Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Iron(III) Chloride Modulated Selective 1,2-*trans* Glycosylation Based on Glycosyl Trichloroacetimidate Donors and its Application in Orthogonal Glycosylation

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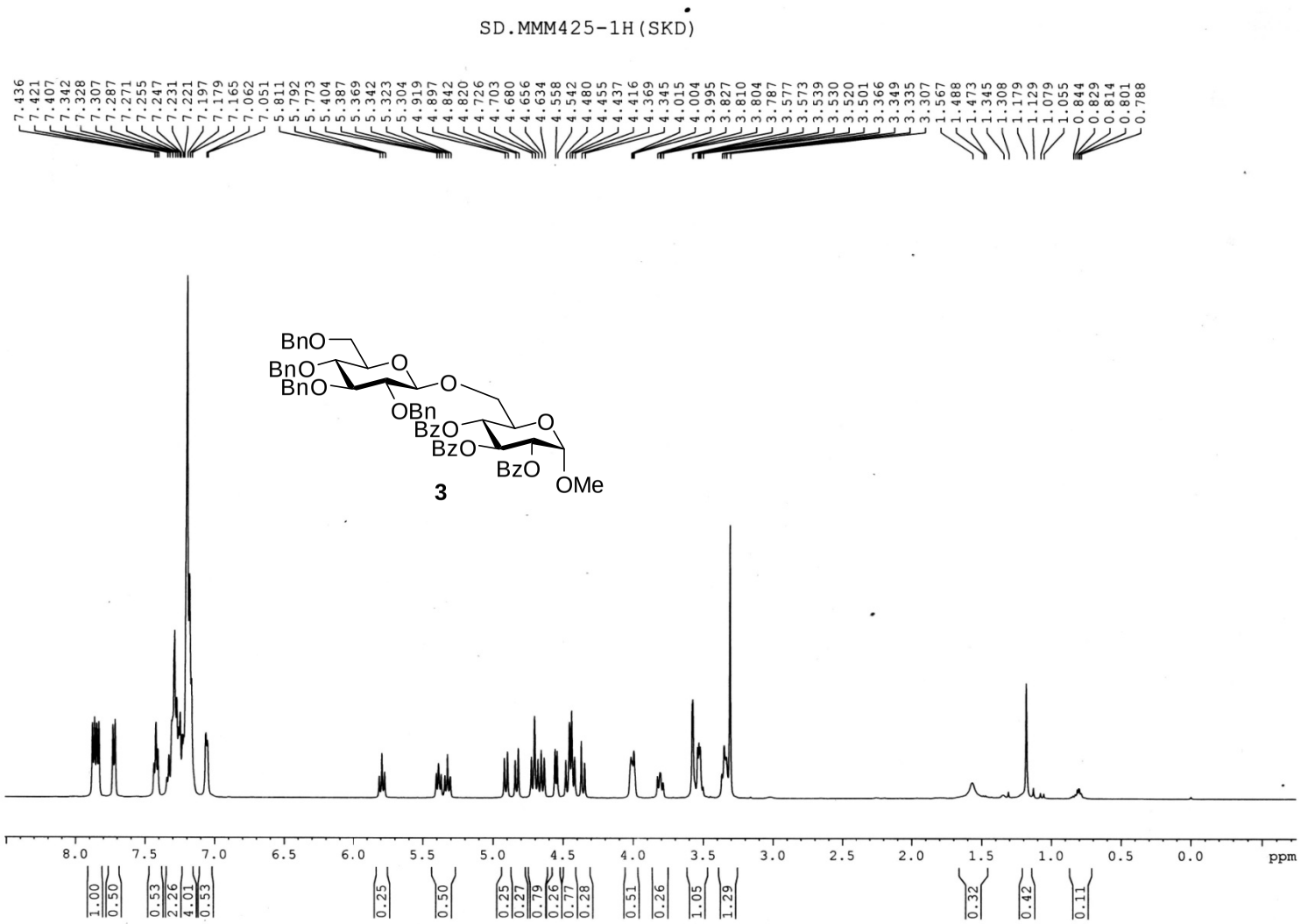
Table of Content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7.231
7.221
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7.165
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7.051
5.811
5.792
5.773
5.404
5.387
5.369
5.342
5.323
5.304
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4.820
4.726
4.703
4.680
4.656
4.634
4.558
4.542
4.480
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4.437
4.416
4.369
4.345
4.015
4.004
3.995
3.827
3.810
3.804
3.787
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3.573
3.539
3.530
3.520
3.501
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0.814
0.801
0.788
BnO
BnO
BnO
O
O
OBn
BzO
BzO
BzO
O
OMe
3
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7.5
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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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1.5
1.0
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0.0
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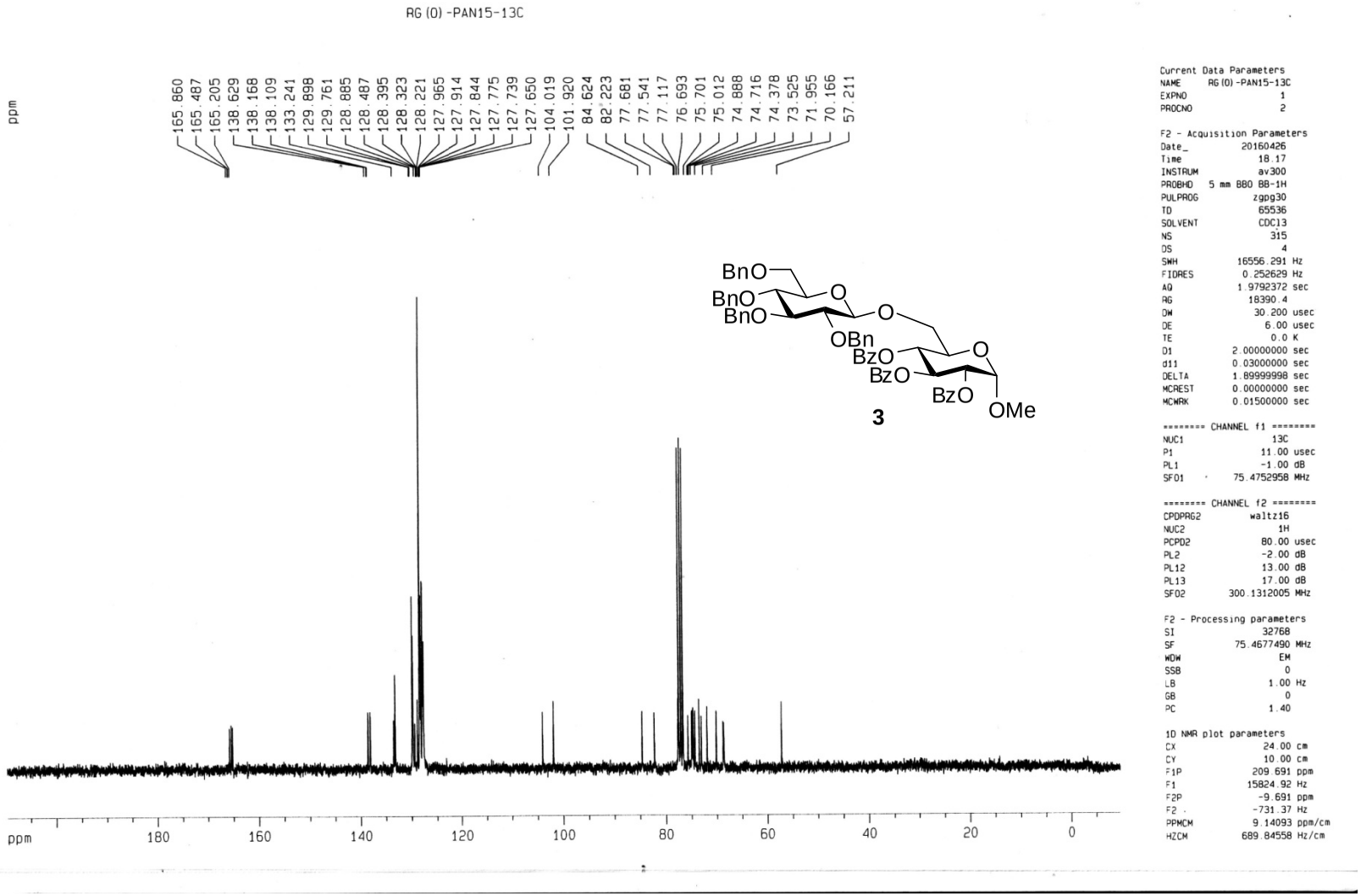
0.11



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PROCNO	2

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TD	65536
SOLVENT	CDCl3
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FIDRES	0.252629 Hz
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RG	18390.4
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DE	6.00 usec
TE	0.0 K
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d11	0.03000000 sec
DELTA	1.89999998 sec
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MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	11.00 usec
PL1	-1.00 dB
SFO1	75.4752958 MHz

======== CHANNEL f2 ========

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NUC2	1H
PCPD2	80.00 usec
PL2	-2.00 dB
PL12	13.00 dB
PL13	17.00 dB
SFO2	300.1312005 MHz

F2 - Processing parameters

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LB	1.00 Hz
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1D NMR plot parameters

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F1	15824.92 Hz
F2P	-9.691 ppm
F2	-731.37 Hz
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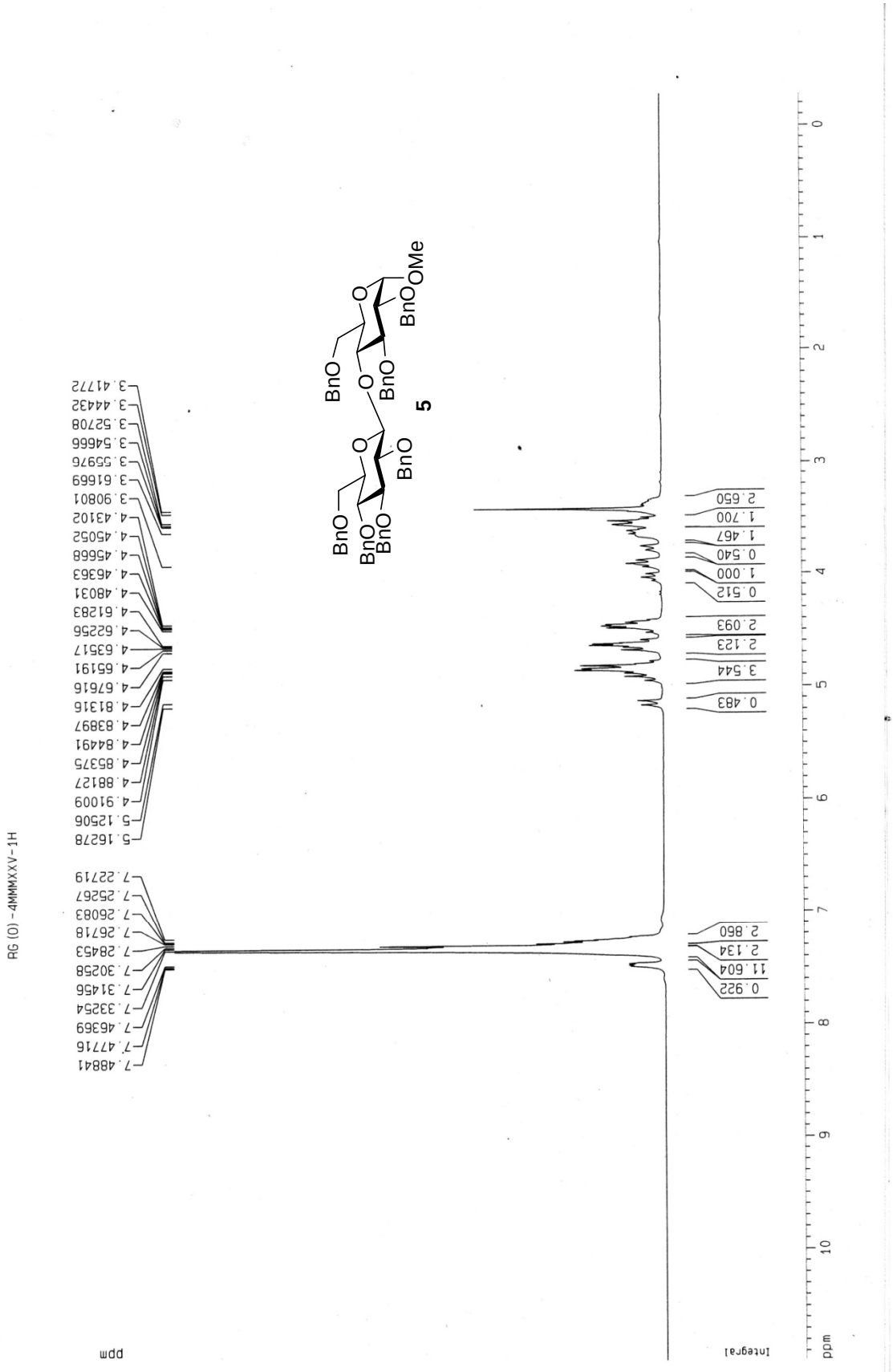
HZCM	689.84558 Hz/cm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7.22719
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5.12506
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4.88127
4.85375
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1.700
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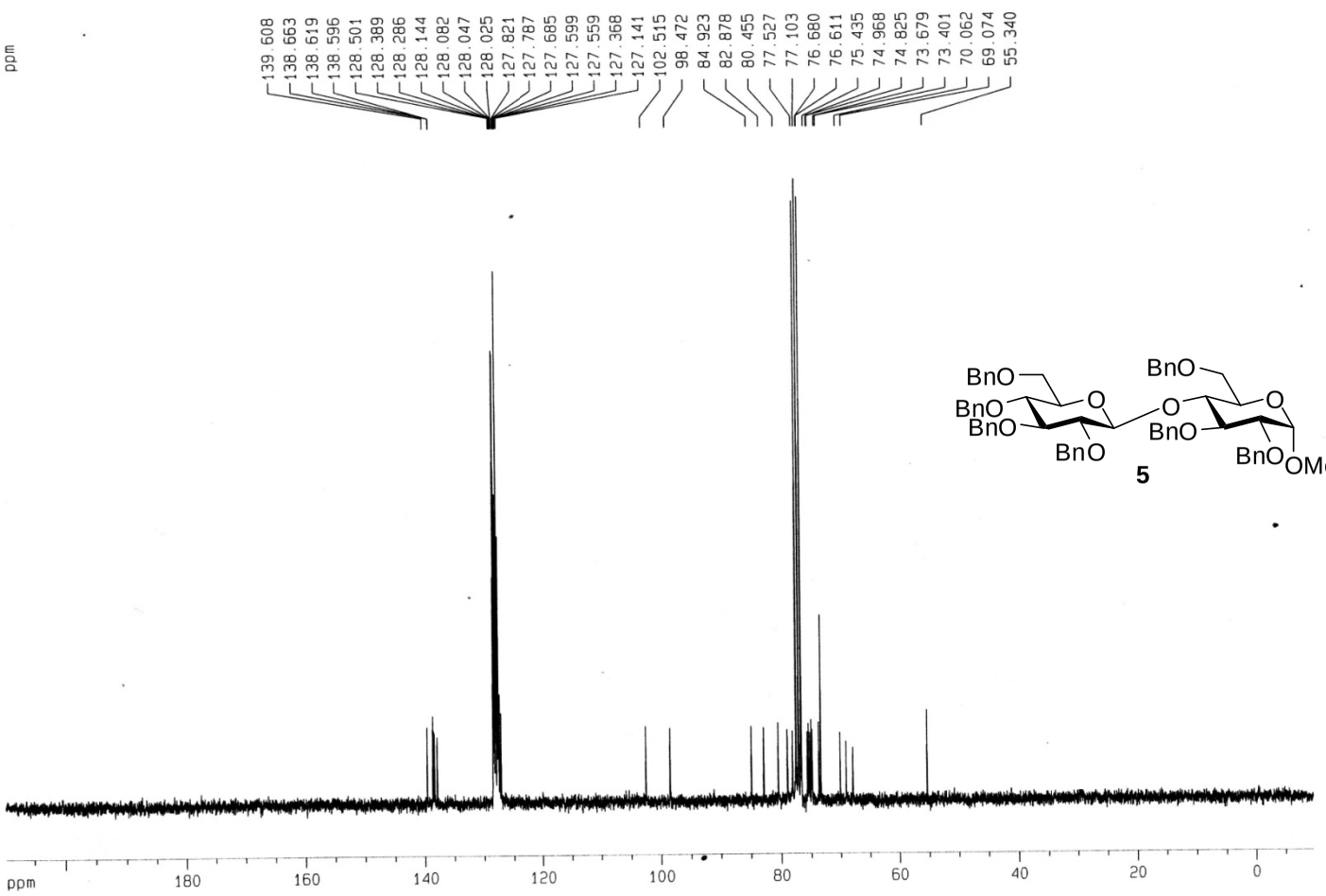
BnO
BnO
BnO
BnO
BnO
BnO
OMe
5

RG (0) -4MMMGlu-13C



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TD                   65536
SOLVENT              CDCl3
NS                     307
DS                       4
SWH              16556.291 Hz
FIDRES           0.252629 Hz
AQ               1.9792372 sec
RG                  18390.4
DW                 30.200 usec
DE                  6.00 usec
TE                     0.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                 11.00 usec
PL1                 -1.00 dB
SF01          75.4752958 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 -2.00 dB
PL12                13.00 dB
PL13                17.00 dB
SF02         300.1312005 MHz

F2 - Processing parameters
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SF            75.4677490 MHz
WDW                       EM
SSB                        0
LB                  1.00 Hz
GB                         0
PC                     1.40

1D NMR plot parameters
CX                  24.00 cm
CY                  10.00 cm
F1P               209.691 ppm
F1              15824.92 Hz
F2P                -9.691 ppm
F2               -731.37 Hz
PPMCM           9.14093 ppm/cm
HZCM          689.84558 Hz/cm
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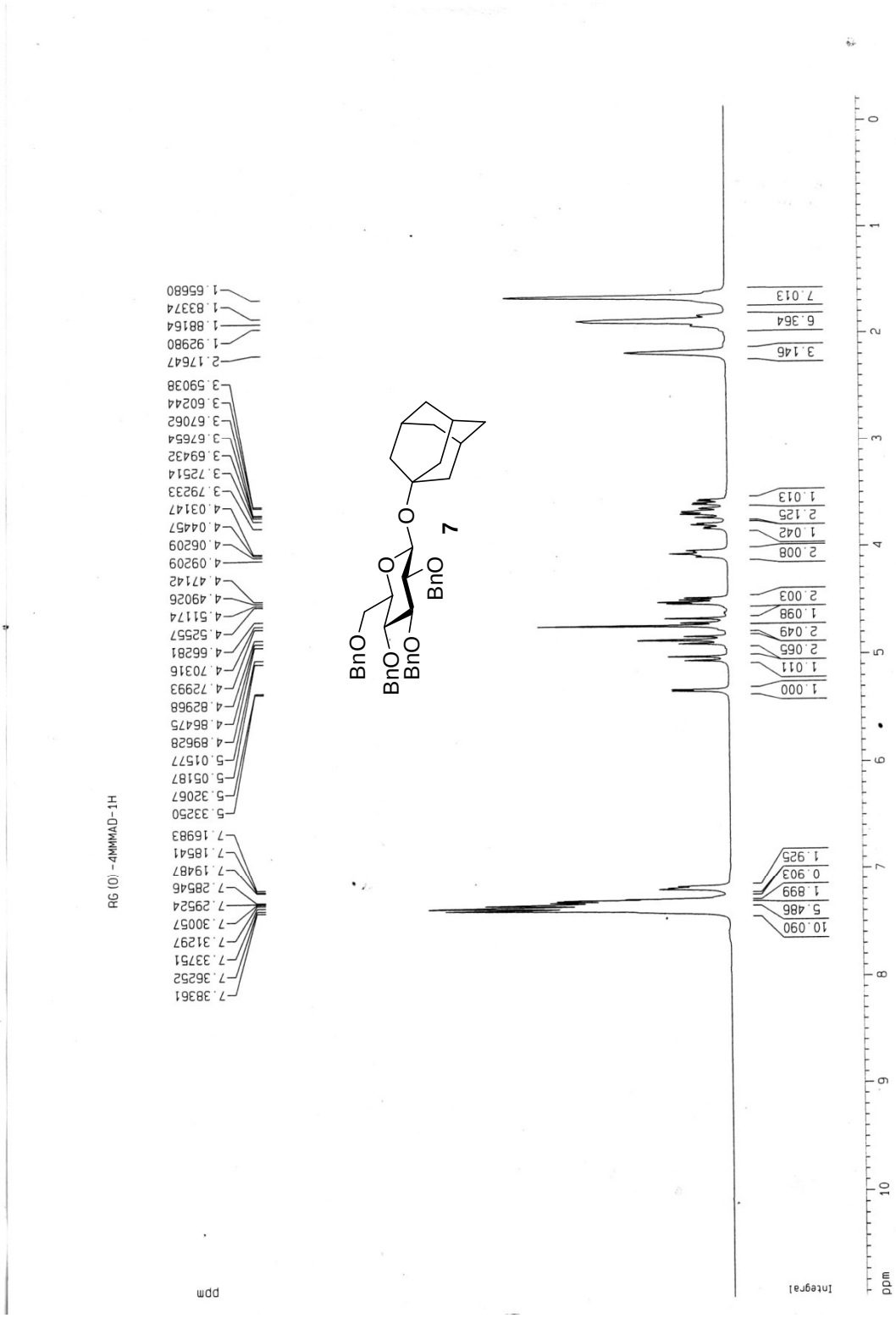
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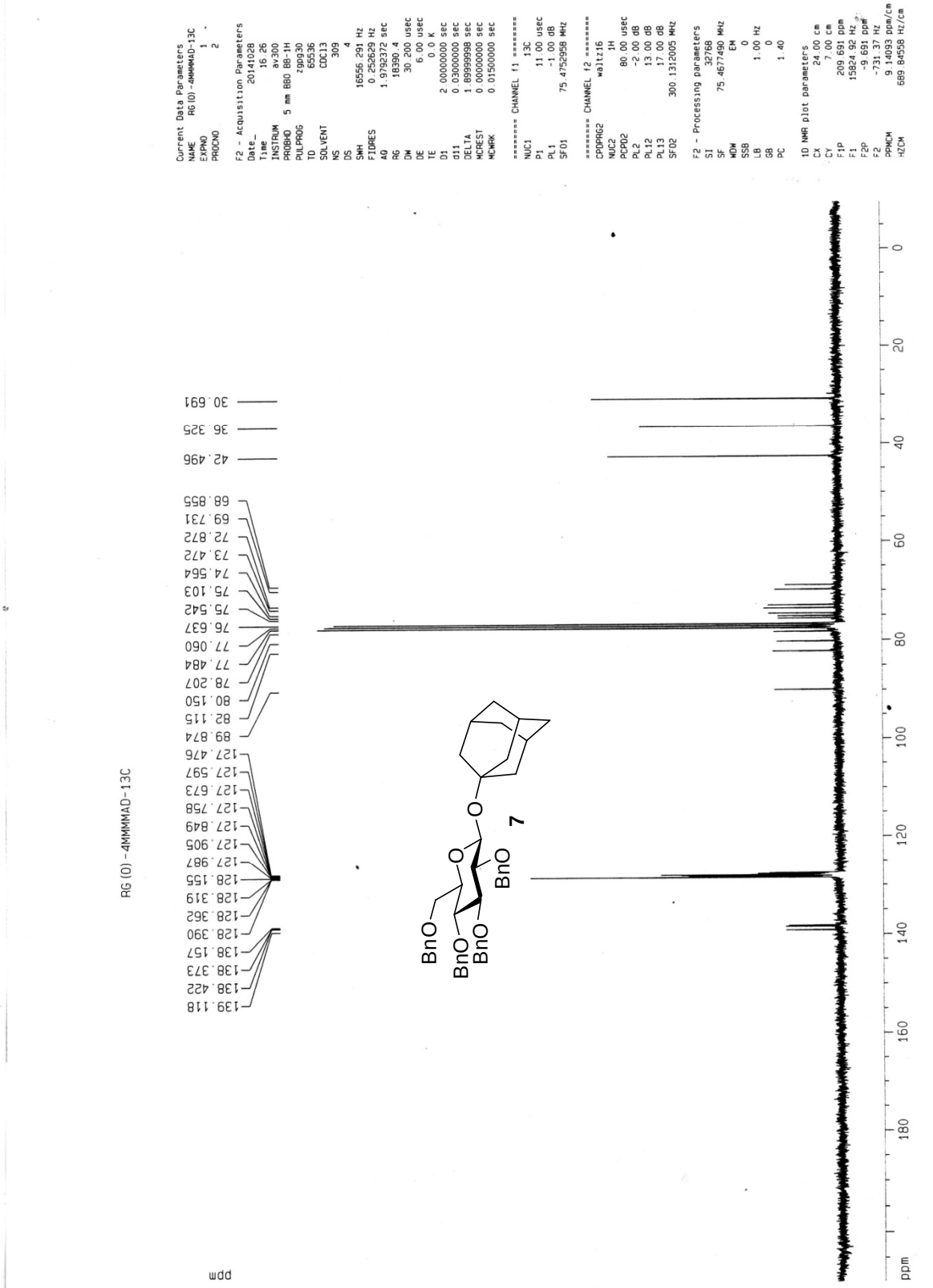
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BnO
BnO
BnO
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O
BnO
7
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PROCNO 2
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 309
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 18390.4
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SF01 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 7.00 cm
F1P 209.691 ppm
F1 15824.92 Hz
F2P -9.691 ppm
F2 -731.37 Hz
PPMCM 9.14093 ppm/cm
HZCM 689.84558 Hz/cm
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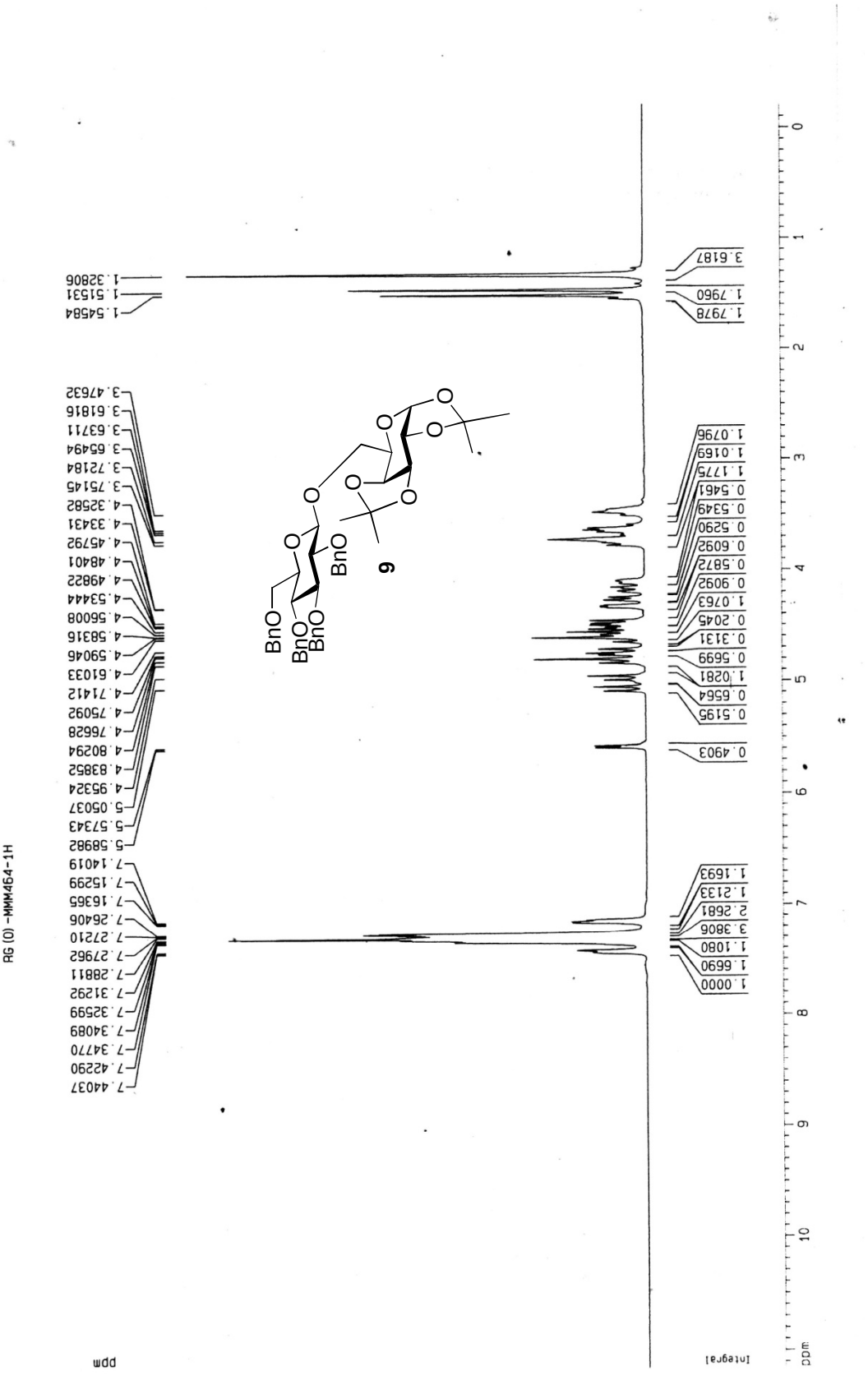
60
80
100
120
140
160
180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Integral
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BnO
BnO
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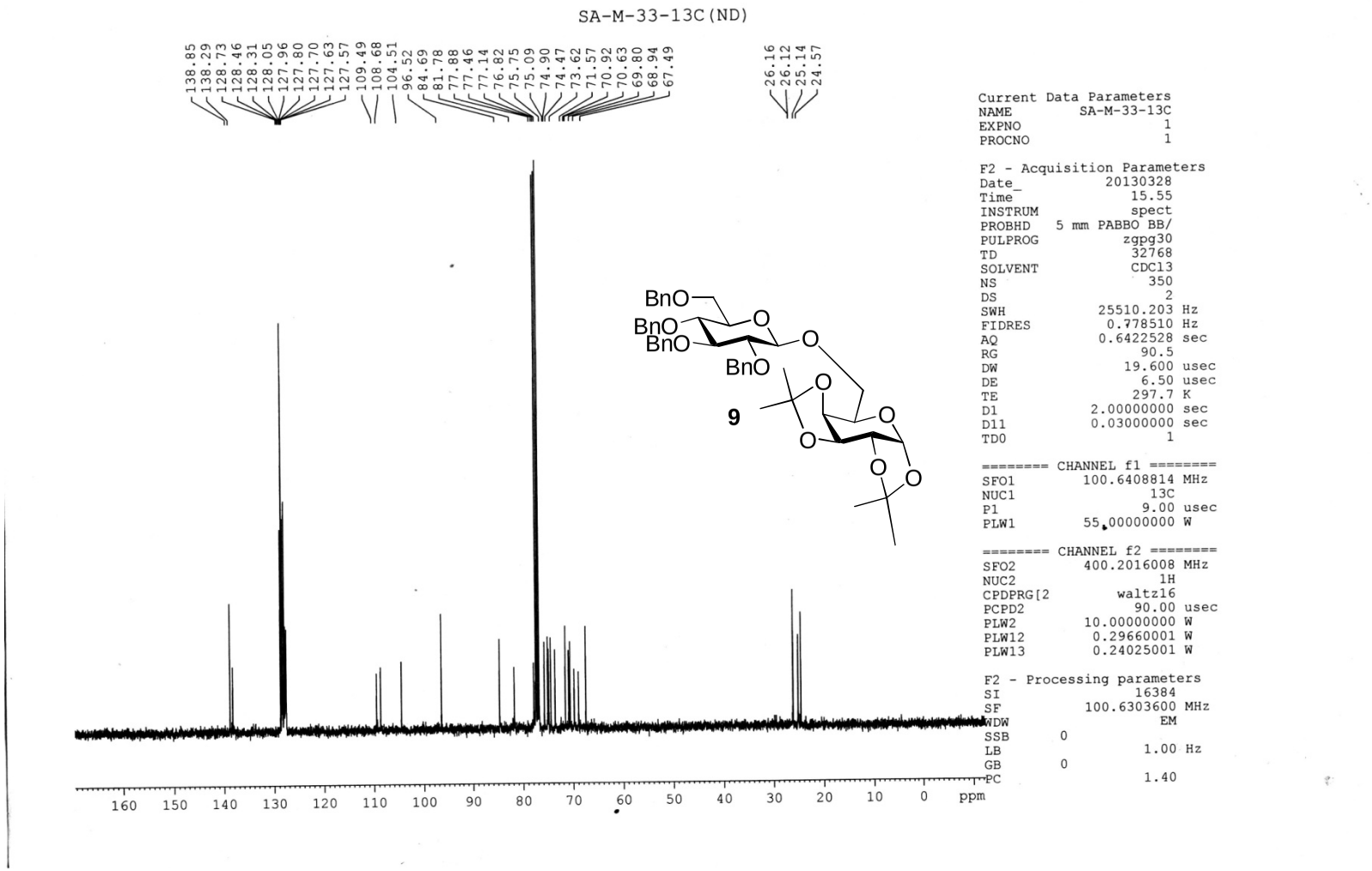
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96.52
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77.88
77.46
77.14
76.82
75.75
75.09
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O
O
O
9
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150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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PROCNO 1
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 350
DS 2
SWH 25510.203 Hz
FIDRES 0.778510 Hz
AQ 0.6422528 sec
RG 90.5
DW 19.600 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6408814 MHz
NUC1 13C
P1 9.00 usec
PLW1 55.00000000 W
======== CHANNEL f2 ========
SFO2 400.2016008 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 10.00000000 W
PLW12 0.29660001 W
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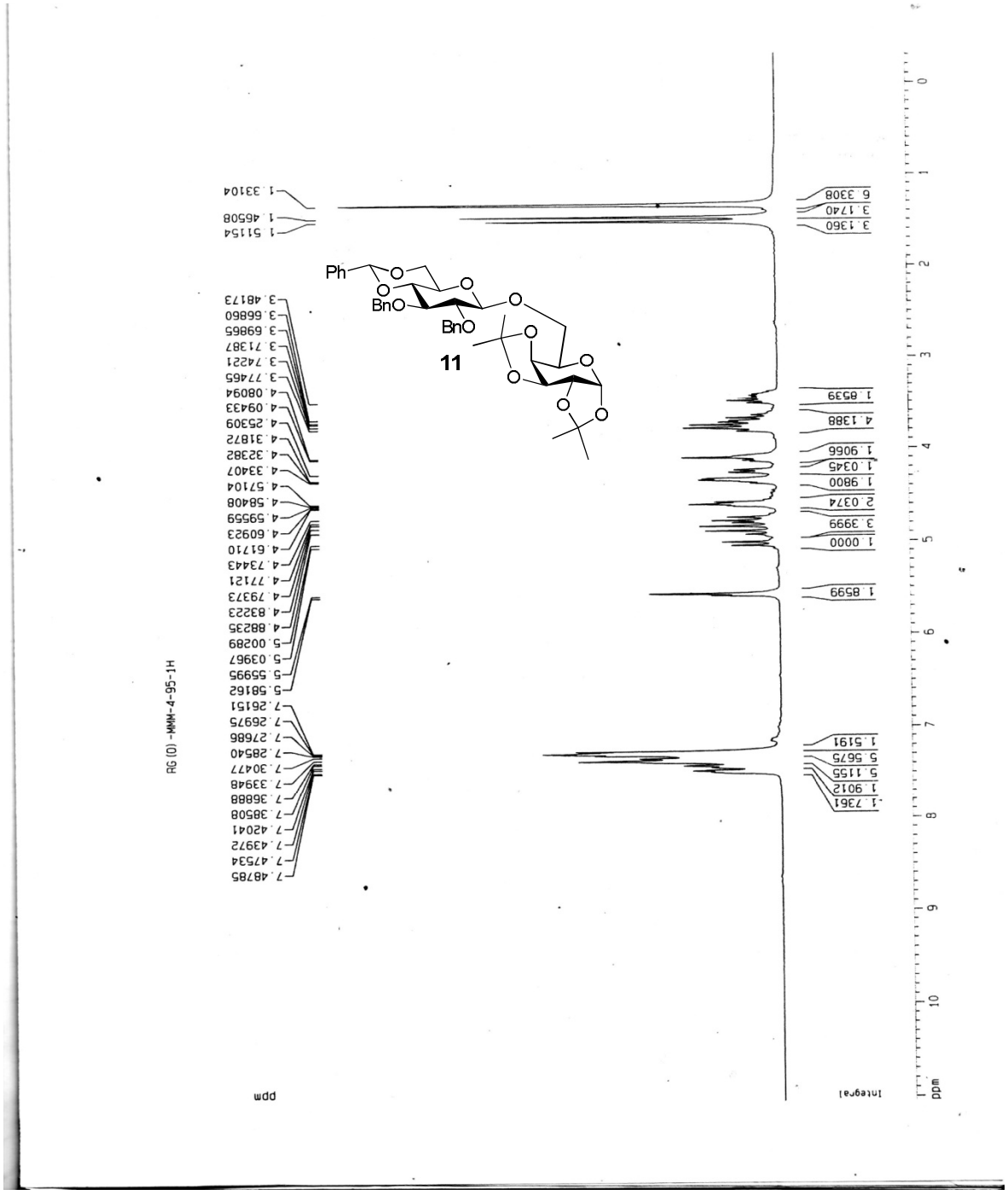
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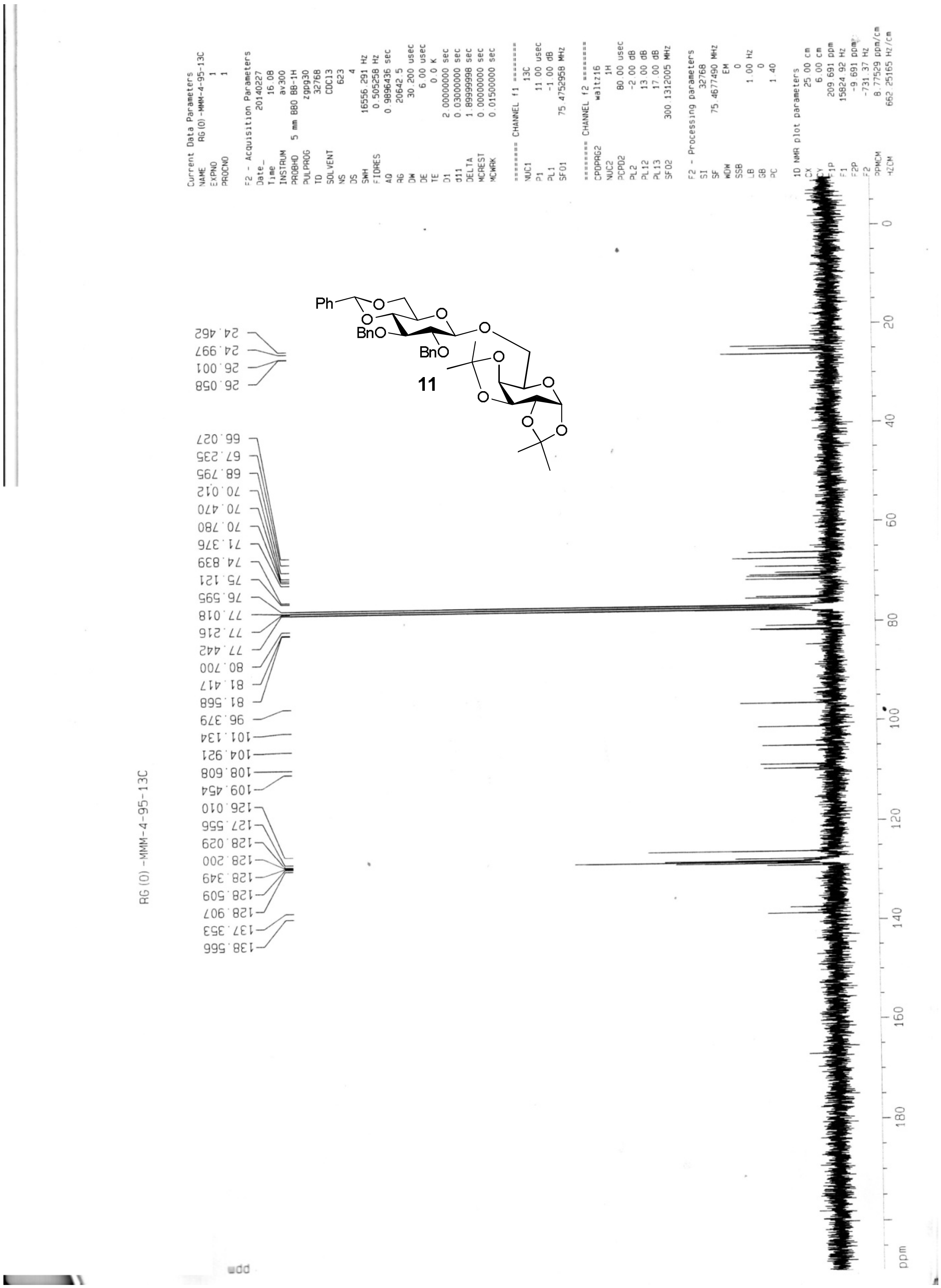
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PROCNO 1
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 623
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SWH 16556.291 Hz
FIDRES 0.505258 Hz
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RG 20642.5
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DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 6.00 cm
F1P 209.691 ppm
F1 15824.92 Hz
F2P -9.691 ppm
F2 -731.37 Hz
PPMCM 8.77529 ppm/cm
HZCM 662.25165 Hz/cm
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70.780
71.376
74.839
75.121
76.595
77.018
77.216
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81.417
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96.379
101.134
104.921
108.608
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Ph
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O
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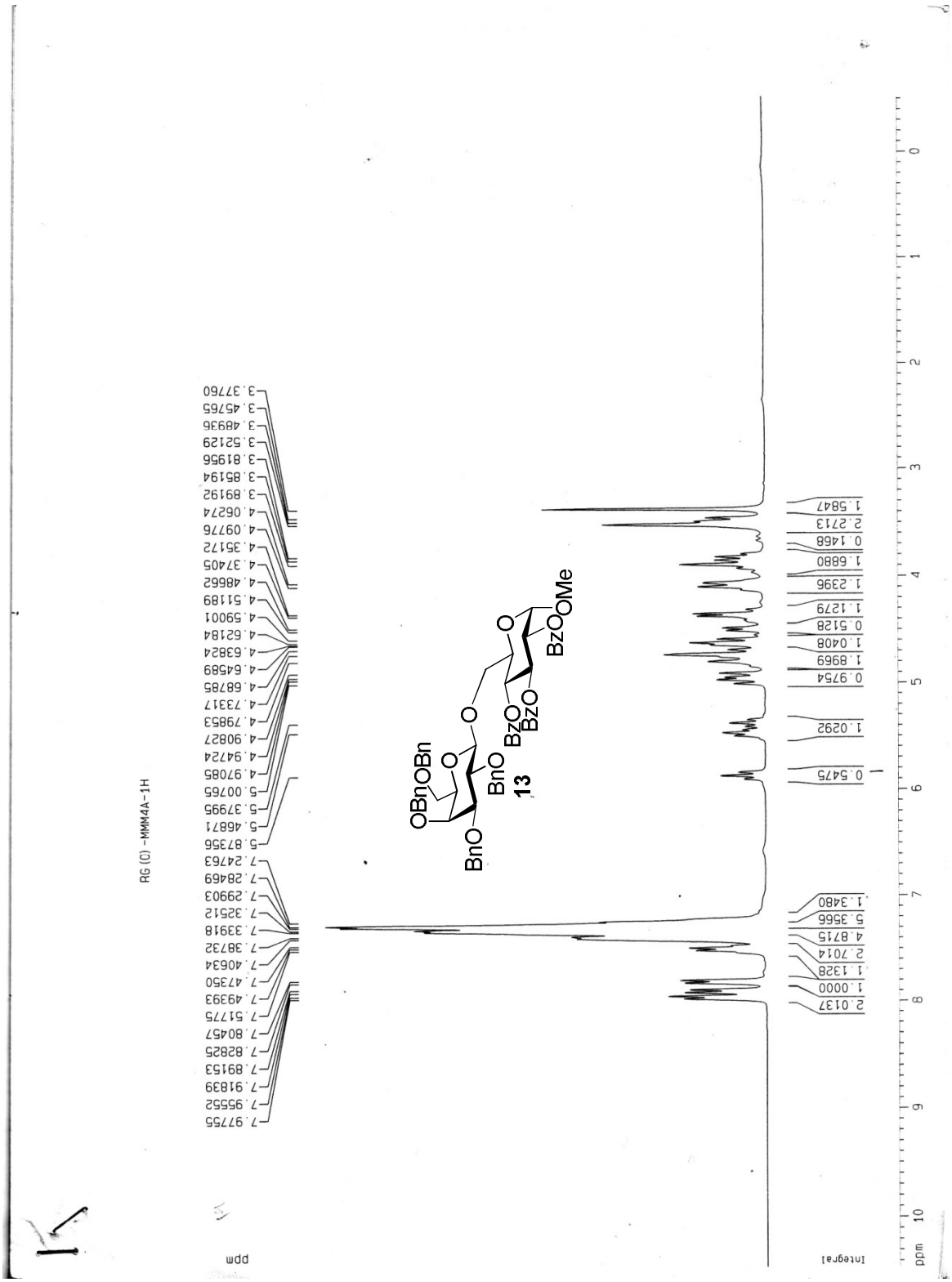
ppm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BzO
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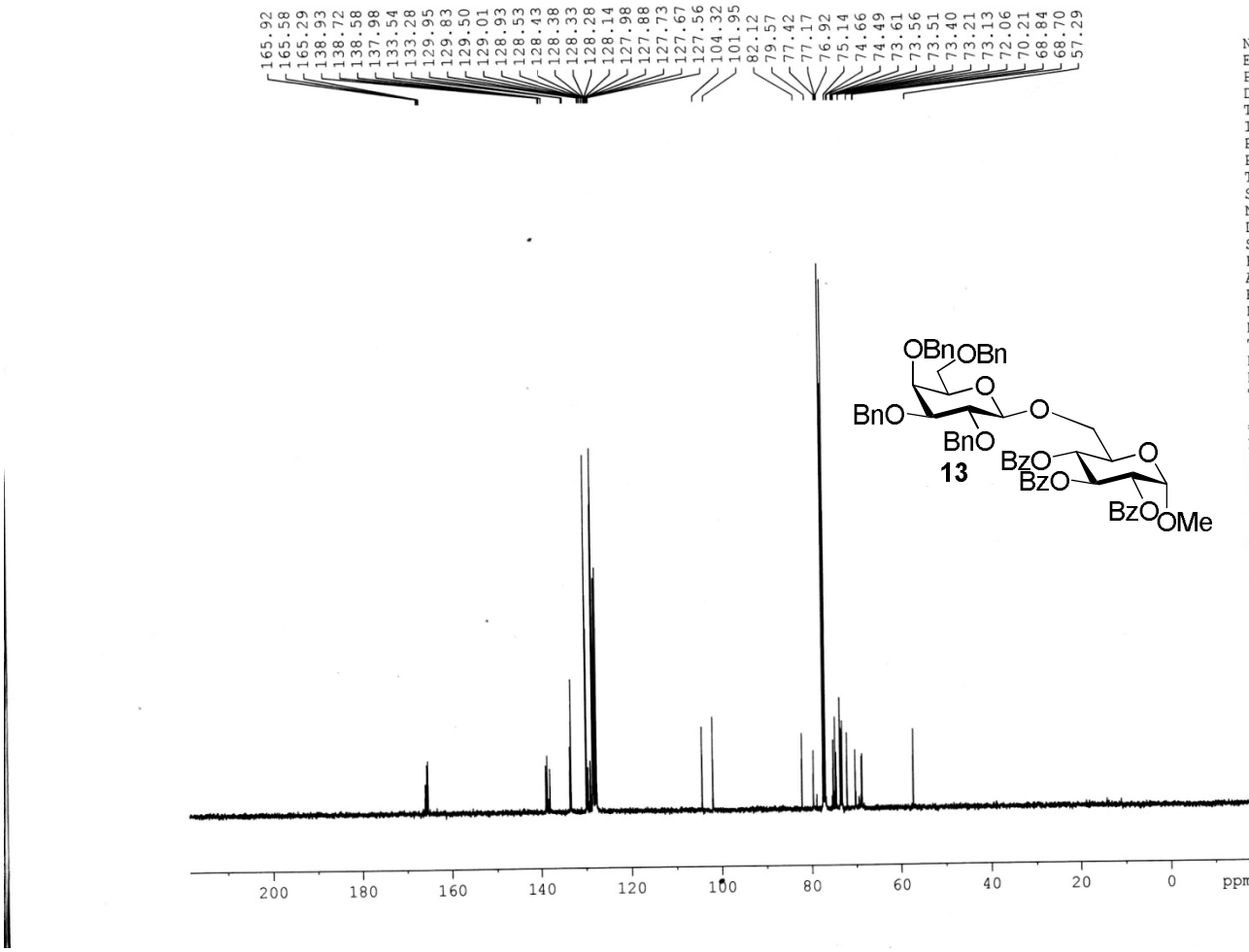
BzO
OMe
ppm
Integral
ppm

