

Supporting Information

Total syntheses of disulphated glycosphingolipid SB1a and the related monosulphated SM1a

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Hideharu Ishida,^a Ten Feizi,^c and Makoto Kiso,^{*,a,b}**

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and

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Du Cane Road, London W12 0NN, UK*

Contents

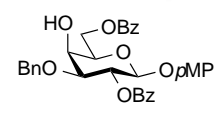
1. Copies of ¹H and ¹³C NMR spectra of new compounds

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7.430
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7.194
7.188
7.174
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6.587
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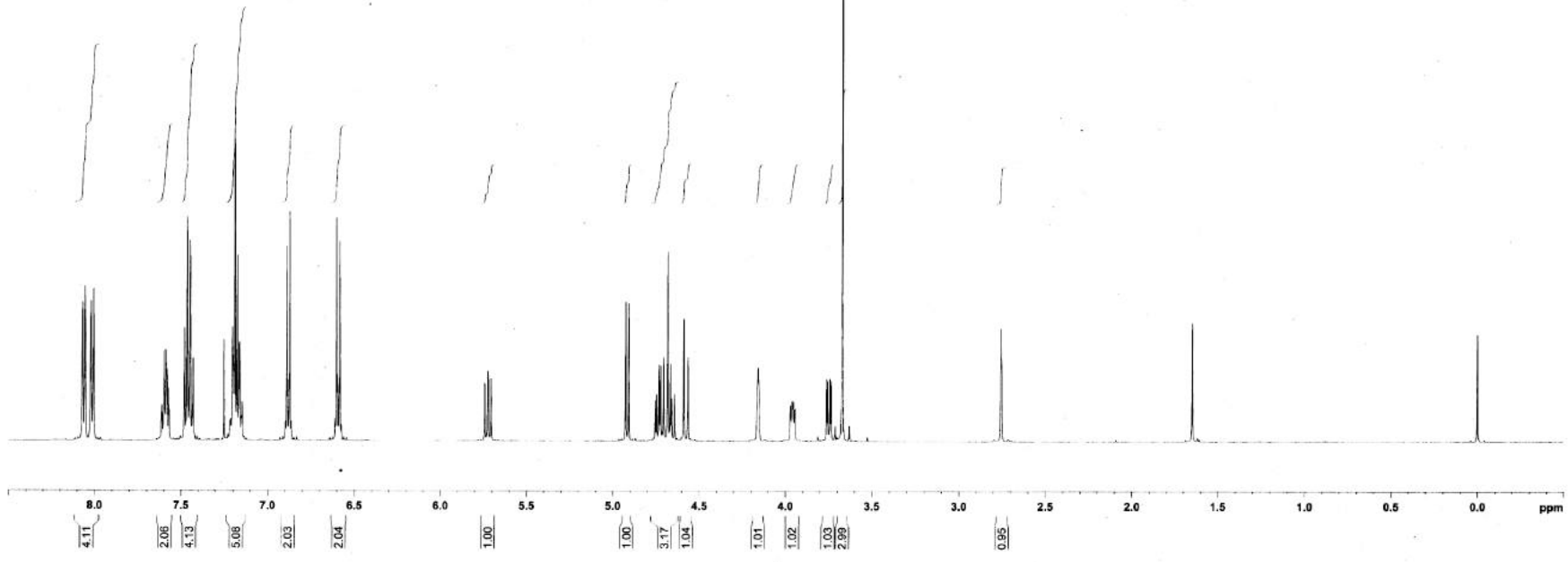
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3.755
3.742
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2.755



9



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165.32

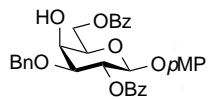
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118.77
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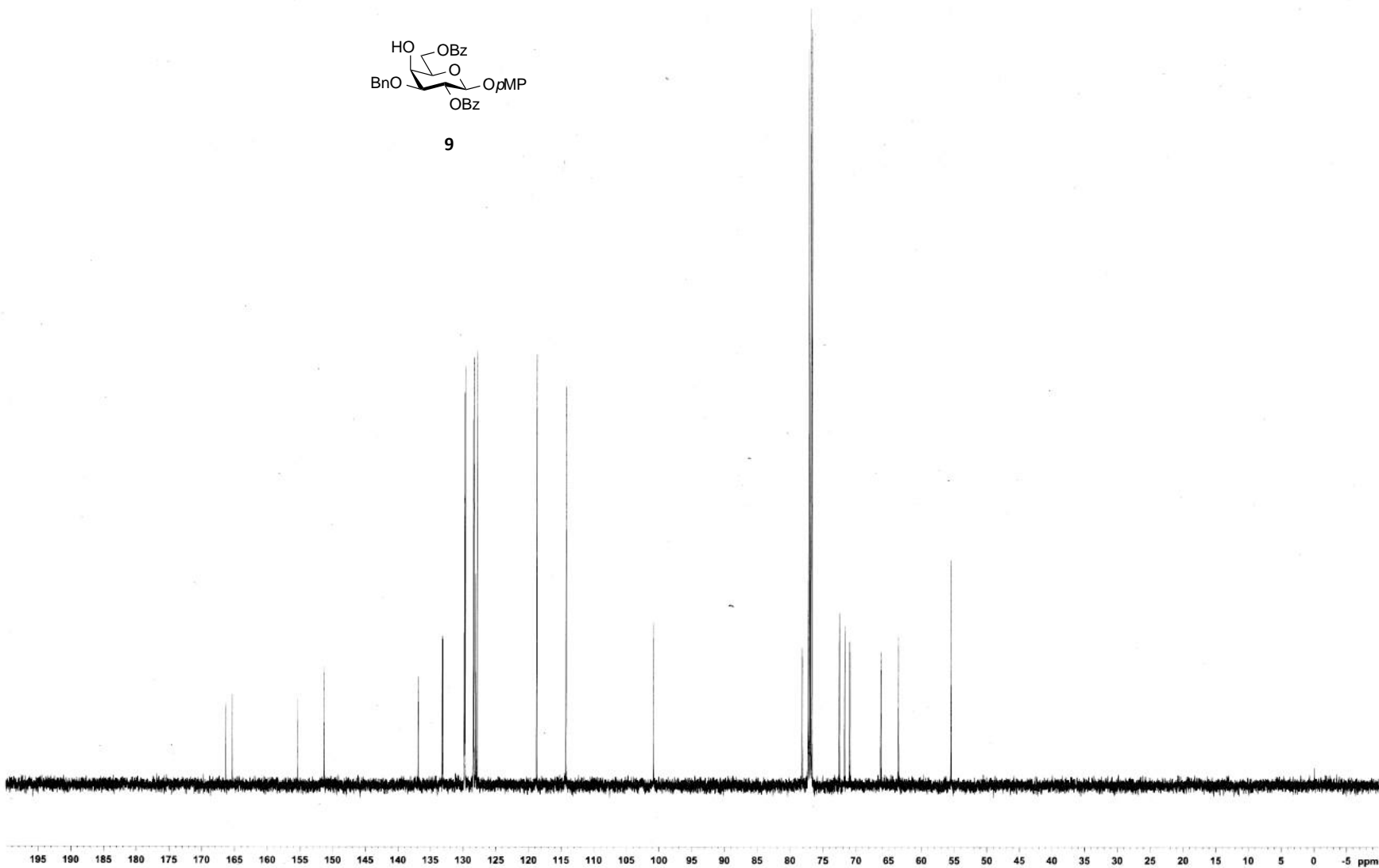
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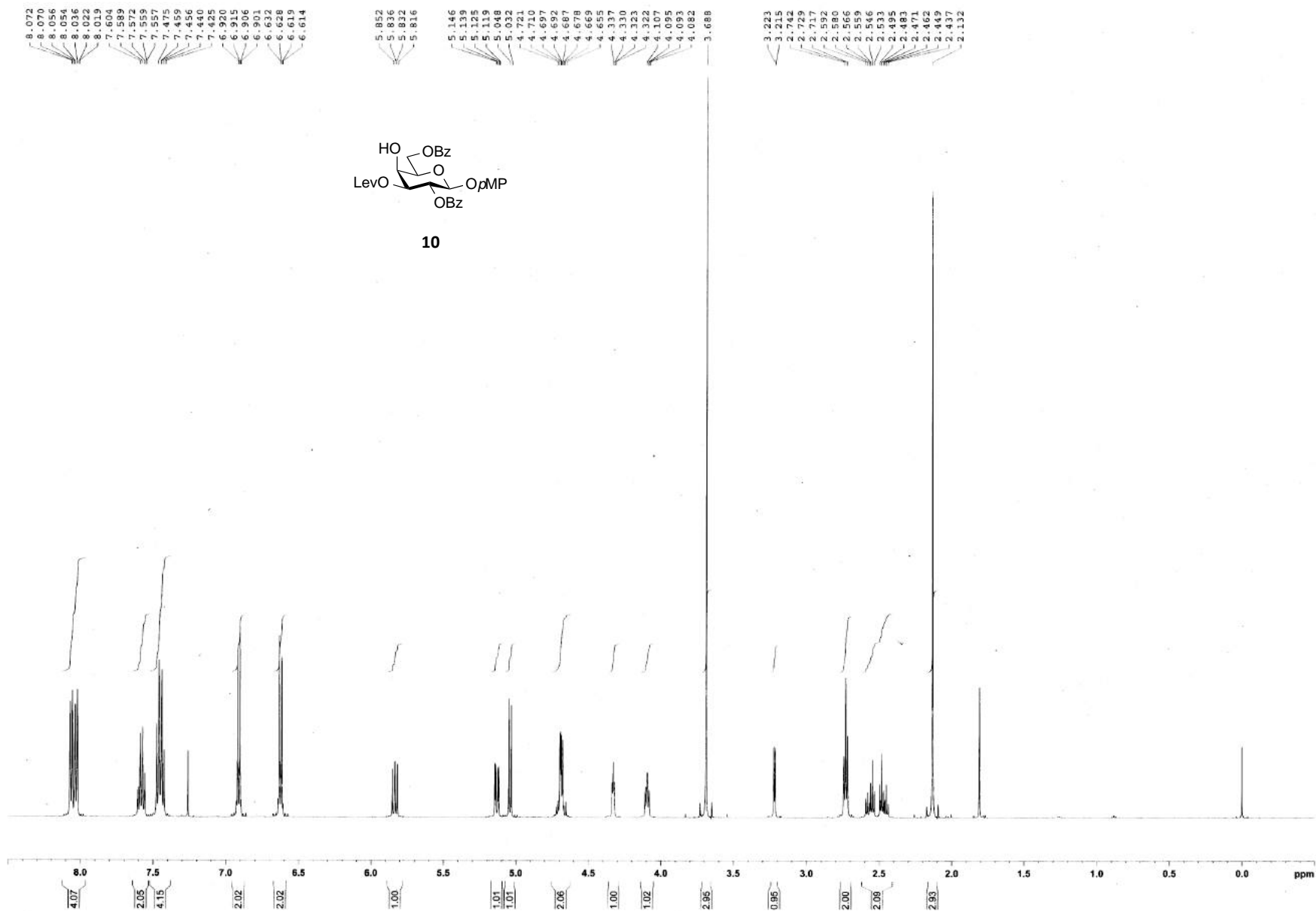
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71.75
70.99
66.19
63.55

55.51



9





—208.00

—171.89

—166.25

—165.28

—155.53

—151.21

—133.25

—133.19

—129.78

—129.74

—129.53

—128.43

—128.40

—118.88

—114.33

—101.03

—74.08

—72.81

—69.41

—66.64

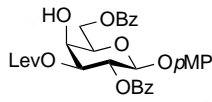
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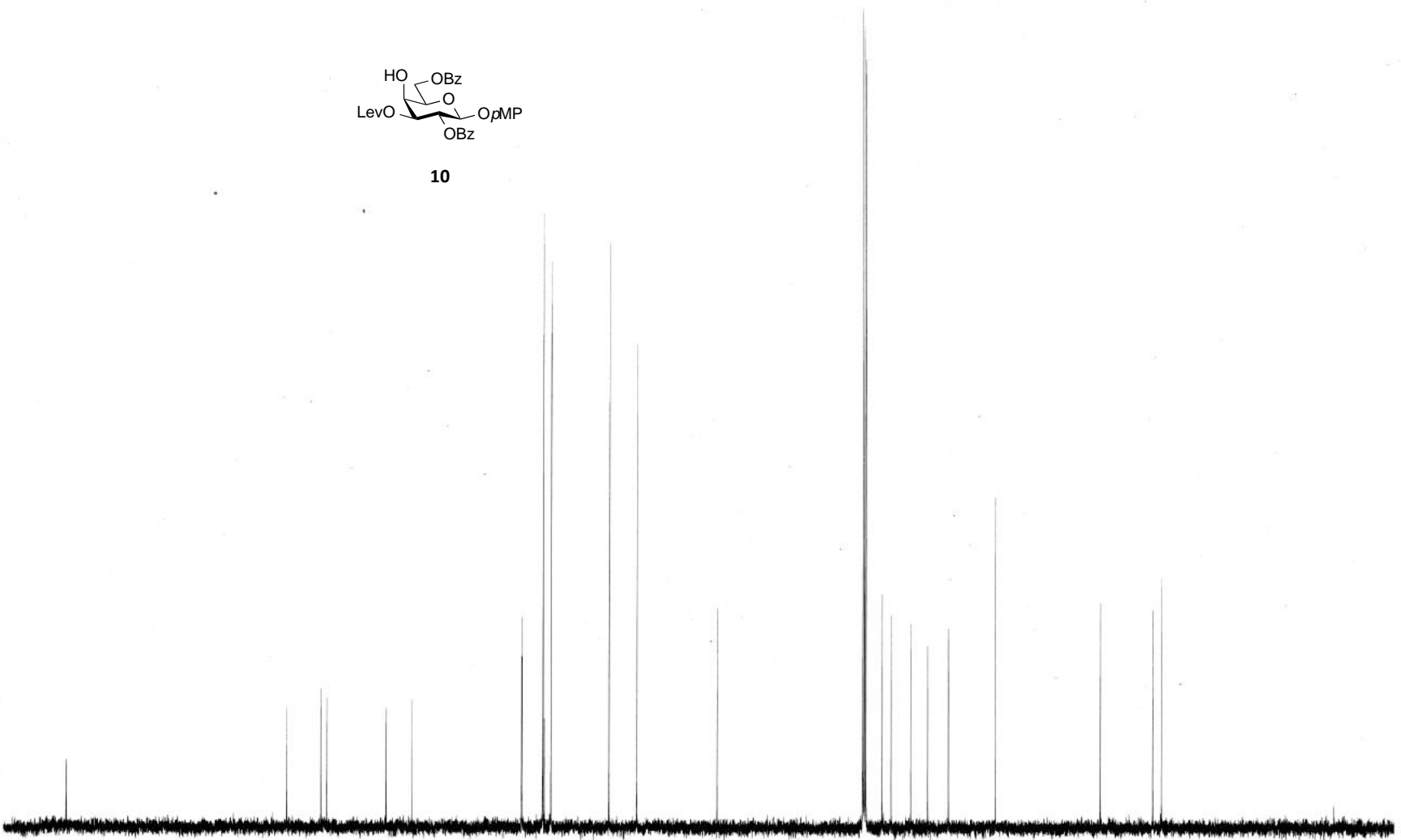
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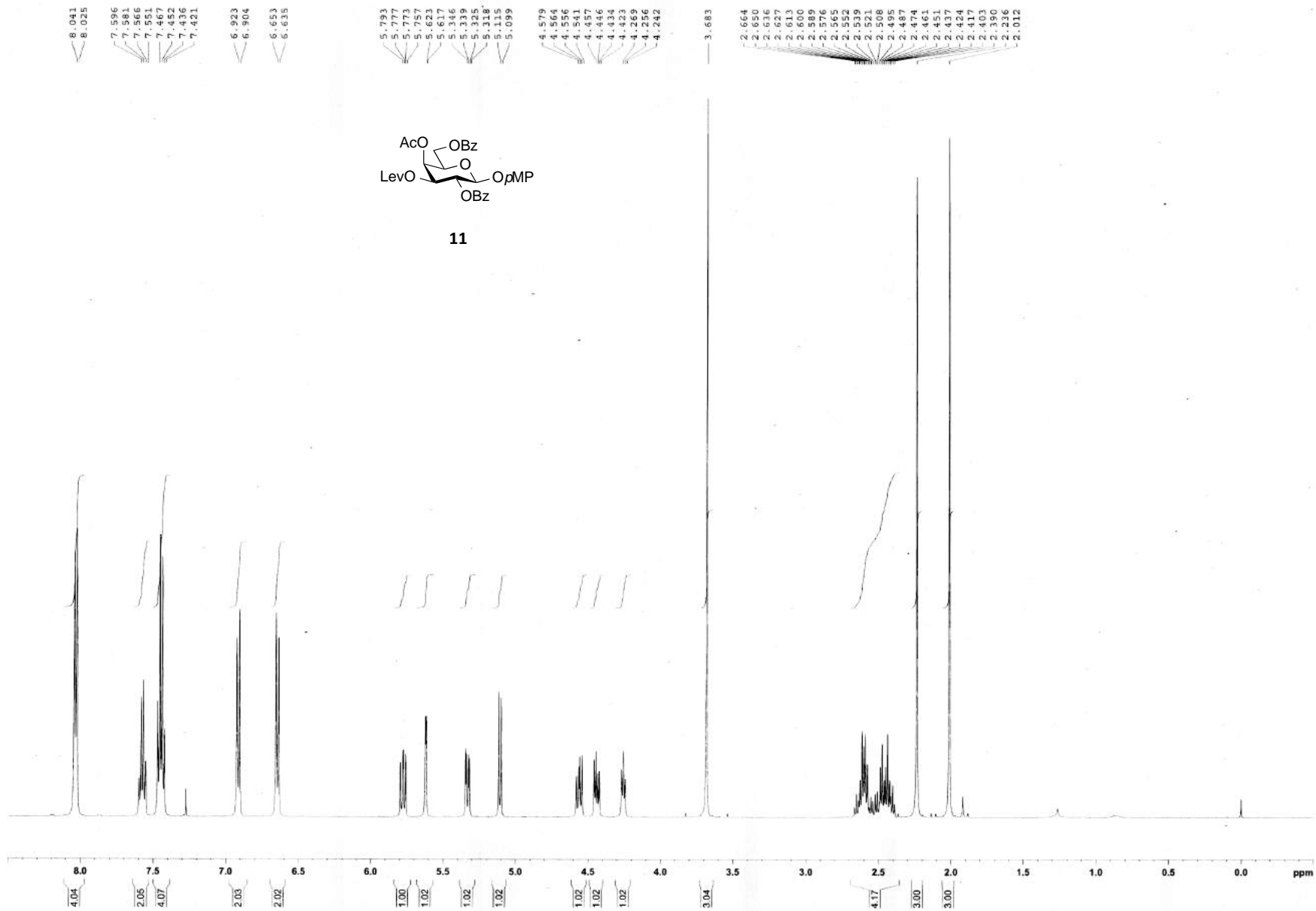
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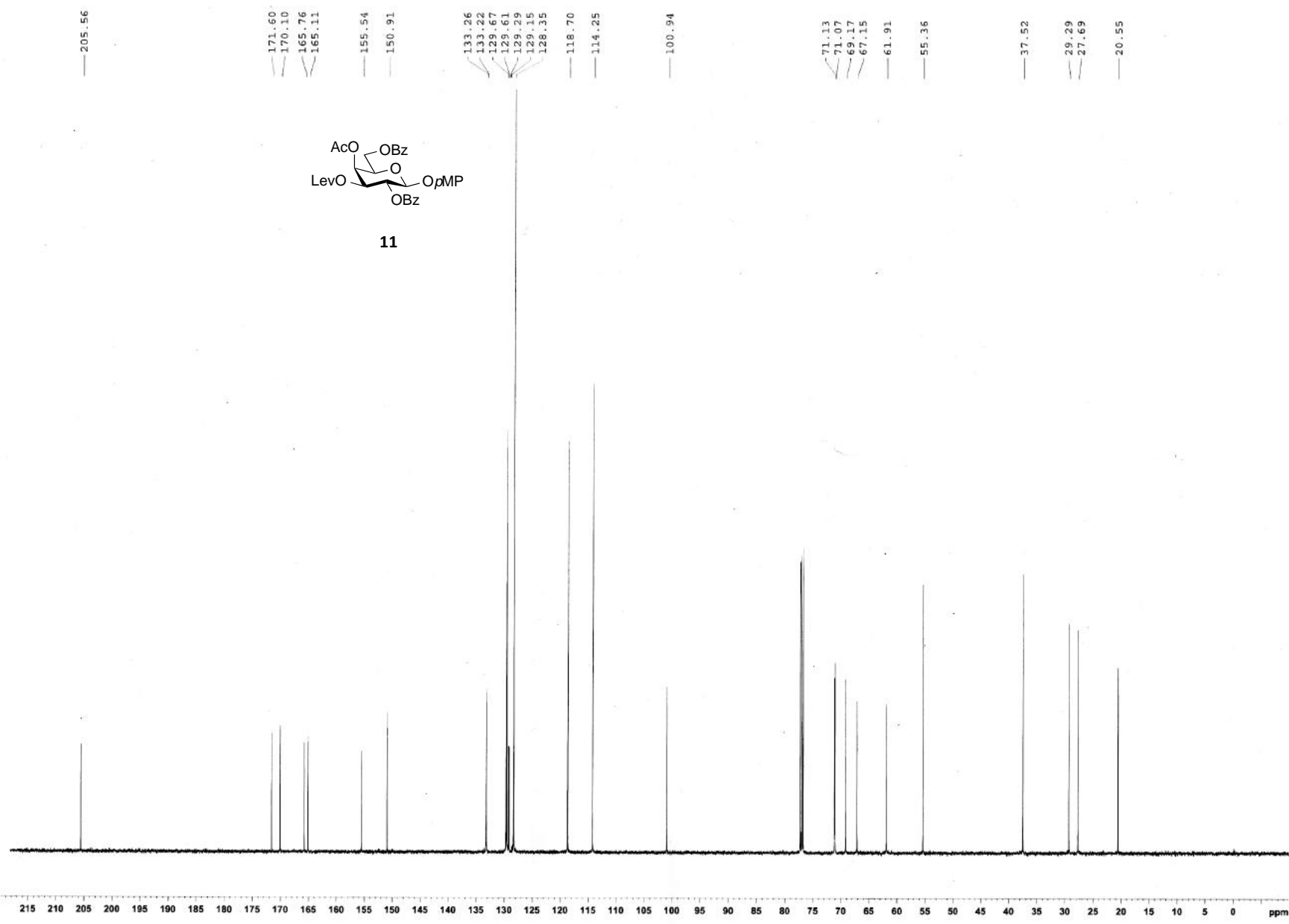


