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A metal-free synthetic approach to peptide-based iminosugar clusters as novel multivalent glycosidase inhibitors

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Supporting Information

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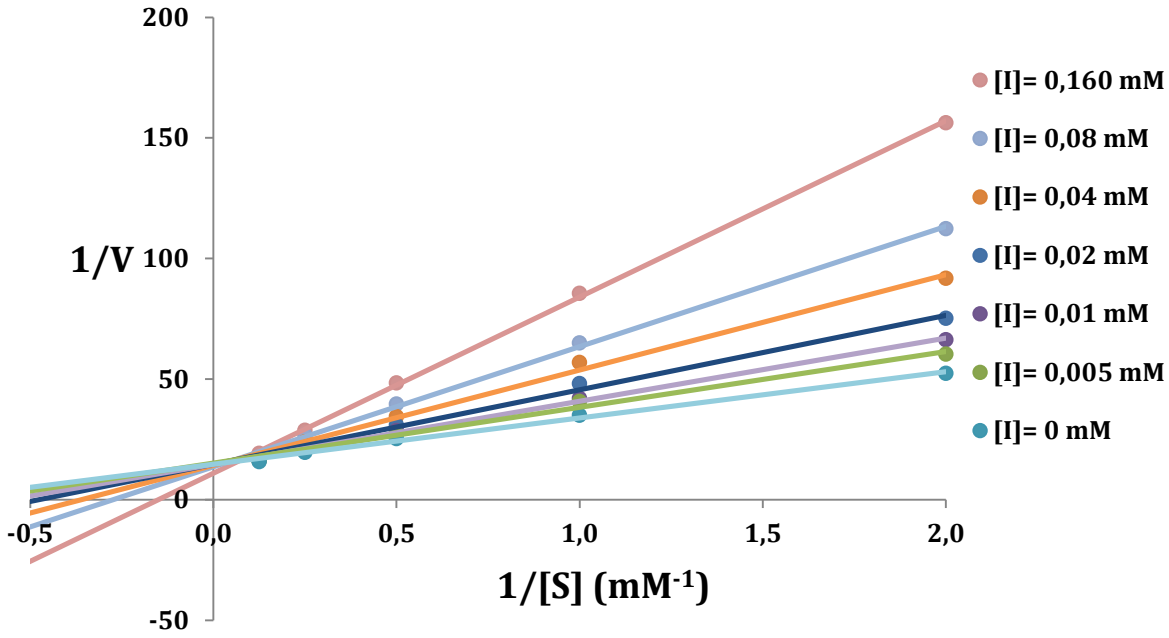


Figure S1. Lineweaver-Burk plot for K_i determination (58.7 ± 8.2 μM) of **14** against Jack bean α-mannosidase (pH 5.5).

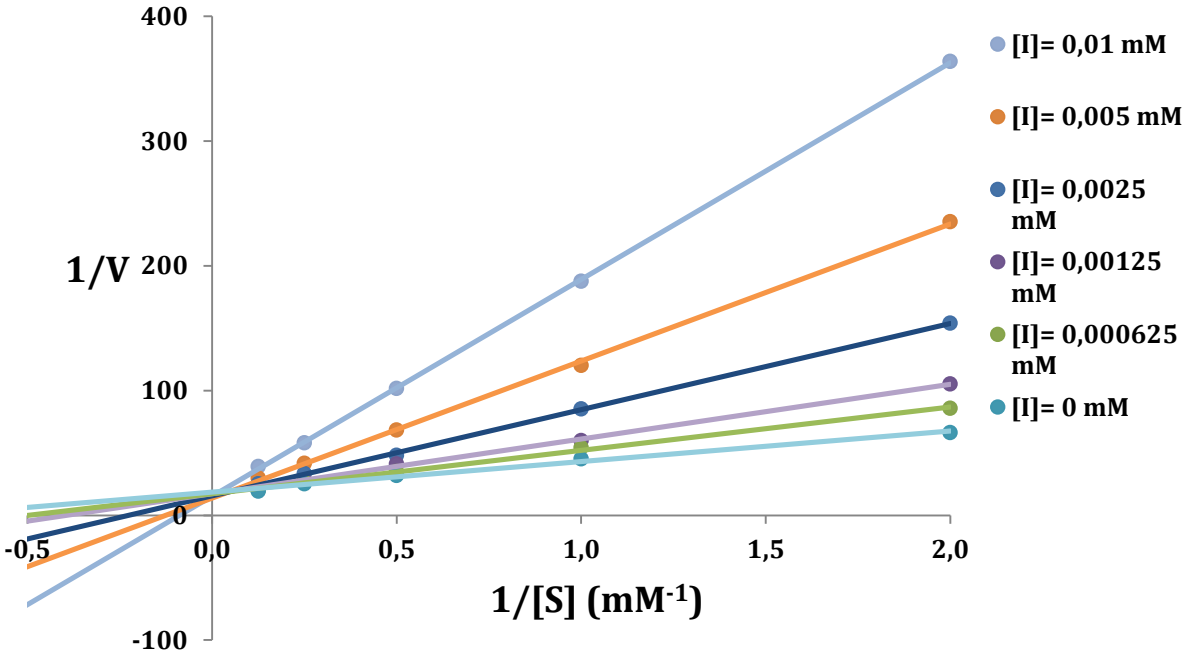


Figure S2. Lineweaver-Burk plot for K_i determination (3.2 ± 0.33 μM) of **15** against Jack bean α-mannosidase (pH 5.5).

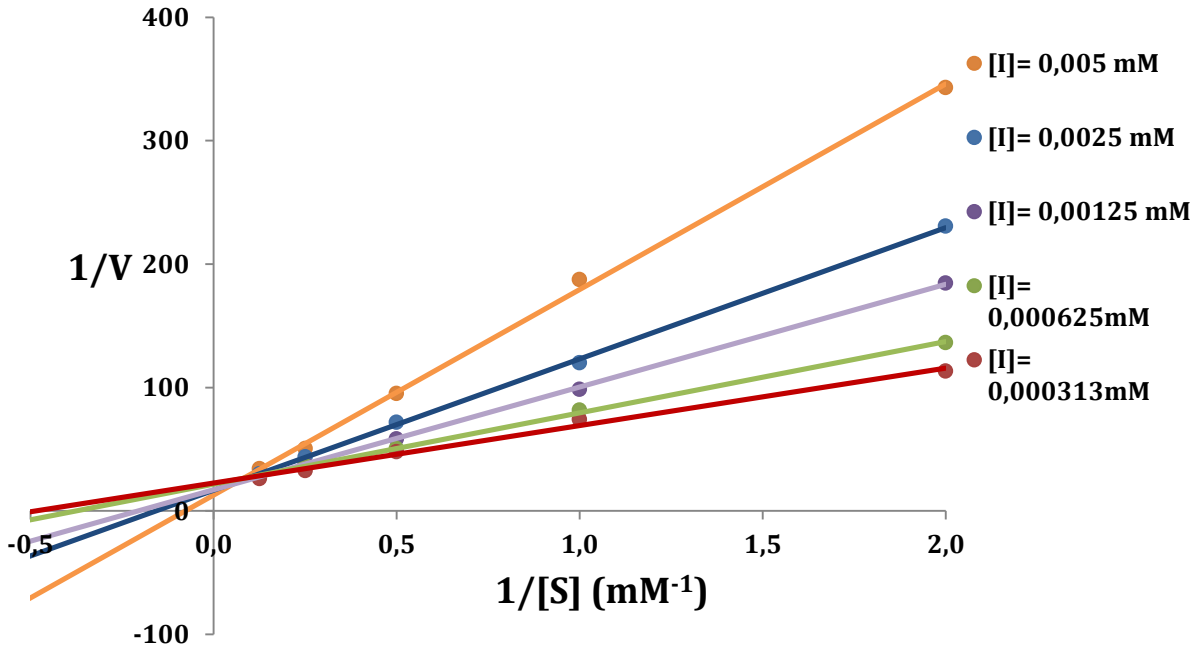


Figure S3. Lineweaver-Burk plot for K_i determination (1.9 ± 0.45 μM) of **16** against Jack bean α-mannosidase (pH 5.5).

