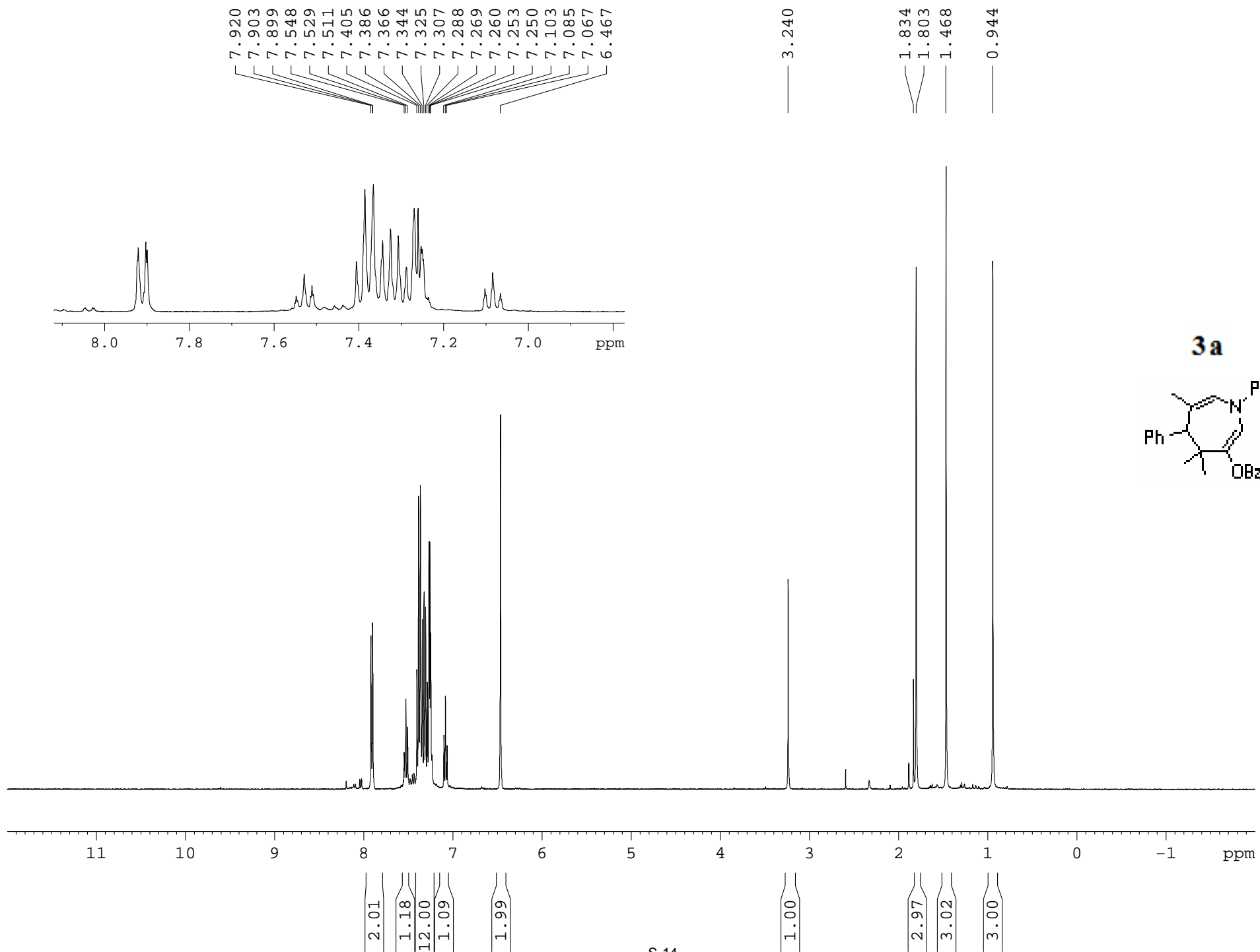


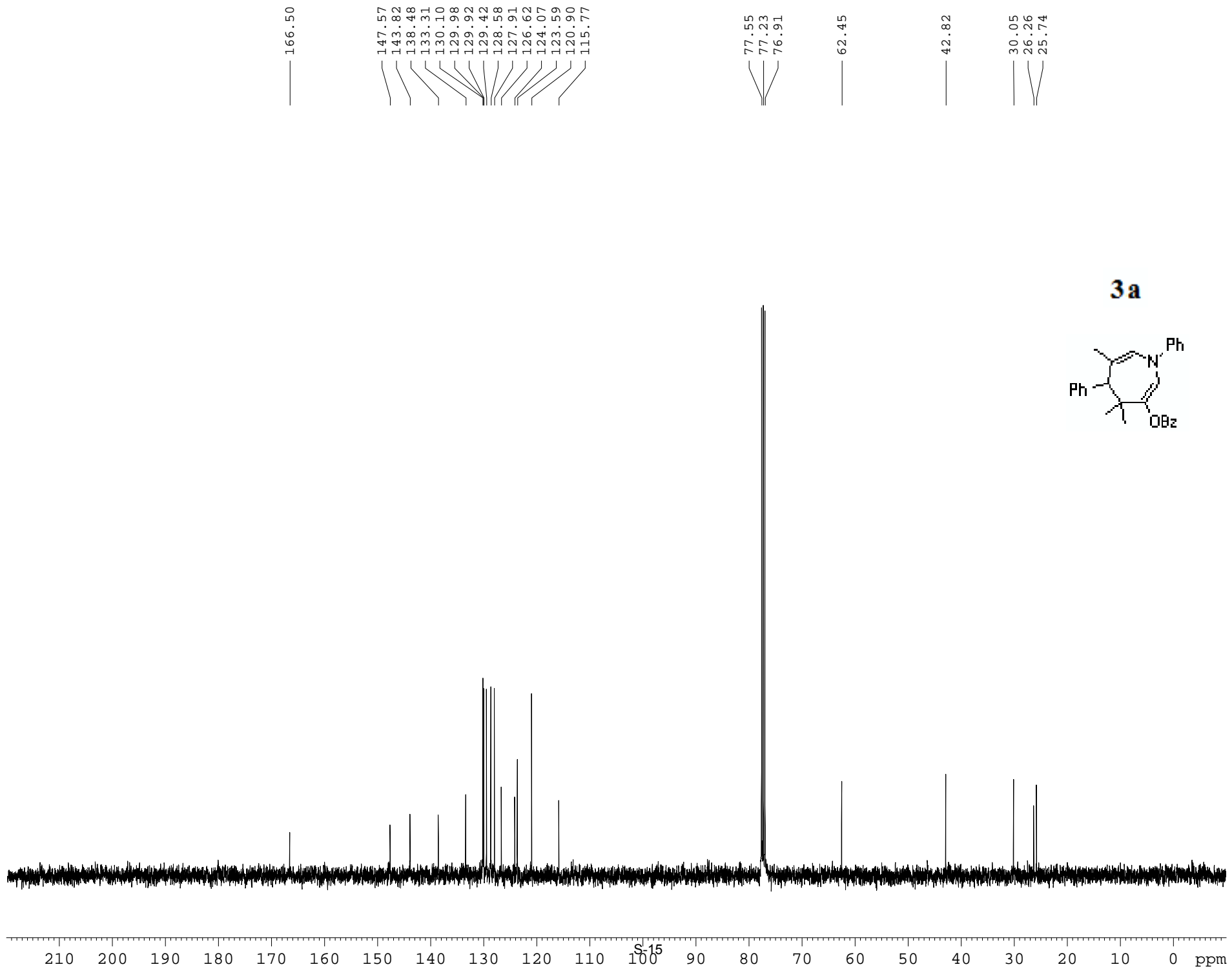
Synthesis of Azepines by a Gold-Catalyzed Intermolecular [4+3]-Annulation

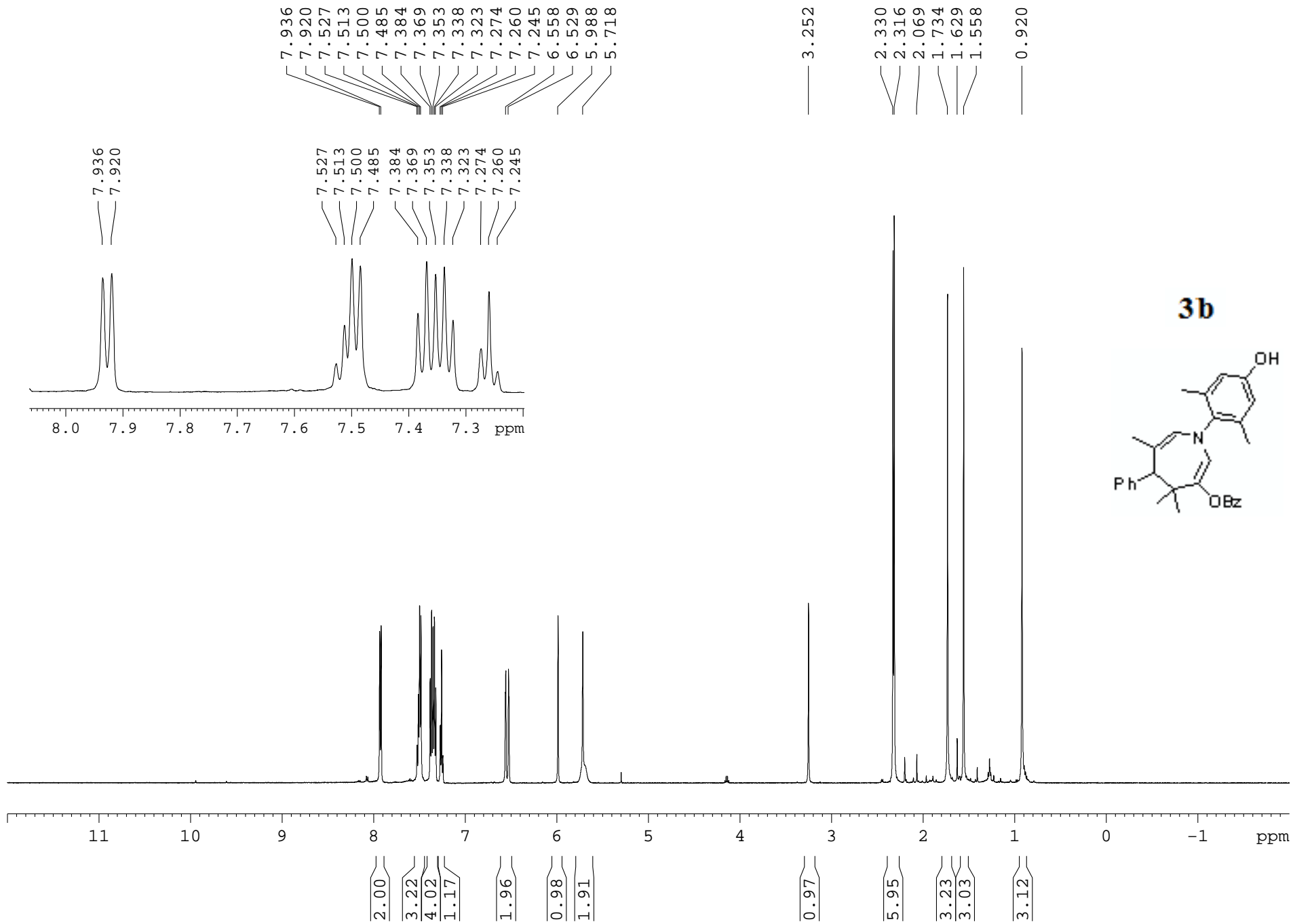
Nathan D. Shapiro and F. Dean Toste*

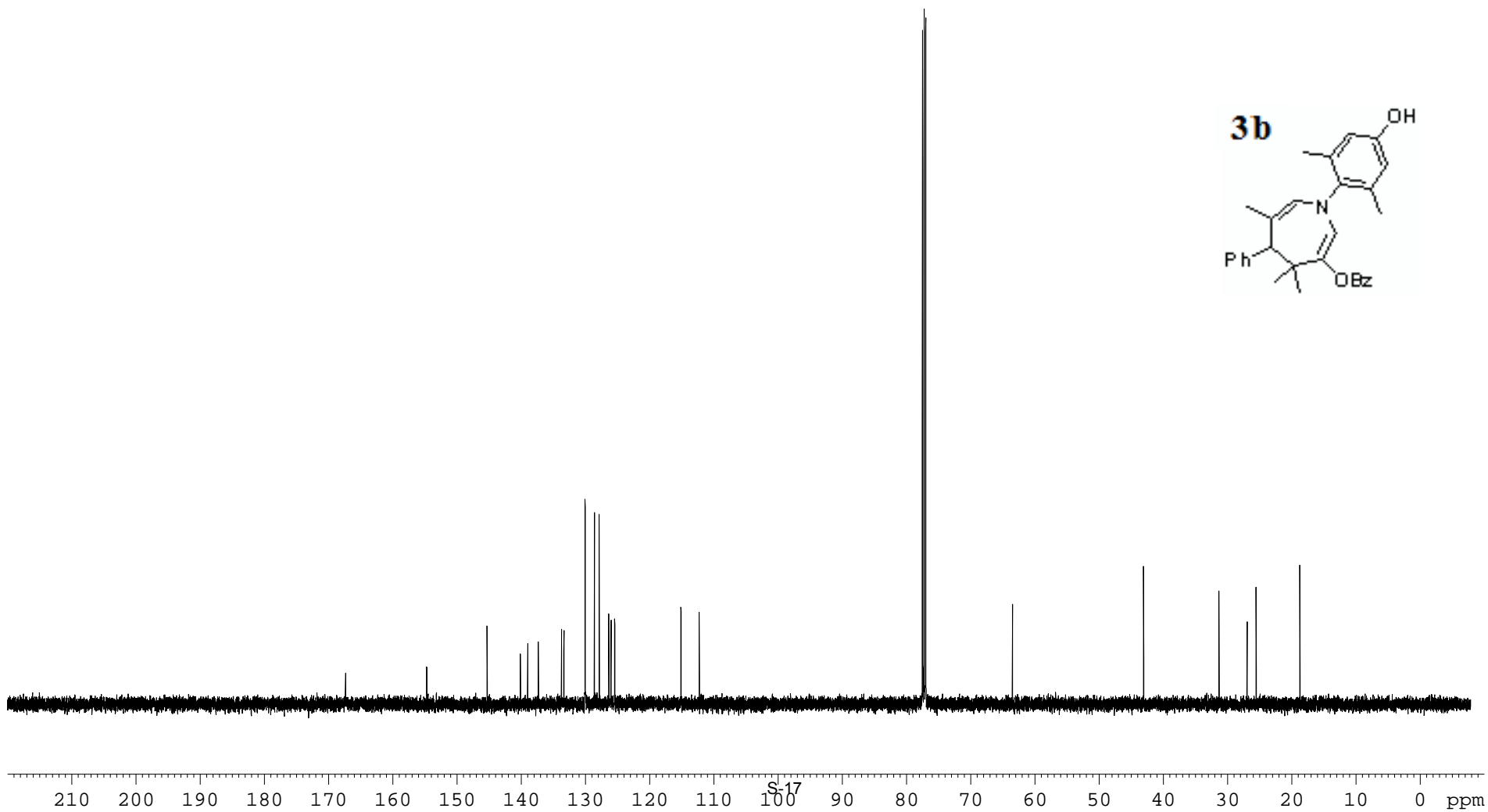
Department of Chemistry, University of California, Berkeley, California 94720

NMR spectra

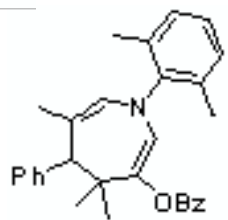








3c



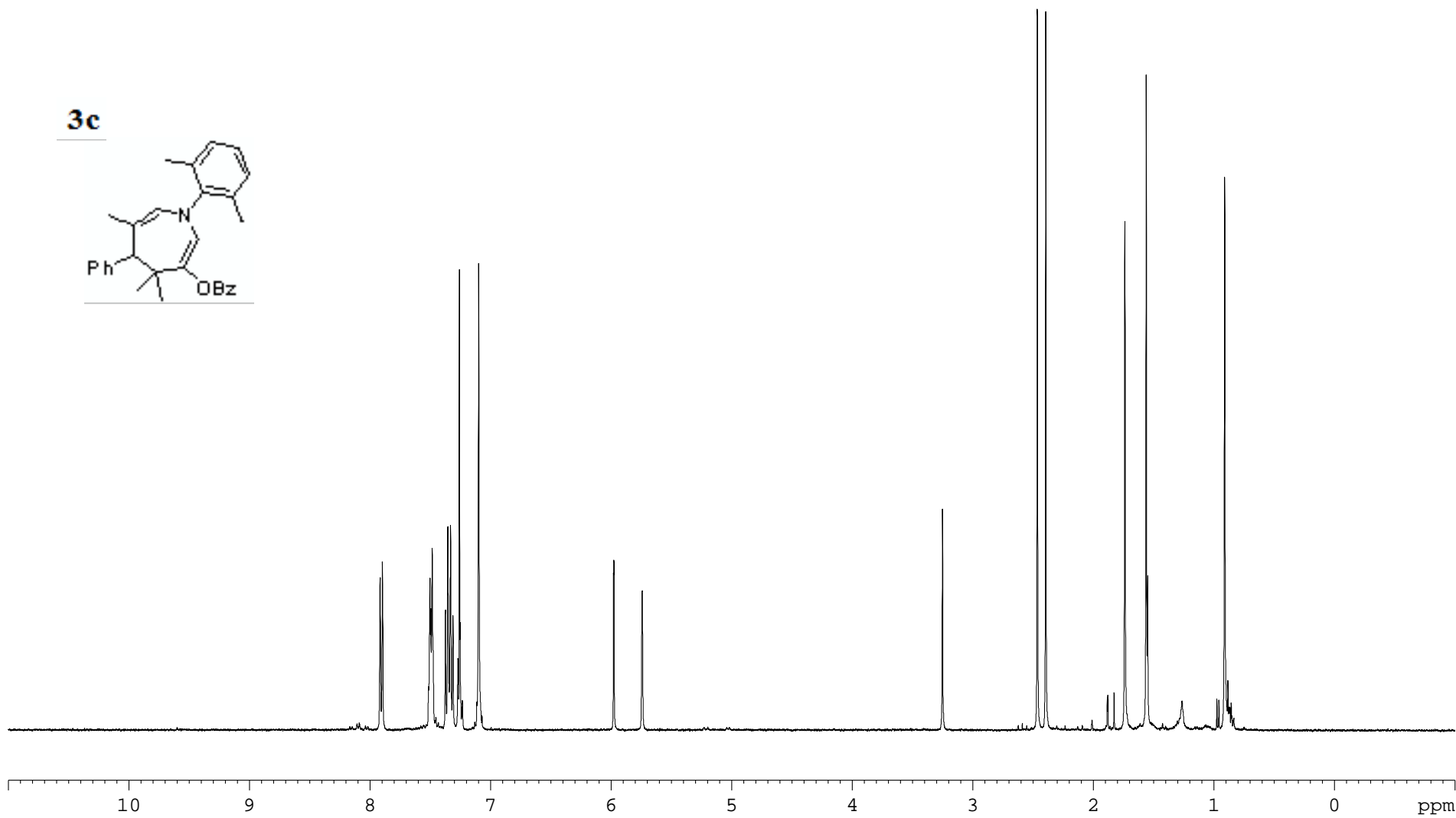
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7.899
7.504
7.497
7.486
7.375
7.356
7.333
7.313
7.271
7.260
7.254
7.100
5.980
5.977
5.744

3.252

2.465
2.395

1.739
1.562
1.550

0.911



2.01

3.11

4.02

2.35

2.99

1.00

1.00

0.99

2.93

2.95

3.10

3.00

3.03

166.93
162.60
146.80
145.39
137.66
135.98
133.99
133.23
130.28
130.15
130.11
129.03
128.98
128.59
127.94
127.68
126.45
125.51
124.89
112.45

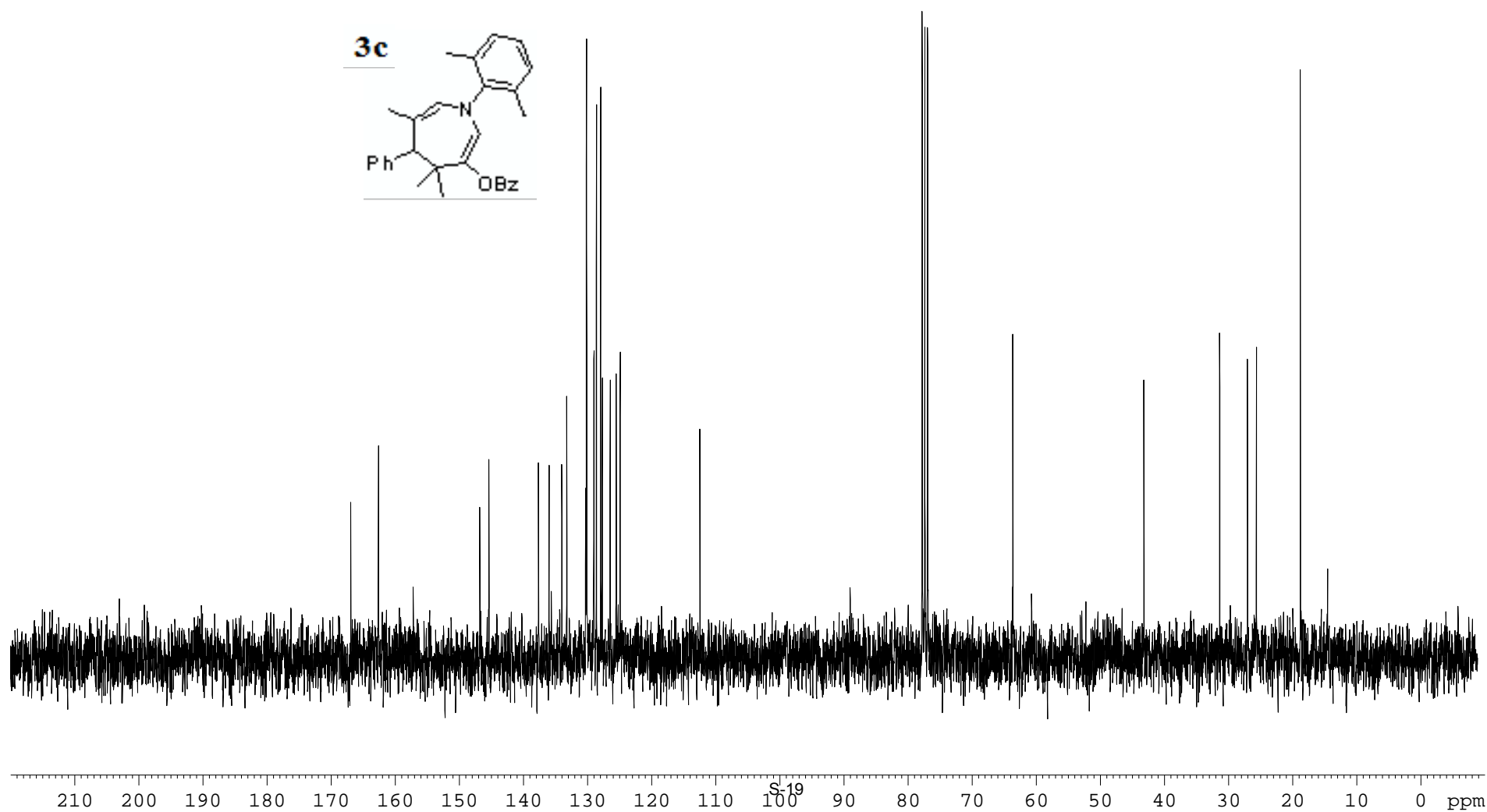
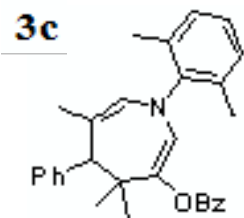
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77.35
76.93

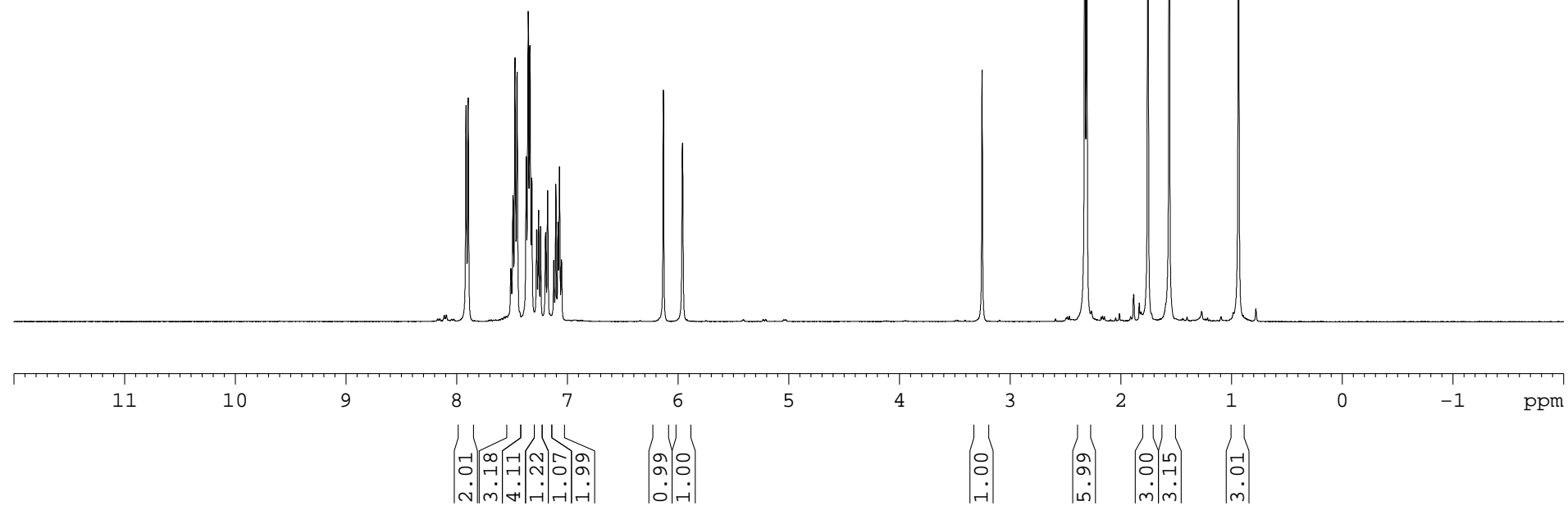
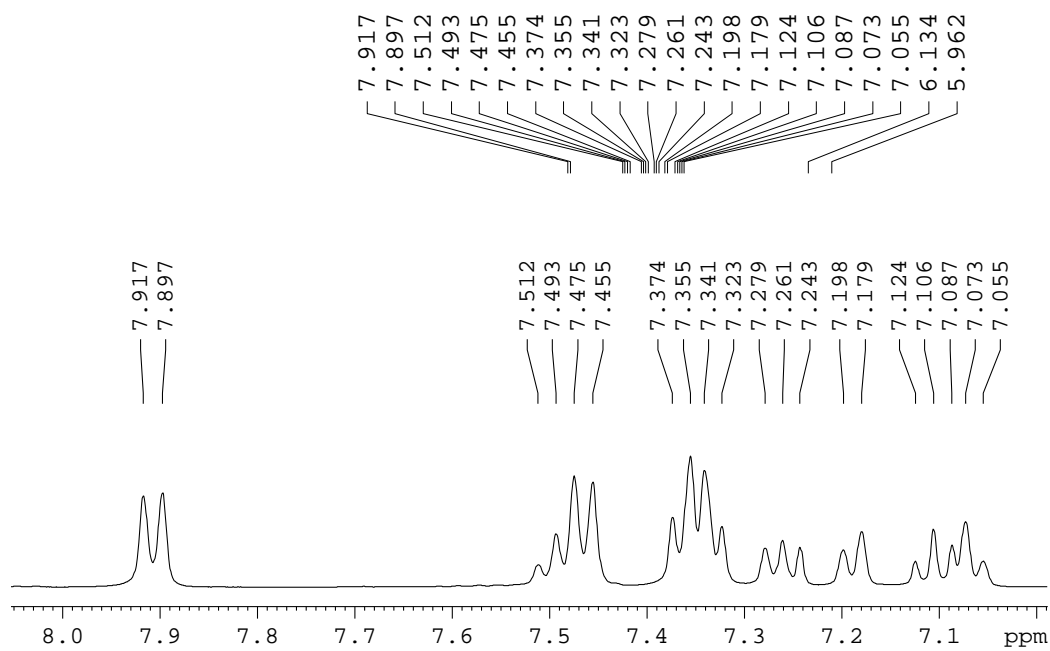
63.63

