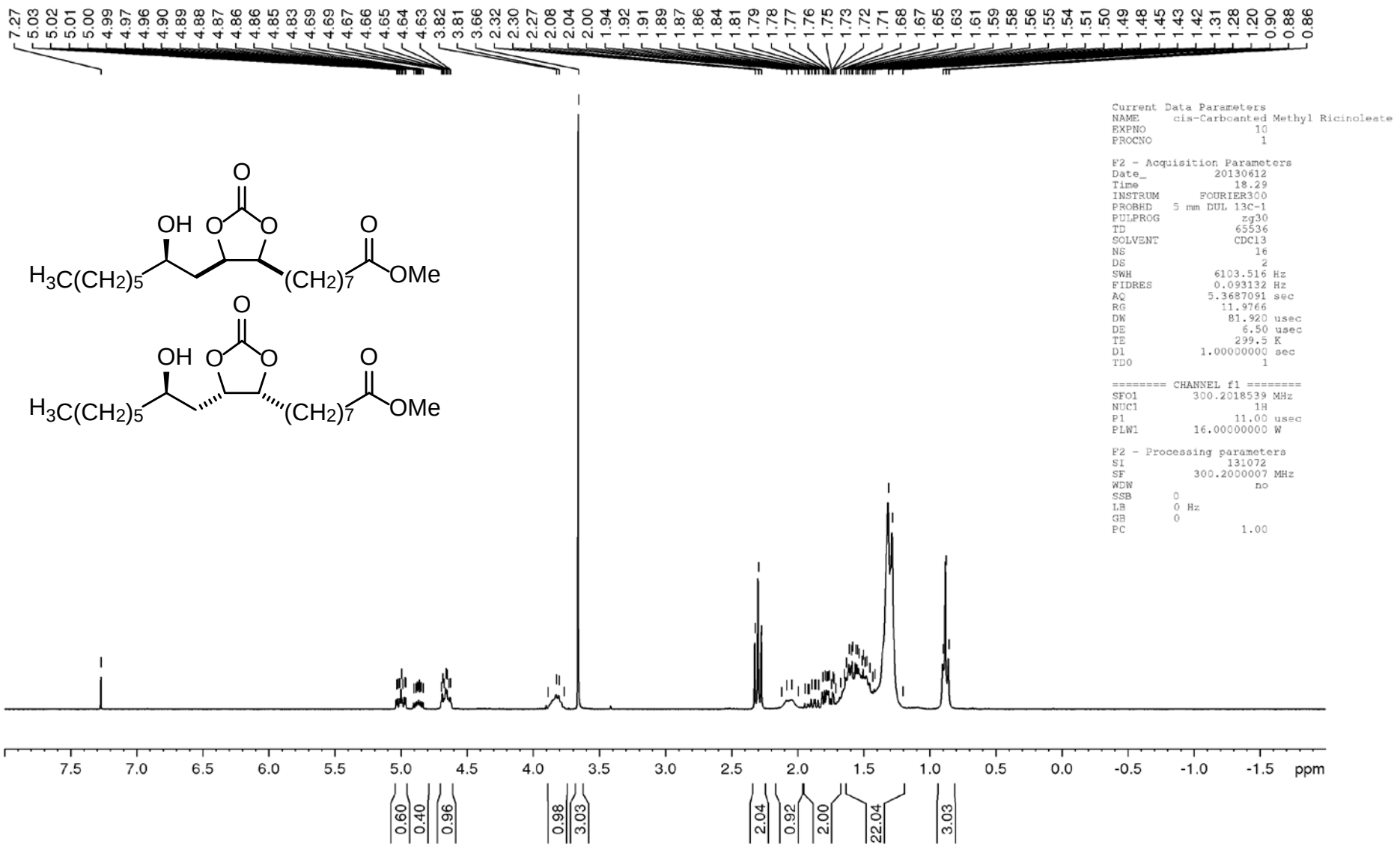


^{13}C NMR *trans*-Methyl 12-(5-octyl-2-oxo-1,3-dioxolan-4-yl)dodecanoate (*trans*-**3e**)

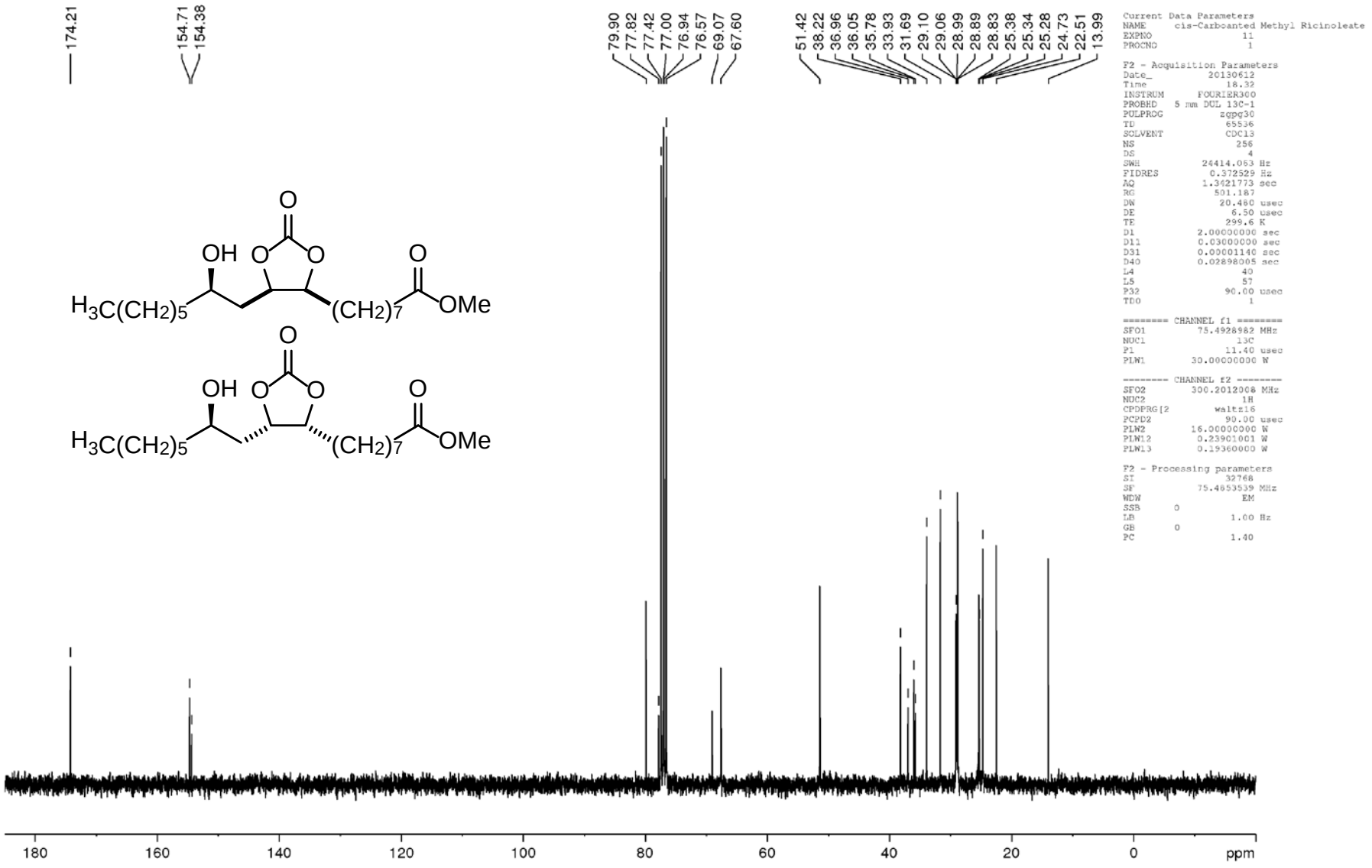



```
Current Data Parameters
NAME      trans-Carbonated Methyl Erucate
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130607
Time              10.07
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           21097.047 Hz
FIDRES        0.643831 Hz
AQ            0.7766016 sec
RG                32768
DW               23.700 usec
DE                6.00 usec
TE               295.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1
SFO1         75.4771825 MHz
NUC1                13C
P1                9.60 usec
PLW1         -1.00000000 W
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2          waltz16
PCPD2            100.00 usec
PLW2         -1.00000000 W
PLW12        -1.00000000 W
PLW13        -1.00000000 W

F2 - Processing parameters
SI                32768
SF           75.4677534 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{1}H NMR *cis*-Methyl 8-(5-((2*R*)-hydroxyoctyl)-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3f**)

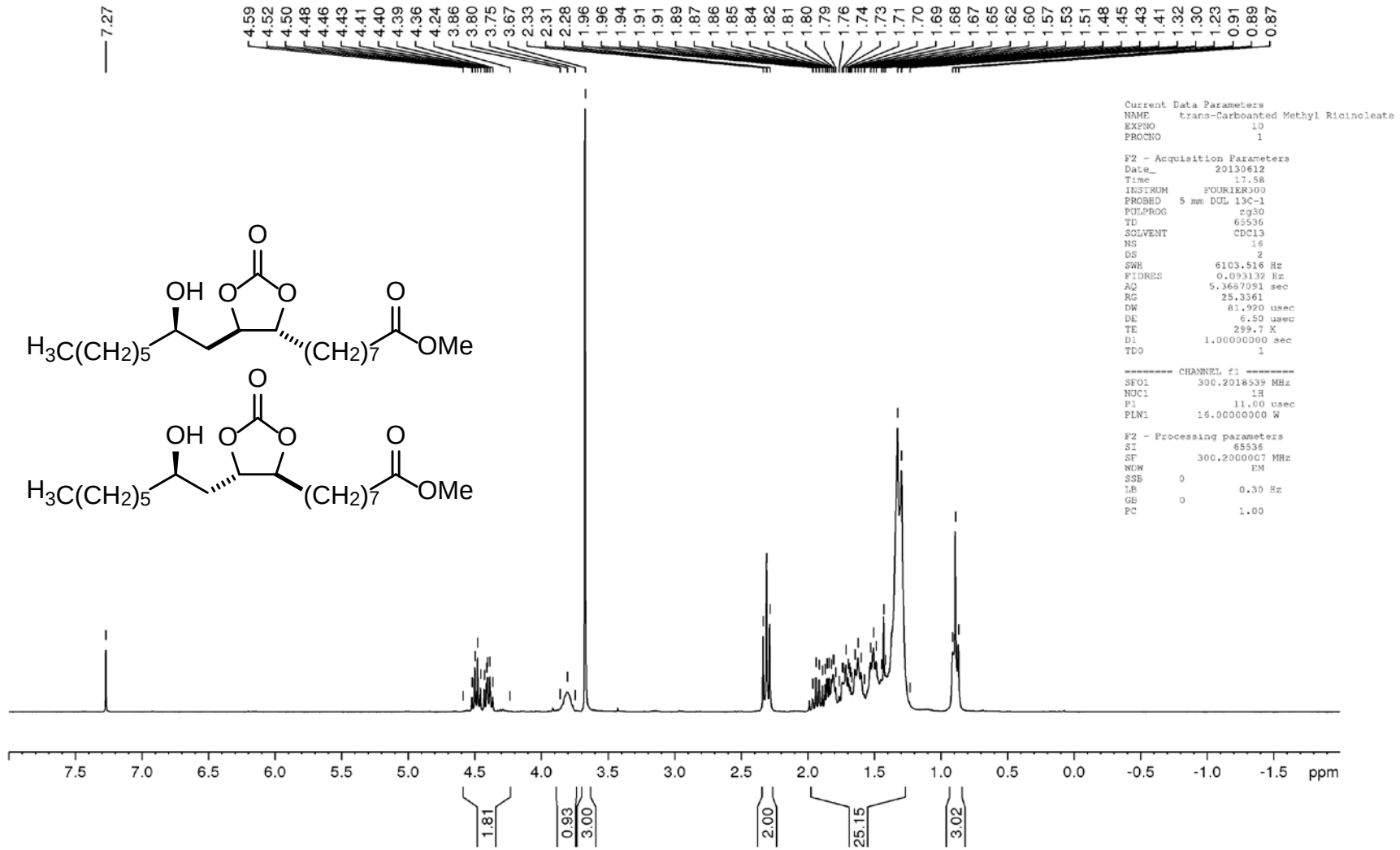


^{13}C NMR *cis*-Methyl 8-(5-((2*R*)-hydroxyoctyl)-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3f**)

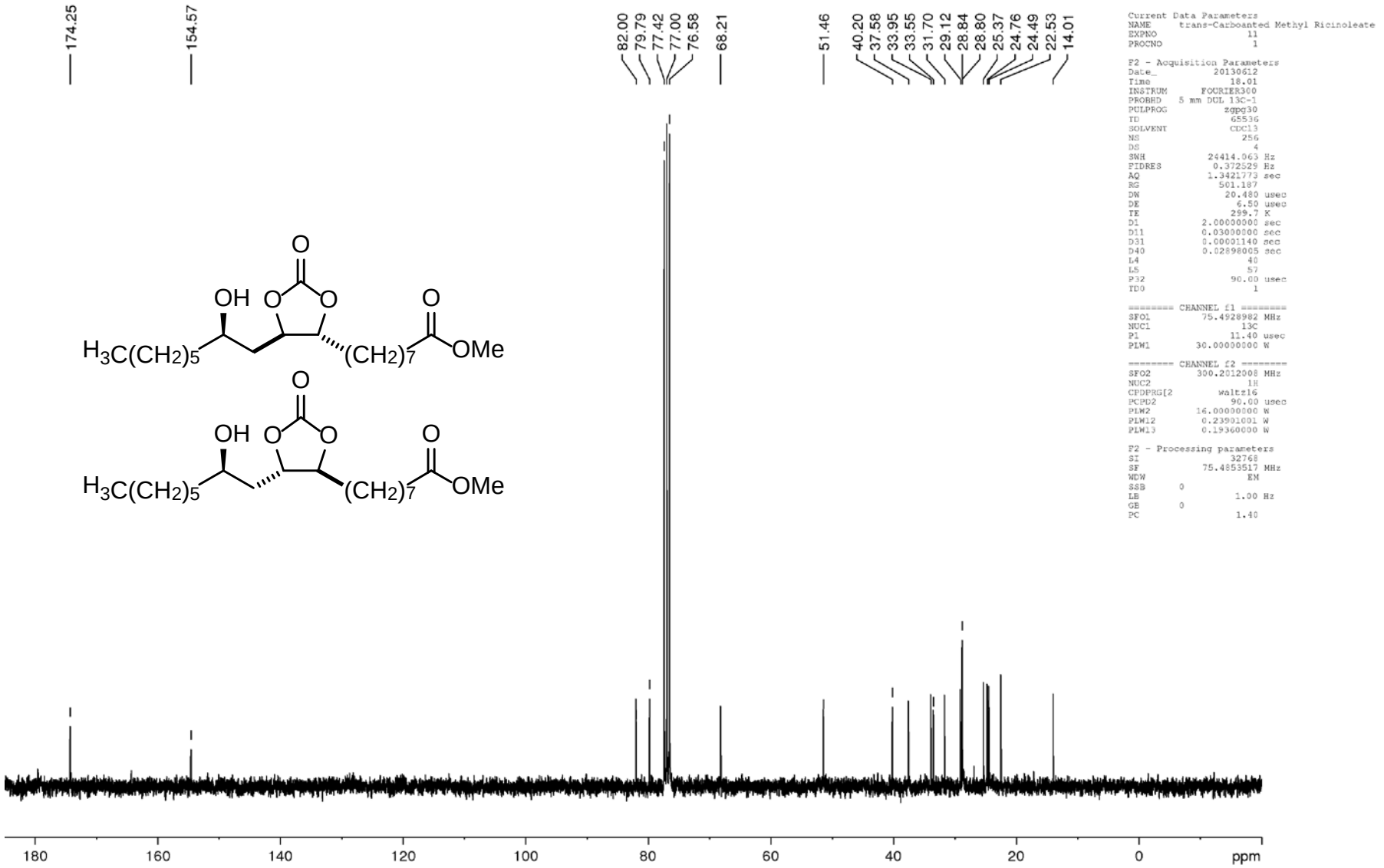



```
Current Data Parameters
NAME      cis-Carboanted Methyl Ricinoleate
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130612
Time              18.32
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24414.063 Hz
FIDRES        0.372529 Hz
AQ            1.3421773 sec
RG              501.187
DW             20.480 usec
DE              6.50 usec
TE              299.6 K
D1            2.00000000 sec
D11           0.03000000 sec
D31           0.00001140 sec
D40           0.02898005 sec
L4                   40
L5                   57
P32             90.00 usec
TD0                   1

======== CHANNEL f1 ========
SFO1          75.4928982 MHz
NUC1                 13C
P1              11.40 usec
PLW1         30.00000000 W

======== CHANNEL f2 ========
SFO2         300.2012008 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2           90.00 usec
PLW2         16.00000000 W
PLW12         0.23901001 W
PLW13         0.19360000 W

F2 - Processing parameters
SI                32768
SF           75.4853539 MHz
WDW                  EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```

^{1}H NMR *trans*-Methyl 8-(5-((2*R*)-hydroxyoctyl)-2-oxo-1,3-dioxolan-4-yl)octanoate (*trans*-**3f**)

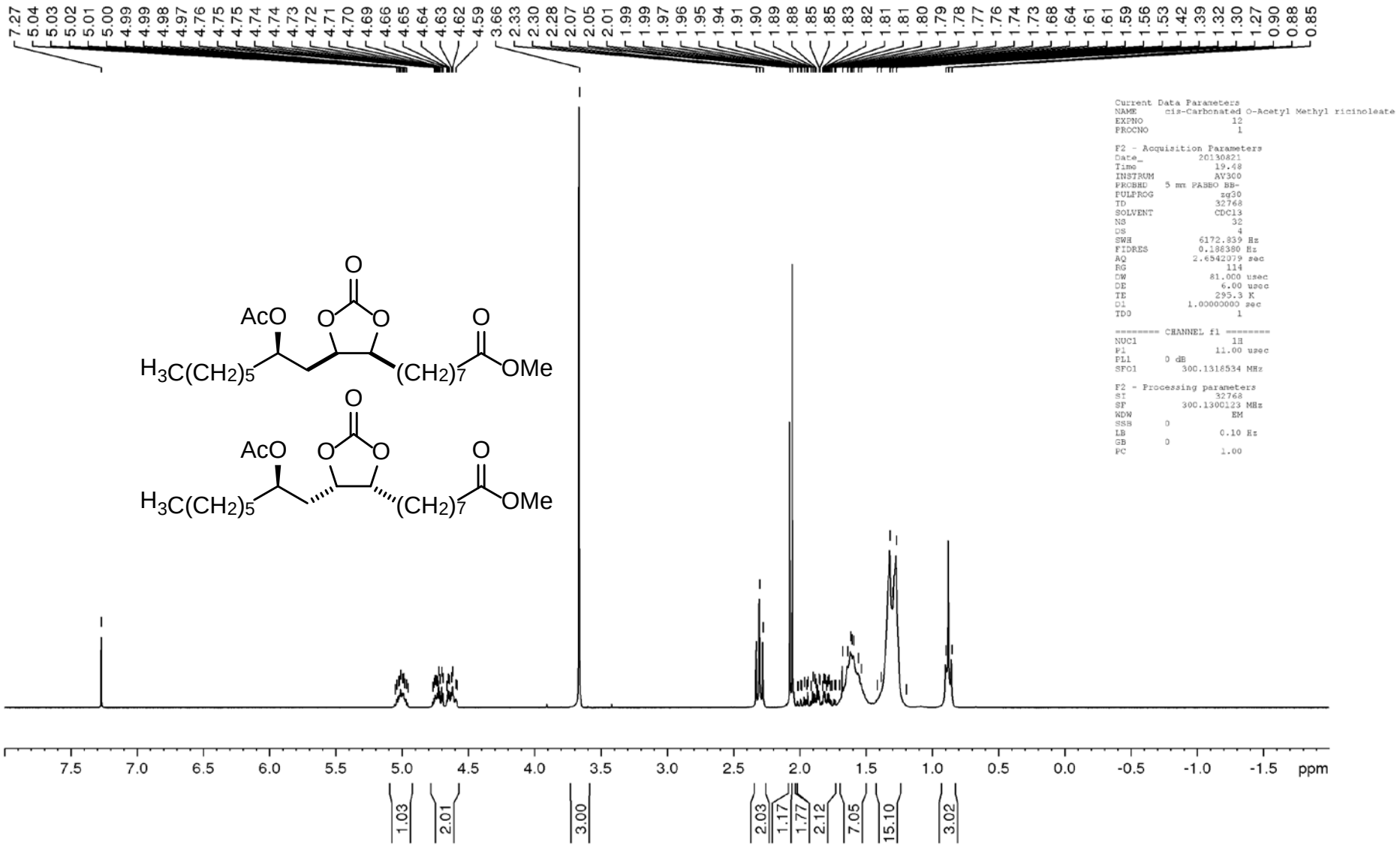


^{13}C NMR *trans*-Methyl 8-(5-((2*R*)-hydroxyoctyl)-2-oxo-1,3-dioxolan-4-yl)octanoate (*trans*-**3f**)