KBA.SJG1-13C(SKD)



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PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	0.5505524 sec
RG	32
DW	16.800 usec
DE	6.50 usec
TE	299.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.88 usec
PL1	0.50 dB
PL1W	82.16106415 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.50 dB
PL13	20.00 dB
PL2W	15.50318813 W
PL12W	0.43693921 W
PL13W	0.19517358 W
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SI	16384
SF	125.7577766 MHz
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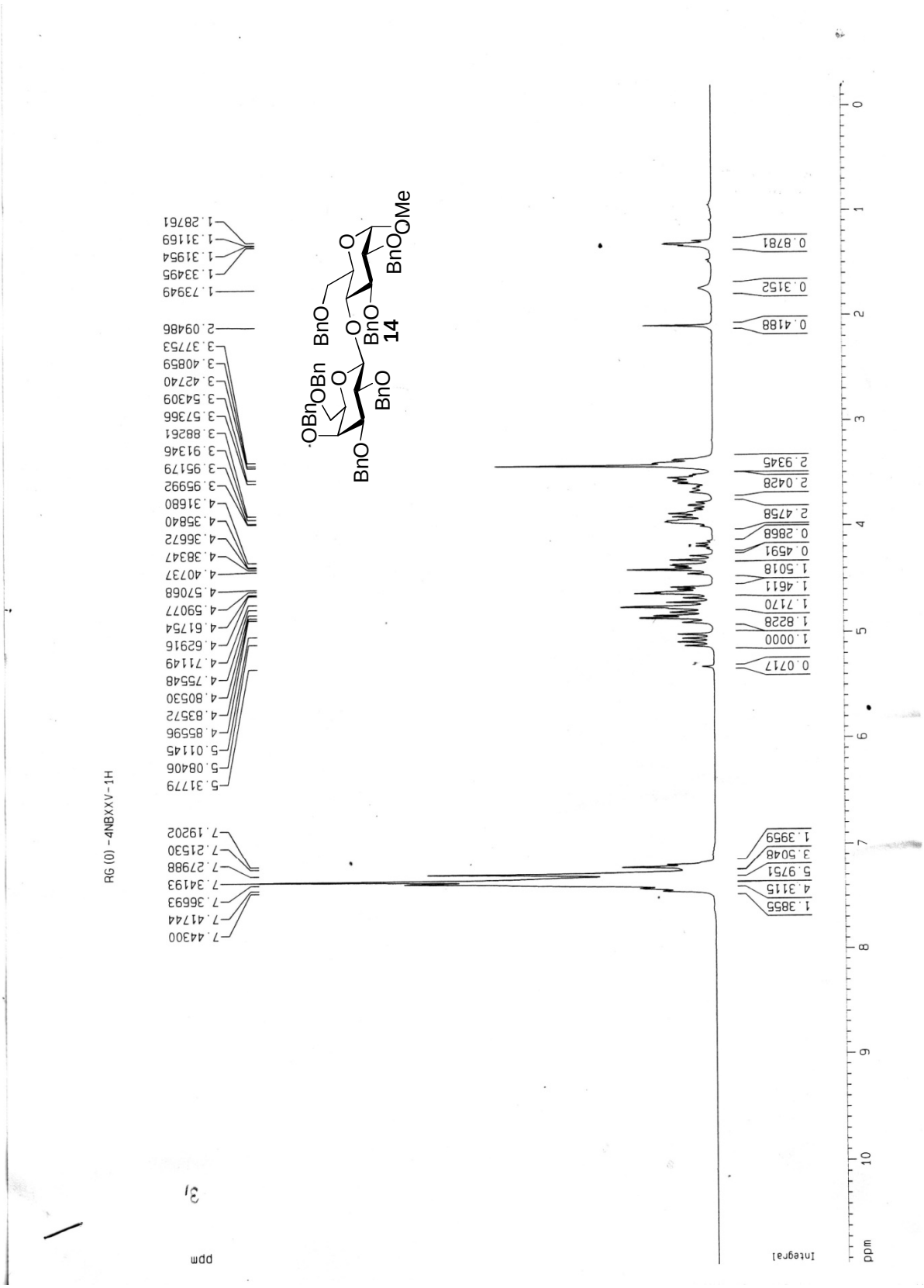
GB	0
PC	1.40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Integral
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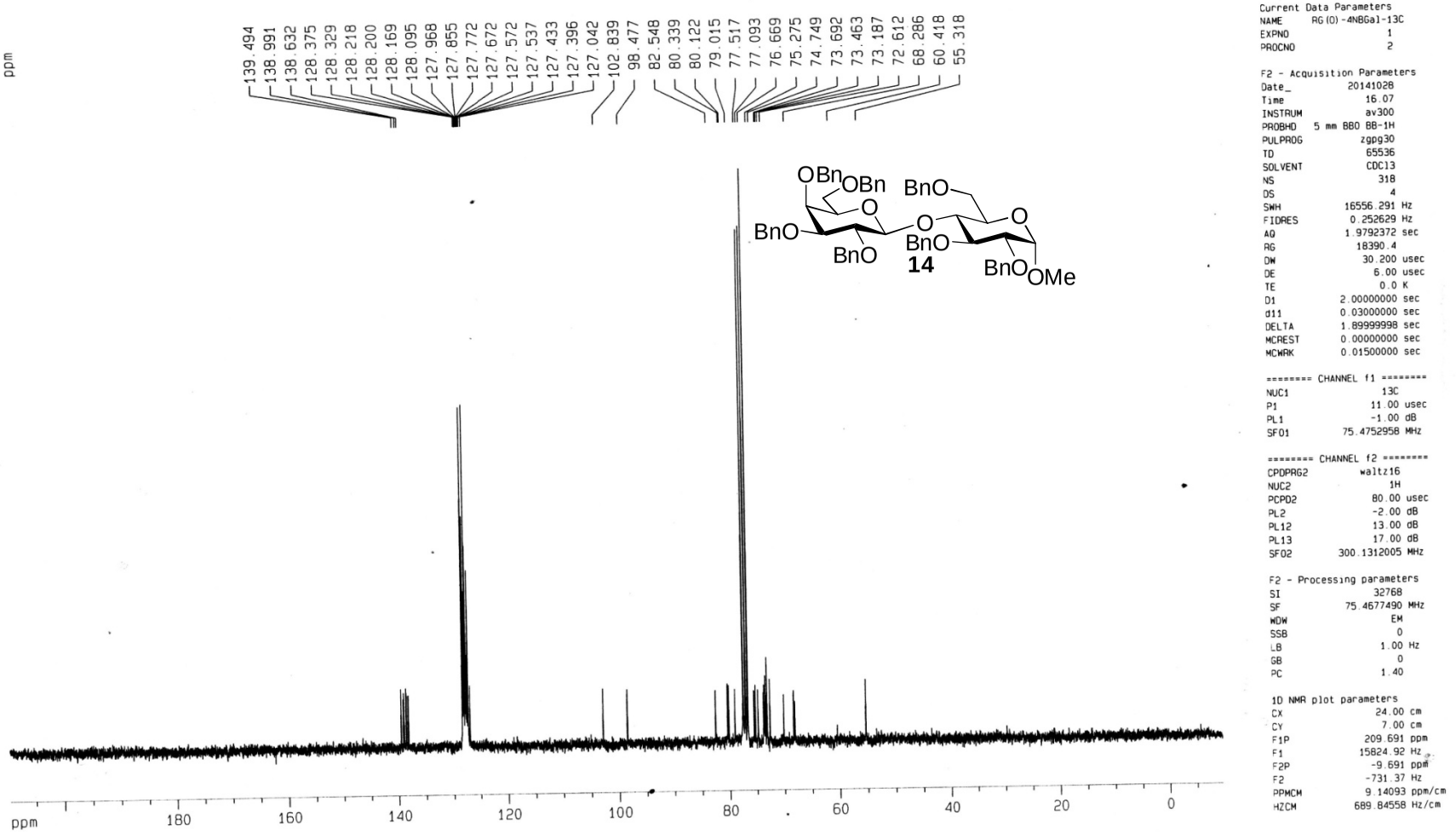
OBn
OMe

RG(0)-4NBGal-13C



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EXPNO	1
PROCNO	2

F2 - Acquisition Parameters

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Time	16.07
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PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	318
DS	4
SWH	16556.291 Hz
FIDRES	0.252629 Hz
AQ	1.9792372 sec
RG	18390.4
DW	30.200 usec
DE	6.00 usec
TE	0.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	11.00 usec
PL1	-1.00 dB
SFO1	75.4752958 MHz

======== CHANNEL f2 ========

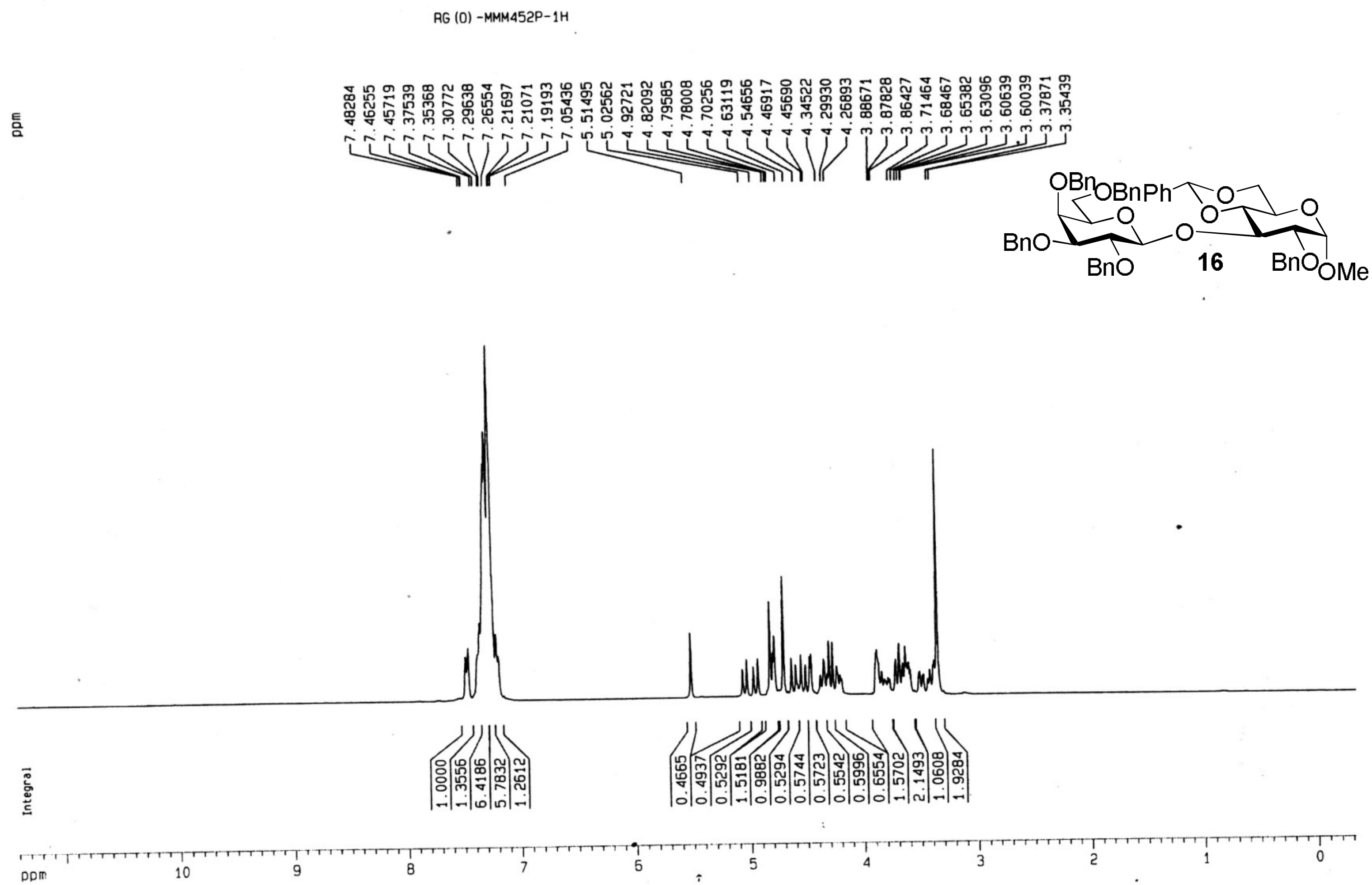
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-2.00 dB
PL12	13.00 dB
PL13	17.00 dB
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	24.00 cm
CY	7.00 cm
F1P	209.691 ppm
F1	15824.92 Hz
F2P	-9.691 ppm
F2	-731.37 Hz
PPMCM	9.14093 ppm/cm
HZCM	689.84558 Hz/cm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7.19193
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5.02562
4.92721
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BnO
BnO
16
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OMe
Integral
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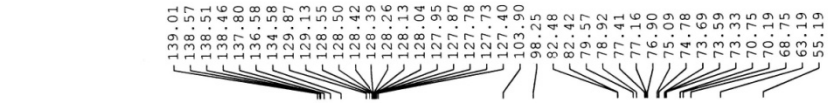
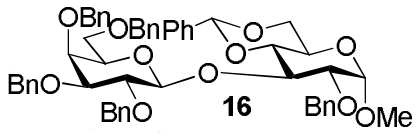
SA704-13C(SKD)





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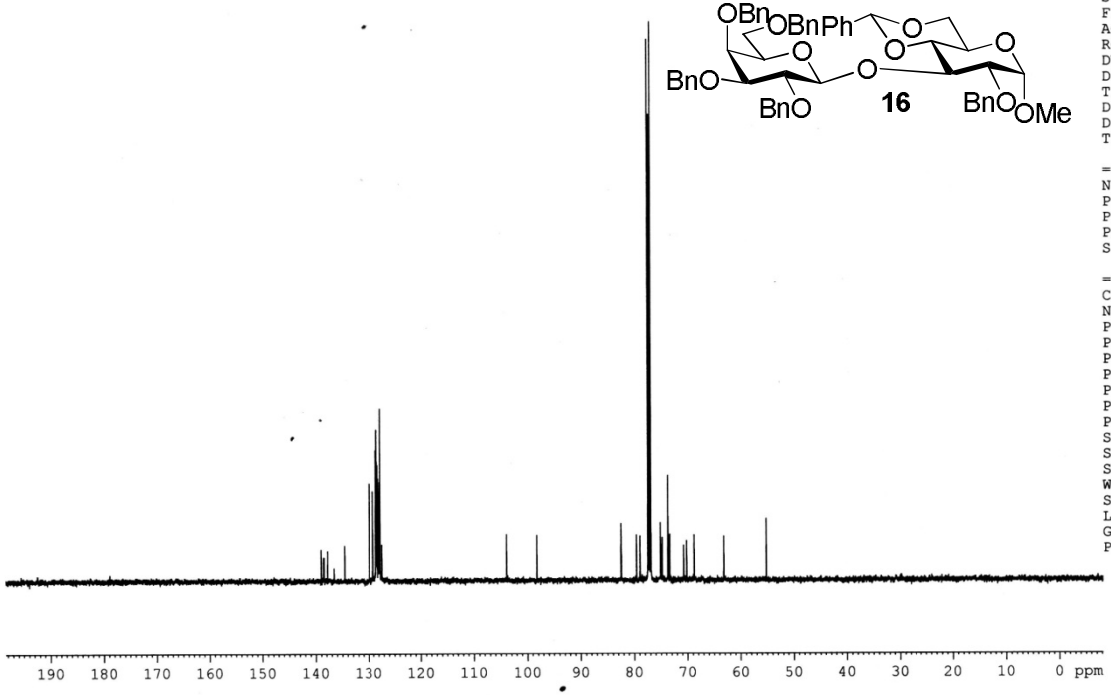
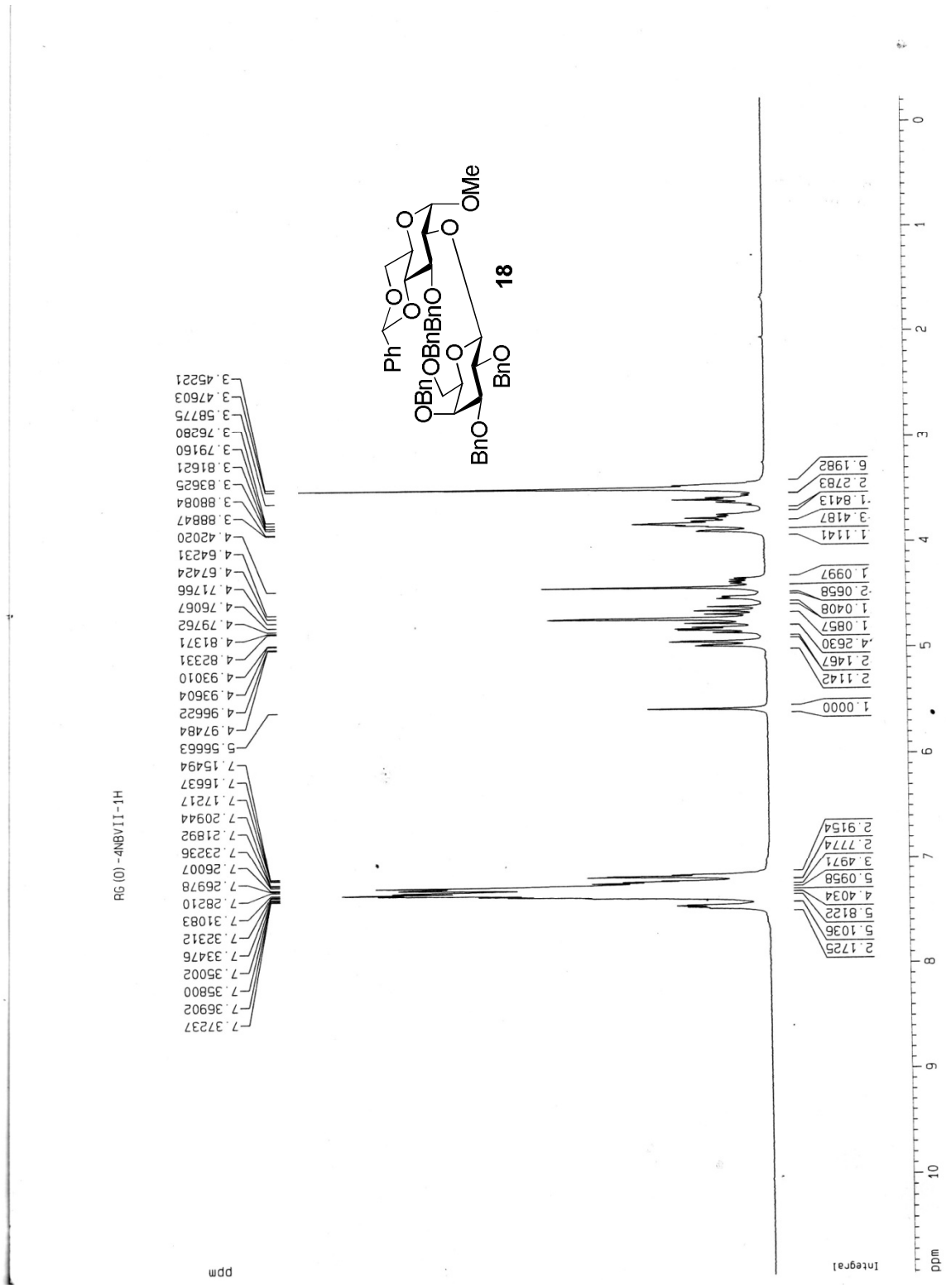
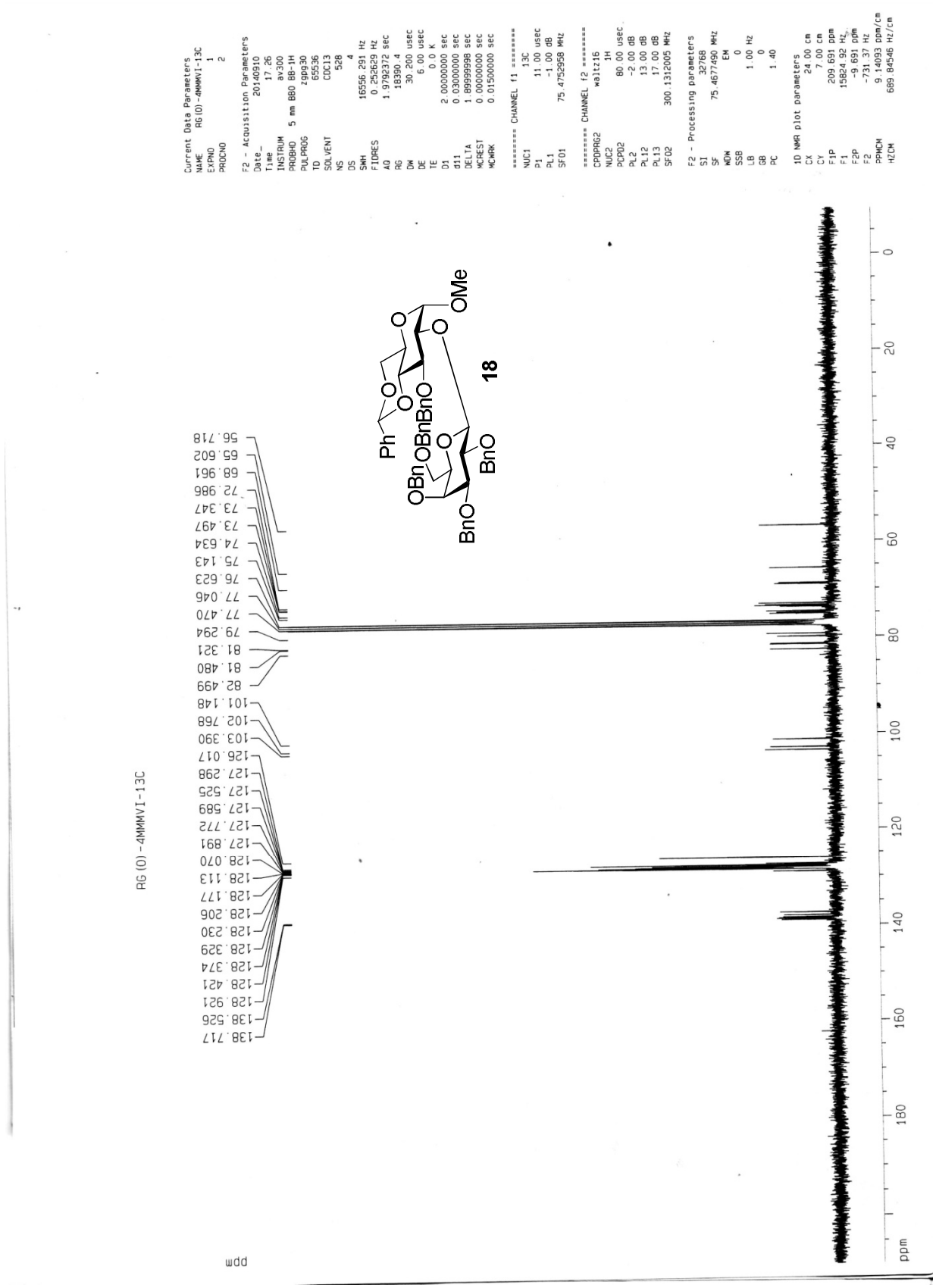
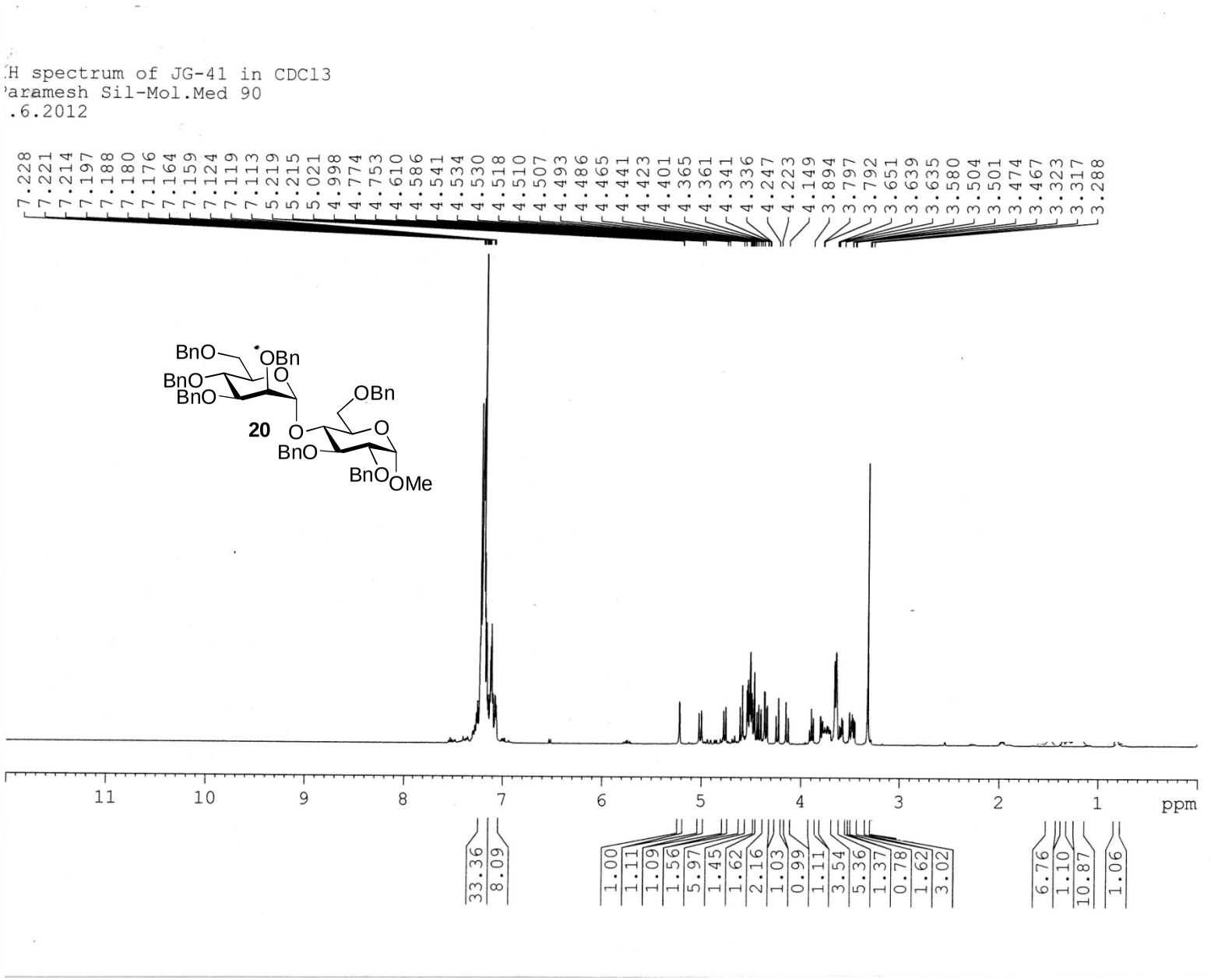
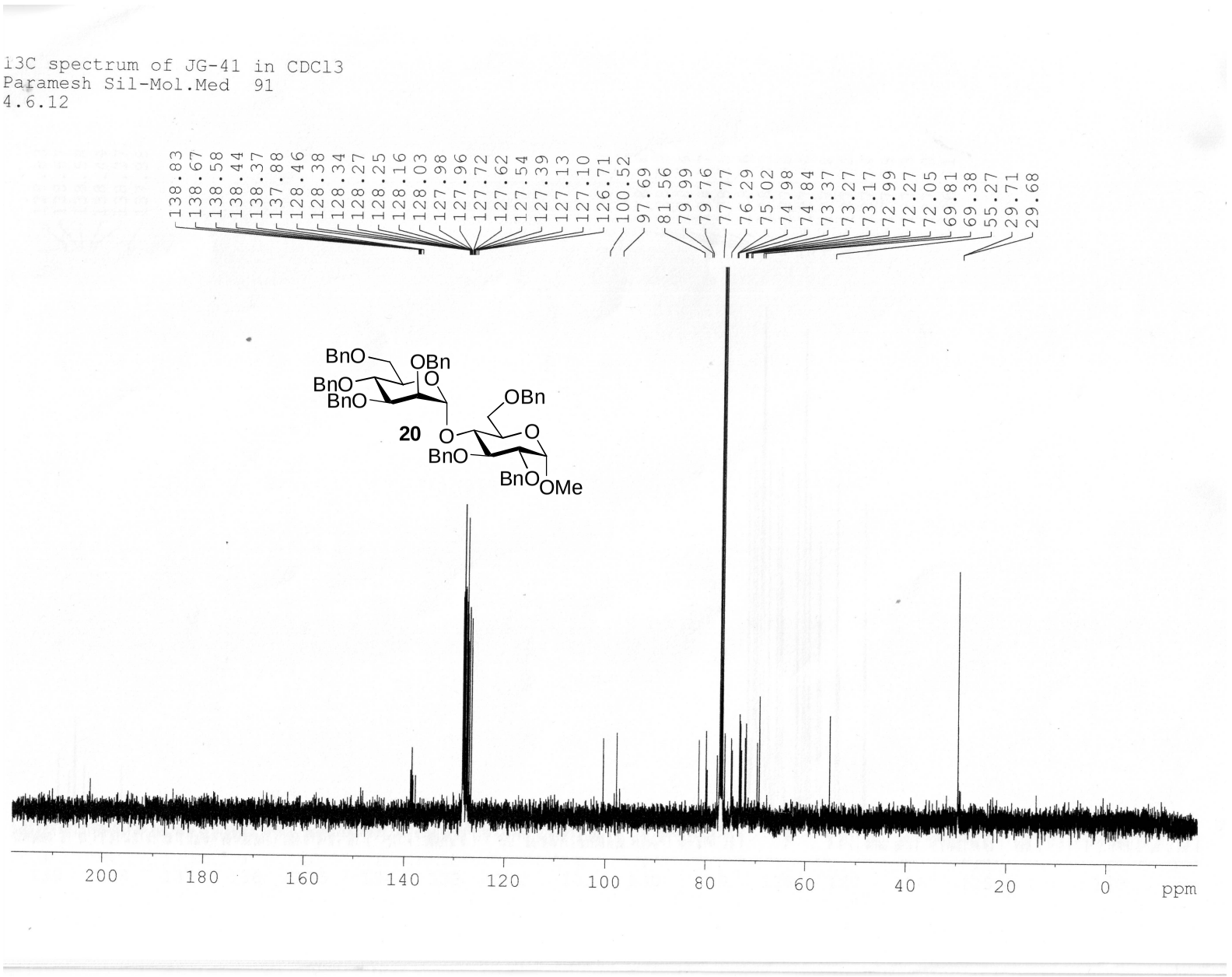
TD	32768
SOLVENT	CDCl3
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	0.5505524 sec
RG	32
DW	16.800 usec
DE	6.50 usec
TE	298.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.88 usec
PL1	0.50 dB
PL1W	82.16106415 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.50 dB
PL13	20.00 dB
PL2W	15.50318813 W
PL12W	0.43693921 W
PL13W	0.19517358 W
SFO2	500.1320005 MHz
SI	16384
SF	125.7577735 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

