

Supporting Information

Total Synthesis of Squafosacin F: Stereodivergent Approach to Mono-tetrahydrofuran

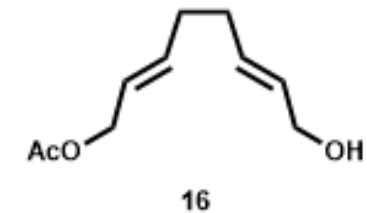
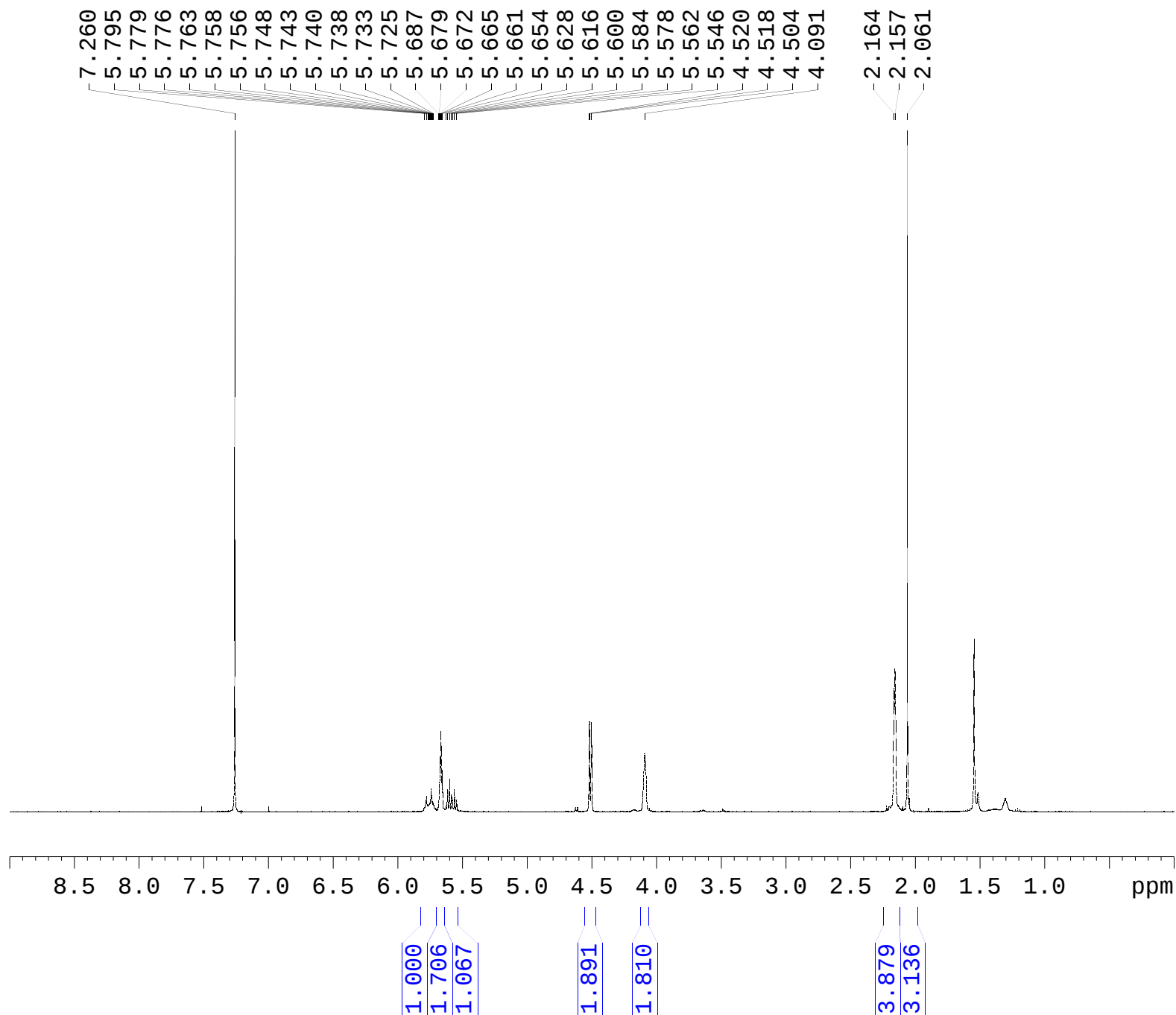
Acetogenins

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Miyaoka*

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Current Data Parameters
 NAME Compound 16
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160603
 Time 16.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 104.97
 DW 62.400 usec
 DE 6.50 usec
 TE 299.9 K
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 TD0 1

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 NUC1 1H
 P1 10.00 usec
 PLW1 16.50000000 W

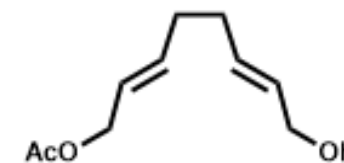
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—170.876

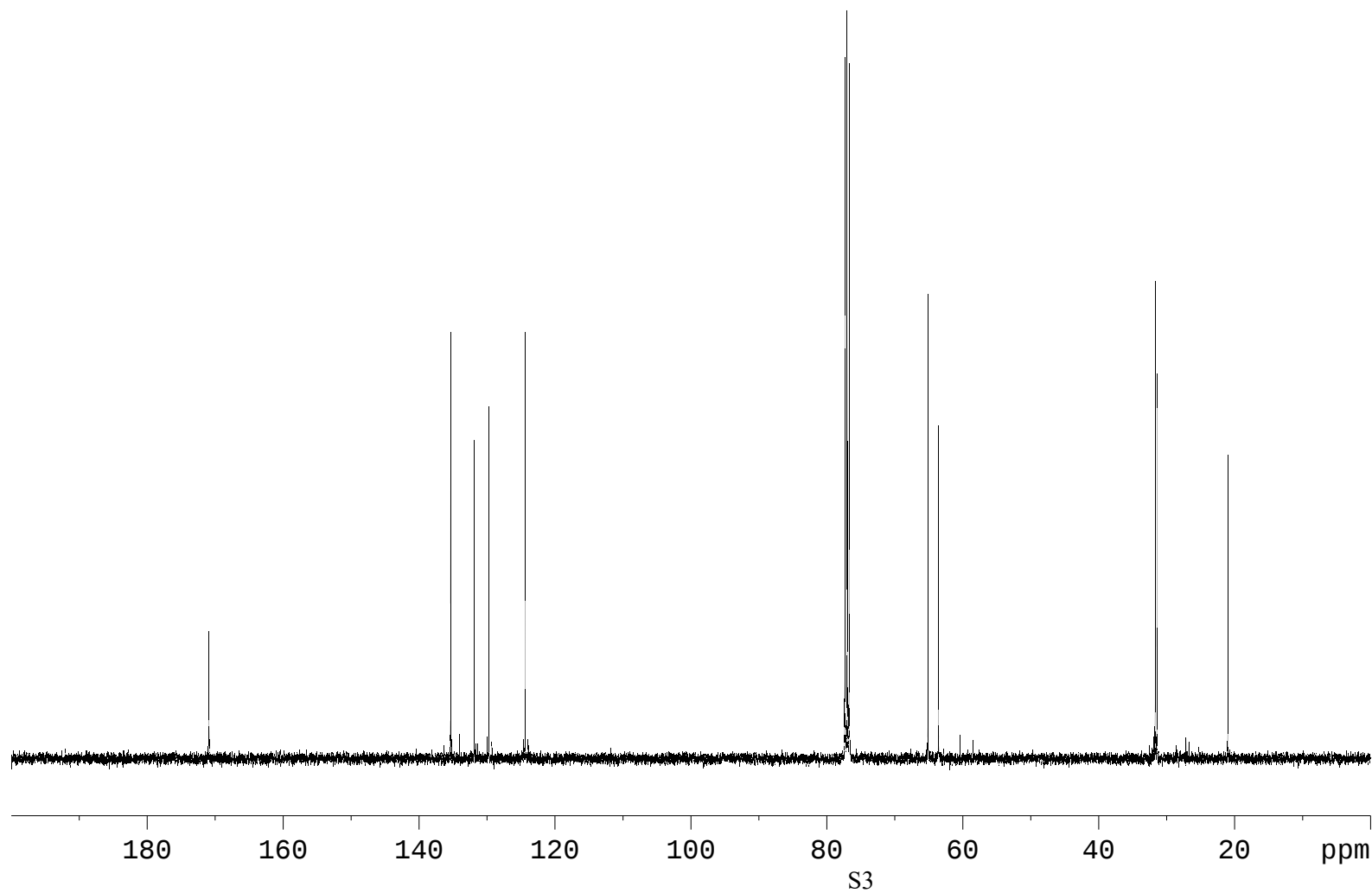
135.355
131.850
129.701
124.391

77.314
76.996
76.679
65.107
63.564

31.664
31.405
—20.969



16

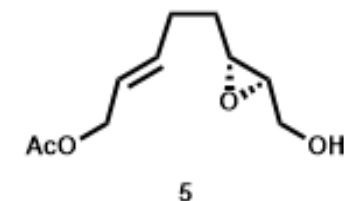
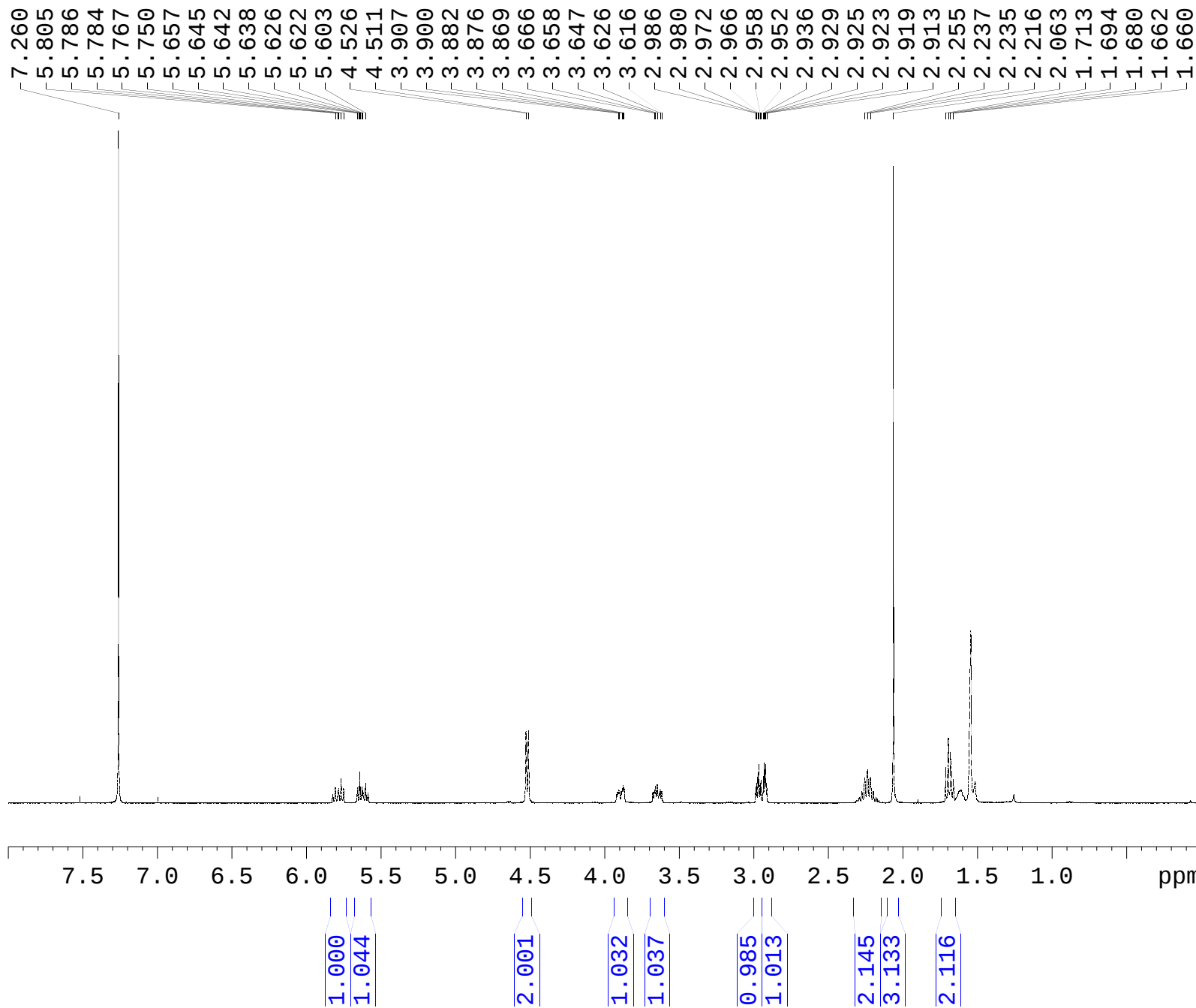


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PROCNO 1

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TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.25
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6354031 MHz
NUC1 13C
P1 10.00 usec
PLW1 63.50000000 W

===== CHANNEL f2 =====
SF02 400.1816007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.50000000 W
PLW12 0.20370001 W
PLW13 0.16500001 W