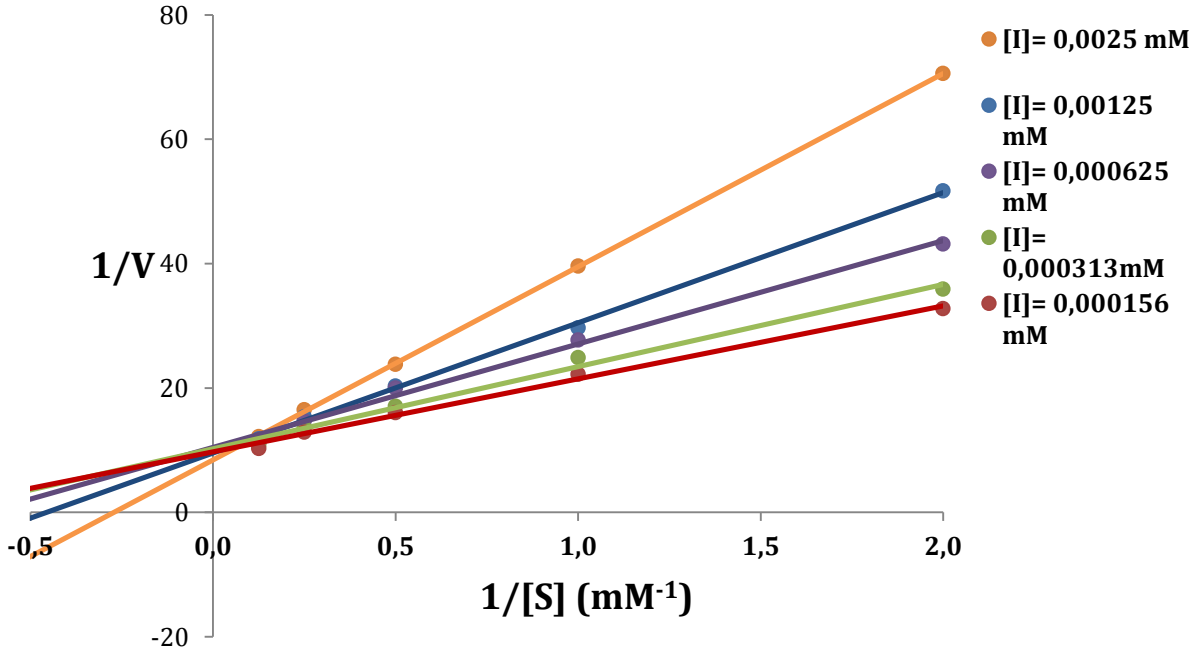
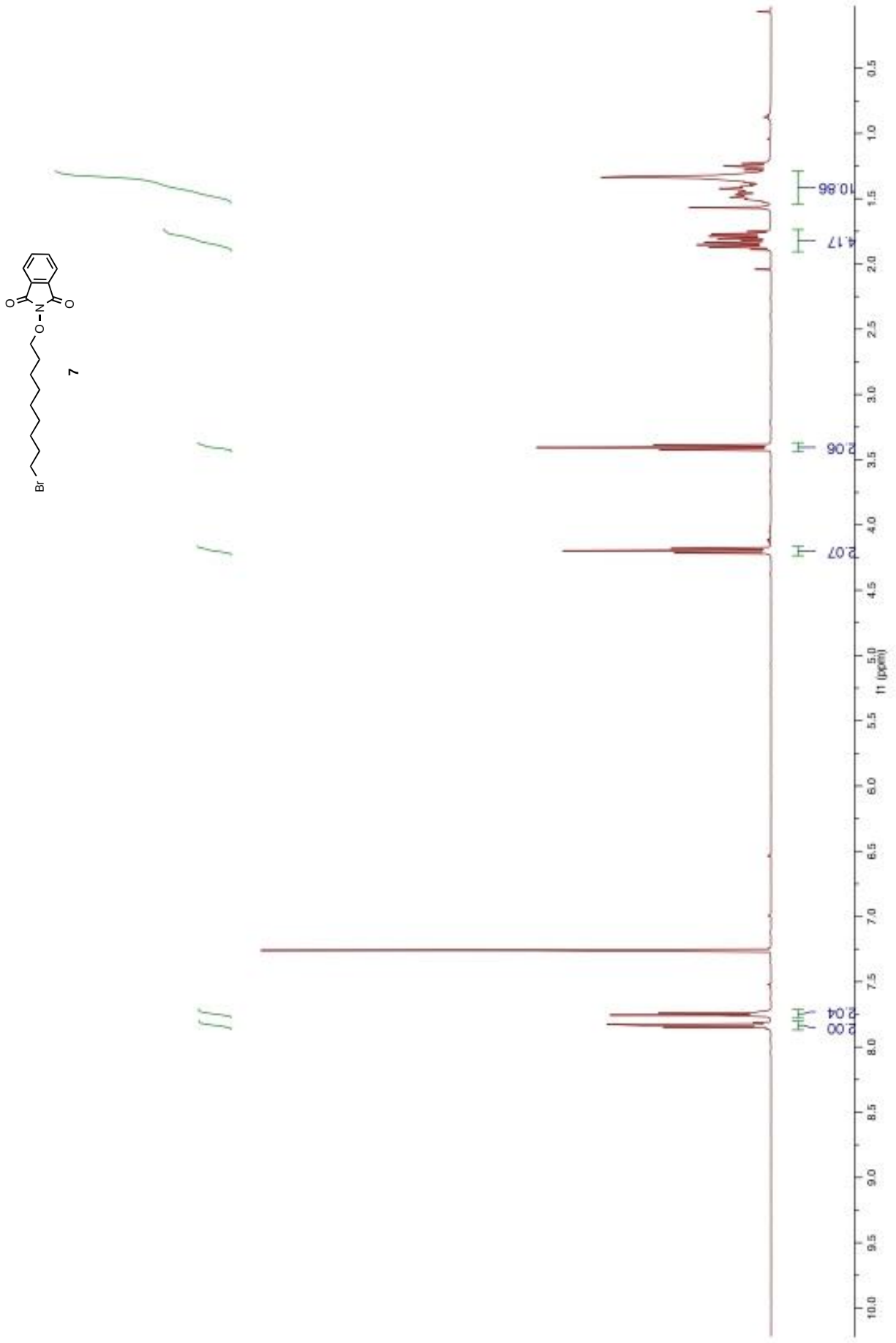
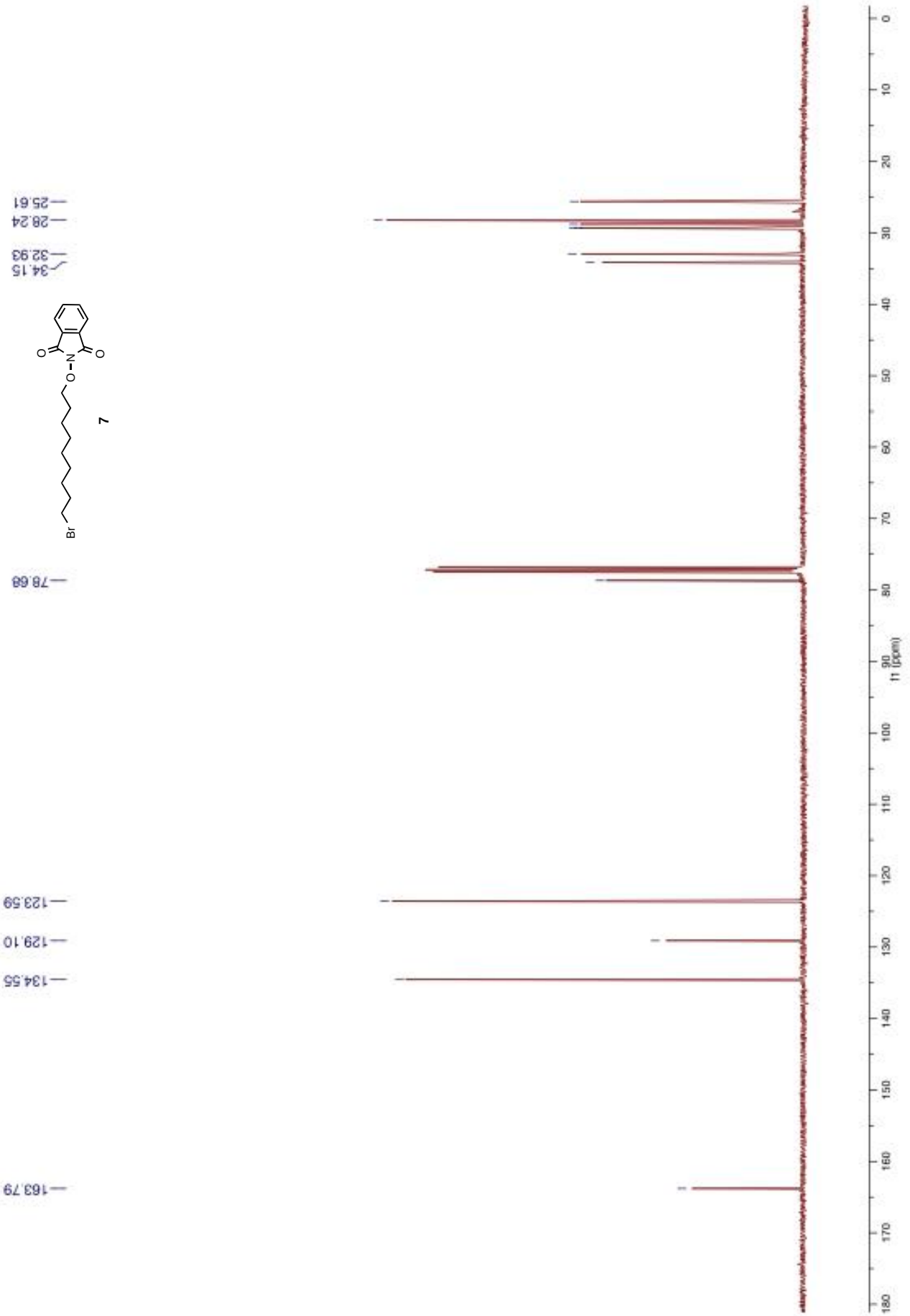
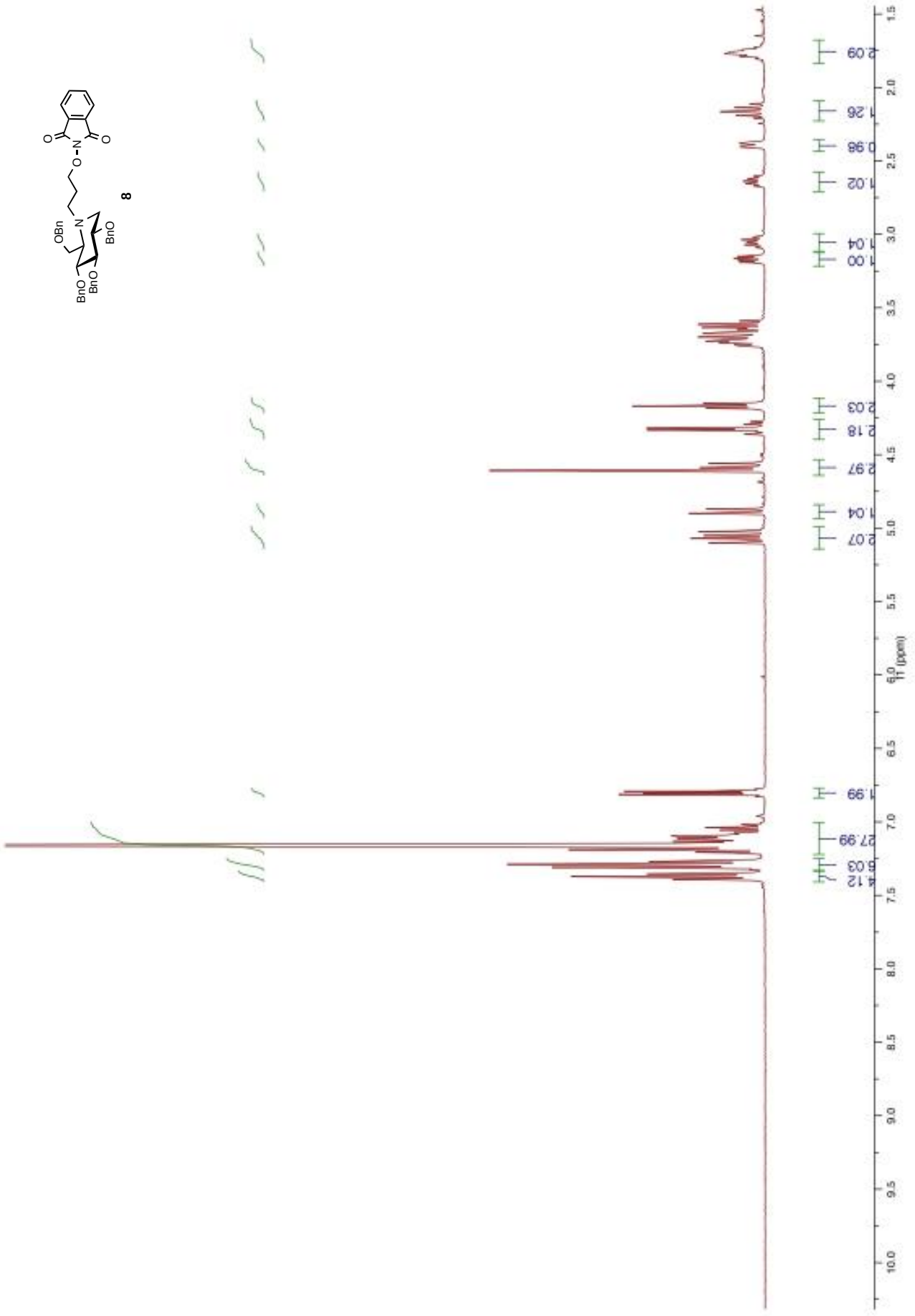
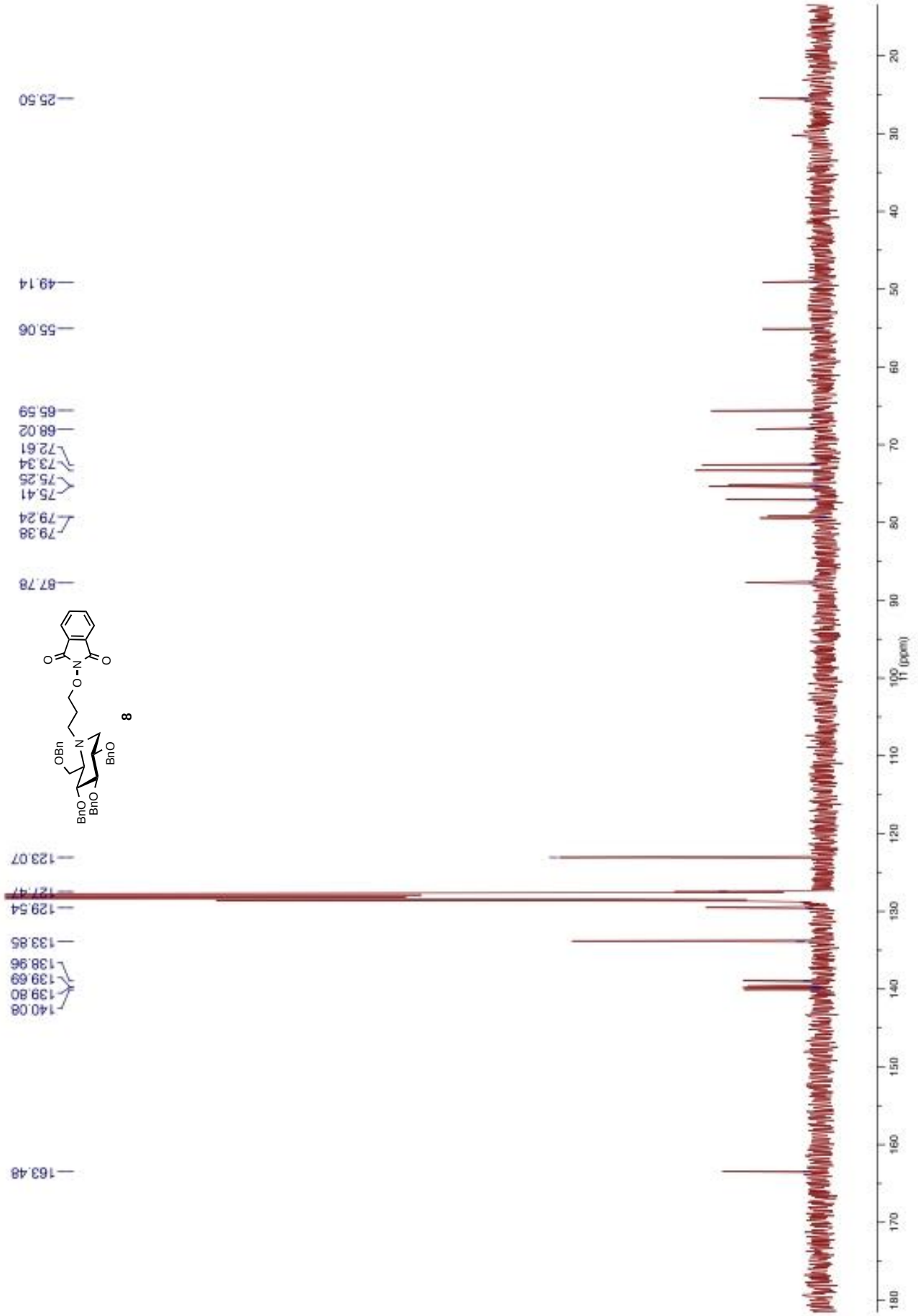