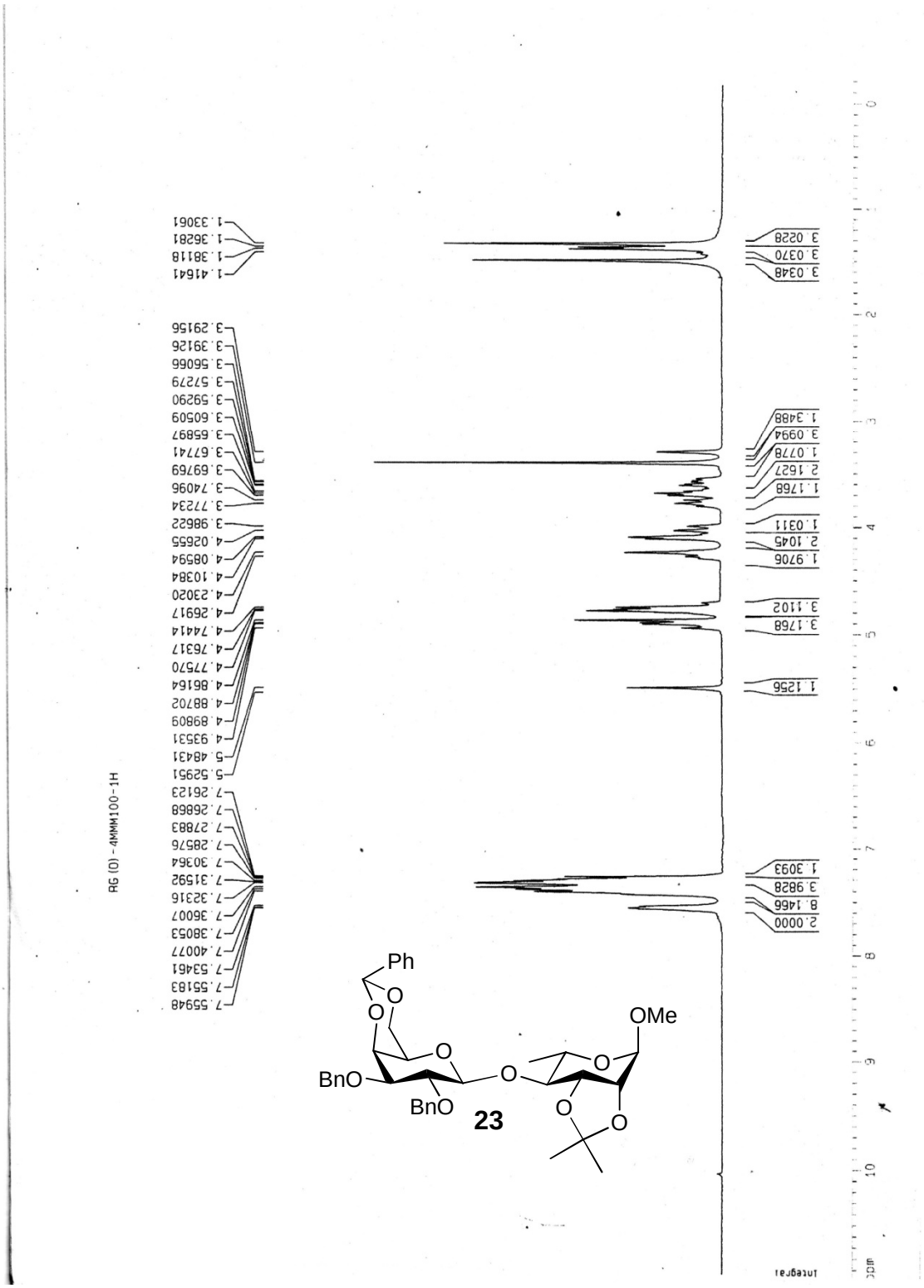


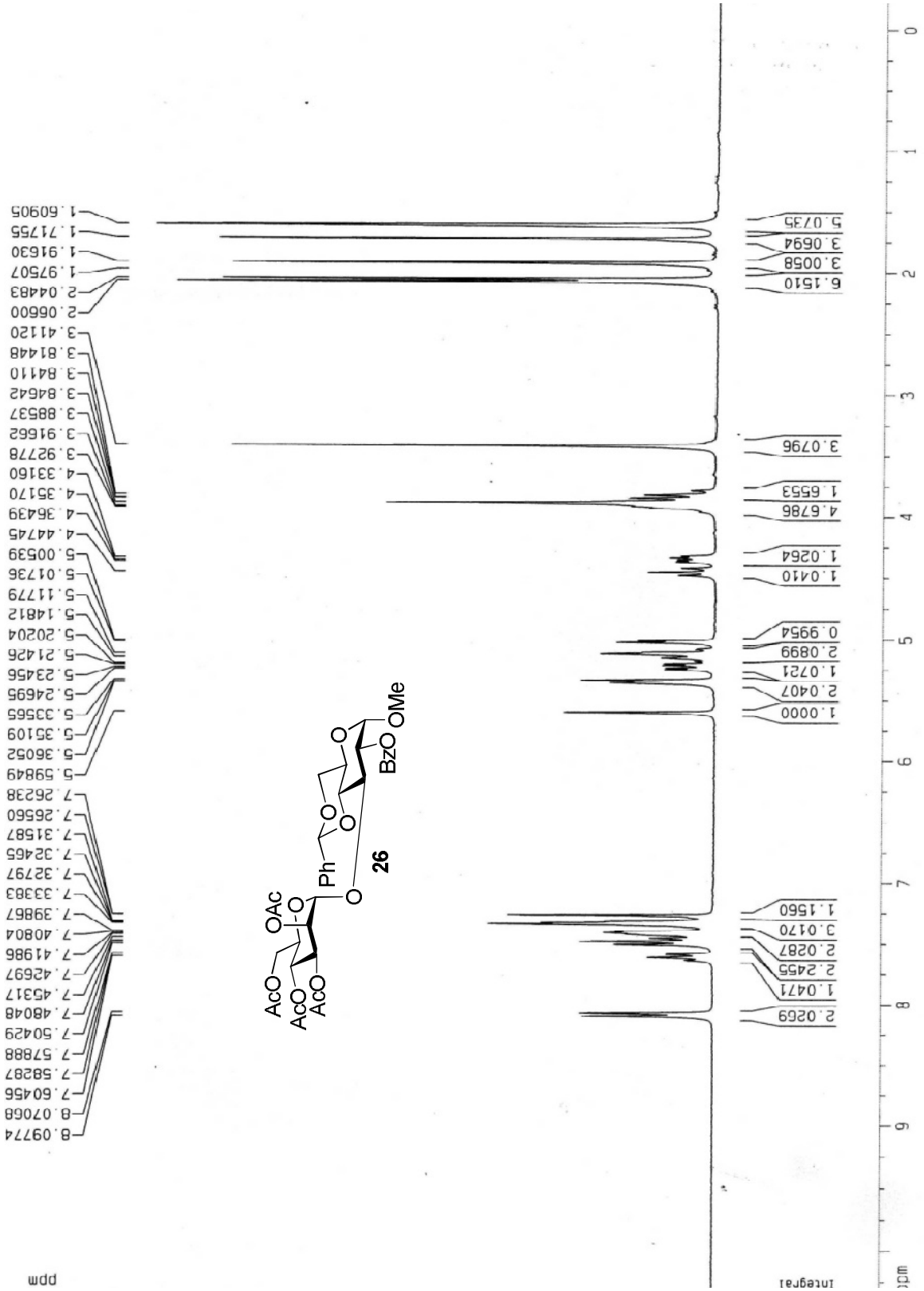

RG(0)-4NBVII-1H
ppm
Integral
18
Ph
OBn
OBnBnO
BnO
BnO
OMe

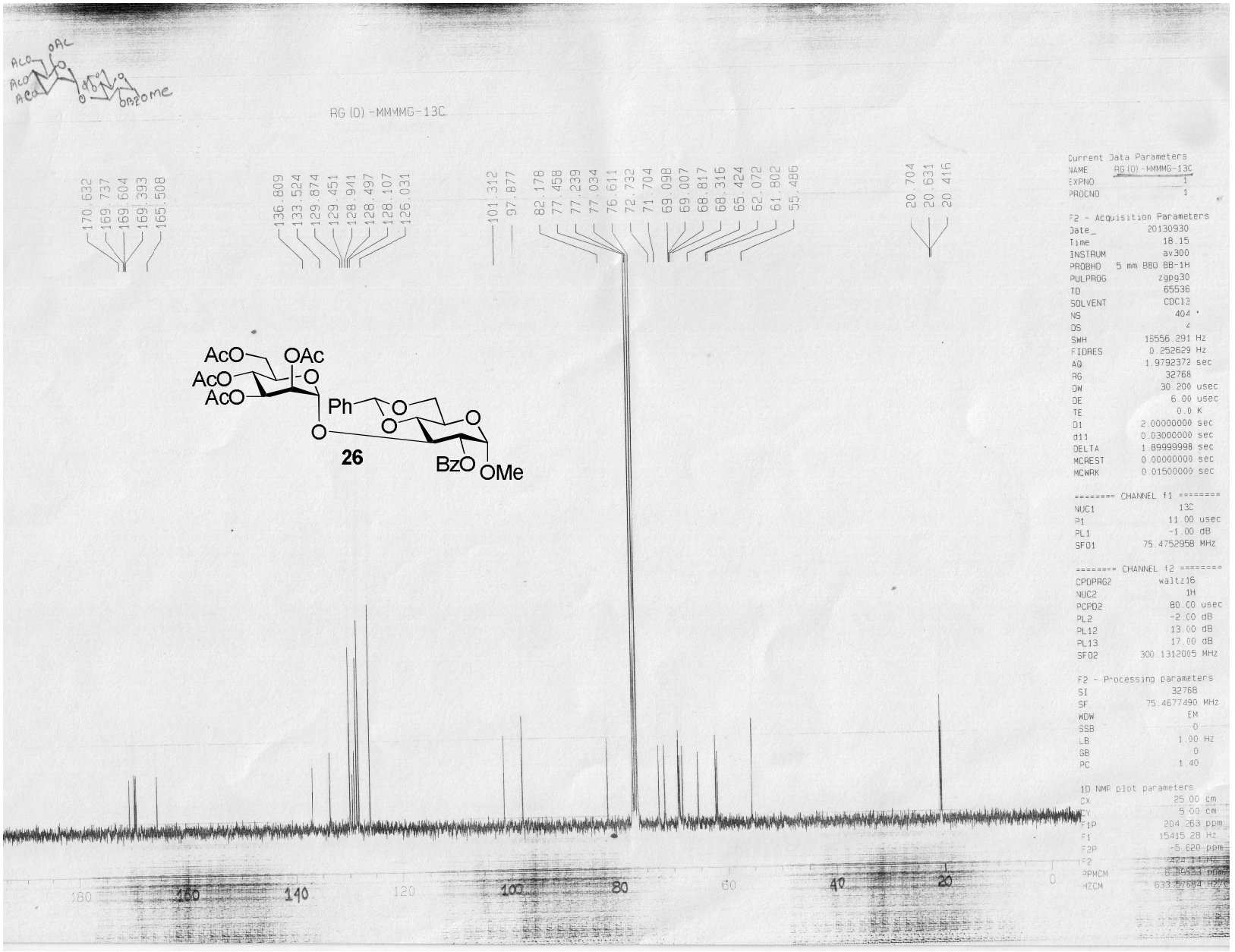

RG(0)-4MMMVI-13C
ppm
138.717
138.526
128.921
128.421
128.374
128.329
128.230
128.206
128.177
128.113
128.070
127.891
127.772
127.589
127.525
127.298
126.017
103.390
102.768
101.148
82.499
81.480
81.321
79.294
77.470
77.046
76.623
75.143
74.634
73.497
73.347
72.986
68.961
65.602
56.718
Ph
OBn
OBn
BnO
BnO
OMe
18
Current Data Parameters
NAME RG(0)-4MMMVI-13C
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20140910
Time 17.26
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 528
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 18390.4
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 7.00 cm
F1P 209.691 ppm
F1 15824.92 Hz
F2P -9.691 ppm
F2 -731.37 Hz
PPMCM 9.14093 ppm/cm
HZCM 689.84546 Hz/cm
ppm
0
20
40
60
80
100
120
140
160
180

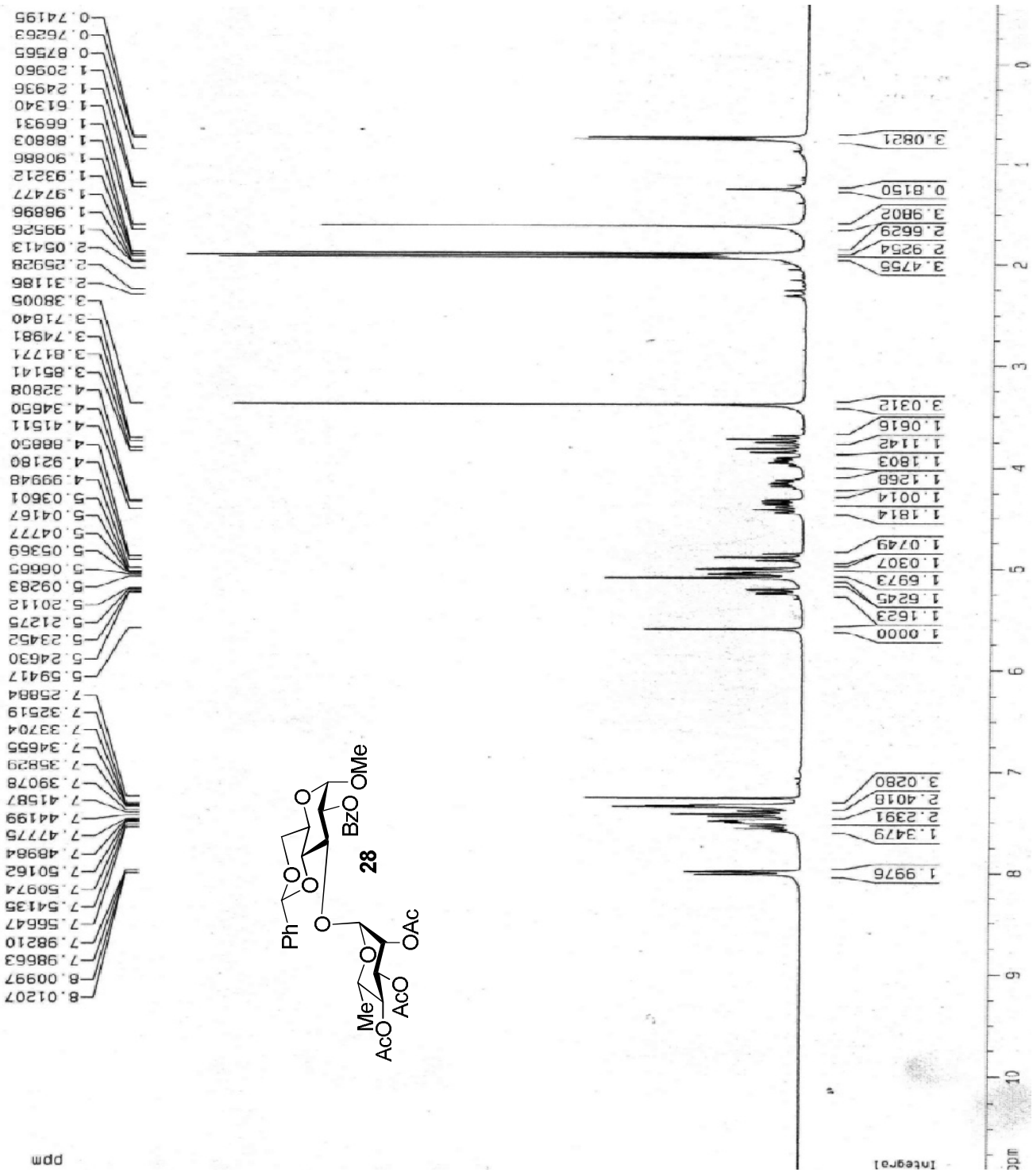

H spectrum of JG-41 in CDCl3
aramesh Sil-Mol.Med 90
.6.2012
7.228
7.221
7.214
7.197
7.188
7.180
7.176
7.164
7.159
7.124
7.119
7.113
5.219
5.215
5.021
4.998
4.774
4.753
4.610
4.586
4.541
4.534
4.530
4.518
4.510
4.507
4.493
4.486
4.465
4.441
4.423
4.401
4.365
4.361
4.341
4.336
4.247
4.223
4.149
3.894
3.797
3.792
3.651
3.639
3.635
3.580
3.504
3.501
3.474
3.467
3.323
3.317
3.288
BnO
OBn
BnO
BnO
O
OBn
20
O
O
BnO
BnO
OMe
11
10
9
8
7
6
5
4
3
2
1
ppm
33.36
8.09
1.00
1.11
1.09
1.56
5.97
1.45
1.62
2.16
1.03
0.99
1.11
3.54
5.36
1.37
0.78
1.62
3.02
6.76
1.10
10.87
1.06

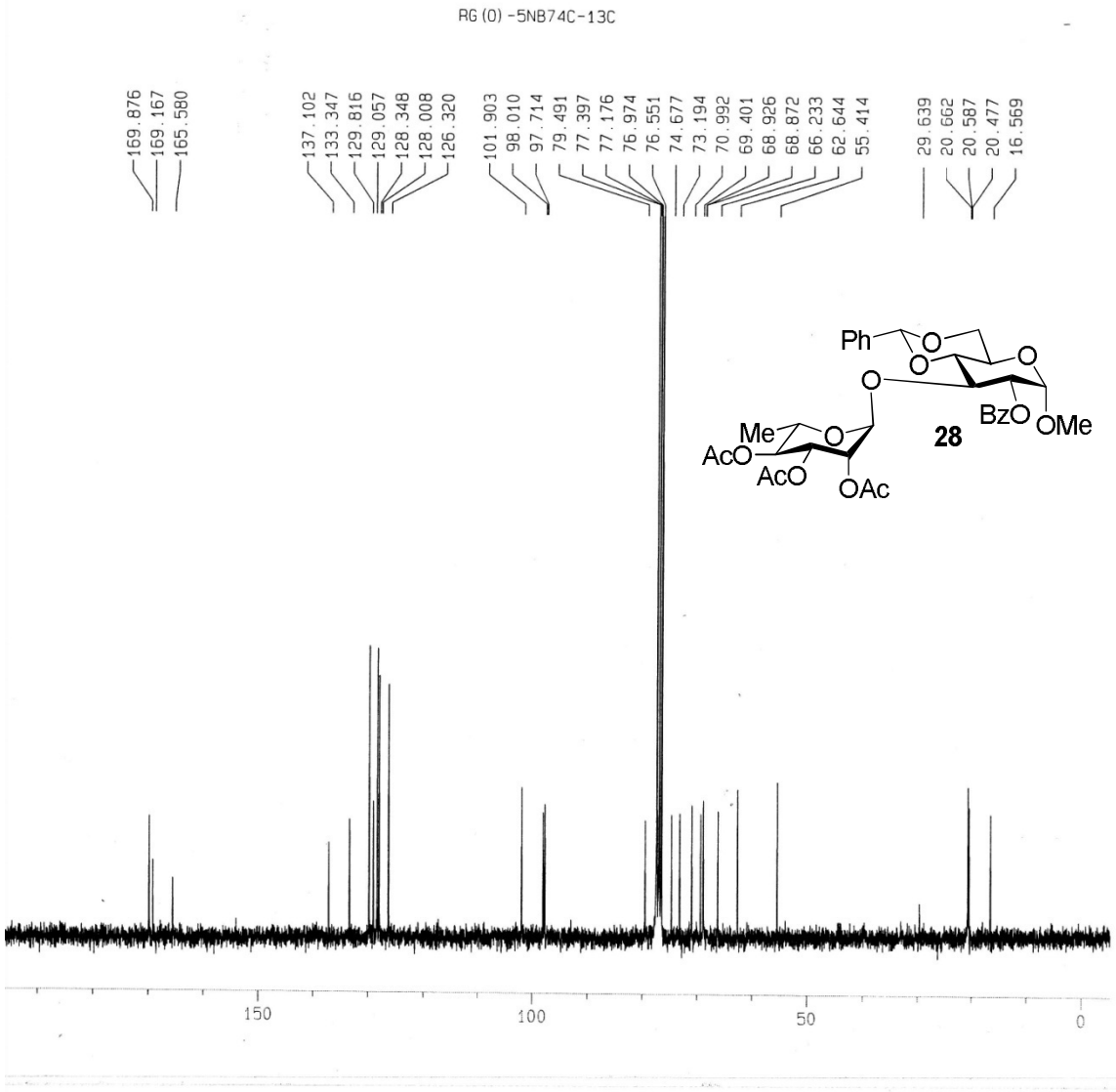

13C spectrum of JG-41 in CDCl3
Paramesh Sil-Mol.Med 91
4.6.12
138.83
138.67
138.58
138.44
138.37
137.88
128.46
128.38
128.34
128.27
128.25
128.16
128.03
127.98
127.96
127.72
127.62
127.54
127.39
127.13
127.10
126.71
100.52
97.69
81.56
79.99
79.76
77.77
76.29
75.02
74.98
74.84
73.37
73.27
73.17
72.99
72.27
72.05
69.81
69.38
55.27
29.71
29.68
BnO
OBn
BnO
O
BnO
OBn
20
O
O
BnO
BnO
OMe
200
180
160
140
120
100
80
60
40
20
0
ppm


RG (0) - 4MMM100-1H
integral
Ph
OMe
BnO
BnO
23


26
OMe
BzO
Ph
OAc
AcO
AcO
AcO
ppm
integral


RG (0) -MMMMG-13C
170.632
169.737
169.604
169.393
165.508
136.809
133.524
129.874
129.451
128.941
128.497
128.107
126.031
101.312
97.877
82.178
77.458
77.239
77.034
76.611
72.732
71.704
69.098
69.007
68.817
68.316
65.424
62.072
61.802
55.486
20.704
20.631
20.416
AcO
OAc
AcO
AcO
Ph
O
O
O
O
BzO
OMe
26
Current Data Parameters
NAME RG(0)-MMMMG-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130930
Time 18.15
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 404
DS 4
SWH 15556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 32768
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SF01 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 5.00 cm
F1P 204.263 ppm
F1 15415.28 Hz
F2P -5.620 ppm
F2 424.14 Hz
PPMCM 8.26553 ppm
HZCM 633.57684 Hz/cm
180
160
140
120
100
80
60
40
20
0


28
Ph
BzO
OMe
OAc
AcO
AcO
Me
ppm
Integral



Current Data Parameters
NAME RG(0)-5NB74C-13C
EXPNO 2
PROCNO 1

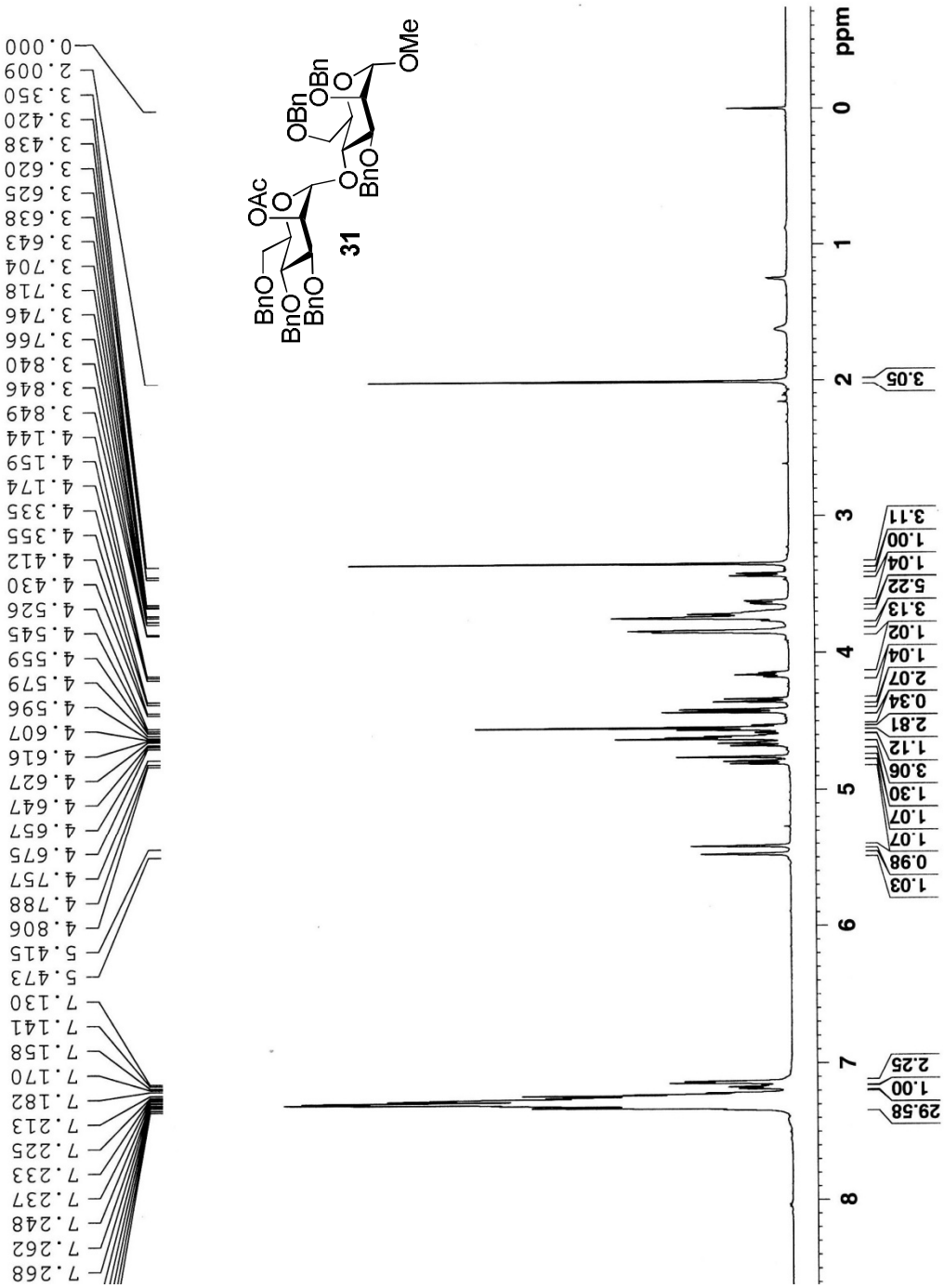
F2 - Acquisition Parameters
Date_ 20110630
Time 16.22
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65576
SOLVENT CDCl3
NS 761
DS 4
SWH 17985.611 Hz
FIDRES 0.274271 Hz
AQ 1.8230628 sec
RG 23170.5
DW 27.800 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

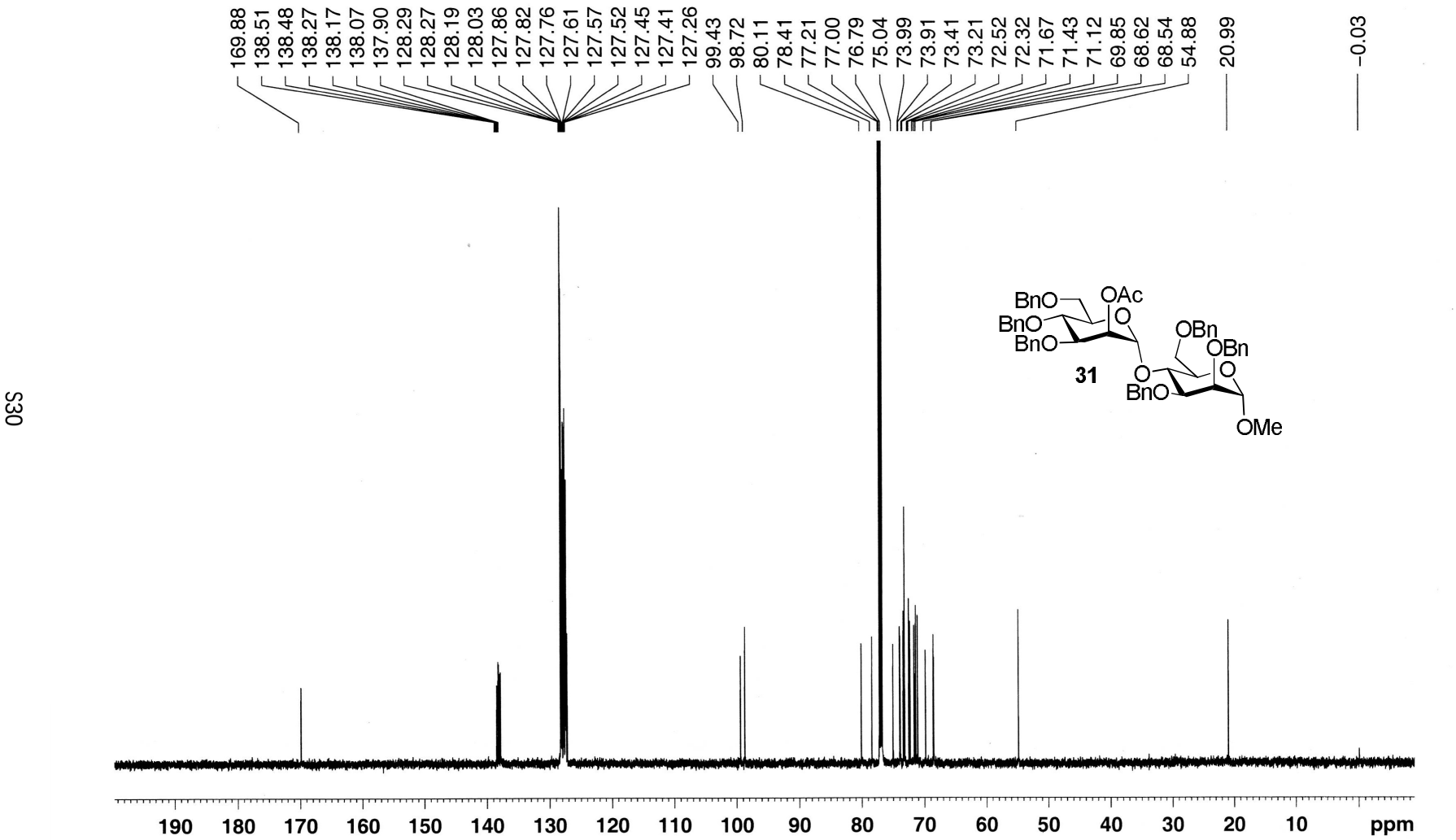
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.75 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

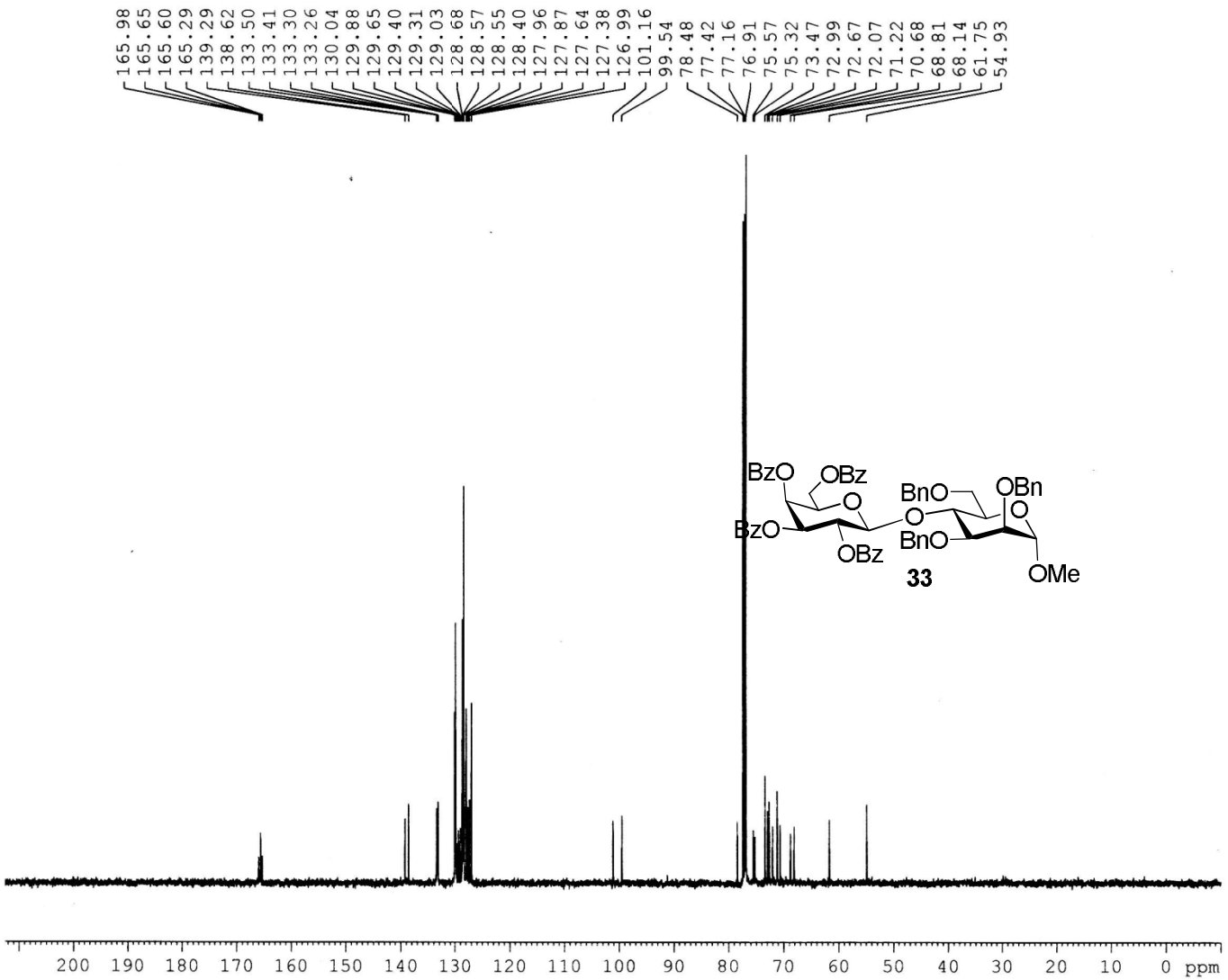
F2 - Processing parameters
SI 16384
SF 75.4677531 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 205.583 ppm
F1 15514.90 Hz
F2P -5.231 ppm
F2 -394.76 Hz
PPMCM 10.54070 ppm/cm
HZCM 795.48297 Hz/cm

