*Supporting Information*

# Asymmetric Synthesis of (-)-Muricatacin's Analogue (4*S*,5*R*)-5-Hydroxy-4-octadecanolide Exhibiting the Cytotoxicity against Esophageal Cancer Cells

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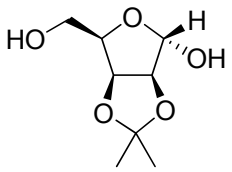
## General Materials and Methods.

Chemicals used in reactions were of reagent grade and were used without further purification except where noted. All solvents used in reaction were obtained from E. Merck or Acros and were dried by stander procedures[1] before use. Solvents for spectral instruments were spectroscopy grade and were purchased from E. Merck. Solvents used for extraction and chromatography were of technical grade and were distilled prior to use. Reactions were monitored by thin-layer chromatography performed on 0.25 mm TLC aluminium plates of Silica Gel 60 $F_{524}$ (E. Merck) and compound spots were visualized by UV light (254 nm) and by staining with a solution of $Ce(NH_4)_2(NO_3)_6$ (0.5 g) and $(NH_4)_6Mo_7O_4H_2O$ (24.0 g) in 6% $H_2SO_4$ (500 mL). Flash chromatography[2] was carried out using E. Merck Silica Gel 60 (230-400 mesh, 111567.9025).

Melting points are uncorrected and were measured with a Yanagimoto Micromelting Point Apparatus. Optical rotations were performed on a Jasco P-1010 polarimeter at the indicated temperatures. Infrared spectra were obtained as neat on KBr plates with a Jasco FTIR-4200 and recorded in $cm^{-1}$. $^1H$ and $^{13}C$ NMR spectra were recorded with a Bruker Avance 300 (300 MHz for $^1H$; 75 MHz for $^{13}C$) and a Bruker Avance II-400 (400 MHz for $^1H$; 100 MHz for $^{13}C$) FT-NMR instruments. Chemical shifts (δ) are reported in ppm relative to tetramethylsilane (δ 0.00) or the residual proton of $CDCl_3$ ($\delta_H$ 7.26, $\delta_C$ 77.0) as

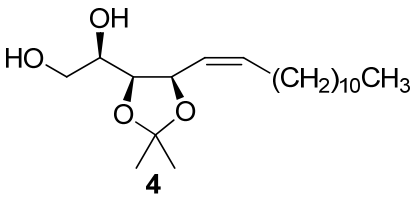
internal standard. COSY, HMQC, and HMBC spectra were applied to the detailed NMR assignments. Stereochemistry of compounds was determined using NOESY. High resolution mass spectra (HRMS) were recorded on a Bruker Daltonics Esquire 2000 mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

## Experimental Procedures




**3**

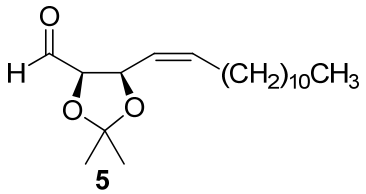
**2,3-*O*-isopropylidene-α-D-lyxofuranose** (**3**) To a stirred suspension of D-(-)-lyxose (0.586 g, 3.90 mmol) in anhydrous acetone (19.5 mL, 0.2 M) was added dropwise conc. $H_2SO_4$ (22 μL, 0.39 mmol) at 0 $^oC$. After stirring at 0 $^oC$ for 10 min, the reaction mixture was continually stirred at room temperature for additional 2 h until a clear solution was achieved. The mixture was neutralized with solid $Ba(OH)_2$ at 0 $^oC$. The solid was filtered out through a short pad of Celite and the Celite pad was washed with ethyl acetate (15 mL). The filtrate was concentrated under reduced pressure to give a colorless syrup residue. The residue was purified via flash column chromatography on silica gel using ethyl acetate and *n*-hexane (2:1 v/v) as the eluent to obtain 0.637 g of white solid **3** as a single α-isomer in 86% yield: $R_f$ = 0.5 (ethyl acetate); mp = 81-83 $^oC$; $[\alpha]^{28}_D$ +28.0 (c = 1.2, $CHCl_3$) [lit.[8] mp = 80-82 $^oC$; $[\alpha]^{21}_D$ +23.0 ($H_2O$)]; FT-IR (neat) $\nu_{max}$ 3398, 2985, 2941, 1646, 1540, 1456, 1375, 1210, 1057, 861, 578, 513, $cm^{-1}$; $^1H$ NMR (300 MHz, $CDCl_3$): δ 5.44 (d, *J* = 2.1 Hz, 1H) , 4.83 (dd, *J* = 6.0, 3.9 Hz, 1H) , 4.64 (d, *J* = 6.0 Hz, 1H), 4.28 (dd, *J* = 9.0, 4.8 Hz, 1H) , 4.01-3.88 (m, 2H), 2.70 (d, *J* = 2.1 Hz, 1H), 2.28 (dd, *J* = 7.2, 4.8 Hz, 1H), 1.47 (s, 3H), 1.32 (s, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 112.6 (C), 100.7 (CH), 85.6 (CH), 80.1 (CH), 80.0 (CH), 60.9 ($CH_2$), 25.8 ($CH_3$), 24.5 ($CH_3$); HRMS-ESI $[M + Na]^+$ Calcd for $C_8H_{14}O_5Na$ 213.0738, Found 213.0733.




**4**

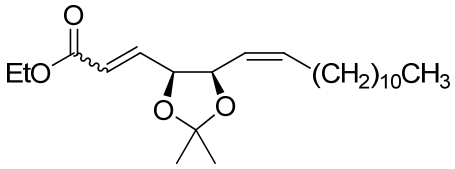
**(4*S*,5*R*)-2,2-Dimethyl-4-((1*R*)-1,2-dihydroxyethyl)-5-((1*Z*)-1-tridecenyl)-1,3-dioxolane** (**4**) Dodecyltriphenylphosphonium bromide (1.755 g, 3.47 mmol) was treated with potassium bis(trimethylsilyl)amide (3.47 mmol, 0.5 M in toluene) at 0 °C. The reaction mixture was kept stirring at