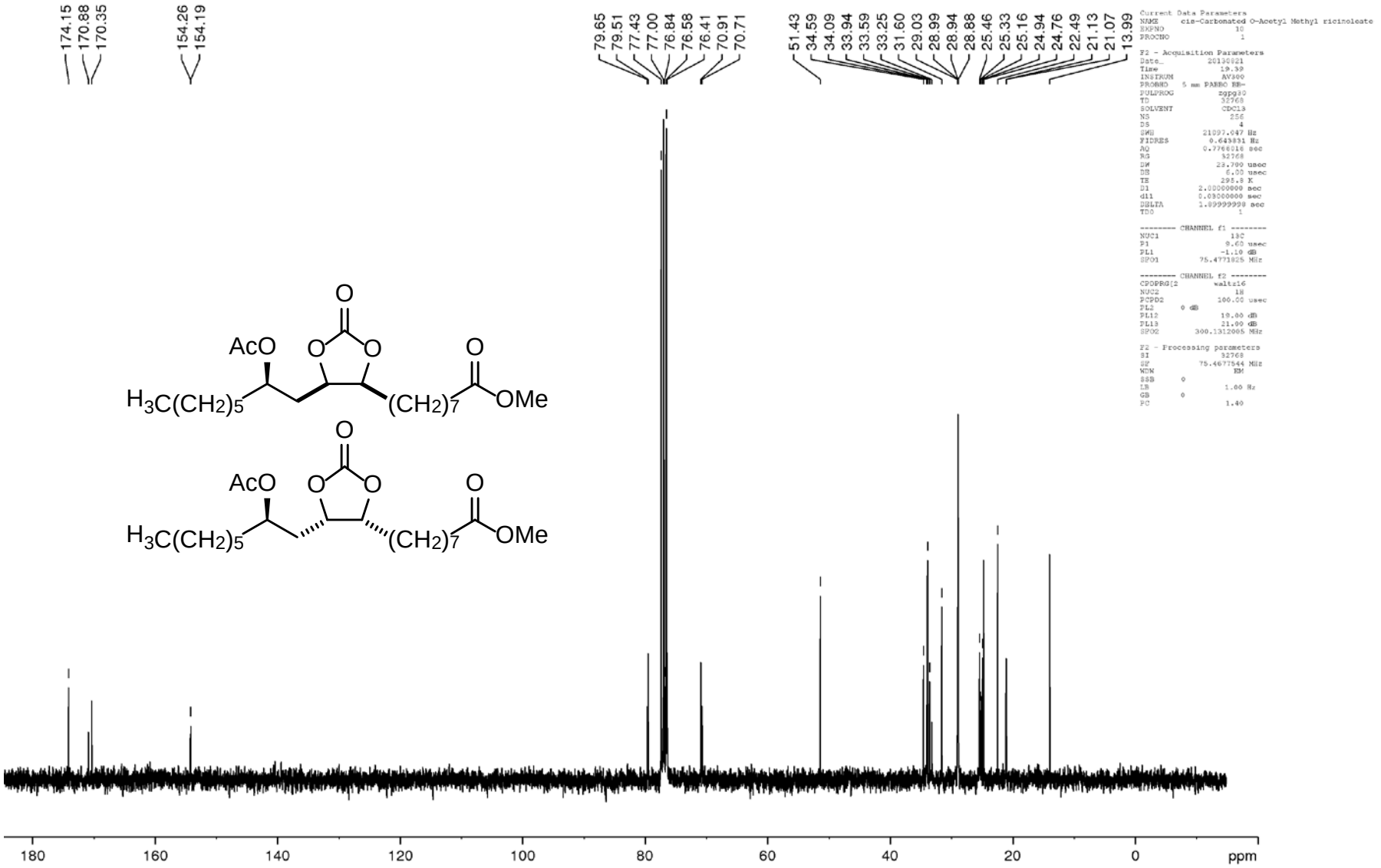



```
Current Data Parameters
NAME      trans-Carboanted Methyl Ricinoleate
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130612
Time              18.01
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24414.063 Hz
FIDRES        0.372529 Hz
AQ            1.3421773 sec
RG              501.187
DW               20.480 usec
DE                6.50 usec
TE              299.7 K
D1            2.00000000 sec
D11           0.03000000 sec
D31           0.00001140 sec
D40           0.02898005 sec
L4                   40
L5                   57
P32               90.00 usec
TD0                   1

======== CHANNEL f1 ========
SFO1          75.4928982 MHz
NUC1              13C
P1                11.40 usec
PLW1        30.00000000 W

======== CHANNEL f2 ========
SFO2         300.2012008 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        16.00000000 W
PLW12        0.23901001 W
PLW13        0.19360000 W

F2 - Processing parameters
SI                32768
SF           75.4853517 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

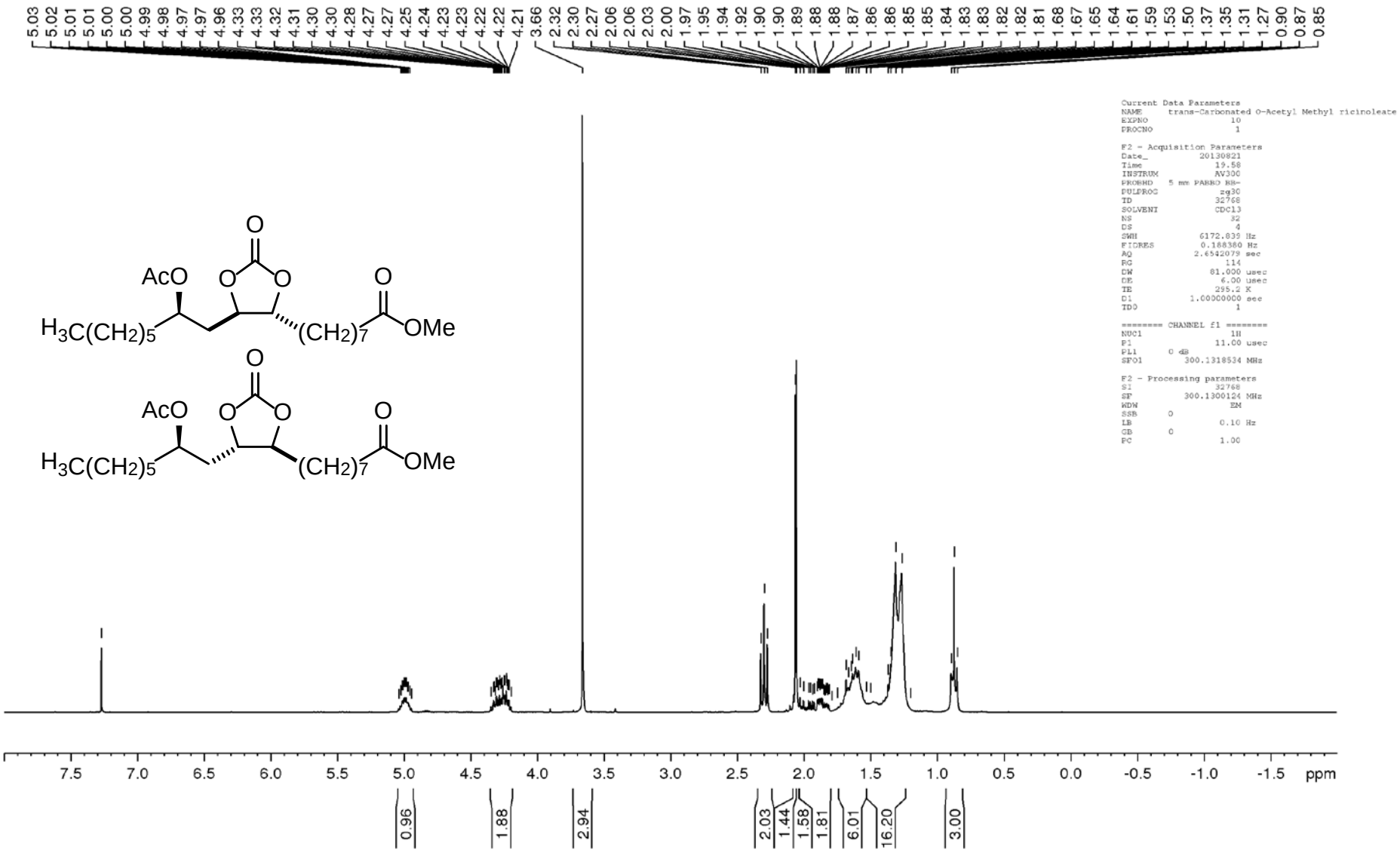
^{1}H NMR *cis* Methyl 8-(5-((2*R*)-acetoxyoctyl)-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3g**)



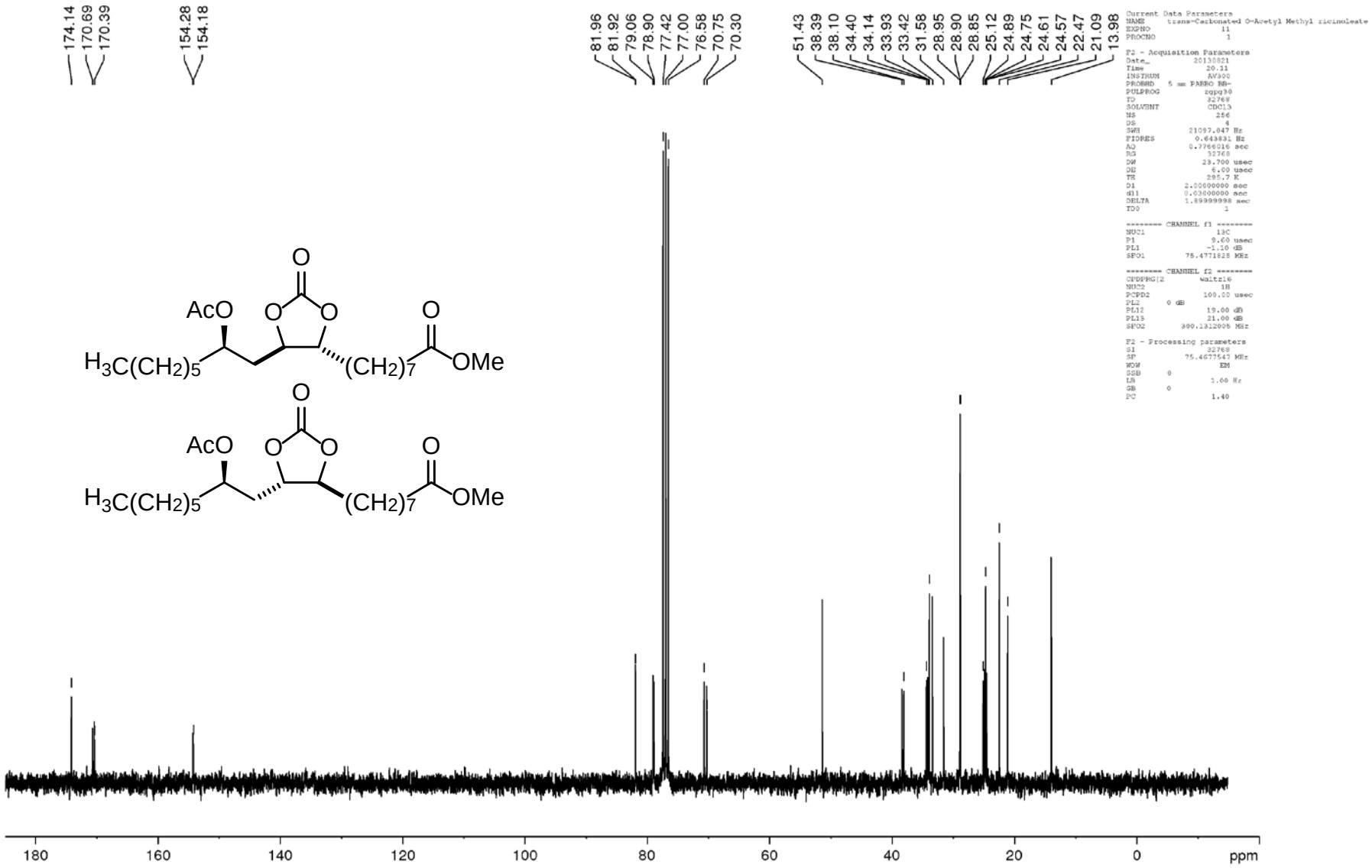
^{13}C NMR *cis*-Methyl 8-(5-((2*R*)-acetoxyoctyl)-2-oxo-1,3-dioxolan-4-yl)octanoate (*cis*-**3g**)



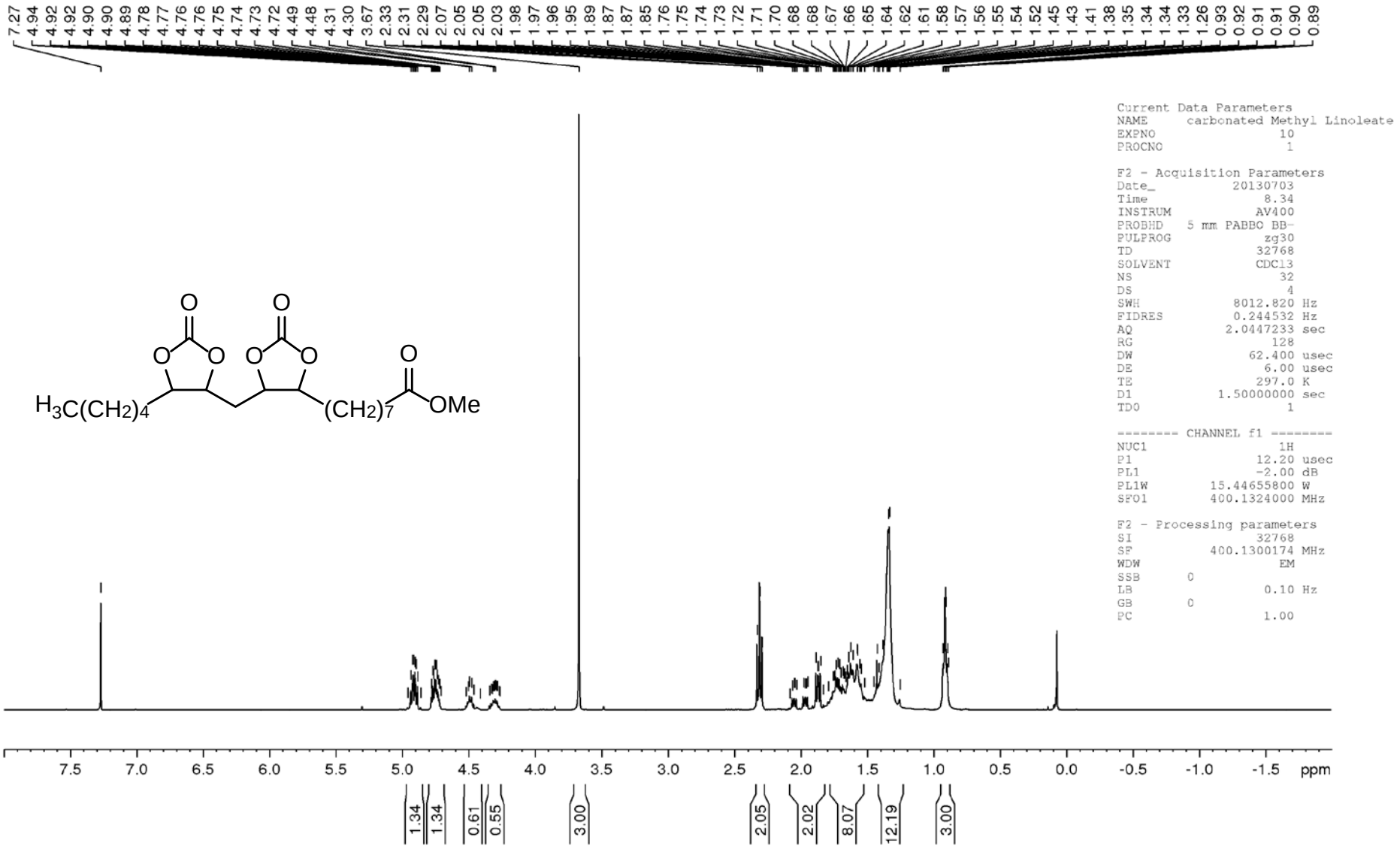
^{1}H NMR *trans*-Methyl 8-(5-((2*R*)-acetoxyoctyl)-2-oxo-1,3-dioxolan-4-yl)octanoate (*trans*-**3g**)



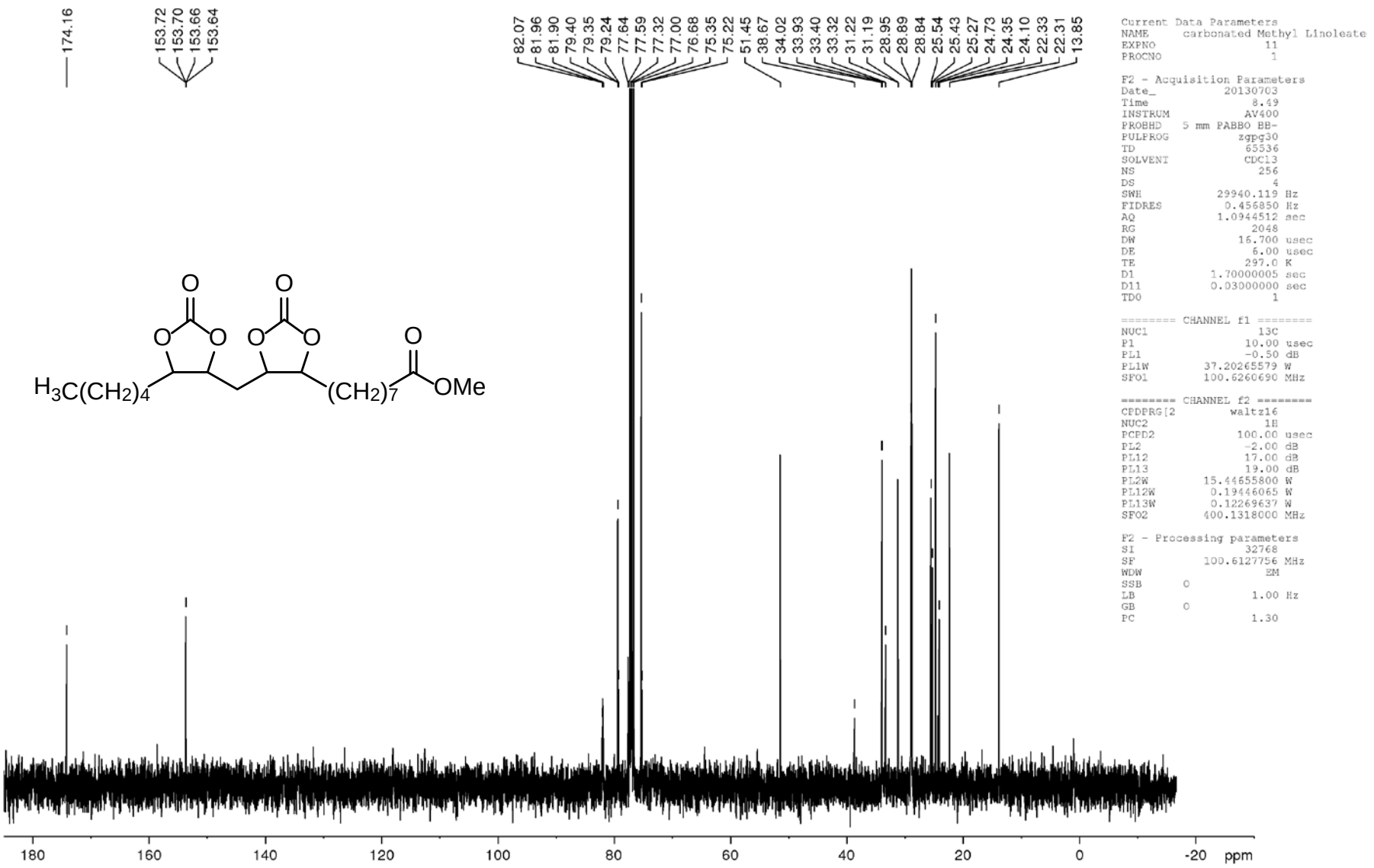
^{13}C NMR *trans*-Methyl 8-(5-((2R)-acetoxyoctyl)-2-oxo-1,3-dioxolan-4-yl)octanoate (*trans*-**3g**)



^{1}H NMR Methyl 8-(2-oxo-5-((2-oxo-5-pentyl-1,3-dioxolan-4-yl)methyl)-1,3-dioxolan-4-yl)octanoate (**3g**)



^{13}C NMR Methyl 8-(2-oxo-5-((2-oxo-5-pentyl-1,3-dioxolan-4-yl)methyl)-1,3-dioxolan-4-yl)octanoate (**3g**)




