Supporting Information

for

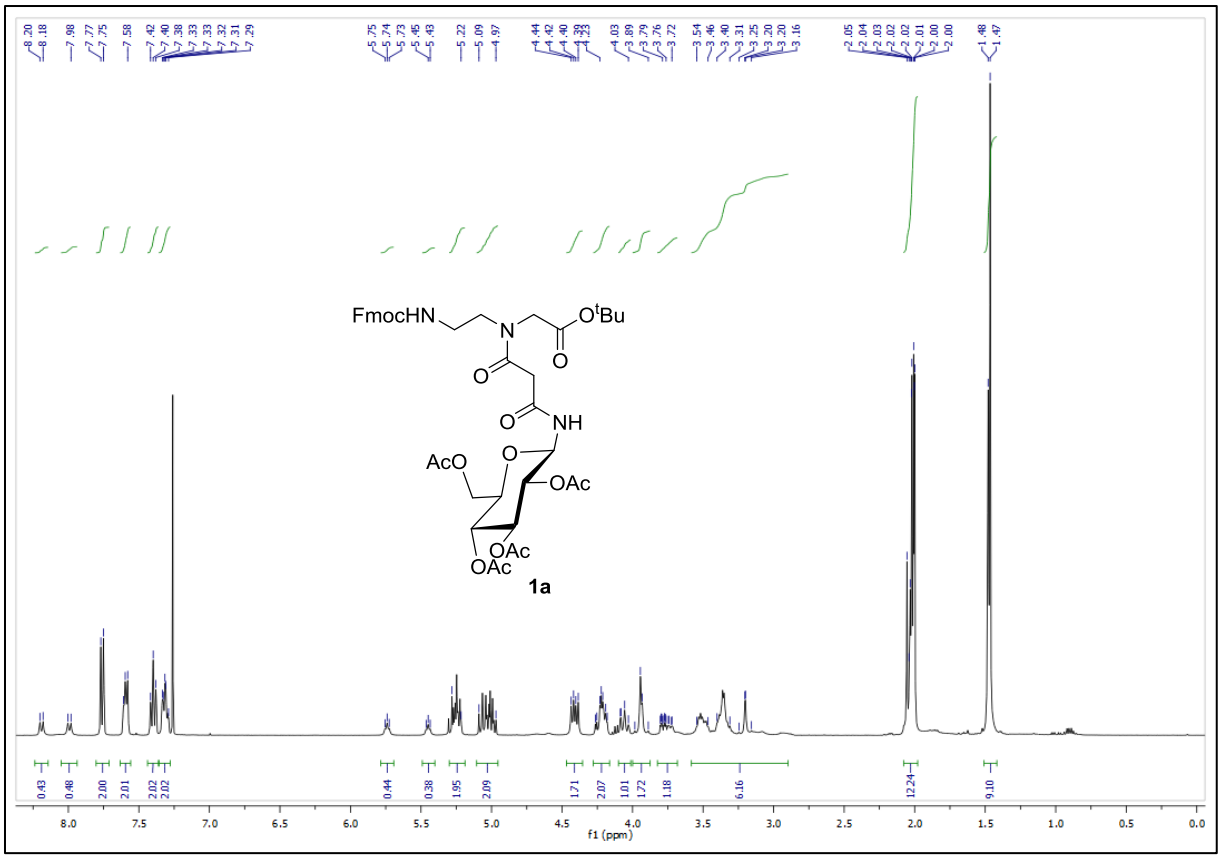
Synthesis and NMR-studies of malonyl-linked glycoconjugates of *N*-(2-aminoethyl)glycine. Building blocks for the construction of combinatorial glycopeptide libraries

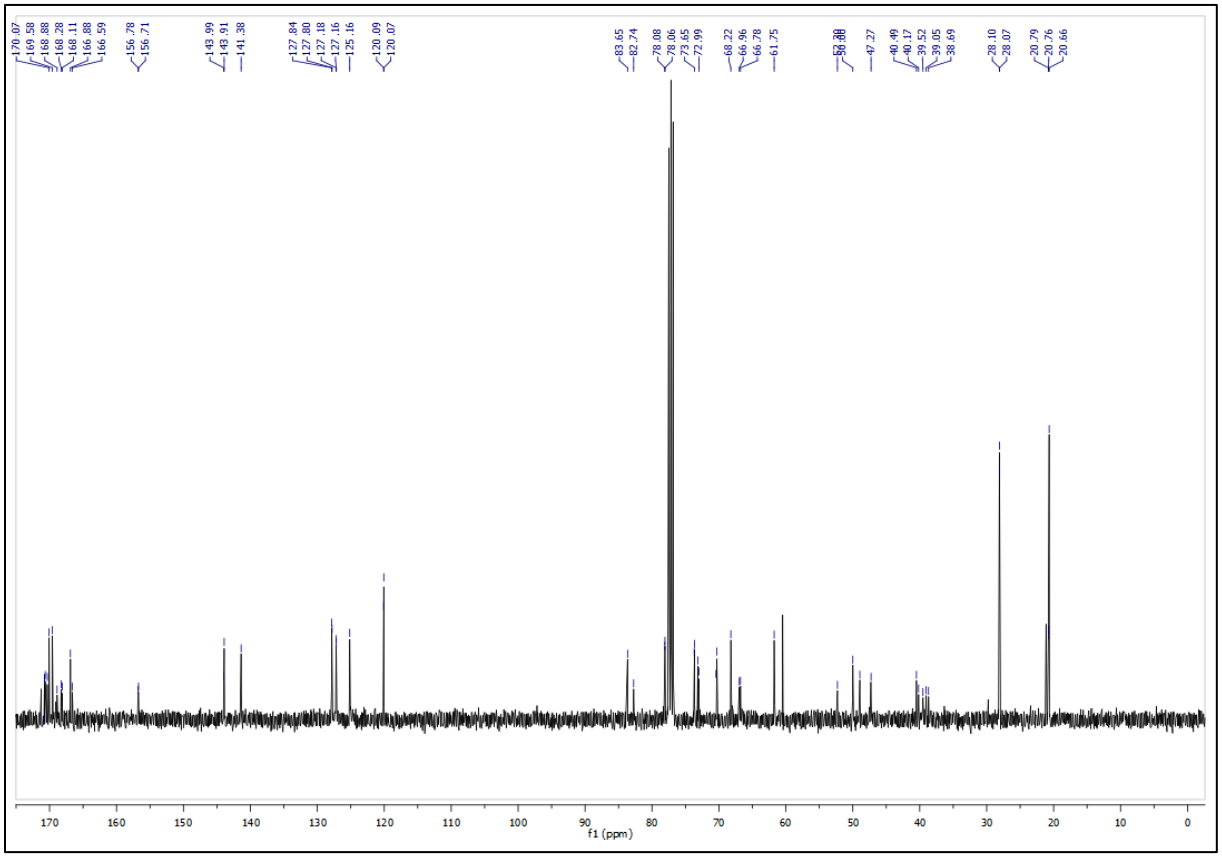
Markus Nörrlinger, Sven Hafner and Thomas Ziegler*

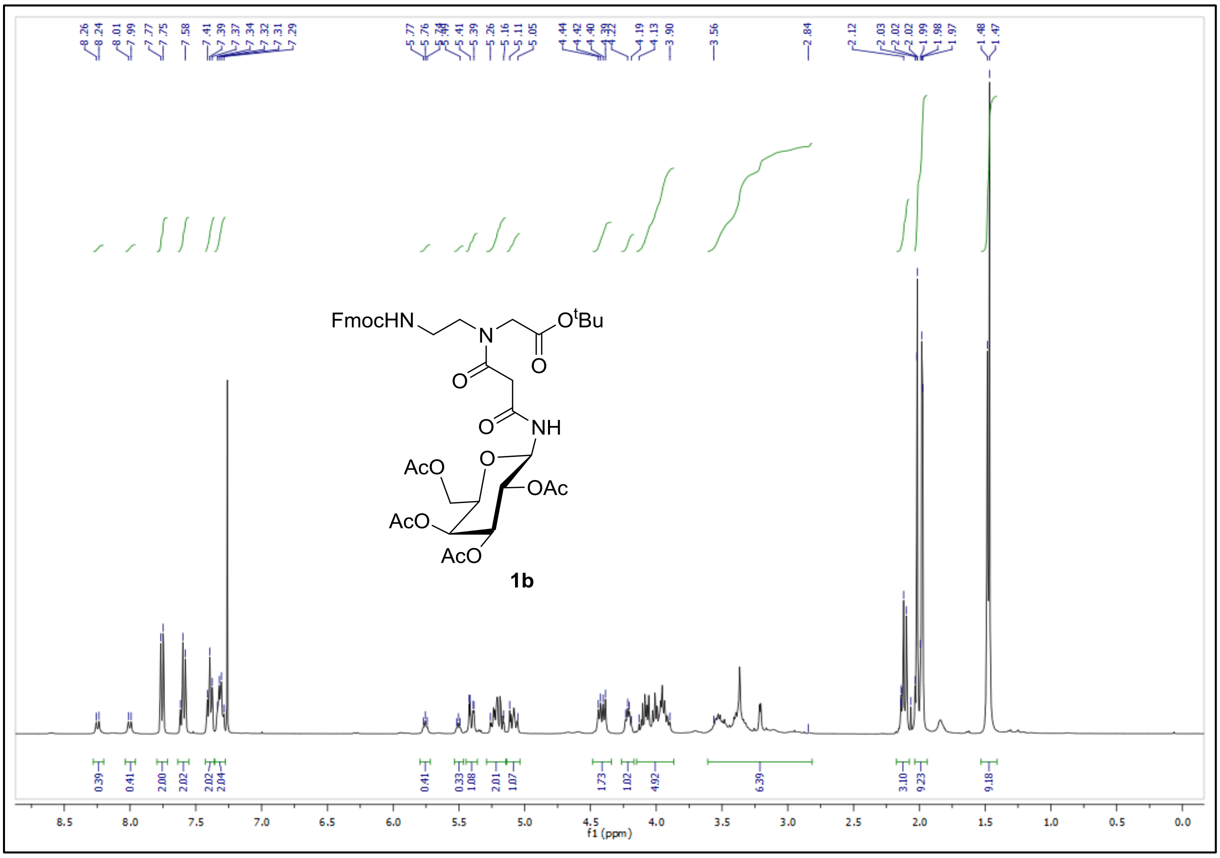
Address: Institute of Organic Chemistry, University of Tuebingen, Auf der Morgenstelle 18, 72076 Tuebingen, Germany