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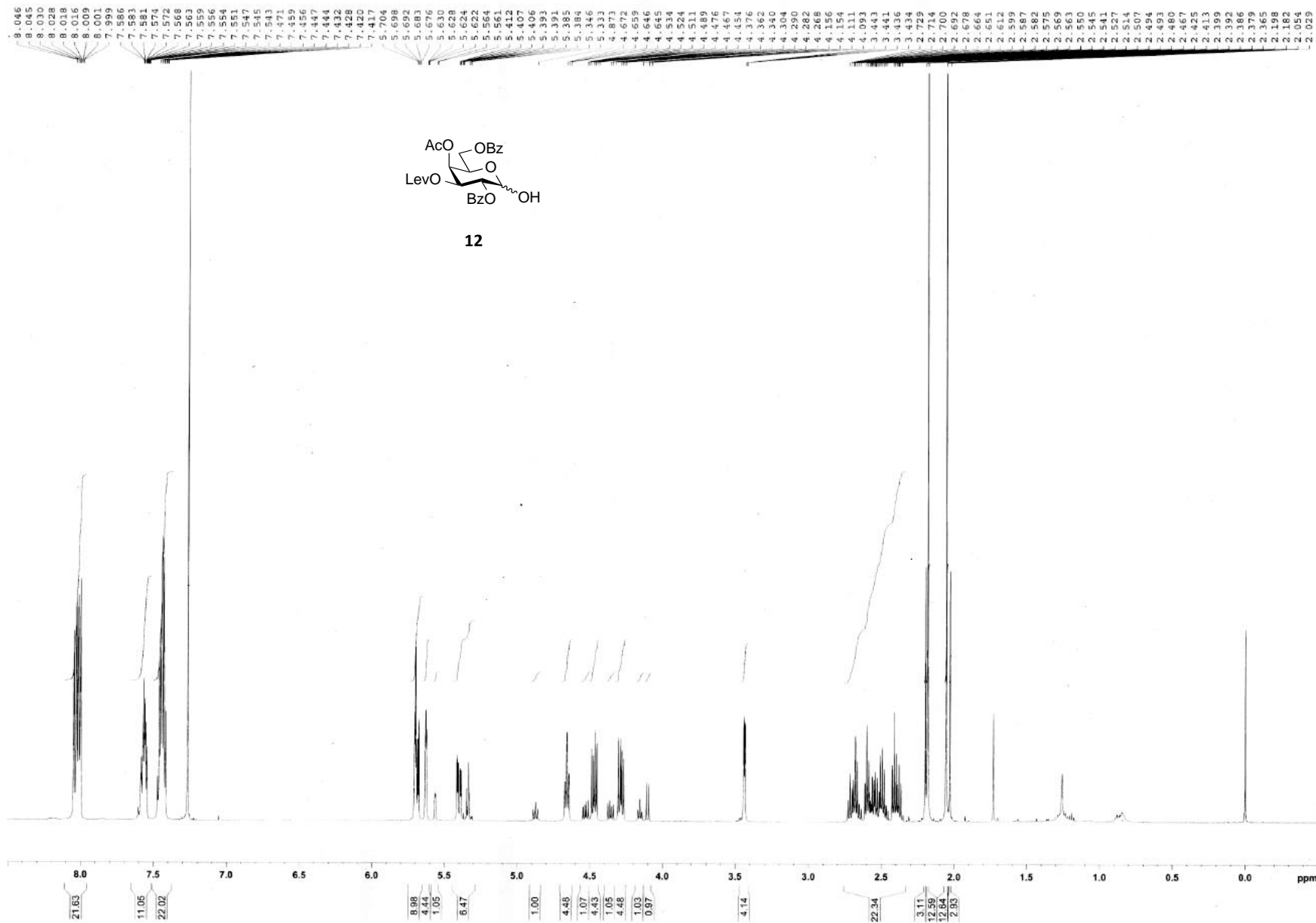
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11

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—206.01

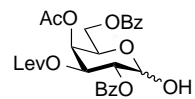
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166.01

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128.43

96.17
90.85

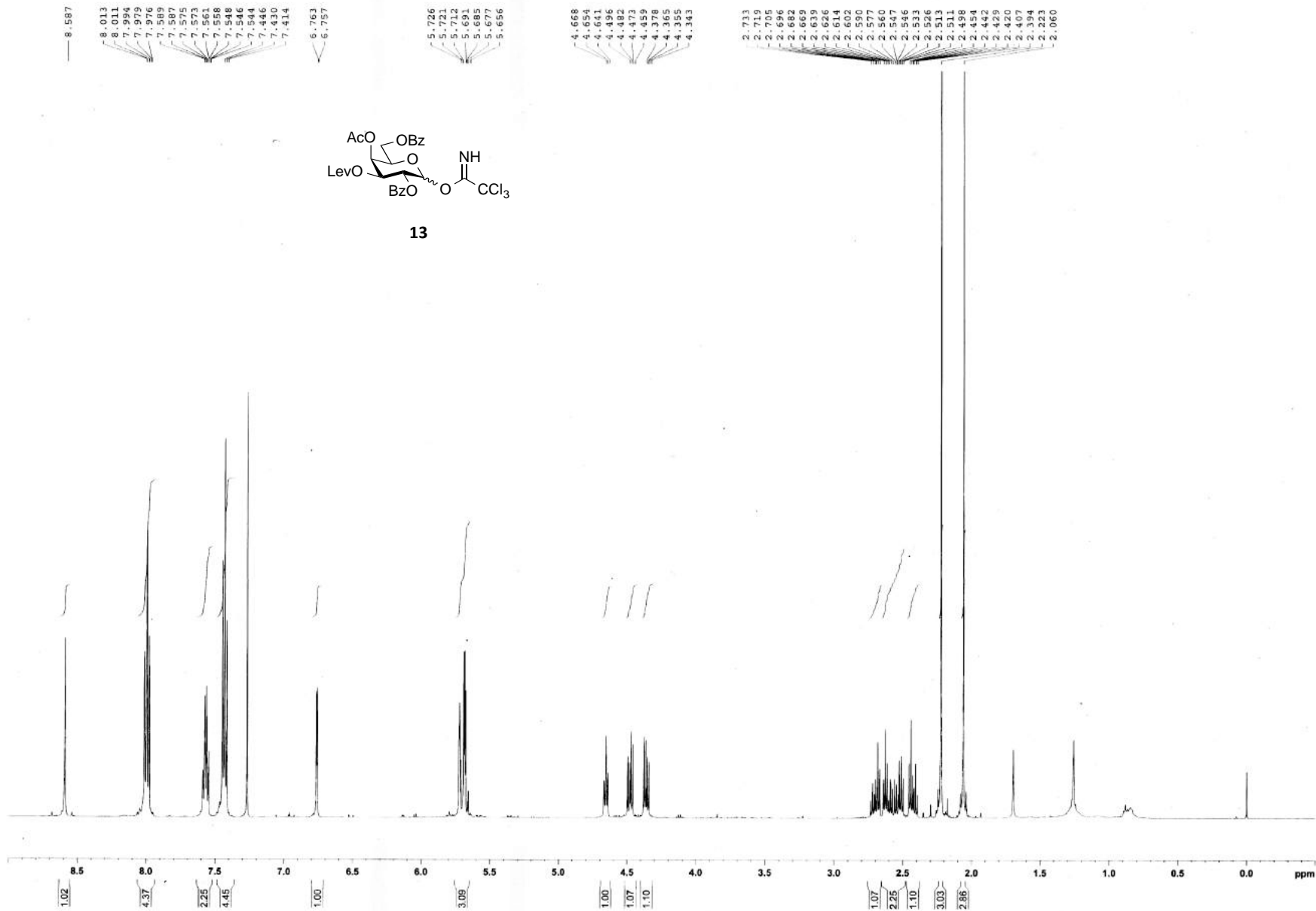
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68.44
67.48
67.38
66.37
62.09
61.78

37.74
37.66
29.56
29.47
27.80
27.70
20.68
20.64



12

215 210 205 200 195 190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 ppm



—205.76

171.74
170.06
165.84
165.54
160.50

133.57
133.26
129.87
129.69
129.30
128.73
128.45
128.38

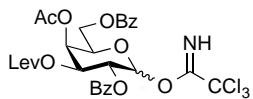
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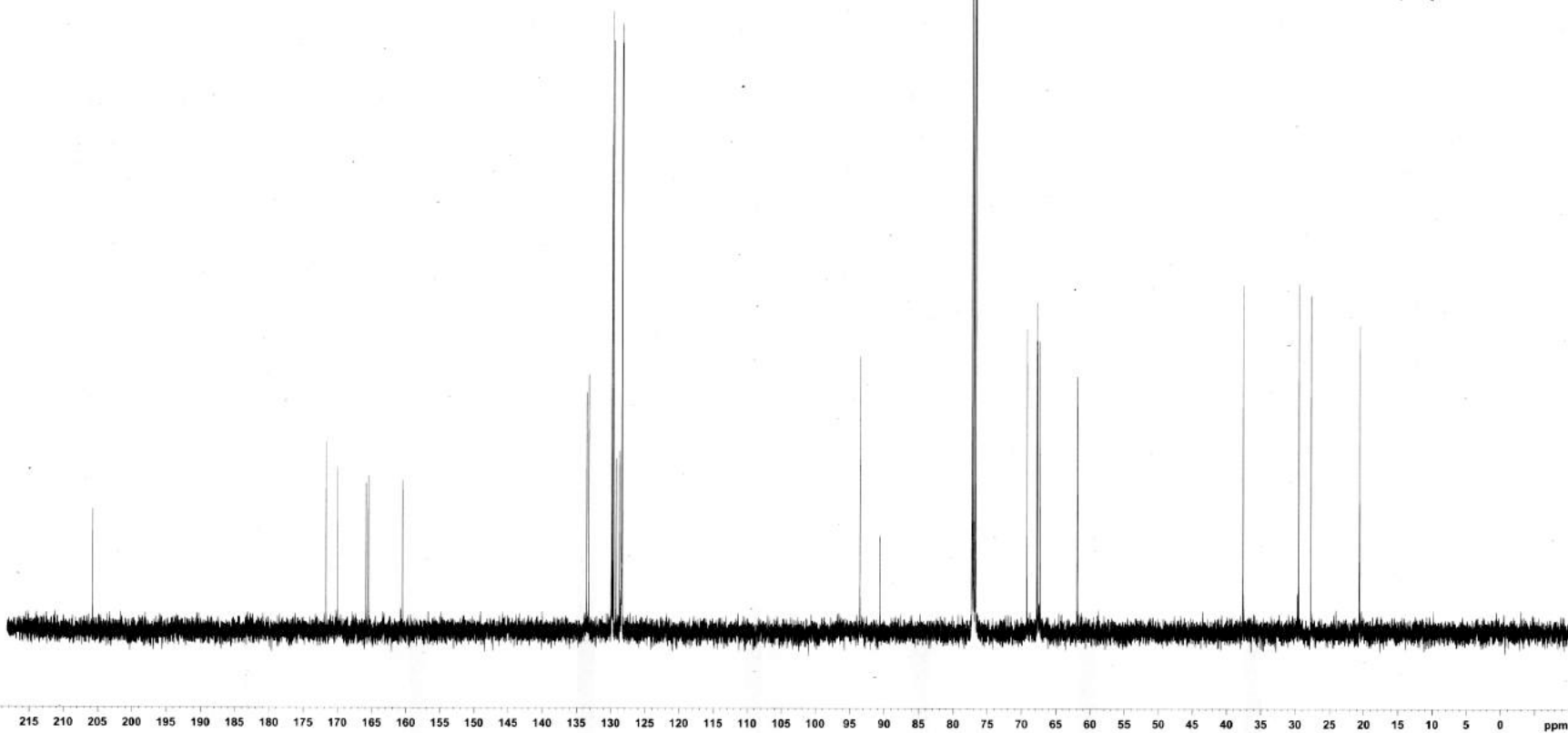
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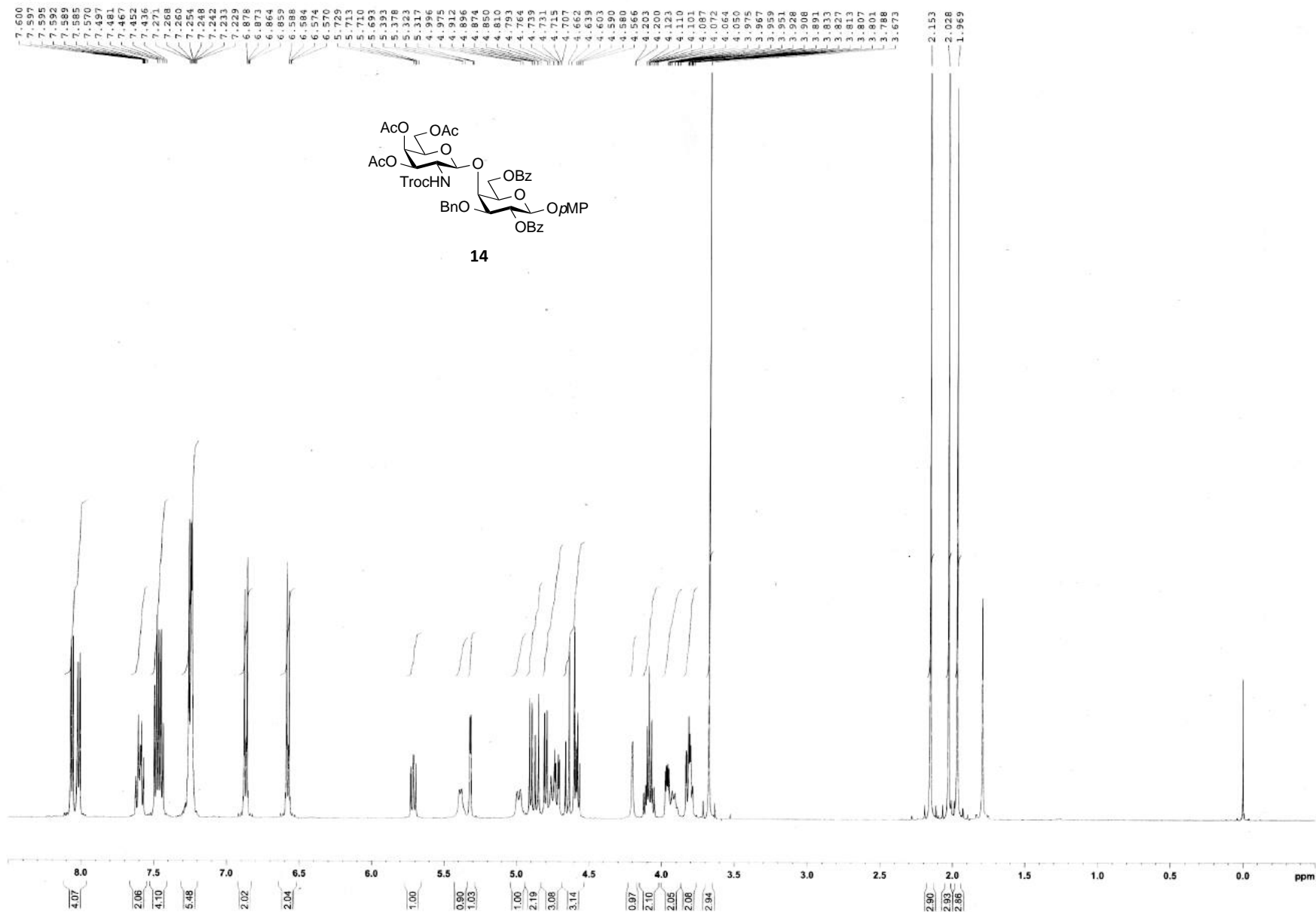
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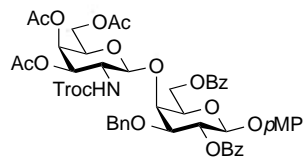