43.18

31.35
27.02
25.62

18.78
14.52



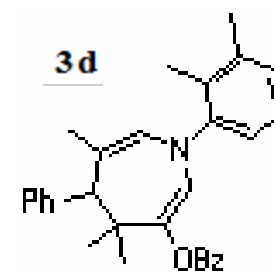


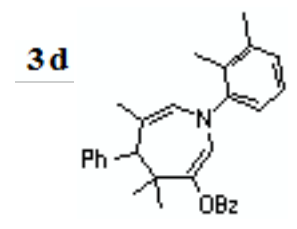
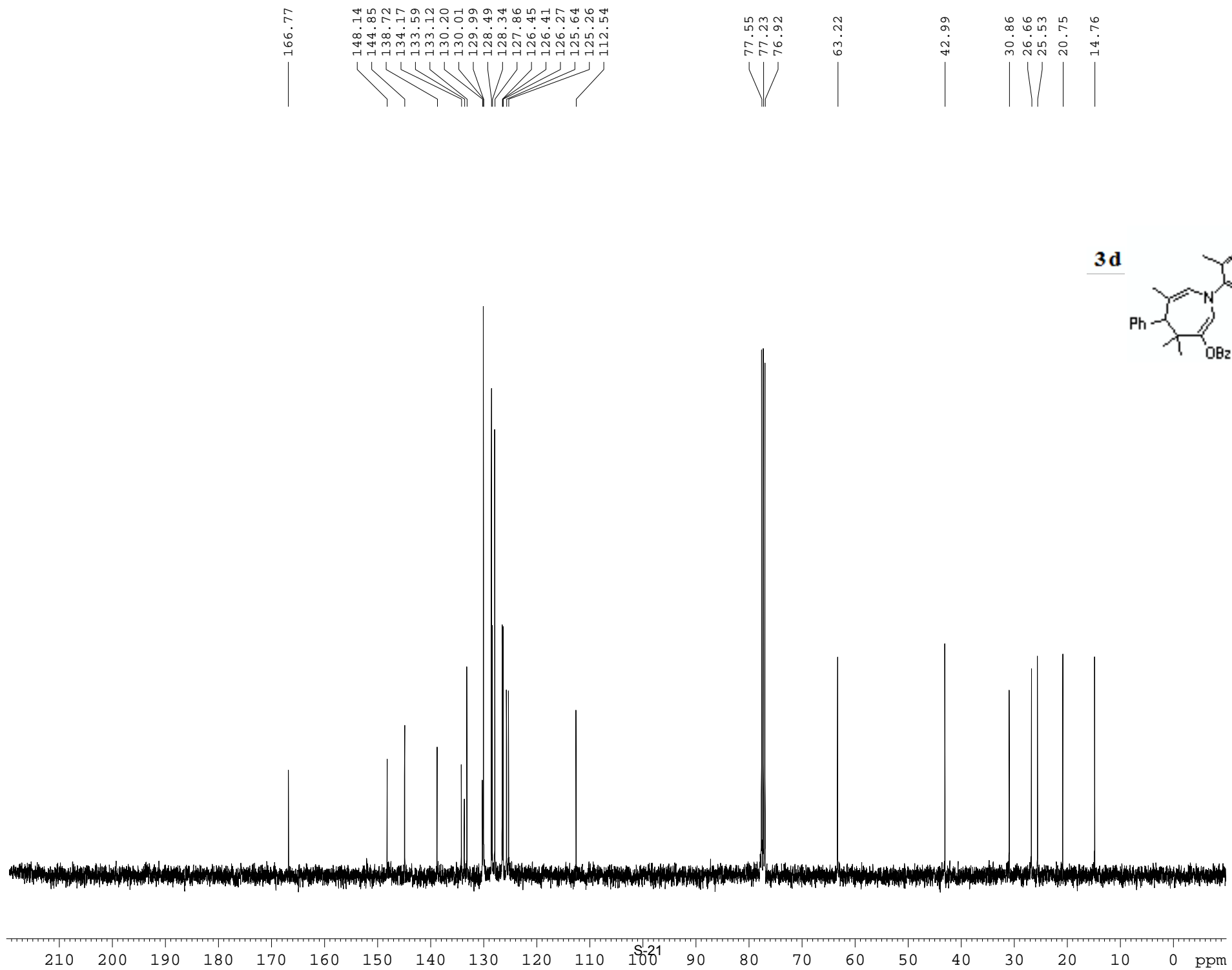
3.254

2.327
2.310

1.756
1.564

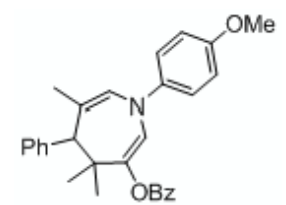
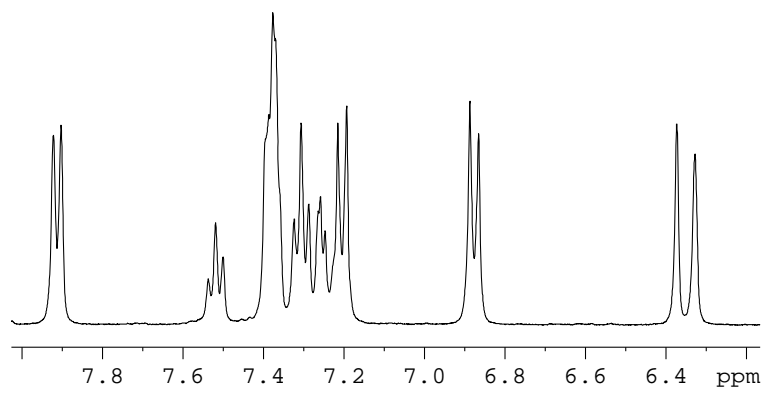
0.938



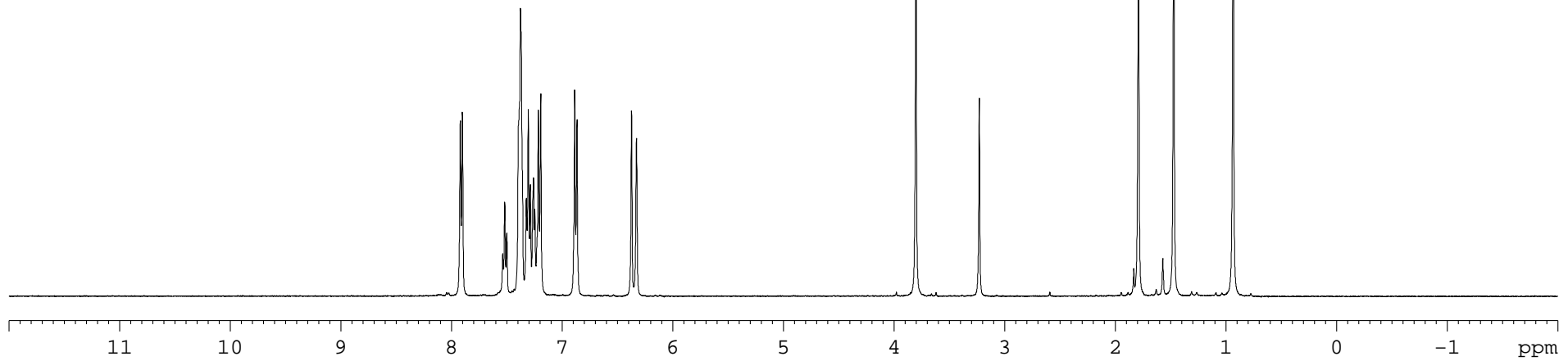


7.921
7.903
7.538
7.520
7.502
7.388
7.378
7.325
7.307
7.289
7.260
7.248
7.216
7.194
6.888
6.866
6.375
6.329

3.802
3.230
1.791
1.472
0.935



3e



1.97
1.09
3.94
2.04
1.17
2.02
2.01
1.97
3.02
1.00
3.07
2.98
2.96

166.63
156.43
144.20
141.78
136.83
133.24
130.06
129.89
128.54
127.87
126.52
124.98
124.13
123.20
114.62
114.53

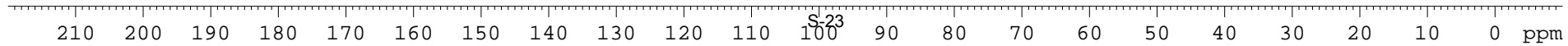
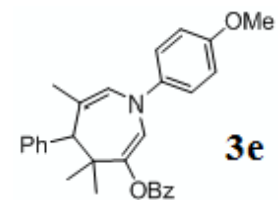
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77.23
76.98

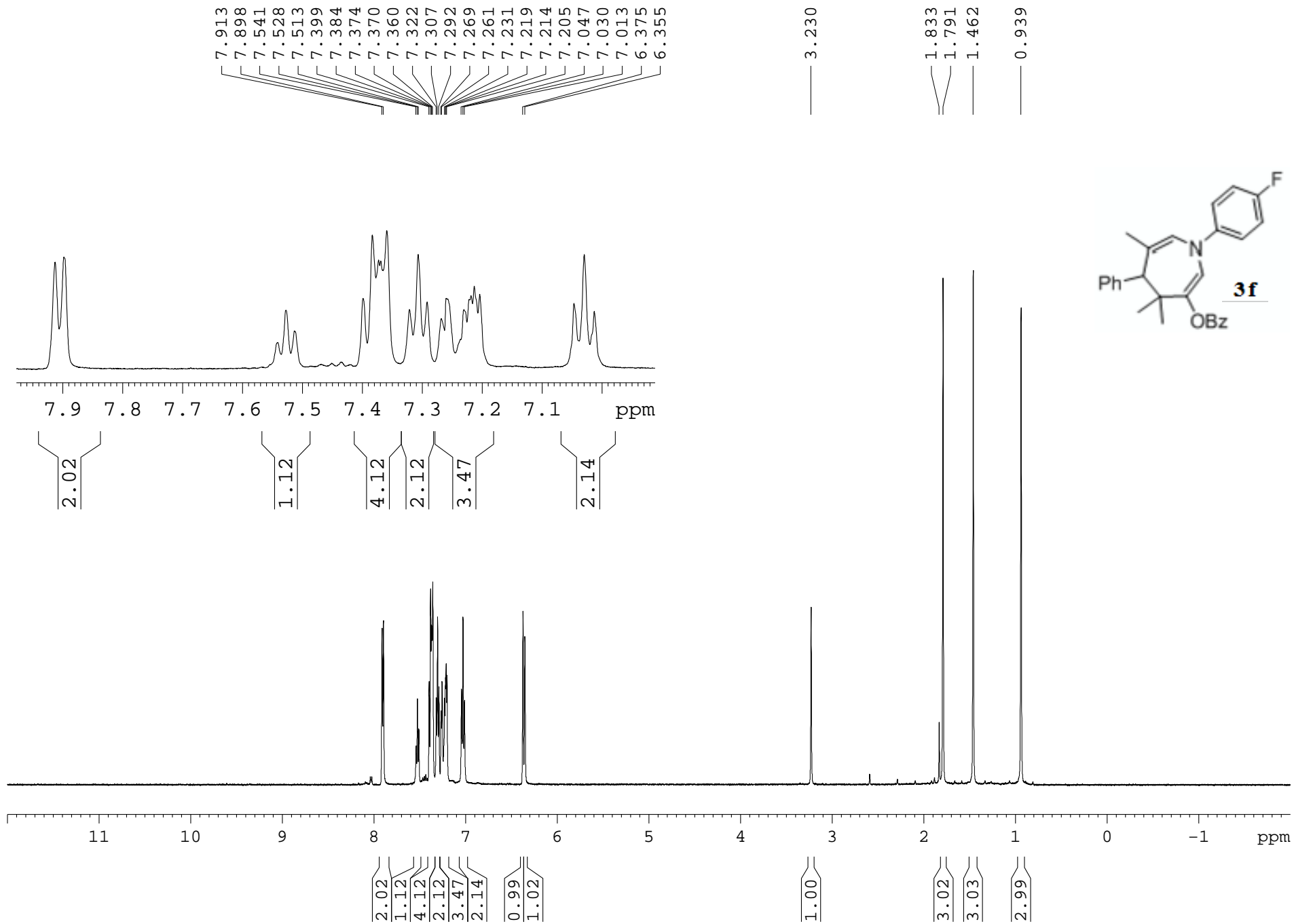
62.71

55.78

42.88

30.45
26.40
25.72





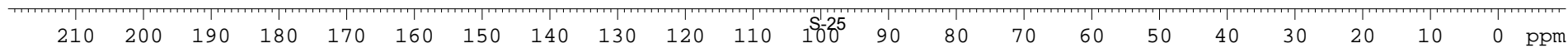
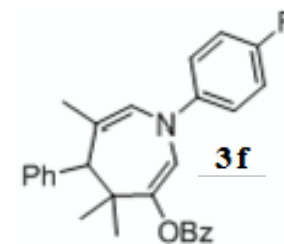
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160.41
158.48
144.12
144.09
143.83
138.11
133.34
130.08
129.93
129.88
128.59
127.93
126.64
124.36
123.74
122.90
122.84
116.12
115.94
115.64

77.48
77.23
76.97

62.48

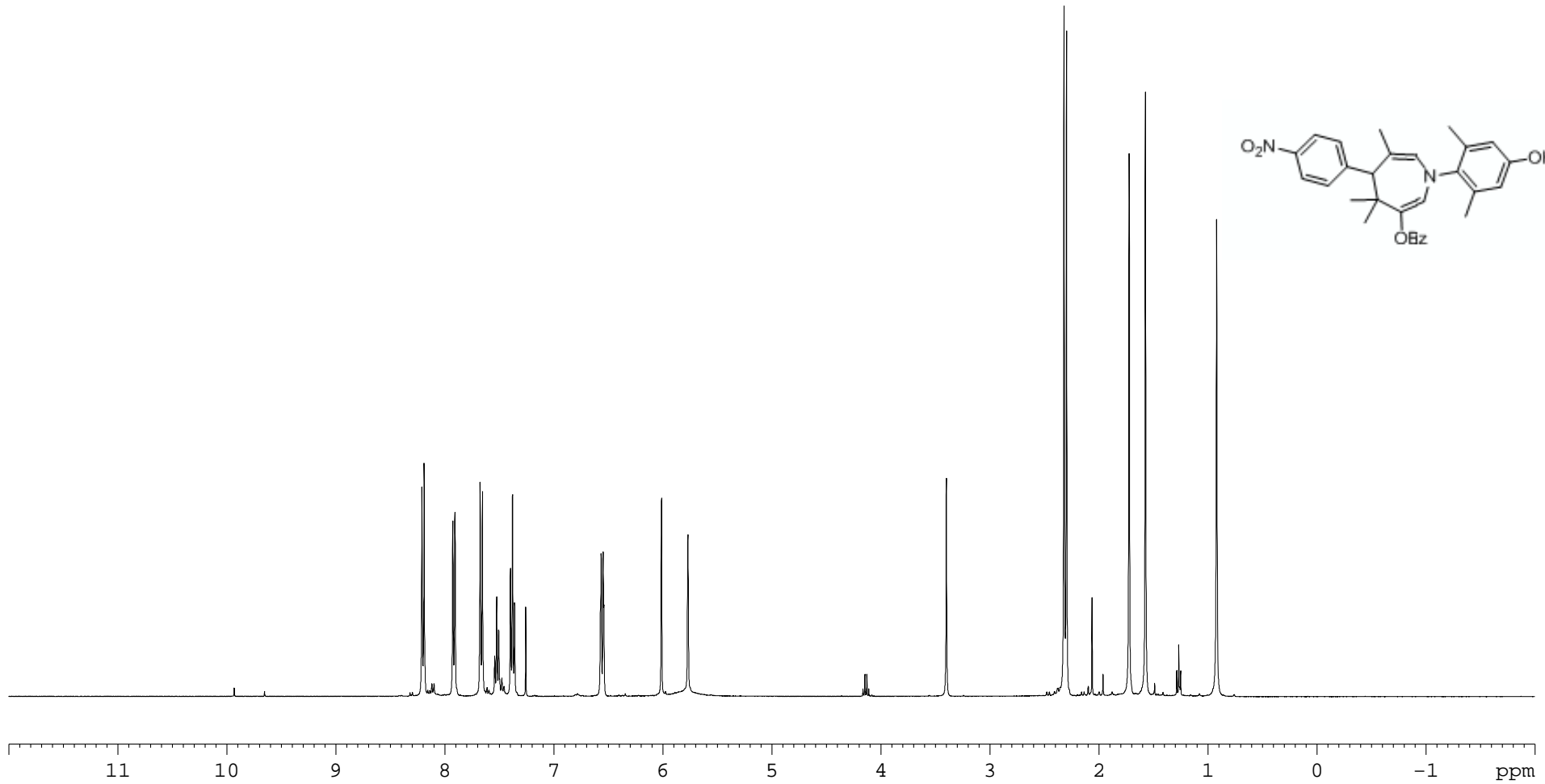
42.85

30.17
26.29
25.67



8.213
8.191
7.928
7.910
7.908
7.679
7.657
7.545
7.526
7.508
7.400
7.381
7.362
7.260
6.568
6.550
6.017
6.014
5.772

3.401
2.322
2.299
2.064
1.724
1.575
1.270
0.922



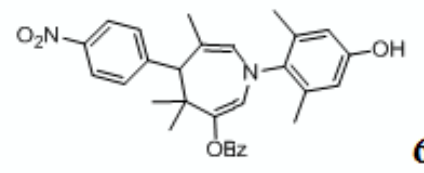
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2.06
2.12
1.19
2.09

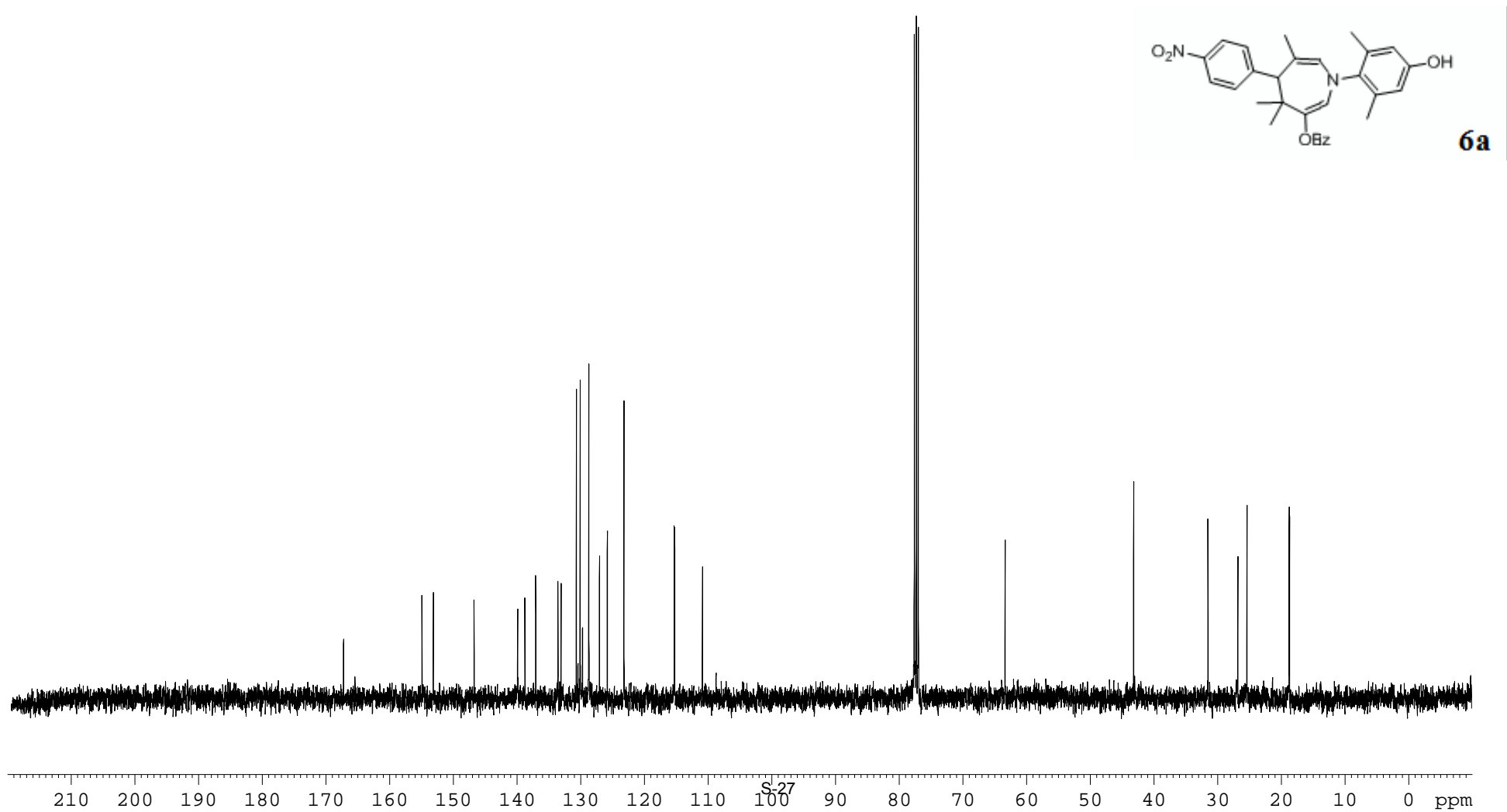
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1.07
1.27

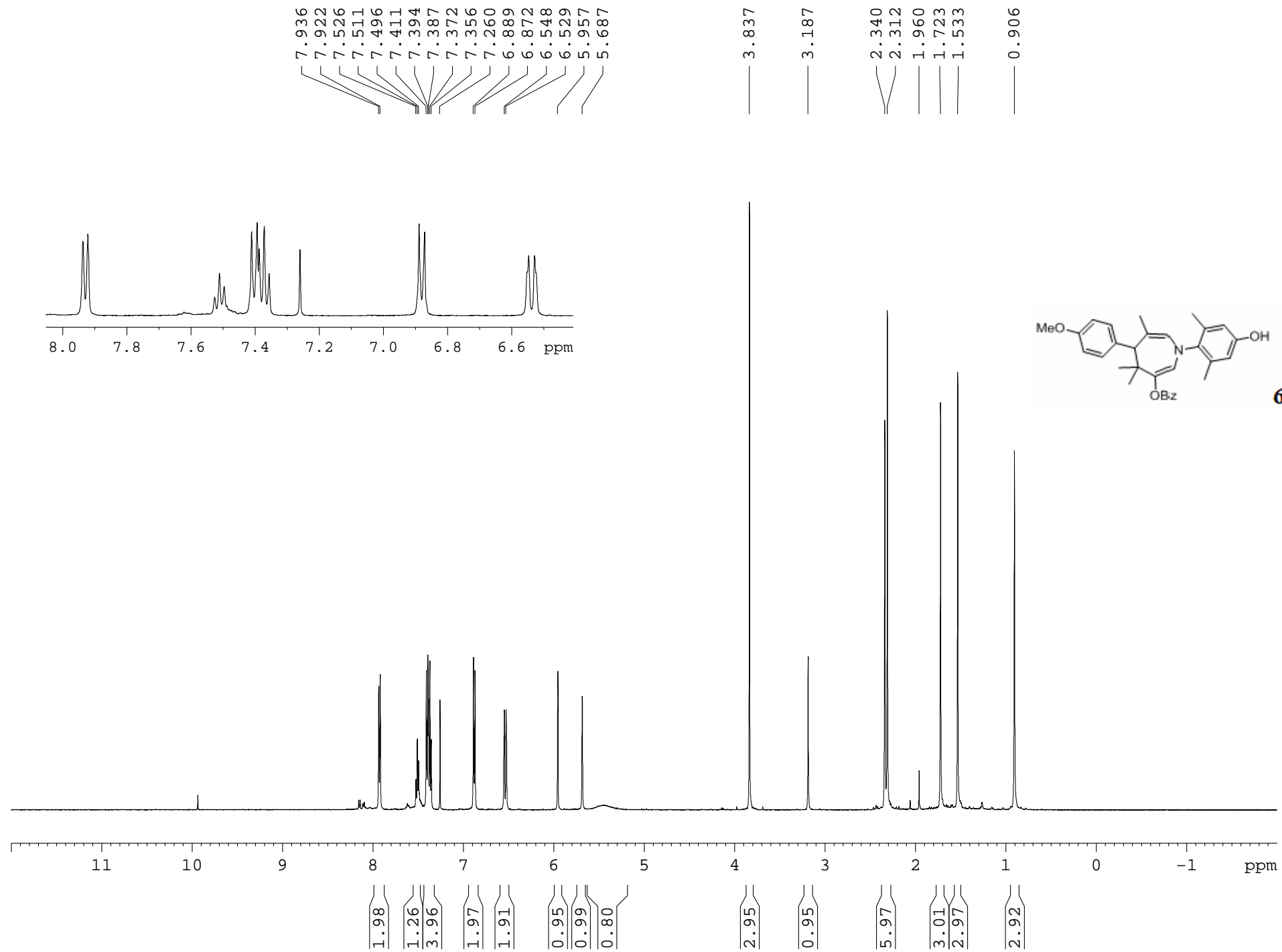
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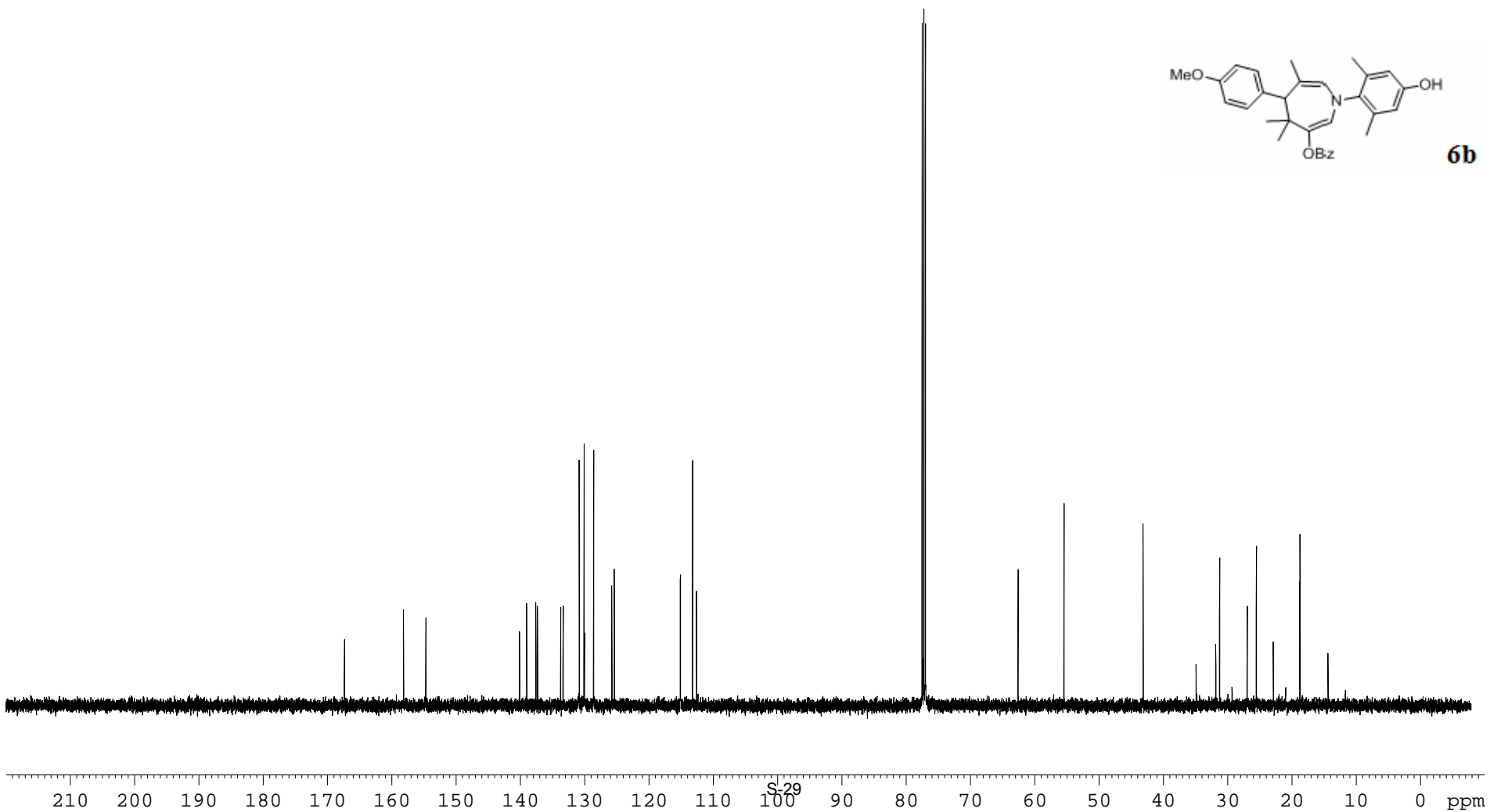
6.10
3.15
3.18