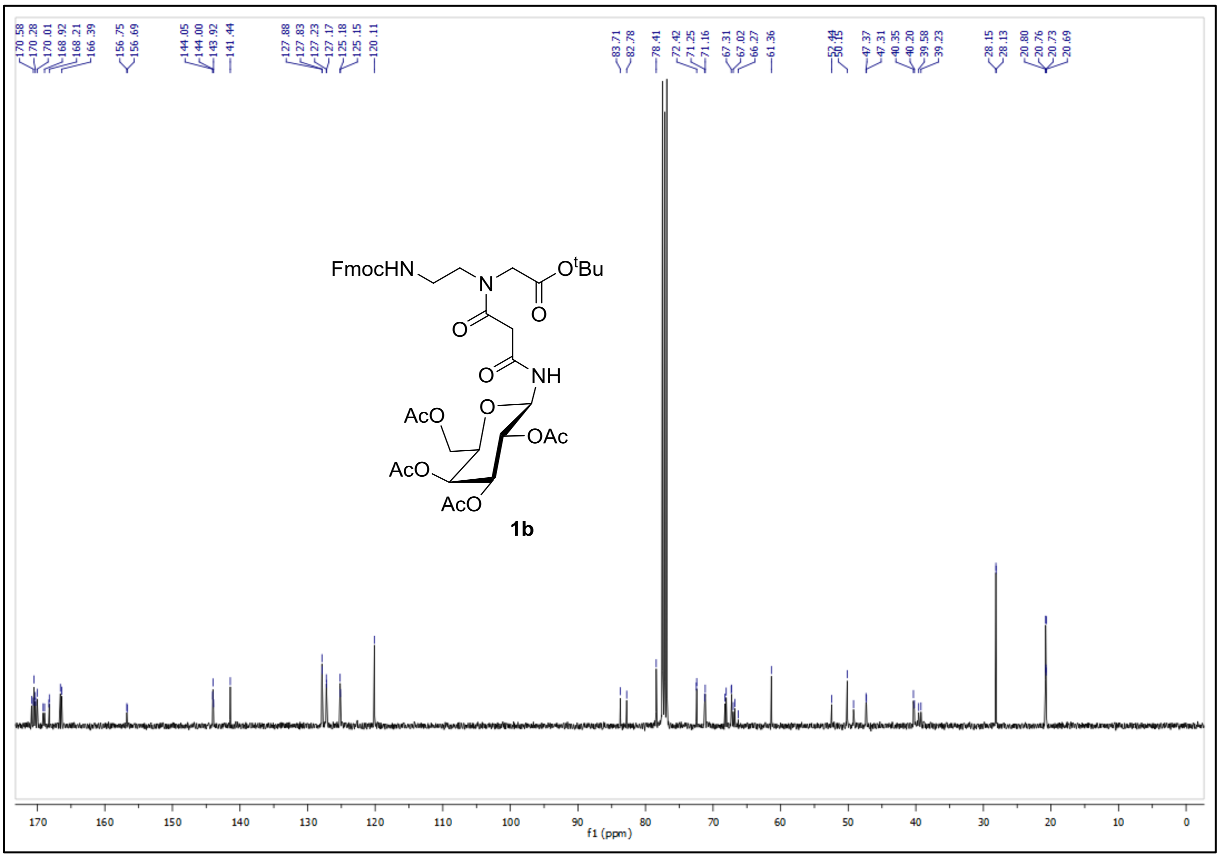
Email: Thomas Ziegler - thomas.ziegler@uni-tuebingen.de
*Corresponding author

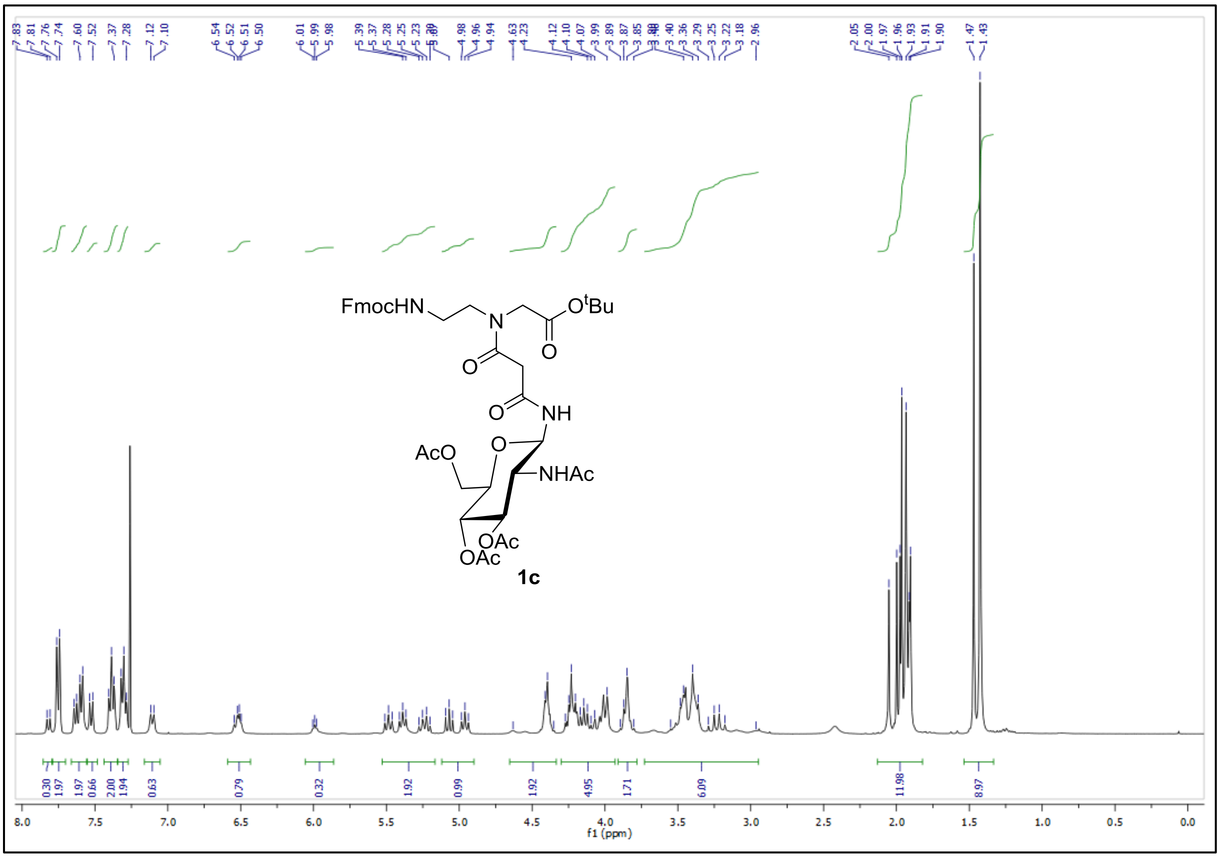
NMR spectra of building blocks 1a–d, 2a–d, 3, 4 and 7; 2D NMR spectra of building block 1a

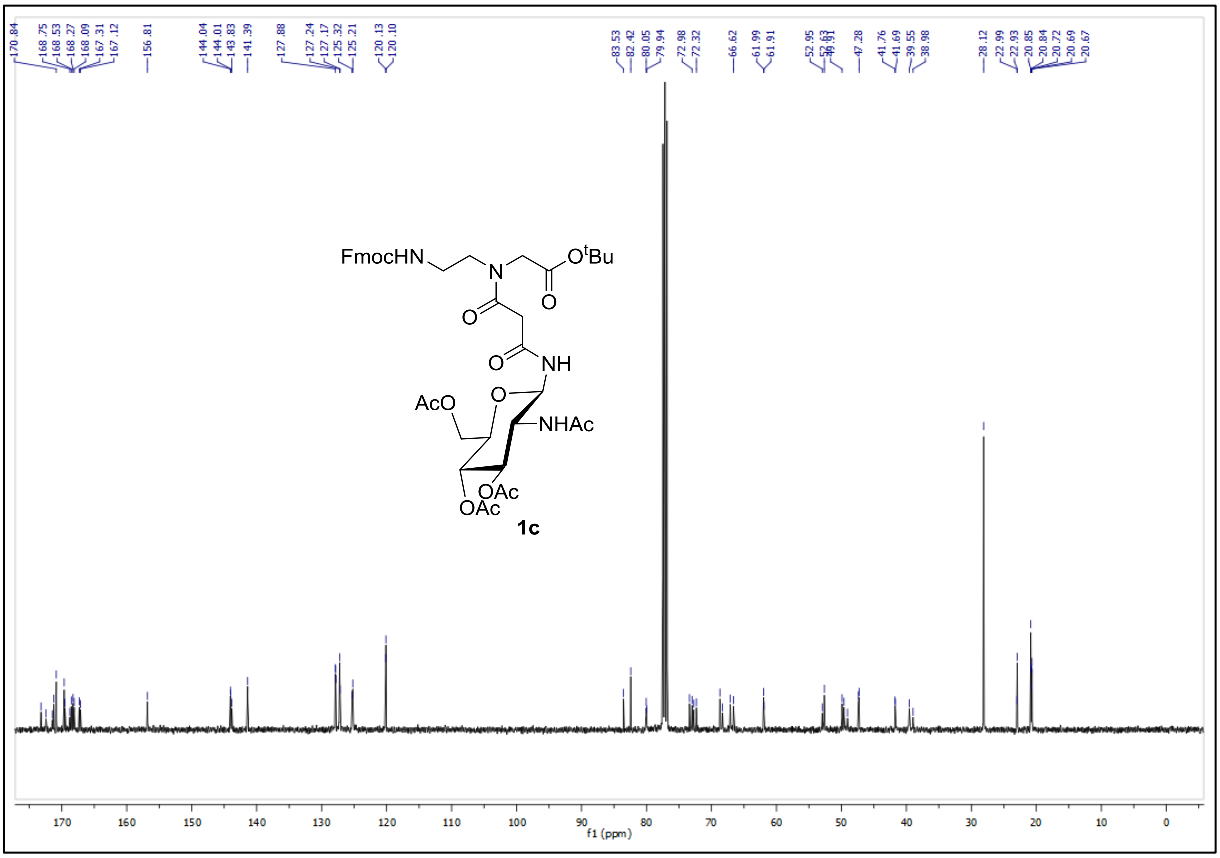

FmocHN
N
O
O
O
O
NH
O
AcO
OAc
OAc
OAc
O
O
tBu
1a
f1 (ppm)