```
Current Data Parameters
NAME      carbonated Methyl Linoleate
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_              20130703
Time                  8.49
INSTRUM             AV400
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      4
SWH             29940.119 Hz
FIDRES          0.456850 Hz
AQ              1.0944512 sec
RG                   2048
DW                 16.700 usec
DE                  6.00 usec
TE                 297.0 K
D1            1.70000005 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                -0.50 dB
PL1W         37.20265579 W
SFO1        100.6260690 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 -2.00 dB
PL12                17.00 dB
PL13                19.00 dB
PL2W         15.44655800 W
PL12W         0.19446065 W
PL13W         0.12269637 W
SFO2        400.1318000 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127756 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.30
```

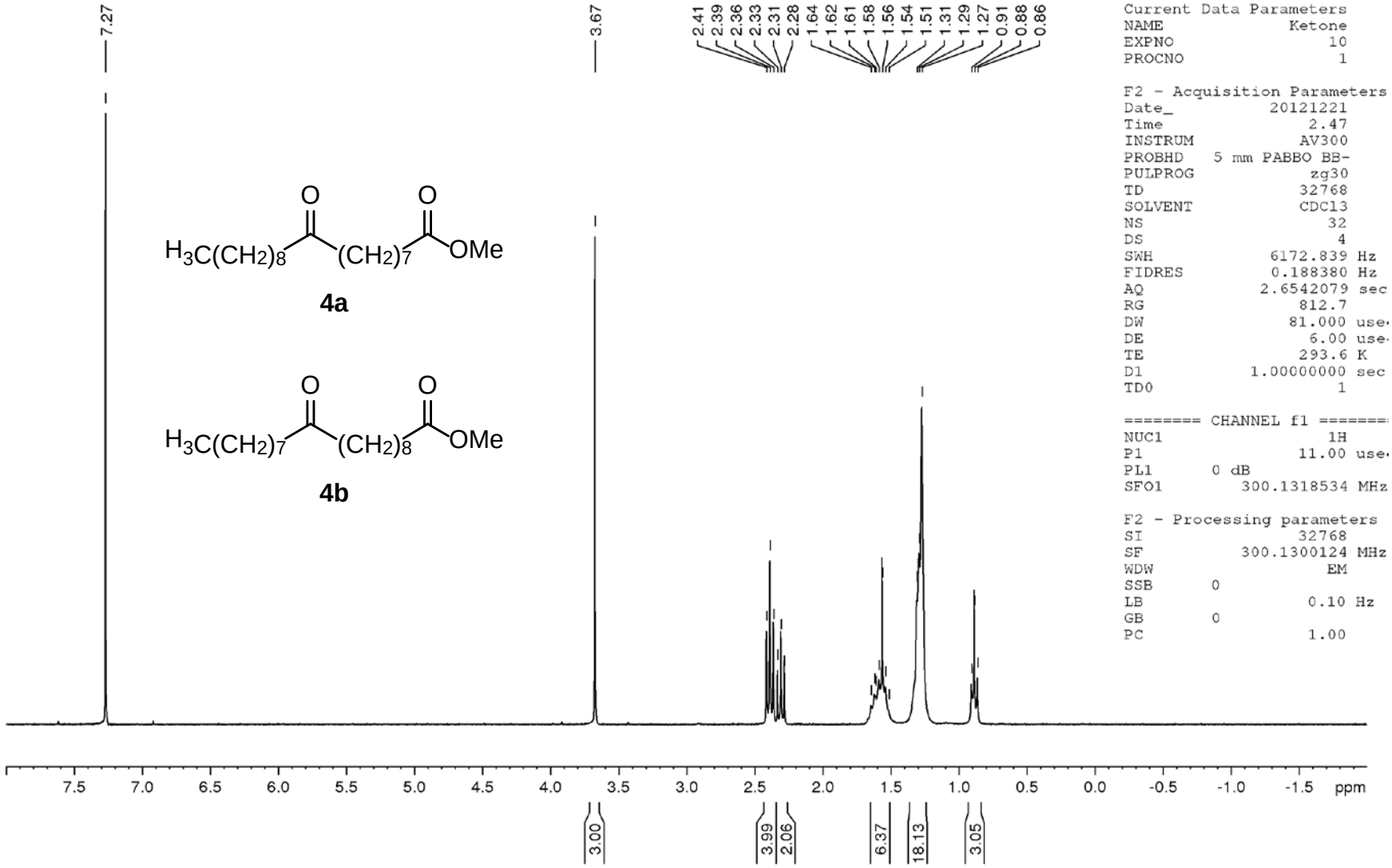
4. Analytic data of by-products

Methyl 9-oxooctadecanoate (**4a**)[9] and Methyl 10-oxooctadecanoate (**4b**)[10]

The formation of ketone **4a** and **4b**, respectively was observed in varying amounts during the conversion of *cis*-**2a** and CO_2 while screening of catalyst and co-catalyst as well evaluation of the reaction conditions.

As a mixture of isomers **4a**:**4b**= 50:50; R_f (*c*Hex:EtOAc= 1:1)= 0.74; ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ= 0.88 (t, $^3J_{H,H}$ = 6.7 Hz, 3H), 1.27-1.31 (m, 18H), 1.51-1.64 (m, 6H), 2.31 (t, $^3J_{H,H}$ = 7.5 Hz, 2H), 2.39 (t, $^3J_{H,H}$ = 7.5 Hz, 4H), 3.67 (s, 3H) ppm; $^{13}C\{^1H\}$ NMR (75 MHz, $CDCl_3$, 22 °C): δ= 14.05 (CH_3), 22.62 (CH_2), 23.69 (CH_2) , 23.76 (CH_2) , 23.83 (CH_2) 24.81 (CH_2), 24.85 (CH_2), 28.89 (CH_2), 28.99 (CH_2), 29.02 (CH_2), 29.10 (CH_2), 29.12 (CH_2), 29.16 (CH_2), 29.22 (CH_2), 29.33 (CH_2), 29.38 (CH_2), 31.77 (CH_2), 31.81 (CH_2), 33.99 (CH_2), 34.01 (CH_2), 42.66 (CH_2), 42.70 (CH_2), 42.79 (CH_2), 51.40 (OCH_3), 174.19 (C=O), 174.23 (C=O), 211.55 (C=O, isomer **4b**), 211.62 (C=O, isomer **4a**);[7] MS (EI): *m/z* (%): 312 (1), 281 (16), 214 (13), 207 (18), 200 (22), 185 (19), 170 (23), 168 (16), 164 (9), 158 (16), 157 (28) 156 (33), 155 (21), 153 (11), 144 (11), 143 (33) 142 (21), 141 (20), 140 (18), 139 (15), 153 (11), 130 (11), 125 (51), 111 (35), 97 (45), 95 (20), 83 (43), 71 (79), 69 (41), 55 (100), 43 (78), 41 (54).

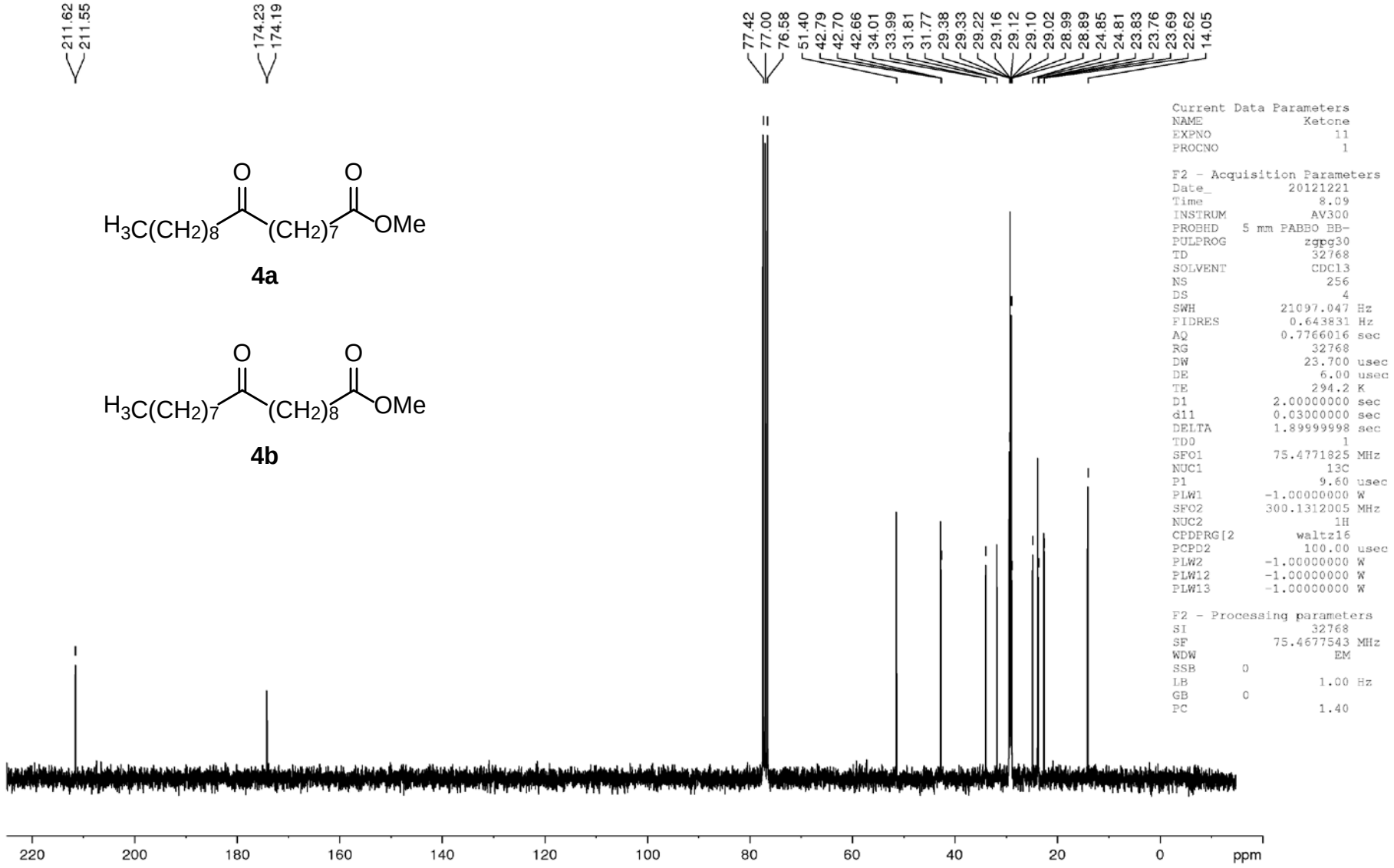
^{1}H NMR Methyl 9-oxooctadecanoate (**4a**) and Methyl 10-oxoocta-decanoate (**4b**)



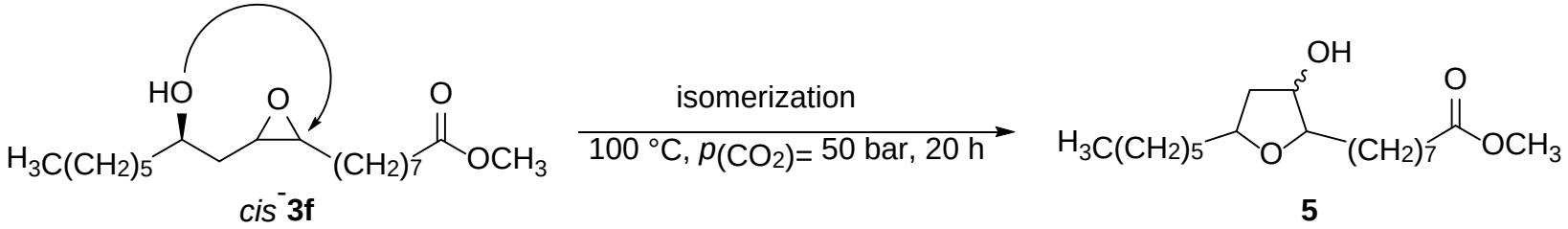
4a

4b

^{13}C-NMR Methyl 9-oxooctadecanoate (**4a**) and Methyl 10-oxooctadecanoate (**4b**)



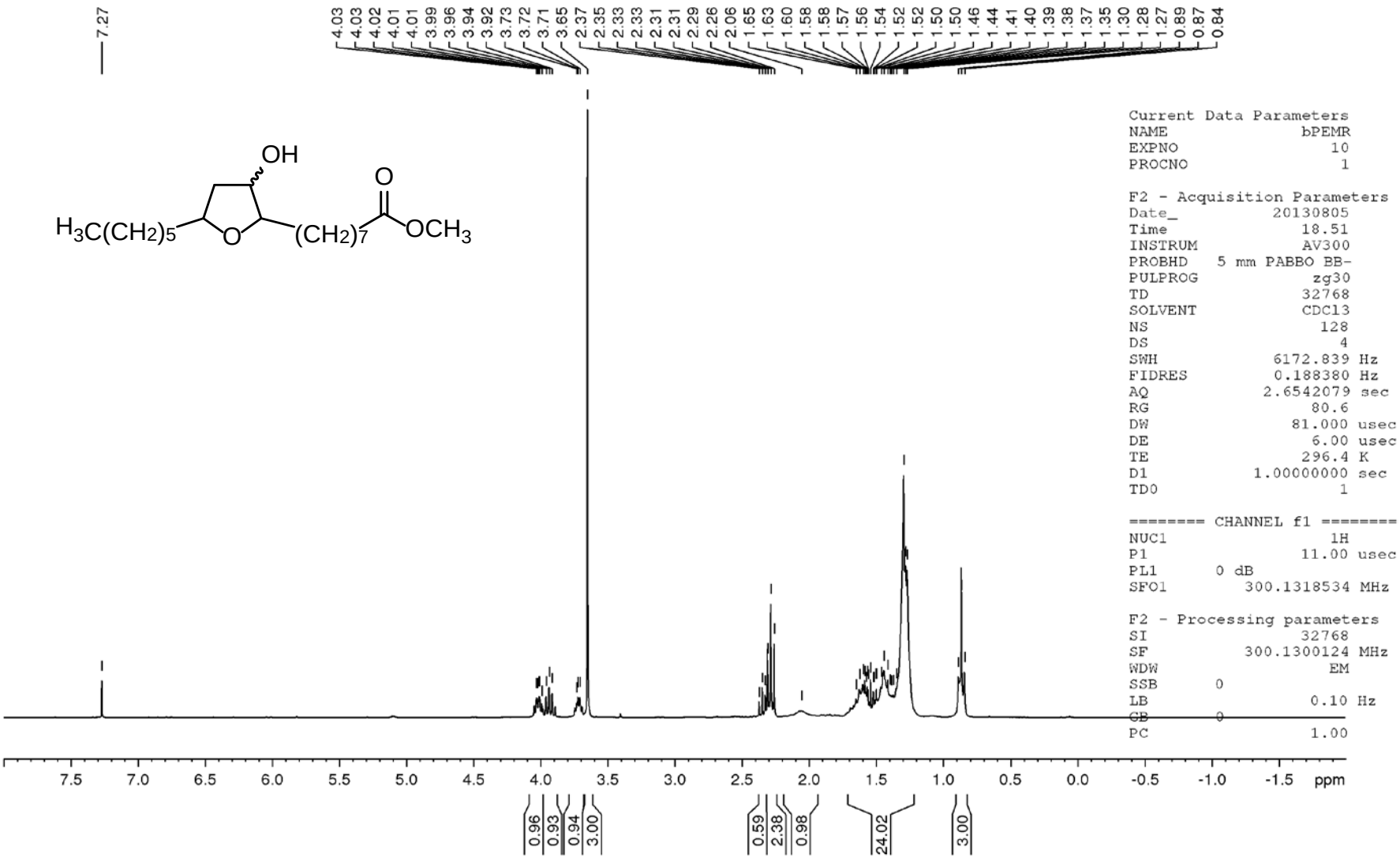
Methyl 8-(5-hexyl-3-hydroxytetrahydrofuran-2-yl)octanoate (**5**)



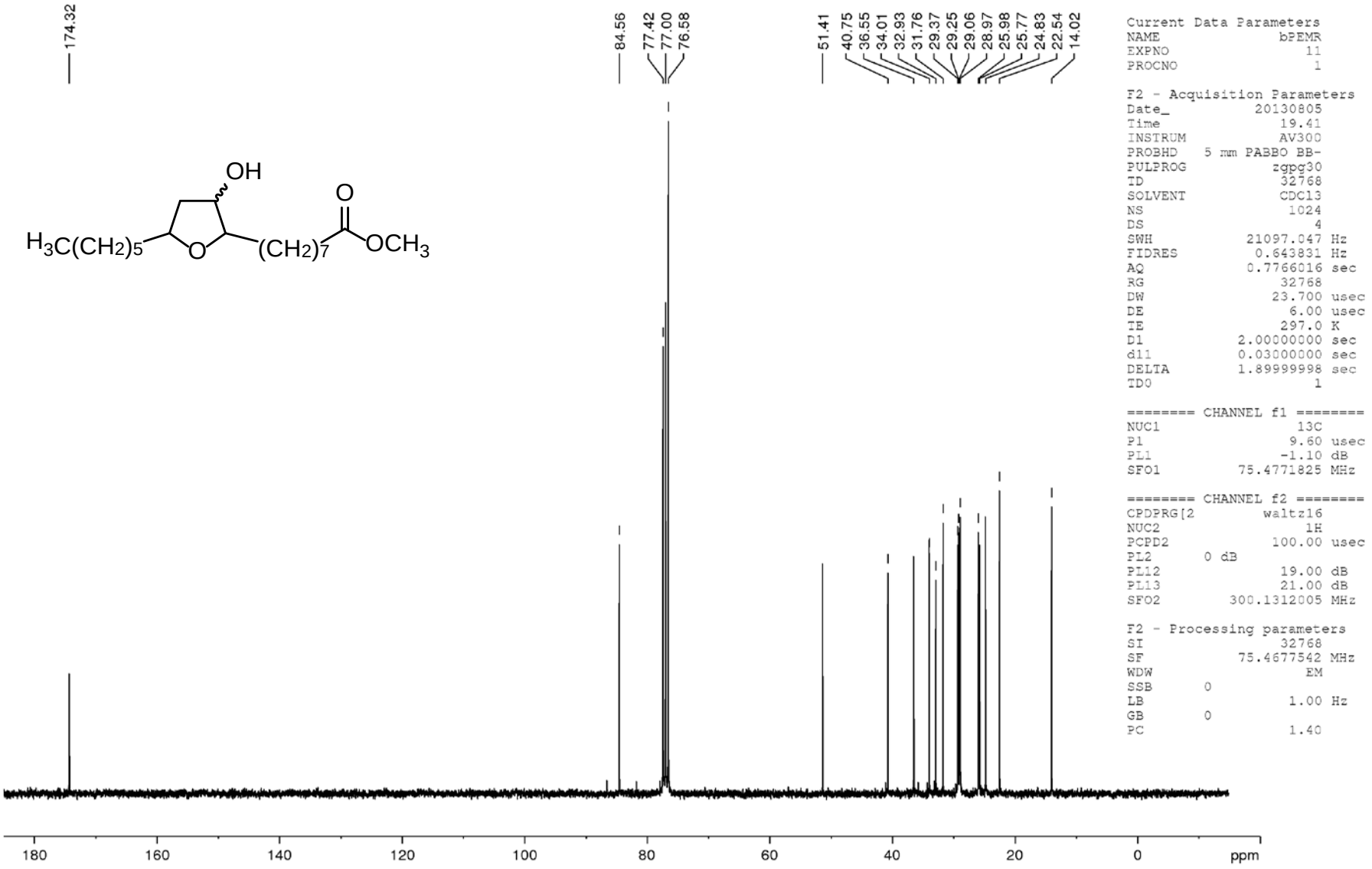
cis-**3f** **5**

5: As a mixture of diastereoisomers (*dr*=50:50); R_f (*c*Hex:EtOAc= 5:1)= 0.35; ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ= 0.87 (t, $^{3}J_{H,H}$ = 6.8 Hz, 3H), 1.27-1.73 (m, 24H), 2.06 (s, br., 1H), 2.26–2.37 (m, 3H), 3.65 (s, 3H), 3.69–3.75 (m, 1H), 3.89–3.98 (m, 1H), 3.99–4.05 (m, 1H) ppm; $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 22 °C): δ= 14.02 (CH_3), 22.54 (CH_2), 24.83 (CH_2), 25.77 (CH_2), 25.98 (CH_2), 28.97 (CH_2), 29.06 (CH_2), 29.25 (CH_2), 29.37 (CH_2), 31.76 (CH_2), 32.93 (CH_2), 34.01 (CH_2), 36.55 (CH_2), 40.75 (CH_2), 51.41 (OCH_3), 76.57 (CH), 77.02 (CH), 84.55 (CH), 174.32 (C=O); MS (EI): *m/z* (%): 310 (2), 294 (1), 279 (3), 225 (24), 193 (11), 187 (43), 156 (10), 155 (100), 109 (16), 95 (10), 81 (12), 69 (11), 67 (13), 57 (18), 55 (21), 43 (12), 41 (11).

^{1}H NMR Methyl 8-(5-hexyl-3-hydroxytetrahydrofuran-2-yl)octanoate (**5**)



^{13}C NMR Methyl 8-(5-hexyl-3-hydroxytetrahydrofuran-2-yl)octanoate (**5**)