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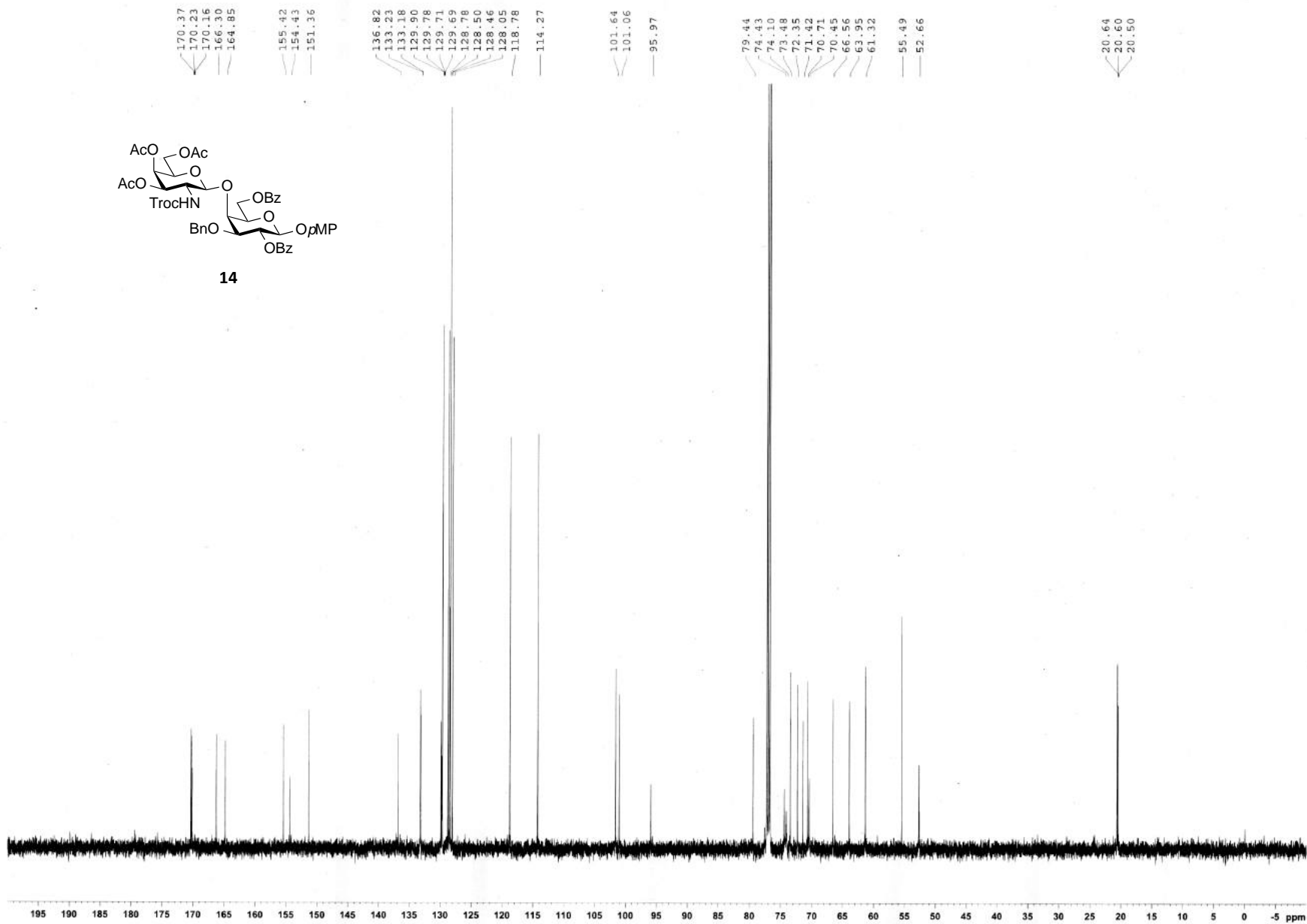


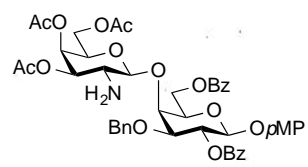
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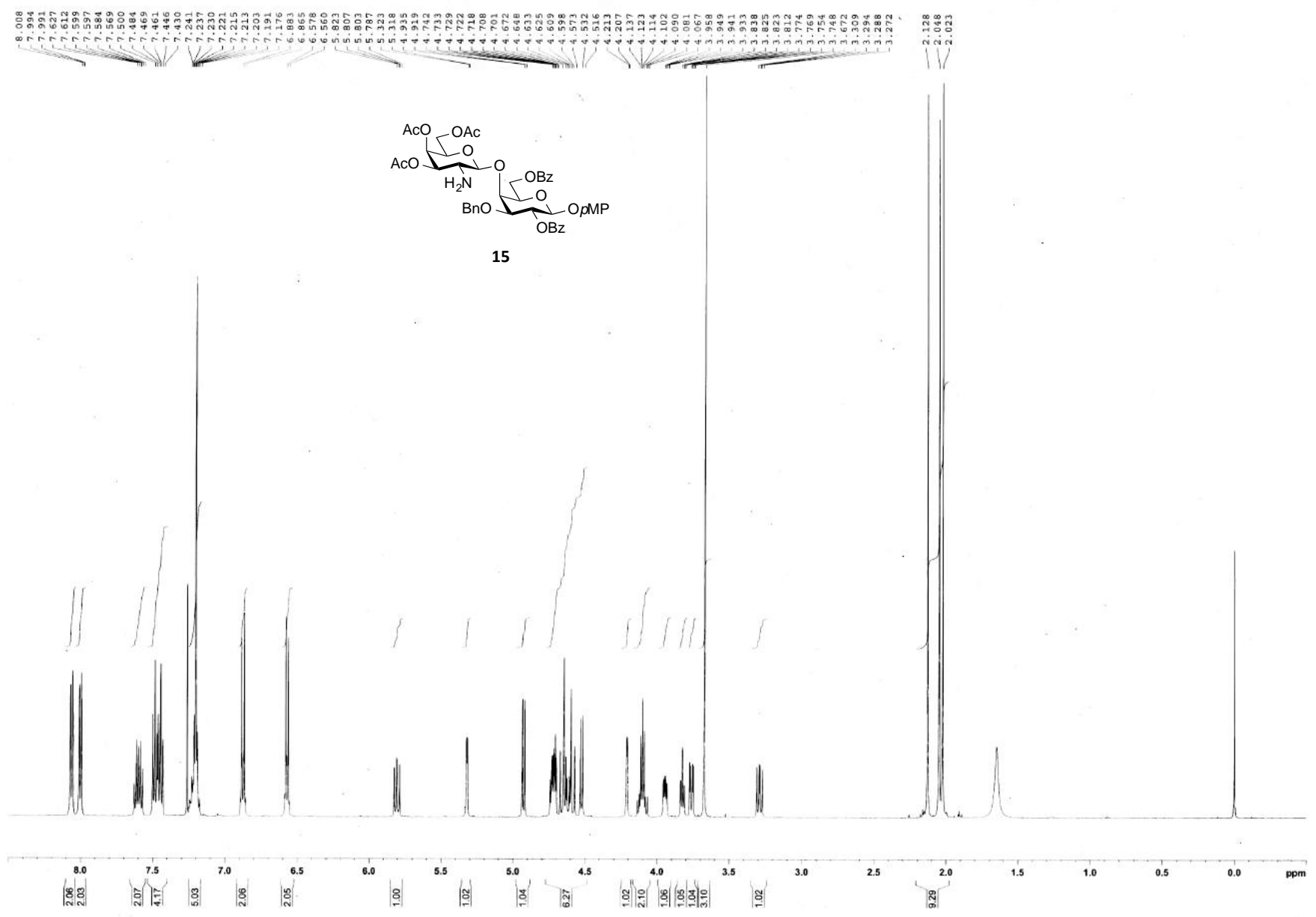


14





15



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170.33
166.59
165.18

155.38
151.36

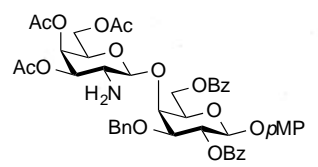
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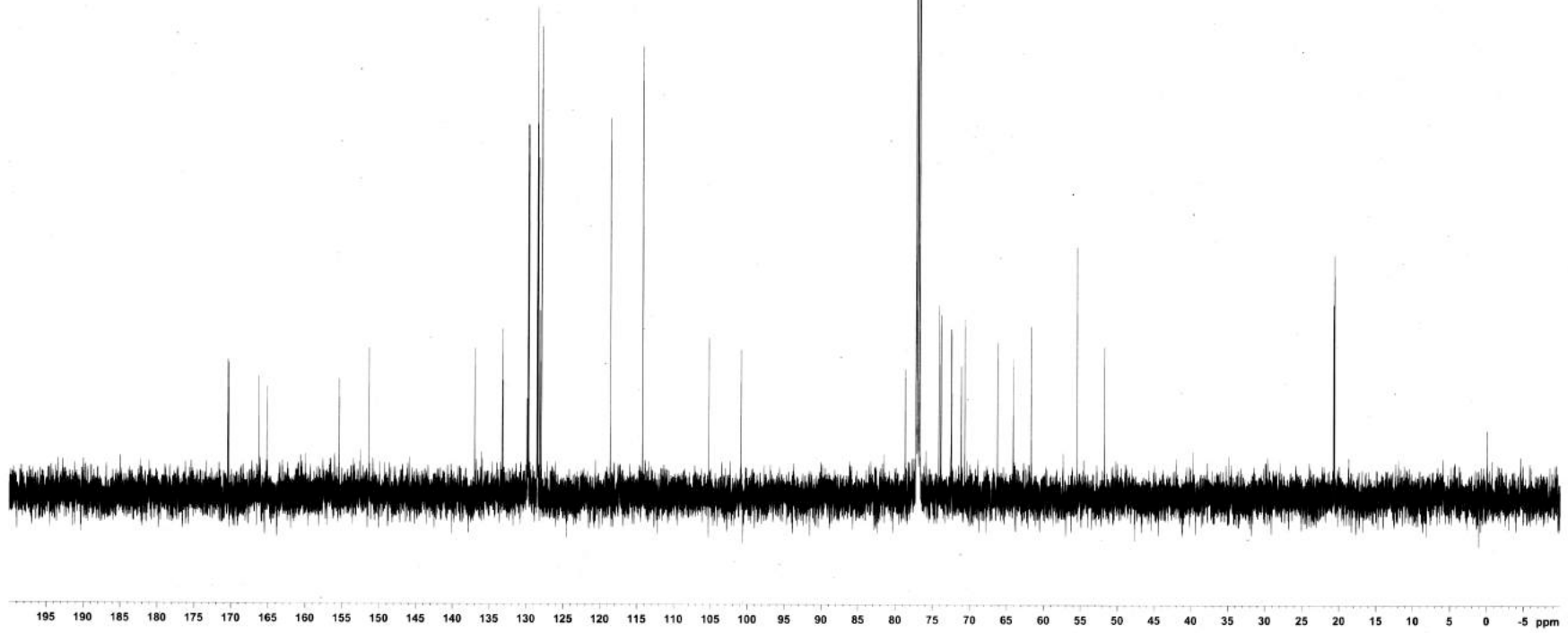
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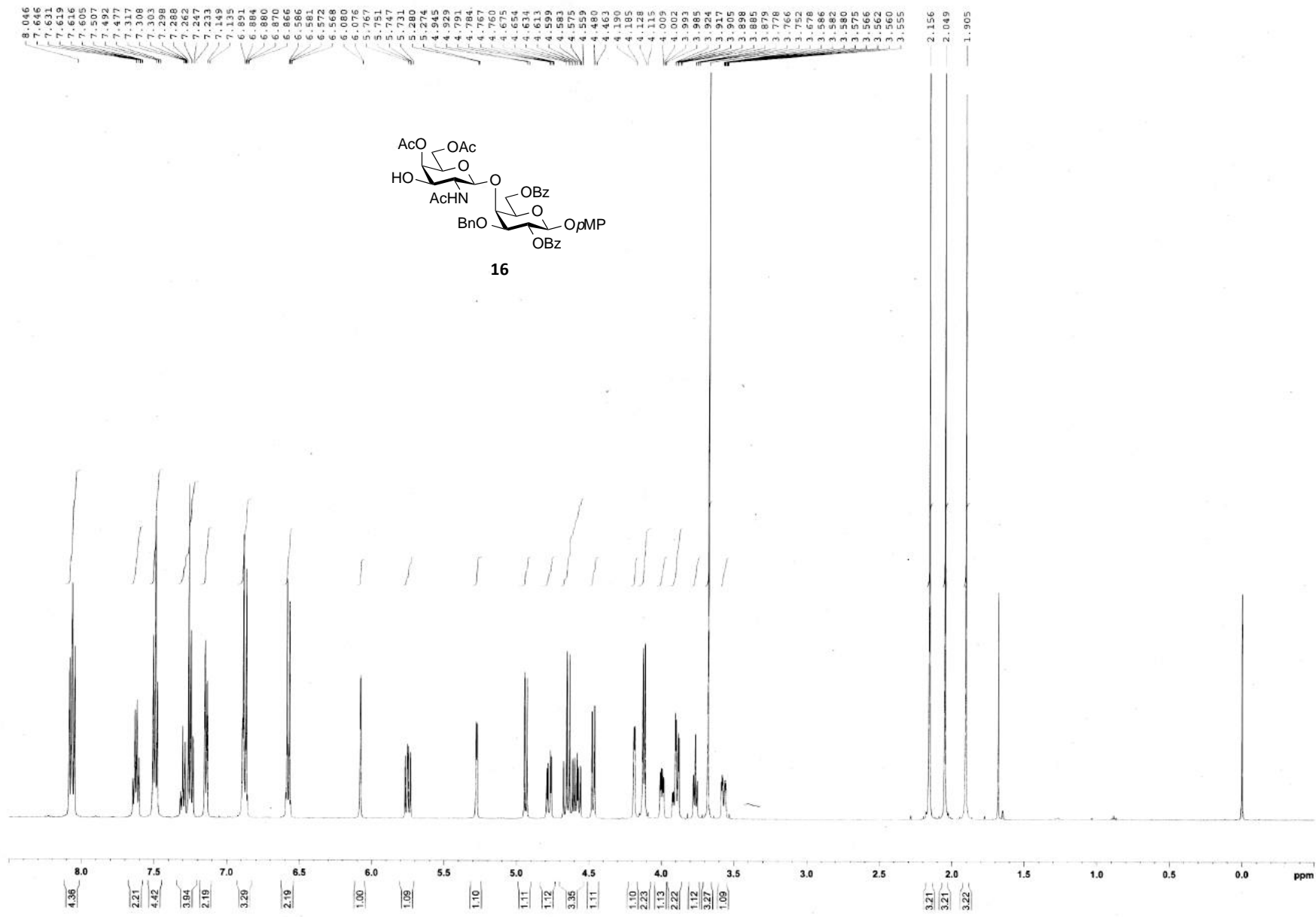
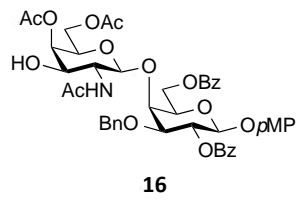
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20.75
20.67
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15





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170.41
166.36
165.08

155.51
151.16

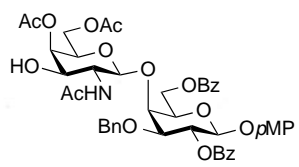
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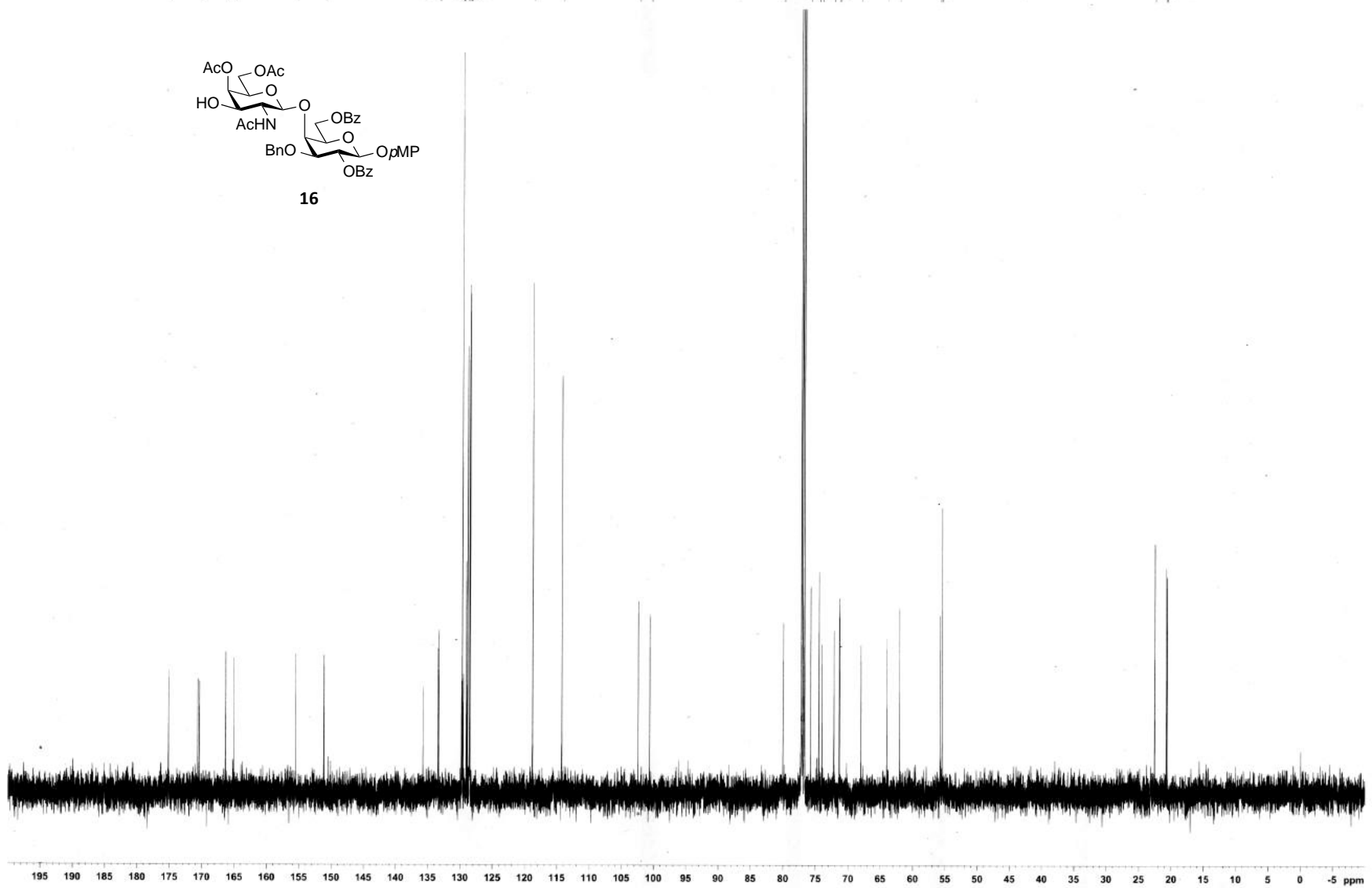
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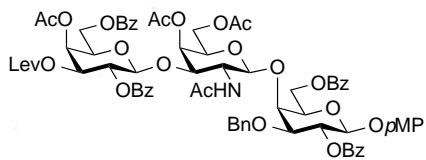