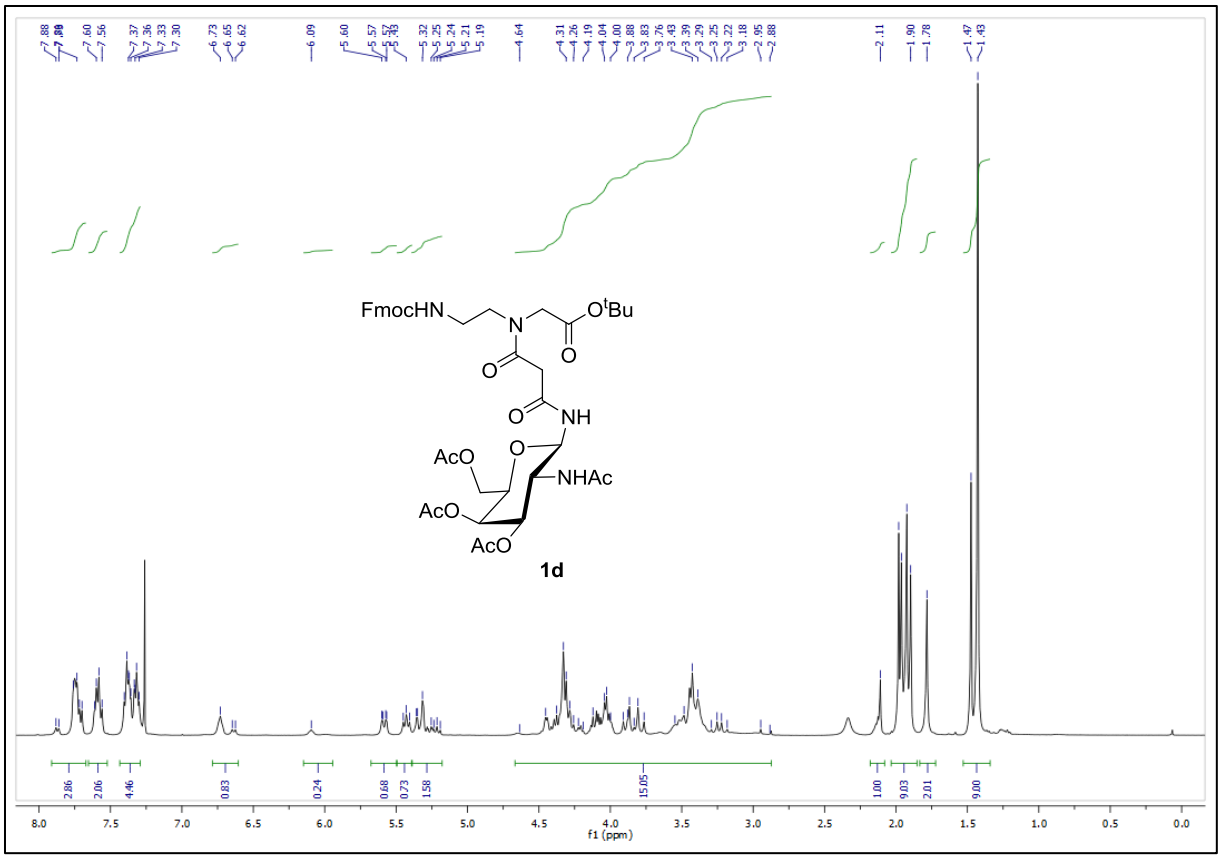

f1 (ppm)

