Supporting Information for

Regioselective Opening of *Myo*-Inositol Orthoesters: Mechanism and Synthetic Utility

Himali Y. Godage,[†] Andrew M. Riley,[†] Timothy J. Woodman,[†] Mark P. Thomas,[†] Mary F. Mahon,[‡] Barry V. L. Potter[†]*

[†]Wolfson Laboratory of Medicinal Chemistry, Department of Pharmacy and Pharmacology, University of Bath, Bath, BA2 7AY, UK

[‡] X-Ray Crystallographic Suite, Department of Chemistry, University of Bath, Bath, BA2 7AY, UK

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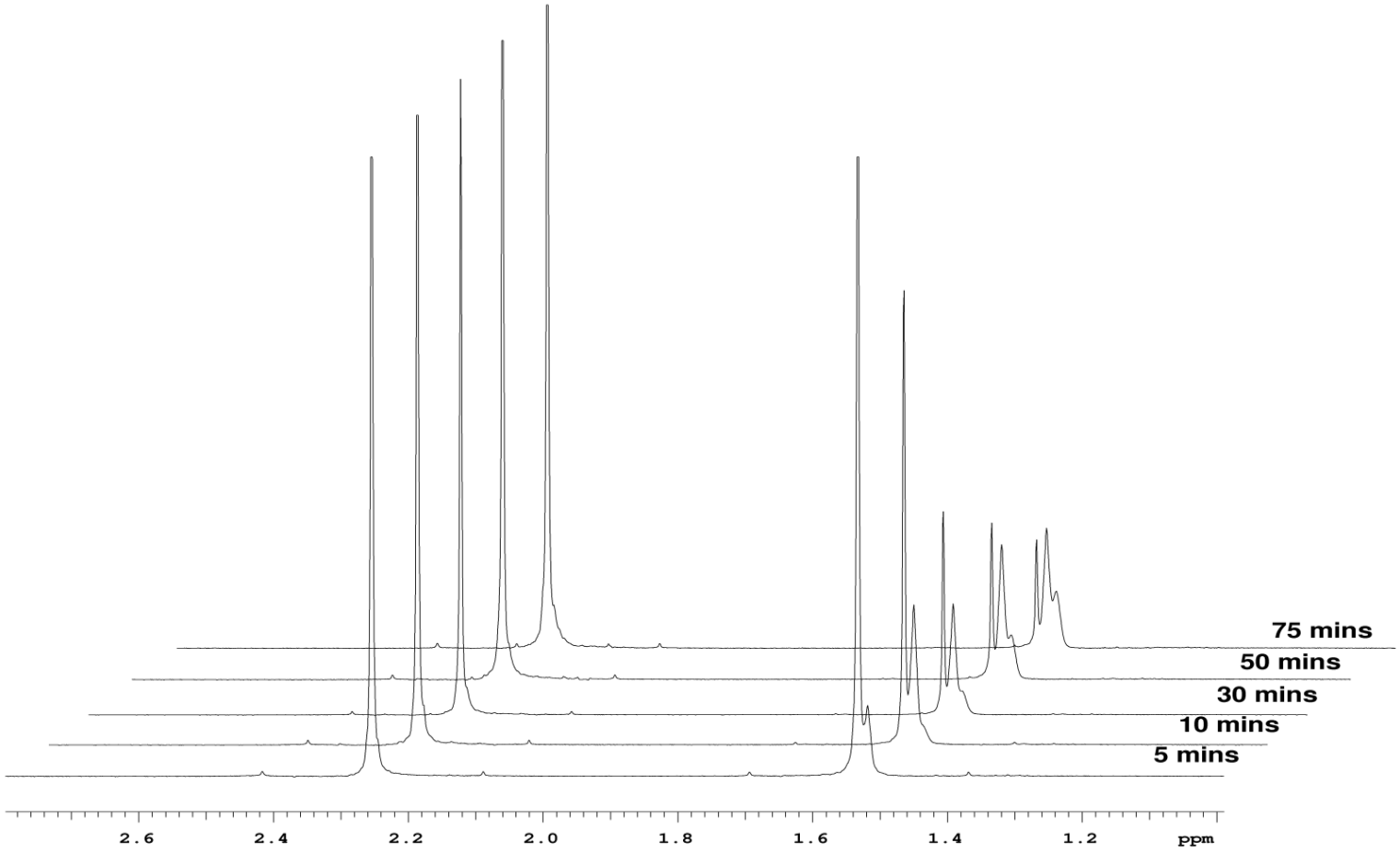


Figure 1 Stack plot of the ^{1}H NMR spectrum of orthoacetate **2** in *d*-TFA/*d*-$CHCl_3$ over 3 h

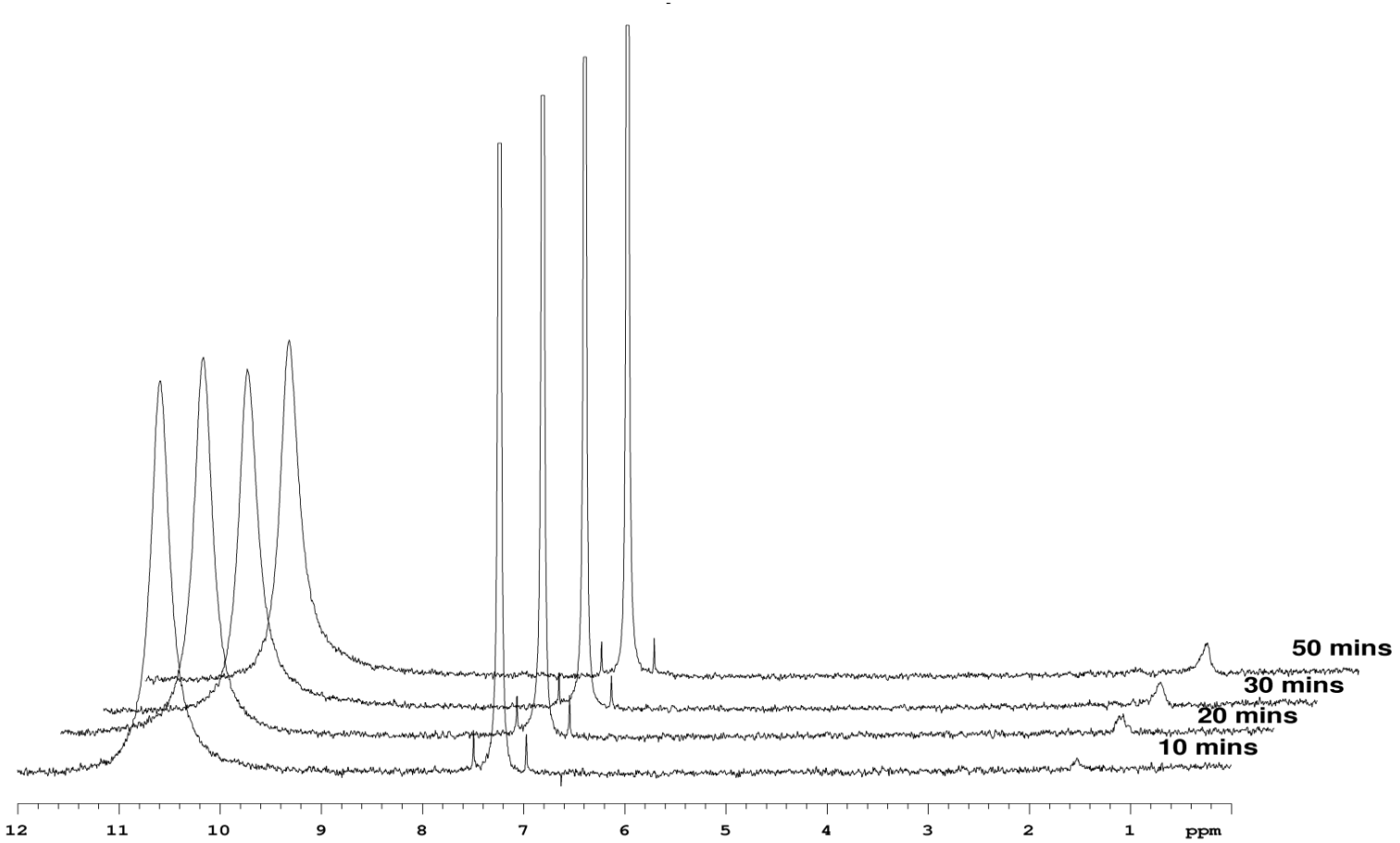


Figure 2 Stack plot of the ^{2}H NMR spectrum of orthoacetate **2** in *d*-TFA/*d*-$CHCl_3$ over 50 mins

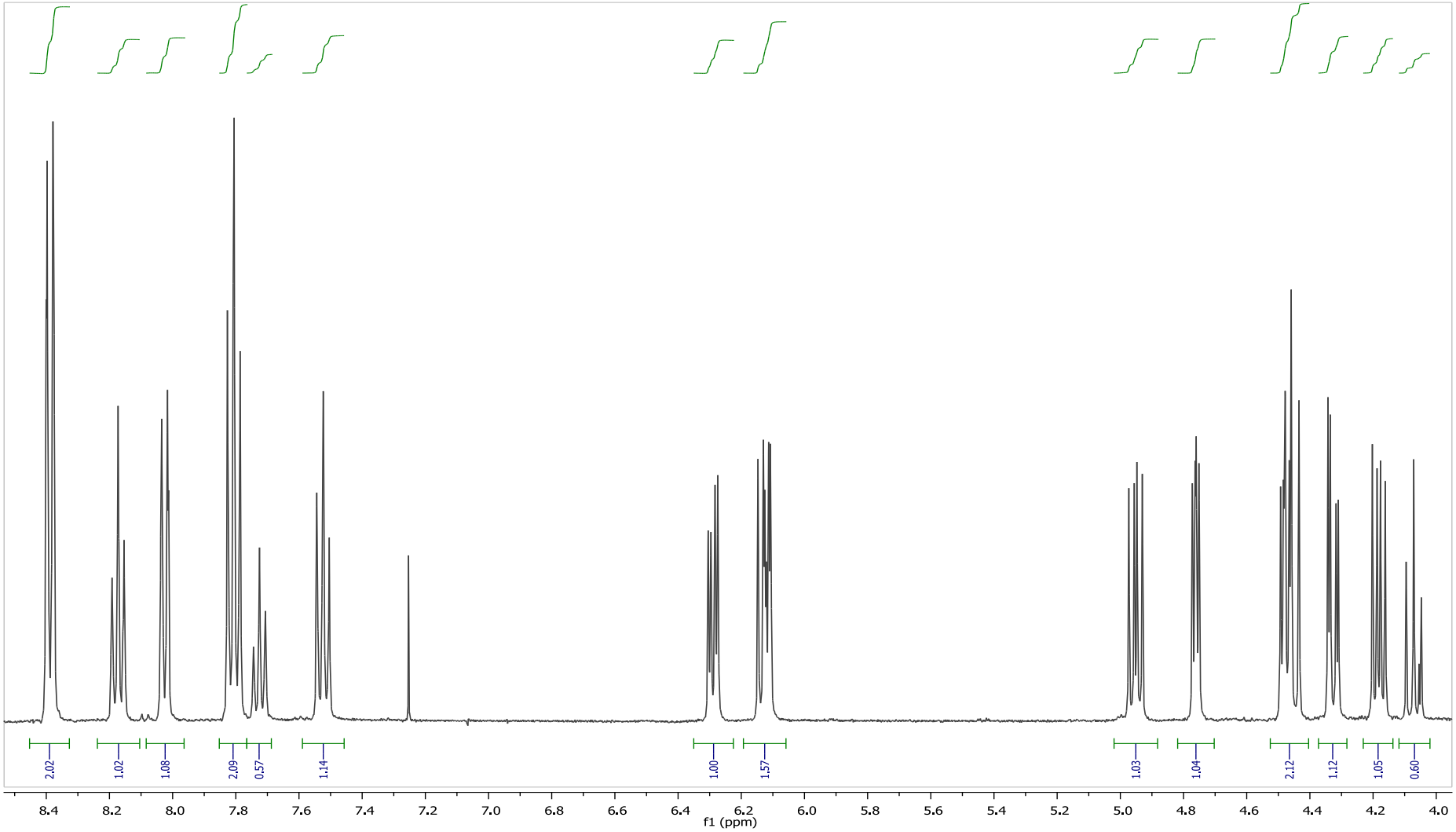


Figure 3 Proton NMR of the1,2-bridged intermediate (±)-**15** and product **6**

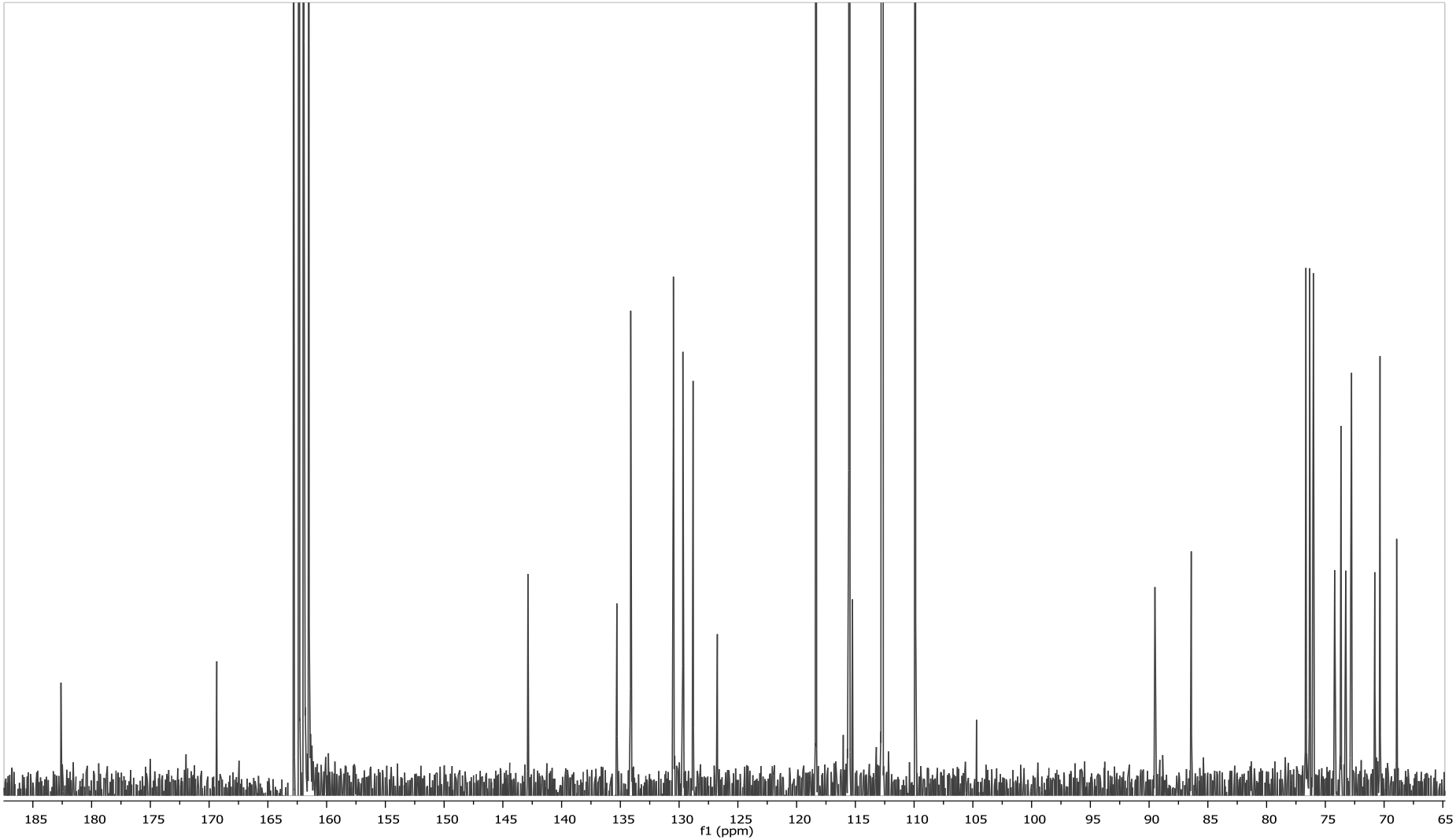


Figure 4 Carbon NMR spectrum of the1,2-bridged intermediate (±)-**15** and product **6**

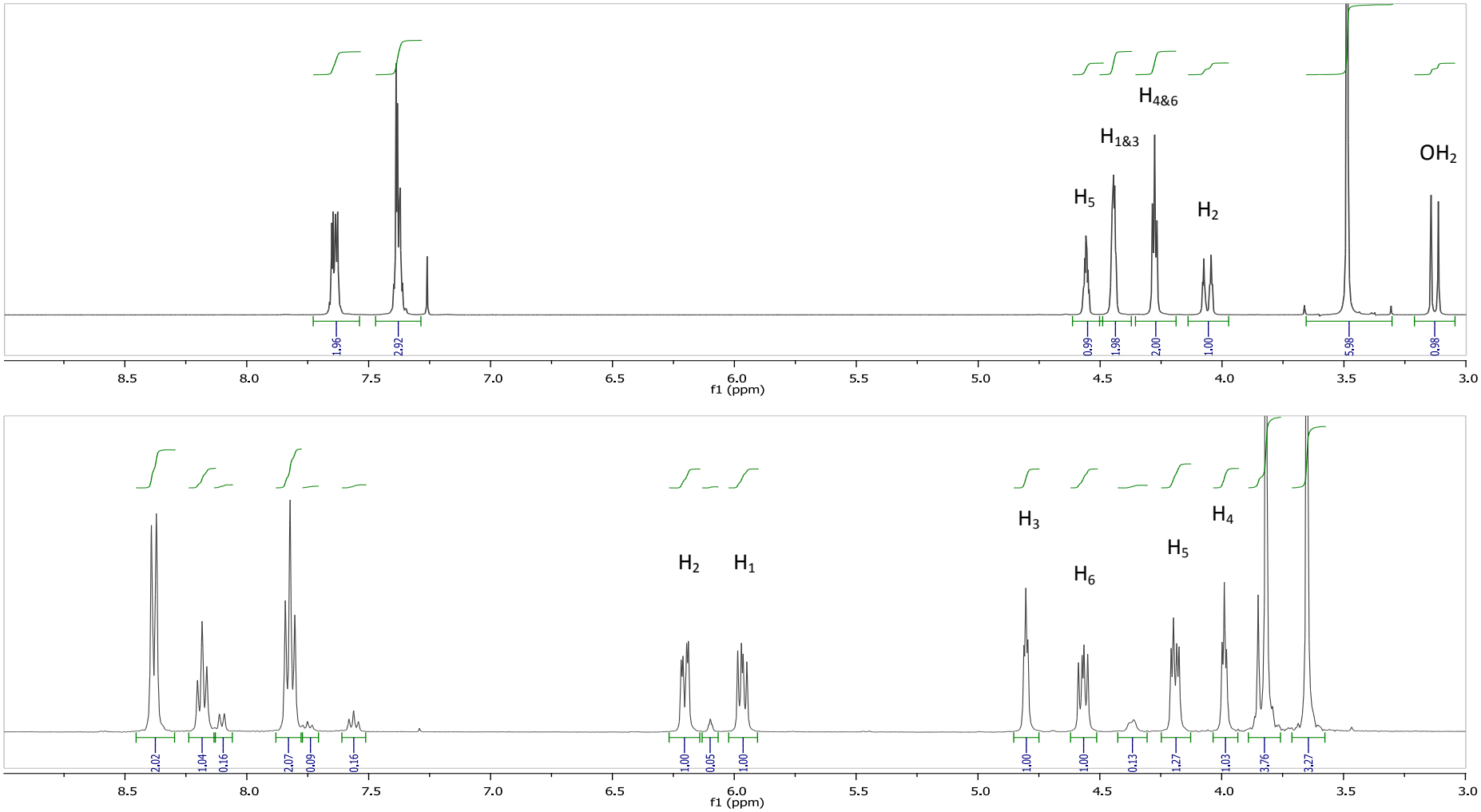


Figure 5 (A) Proton NMR of starting material *myo*-inositol 4,6-di-*O*-Me 1,3,5-orthobenzoate **16**;

(B) Proton NMR of the1,2-bridged intermediate (±)-**17** with very small amount of product **18**