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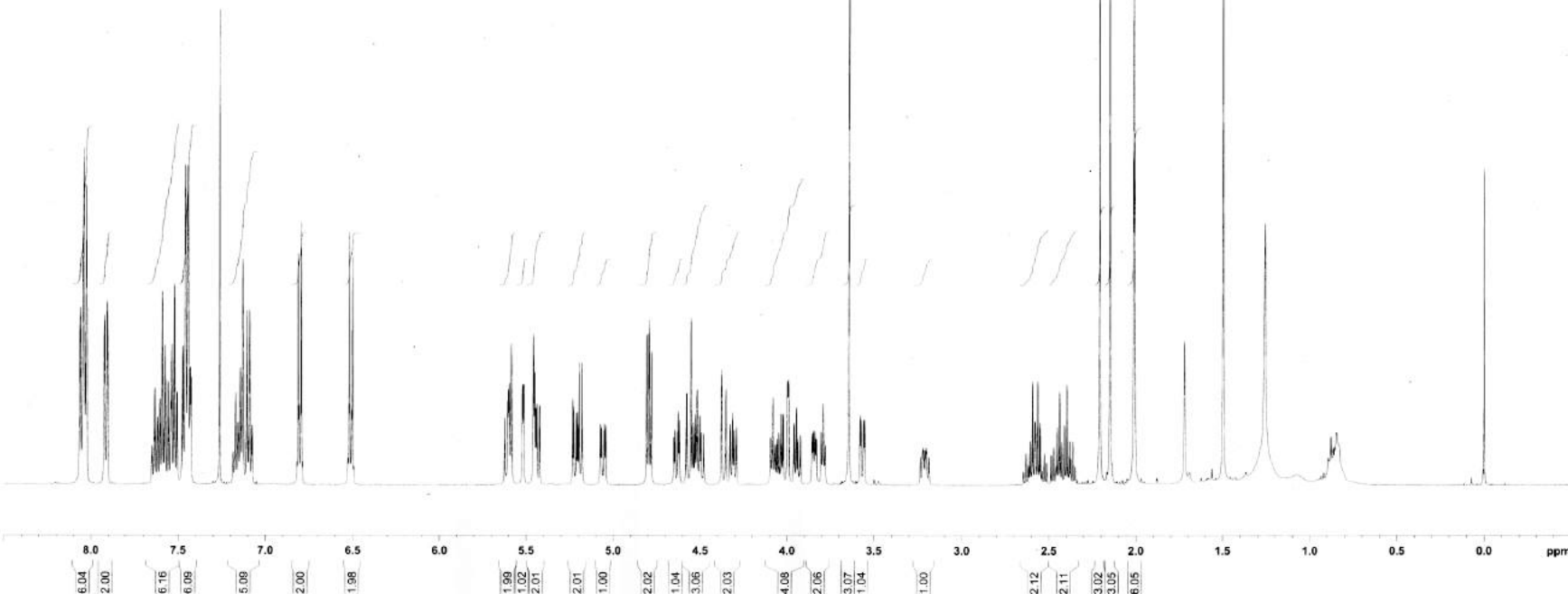


195 190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 ppm

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8.022
7.921
7.907
7.904
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7.604
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7.505
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5.423
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5.196
5.180
5.073
5.066
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4.792
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4.643
4.626
4.619
4.577
4.552
4.539
4.529
4.517
4.502
4.495
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4.352
4.328
4.314
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4.082
4.047
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4.024
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3.993
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3.924
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3.804
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2.579
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2.438
2.402
2.397
2.100
2.100



18



—205.67

172.63
171.71
170.47
170.28
169.91
166.25
165.84
165.10
164.97

—155.33

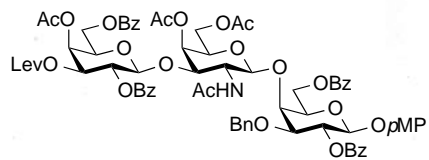
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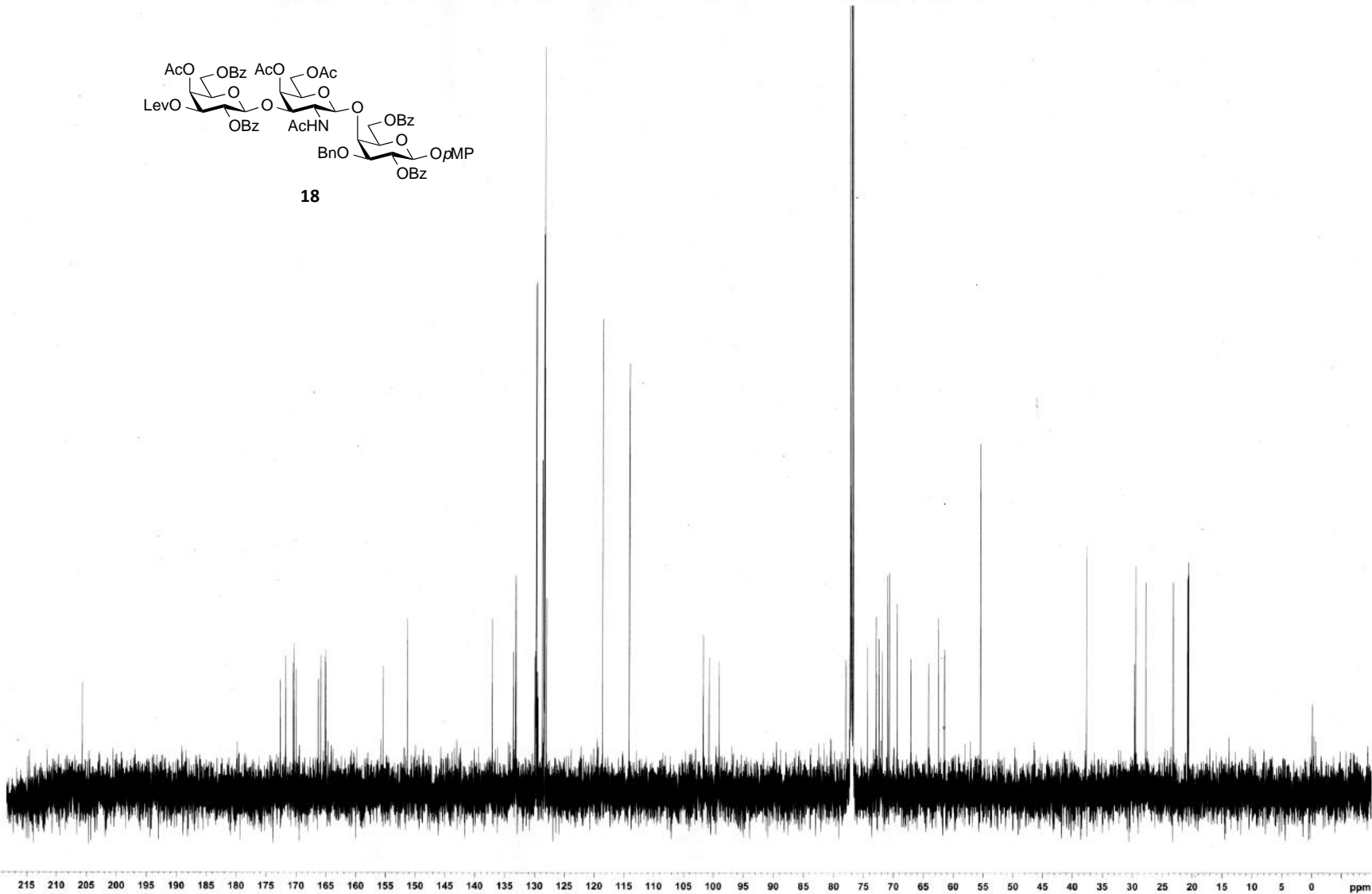
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55.46

—37.70

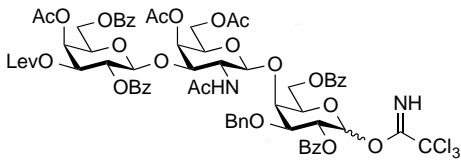
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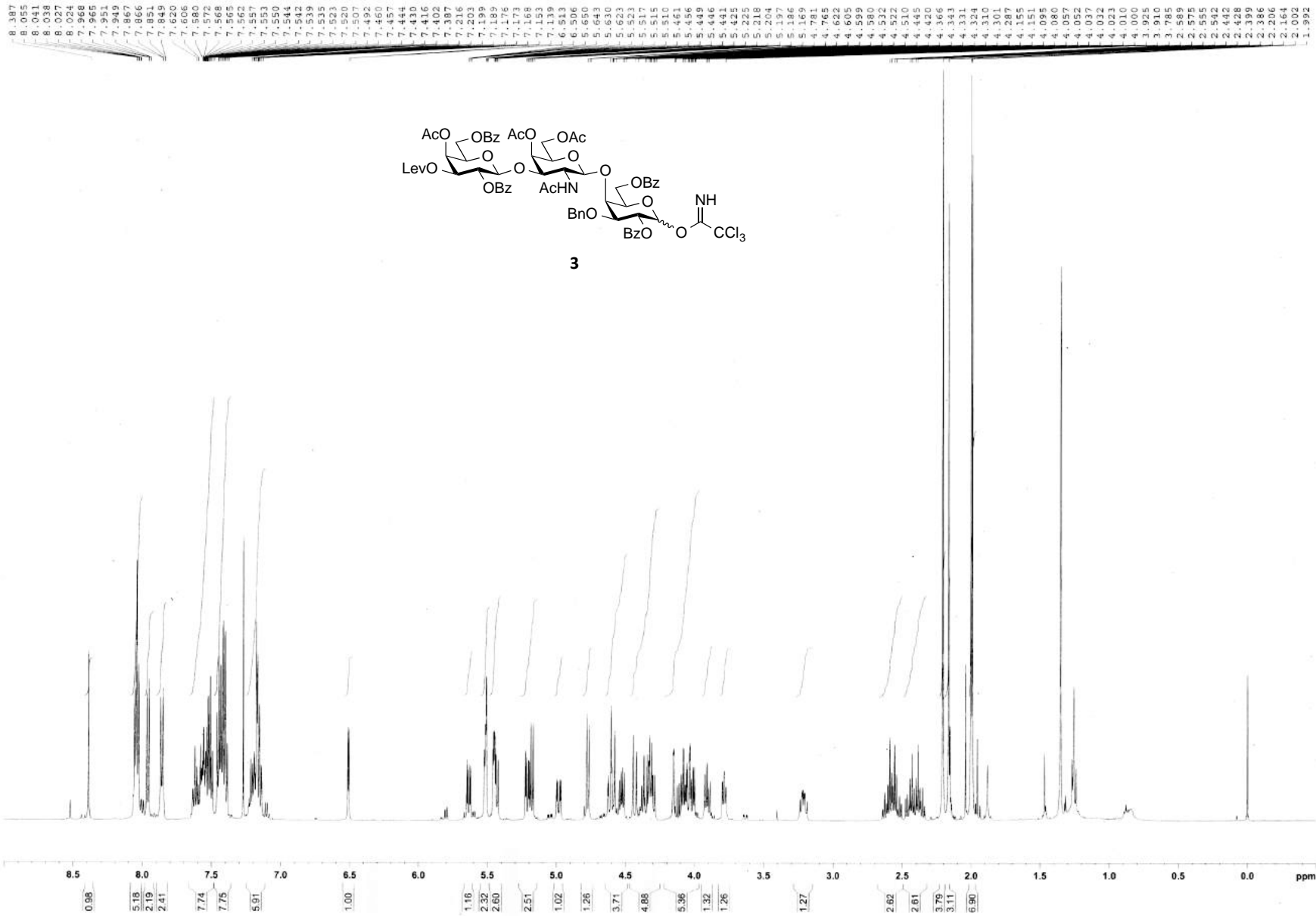
18



215 210 205 200 195 190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 ppm



3



—205.65

172.08
171.66
170.43
170.21
169.89
166.21
165.79
165.30
164.91
160.21

137.10
133.47
133.30
133.14
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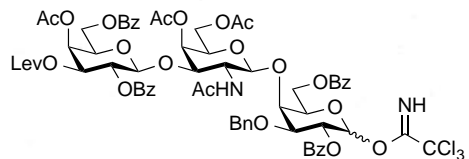
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—37.63

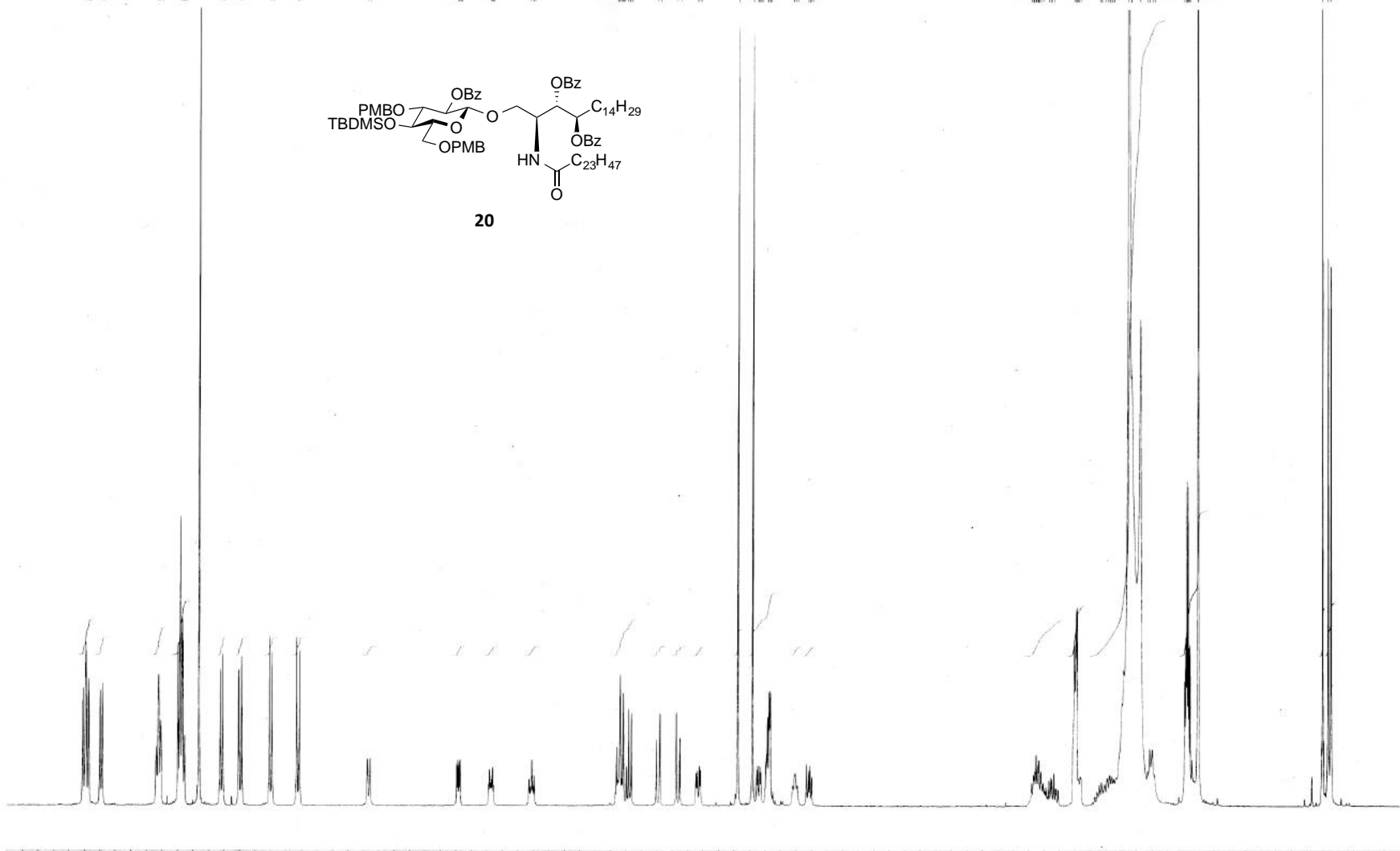
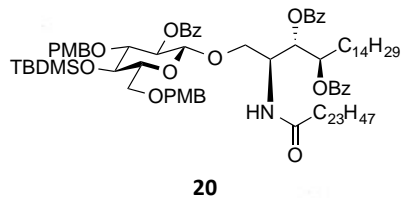
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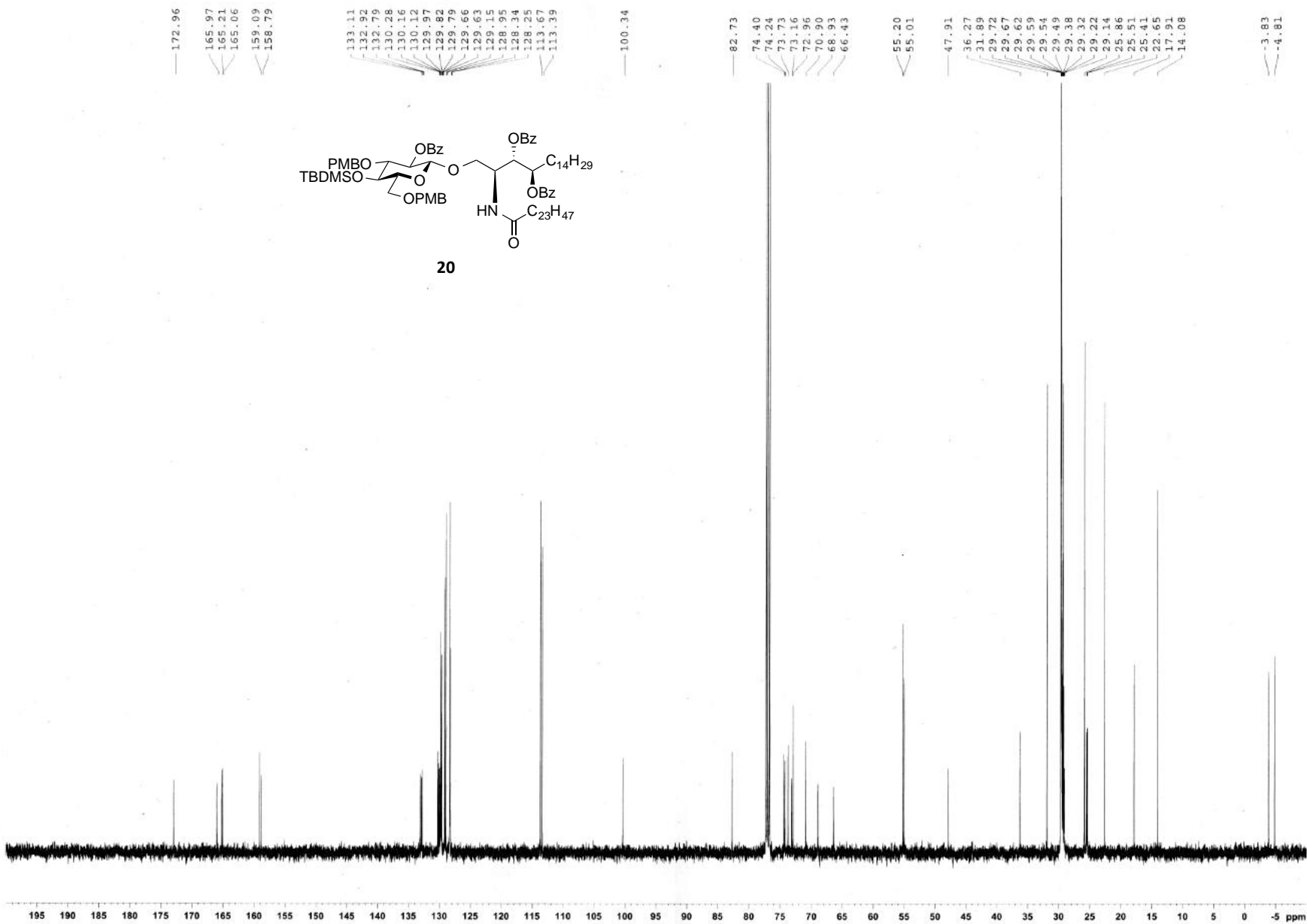
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 7.971
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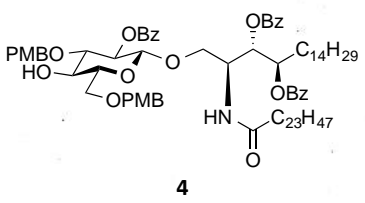