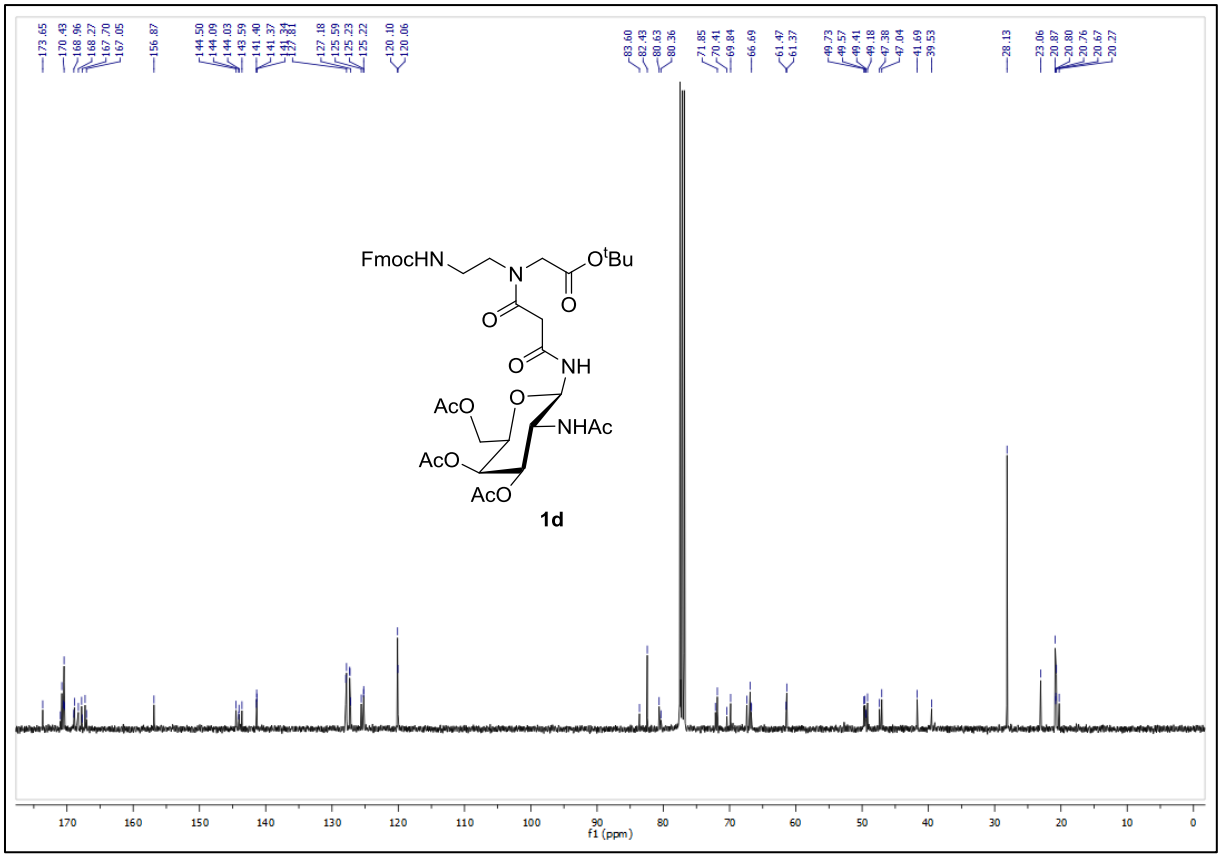


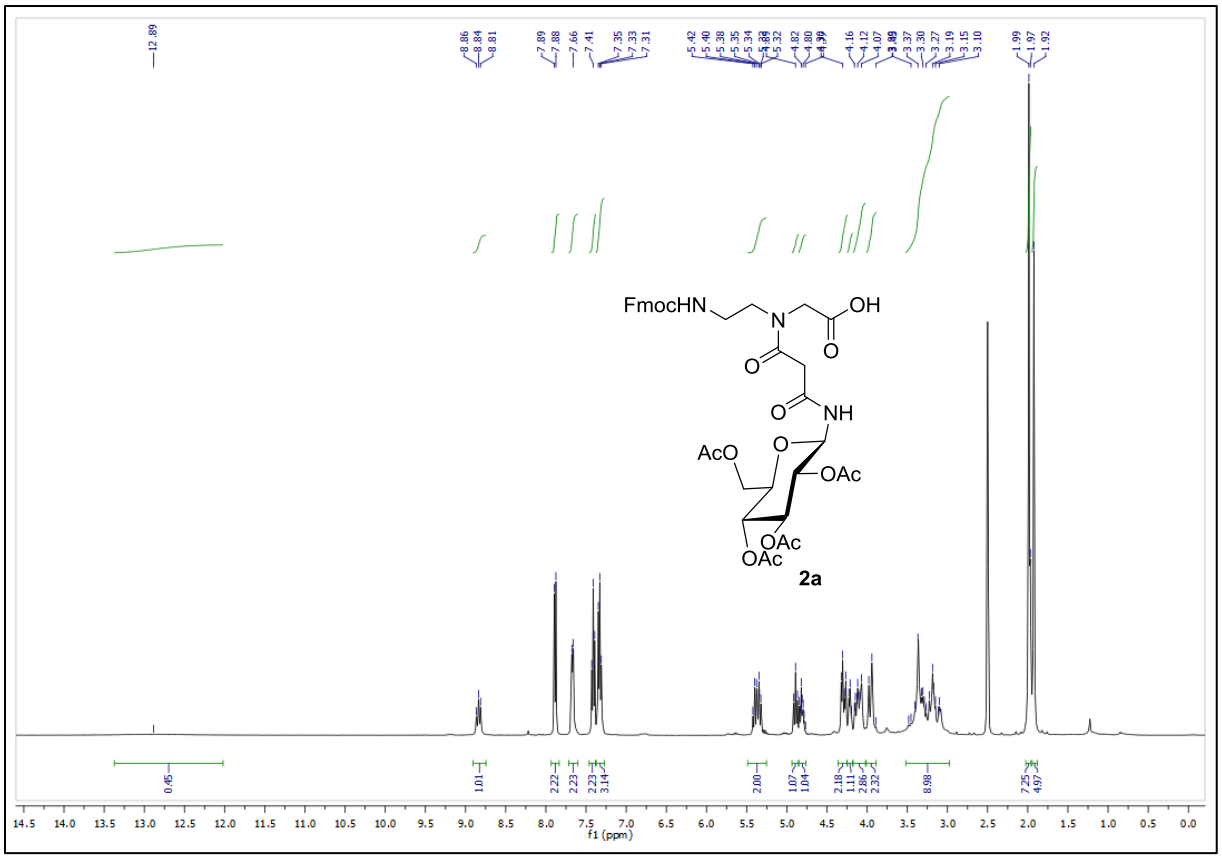


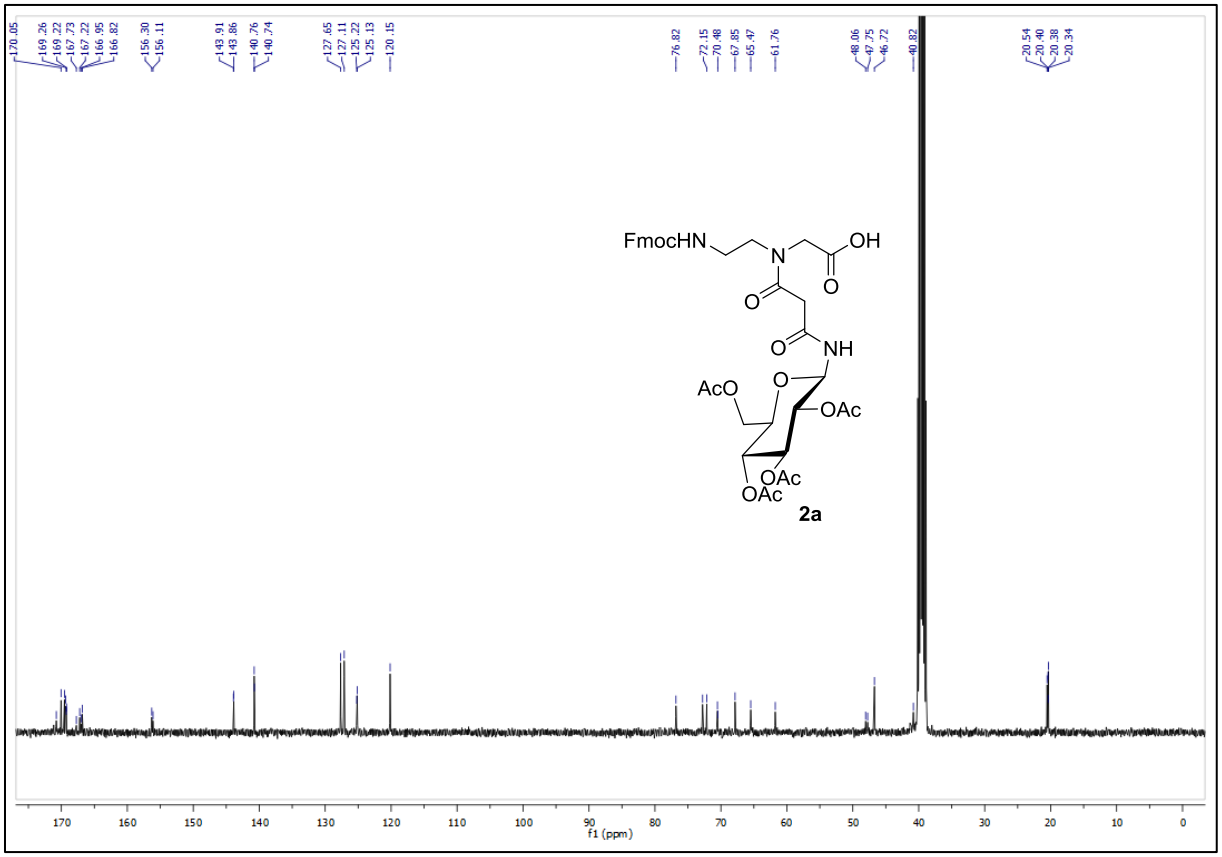

FmocHN
N
O^{t}Bu
O
O
O
NH
AcO
O
NHAc
OAc
OAc
1c
f1 (ppm)

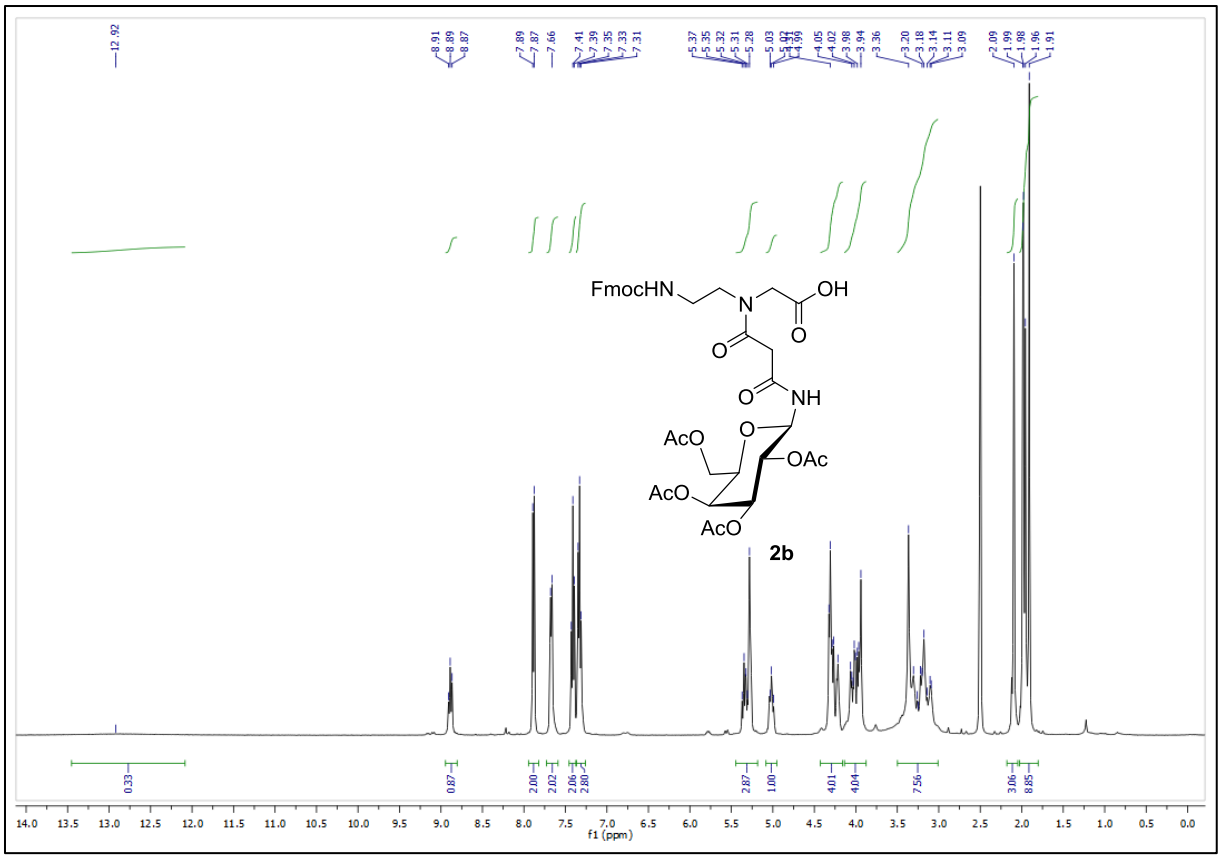

FmocHN
N
O^{t}Bu
O
O
O
NH
AcO
O
NHAc
OAc
OAc
1c
f1 (ppm)

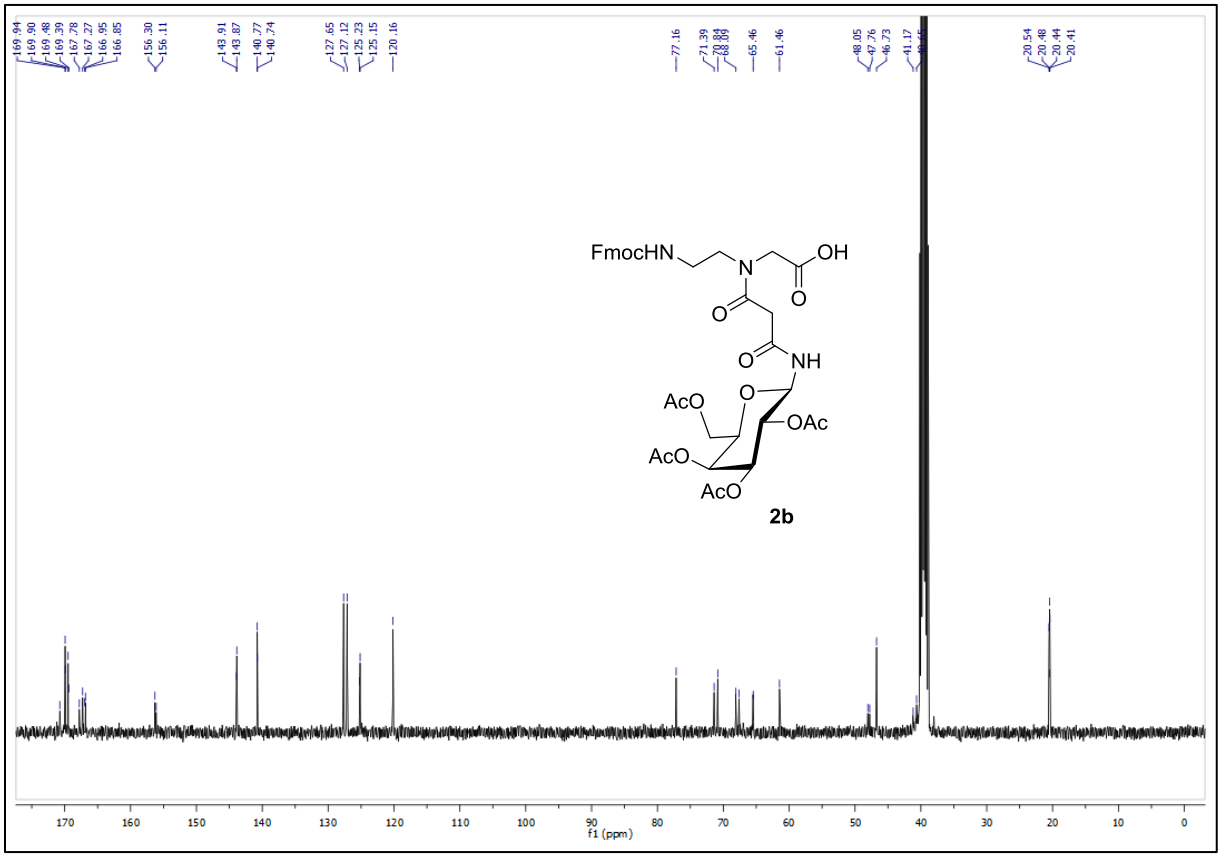

FmocHN
N
O
O
O
O
NH
O
AcO
NHAc
AcO
AcO
1d
f1 (ppm)