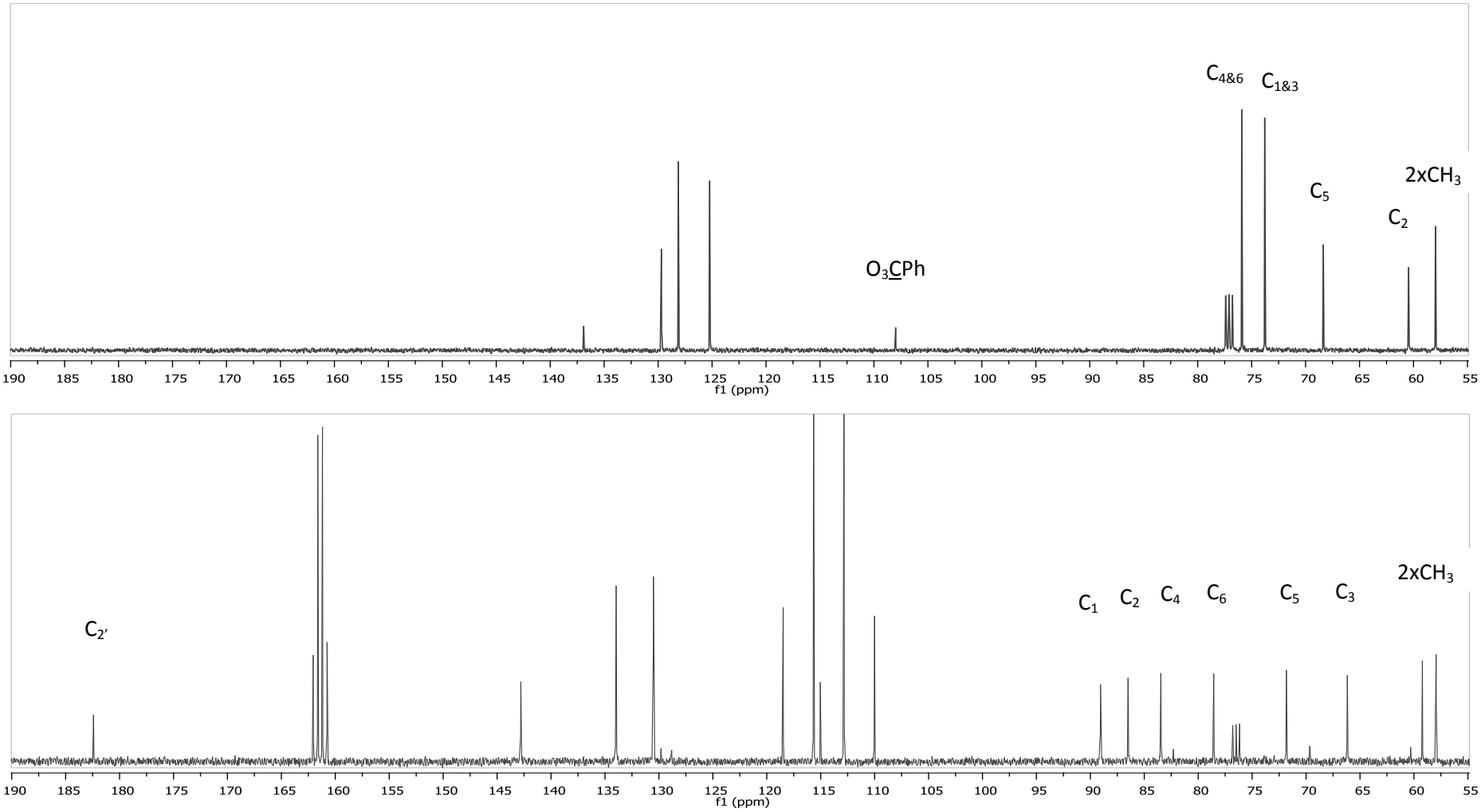


Figure 6 (A) Carbon NMR of starting material *myo*-inositol 4,6-di-*O*-Me 1,3,5-orthobenzoate **16;**

(B) Carbon NMR of the1,2-bridged intermediate (±)-**17** with very small amount of product **18**

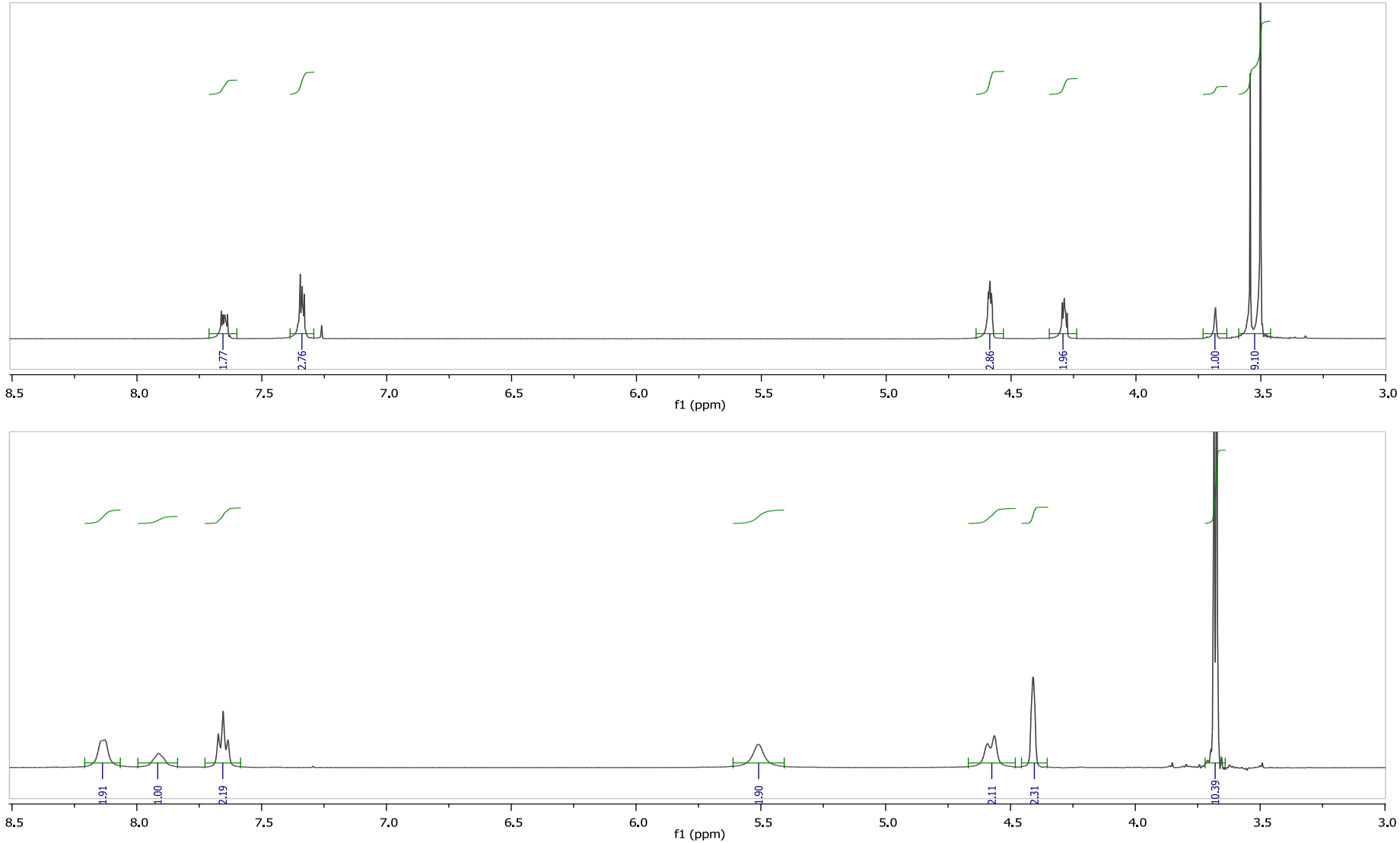


Figure 7 Comparison of ^{1}H NMR spectrum of **24** (A) in $CDCl_3$ and (B) in CF_3CO_2D and $CDCl_3$

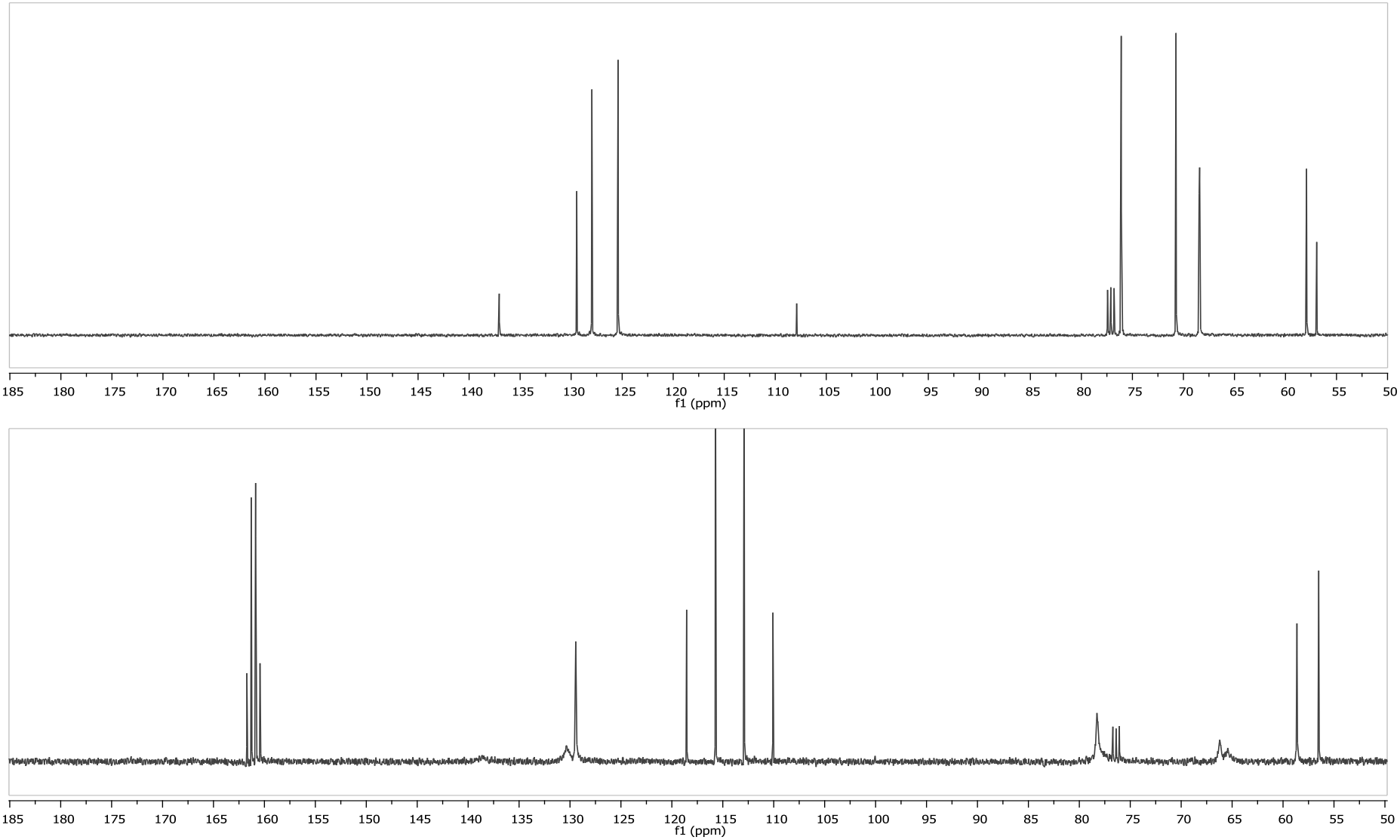


Figure 8 Comparison of ^{13}C NMR spectrum of **24** (A) in $CDCl_3$ and (B) in CF_3CO_2D and $CDCl_3$

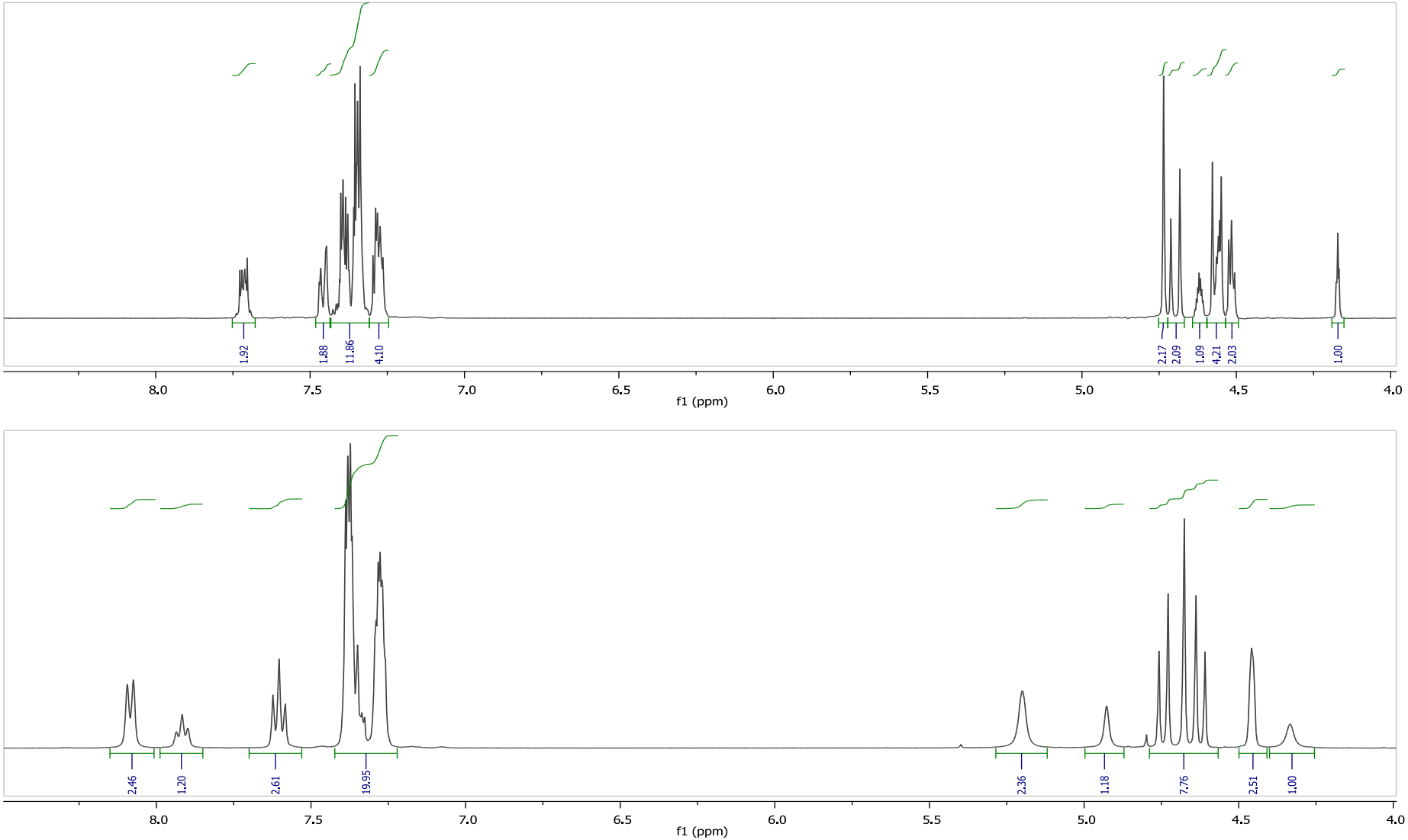


Figure 9 Comparison of ^{1}H NMR spectrum of **25** (A) in $CDCl_3$ and (B) in CF_3CO_2D

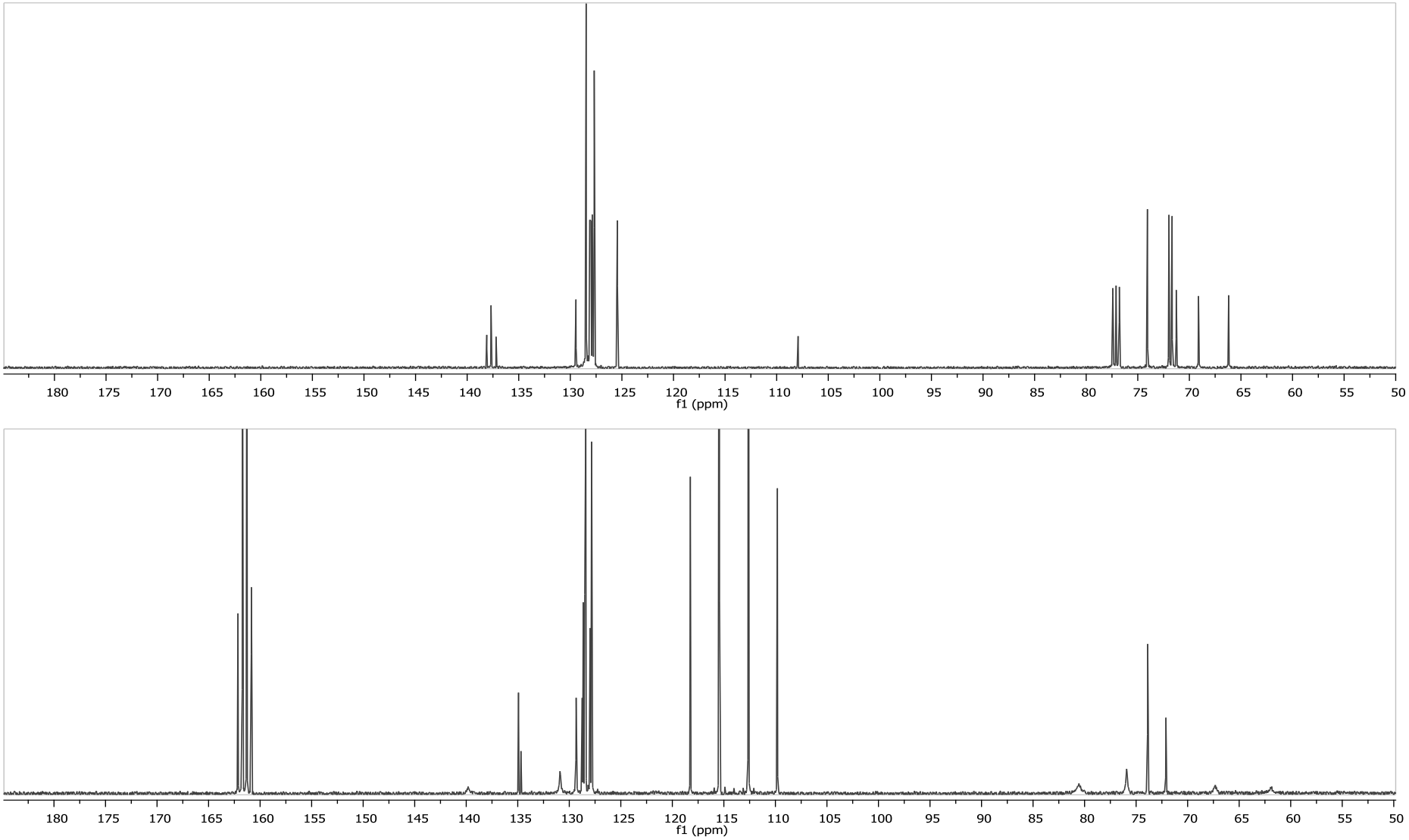
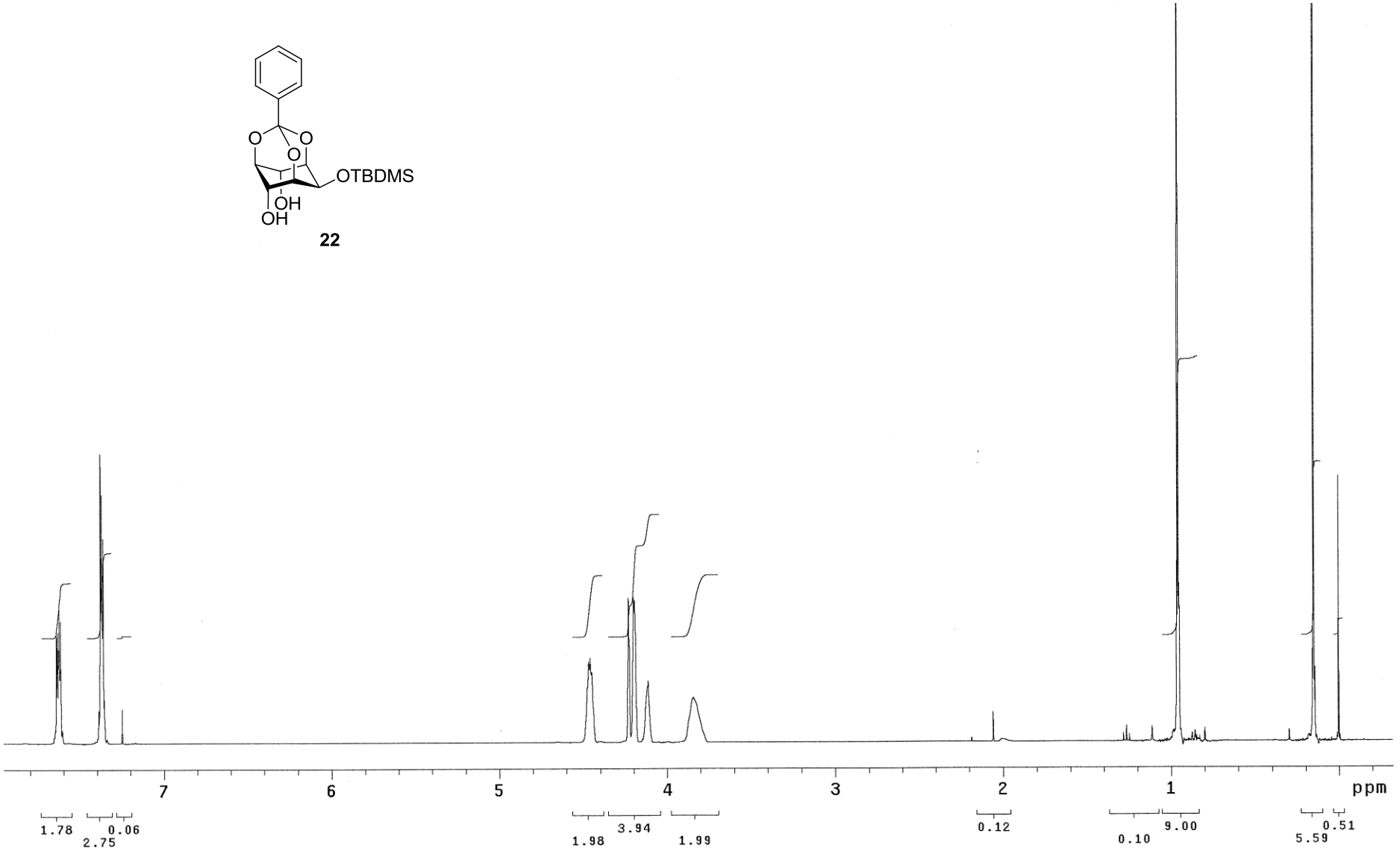