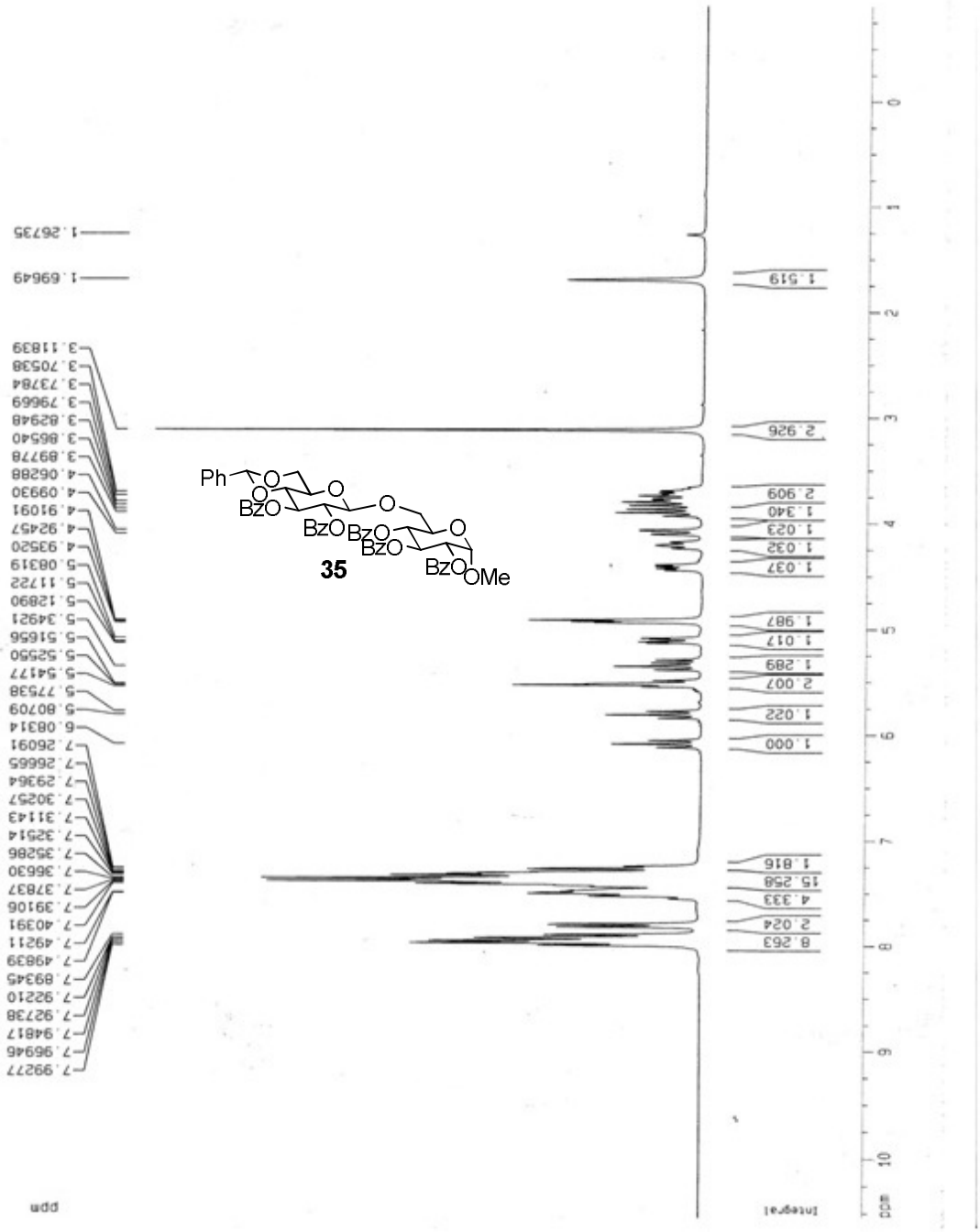

OMe
OBn
OBn
O
BnO
O
OAc
O
BnO
BnO
BnO
31
ppm
0
1
2
3
4
5
6
7
8
3.05
3.11
1.00
1.04
5.22
3.13
1.02
1.04
2.07
0.34
2.81
1.12
3.06
1.30
1.07
1.07
0.98
1.03
29.58
1.00
2.25
0.000
2.009
3.350
3.420
3.438
3.620
3.625
3.638
3.643
3.704
3.718
3.746
3.766
3.840
3.846
3.849
4.144
4.159
4.174
4.335
4.355
4.412
4.430
4.526
4.545
4.559
4.579
4.596
4.607
4.616
4.627
4.647
4.657
4.675
4.757
4.788
4.806
5.415
5.473
7.130
7.141
7.158
7.170
7.182
7.213
7.225
7.233
7.237
7.248
7.262
7.268

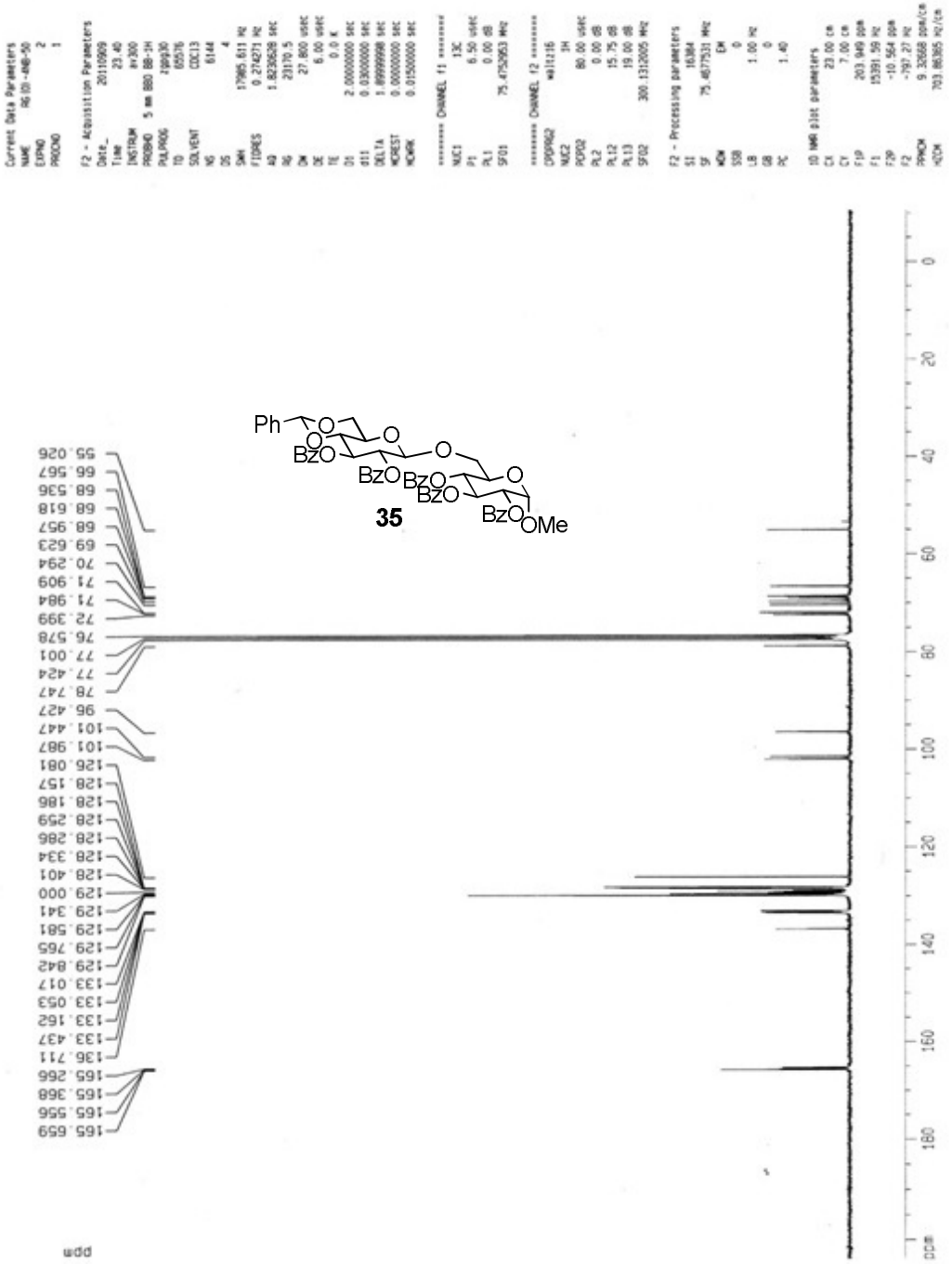

169.88
138.51
138.48
138.27
138.17
138.07
137.90
128.29
128.27
128.19
128.03
127.86
127.82
127.76
127.61
127.57
127.52
127.45
127.41
127.26
99.43
98.72
80.11
78.41
77.21
77.00
76.79
75.04
73.99
73.91
73.41
73.21
72.52
72.32
71.67
71.43
71.12
69.85
68.62
68.54
54.88
20.99
-0.03
BnO
OAc
BnO
BnO
OBn
OBn
O
31
O
BnO
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3.251
3.614
3.620
3.759
3.763
3.767
3.943
4.252
4.272
4.365
4.380
4.597
4.617
4.671
4.691
4.702
4.713
4.912
4.932
4.982
4.996
5.716
5.871
5.877
7.184
7.213
7.226
7.238
7.252
7.273
7.286
7.298
7.311
7.320
7.333
7.349
7.353
7.360
7.366
7.379
7.410
7.444
7.457
7.492
7.502
7.556
7.750
7.762
7.881
BzO
OBz
O
BzO
OBz
BnO
O
BnO
OBn
O
OMe
33
0 ppm
1
2
3
4
5
6
7
8
1.97
1.96
1.87
1.90
1.05
2.34
2.02
1.43
7.64
7.70
6.10
1.17
0.92
1.00
0.92
0.91
0.92
2.93
1.07
2.05
1.72
0.93
0.98
1.00
1.82
0.88
2.84



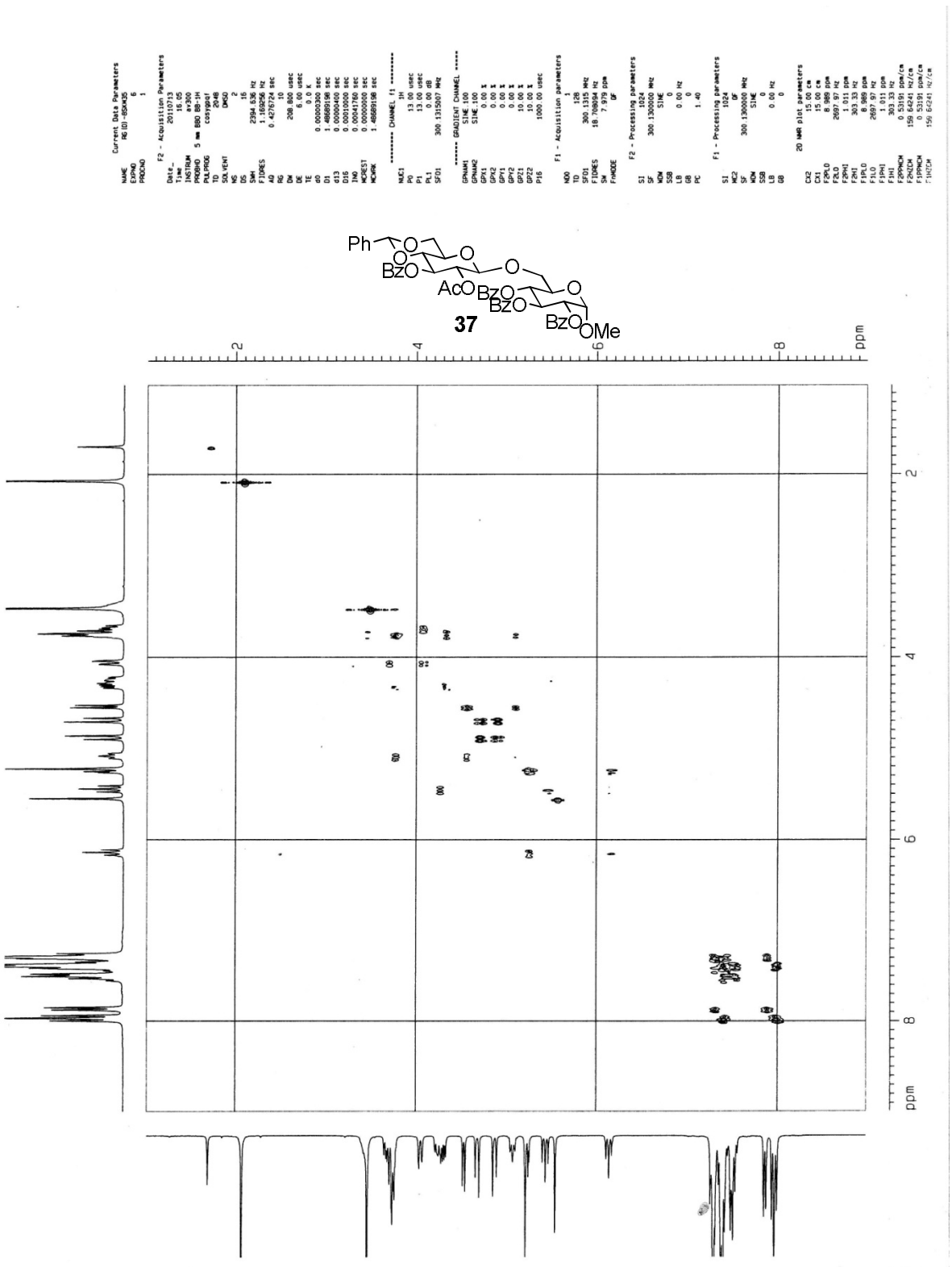
NAME	KM-543-13C
EXPNO	1
PROCNO	1
Date_	20110110
Time	15.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	32768
SOLVENT	CDC13
NS	1024
DS	4
SWH	36231.883 Hz
FIDRES	1.105709 Hz
AQ	0.4522484 sec
RG	32
DW	13.800 use
DE	6.50 use
TE	300.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 =======	
NUC1	13C
P1	9.88 use
PL1	0.50 dB
PL1W	82.16106415 W
SFO1	125.7703643 MHz
======== CHANNEL f2 =======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 use
PL2	1.00 dB
PL12	16.50 dB
PL13	20.00 dB
PL2W	15.50318813 W
PL12W	0.43693921 W
PL13W	0.19517358 W
SFO2	500.1320005 MHz
SI	16384
SF	125.7577718 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

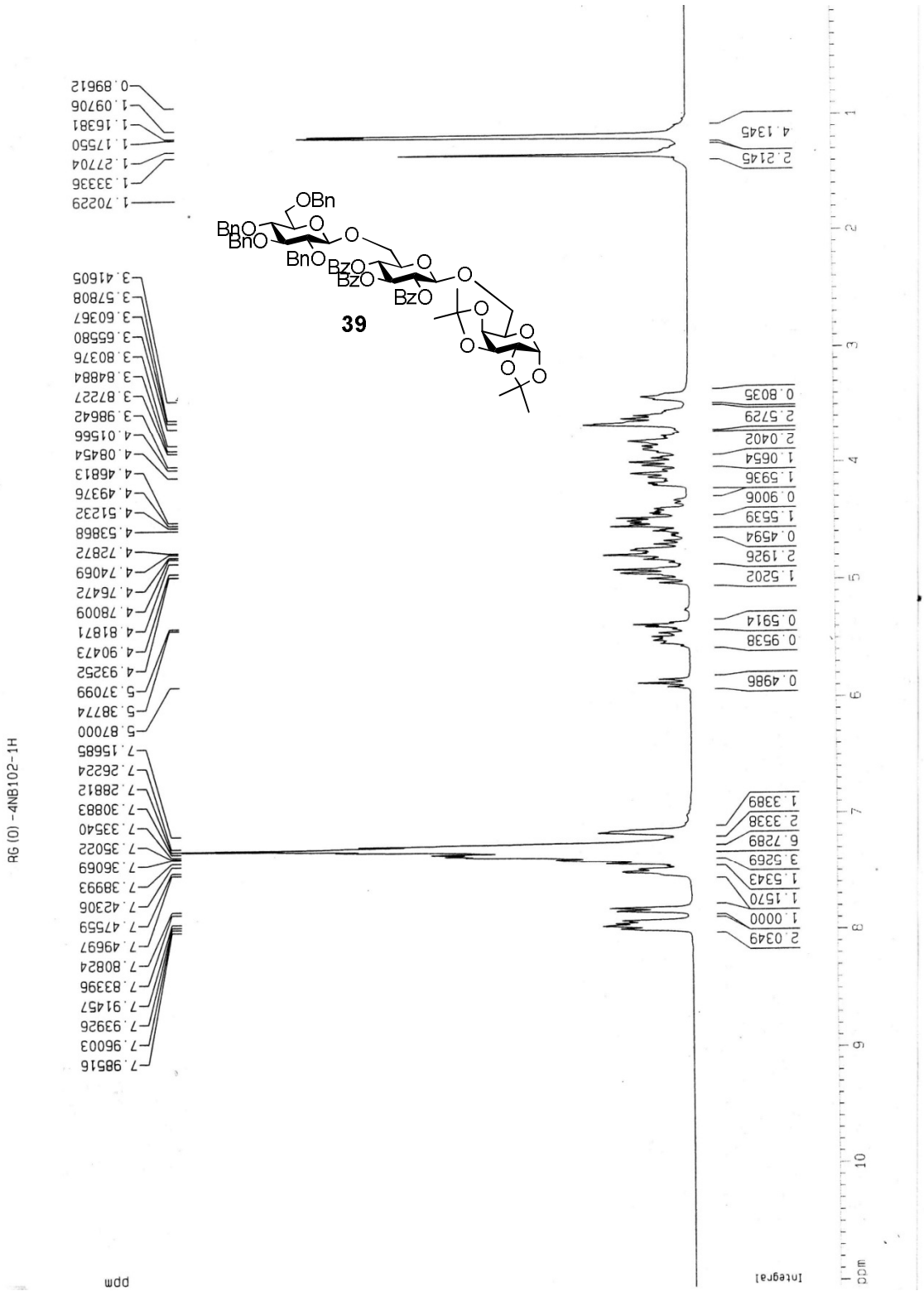

Ph
O
O
BzO
O
BzO
BzO
O
BzO
BzO
OMe
35
integral
ppm

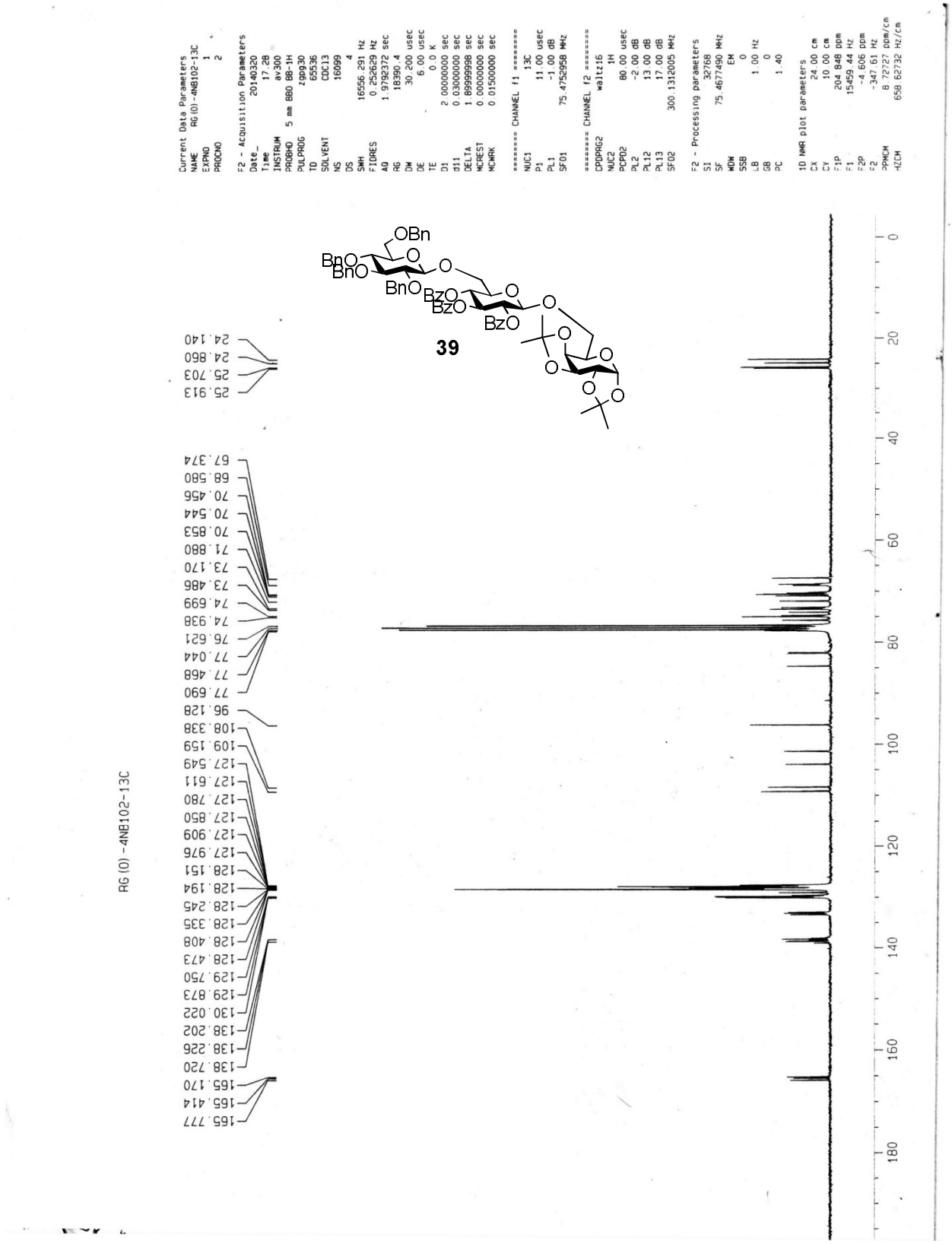

Ph
BzO
BzO
BzO
BzO
BzO
OMe
35
ppm

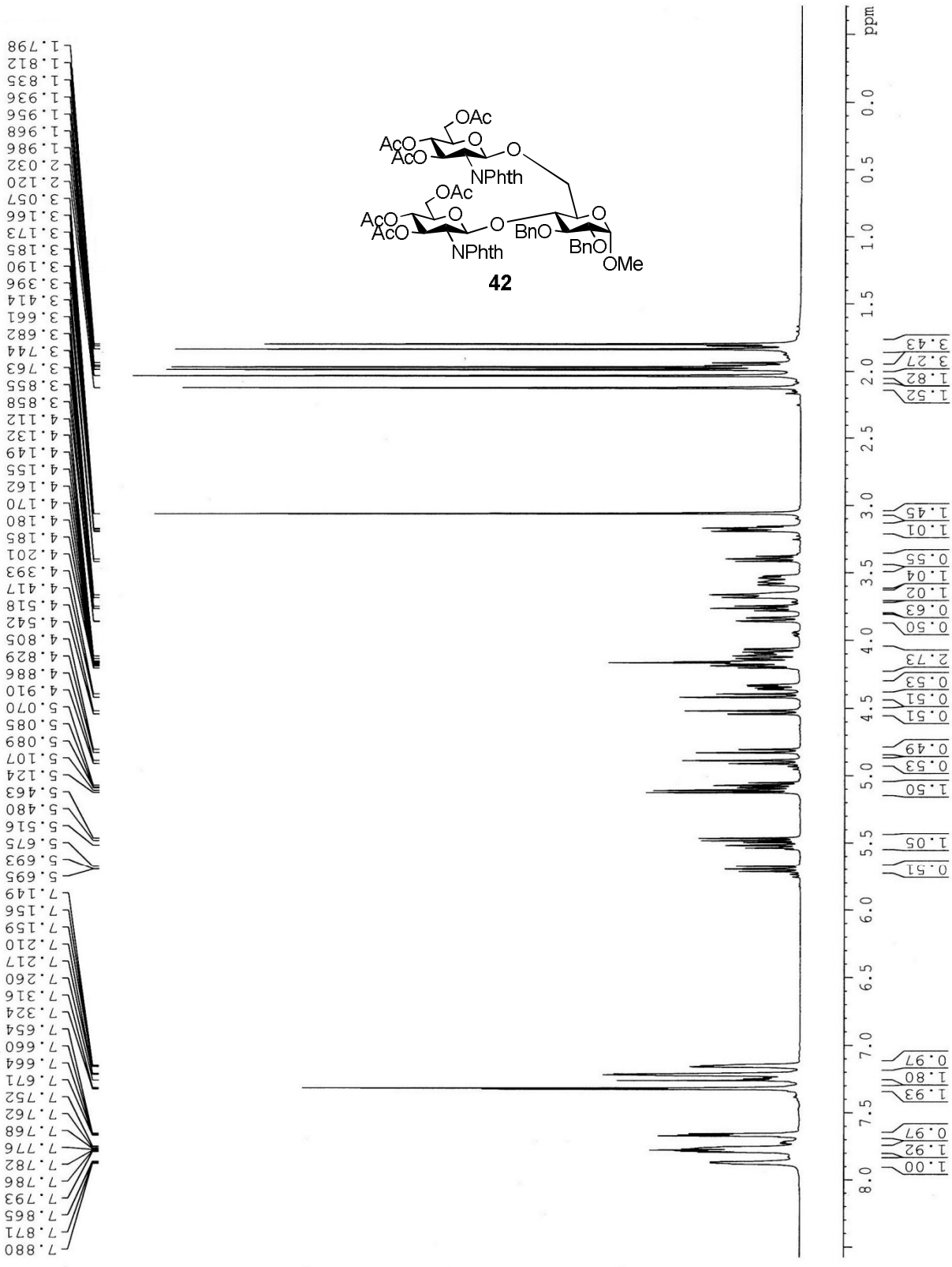
Ph
O
O
BzO
AcO
BzO
BzO
BzO
OMe
37
1.69519
2.07136
3.45896
3.70511
3.73292
3.73926
3.75399
3.76239
3.77116
4.04000
4.28503
4.52606
4.55249
4.66846
4.70871
4.86305
4.90328
5.22585
5.25554
5.41330
5.44618
5.47891
5.52994
6.14707
7.25917
7.28811
7.29793
7.30208
7.31418
7.37792
7.38410
7.39568
7.40150
7.41962
7.48565
7.51088
7.84933
7.85297
7.87725
7.94057
7.96772
7.97142
7.99674
ppm
0.5705
3.0321
3.7593
1.3889
2.7389
1.0102
2.0555
0.9990
1.0160
1.0171
1.0110
1.4282
0.6109
1.0188
1.0179
1.0000
7.0314
8.3536
4.1363
2.0160
4.0445
Integral
ppm

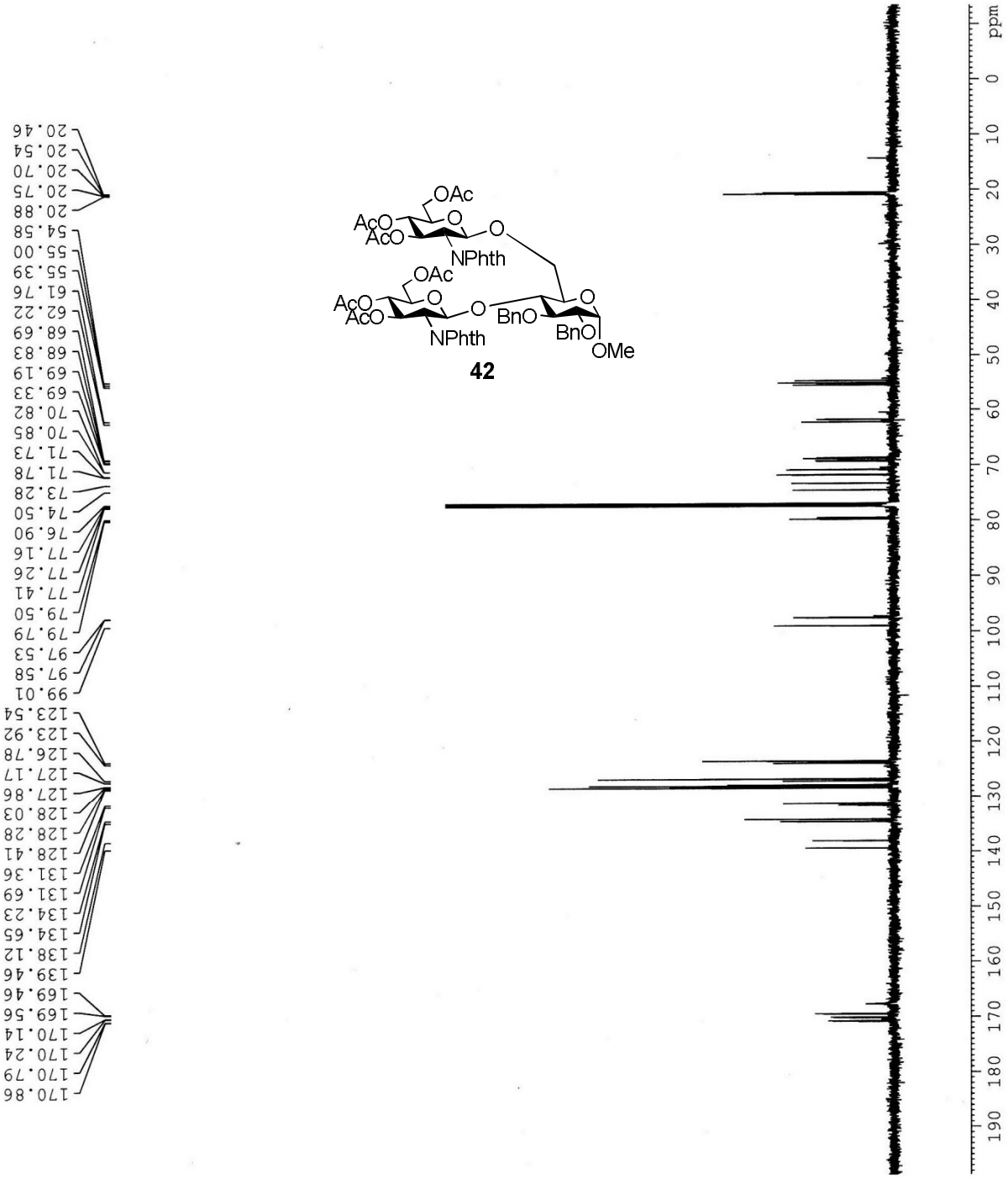
Current Data Parameters
NAME RG(0)-BSKM35
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110713
Time 16.44
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65576
SOLVENT DMSO
NS 666
DS 4
SWH 17985.611 Hz
FIDRES 0.274271 Hz
AQ 1.8230628 sec
RG 23170.5
DW 27.800 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.75 dB
PL13 19.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 16384
SF 75.4677531 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 23.00 cm
CY 7.00 cm
F1P 204.772 ppm
F1 15453.68 Hz
F2P -9.431 ppm
F2 -711.75 Hz
PPMCM 9.31318 ppm/cm
HZCM 702.84448 Hz/cm
Ph
BzO
AcO
BzO
BzO
BzO
OMe
37
20.879
55.430
66.237
68.349
68.534
69.406
70.494
72.031
72.624
74.100
76.593
77.016
77.439
78.367
81.391
96.740
101.203
101.773
125.965
127.621
127.796
128.230
128.257
128.375
128.429
128.869
128.995
129.030
129.613
129.820
129.887
133.032
133.310
133.451
137.119
138.166
165.294
165.703
165.774
169.378
ppm
0
20
40
60
80
100
120
140
160
180
ppm


Ph
BzO
AcO
BzO
BzO
BzO
OMe
37
ppm
ppm

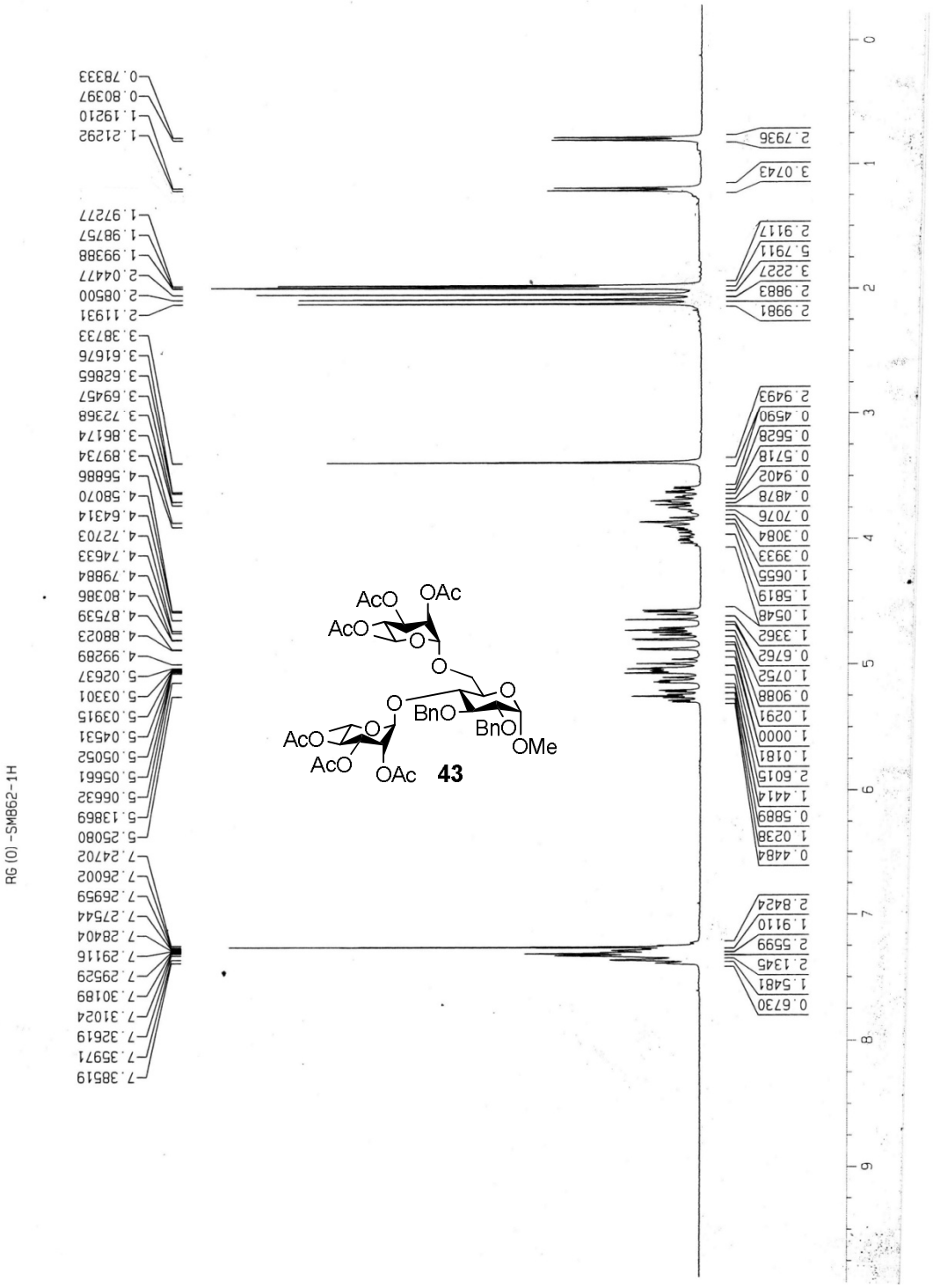

RG (D) -4NB102-1H
ppm
Integral
39
OBn
BnO
BnO
BnO
BzO
BzO
BzO

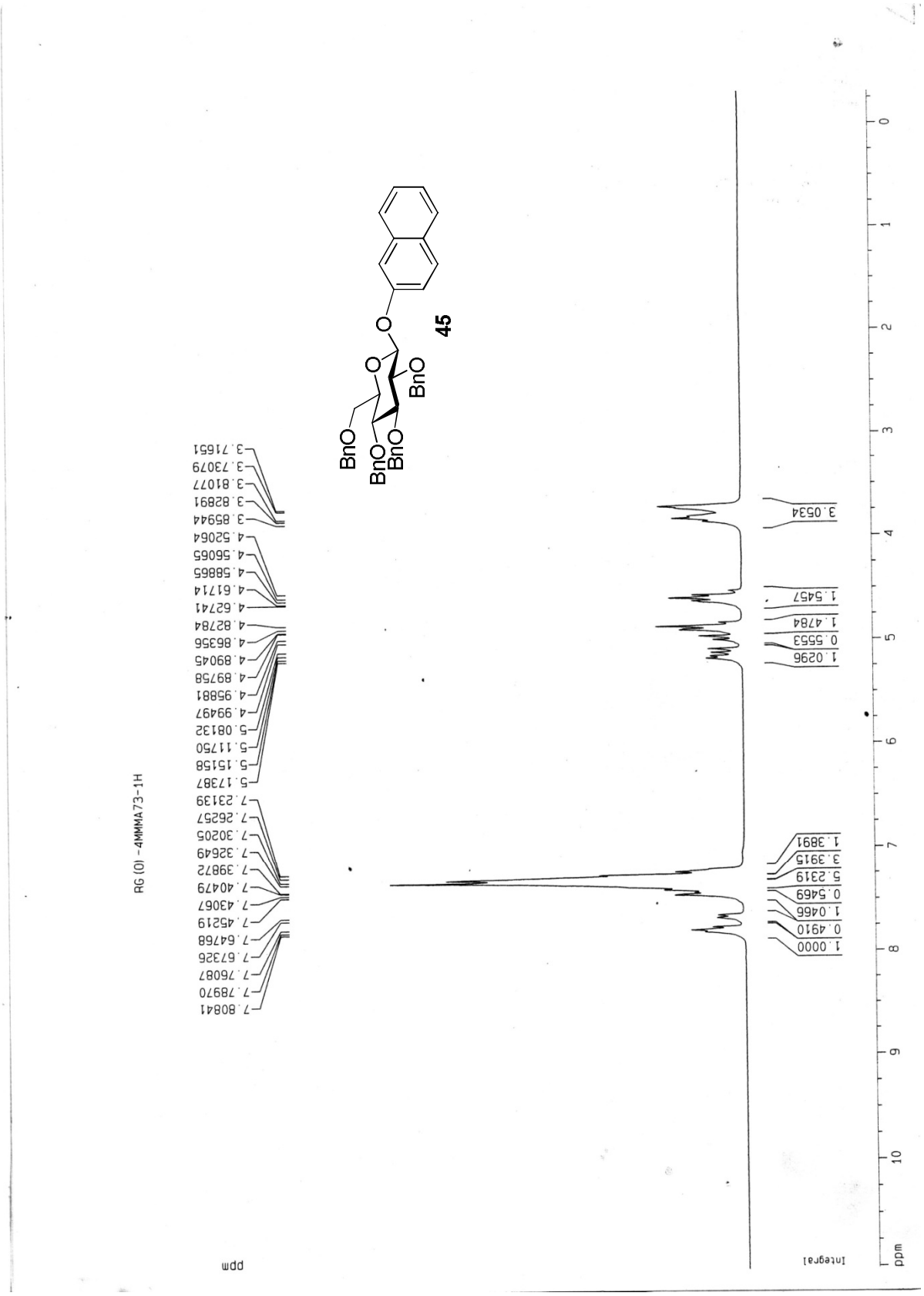

RG(0)-4NB102-13C
39
OBn
BnO
BnO
BnO
BzO
BzO
BzO
Current Data Parameters
NAME RG(0)-4NB102-13C
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20140320
Time 17.28
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16099
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 18390.4
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SF01 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 10.00 cm
F1P 204.848 ppm
F1 15459.44 Hz
F2P -4.606 ppm
F2 -347.61 Hz
PPMCM 8.72727 ppm/cm
HZCM 658.62732 Hz/cm
24.140
24.860
25.703
25.913
67.374
68.580
70.456
70.544
70.853
71.880
73.170
73.486
74.699
74.938
76.621
77.044
77.468
77.690
96.128
108.338
109.159
127.549
127.611
127.780
127.850
127.909
127.976
128.151
128.194
128.245
128.335
128.408
128.473
129.750
129.873
130.022
138.202
138.226
138.720
165.170
165.414
165.777
0
20
40
60
80
100
120
140
160
180