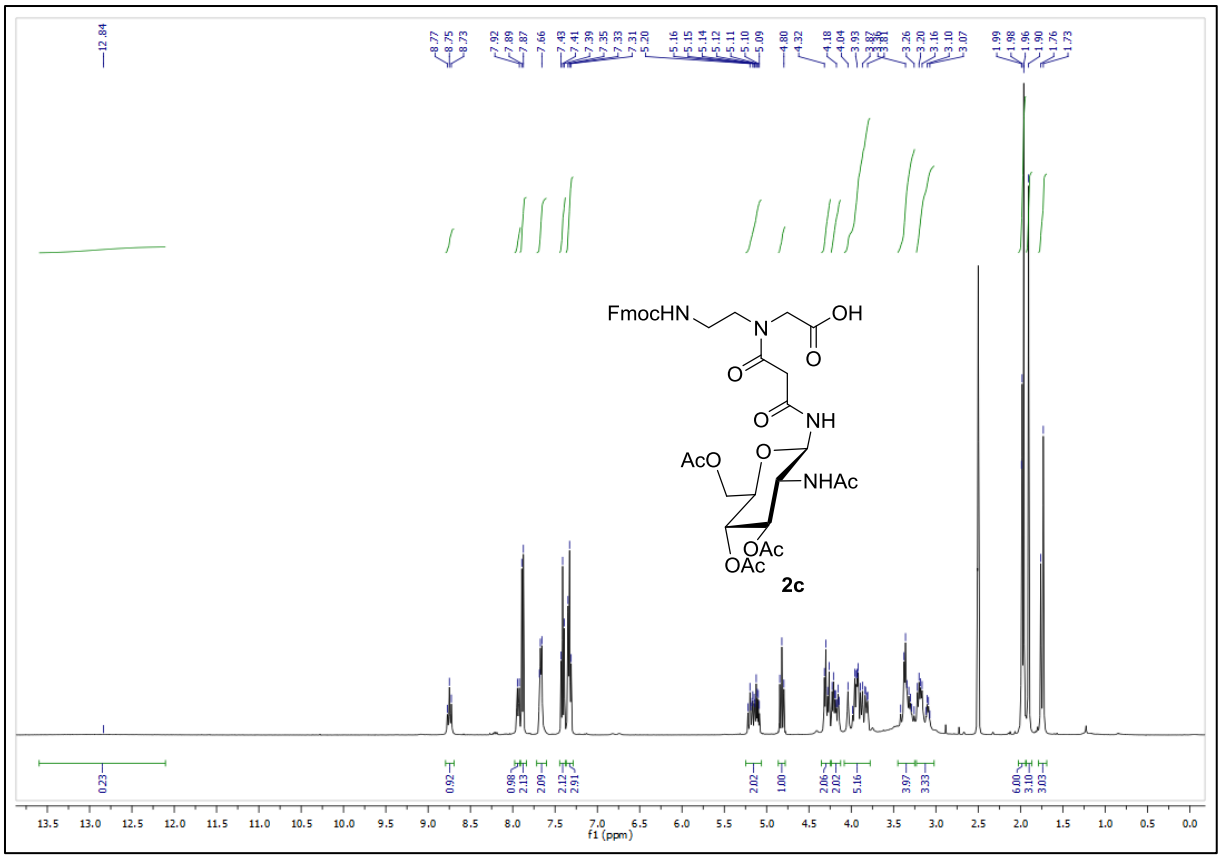

FmocHN
N
O
O
O
O
NH
O
AcO
NHAc
AcO
AcO
1d
f1 (ppm)

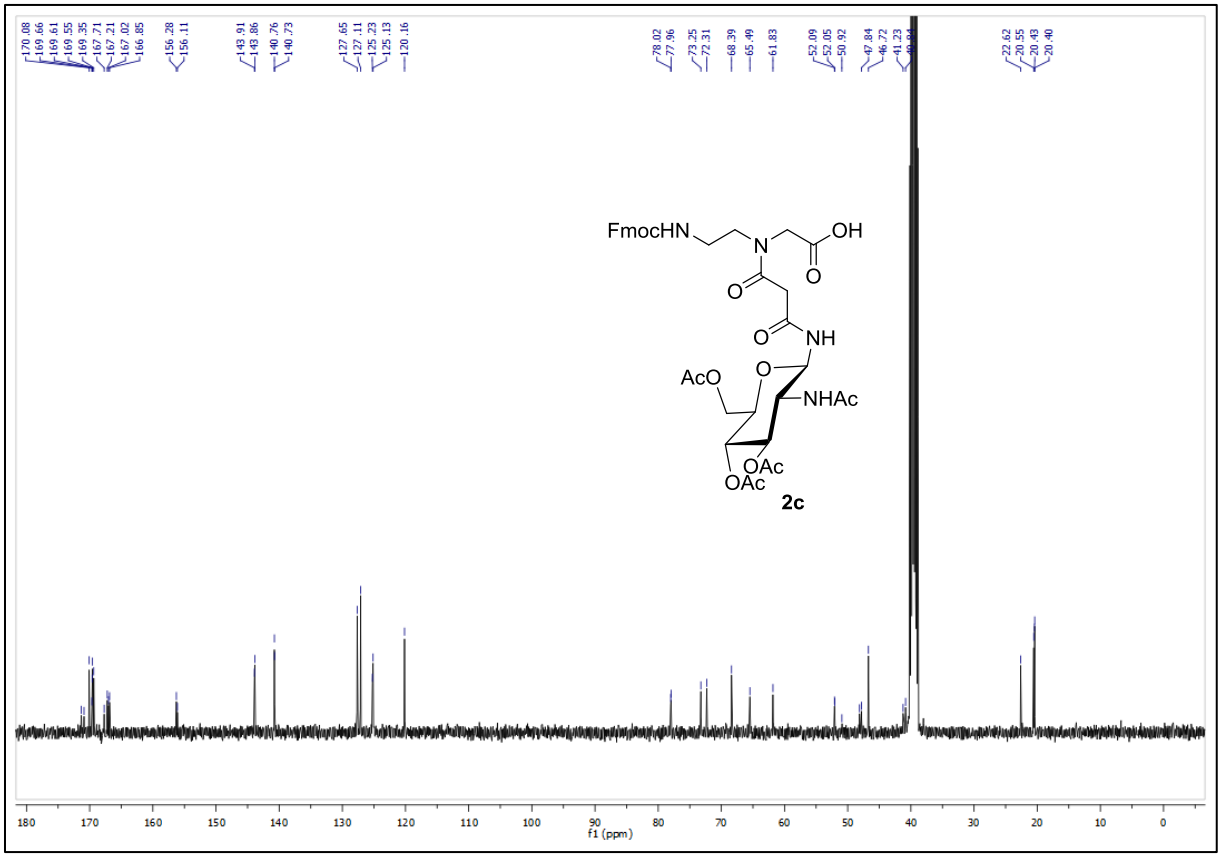

FmocHN
N
OH
O
O
O
NH
AcO
O
OAc
OAc
OAc
2a
f1 (ppm)

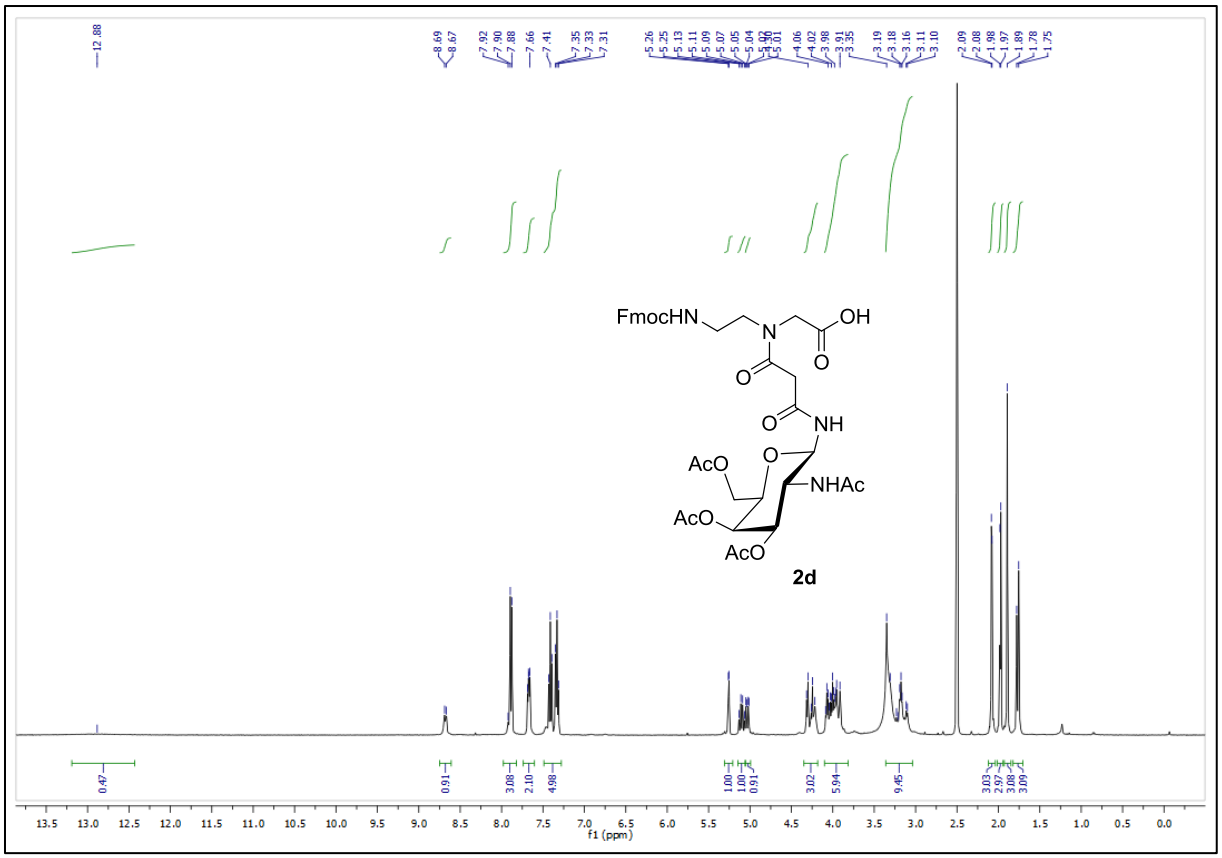

FmocHN
N
OH
O
O
O
NH
AcO
O
OAc
OAc
OAc
2a
f1 (ppm)