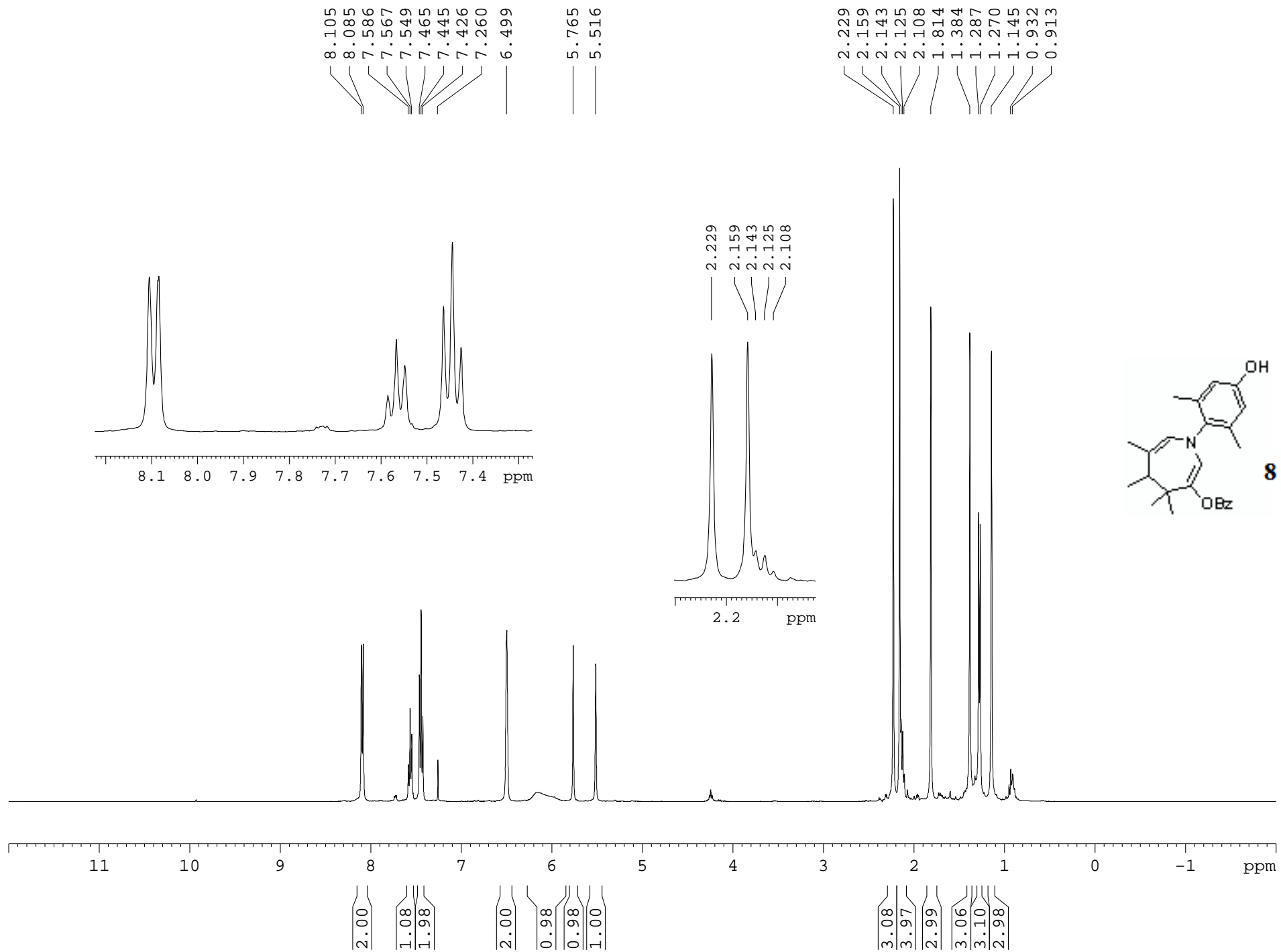
3.06

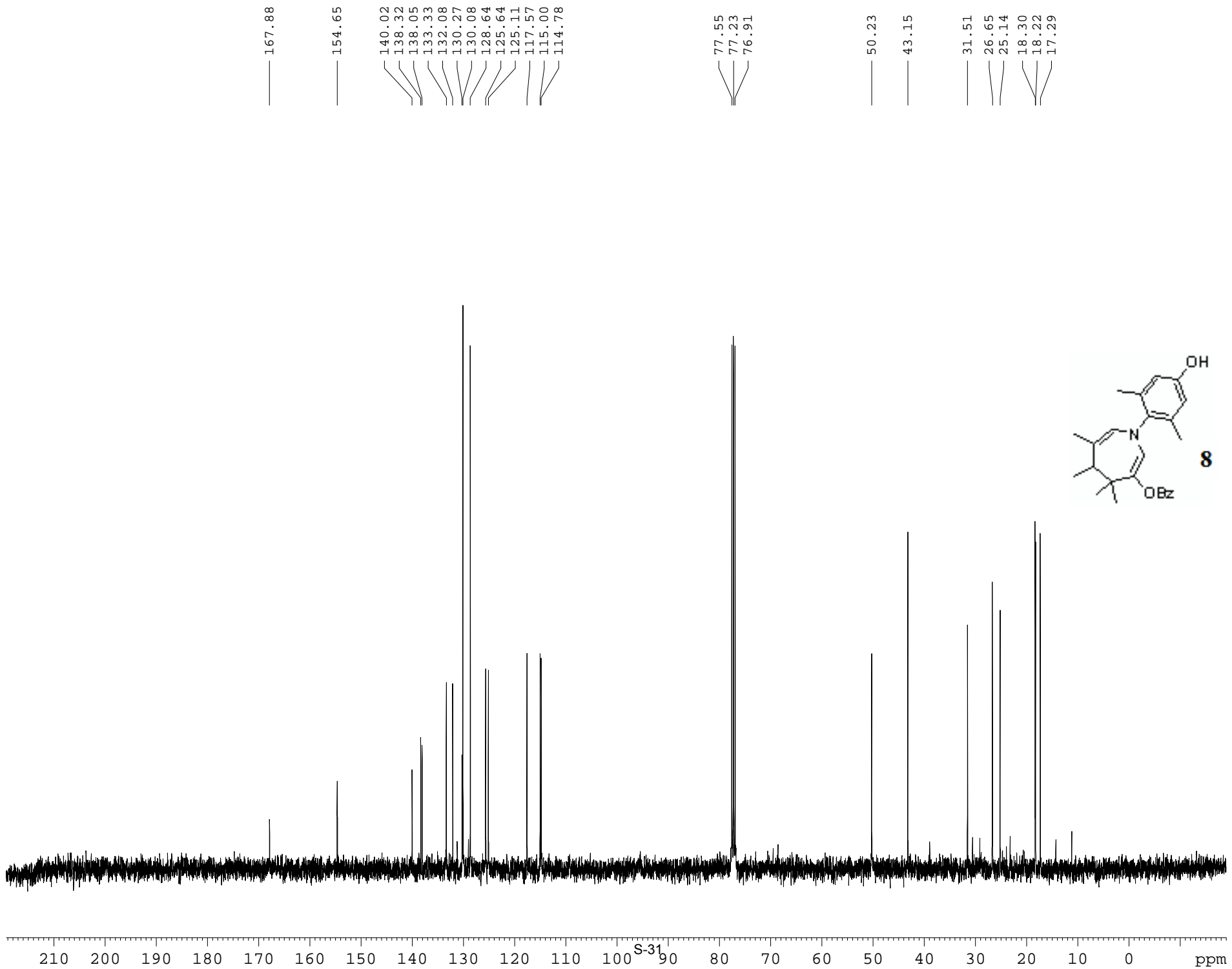


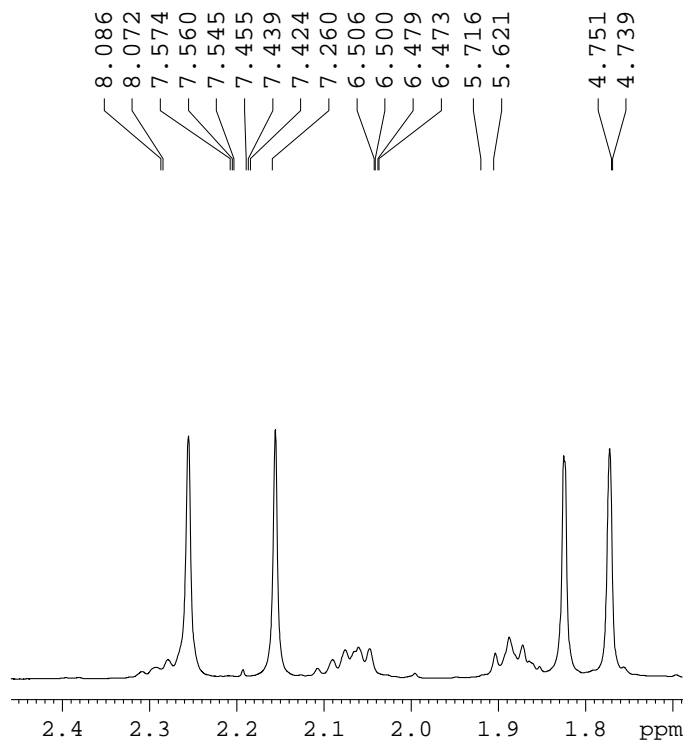
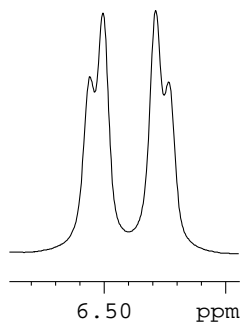








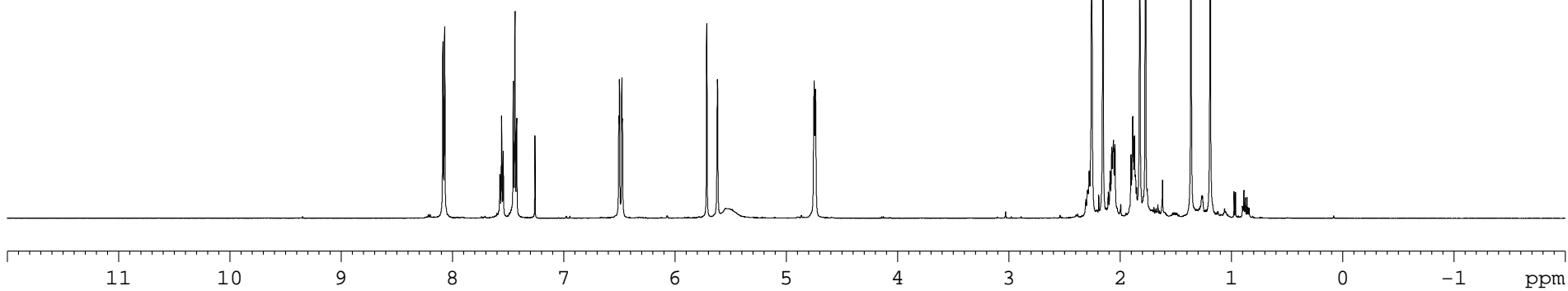




8.086
8.072
7.574
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7.455
7.439
7.424
7.260
6.506
6.500
6.479
6.473
5.716
5.621

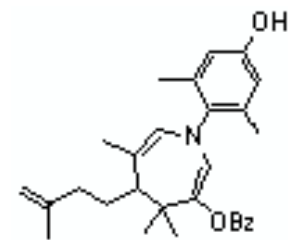
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4.739

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2.279
2.256
2.156
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2.090
2.076
2.060
2.047
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1.888
1.872
1.853
1.825
1.773
1.619
1.363
1.191
0.977
0.888

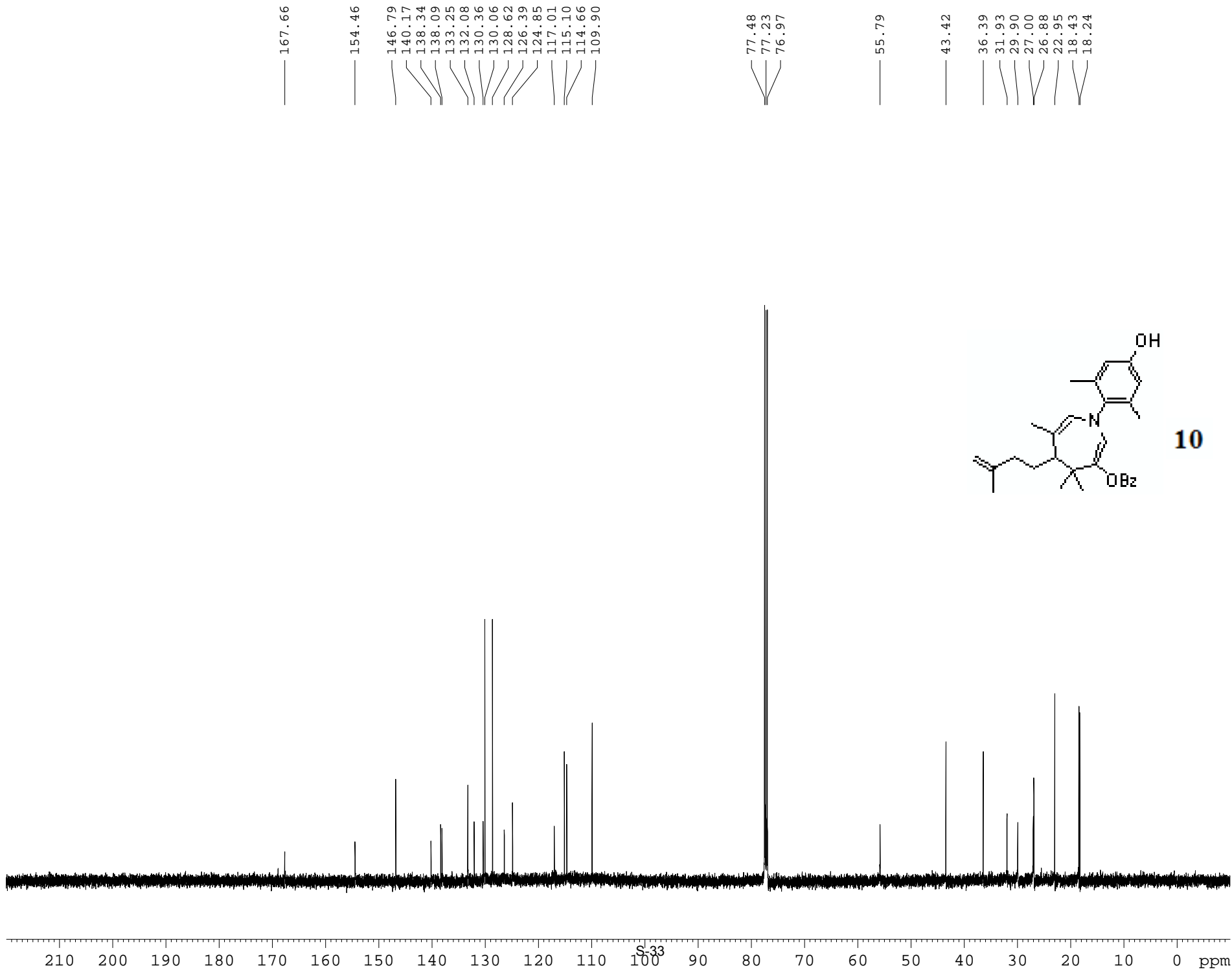


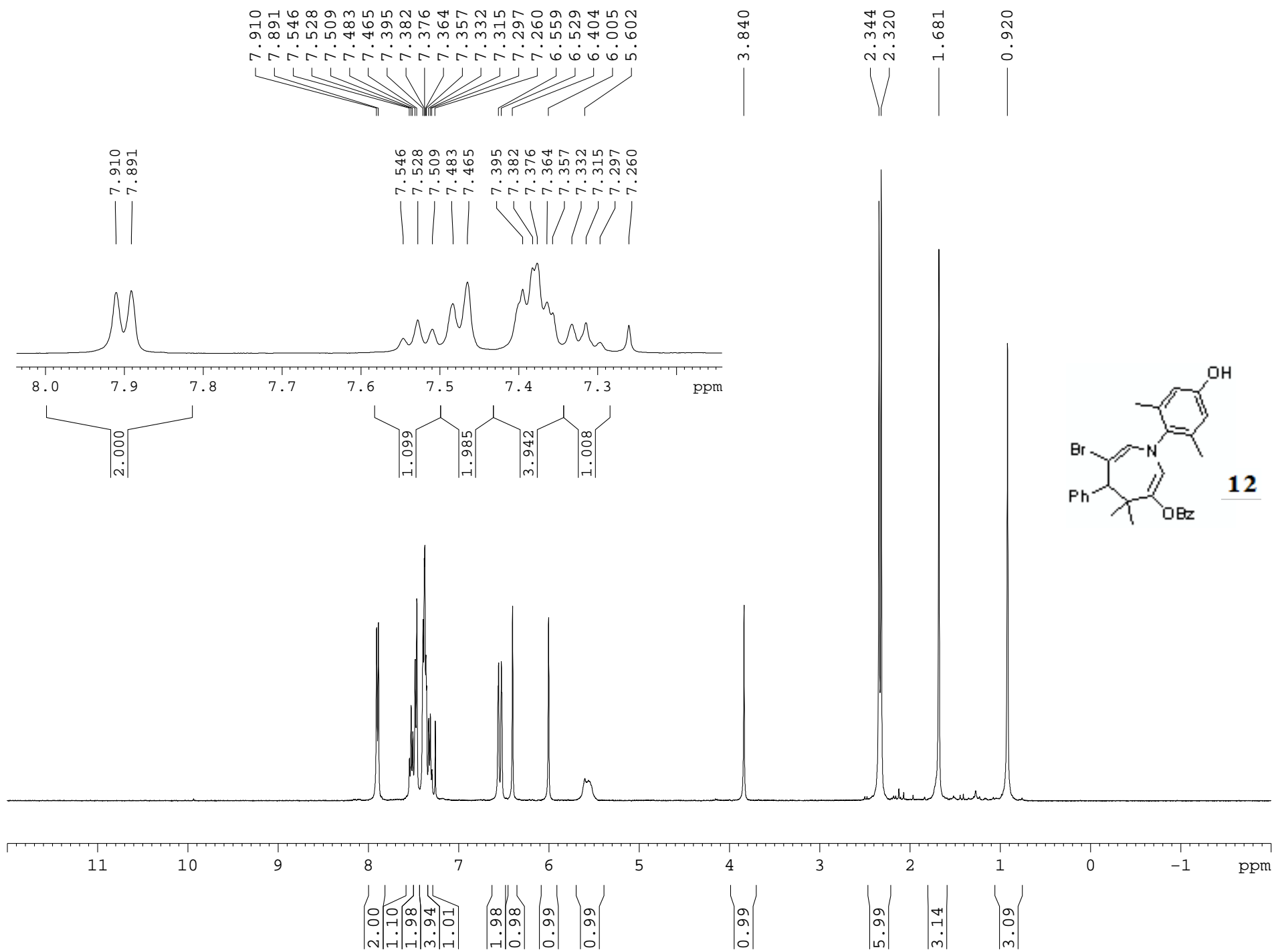
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1.02
1.06
0.82
2.08

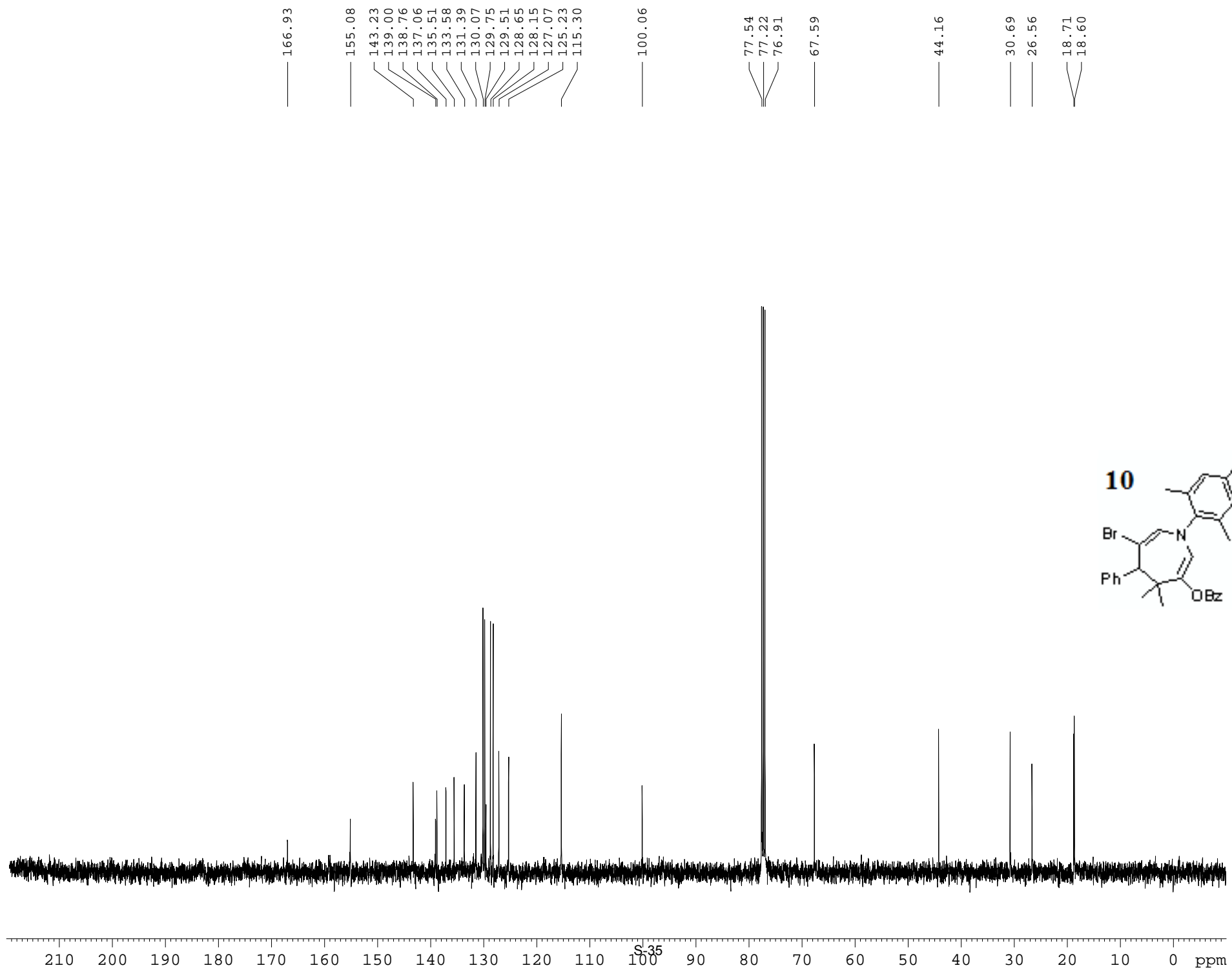
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2.99
2.36
2.15
3.02
3.33
3.11
3.15

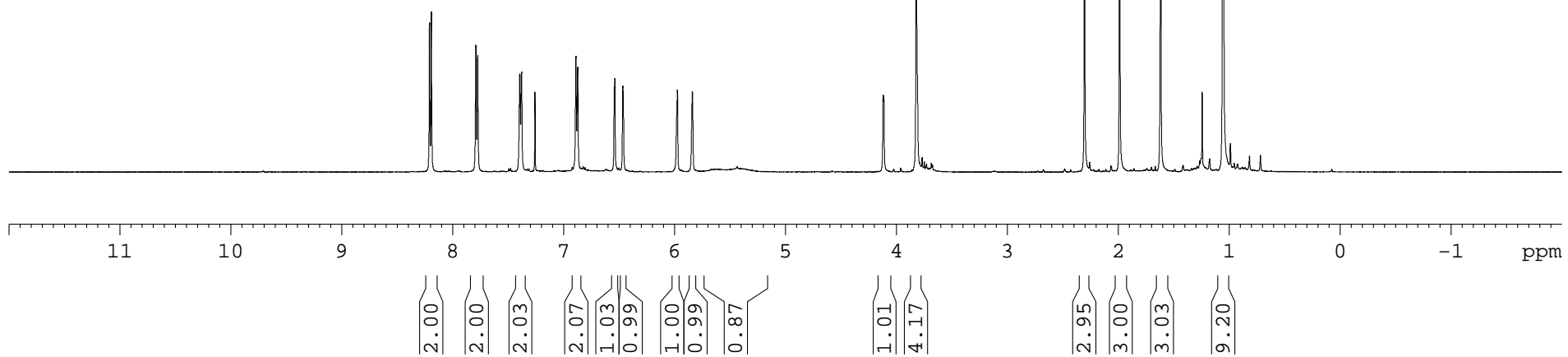
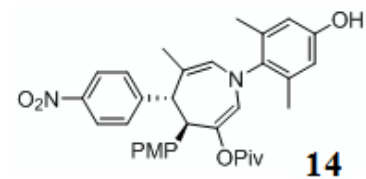
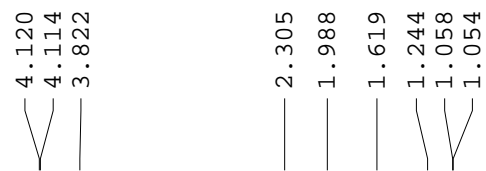
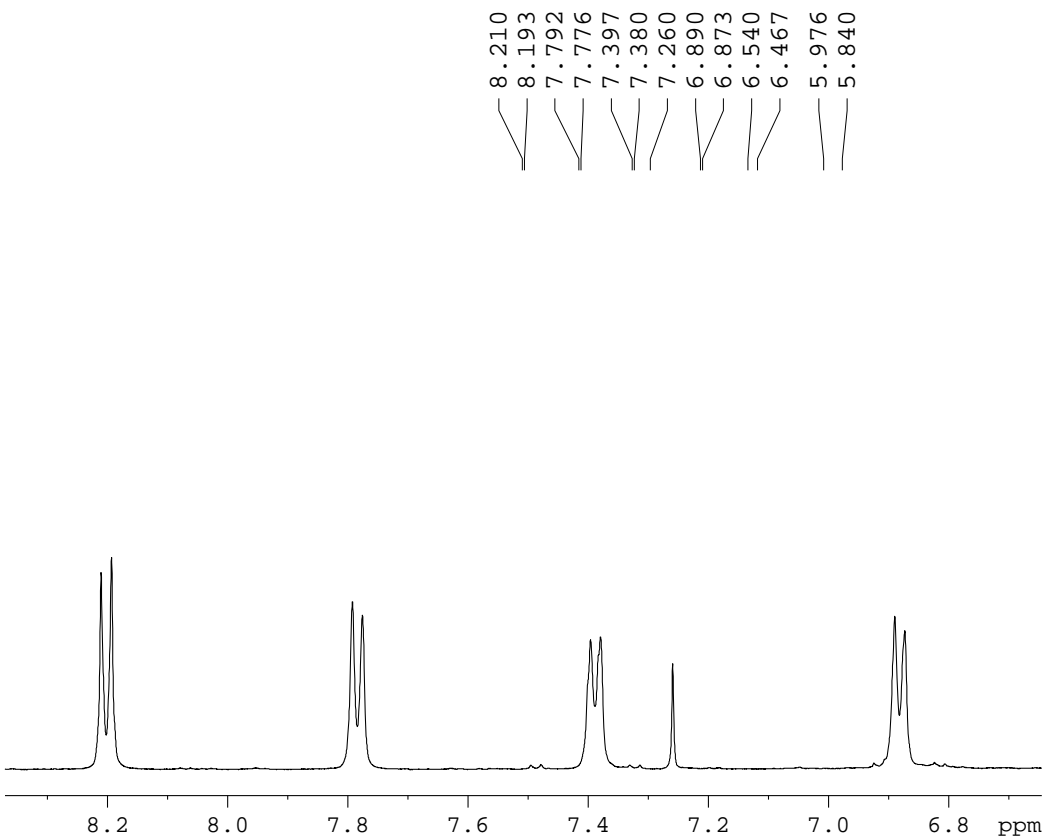


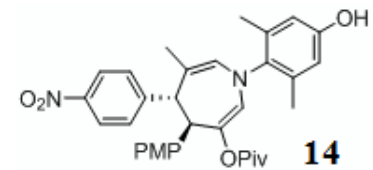
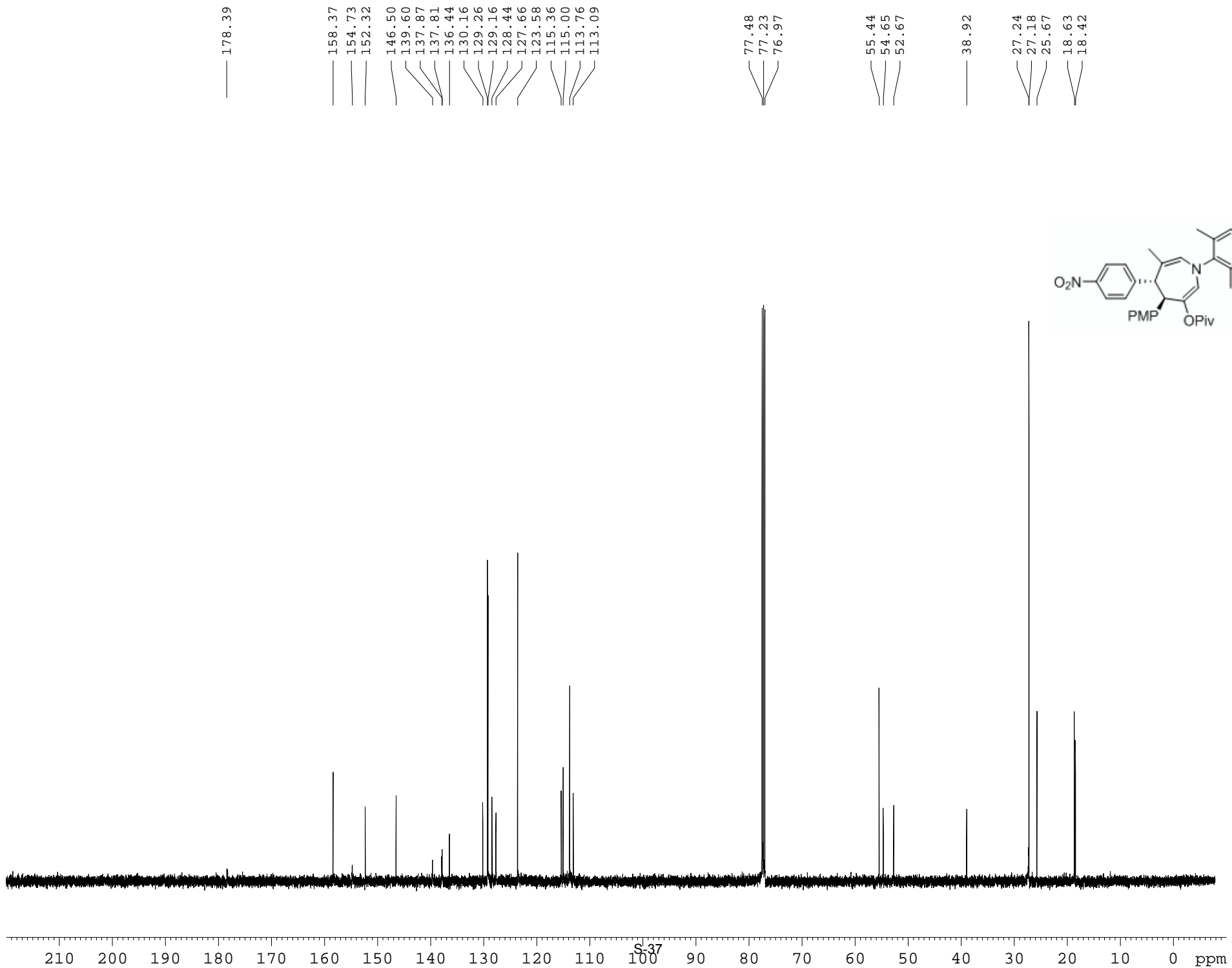
10