OAc
AcO
AcO
O
O
NPhth
OAc
AcO
AcO
O
O
NPhth
BnO
O
BnO
OMe
42
ppm

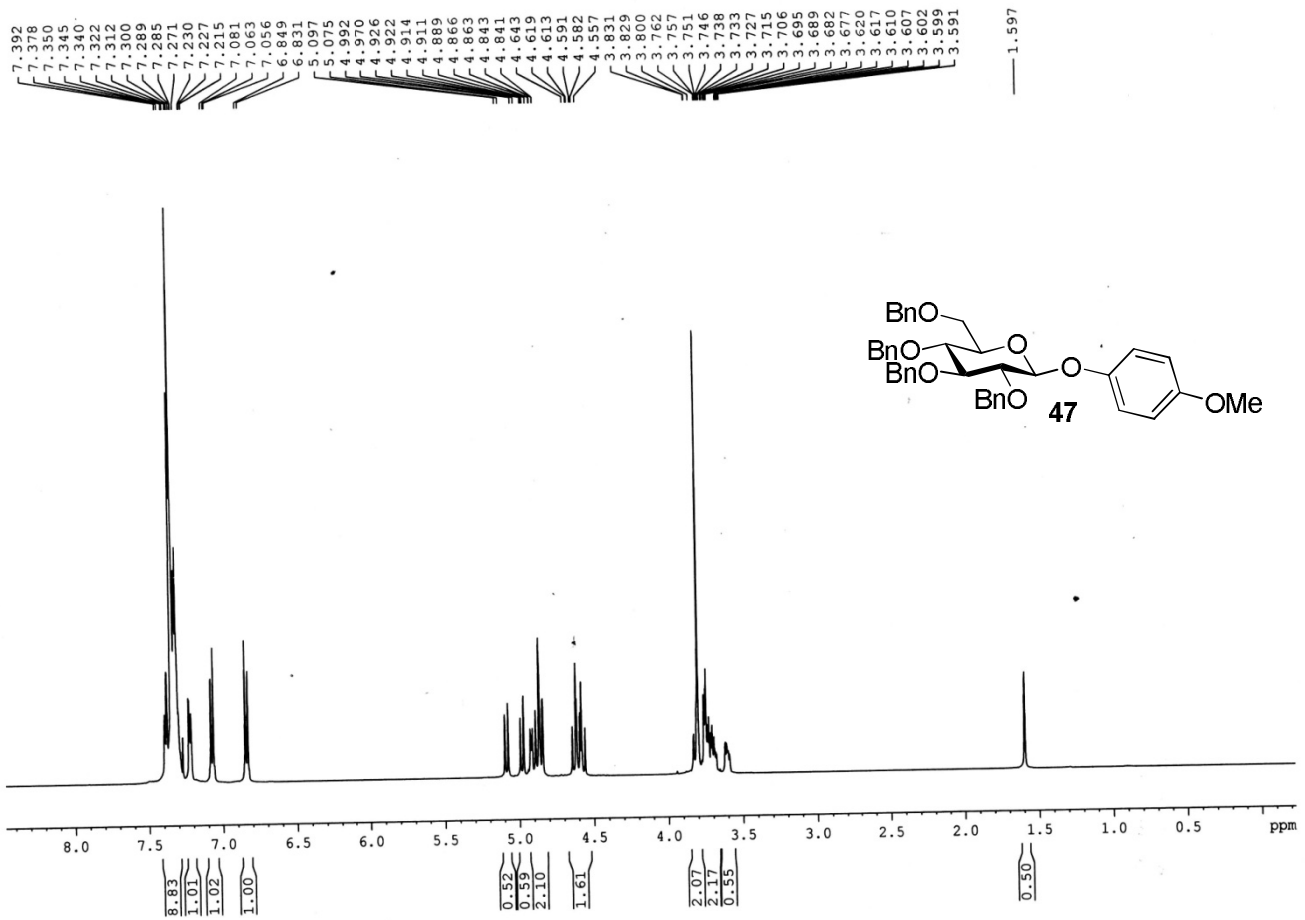

20.46
20.54
20.70
20.75
20.88
54.58
55.00
55.39
61.76
62.22
68.69
68.83
69.19
69.33
70.82
70.85
71.73
71.78
73.28
74.50
76.90
77.16
77.26
77.41
79.50
79.79
97.53
97.58
99.01
123.54
123.92
126.78
127.17
127.86
128.03
128.28
128.41
131.36
131.69
134.23
134.65
138.12
139.46
169.46
169.56
170.14
170.24
170.79
170.86
OAc
AcO
AcO
O
NPhth
BnO
BnO
OMe
ppm
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

42


RG (0) -SM862-1H
AcO
OAc
AcO
O
O
O
BnO
O
BnO
OMe
AcO
O
AcO
OAc
43


45
BnO
BnO
BnO
BnO
RG (0) - 4MMMA73-1H
ppm
Integral
1.0000
0.4910
1.0466
0.5469
5.2319
3.3915
1.3891
1.0296
0.5553
1.4784
1.5457
3.0534

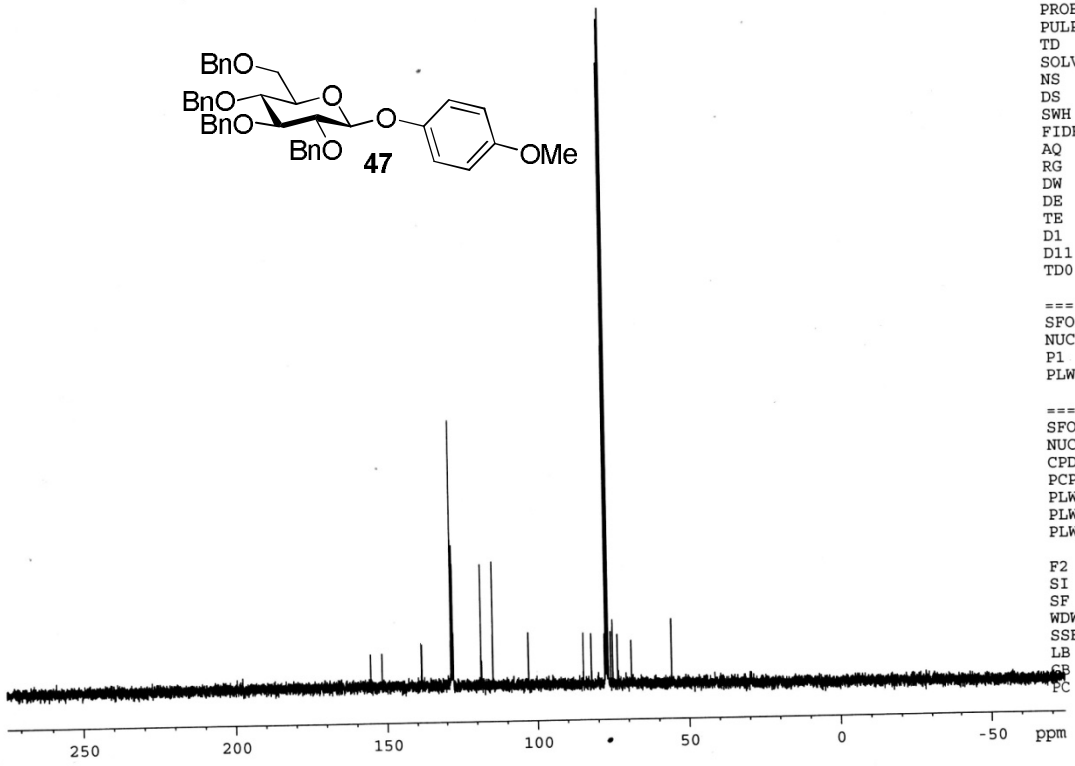
SA.M73-1H(SKD)


7.392
7.378
7.350
7.345
7.340
7.322
7.312
7.300
7.289
7.285
7.271
7.230
7.227
7.215
7.081
7.063
7.056
6.849
6.831
5.097
5.075
4.992
4.970
4.926
4.922
4.914
4.911
4.889
4.866
4.863
4.843
4.841
4.643
4.619
4.613
4.591
4.582
4.557
3.831
3.829
3.800
3.762
3.757
3.751
3.746
3.738
3.733
3.727
3.715
3.706
3.695
3.689
3.682
3.677
3.620
3.617
3.610
3.607
3.602
3.599
3.591
1.597
BnO
BnO
BnO
BnO
O
O
OMe
47
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
ppm
8.83
1.01
1.02
1.00
0.52
0.59
2.10
1.61
2.07
2.17
0.55
0.50

SA-M-217-13C-DK

155.44
151.68
138.68
138.44
138.33
138.19
128.55
128.47
128.36
128.17
128.11
128.02
127.95
127.89
127.86
127.79
127.71
118.59
114.70
102.96
84.85
82.24
77.92
77.58
77.36
77.16
76.73
75.90
75.22
75.16
73.63
69.07
55.79

47



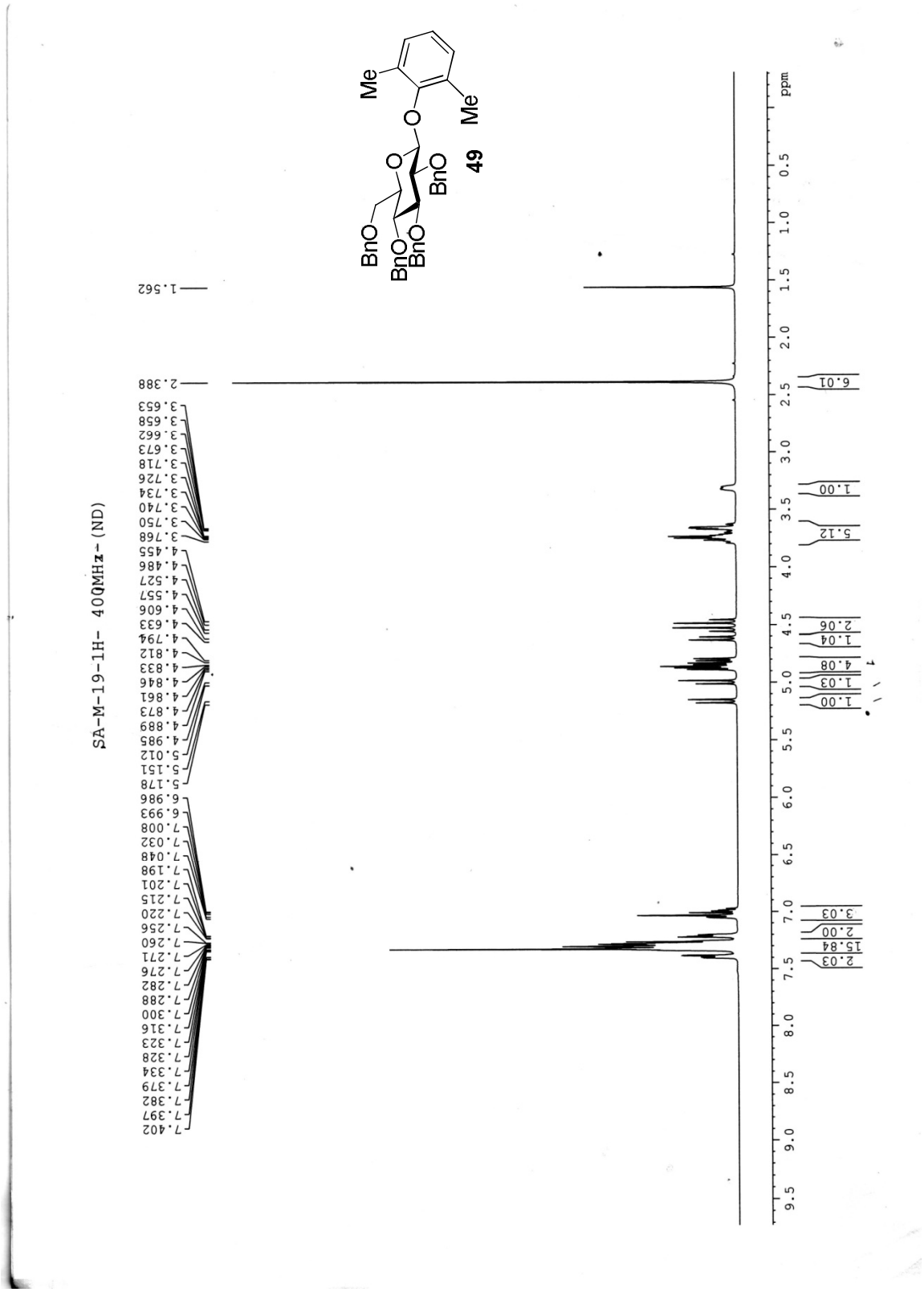
Current Data Parameters
NAME SA-M-217-13C
EXPNO 1
PROCNO 1

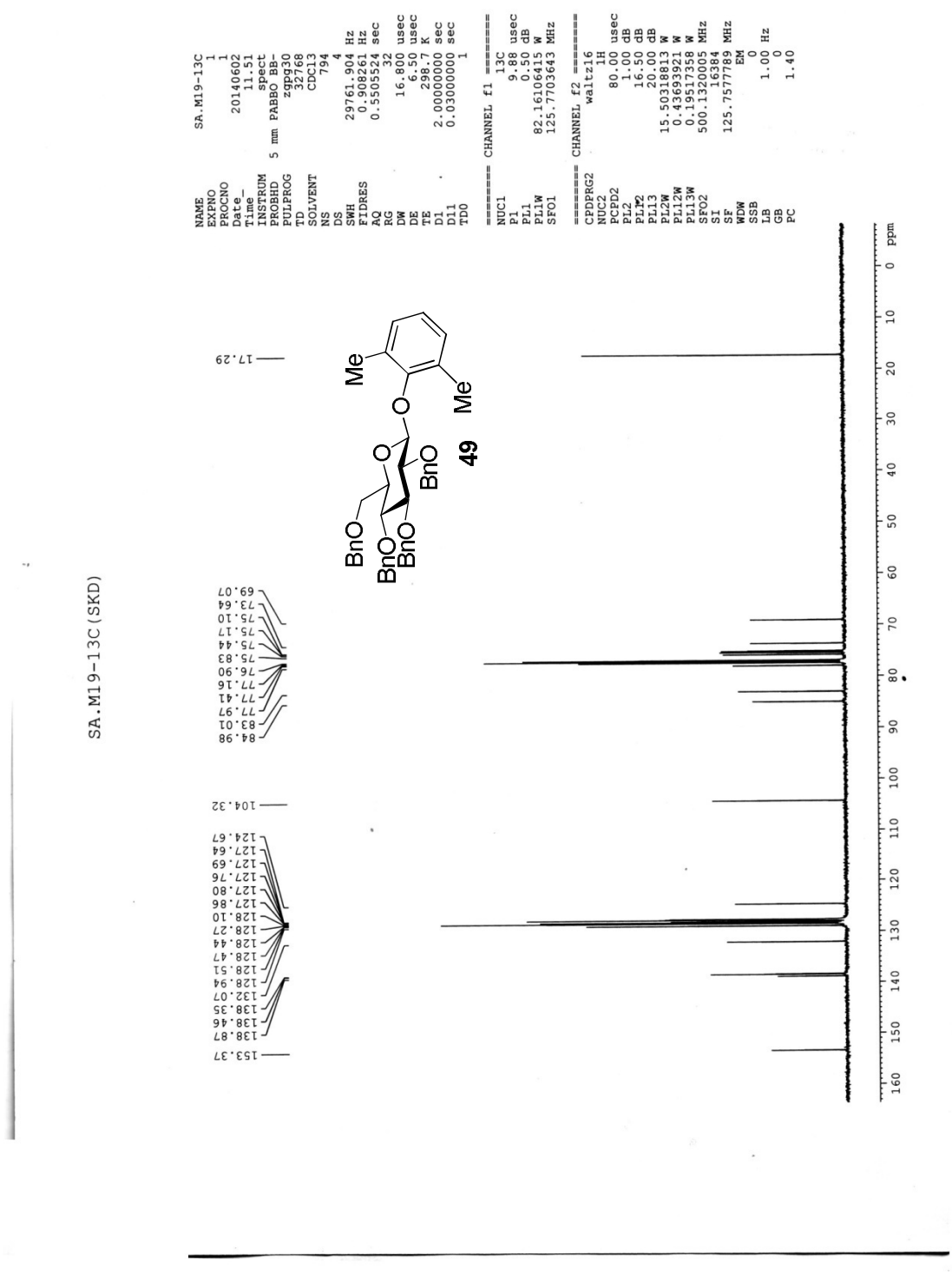
F2 - Acquisition Parameters
Date_ 20130509
Time 19.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1665
DS 4
SWH 26315.789 Hz
FIDRES 0.803094 Hz
AQ 0.6225920 sec
RG 210.78
DW 19.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

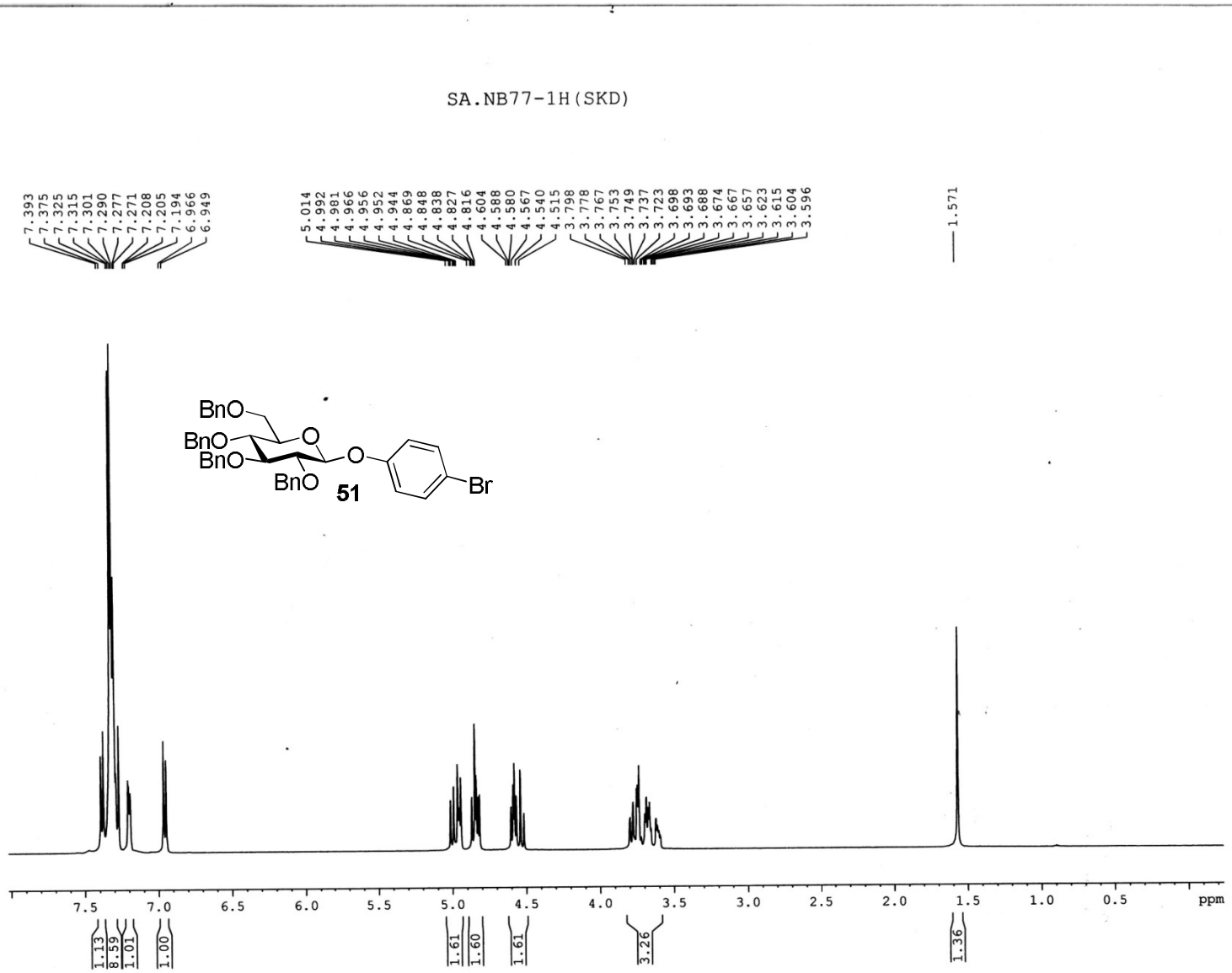
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.25 usec
PLW1 34.00000000 W

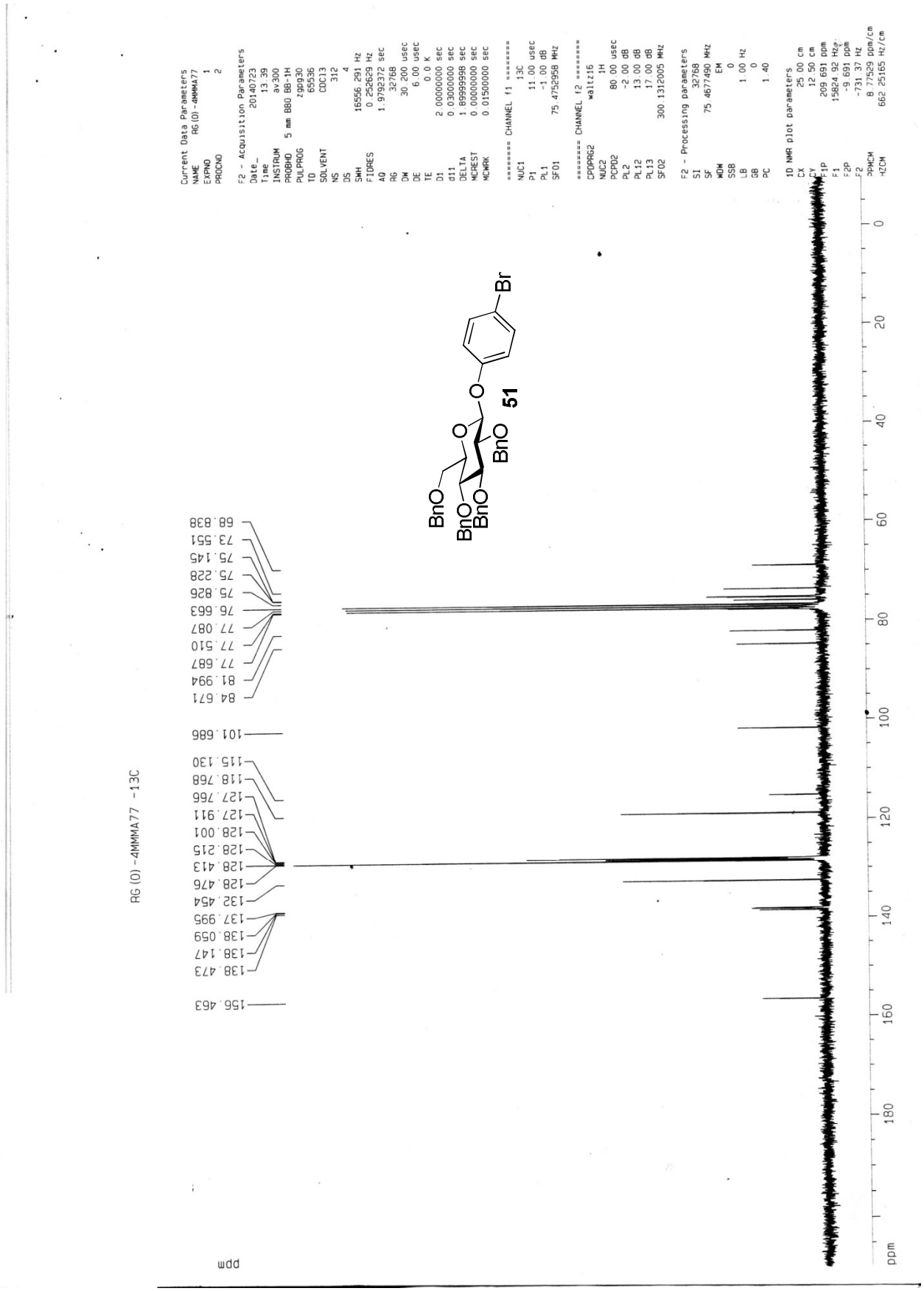
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 6.99840021 W
PLW12 0.17545000 W
PLW13 0.14211001 W

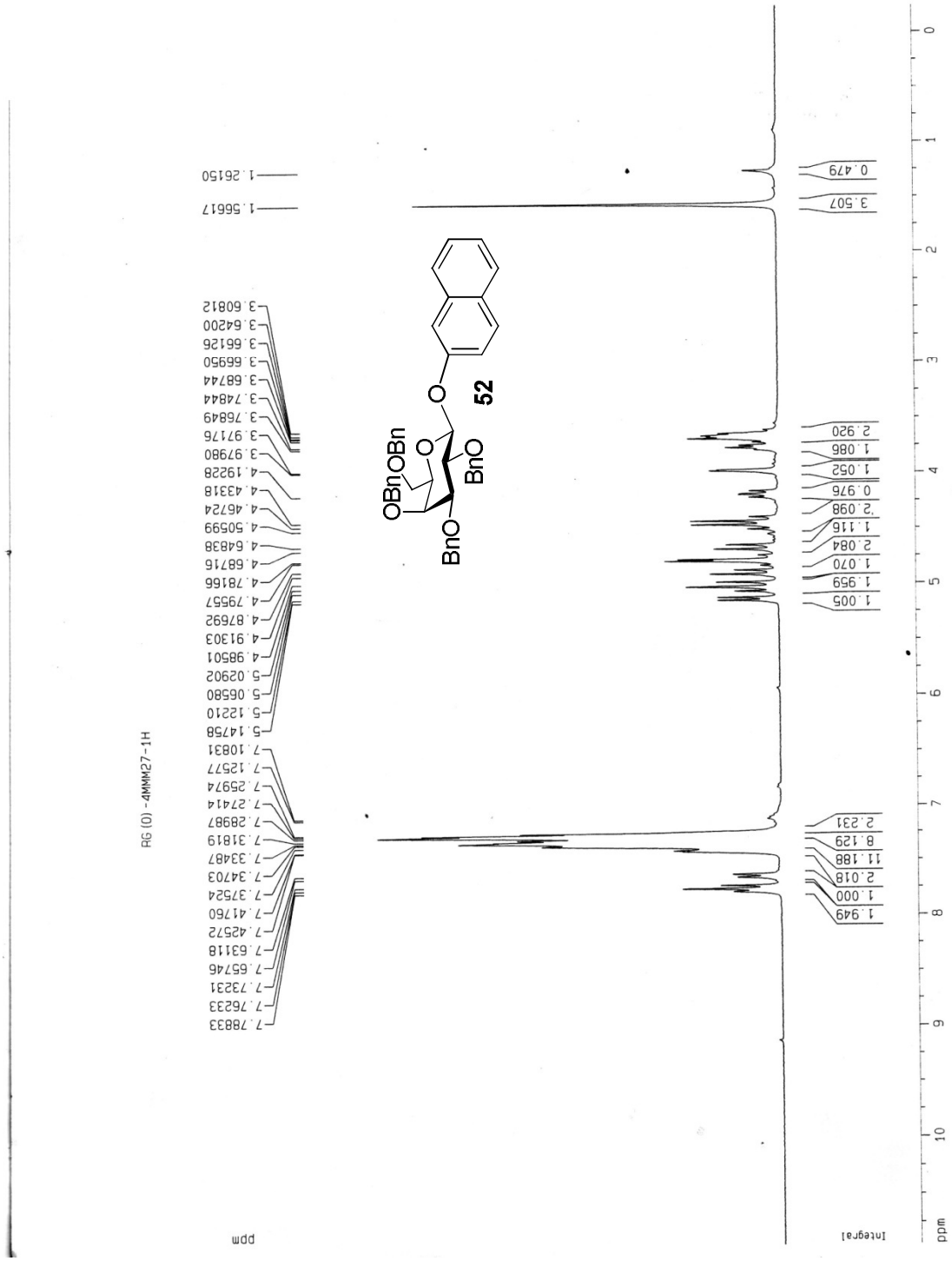
F2 - Processing parameters
SI 32768
SF 75.4677383 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


SA-M-19-1H- 400MHz-(ND)
Me
Me
BnO
BnO
BnO
BnO
49
ppm


SA.M19-13C (SKD)
NAME SA.M19-13C
EXPNO 1
PROCNO 1
Date_ 20140602
Time 11.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 794
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1 13C
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
CHANNEL f2 1H
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577789 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
17.29
69.07
73.64
75.10
75.17
75.44
75.83
76.90
77.16
77.41
77.97
83.01
84.98
104.32
124.67
127.64
127.69
127.76
127.80
127.86
128.10
128.27
128.44
128.47
128.51
128.94
132.07
138.35
138.46
138.87
153.37
Me
Me
O
O
BnO
BnO
BnO
BnO
49
ppm


SA.NB77-1H(SKD)
7.393
7.375
7.325
7.315
7.301
7.290
7.277
7.271
7.208
7.205
7.194
6.966
6.949
5.014
4.992
4.981
4.966
4.956
4.952
4.944
4.869
4.848
4.838
4.827
4.816
4.604
4.588
4.580
4.567
4.540
4.515
3.798
3.778
3.767
3.753
3.749
3.737
3.723
3.698
3.693
3.688
3.674
3.667
3.657
3.623
3.615
3.604
3.596
1.571
BnO
BnO
BnO
BnO
O
O
Br
51
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
ppm
1.13
8.59
1.01
1.00
1.61
1.60
1.61
3.26
1.36


RG (0) -4MMMA77 -13C
ppm
84.671
81.994
77.687
77.510
77.087
76.663
75.826
75.228
75.145
73.551
68.838
101.686
115.130
118.768
127.766
127.911
128.001
128.215
128.413
128.476
132.454
137.995
138.059
138.147
138.473
156.463
BnO
BnO
BnO
BnO
Br
51
Current Data Parameters
NAME RG(0)-4MMMA77
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20140723
Time 13.39
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 312
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 32768
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 25.00 cm
CY 12.50 cm
F1P 209.691 ppm
F1 15824.92 Hz
F2P -9.691 ppm
F2 -731.37 Hz
PPMCM 8.77529 ppm/cm
HZCM 662.25165 Hz/cm
ppm


RG (0) -4MM27-1H
ppm
Integral
52
OBnOBn
BnO
BnO
7.78833
7.76233
7.73231
7.65746
7.63118
7.42572
7.41760
7.37524
7.34703
7.33487
7.31819
7.28987
7.27414
7.25974
7.12577
7.10831
5.14758
5.12210
5.06580
5.02902
4.98501
4.91303
4.87692
4.79557
4.78166
4.68715
4.64838
4.50599
4.46724
4.43318
4.19228
3.97980
3.97176
3.76849
3.74844
3.68744
3.66950
3.66126
3.64200
3.60812
1.56617
1.26150
0.479
3.507
2.920
1.086
1.052
0.976
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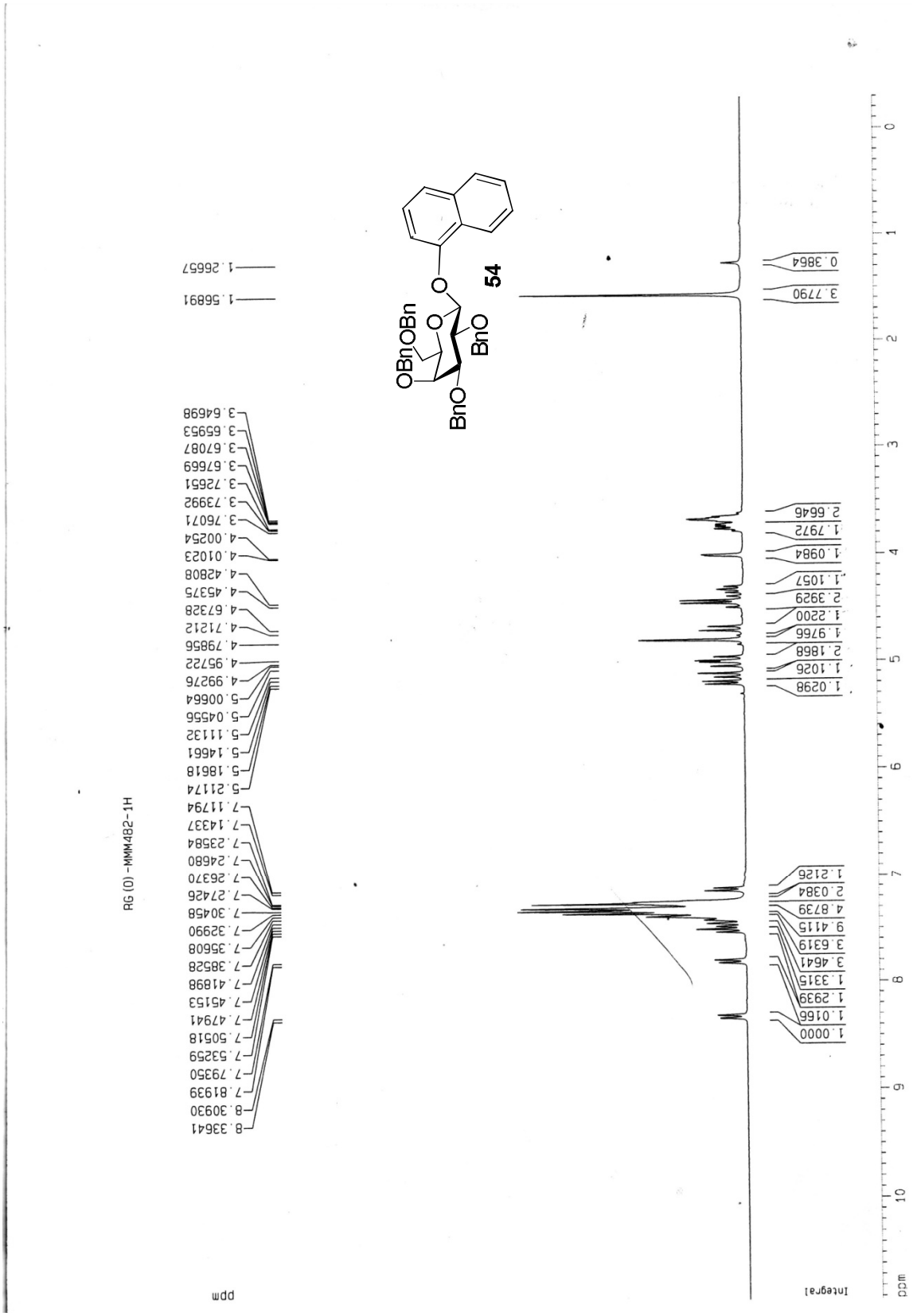
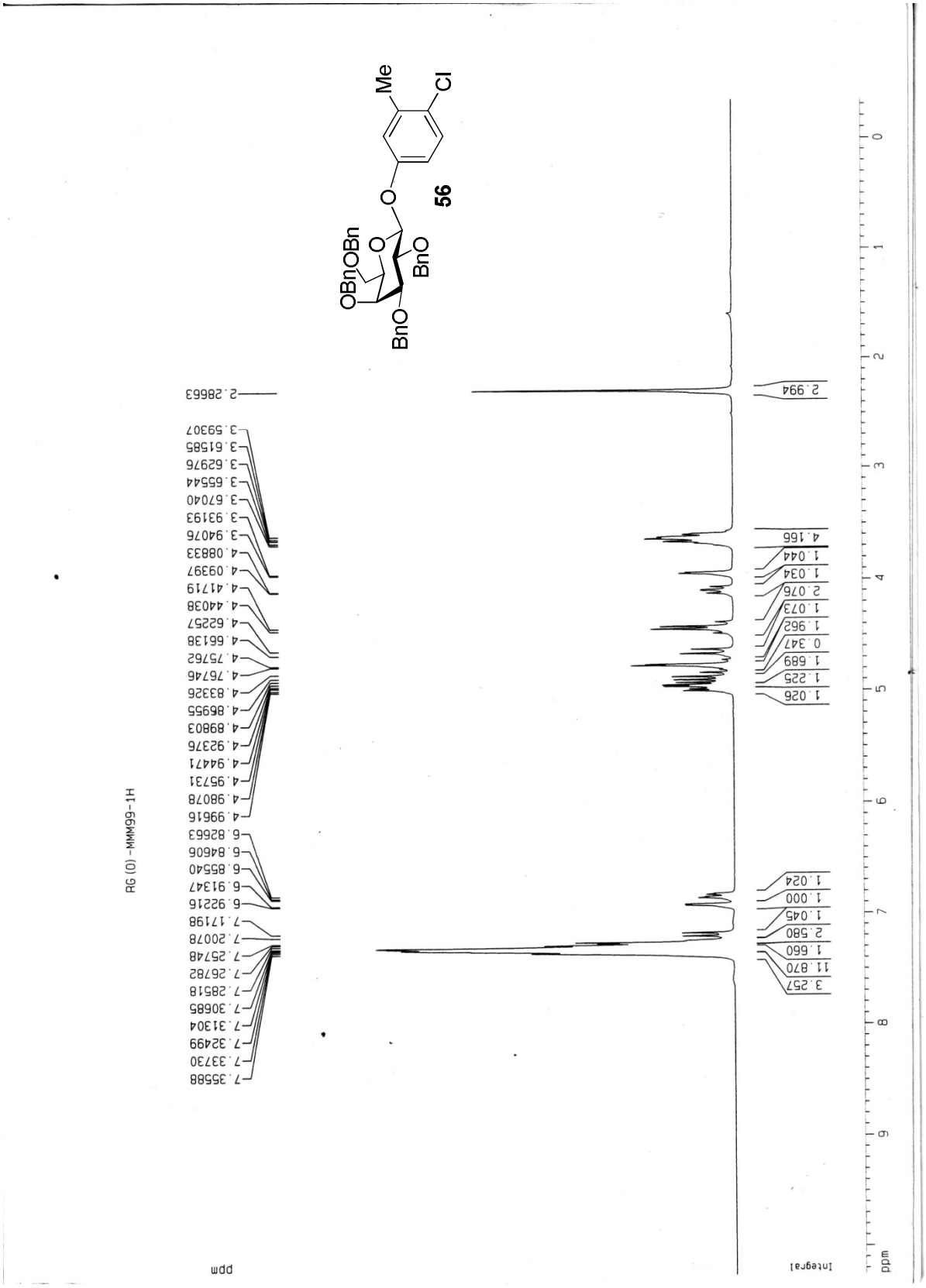
1.116
2.084
1.070
1.959
1.005
2.231
8.129
11.188
2.018
1.000
1.949