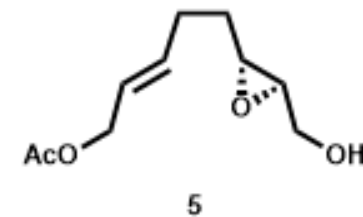
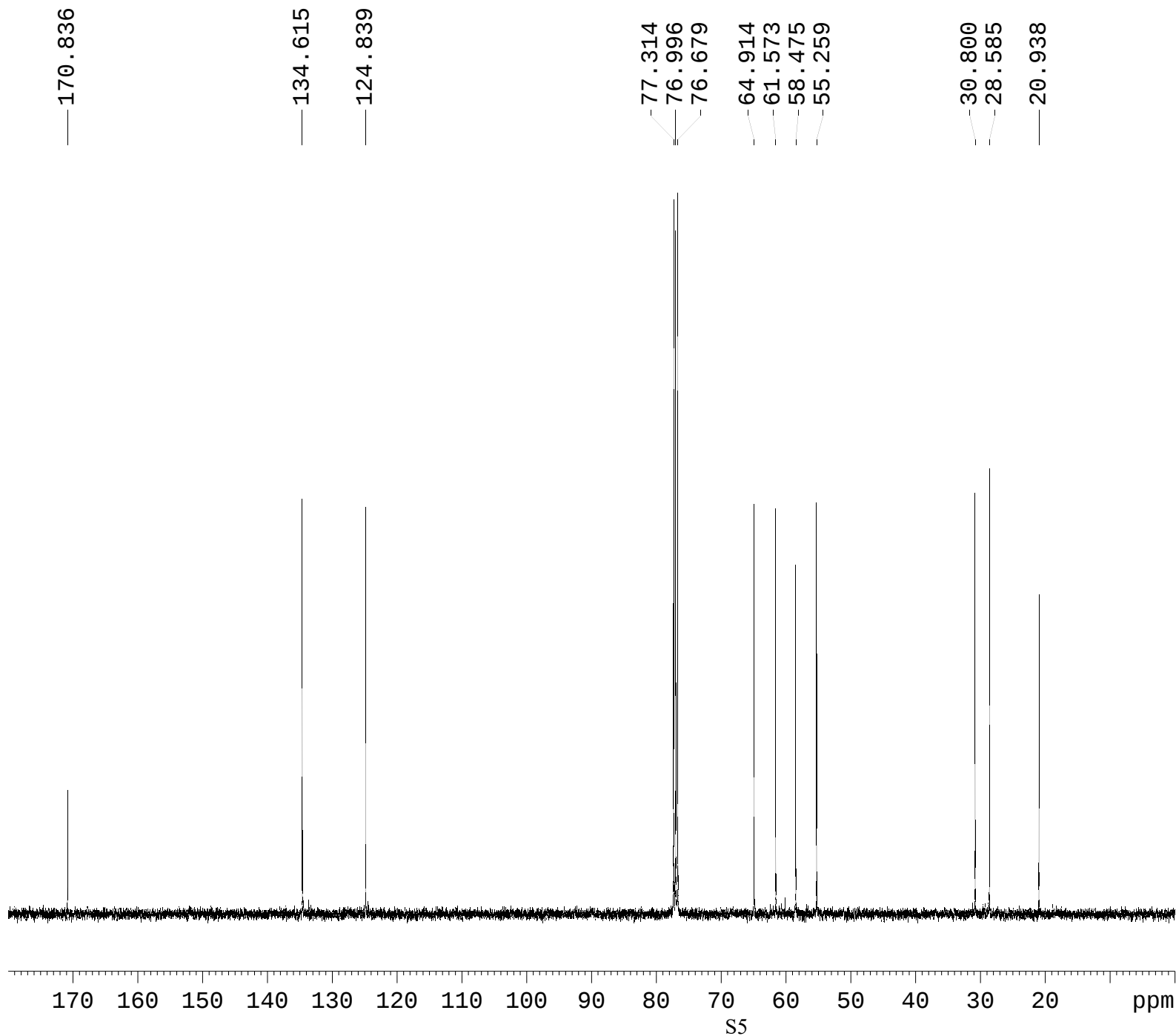


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 PROCNO 1

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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 165.31
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1824713 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.50000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1800095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



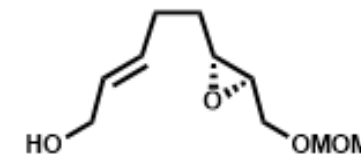
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.25
 DW 20.800 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

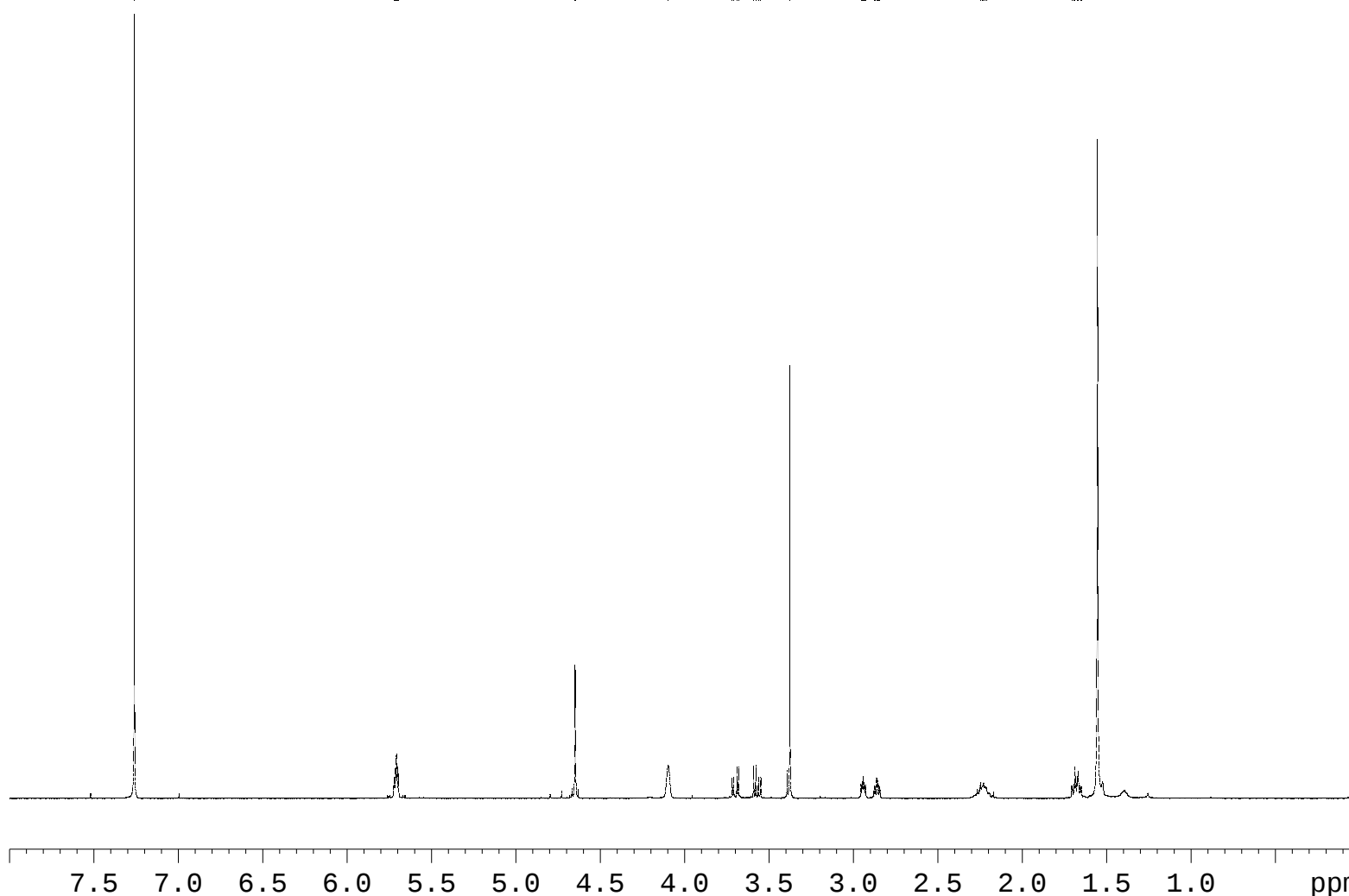
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 NUC1 13C
 P1 10.00 usec
 PLW1 63.50000000 W

===== CHANNEL f2 =====
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 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.50000000 W
 PLW12 0.20370001 W
 PLW13 0.16500001 W

7.260
5.721
5.718
5.713
5.708
5.706
5.701
5.695
4.650
4.647
4.097
3.718
3.709
3.689
3.680
3.591
3.578
3.562
3.549
3.376
2.955
2.949
2.945
2.940
2.936
2.932
2.926
2.876
2.871
2.862
2.857
2.848
2.842
2.247
2.235
2.229
2.219
2.213
1.706
1.702
1.693
1.687
1.674
1.669
1.655
1.649



6



1.826

2.000

1.945

1.045

1.038

2.902

0.995

0.991

2.009

2.026

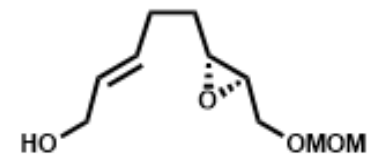
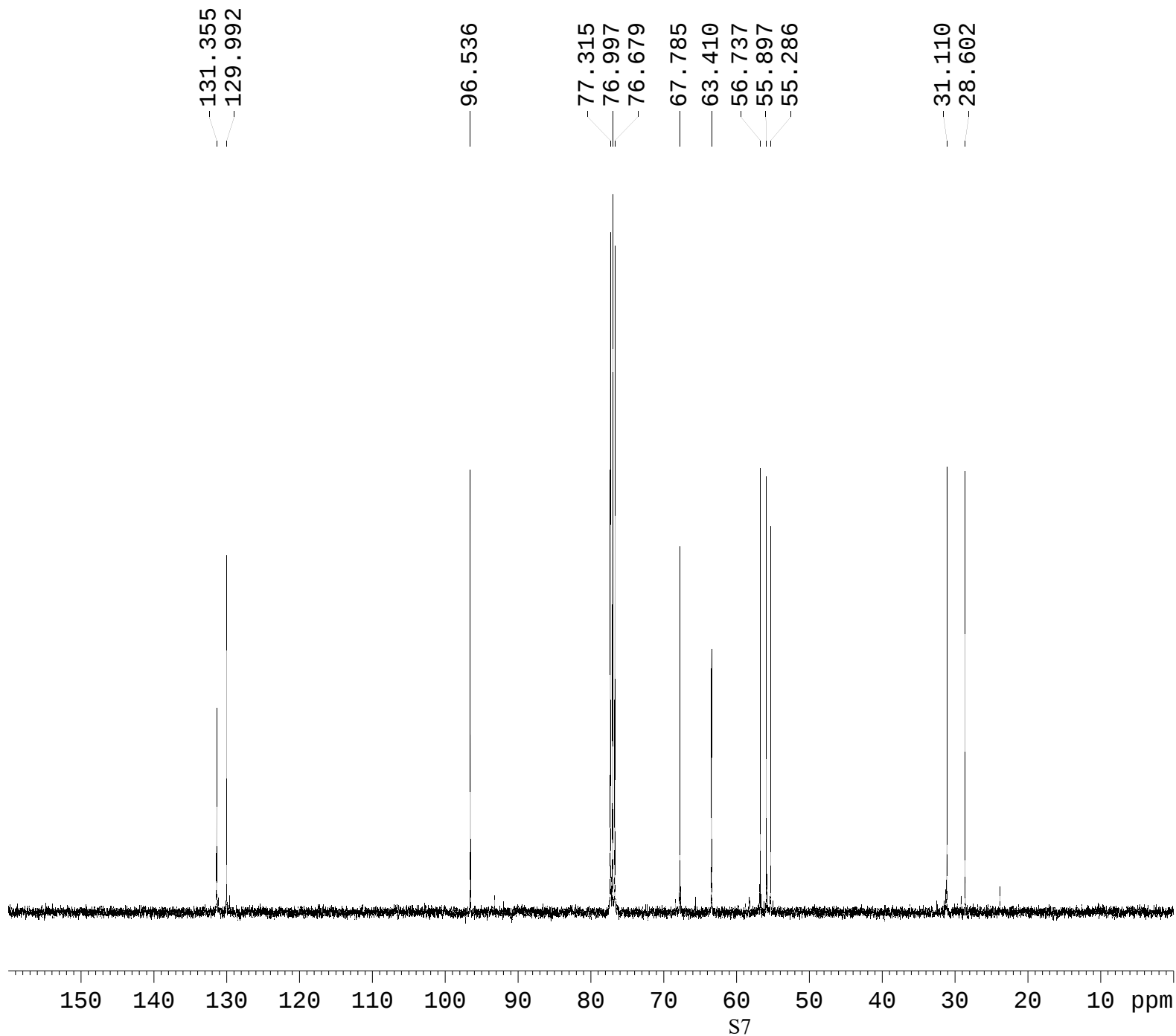
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EXPNO 1
PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 165.31
DW 62.400 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1824713 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.50000000 W

F2 - Processing parameters
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SF 400.1800094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S6