Figure 10 Comparison of ^{13}C NMR spectrum of **25** (A) in $CDCl_3$ and (B) in CF_3CO_2D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O
O
OTBDMS
OH
OH
22
7
6
5
4
3
2
1
ppm
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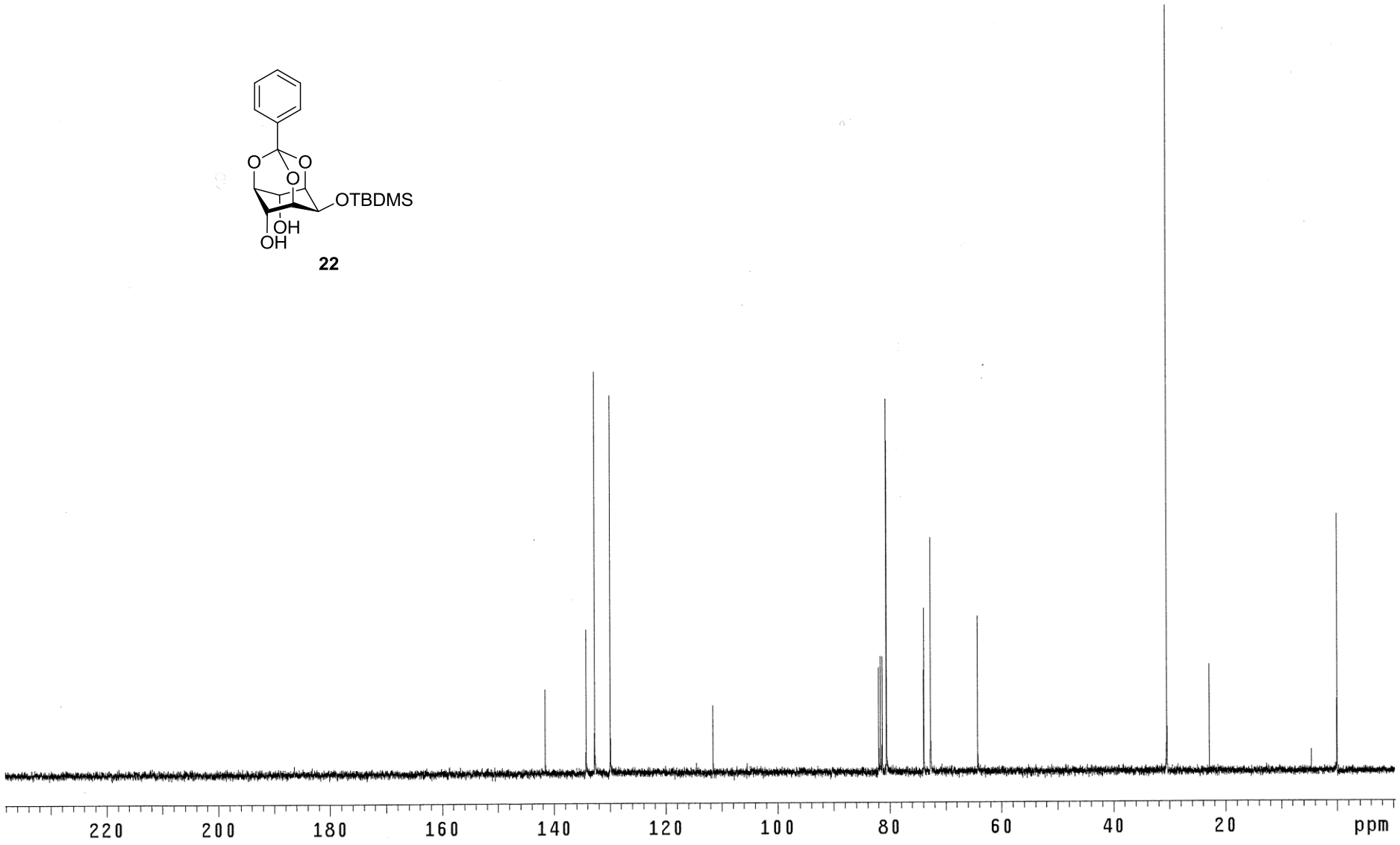
2.75
0.06
1.98
3.94
1.99
0.12
0.10
9.00
5.59
0.51



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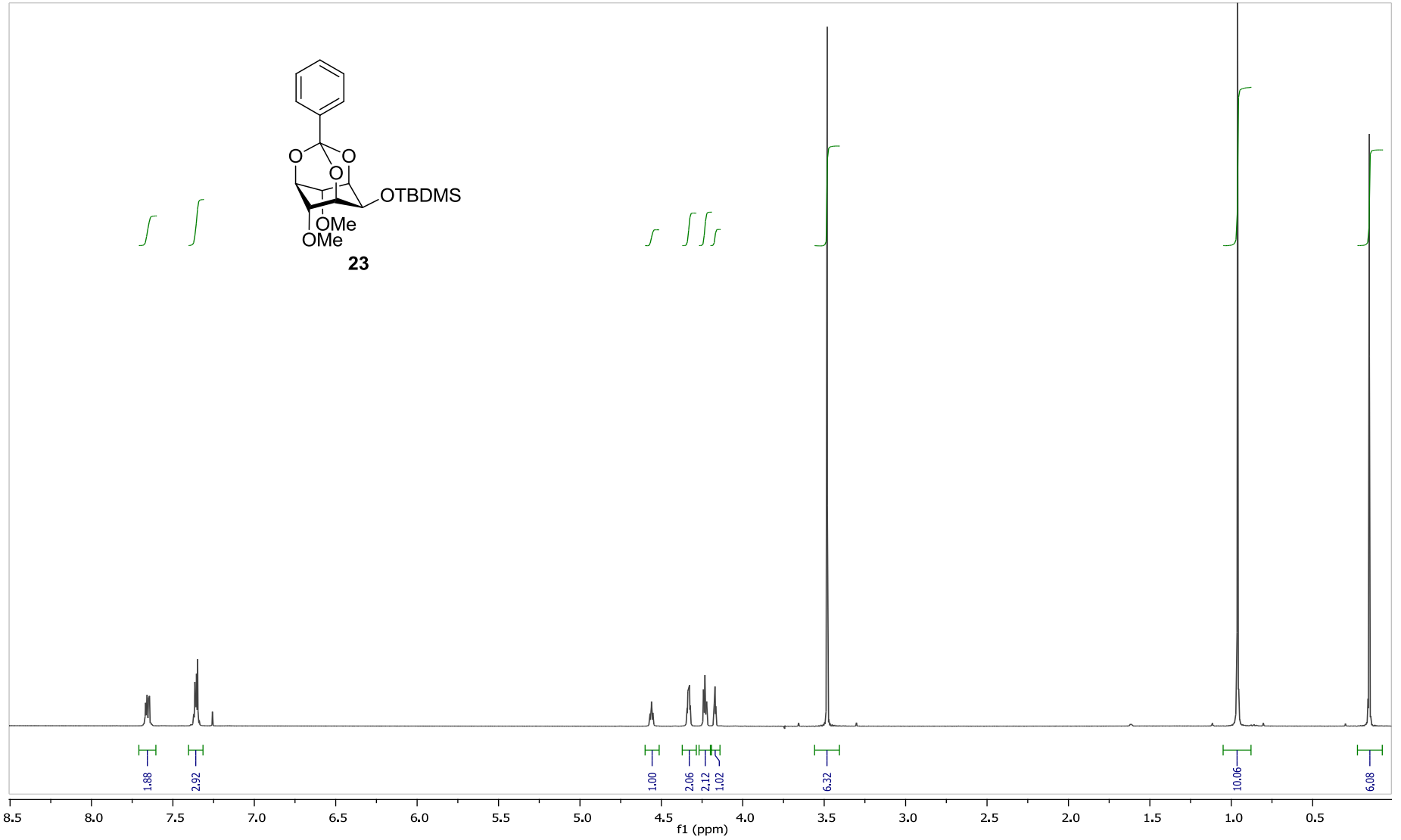
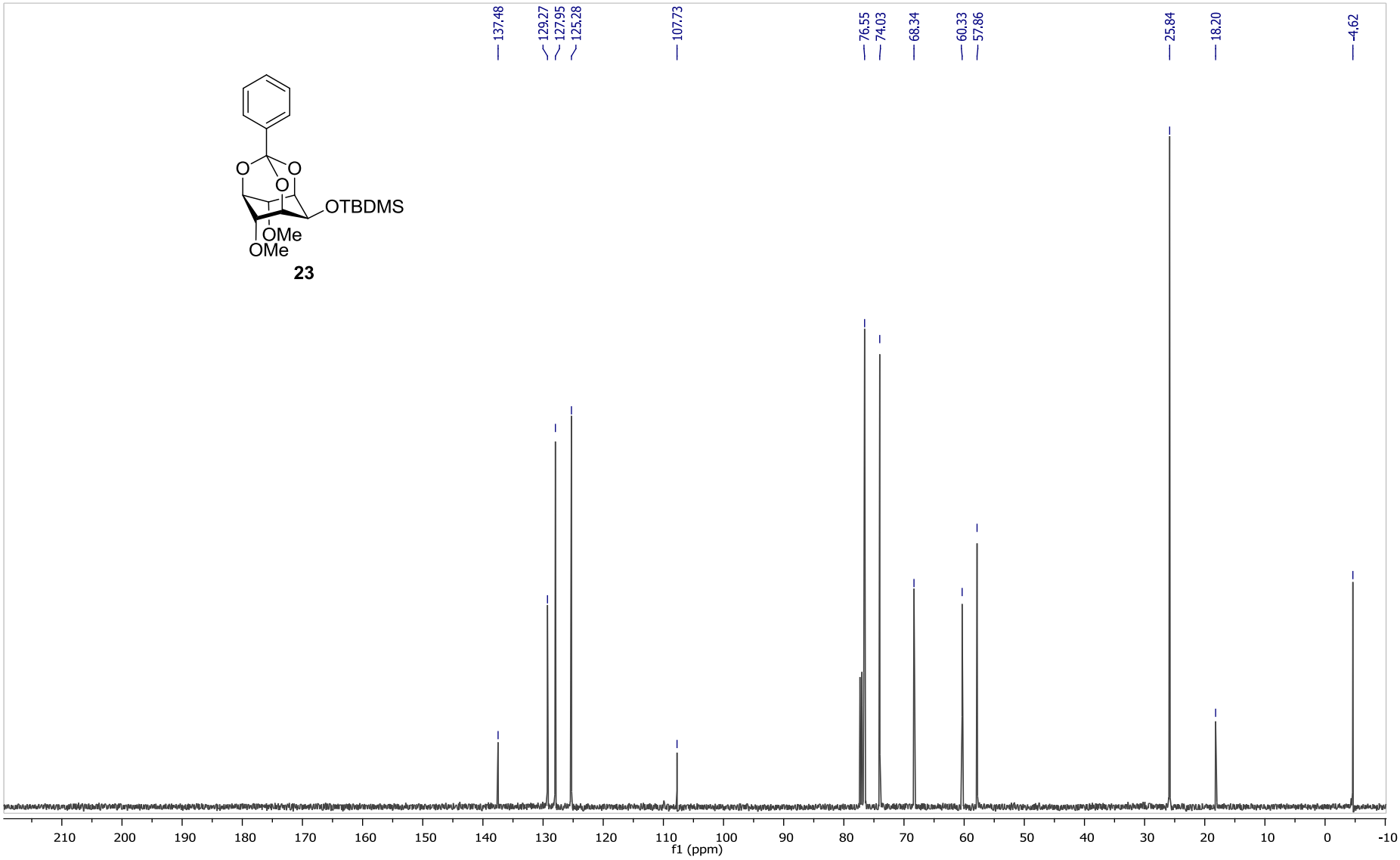

OTBDMS
OMe
OMe
23
1.88
2.92
1.00
2.06
2.12
1.02
6.32
10.06
6.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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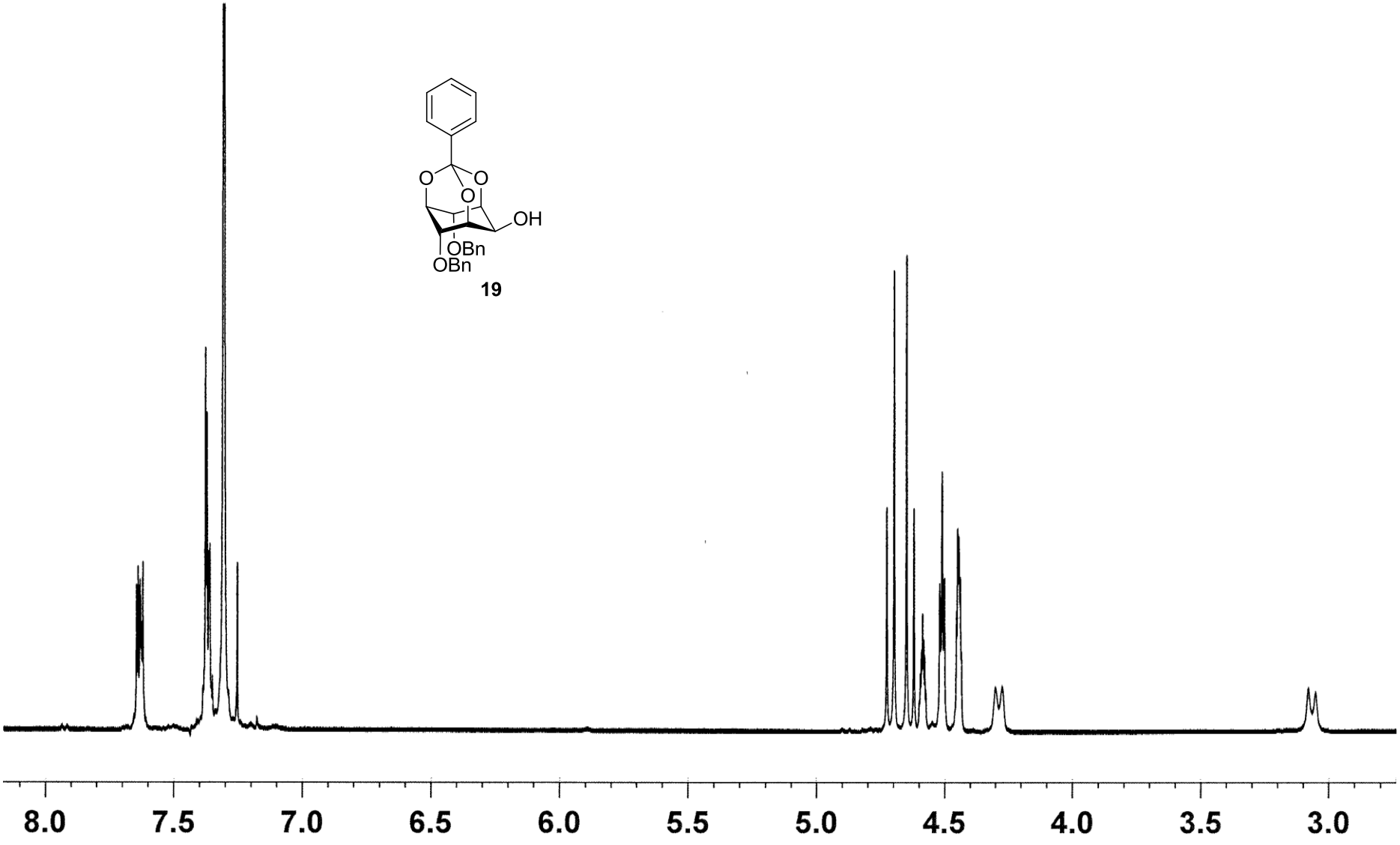
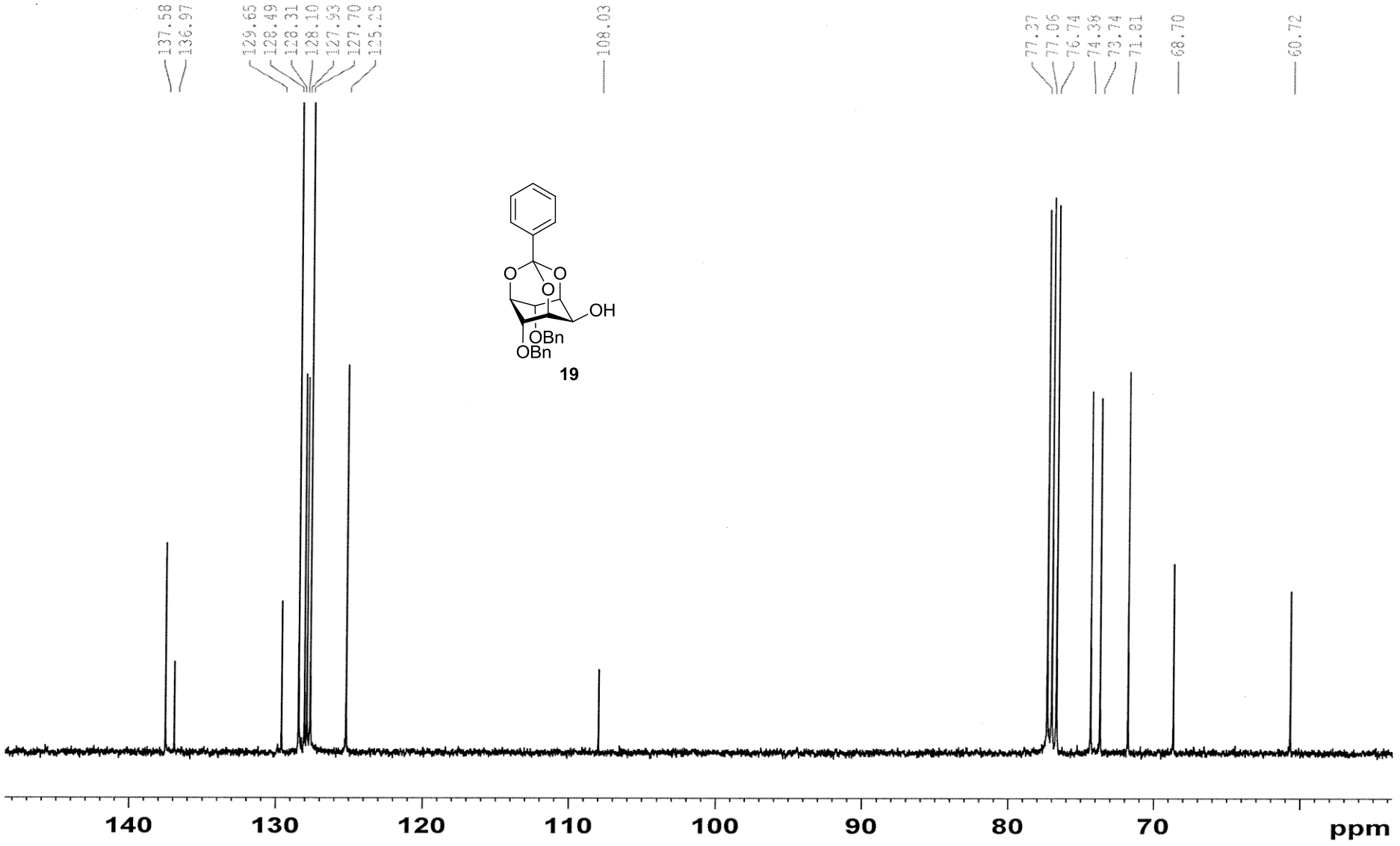
129.27
127.95
125.28
107.73
76.55
74.03
68.34
60.33
57.86
25.84
18.20
-4.62
OTBDMS
OMe
OMe
23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