```
Current Data Parameters
NAME                  bPEMR
EXPNO                    11
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130805
Time                  19.41
INSTRUM               AV300
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              21097.047 Hz
FIDRES            0.643831 Hz
AQ               0.7766016 sec
RG                    32768
DW                23.700 usec
DE                 6.00 usec
TE                 297.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.60 usec
PL1                 -1.10 dB
SFO1            75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2              100.00 usec
PL2        0 dB
PL12                19.00 dB
PL13                21.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF              75.4677542 MHz
WDW                      EM
SSB        0
LB                   1.00 Hz
GB         0
PC                   1.40
```

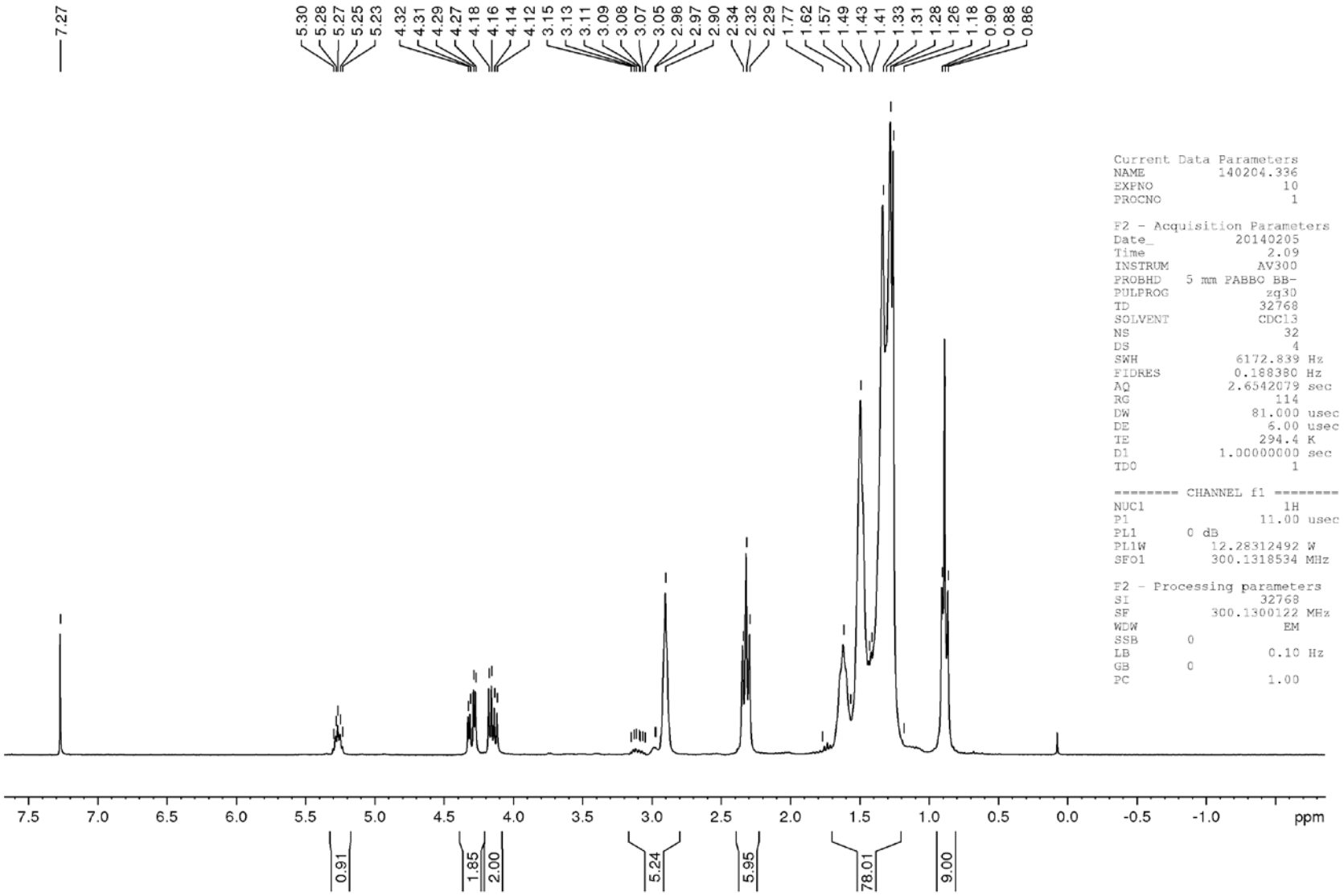
5. NMR spectra and analytic data of epoxidized and carbonated oils

Reference spectra of epoxidzied oils **6** are attached.

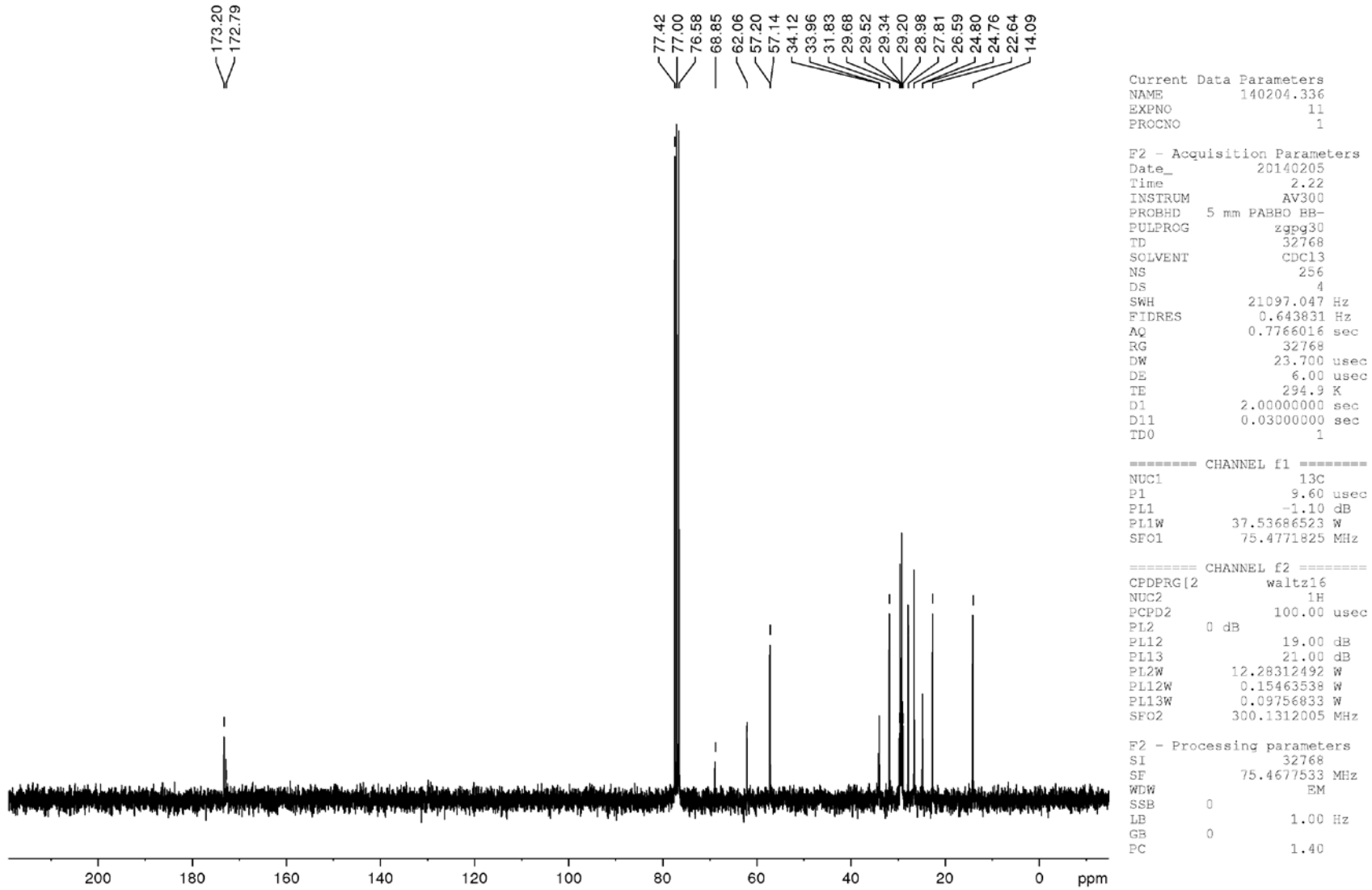
Carbonated high-oleic sunflower oil (**7a**)

Analytic data of **6a**: ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.86–0.90 (m, 9H), 1.18–1.77 (m, 78H), 2.32 (t, $^{3}J_{H,H}$= 7.5 Hz, 6H), 2.90–3.15 (m, 5H), 4.15 (dd, $^{2}J_{H,H}$= 11.9 Hz, $^{3}J_{H,H}$= 5.9 Hz, 2H), 4.30 (dd, $^{2}J_{H,H}$= 11.9 Hz, $^{3}J_{H,H}$= 4.2 Hz, 2H), 5.23–5.30 (m, 1H) ppm; $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 22 °C): δ= 14.09 (CH_3), 22.64 (CH_2), 24.76–34.12 (multiple signals, CH_2), 57.14 (CH), 57.20 (CH), 62.60 (CH_2), 68.85 (CH), 172.79 (C=O), 173.20 (C=O) ppm.

^{1}H NMR Epoxidized high-oleic sunflower oil (**6a**)

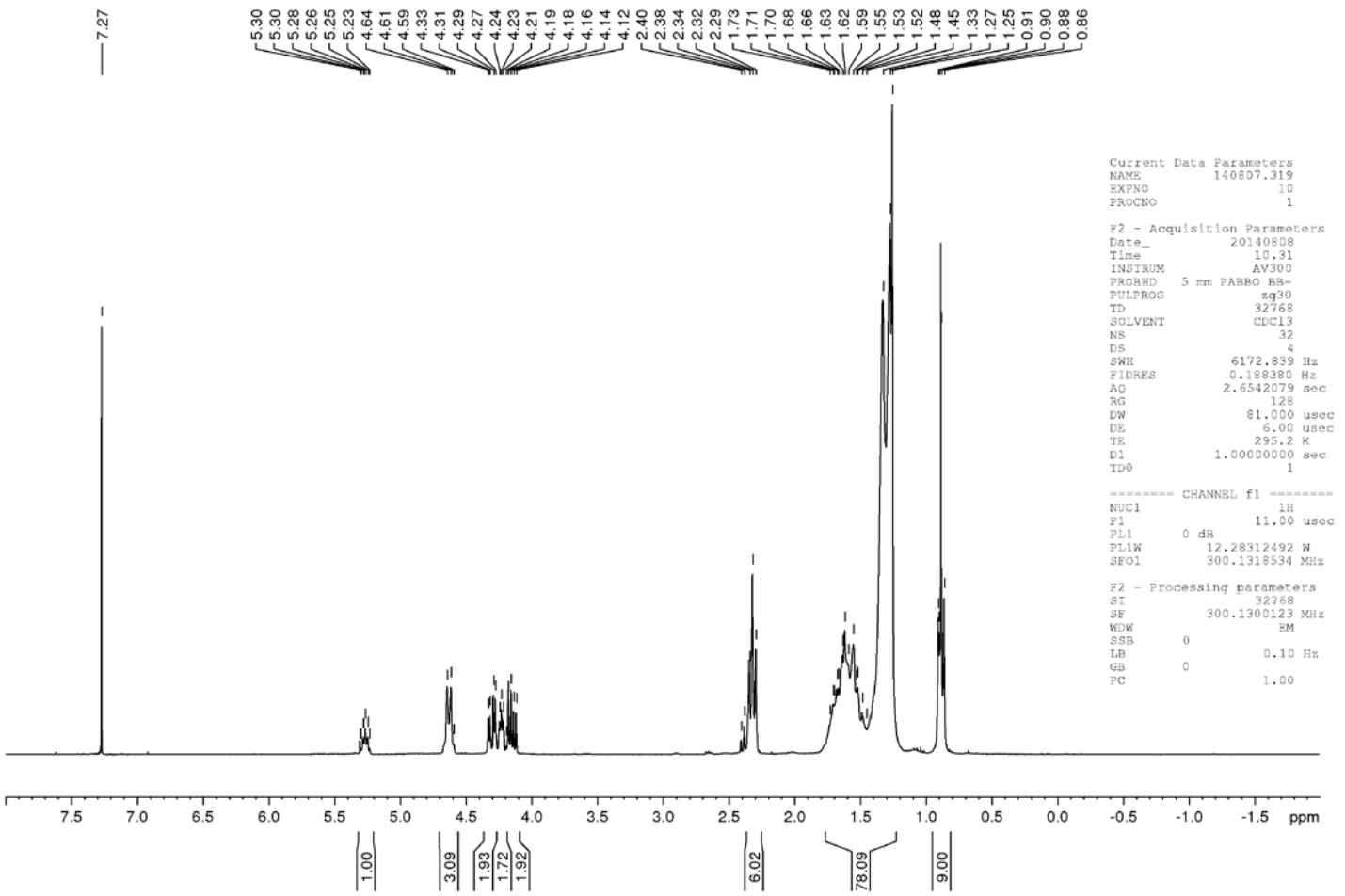


^{13}C NMR Epoxidized high-oleic sunflower oil (**6a**)

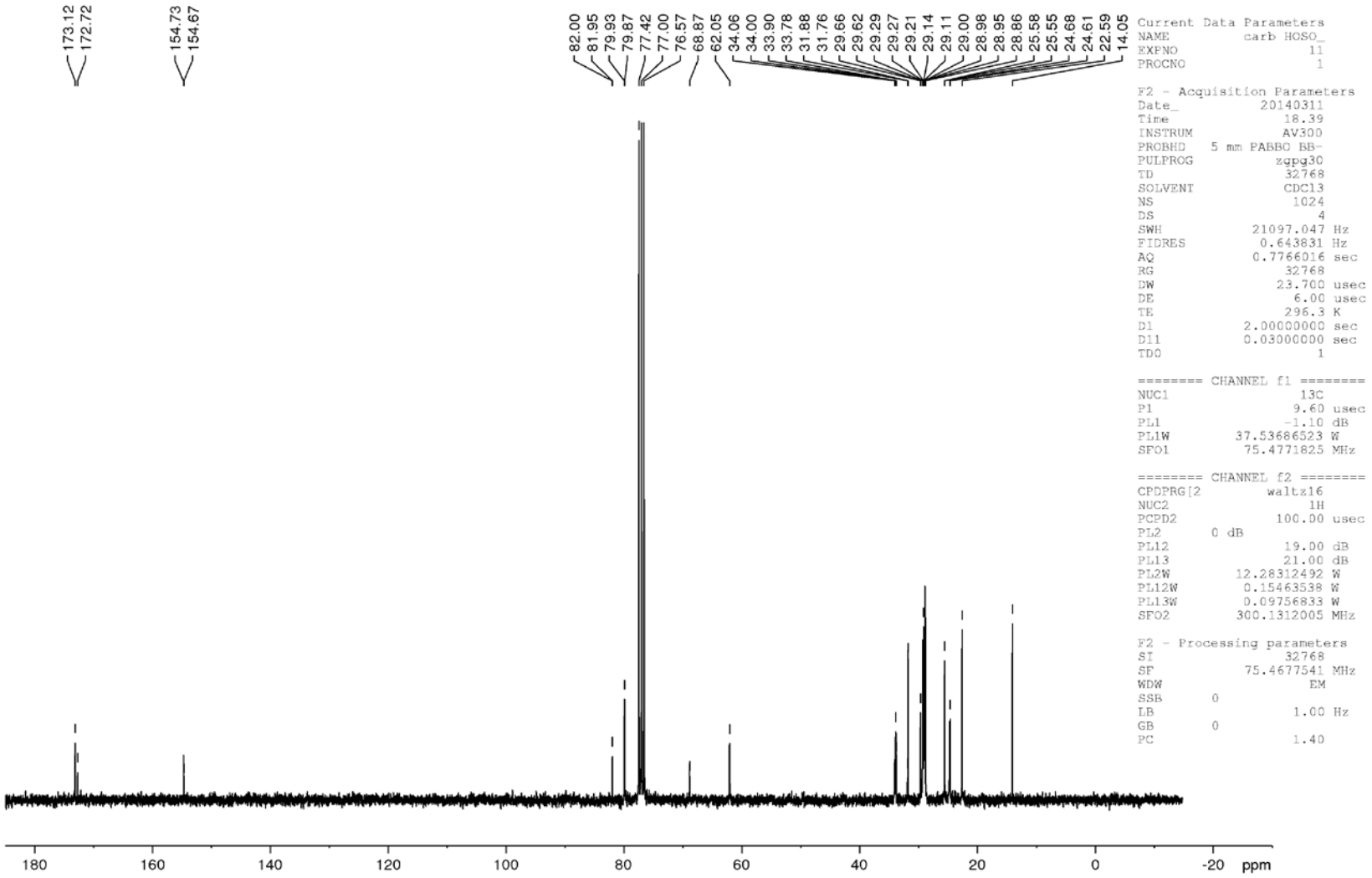



```
Current Data Parameters
NAME          140204.336
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140205
Time                2.22
INSTRUM            AV300
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           21097.047 Hz
FIDRES         0.643831 Hz
AQ            0.7766016 sec
RG                32768
DW               23.700 usec
DE                6.00 usec
TE               294.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.60 usec
PL1                -1.10 dB
PL1W        37.53686523 W
SFO1         75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2       0 dB
PL12                19.00 dB
PL13                21.00 dB
PL2W        12.28312492 W
PL12W        0.15463538 W
PL13W        0.09756833 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677533 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

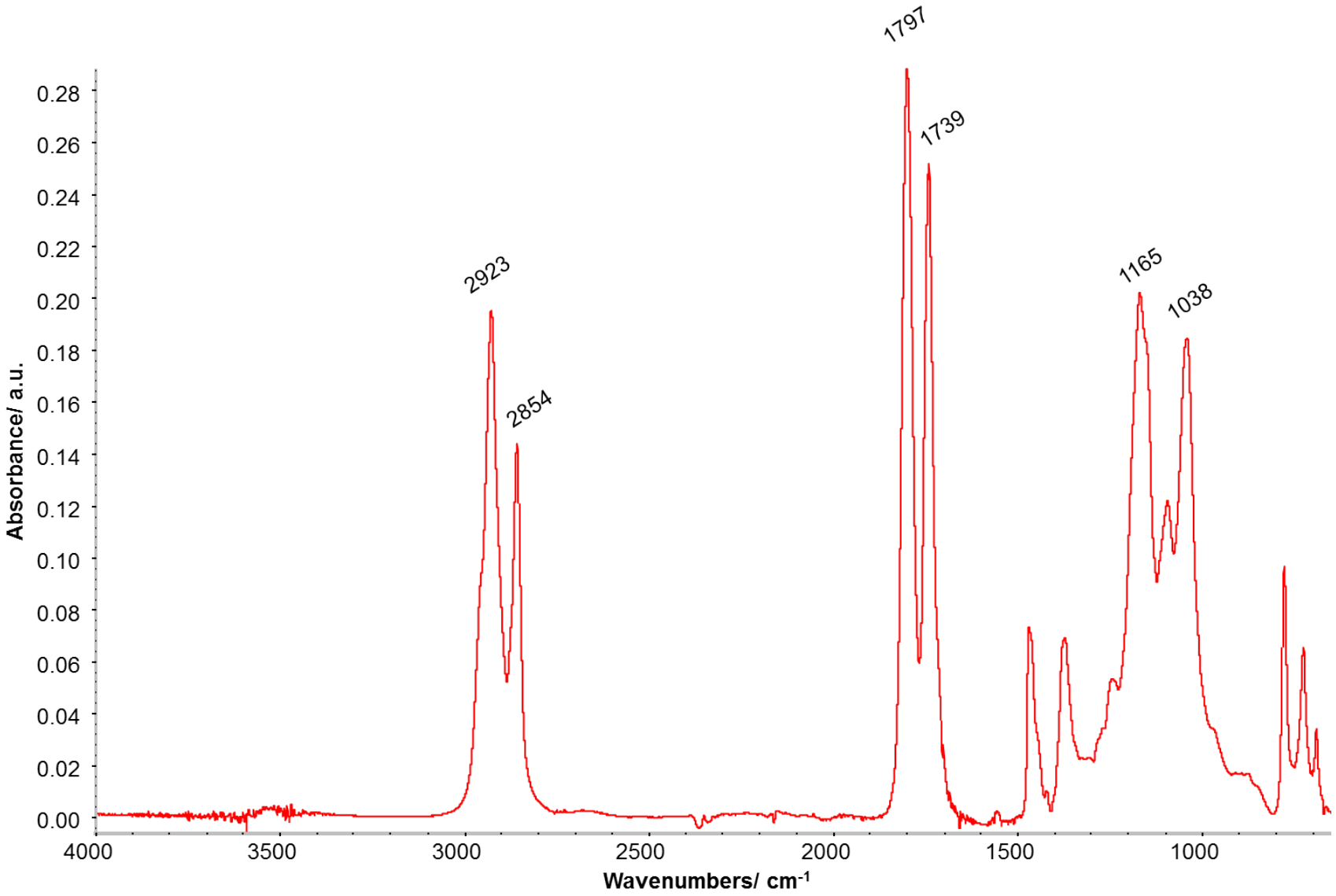
^{1}H NMR Carbonated high-oleic sunflower oil (**7a**)



^{13}C NMR Carbonated high-oleic sunflower oil (**7a**)