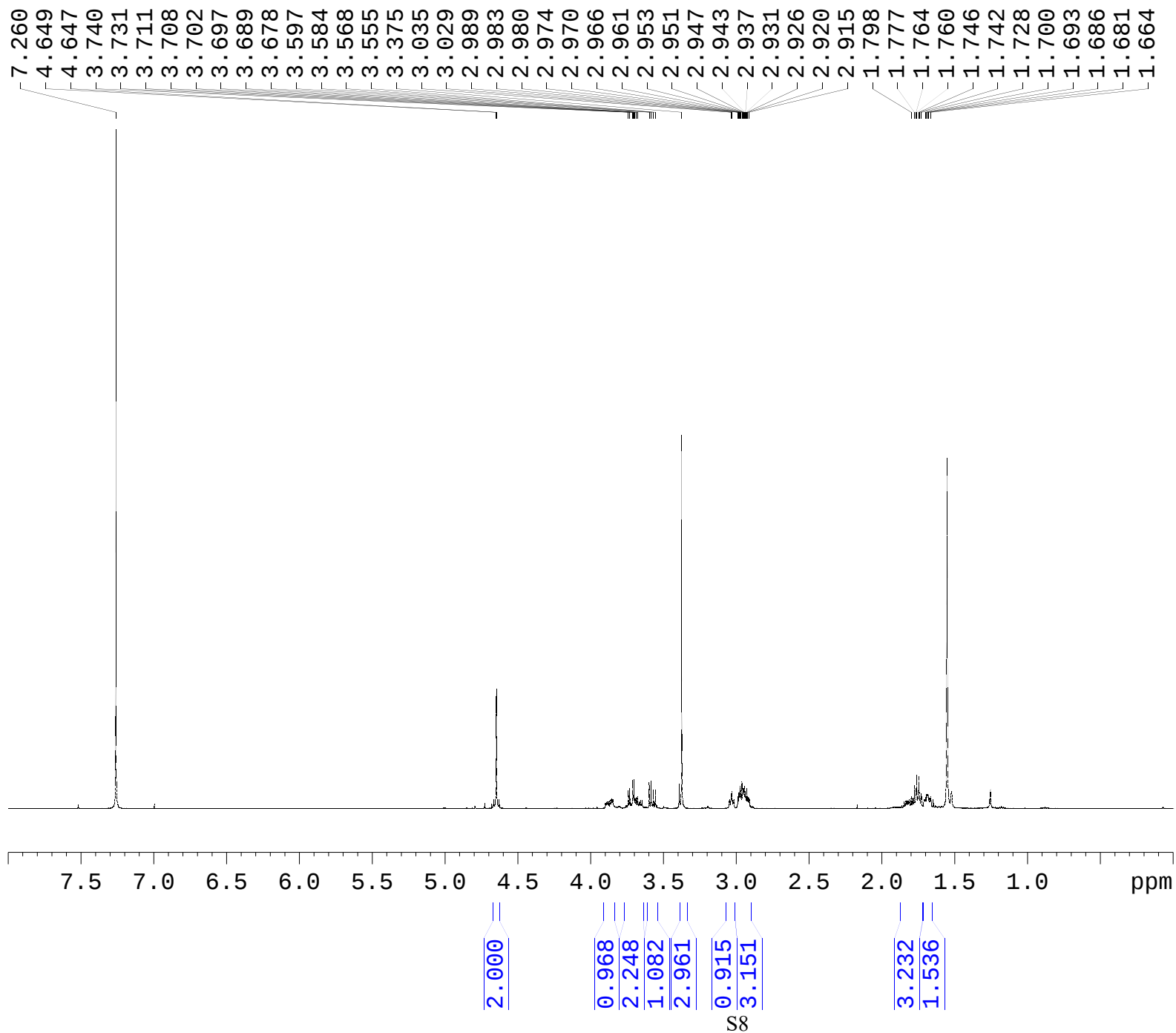
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Current Data Parameters
NAME Compound 6
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 15.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.25
DW 20.800 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6354031 MHz
NUC1 13C
P1 10.00 usec
PLW1 63.50000000 W

===== CHANNEL f2 =====
SF02 400.1816007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.50000000 W
PLW12 0.20370001 W
PLW13 0.16500001 W



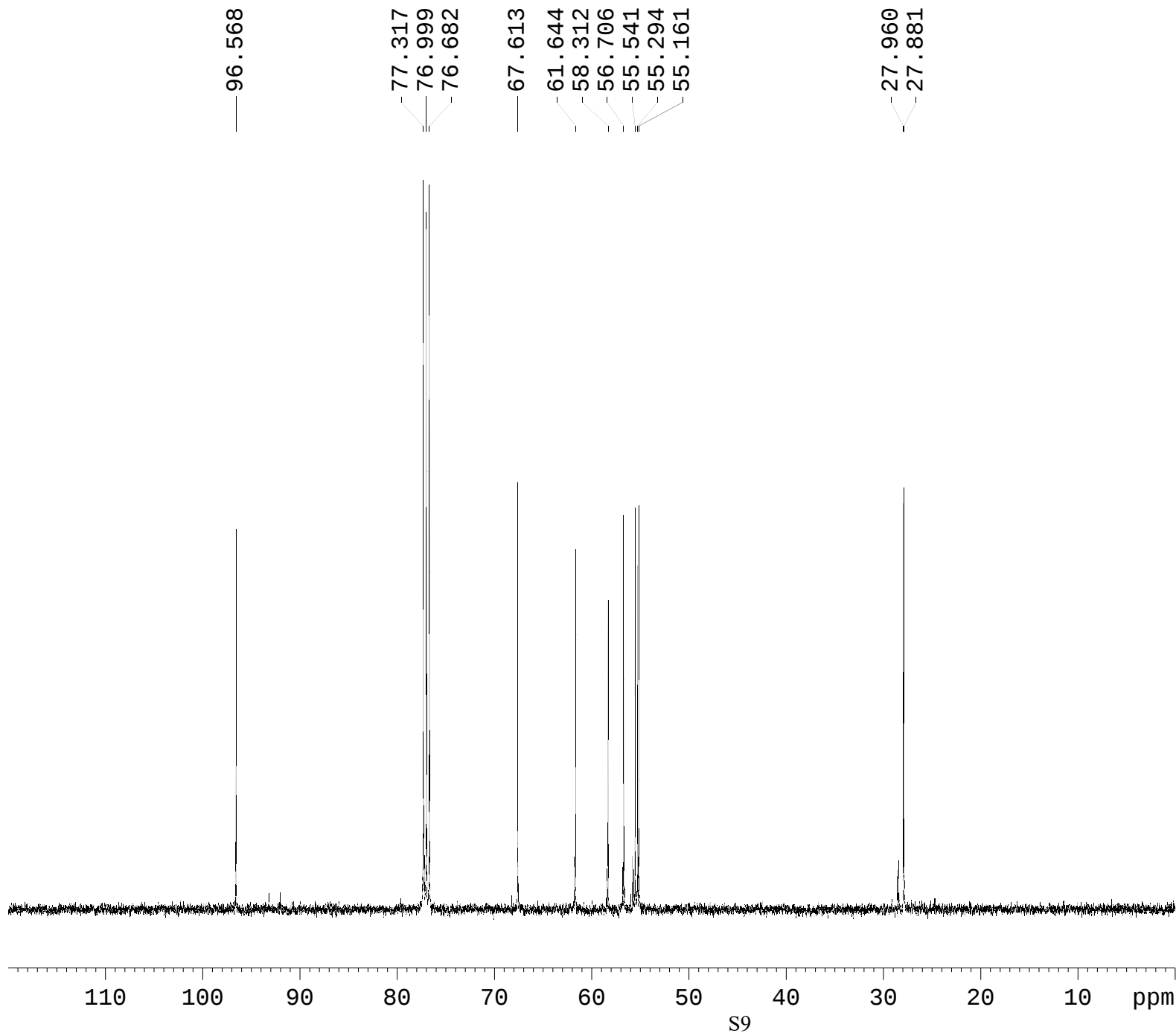
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Current Data Parameters
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
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 Time 12.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 165.31
 DW 62.400 usec
 DE 6.50 usec
 TE 300.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1824713 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.50000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1800097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



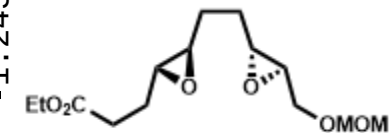
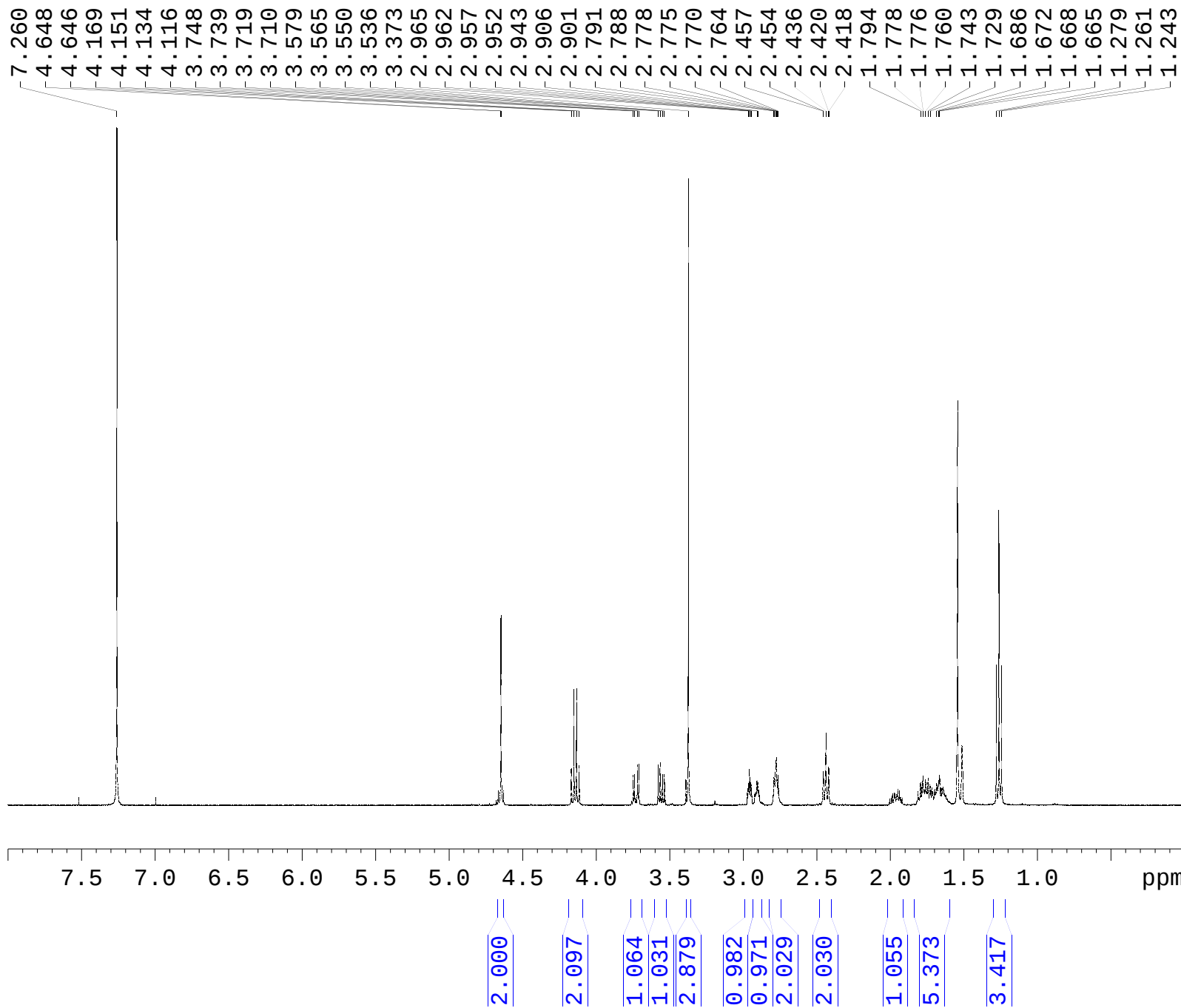
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Current Data Parameters
NAME Compound 17
EXPNO 1
PROCNO 1

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.25
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6354031 MHz
NUC1 13C
P1 10.00 usec
PLW1 63.50000000 W

===== CHANNEL f2 =====
SF02 400.1816007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.50000000 W
PLW12 0.20370001 W
PLW13 0.16500001 W



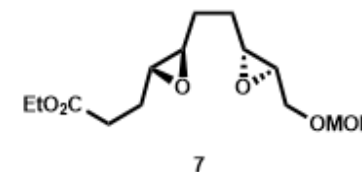
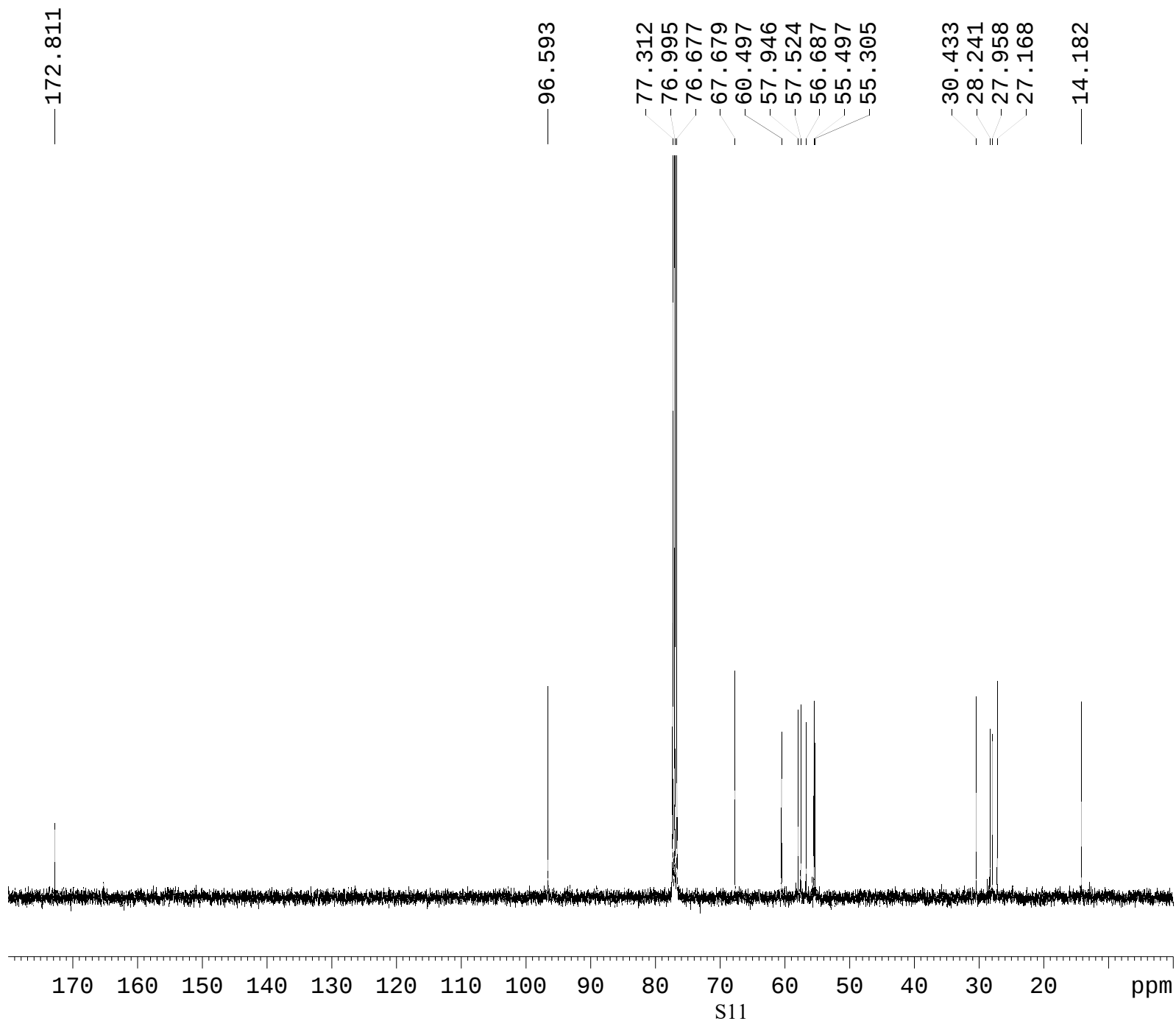
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Current Data Parameters
 NAME Compound 7
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160622
 Time 17.58
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 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 165.31
 DW 62.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1824713 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.50000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1800095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