O
O
O
OH
OBn
OBn
19
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0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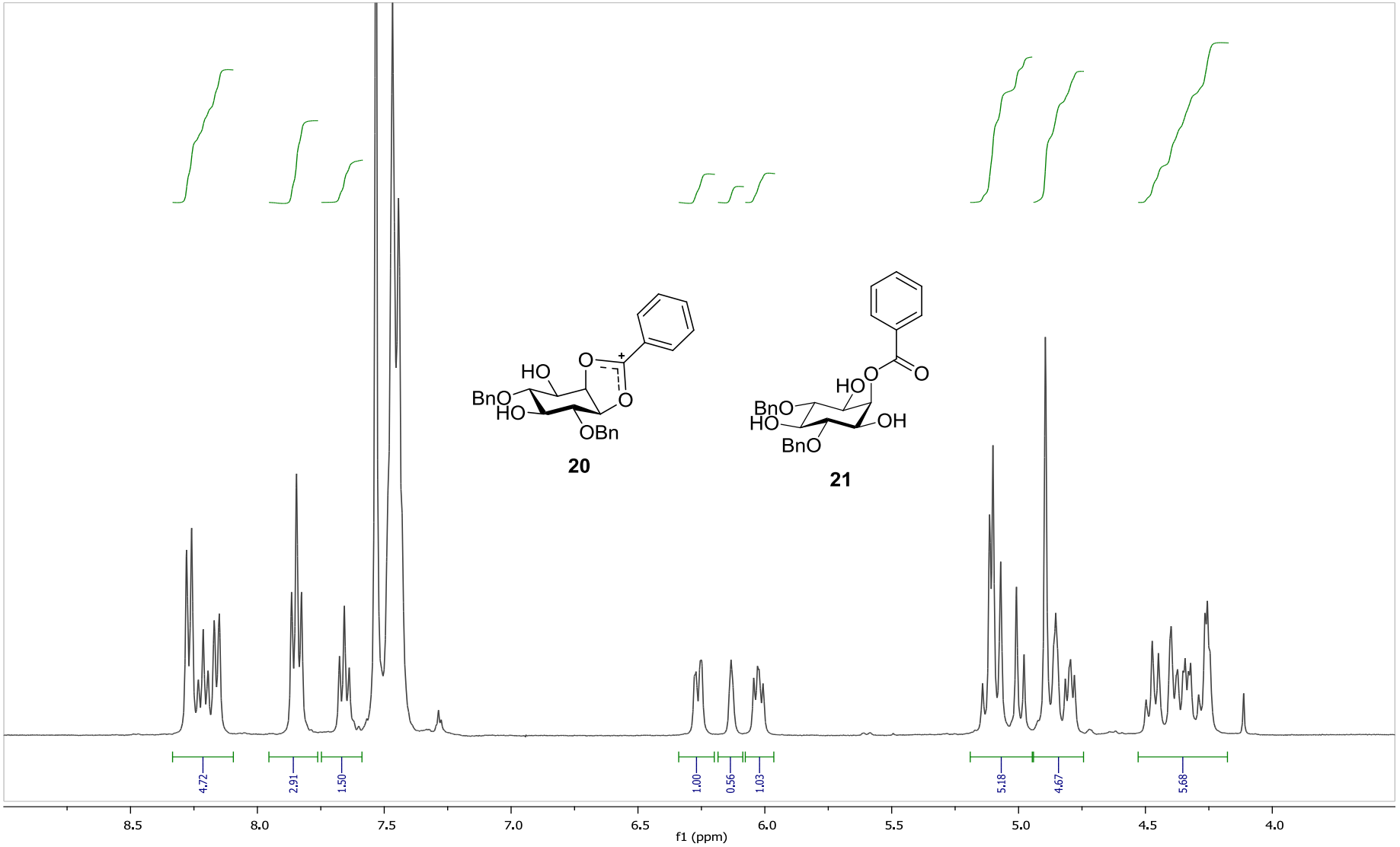
136.97
129.65
128.49
128.31
128.10
127.93
127.70
125.25
108.03
77.37
77.06
76.74
74.38
73.74
71.81
68.70
60.72
O
O
O
OH
OBn
OBn
19
140
130
120
110
100
90
80
70
ppm