RG(D)-MMM482-1H
ppm
Integral
OBnOBn
BnO
BnO
54


Me
Cl
O
OBn
O
BnO
BnO
56
RG (0) -MMM99-1H
ppm
Integral
2.99
4.166
1.044
1.034
2.076
1.073
1.962
0.347
1.689
1.225
1.026
3.257
11.870
1.660
2.580
1.045
1.000
1.024
2.28663
3.59307
3.61585
3.62976
3.65544
3.67040
3.93193
3.94076
4.08833
4.09397
4.41719
4.44038
4.62257
4.66138
4.75762
4.76746
4.83326
4.86955
4.89803
4.92376
4.94471
4.95731
4.98078
4.99616
6.82663
6.84606
6.85540
6.91347
6.92216
7.17198
7.20078
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7.26782
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7.30685
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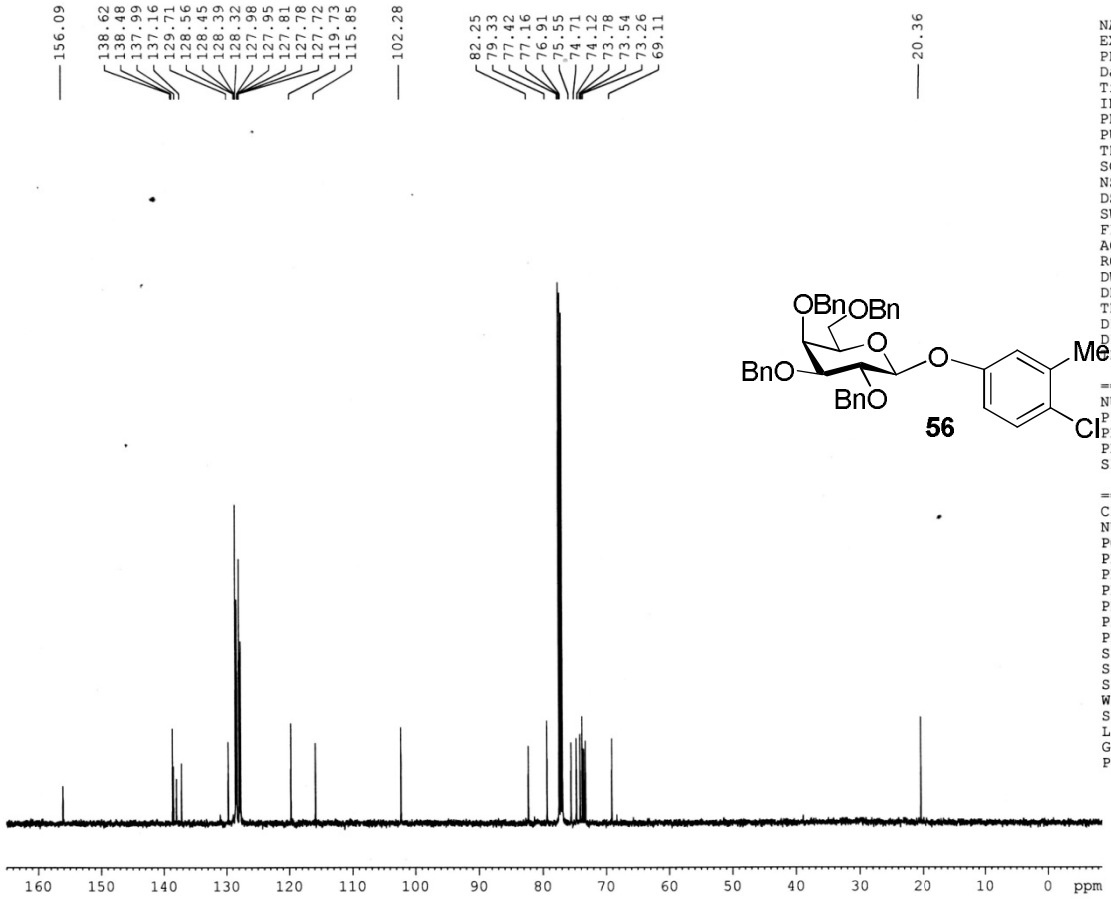
7.35588

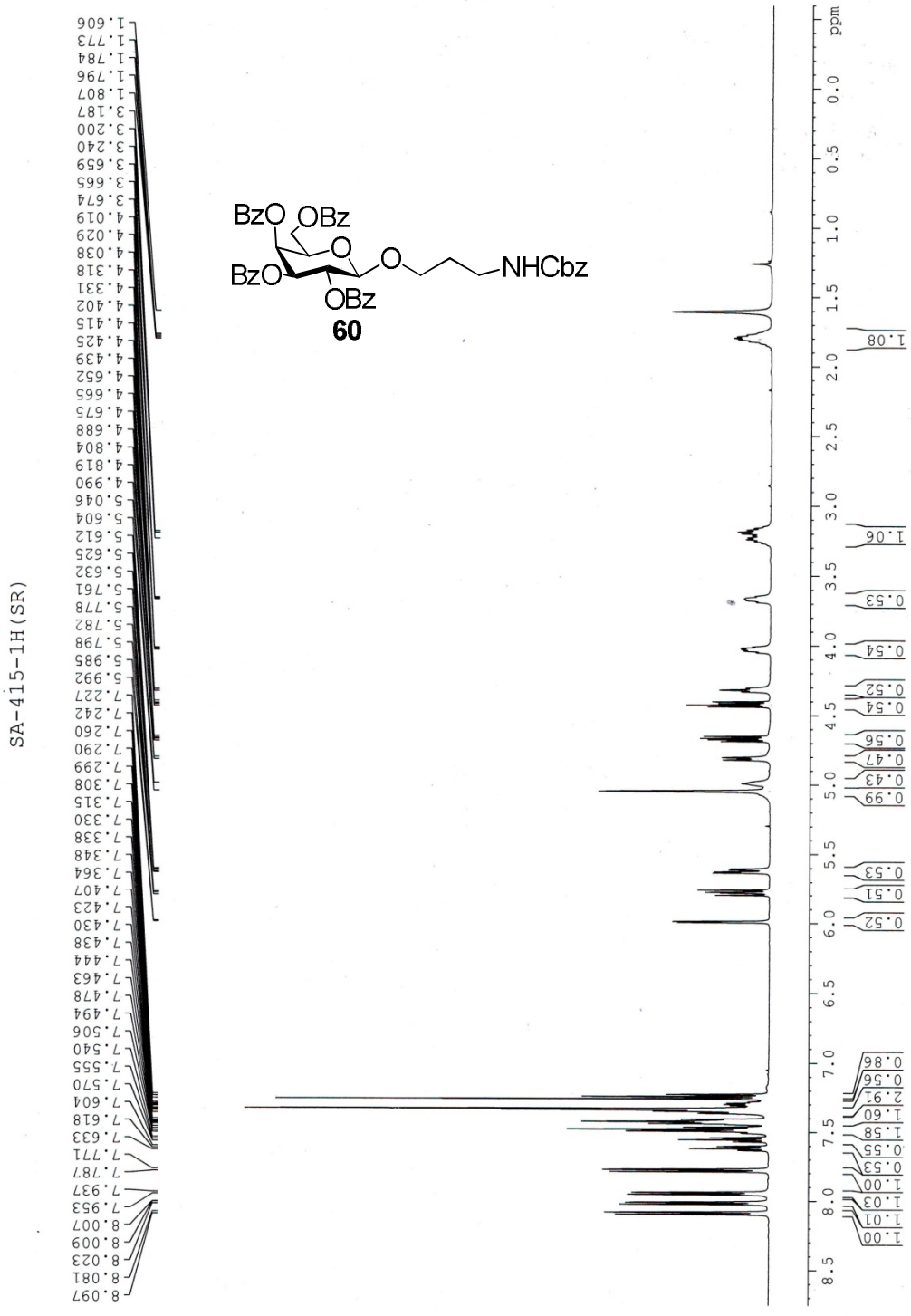
KBA.SJGO-13C(SKD)

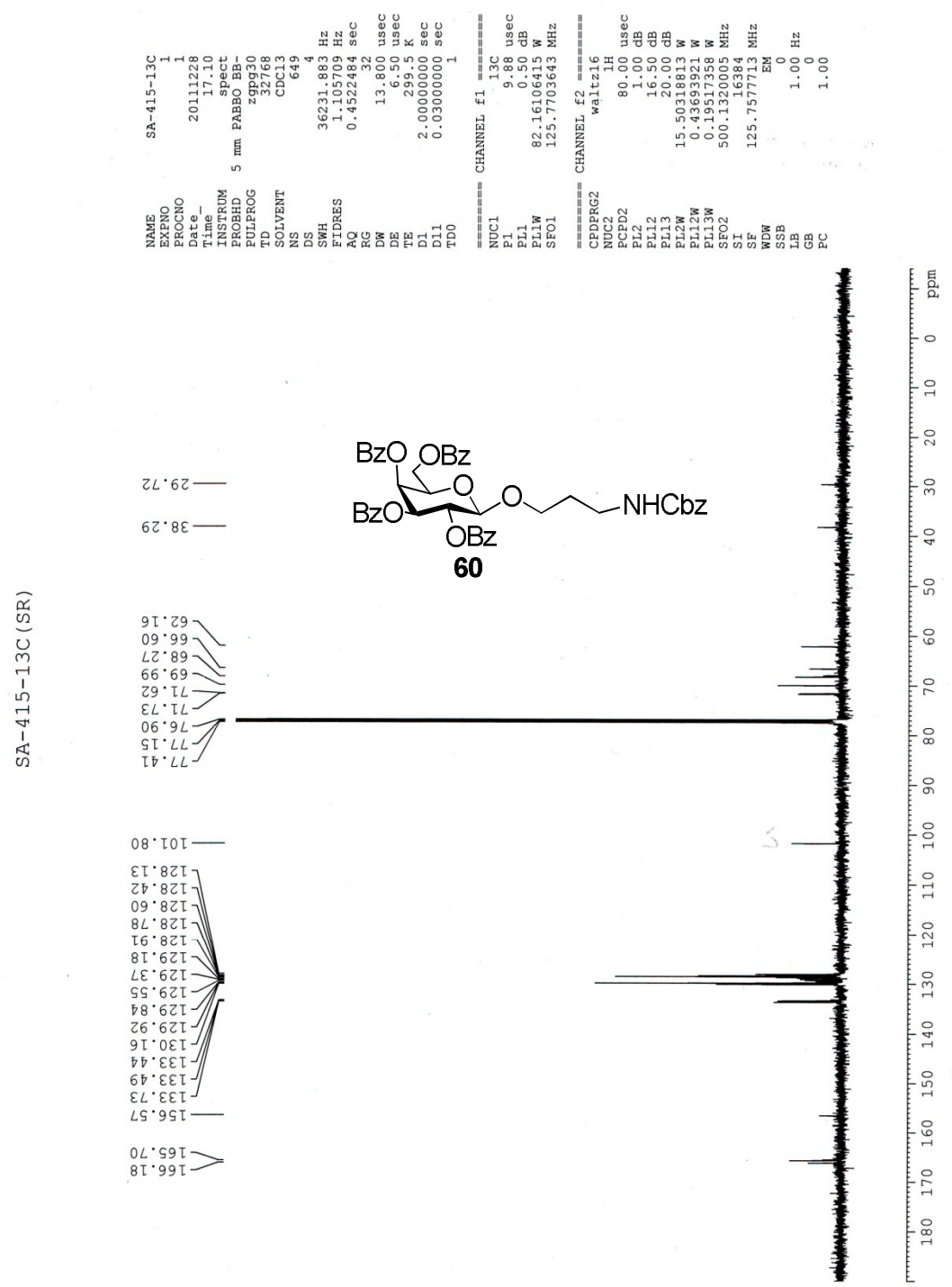


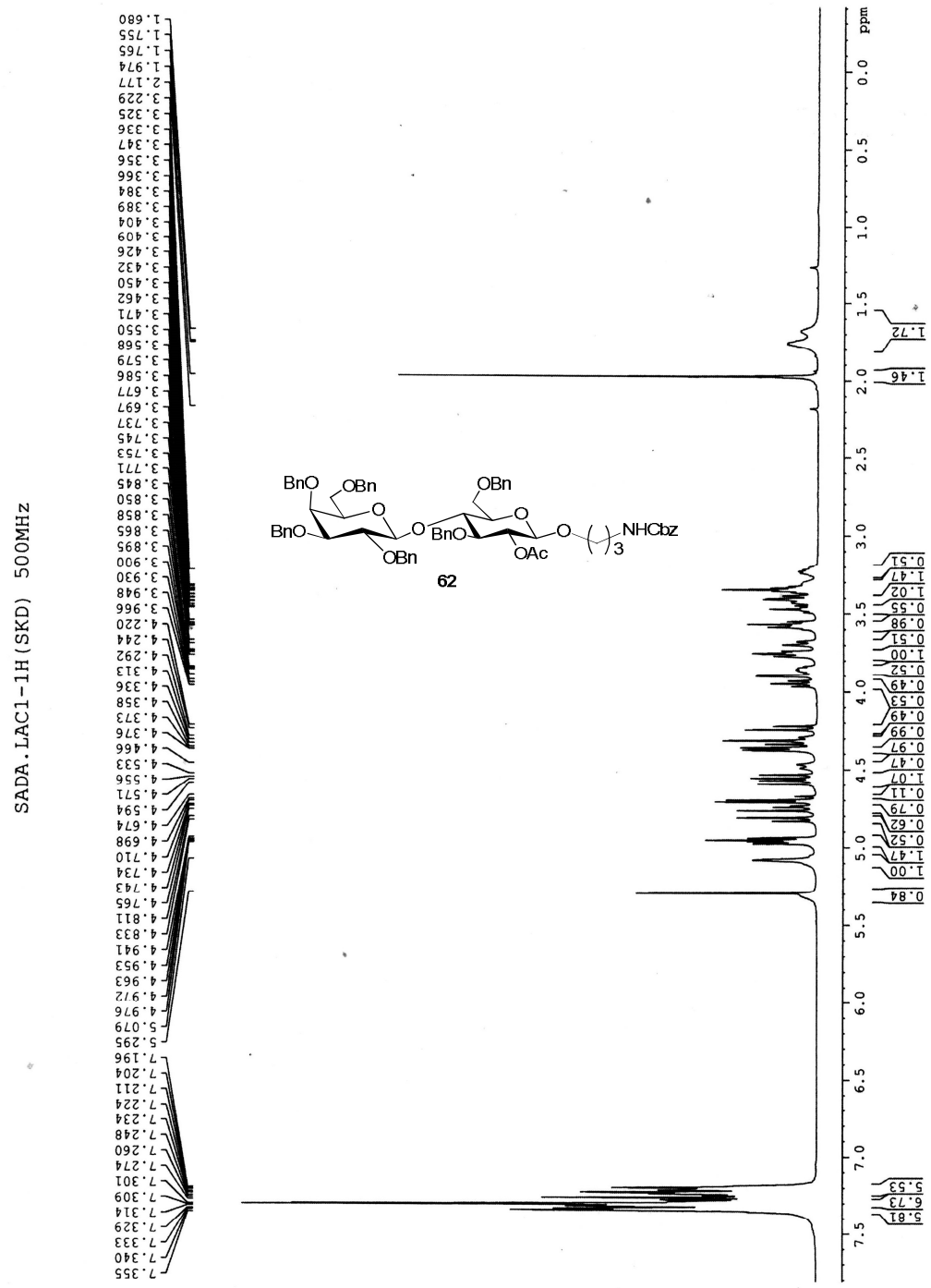
56

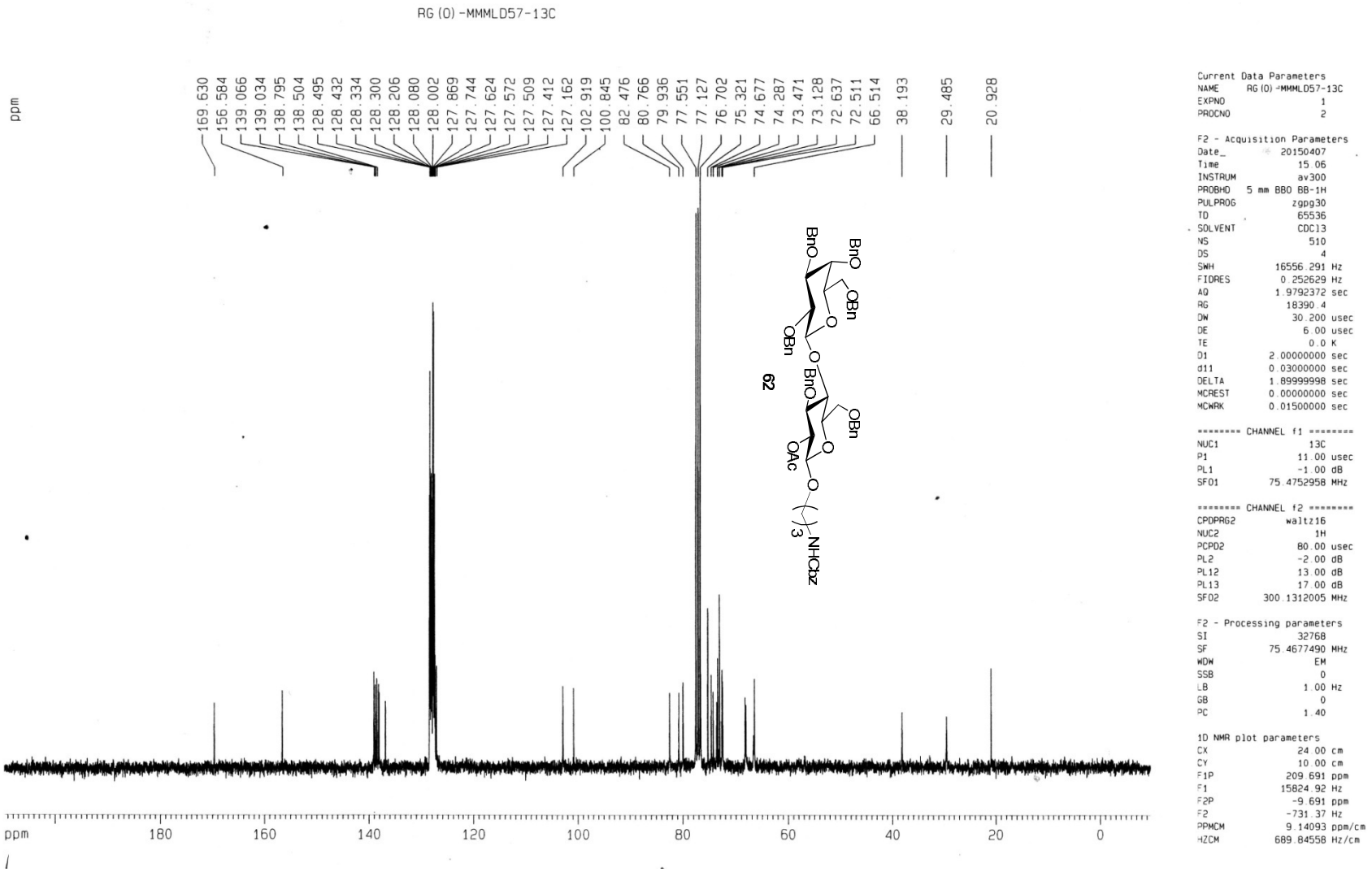
NAME	KBA.SJGO-13C
EXPNO	1
PROCNO	1
Date_	20130905
Time	14.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	989
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	0.5505524 sec
RG	32
DW	16.800 usec
DE	6.50 usec
TE	299.2 K
D1	2.00000000 sec
D11	0.03000000 sec
D0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.88 usec
PL1	0.50 dB
PL1W	82.16106415 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.50 dB
PL13	20.00 dB
PL2W	15.50318813 W
PL12W	0.43693921 W
PL13W	0.19517358 W
SFO2	500.1320005 MHz
SI	16384
SF	125.7577735 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

RG (o) -MMM-4-84
ppm
Integral
Me
Me
O
OBn
OBn
O
BnO
BnO
57
7.38944
7.38470
7.36231
7.35634
7.34449
7.33568
7.32670
7.31272
7.30133
7.29549
7.28879
7.27741
7.26213
7.19253
7.18538
6.99927
6.98011
5.12501
5.08872
5.02735
4.98825
4.91700
4.88072
4.78841
4.76705
4.73974
4.66250
4.62338
4.34874
3.93419
3.92580
3.63056
3.62351
3.61143
3.60105
3.50594
3.45261
3.41117
2.35515
3.2259
1.0655
1.0912
0.5305
0.5387
1.0524
0.5511
0.3652
1.2590
0.5530
0.5465
0.5468
1.6065
1.0000
0.5515
3.8749
3.2733
1.7305


SA-415-1H(SR)
BzO
OBz
O
BzO
O
NHCbz
OBz
60
ppm


SA-415-13C (SR)
NAME SA-415-13C
EXPNO 1
PROCNO 1
Date_ 20111228
Time_ 17.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 649
DS 4
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.4522484 sec
RG 32
DW 13.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577713 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
BzO
OBz
O
BzO
OBz
O
NHCbz
60
29.72
38.29
62.16
66.60
68.27
69.99
71.62
71.73
76.90
77.15
77.41
101.80
128.13
128.42
128.60
128.78
128.91
129.18
129.37
129.55
129.84
129.92
130.16
133.44
133.49
133.73
156.57
165.70
166.18
ppm


SADA.LAC1-1H(SKD) 500MHz
BnO
OBn
O
BnO
OBn
O
BnO
OBn
O
OAc
O
NHCbz
3
62
ppm



Current Data Parameters

NAME	RG (0) -MMMLD57-13C
EXPNO	1
PROCNO	2

F2 - Acquisition Parameters

Date_	20150407
Time	15.06
INSTRUM	av300
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	510
DS	4
SWH	16556.291 Hz
FIDRES	0.252629 Hz
AQ	1.9792372 sec
RG	18390.4
DW	30.200 usec
DE	6.00 usec
TE	0.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	11.00 usec
PL1	-1.00 dB
SFO1	75.4752958 MHz

======== CHANNEL f2 ========

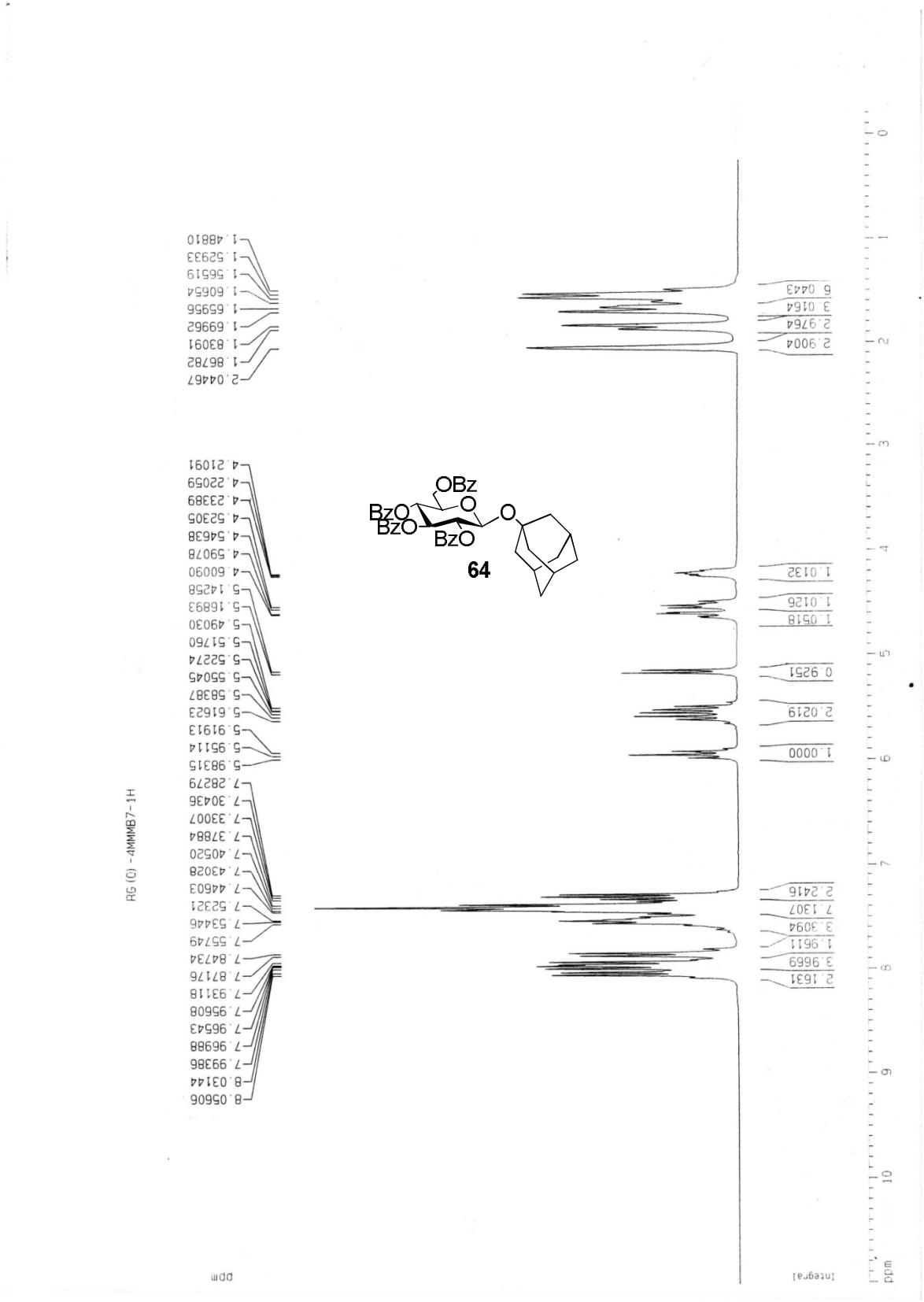
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-2.00 dB
PL12	13.00 dB
PL13	17.00 dB
SFO2	300.1312005 MHz

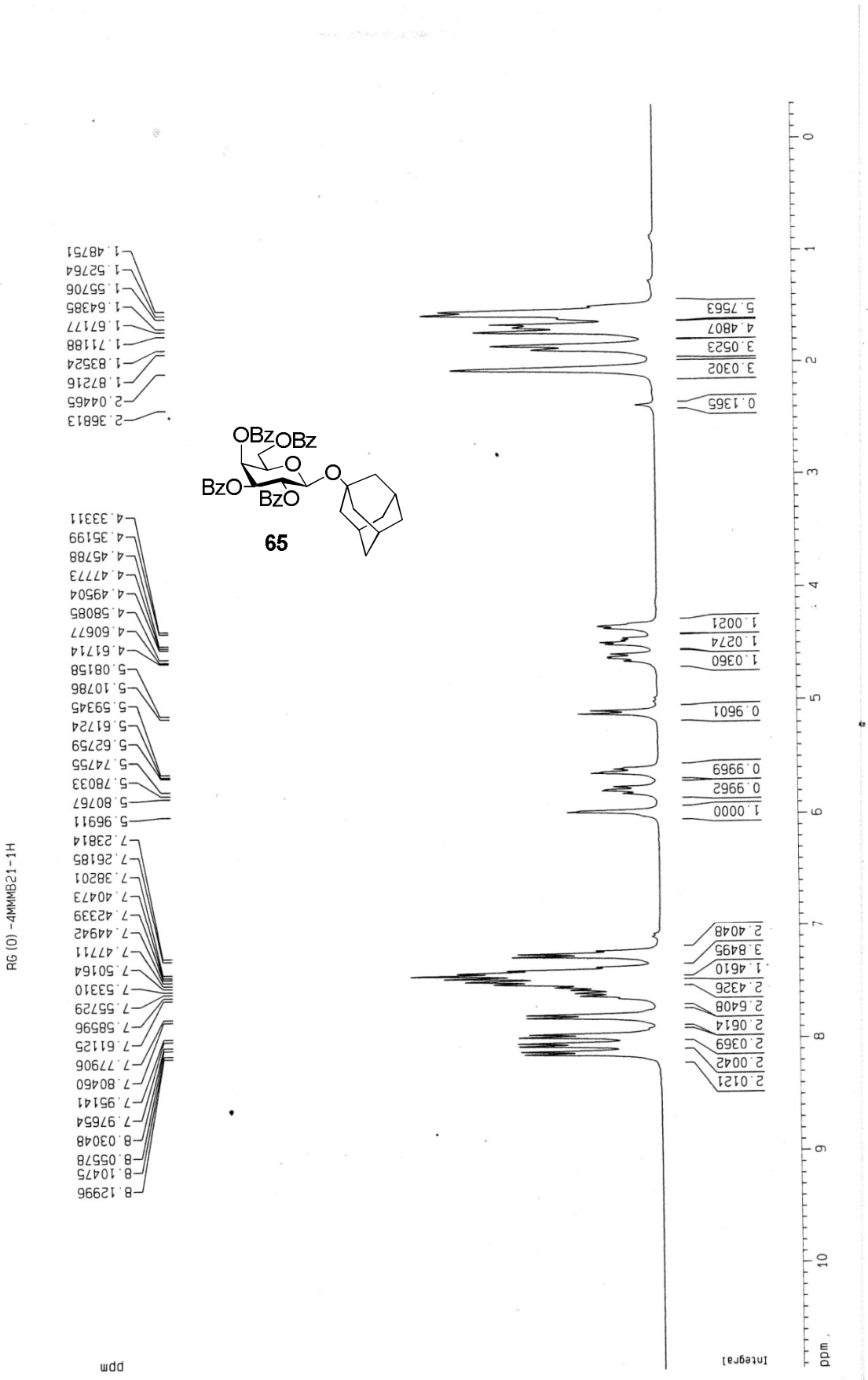
F2 - Processing parameters

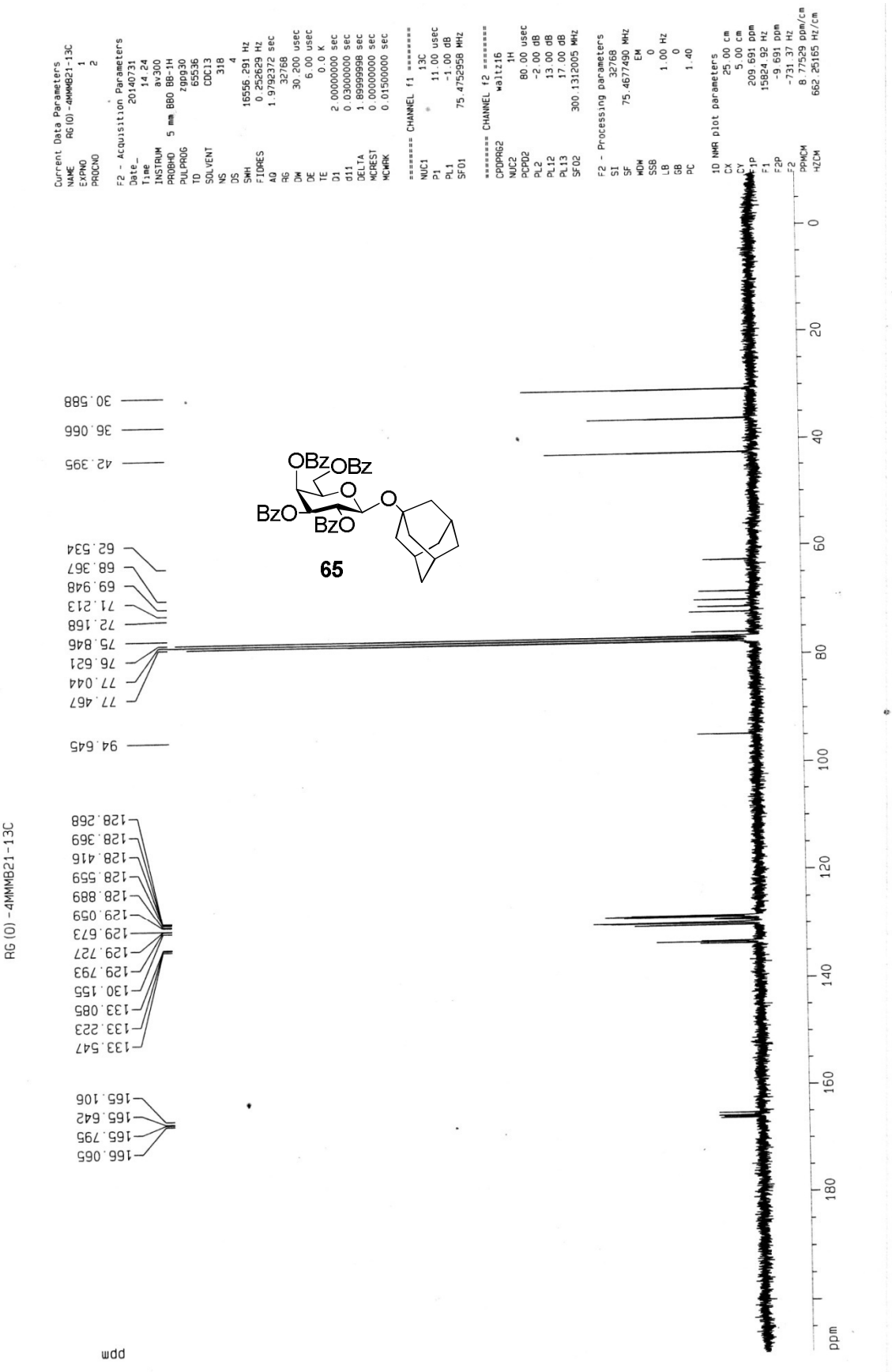
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