0 °C for 1 h and then solid **3** (188 mg, 0.99 mmol) was quickly added to the above solution. After stirring at 0 °C for 10 min, the reaction mixture was stirred at room temperature for additional 6 h. To this mixture was carefully added cold water at 0 °C and the mixture was extracted with ethyl acetate, dried, filtered and evaporated under reduced pressure to give a yellow syrup. This syrup was purified by flash column chromatography on silica gel using hexane and ethyl acetate (1:4 v/v) as the eluent to give 0.865 g of white solid **4** as a *Z*-stereoisomer in 81% yield: $R_f$ = 0.2 (ethyl acetate : *n*-hexane = 1:4 (v/v)); mp = 63-65 $^{o}$C; $[\alpha]^{28}_{D}$ –35.9 (c = 1.1, $CHCl_3$); FT-IR (neat) $\nu_{max}$ 3432, 2924, 2854, 1742, 1655, 1464, 1378, 1215, 1059, 882, 721, 514 $cm^{-1}$; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 5.74-5.50 (m, 2H), 5.00 (t, *J* = 7.5 Hz, 1H), 4.13 (t, *J* = 4.8 Hz, 1H), 3.68-3.54 (m, 3H), 2.57 (bs, 1H), 2.36 (bs, 1H), 2.17-1.97 (m, 2H), 1.51 (s, 3H), 1.39, (s, 3H), 1.25 (bs, 20H), 0.87 (t, *J* = 5.1 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 135.8 (CH), 124.6 (CH), 108.5 (C), 77.7 (CH), 73.0 (CH), 69.9 (CH), 64.3 ($CH_2$), 31.9 ($CH_2$), 29.6 ($CH_2$), 29.6 ($CH_2$), 29.5 ($CH_2$), 29.4 ($CH_2$), 29.3 ($CH_2$), 29.2 ($CH_2$), 27.7 ($CH_2$), 27.3 ($CH_3$), 24.9 ($CH_3$), 22.6 ($CH_2$), 14.1 ($CH_3$); HRMS-ESI $[M + Na]^+$ Calcd for $C_{20}H_{38}O_4Na$ 365.2662, Found 365.2667.



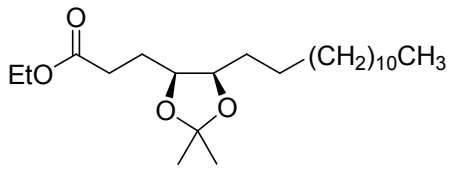

**5**

**(4*S*,5*R*)-2,2-Dimethyl-4-formyl-5-((1*Z*)-1-tridecenyl)-1,3-dioxolane (5)** To a solution of diol **4** (102 mg, 0.30 mmol) in EtOH/$H_2O$ (1 mL, 2:1 (v/v)) was added sodium metaperiodate (127 mg, 0.60 mmol) in one portion at 0 $^{o}$C. The reaction mixture was stirred for another 10 min at 0 $^{o}$C before the ice bath was removed and then stirring was continued at room temperature for 3 h. After starting material being consumed, the reaction mixture was filtered to remove the solid compounds. The filtrate was concentrated in vacuo without further purification to yield 86 mg of aldehyde compound **5** as a syrup compound in 93 % yield: $R_f$ = 0.75 (ethyl acetate : *n*-hexane = 1:1 (v/v)); $[\alpha]^{27}_{D}$ –29.7$^{o}$ (c = 0.3, $CHCl_3$); FT-IR (neat) $\nu_{max}$ 2986, 2925, 1738, 1658, 1463, 1377, 1242, 1217, 1161, 1065, 868, 799, 722; $^{1}$H NMR (300 MHz, $CDCl_3$): δ 9.43 (d, *J* = 3.3 Hz, 1H), 5.63-5.54 (m, 1H), 5.24 (t, *J* = 11.1 Hz, 1H), 5.08 (t, *J* = 7.8 Hz, 1H), 4.25 (dd, *J* = 7.8, 3.3 Hz, 1H), 2.08-1.89 (m, 2H), 1.50 (s, 3H), 1.33 (s, 3H), 1.18 (bs, 18H), 0.79 (t, *J* = 6.3 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) δ 199.3 (CH), 136.1 (CH), 122.7 (CH), 110.5 (C), 82.1 (CH), 74.5 (CH), 31.6 ($CH_2$), 29.4 ($CH_2$), 29.4 ($CH_2$), 29.3 ($CH_2$), 29.2 ($CH_2$), 29.1 ($CH_2$), 28.9 ($CH_2$), 28.9 ($CH_2$), 27.8 ($CH_2$), 27.1 ($CH_3$), 25.0 ($CH_3$), 22.4 ($CH_2$), 13.8 ($CH_3$); HRMS-ESI $[M + Na]^+$ Calcd for 333.2400**,** Found 333.2388.



6

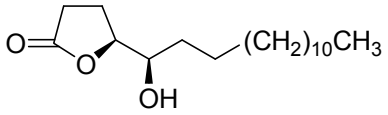
**(4*S*,5*R*)-2,2-Dimethyl-4-((1*E*)-ethoxycarbonylethenyl)-5-((1*Z*)-1-tridecenyl)-1,3-dioxolane (6-2E) and (4*S*,5*R*)-2,2-Dimethyl-4-((1*Z*)-ethoxycarbonylethenyl)-5-((1*Z*)-1-tridecenyl)-1,-3-dioxolane (6-2Z)** To a solution of the crude aldehyde (398 mg, 1.28 mmol) in dry $CH_2Cl_2$ (7.8 mL, 0.165 M) was added the methyl(triphenylphosporanilidine)acetate (940 mg, 2.56 mmol) at 0 $^oC$. After 10 min at 0 $^oC$, the resulting solution was allowed to stir at room temperature for another 3 h. The solvent was removed under reduced pressure to afford a syrup residue which was purified by column chromatography using EtOAc/*n*-hexane (1:20 v/v) as the eluent to afford 400 mg of a syrup dienester **6** as a ca. 3.2:1.0 mixture of *E*- and *Z*-stereoisomers in 82% yield: $R_f$ = 0.5 (ethyl acetate : *n*-hexane = 1:20 (v/v)); FT-IR (neat) $\nu_{max}$ 2925, 2854, 1719, 1644, 1466, 1370, 1188, 1049, 874, 721, 508 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$): δ (**6-2E)** 6.78 (dd, *J* = 15.6, 5.6 Hz, 1H), 6.03 (dd, *J* = 15.6, 1.6 Hz, 1H), 5.71-5.61 (m, 1H), 5.32-5.24 (m, 1H), 5.07-5.02 (m, 1H), 4.69 (dt, *J* = 4.8, 1.6 Hz, 1H), 4.18 (q, *J* = 7.2 Hz, 2H), 2.18-1.92 (m, 2H), 1.53 (s, 3H), 1.40 (s, 3H), 1.39-1.25 (m, 18H), 0.86 (t, *J* = 6.8 Hz, 3H); (**6-2Z)** 6.19 (dd, *J* = 12.0, 8.0 Hz, 1H), 5.84 (dd, *J* = 12.0, 1.6 Hz, 1H), 5.56-5.50 (m, 1H), 5.22-5.16 (m, 1H), 5.07-5.02 (m, 1H), 4.69 (dt, *J* = 4.8, 1.6 Hz, 1H), 4.14 (q, *J* = 6.8 Hz, 2H), 2.18-1.92 (m, 2H), 1.52 (s, 3H), 1.39 (s, 3H), 1.39-1.25 (m, 18H), 0.86 (t, *J* = 6.8 Hz, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 165.9 (C), 144.0 (CH), 135.5 (CH), 135.0 (CH), 125.1 (CH), 124.6 (CH), 122.6 (CH), 121.2 (CH), 119.1 (CH), 109.2 (C), 77.2 (CH), 75.4 (CH), 74.6 (CH), 74.2 (CH), 60.4 ($CH_2$), 60.3 ($CH_2$), 31.6 ($CH_2$), 31.5 ($CH_2$), 29.6 ($CH_2$), 29.4 ($CH_2$), 29.3 ($CH_2$), 29.3 ($CH_2$), 29.2 ($CH_2$), 29.0 ($CH_2$), 28.7 ($CH_2$), 28.1 ($CH_2$), 27.8 ($CH_2$), 27.6 ($CH_2$), 27.5 ($CH_2$), 25.4($CH_3$), 22.6 ($CH_2$), 14.2 ($CH_3$), 14.1 ($CH_3$); HRMS-ESI $[M + Na]^+$ Calcd for $C_{23}H_{40}O_4Na$ 403.2819, Found 403.2820.