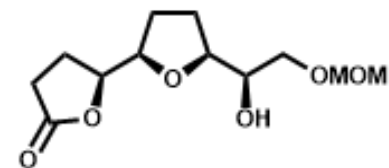
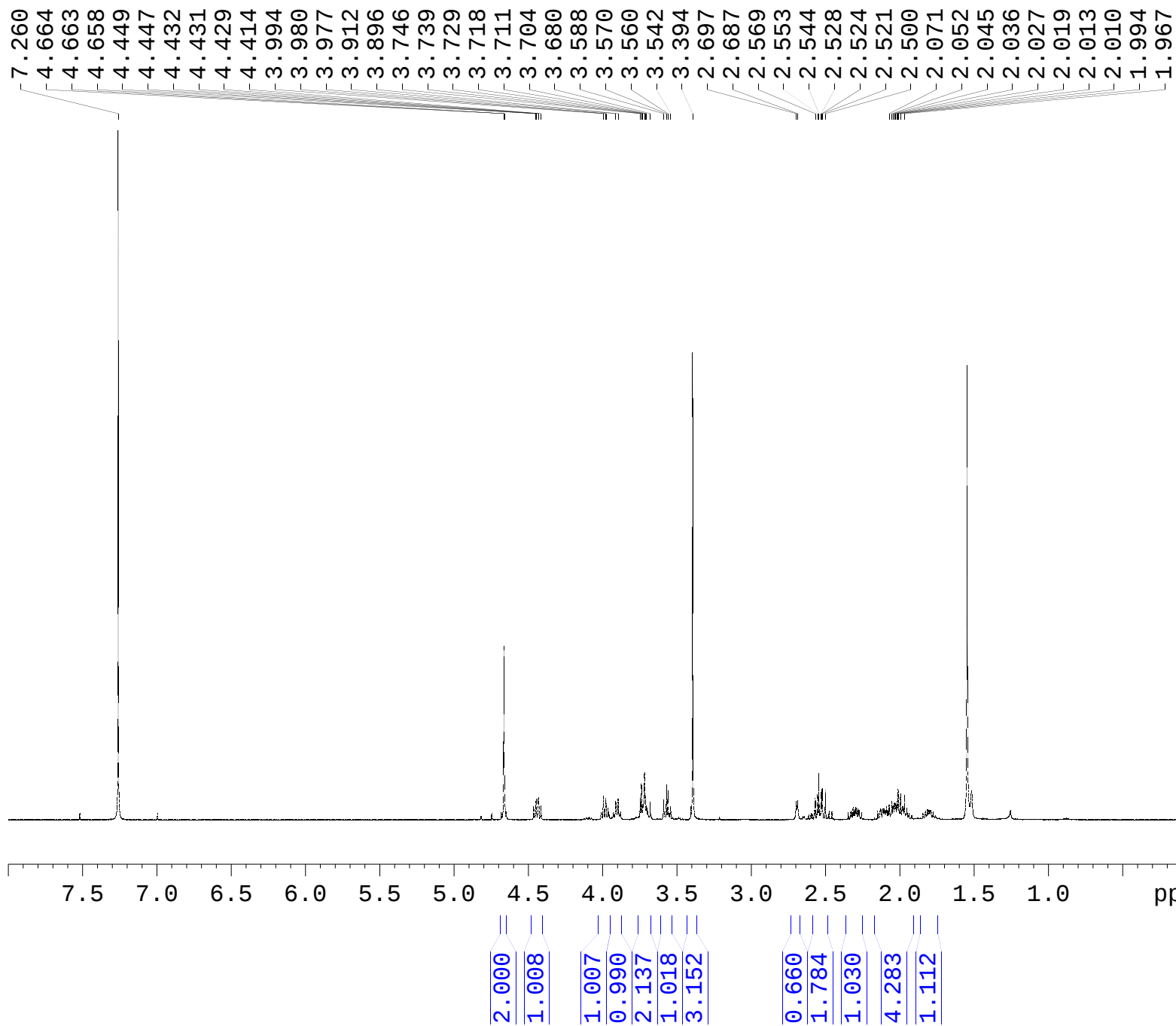


Current Data Parameters
 NAME Compound 7
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160622
 Time 19.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.25
 DW 20.800 usec
 DE 6.50 usec
 TE 300.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 100.6354031 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 63.50000000 W

===== CHANNEL f2 =====
 SF02 400.1816007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.50000000 W
 PLW12 0.20370001 W
 PLW13 0.16500001 W



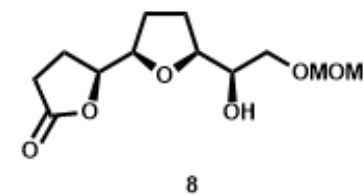
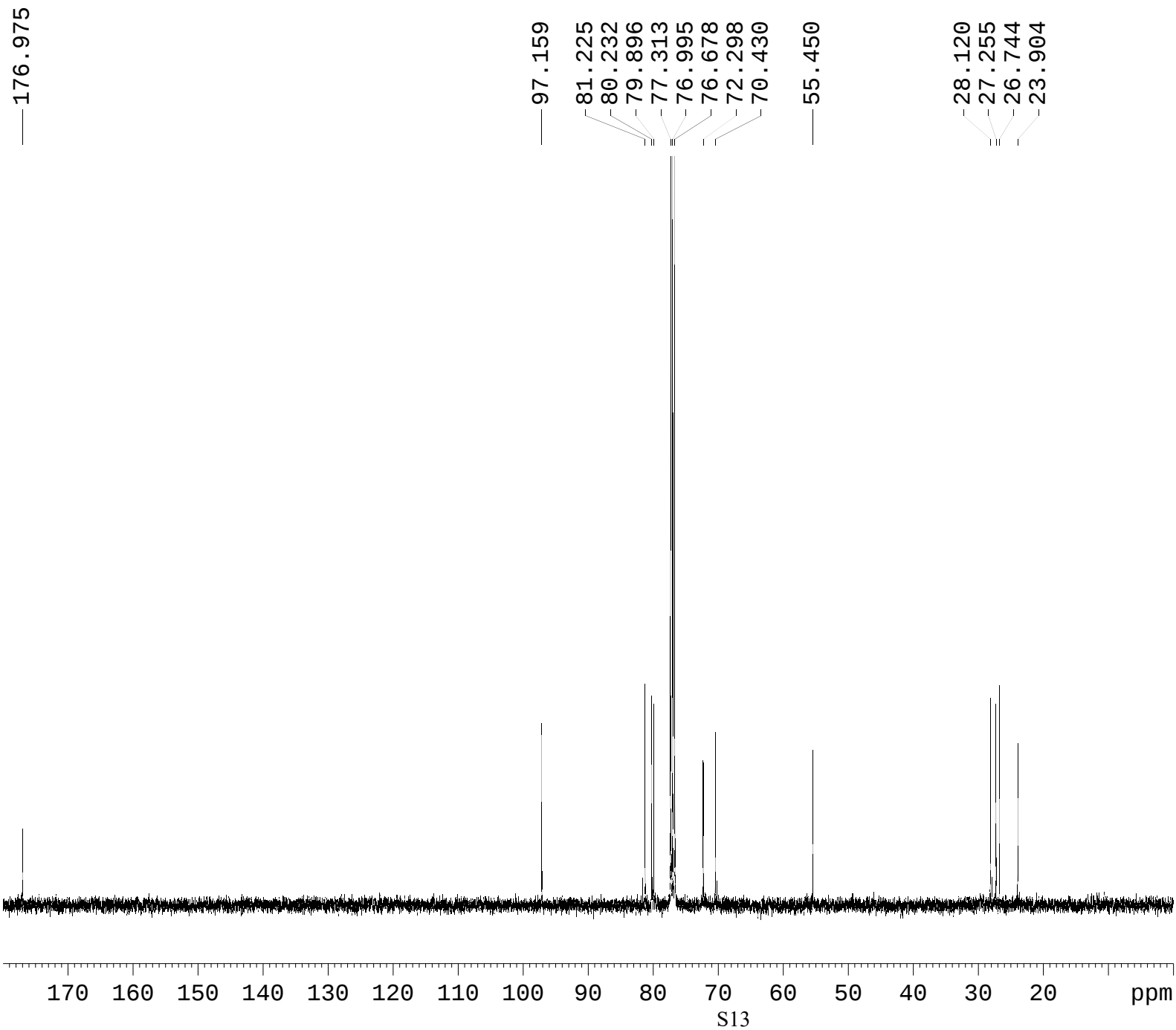
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Current Data Parameters
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PROCNO 1

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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 184.75
DW 62.400 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1824713 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1800097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

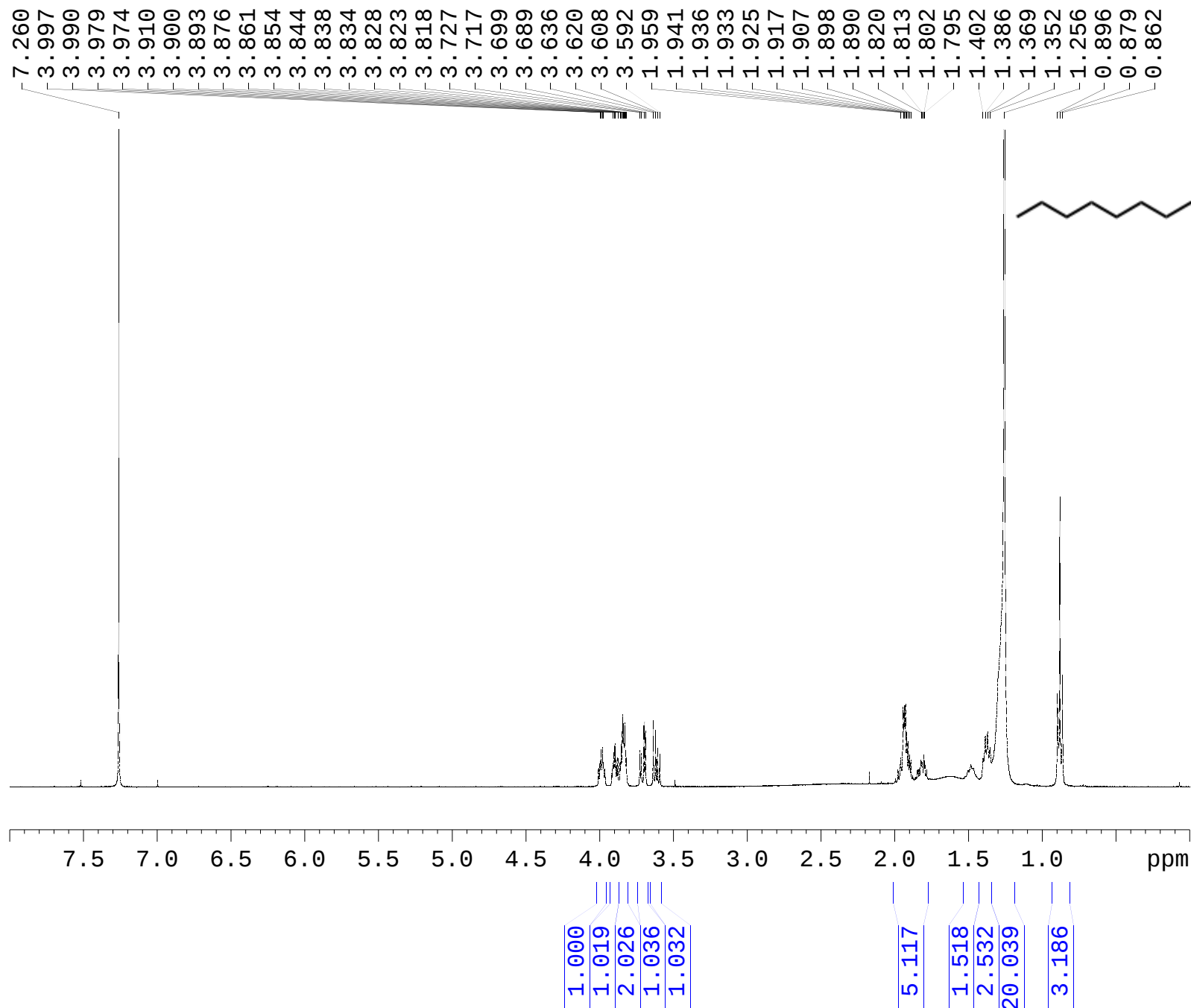


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 NAME Compound 8
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 PROCNO 1

