Supporting Information to

Development of a competitive binding assay for the *Burkholderia cenocepacia* lectin BC2L-A and structure activity relationship of natural and synthetic inhibitors

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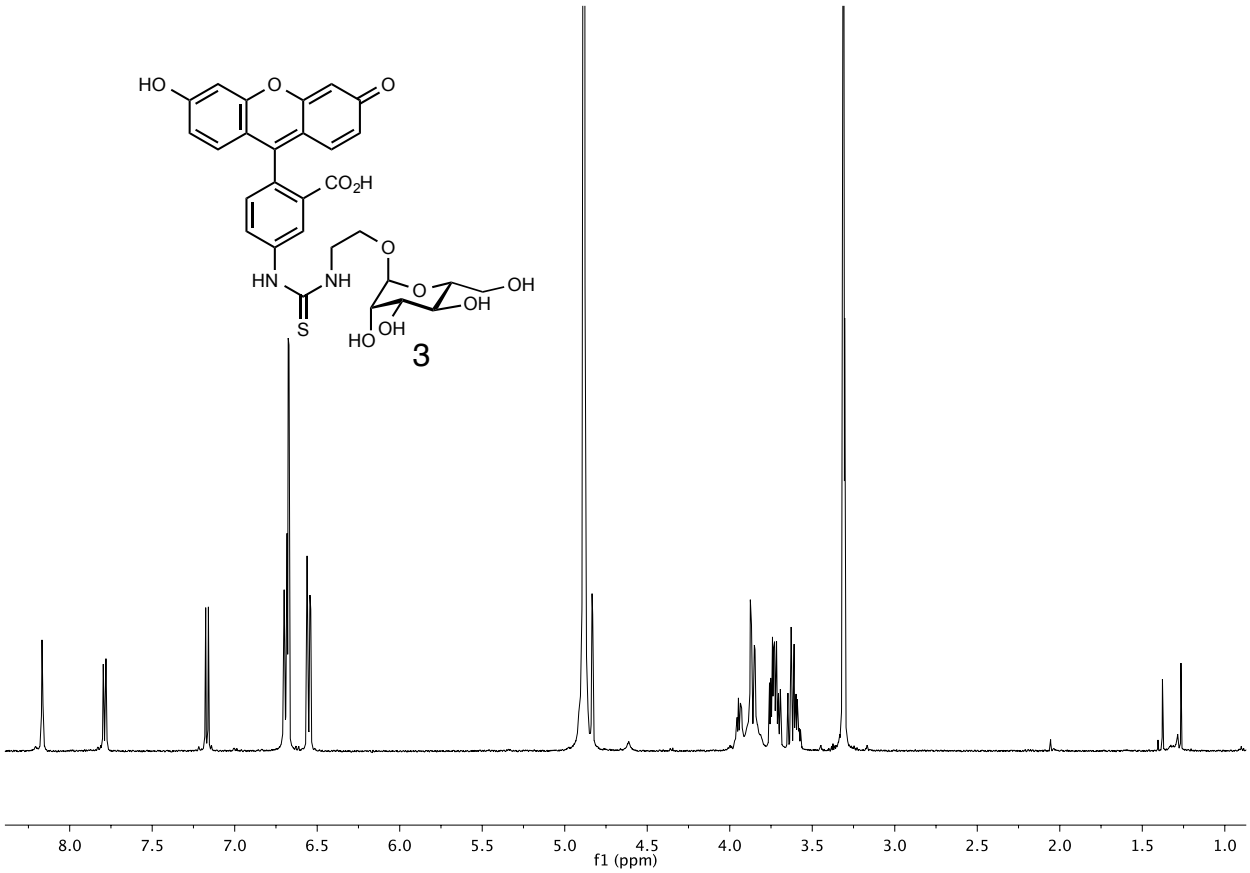
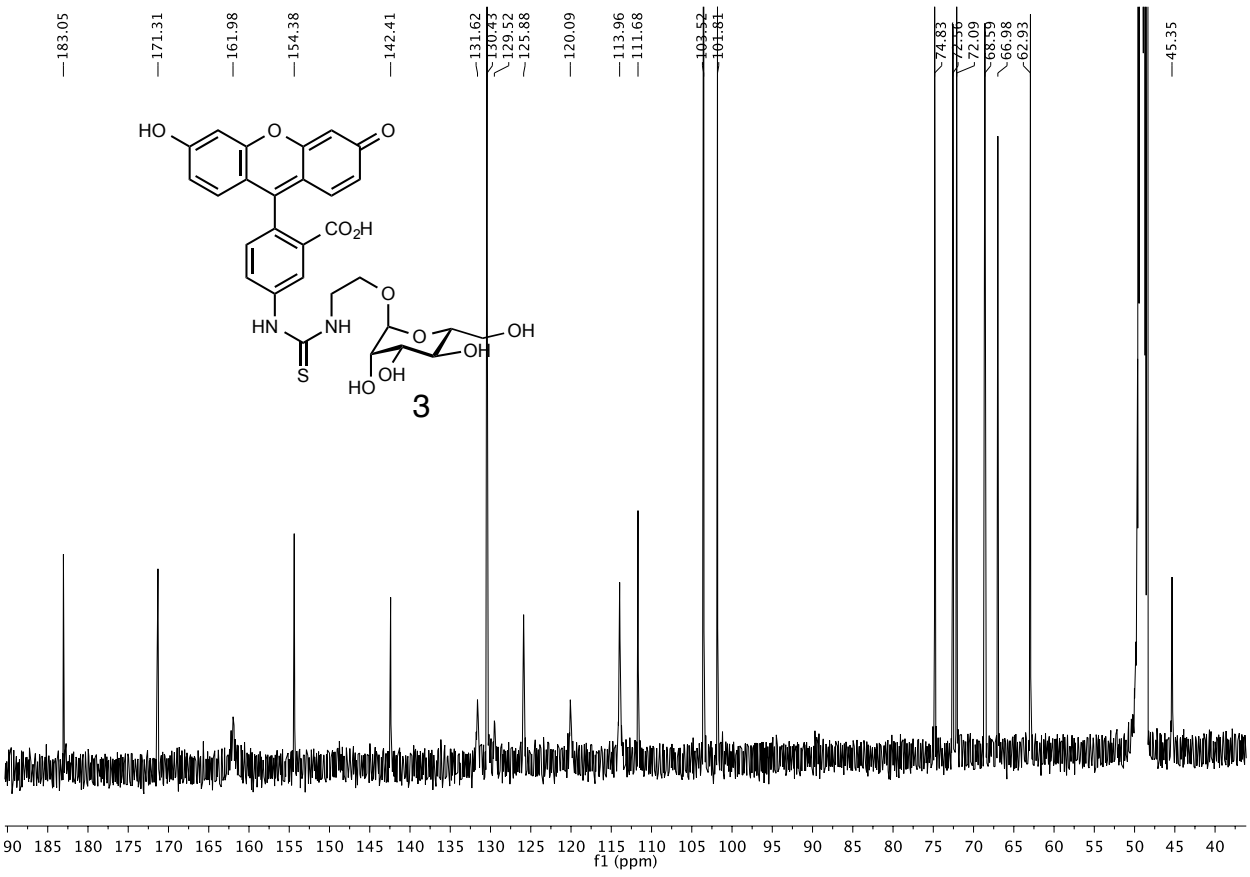
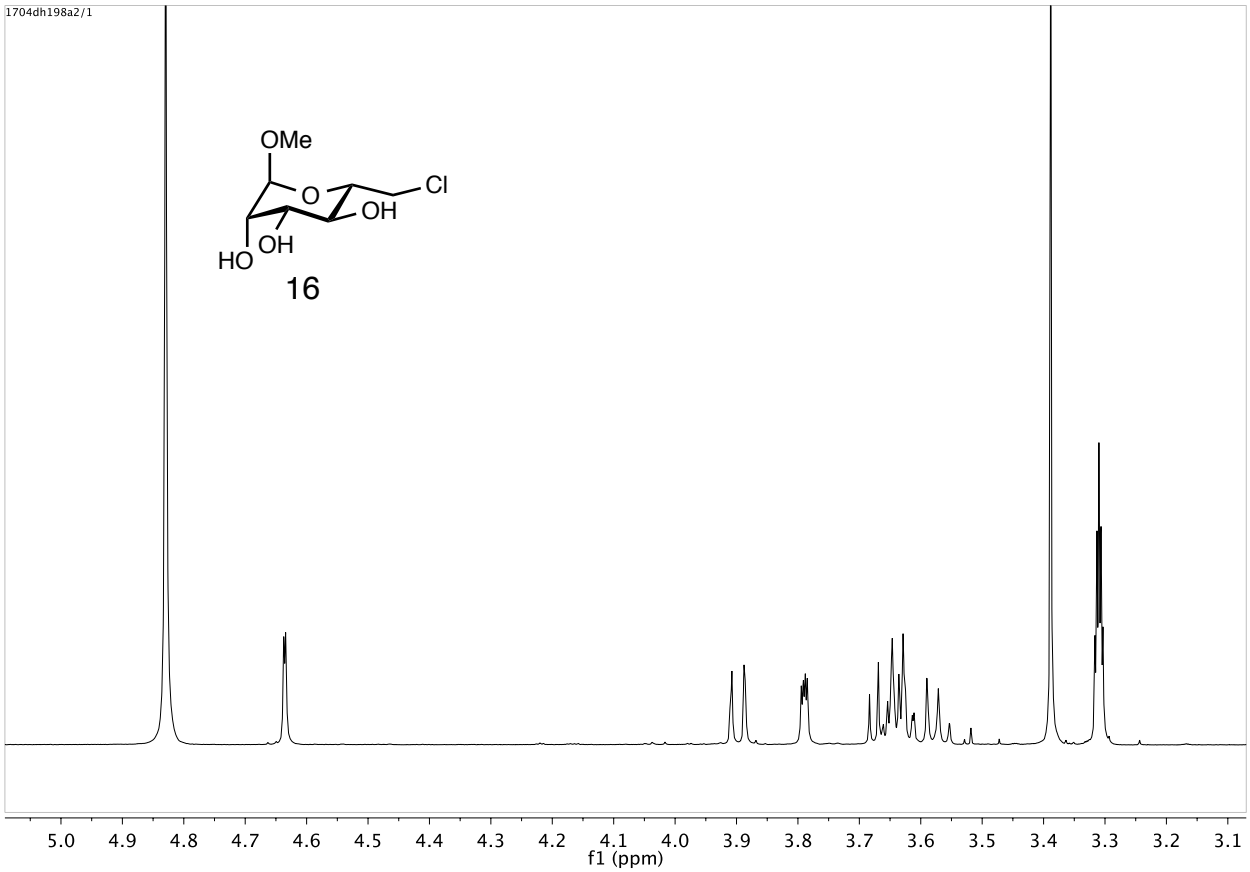
^{1}H-NMR, ^{13}C-NMR and ^{19}F-NMR traces of synthesized compounds



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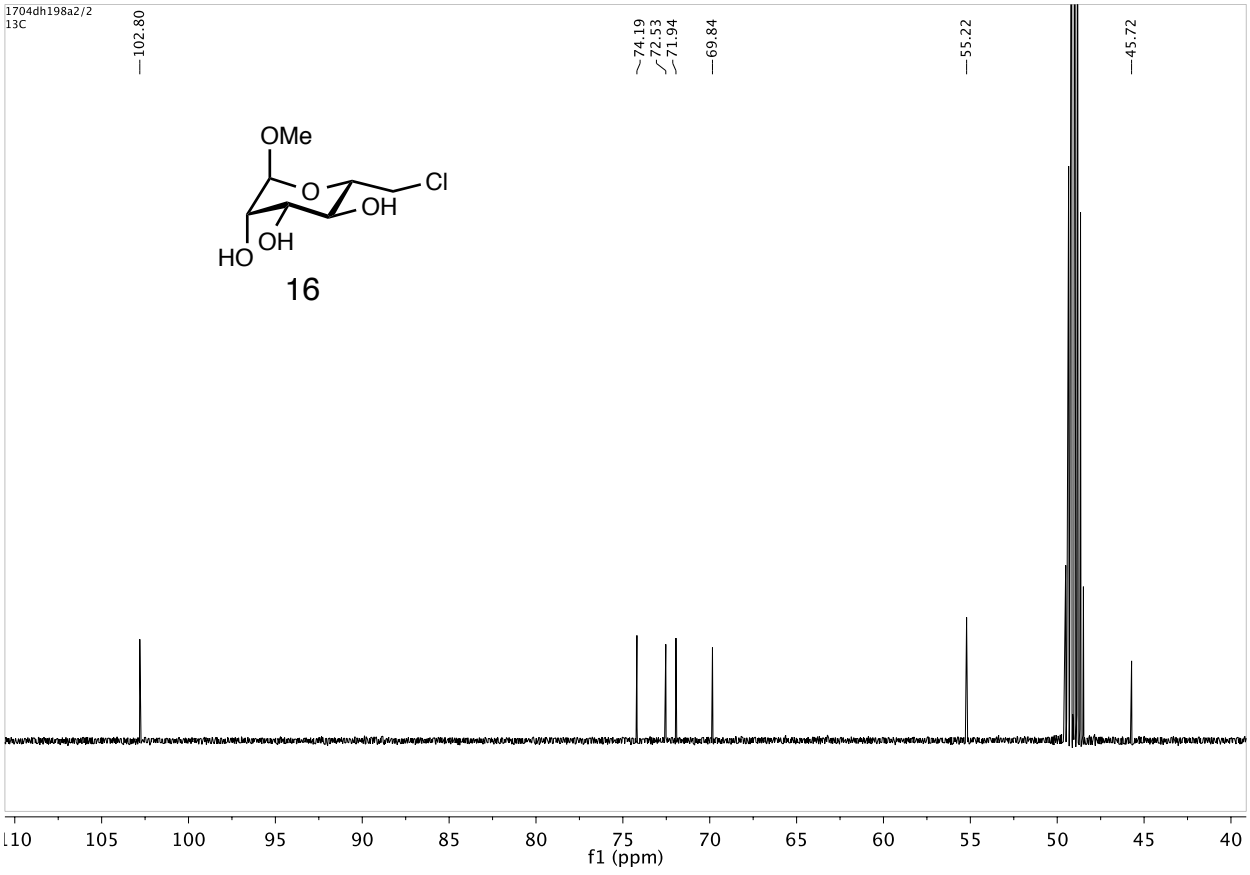
f1 (ppm)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HO
OH
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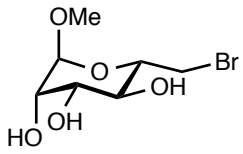
f1 (ppm)

0407dh198b.1.fid



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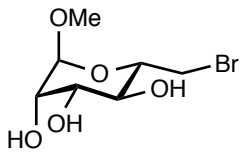