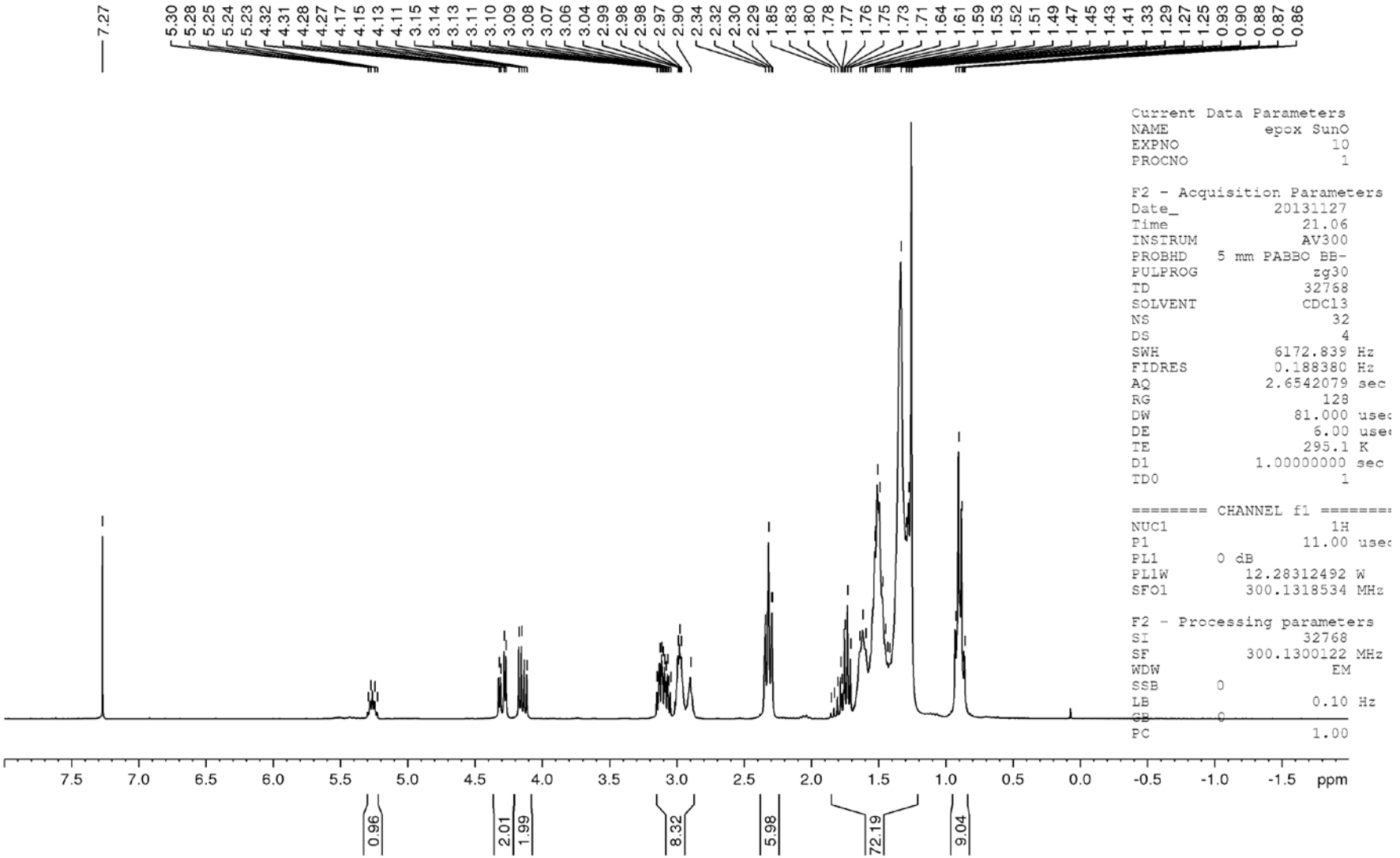
ATR FTIR Carbonated high-oleic sunflower oil (**7a**)



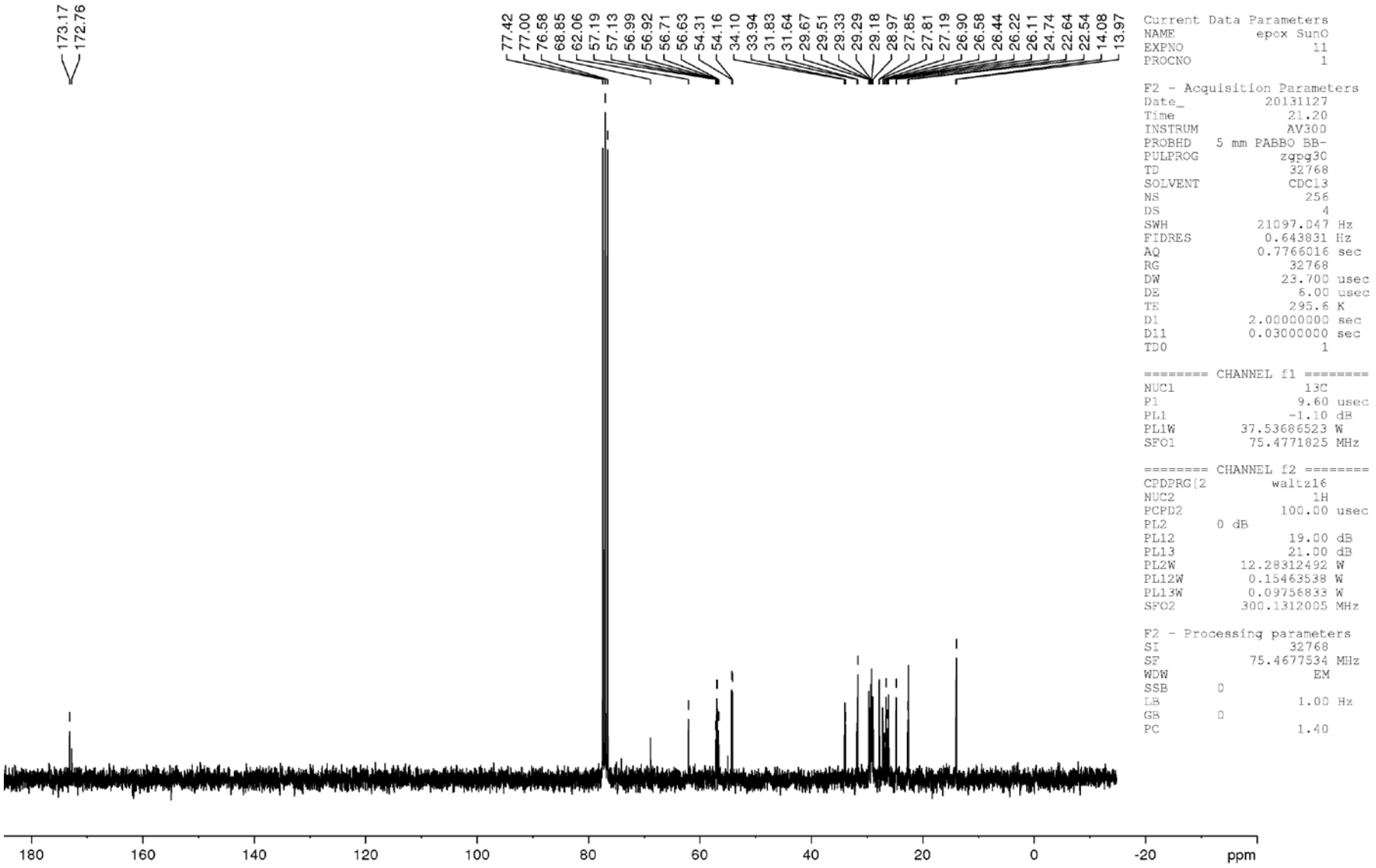
Carbonated sunflower oil (**7b**)

Analytic data of **6b**: ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.86–0.93 (m, 9H), 1.25–1.85 (m, 72H), 2.29–2.34 (m, 6H) 2.89–3.15 (m, 8H), 4.14 (dd, $^{2}J_{H,H}$= 11.9 Hz, $^{3}J_{H,H}$= 5.8 Hz, 2H), 4.30 (dd, $^{2}J_{H,H}$= 11.9 Hz, $^{3}J_{H,H}$= 4.4 Hz, 2H), 5.23–5.30 (m, 1H) ppm; $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 22 °C): δ= 13.97 (CH_3), 14.08 (CH_3), 22.54–34.10 (multiple signals, CH_2), 54.16 (CH), 54.31 (CH), 56.63–57.19 (multiple signals, CH), 62.06 (CH_2), 68.85 (CH), 172.76 (C=O), 173.17 (C=O).

^{1}H NMR Epoxidized sunflower oil (**6b**)

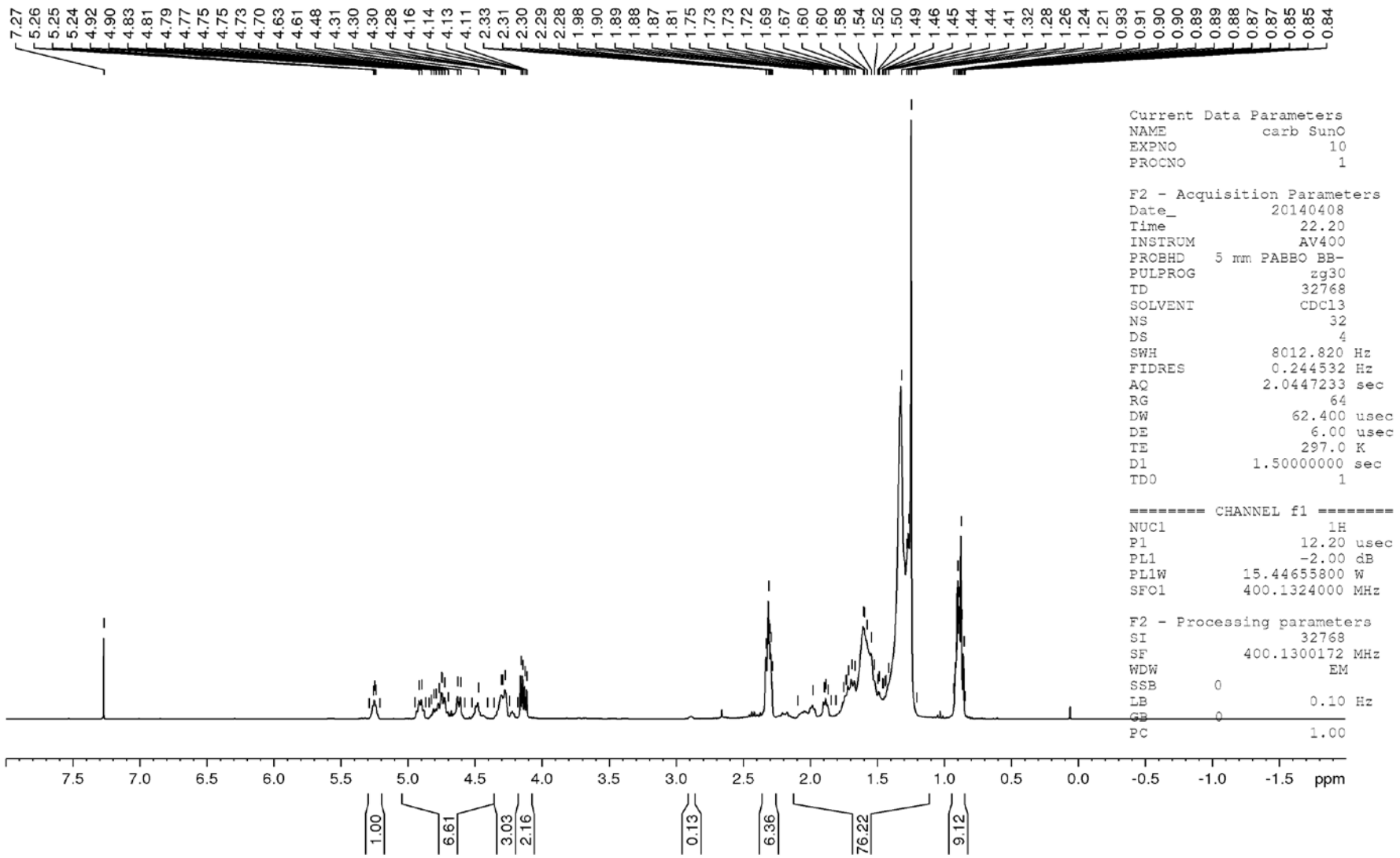


^{13}C NMR Epoxidized sunflower oil (**6b**)

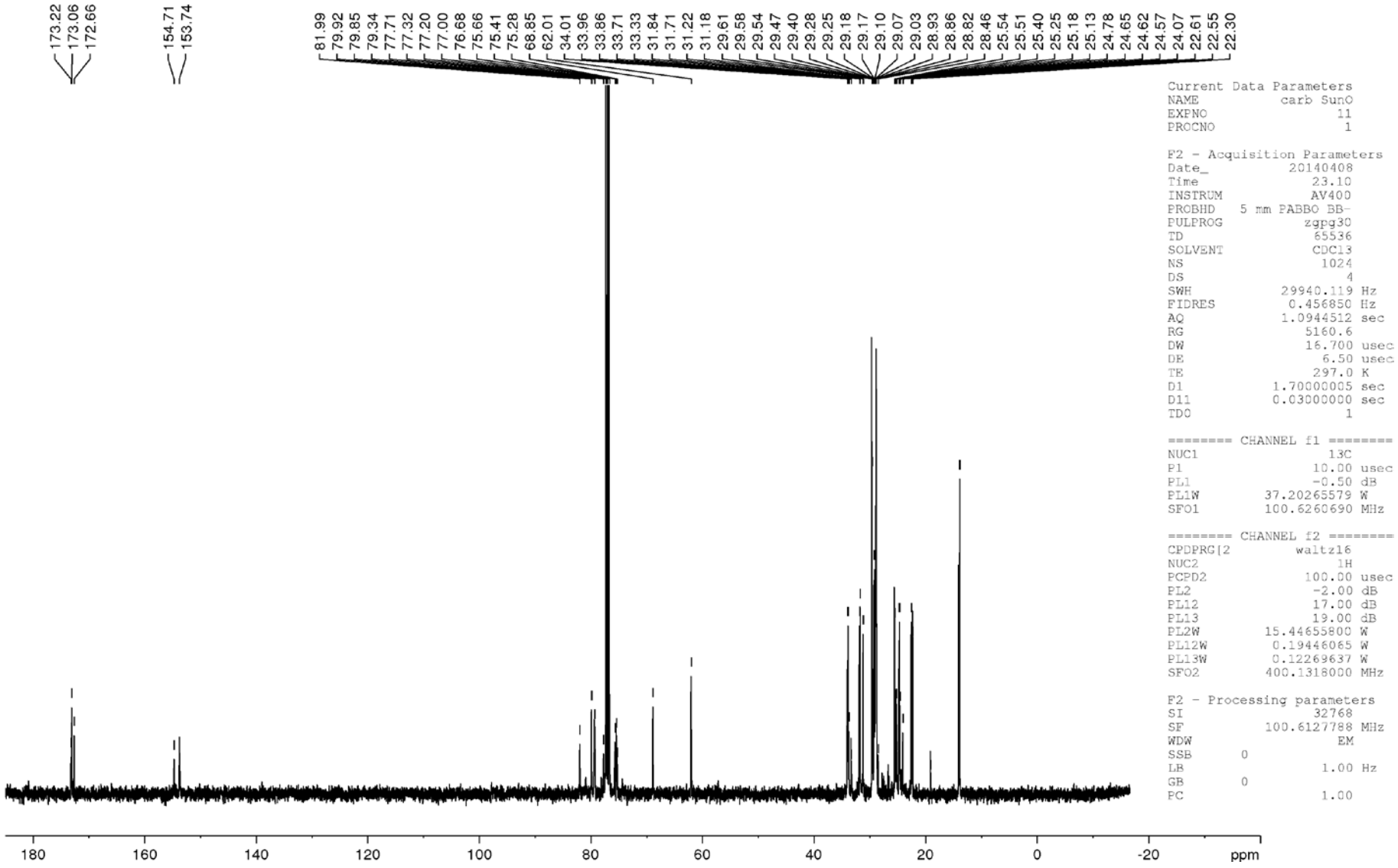



```
Current Data Parameters
NAME                 epox SunO
EXPNO                       11
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20131127
Time                     21.20
INSTRUM                  AV300
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                        256
DS                          4
SWH                 21097.047 Hz
FIDRES               0.643831 Hz
AQ                   0.7766016 sec
RG                      32768
DW                     23.700 usec
DE                      6.00 usec
TE                     295.6 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.60 usec
PL1                      -1.10 dB
PL1W               37.53686523 W
SFO1                75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                   100.00 usec
PL2          0 dB
PL12                     19.00 dB
PL13                     21.00 dB
PL2W               12.28312492 W
PL12W               0.15463538 W
PL13W               0.09756833 W
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                      32768
SF                 75.4677534 MHz
WDW                        EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

^{1}H NMR Carbonated sunflower oil (**7b**)

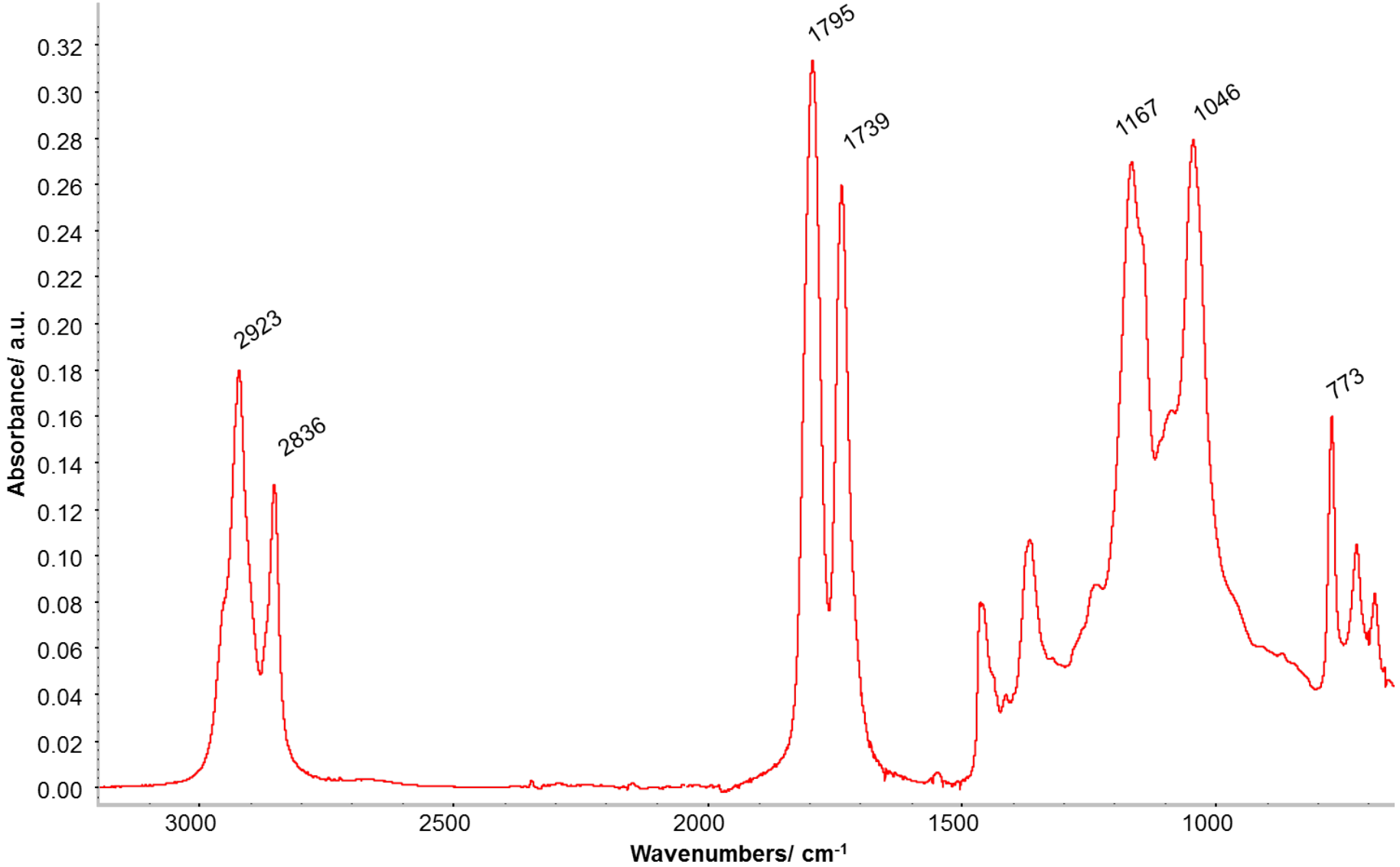


^{13}C NMR Carbonated sunflower oil (**7b**)




```
Current Data Parameters
NAME                  carb SunO
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20140408
Time                     23.10
INSTRUM                  AV400
PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                         1024
DS                            4
SWH                 29940.119 Hz
FIDRES               0.456850 Hz
AQ                   1.0944512 sec
RG                      5160.6
DW                     16.700 usec
DE                      6.50 usec
TE                     297.0 K
D1                  1.70000005 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                       10.00 usec
PL1                      -0.50 dB
PL1W               37.20265579 W
SFO1               100.6260690 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                   100.00 usec
PL2                      -2.00 dB
PL12                     17.00 dB
PL13                     19.00 dB
PL2W               15.44655800 W
PL12W               0.19446065 W
PL13W               0.12269637 W
SFO2               400.1316000 MHz