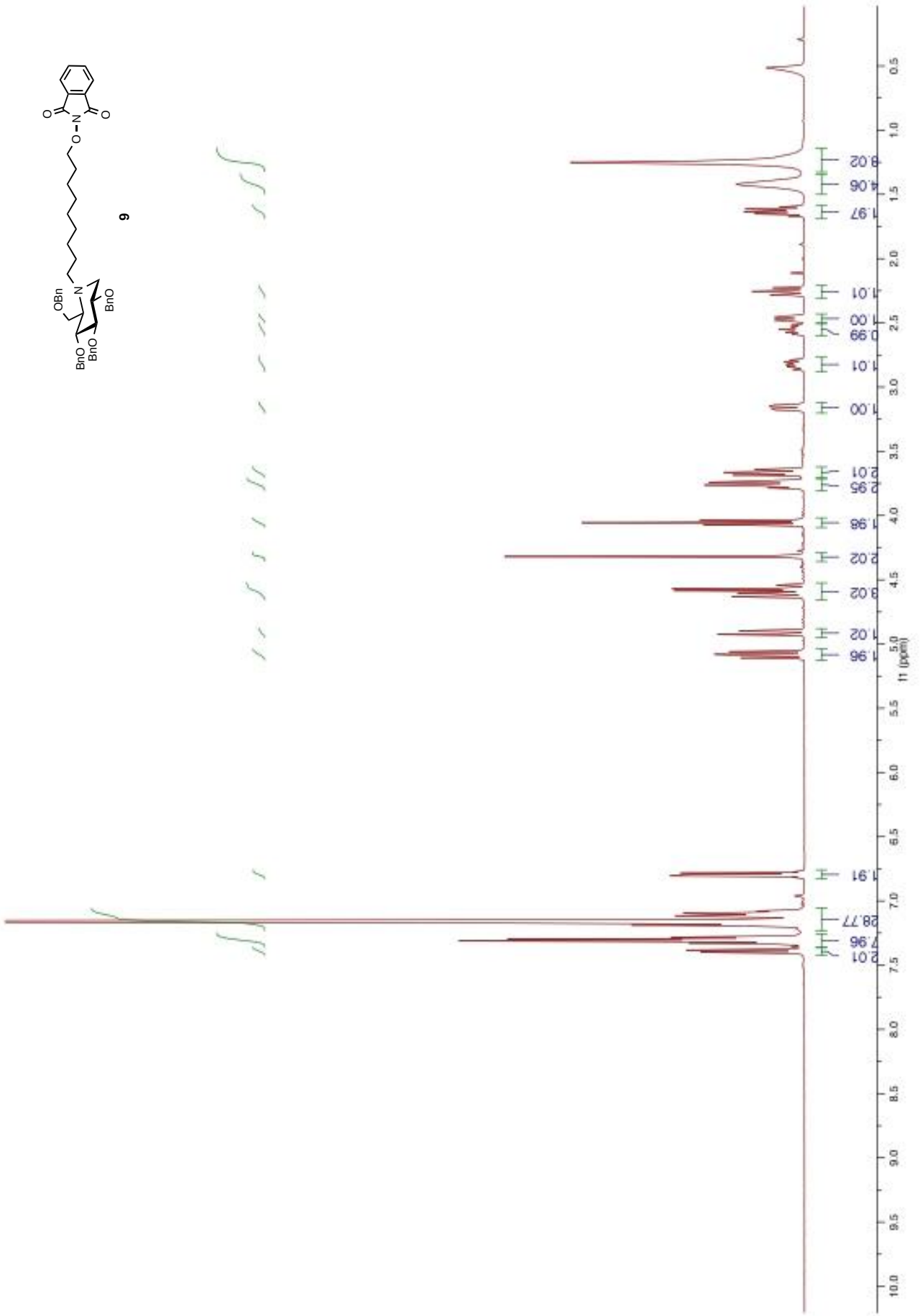
Figure S4. Lineweaver-Burk plot for K_i determination (1.3 ± 0.33 μM) of **17** against Jack bean α-mannosidase (pH 5.5).