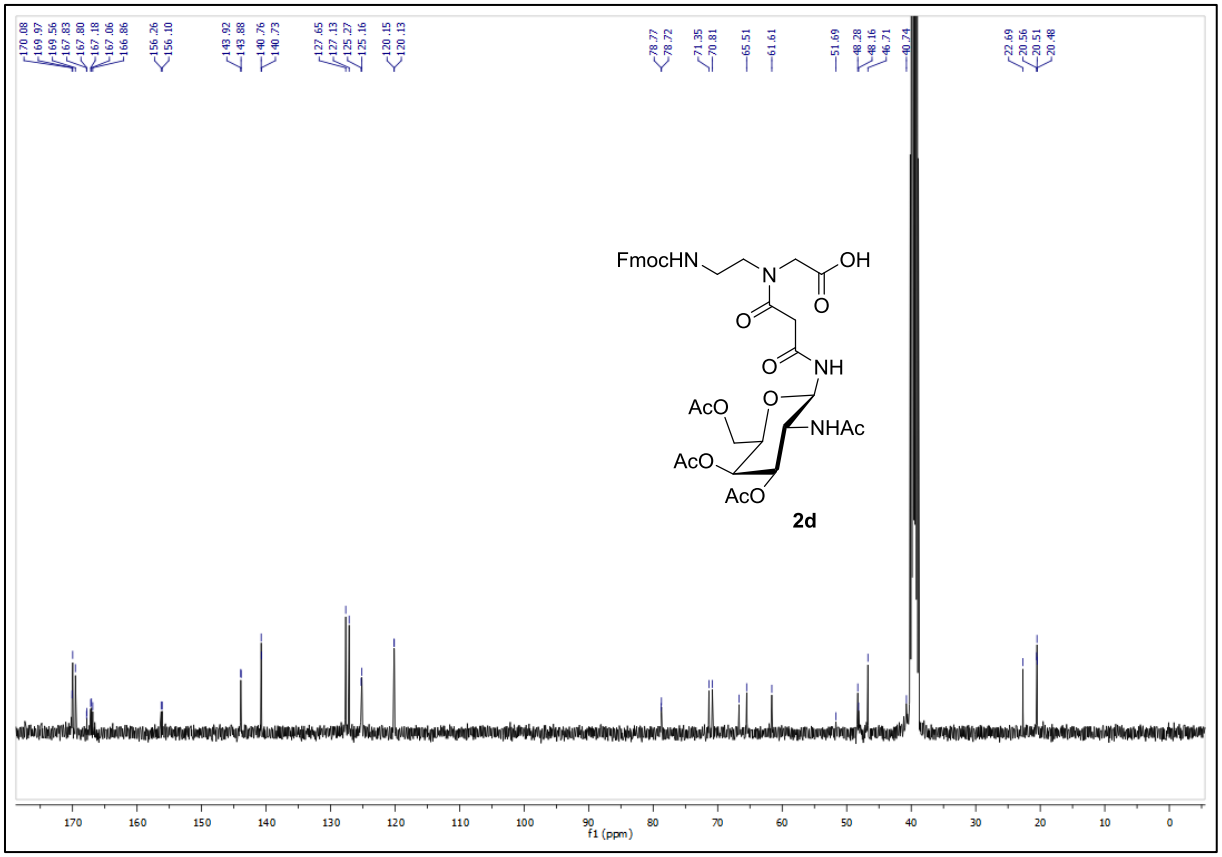

FmocHN
N
OH
O
O
O
NH
O
AcO
OAc
AcO
AcO
2b
f1 (ppm)

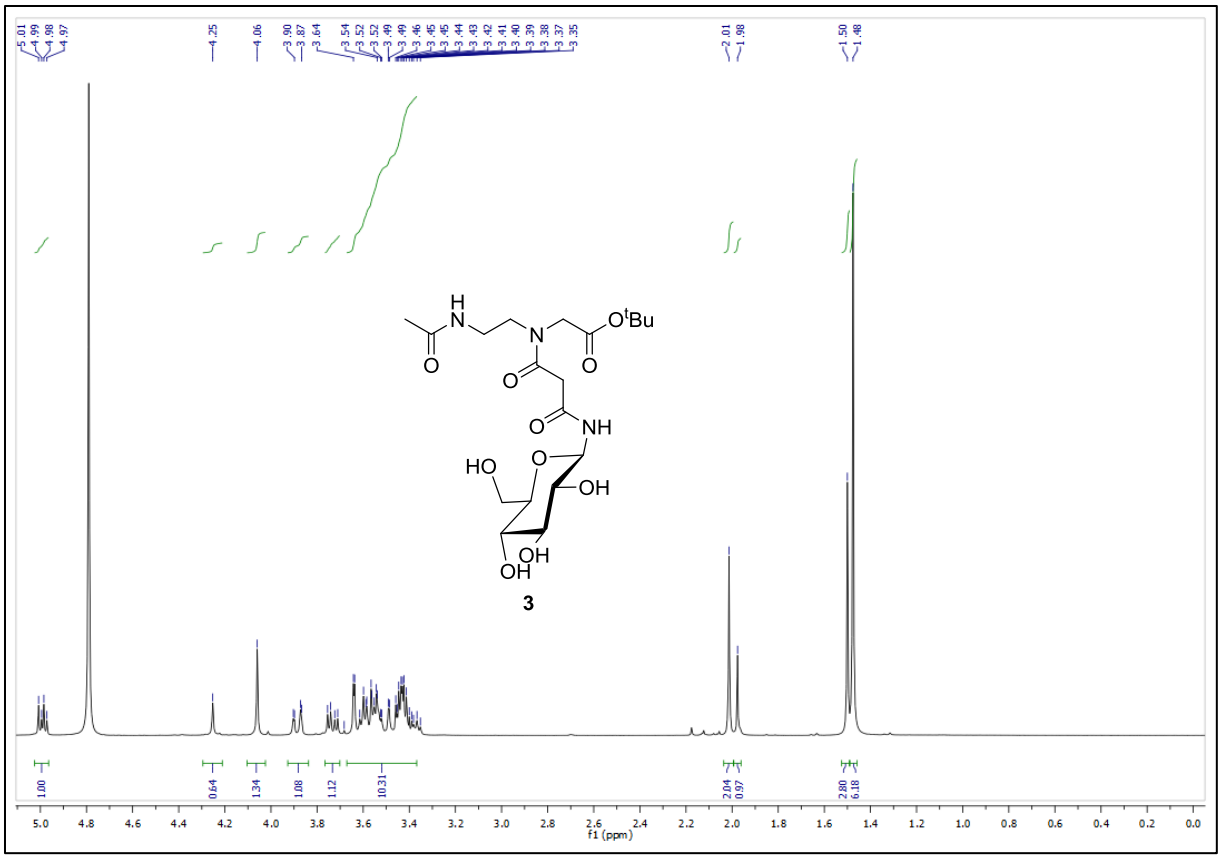

FmocHN
N
OH
O
O
O
NH
O
AcO
OAc
AcO
AcO
2b
f1 (ppm)

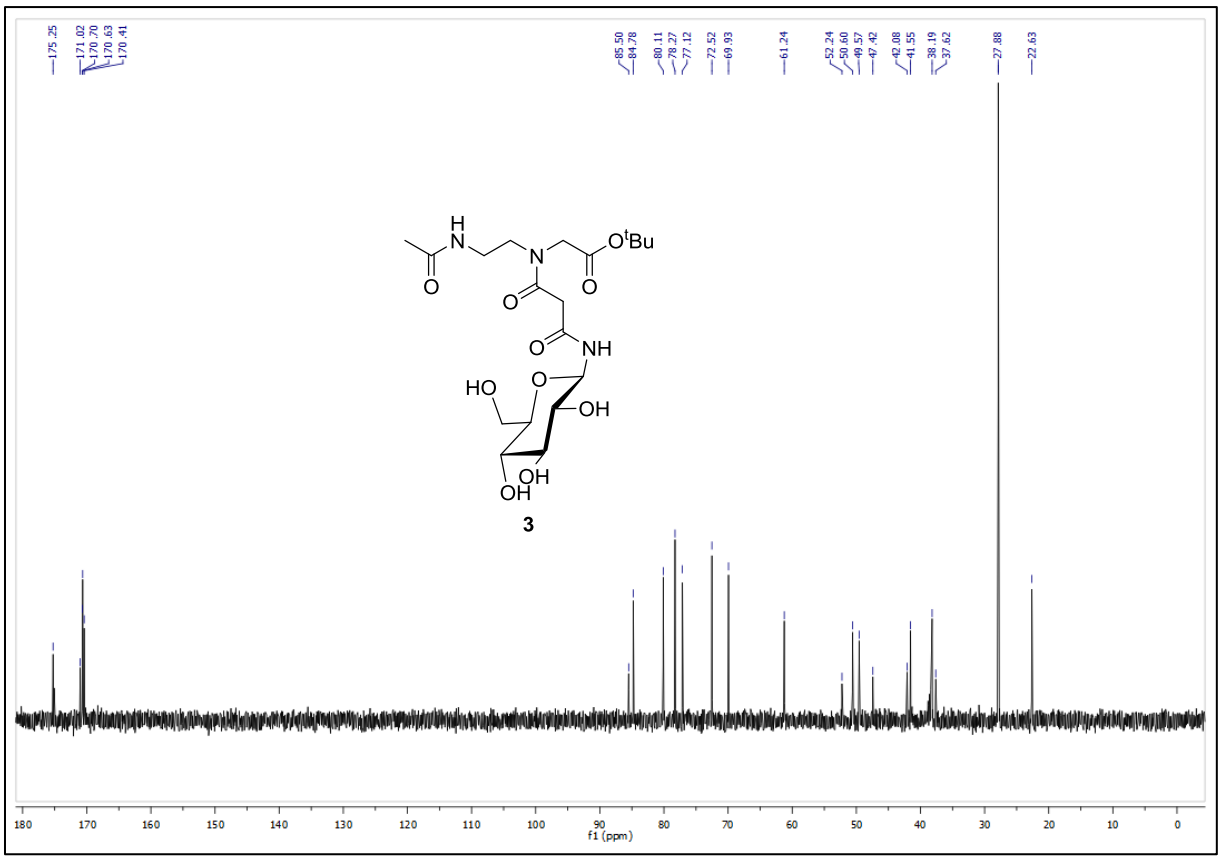

FmocHN
N
OH
O
O
O
NH
AcO
O
NHAc
OAc
OAc
2c
f1 (ppm)