7

**(4*S*,5*R*)-2,2-Dimethyl-4-methoxycarbonylethyl-5-tridecyl-1,3-dioxolane (7)** To a solution of **6** (400 mg, 1.05 mmol) in 5.3 mL of ethyl acetate at room temperature was added activated 10% Pd/C (38 mg). The reaction mixture was stirred for 1 h under a hydrogen atmosphere (60 psi) at the same temperature. After the reaction was complete, monitored by TLC (ethyl acetatec:*n*-hexane = 1:1 (v/v), $R_f$ = 0.7), it was

filtered through a short pad of Celite and the Celite pad was washed with ethyl acetate (15 mL). The filtrate obtained was concentrated in vacuo without further purification to yield saturated ester **7** as a syrup compound in 99% yield: $R_f$ = 0.25 (ethyl acetate:*n*-hexane = 1:20 (v/v)); $[\alpha]^{28}_D$ –14.5 (c 0.9, $CHCl_3$); FT-IR (neat) $\nu_{max}$ 3539, 2917, 2849, 1737, 1465, 1370, 1182, 1065, 877, 718 $cm^{-1}$; $^1H$ NMR (400 MHz, $CDCl_3$): δ 4.12 (q, *J* = 6.8, 2H), 4.10-40.0 (m, 2H), 2.60-2.30 (m, 2H), 1.80-1.60 (m, 2H), 1.40 (s, 3H), 1.31 (s, 3H), 1.24 (bs, 24H), 0.86 (t, *J* = 6.6 Hz, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 173.5 (C), 107.5 (C), 77.9 (CH), 76.8 (CH), 60.3 ($CH_2$), 32.0 ($CH_2$), 30.9 ($CH_2$), 30.8 ($CH_2$), 29.7 ($CH_2$), 29.7 ($CH_2$), 29.7 ($CH_2$), 29.6 ($CH_2$), 29.6 ($CH_2$), 29.5 ($CH_2$), 29.4 ($CH_2$), 26.4 ($CH_2$), 25.4 ($CH_2$), 22.7 ($CH_2$), 28.6 ($CH_3$), 25.9 ($CH_3$), 14.2 ($CH_3$), 14.1 ($CH_3$); HRMS-ESI $[M + Na]^+$ Calcd for $C_{23}H_{44}O_4Na$ 407.3132, Found 407.3134.

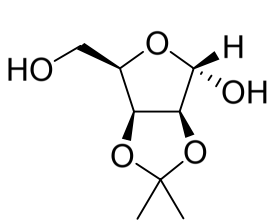



**2**

**(*S*)-(+)-5-((1*R*)-1-hydroxytetradecyl)-dihydrofuran-2(3*H*)-one (2)** To a solution of the ethyl ester **7** (60 mg, 0.16 mmol) in THF/$H_2O$ (3.9 mL, 10:3 v/v) was added conc. HCl (0.65 mL, 7.80 mmol) at 0 °C. After stirring at 0 °C for 10 min, the reaction mixture was kept stirring at 30 °C for additional 3 h. After the mixture was diluted with $Et_2O$, the solution was neutralized with saturated aqueous $NaHCO_3$ solution and then the neutralized aqueous layer was extracted with $Et_2O$, and the organic layer was washed with brine, dried over $MgSO_4$, and concentrated in vacuo. The residue was chromatographed on a silica gel column (ethyl acetate:*n*-hexane = 1:3) to obtain 41 mg of the product **2** as a white solid compound in 88% yield: $R_f$ = 0.2 (ethyl acetate:*n*-hexane = 1:3 (v/v)); mp = 48-50 °C; $[\alpha]^{28}_D$ +10.0 (c 0.4, $CHCl_3$); FT-IR (neat) $\nu_{max}$ 3539, 3413, 2954, 2917, 2848, 2360, 2341, 1757, 1460, 1189 $cm^{-1}$; $^1H$ NMR (300 MHz, $CDCl_3$): δ 4.44 (td, *J* = 7.2 Hz, 1H), 4.00-3.90 (m, 1H), 2.70-2.40 (m, 2H), 2.40-2.00. (m, 2H), 1.86 (s, 1H), 1.70-1.40 (m, 2H), 1.26 (bs, 22H), 0.88 (t, *J* = 6.0 Hz, 3H); $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 177.6 (C), 82.9 (CH), 71.3 (CH), 31.9 ($CH_2$), 31.8 ($CH_2$), 29.7 ($CH_2$), 29.6 ($CH_2$), 29.6 ($CH_2$), 29.5 ($CH_2$), 29.5 ($CH_2$), 29.5 ($CH_2$) 29.32 ($CH_2$), 28.7 ($CH_2$), 25.6 ($CH_2$), 22.7 ($CH_2$), 21.0 ($CH_2$), 14.1 ($CH_3$); HRMS-ESI $[M + Na]^+$ Calcd for $C_{18}H_{34}O_3Na$ 321.2400, Found 321.2400.