HO
O
+
BnO
HO
O
OBn
20
HO
O
O
BnO
HO
OH
BnO
21
4.72
2.91
1.50
1.00
0.56
1.03
5.18
4.67
5.68
8.5
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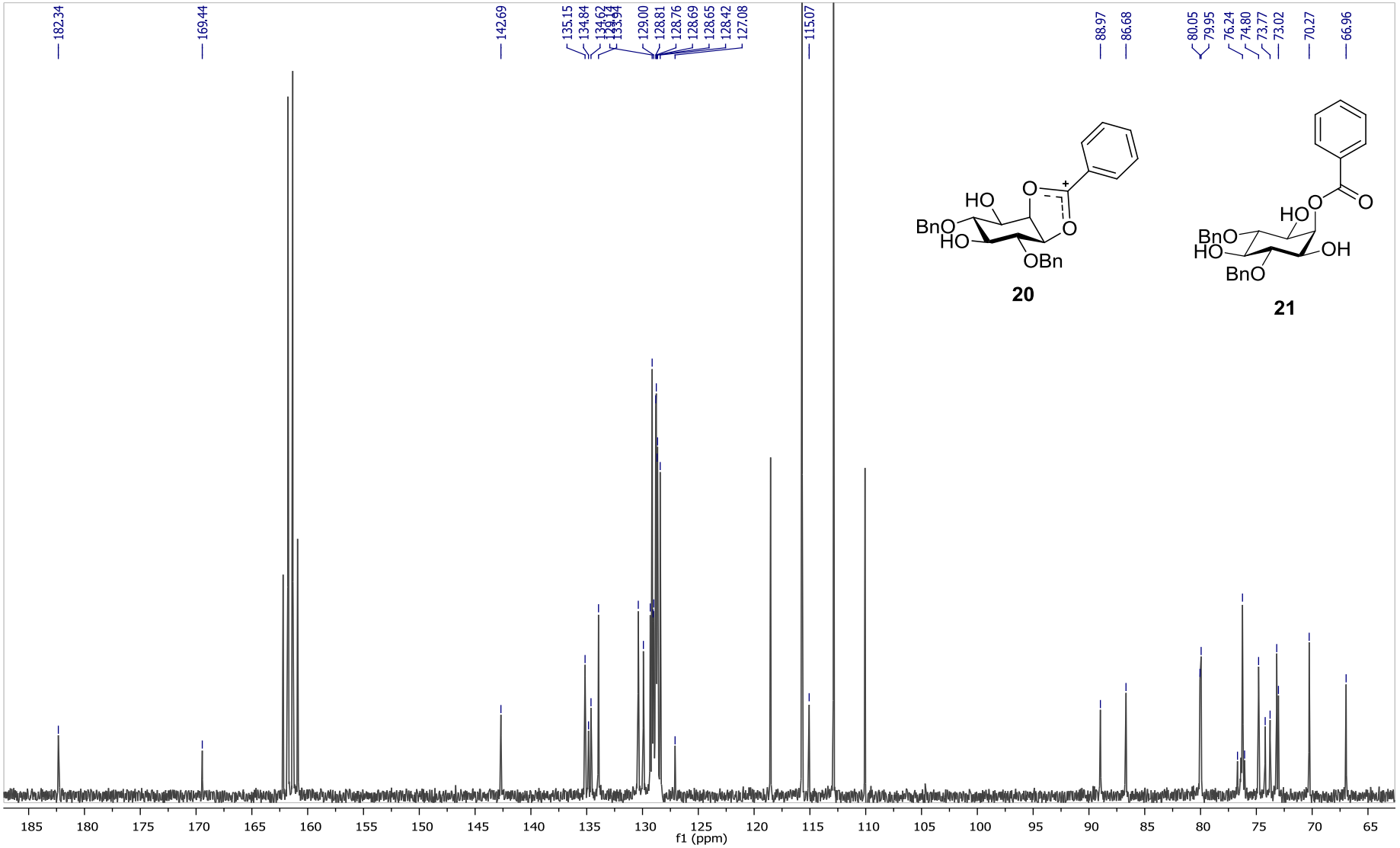
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
f1 (ppm)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169.44
142.69
135.15
134.84
134.62
133.94
129.00
128.81
128.76
128.69
128.65
128.42
127.08
115.07
88.97
86.68
80.05
79.95
76.24
74.80
73.77
73.02
70.27
66.96
HO
O
BnO
HO
OBn
20
O
HO
BnO
HO
OH
BnO
21
185
180
175
170
165
160
155
150
145
140
135
130
125
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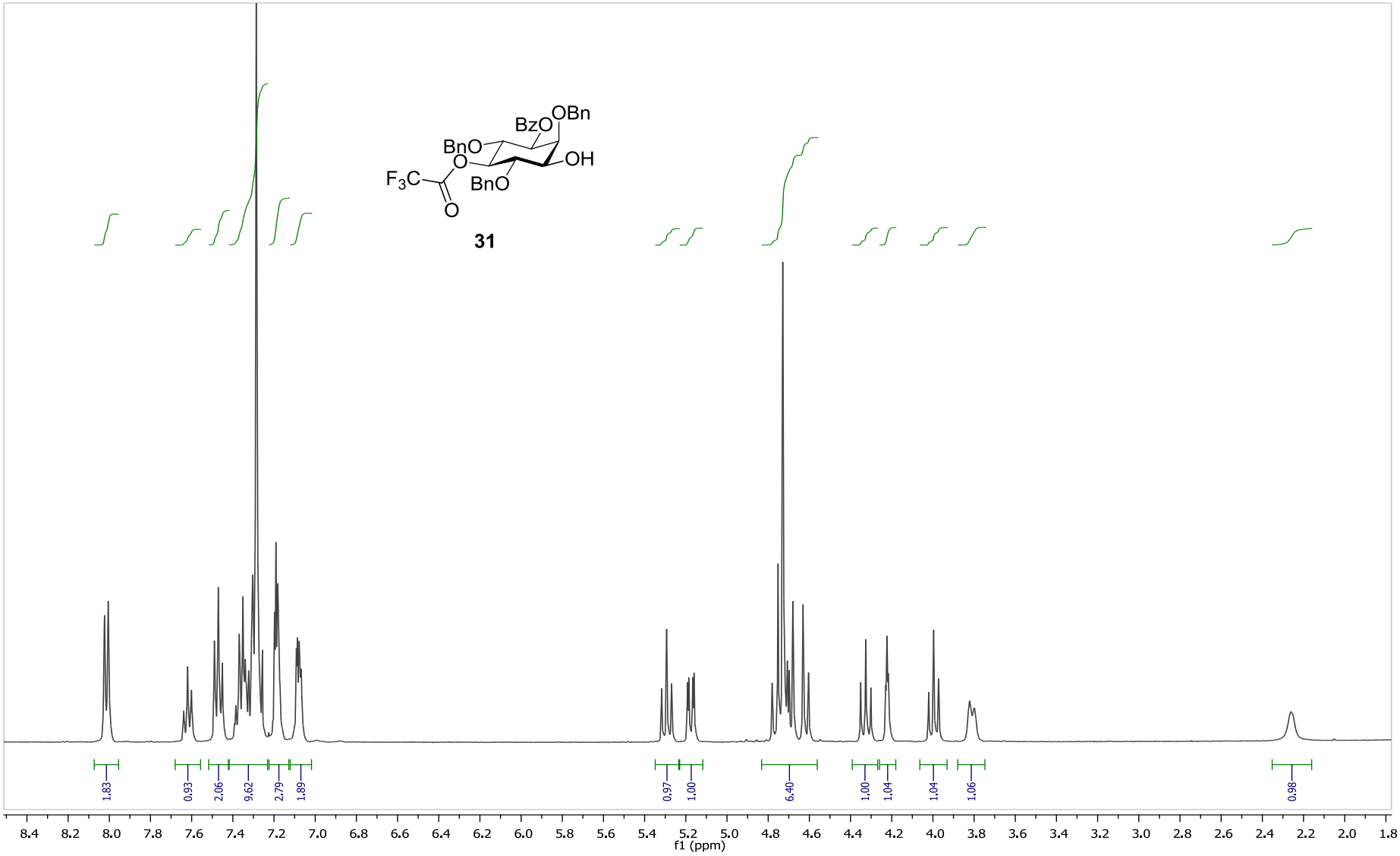
95
90
85
80
75
70
65
f1 (ppm)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OBn
BnO
OH
O
F3C
BnO
O
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2.06
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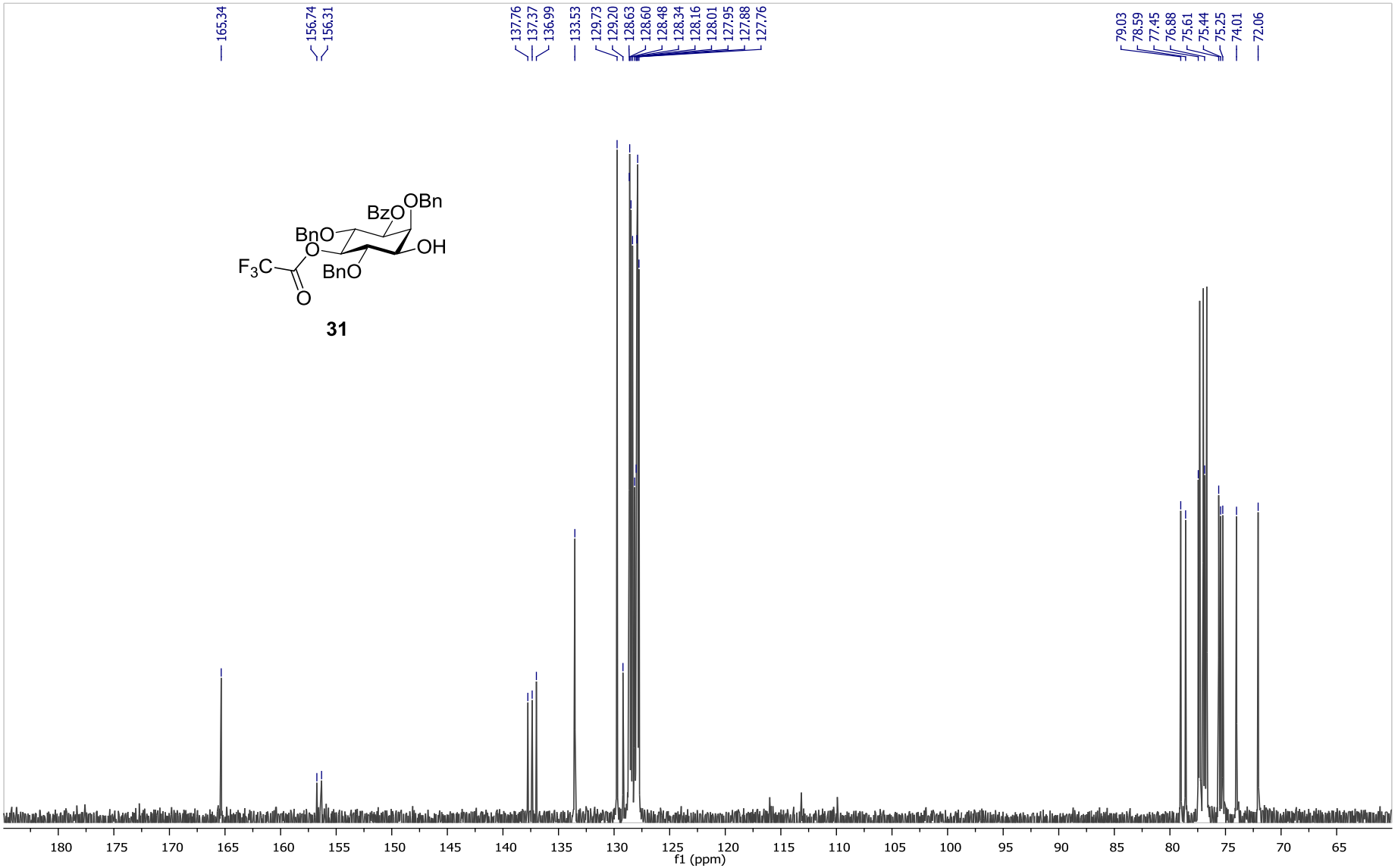
2.79
1.89
0.97
1.00
6.40
1.00
1.04
1.04
1.06
0.98
8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8
f1 (ppm)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156.74
156.31
137.76
137.37
136.99
133.53
129.73
129.20
128.63
128.60
128.48
128.34
128.16
128.01
127.95
127.88
127.76
79.03
78.59
77.45
76.88
75.61
75.44
75.25
74.01
72.06
BzO
OBn
BnO
O
OH
F3C
BnO
O
31
180
175
170
165
160
155
150
145
140
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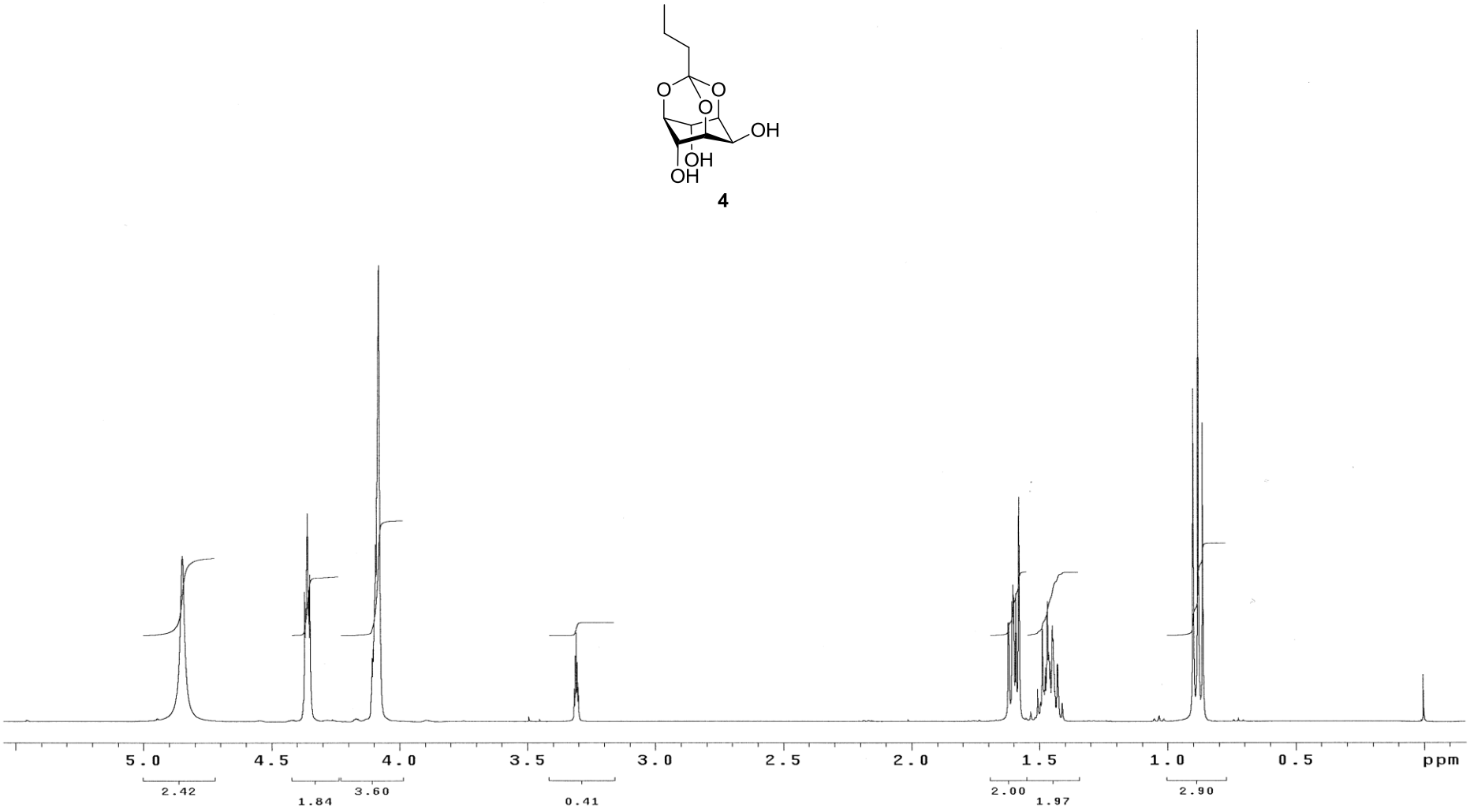
130
125
120
115
110
105
100
95
90
85
80
75
70
65
f1 (ppm)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O
O
OH
OH
OH
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5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
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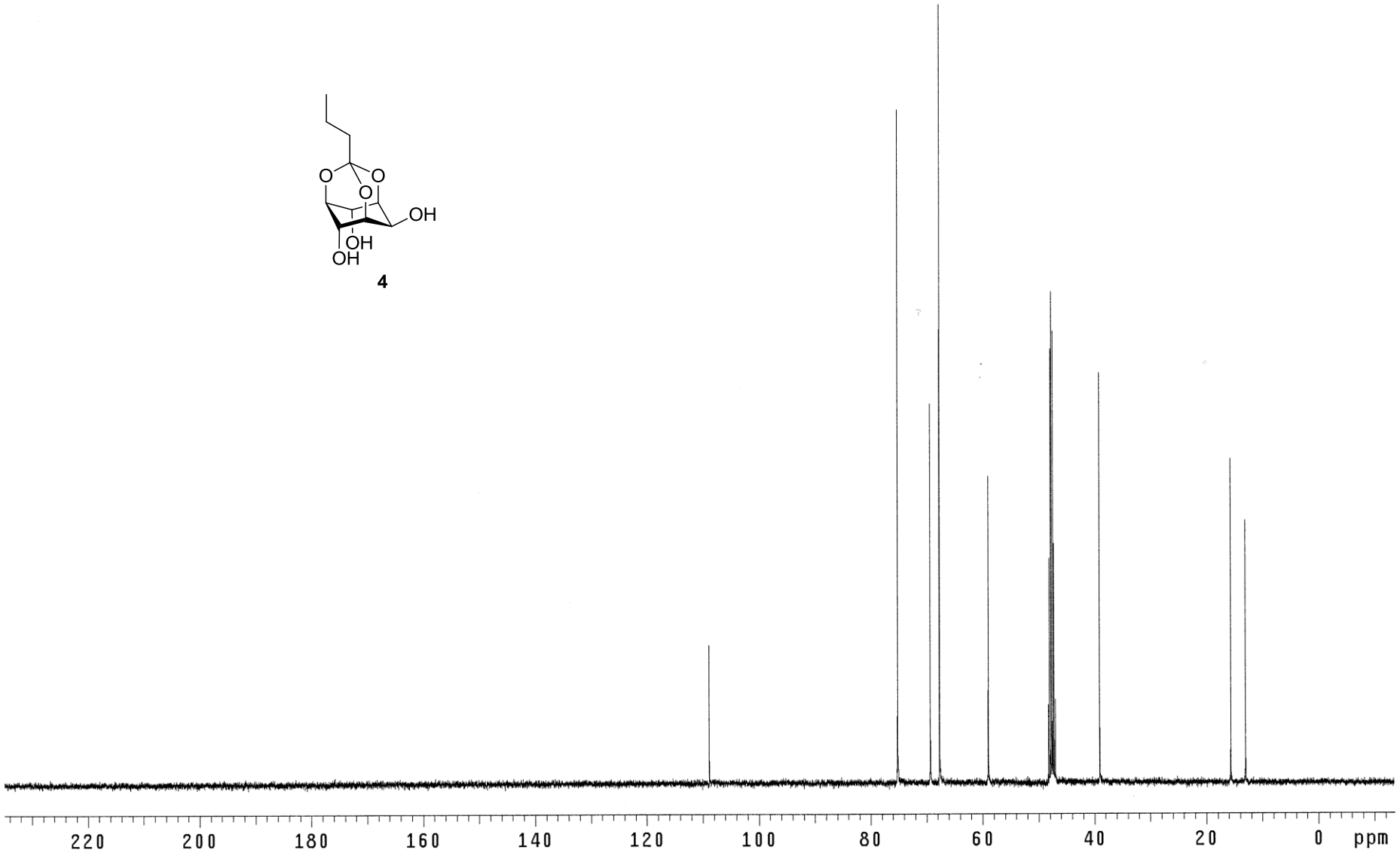
3.60
0.41
2.00
1.97
2.90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OH
OH
OH
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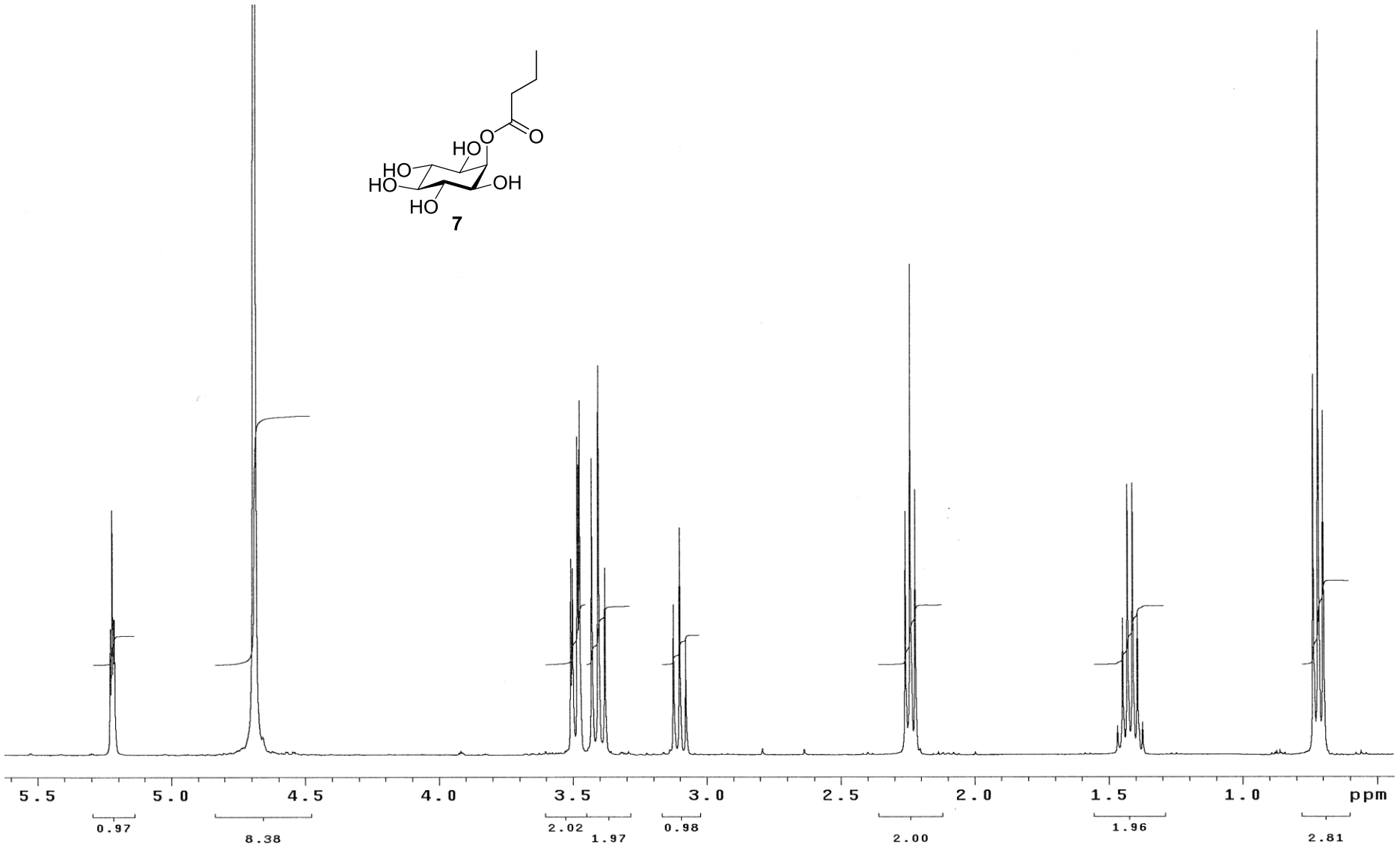
200
180
160
140
120
100
80
60
40
20
0
ppm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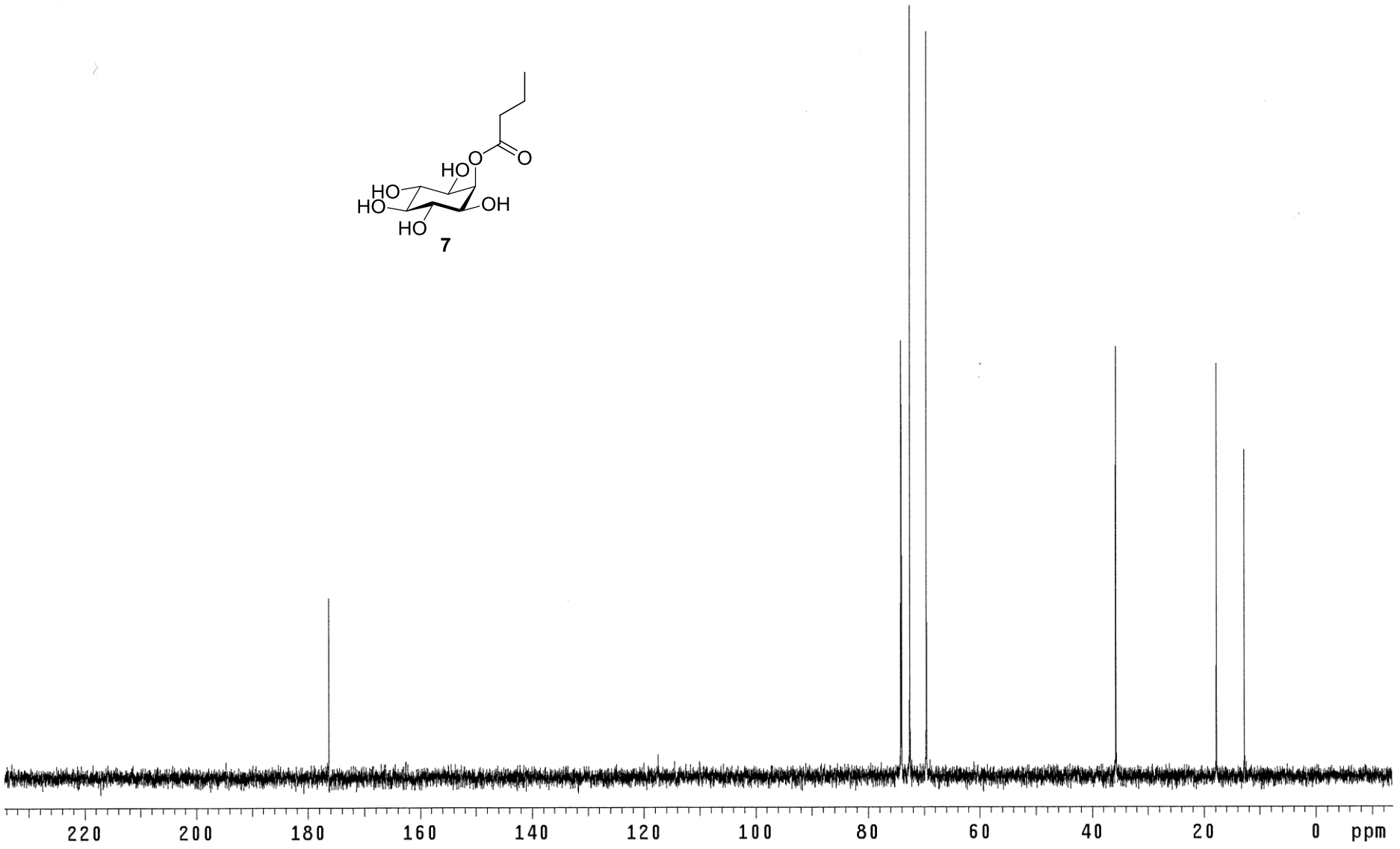
2.81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HO
HO
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O
OH
7
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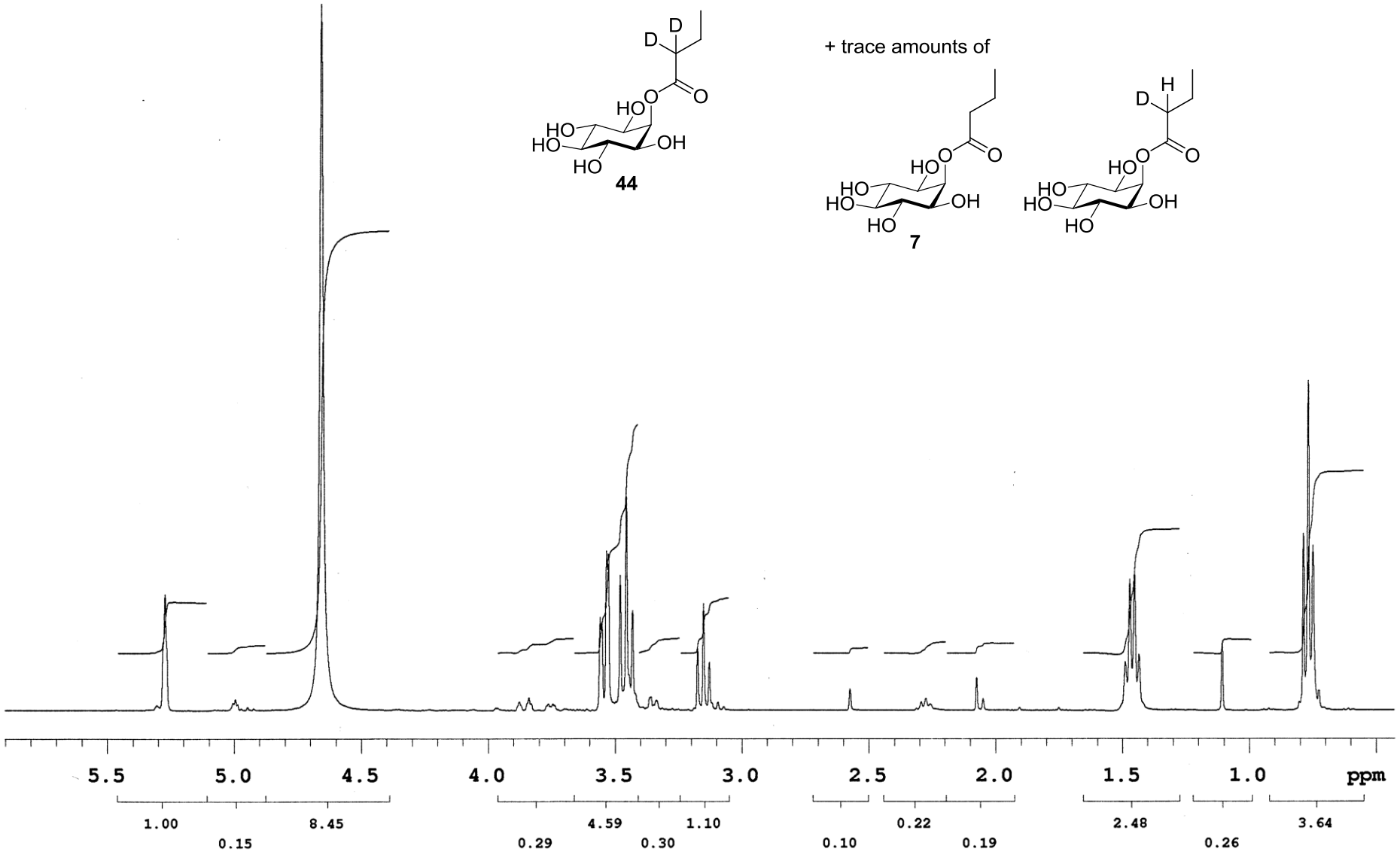
200
180
160
140
120
100
80
60
40
20
0
ppm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D
O
O
HO
HO
HO
OH
HO
44
+ trace amounts of
O
O
HO
HO
HO
OH
HO
7
H
D
O
O
HO
HO
HO
OH
HO
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
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0.10
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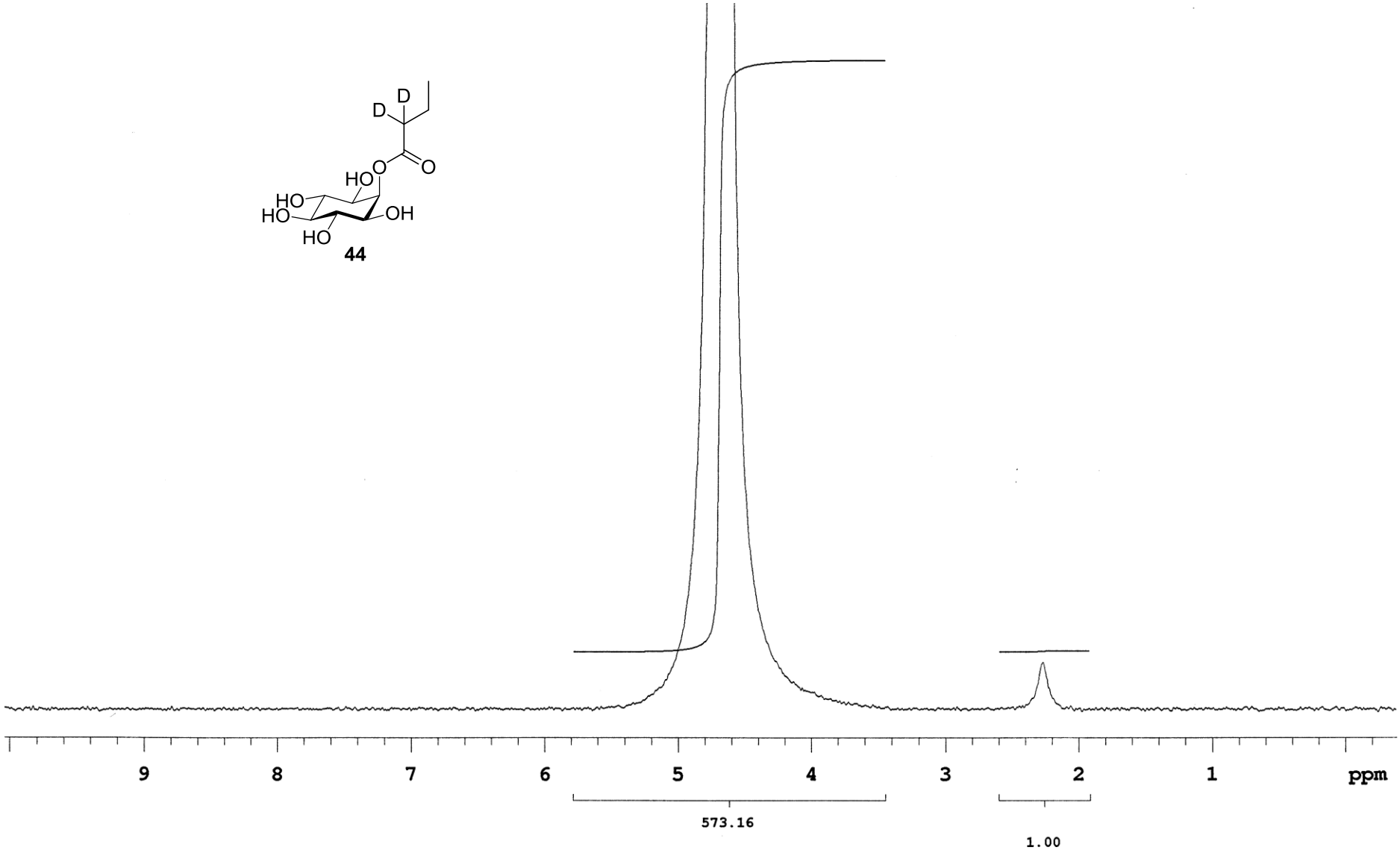
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4
3
2
1
ppm
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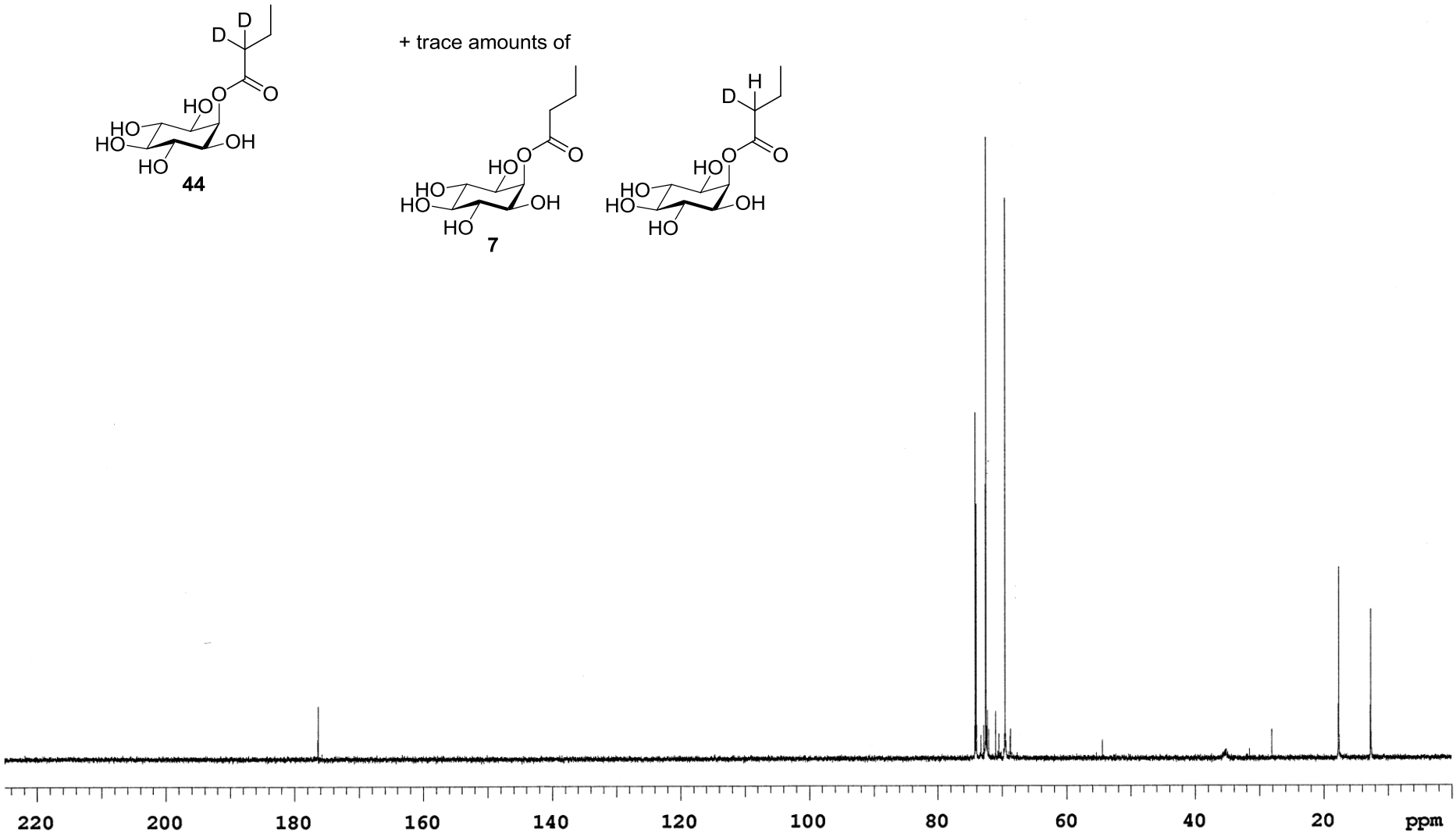
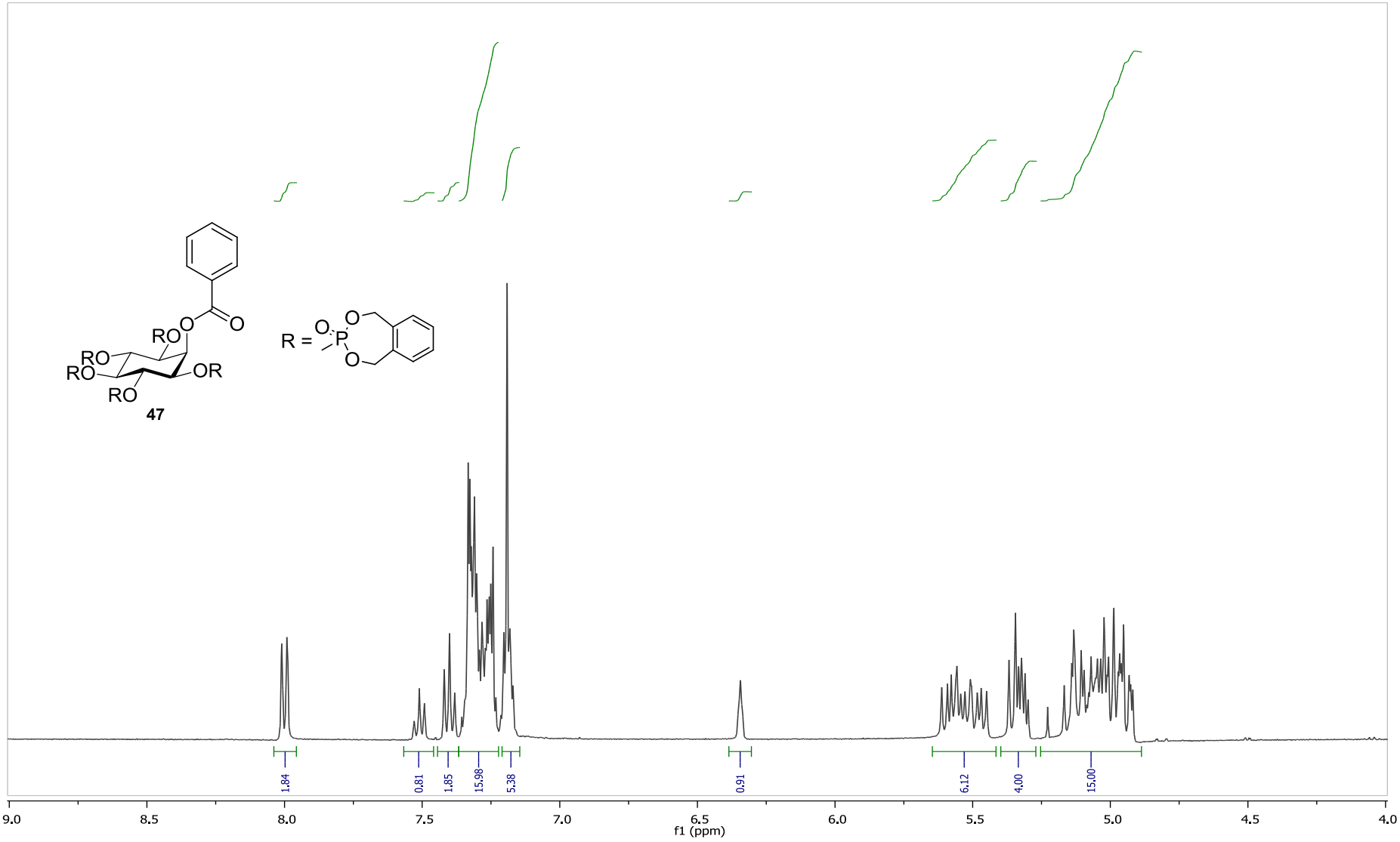
1.00