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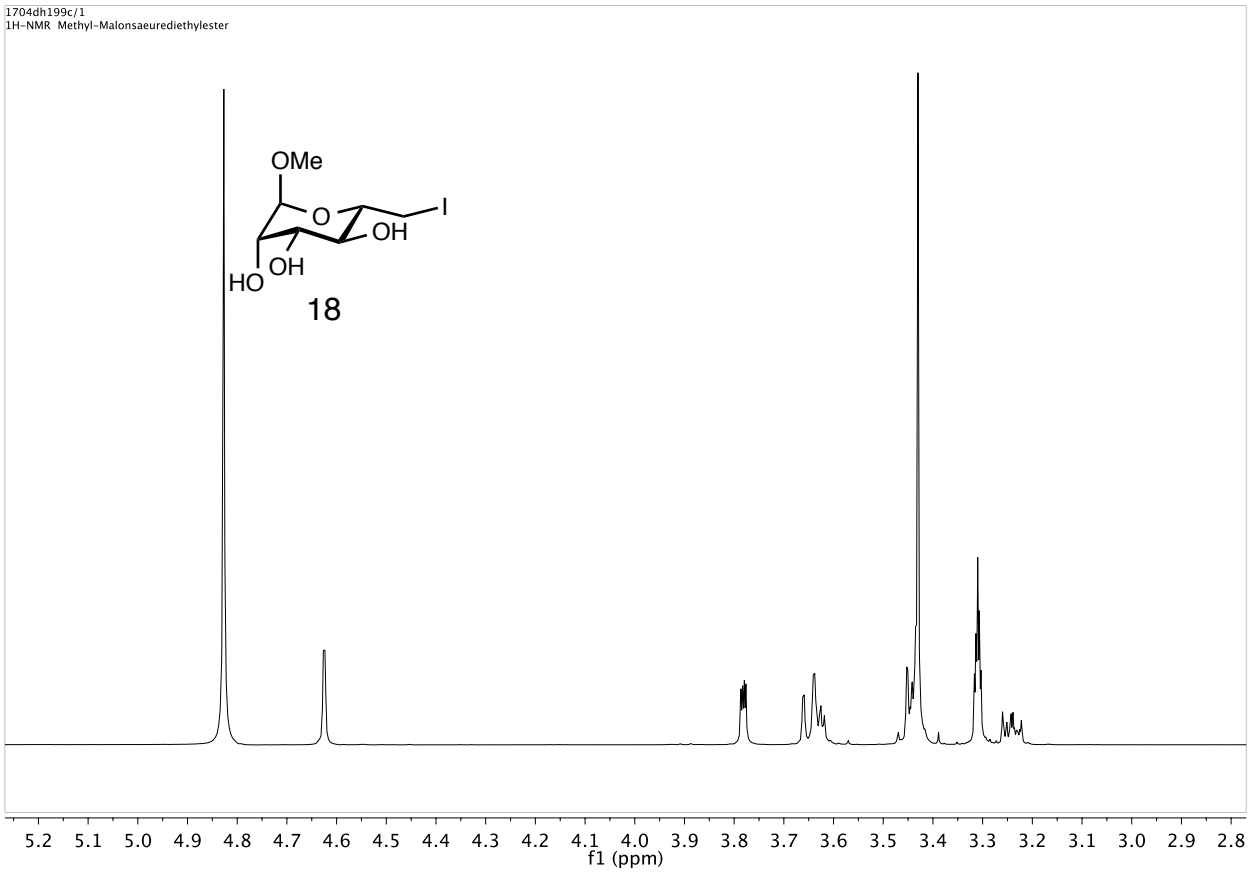
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1H-NMR Methyl-Malonsaeurediethylester
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O
I
OH
HO
OH
18
5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8
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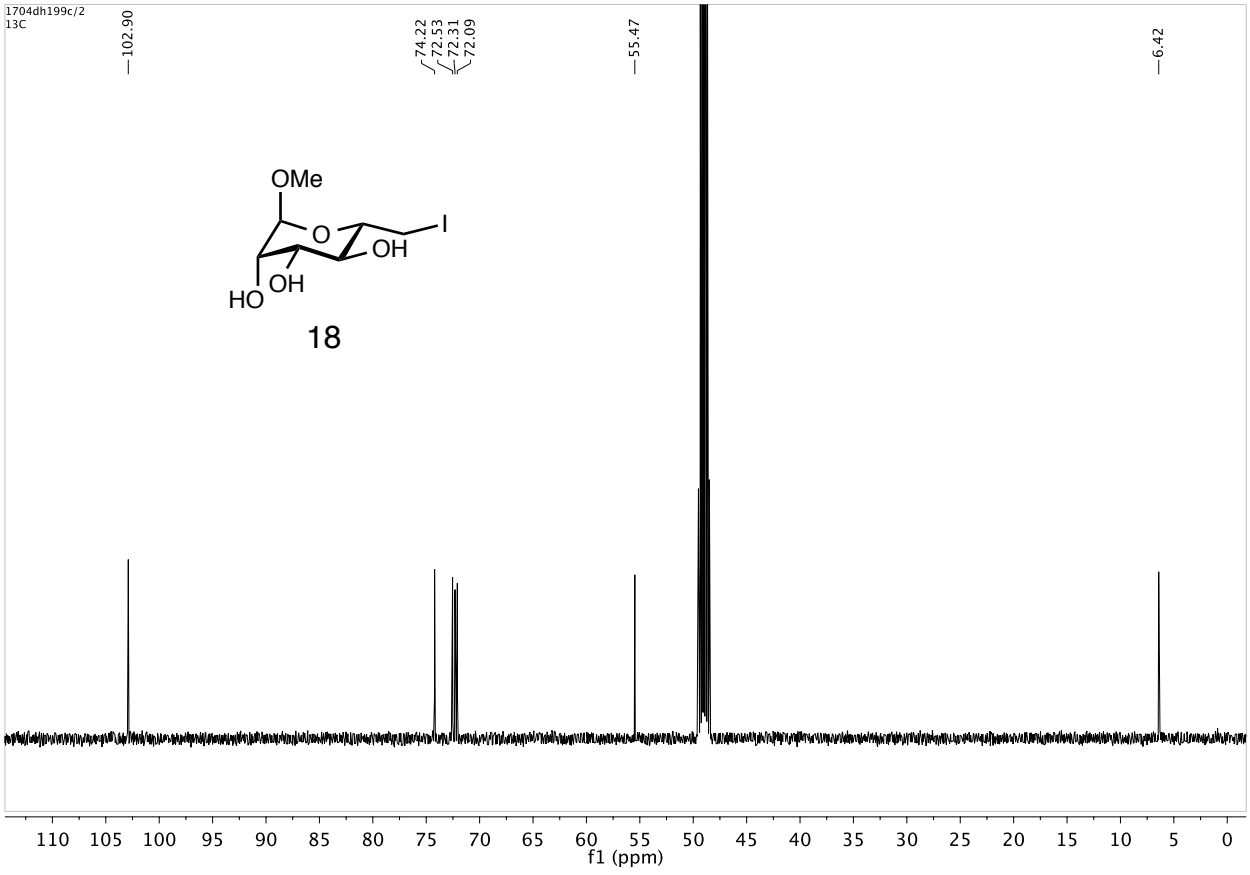
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HO
OH
18
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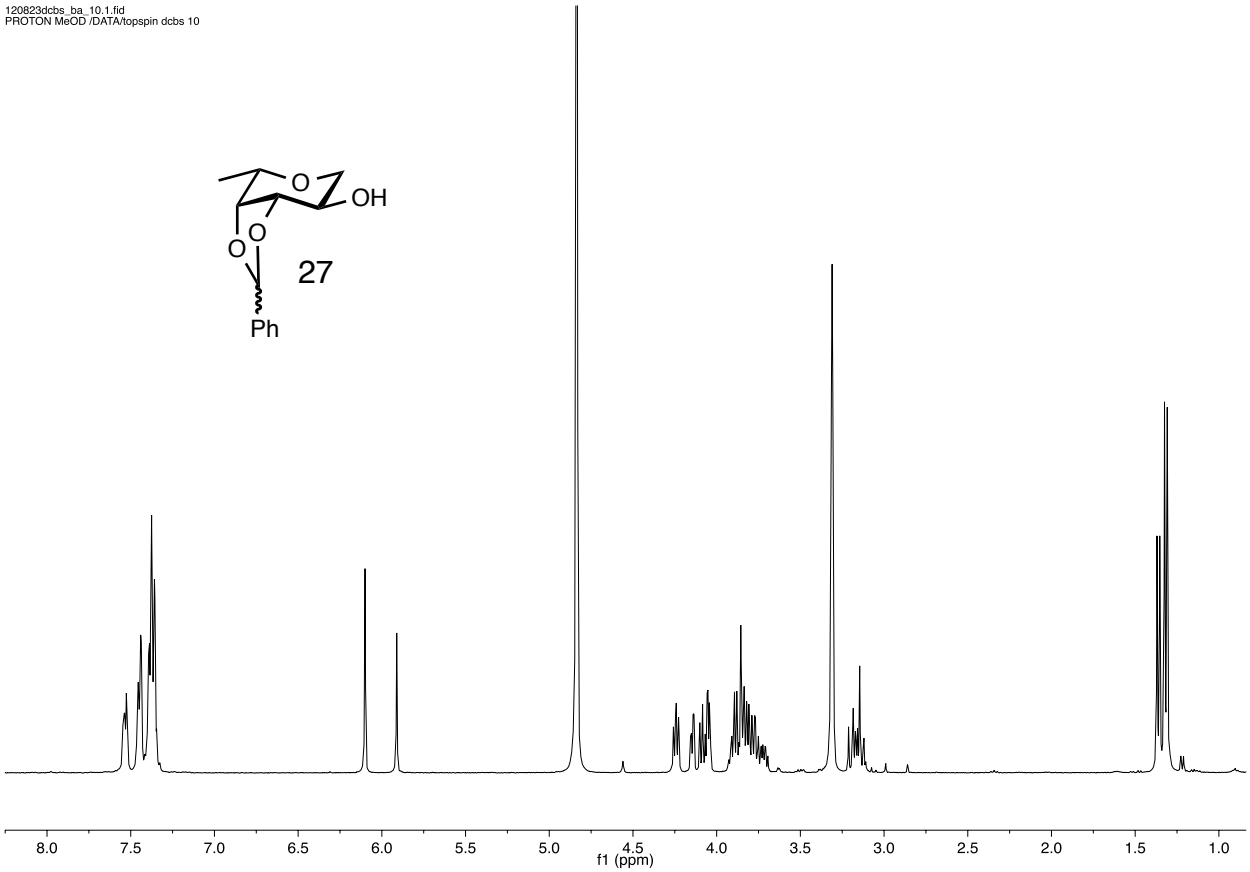
f1 (ppm)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OH
O
O
27
Ph
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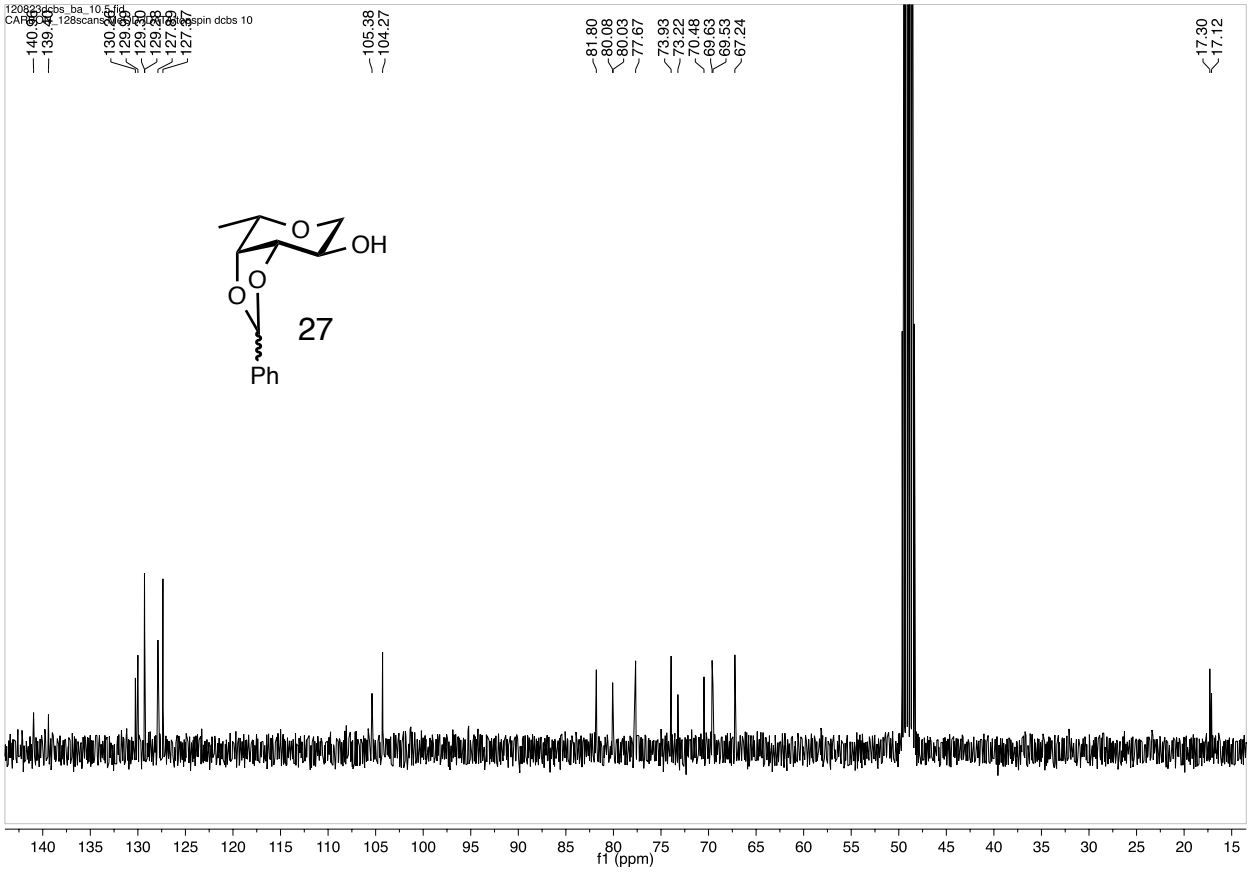