**References**

1. D. D. Perrin, W. L. F. Armarego and D. R. Perrin, *Purification of Laboratory Chemicals*, 2nd ed., Pergamon Press: New York, 1980.
2. W. C. Still, M. Kahn and A. Mitra, *J. Org. Chem.*, 1978, **43**, 2923.




**3**

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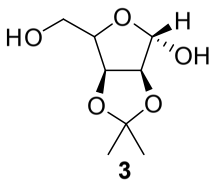


**3**

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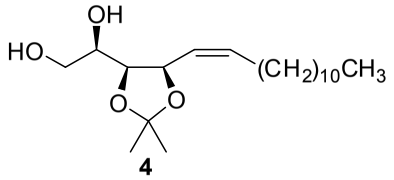


**4**

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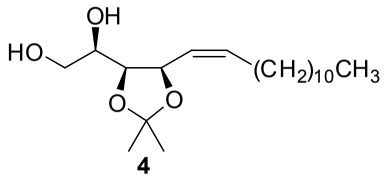


4

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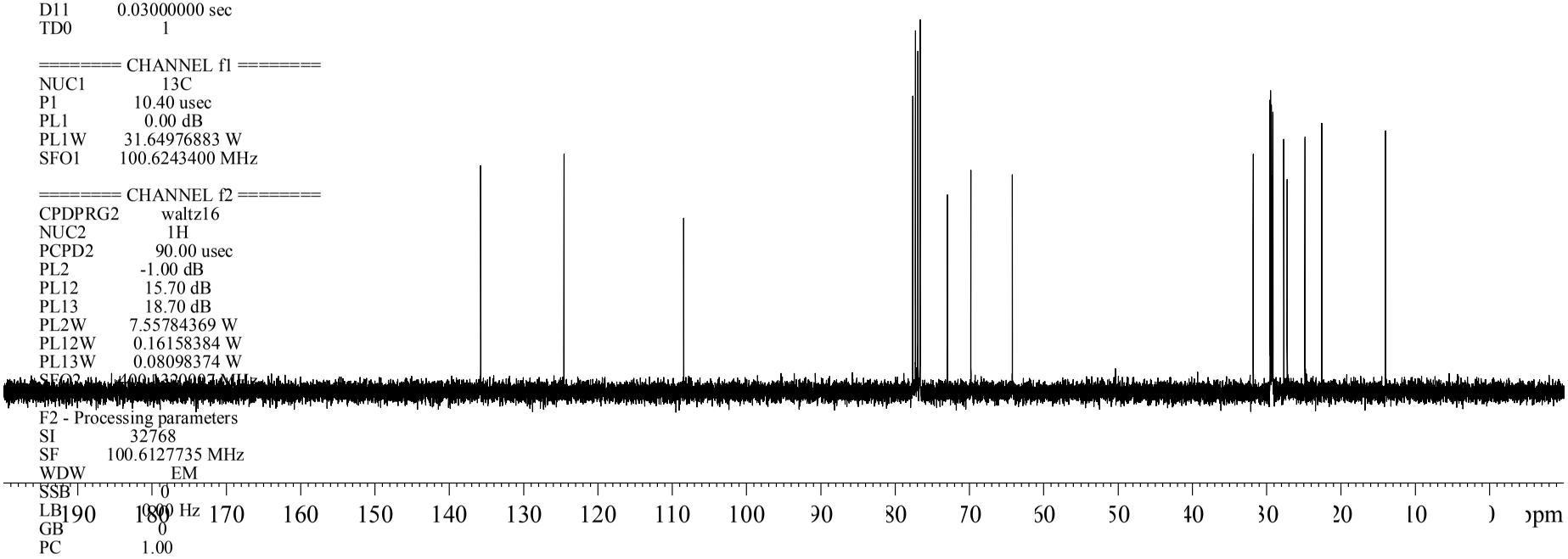
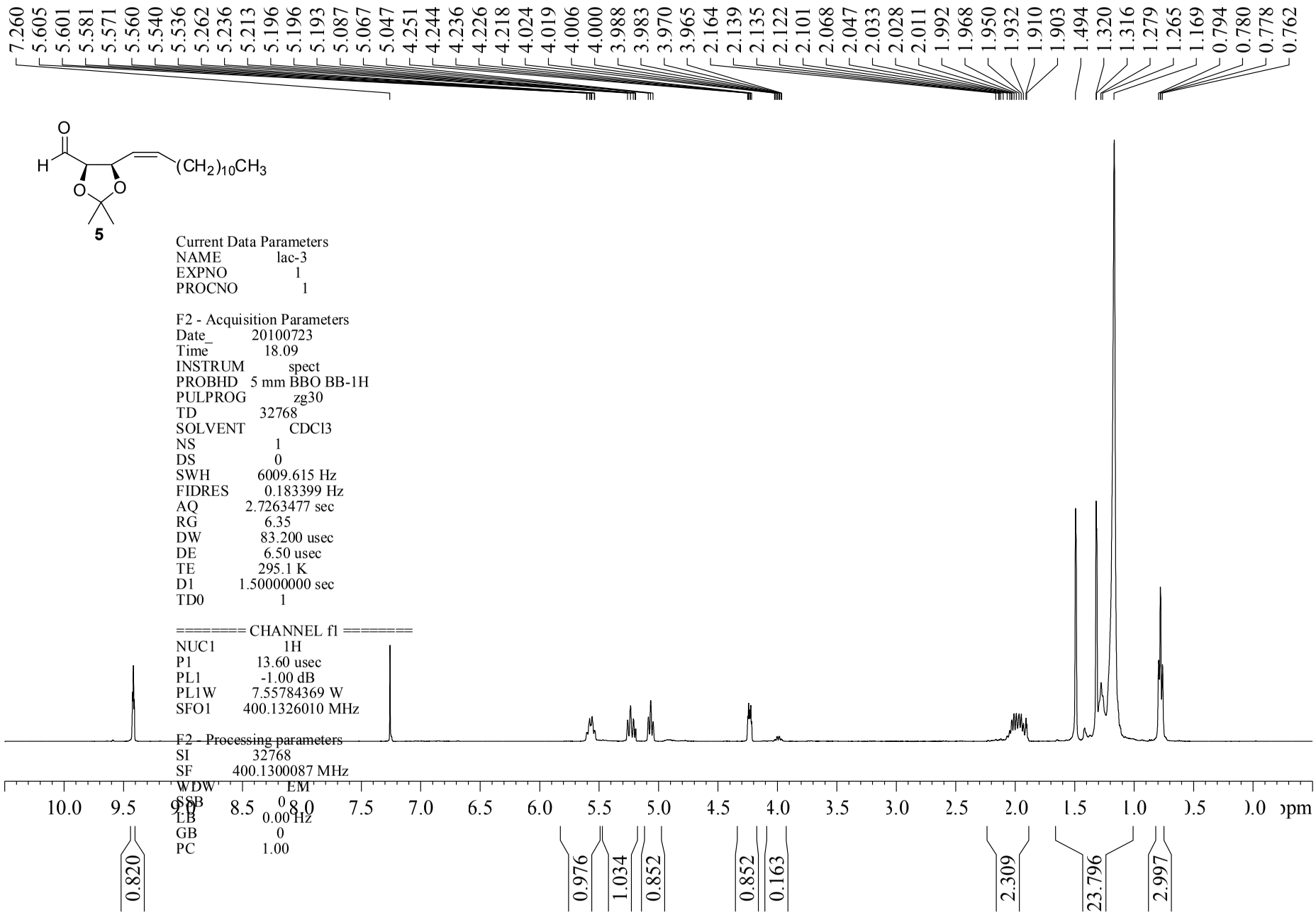
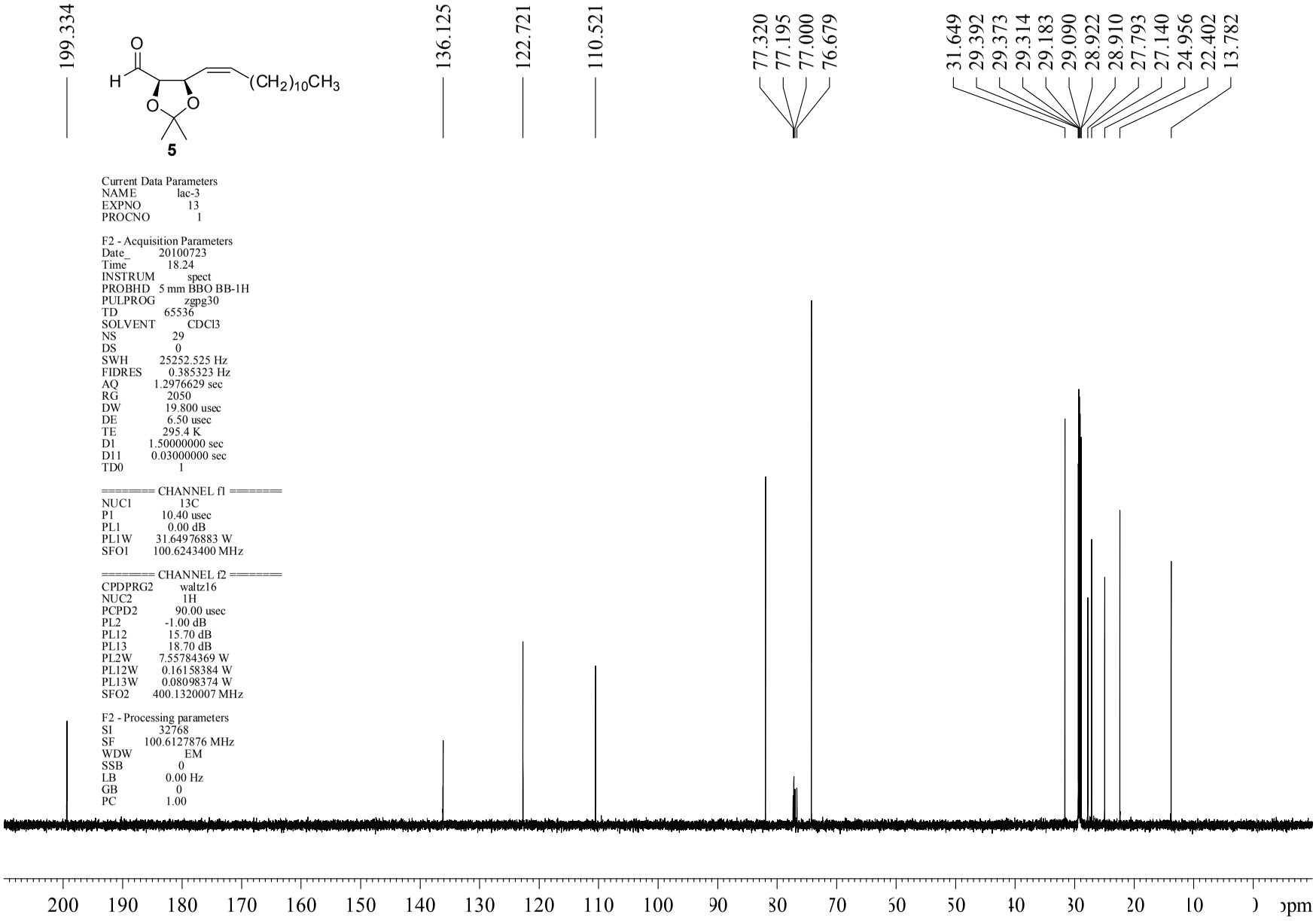
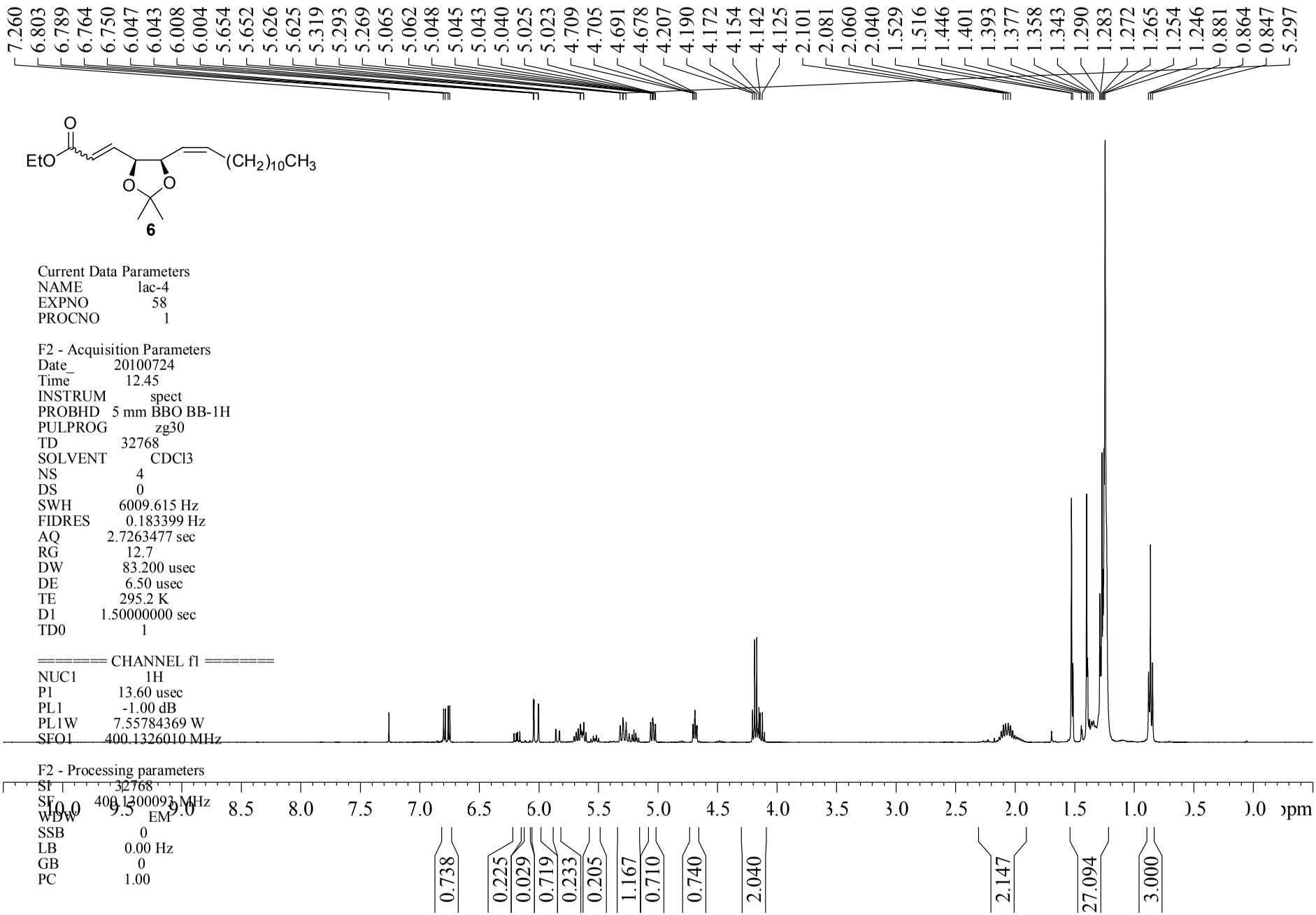
PL12W 0.16158384 W
PL13W 0.08098374 W
SFO2 400.1320097 MHz