D
D
O
O
HO
HO
HO
OH
HO
44
+ trace amounts of
O
O
HO
HO
HO
OH
HO
7
H
D
O
O
HO
HO
HO
OH
HO
220
200
180
160
140
120
100
80
60
40
20
ppm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RO
RO
RO
O
O
OR
47
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O
P
O
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0.81
1.85
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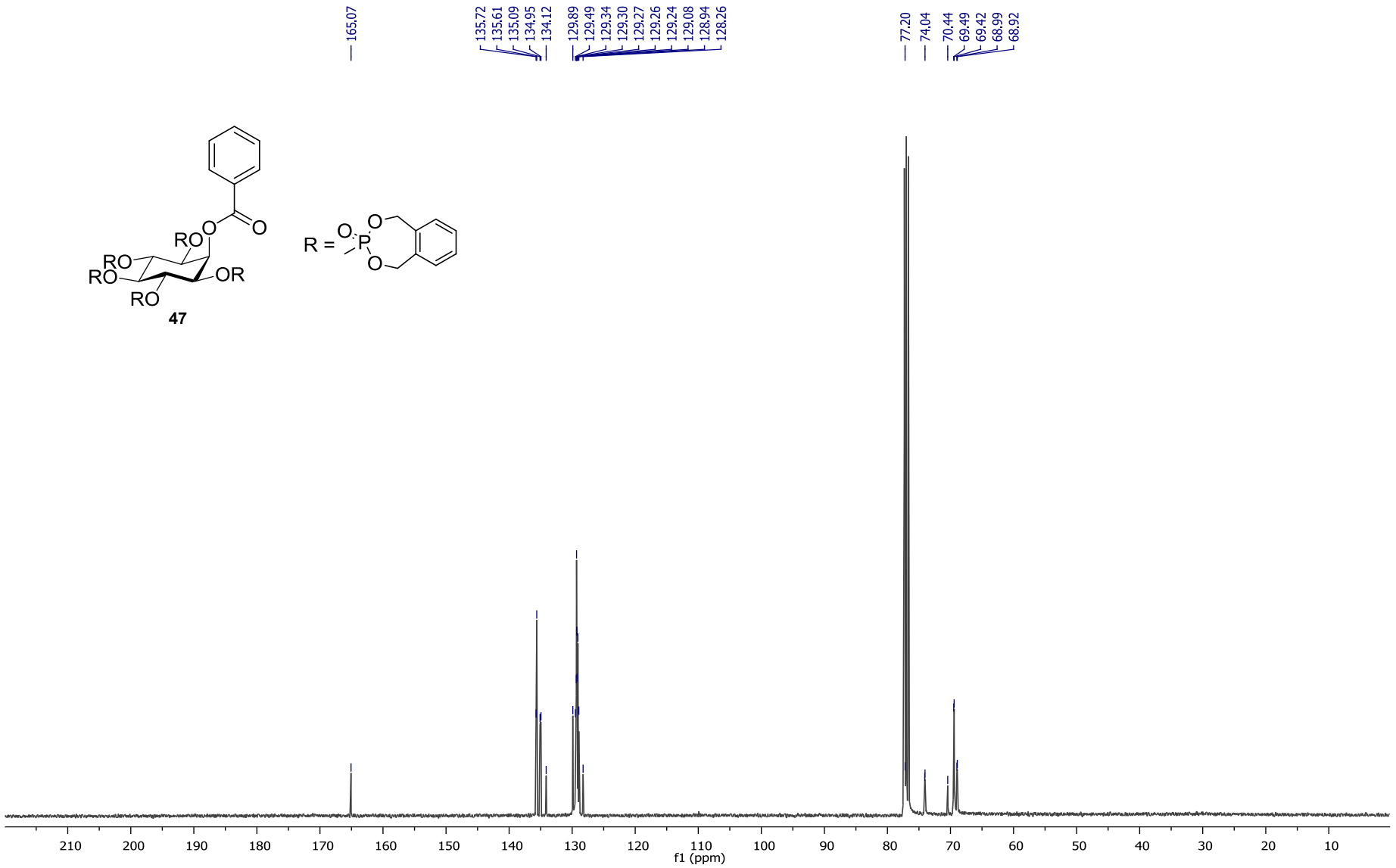
5.38
0.91
6.12
4.00
15.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
f1 (ppm)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135.72
135.61
135.09
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129.89
129.49
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129.27
129.26
129.24
129.08
128.94
128.26
77.20
74.04
70.44
69.49
69.42
68.99
68.92
RO
RO
RO
RO
OR
O
O
R =
O
P
O
O
47
210
200
190
180
170
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150
140
130
120
110
100
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80
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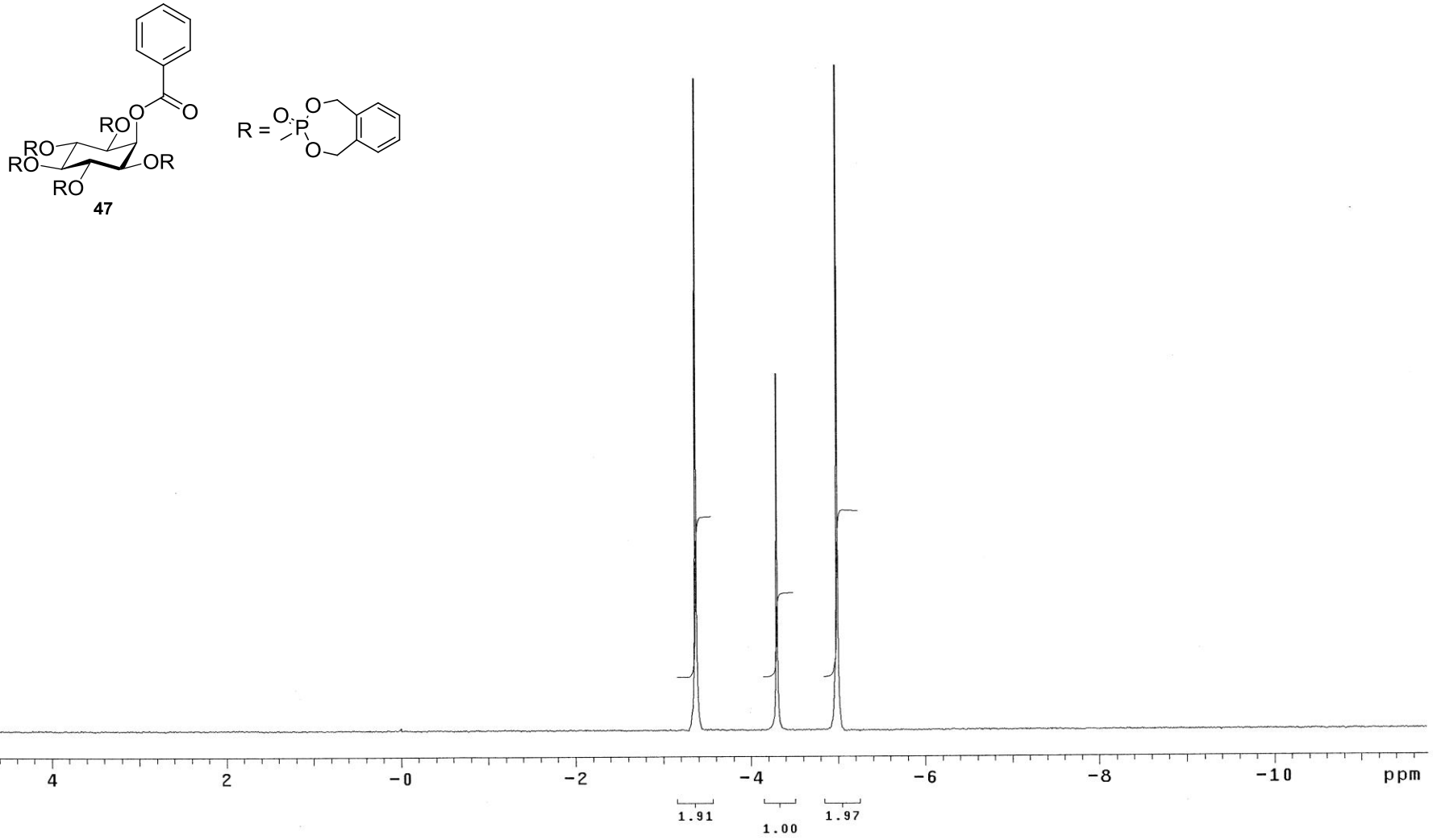
60
50
40
30
20
10
f1 (ppm)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RO
RO
RO
OR
O
O
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R =
O
O
P
O
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2
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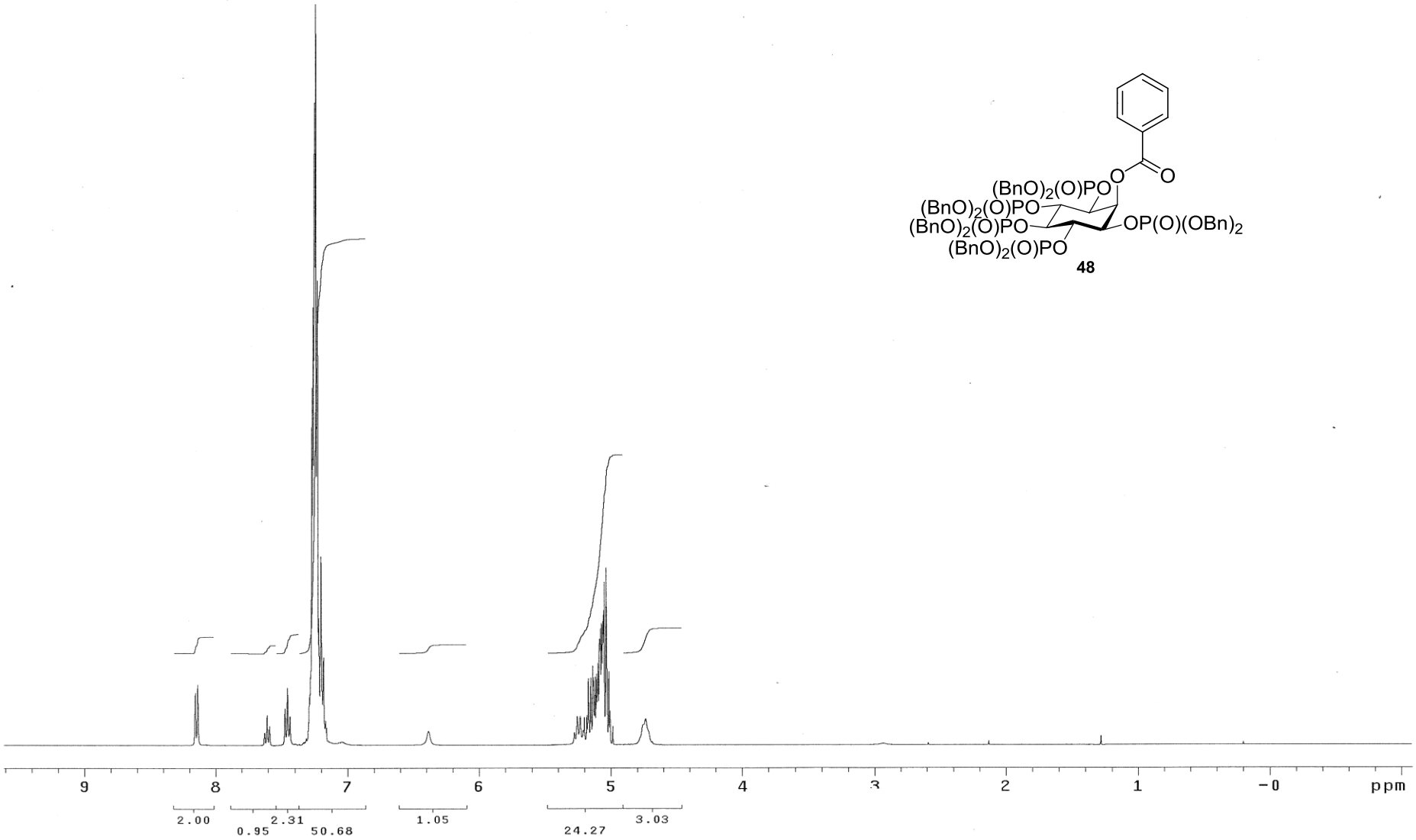
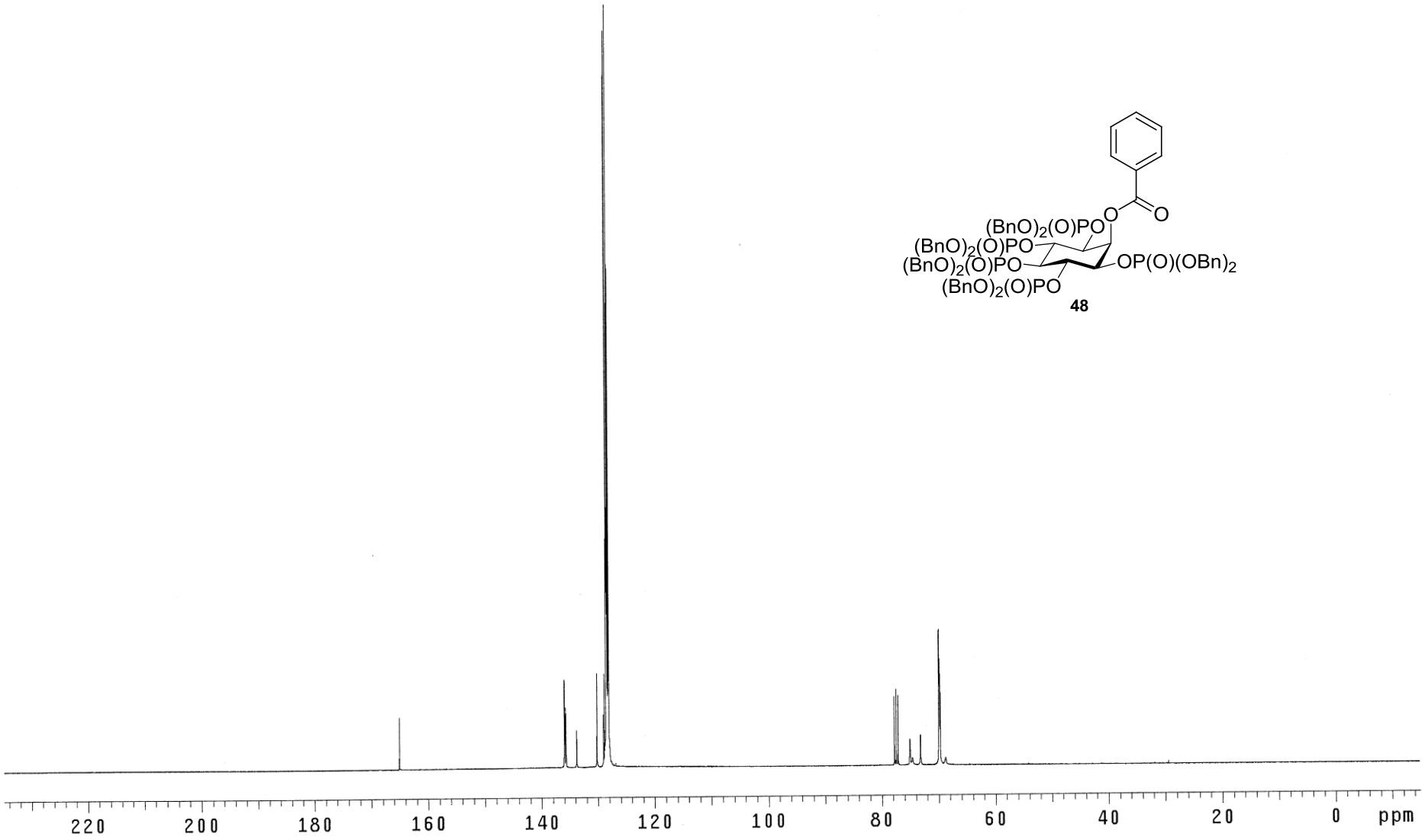
-2
-4
-6
-8
-10
ppm
1.91
1.00
1.97