F2 - Acquisition Parameters
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 Time 18.29
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.25
 DW 20.800 usec
 DE 6.50 usec
 TE 299.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 100.6354031 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 63.50000000 W

===== CHANNEL f2 =====
 SF02 400.1816007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 16.50000000 W
 PLW12 0.20370001 W
 PLW13 0.16500001 W

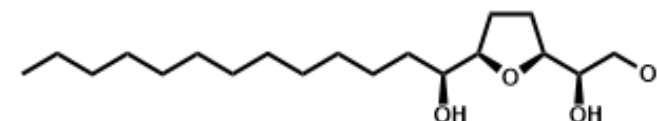
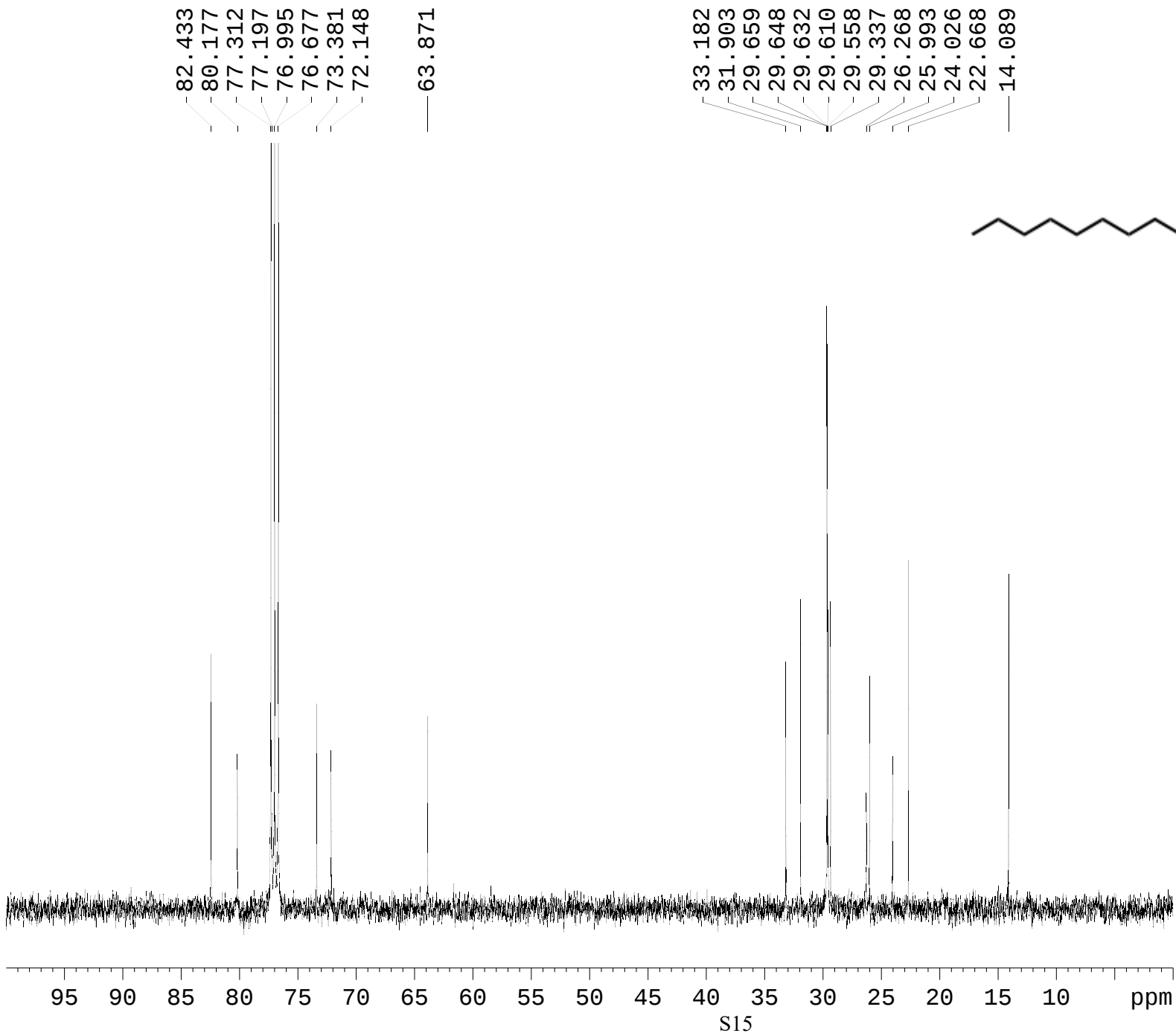


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 PROCNO 1

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 PULPROG zg30
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 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 104.97
 DW 62.400 usec
 DE 6.50 usec
 TE 299.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1824713 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.50000000 W

F2 - Processing parameters
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 SF 400.1800097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



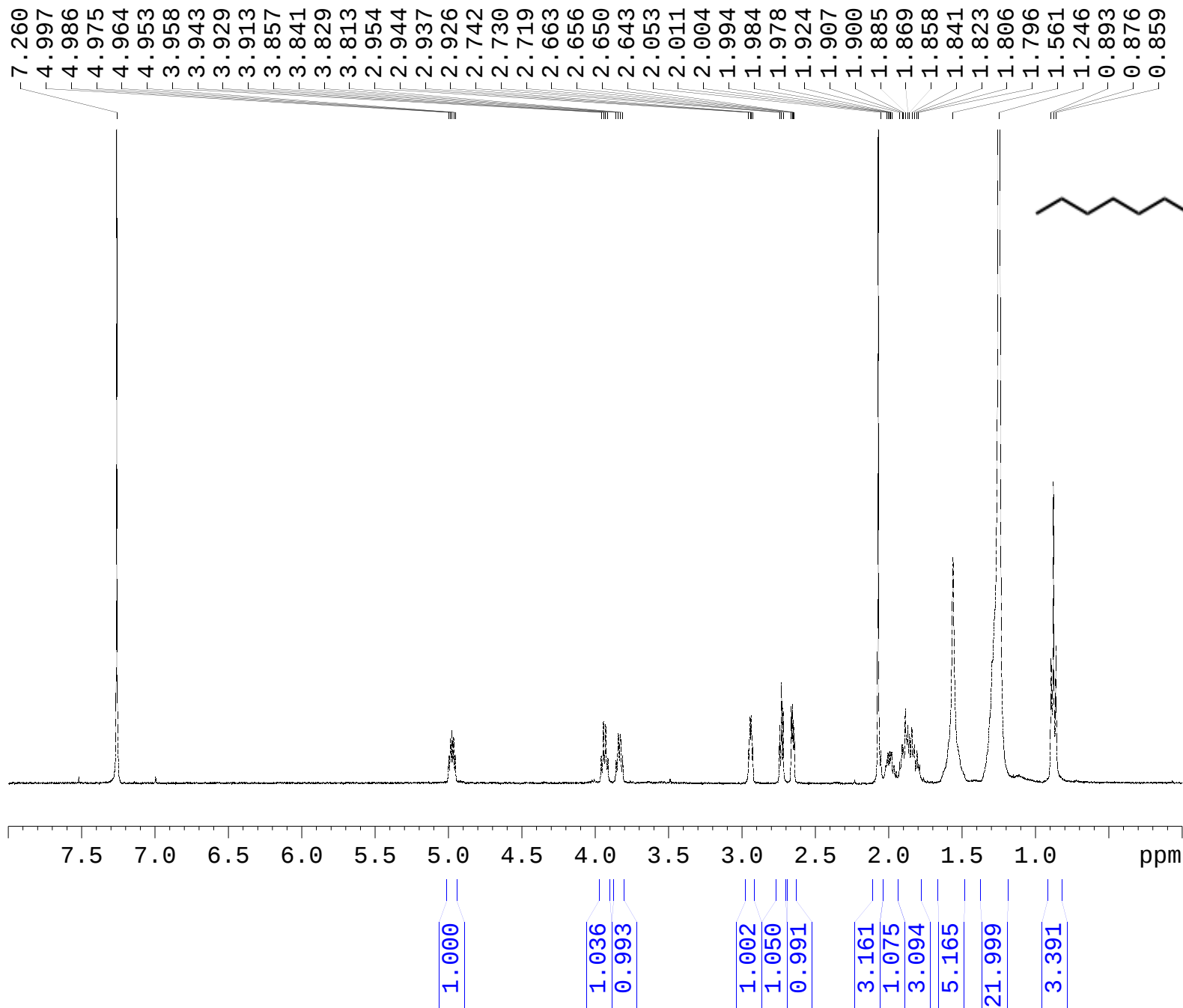
10

Current Data Parameters
NAME Compound 10
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 16.31
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.25
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6354031 MHz
NUC1 13C
P1 10.00 usec
PLW1 63.50000000 W

===== CHANNEL f2 =====
SF02 400.1816007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.50000000 W
PLW12 0.20370001 W
PLW13 0.16500001 W



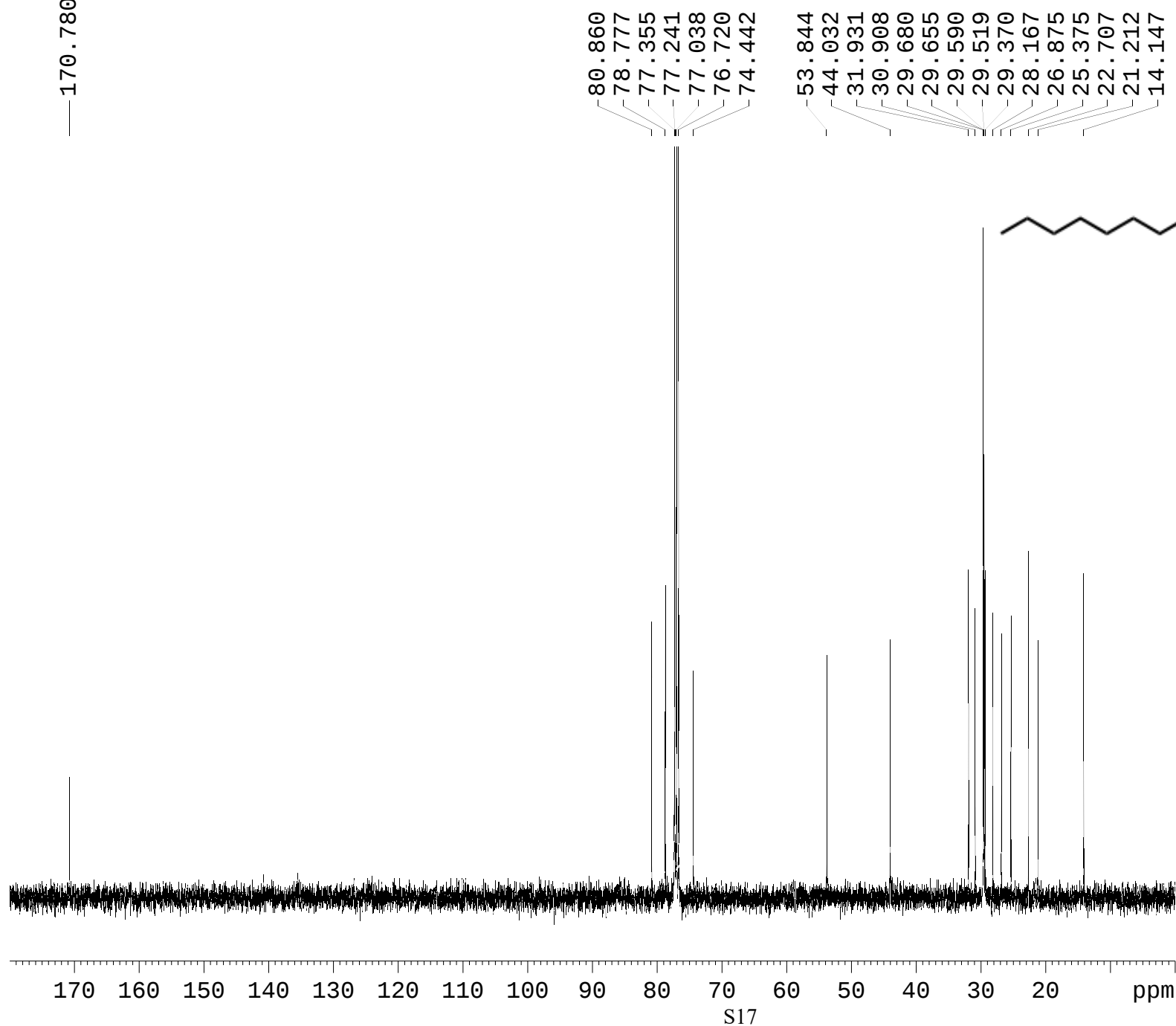
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 PROCNO 1

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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 103.11
 DW 60.800 usec
 DE 6.50 usec
 TE 293.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PLW1 17.00000000 W
 SF01 400.1324710 MHz