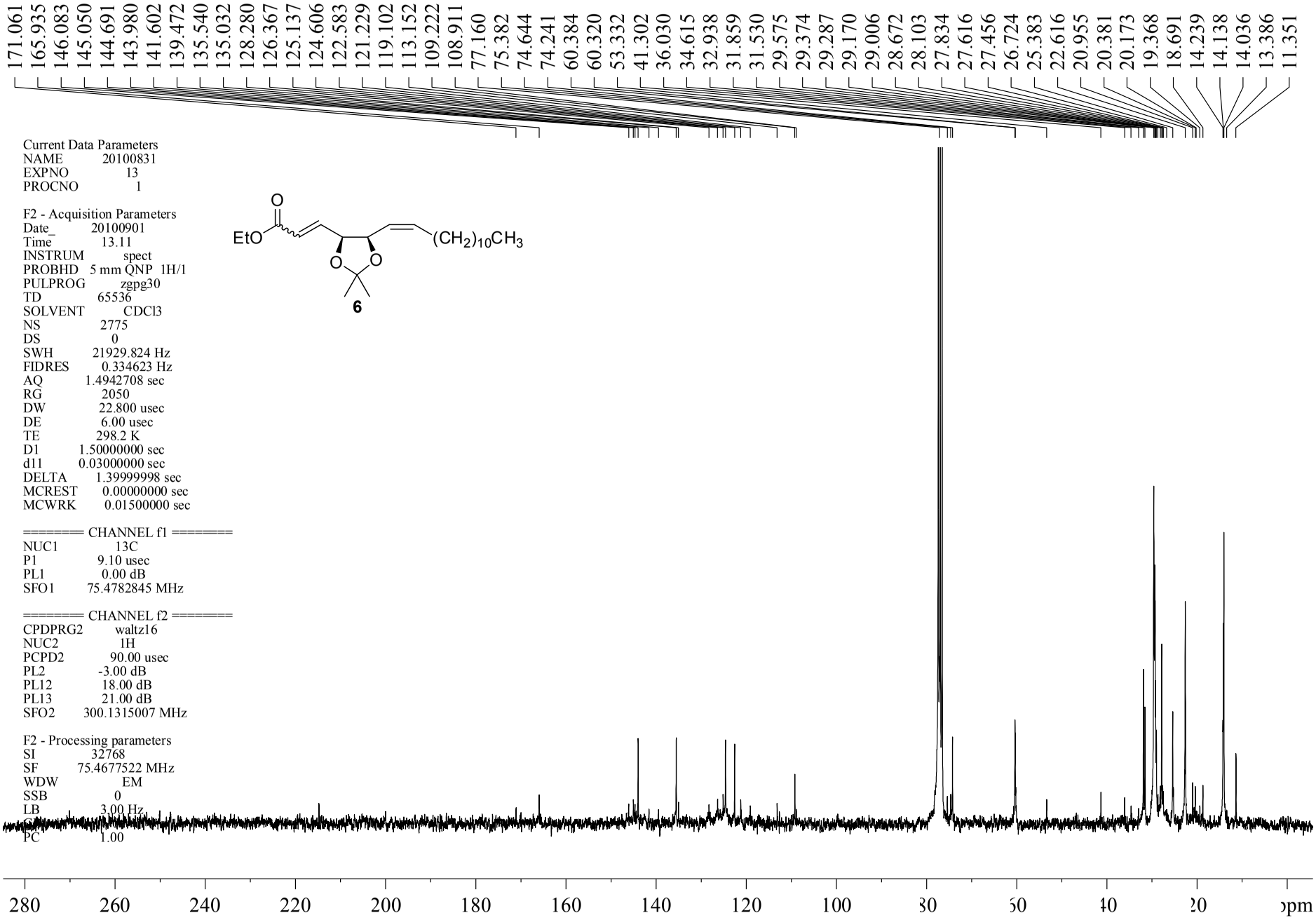
F2 - Processing parameters
SI 32768
SF 100.6127735 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