(BnO)2(O)PO
(BnO)2(O)PO
(BnO)2(O)PO
(BnO)2(O)PO
OP(O)(OBn)2
O
O
48
9
8
7
6
5
4
3
2
1
-0
ppm
2.00
0.95
2.31
50.68
1.05
24.27
3.03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(BnO)2(O)PO
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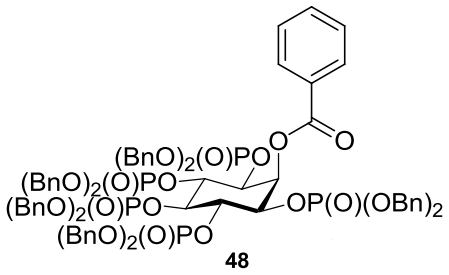
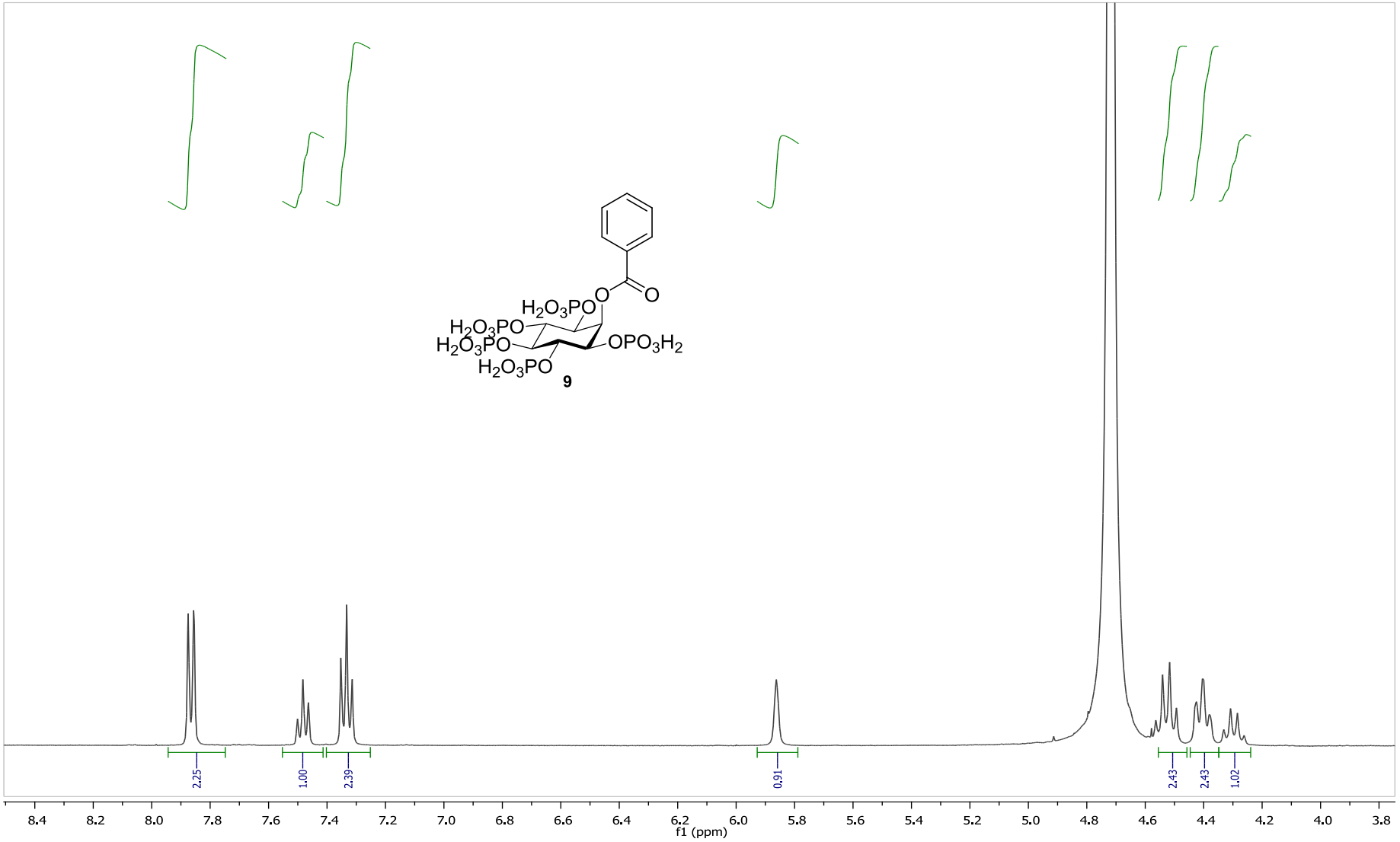
100
80
60
40
20
0
ppm

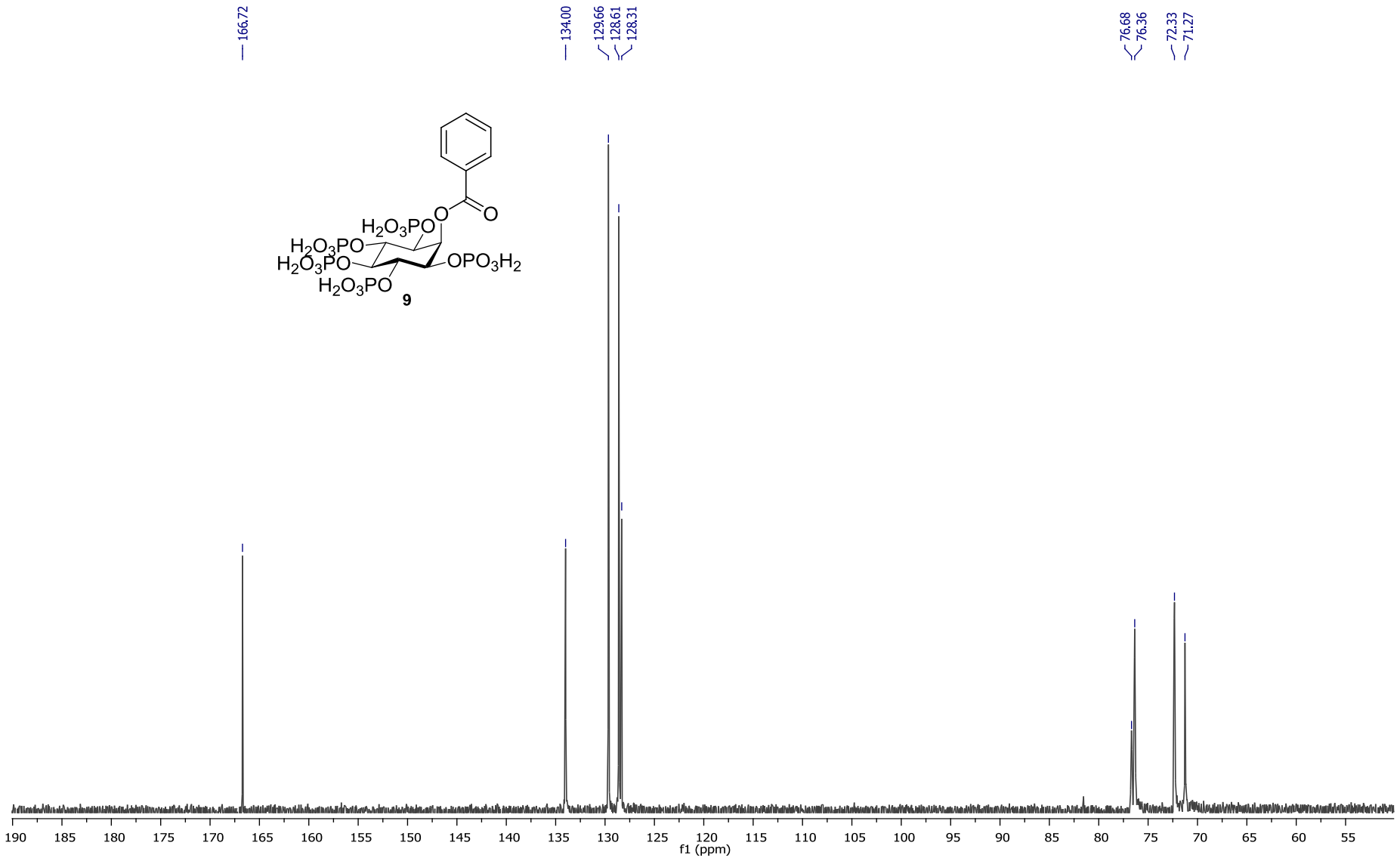
48

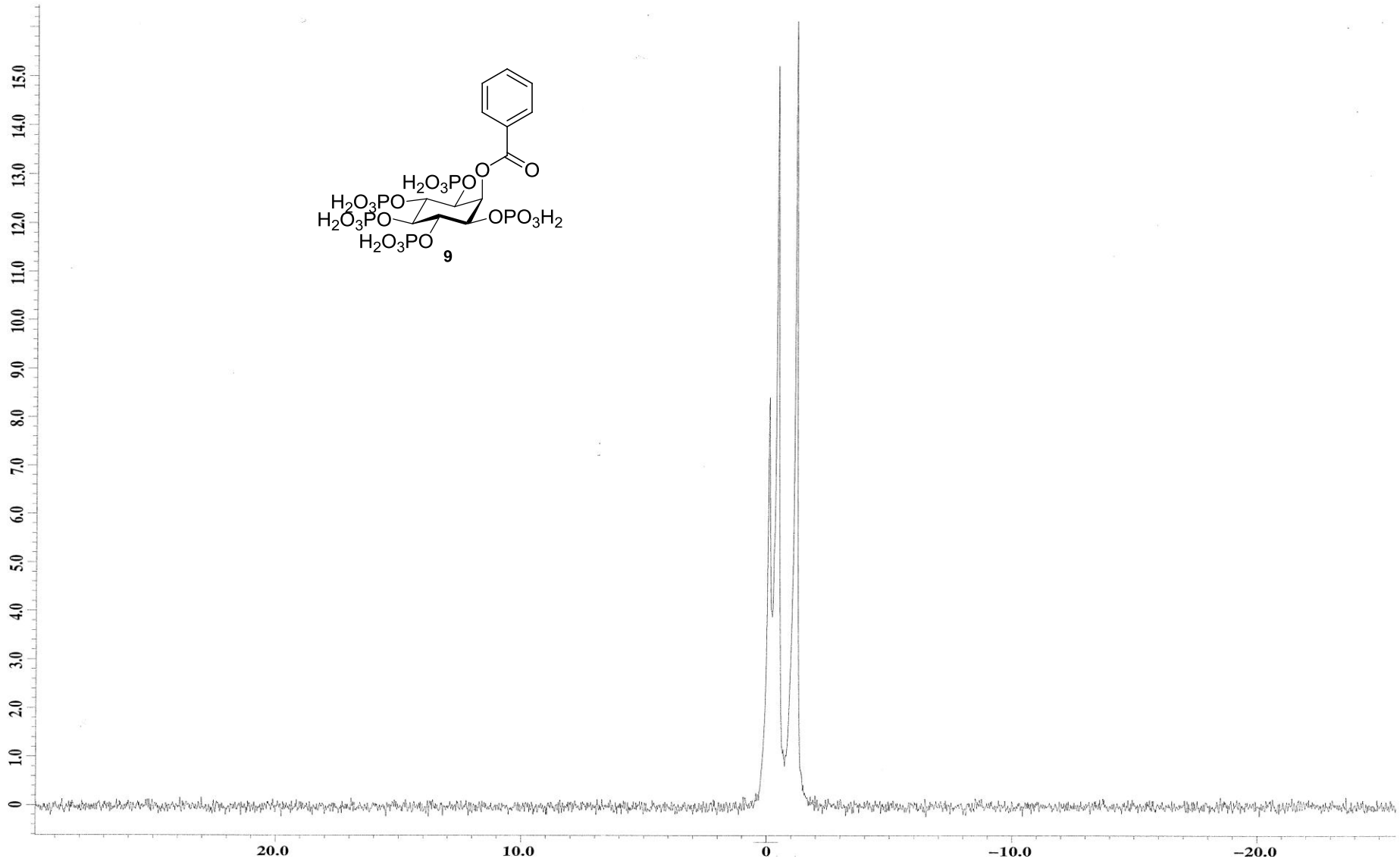

(BnO)2(O)PO
(BnO)2(O)PO
(BnO)2(O)PO
(BnO)2(O)PO
OP(O)(OBn)2
O
O

48

20
15
10
5
0
-5
-10
-15
ppm


H_2O_3PO
H_2O_3PO
H_2O_3PO
H_2O_3PO
OPO_3H_2
O
O
9
2.25
1.00
2.39
0.91
2.43
2.43
1.02
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
4.4
4.2
4.0
3.8
f1 (ppm)


166.72
134.00
129.66
128.61
128.31
76.68
76.36
72.33
71.27
H_2O_3PO
H_2O_3PO
H_2O_3PO
H_2O_3PO
OPO_3H_2
O
O
9
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
f1 (ppm)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H_2O_3PO
H_2O_3PO
H_2O_3PO
OPO_3H_2
O
O
9
15.0
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13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
20.0
10.0
0
−10.0
−20.0

X-ray Crystallographic data for Compound 7

Table 1. Crystal data and structure refinement for Compound **7**.

Identification code	k11farm8
Empirical formula	C10 H18 O7
Formula weight	250.24
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/a
Unit cell dimensions	a = 11.0090(3)Å alpha = 90°
	b = 9.0330(3)Å beta = 105.775(1)°
	c = 12.5370(4)Å gamma = 90°
Volume	1199.78(6) $Å^3$
Z	4
Density (calculated)	1.385 Mg/m^3
Absorption coefficient	0.118 mm^{-1}
F(000)	536
Crystal size	0.40 x 0.40 x 0.10 mm
Theta range for data collection	4.06 to 27.42°
Index ranges	-14<=h<=14; -11<=k<=11; -16<=l<=16
Reflections collected	16216
Independent reflections	2710 [R(int) = 0.0541]
Reflections observed (>2sigma)	2156
Data Completeness	0.990
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.972 and 0.843
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2710 / 14 / 178
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0429 wR2 = 0.1104
R indices (all data)	R1 = 0.0560 wR2 = 0.1212
Largest diff. peak and hole	0.276 and -0.193 $eÅ^{-3}$

Notes:

C9 and C10 each disordered over 2 sites in a 70:30 ratio. ADP restraints applied to minor fractional atoms to assist convergence.
Extensive hydrogen-bonding the gross structure – to form sheets parallel to the *ab* place, which interdigitate as they stack along the *c* axis.

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O3-H3	0.820	1.973	153.53	2.732	O4 [-x+2, -y+1, -z]
O4-H4	0.820	1.916	167.84	2.724	O6 [x+1/2, -y+1/2, z]
O5-H5	0.820	2.024	162.35	2.816	O2 [x, y-1, z]
O6-H6	0.820	2.208	132.41	2.827	O5 [x-1/2, -y+1/2, z]
O6-H6	0.820	2.411	110.14	2.801	O7
O7-H7	0.820	1.977	172.69	2.792	O3 [x-1/2, -y+3/2, z]

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
O(1)	8087(1)	7094(1)	2482(1)	35(1)
O(2)	7383(2)	9403(1)	2048(1)	60(1)
O(3)	9179(1)	6817(1)	724(1)	38(1)
O(4)	9628(1)	3734(1)	882(1)	40(1)
O(5)	8576(1)	2188(1)	2402(1)	46(1)
O(6)	6142(1)	3067(1)	2425(1)	44(1)
O(7)	5593(1)	6097(1)	2190(1)	47(1)
C(1)	7371(1)	6544(2)	1407(1)	31(1)
C(2)	6394(1)	5452(2)	1606(1)	33(1)
C(3)	7038(1)	4142(2)	2289(1)	31(1)
C(4)	7921(1)	3365(2)	1727(1)	32(1)
C(5)	8899(1)	4431(2)	1519(1)	30(1)
C(6)	8269(1)	5768(2)	861(1)	30(1)
C(7)	7962(2)	8521(2)	2717(1)	41(1)
C(8)	8616(2)	8875(2)	3904(2)	58(1)
C(9)	7757(3)	9738(4)	4472(3)	69(1)
C(10)	6571(5)	9075(8)	4482(6)	84(2)
C(9A)	8030(8)	8354(10)	4647(6)	68(2)
C(10A)	6769(14)	8540(20)	4597(19)	100(6)

Table 3. Bond lengths [Å] and angles [^{o}] for **7**.

O(1)-C(7)	1.3380(18)	O(1)-C(1)	1.4511(17)
O(2)-C(7)	1.206(2)	O(3)-C(6)	1.4228(16)
O(3)-H(3)	0.8200	O(4)-C(5)	1.4244(16)
O(4)-H(4)	0.8200	O(5)-C(4)	1.4267(18)
O(5)-H(5)	0.8200	O(6)-C(3)	1.4268(16)
O(6)-H(6)	0.8200	O(7)-C(2)	1.4162(17)
O(7)-H(7)	0.8200	C(1)-C(6)	1.5185(19)
C(1)-C(2)	1.529(2)	C(1)-H(1)	0.9800
C(2)-C(3)	1.518(2)	C(2)-H(2)	0.9800
C(3)-C(4)	1.5192(19)	C(3)-H(3A)	0.9800
C(4)-C(5)	1.5187(19)	C(4)-H(4A)	0.9800
C(5)-C(6)	1.5197(19)	C(5)-H(5A)	0.9800
C(6)-H(6A)	0.9800	C(7)-C(8)	1.501(2)
C(8)-C(9A)	1.354(7)	C(8)-C(9)	1.541(4)
C(8)-H(8A)	0.9700	C(8)-H(8B)	0.9700
C(9)-C(10)	1.440(6)	C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700	C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600	C(10)-H(10C)	0.9600
C(9A)-C(10A)	1.383(14)	C(9A)-H(9A1)	0.9700
C(9A)-H(9A2)	0.9700	C(10A)-H(10D)	0.9600
C(10A)-H(10E)	0.9600	C(10A)-H(10F)	0.9600
C(7)-O(1)-C(1)	118.17(12)	C(6)-O(3)-H(3)	109.5
C(5)-O(4)-H(4)	109.5	C(4)-O(5)-H(5)	109.5
C(3)-O(6)-H(6)	109.5	C(2)-O(7)-H(7)	109.5
O(1)-C(1)-C(6)	108.70(11)	O(1)-C(1)-C(2)	107.32(11)
C(6)-C(1)-C(2)	110.38(11)	O(1)-C(1)-H(1)	110.1
C(6)-C(1)-H(1)	110.1	C(2)-C(1)-H(1)	110.1
O(7)-C(2)-C(3)	106.79(12)	O(7)-C(2)-C(1)	112.52(12)
C(3)-C(2)-C(1)	110.73(11)	O(7)-C(2)-H(2)	108.9
C(3)-C(2)-H(2)	108.9	C(1)-C(2)-H(2)	108.9
O(6)-C(3)-C(2)	111.47(12)	O(6)-C(3)-C(4)	106.92(11)

C(2)-C(3)-C(4)	110.92(12)	O(6)-C(3)-H(3A)	109.2
C(2)-C(3)-H(3A)	109.2	C(4)-C(3)-H(3A)	109.2
O(5)-C(4)-C(5)	107.85(11)	O(5)-C(4)-C(3)	110.67(12)
C(5)-C(4)-C(3)	111.09(11)	O(5)-C(4)-H(4A)	109.1
C(5)-C(4)-H(4A)	109.1	C(3)-C(4)-H(4A)	109.1
O(4)-C(5)-C(4)	110.52(11)	O(4)-C(5)-C(6)	106.84(11)
C(4)-C(5)-C(6)	110.89(11)	O(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5A)	109.5	C(6)-C(5)-H(5A)	109.5
O(3)-C(6)-C(1)	108.20(11)	O(3)-C(6)-C(5)	111.28(11)
C(1)-C(6)-C(5)	112.29(11)	O(3)-C(6)-H(6A)	108.3
C(1)-C(6)-H(6A)	108.3	C(5)-C(6)-H(6A)	108.3
O(2)-C(7)-O(1)	123.38(15)	O(2)-C(7)-C(8)	124.67(15)
O(1)-C(7)-C(8)	111.95(15)	C(9A)-C(8)-C(7)	114.8(4)
C(9A)-C(8)-C(9)	52.5(4)	C(7)-C(8)-C(9)	112.16(19)
C(9A)-C(8)-H(8A)	136.0	C(7)-C(8)-H(8A)	109.2
C(9)-C(8)-H(8A)	109.2	C(9A)-C(8)-H(8B)	58.7
C(7)-C(8)-H(8B)	109.2	C(9)-C(8)-H(8B)	109.2
H(8A)-C(8)-H(8B)	107.9	C(10)-C(9)-C(8)	117.8(4)
C(10)-C(9)-H(9A)	107.9	C(8)-C(9)-H(9A)	107.9
C(10)-C(9)-H(9B)	107.9	C(8)-C(9)-H(9B)	107.9
H(9A)-C(9)-H(9B)	107.2	C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5	H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5	H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5	C(8)-C(9A)-C(10A)	126.0(11)
C(8)-C(9A)-H(9A1)	105.8	C(10A)-C(9A)-H(9A1)	105.8
C(8)-C(9A)-H(9A2)	105.8	C(10A)-C(9A)-H(9A2)	105.8
H(9A1)-C(9A)-H(9A2)	106.2	C(9A)-C(10A)-H(10D)	109.5
C(9A)-C(10A)-H(10E)	109.5	H(10D)-C(10A)-H(10E)	109.5
C(9A)-C(10A)-H(10F)	109.5	H(10D)-C(10A)-H(10F)	109.5
H(10E)-C(10A)-H(10F)	109.5		

Symmetry transformations used to generate equivalent atoms

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **7**. The anisotropic displacement factor exponent takes the form: $-2\ gpi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U$

Atom	U11	U22	U33	U23	U13	U12
O(1)	39(1)	27(1)	39(1)	-4(1)	9(1)	1(1)
O(2)	78(1)	27(1)	68(1)	-2(1)	11(1)	6(1)
O(3)	42(1)	29(1)	52(1)	1(1)	26(1)	-3(1)
O(4)	41(1)	38(1)	50(1)	5(1)	26(1)	10(1)
O(5)	41(1)	27(1)	75(1)	13(1)	25(1)	4(1)
O(6)	37(1)	35(1)	68(1)	-3(1)	28(1)	-8(1)
O(7)	42(1)	46(1)	62(1)	8(1)	29(1)	14(1)
C(1)	31(1)	28(1)	35(1)	-1(1)	10(1)	3(1)
C(2)	27(1)	34(1)	40(1)	-2(1)	12(1)	2(1)
C(3)	29(1)	27(1)	41(1)	-2(1)	15(1)	-4(1)
C(4)	31(1)	24(1)	43(1)	-2(1)	14(1)	-1(1)
C(5)	28(1)	27(1)	37(1)	-1(1)	13(1)	0(1)
C(6)	31(1)	26(1)	35(1)	0(1)	13(1)	-1(1)
C(7)	42(1)	30(1)	53(1)	-8(1)	17(1)	-1(1)
C(8)	57(1)	53(1)	59(1)	-22(1)	8(1)	0(1)
C(9)	87(2)	62(2)	62(2)	-16(2)	29(2)	-1(2)
C(10)	68(3)	112(5)	75(3)	-8(3)	25(2)	4(3)
C(9A)	83(4)	74(4)	47(3)	-6(3)	18(3)	-16(3)
C(10A)	104(7)	107(7)	95(7)	-3(5)	39(5)	-17(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **7**.