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)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69.53
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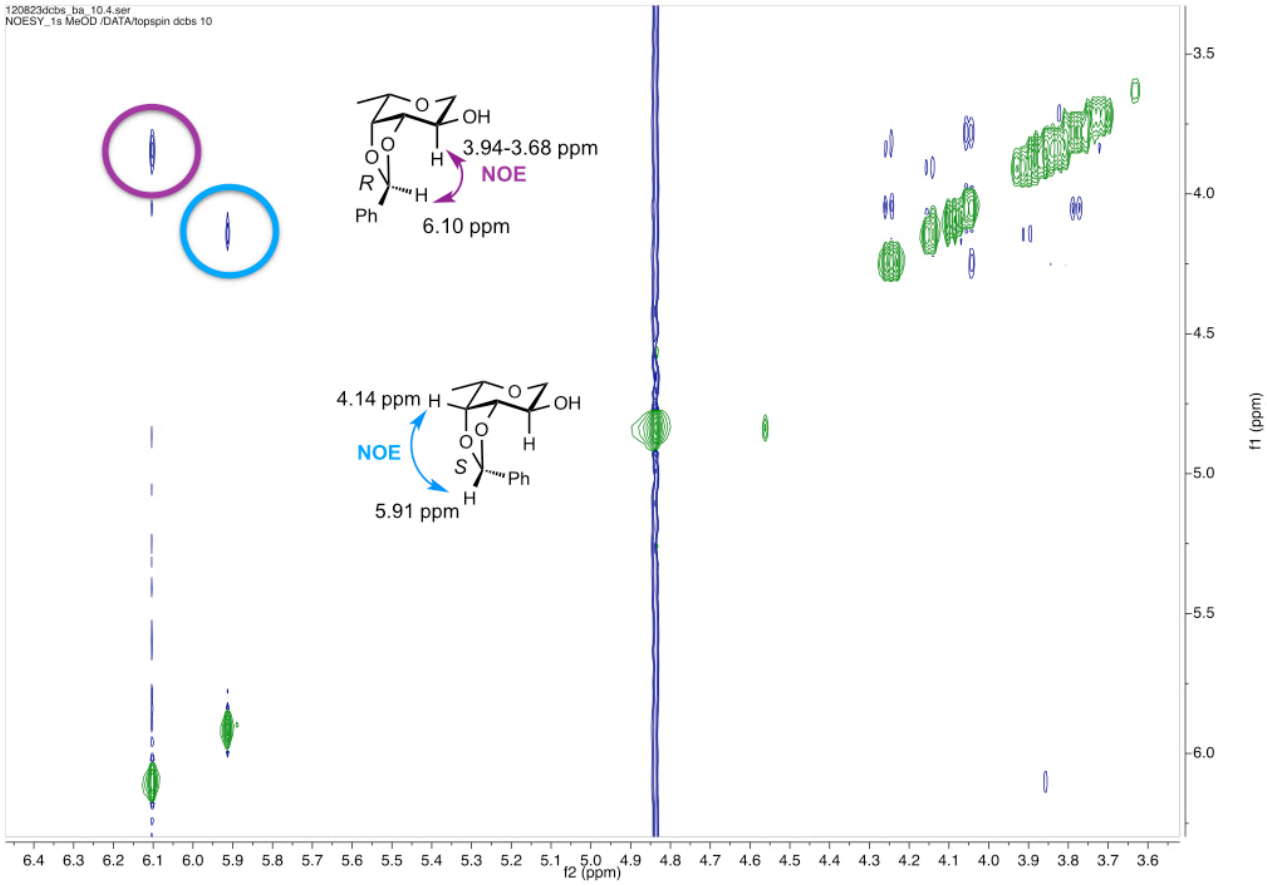
17.12
O
OH
O
O
27
Ph
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)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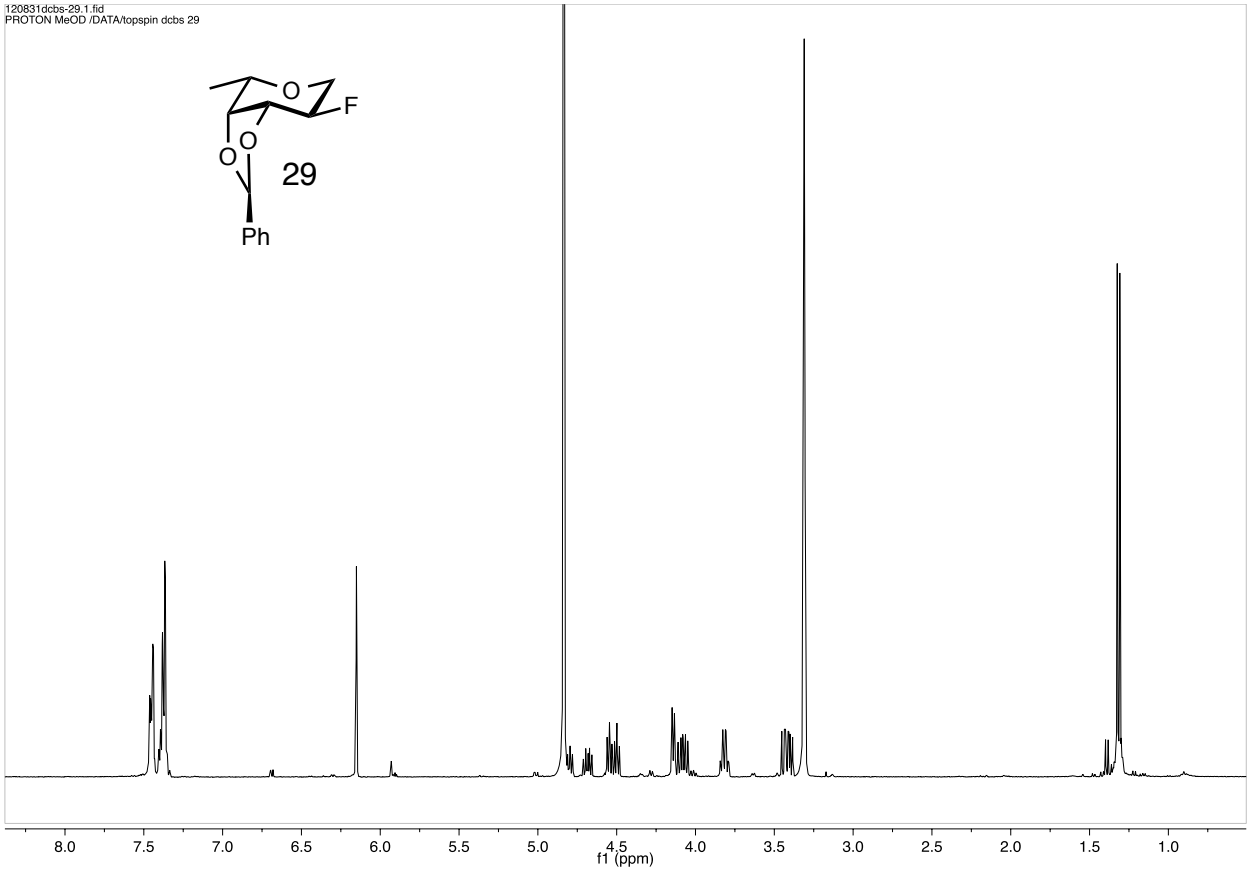
OH
O
O
H
R
H
Ph
3.94-3.68 ppm
NOE
6.10 ppm
4.14 ppm H
O
OH
O
H
NOE
S
Ph
H
5.91 ppm
f2 (ppm)
f1 (ppm)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PROTON MeOD /DATA/topspin dcbs 29
O
F
O
O
29
Ph
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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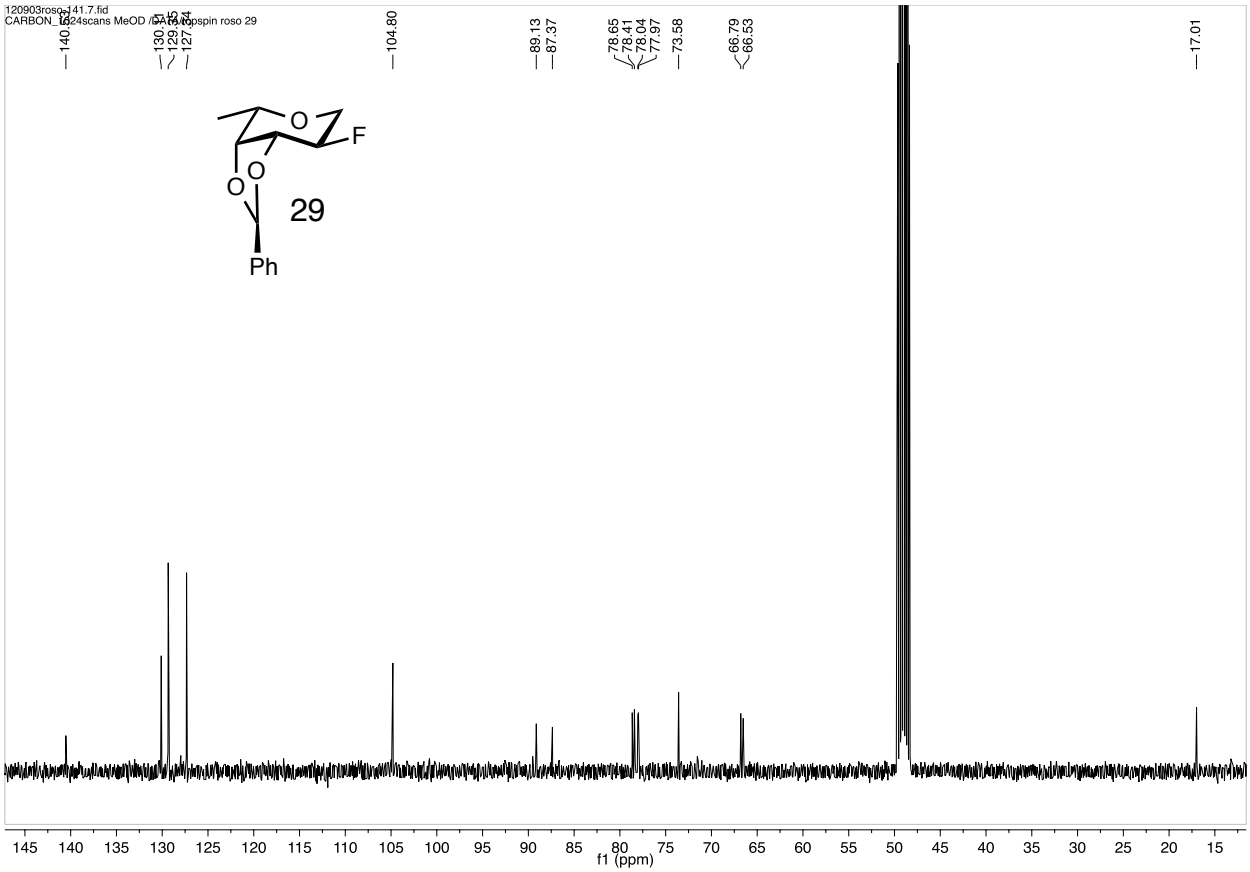
2.0
1.5
1.0