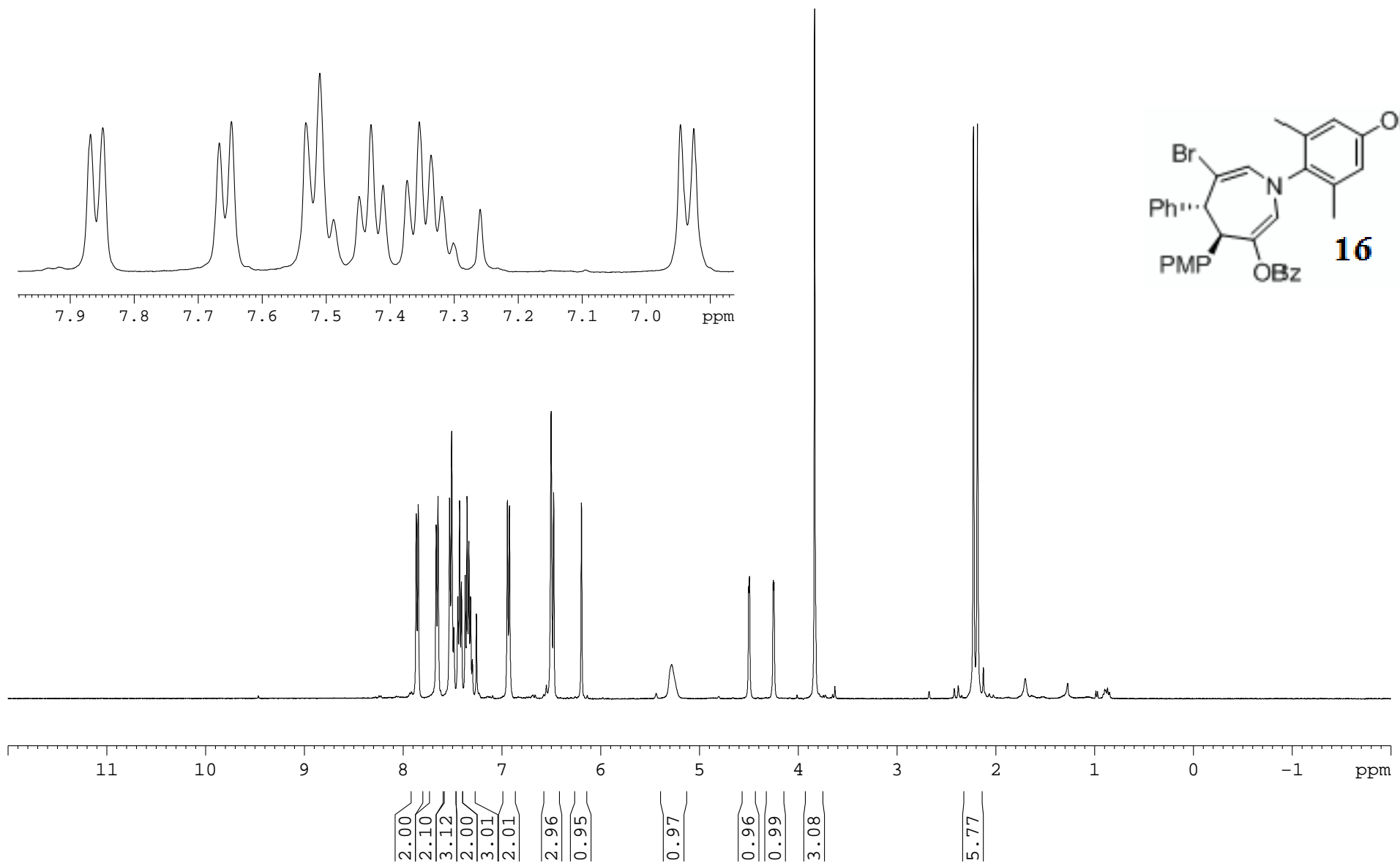
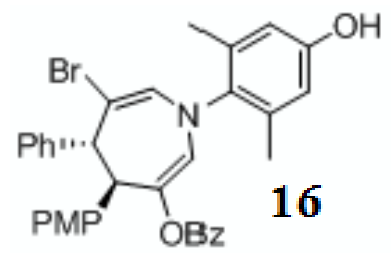
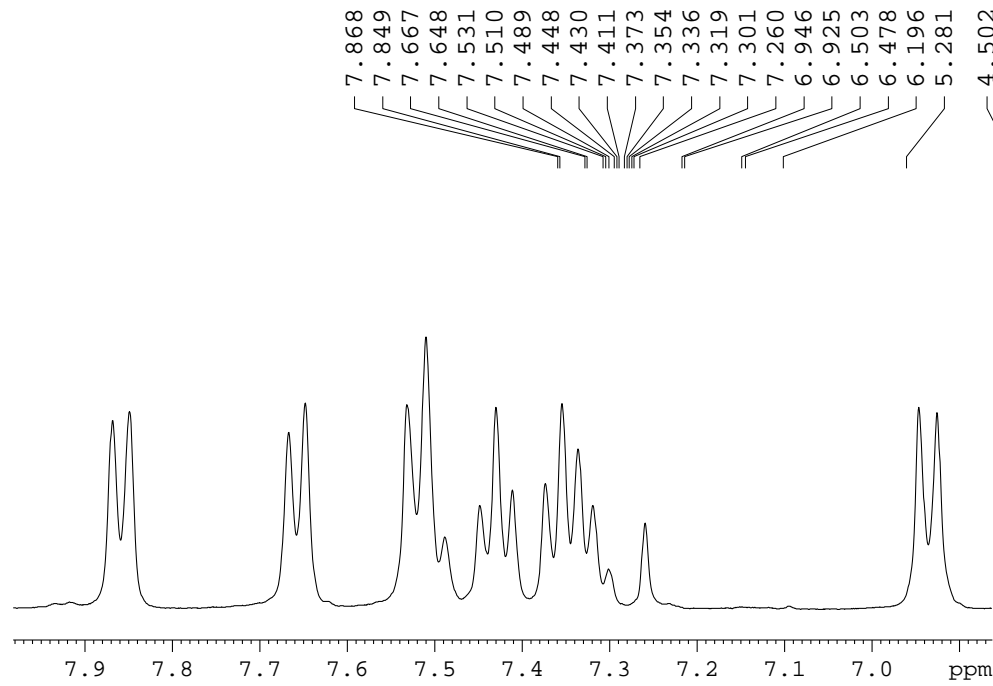


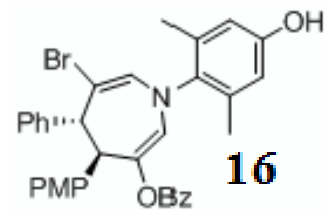
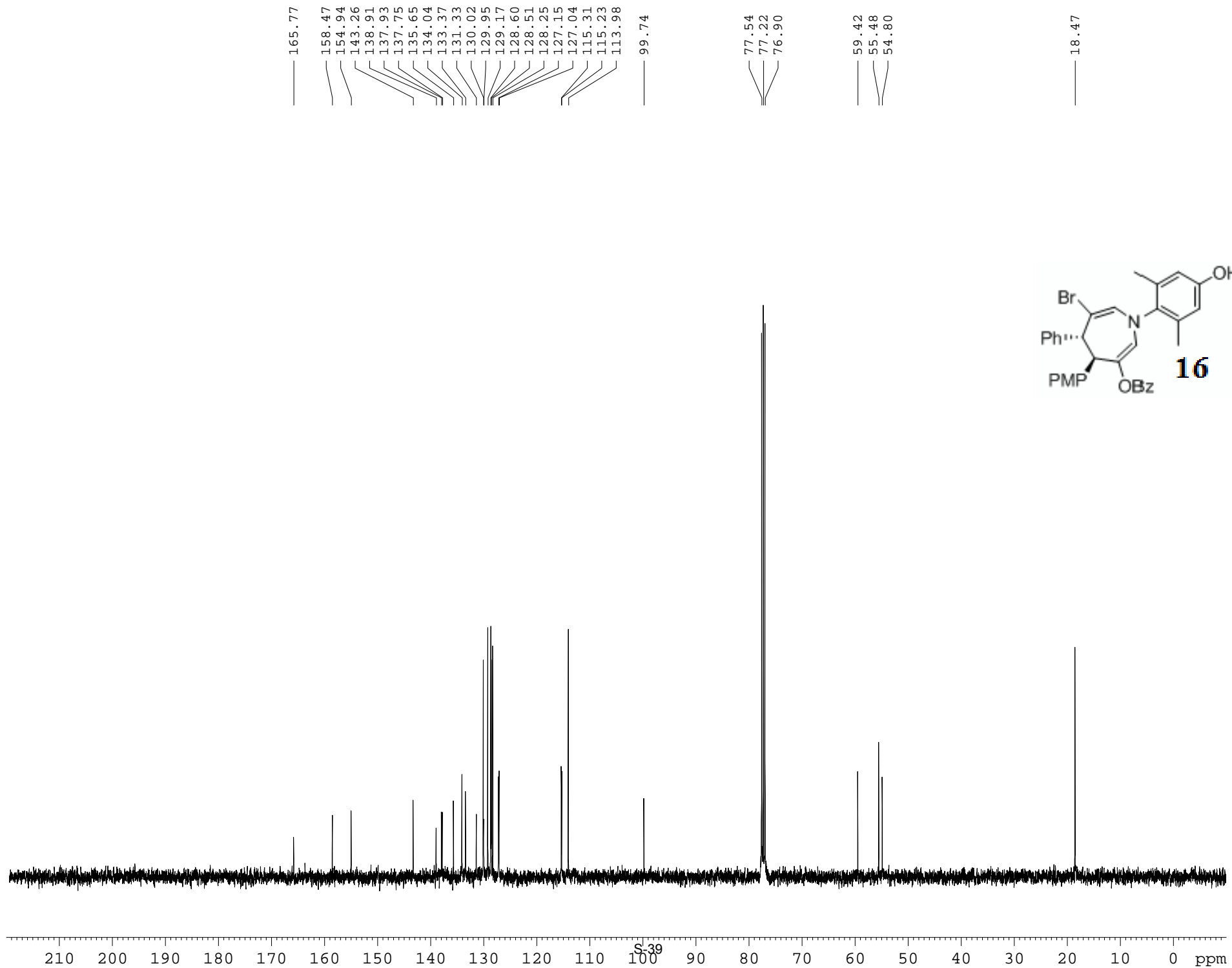


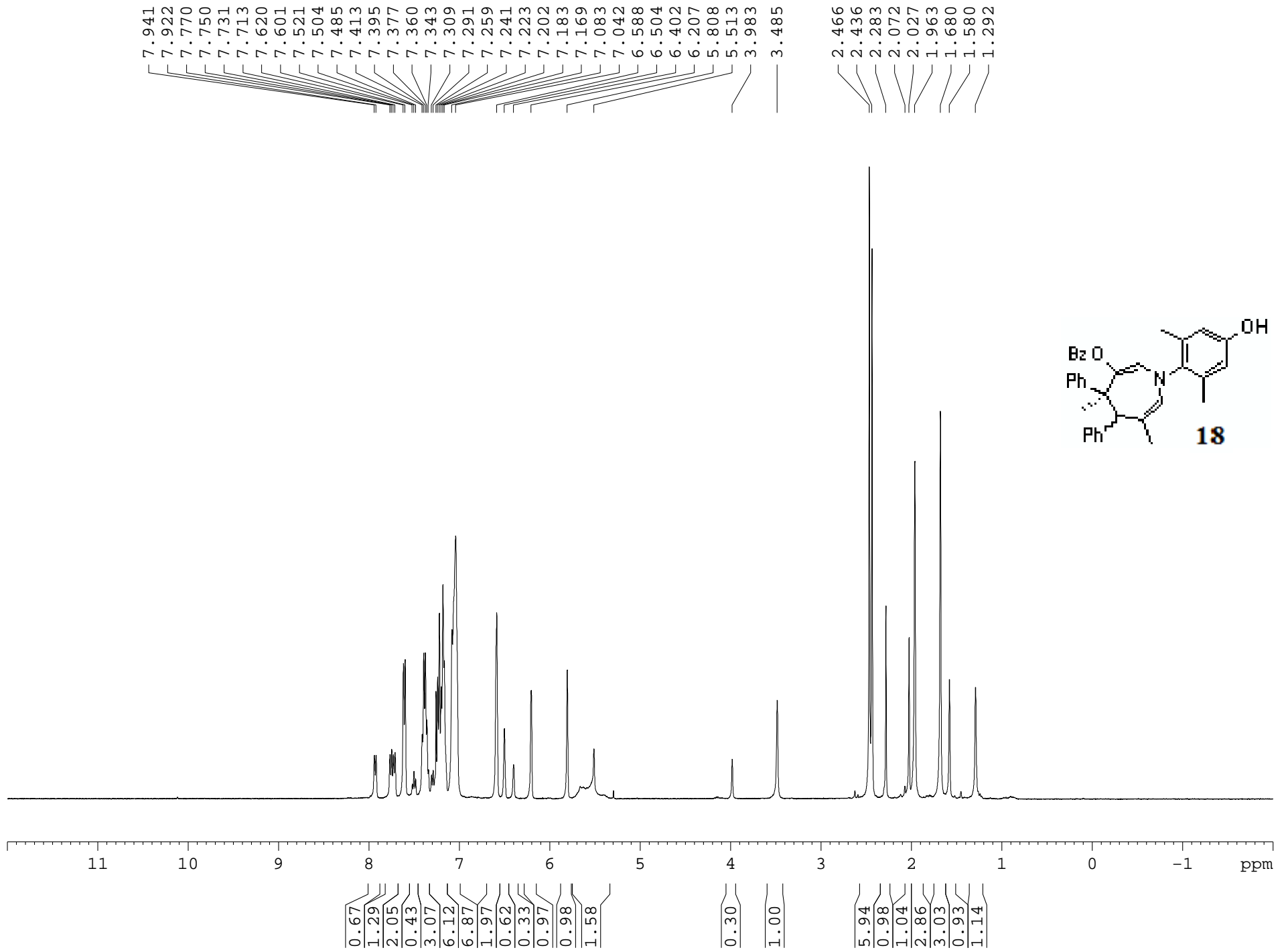


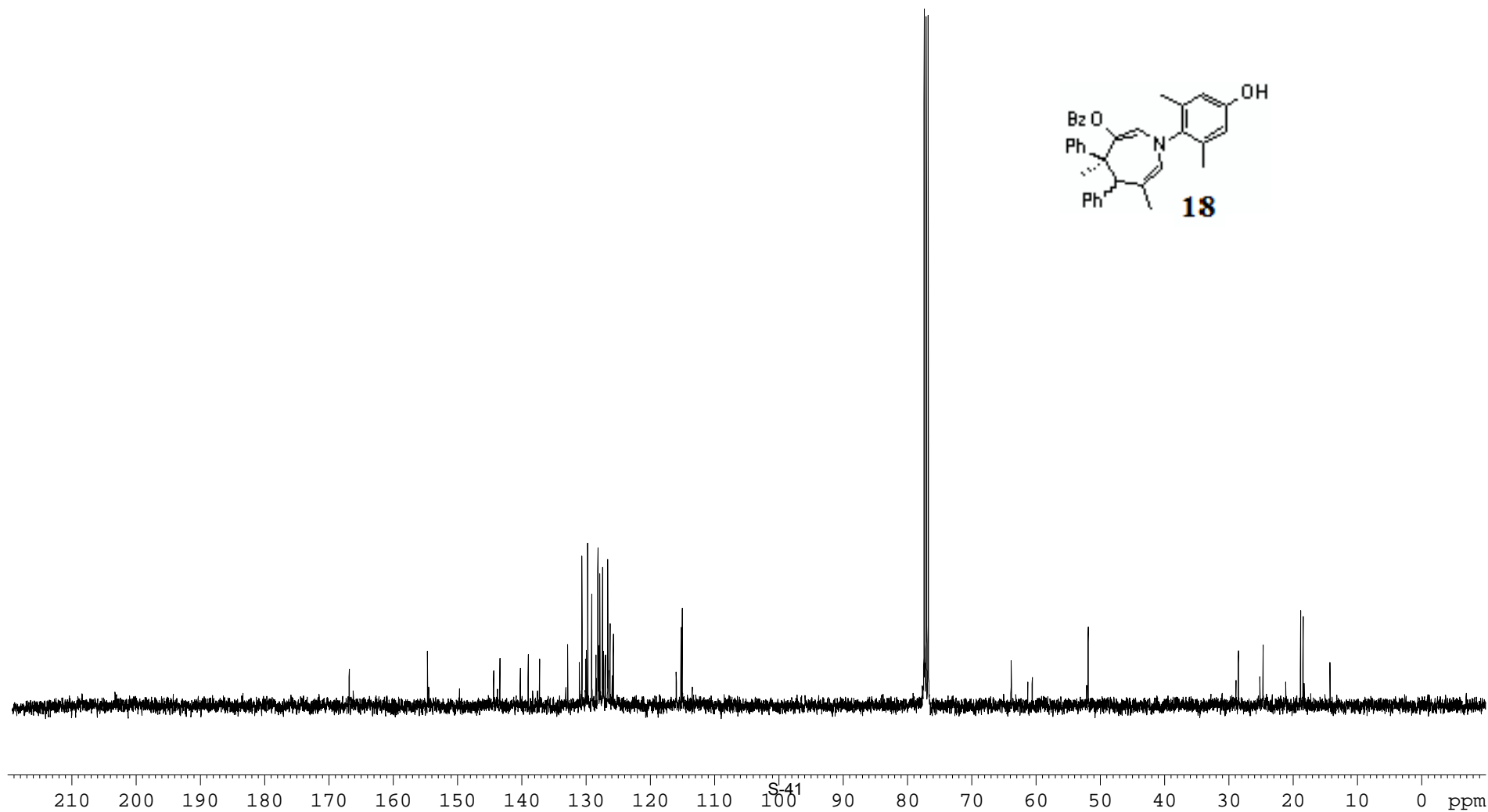




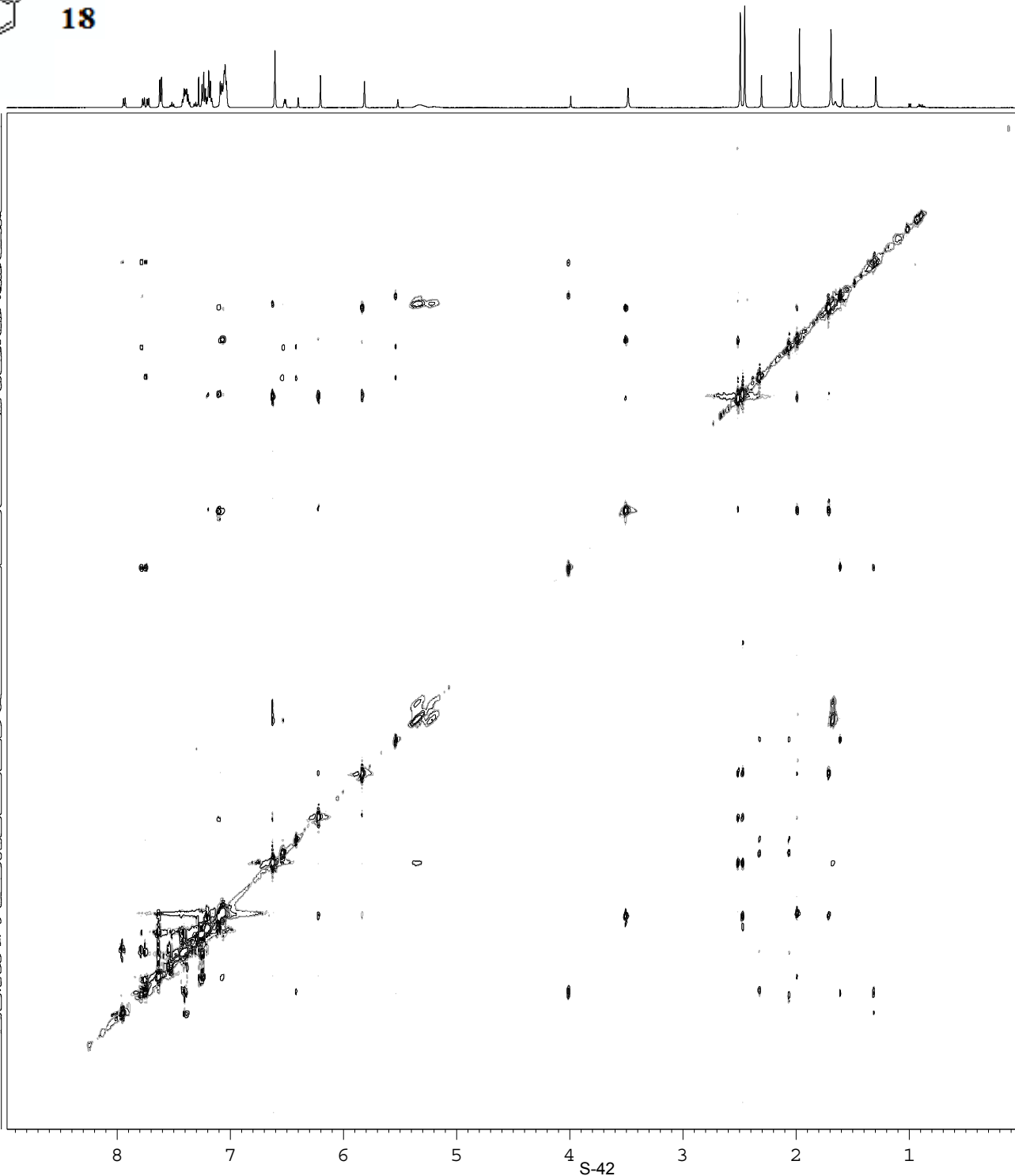
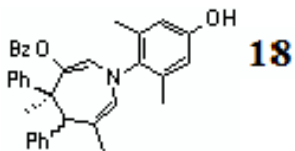








166.78
 166.15
 154.61
 154.38
 149.62
 144.30
 143.72
 143.33
 140.16
 138.92
 138.22
 137.48
 137.16
 133.07
 132.79
 130.97
 130.57
 130.00
 129.87
 129.67
 129.04
 128.39
 128.33
 128.09
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 127.78
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 127.20
 127.14
 126.91
 126.55
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 126.20
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 125.68
 115.89
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 114.96
 113.41
 77.65
 77.38
 77.27
 77.06
 76.75
 63.84
 61.26
 60.56
 52.10
 51.87
 28.87
 28.49
 25.15
 24.63
 21.12
 18.80
 18.42
 18.27
 14.23



Current Data Parameters
 USER nshapiro
 NAME 09-129-noesy-2
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080507
 Time 19.35
 INSTRUM AV-500
 PROBHD 5 mm TBI 1H/31
 PULPROG noesygpph
 TD 4096
 SOLVENT CDC13
 NS 2
 DS 4
 SWH 4496.403 Hz
 FIDRES 1.097755 Hz
 AQ 0.4555252 sec
 RG 88
 DW 111.200 usec
 DE 7.11 usec
 TE 300.0 K
 d0 0.00010139 sec
 D1 4.00000000 sec
 D8 0.66000003 sec
 D16 0.00010000 sec
 IN0 0.00022213 sec
 MCREST 0.00000000 sec
 MCWRK 4.00000000 sec
 TAU 0.32890001 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 7.60 usec
 P2 15.20 usec
 PL1 0.00 dB
 SFO1 500.2322510 MHz

==== GRADIENT CHANNEL ====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPX1 0.00 %
 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 40.00 %
 GPZ2 -40.00 %
 P16 1000.00 usec

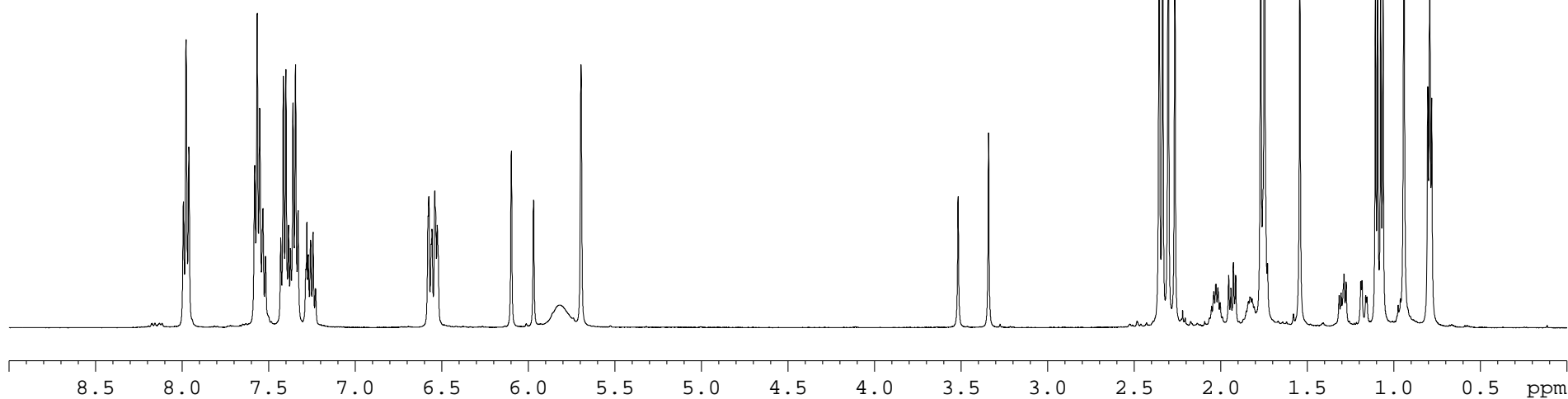
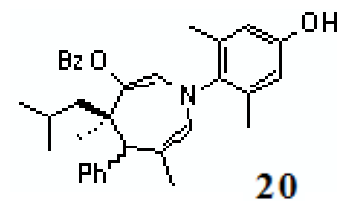
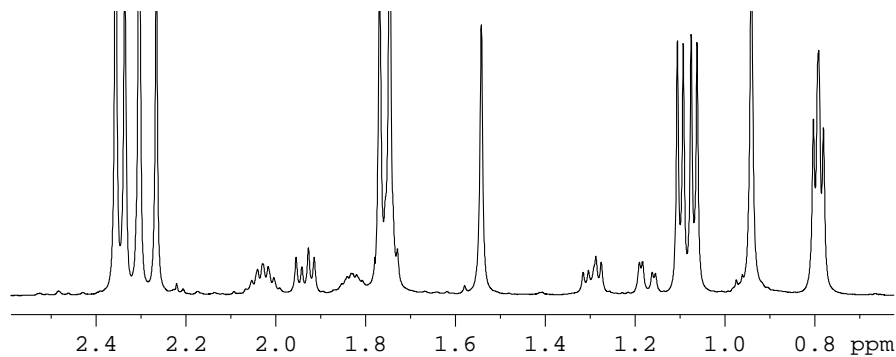
F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 500.2323 MHz
 FIDRES 35.171638 Hz
 SW 9.000 ppm
 FMODE TPPI

F2 - Processing parameters
 SI 2048
 SF 500.2300104 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 2048
 MC2 TPPI
 SF 500.2300104 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

7.978
7.963
7.582
7.567
7.553
7.534
7.519
7.431
7.416
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7.375
7.361
7.346
7.331
7.280
7.272
7.259
7.245
7.230
6.576
6.557
6.541
6.527
6.098
5.970
5.819
5.696

3.518
3.342
2.356
2.336
2.304
2.266
2.220
2.040
2.028
2.017
2.004
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1.942
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1.832
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1.747
1.730
1.580
1.543
1.317
1.305
1.288
1.276
1.191
1.184
1.163
1.107



5.15
8.23
14.03
5.18
1.46
1.10
2.24
2.61
1.00
1.44
4.40
3.40
4.72
3.24
1.63
1.70
1.36
9.63
3.26
1.55
1.23
9.20
5.23
6.60

167.56
166.70
154.86
145.00
144.88
140.25
140.00
138.72
138.27
137.60
137.32
134.79
133.38
133.25
132.78
130.52
130.28
130.21
130.13
129.98
128.60
128.25
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127.87
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125.79
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115.09
112.54
112.32

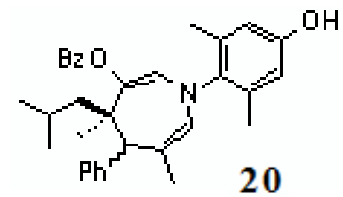
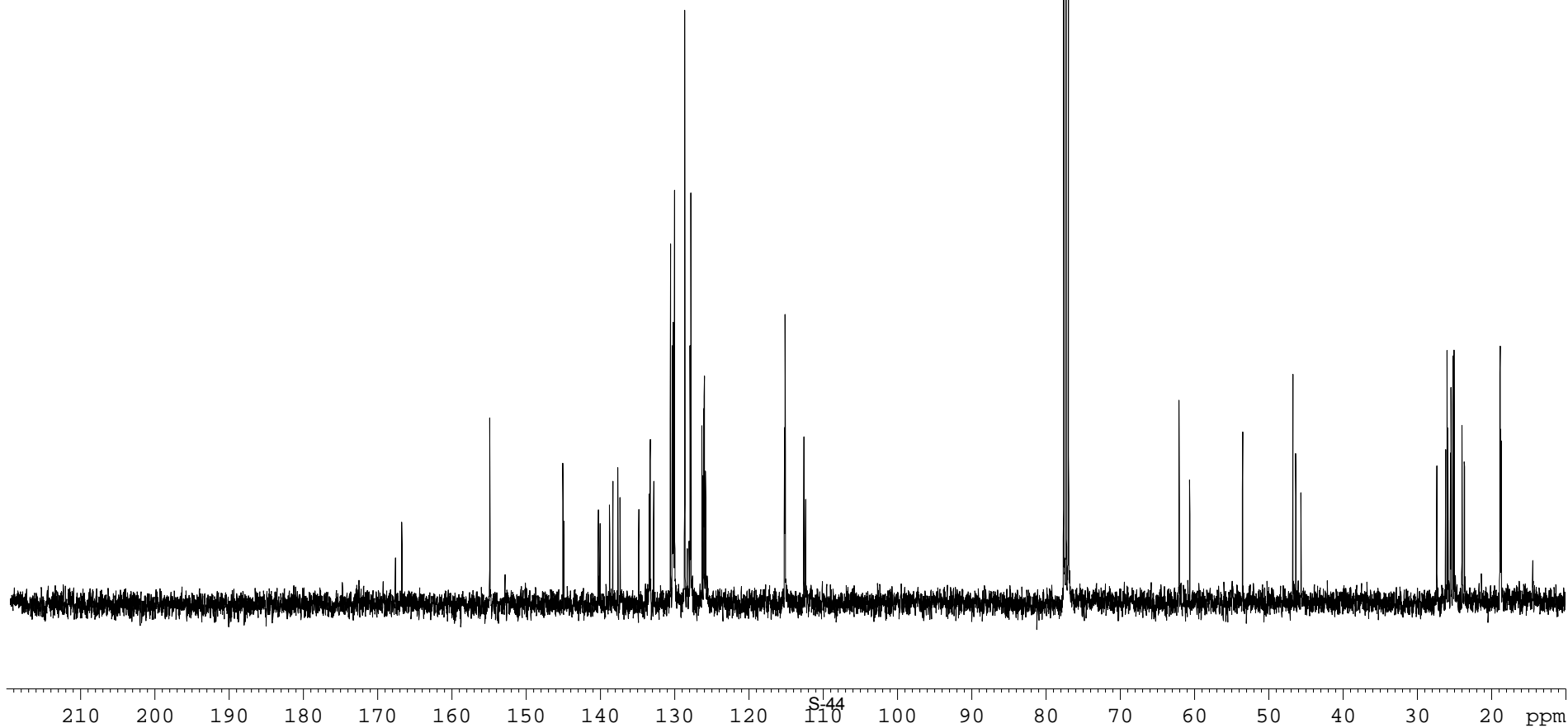
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77.23
76.91