Atom	x	y	z	U(eq)
H(3)	9636	6434	384	46
H(4)	10146	3178	1280	48
H(5)	8107	1470	2345	55
H(6)	5548	3486	2575	53
H(7)	5133	6709	1794	56
H(1)	6948	7366	941	37
H(2)	5877	5090	888	40
H(3A)	7524	4494	3020	37
H(4A)	7426	2959	1017	38
H(5A)	9457	4758	2230	35
H(6A)	7786	5429	125	36
H(8A)	9365	9458	3934	69
H(8B)	8883	7961	4305	69
H(9A)	8231	9918	5234	82
H(9B)	7580	10695	4112	82
H(10A)	6133	9716	4864	125
H(10B)	6722	8138	4856	125
H(10C)	6066	8930	3734	125
H(9A1)	8499	8749	5360	82
H(9A2)	8176	7294	4684	82
H(10D)	6587	8040	5212	149
H(10E)	6256	8131	3916	149
H(10F)	6588	9575	4629	149

Table 6. Dihedral angles [^{o}] for **7**.

Atom1 - Atom2 - Atom3 - Atom4	Dihedral
C(7) - O(1) - C(1) - C(6)	127.75(13)
C(7) - O(1) - C(1) - C(2)	-112.86(14)
O(1) - C(1) - C(2) - O(7)	57.17(15)
C(6) - C(1) - C(2) - O(7)	175.47(12)
O(1) - C(1) - C(2) - C(3)	-62.26(14)
C(6) - C(1) - C(2) - C(3)	56.04(15)
O(7) - C(2) - C(3) - O(6)	60.76(15)
C(1) - C(2) - C(3) - O(6)	-176.42(11)
O(7) - C(2) - C(3) - C(4)	179.80(11)
C(1) - C(2) - C(3) - C(4)	-57.38(15)
O(6) - C(3) - C(4) - O(5)	-61.53(15)
C(2) - C(3) - C(4) - O(5)	176.74(11)
O(6) - C(3) - C(4) - C(5)	178.70(12)
C(2) - C(3) - C(4) - C(5)	56.96(15)
O(5) - C(4) - C(5) - O(4)	65.15(15)
C(3) - C(4) - C(5) - O(4)	-173.40(11)
O(5) - C(4) - C(5) - C(6)	-176.55(12)
C(3) - C(4) - C(5) - C(6)	-55.11(16)
O(1) - C(1) - C(6) - O(3)	-60.86(14)
C(2) - C(1) - C(6) - O(3)	-178.32(11)
O(1) - C(1) - C(6) - C(5)	62.36(15)
C(2) - C(1) - C(6) - C(5)	-55.10(15)
O(4) - C(5) - C(6) - O(3)	-63.27(14)
C(4) - C(5) - C(6) - O(3)	176.23(11)
O(4) - C(5) - C(6) - C(1)	175.26(11)
C(4) - C(5) - C(6) - C(1)	54.76(16)
C(1) - O(1) - C(7) - O(2)	-7.2(2)
C(1) - O(1) - C(7) - C(8)	172.23(14)
O(2) - C(7) - C(8) - C(9A)	106.3(5)
O(1) - C(7) - C(8) - C(9A)	-73.2(5)

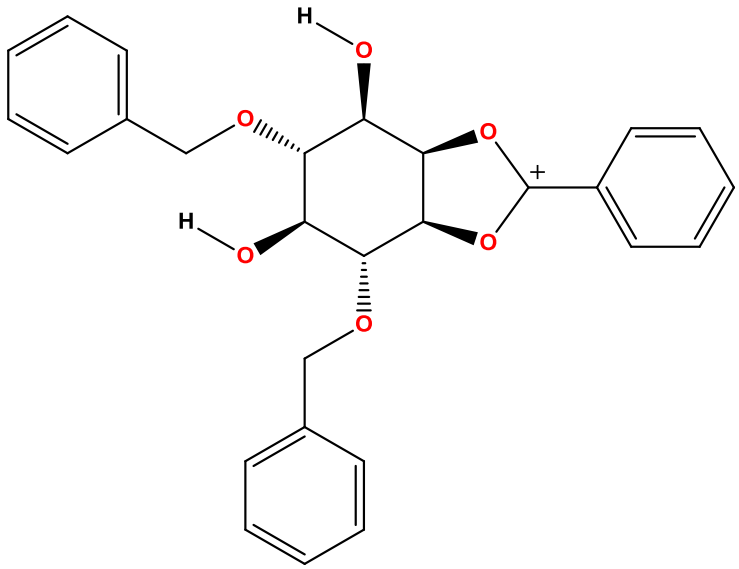
O(2) - C(7) - C(8) - C(9)	48.7(3)
O(1) - C(7) - C(8) - C(9)	-130.7(2)
C(9A) - C(8) - C(9) - C(10)	-47.9(5)
C(7) - C(8) - C(9) - C(10)	57.0(5)
C(7) - C(8) - C(9A) - C(10A)	-50.3(14)
C(9) - C(8) - C(9A) - C(10A)	49.5(12)

Symmetry transformations used to generate equivalent atoms

Computational Data for Compound 20

Methods:-

The Schrödinger software was used to build and minimise the structure below.



The Impact module of the Schrödinger software was used for a number of dynamics runs of 10,000 steps of 0.001 picoseconds at temperatures ranging from 276.15K to 3,276.15K. (This range of temperatures was used in an effort to generate a wide range of conformations in a reasonable length of time.) Every fifth structure, i.e. 2,000 structures, from each dynamics run was saved. Every fifth structure, i.e. 400 structures, from those saved had the coupling constants calculated by the Schrödinger software. These were studied to determine for which structures the

calculated coupling constants most closely matched the observed coupling constants. From a preliminary scan seven structures were selected. These structures and the ten structures either side of these were studied in detail. The results for the structure that most closely matched the observed results are shown below in Table 1.

Table 1 Comparison of observed and calculated coupling constants for Dioxolenium ion **20**

	1,2	**2,3**	**3,4**	**4,5**	**5,6**	**6,1**
J_{Obs}	9.0	2.9-3.4	4.0	3.7	8.7	6.0
J_{Calc}	7.4	5.9	2.7	1.1	9.8	5.5
Dihedral	7.03	-26.10	-70.70	122.14	172.32	151.58

Figure 11 below shows the gross conformation of the hexane ring. The 1,6 bond is horizontal in the foreground and C2 is directly behind C1. For the sake of clarity the aromatic rings are shown as lines in a different colour. The Figure 12 shows the dihedral angles. Figure 13 and Figure 14 are different views of the compound.

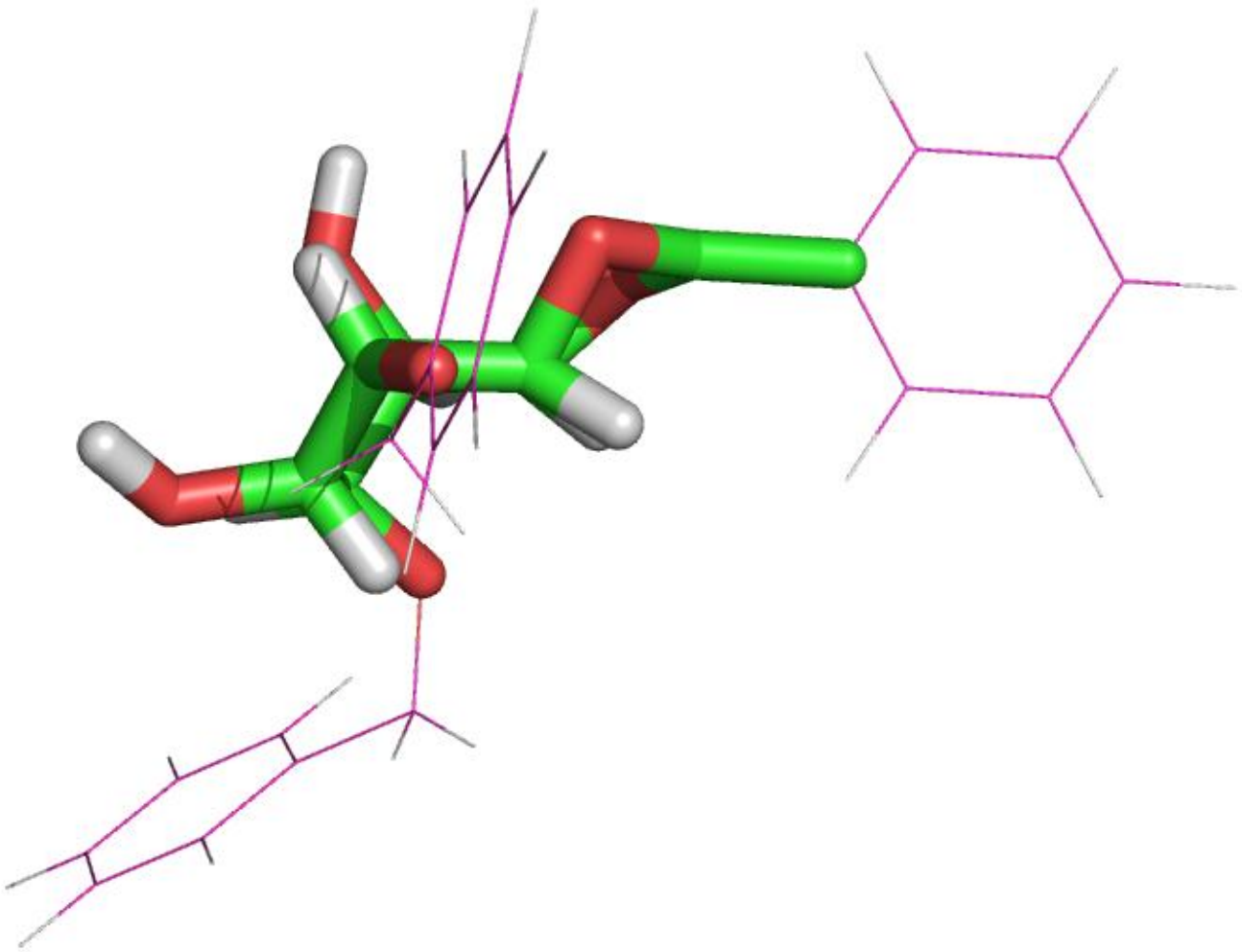


Figure 11

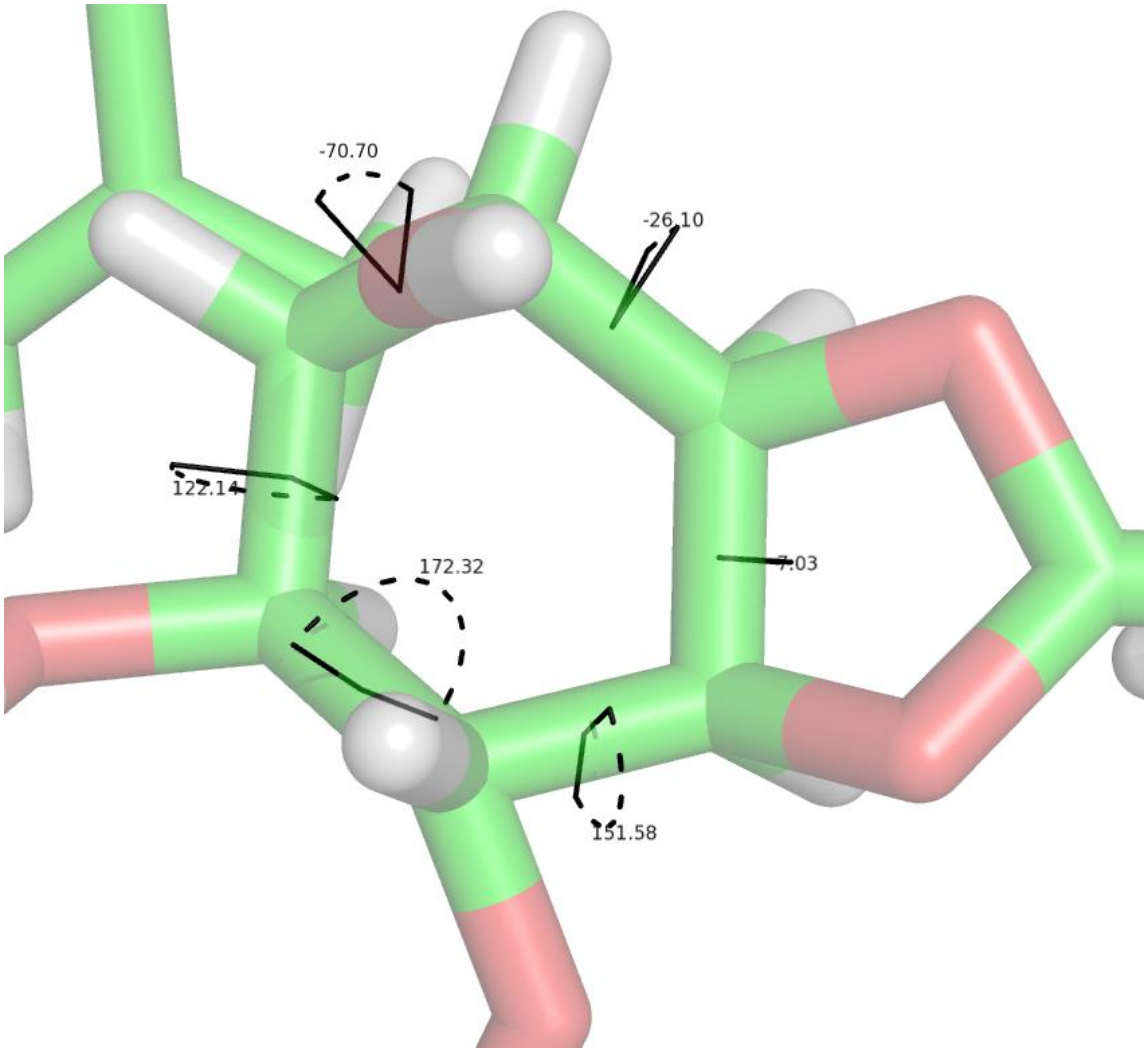


Figure 12

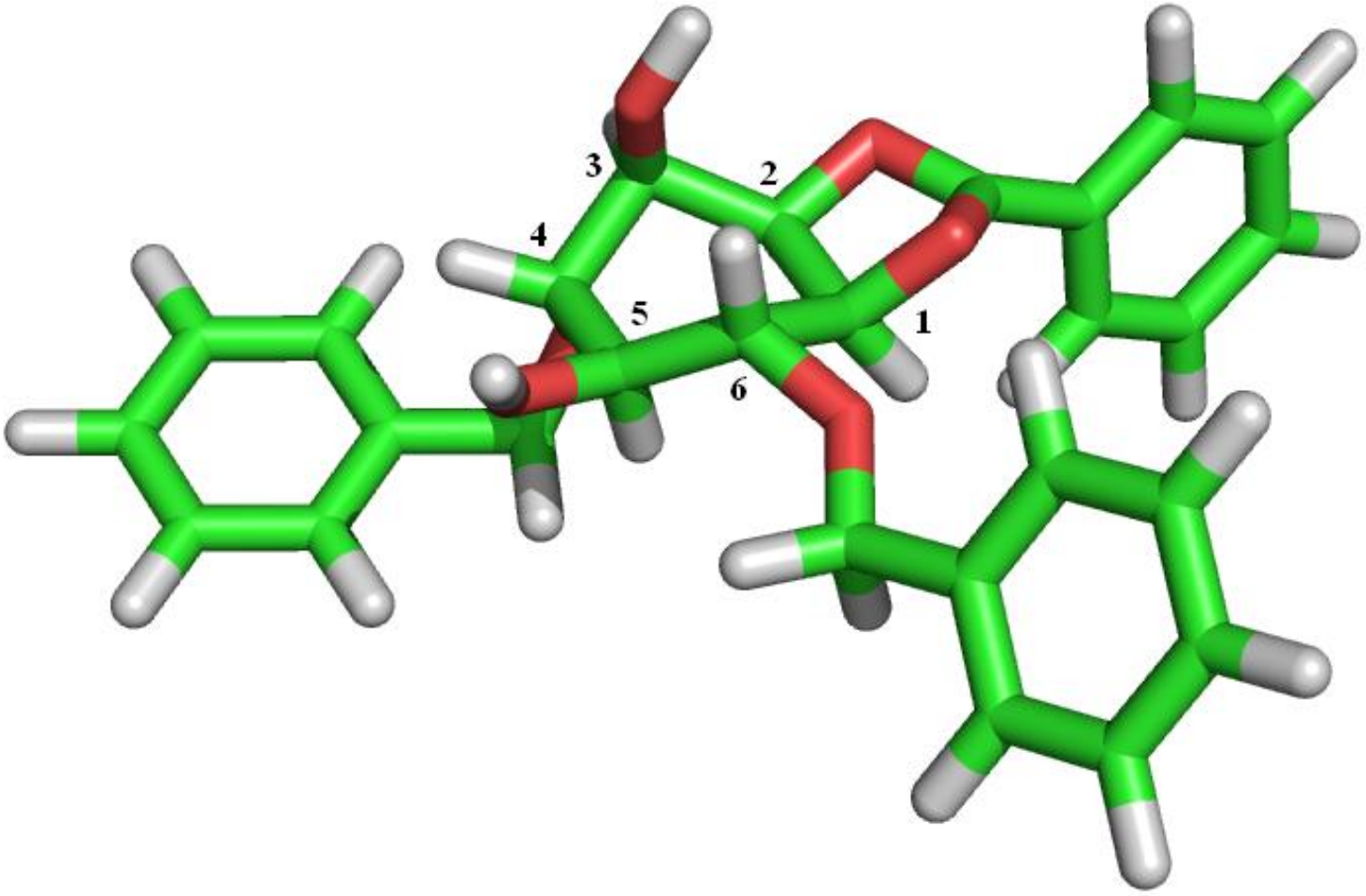


Figure 13

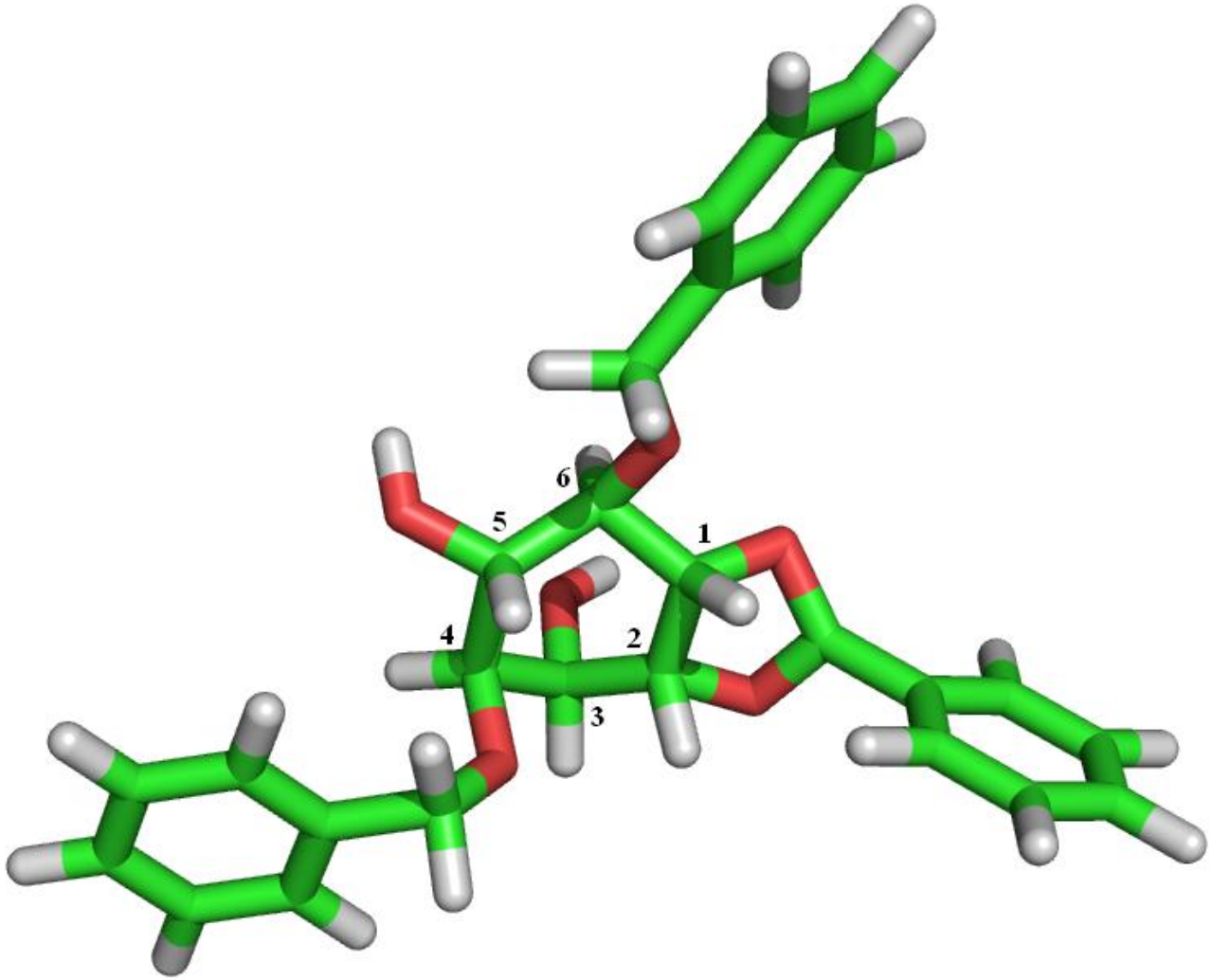


Figure 14