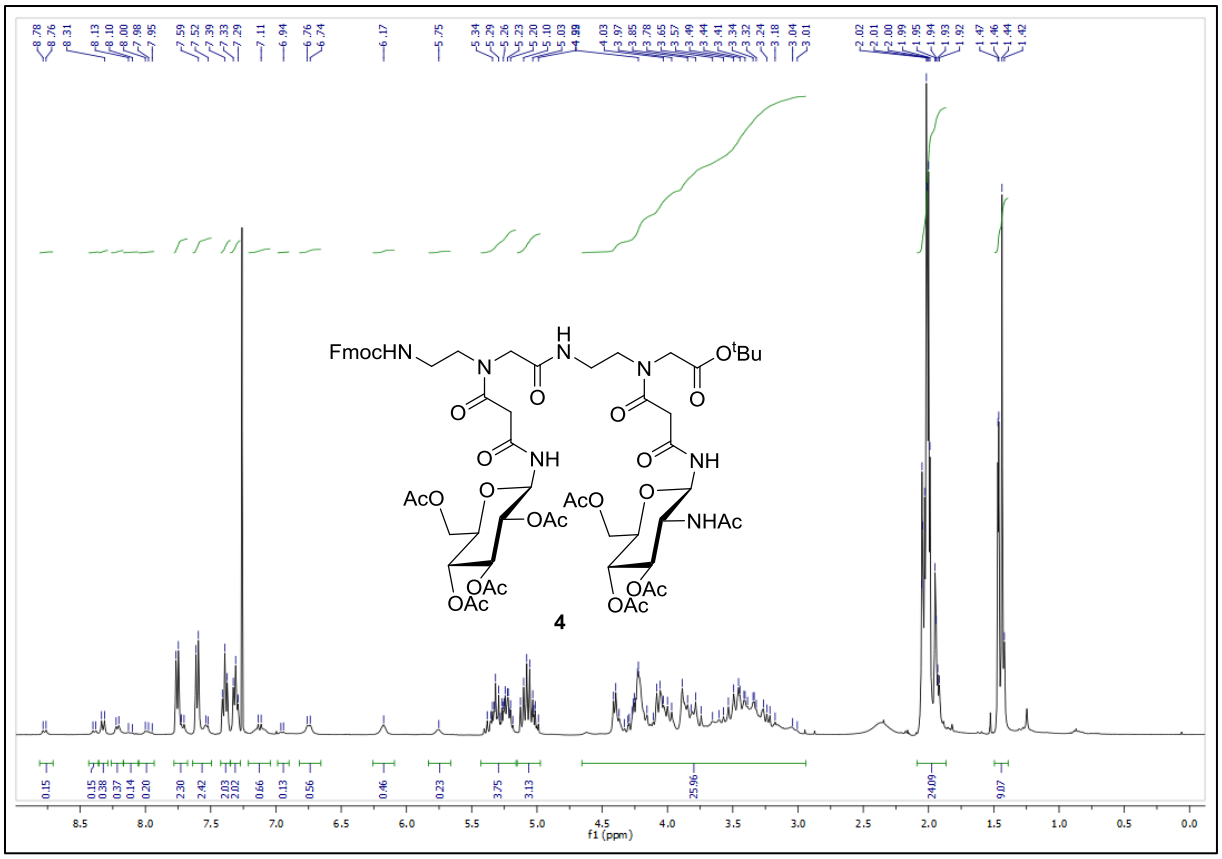

FmocHN
N
OH
O
O
O
NH
AcO
O
NHAc
OAc
OAc
2c
f1 (ppm)

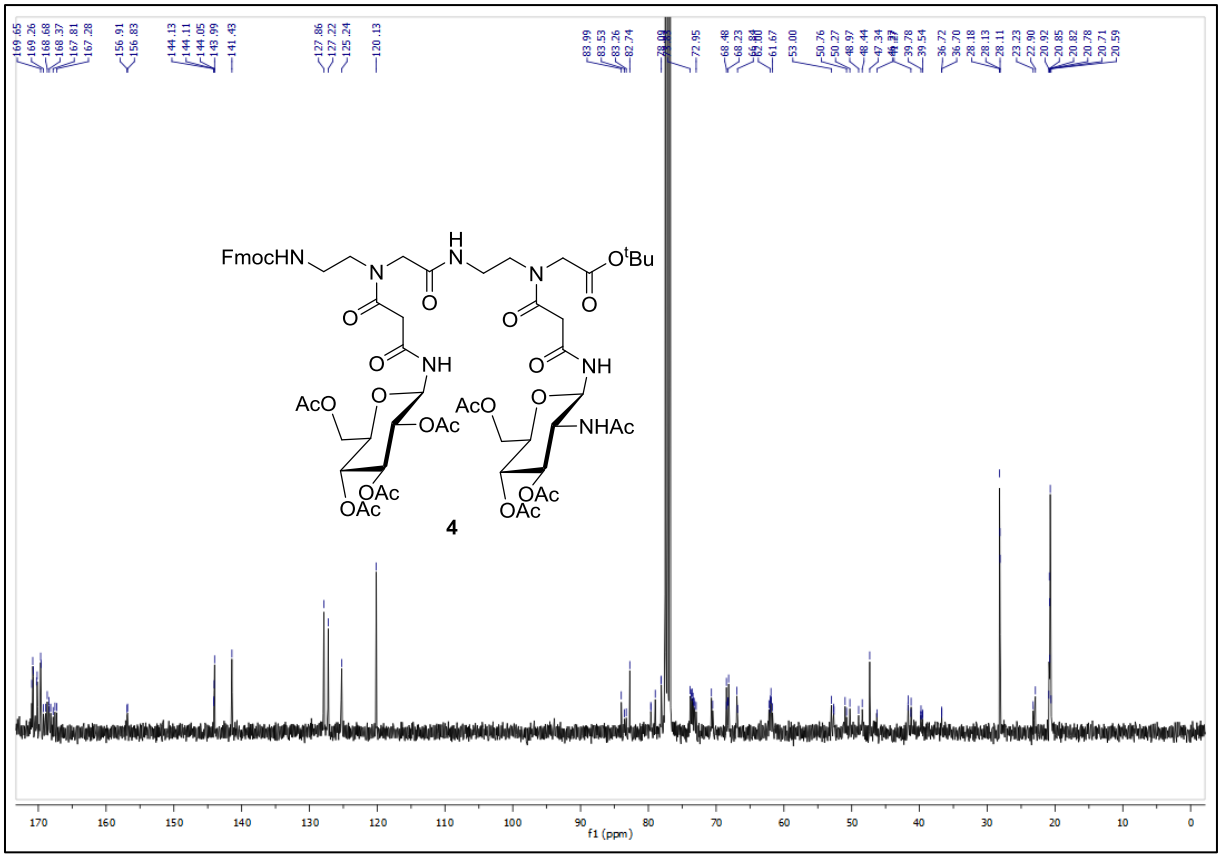

FmocHN
N
OH
O
O
O
NH
O
AcO
NHAc
AcO
AcO
2d
f1 (ppm)