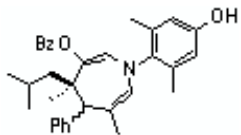
62.01
60.58

53.45

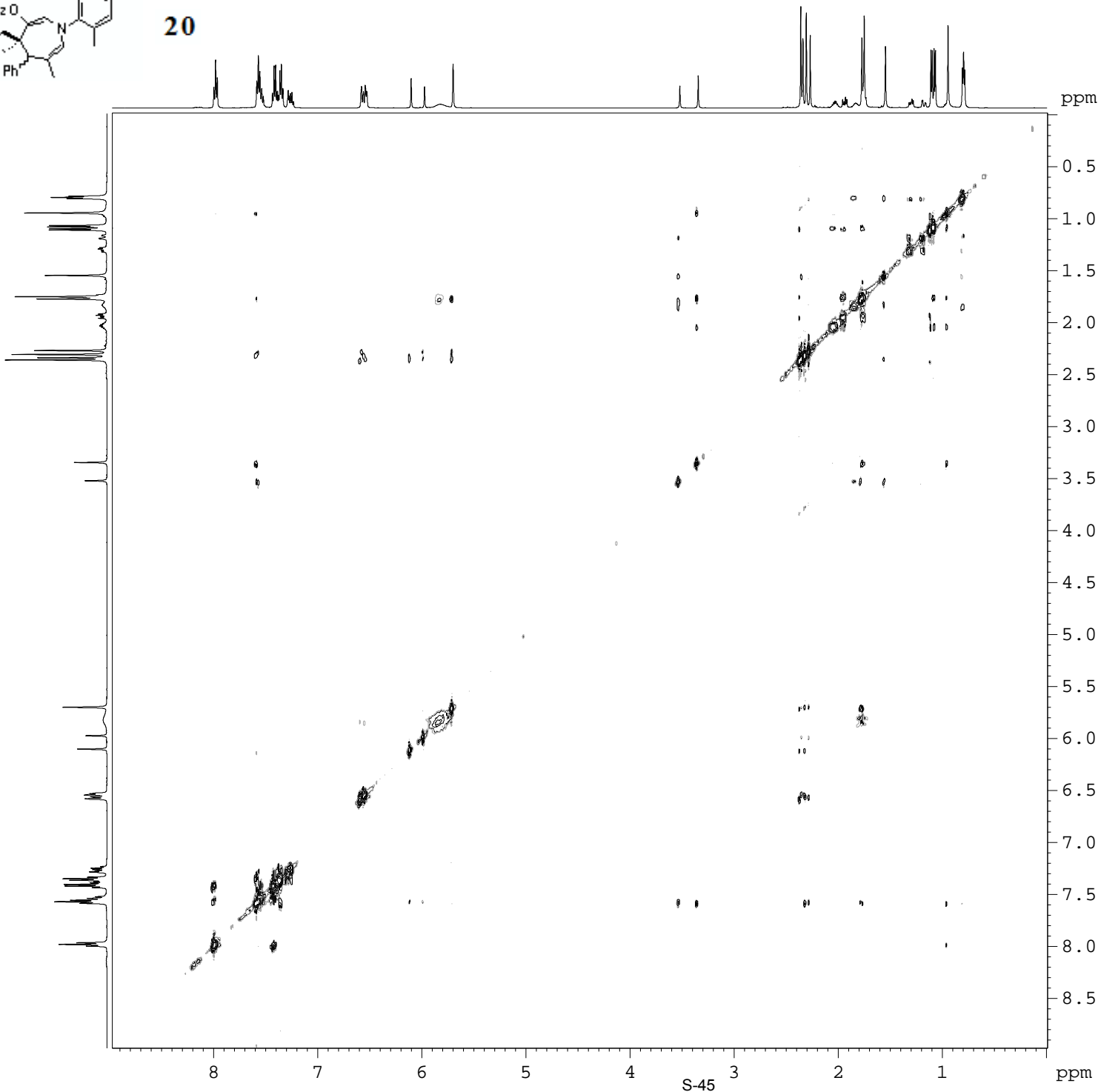
46.67
46.29
45.60

27.29
26.11
25.91
25.79
25.45
25.37
25.11
24.97
23.90
23.58
18.79
18.76





20



Current Data Parameters
 NAME 09-076-noesy
 EXPNO 11
 PROCNO 1
 DU /u
 USER nshapiro

F2 - Acquisition Parameters
 Date_ 20080507
 Time 19.05
 INSTRUM AV-500
 PROBHD 5 mm TBI 1H/31
 PULPROG noesygpph
 TD 4096
 SOLVENT CDCl3
 NS 2
 DS 4
 SWH 4496.403 Hz
 FIDRES 1.097755 Hz
 AQ 0.4556364 sec
 RG 88
 DW 111.200 use
 DE 7.11 use
 TE 300.0 K
 d0 0.00010139 sec
 D1 5.00000000 sec
 D8 0.52999997 sec
 D16 0.00010000 sec
 IN0 0.00022213 sec
 MCREST 0.00000000 sec
 MCWRK 5.00000000 sec
 TAU 0.26389998 sec

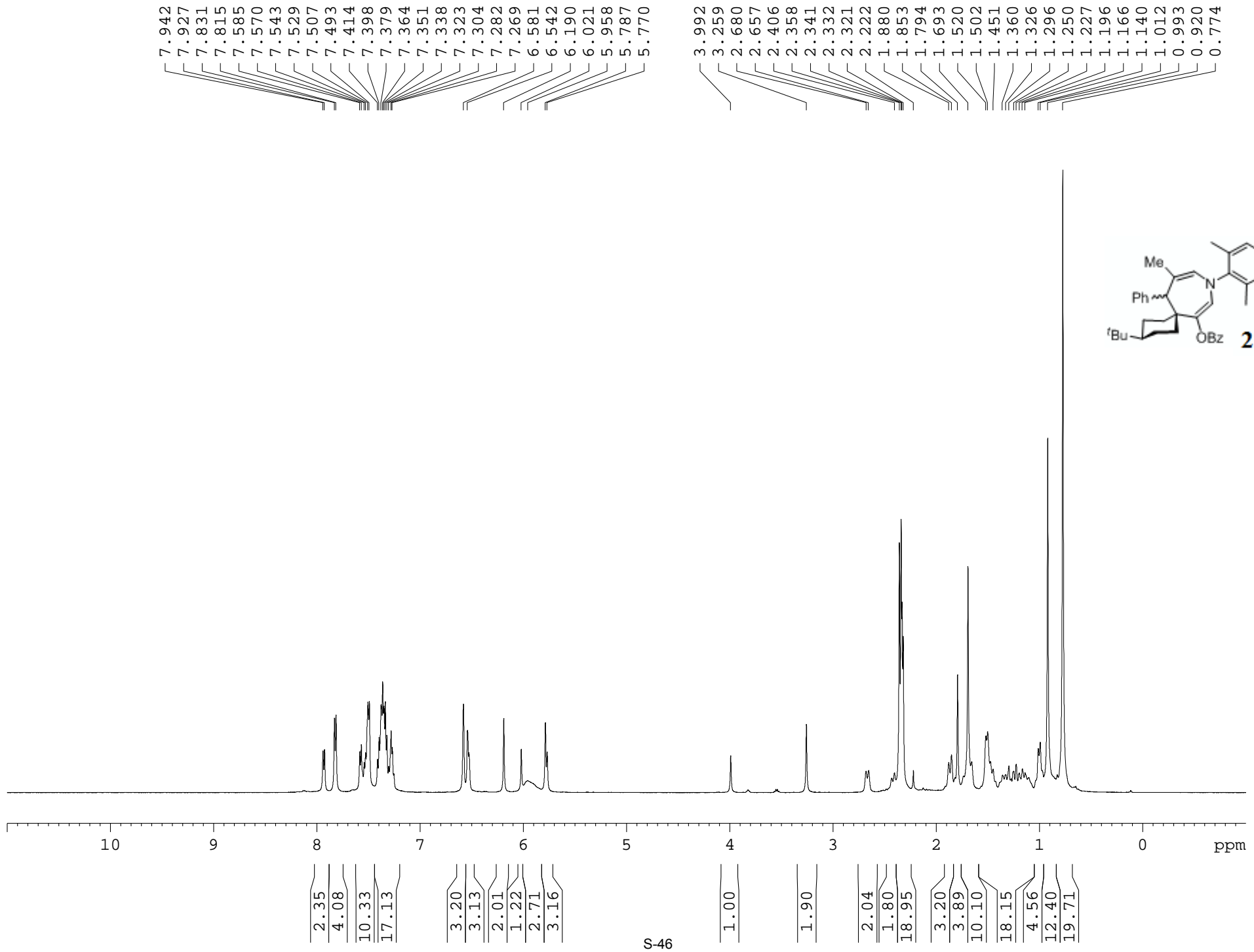
==== CHANNEL f1 =====
 NUC1 1H
 P1 7.60 use
 P2 15.20 use
 PL1 0.00 dB
 SFO1 500.2322510 MHz

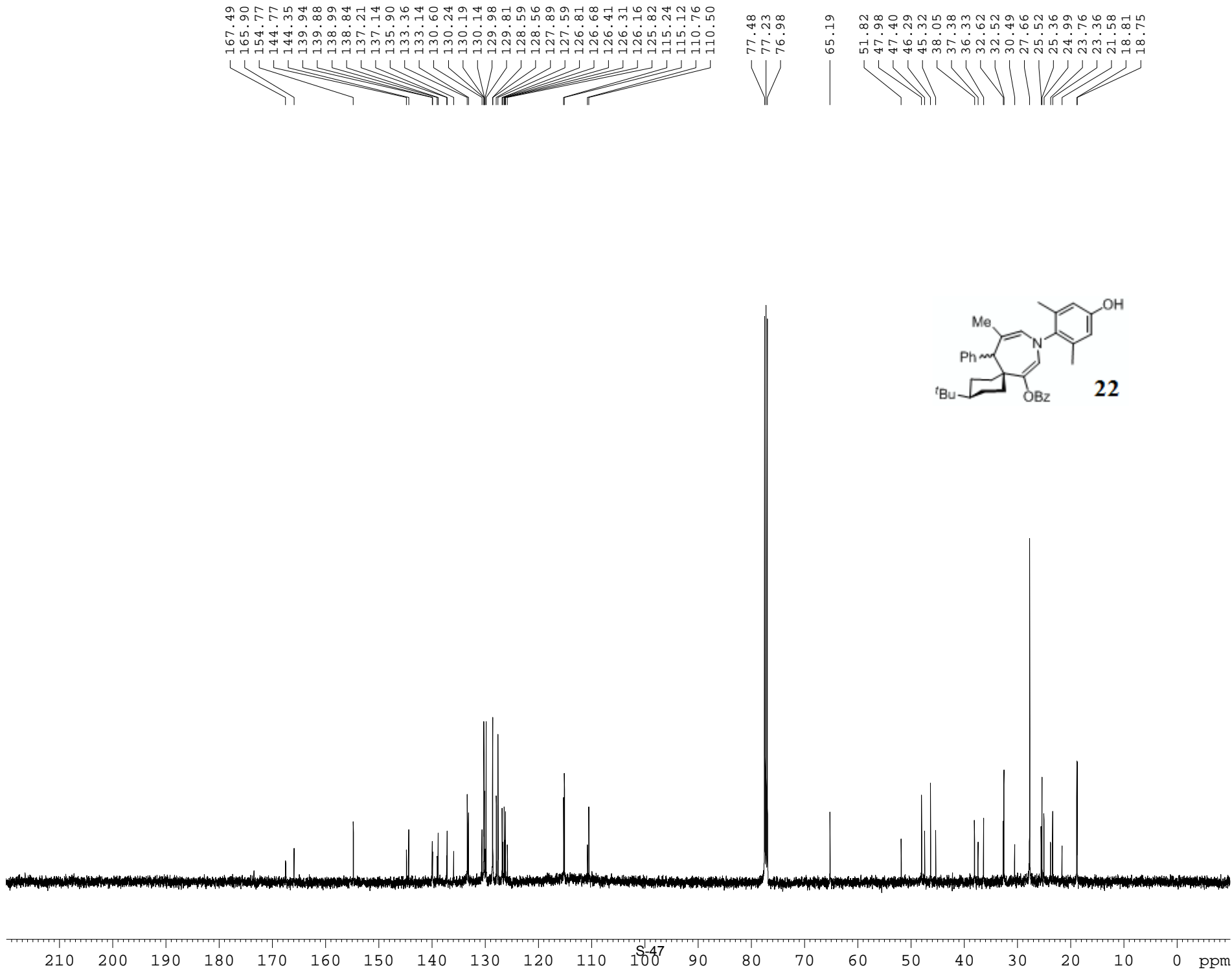
==== GRADIENT CHANNEL ===
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPX1 0.00 %
 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 40.00 %
 GPZ2 -40.00 %
 P16 1000.00 use

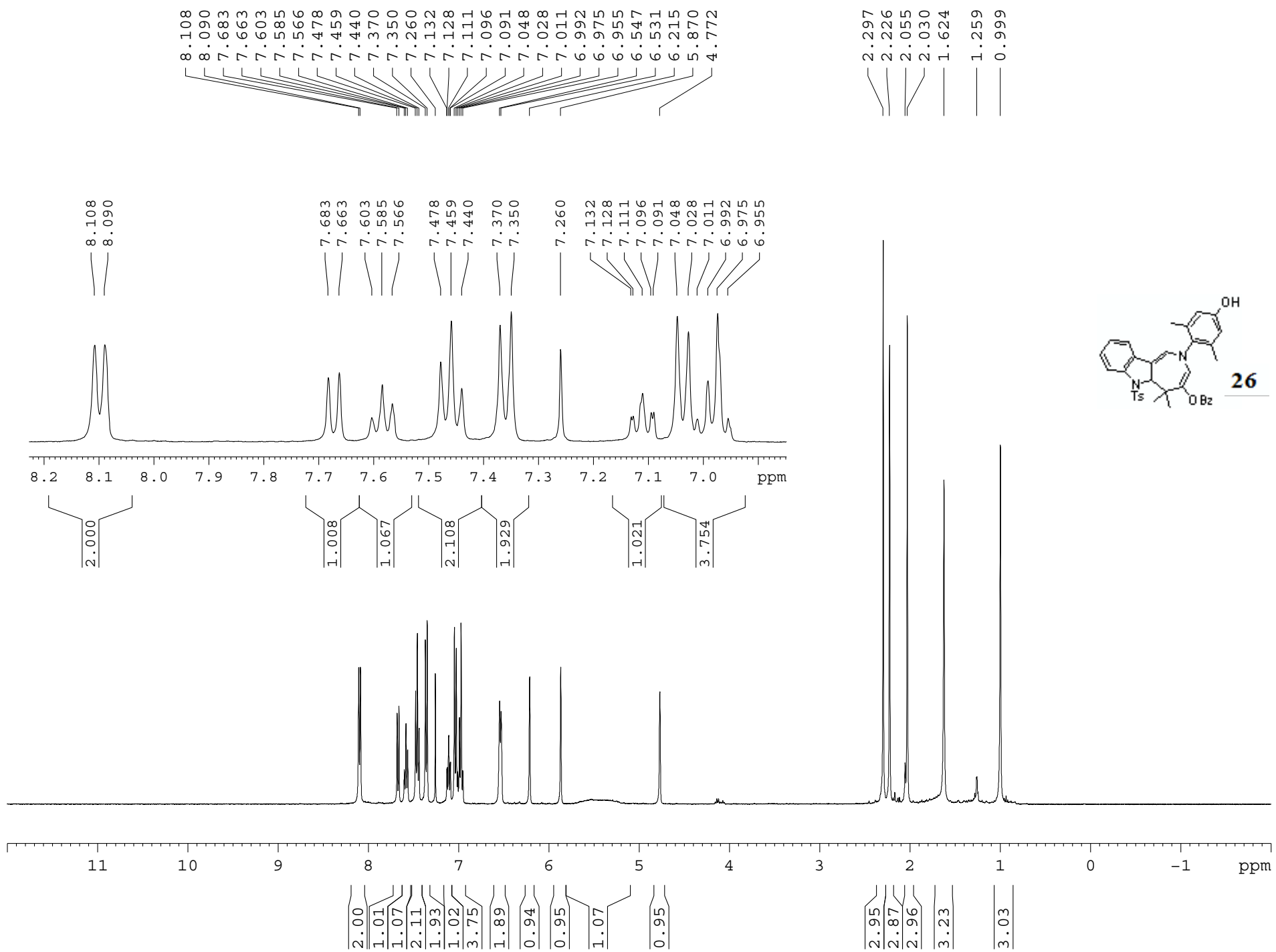
F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 500.2323 MHz
 FIDRES 35.171638 Hz
 SW 9.000 ppm
 FnmODE TPPI

F2 - Processing parameters
 SI 2048
 SF 500.2300104 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 2048
 MC2 TPPI
 SF 500.2300104 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0







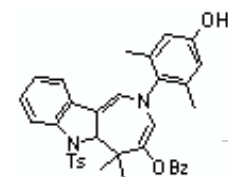
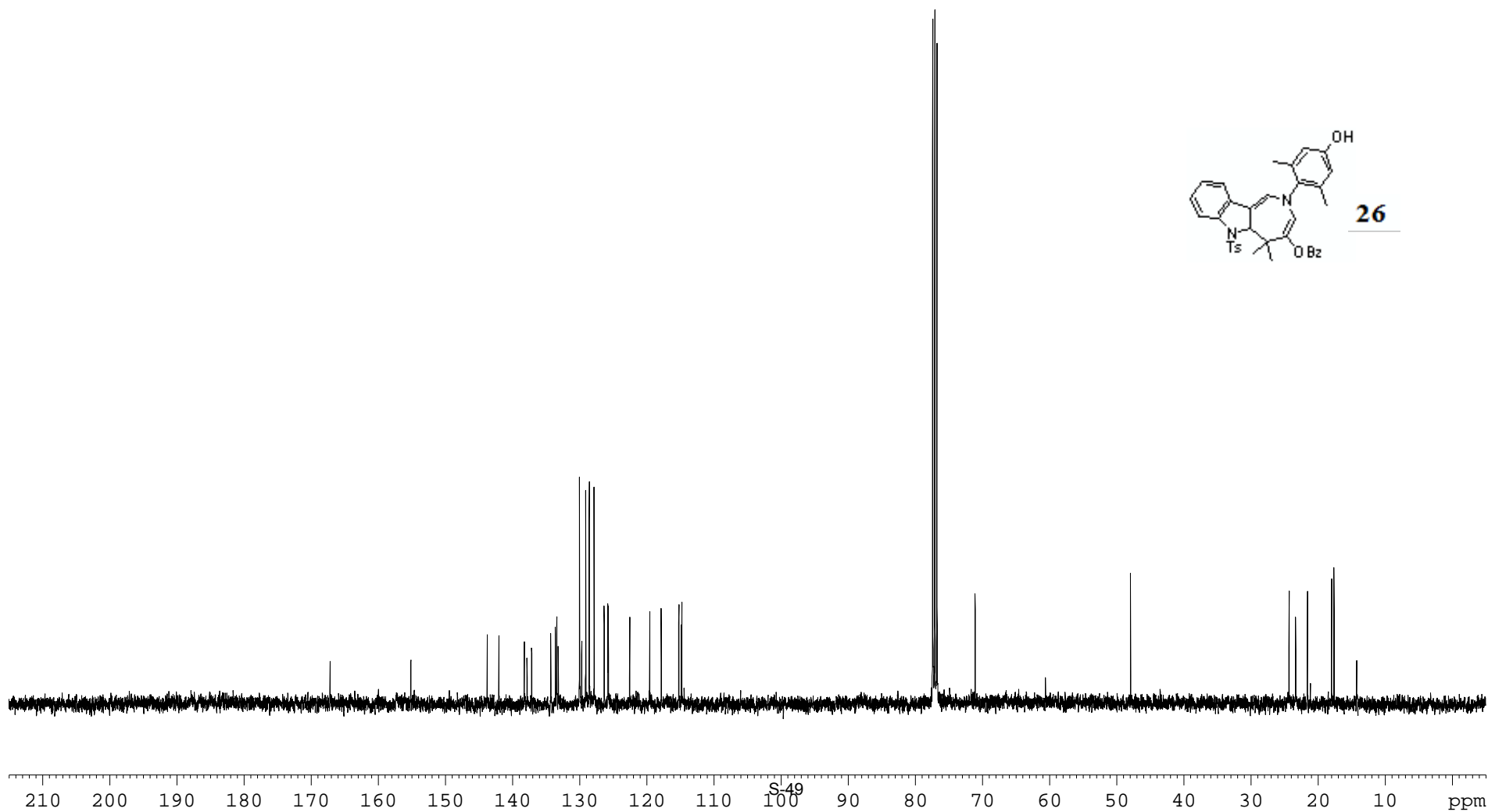
167.17
155.13
143.76
142.03
138.24
137.84
137.14
134.30
133.62
133.41
133.20
130.02
129.69
129.10
128.57
127.85
126.34
125.79
125.73
122.52
119.54
117.84
115.21
114.88
114.77

77.39
77.08
76.76
71.07

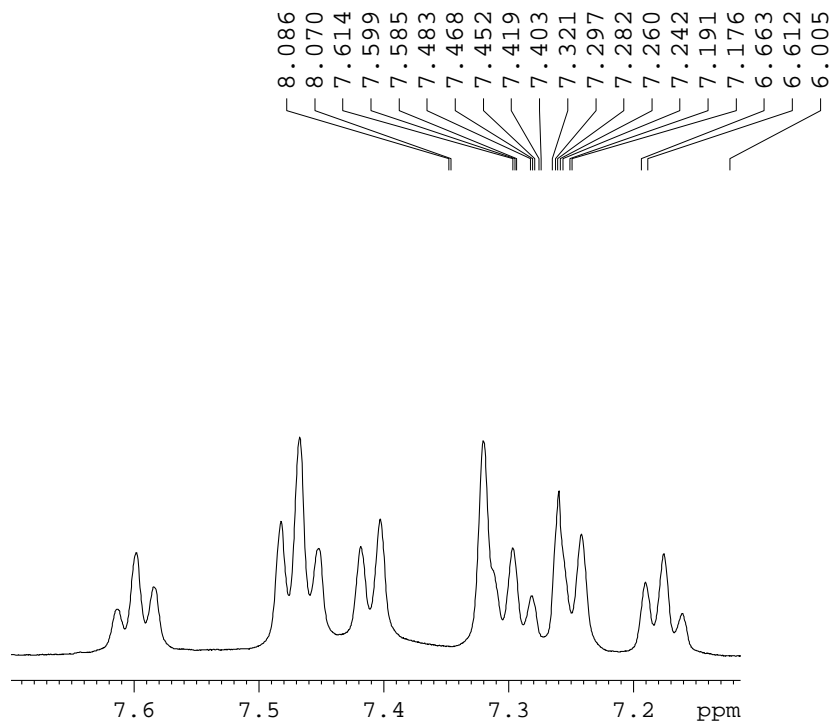
60.60

47.92

24.30
23.32
21.55
21.12
17.96
17.61
14.22



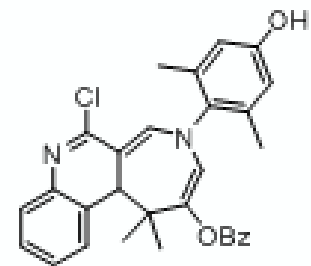
26



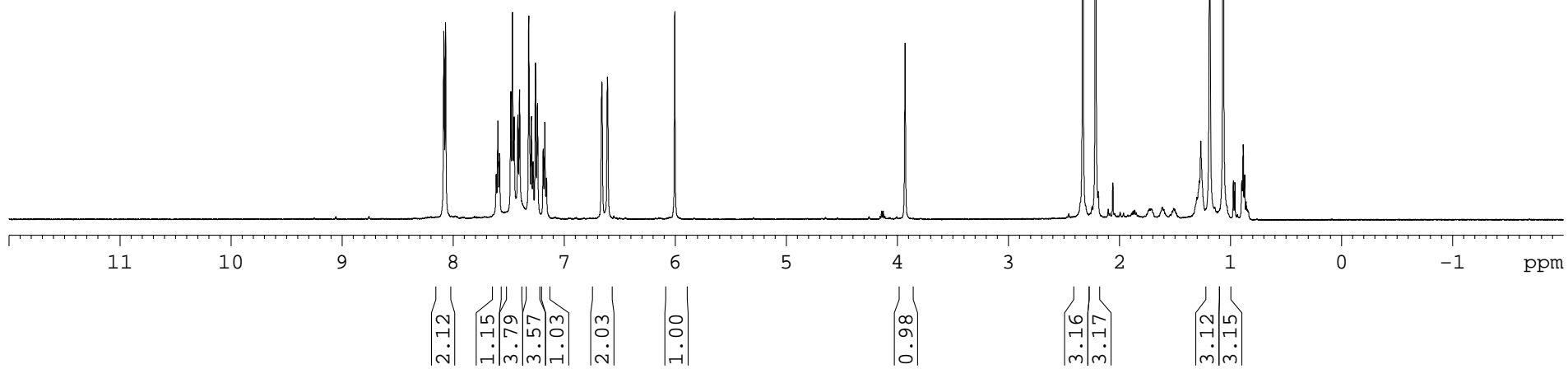
3.932

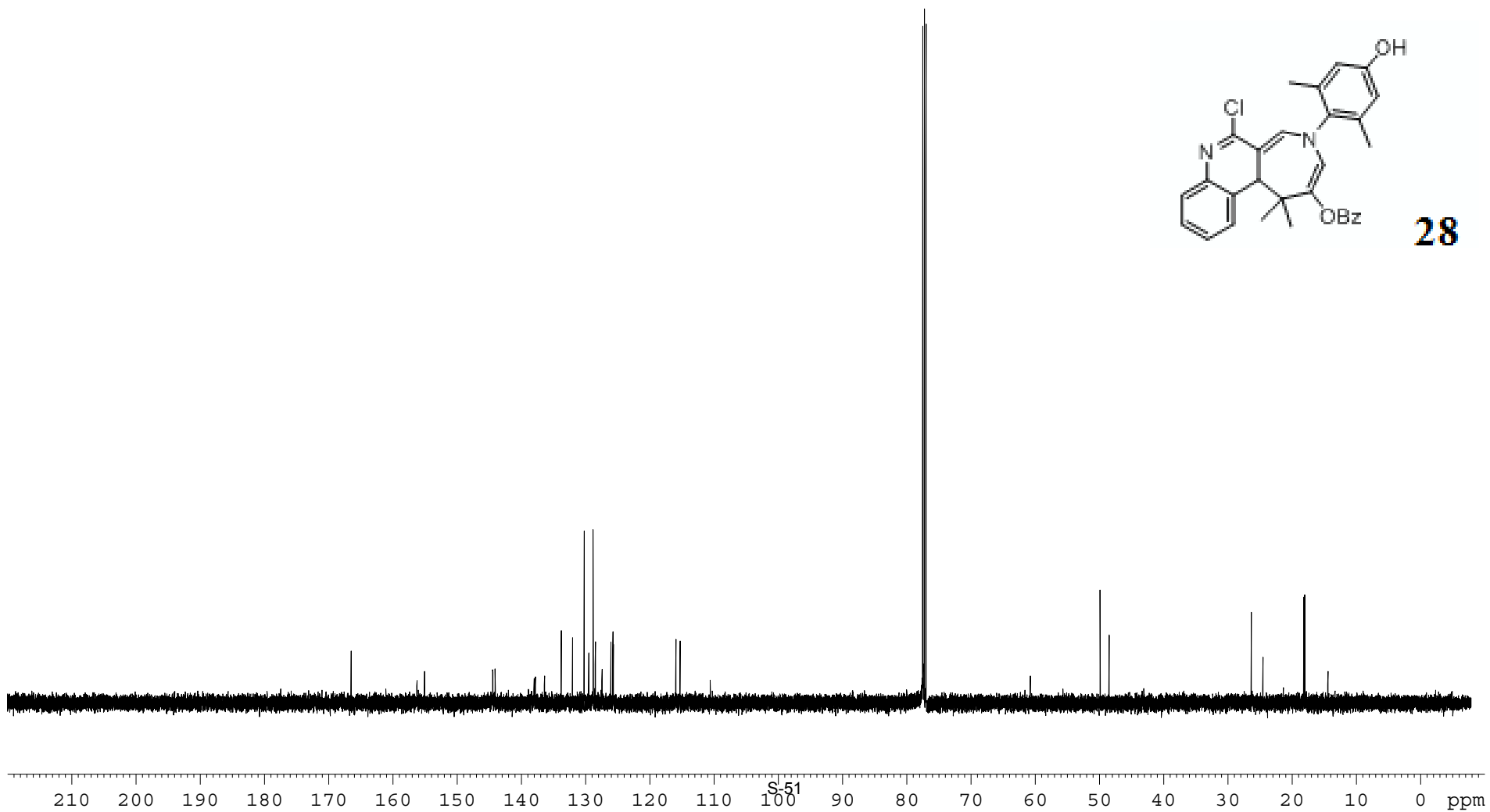
2.330
2.215

1.268
1.188
1.066
0.886

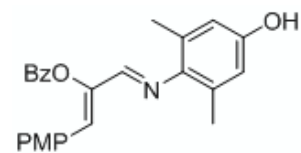
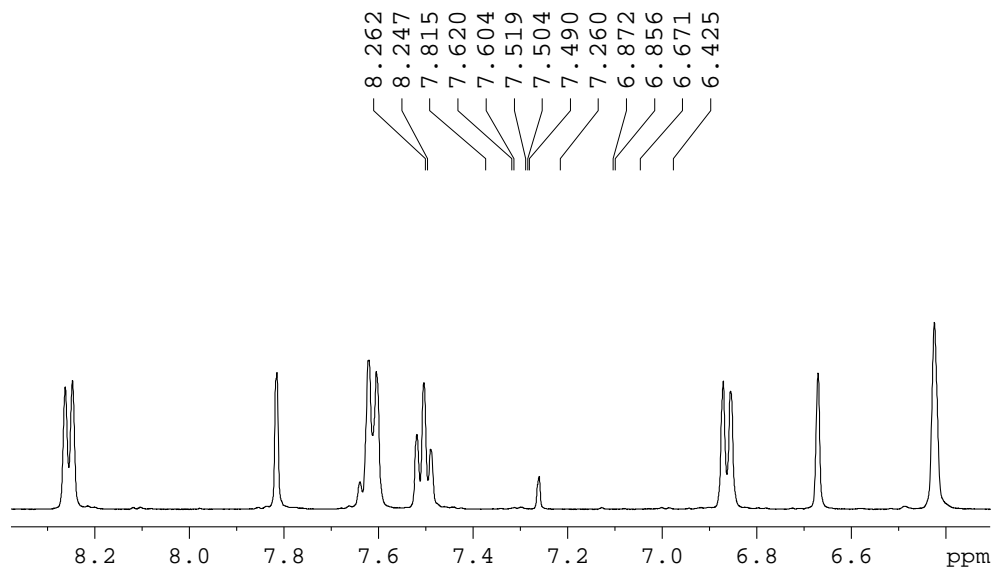