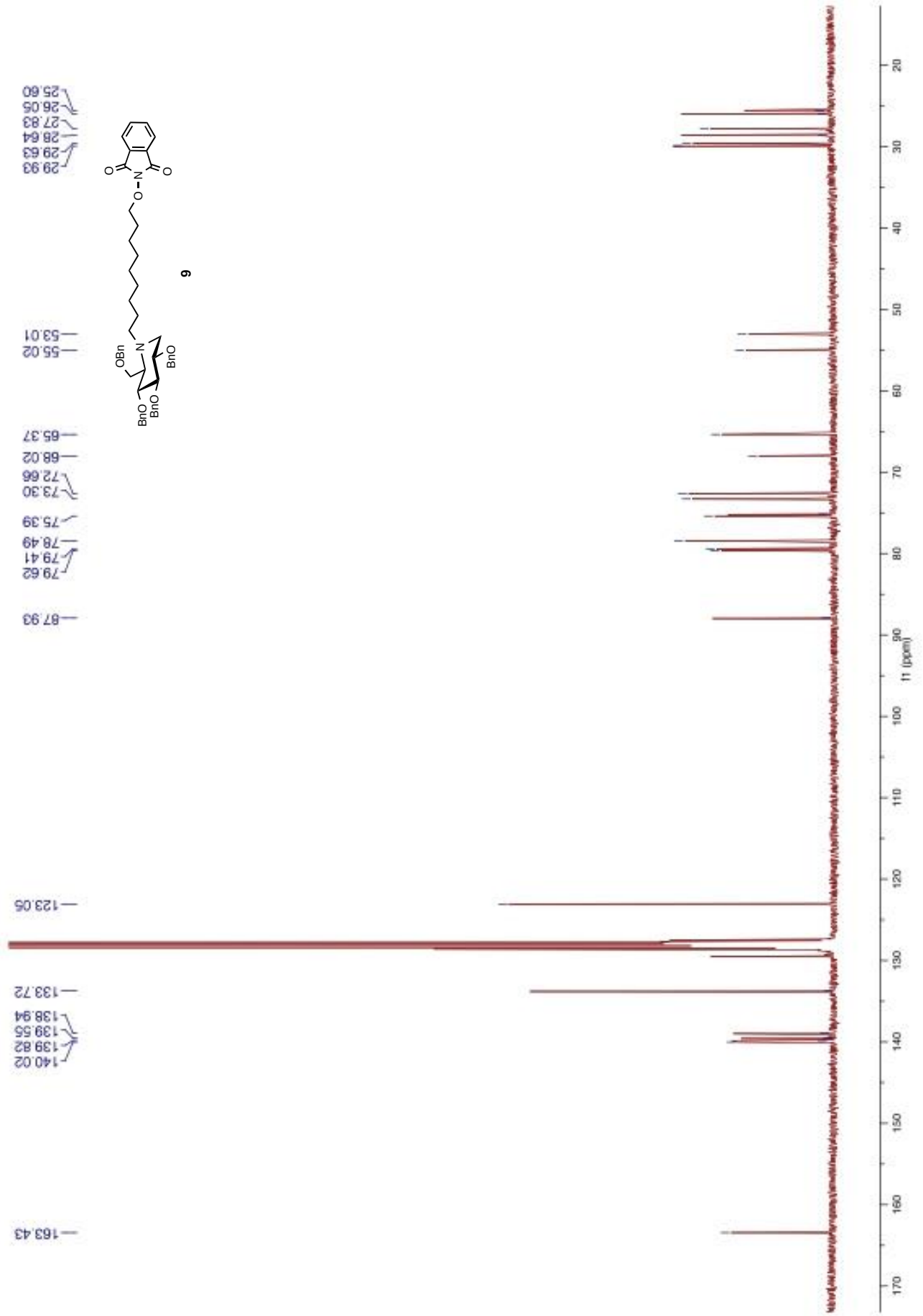

O
N
O
O
O
Br
7
10.86
4.17
2.06
2.07
2.00
2.04
f1 (ppm)


25.61
28.24
32.93
34.15
78.68
123.59
129.10
134.55
163.79
7
Br
O
N
O
O
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
f1 (ppm)


8
OBn
BnO
BnO
BnO
f1 (ppm)


25.50
49.14
55.06
65.59
68.02
72.61
73.34
75.25
75.41
79.24
79.38
87.78
123.07
127.47
129.54
133.85
138.96
139.69
139.80
140.08
163.48
8
f1 (ppm)