f1 (ppm)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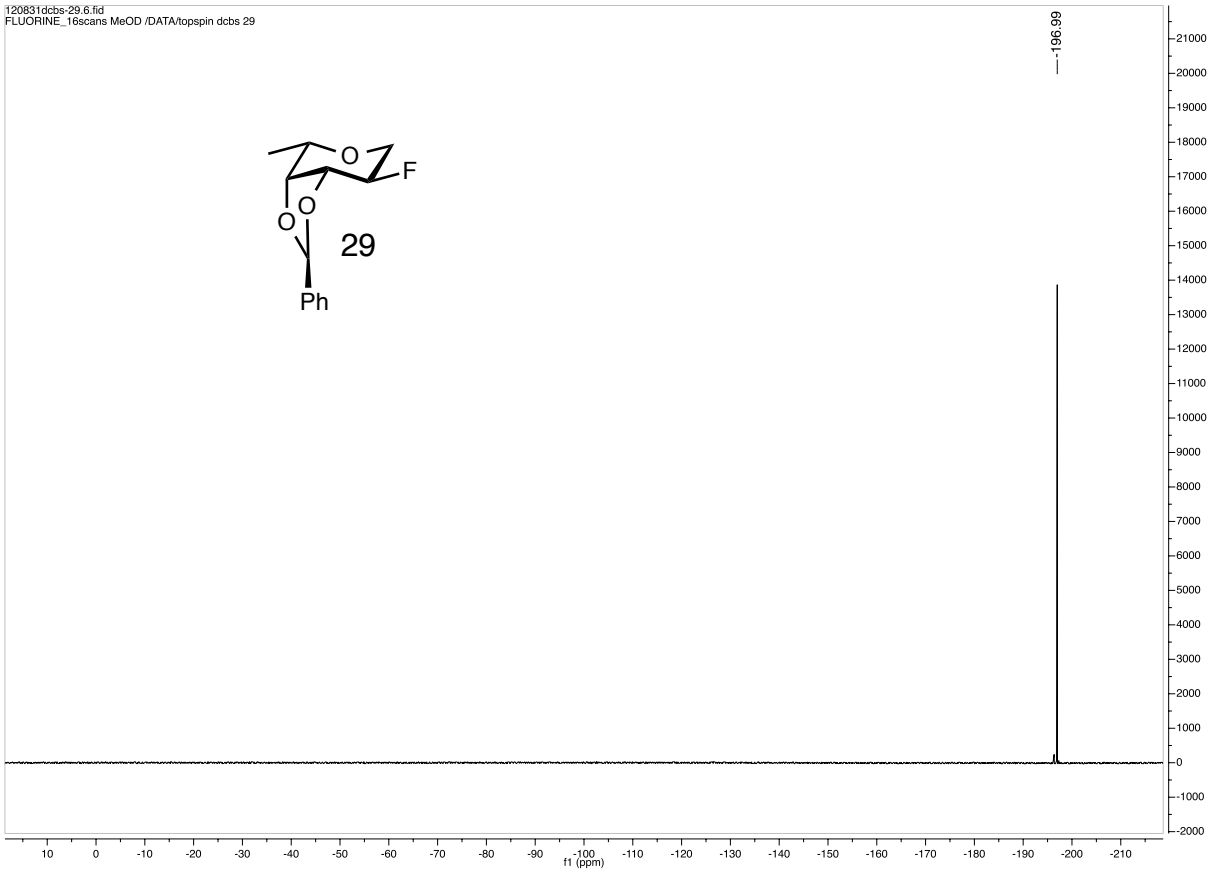
130.15
129.45
127.24
104.80
89.13
87.37
78.65
78.41
78.04
77.97
73.58
66.79
66.53
17.01
O
F
O
O
29
Ph
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)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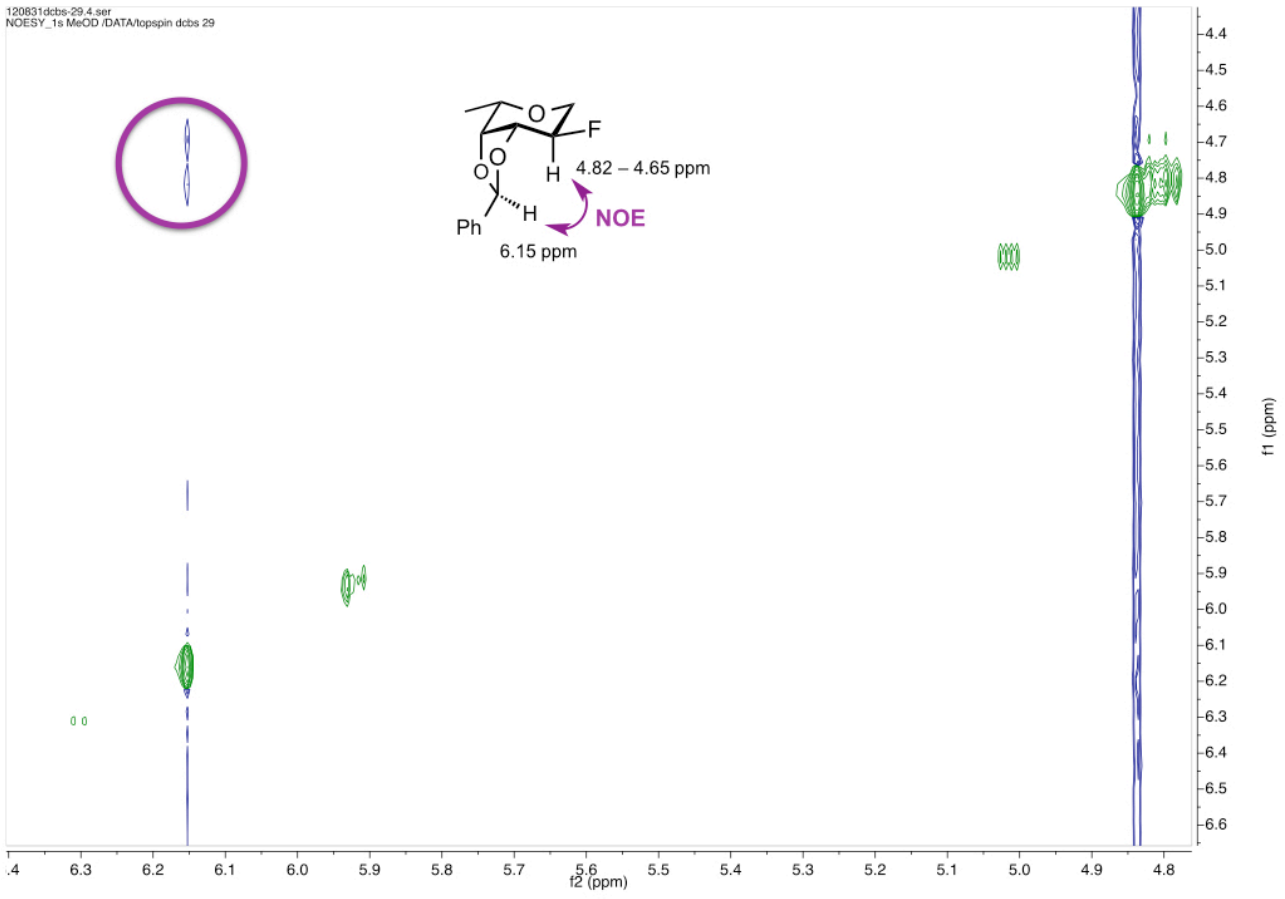
-196.99
O
F
O
O
29
Ph
f1 (ppm)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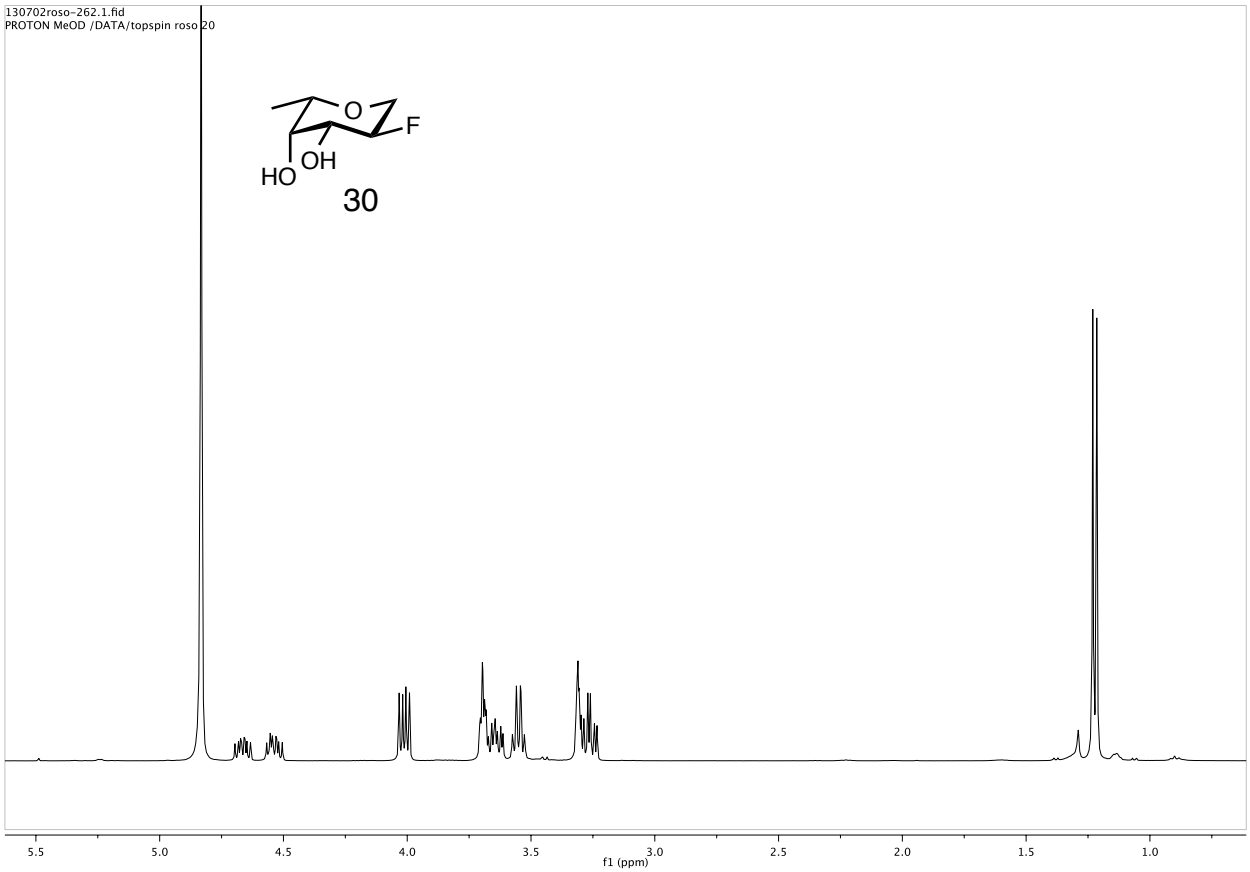
O
F
O
O
H
Ph
H
4.82 – 4.65 ppm
NOE
6.15 ppm
f2 (ppm)
f1 (ppm)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F
HO
OH
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3.0
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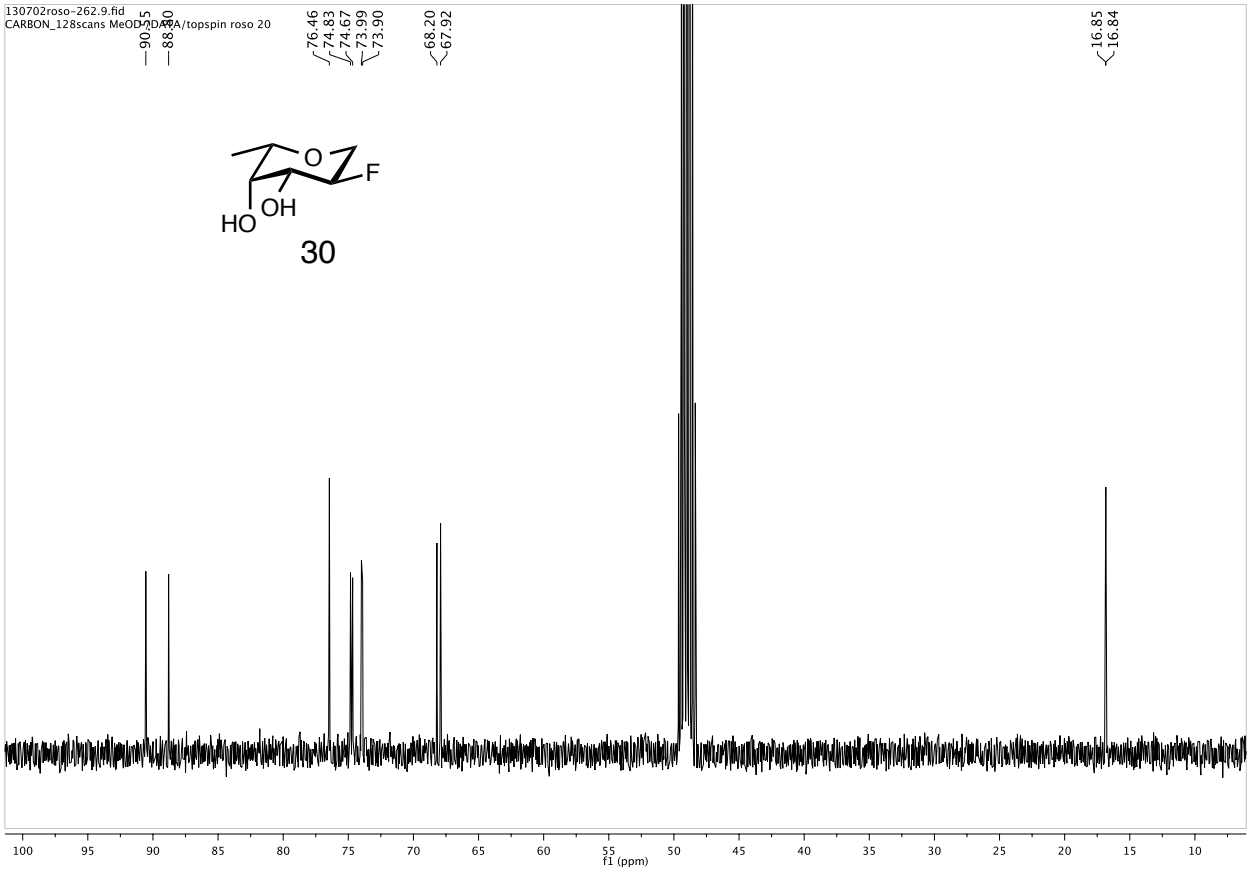
2.0
1.5
1.0
f1 (ppm)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73.90