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 1.00
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 1.00
 4.06
 1.03
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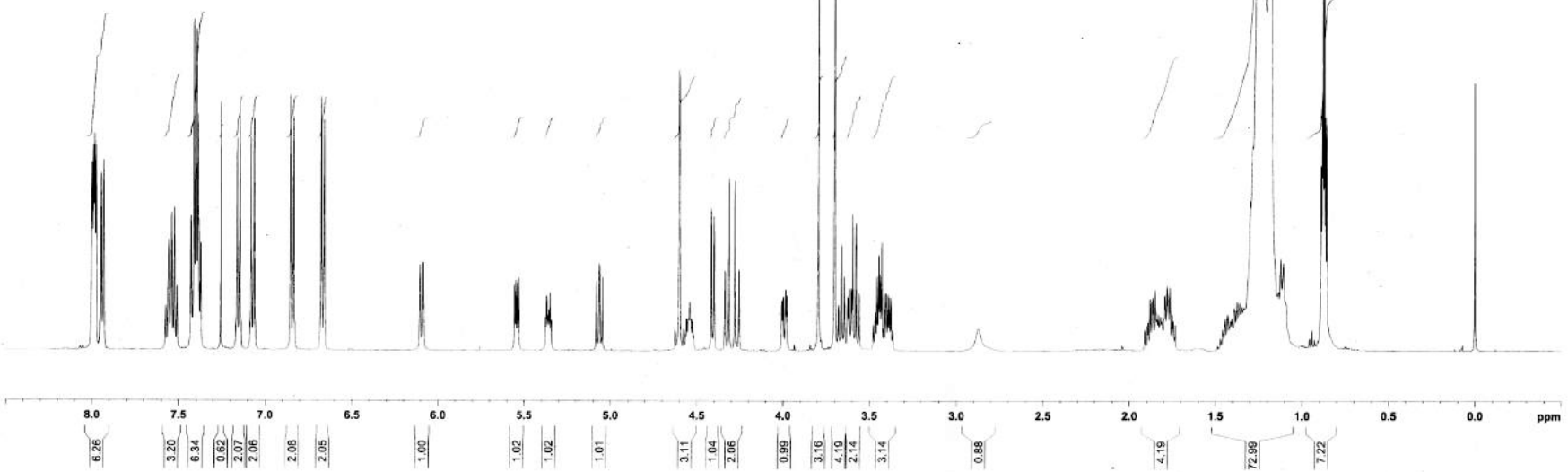
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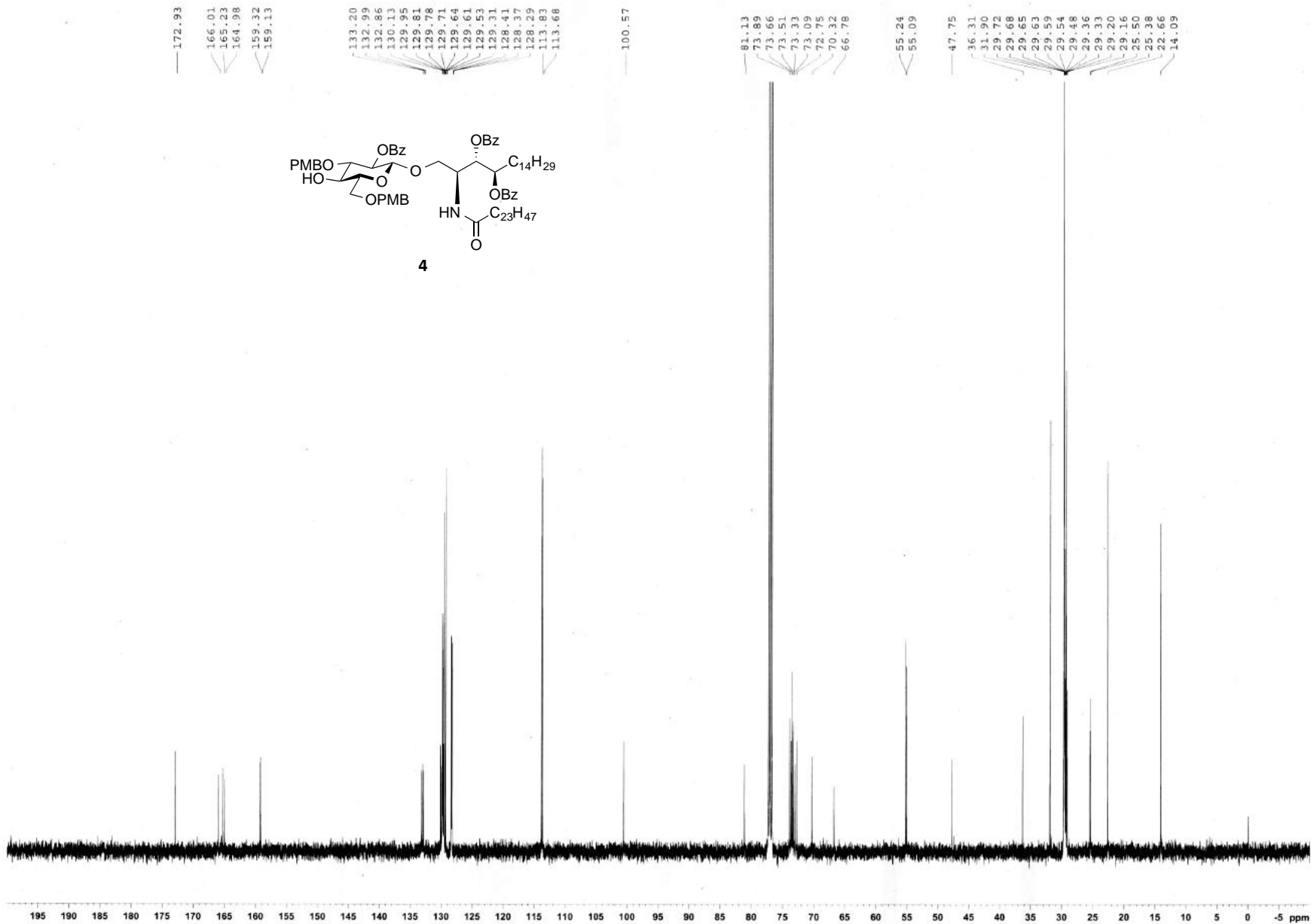


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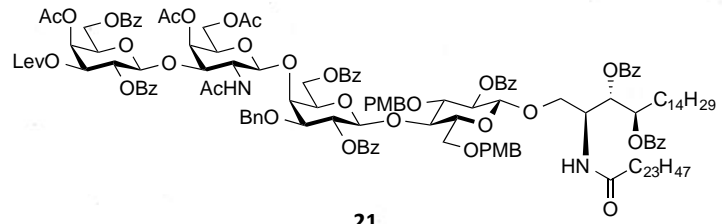


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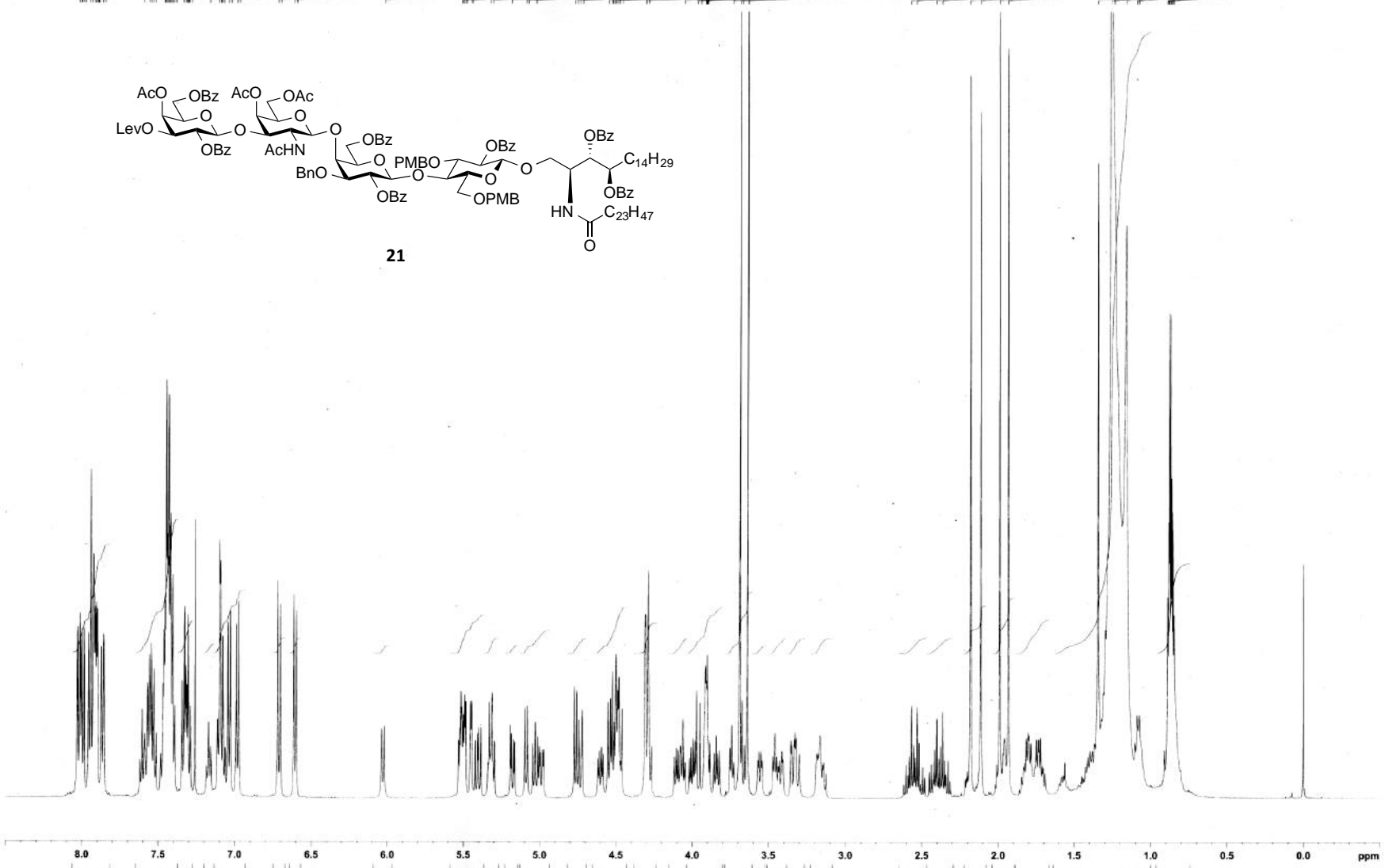




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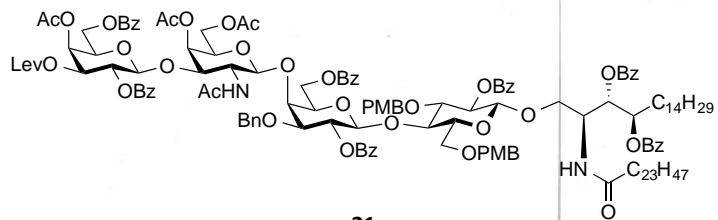
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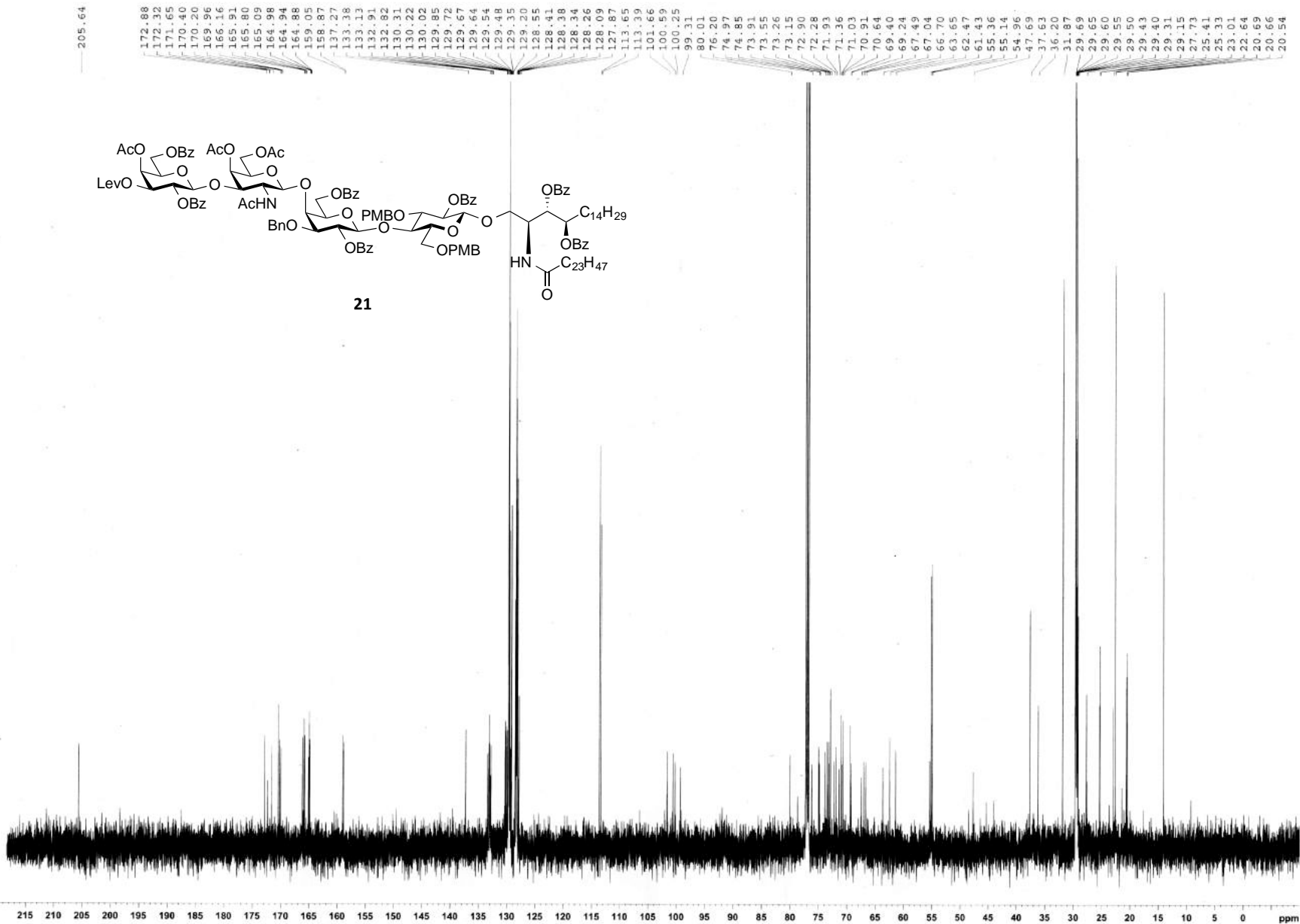
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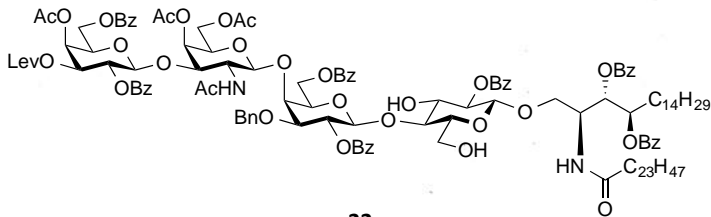
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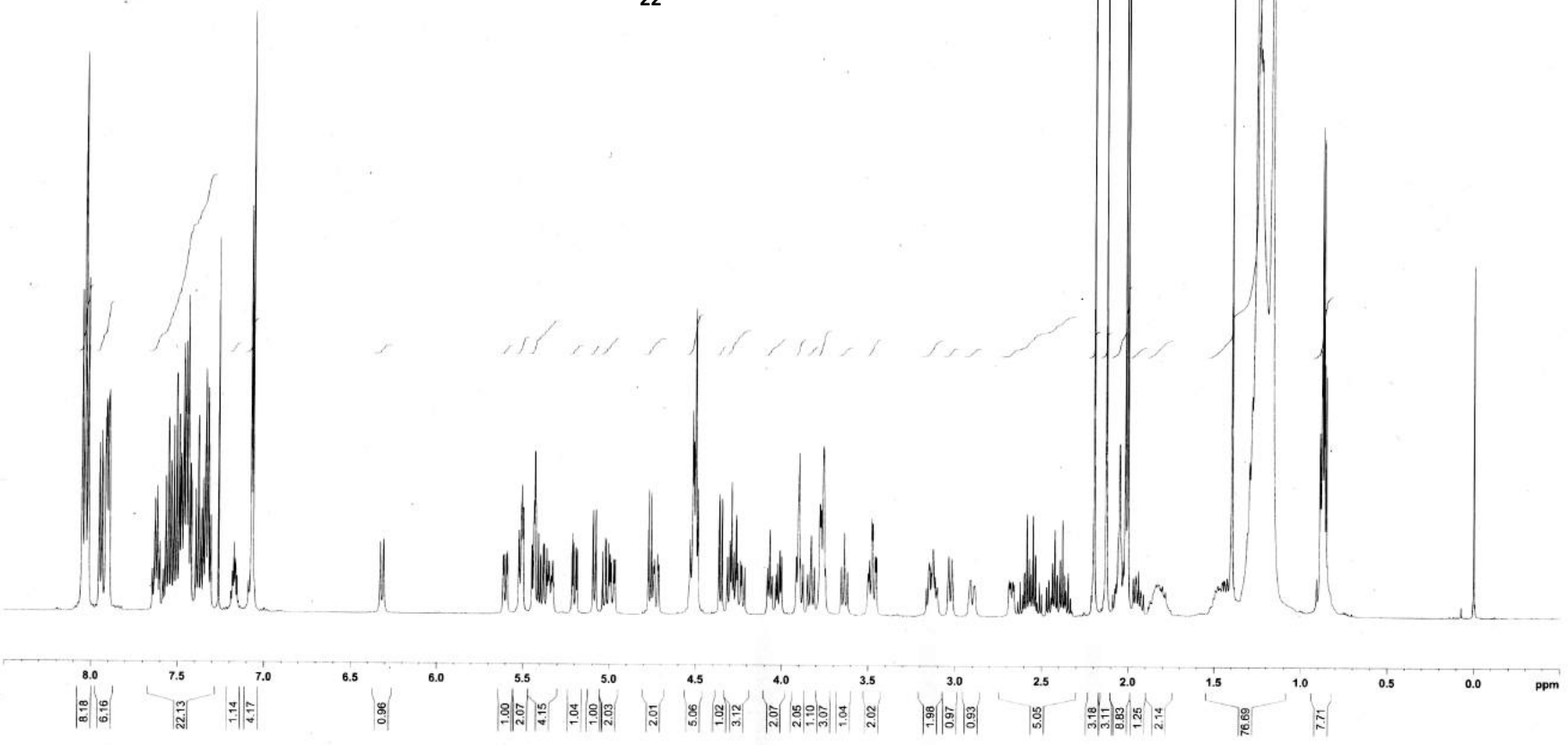
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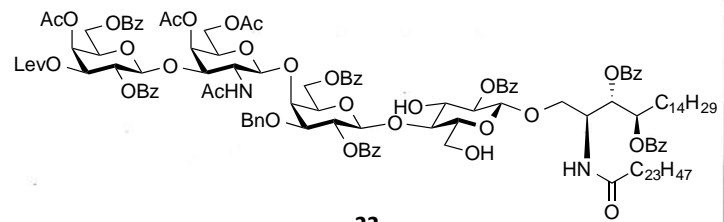