9
OBn
BnO
BnO
BnO
8.02
4.06
1.97
1.01
1.00
0.99
1.01
1.00
2.01
2.95
1.98
2.02
3.02
1.02
1.96
1.91
28.77
7.96
2.01
f1 (ppm)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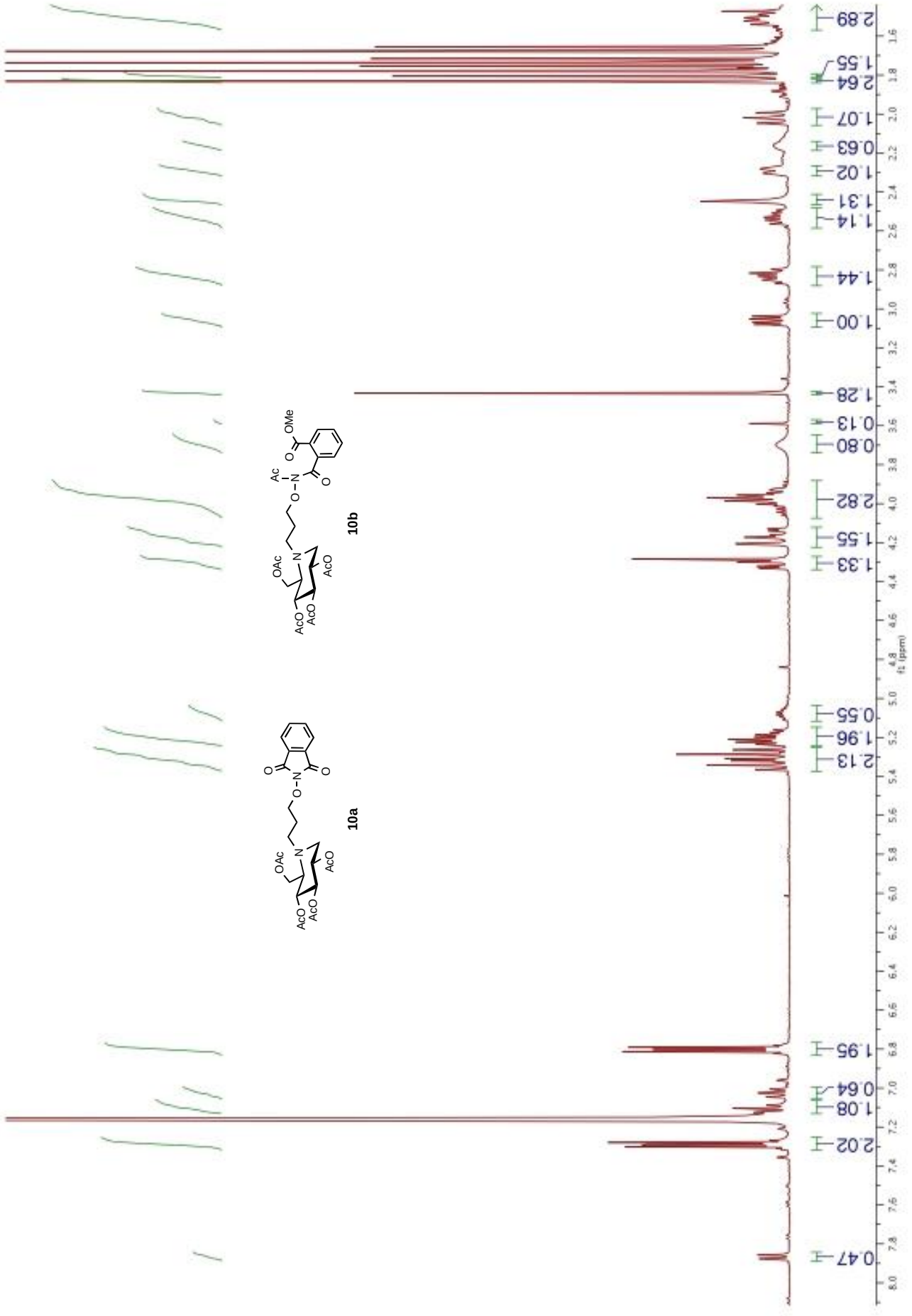
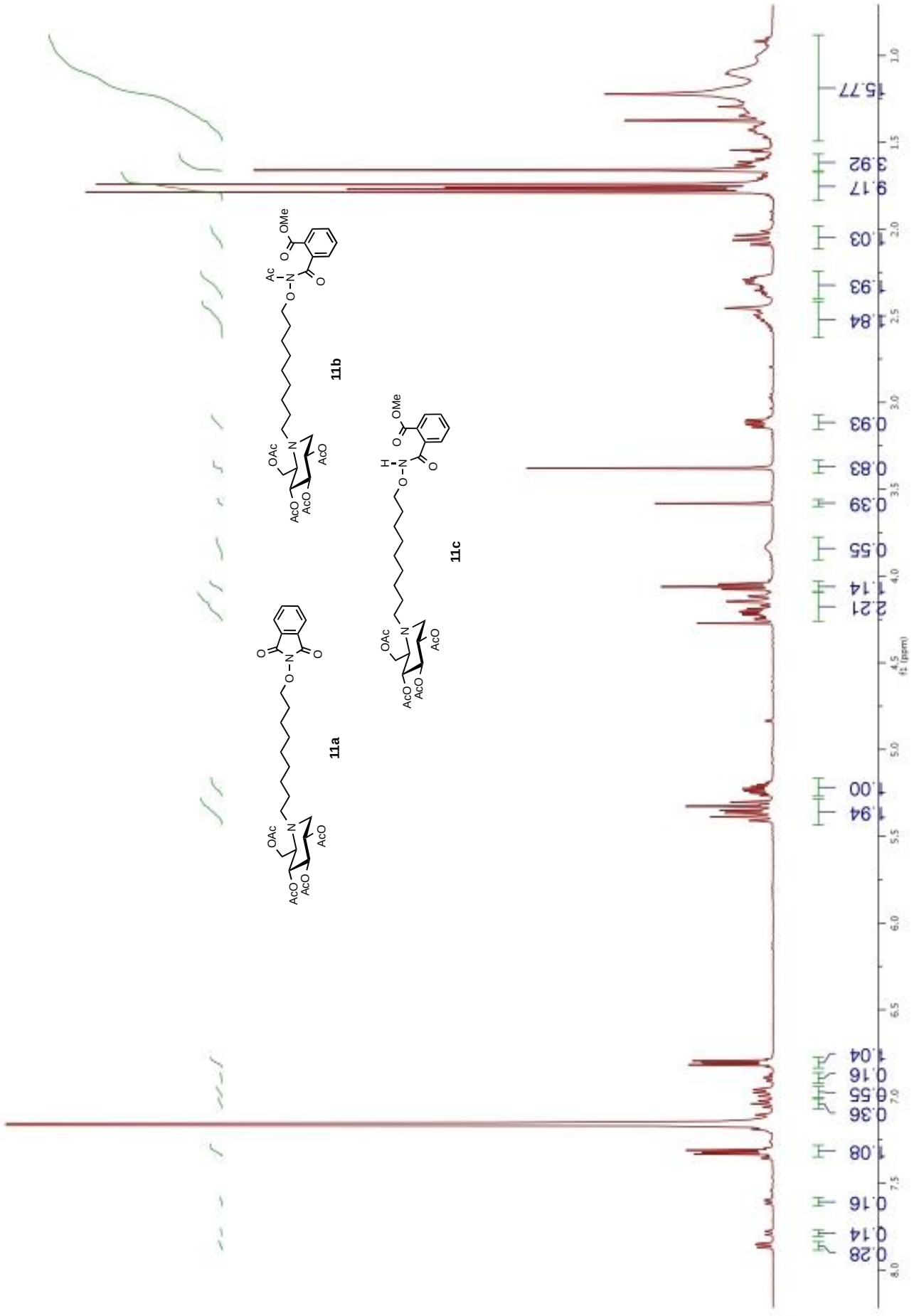
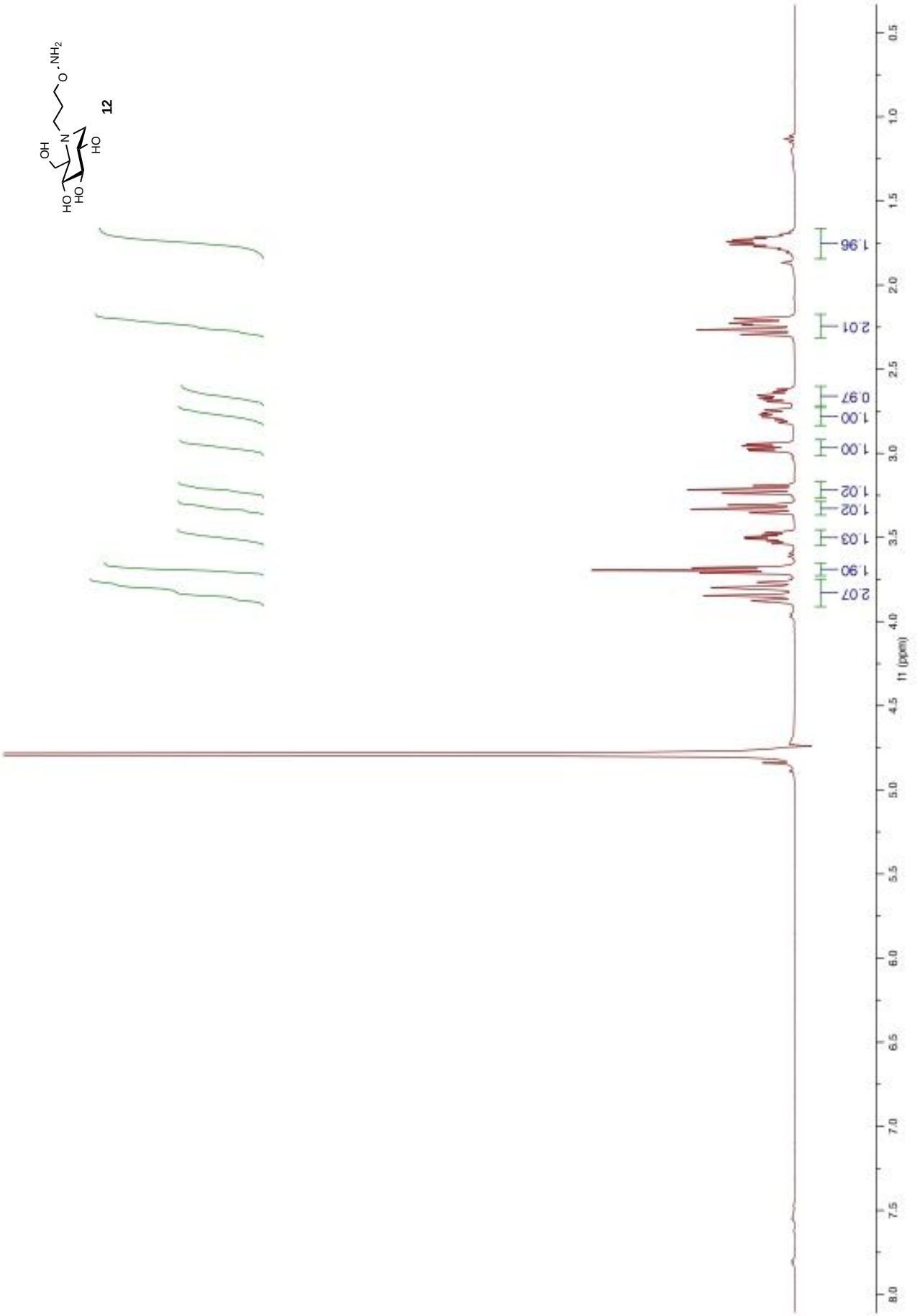
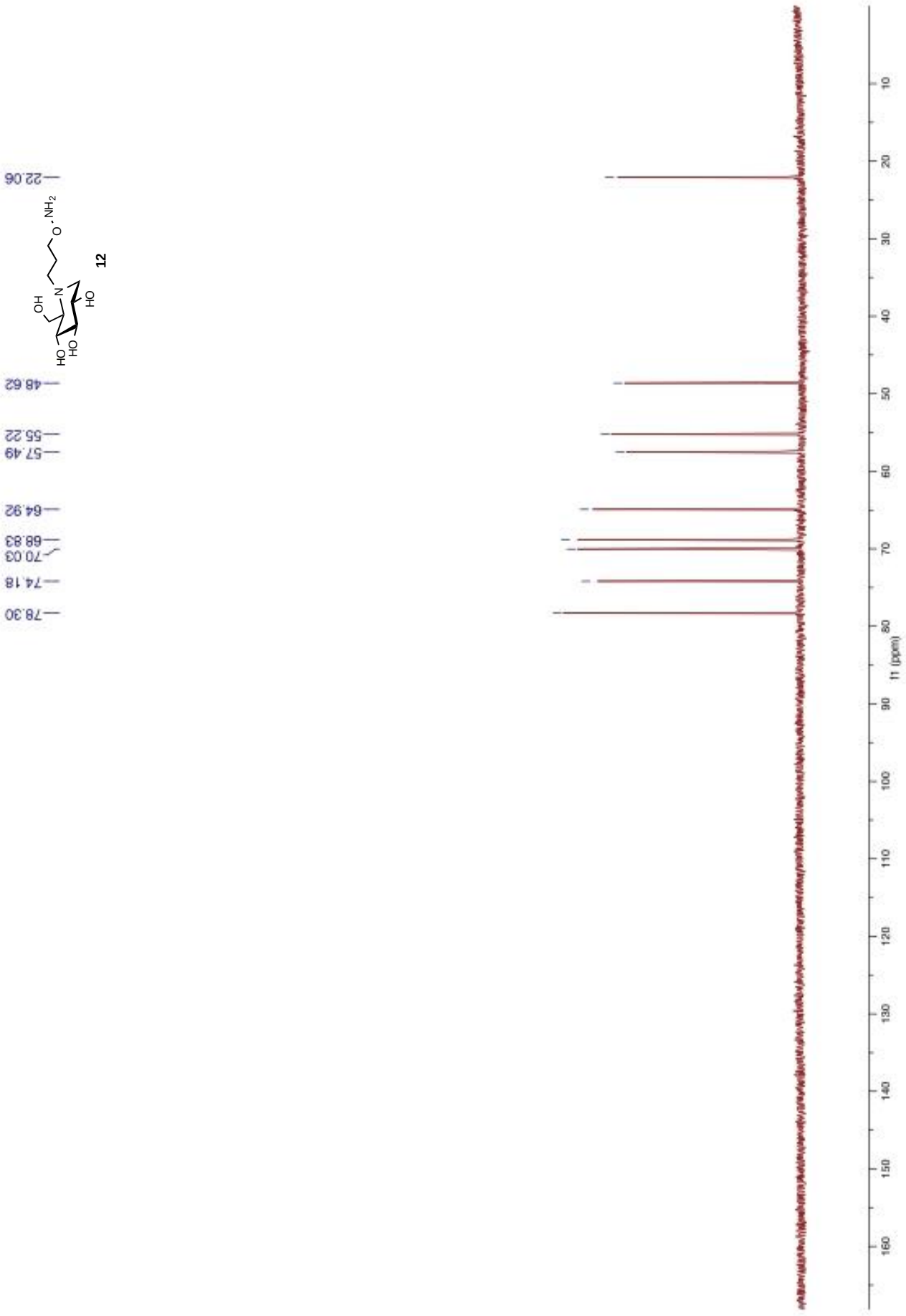
139.82
139.55
138.94
133.72
123.05
87.93
79.62
79.41
78.49
75.39
73.30
72.66
68.02
65.37
55.02
53.01
29.93
29.63
28.64
27.83
26.05
25.60
OBn
BnO
BnO
BnO
N
O
N
O
O
O
6
f1 (ppm)