68.20
67.92
16.85
16.84
O
F
HO
OH
30
100
95
90
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75
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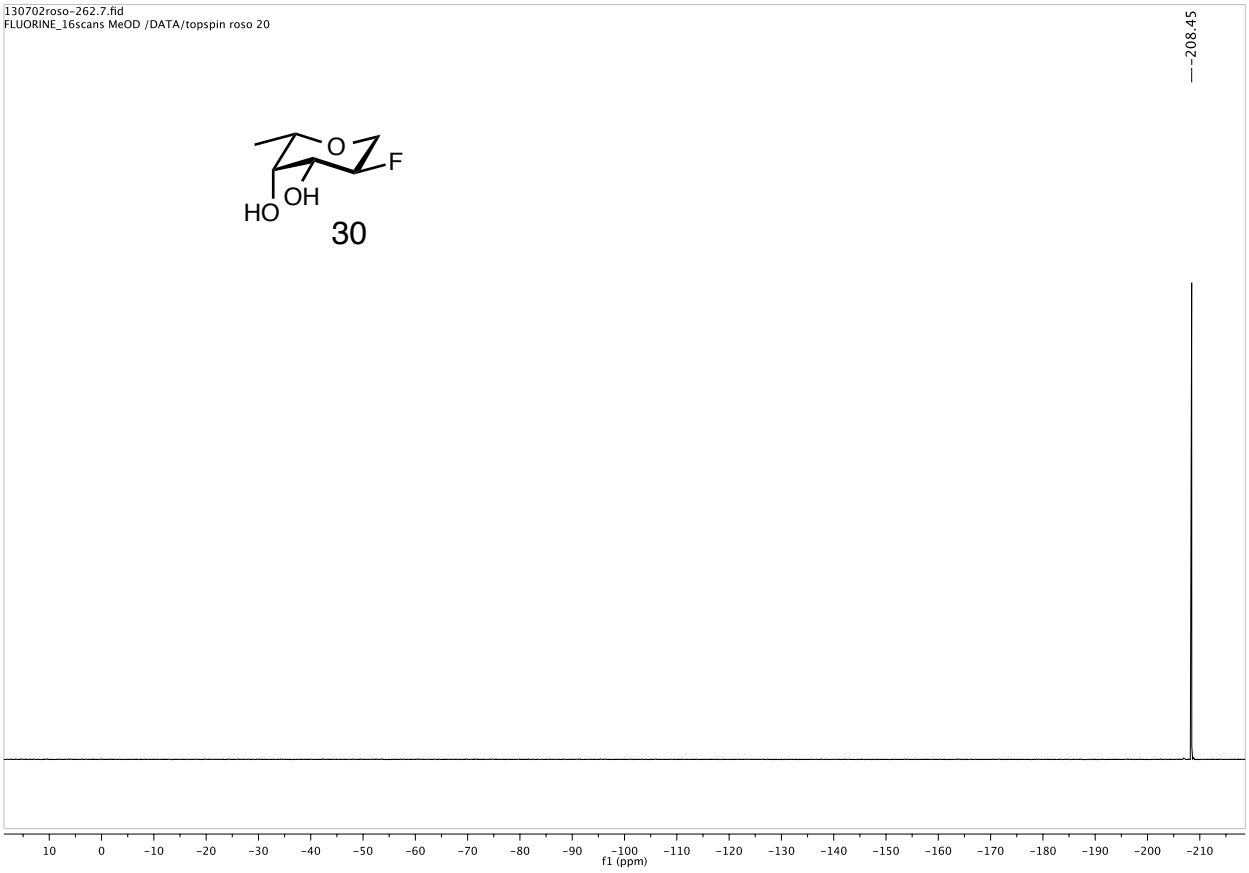
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)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O
F
HO
OH
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10
0
-10
-20
-30
-40
-50
-60
-70
-80
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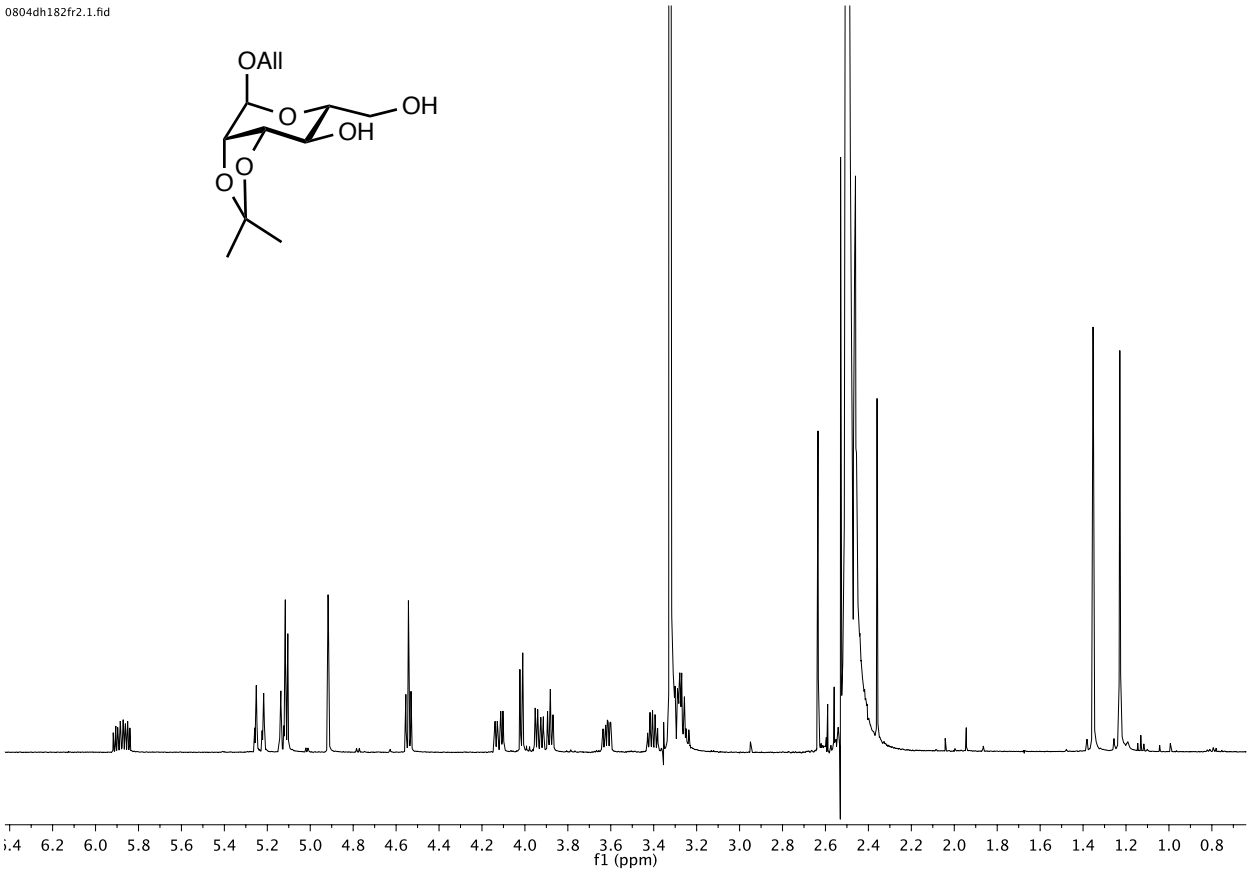
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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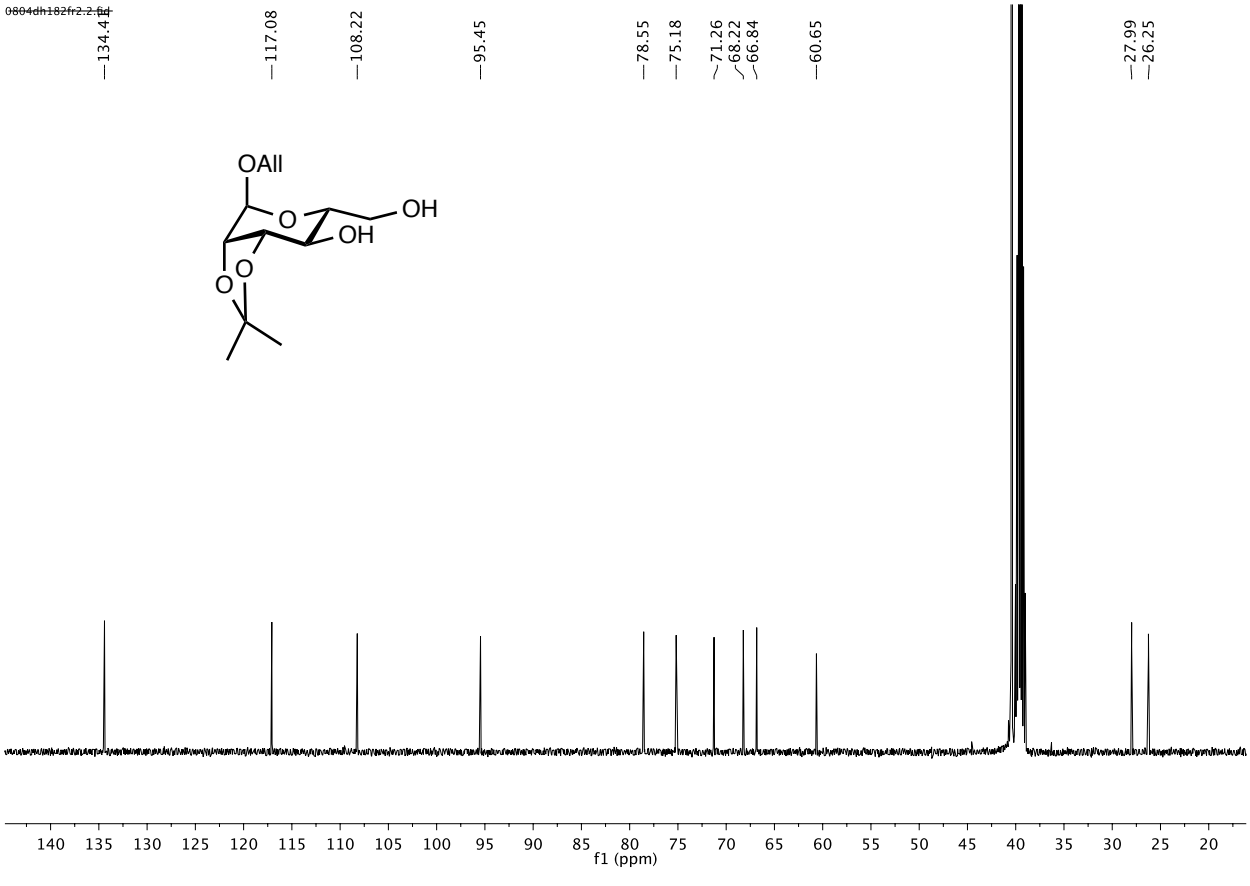
OAll
O
OH
OH
O
O
6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8
f1 (ppm)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108.22