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22





22

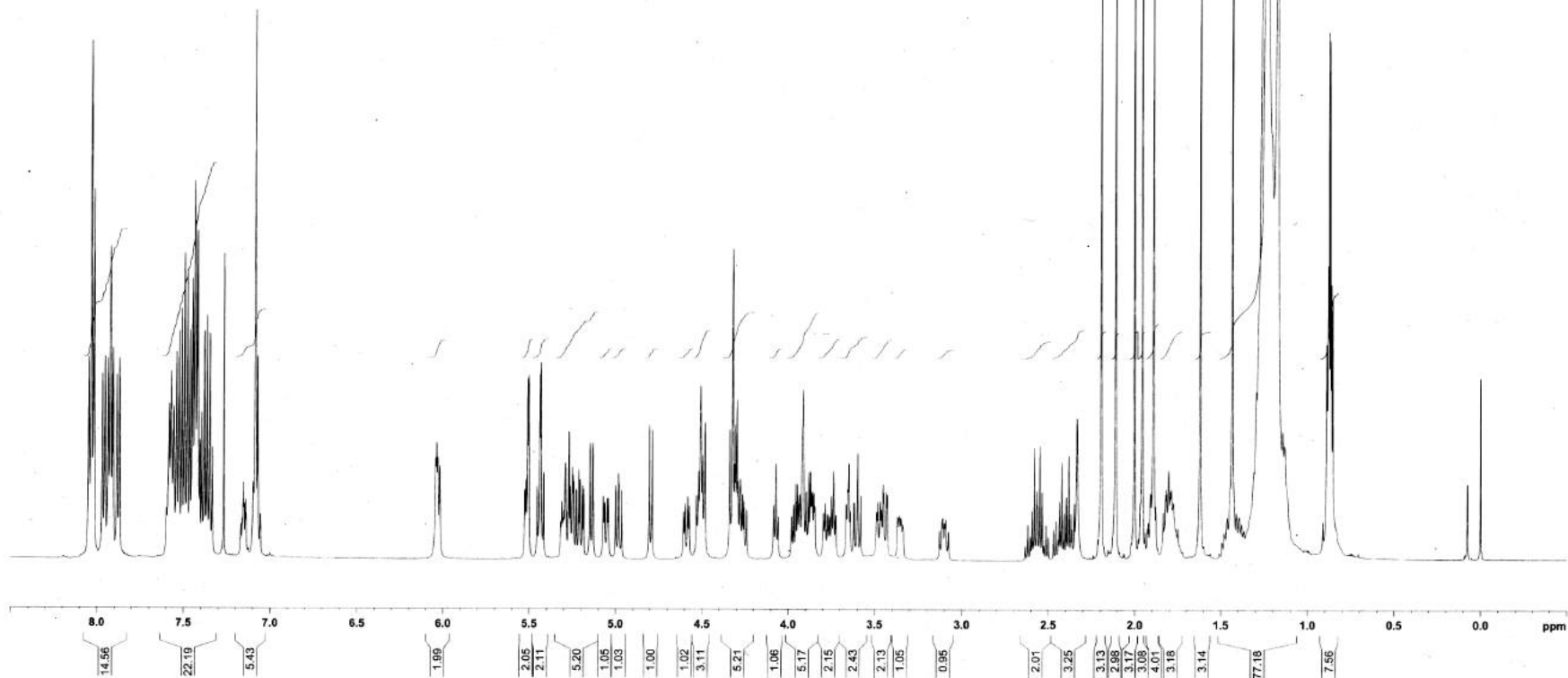
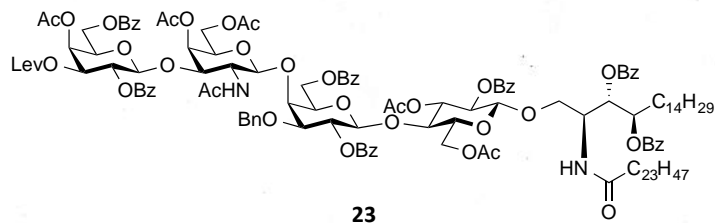
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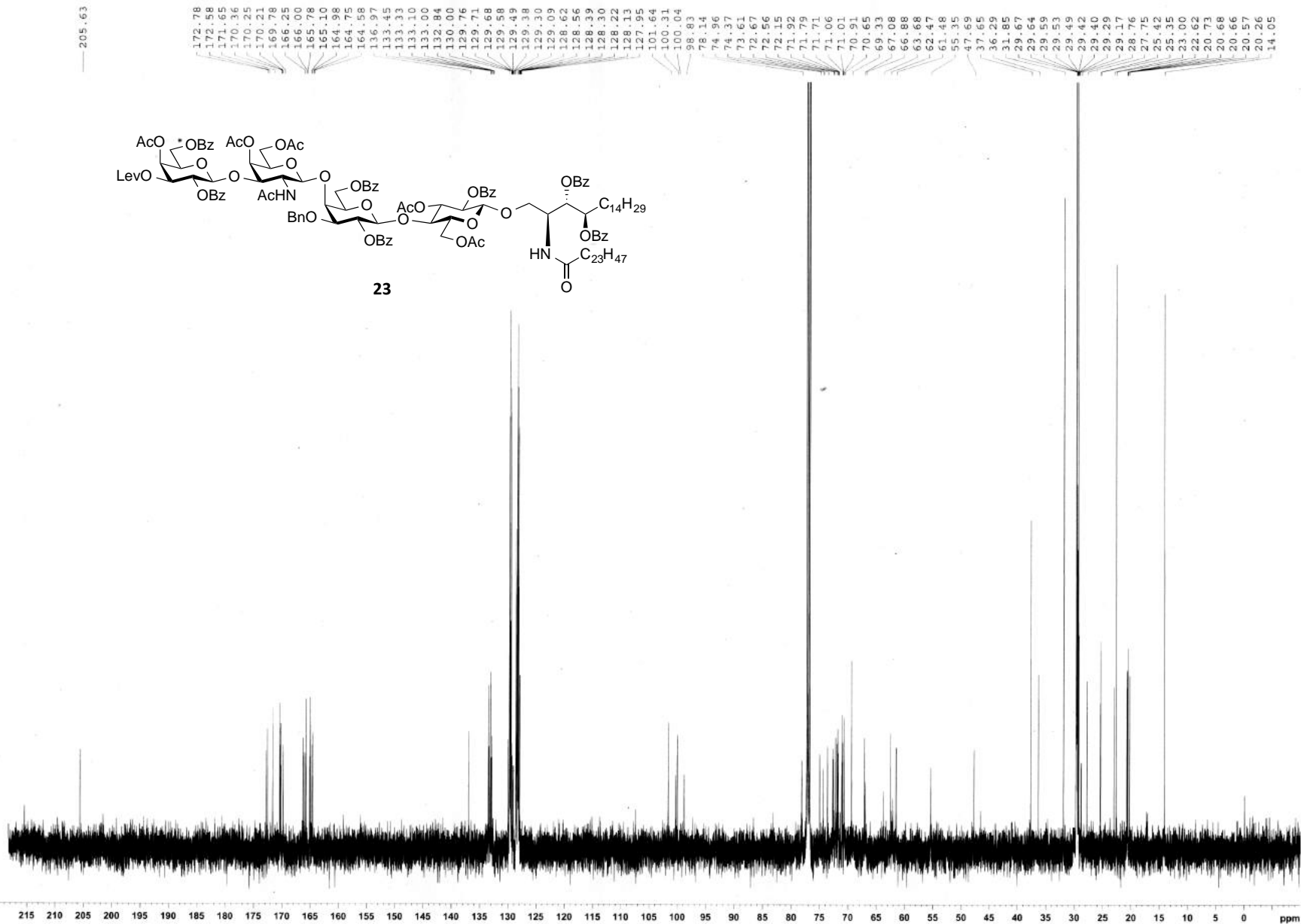
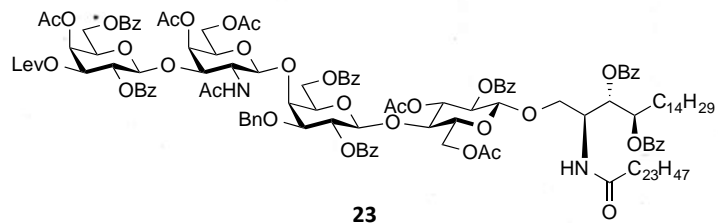
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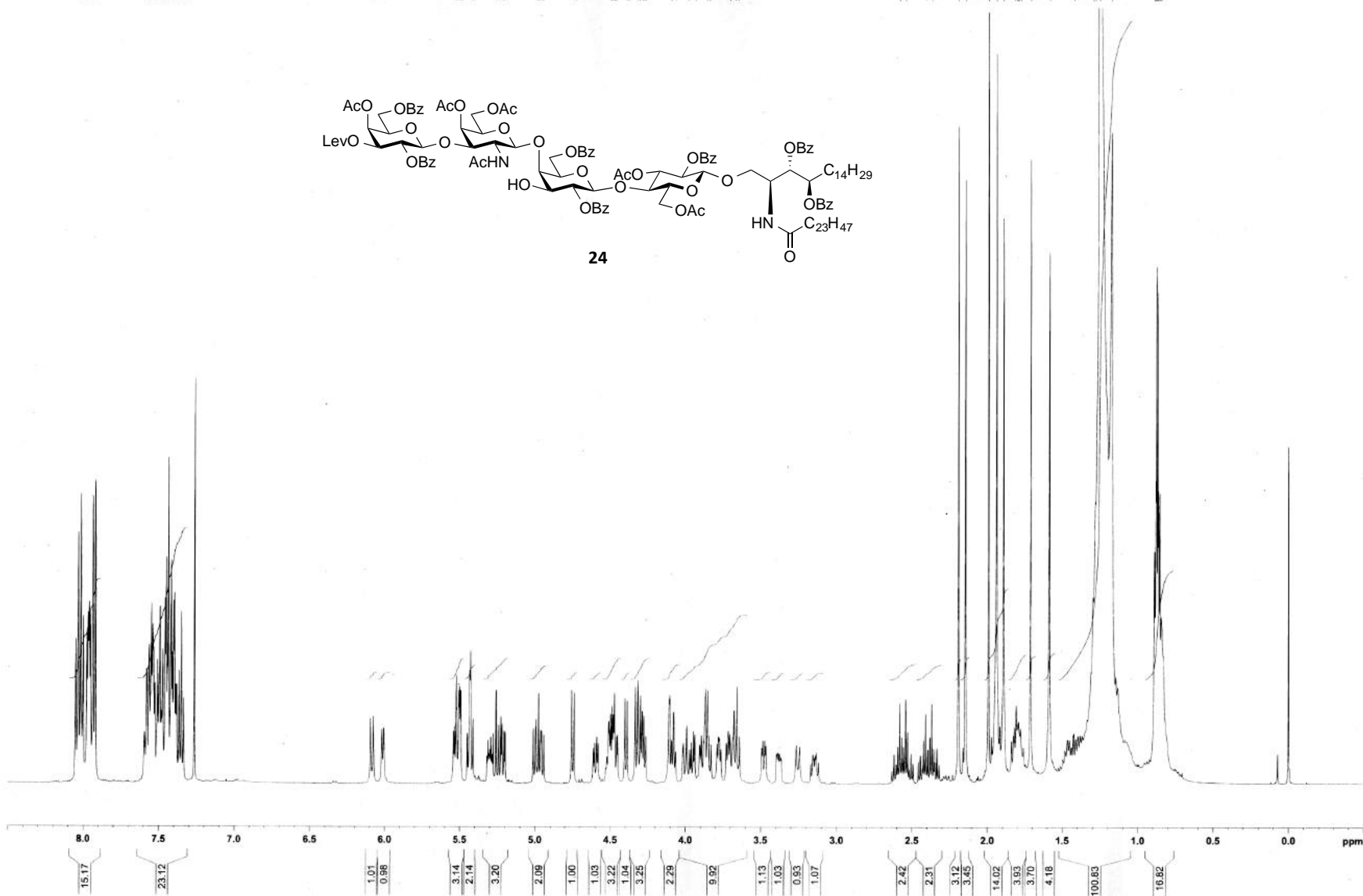
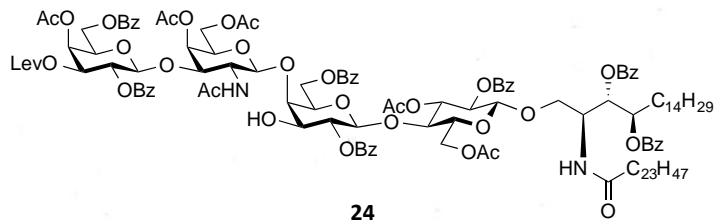
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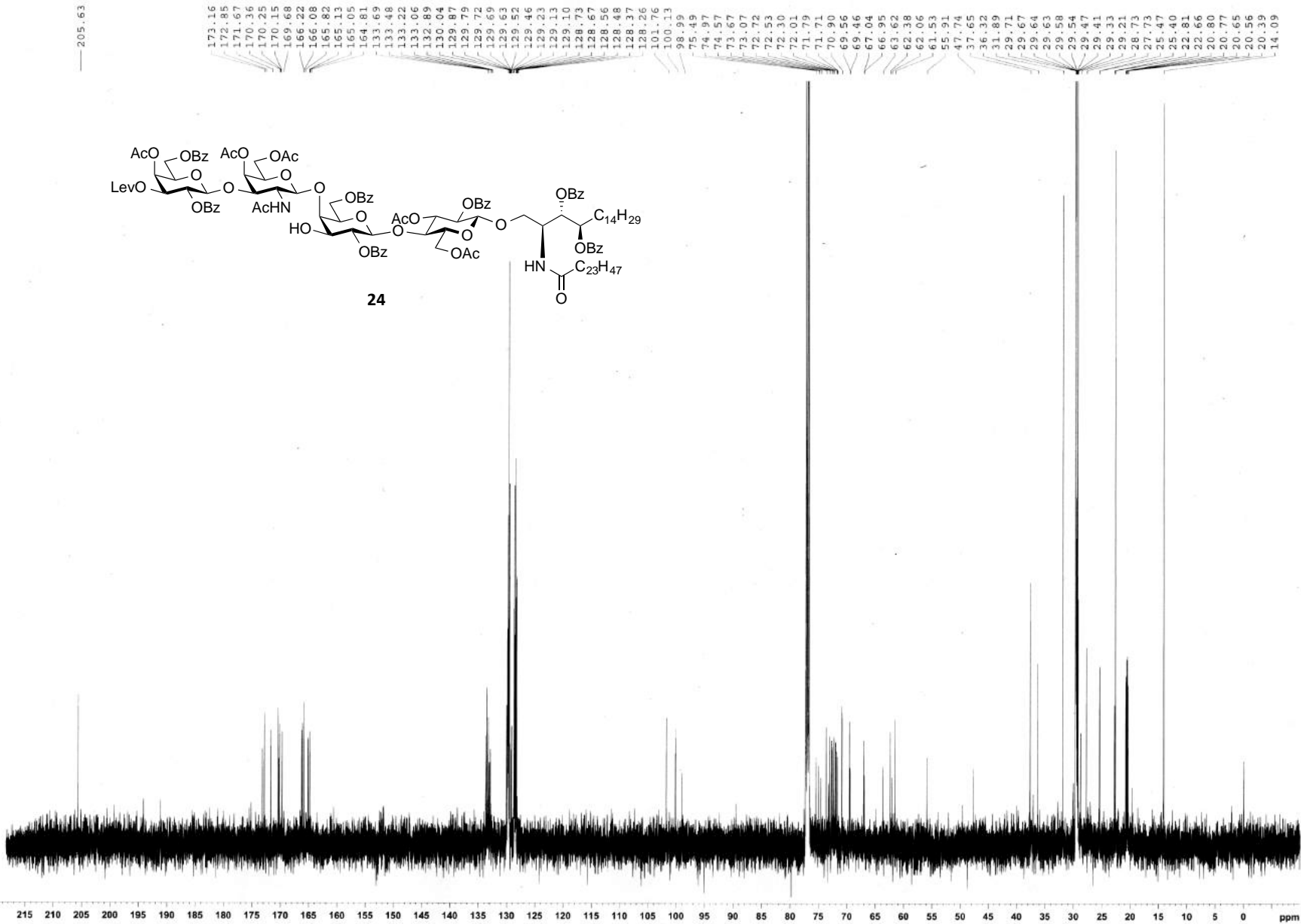
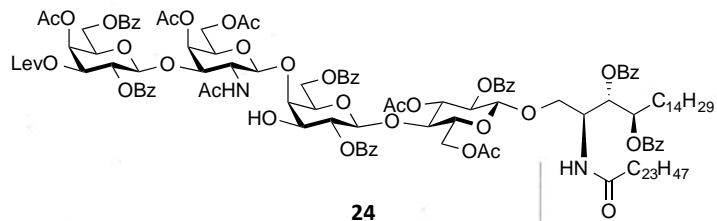
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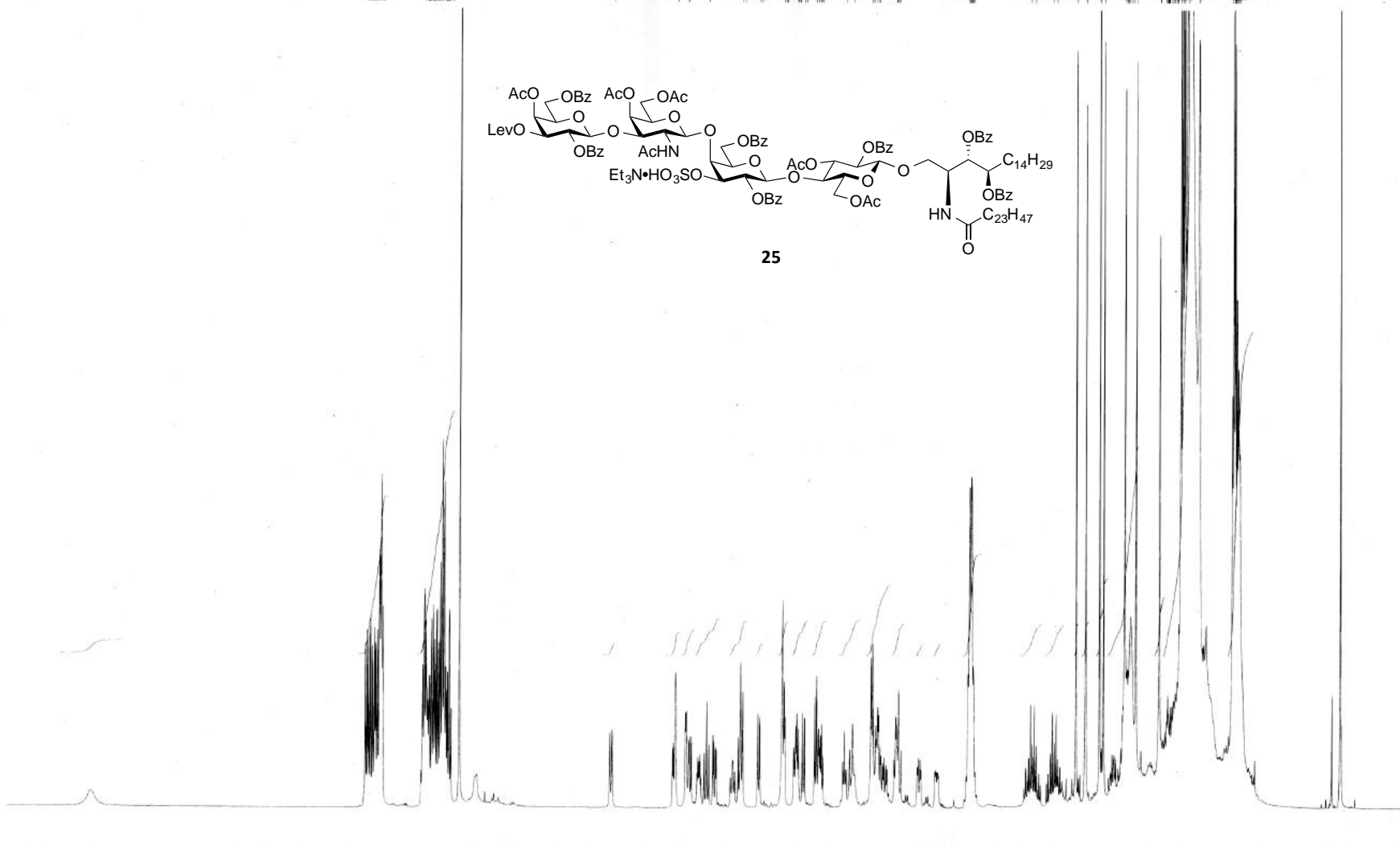
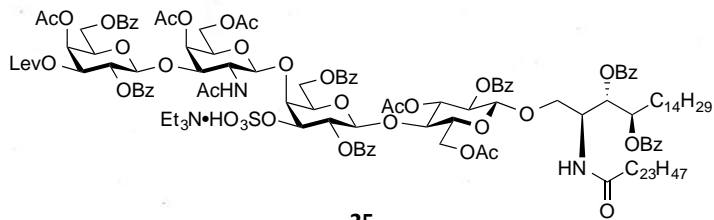