2.89
1.55
2.64
1.07
0.63
1.02
1.31
1.14
1.44
1.00
1.28
0.13
0.80
2.82
1.55
1.33
0.55
1.96
2.13
1.95
0.64
1.08
2.02
0.47
f1 (ppm)
10b
10a


11a
11b
11c
15.77
3.92
9.17
2.03
1.93
1.84
0.93
0.83
0.39
0.55
2.21
1.14
1.00
1.94
1.04
0.16
0.55
0.36
1.08
0.16
0.14
0.28
f1 (ppm)


12
OH
HO
HO
HO
N
O
NH2
1.96
2.01
0.97
1.00
1.00
1.02
1.02
1.03
1.90
2.07
f1 (ppm)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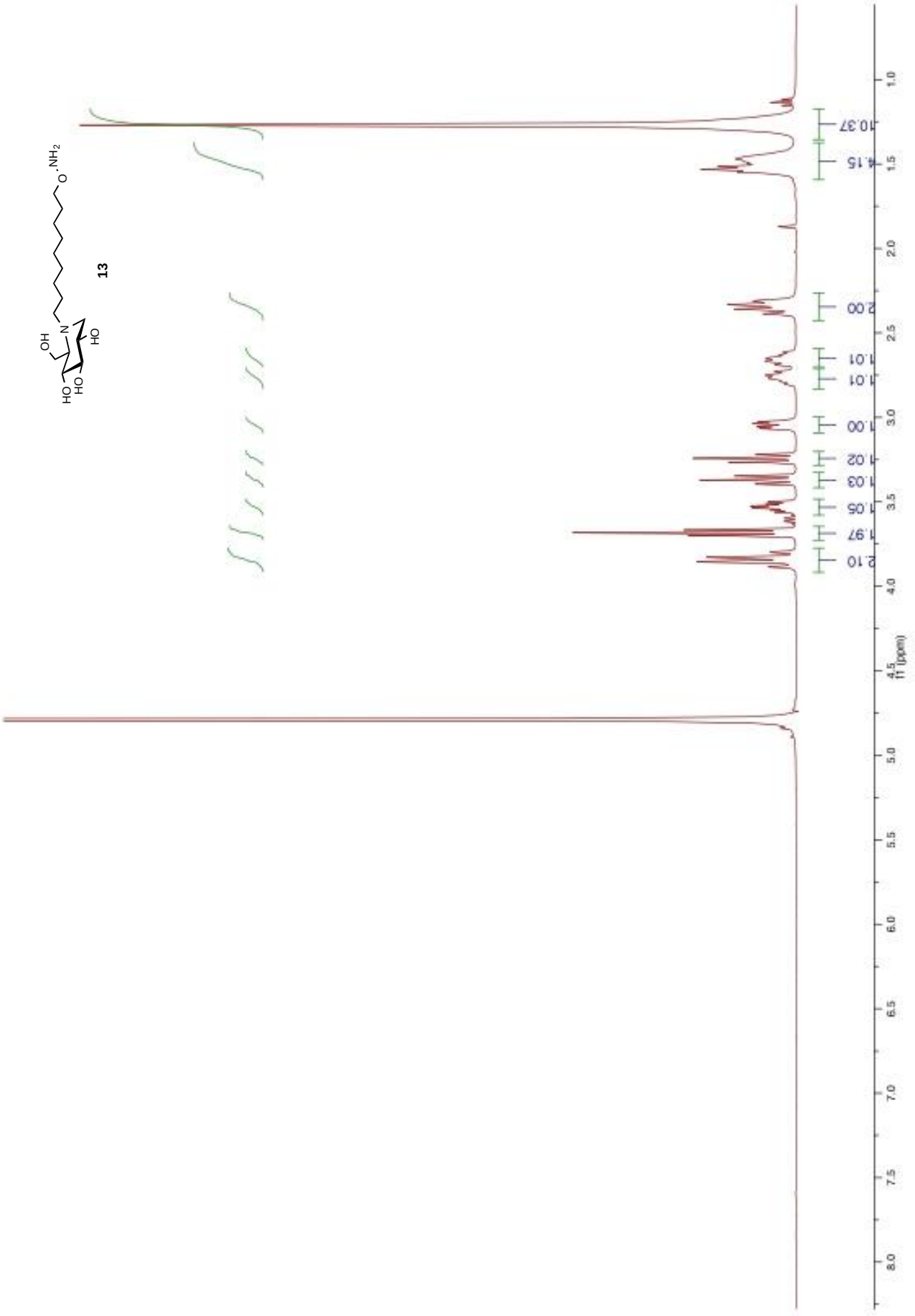
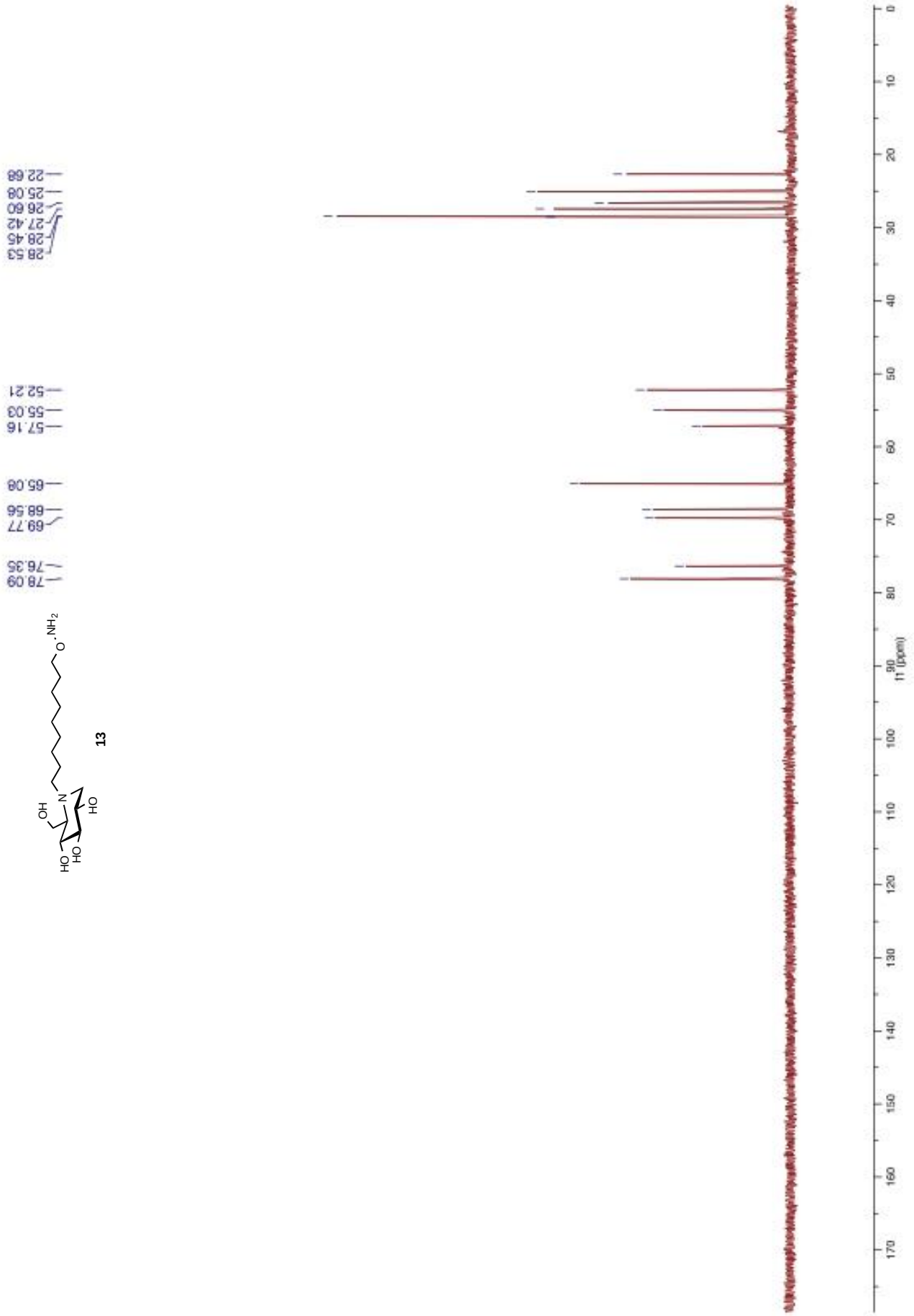
70.03
74.18
78.30
12
f1 (ppm)