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78.55
75.18
71.26
68.22
66.84
60.65
27.99
26.25
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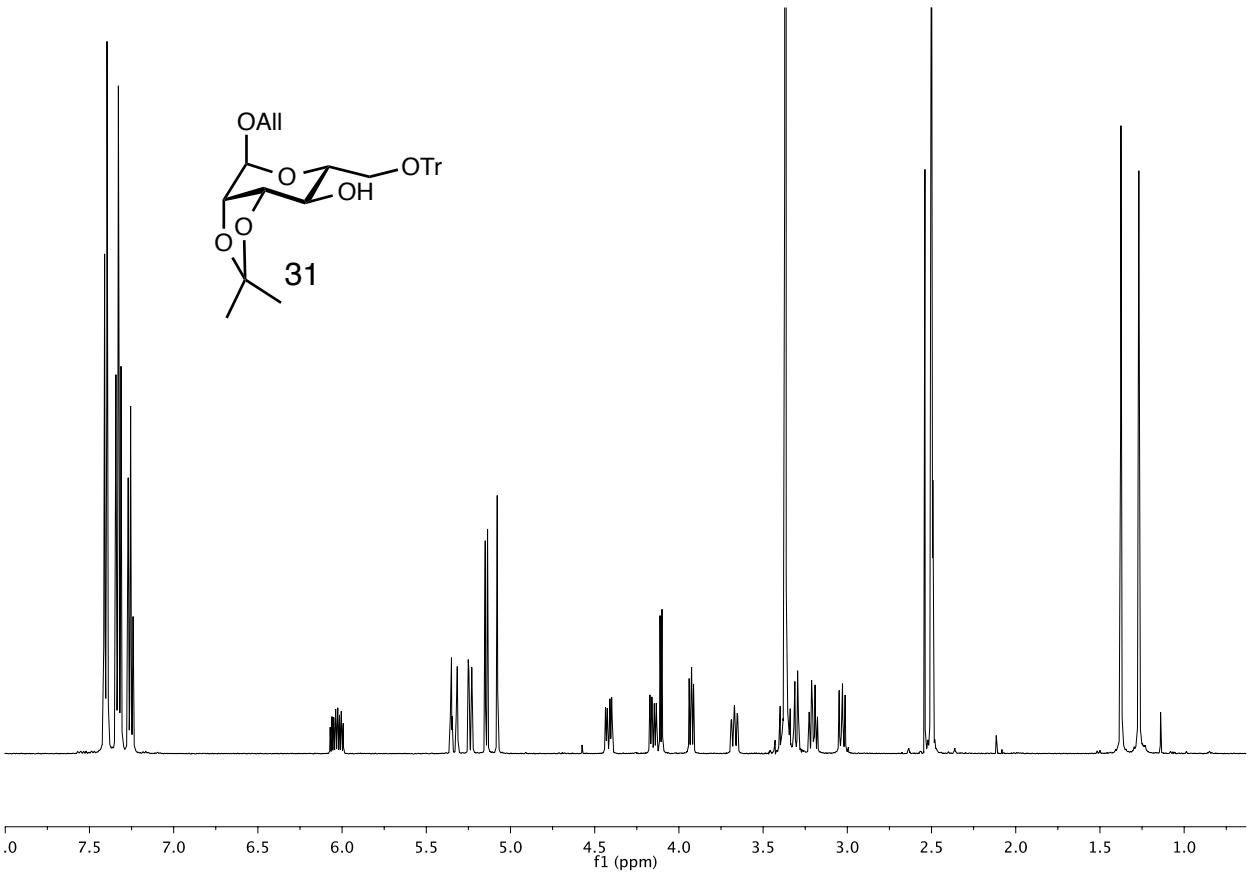
O
OH
OH
O
O
140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20
f1 (ppm)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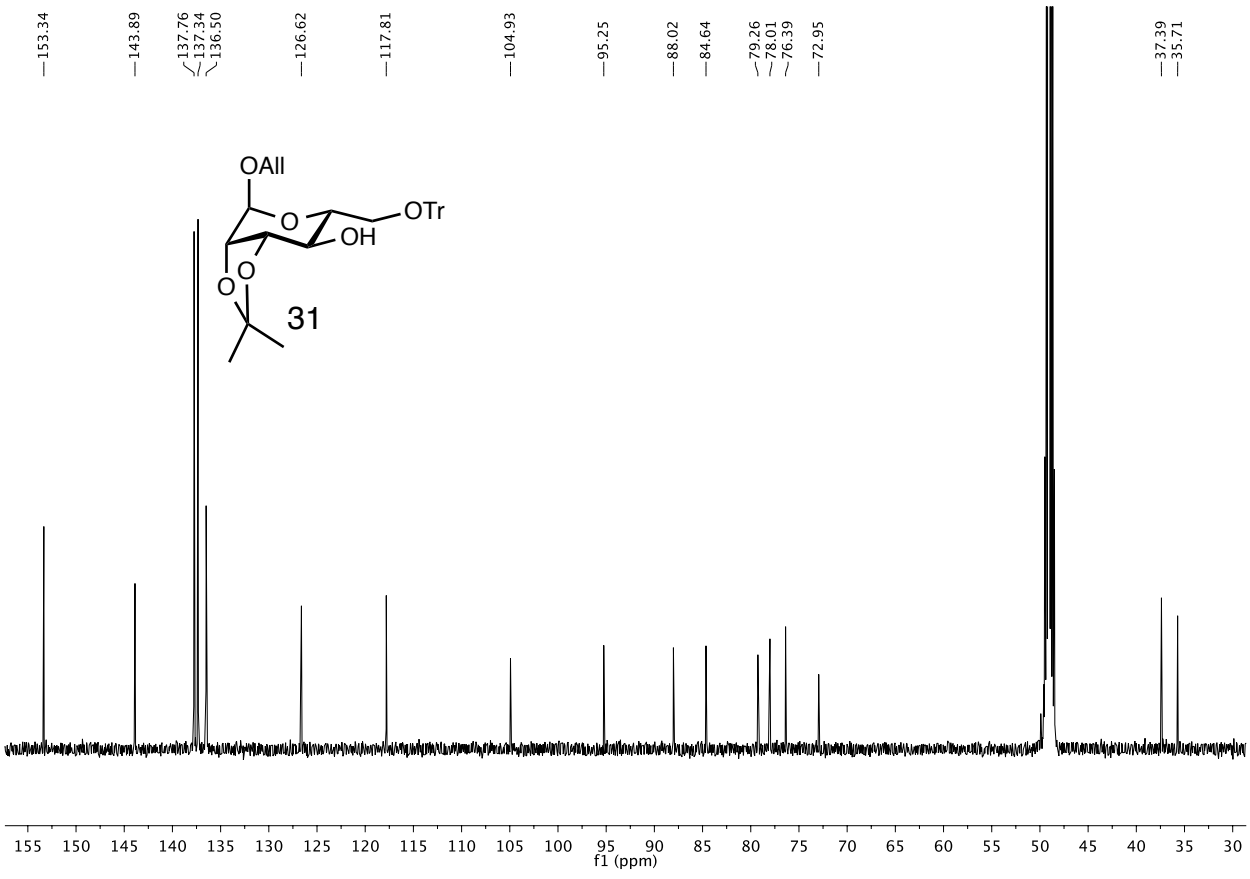
O
OTr
OH
O
O
31
f1 (ppm)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88.02
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O
OTr
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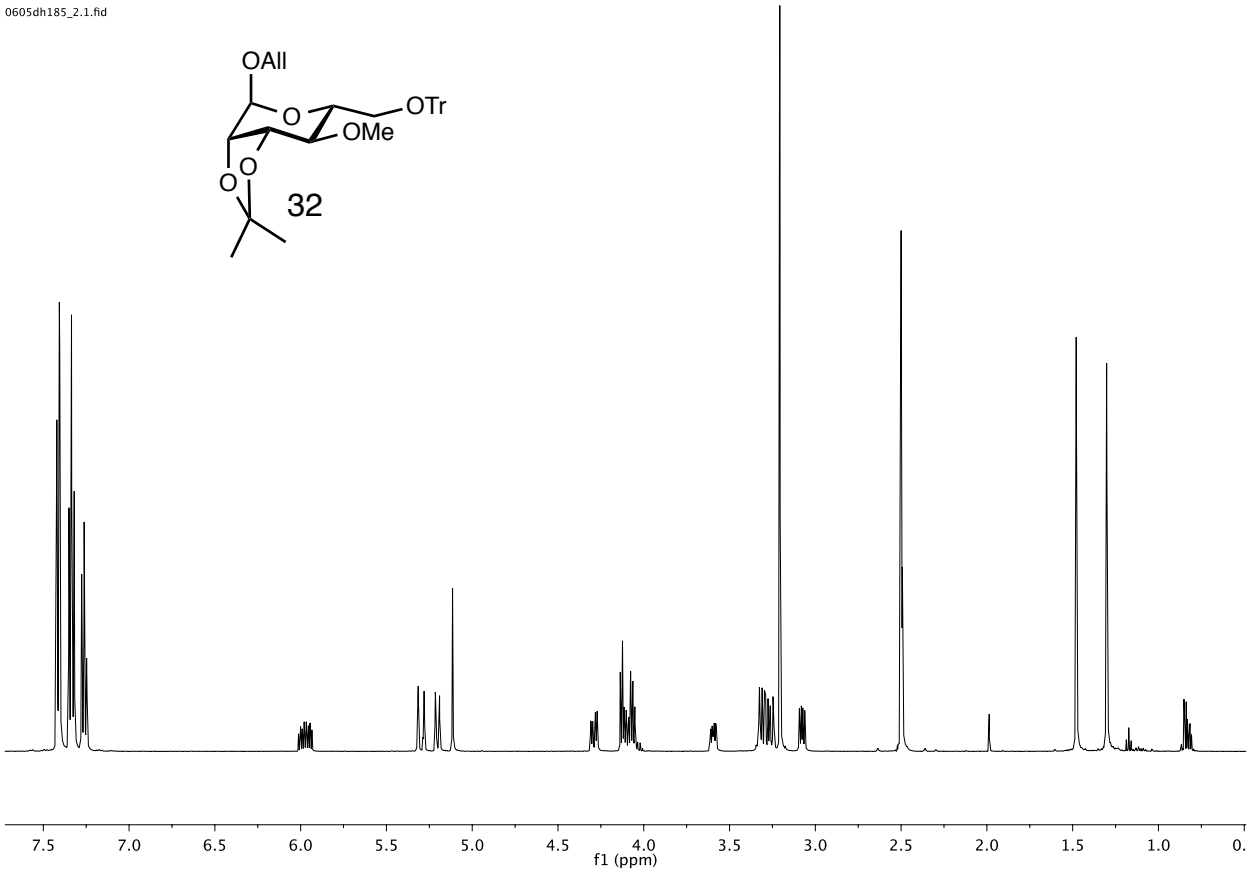
O
O
31
f1 (ppm)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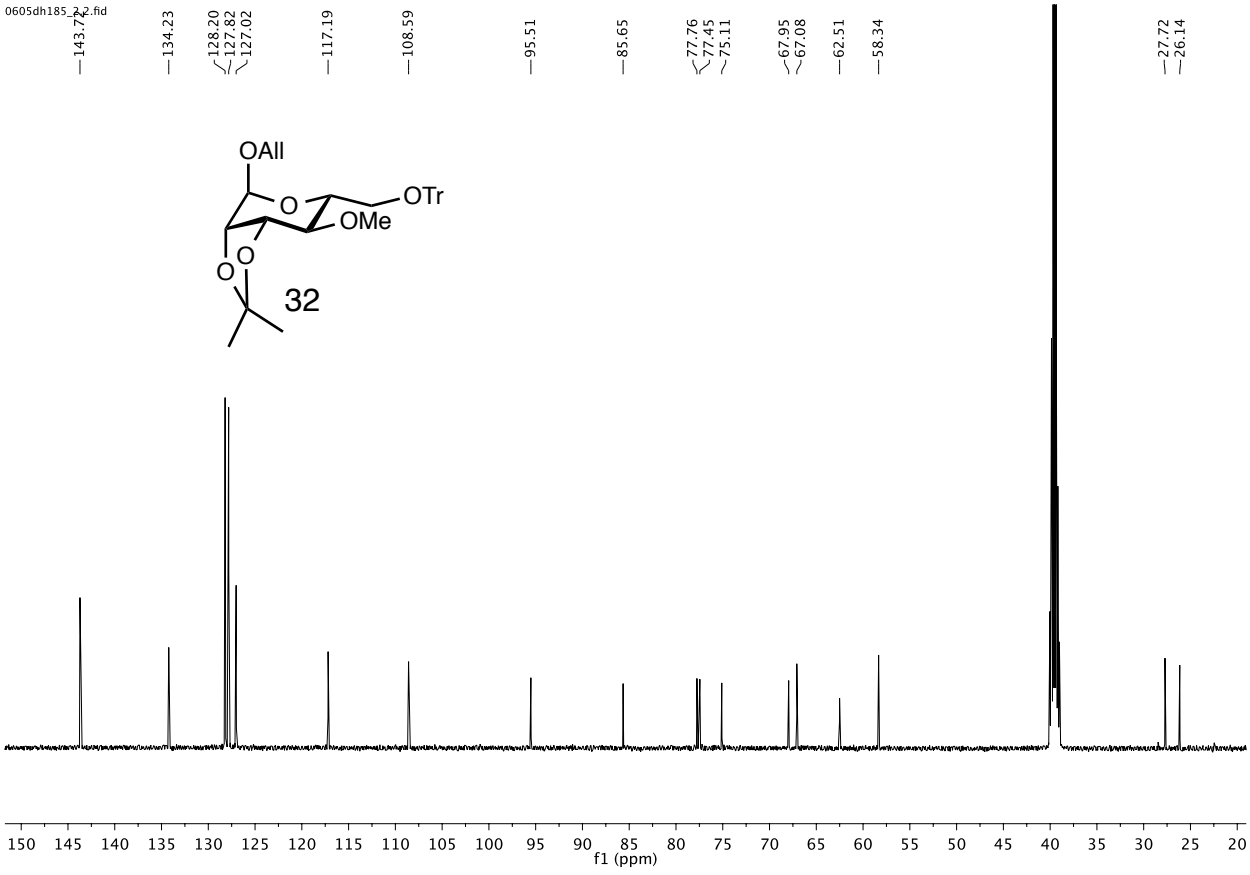
f1 (ppm)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117.19