28

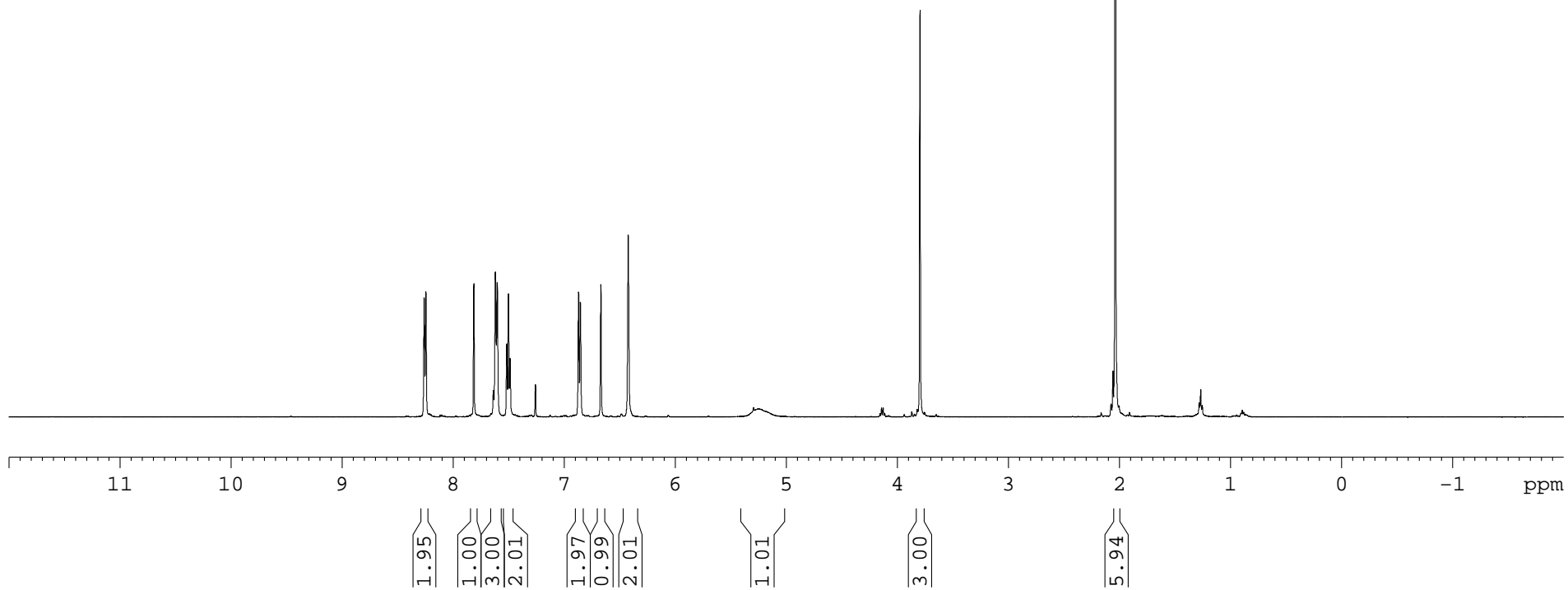


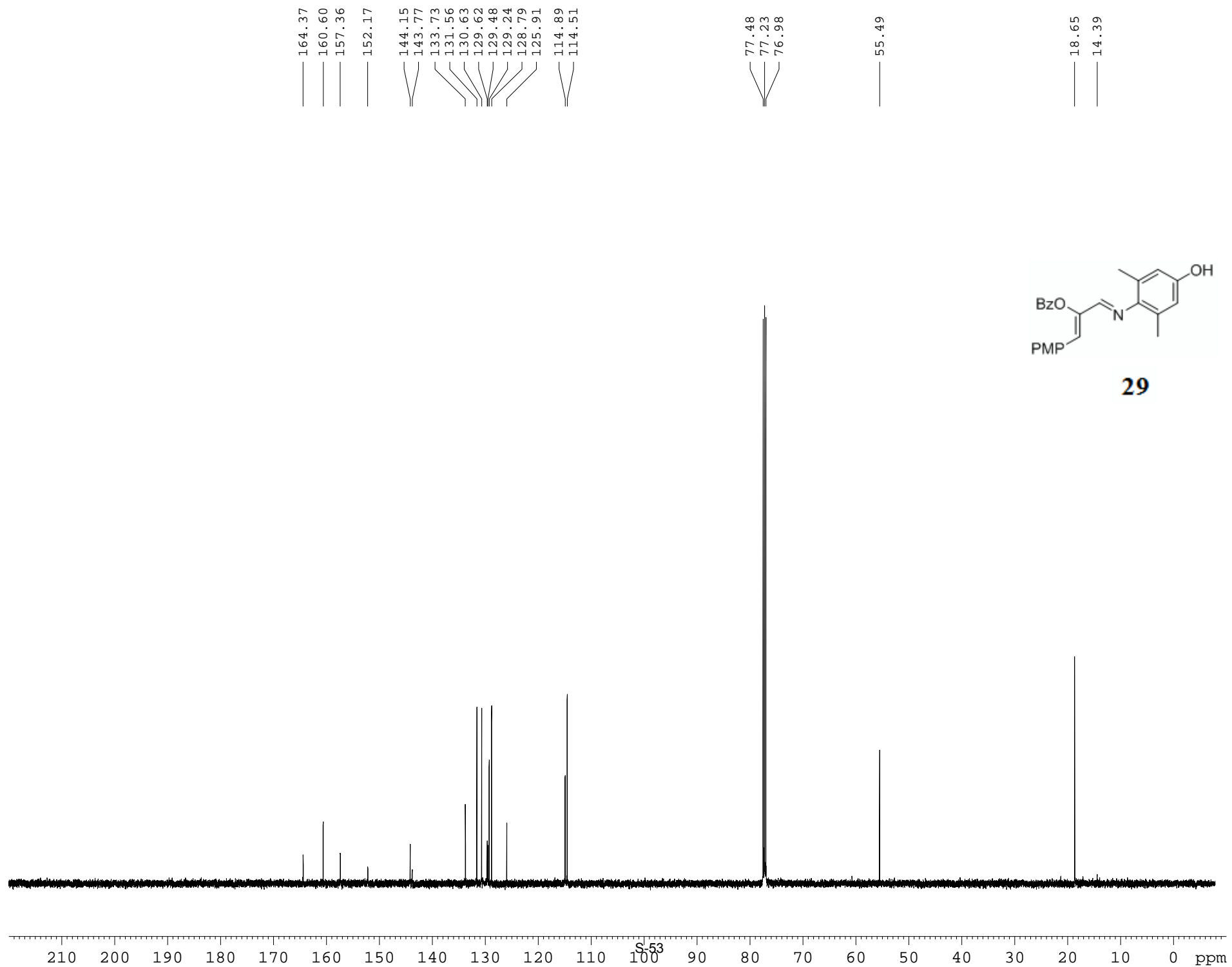


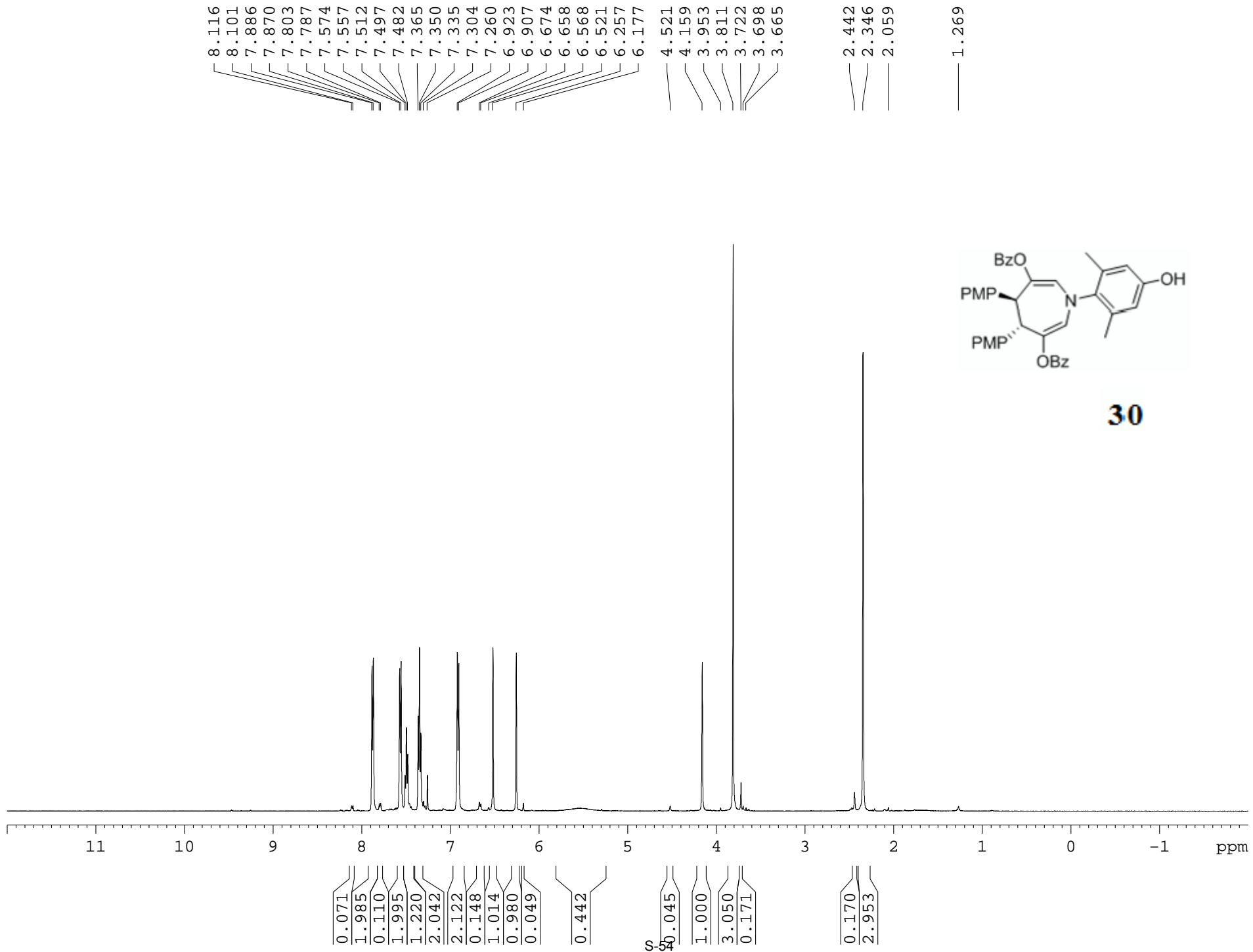
28

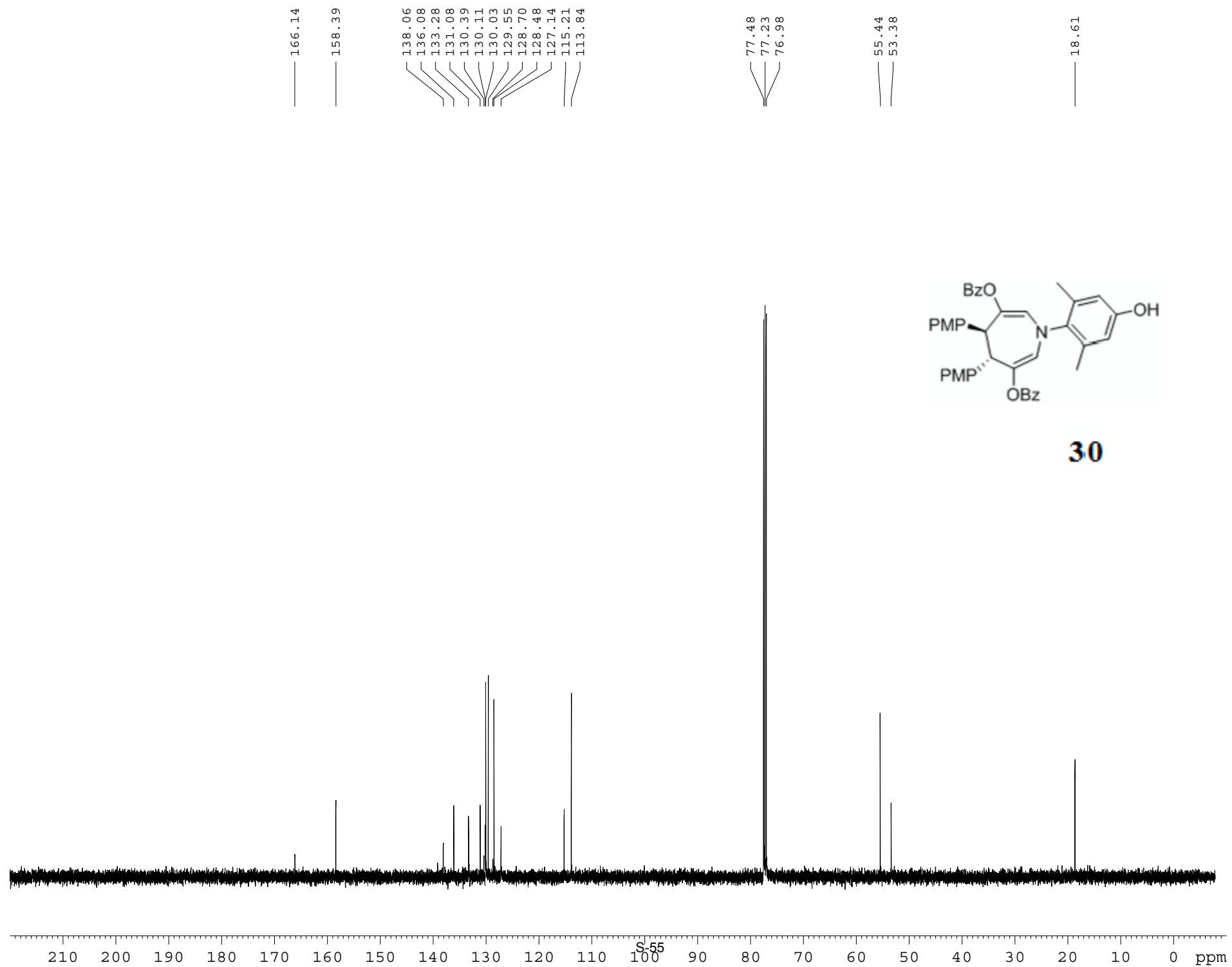


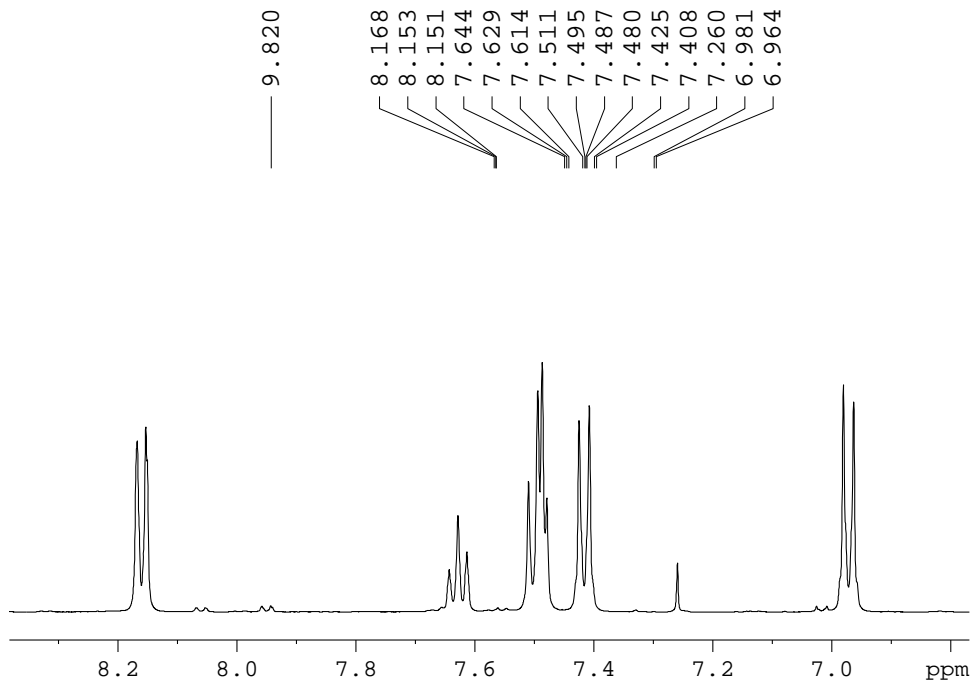
29



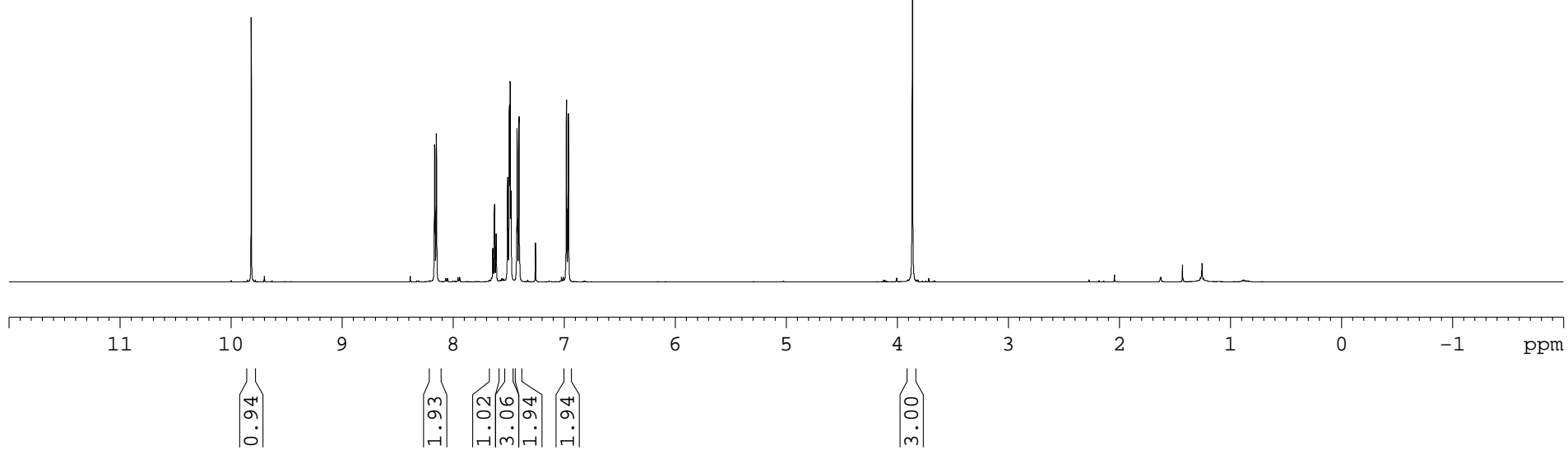
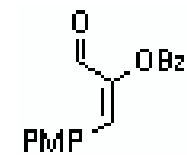


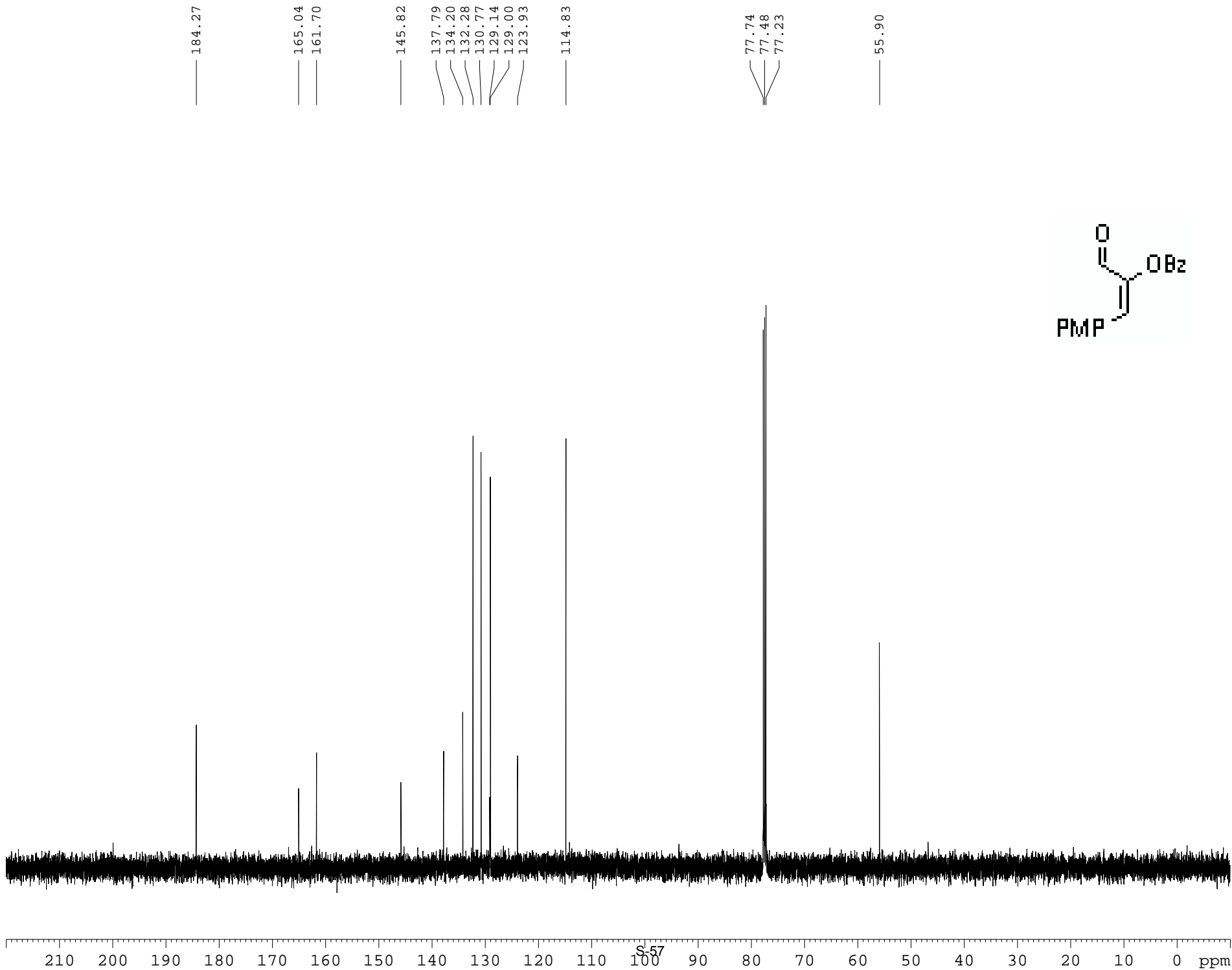


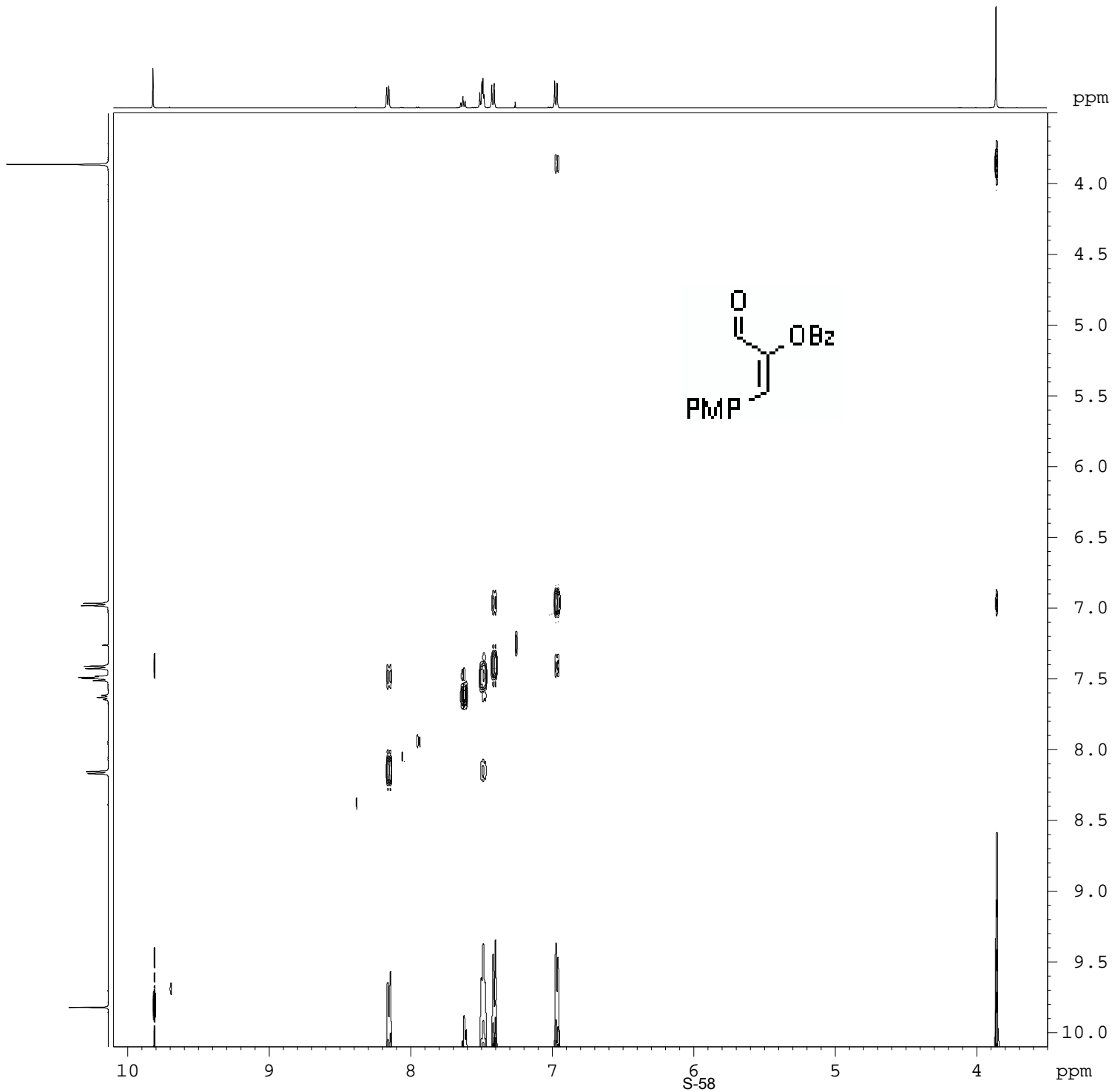




3.865







Current Data Parameters
 NAME 09-149A
 EXPNO 11
 PROCNO 1
 DU /u
 USER nshapiro

F2 - Acquisition Parameters
 Date_ 20080501
 Time 13.22
 INSTRUM AV-500
 PROBHD 5 mm TBI 1H/31
 PULPROG noesygpph
 TD 4096
 SOLVENT CDC13
 NS 1
 DS 4
 SWH 3591.954 Hz
 FIDRES 0.876942 Hz
 AQ 0.5703524 sec
 RG 60
 DW 139.200 usec
 DE 7.11 usec
 TE 300.0 K
 d0 0.00012915 sec
 D1 5.00000000 sec
 D8 2.099999990 sec
 D16 0.00010000 sec
 IN0 0.00027765 sec
 MCREST 0.00000000 sec
 MCWRK 5.00000000 sec
 TAU 1.04890001 sec

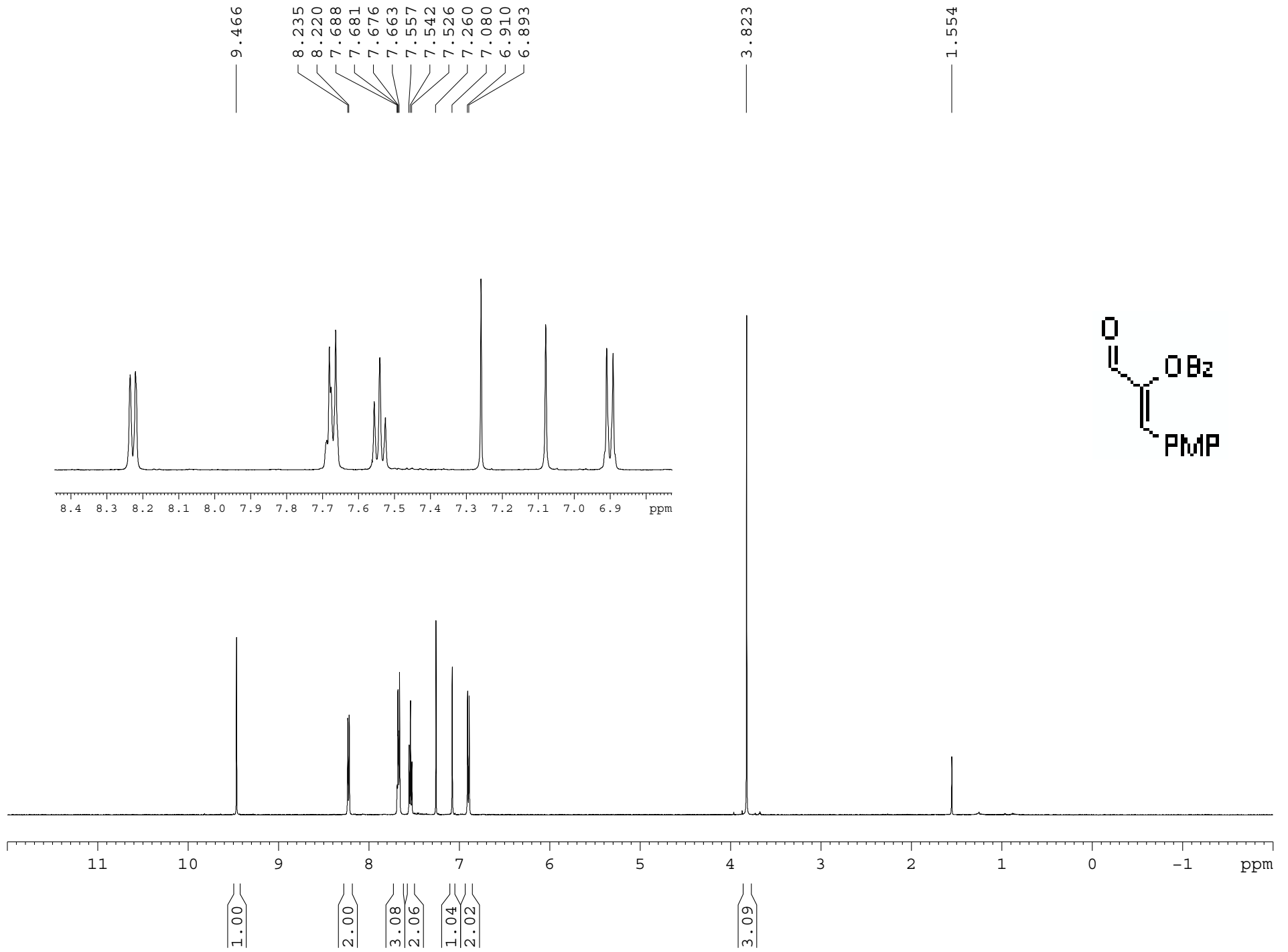
==== CHANNEL f1 =====
 NUC1 1H
 P1 7.60 usec
 P2 15.20 usec
 PL1 0.00 dB
 SFO1 500.2333515 MHz