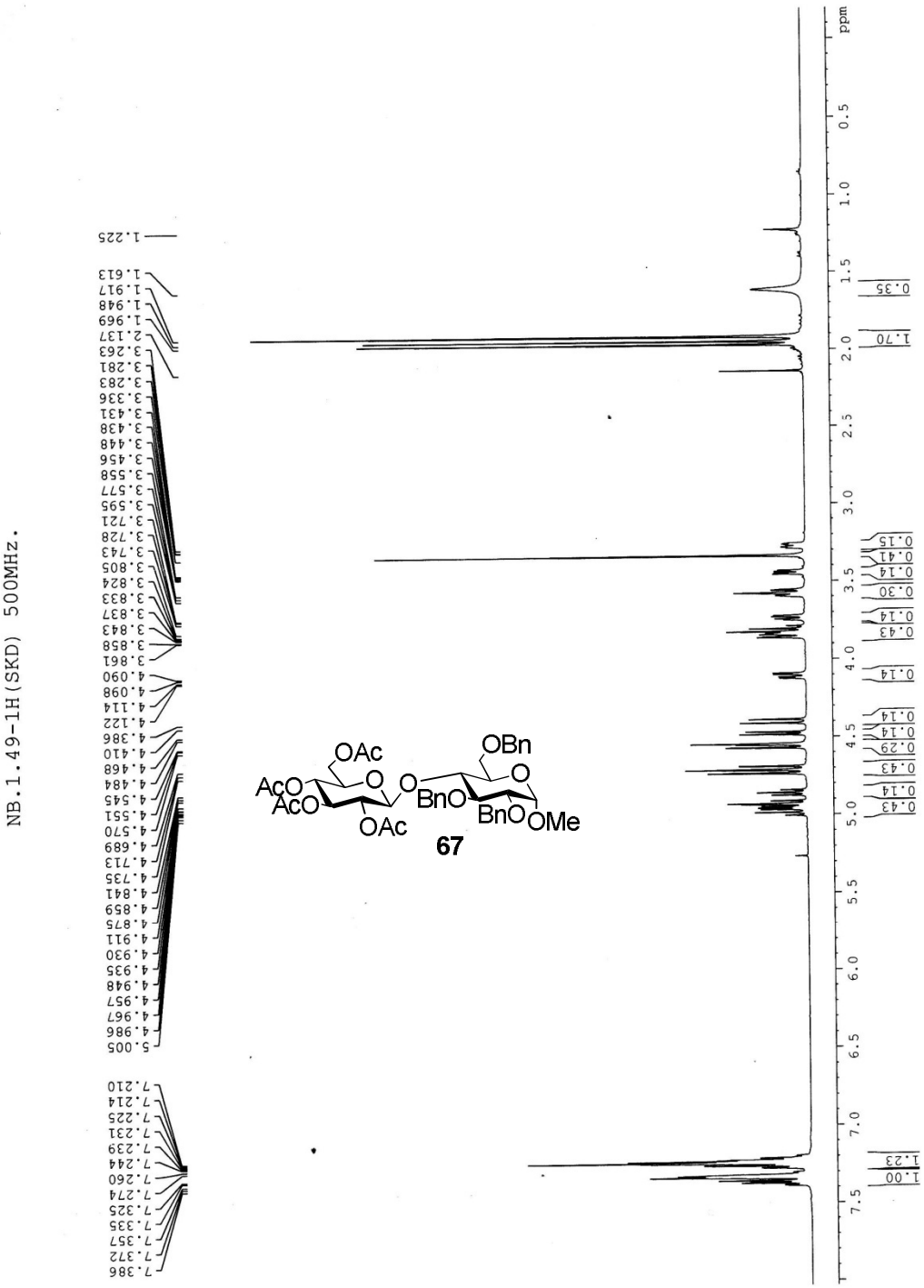
1D NMR plot parameters

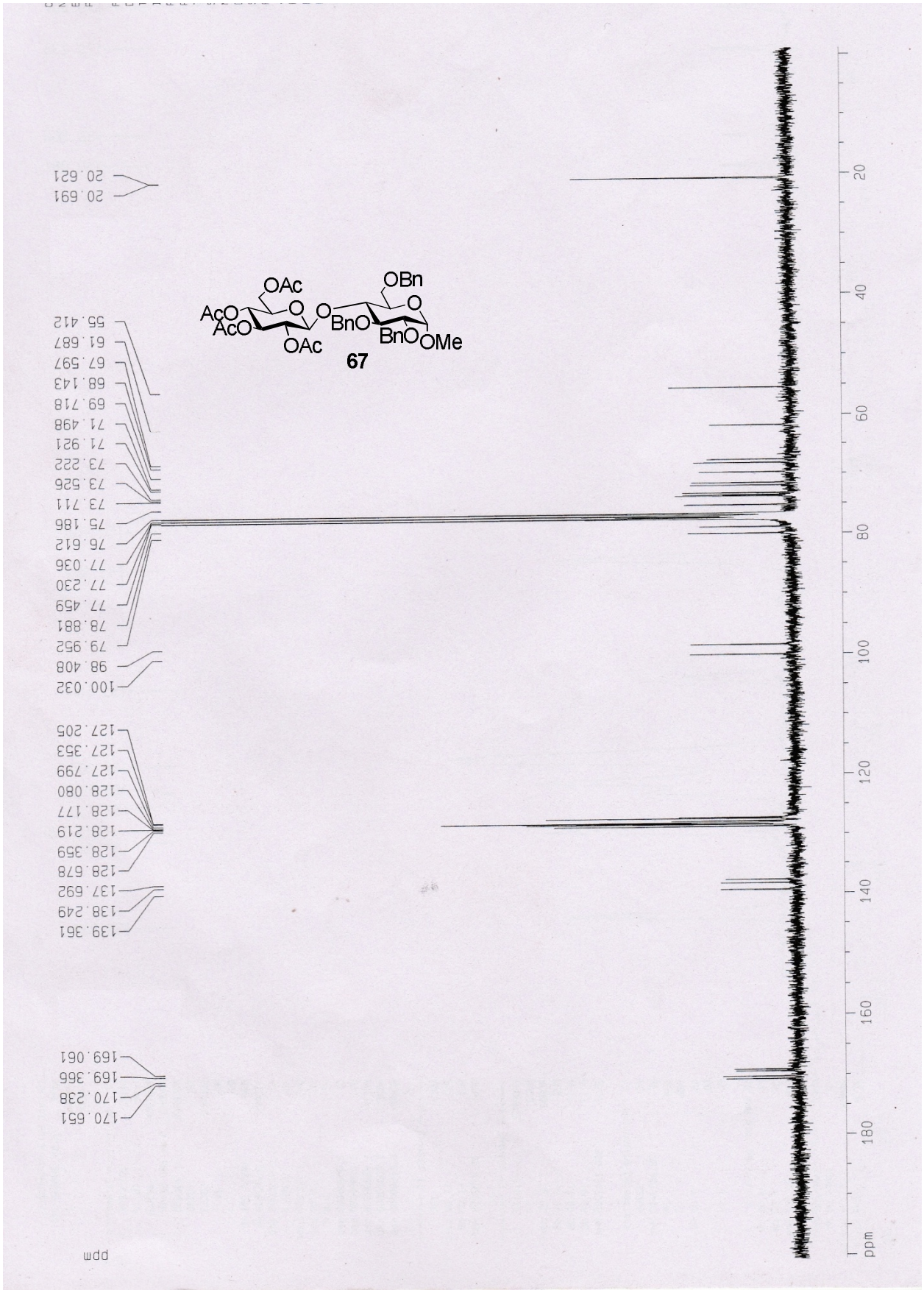
CX	24.00 cm
CY	10.00 cm
F1P	209.691 ppm
F1	15824.92 Hz
F2P	-9.691 ppm
F2	-731.37 Hz
PPMCM	9.14093 ppm/cm
HZCM	689.84558 Hz/cm

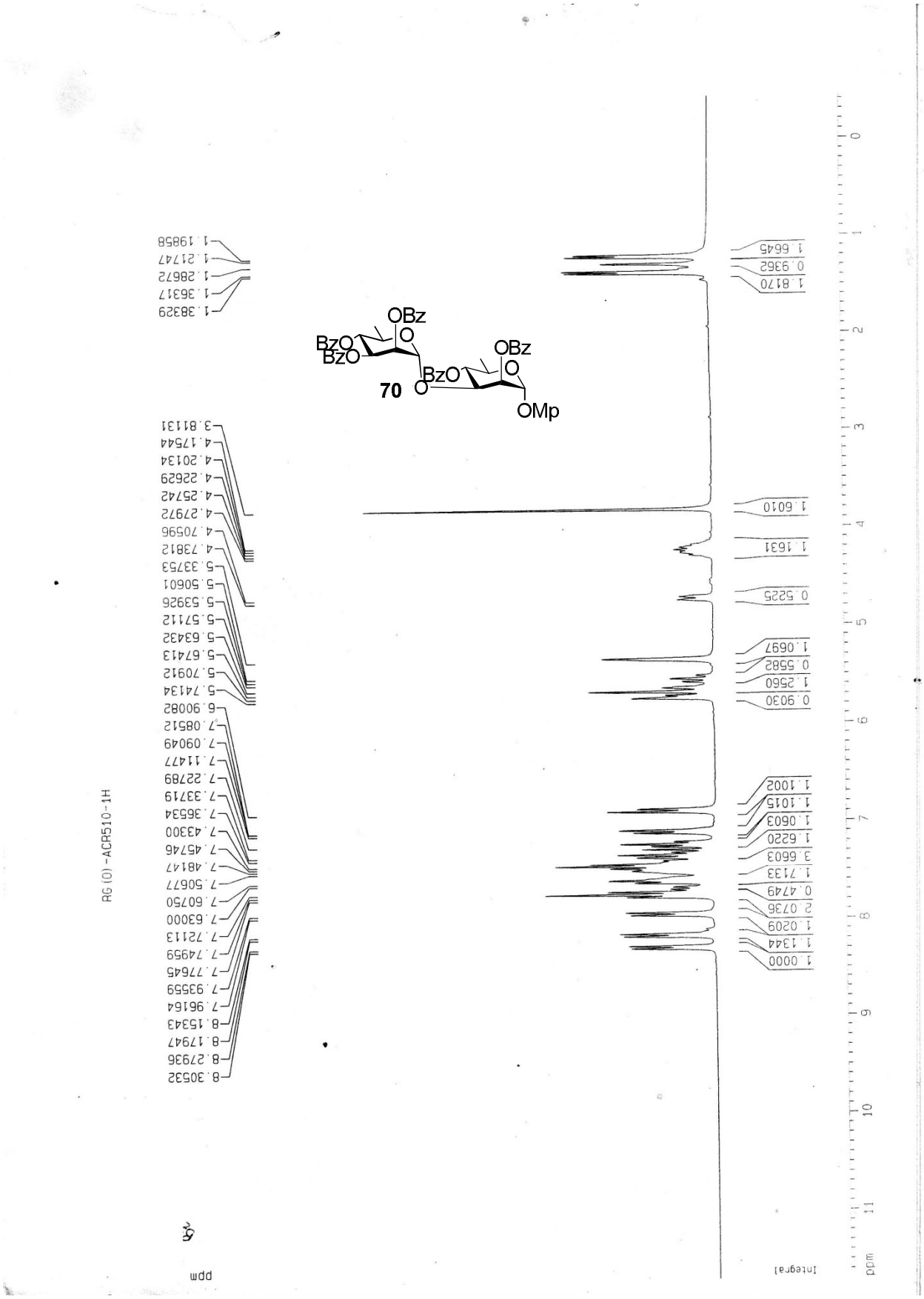

RG (D) -4MMB7-1H
ppm
Integral
OBz
BzO
BzO
BzO
O
O
64

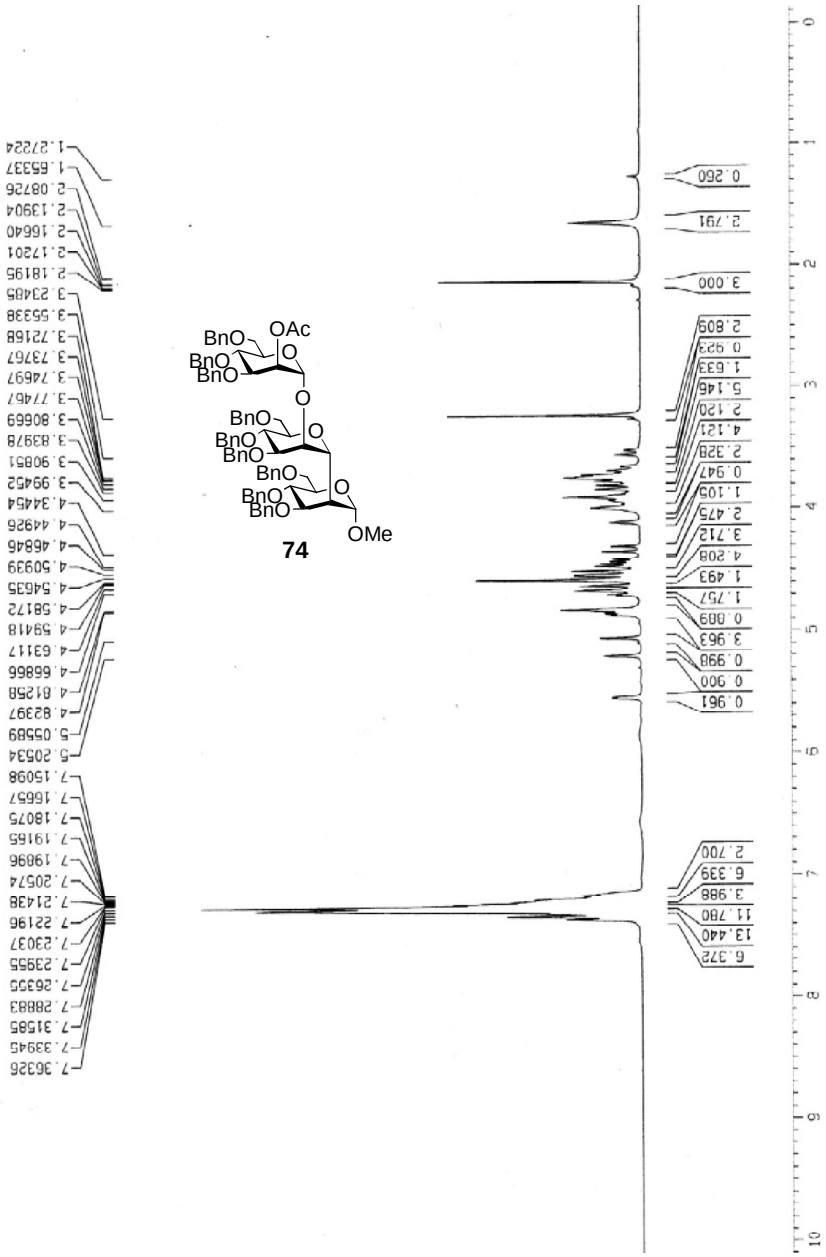

RG (0) -4MMMB21-1H
ppm
Integral
OBz
OBz
O
O
BzO
BzO
65


RG(0)-4MMB21-13C
ppm
30.588
36.066
42.395
62.534
68.367
69.948
71.213
72.168
75.846
76.621
77.044
77.467
94.645
128.268
128.369
128.416
128.559
128.889
129.059
129.673
129.727
129.793
130.155
133.085
133.223
133.547
165.106
165.642
165.795
166.065
OBz
OBz
O
O
BzO
BzO
65

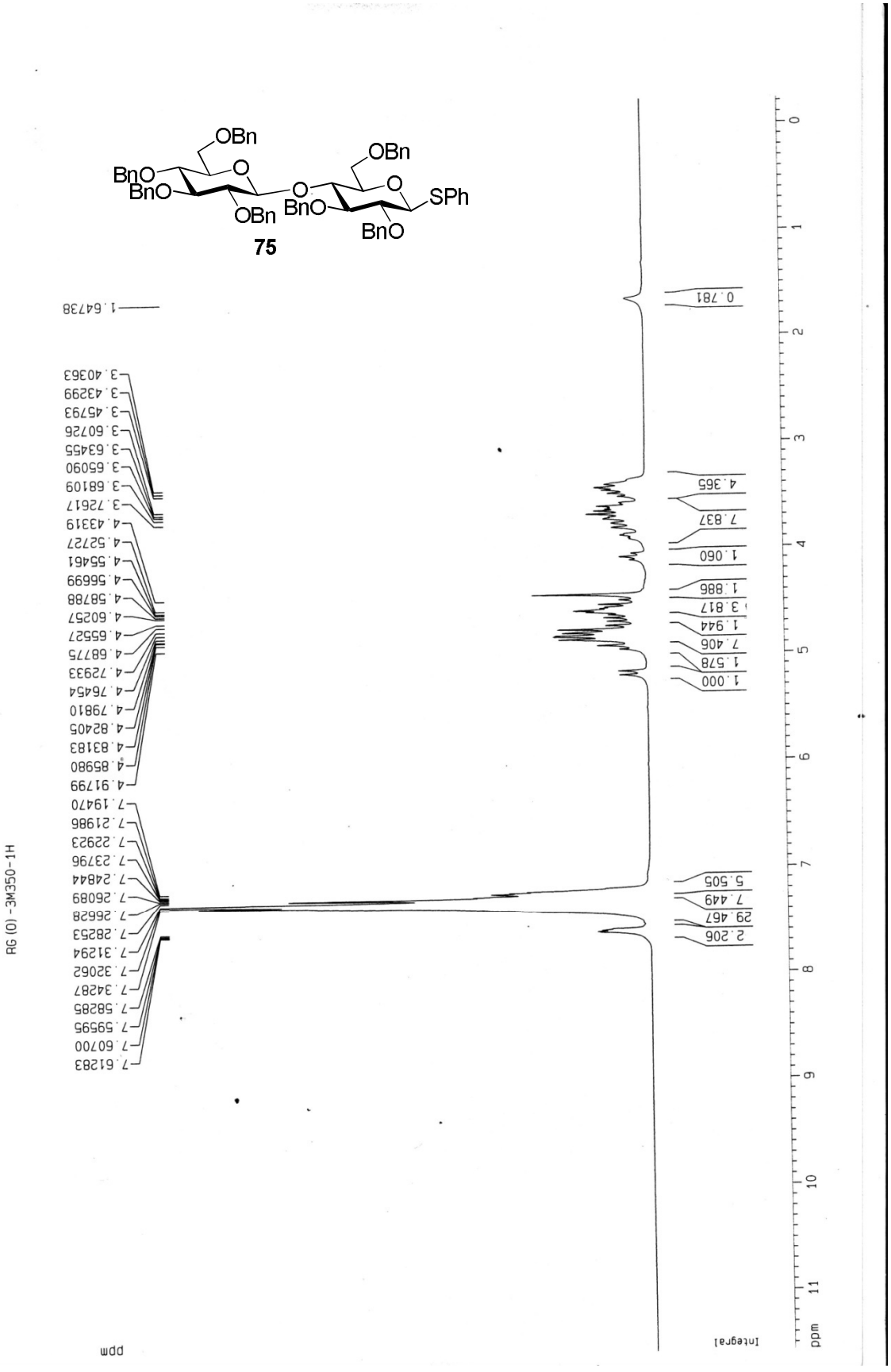

NB.1.49-1H(SKD) 500MHz.
OAc
AcO
AcO
O
O
OAc
OBn
BnO
O
BnO
OMe
67
ppm

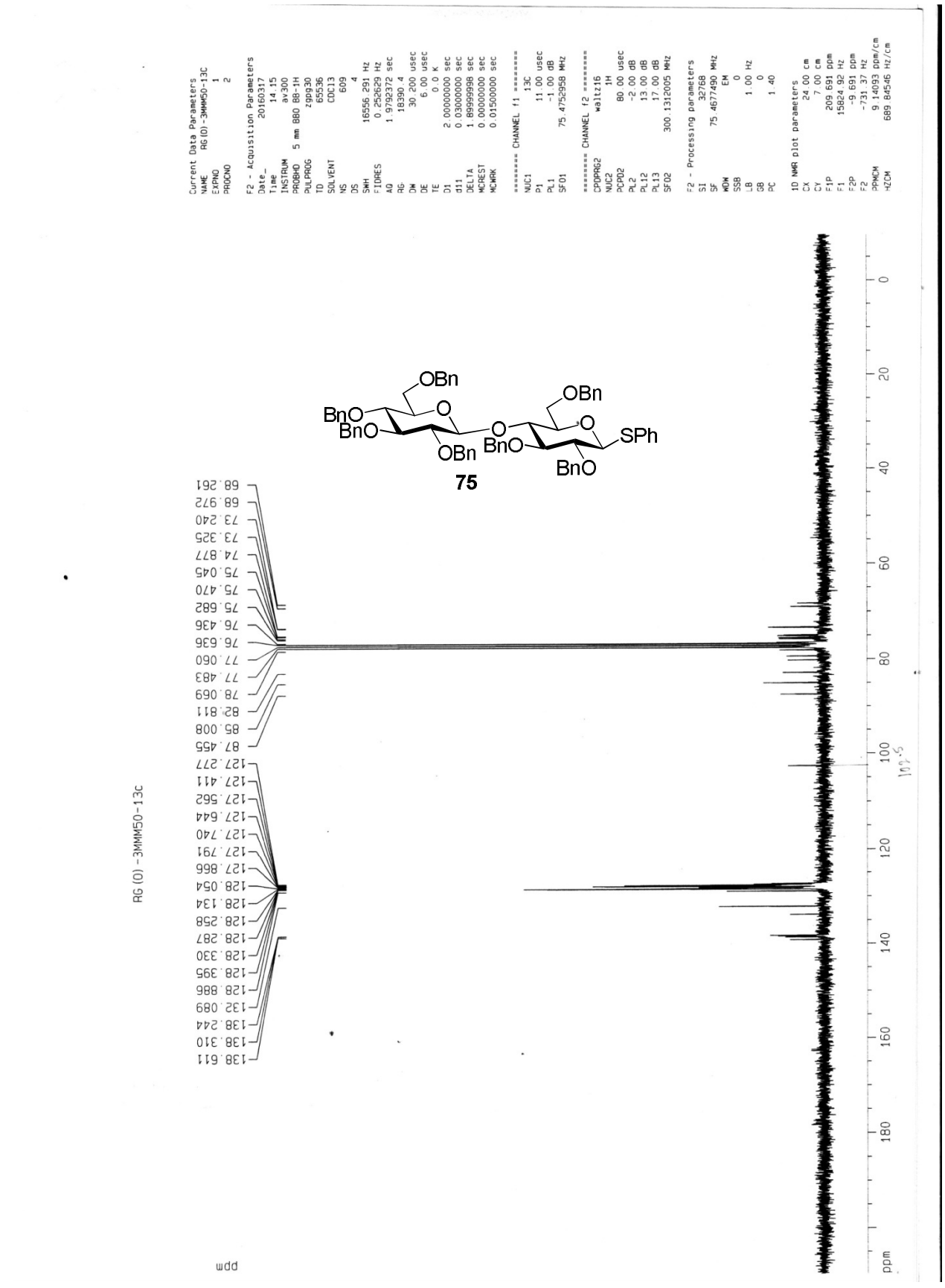

20.621
20.691
55.412
61.687
67.597
68.143
69.718
71.498
71.921
73.222
73.526
73.711
75.186
76.612
77.036
77.230
77.459
78.881
79.952
98.408
100.032
127.205
127.353
127.799
128.080
128.177
128.219
128.359
128.678
137.692
138.249
139.361
169.061
169.366
170.238
170.651
OAc
AcO
AcO
O
O
OAc
OBn
O
BnO
BnO
OMe
67
20
40
60
80
100
120
140
160
180
ppm

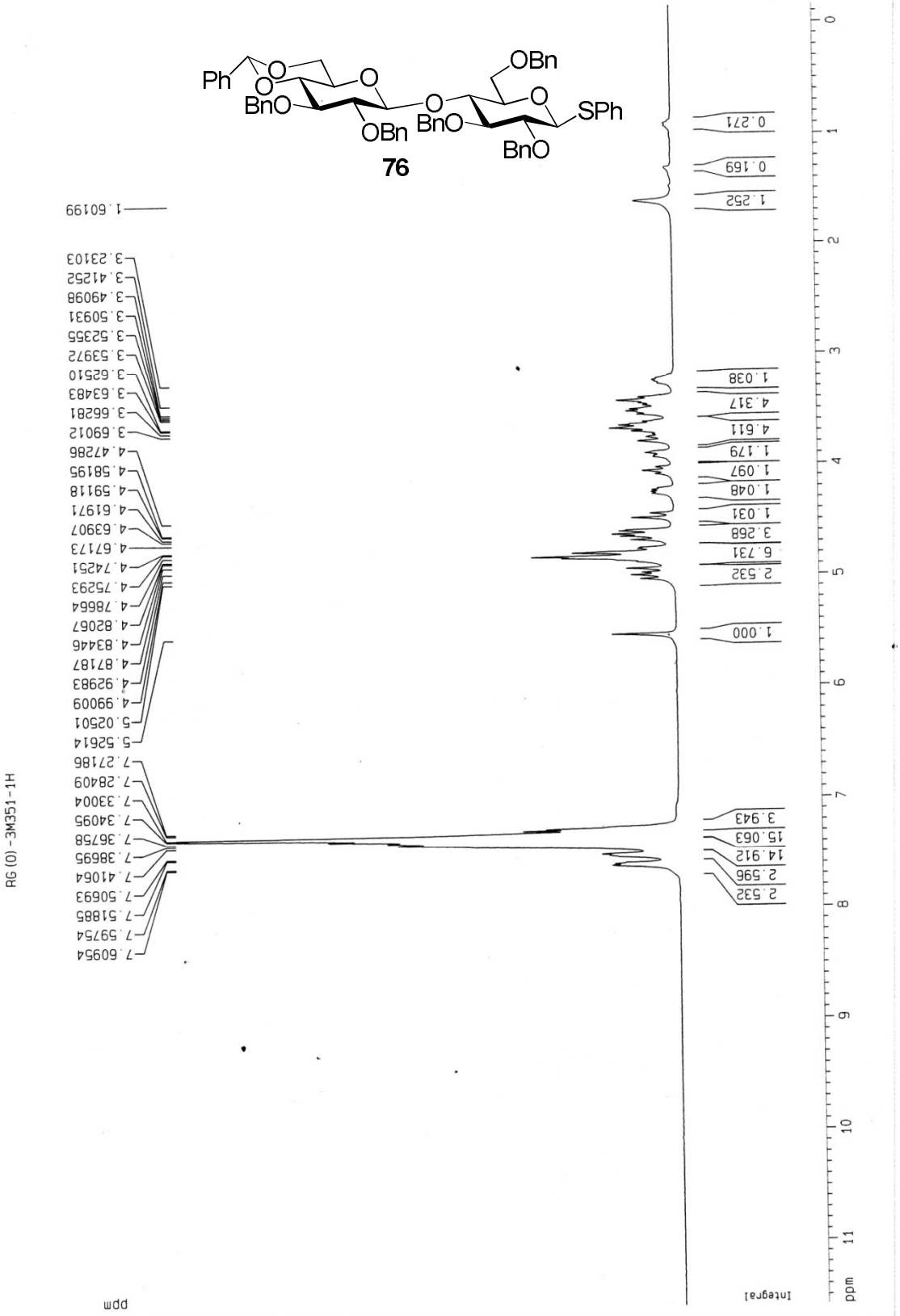

70
OBz
BzO
BzO
OBz
BzO
O
OMp
RG(0)-ACR510-1H
ppm
Integral



74


OBn
BnO
BnO
OBn
O
O
OBn
BnO
O
SPh
BnO
75
RG (0) - 3M350-1H
ppm
Integral

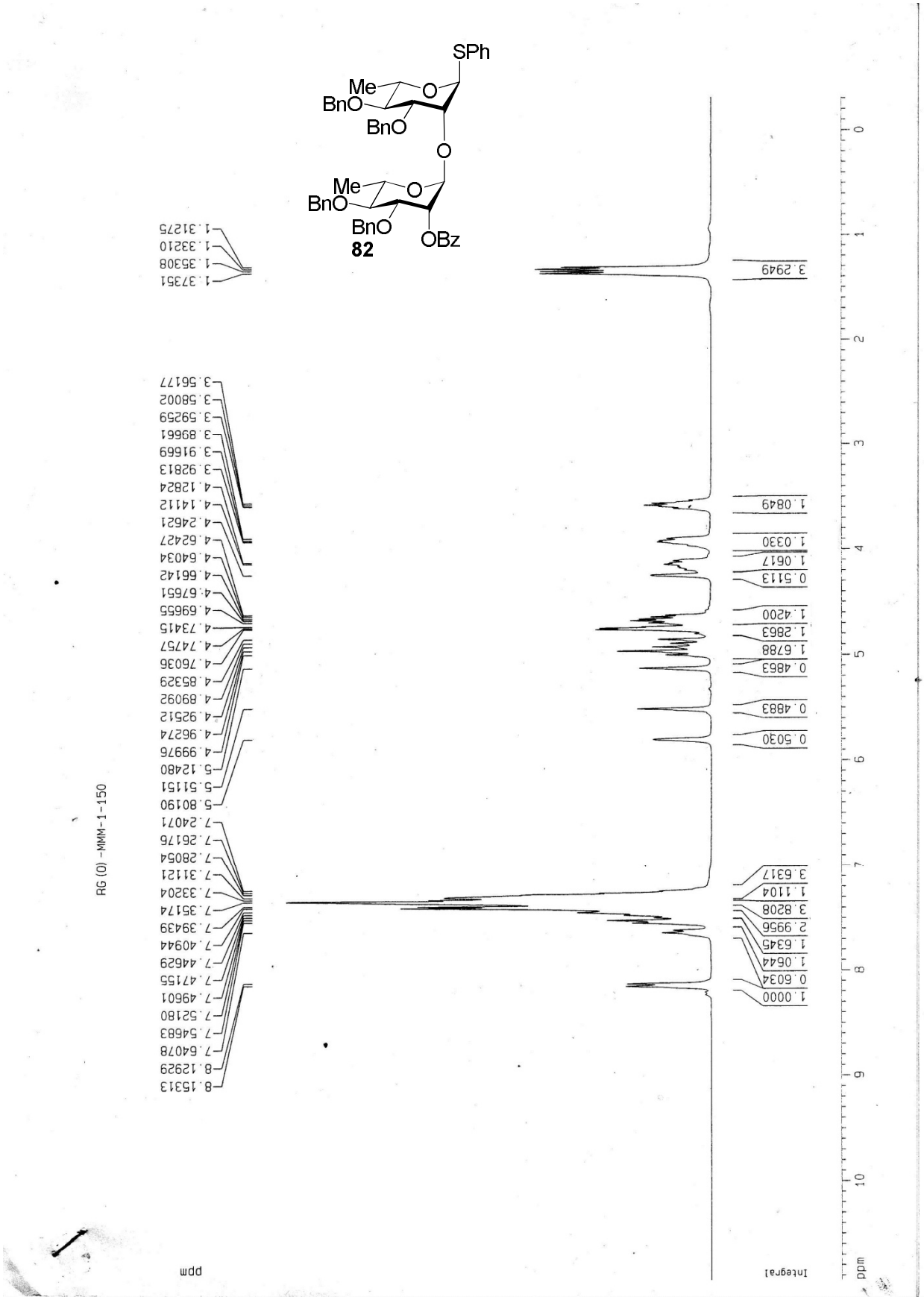

RG (0) -3MM50-13c
ppm
Current Data Parameters
NAME RG(0)-3MM50-13C
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20160317
Time 14.15
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 609
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 18390.4
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 7.00 cm
F1P 209.691 ppm
F1 15824.92 Hz
F2P -9.691 ppm
F2 -731.37 Hz
PPMCM 9.14093 ppm/cm
HZCM 689.84546 Hz/cm
OBn
BnO
BnO
O
OBn
O
BnO
OBn
O
SPh
BnO
75
68.261
68.972
73.240
73.325
74.877
75.045
75.470
75.682
76.436
76.636
77.060
77.483
78.069
82.811
85.008
87.455
127.277
127.411
127.562
127.644
127.740
127.791
127.866
128.054
128.134
128.258
128.287
128.330
128.395
128.886
132.089
138.244
138.310
138.611

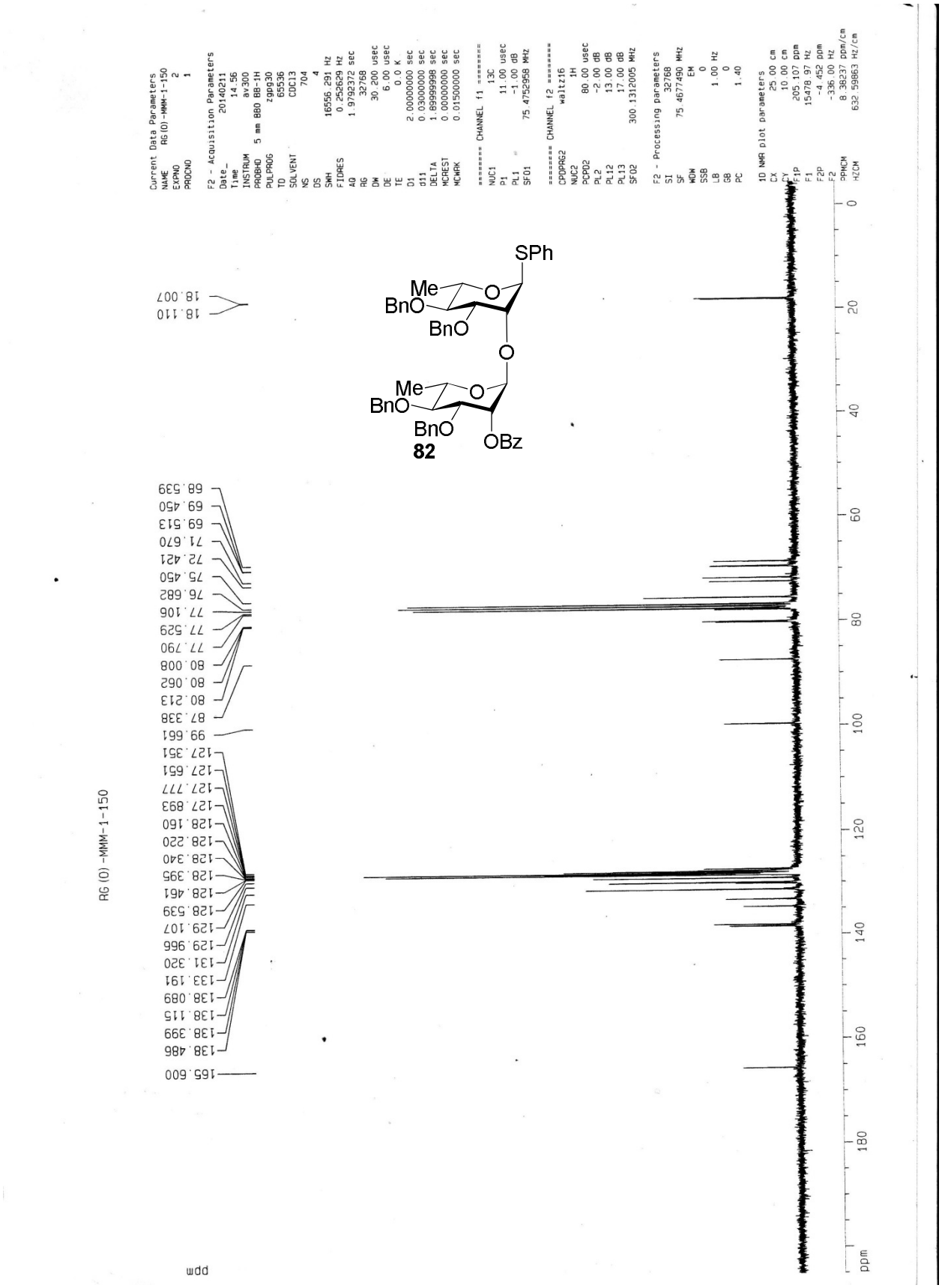

Ph
O
O
O
BnO
OBn
O
OBn
BnO
O
SPh
BnO
76
RG (0) -3M351-1H
ppm
Integral

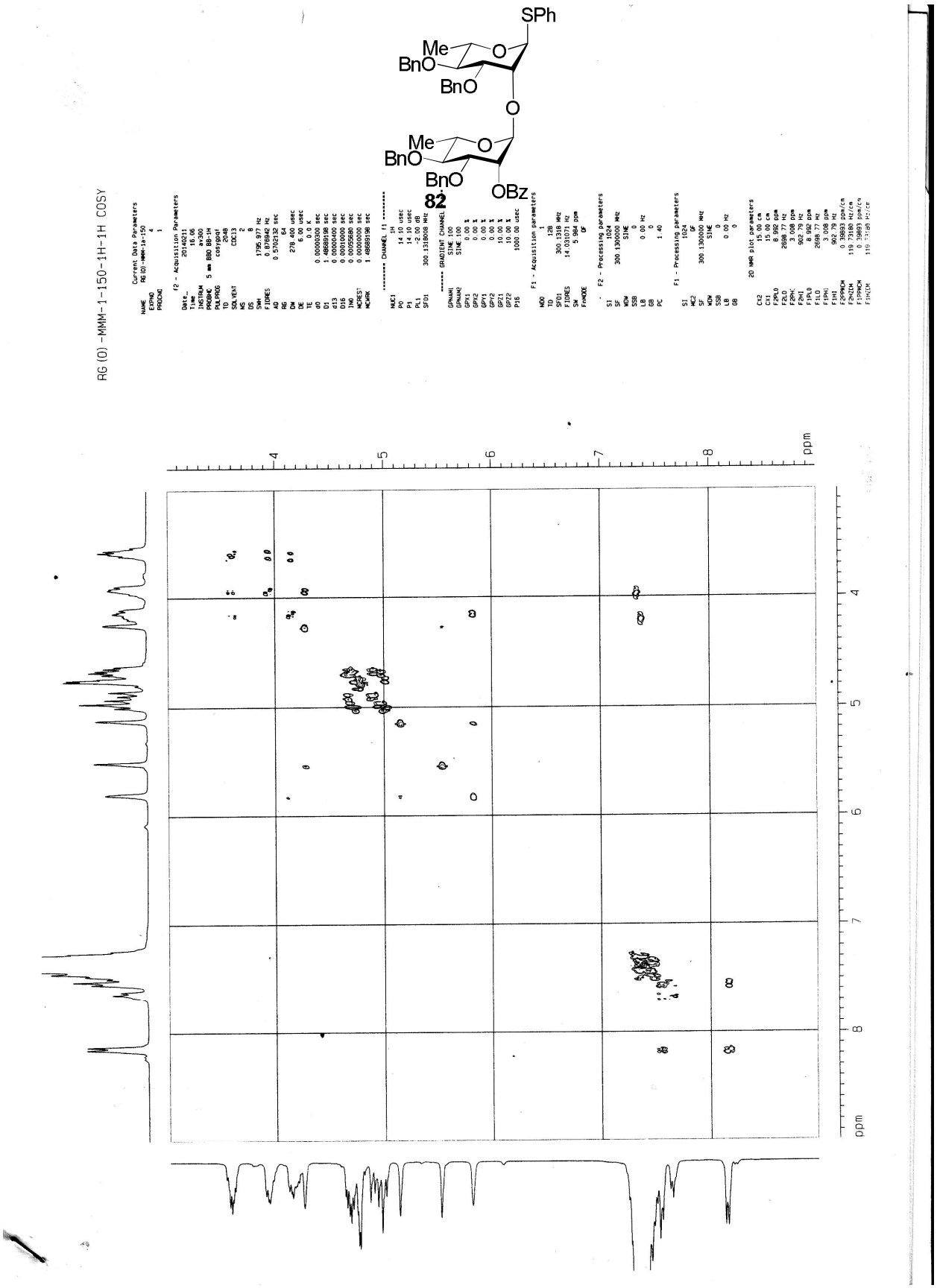
Current Data Parameters
NAME RG(0)-3MM51-13C
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20160331
Time 11.49
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16722
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 18390.4
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SFO1 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 10.00 cm
F1P 209.691 ppm
F1 15824.92 Hz
F2P -9.691 ppm
F2 -731.37 Hz
PPMCM 9.14093 ppm/cm
HZCM 689.84558 Hz/cm
Ph
O
O
BnO
O
OBn
O
BnO
OBn
O
SPh
BnO
76
RG (0) -3MM51-13C
62.361
68.162
70.751
73.343
74.933
75.351
75.527
75.591
76.624
77.047
77.250
77.471
79.279
82.466
84.866
87.539
102.594
126.058
127.354
127.529
127.663
127.775
127.849
127.933
127.985
128.234
128.327
128.396
128.664
128.922
129.020
129.769
132.117
138.201
138.518
ppm
ppm