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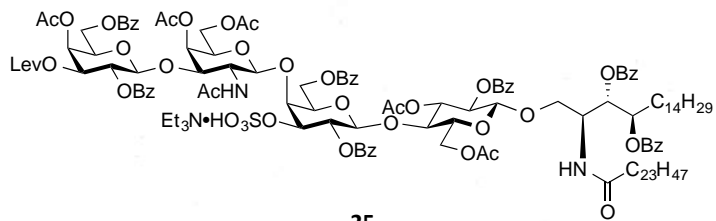
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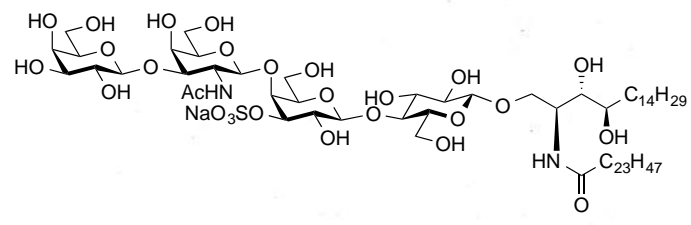
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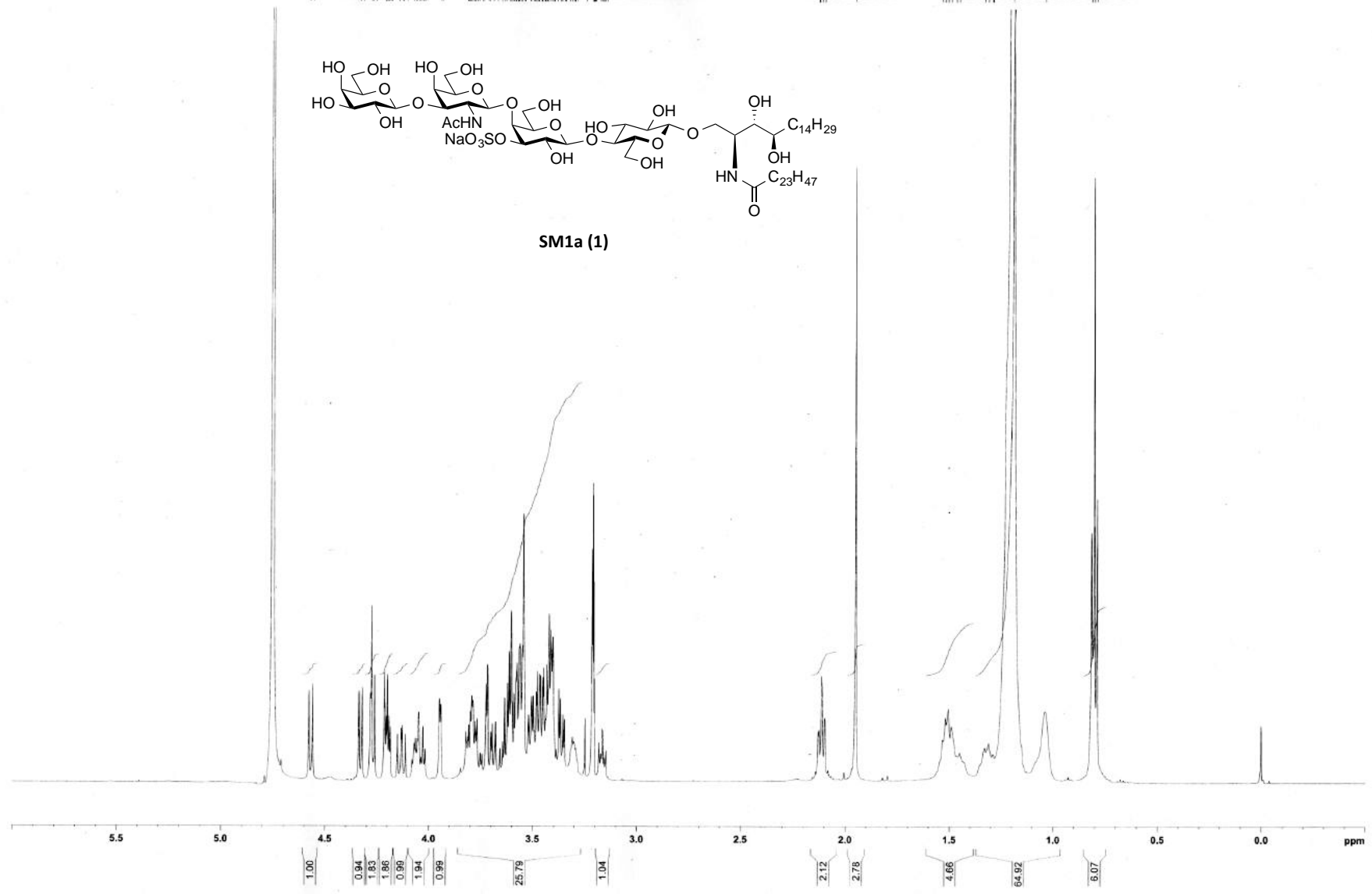
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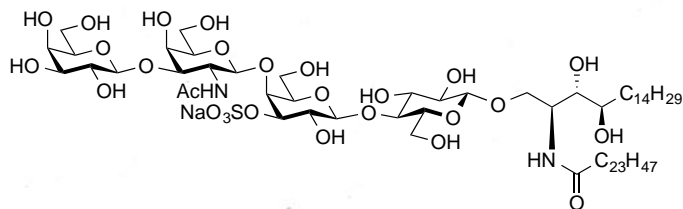
SM1a (1)



zgig30

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SM1a (1)

Current Data Parameters
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PROCNO 1

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Time 10.09
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TD 65356
SOLVENT DMSO
NS 30094
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SMH 48076.922 Hz
FIDRES 0.735618 Hz
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DE 18.00 usec
TE 293.2 K
D1 2.00000000 sec
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TD0 1

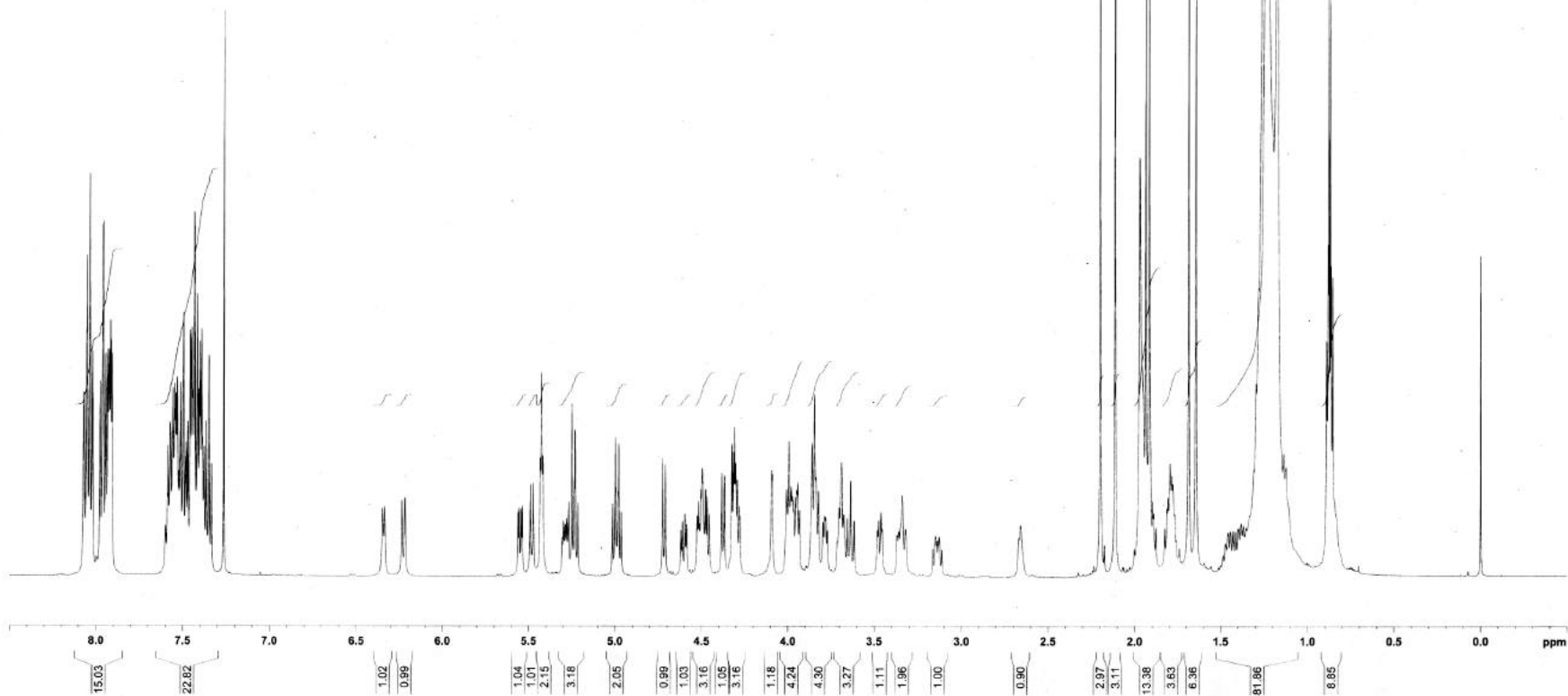
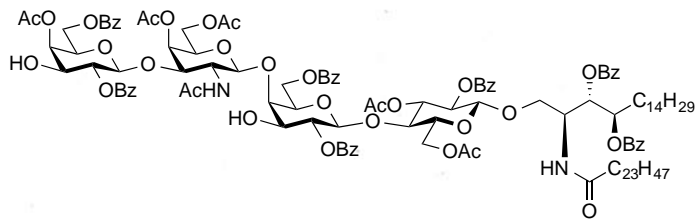
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PLW1 159.58999634 W

==== CHANNEL f2 =====
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NUC2 1H
CFDRG[2] waltz16
PCPD2 100.00 usec
PLW2 7.53359985 W
PLW12 0.03616600 W

F2 - Processing parameters
SI 32768
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LB 1.00 Hz
GB 0
PC 1.40