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 SF 400.1300101 MHz
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 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

—170.780



11

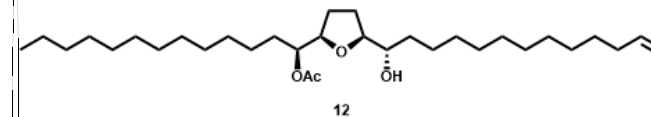
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NAME Compound 11
EXPNO 1
PROCNO 1

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Time 17.24
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PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 204.44
DW 20.800 usec
DE 6.50 usec
TE 293.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PLW1 85.00000000 W
SF01 100.6228293 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 17.00000000 W
PLW12 0.20987999 W
PLW13 0.17000000 W
SF02 400.1316005 MHz

7.260
5.842
5.816
5.799
5.774
5.041
5.027
5.009
4.963
4.934
4.908
3.998
3.983
3.971
3.956
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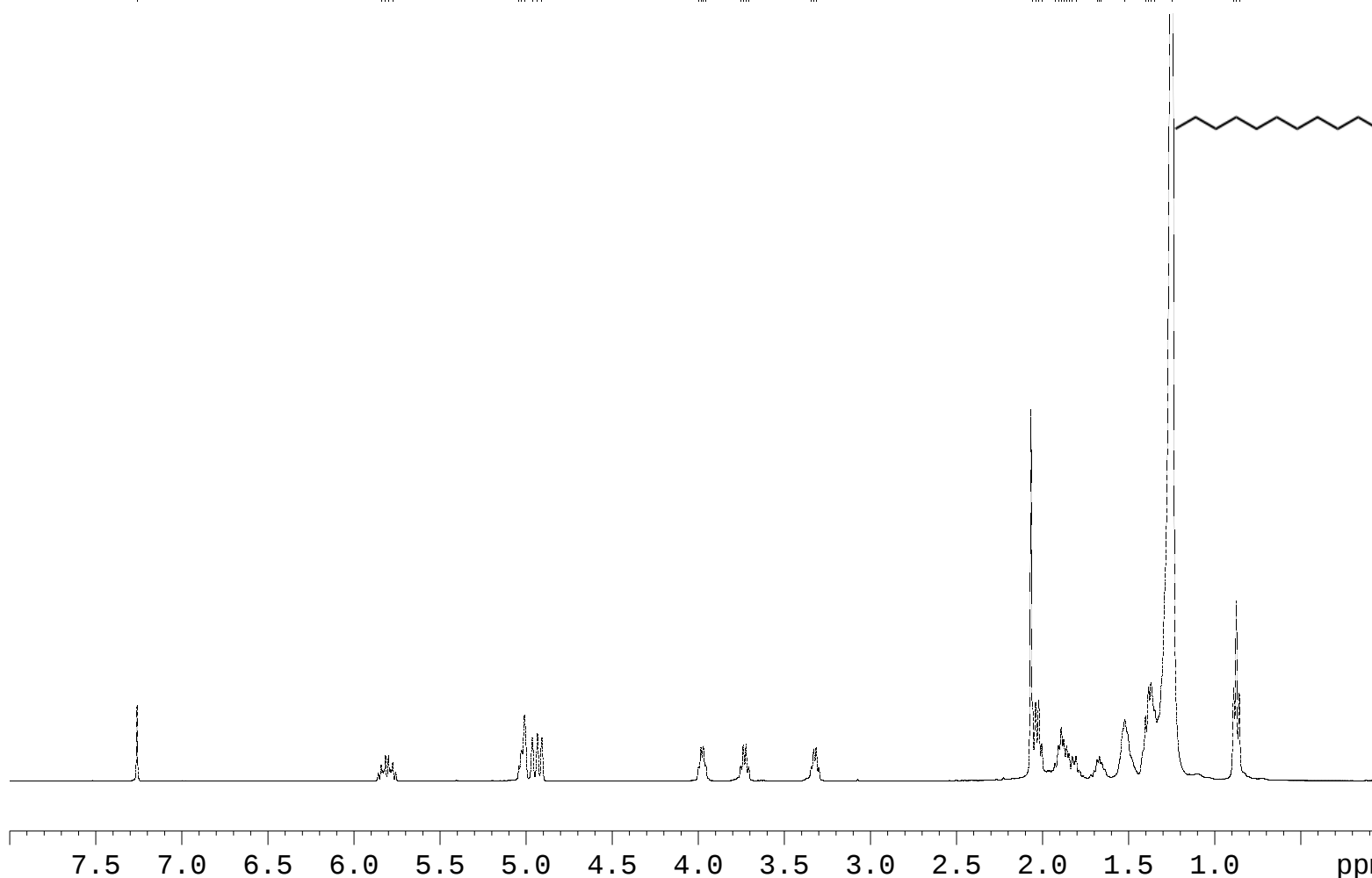


Current Data Parameters
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EXPNO 2
PROCNO 1

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Time 8.27
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 52.09
DW 60.800 usec
DE 6.50 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PLW1 17.00000000 W
SF01 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.000

3.044

1.032

1.009

0.985

5.785

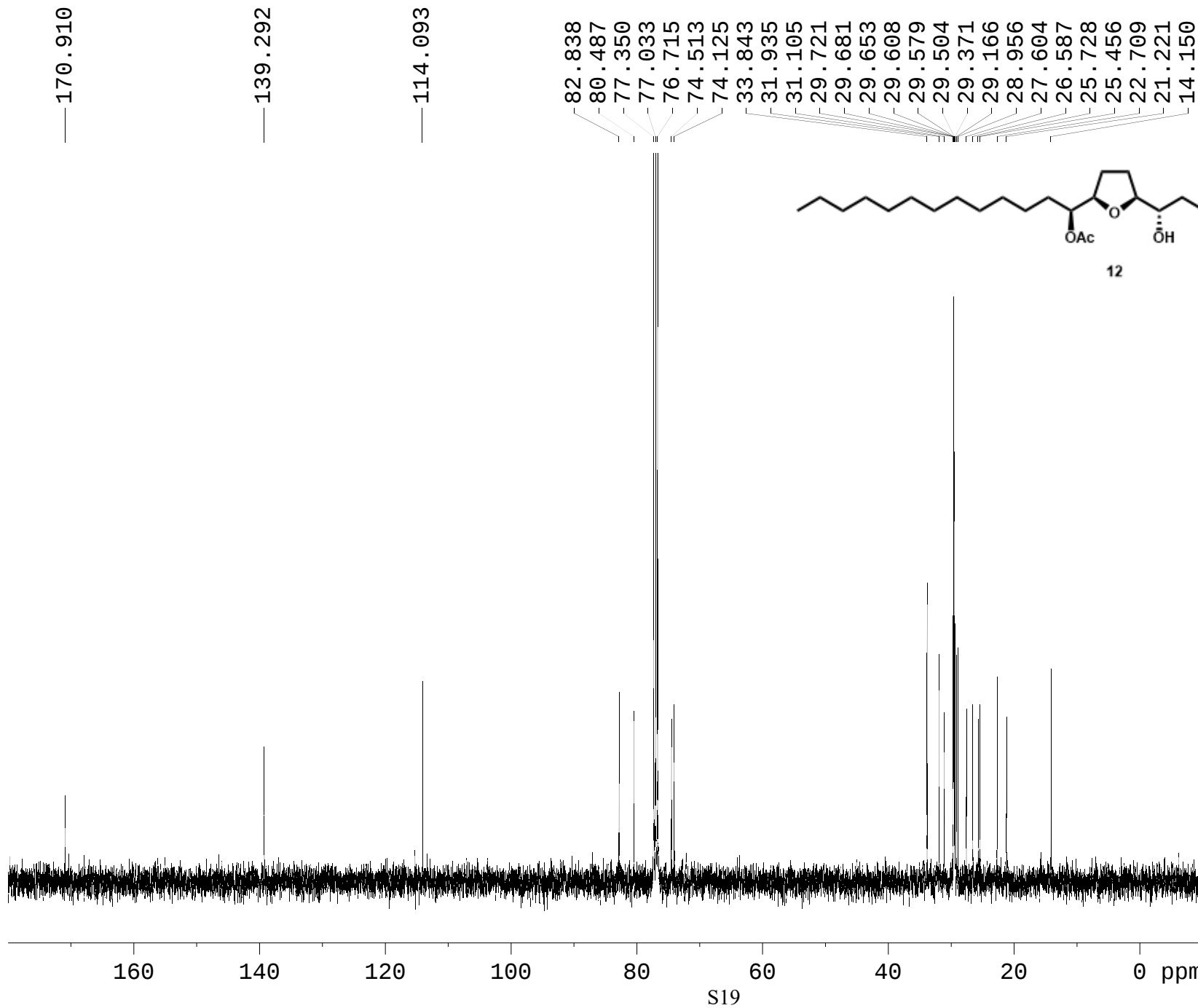
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3.288

40.479

3.559



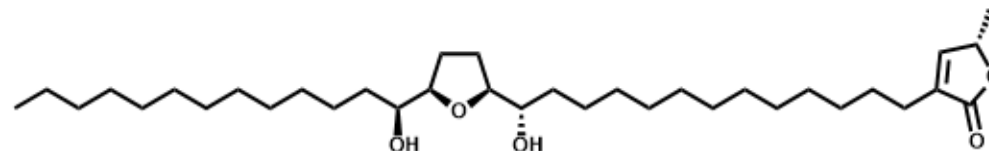
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 204.44
DW 20.800 usec
DE 6.50 usec
TE 293.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PLW1 85.00000000 W
SF01 100.6228293 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 17.00000000 W
PLW12 0.20987999 W
PLW13 0.17000000 W
SF02 400.1316005 MHz

7.260
6.981
6.978
4.998
4.994
4.984
4.981
3.905
3.899
3.833
3.826
3.823
3.820
3.814
3.810
3.807
3.450
3.440
2.276
2.272
2.261
2.248
2.245
2.241
1.955
1.952
1.946
1.939
1.930
1.926
1.917
1.778
1.760
1.557
1.542
1.527
1.487
1.475
1.467
1.458
1.409
1.396
1.254
0.891
0.878
0.863



1

Current Data Parameters
NAME Compound 1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190515
Time 19.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 168.92
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 500.2330891 MHz
NUC1 1H
P1 11.00 usec
PLW1 27.00000000 W

F2 - Processing parameters
SI 65536
SF 500.2300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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 ppm

1.000

0.996

1.389

2.848

1.403

2.210

2.320

2.932

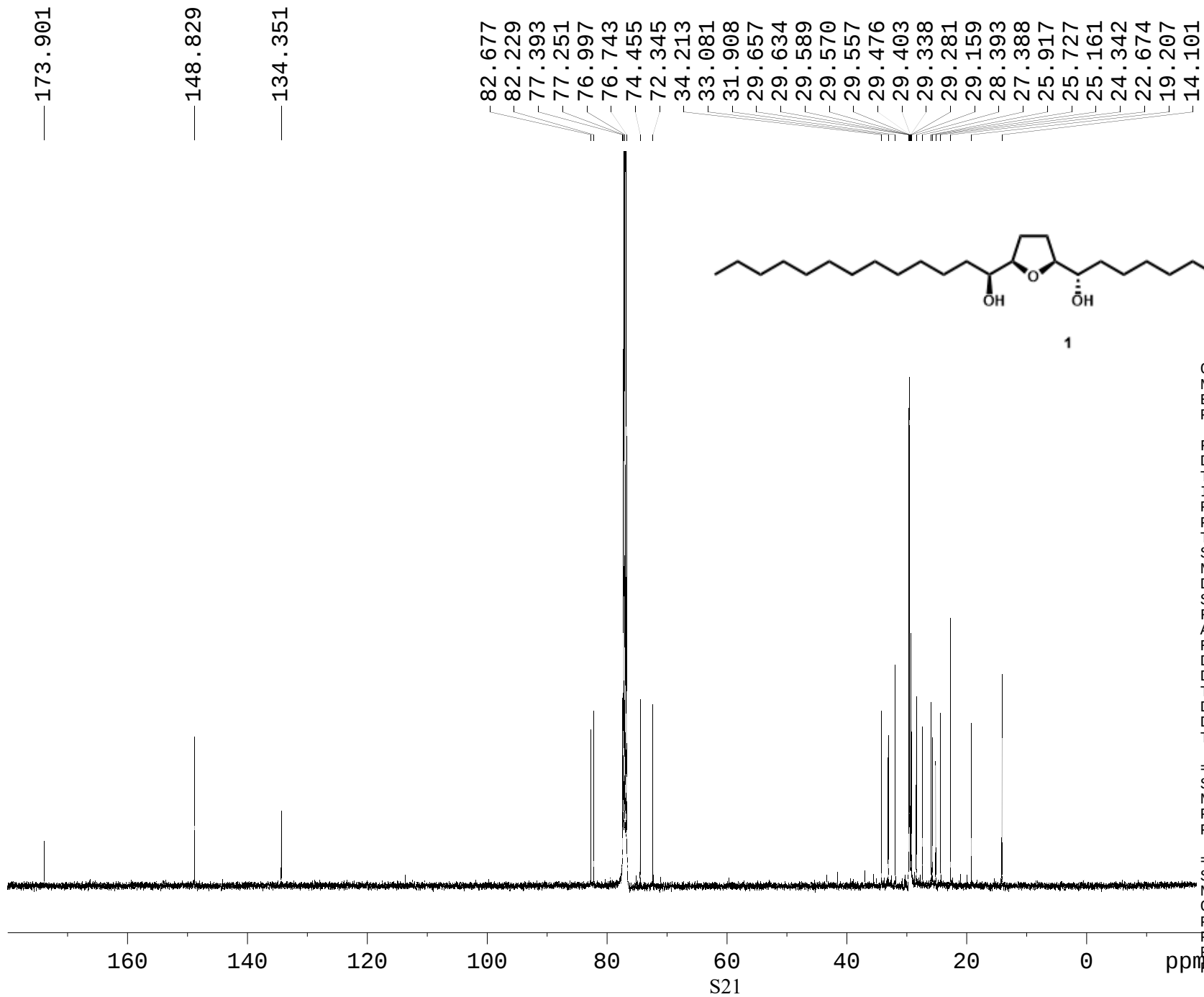
2.888

15.942

7.985

57.806

5.780



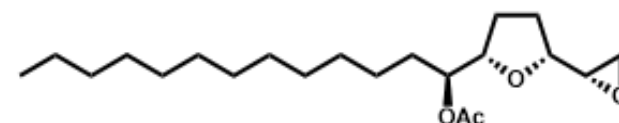
Current Data Parameters
 NAME Compound 1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190516
 Time 9.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 16000
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 190.86
 DW 16.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 125.7955112 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 88.00000000 W

===== CHANNEL f2 =====
 SF02 500.2320009 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 27.00000000 W
 PLW12 0.51046997 W
 PLW13 0.32670000 W

7.260
4.875
4.861
4.855
4.842
4.069
4.065
4.051
4.049
3.918
3.913
3.901
3.896
3.010
3.003
3.000
2.998
2.993
2.992
2.988
2.981
2.796
2.786
2.784
2.774
2.586
2.580
2.574
2.567
2.087
2.025
2.014
2.001
1.990
1.985
1.763
1.646
1.644
1.637
1.554
1.295
1.279
1.247
0.894
0.878
0.860



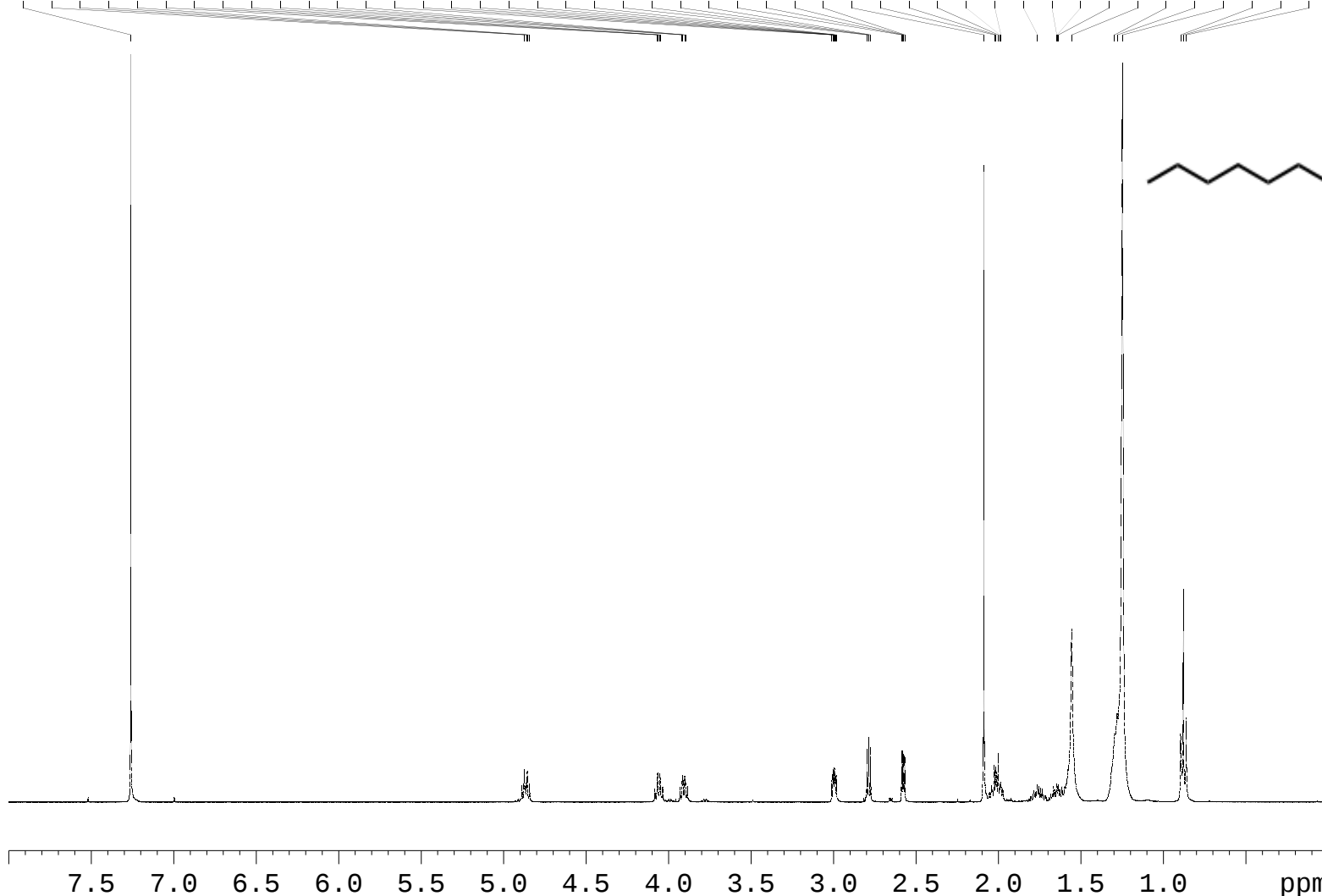
14

Current Data Parameters
NAME Compound 14
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190708
Time 21.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1824713 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.00000000 W

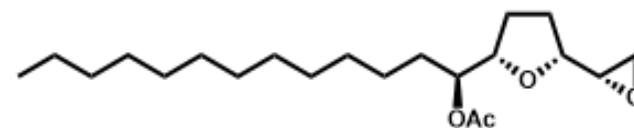
F2 - Processing parameters
SI 65536
SF 400.1800094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.000
0.986
0.975
1.000
1.008
0.981
3.165
2.193
2.229
6.224
22.135
3.171

—170.874

80.102
78.926
77.314
77.199
76.996
76.679
75.116
53.063
45.341
31.863
30.979
29.607
29.579
29.504
29.433
29.296
27.830
27.648
25.363
22.634
21.145
14.065



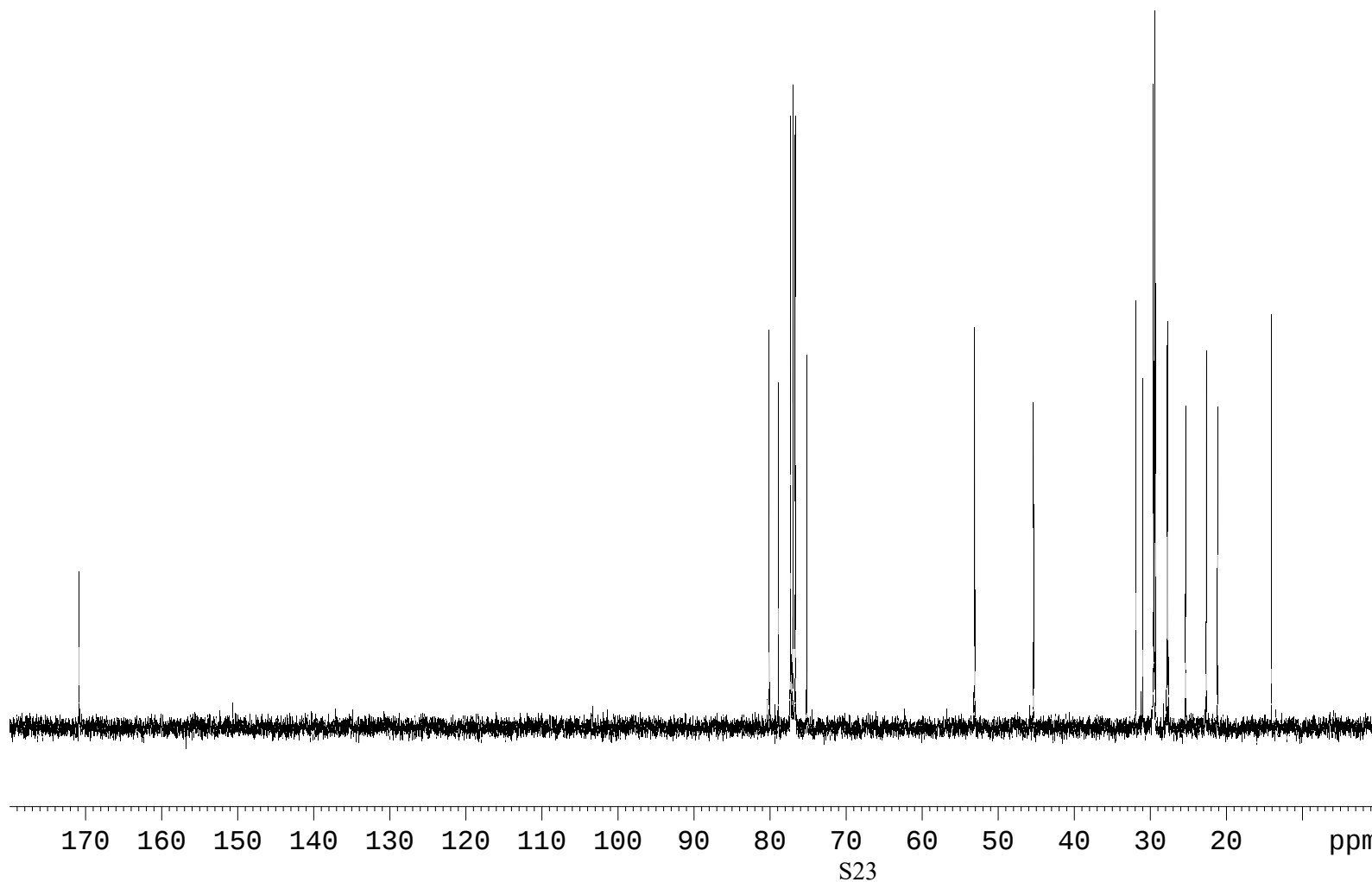
14

Current Data Parameters
NAME Compound 14
EXPNO 1
PROCNO 1

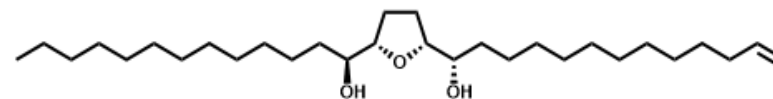
F2 - Acquisition Parameters
Date_ 20190708
Time 21.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6354031 MHz
NUC1 13C
P1 10.00 usec
PLW1 70.00000000 W

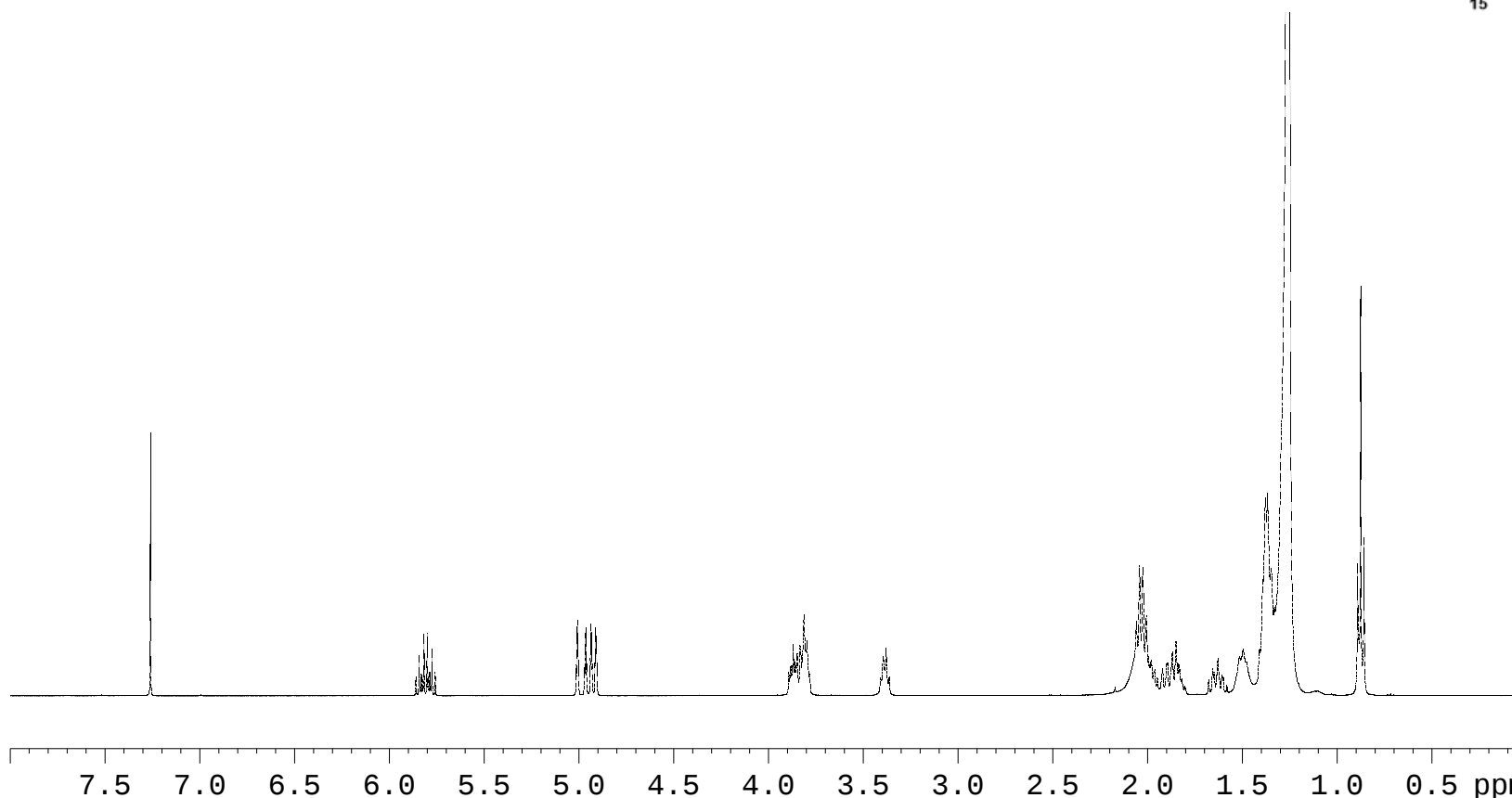
===== CHANNEL f2 =====
SF02 400.1816007 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 17.00000000 W
PLW12 0.20987999 W
PLW13 0.10557000 W