108.59
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77.76
77.45
75.11
67.95
67.08
62.51
58.34
27.72
26.14
OAll
O
OTr
OMe
O
O
32
150
145
140
135
130
125
120
115
110
105
100
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85
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65
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45
40
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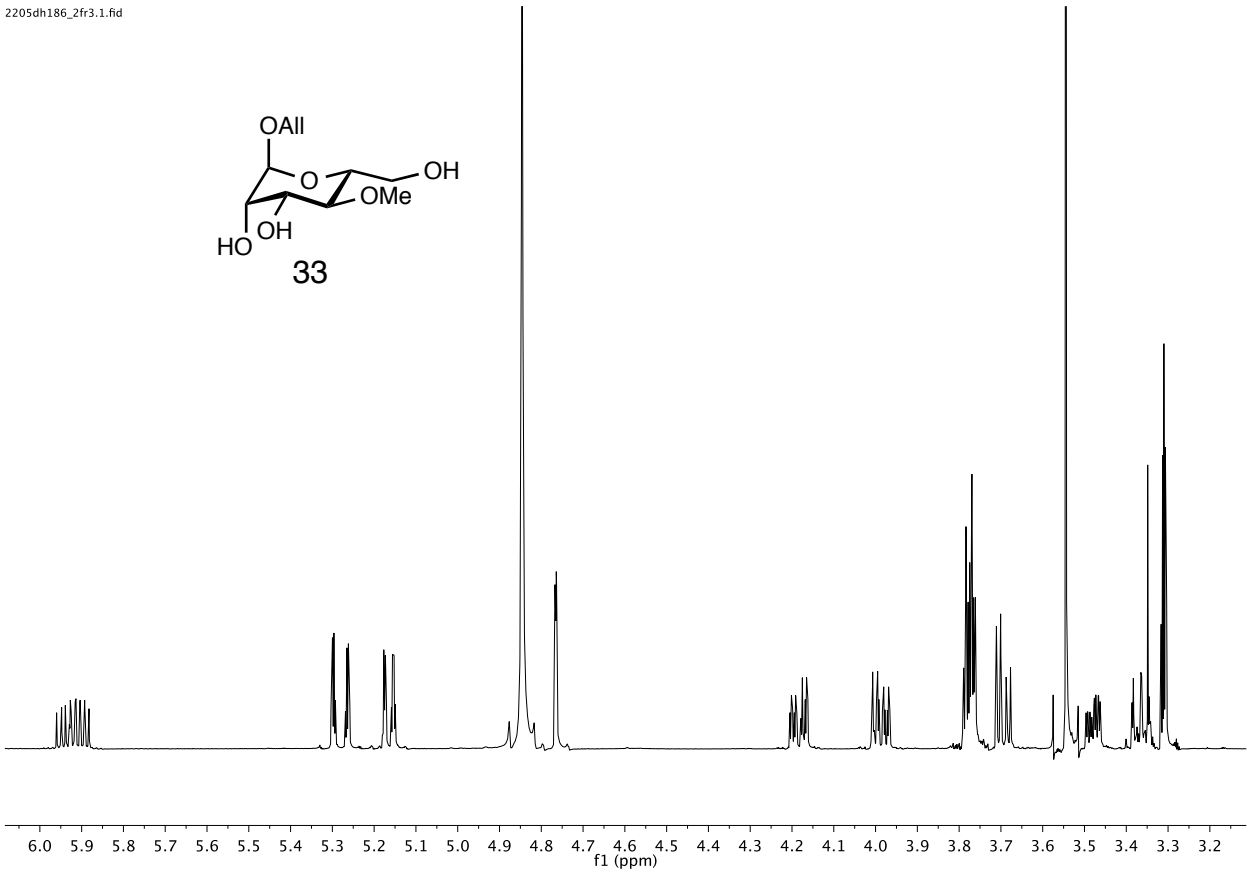
30
25
20
f1 (ppm)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HO
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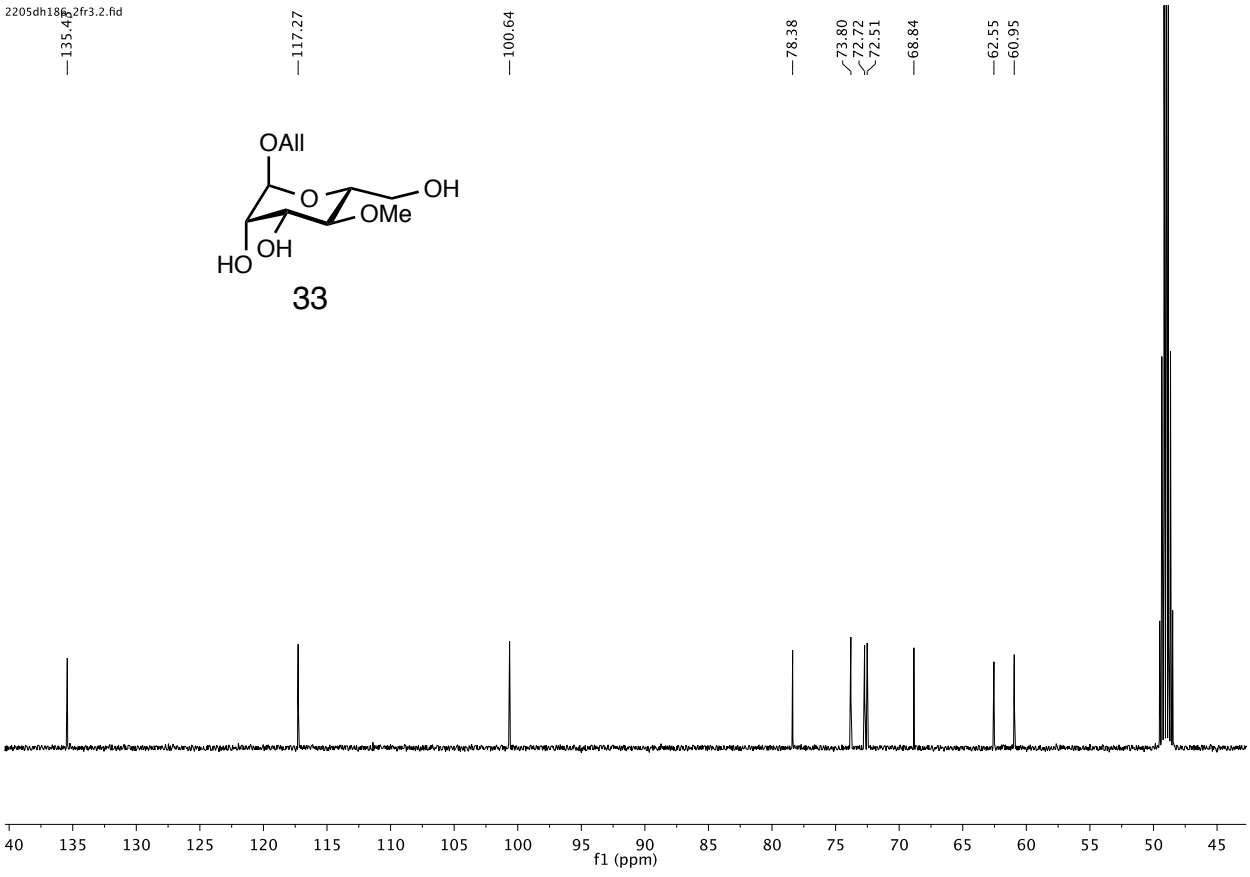
6.0 5.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2
f1 (ppm)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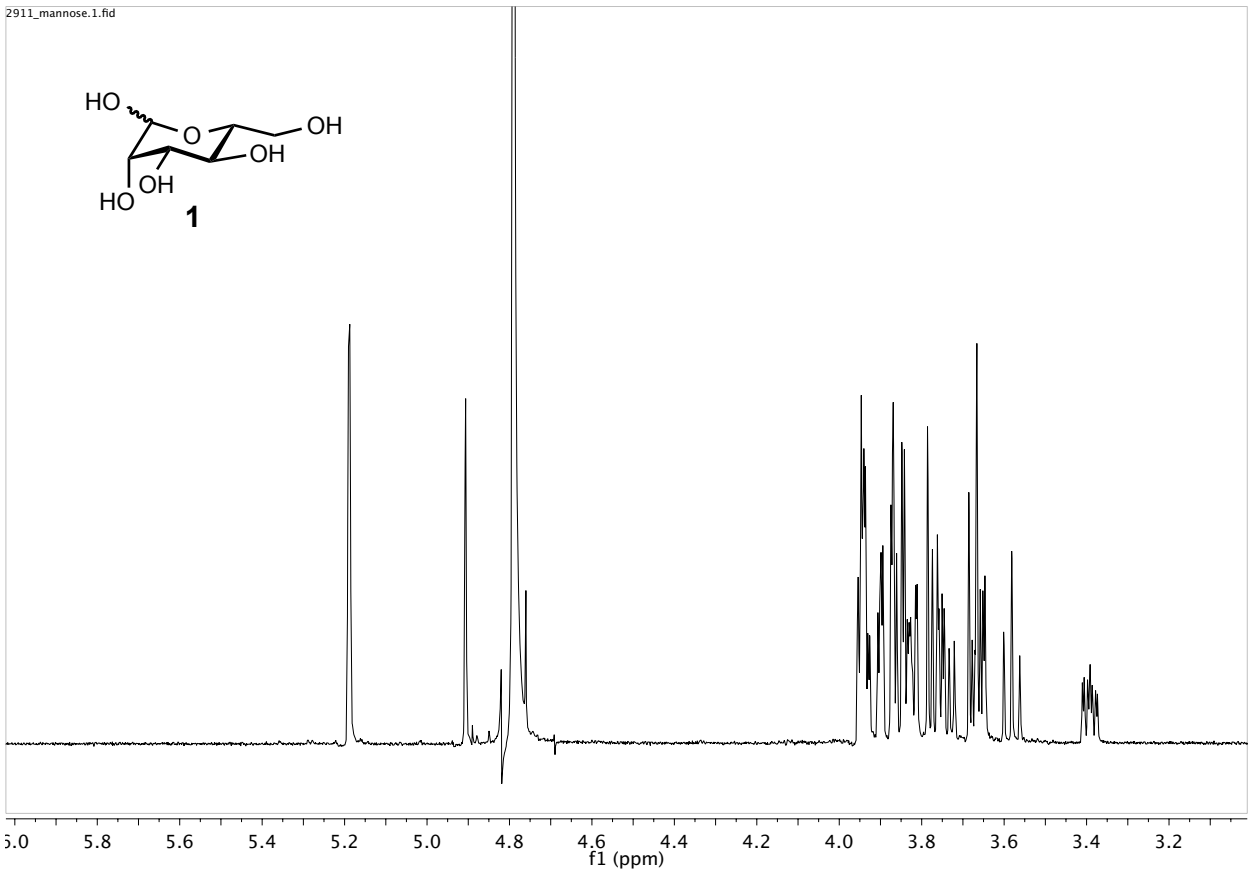