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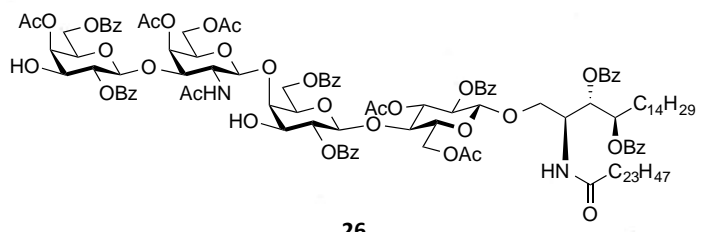
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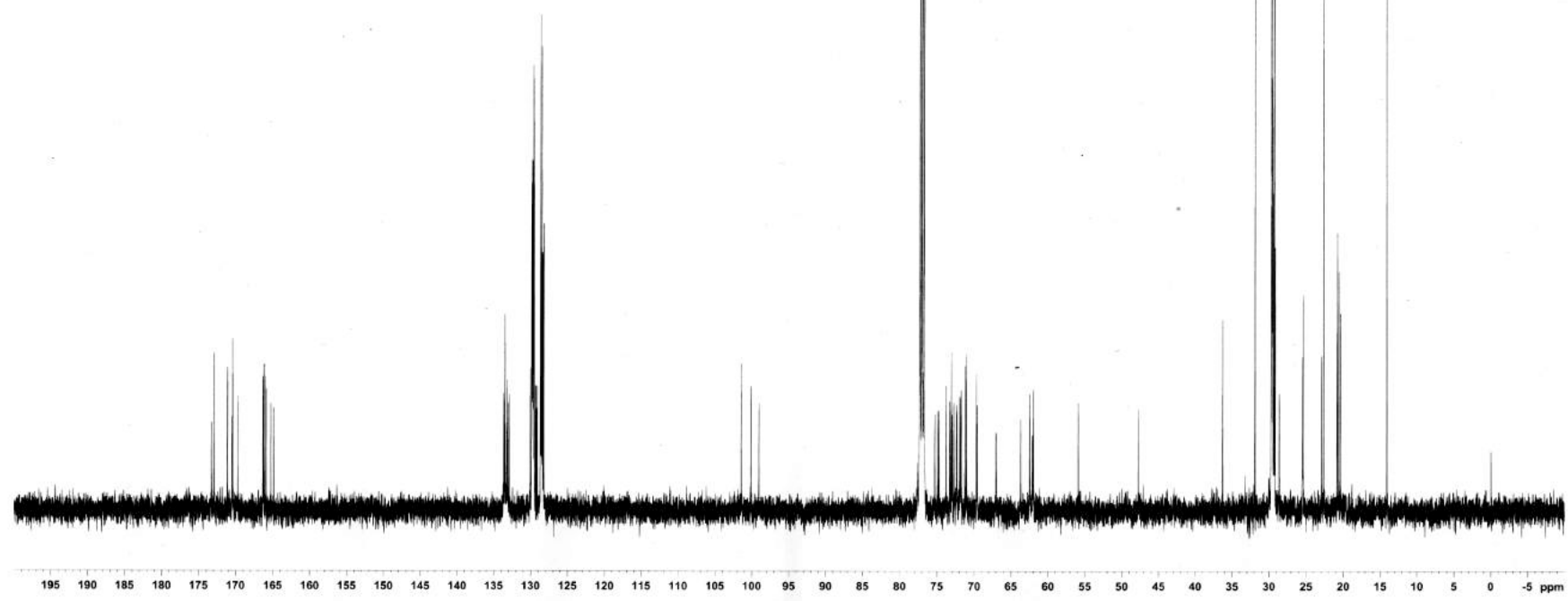
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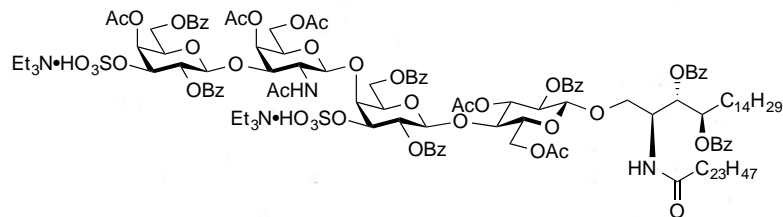
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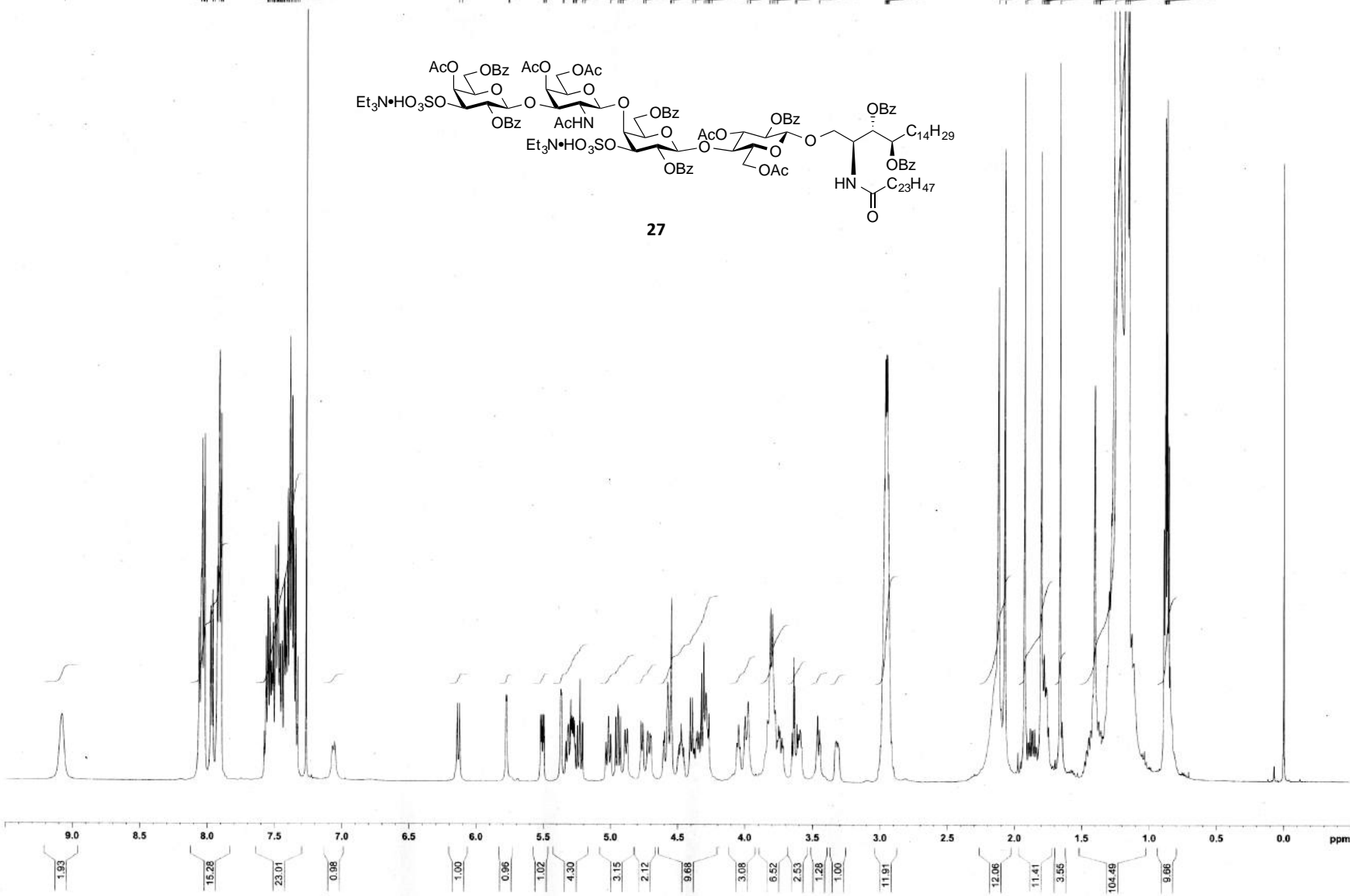
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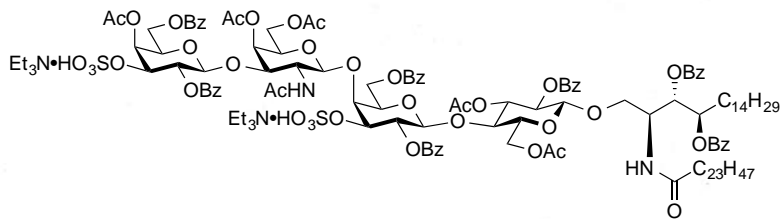


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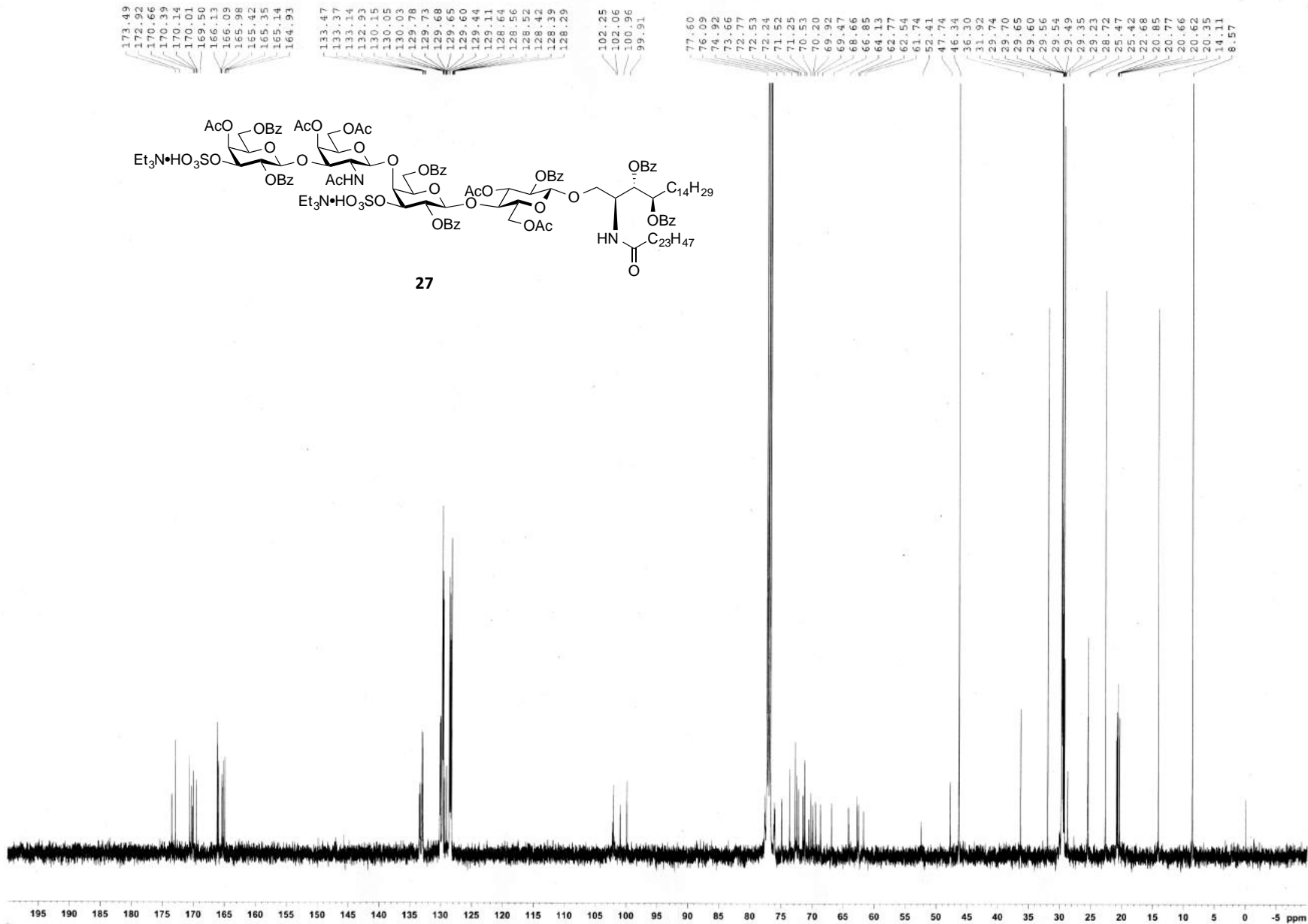
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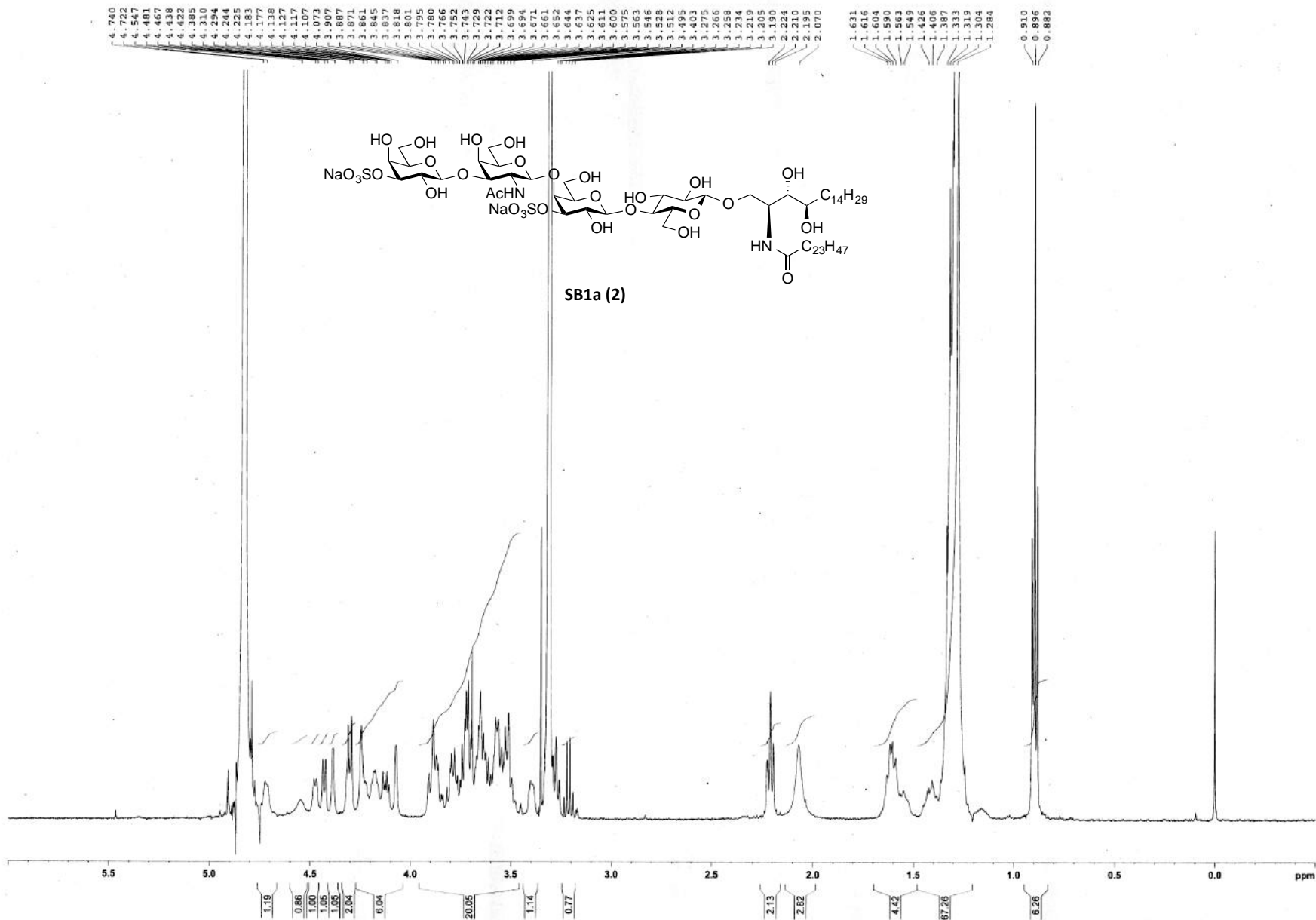
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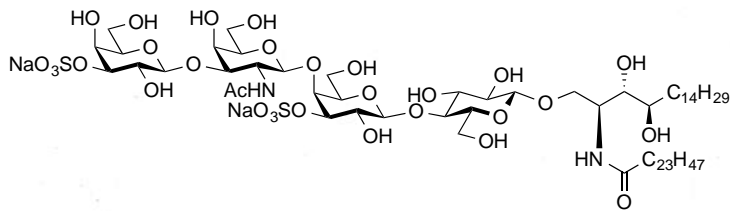




zgig30

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SB1a (2)

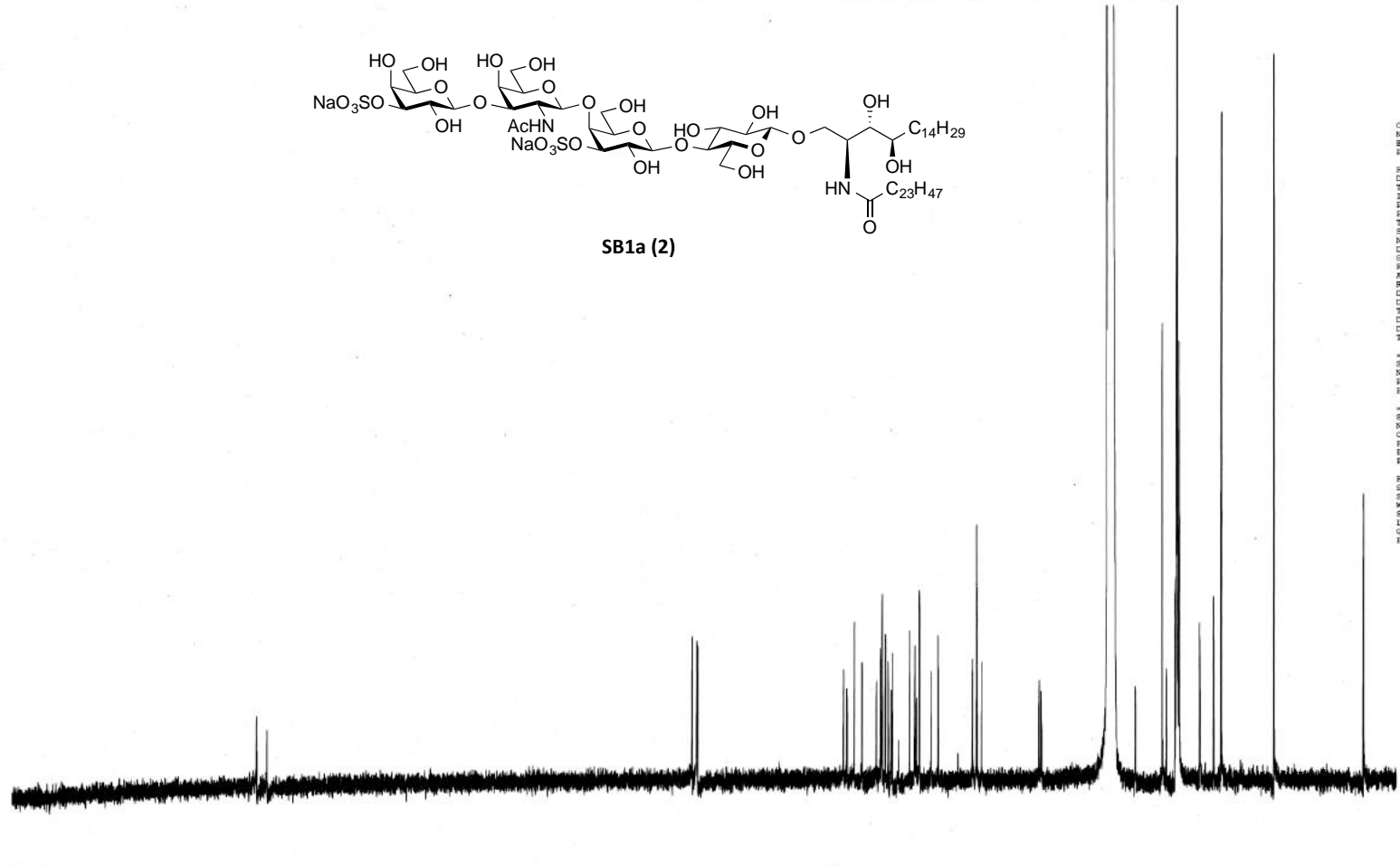
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EXPNO 100013
PROCNO 1

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Time 10.56
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PULPROG zgig30
TD 65356
SOLVENT DMSO
NS 32459
DS 8
SWH 48676.922 Hz
FIDRES 0.735616 Hz
AQ 0.6797024 sec
RG 203
OR 10.400 usec
DE 18.90 usec
TE 293.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

***** CHANNEL f1 *****
SFO1 201.2179973 MHz
NUC1 13C
P1 10.40 usec
PLW1 159.58999634 W

***** CHANNEL f2 *****
SFO2 800.1532006 MHz
NUC2 1H
CPOPRGf2 waltz16
PCPD2 100.00 usec
PLW2 7.53359985 W
PLW12 0.03616600 W

F2 - Processing parameters
SI 32768
SF 201.1979694 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm