

Synthesis of C-Glycoside Analogues of β -Galactosamine-(1->4)-3-O-Methyl-D-Chiro-Inositol and Assay as Activator of Protein Phosphatases PDHP and PP2C α

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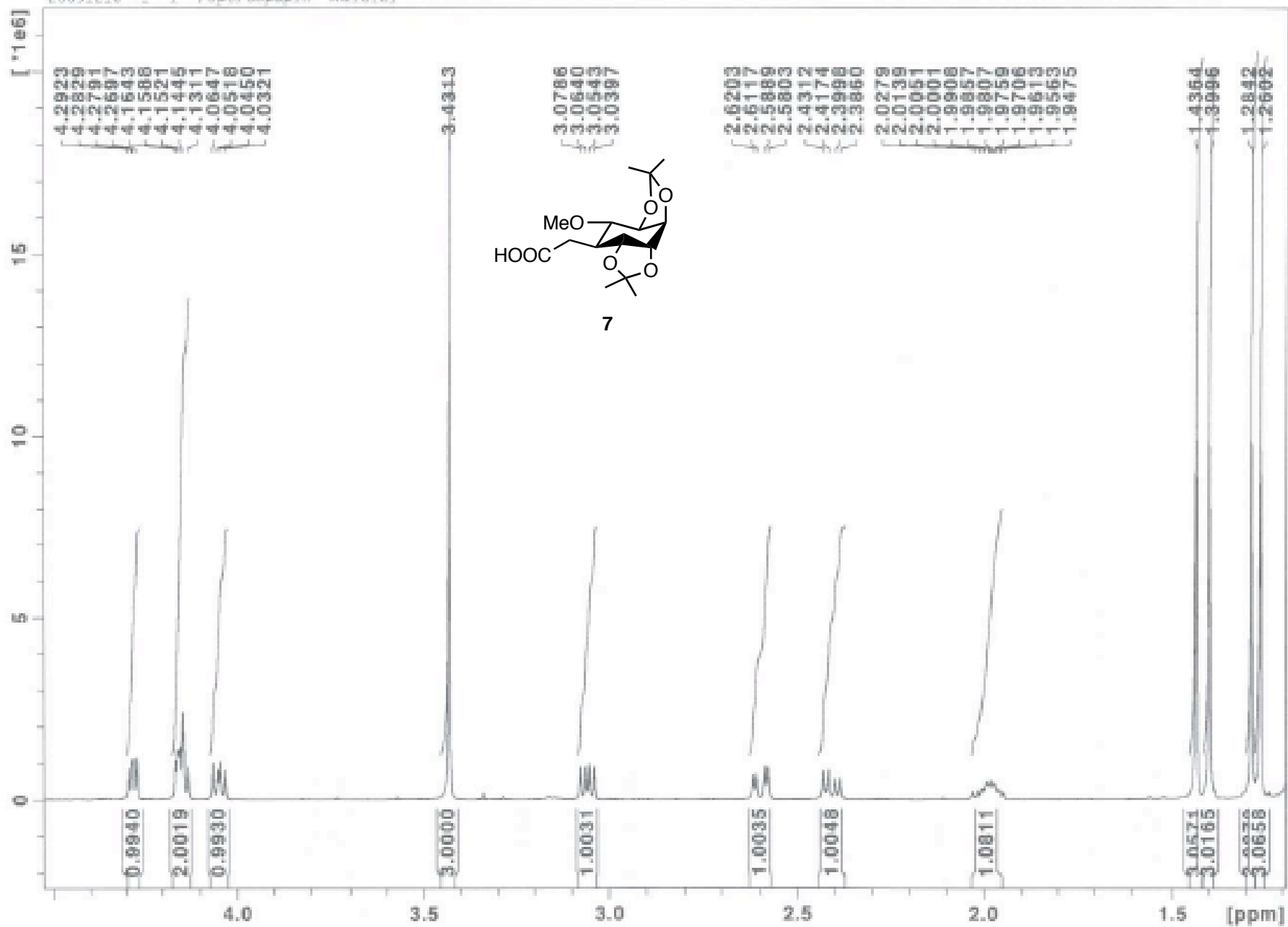
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SUPPORTING INFORMATION

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100.000
103.219
103.266

80.305
80.370
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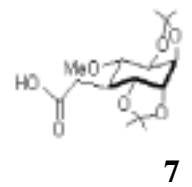
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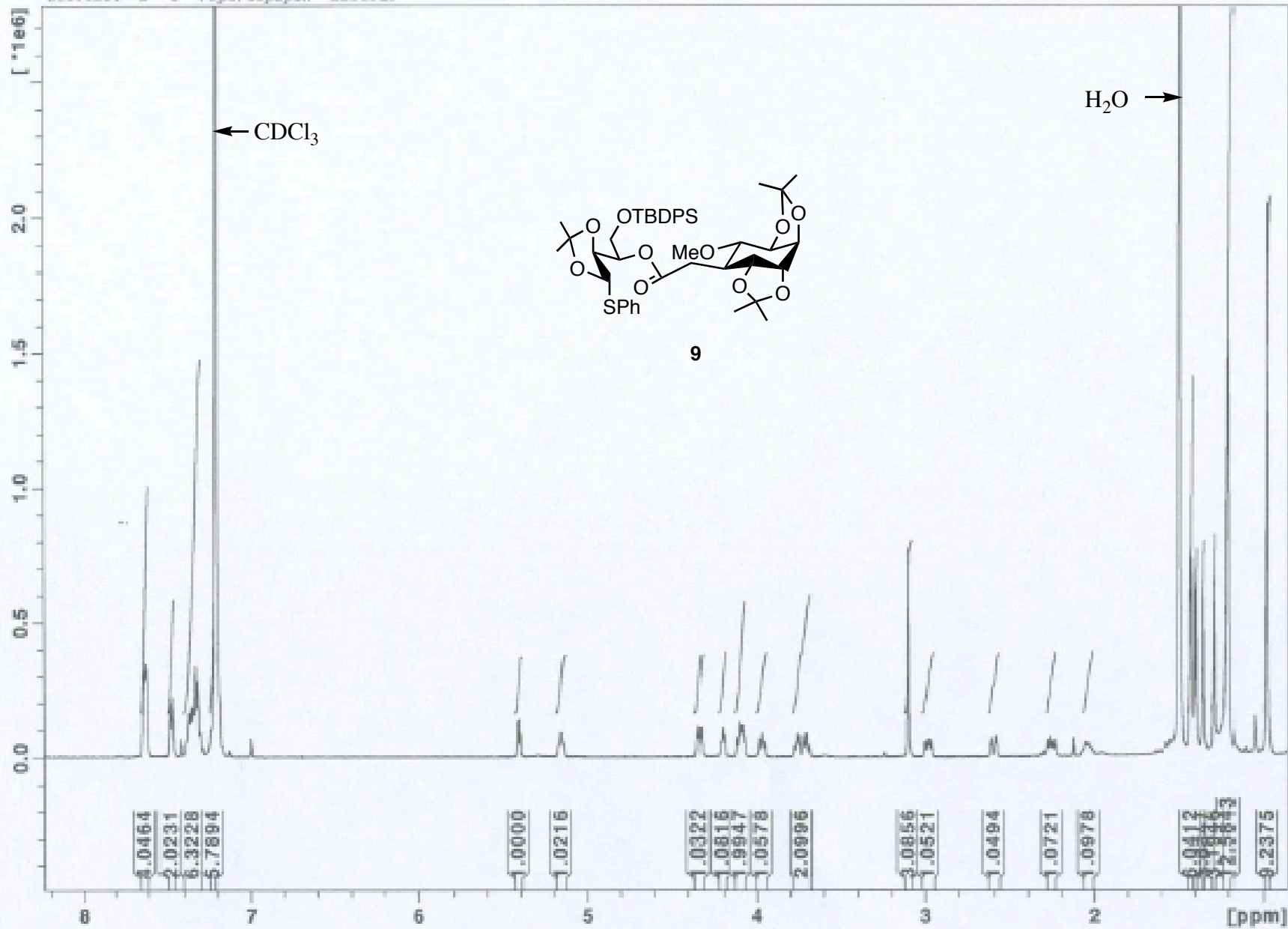
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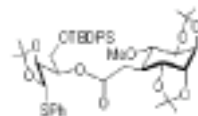
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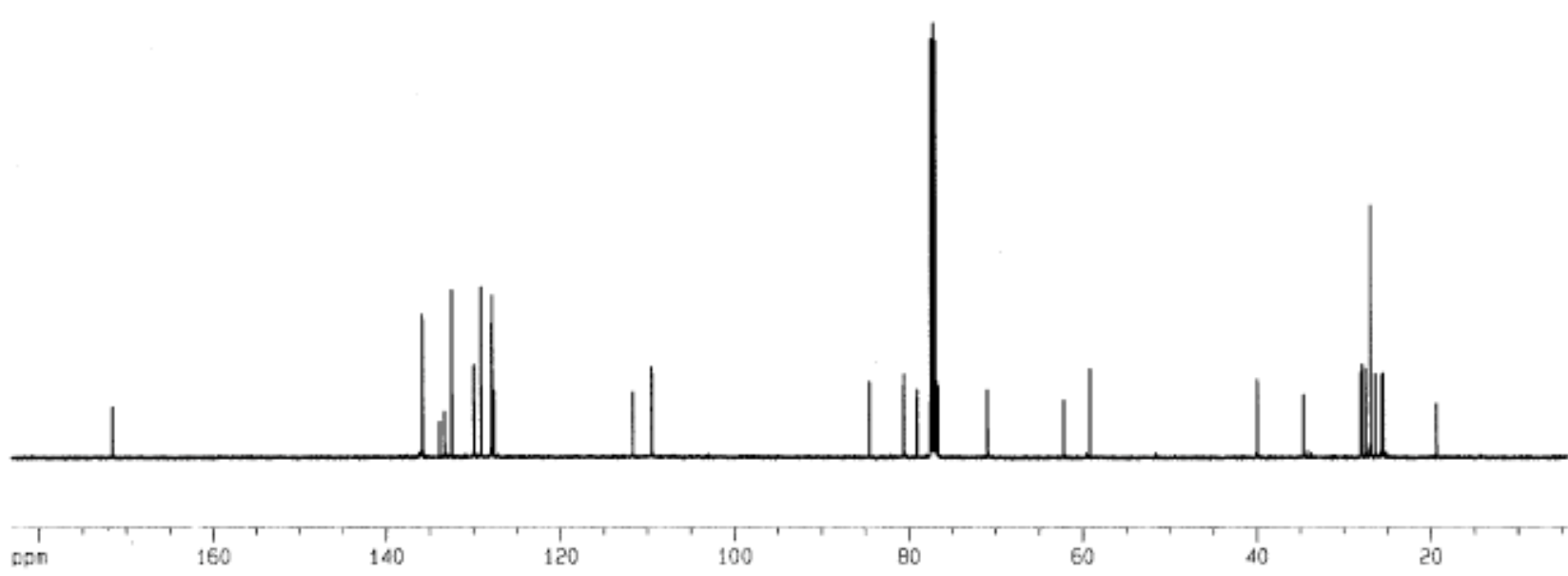
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109.516

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50.660
80.597
79.023
77.485
77.231
75.976
76.834
75.699
70.987
62.180
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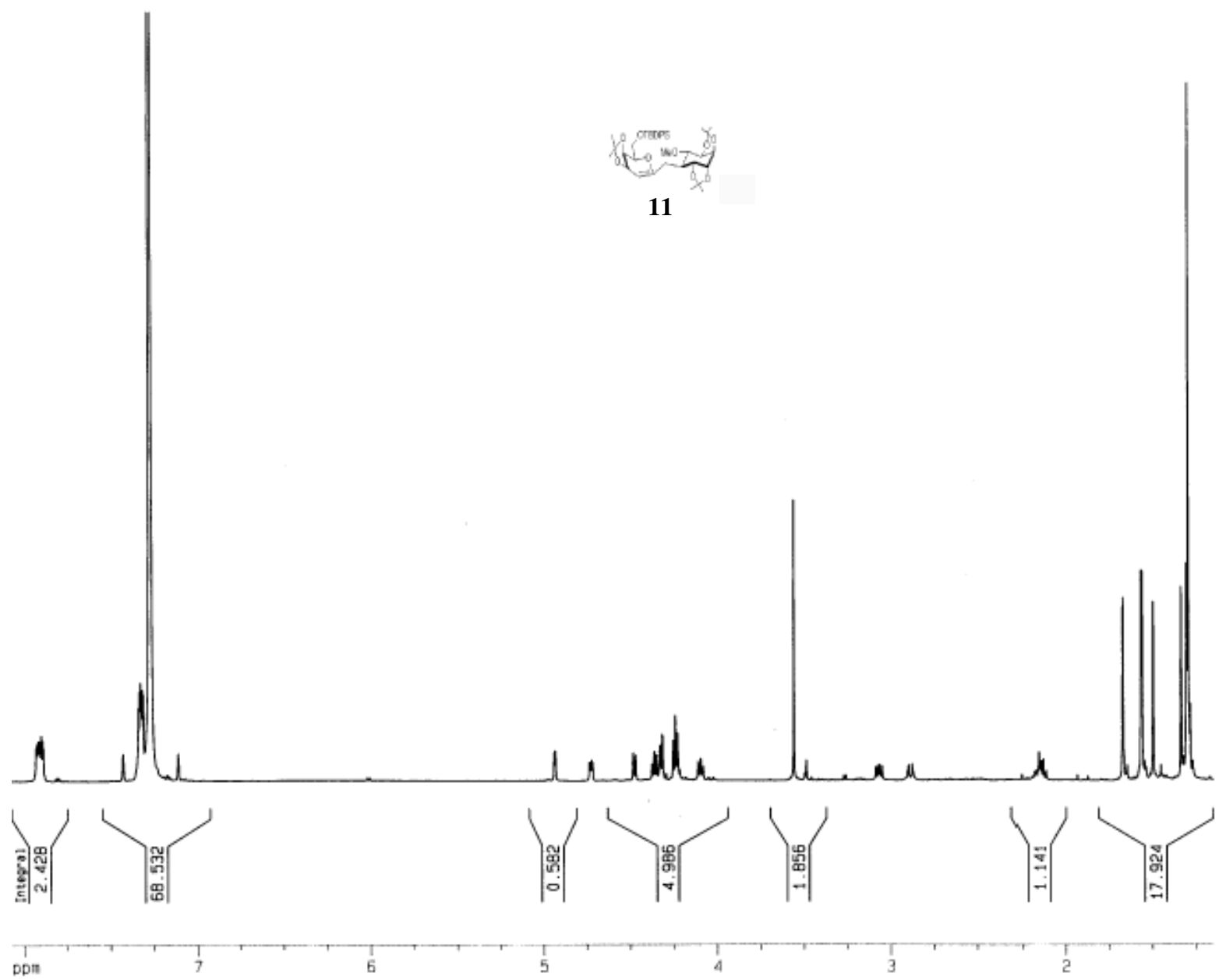


9





11



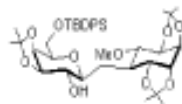
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 PULPROG zg30
 TO 32768
 SOLVENT C6D6
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
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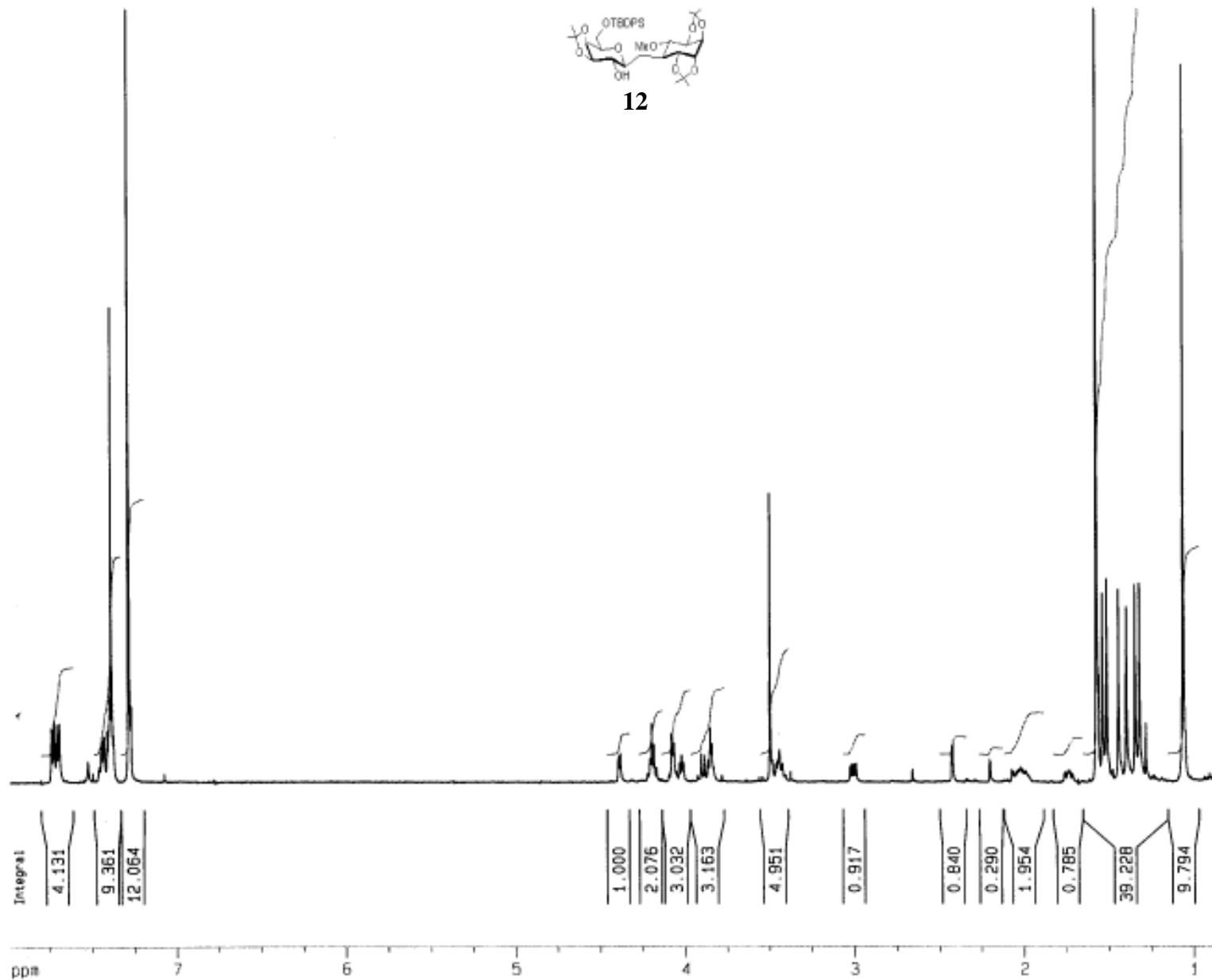
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 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
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 CY 85.17 cm
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 F1 4037.66 Hz
 F2P 1.151 ppm
 F2 575.40 Hz
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 HZCM 157.37521 Hz/cm



12



Current Data Parameters

NAME 12040601
EXPNO 15
PROCNO 1

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INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 32768
SOLVENT C6D6
NS 8
DS 2
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FIDRES 0.244532 Hz
AQ 2.0448356 sec
RG 25.4
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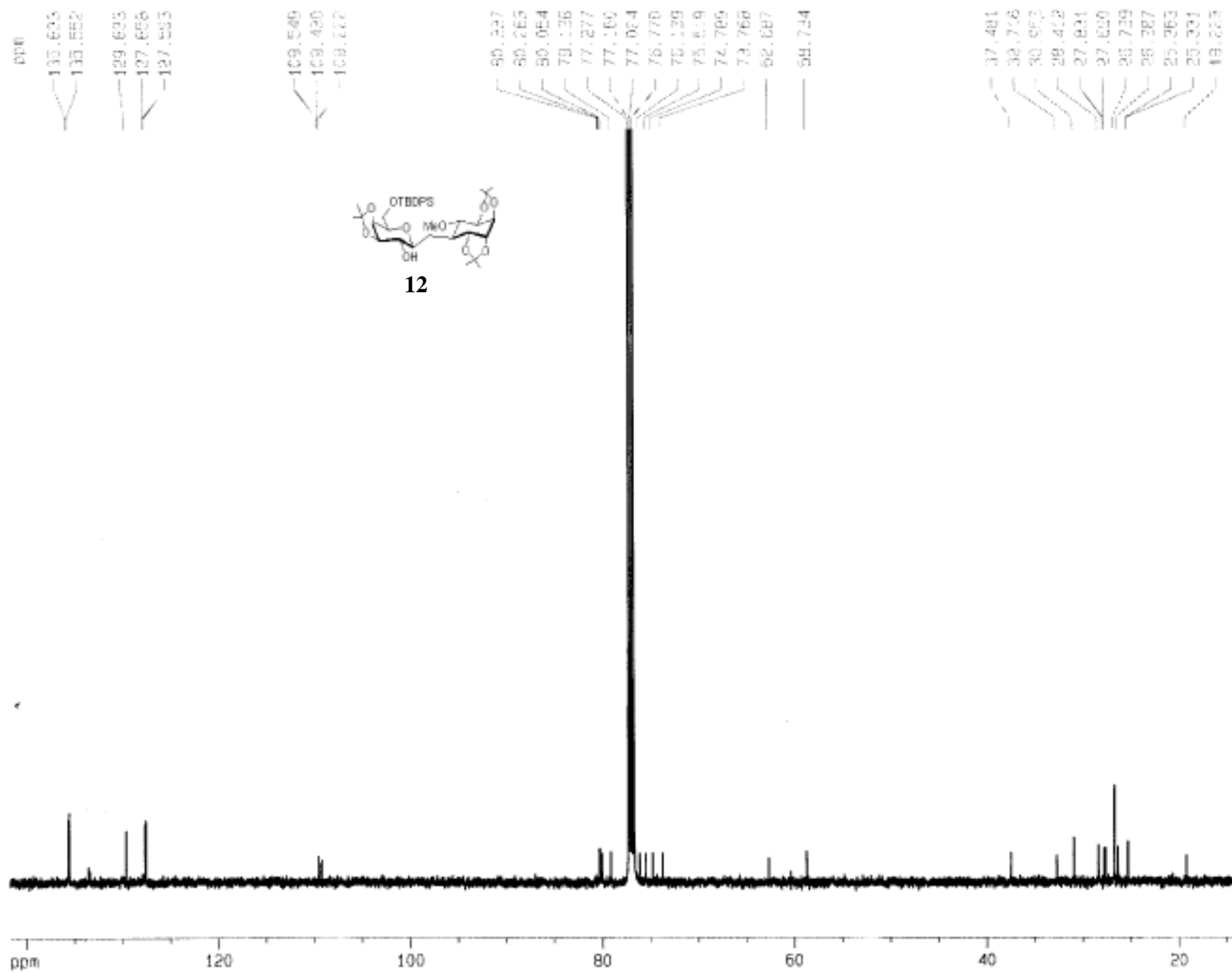
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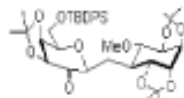
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LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

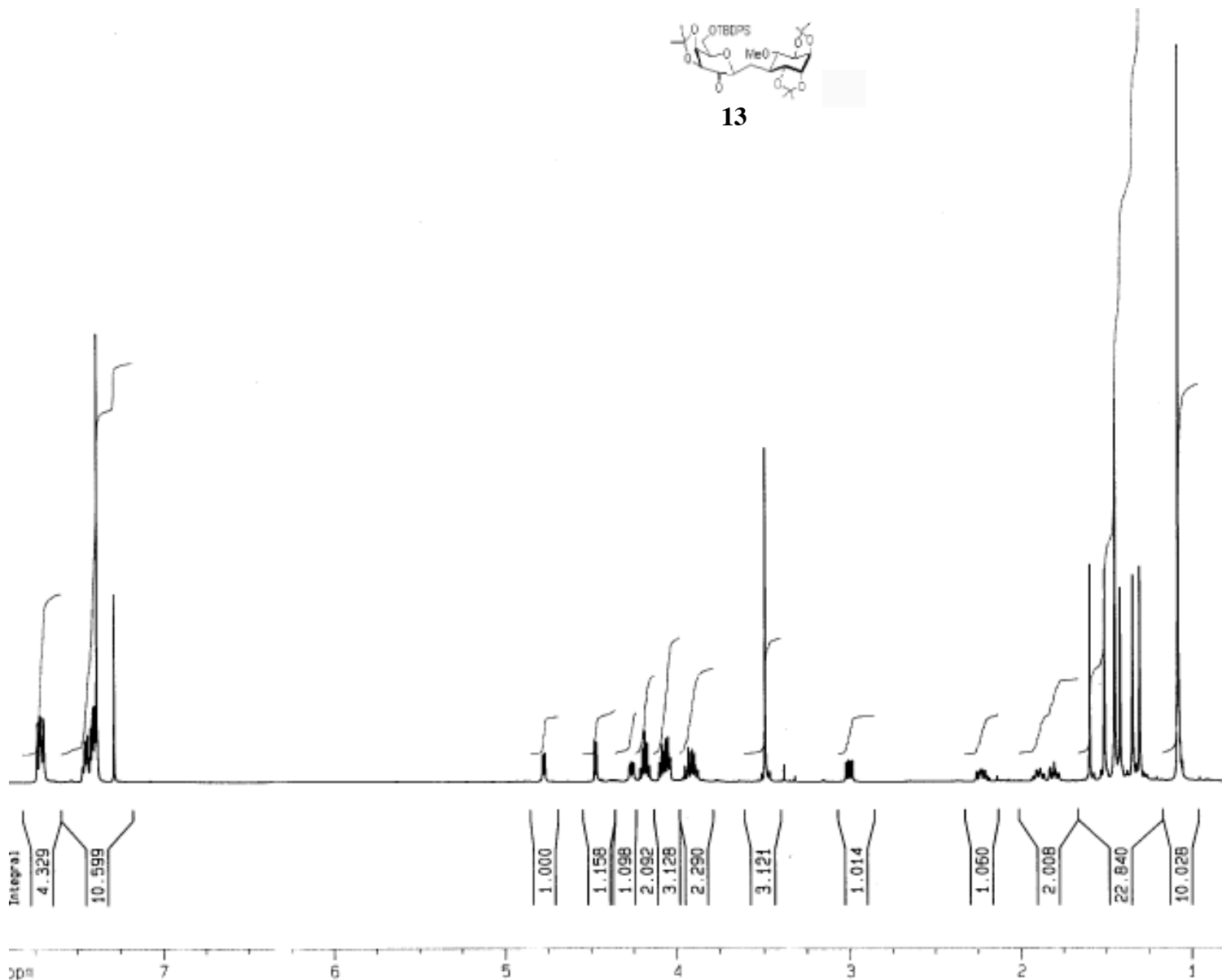
CX 22.00 cm
CY 34.48 cm
F1P 7.984 ppm
F1 3992.86 Hz
F2P 0.852 ppm
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PPMCM 0.32418 ppm/cm
HZCM 162.13031 Hz/cm



12



13



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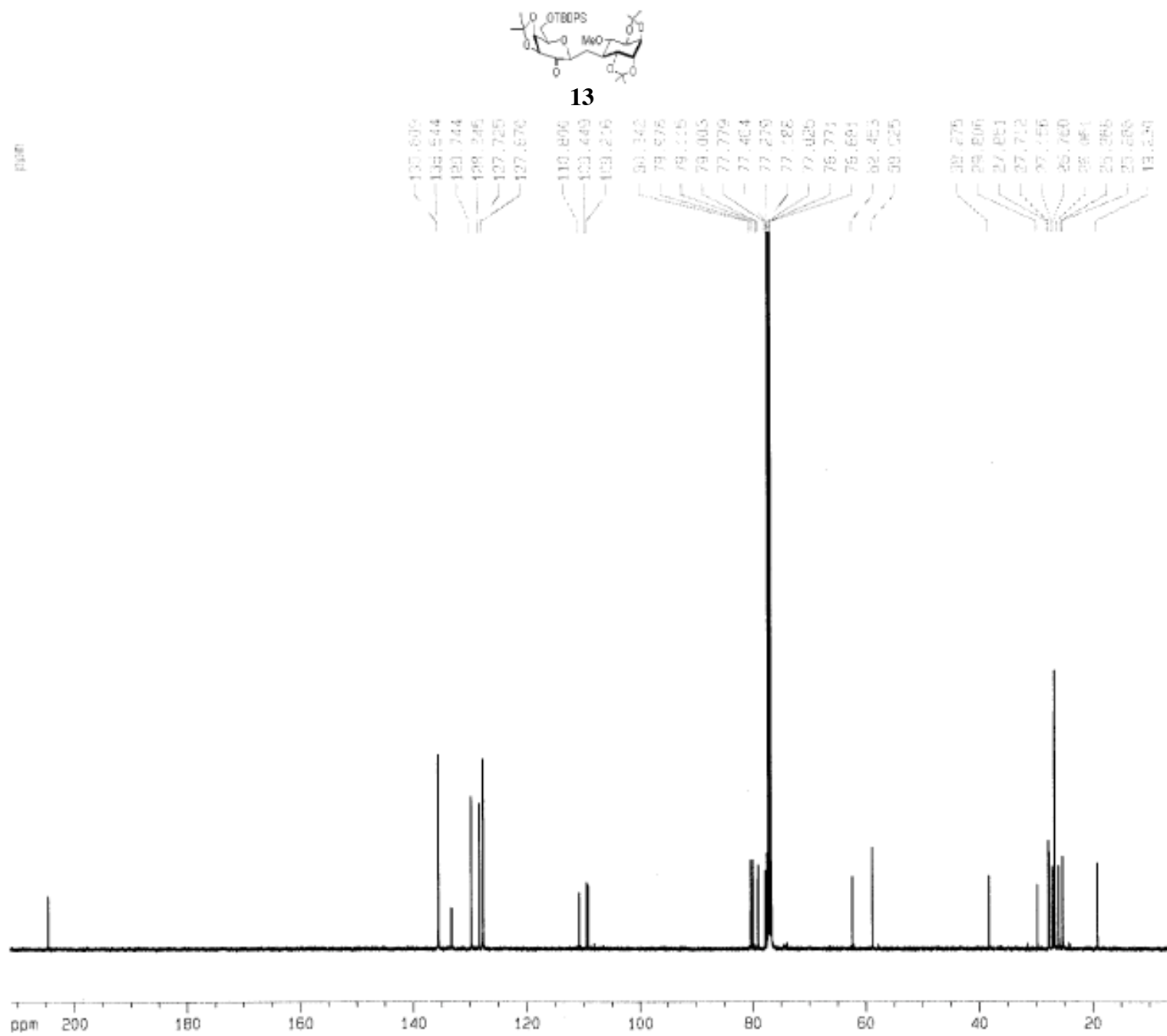
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 PULPROG zg30
 TD 32768
 SOLVENT C6D6
 NS 8
 DS 2
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 FIDRES 0.244532 Hz
 AQ 2.0448356 sec
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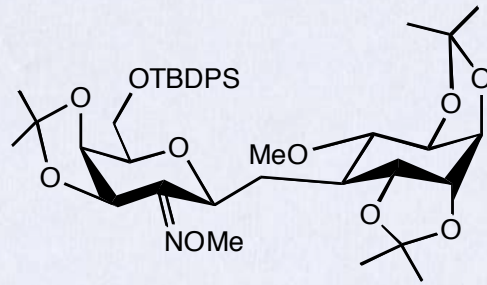
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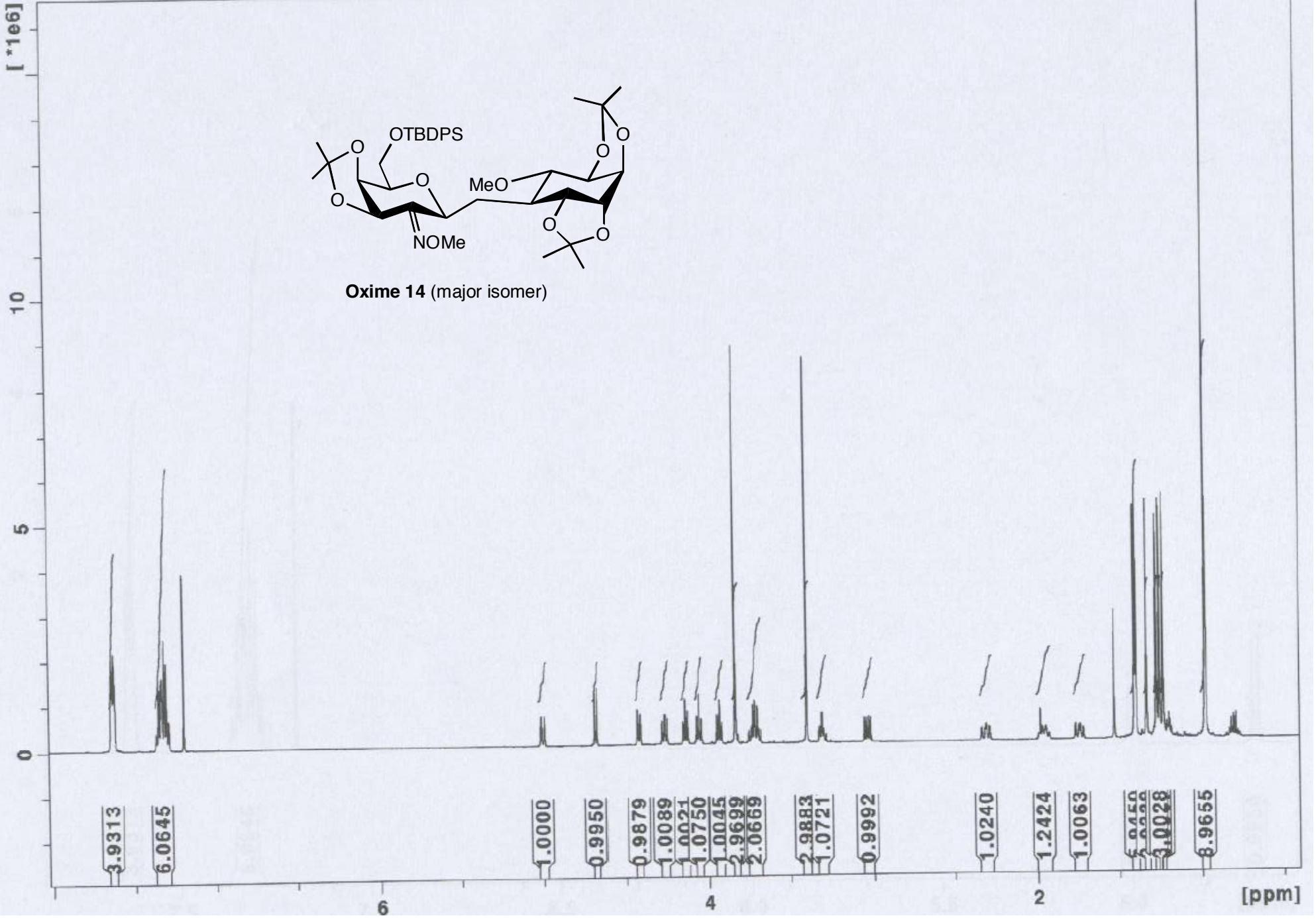
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 F1 3962.54 Hz
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 F2 385.57 Hz
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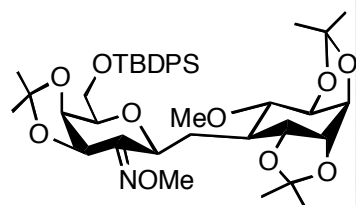
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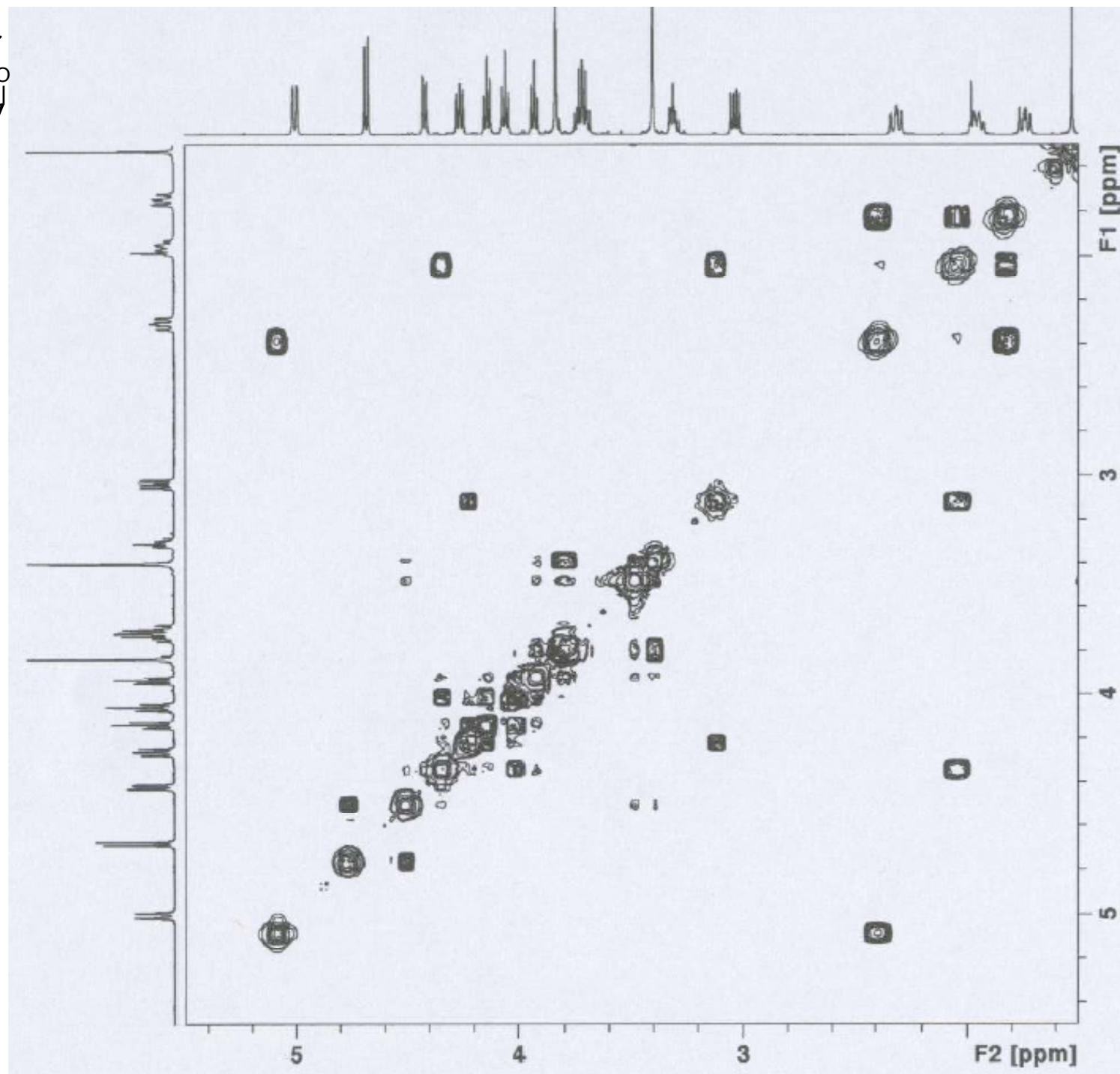


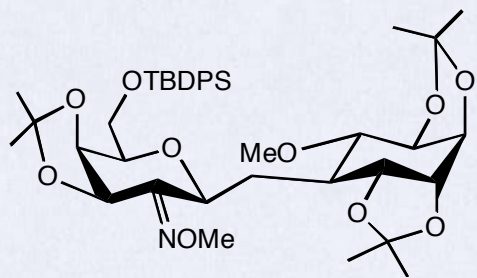
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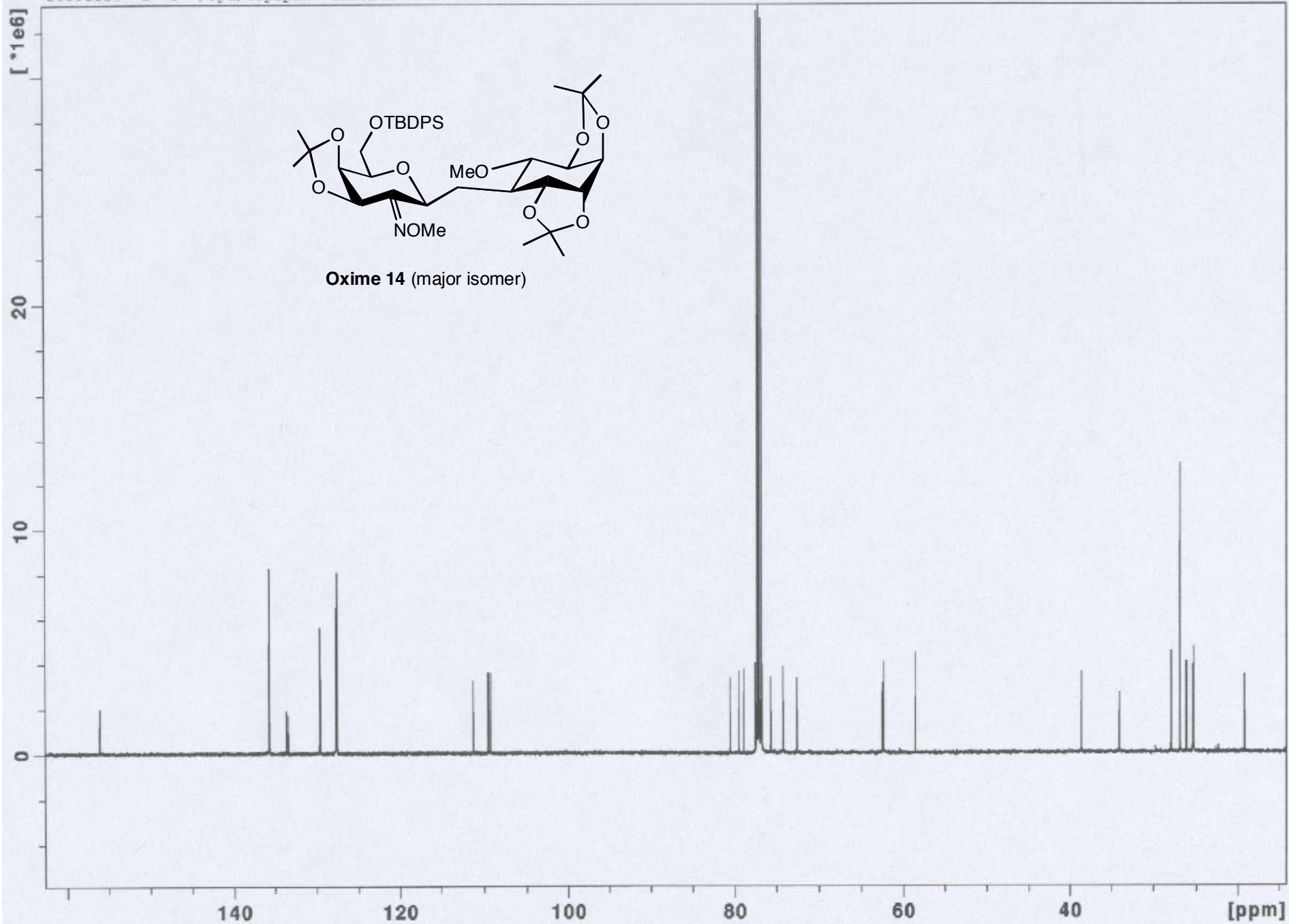


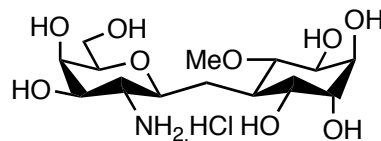
Oxime 14 (major isomer)



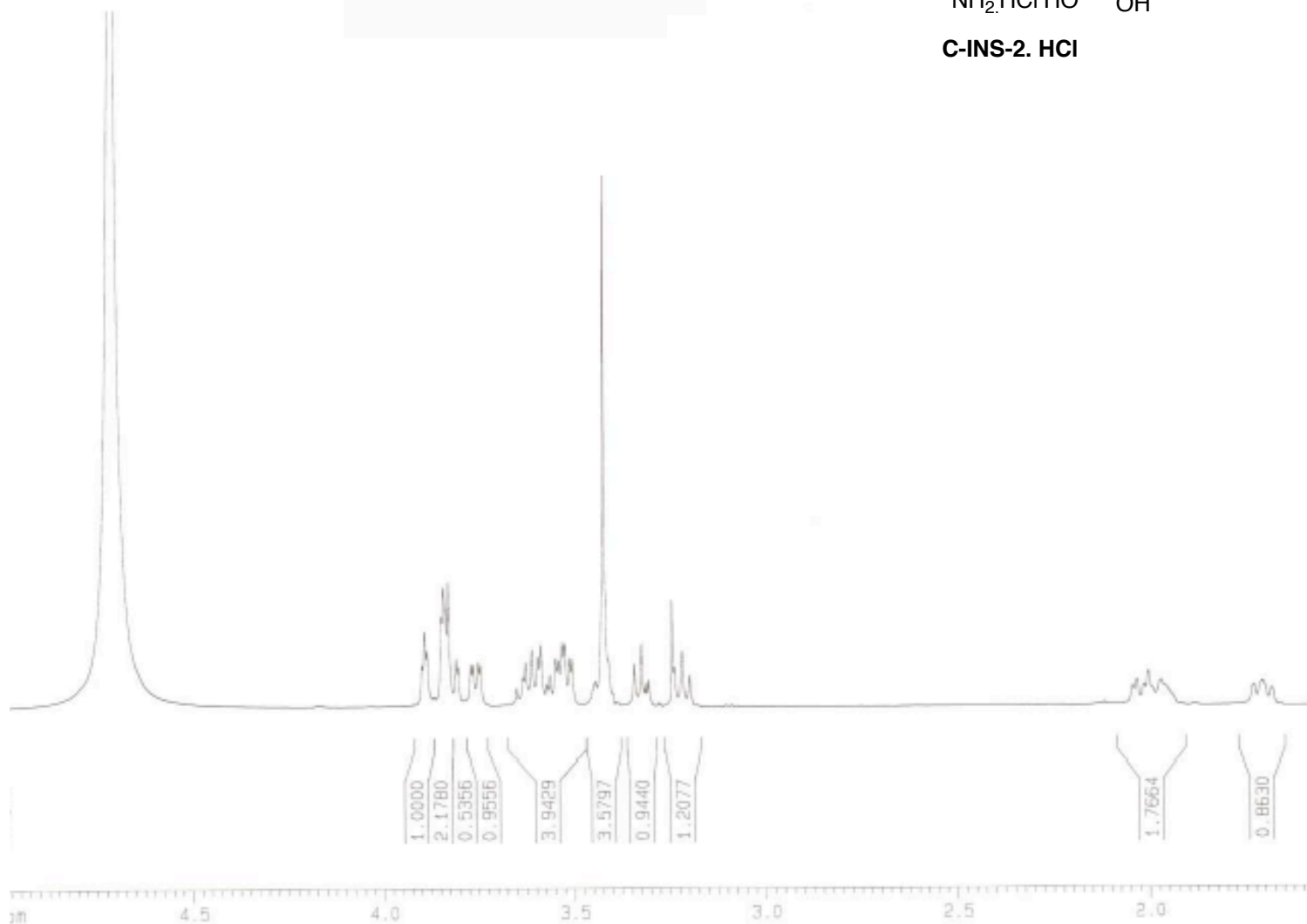


Oxime 14 (major isomer)





C-INS-2.HCl



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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
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 INSTRUM spect
 PROBHD 5 mm CPDCH 13C
 PULPROG zg30
 TD 32768
 SOLVENT C6D6
 NS 8
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 2.0448356 sec
 RG 35.9
 DM 62.400 usec
 DE 6.00 usec
 TE 303.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

----- CHANNEL f1 -----
 NUC1 1H
 P1 9.25 usec
 PL1 -0.50 dB
 SFO1 500.1330895 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300000 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
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 CY 16.38 cm
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 F1 2510.70 Hz
 F2P 1.563 ppm
 F2 701.09 Hz
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 HZCM 78.58234 Hz/cm

ppm

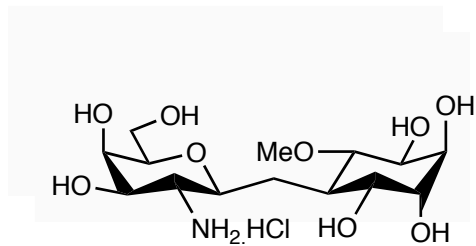
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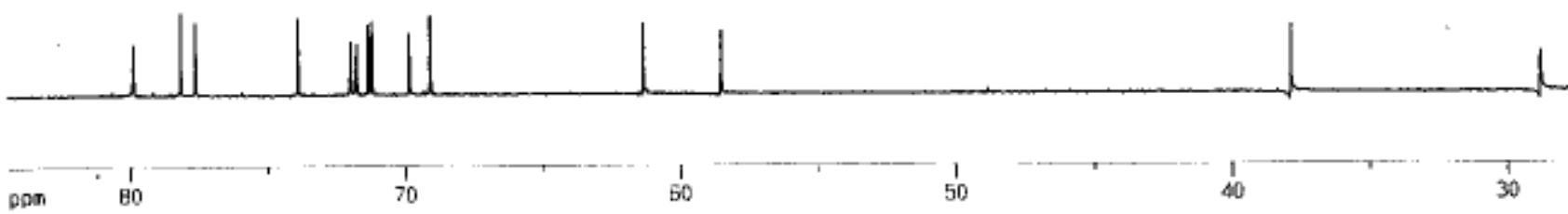
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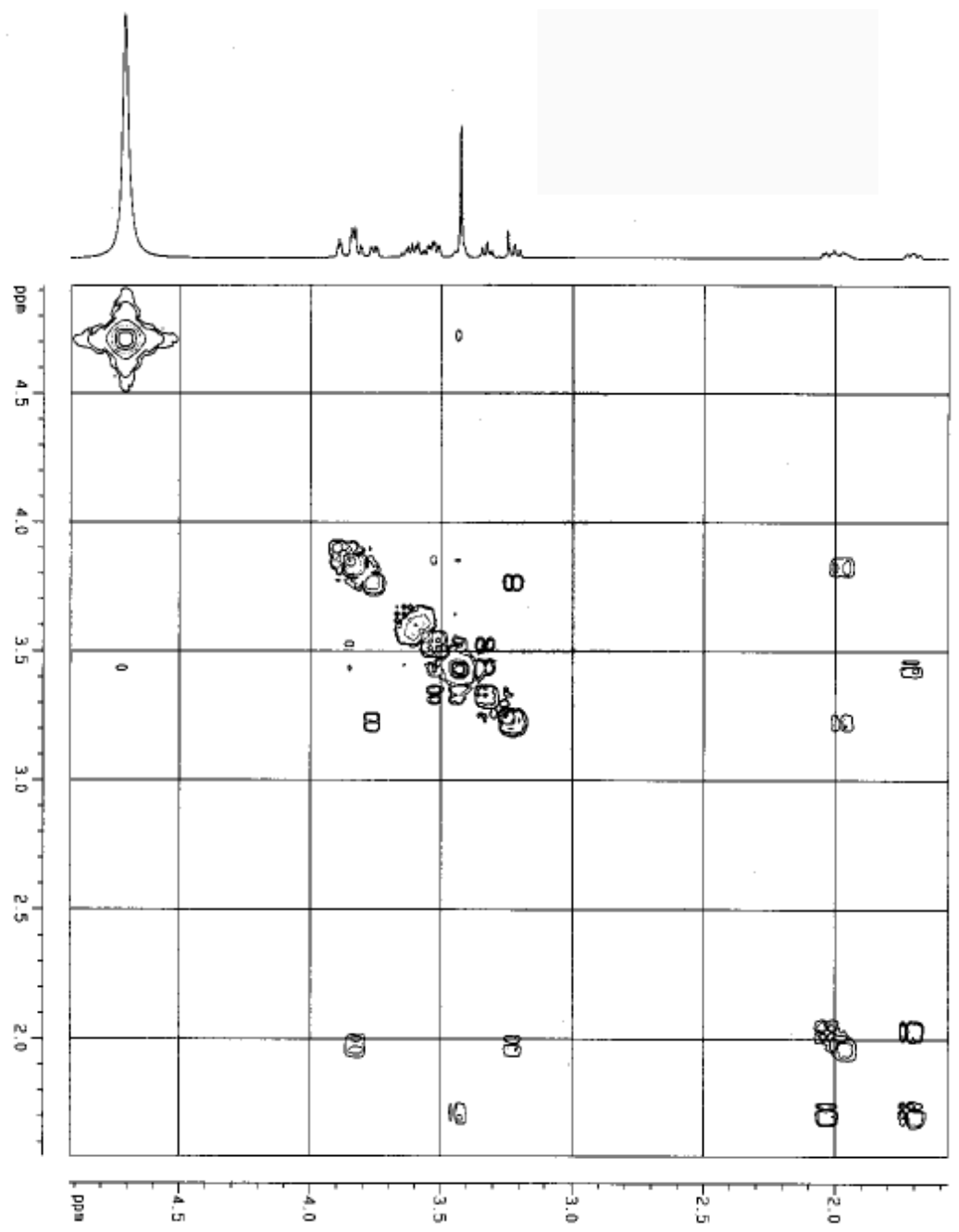
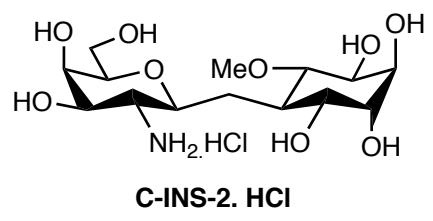
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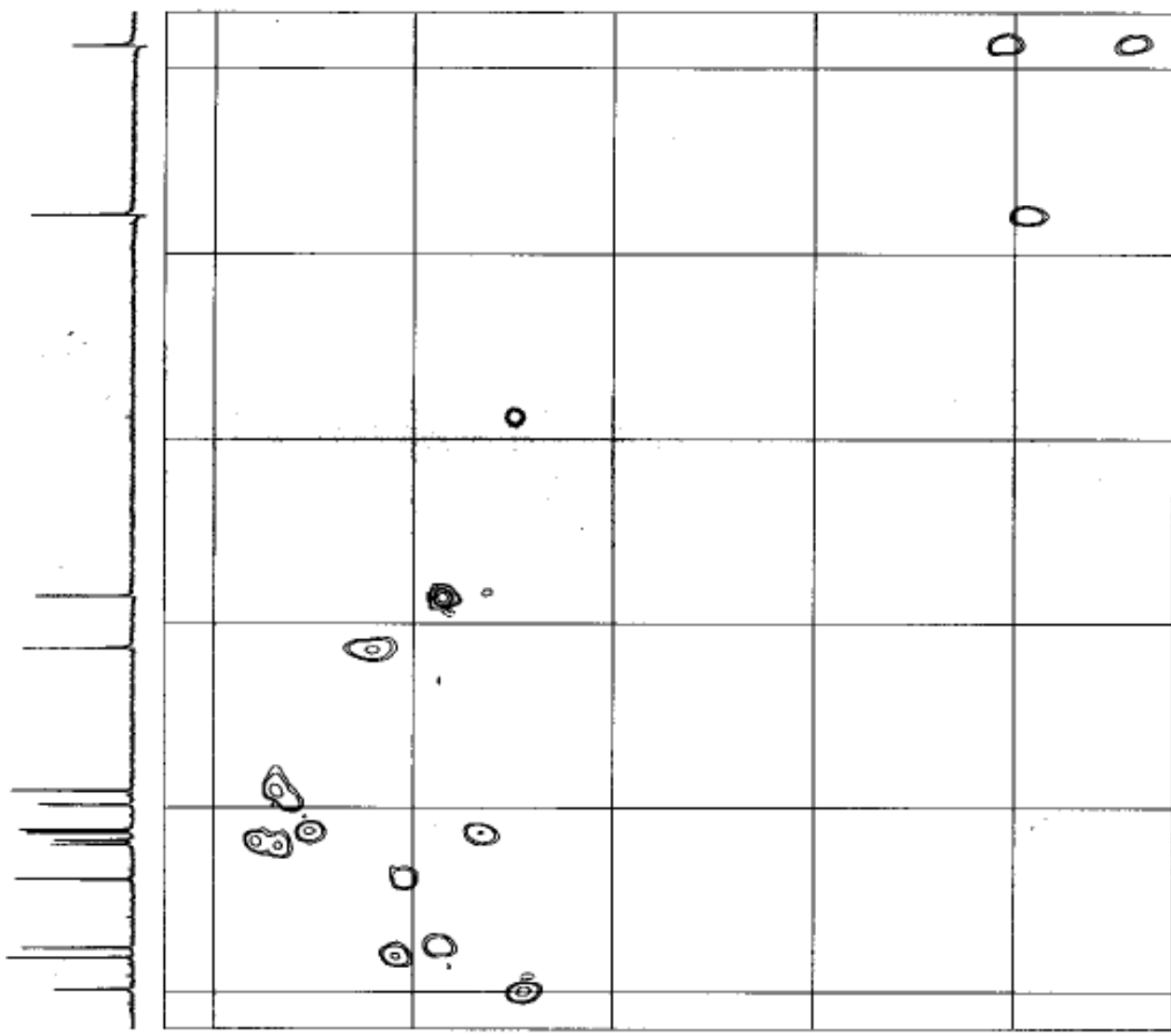
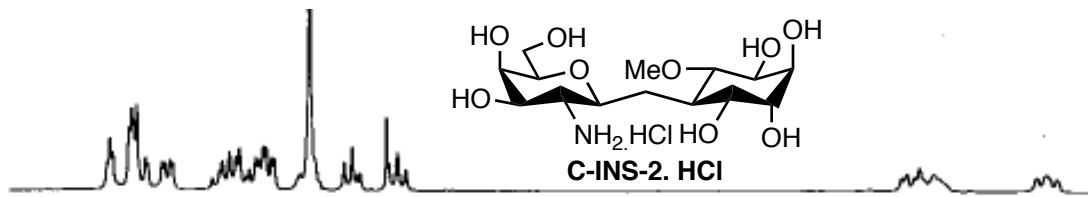
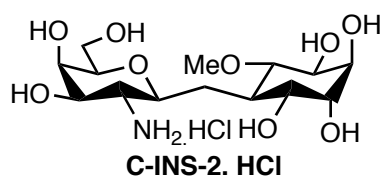
26.4283



C-INS-2.HCl







ppm 3.5 3.0 2.5 2.0

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 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080202
 Time 11.30
 INSTRUM spect
 PROBRW 5 MHz CPDCH 1.0
 PULPROG zgpg30
 TO 1024
 SOLVENT DMSO
 NS 2
 DS 16
 SWH 1070.857 Hz
 FIDRES 0.53047 Hz
 AQ 0.678028 sec
 RG 1024.4
 SN 75.858 dB
 SC 0.00 mm
 SS 0.00 s
 DQ02 1.0000000
 AQ 0.0000000 Hz
 EQ 1.0000000 Hz
 RQ 0.0010414 Hz
 SFO 500.13644 MHz
 FID 0.0000000 Hz
 F10 0.0001000 Hz
 F14 0.0012490 Hz
 SFL 0.0007184 Hz
 SFO 500.13644 MHz
 ACSF 0.0000000 Hz
 ACBS 0.2400001 Hz
 STICK 0

----- Channel f1 -----
 NUC1 31
 P1 0.25000000
 PC 10.000000
 PL1 0.000000
 SFO1 500.13644 MHz

----- Channel f2 -----
 CPDPRG2 zgpg30
 NUC2 13C
 P2 0.25000000
 PC 10.000000
 PL2 0.000000
 PL12 0.000000
 SFO2 101.626180 MHz

----- CHANNEL CHANNEL -----
 CPDPRG1 zgpg30
 CPDPRG2 zgpg30
 GPC1 0.00 Hz
 GPC2 0.00 Hz
 GPC3 0.00 Hz
 GPC4 0.00 Hz
 GPC5 0.00 Hz
 GPC6 0.00 Hz
 GPC7 0.00 Hz
 GPC8 0.00 Hz
 GPC9 0.00 Hz
 GPC10 0.00 Hz
 GPC11 0.00 Hz
 GPC12 0.00 Hz
 GPC13 0.00 Hz
 GPC14 0.00 Hz
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 GPC16 0.00 Hz
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 GPC20 0.00 Hz
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 GPC25 0.00 Hz
 GPC26 0.00 Hz
 GPC27 0.00 Hz
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 GPC34 0.00 Hz
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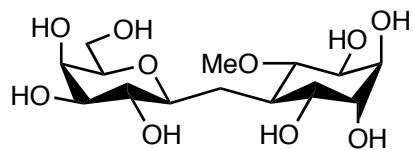
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 RG 1024.4
 SN 75.858 dB
 SC 0.00 mm
 SS 0.00 s
 DQ02 1.0000000

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 GB 0
 PC 1.00

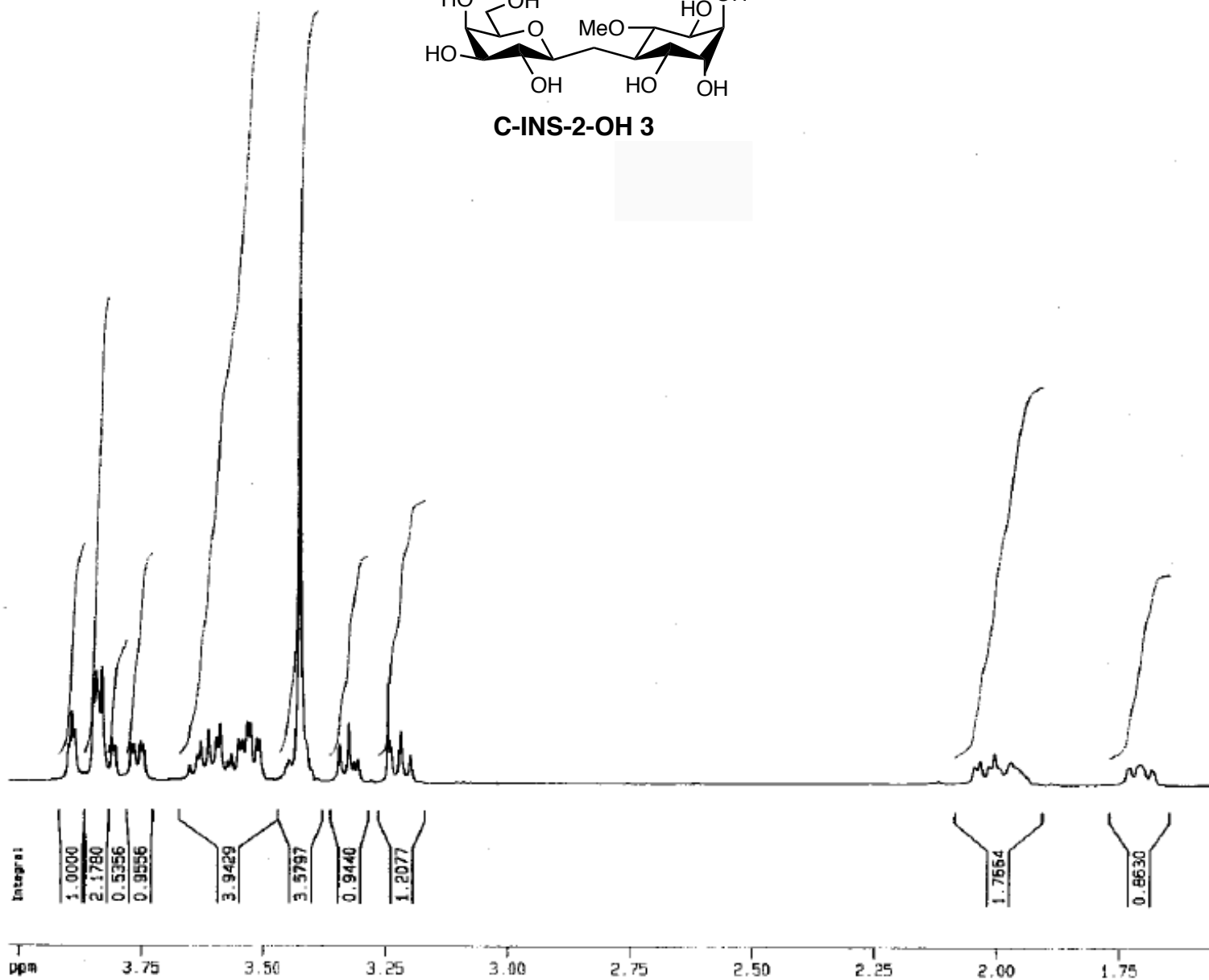
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 PC 1.00

2D NMR list parameters
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 FWH0 4.100 MHz
 FWH1 2062.00 Hz
 FWH2 5.100 MHz
 FWH3 700.00 Hz
 FWH4 50.000 MHz
 FWH5 10000.00 Hz
 FWH6 27.000 MHz
 FWH7 1000.00 Hz
 FWH8 0.1000 MHz/cm
 FWH9 70.0000 MHz/cm
 FWH10 0.1000 MHz/cm
 FWH11 400.0000 MHz/cm

30
40
50
60
70
ppm



C-INS-2-OH 3



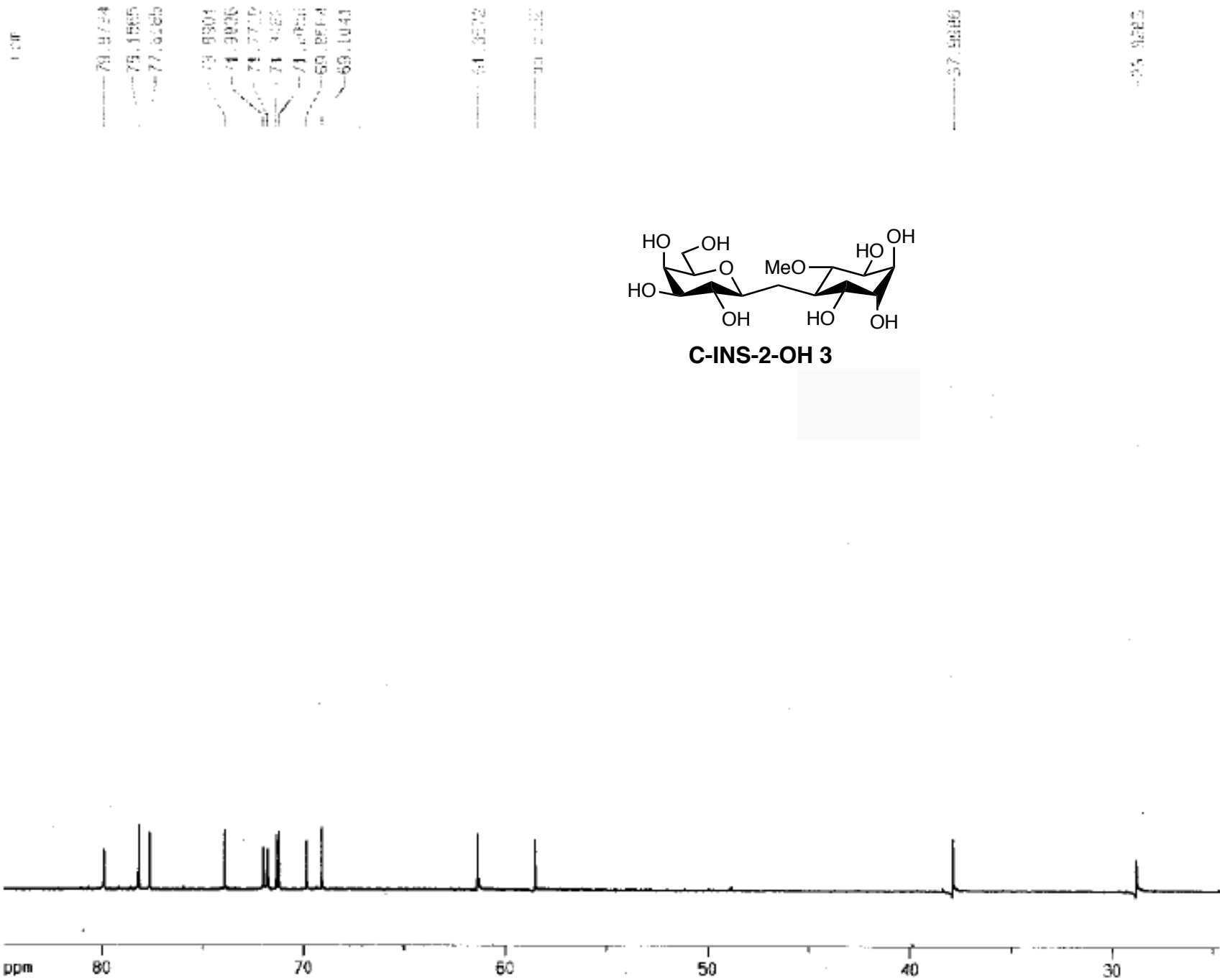
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 PROCNO 1

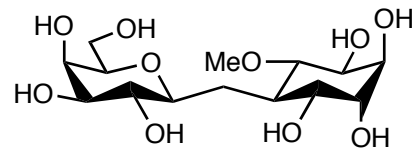
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 PULPROG zg30
 TD 32768
 SOLVENT C606
 NS 8
 OS 2
 SWH 8012.820 Hz
 FIDRES 0.24632 Hz
 AQ 2.0448356 sec
 RG 35.9
 DM 62.400 usec
 DE 6.00 usec
 TE 303.0 K
 D1 1.0000000 sec
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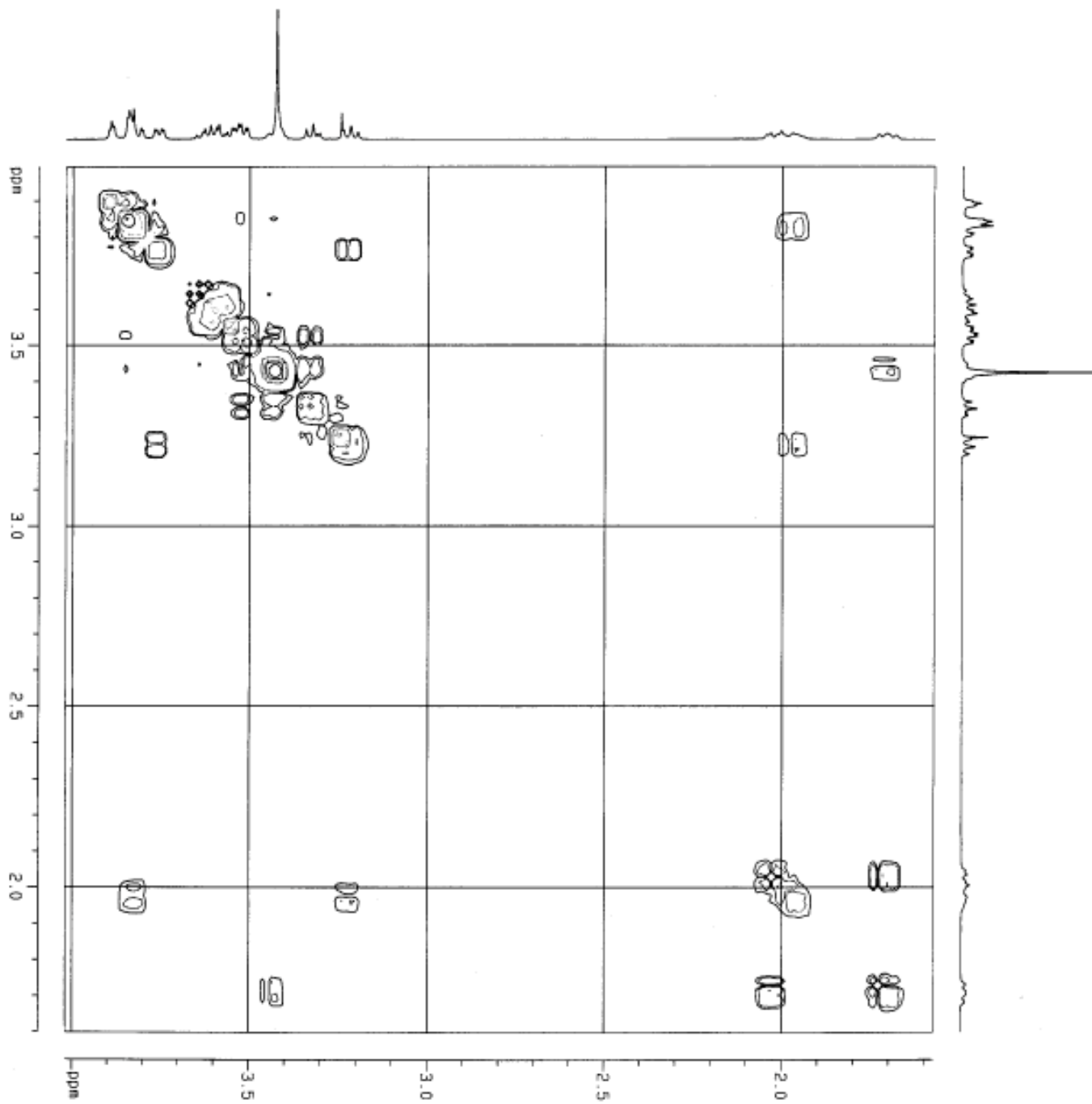
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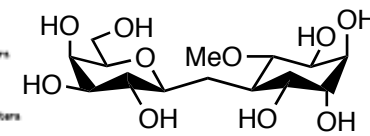
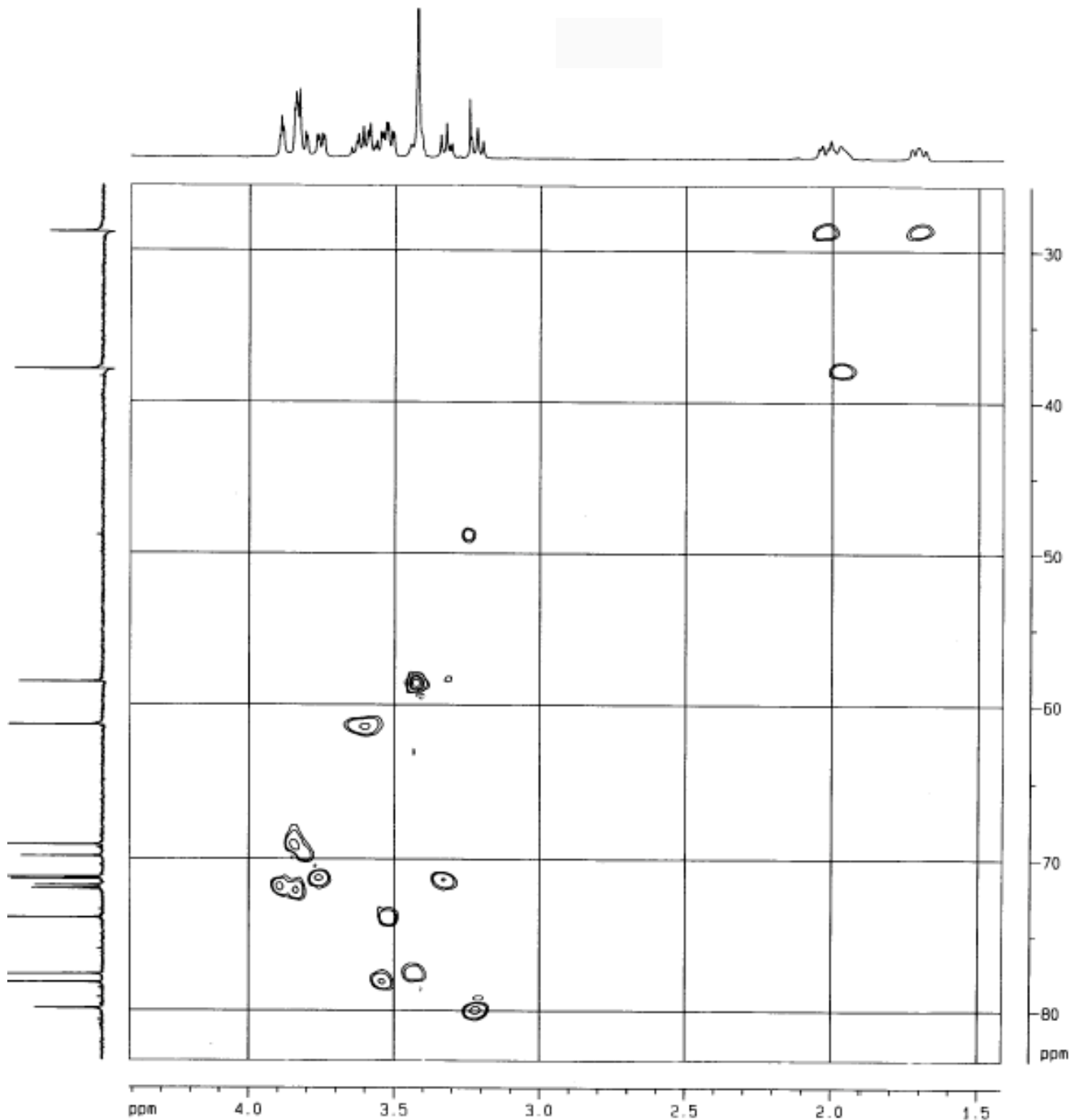
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 CV 15.38 cm
 F1P 4.020 ppm
 F1 2010.70 Hz
 F2P 1.559 ppm
 F2 779.54 Hz
 PPMCH 0.11189 ppm/cm
 HZCM 55.96159 Hz/cm





C-INS-2-OH 3





C-INS-2-OH 3

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Current Data Parameters
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EXPNO    7
PROCNO   1

F2 - Acquisition Parameters
Date_     20080308
Time      18.58
INSTRUM   spect
PROBHD    5 mm CPXCI 13C
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        2
DS        16
SWH        8000.000 Hz
F2FREQ    5.5640170
AQ        0.0180290 sec
RG        38200.4
SR        19.000 MHz
DE        6.00 MHz
TE        303.2 K
CQF2      145.0000000
DE        0.0000000 MHz
DI        1.0000000 sec
DQ        0.0017045 sec
d11       0.0000000 sec
d12       0.0000000 sec
d15       0.0000000 sec
DELTA1A   0.0010000 sec
DELTA1B   0.0007100 sec
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ACQRES    0.0000000 sec
AQCRES    0.0000001 sec
STRTPT    64

***** CHANNEL f1 *****
NUC1       13C
P1         9.25 MHz
PR         18.50 MHz
PL1        0.00 dB
PL2        0.00 dB
PL3        0.00 dB
PL4        0.00 dB
PL5        0.00 dB
PL6        0.00 dB
PL7        0.00 dB
PL8        0.00 dB
PL9        0.00 dB
PL10       0.00 dB
PL11       0.00 dB
PL12       0.00 dB
PL13       0.00 dB
PL14       0.00 dB
PL15       0.00 dB
PL16       0.00 dB
PL17       0.00 dB
PL18       0.00 dB
PL19       0.00 dB
PL20       0.00 dB
PL21       0.00 dB
PL22       0.00 dB
PL23       0.00 dB
PL24       0.00 dB
PL25       0.00 dB
PL26       0.00 dB
PL27       0.00 dB
PL28       0.00 dB
PL29       0.00 dB
PL30       0.00 dB
PL31       0.00 dB
PL32       0.00 dB
PL33       0.00 dB
PL34       0.00 dB
PL35       0.00 dB
PL36       0.00 dB
PL37       0.00 dB
PL38       0.00 dB
PL39       0.00 dB
PL40       0.00 dB
PL41       0.00 dB
PL42       0.00 dB
PL43       0.00 dB
PL44       0.00 dB
PL45       0.00 dB
PL46       0.00 dB
PL47       0.00 dB
PL48       0.00 dB
PL49       0.00 dB
PL50       0.00 dB
PL51       0.00 dB
PL52       0.00 dB
PL53       0.00 dB
PL54       0.00 dB
PL55       0.00 dB
PL56       0.00 dB
PL57       0.00 dB
PL58       0.00 dB
PL59       0.00 dB
PL60       0.00 dB
PL61       0.00 dB
PL62       0.00 dB
PL63       0.00 dB
PL64       0.00 dB
PL65       0.00 dB
PL66       0.00 dB
PL67       0.00 dB
PL68       0.00 dB
PL69       0.00 dB
PL70       0.00 dB
PL71       0.00 dB
PL72       0.00 dB
PL73       0.00 dB
PL74       0.00 dB
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PL76       0.00 dB
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PL80       0.00 dB
PL81       0.00 dB
PL82       0.00 dB
PL83       0.00 dB
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PL87       0.00 dB
PL88       0.00 dB
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PL92       0.00 dB
PL93       0.00 dB
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PL96       0.00 dB
PL97       0.00 dB
PL98       0.00 dB
PL99       0.00 dB
PL100      0.00 dB

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CPDPRG2   gpcp
NUC2       13C
P2         9.25 MHz
PR         18.50 MHz
PL2        0.00 dB
PL3        0.00 dB
PL4        0.00 dB
PL5        0.00 dB
PL6        0.00 dB
PL7        0.00 dB
PL8        0.00 dB
PL9        0.00 dB
PL10       0.00 dB
PL11       0.00 dB
PL12       0.00 dB
PL13       0.00 dB
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PL15       0.00 dB
PL16       0.00 dB
PL17       0.00 dB
PL18       0.00 dB
PL19       0.00 dB
PL20       0.00 dB
PL21       0.00 dB
PL22       0.00 dB
PL23       0.00 dB
PL24       0.00 dB
PL25       0.00 dB
PL26       0.00 dB
PL27       0.00 dB
PL28       0.00 dB
PL29       0.00 dB
PL30       0.00 dB
PL31       0.00 dB
PL32       0.00 dB
PL33       0.00 dB
PL34       0.00 dB
PL35       0.00 dB
PL36       0.00 dB
PL37       0.00 dB
PL38       0.00 dB
PL39       0.00 dB
PL40       0.00 dB
PL41       0.00 dB
PL42       0.00 dB
PL43       0.00 dB
PL44       0.00 dB
PL45       0.00 dB
PL46       0.00 dB
PL47       0.00 dB
PL48       0.00 dB
PL49       0.00 dB
PL50       0.00 dB
PL51       0.00 dB
PL52       0.00 dB
PL53       0.00 dB
PL54       0.00 dB
PL55       0.00 dB
PL56       0.00 dB
PL57       0.00 dB
PL58       0.00 dB
PL59       0.00 dB
PL60       0.00 dB
PL61       0.00 dB
PL62       0.00 dB
PL63       0.00 dB
PL64       0.00 dB
PL65       0.00 dB
PL66       0.00 dB
PL67       0.00 dB
PL68       0.00 dB
PL69       0.00 dB
PL70       0.00 dB
PL71       0.00 dB
PL72       0.00 dB
PL73       0.00 dB
PL74       0.00 dB
PL75       0.00 dB
PL76       0.00 dB
PL77       0.00 dB
PL78       0.00 dB
PL79       0.00 dB
PL80       0.00 dB
PL81       0.00 dB
PL82       0.00 dB
PL83       0.00 dB
PL84       0.00 dB
PL85       0.00 dB
PL86       0.00 dB
PL87       0.00 dB
PL88       0.00 dB
PL89       0.00 dB
PL90       0.00 dB
PL91       0.00 dB
PL92       0.00 dB
PL93       0.00 dB
PL94       0.00 dB
PL95       0.00 dB
PL96       0.00 dB
PL97       0.00 dB
PL98       0.00 dB
PL99       0.00 dB
PL100      0.00 dB

***** CHANNEL f3 *****
NAME      2000028
EXPNO    7
PROCNO   1

F1 - Acquisition parameters
NUC       13C
TD        65536
SOLVENT   DMSO
NS        2
DS        16
SWH        8000.000 Hz
F2FREQ    5.5640170
AQ        0.0180290 sec
RG        38200.4
SR        19.000 MHz
DE        6.00 MHz
TE        303.2 K
CQF1      145.0000000
DE        0.0000000 MHz
DI        1.0000000 sec
DQ        0.0017045 sec
d11       0.0000000 sec
d12       0.0000000 sec
d15       0.0000000 sec
DELTA1A   0.0010000 sec
DELTA1B   0.0007100 sec
LNO       0.0000000 sec
ACQRES    0.0000000 sec
AQCRES    0.0000001 sec
STRTPT    64

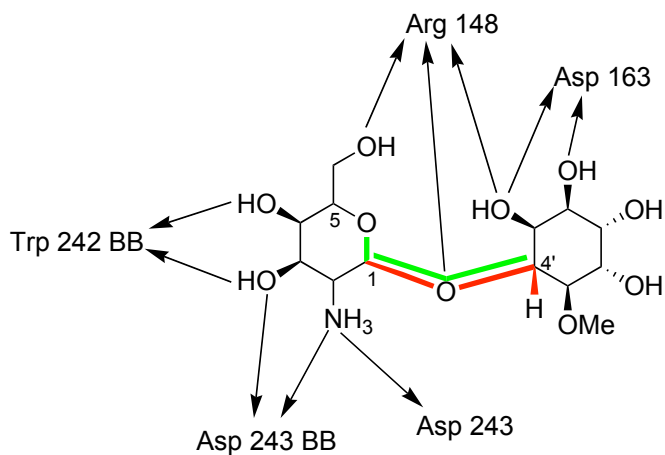
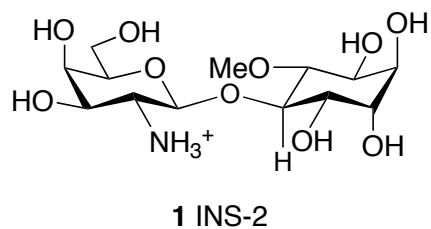
F2 - Processing parameters
SI        32768
SF        500.136000 MHz
WDW       EM
SSB       0
GB        0
PC        1.40