13
OH
N
HO
HO
HO
HO
O
NH2
10.37
4.15
2.00
1.01
1.01
1.00
1.02
1.03
1.05
1.97
2.10
f1 (ppm)


22.68
25.08
26.60
27.42
28.45
28.53
52.21
55.03
57.16
65.08
68.56
69.77
76.35
78.09
13
f1 (ppm)

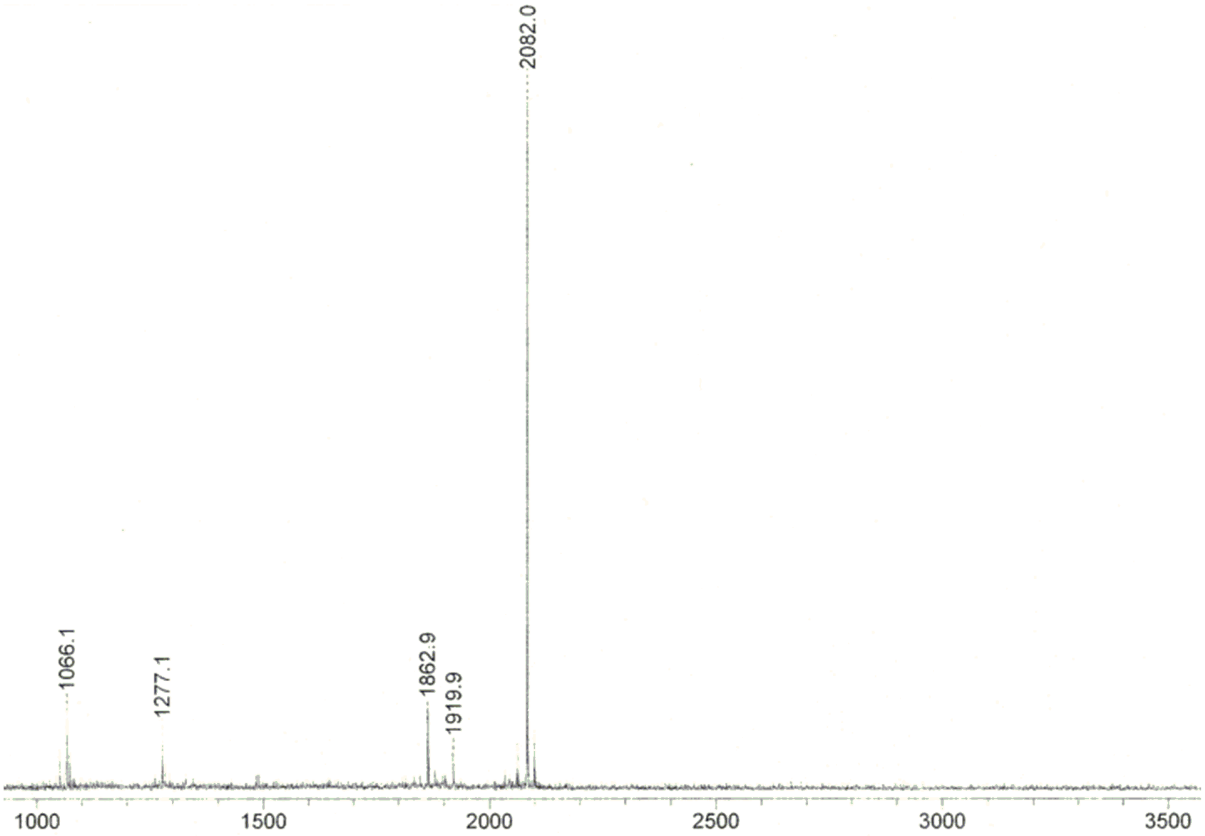


Figure S5. MALDI-TOF spectrum of the cyclic iminosugar cluster **14**.

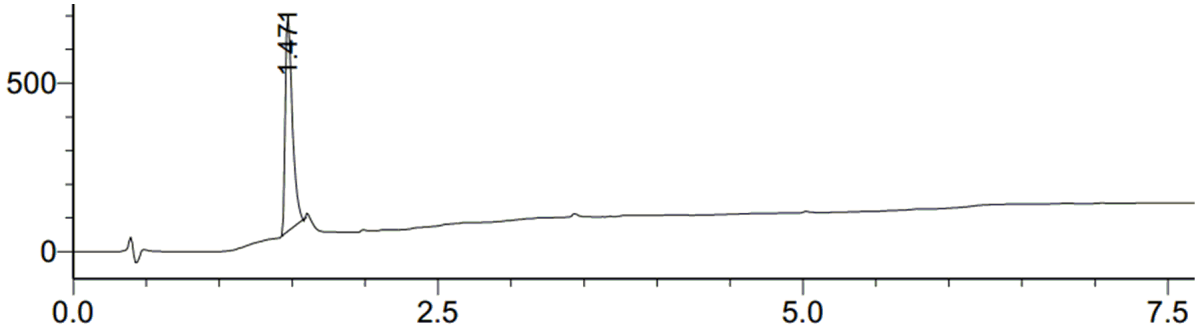


Figure S6. LC chromatogram of the cyclic iminosugar cluster **14**.

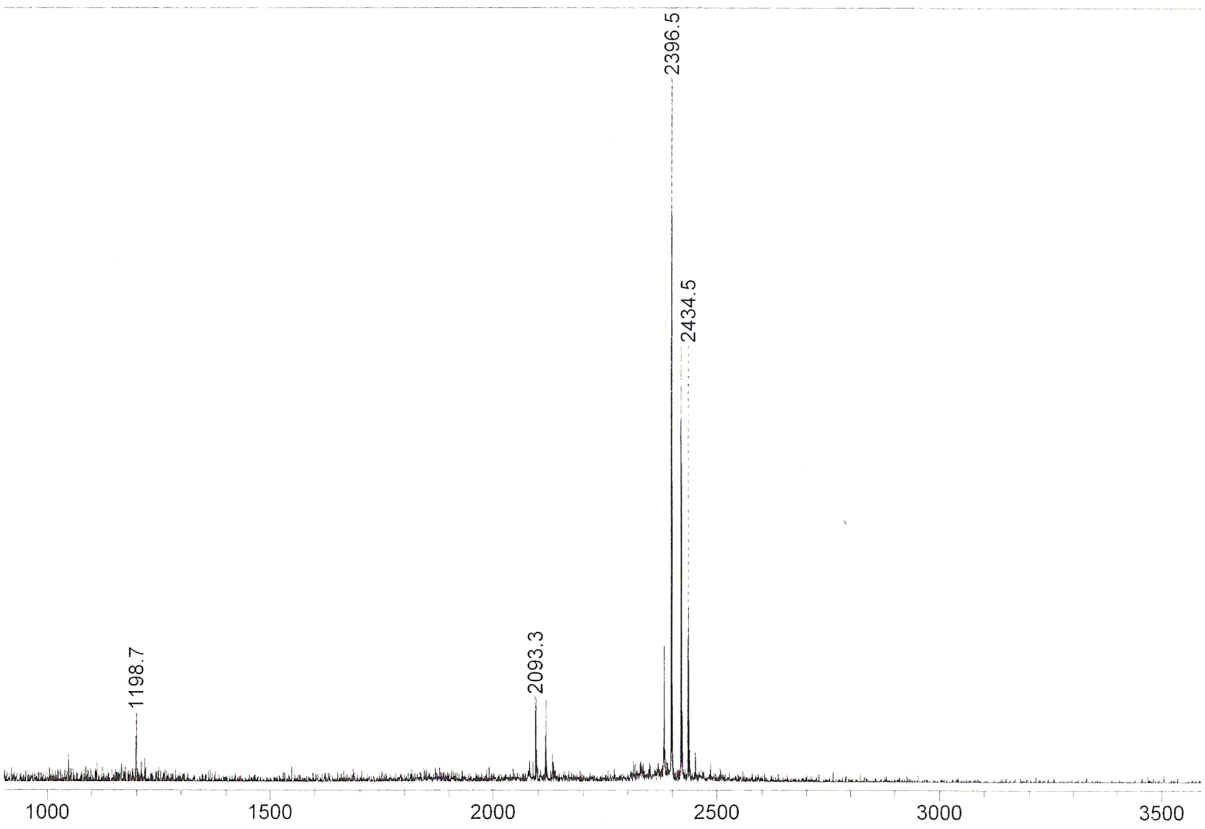


Figure S7. MALDI-TOF spectrum of the cyclic iminosugar cluster **15**.

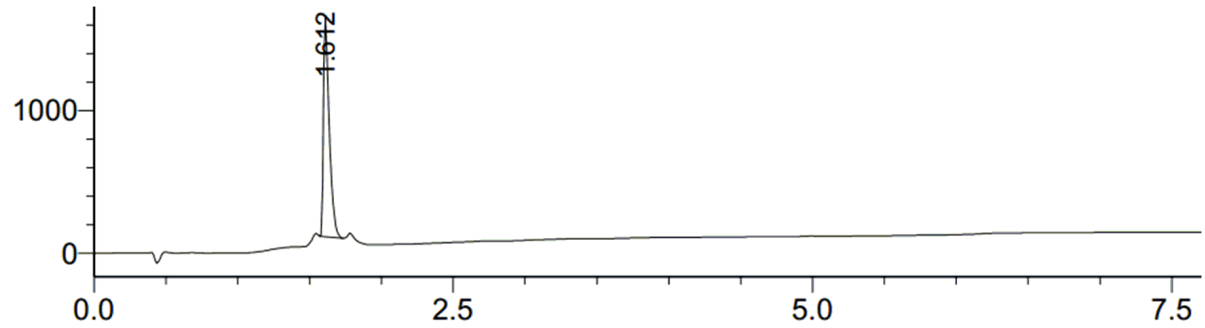


Figure S8. LC chromatogram of the cyclic iminosugar cluster **15**.