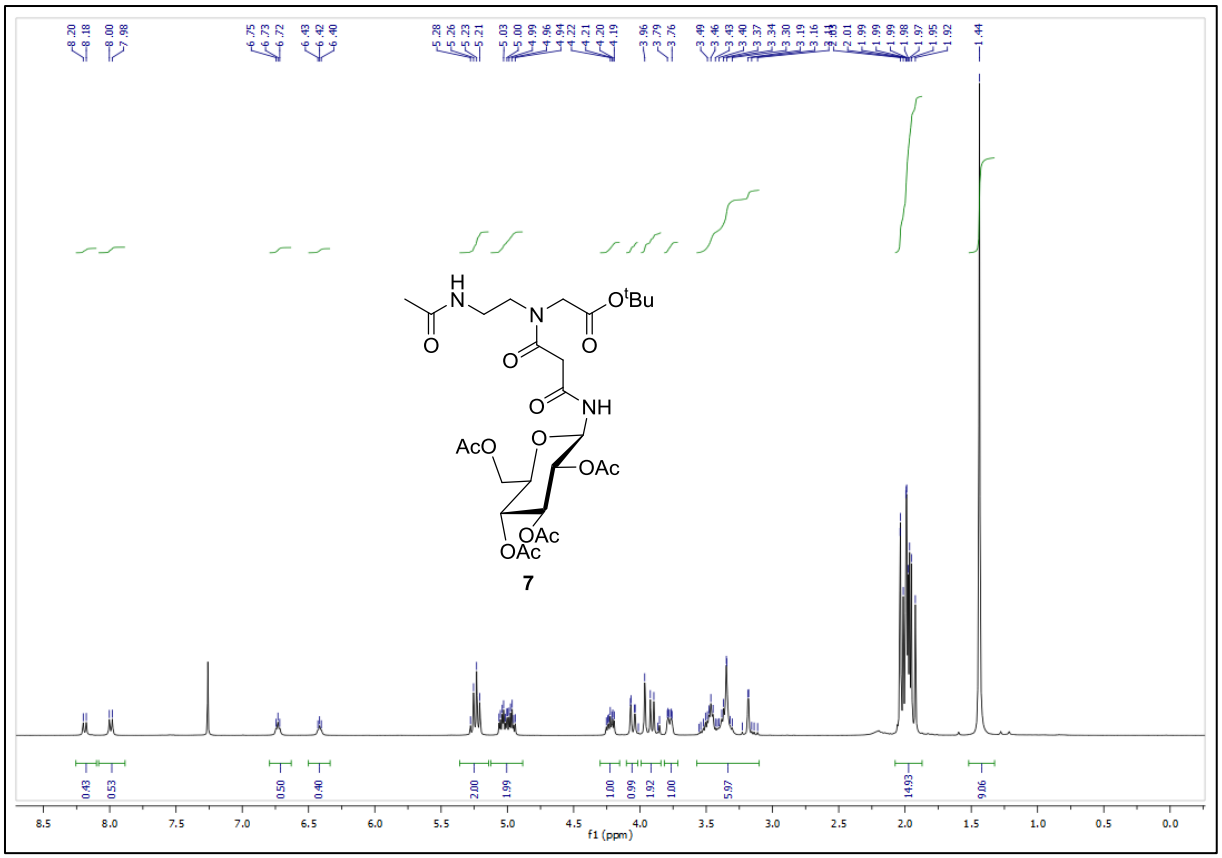

FmocHN
N
OH
O
O
O
NH
O
AcO
NHAc
AcO
AcO
2d
f1 (ppm)

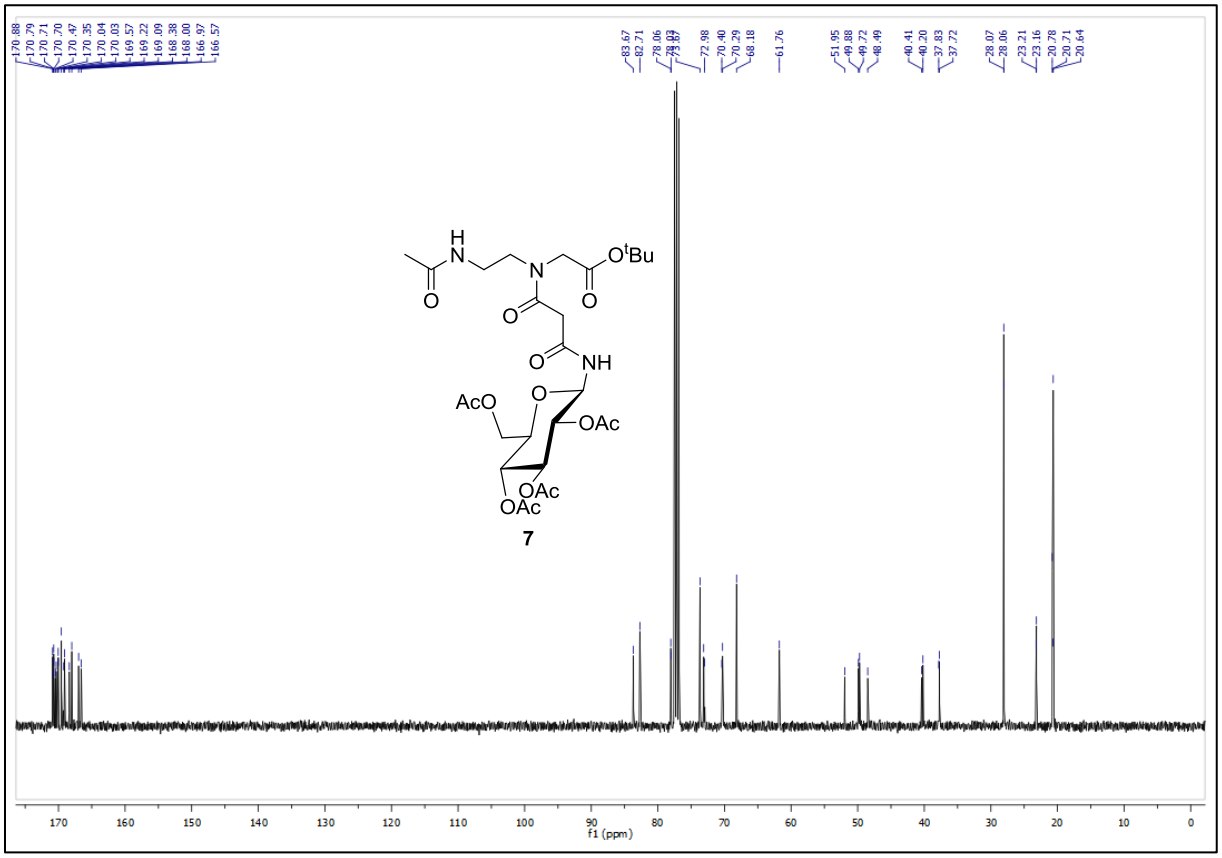

5.01
4.99
4.98
4.97
4.25
4.06
3.90
3.87
3.64
3.54
3.52
3.52
3.49
3.49
3.46
3.45
3.45
3.44
3.43
3.42
3.41
3.40
3.39
3.38
3.37
3.35
2.01
1.98
1.50
1.48
1.00
0.64
1.34
1.08
1.12
10.31
2.04
0.97
2.80
6.18
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
f1 (ppm)
H
N
O
O
N
O
O
O
O
O
O
NH
HO
O
OH
OH
OH
3


175.25
171.02
170.70
170.63
170.41
85.50
84.78
80.11
78.27
77.12
72.52
69.93
61.24
52.24
50.60
49.57
47.42
42.08
41.55
38.19
37.62
27.88
22.63
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
H
N
O
O
N
O
O
O
O
O
O
NH
HO
O
OH
OH
OH
3

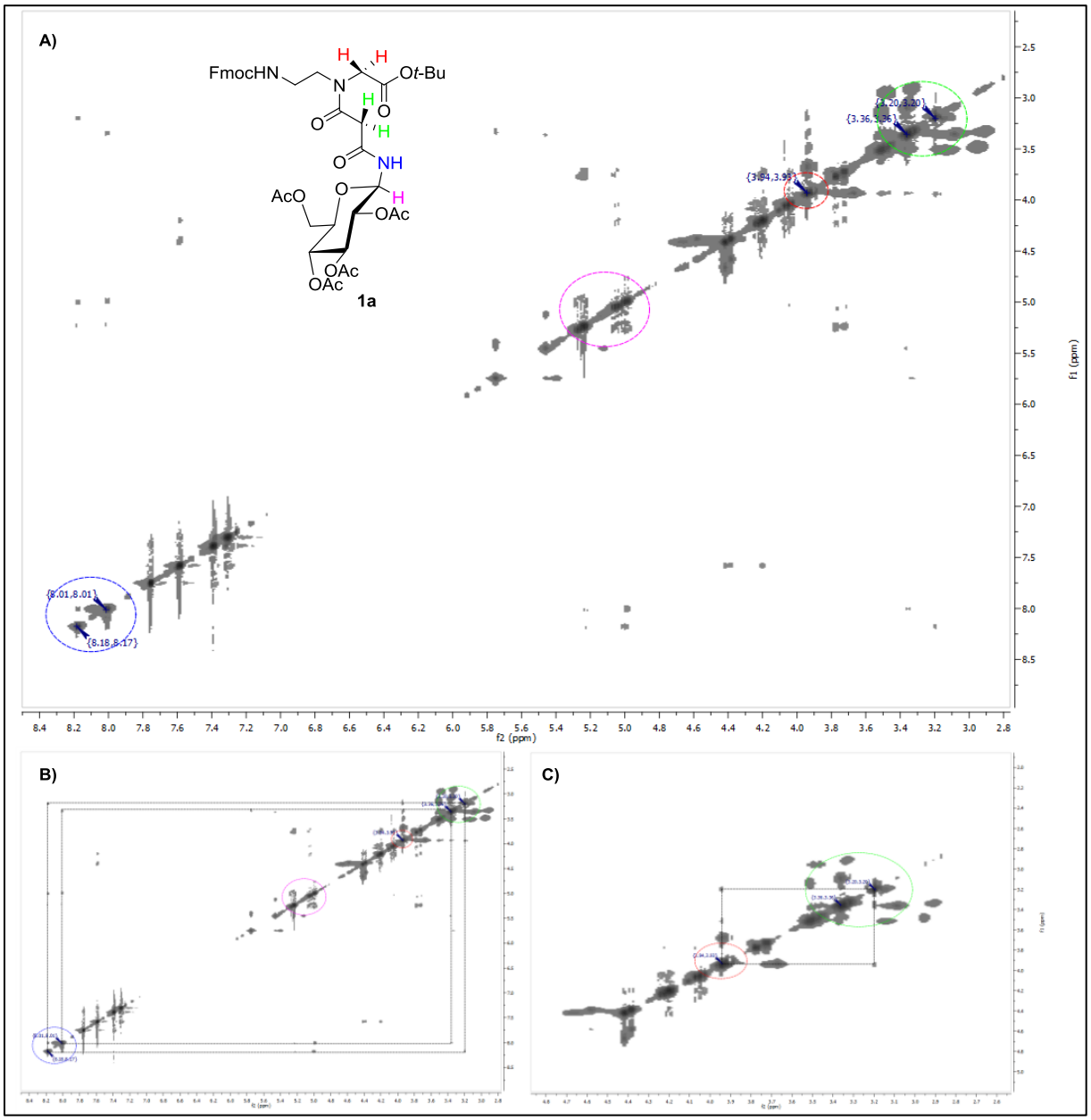

FmocHN
H
N
O^{t}Bu
NH
AcO
OAc
NHAc
4
f1 (ppm)


FmocHN
H
N
O^{t}Bu
NH
AcO
OAc
NHAc
4
f1 (ppm)


7


7

2D NMR Spectra of building block 1a



A) 2D-NOESY (600 MHz; τ_m = 450 ms) spectrum of building block **1a** in $CDCl_3$; **B)** Crosspeaks of the amidic doublets (blue) and the malonyl protons (green); **C)** Crosspeaks of the methylene protons of the PNA backbone (red) and the malonyl protons (green).