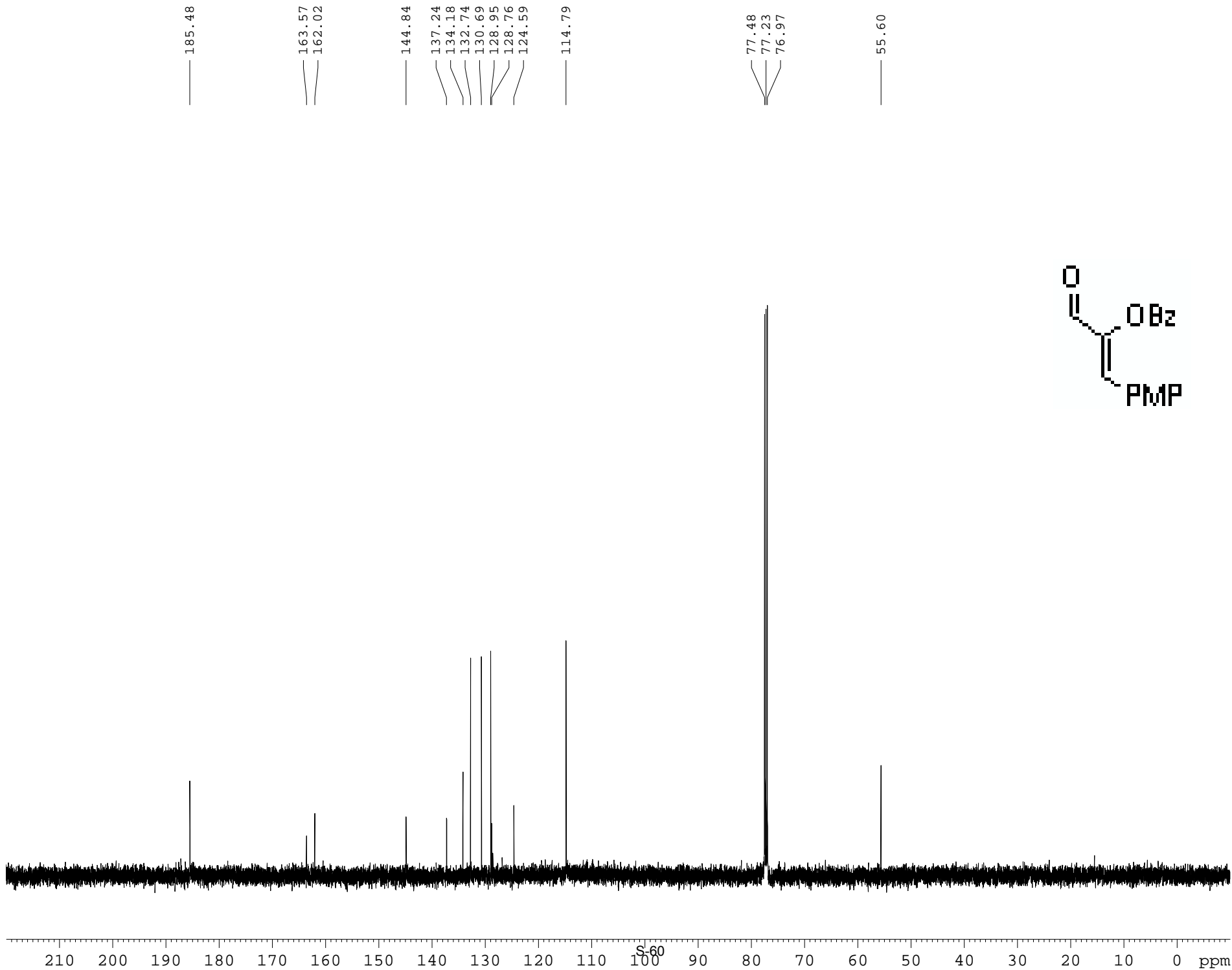
===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPX1 0.00 %
 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 40.00 %
 GPZ2 -40.00 %
 P16 1000.00 usec

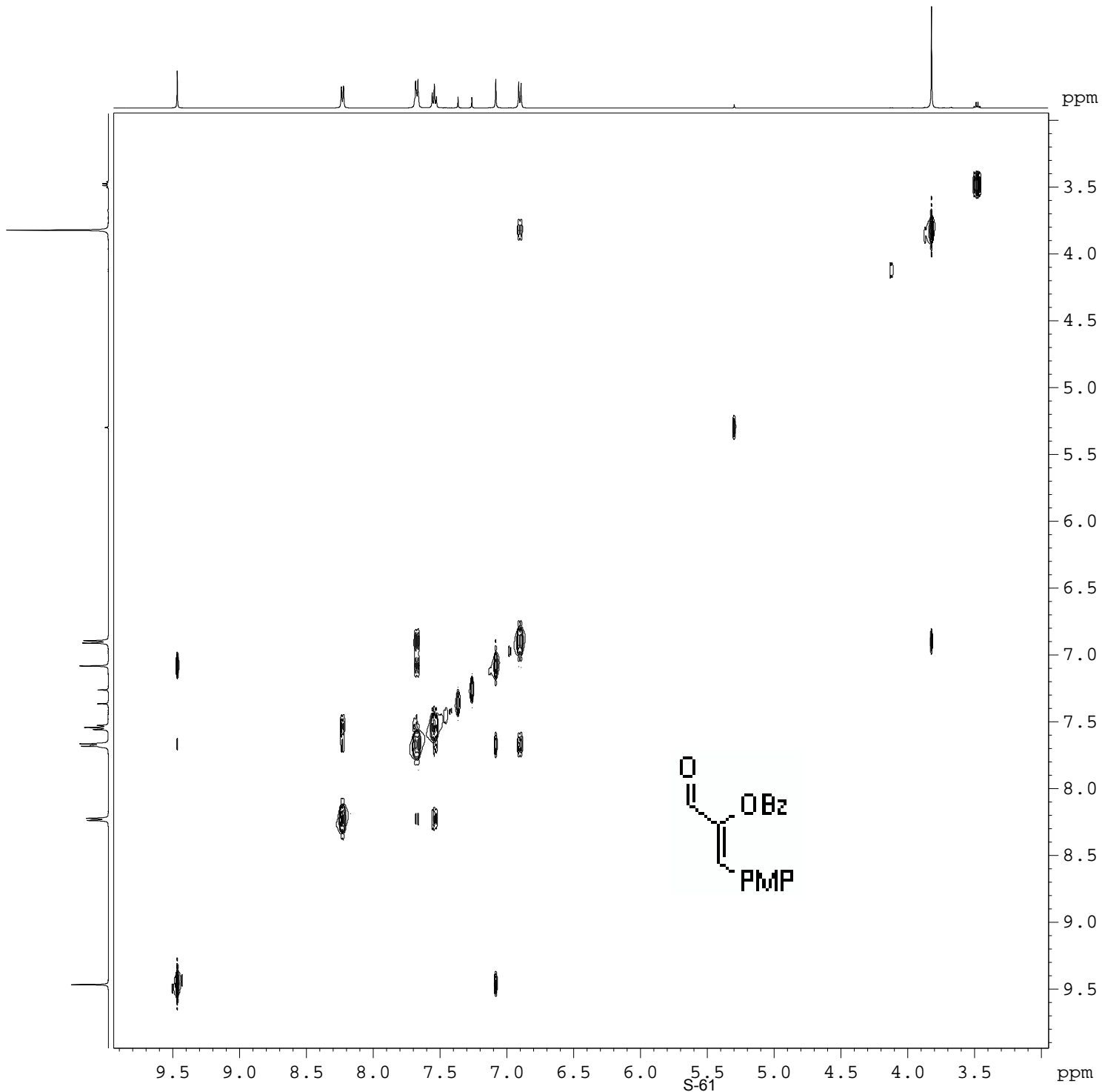
F1 - Acquisition parameters
 ND0 1
 TD 128
 SFO1 500.2334 MHz
 FIDRES 28.137943 Hz
 SW 7.200 ppm
 FnmODE TPPI

F2 - Processing parameters
 SI 2048
 SF 500.2300104 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 2048
 MC2 TPPI
 SF 500.2300104 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0







Current Data Parameters
 NAME 09-149C-2
 EXPNO 11
 PROCNO 1
 DU /u
 USER nshapiro

F2 - Acquisition Parameters
 Date_ 20080501
 Time_ 12.43
 INSTRUM AV-500
 PROBHD 5 mm TBI 1H/31
 PULPROG noesygpph
 TD 4096
 SOLVENT CDCl3
 NS 2
 DS 8
 SWH 3501.401 Hz
 FIDRES 0.854834 Hz
 AQ 0.5851016 sec
 RG 222
 DW 142.800 usec
 DE 7.11 usec
 TE 300.0 K
 d0 0.00013312 sec
 D1 5.00000000 sec
 D8 2.09999990 sec
 D16 0.00010000 sec
 IN0 0.00028559 sec
 MCREST 0.00000000 sec
 MCWRK 5.00000000 sec
 TAU 1.04890001 sec

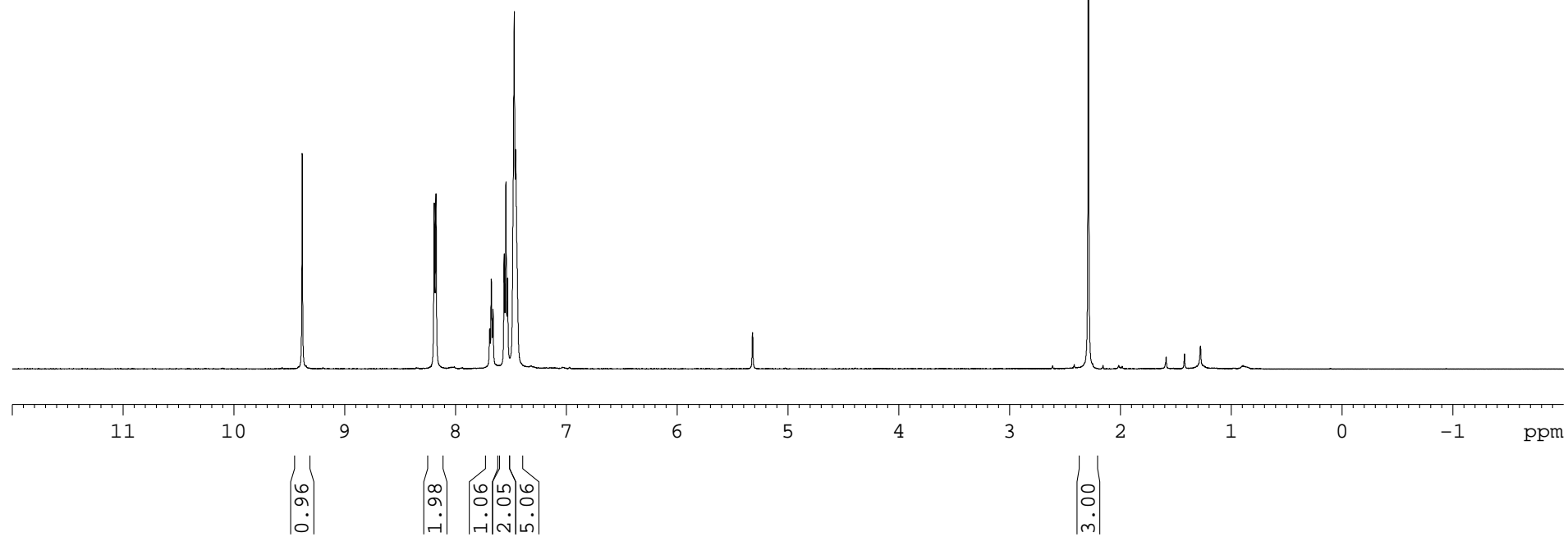
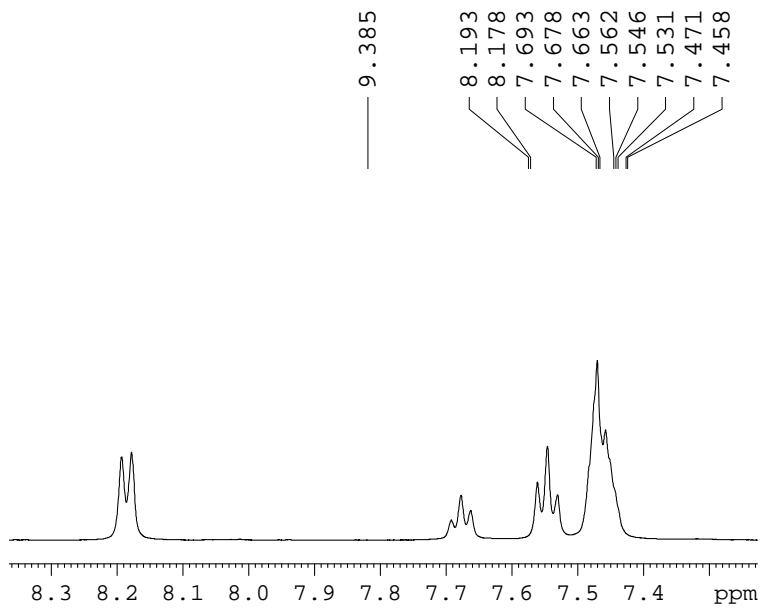
==== CHANNEL f1 =====
 NUC1 1H
 P1 7.60 usec
 P2 15.20 usec
 PL1 0.00 dB
 SFO1 500.2332515 MHz

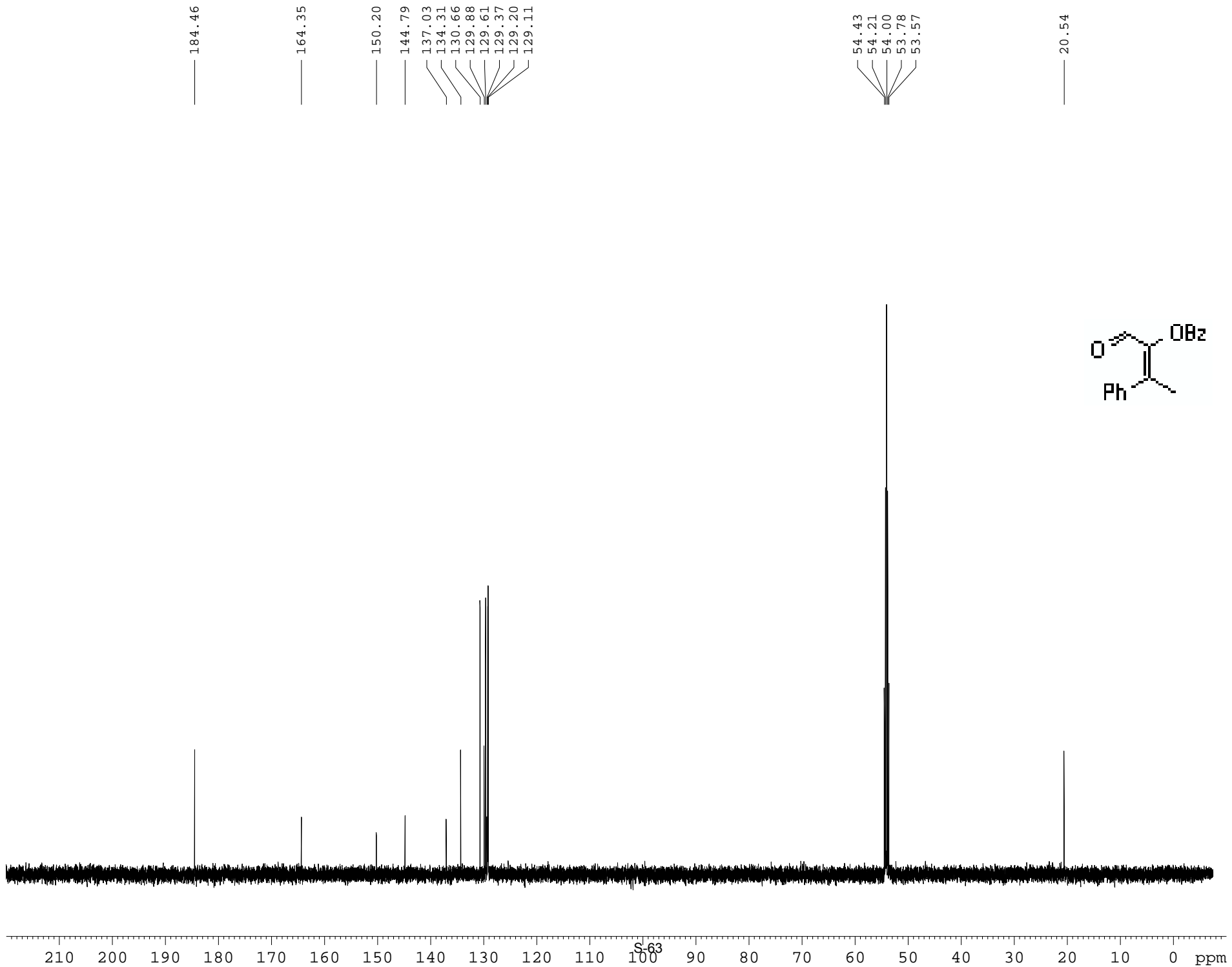
===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPX1 0.00 %
 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 40.00 %
 GPZ2 -40.00 %
 P16 1000.00 usec

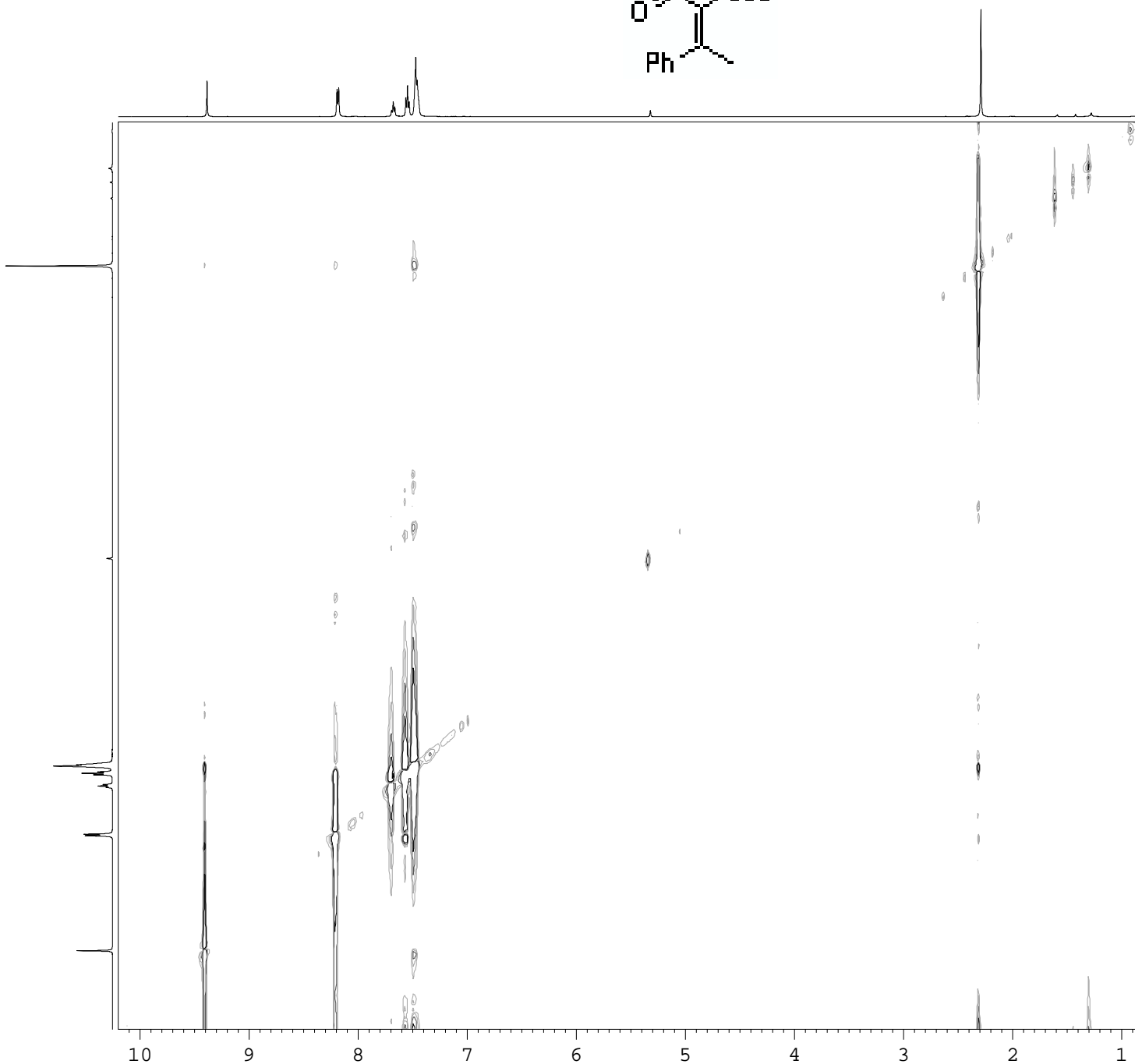
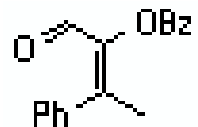
F1 - Acquisition parameters
 NDO 1
 TD 128
 SFO1 500.2333 MHz
 FIDRES 27.355888 Hz
 SW 7.000 ppm
 FnmODE TPPI

F2 - Processing parameters
 SI 2048
 SF 500.2300289 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 4.00

F1 - Processing parameters
 SI 2048
 MC2 TPPI
 SF 500.2300288 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0







```

Current Data Parameters
NAME          09-132A
EXPNO         11
PROCNO        1
DU            /u
USER          nshapiro

ppm F2 - Acquisition Parameters
Date_         20080427
Time          10.21
1.0 INSTRUM   DRX-500
PROBHD       5 mm BBO BB-1H
PULPROG      noesygpph
1.5 TD        2048
SOLVENT      CDCl3
NS            1
DS            4
2.0 SWH       5000.000 Hz
FIDRES       2.441406 Hz
AQ           0.2048500 sec
2.5 RG        128
DW           100.000 usec
DE           7.11 usec
3.0 TE        293.0 K
d0           0.00008444 sec
D1           6.00000000 sec
D8           2.73000002 sec
3.5 D16       0.00020000 sec
INO         0.00019995 sec
MCREST       0.00000000 sec
4.0 MCWRK     6.00000000 sec
TAU         1.36380005 sec

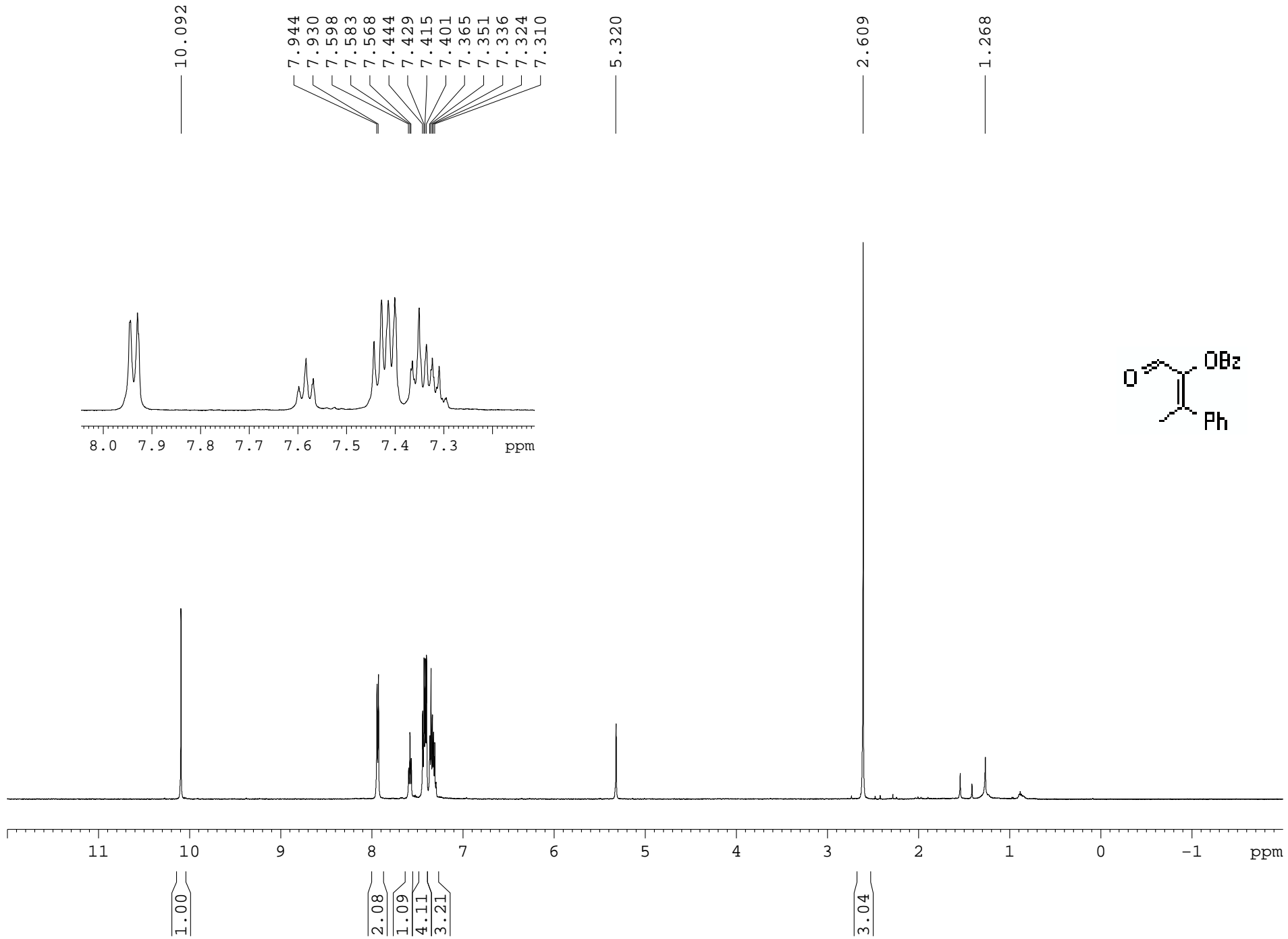
===== CHANNEL f1 =====
4.5 NUC1       1H
P1           12.20 usec
P2           24.40 usec
5.0 PL1        -5.00 dB
SFO1         500.1327507 MHz

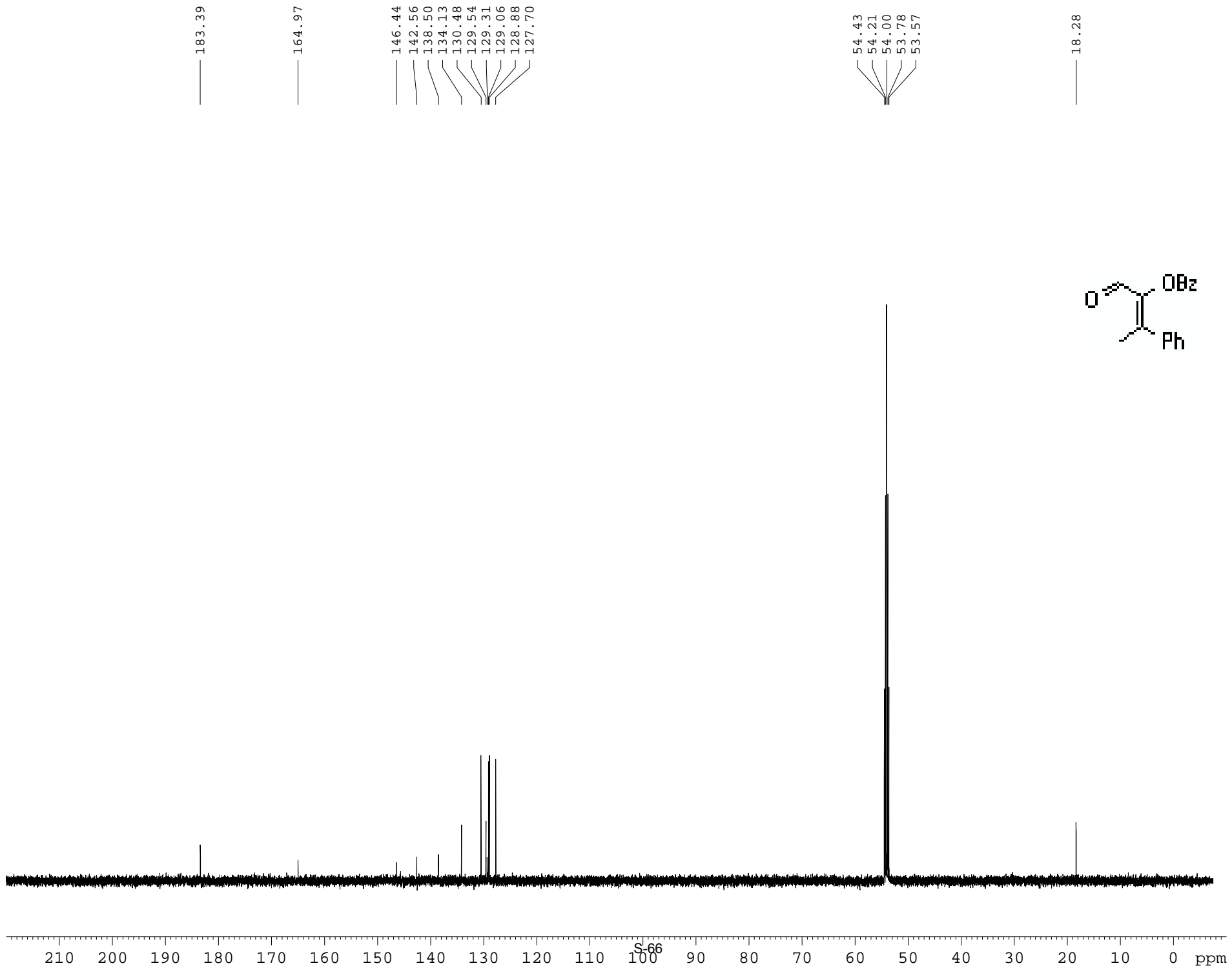
===== GRADIENT CHANNEL =====
5.5 GPNAM1     SINE.100
GPNAM2       SINE.100
6.0 GPX1        0.00 %
GPX2         0.00 %
GPY1         0.00 %
GPY2         0.00 %
6.5 GPZ1        40.00 %
GPZ2        -40.00 %
P16          1000.00 usec

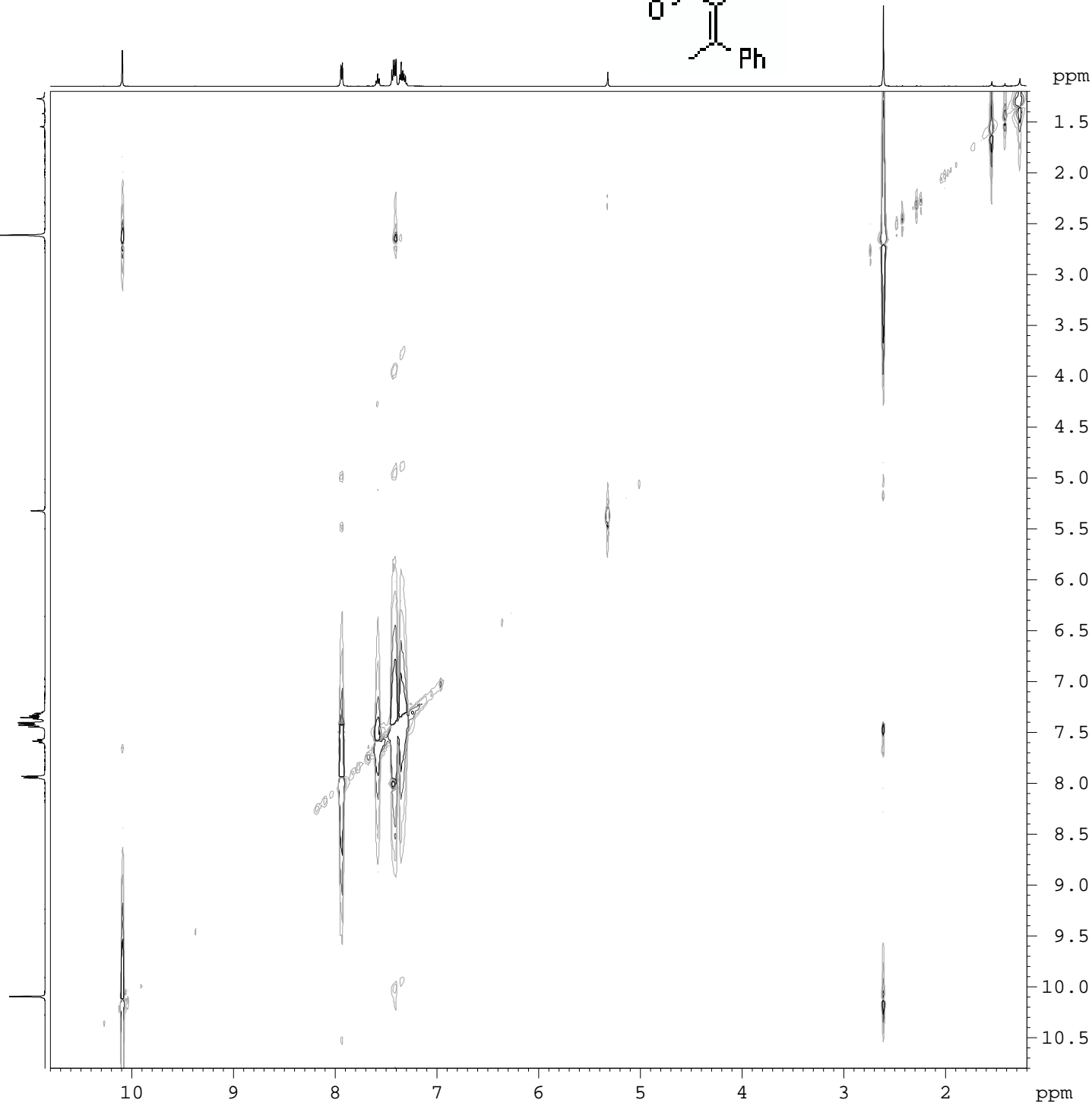
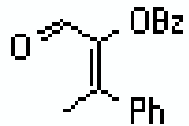
7.0 F1 - Acquisition parameters
ND0          1
TD           256
7.5 SFO1       500.1328 MHz
FIDRES       19.536135 Hz
SW           10.000 ppm
FnMODE       TPPI
8.0 F2 - Processing parameters
SI           1024
8.5 SF         500.1300127 MHz
WDW          QSINE
SSB          2
9.0 LB         0.00 Hz
GB           0
PC           5.00

9.5 F1 - Processing parameters
SI           256
MC2          TPPI
9.0 SF         500.1300128 MHz
WDW          QSINE
SSB          2
LB           0.00 Hz
GB           0

```







Current Data Parameters
 NAME 09-132B
 EXPNO 11
 PROCNO 1
 DU /u
 USER nshapiro

F2 - Acquisition Parameters
 Date_ 20080427
 Time 11.13
 INSTRUM DRX-500
 PROBHD 5 mm BBO BB-1H
 PULPROG noesygpph
 TD 2048
 SOLVENT CDCl3
 NS 2
 DS 4
 SWH 5000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 128
 DW 100.000 use
 DE 7.11 use
 TE 293.0 K
 d0 0.00008444 sec
 D1 4.00000000 sec
 D8 2.11999989 sec
 D16 0.00020000 sec
 IN0 0.00019995 sec
 MCREST 0.00000000 sec
 MCWRK 4.00000000 sec
 TAU 1.05879998 sec

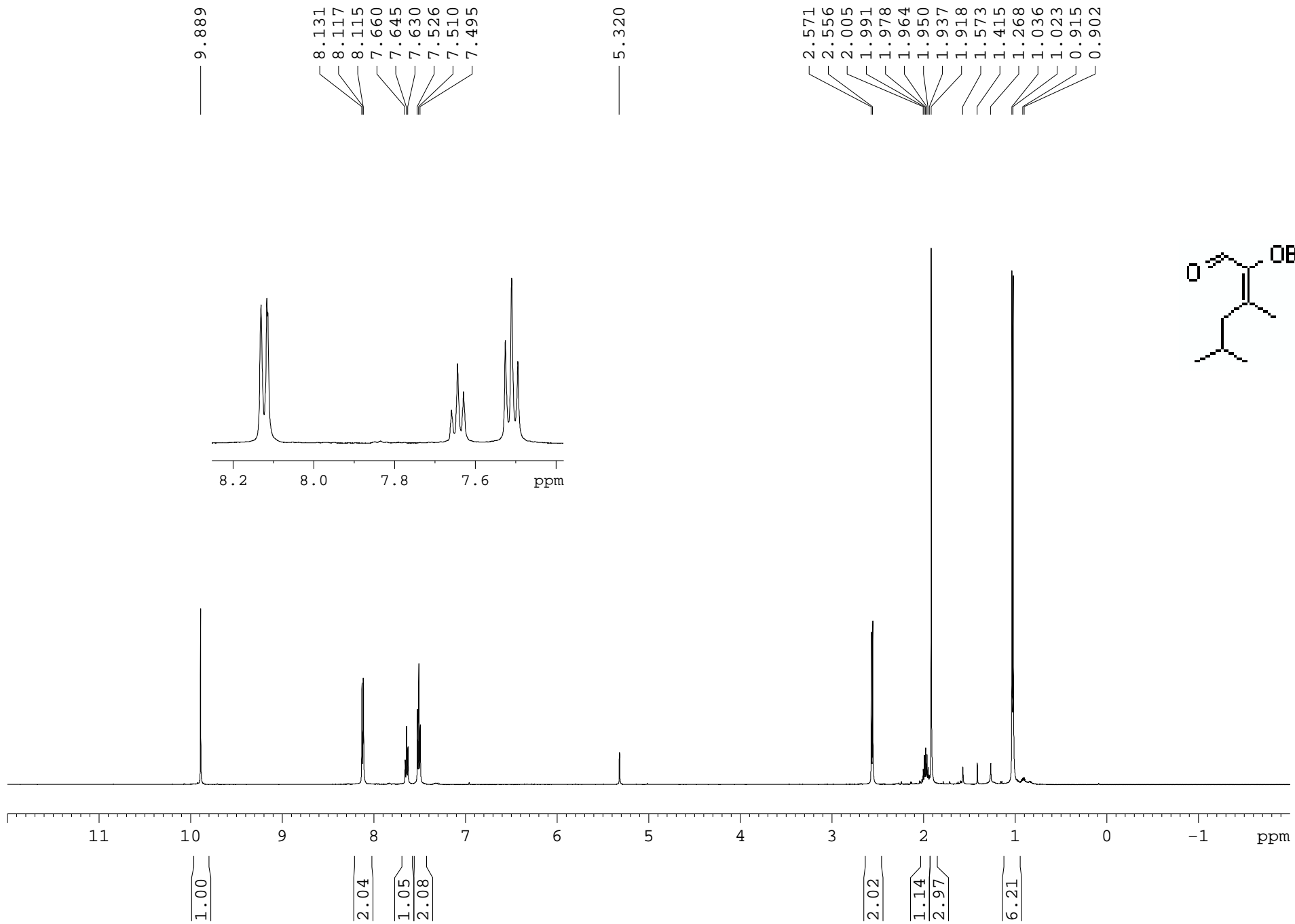
==== CHANNEL f1 =====
 NUC1 1H
 P1 12.20 use
 P2 24.40 use
 PL1 -5.00 dB
 SFO1 500.1330008 MHz

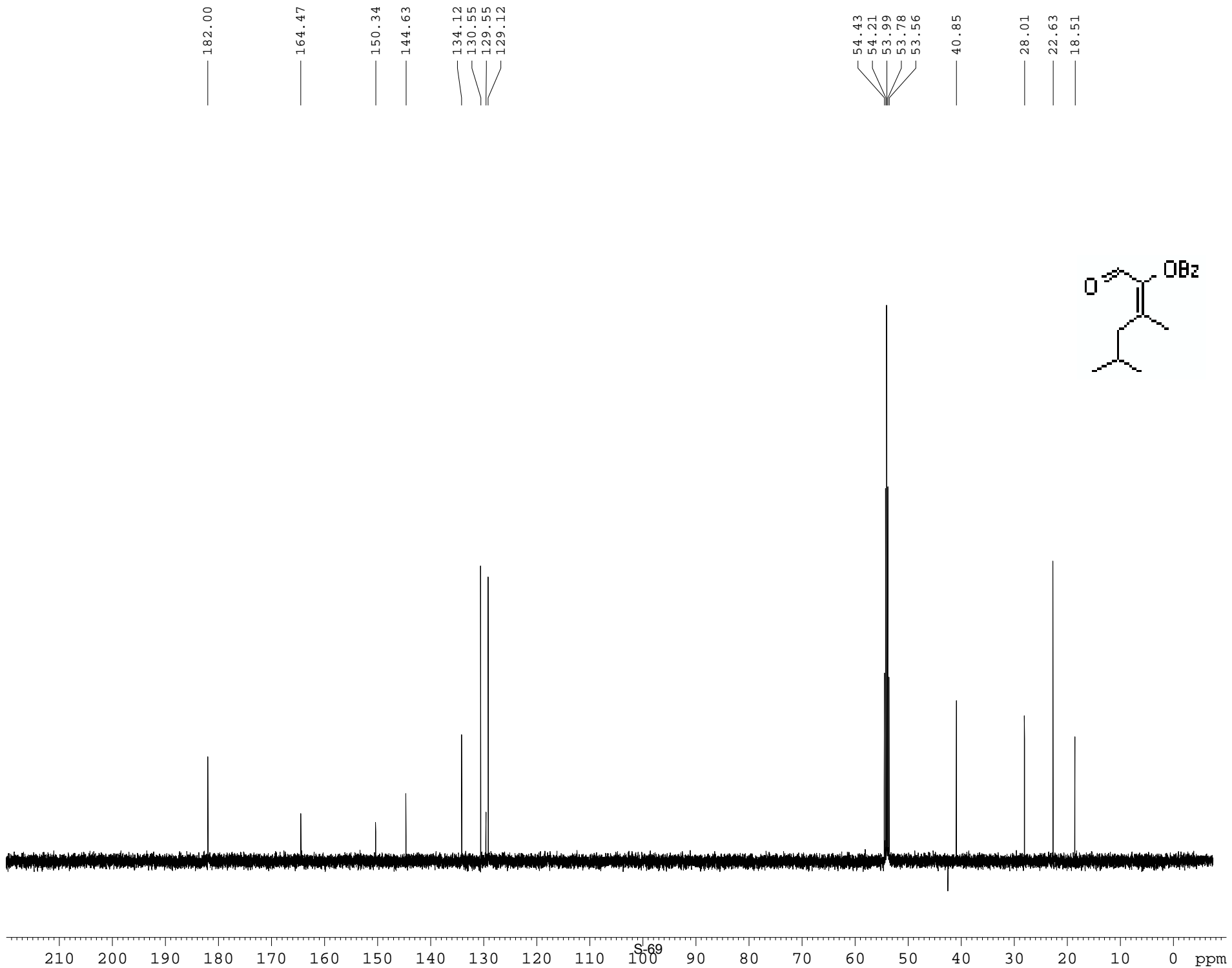
==== GRADIENT CHANNEL ===
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPX1 0.00 %
 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 40.00 %
 GPZ2 -40.00 %
 P16 1000.00 use

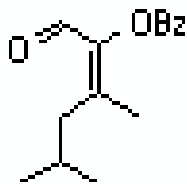
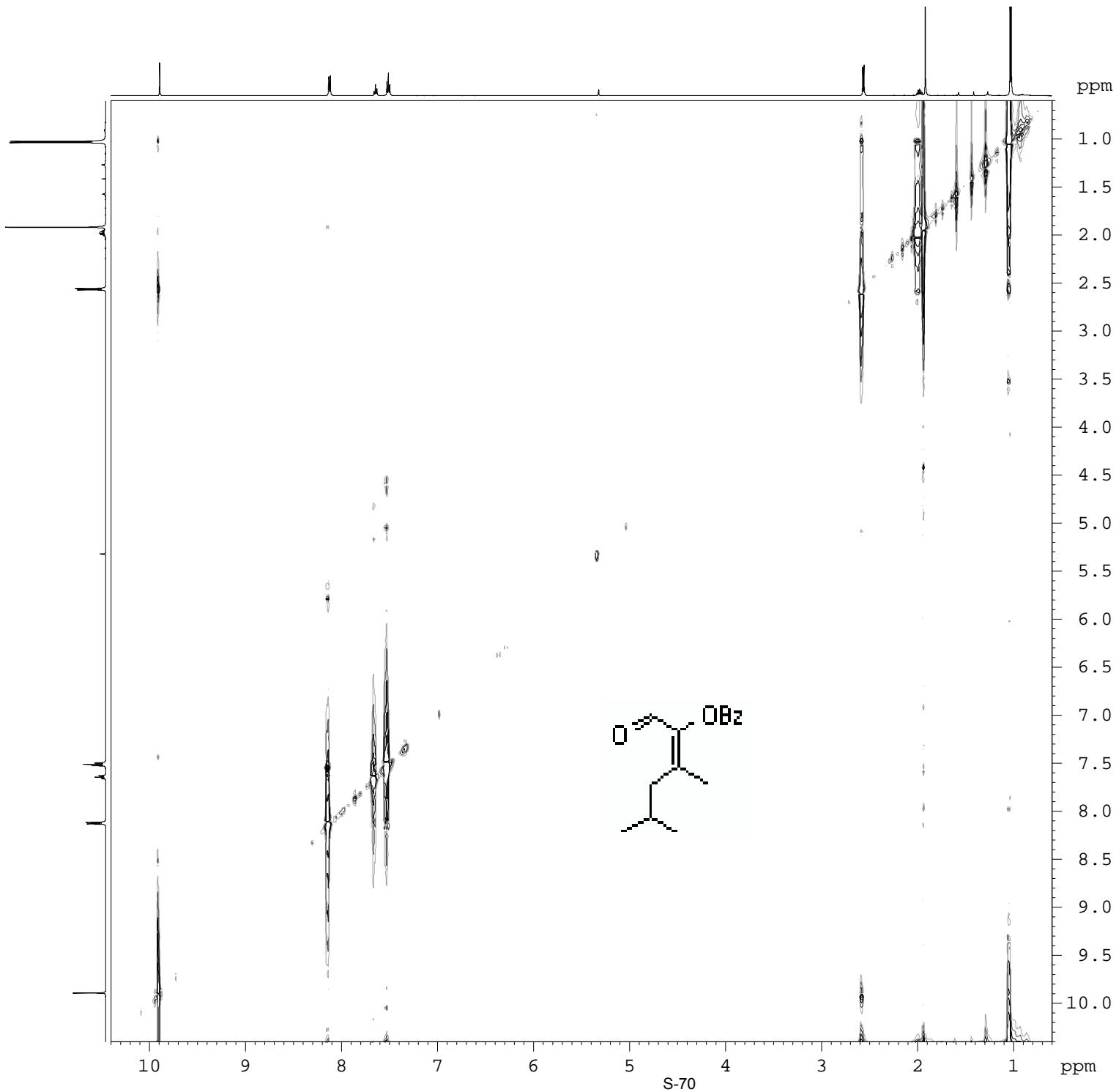
F1 - Acquisition parameters
 ND0 1
 TD 256
 SFO1 500.133 MHz
 FIDRES 19.536135 Hz
 SW 10.000 ppm
 FnMODE TPPI

F2 - Processing parameters
 SI 1024
 SF 500.1300127 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 5.00

F1 - Processing parameters
 SI 256
 MC2 TPPI
 SF 500.1300128 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0







Current Data Parameters
 NAME 09-133A
 EXPNO 11
 PROCNO 1
 DU /u
 USER nshapiro

F2 - Acquisition Parameters
 Date_ 20080427
 Time 12.22
 INSTRUM DRX-500
 PROBHD 5 mm BBO BB-1H
 PULPROG noesygpcp
 TD 2048
 SOLVENT CDCl3
 NS 1
 DS 4
 SWH 5000.000 Hz
 FIDRES 2.441406 Hz
 AQ 0.2048500 sec
 RG 128
 DW 100.000 usec
 DE 7.11 usec
 TE 293.0 K
 d0 0.00008444 sec
 D1 5.00000000 sec
 D8 1.29999995 sec
 D16 0.00020000 sec
 INO 0.00019995 sec
 MCREST 0.00000000 sec
 MCWRK 5.00000000 sec
 TAU 0.64879996 sec

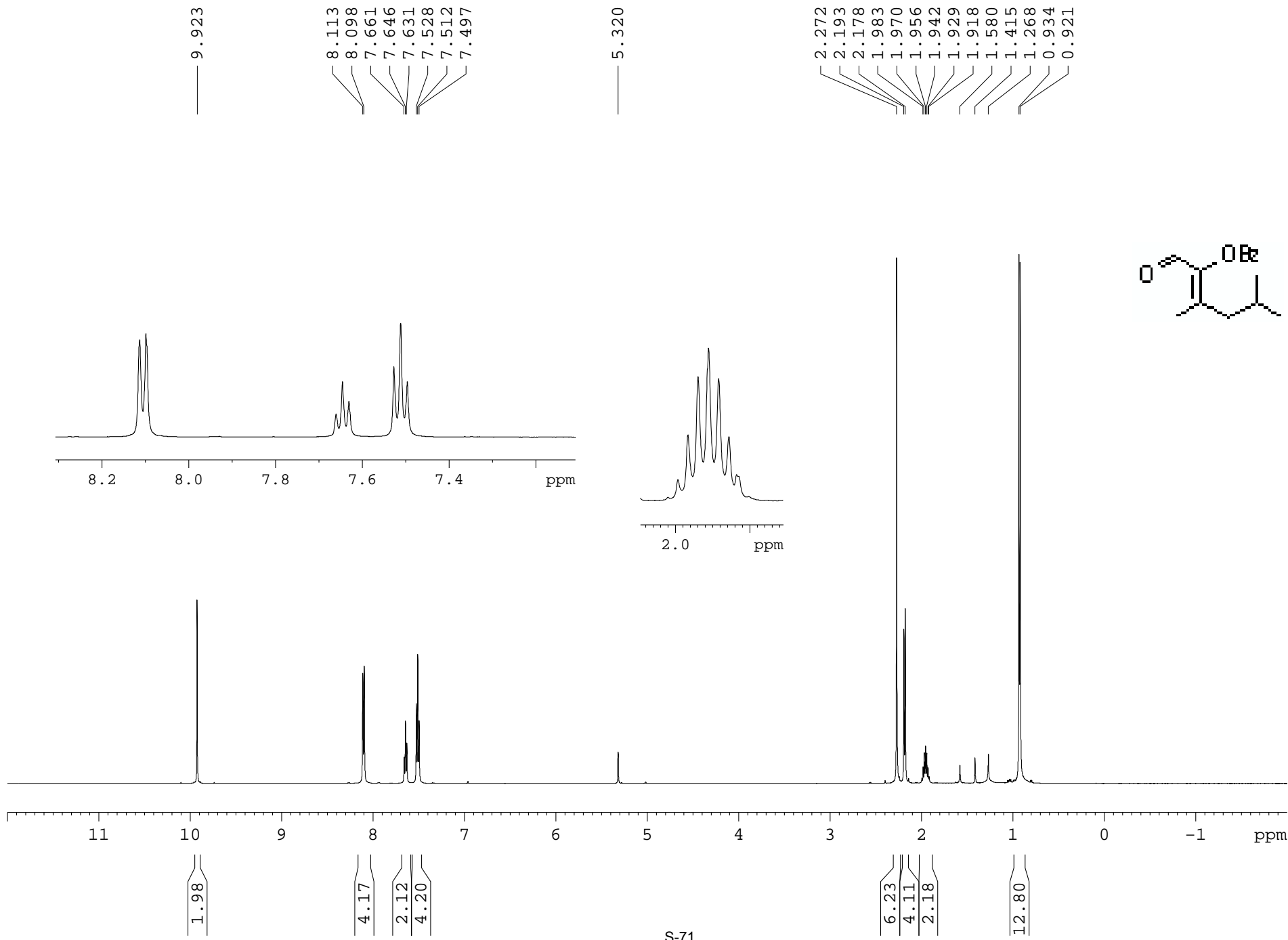
==== CHANNEL f1 =====
 NUC1 1H
 P1 12.20 usec
 P2 24.40 usec
 PL1 -5.00 dB
 SFO1 500.1327507 MHz

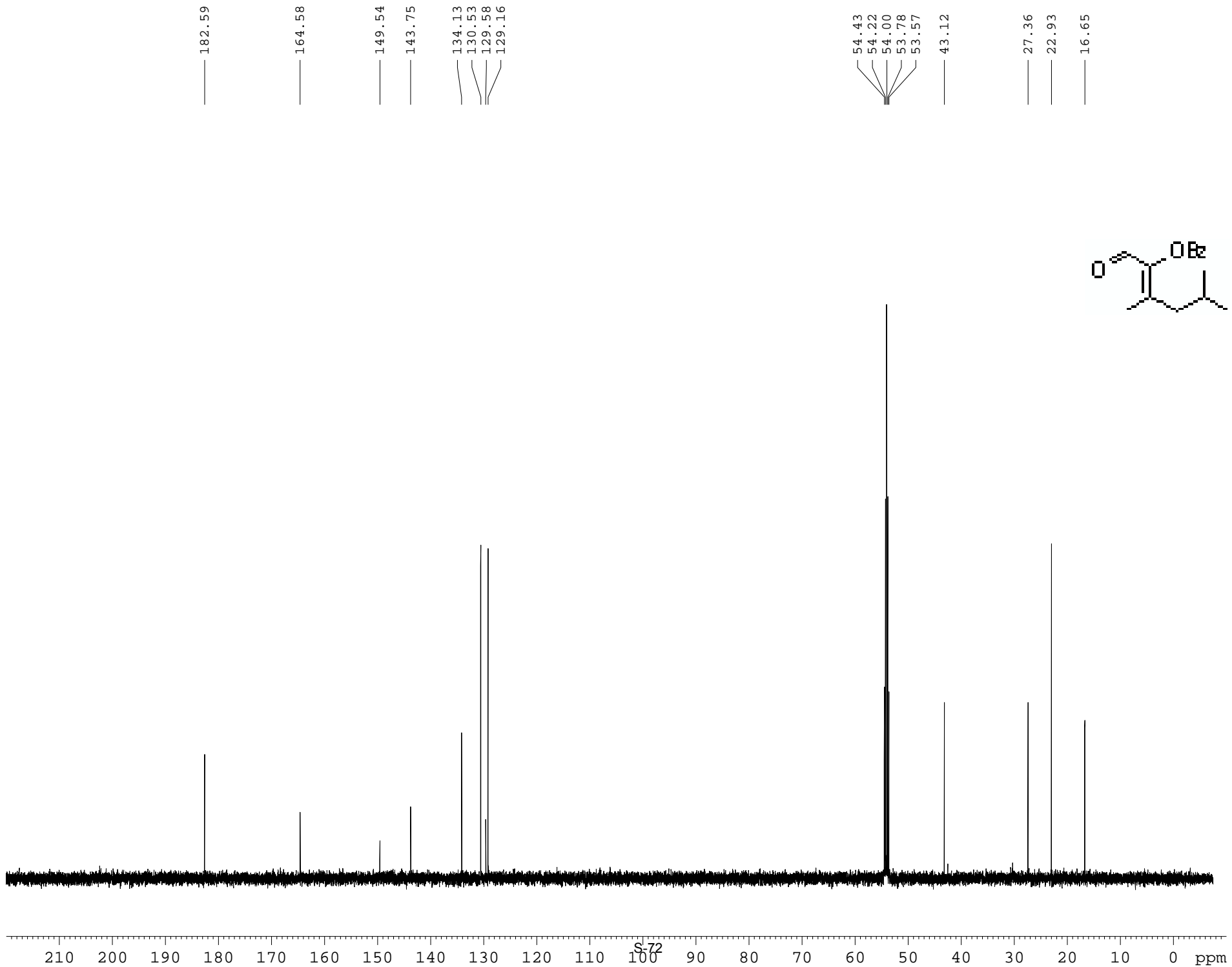
==== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GPNAM2 SINE.100
 GPX1 0.00 %
 GPX2 0.00 %
 GPY1 0.00 %
 GPY2 0.00 %
 GPZ1 40.00 %
 GPZ2 -40.00 %
 P16 1000.00 usec

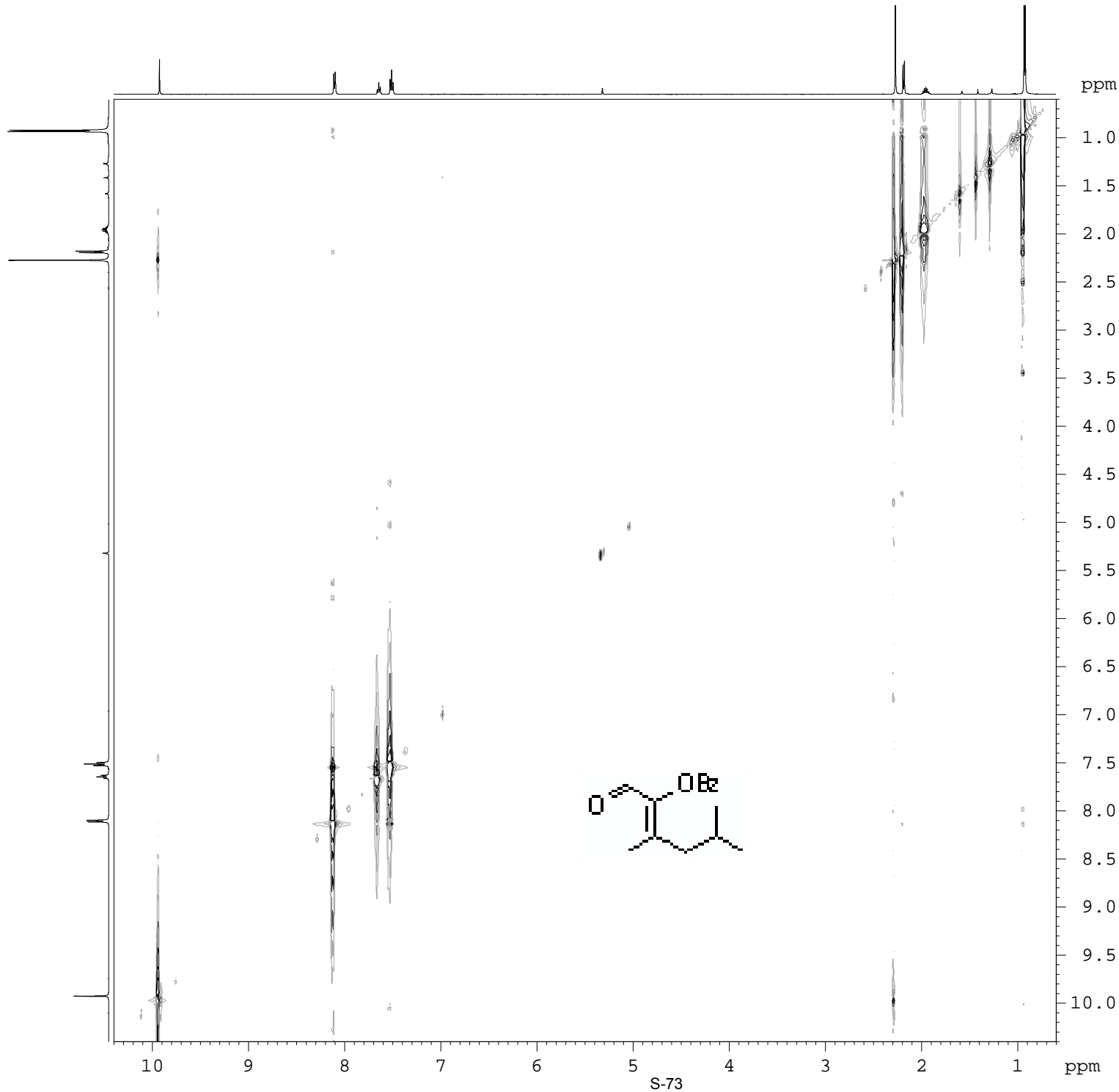
F1 - Acquisition parameters
 ND0 1
 TD 256
 SFO1 500.1328 MHz
 FIDRES 19.536135 Hz
 SW 10.000 ppm
 FhMODE TPPI

F2 - Processing parameters
 SI 1024
 SF 500.1300127 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 5.00

F1 - Processing parameters
 SI 256
 MC2 TPPI
 SF 500.1300128 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0







```

Current Data Parameters
NAME          09-133B
EXPNO         11
PROCNO        1
DU            /u
USER          nshapiro

F2 - Acquisition Parameter:
Date_         20080427
Time          14.10
INSTRUM       DRX-500
PROBHD        5 mm BBO BB-1H
PULPROG       noesygpph
TD            2048
SOLVENT       CDCl3
NS            2
DS            4
SWH           5000.000 Hz
FIDRES        2.441406 Hz
AQ            0.2048500 se
RG            128
DW            100.000 us
DE            7.11 us
TE            293.0 K
d0            0.00008444 se
D1            5.00000000 se
D8            1.33000004 se
D16           0.00020000 se
INO           0.00019995 se
MCREST        0.00000000 se
MCWRK         5.00000000 se
TAU           0.66380000 se

===== CHANNEL f1 =====
NUC1           1H
P1             12.20 us
P2             24.40 us
PL1            -5.00 dB
SF01           500.1327507 MHz

===== GRADIENT CHANNEL ==
GPNAM1        SINE.100
GPNAM2        SINE.100
GPX1           0.00 %
GPX2           0.00 %
GPY1           0.00 %
GPY2           0.00 %
GPZ1           40.00 %
GPZ2          -40.00 %
P16           1000.00 us

F1 - Acquisition parameter:
ND0            1
TD             256
SF01           500.1328 MHz
FIDRES         19.536135 Hz
SW             10.000 ppi
FnMODE         TPPI

F2 - Processing parameters
SI             1024
SF             500.1300127 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
PC             5.00

F1 - Processing parameters
SI             256
MC2            TPPI
SF             500.1300128 MHz
WDW            QSINE
SSB            2
LB             0.00 Hz
GB             0
  
```