F3 - Processing parameters
SI        32768
SF        125.761700 MHz
WDW       EM
SSB       0
GB        0
PC        1.40

2D NMR parameters
CQ2      125.761700 MHz
CQ1      125.761700 MHz
SF        500.136000 MHz
WDW       EM
SSB       0
GB        0
PC        1.40
F2FREQ    5.5640170 MHz
F1FREQ    125.761700 MHz
F2AQ      0.0180290 sec
F1AQ      0.0180290 sec
F2RG      38200.4
F1RG      38200.4
F2SR      19.000 MHz
F1SR      125.761700 MHz
F2DE      6.00 MHz
F1DE      6.00 MHz
F2TE      303.2 K
F1TE      303.2 K
F2CQF2    145.0000000 MHz
F1CQF2    145.0000000 MHz
F2DE      0.0000000 MHz
F1DE      0.0000000 MHz
F2DI      1.0000000 sec
F1DI      1.0000000 sec
F2DQ      0.0017045 sec
F1DQ      0.0017045 sec
F2d11     0.0000000 sec
F1d11     0.0000000 sec
F2d12     0.0000000 sec
F1d12     0.0000000 sec
F2DELTA1A 0.0010000 sec
F1DELTA1A 0.0010000 sec
F2DELTA1B 0.0007100 sec
F1DELTA1B 0.0007100 sec
F2LNO     0.0000000 sec
F1LNO     0.0000000 sec
F2ACQRES  0.0000000 sec
F1ACQRES  0.0000000 sec
F2AQCRES  0.0000001 sec
F1AQCRES  0.0000001 sec
F2STRTPT  64
F1STRTPT  64

```

INS-2 / PP2C α

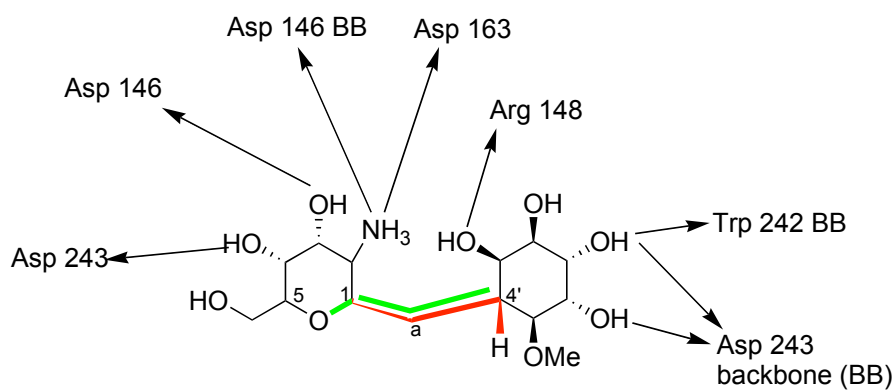
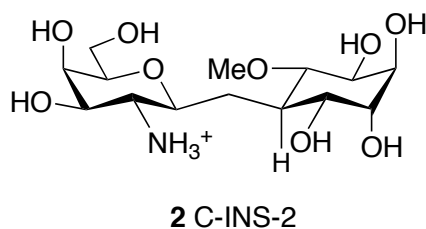


Intersaccharide torsions

$$C1-O-C4'-H4' = +63.7$$

$$O5-C1-O-C4' = +270.0$$

C-INS-2 / PP2C α

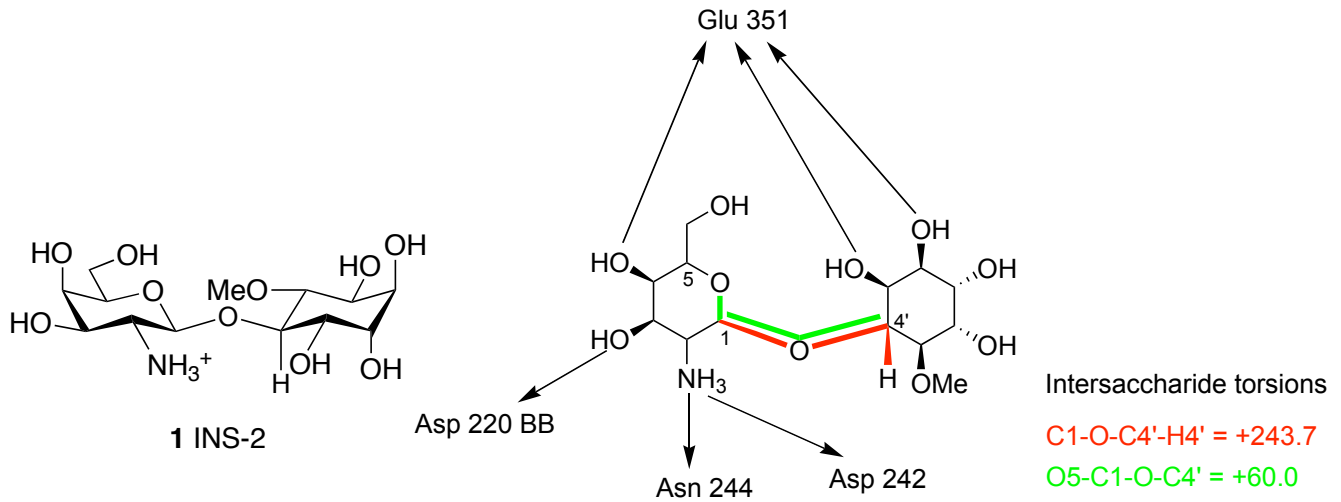


Intersaccharide torsions

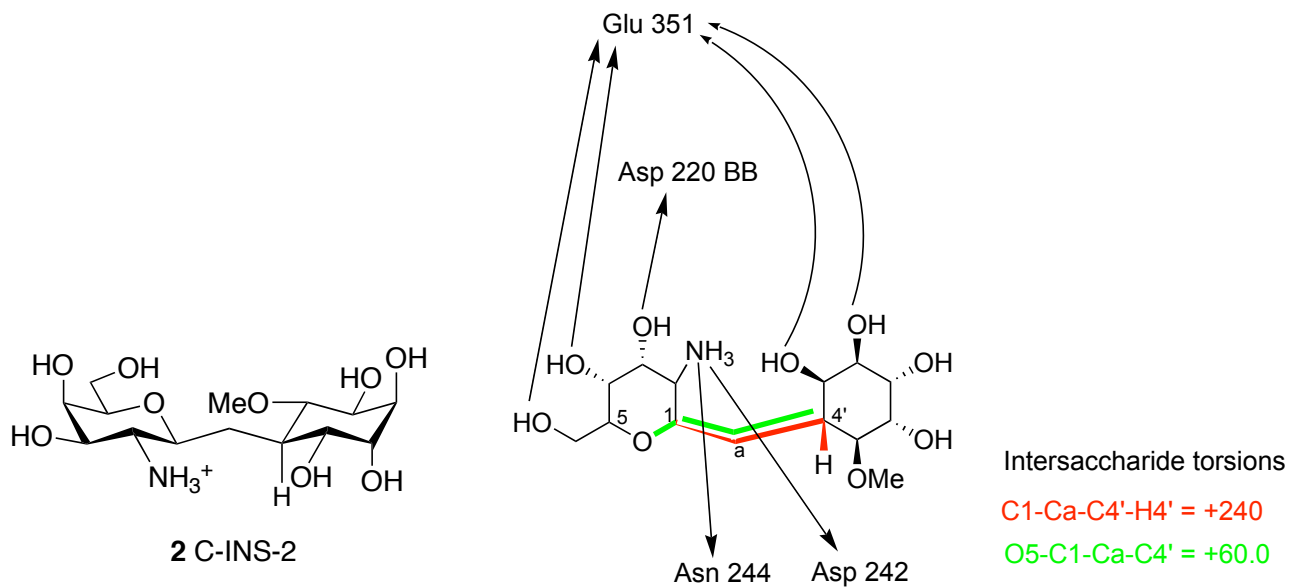
$$C1-Ca-C4'-H4' = +210$$

$$O5-C1-Ca-C4' = +300.0$$

INS-2 / PDHP



C-INS-2 / PDHP



Compound	Protein				
INS-2	PDHP				
#	D-score	PMF	G-score	Chemscore	C-score
9	-150.98	-89.1	-164.66	-14.94	5
5	-148.67	-92.73	-161.87	-15.71	5
3	-76.99	-78.12	-166.27	-19.45	4
4	-78.88	-77.05	-161.62	-19.45	4
16	-153.12	-82.34	-154.71	-15.1	4
1	-68.28	-72.51	-177.4	-14.43	3
2	-69.33	-70.08	-173.37	-16.22	3
6	-71.4	-71.65	-166.53	-16.81	3
7	-72.52	-70.34	-164.95	-16.68	3
11	-97.07	-69.13	-158.18	-15.51	3

Compound	Protein				
C-INS-2	PDHP				
#	D-score	PMF	G-score	Chemscore	C-score
11	-140.04	-78.86	-176.11	-20.27	4
1	-82.91	-70.55	-189.08	-24.76	4
28	-140	-67.16	-157.91	-16.5	3
20	-84.83	-64.62	-203.05	-20.53	3
19	-84.11	-64.6	-201.93	-20.53	3
3	-79.56	-70.44	-187.85	-20.71	3
18	-92.9	-66.3	-183.17	-19.22	2
9	-86.51	-66.71	-204.87	-18.99	2
7	-76.18	-70.3	-164.16	-17.18	2
13	-75.76	-68.48	-157.13	-18.58	2

Compound	Protein				
INS-2	PP2C				
#	D-score	PMF	G-score	Chemscore	C-score
1	-112.09	-49.56	-113.55	-13.31	5
2	-105.23	-47.14	-108.63	-12.99	5
3	-124.46	-57.53	-143.23	-11.5	4
6	-100.2	-46.54	-127.09	-9.89	4
4	-100.07	-48.23	-118.44	-9.9	4
7	-75.16	-49.26	-110.95	-12.82	4
14	-105.6	-45.81	-136.61	-9.4	3
12	-106.14	-47.85	-134.99	-8.57	3
13	-112.39	-49.73	-132.54	-9.62	3
27	-78.34	-47.29	-121.75	-12.16	3

Compound	Protein					
C-INS-2	PP2C					
#	D-score	PMF	G-score	Chemscore	C-score	
3	.138.63	-76.8	-181.3	-22.25	4	
11	-148.27	-54.26	-174.01	-22.2	4	
5	-138.35	-70.09	-173.06	-18.99	4	
6	-147.32	-67.03	-172.31	-18.84	4	
7	-159.73	-122.37	-153.37	-16.49	4	
9	-150.05	-118.65	-148.53	-16.53	4	
19	-178.87	-137.69	-184.77	-13.83	3	
10	-138.96	-70.16	-172.78	-18.1	3	
4	-134.37	-72.75	-166.34	-23.44	3	
8	-129.4	-69.25	-167.35	-19.93	3	

Compound	Protein					
C-INS-2-OH	PDHP					
#	D-score	PMF	G-score	Chemscore	C-score	
10	-142.38	-84.6	-132.27	-15.47	5	
20	-131.09	-66.89	-145.72	-16.43	4	
4	-128.97	-29.67	-141.88	-15.05	4	
19	-146.21	-79.93	-138.5	-15.22	4	
3	-123.45	-62.72	-136.04	-15.46	4	
2	-124.82	-60.05	-135.04	-16.42	4	
1	-89.47	-46.22	-135.44	-17.29	3	
8	-90.62	-75.73	-133.73	-8.47	3	
9	-89.73	-75.53	-128.27	-11.16	3	
25	-165.72	-100.27	-96.39	-14.26	3	

Compound	Protein					
C-INS-2-OH	PP2C					
#	D-score	PMF	G-score	Chemscore	C-score	
1	-127.56	-65.27	-154.89	-17.98	5	
10	-141.16	-62.76	-153.02	-21.32	4	
18	-116.05	-72.64	-122.15	-17.5	4	
14	-127.66	-82.38	-161.29	-10.64	3	
19	-117.88	-87.04	-145.18	-10.03	3	
3	-93.6	-43.58	-121.2	-20.06	3	
12	-95.31	-64.84	-116.56	-17.23	3	
11	-95.13	-64.36	-116.55	-17.23	3	
2	-93.11	-67.03	-108.63	-18.77	3	
6	-63.53	-31.34	-78.56	-16.62	2	