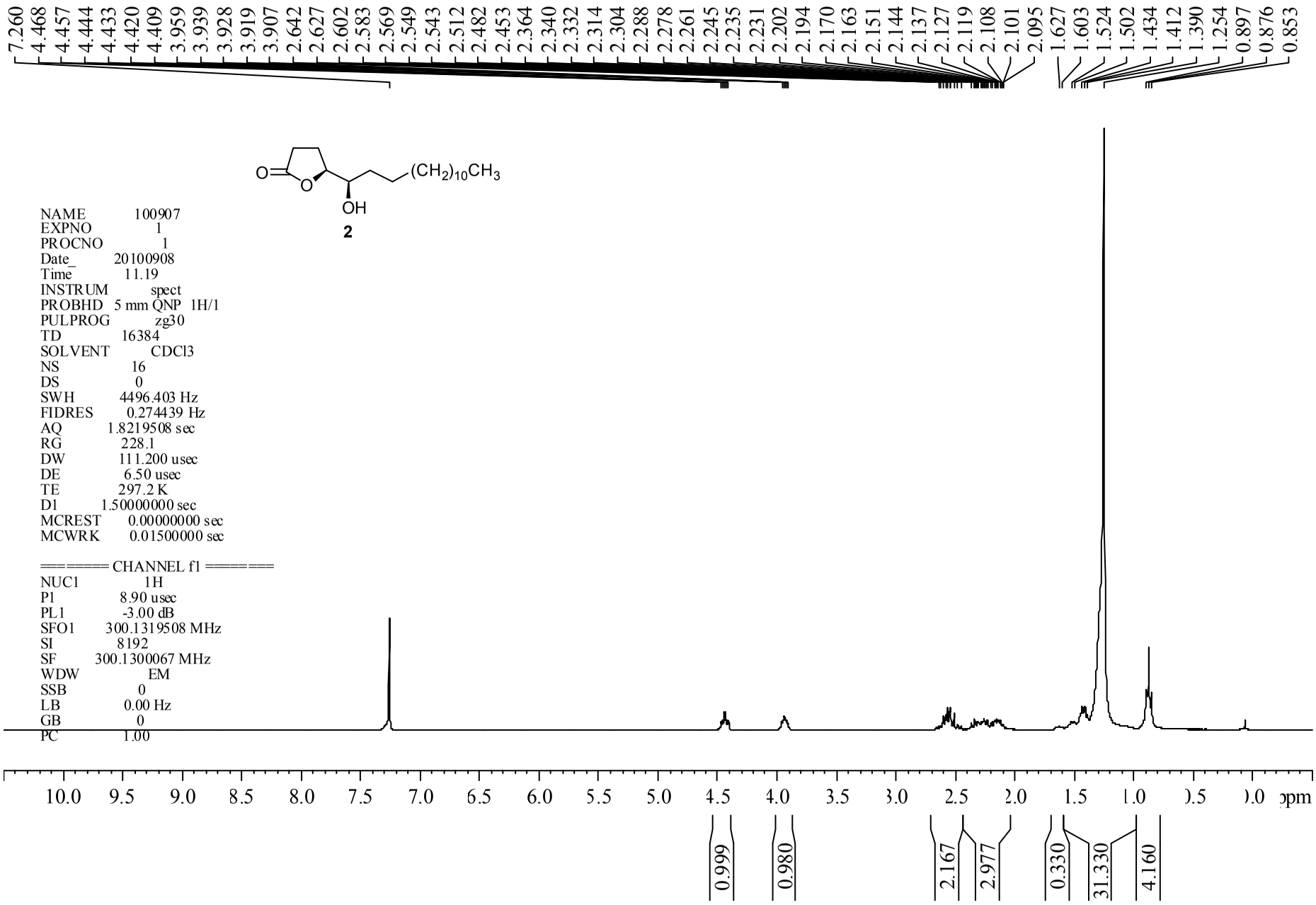


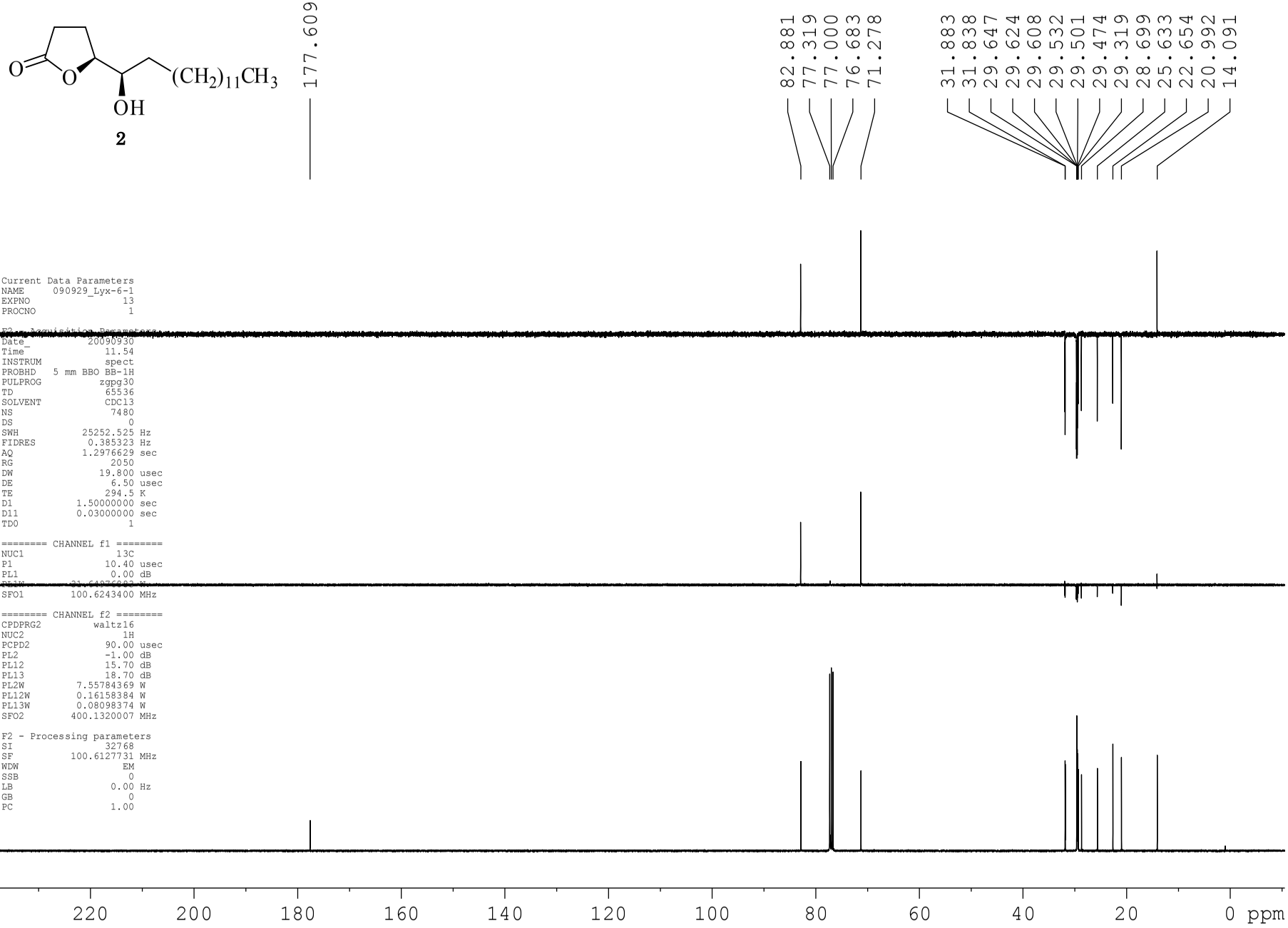

7.260
5.605
5.601
5.581
5.571
5.560
5.540
5.536
5.262
5.236
5.213
5.196
5.196
5.193
5.087
5.067
5.047
4.251
4.244
4.236
4.226
4.218
4.024
4.019
4.006
4.000
3.988
3.983
3.970
3.965
2.164
2.139
2.135
2.122
2.101
2.068
2.047
2.033
2.028
2.011
1.992
1.968
1.950
1.932
1.910
1.903
1.494
1.320
1.316
1.279
1.265
1.169
0.794
0.780
0.778
0.762
O
H
O
O
(CH2)10CH3
5
Current Data Parameters
NAME lac-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100723
Time 18.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 6.35
DW 83.200 usec
DE 6.50 usec
TE 295.1 K
D1 1.50000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
PL1W 7.55784369 W
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 32768
SF 400.1300087 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.820
0.976
1.034
0.852
0.852
0.163
2.309
23.796
2.997


199.334
136.125
122.721
110.521
77.320
77.195
77.000
76.679
31.649
29.392
29.373
29.314
29.183
29.090
28.922
28.910
27.793
27.140
24.956
22.402
13.782
O
H
O
O
(CH2)10CH3
5
Current Data Parameters
NAME lac-3
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100723
Time 18.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 29
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 295.4 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.40 usec
PL1 0.00 dB
PL1W 31.64976883 W
SFO1 100.6243400 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.70 dB
PL13 18.70 dB
PL2W 7.55784369 W
PL12W 0.16158384 W
PL13W 0.08098374 W
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127876 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.260
6.803
6.789
6.764
6.750
6.047
6.043
6.008
6.004
5.654
5.652
5.626
5.625
5.319
5.293
5.269
5.065
5.062
5.048
5.045
5.043
5.040
5.025
5.023
4.709
4.705
4.691
4.678
4.207
4.190
4.172
4.154
4.142
4.125
2.101
2.081
2.060
2.040
1.529
1.516
1.446
1.401
1.393
1.377
1.358
1.343
1.290
1.283
1.272
1.265
1.254
1.246
0.881
0.864
0.847
5.297
EtO
O
O
O
(CH2)10CH3
6
Current Data Parameters
NAME lac-4
EXPNO 58
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100724
Time 12.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 12.7
DW 83.200 usec
DE 6.50 usec
TE 295.2 K
D1 1.50000000 sec
TD0 1
======= CHANNEL f1 =======
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
PL1W 7.55784369 W
SFO1 400.1326010 MHz
F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.738
0.225
0.029
0.719
0.233
0.205
1.167
0.710
0.740
2.040
2.147
27.094
3.000


171.061
165.935
146.083
145.050
144.691
143.980
141.602
139.472
135.540
135.032
128.280
126.367
125.137
124.606
122.583
121.229
119.102
113.152
109.222
108.911
77.160
75.382
74.644
74.241
60.384
60.320
53.332
41.302
36.030
34.615
32.938
31.859
31.530
29.575
29.374
29.287
29.170
29.006
28.672
28.103
27.834
27.616
27.456
26.724
25.383
22.616
20.955
20.381
20.173
19.368
18.691
14.239
14.138
14.036
13.386
11.351
Current Data Parameters
NAME 20100831
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100901
Time 13.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2775
DS 0
SWH 21929.824 Hz
FIDRES 0.334623 Hz
AQ 1.4942708 sec
RG 2050
DW 22.800 usec
DE 6.00 usec
TE 298.2 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 9.10 usec
PL1 0.00 dB
SFO1 75.4782845 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 21.00 dB
SFO2 300.1315007 MHz
F2 - Processing parameters
SI 32768
SF 75.4677522 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
EtO
O
O
(CH2)10CH3
6
280
260
240
220
200
180
160
140
120
100
80
60
40
20
ppm


7.260
4.468
4.457
4.444
4.433
4.420
4.409
3.959
3.939
3.928
3.919
3.907
2.642
2.627
2.602
2.583
2.569
2.549
2.543
2.512
2.482
2.453
2.364
2.340
2.332
2.314
2.304
2.288
2.278
2.261
2.245
2.235
2.231
2.202
2.194
2.170
2.163
2.151
2.144
2.137
2.127
2.119
2.108
2.101
2.095
1.627
1.603
1.524
1.502
1.434
1.412
1.390
1.254
0.897
0.876
0.853
O
O
OH
(CH2)10CH3
2
NAME 100907
EXPNO 1
PROCNO 1
Date_ 20100908
Time 11.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 4496.403 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 228.1
DW 111.200 usec
DE 6.50 usec
TE 297.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.90 usec
PL1 -3.00 dB
SFO1 300.1319508 MHz
SI 8192
SF 300.1300067 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.999
0.980
2.167
2.977
0.330
31.330
4.160


O
O
OH
(CH2)11CH3
2
177.609
82.881
77.319
77.000
76.683
71.278
31.883
31.838
29.647
29.624
29.608
29.532
29.501
29.474
29.319
28.699
25.633
22.654
20.992
14.091
Current Data Parameters
NAME 090929_Lyx-6-1
EXPNO 13
PROCNO 1
Date_ 20090930
Time 11.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 7480
DS 0
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 294.5 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.40 usec
PL1 0.00 dB
SFO1 100.6243400 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 15.70 dB
PL13 18.70 dB
PL2W 7.55784369 W
PL12W 0.16158384 W
PL13W 0.08098374 W
SFO2 400.1320007 MHz
F2 - Processing parameters
SI 32768
SF 100.6127731 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
220
200
180
160
140
120
100
80
60
40
20
0 ppm