F2 - Processing parameters
SI                           32768
SF                 100.6127788 MHz
WDW                             EM
SSB                  0
LB                       1.00 Hz
GB                   0
PC                       1.00
```

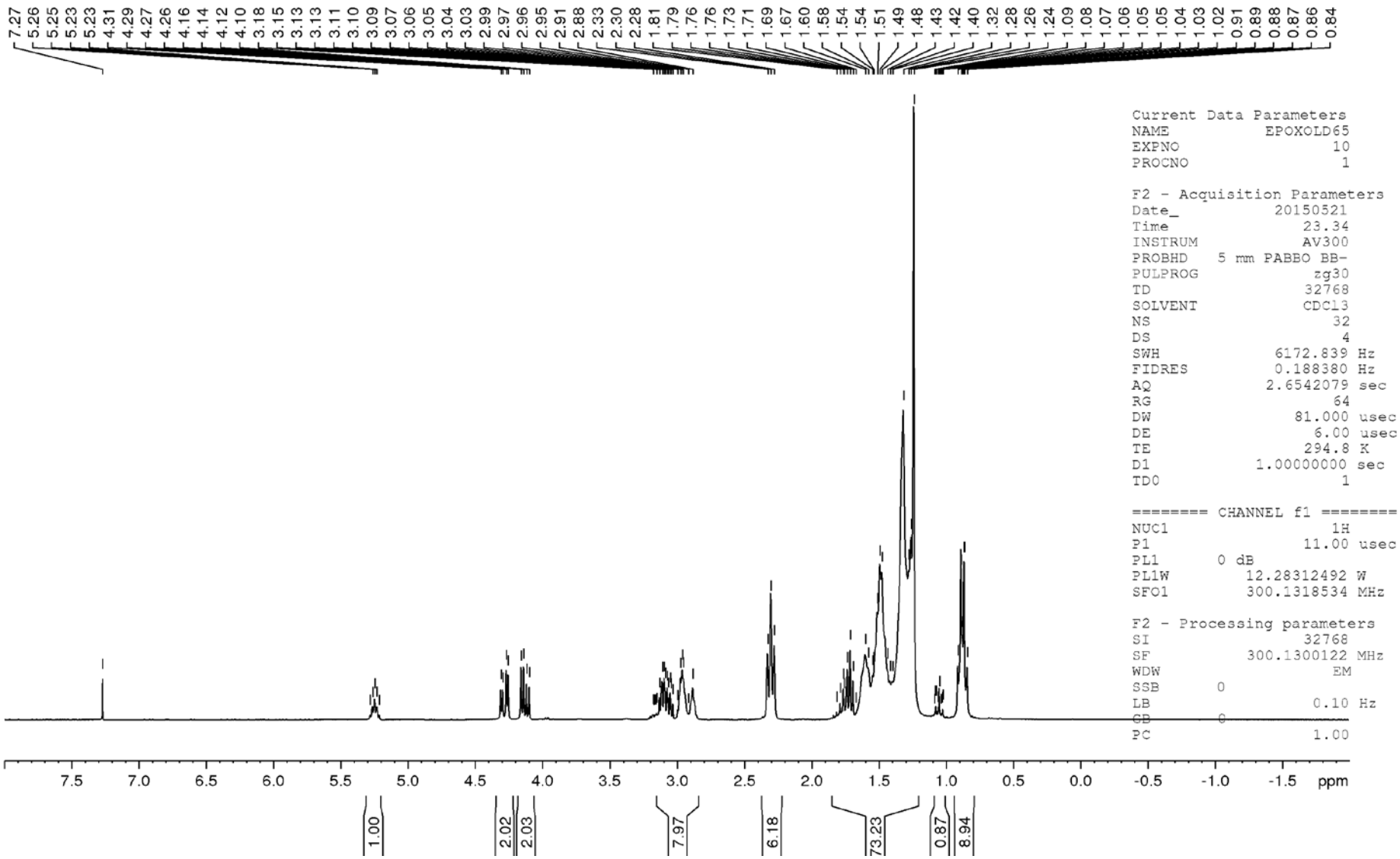
ATR FTIR carbonated sunflower oil (**cFAT2b**)



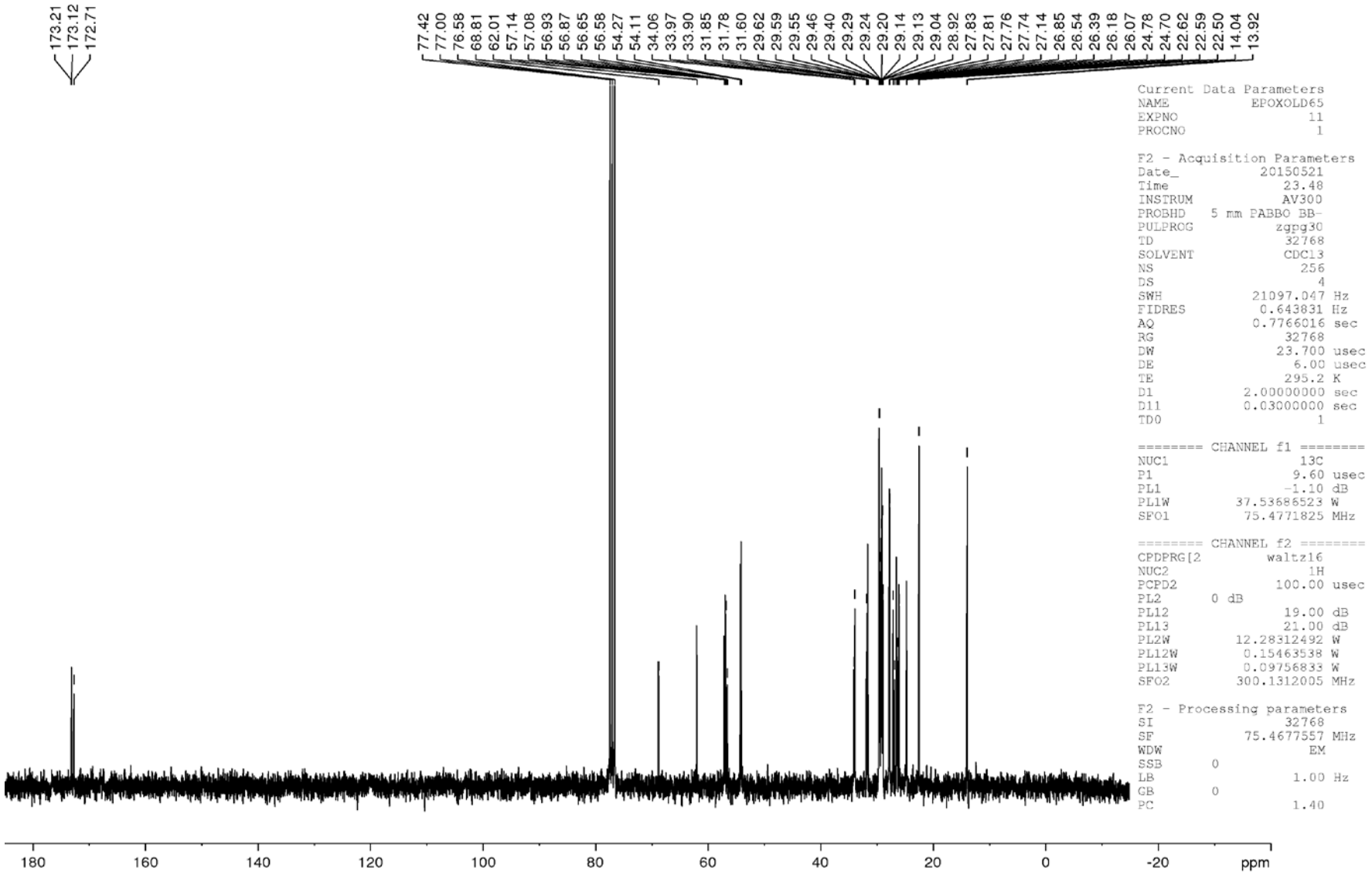
Carbonated EPOXOL D65 (**7c**)

Analytic data of **6c**: ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.84–0.91 (m, 9H), 1.02–1.09 (m, 1H), 1.24–1.81 (m, 73H), 2.28–2.32 (m, 6H), 2.88–3.18 (m, 8H), 4.14 (dd, *J*= 11.9 Hz, 6.1 Hz, 2H), 4.28 (dd, *J*= 11.9 Hz, 4.3 Hz, 2H), 5.21–5.28 (m, 1H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 22 °C) δ= 13.92 (CH_3), 14.04 (CH_3) 22.50–34.06 (multiple signals, CH_2), 54.11 (CH), 54.27 (CH), 56.58 (CH), 56.65 (CH), 56.87 (CH), 56.93 (CH), 57.08 (CH), 57.14 (CH), 62.01 (CH_2), 68.81 (CH), 172.71 (C=O), 173.12 (C=O), 173.21 (C=O);

^{1}H NMR EPOXOL D65 (**6c**)

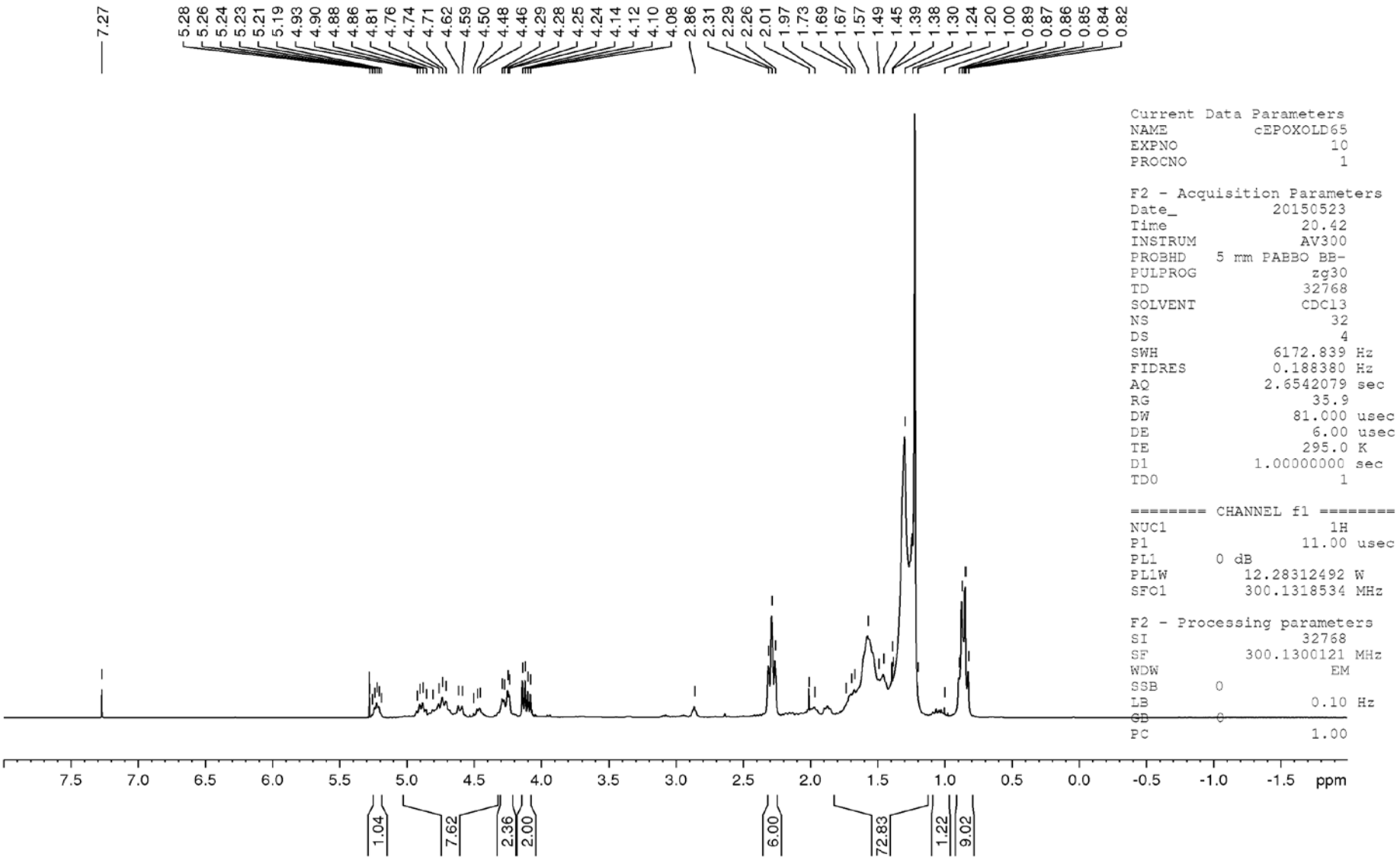


^{13}C NMR EPOXOL D65 (**6c**)

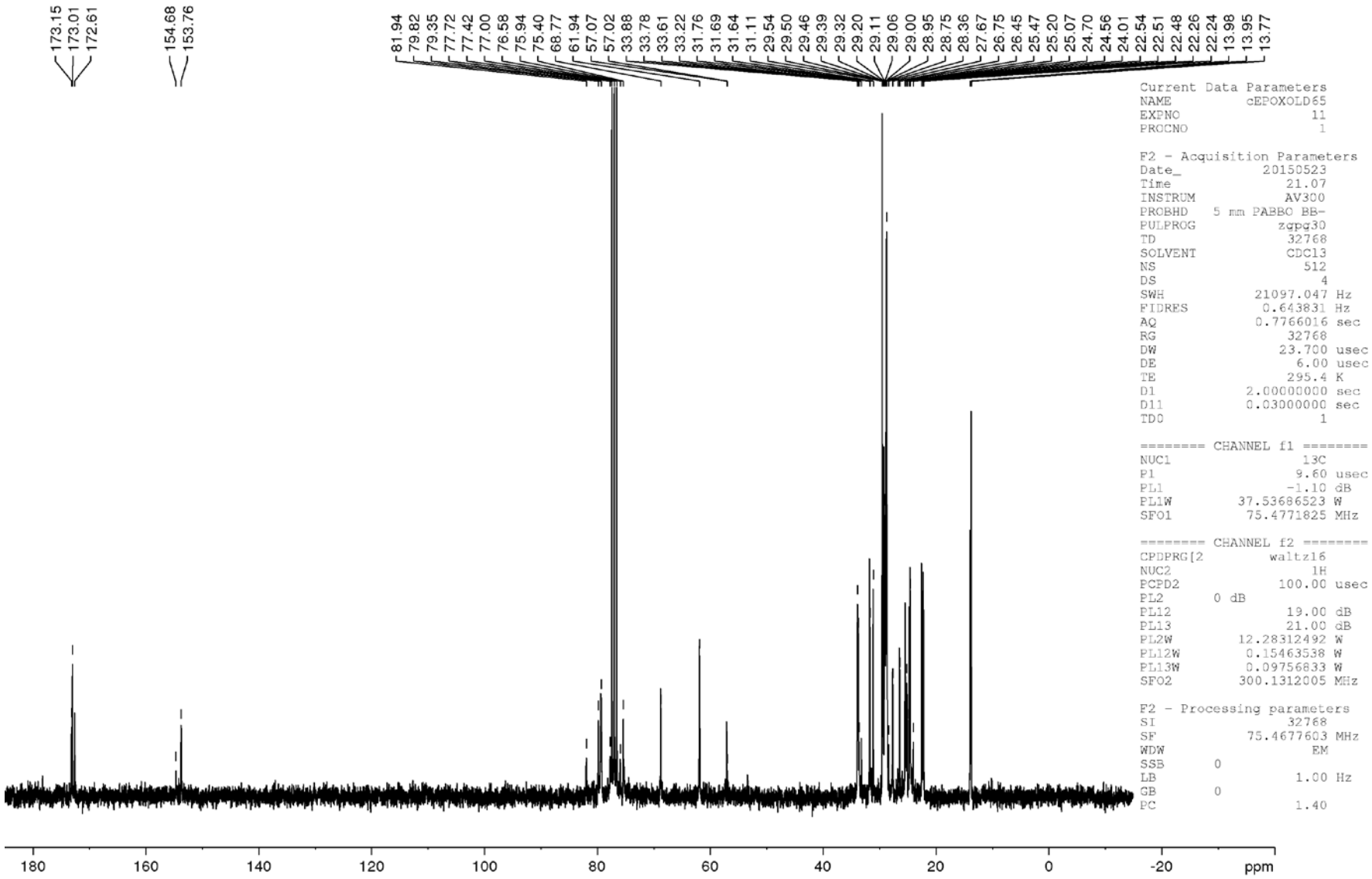



```
Current Data Parameters
NAME                  EPOXOLD65
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20150521
Time                      23.48
INSTRUM                  AV300
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                        32768
SOLVENT                  CDCl3
NS                          256
DS                            4
SWH                21097.047 Hz
FIDRES              0.643831 Hz
AQ                  0.7766016 sec
RG                        32768
DW                     23.700 usec
DE                      6.00 usec
TE                      295.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                        9.60 usec
PL1                      -1.10 dB
PL1W              37.53686523 W
SFO1               75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                   100.00 usec
PL2          0 dB
PL12                     19.00 dB
PL13                     21.00 dB
PL2W              12.28312492 W
PL12W              0.15463538 W
PL13W              0.09756833 W
SFO2              300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                 75.4677557 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

^{1}H NMR carbonated EPOXOL D65 (**7c**)

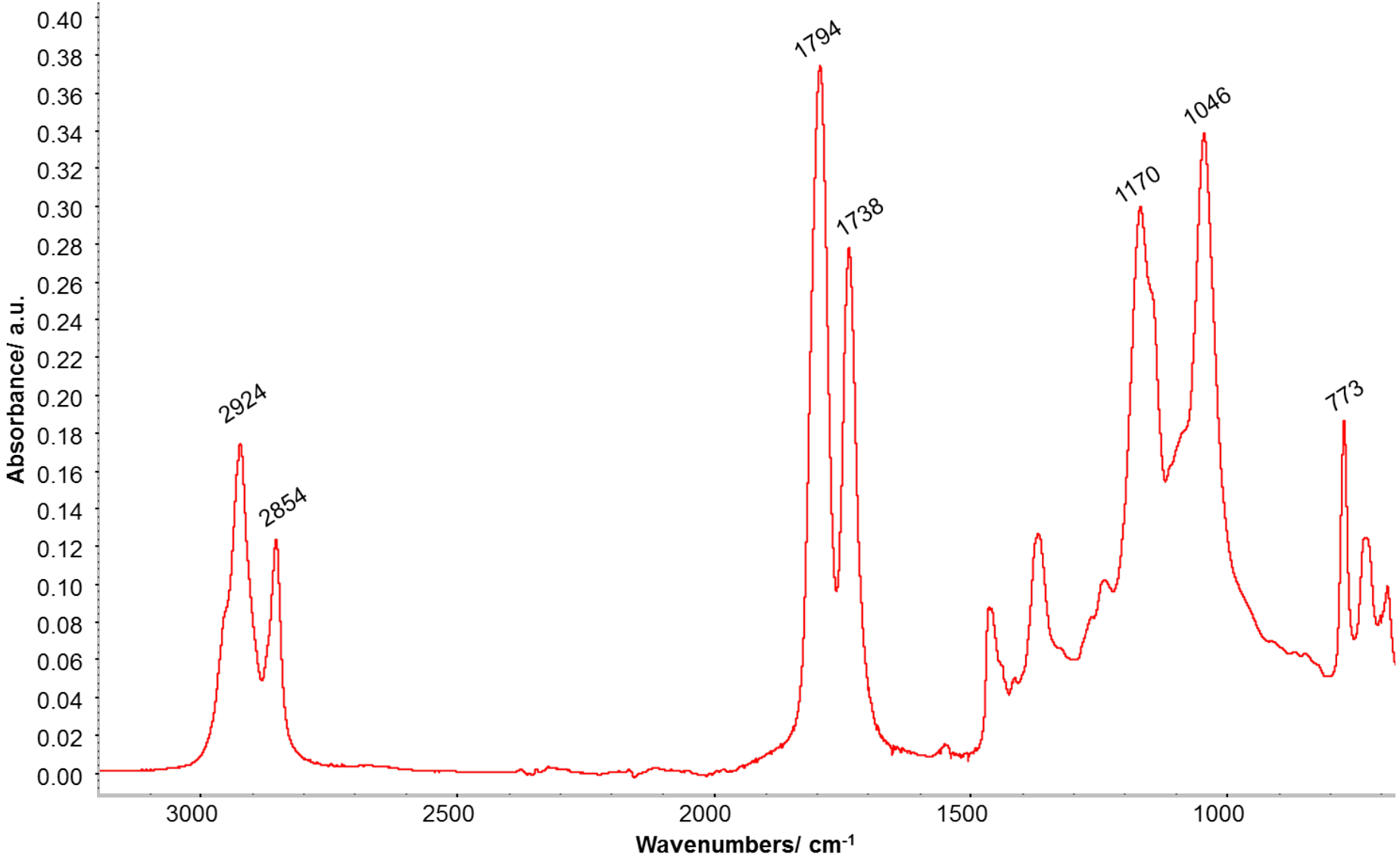


^{13}C NMR carbonated EPOXOL D65 (**7c**)




```
Current Data Parameters
NAME                  cEPOXOLD65
EXPNO                         11
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20150523
Time                       21.07
INSTRUM                    AV300
PROBHD     5 mm PABBO BB-
PULPROG                  zgpg30
TD                         32768
SOLVENT                    CDCl3
NS                           512
DS                             4
SWH                  21097.047 Hz
FIDRES                0.643831 Hz
AQ                    0.7766016 sec
RG                         32768
DW                        23.700 usec
DE                         6.00 usec
TE                        295.4 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                         9.60 usec
PL1                       -1.10 dB
PL1W                37.53686523 W
SFO1                 75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2             0 dB
PL12                      19.00 dB
PL13                      21.00 dB
PL2W                12.28312492 W
PL12W                0.15463538 W
PL13W                0.09756833 W
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                   75.4677603 MHz
WDW                           EM
SSB             0
LB                         1.00 Hz
GB              0
PC                         1.40
```

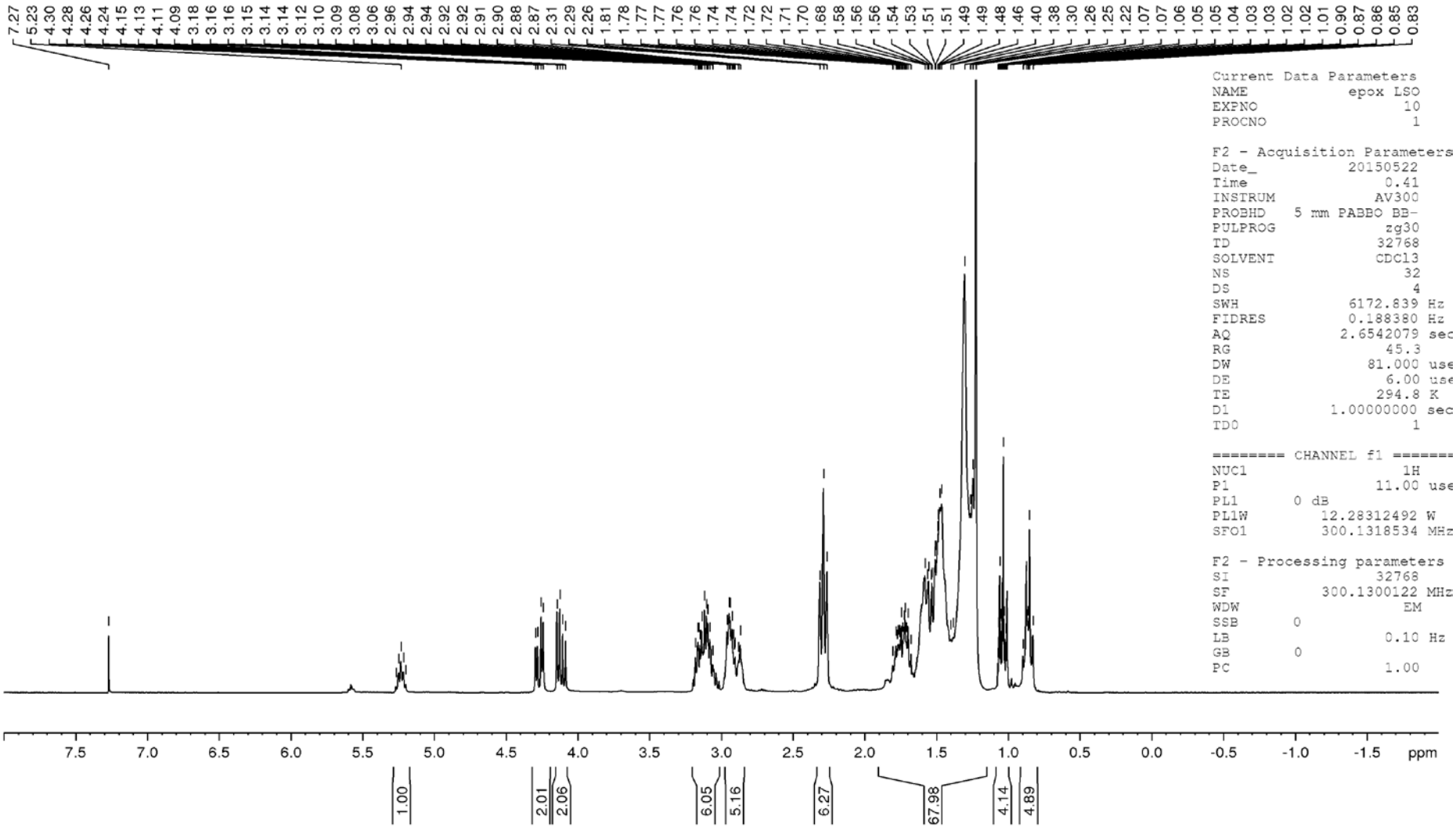
ATR FTIR carbonated EPOXOL D65 (**7c**)



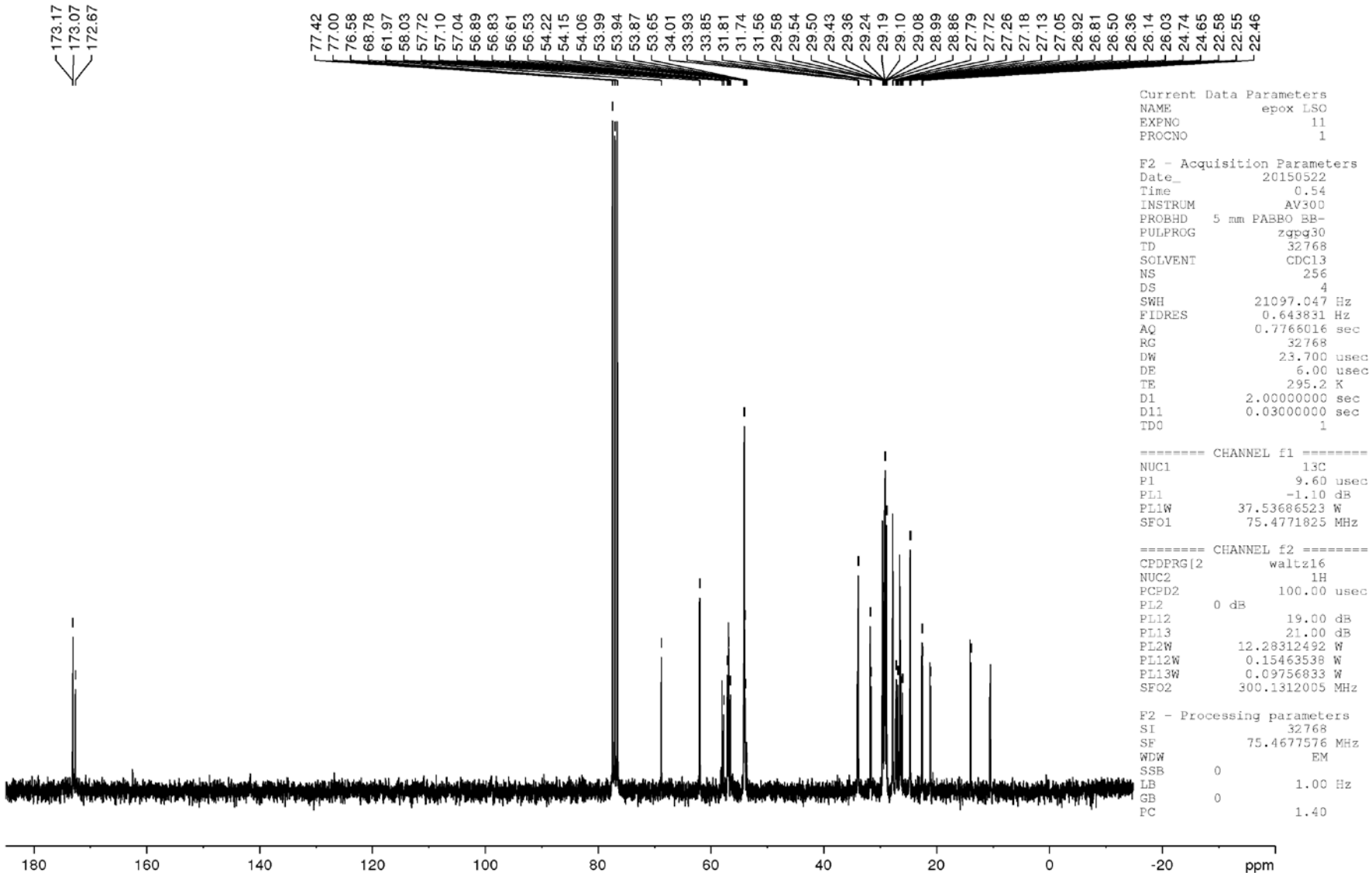
Carbonated linseed oil (**7d**)

Analytic data of **6d**: ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ = 0.83–0.90 (m, 5H), 1.01–1.07 (m, 4H), 1.22–1.78 (m, 68H), 2.26–2.31 (m, 6H), 2.87–2.96 (m, 5H), 3.08–3.18 (m, 6H), 4.12 (dd, *J*= 11.9 Hz, 5.9 Hz, 2H), 4.27 (dd, *J*= 11.9 Hz, 4.3 Hz, 2H), 5.20–5.27 (m, 1H); $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 22 °C) δ= 10.39 (CH_3), 10.51 (CH_3), 13.89 (CH_3), 14.01 (CH_3), 21.03–34.01 (multiple signals, CH_2), 53.65–54.22 (multiple signals, CH), 56.53–58.03 (multiple signals, CH), 61.97 (CH_2), 68.77 (CH), 172.67 (C=O), 173.07 (C=O), 173.17 (C=O).

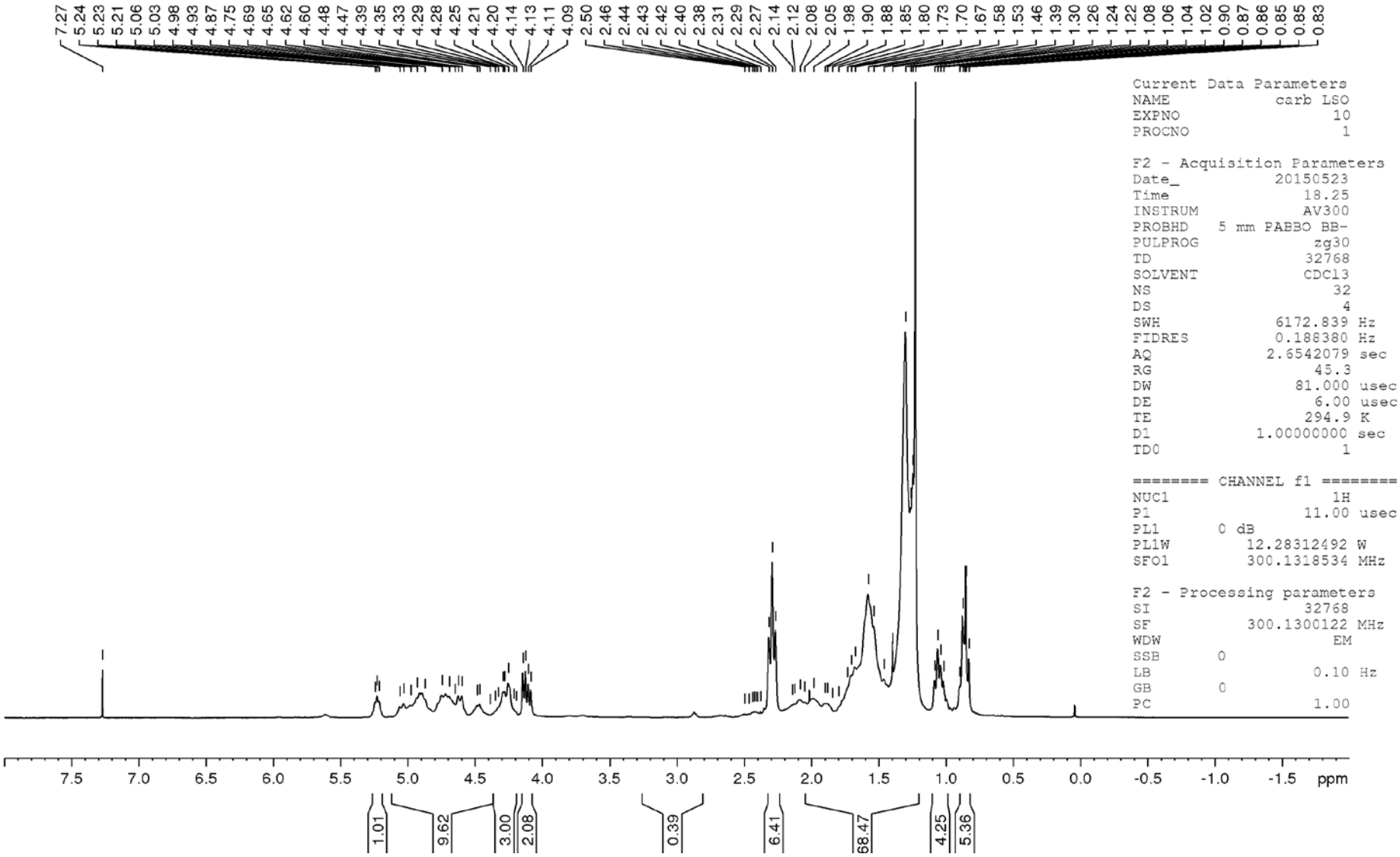
^{1}H NMR Epoxidized linseed oil (**6d**)



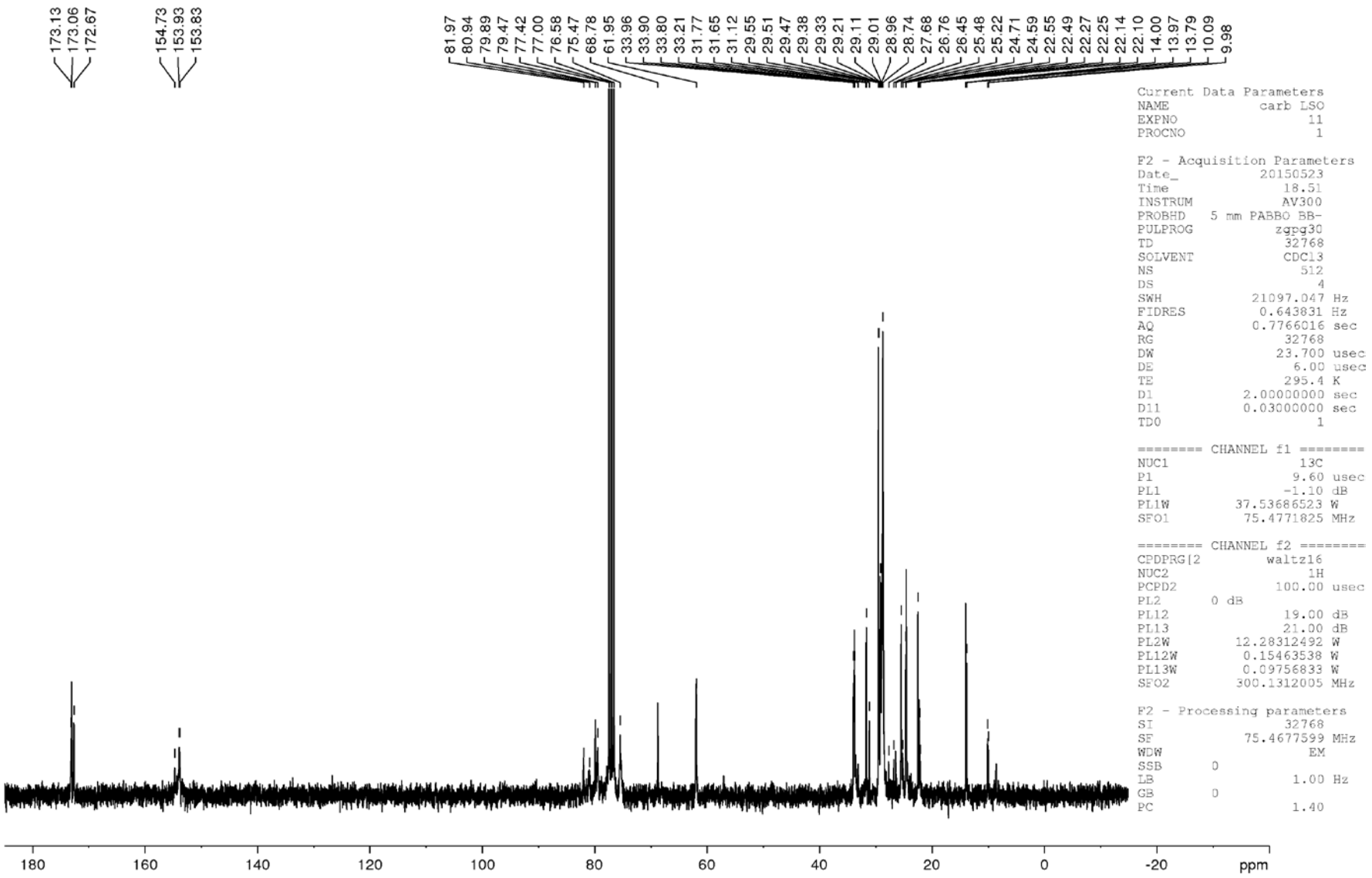
^{13}C NMR Epoxidized linseed oil (**6d**)



^{1}H NMR Carbonated linseed oil (**7d**)

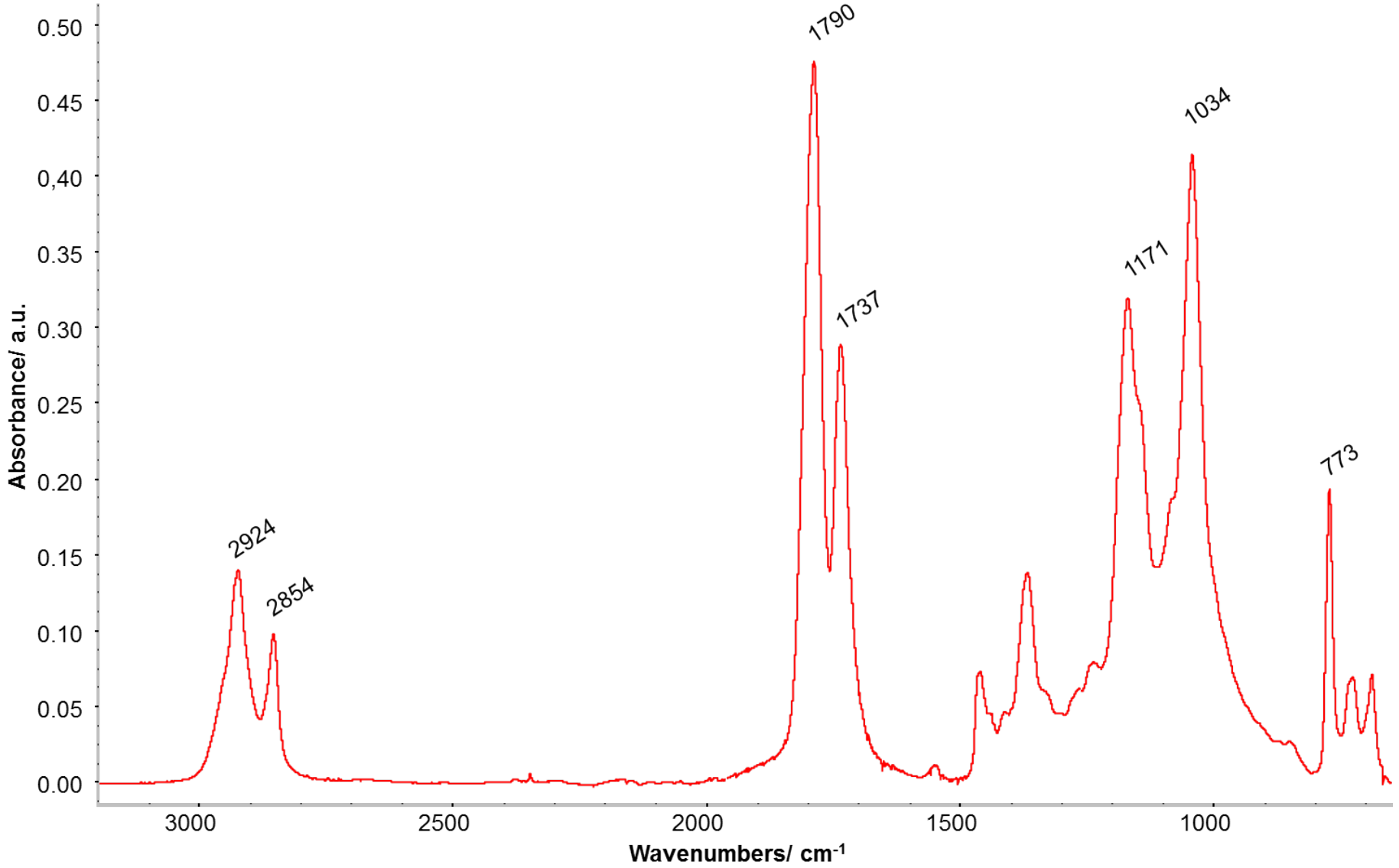


^{13}C NMR Carbonated linseed oil (**7d**)




```
Current Data Parameters
NAME                  carb LSO
EXPNO                       11
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150523
Time                   18.51
INSTRUM                AV300
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                      32768
SOLVENT                CDCl3
NS                        512
DS                          4
SWH                21097.047 Hz
FIDRES              0.643831 Hz
AQ                  0.7766016 sec
RG                      32768
DW                     23.700 usec
DE                      6.00 usec
TE                     295.4 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.60 usec
PL1                      -1.10 dB
PL1W               37.53686523 W
SFO1                75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                       1H
PCPD2                   100.00 usec
PL2            0 dB
PL12                     19.00 dB
PL13                     21.00 dB
PL2W               12.28312492 W
PL12W               0.15463538 W
PL13W               0.09756833 W
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                      32768
SF                 75.4677599 MHz
WDW                        EM
SSB            0
LB                       1.00 Hz
GB             0
PC                       1.40
```