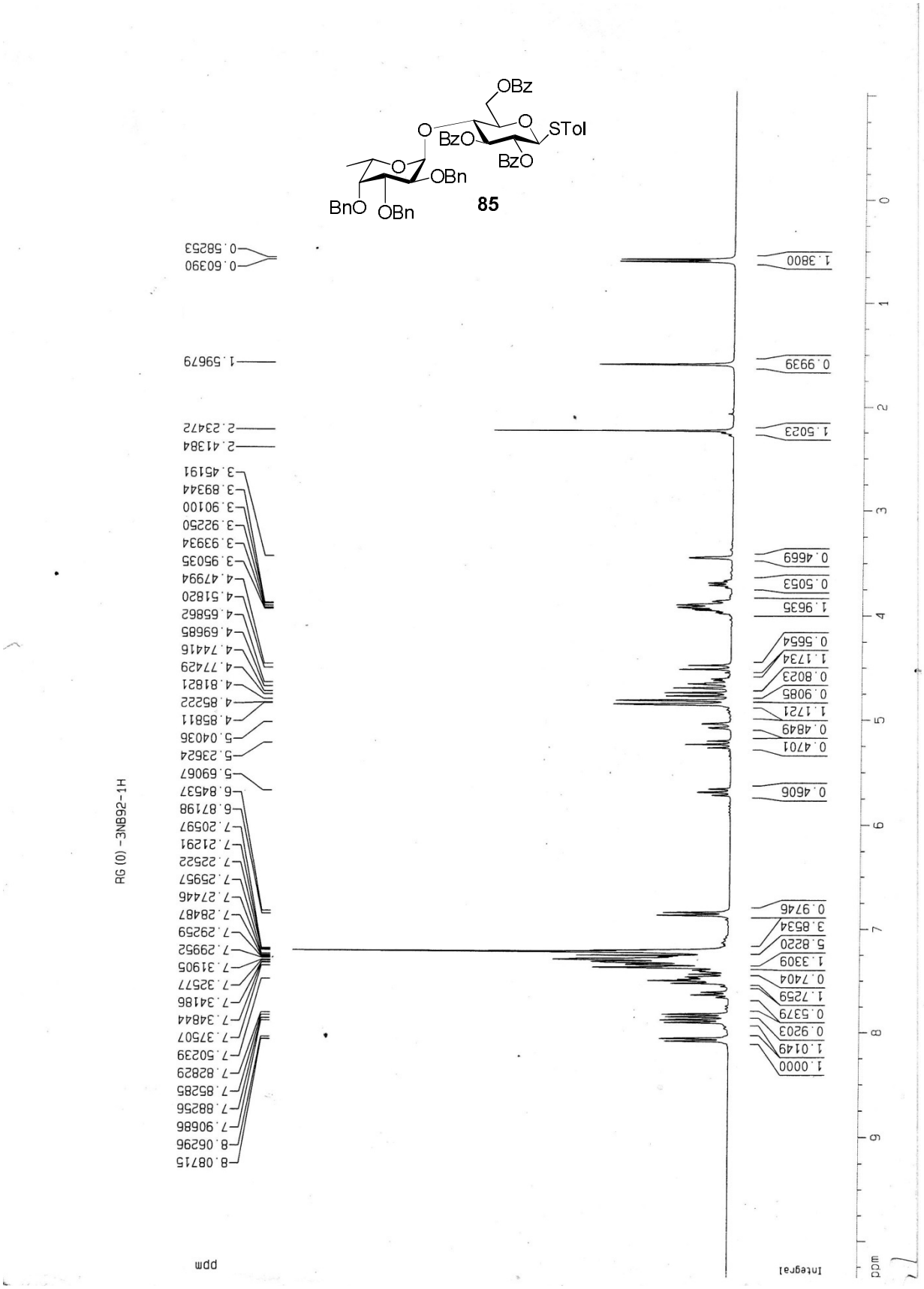
8.078
8.066
8.001
7.989
7.852
7.840
7.548
7.535
7.482
7.457
7.444
7.434
7.431
7.349
7.336
7.324
7.288
7.278
7.267
7.263
7.257
7.249
7.244
7.162
7.159
7.154
7.150
7.141
5.991
5.942
5.939
5.937
5.934
5.727
5.725
5.357
5.355
5.352
4.872
4.844
4.826
4.587
4.567
4.513
4.495
4.452
4.434
4.367
4.347
4.333
4.315
3.869
3.695
3.677
2.103
0.000
ppm
9
8
7
6
5
4
3
2
1
0
2.02
2.56
2.52
3.64
1.49
3.81
3.26
19.04
3.30
1.10
1.54
1.11
0.99
1.00
1.08
1.26
0.88
1.20
1.15
1.14
2.16
1.09
1.08
1.18
1.14
2.14
0.99
3.10
BnO
BnO
BnO
OAc
O
O
BzO
BzO
OBz
O
SPh
79

170.27
165.44
165.36
138.53
138.06
137.93
133.55
133.45
133.25
133.22
132.14
131.54
129.92
129.89
129.82
129.74
129.71
129.34
129.28
129.22
128.86
128.62
128.54
128.47
128.32
128.27
128.23
128.18
128.02
127.90
127.88
127.75
127.65
127.51
127.50
97.97
85.99
78.43
77.21
77.00
76.79
75.09
74.02
73.24
72.04
71.84
71.46
70.48
70.45
68.46
68.44
67.28
66.64
21.06
BnO
BnO
BnO
OAc
O
O
O
BzO
BzO
OBz
O
SPh
79
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

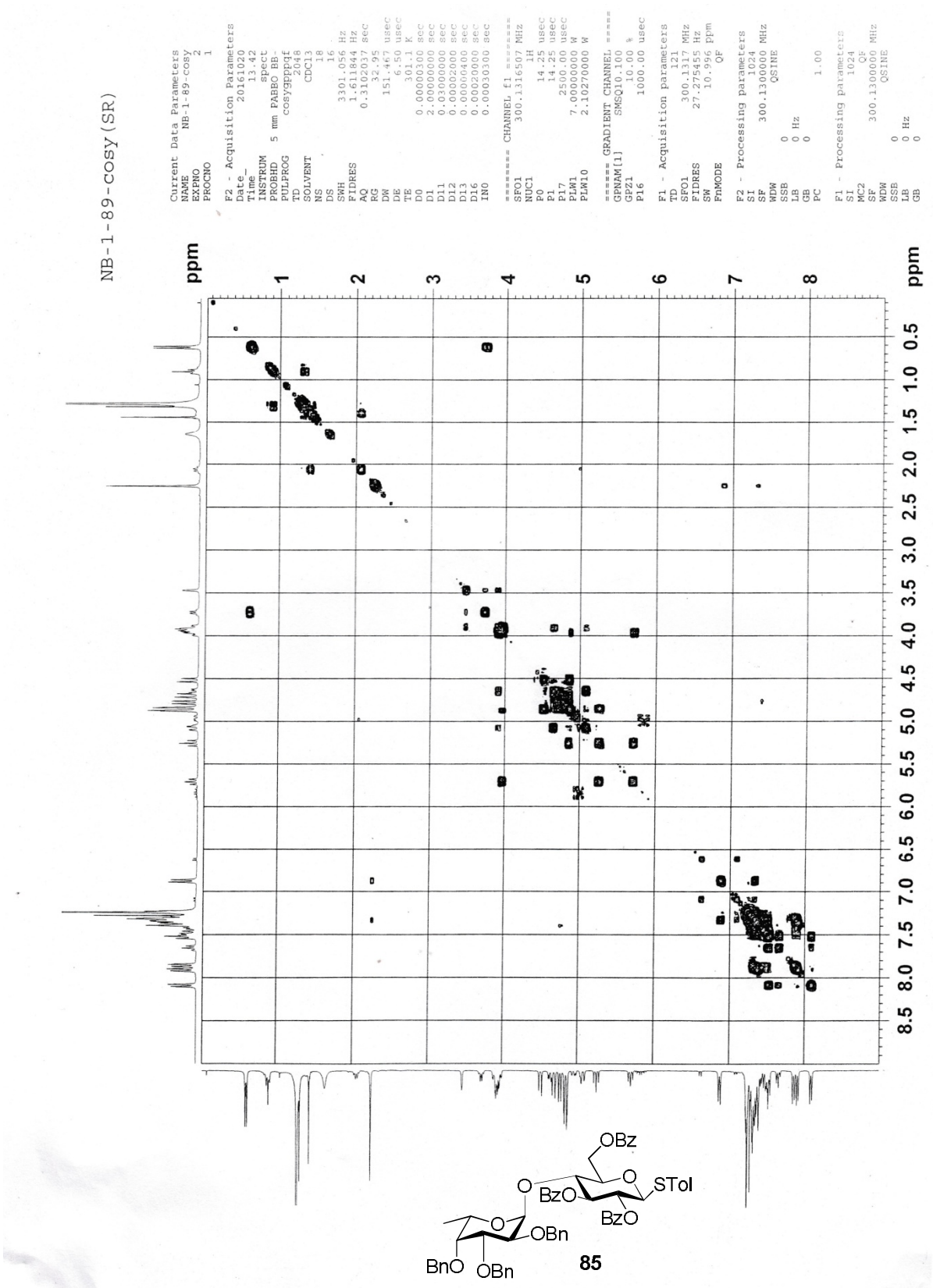

SPh
Me
BnO
BnO
O
O
Me
BnO
BnO
OBz
82
RG (0) -MMM-1-150
ppm
Integral
ppm

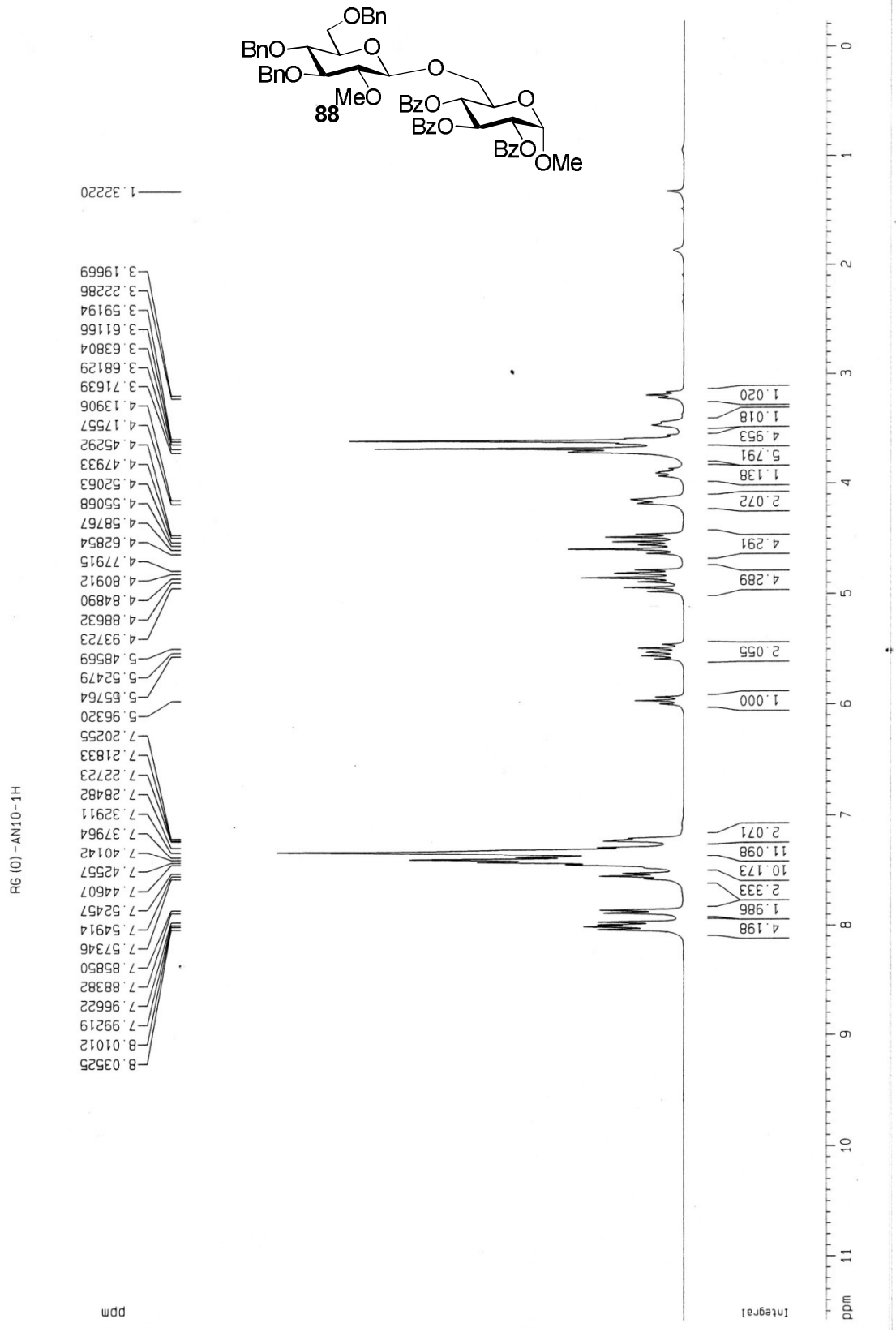

SPh
Me
BnO
BnO
O
Me
BnO
BnO
OBz
82
RG(0)-MMM-1-150
ppm

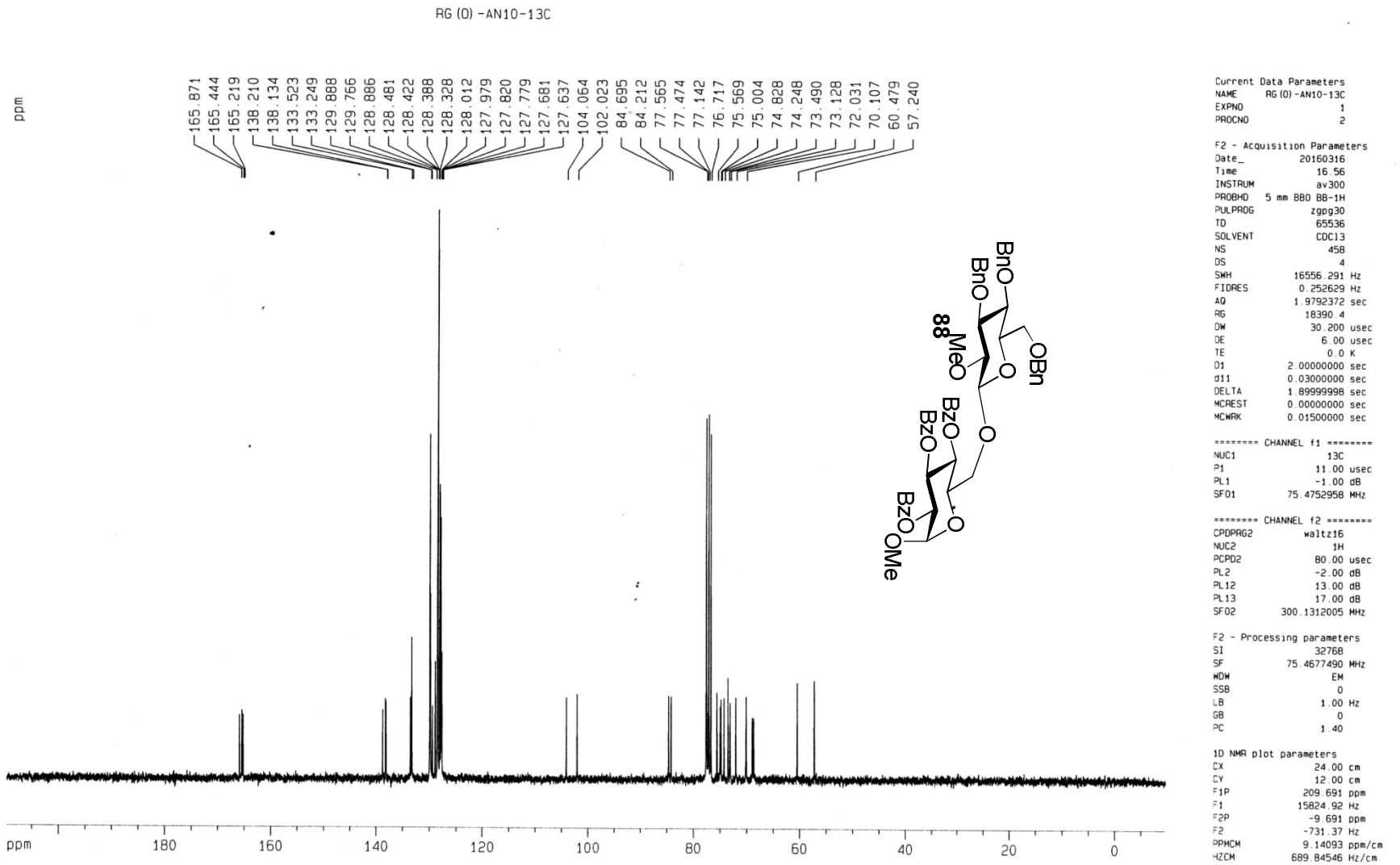

SPh
Me
BnO
O
BnO
O
Me
BnO
O
BnO
OBz
82
RG (0) -MMM-1-150-1H-1H COSY
ppm
ppm


OBz
O
O
STol
BzO
BzO
O
OBn
BnO
OBn
85
RG (0) -3NB92-1H
ppm
Integral

Current Data Parameters
NAME RG(0)-3NB92-13C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111129
Time 14.30
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1783
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 26008
DW 27.800 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.50 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.75 dB
PL13 19.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 16384
SF 75.4677498 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 20.00 cm
F1P 208.000 ppm
F1 15697.29 Hz
F2P -12.087 ppm
F2 -912.17 Hz
PPMCM 11.00434 ppm/cm
HZCM 830.47284 Hz/cm
RG(0)-3NB92-13C
ppm
15.952
21.138
63.085
67.700
72.722
74.342
74.846
75.600
76.593
77.016
77.218
77.439
77.608
77.847
79.209
85.467
100.541
127.463
127.509
127.724
128.117
128.236
128.277
128.374
128.418
129.471
129.783
129.870
133.056
133.119
133.924
138.341
138.634
165.154
165.963
166.018
OBz
O
BzO
O
STol
BzO
O
OBn
BnO
OBn
85
ppm
0
50
100
150


NB-1-89-cosy(SR)
Current Data Parameters
NAME NB-1-89-cosy
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161020
Time_ 13.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpppqf
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 3301.056 Hz
FIDRES 1.611844 Hz
AQ 0.3102037 sec
RG 32.95
DW 151.467 usec
DE 6.50 usec
TE 301.1 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00030300 sec
======== CHANNEL f1 ========
SFO1 300.1316507 MHz
NUC1 1H
P0 14.25 usec
P1 14.25 usec
P17 2500.00 usec
PLW1 7.00000000 W
PLW10 2.10270000 W
====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec
F1 - Acquisition parameters
TD 121
SFO1 300.1317 MHz
FIDRES 27.275455 Hz
SW 10.996 ppm
FnMODE QF
F2 - Processing parameters
SI 1024
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.00
F1 - Processing parameters
SI 1024
MC2 QF
SF 300.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
ppm
1
2
3
4
5
6
7
8
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
ppm
OBz
O
STol
BzO
BzO
O
OBn
BnO
OBn
85


OBn
BnO
BnO
MeO
88
BzO
BzO
BzO
OMe
RG(D)-AN10-1H
ppm
Integral



Current Data Parameters

NAME	RG (0) -AN10-13C
EXPNO	1
PROCNO	2

F2 - Acquisition Parameters

Date_	20160316
Time	16.56
INSTRUM	av300
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	458
DS	4
SWH	16556.291 Hz
FIDRES	0.252629 Hz
AQ	1.9792372 sec
RG	18390.4
DW	30.200 usec
DE	6.00 usec
TE	0.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	13C
P1	11.00 usec
PL1	-1.00 dB
SFO1	75.4752958 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-2.00 dB
PL12	13.00 dB
PL13	17.00 dB
SFO2	300.1312005 MHz

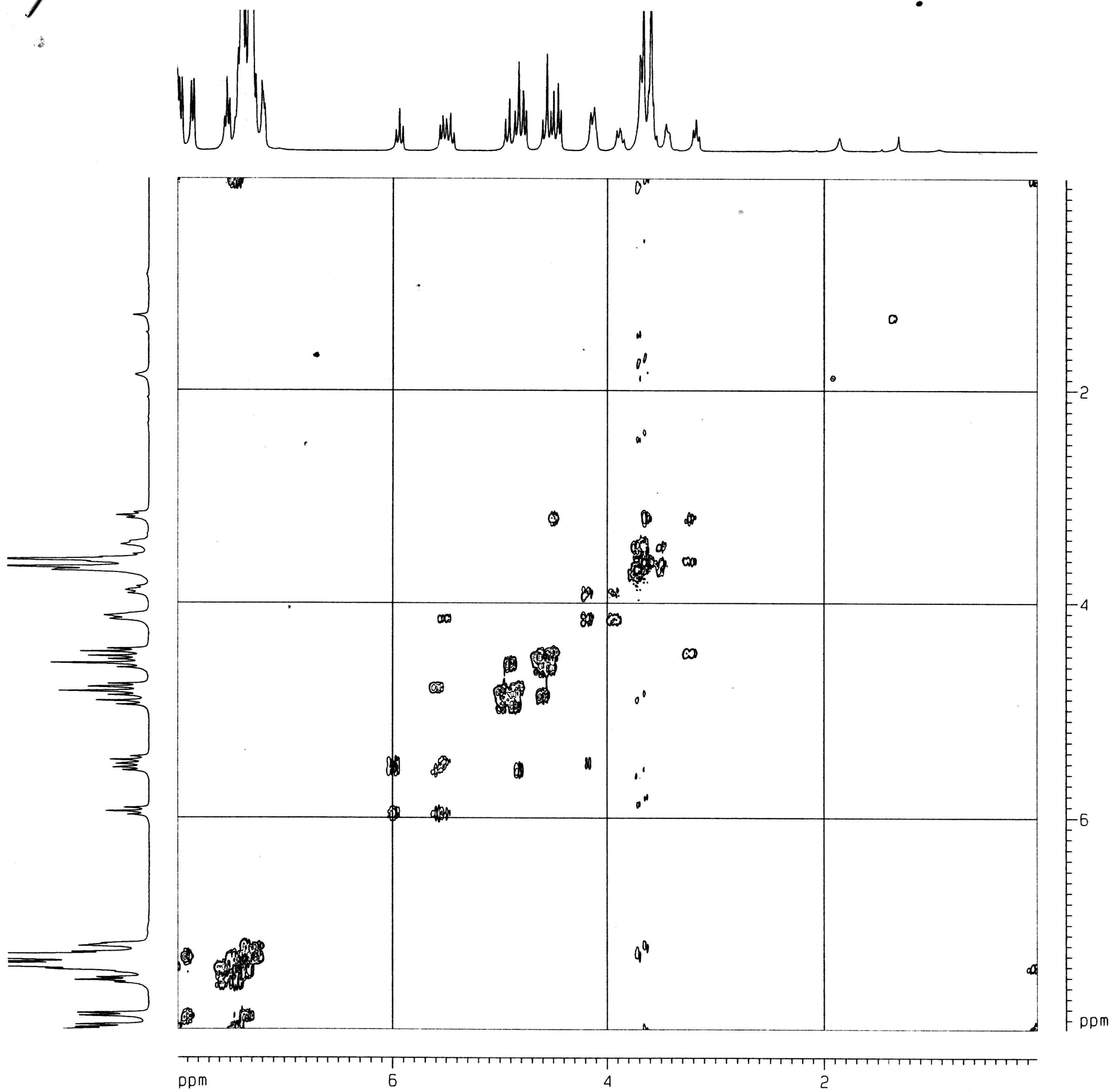
F2 - Processing parameters

SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	24.00 cm
CY	12.00 cm
F1P	209.691 ppm
F1	15824.92 Hz
F2P	-9.691 ppm
F2	-731.37 Hz
PPMCM	9.14093 ppm/cm
HZCM	689.84546 Hz/cm

RG (O) -AN10 1H-1H COSY



Current Data Parameters		
NAME	RG (O) -AN10	
EXPNO	4	
PROCNO	1	

F2 - Acquisition Parameters		
Date_	20160316	
Time	15.50	
INSTRUM	av300	
PROBHD	5 mm BBO BB-1H	
PULPROG	cosygpqf	
TD	2048	
SOLVENT	CDCl3	
NS	2	
DS	8	
SWH	2394.636	Hz
FIDRES	1.169256	Hz
AQ	0.4276724	sec
RG	228.1	
DW	208.800	usec
DE	6.00	usec
TE	0.0	K
d0	0.00000300	sec
D1	1.48689198	sec
d13	0.00000400	sec
D16	0.00010000	sec
IN0	0.00041760	sec
MCREST	0.00000000	sec
MCWRK	1.48689198	sec

======== CHANNEL f1 ========		
NUC1	1H	
P0	14.10	usec
P1	14.10	usec
PL1	-2.00	dB
SFO1	300.1312005	MHz

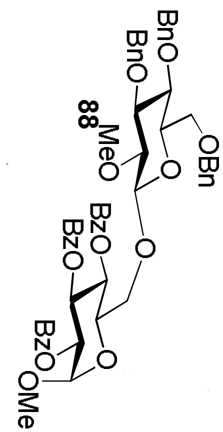
====== GRADIENT CHANNEL =====		
GPNAM1	SINE.100	
GPNAM2	SINE.100	
GPX1	0.00	%
GPX2	0.00	%
GPY1	0.00	%
GPY2	0.00	%
GPZ1	10.00	%
GPZ2	10.00	%
P16	1000.00	usec

F1 - Acquisition parameters		
ND0	1	
TD	128	
SFO1	300.1312	MHz
FIDRES	18.708094	Hz
SW	7.979	ppm
FnMODE	QF	

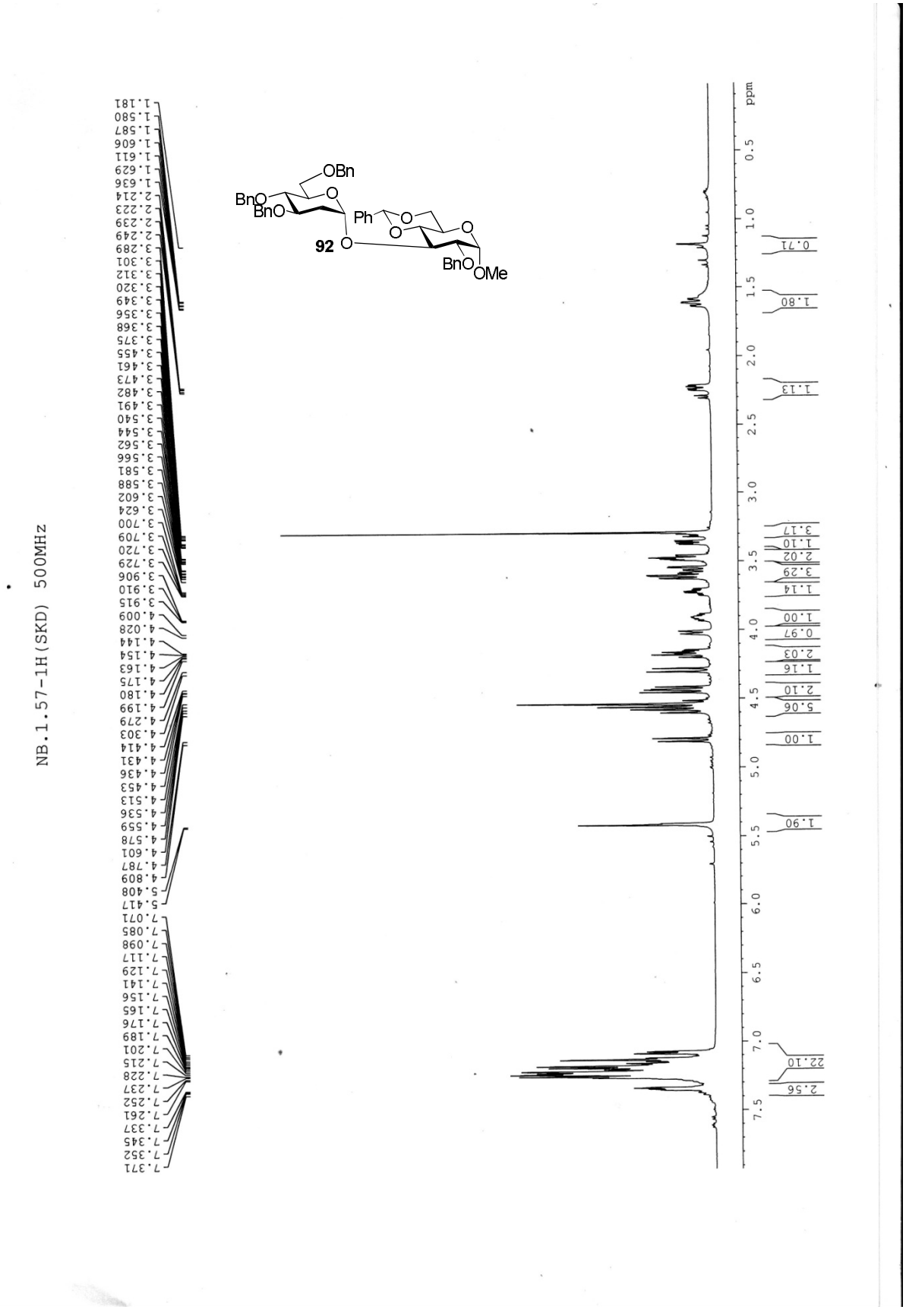
F2 - Processing parameters		
SI	1024	
SF	300.1300000	MHz
WDW	SINE	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.40	

F1 - Processing parameters		
SI	1024	
MC2	QF	
SF	300.1300000	MHz
WDW	SINE	
SSB	0	
LB	0.00	Hz
GB	0	

2D NMR plot parameters		
CX2	15.00	cm
CX1	15.00	cm
F2PLO	7.989	ppm
F2LO	2397.84	Hz
F2PHI	0.011	ppm
F2HI	3.20	Hz
F1PLO	7.989	ppm
F1LO	2397.84	Hz
F1PHI	0.011	ppm
F1HI	3.20	Hz
F2PPMCM	0.53191	ppm/cm
F2HZCM	159.64241	Hz/cm
F1PPMCM	0.53191	ppm/cm
F1HZCM	159.64241	Hz/cm



88


NB.1.57-1H(SKD) 500MHz
OBn
BnO
BnO
Ph
O
O
O
92
O
BnO
OMe
ppm

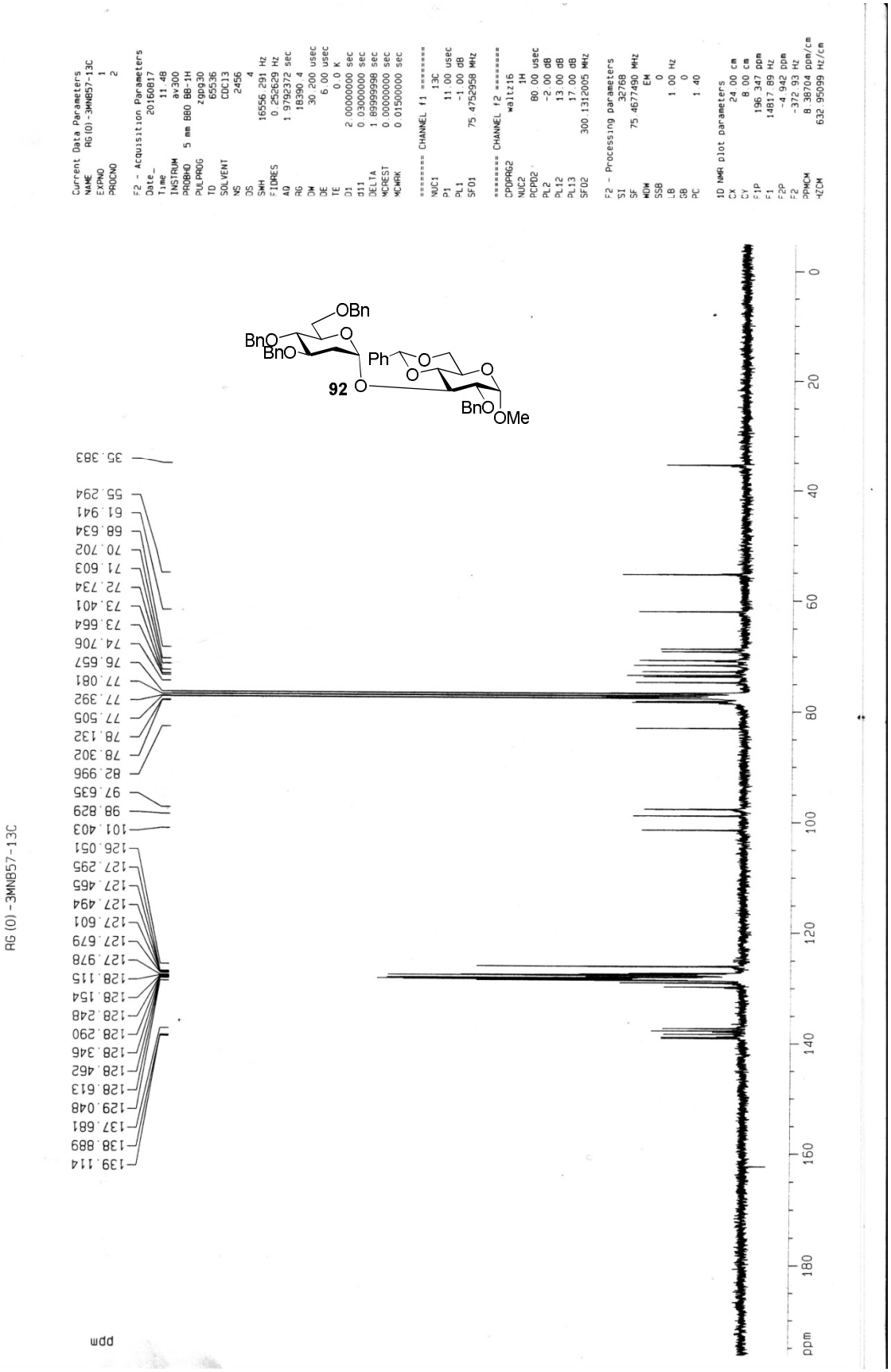

RG(0)-3MNB57-13C
Current Data Parameters
NAME RG(0)-3MNB57-13C
EXPNO 1
PROCNO 2
F2 - Acquisition Parameters
Date_ 20160817
Time 11.48
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2456
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 18390.4
DW 30.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
WCREST 0.00000000 sec
WCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 -1.00 dB
SF01 75.4752958 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 17.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 24.00 cm
CY 8.00 cm
F1P 196.347 ppm
F1 14817.89 Hz
F2P -4.942 ppm
F2 -372.93 Hz
PPMCM 8.38704 ppm/cm
HZCM 632.95099 Hz/cm
OBn
BnO
BnO
Ph
O
92
BnO
OMe
35.383
55.294
61.941
68.634
70.702
71.603
72.734
73.401
73.664
74.706
76.657
77.081
77.392
77.505
78.132
78.302
82.996
97.635
98.829
101.403
126.051
127.295
127.465
127.494
127.601
127.679
127.978
128.115
128.154
128.248
128.290
128.346
128.462
128.613
129.048
137.681
138.889
139.114
ppm
0
20
40
60
80
100
120
140
160
180

Table for crystallographic and structural refinement parameters of compound **7**

Formula	$C_{44}H_{50}O_6$
Formula Weight	674.84
Crystal System	Orthorhombic
Space group	P212121
a/ Å	9.4392(3)
b/Å	12.6456(5)
c/ Å	31.178(1)
α/°	90
β/°	90
γ/°	90
V/ Å3	3721.5(2)
Z	4
D_c/ g cm^{-3}	1.204
μ /mm^{-1}	0.079
F(000)	1448
θ range/°	1.3 - 27.6
Reflections collected	65116
Unique reflections	8626
Reflections $I > 2\sigma(I)$	5376
R_{int}	0.092
goodness-of-fit (F^2)	1.03
$R1$ ($I > 2\sigma(I)$) [a]	0.0605
$wR2(I > 2\sigma(I))$ [a]	0.1635
Δρ min / max /e Å^3	-0.43, 0.36

[a] $R_1 = \Sigma \left| |F_o| - |F_c| \right| / \Sigma |F_o|$, $wR_2 = [\Sigma (w (F_o^2 - F_c^2)^2) / \Sigma w (F_o^2)^2]^{½}$