7.260
5.842
5.817
5.800
5.774
5.010
5.004
4.967
4.962
4.940
4.937
4.934
4.932
4.912
4.909
4.906
3.869
3.847
3.832
3.829
3.812
3.796
3.395
3.379
2.062
2.059
2.056
2.042
2.025
2.023
2.009
2.006
2.003
1.995
1.869
1.850
1.628
1.513
1.495
1.409
1.392
1.377
1.367
1.348
1.330
0.892
0.875
0.857



15

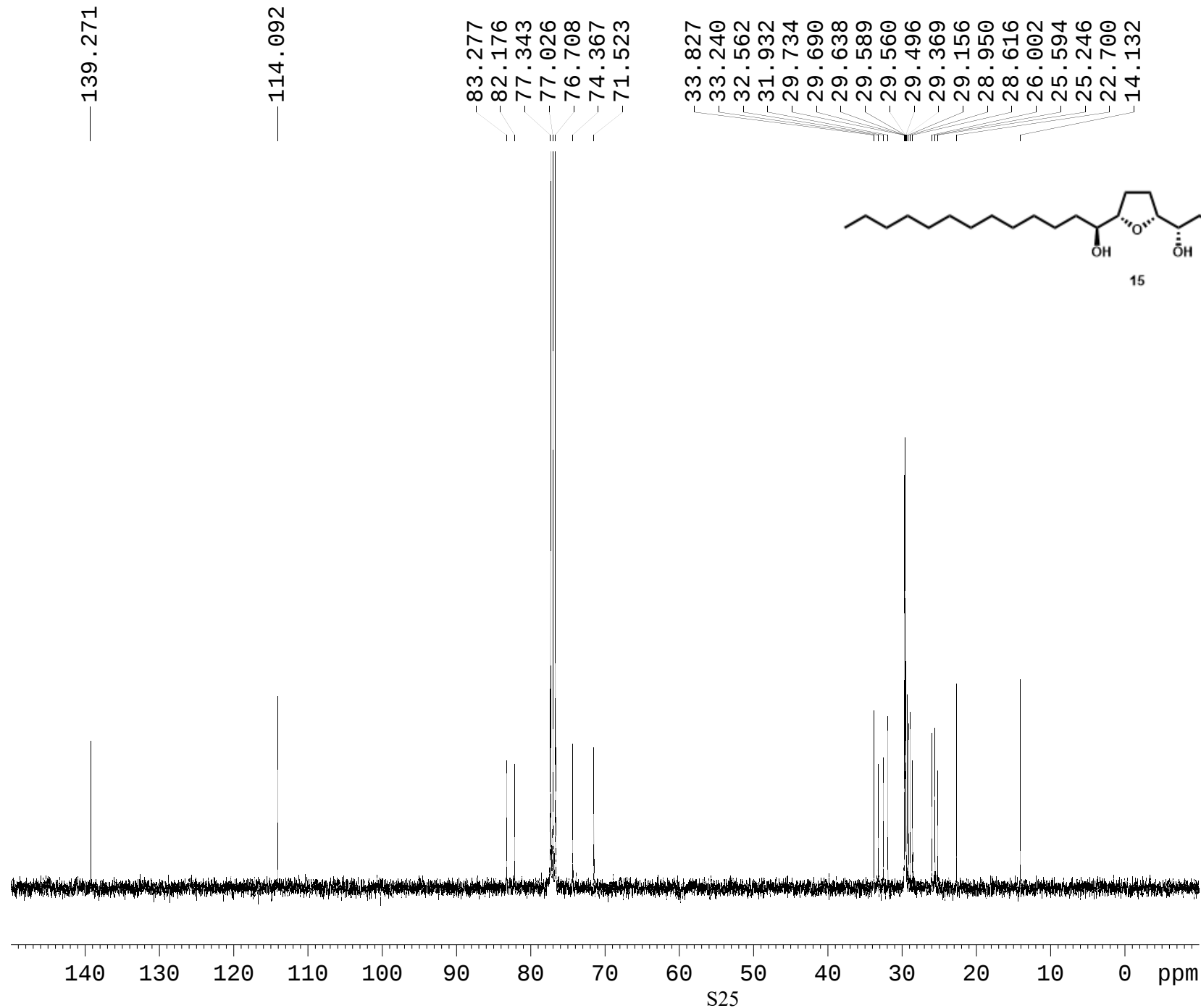


Current Data Parameters
NAME Compound 15
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190716
Time 15.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 64
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 50.8
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1824713 MHz
NUC1 1H
P1 10.00 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1800094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



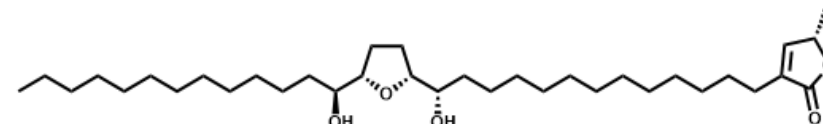
Current Data Parameters
 NAME Compound 15
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190716
 Time 15.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 297.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 100.6354031 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 70.00000000 W

===== CHANNEL f2 =====
 SF02 400.1816007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 17.00000000 W
 PLW12 0.20987999 W
 PLW13 0.10557000 W

6.982
6.979
6.976
6.973
4.995
4.992
4.982
4.978
3.868
3.830
3.827
3.814
3.801
3.393
3.391
3.380
2.277
2.273
2.270
2.259
2.246
2.243
2.239
2.239
1.936
1.922
1.913
1.903
1.897
1.894
1.892
1.873
1.857
1.851
1.634
1.554
1.540
1.525
1.510
1.497
1.487
1.380
1.371
1.360
1.351
1.253
0.889
0.875
0.861



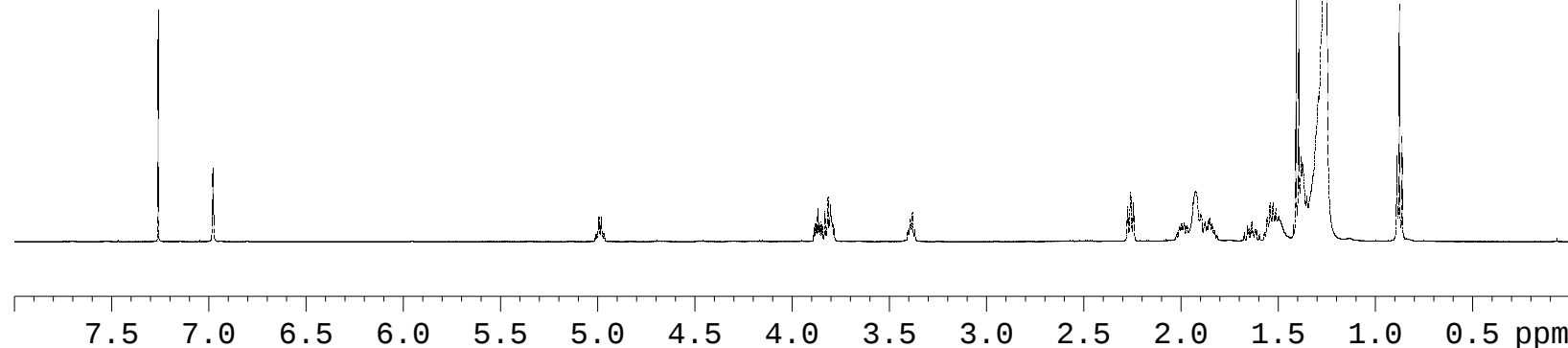
2

Current Data Parameters
NAME Compound 2
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190724
Time 9.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 108.6
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 500.2330891 MHz
NUC1 1H
P1 11.00 usec
PLW1 27.00000000 W

F2 - Processing parameters
SI 65536
SF 500.2300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.000

1.008

3.452

1.181

2.094

7.942

1.323

4.806

52.127

3.724

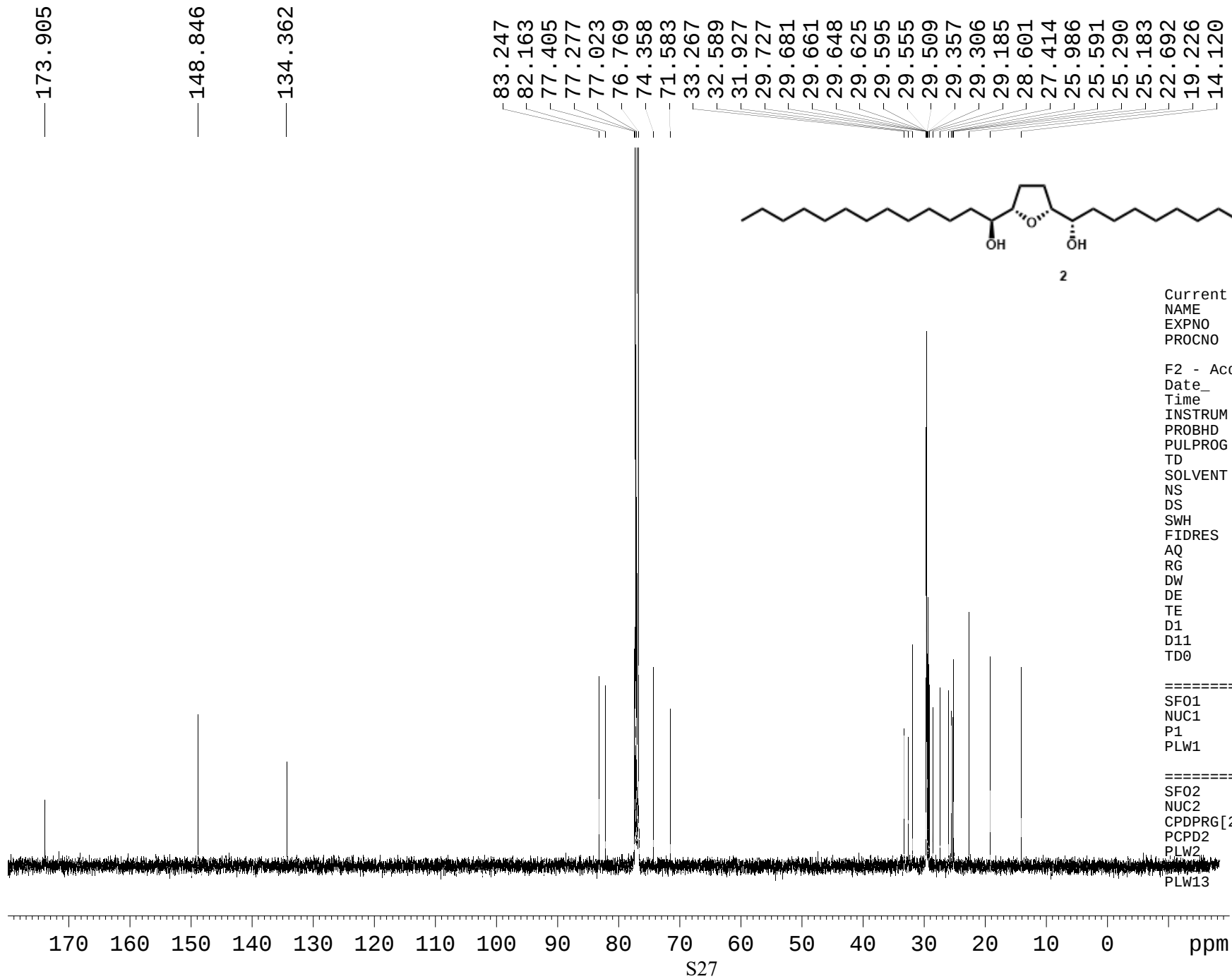


Table S1. Crystal data and structure refinement for compound **9** and CCDC: 1950967

Crystal data	
Chemical formula	C ₁₇ H ₁₈ N ₂ O ₁₀
M_r	410.33
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	90
a, b, c (Å)	5.1460 (2), 10.6897 (3), 31.9749 (11)
V (Å ³)	1758.91 (10)
Z	4
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	1.12
Crystal size (mm)	0.50 × 0.40 × 0.25
Data collection	
Diffractometer	Bruker APEXII CCD area detector diffractometer
Absorption correction	Numerical Crystal Faces plugin in Bruker APEX2 software
$T_{\min}, T_{\max}$	0.68, 0.767
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13143, 3063, 2903
R_{int}	0.034
$(\sin \theta/\lambda)_{\max}$ (Å ⁻¹)	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.031, 0.077, 1.07
No. of reflections	3063
No. of parameters	312
No. of restraints	369
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.17, -0.18
Absolute structure	Flack x determined using 1139 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.06 (9)

Figure S1. Single crystal XRD- for compound **9**, with thermal ellipsoids drawn at the 50% probability level and CCDC: 1950967