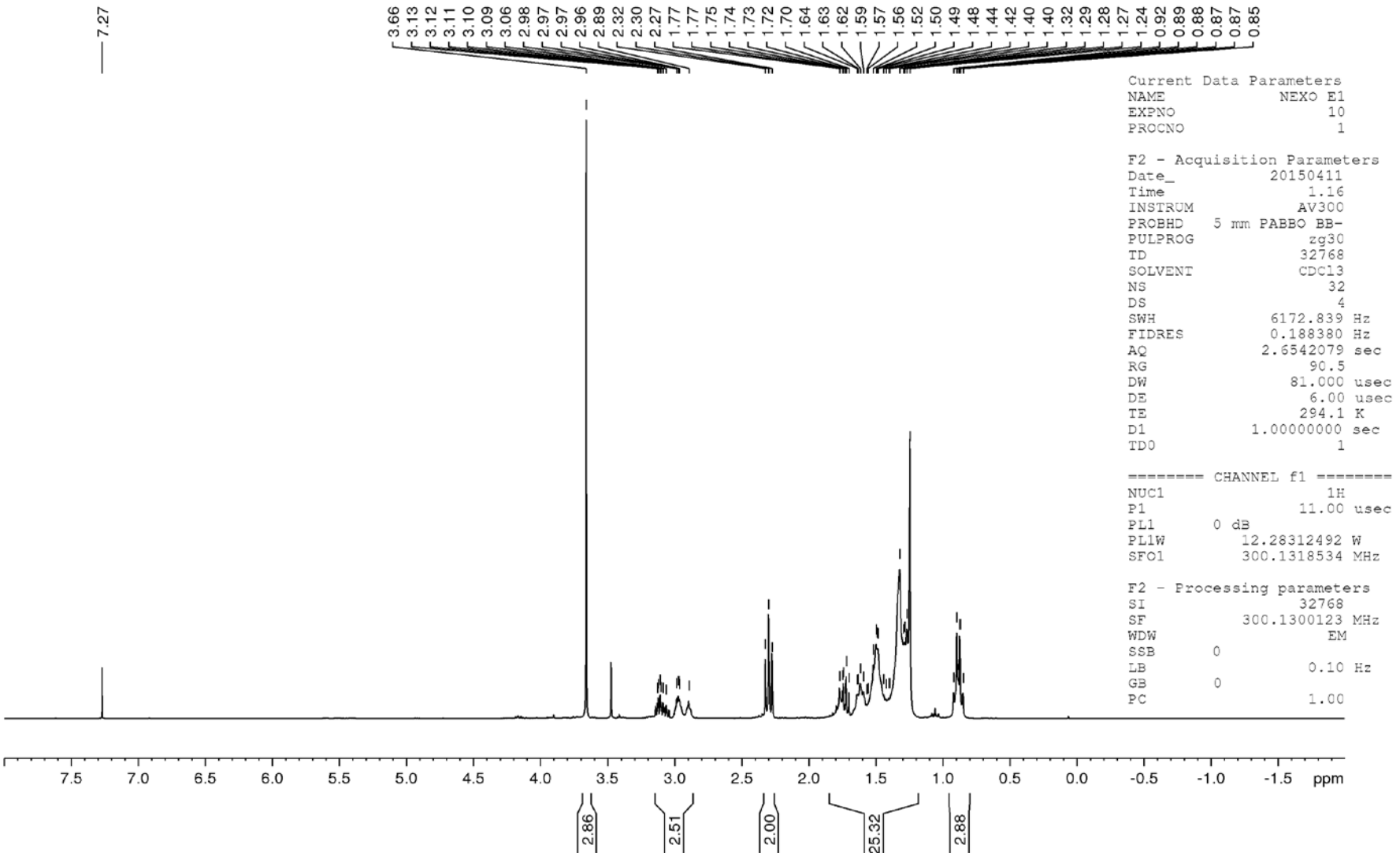
ATR FTIR Carbonated linseed oil (**7d**)



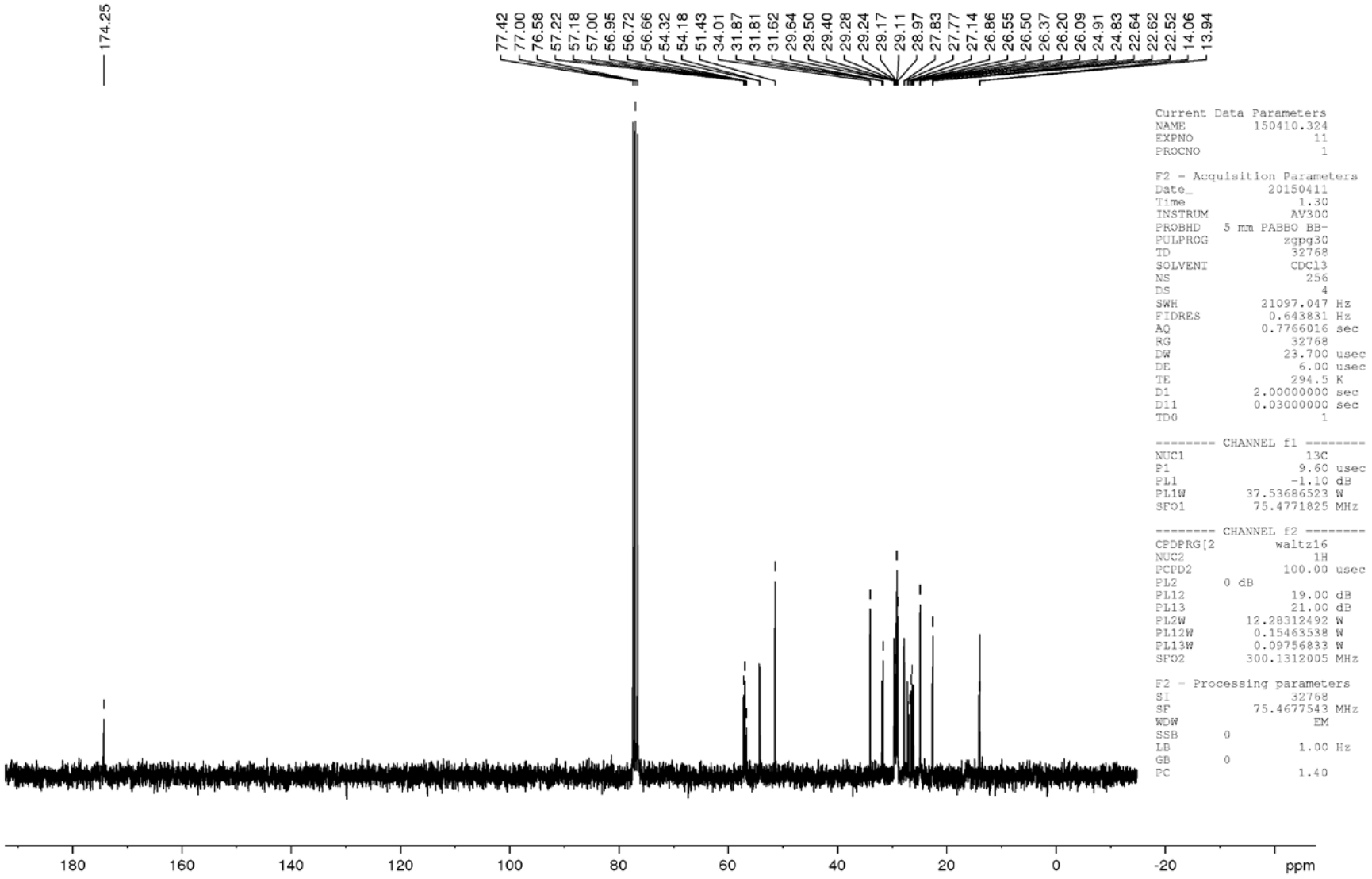
Carbonated methyl soyate NEXO E1 (**7e**)[8]

Analytic data of **6e**: ^{1}H NMR (300 MHz, $CDCl_3$, 22 °C): δ=0.85–0.92 (m, 3H), 1.24–1.77 (m, 25H), 2.30 (t, $^{3}J_{H,H}$= 7.5 Hz, 2H), 2.89–3.13 (m, 3H), 3.66 (s, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$, 22 °C) δ= 13.94 (CH_3), 14.06 (CH_3), 22.52–34.01 (multiple signals, CH_2), 51.43 (CH), 54.18 (CH), 54.32 (CH), 56.66–57.22 (multiple signals, CH), 174.25 (C=O);

^{1}H NMR Epoxidized methyl soyate NEXO E1 (**6e**)

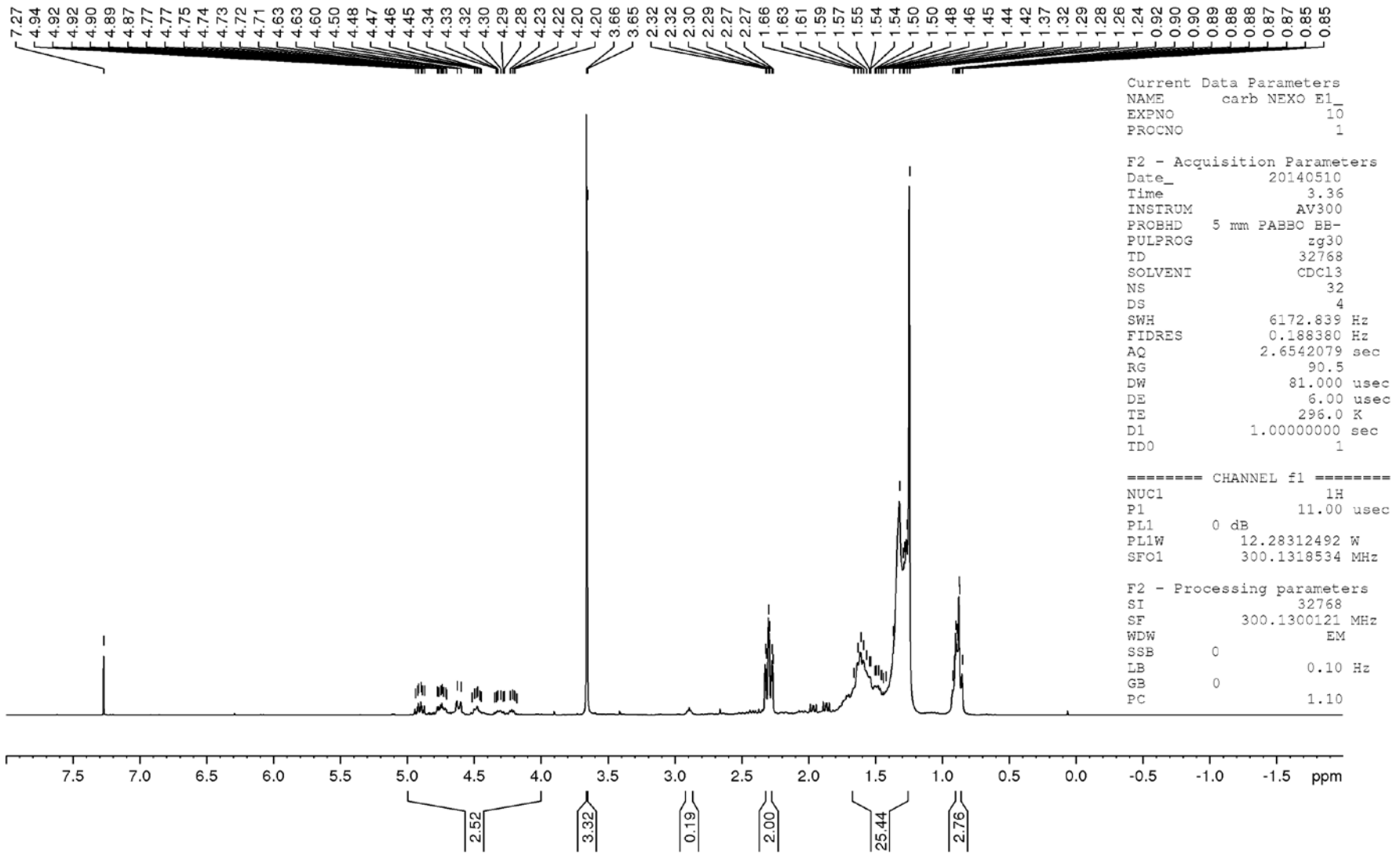


^{13}C NMR Epoxidized methyl soyate NEXO E1 (**6e**)

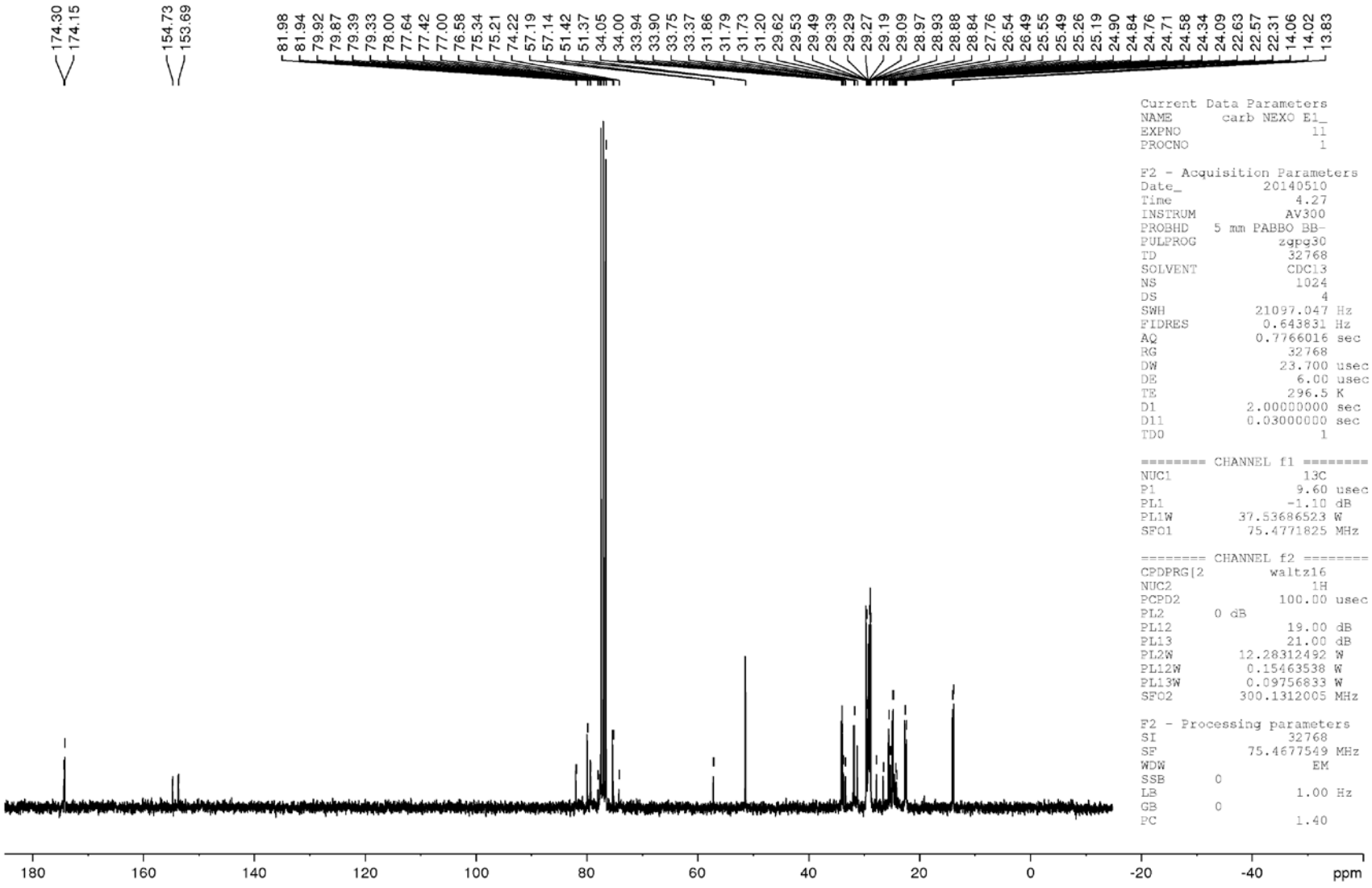



```
Current Data Parameters
NAME          150410.324
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150411
Time                1.30
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           21097.047 Hz
FIDRES         0.643831 Hz
AQ             0.7766016 sec
RG                32768
DW               23.700 usec
DE                6.00 usec
TE                294.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.60 usec
PL1                 -1.10 dB
PL1W         37.53686523 W
SFO1          75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2        0 dB
PL12                19.00 dB
PL13                21.00 dB
PL2W         12.28312492 W
PL12W         0.15463538 W
PL13W         0.09756833 W
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677543 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{1}H NMR Carbonated methyl soyate NEXO E1 (**7e**)

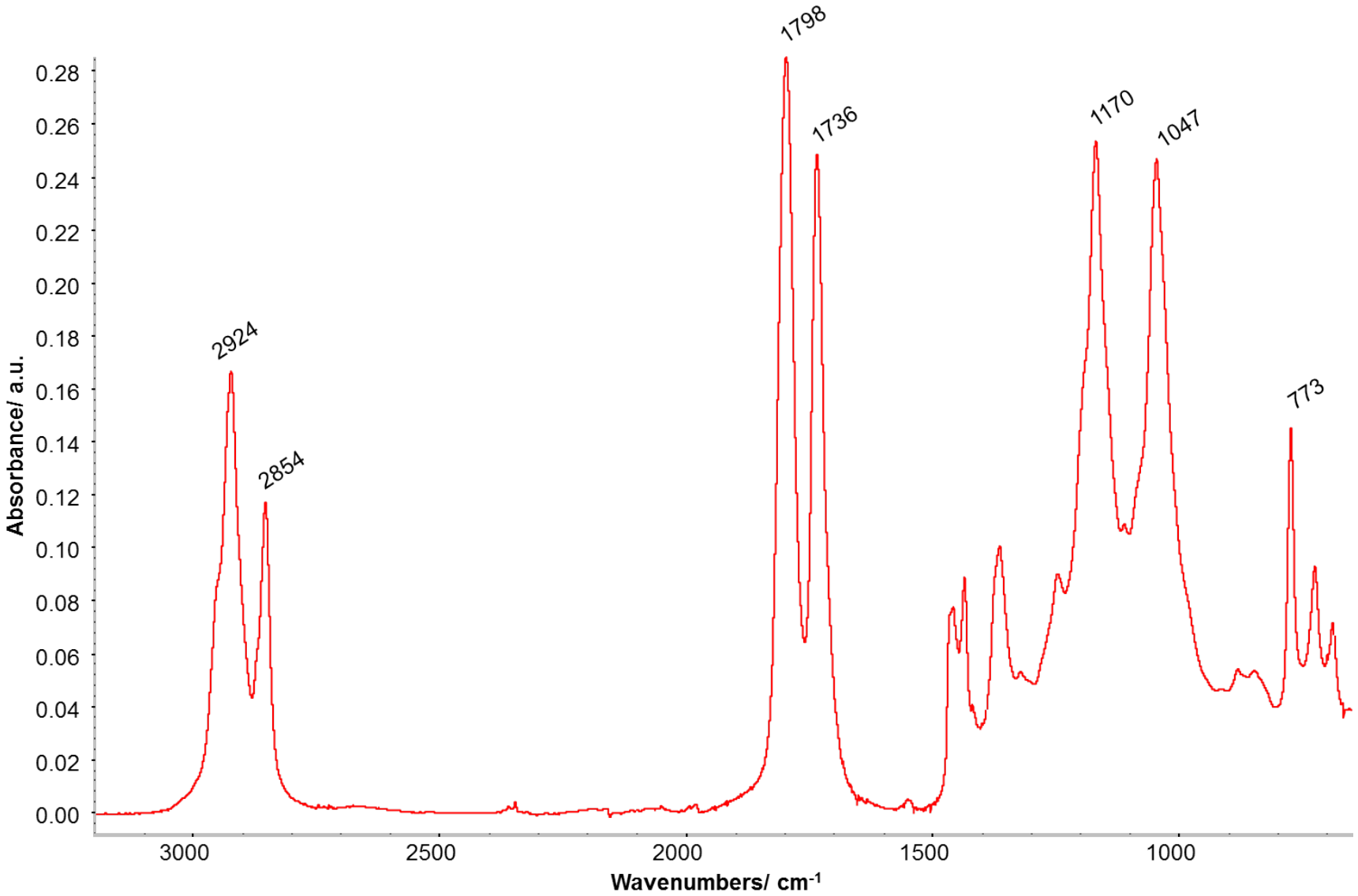


^{13}C NMR Carbonated methyl soyate NEXO E1 (**7e**)




```
Current Data Parameters
NAME       carb NEXO E1_
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20140510
Time               4.27
INSTRUM           AV300
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
NS                1024
DS                   4
SWH          21097.047 Hz
FIDRES        0.643831 Hz
AQ           0.7766016 sec
RG               32768
DW              23.700 usec
DE               6.00 usec
TE              296.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.60 usec
PL1               -1.10 dB
PL1W       37.53686523 W
SFO1        75.4771825 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2           100.00 usec
PL2        0 dB
PL12              19.00 dB
PL13              21.00 dB
PL2W       12.28312492 W
PL12W       0.15463538 W
PL13W       0.09756833 W
SFO2       300.1312005 MHz

F2 - Processing parameters
SI               32768
SF          75.4677549 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

ATR FTIR Carbonated methyl soyate NEXO E1 (**7e**)



6. References

1. A. Behr, N. Tenhumberg and A. Wintzer, *Eur. J. Lipid Sci. Technol.*, 2012, **114**, 905-910.
2. M. Tavasli, D. O'Hagan, C. Pearson and M. C. Petty, *Chem. Commun.*, 2002, DOI: 10.1039/B202891C, 1226-1227.
3. J. Langanke, L. Greiner and W. Leitner, *Green Chem.*, 2013, **15**, 1173-1182.
4. O. Kreye, T. Tóth and M. A. R. Meier, *Eur. Polym. J.*, 2011, **47**, 1804-1816.
5. A. Kazariya and S. Matsumura, *Polymers*, 2012, **4**, 486-500.
6. A. M. Davletbakova, N. Z. Baibulatova, V. A. Dokichev, R. R. Muslukhov, S. G. Yunusova and M. S. Yunusov, *Russ. J. Org. Chem.*, 2001, **37**, 1220-1222.
7. Due to the complex mixture of diastereoisomers a conclusive assignment of resonances was omitted.
8. B. Schäffner, M. Blug, D. Kruse, M. Polyakov, A. Köckritz, A. Martin, P. Rajagopalan, U. Bentrup, A. Brückner, S. Jung, D. Agar, B. Rüngeler, A. Pfennig, K. Müller, W. Arlt, B. Woldt, M. Graß and S. Buchholz, *ChemSusChem*, 2014, **7**, 1133–1139.
9. L. A. Rios, B. A. Llano and W. F. Hoelderich, *Appl. Catal. A*, 2012, **445–446**, 346-350.
10. T. M. Kuo, A. C. Lanser, T. Kaneshiro and C. T. Hou, *J. Am. Oil Chem. Soc.*, 1999, **76**, 709-712.