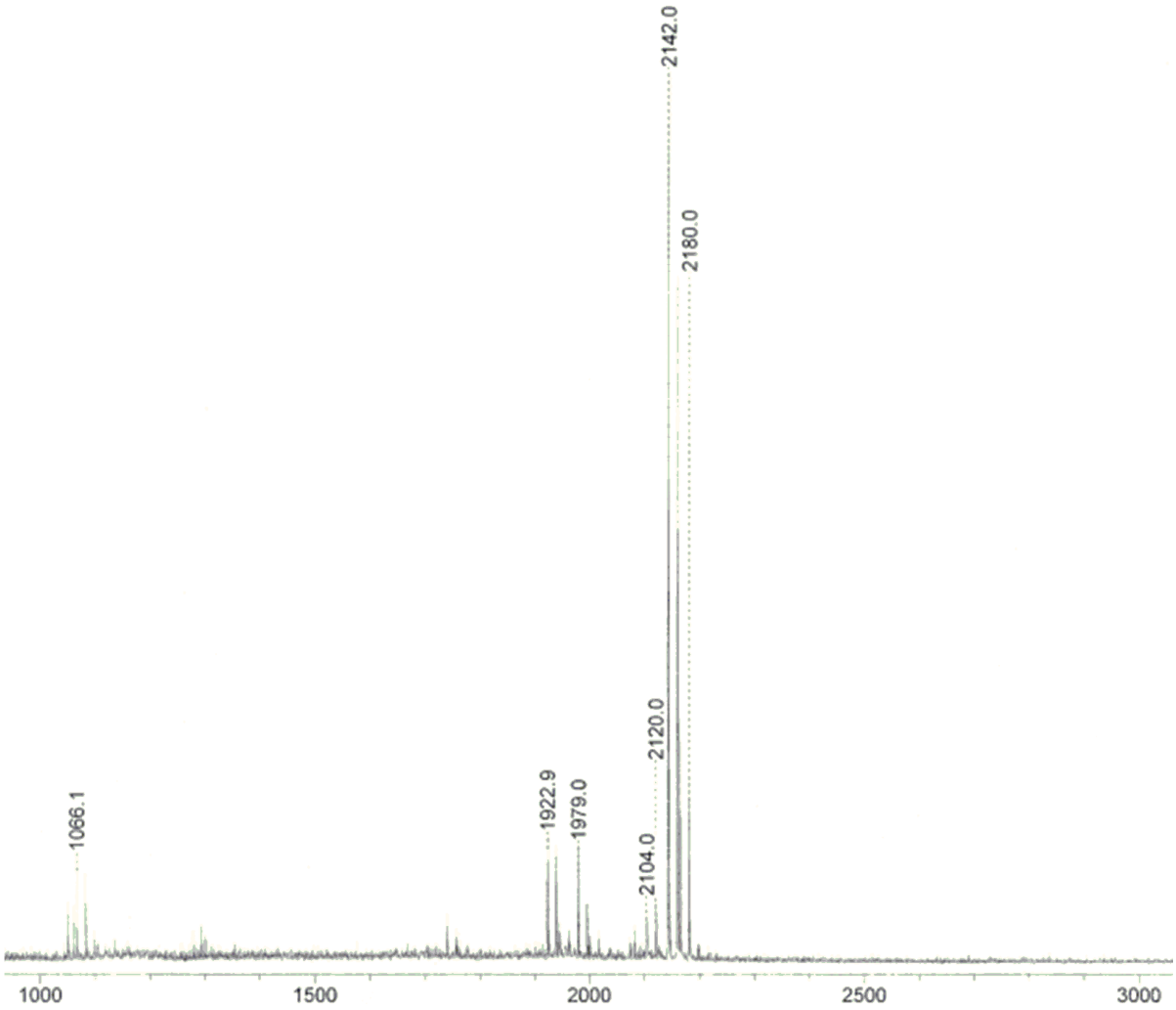


Figure S9. MALDI-TOF spectrum of the linear iminosugar cluster **16**.

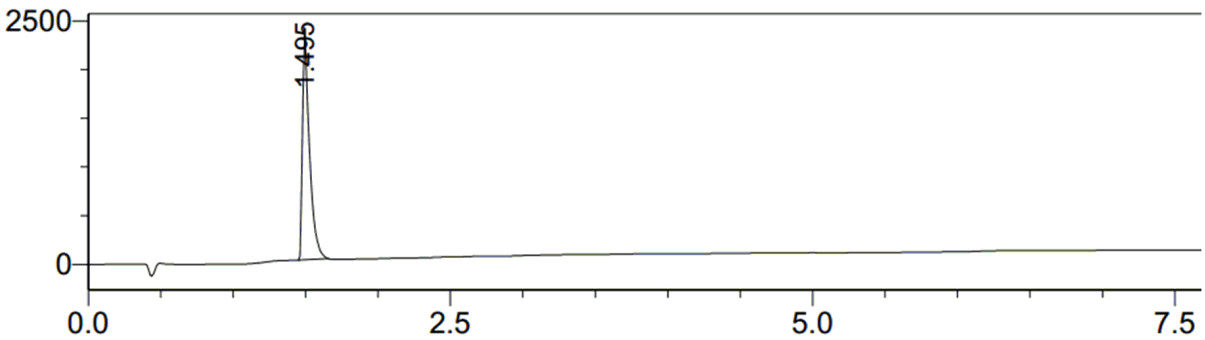


Figure S10. LC chromatogram of the linear iminosugar cluster **16**.

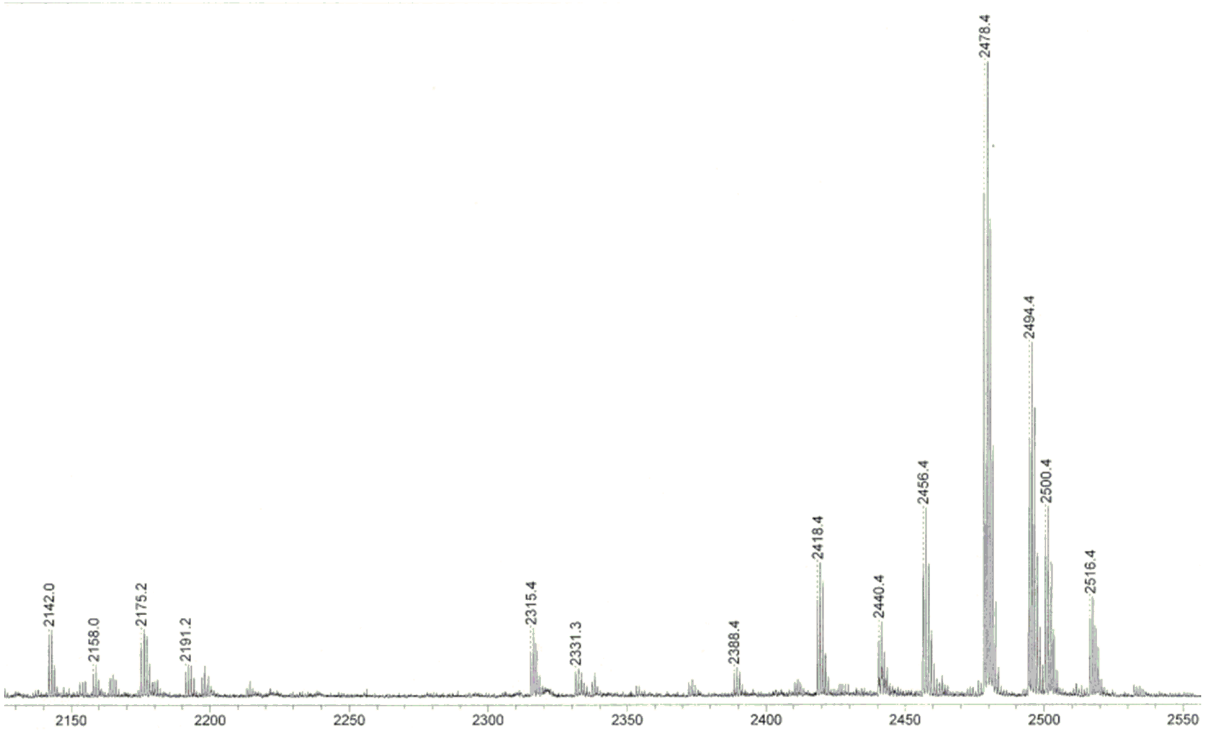


Figure S11. MALDI-TOF spectrum of the linear iminosugar cluster **17**.

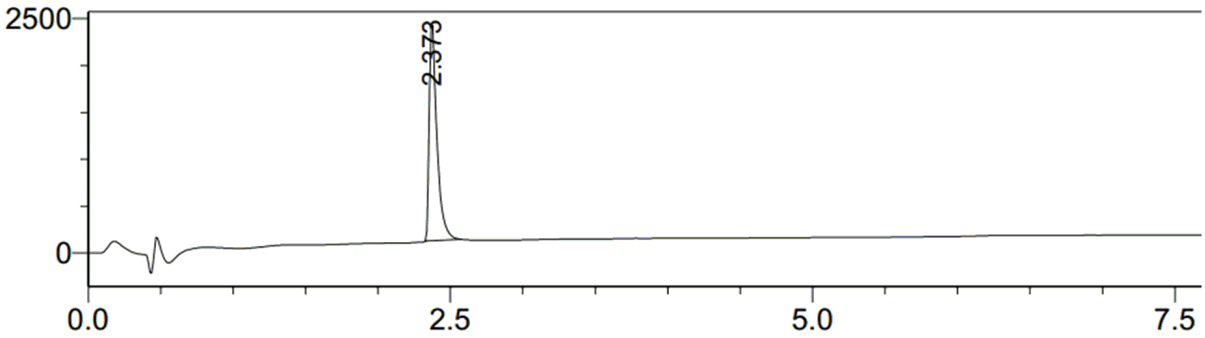


Figure S12. LC chromatogram of the linear iminosugar cluster **17**.