135.43
117.27
100.64
78.38
73.80
72.72
72.51
68.84
62.55
60.95
OAll
O
OH
OMe
HO
OH
33
40 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45
f1 (ppm)

Table S1: Calculation of inhibition constants (K_i) from IC_{50} values

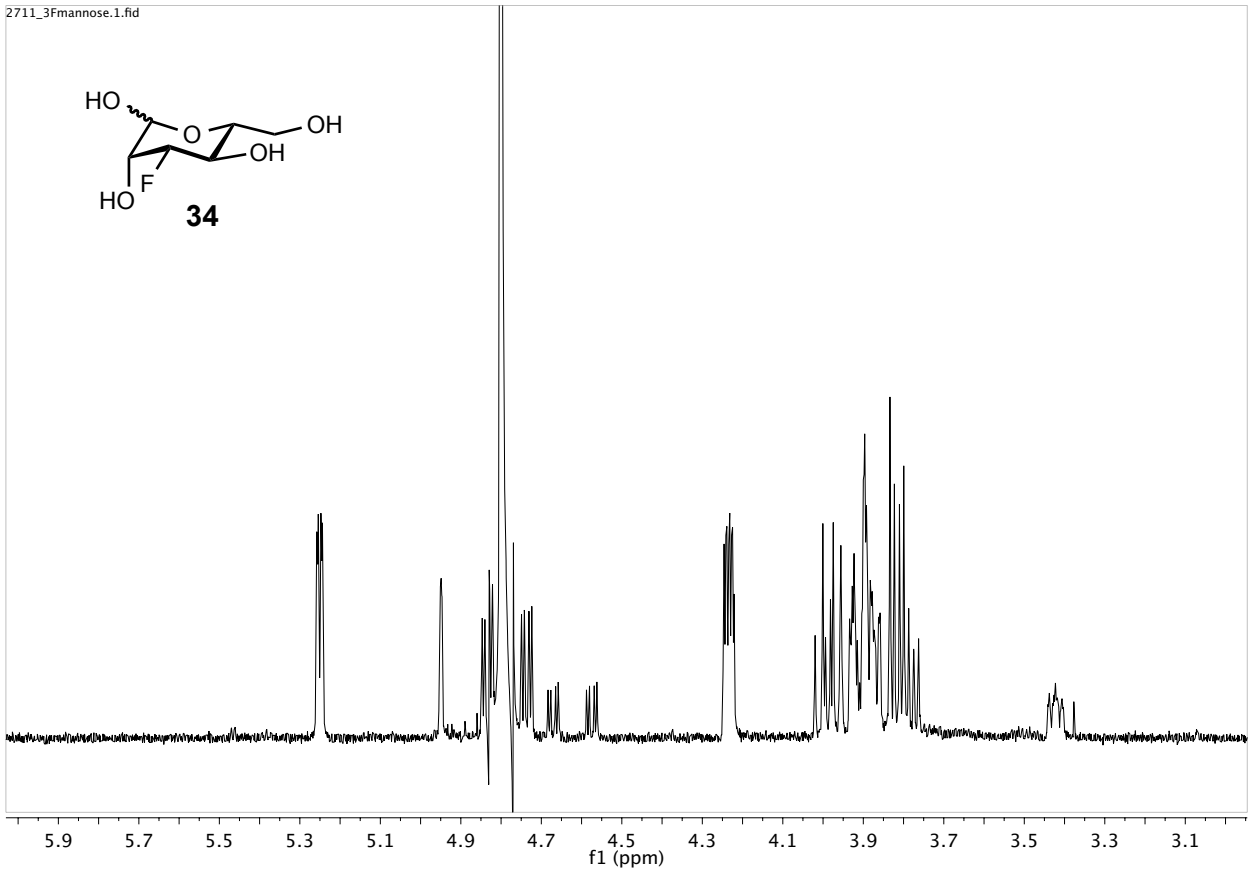
K_d (tracer 3) [µM]	3.1	
concentration of 3 [µM]	0.01	
compound	IC_{50} [µM]	K_i [µM]
1	10.8	10.8
5	498	496.4
10	13	13.0
11	2.9	2.9
12	7.0	7.0
14	14.5	14.5
15	7.4	7.4
20	116	115.6
21	104	103.7
22	64	63.8
25	19	18.9
26	13.8	13.8

Calculation performed using the Cheng-Prusoff equation initially developed for competitive inhibition of enzymes (Cheng, Y.C. and Prusoff, W.H. *Biochem. Pharm.*,1973, 22:3099-108).

^{1}H-NMR trace of **1**



^{1}H-NMR trace of **34**



^{1}H-NMR trace of **35**