Supporting Information to

Development and optimization of a competitive binding assay for the galactophilic low affinity lectin LecA from *Pseudomonas aeruginosa*

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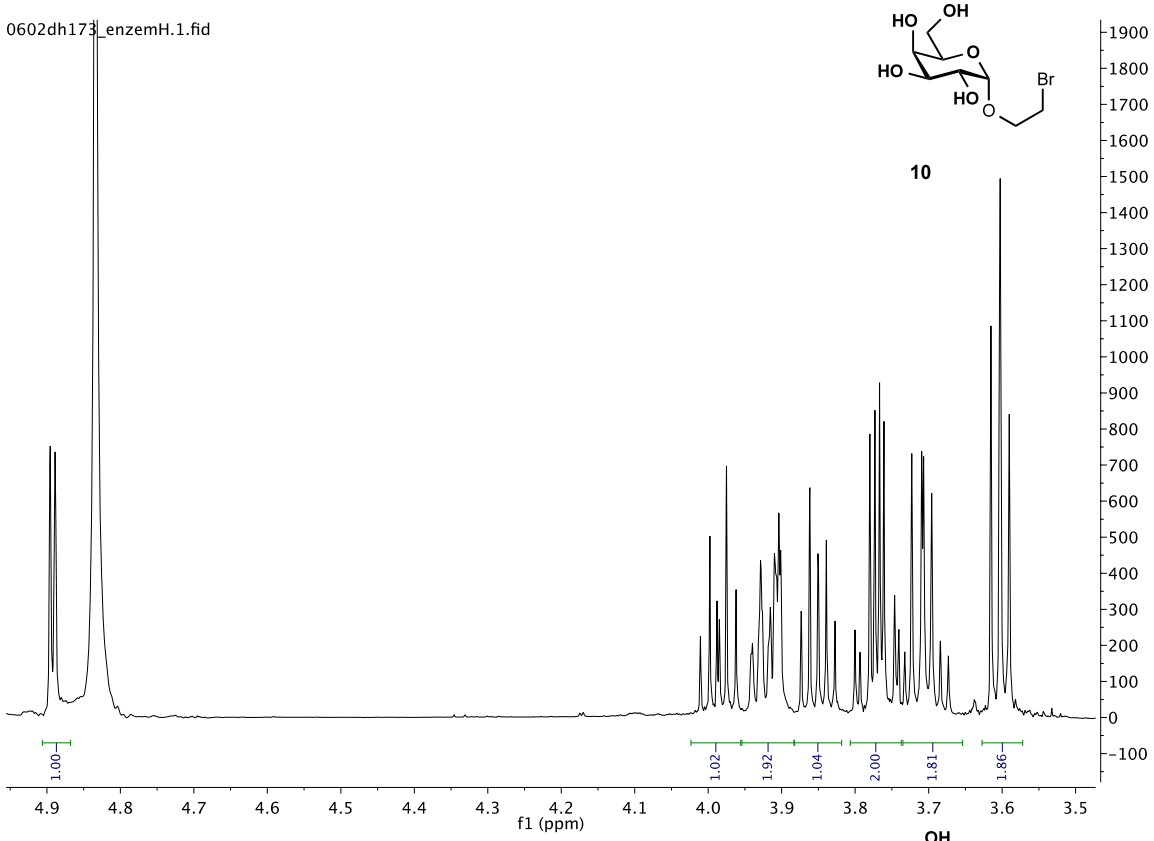
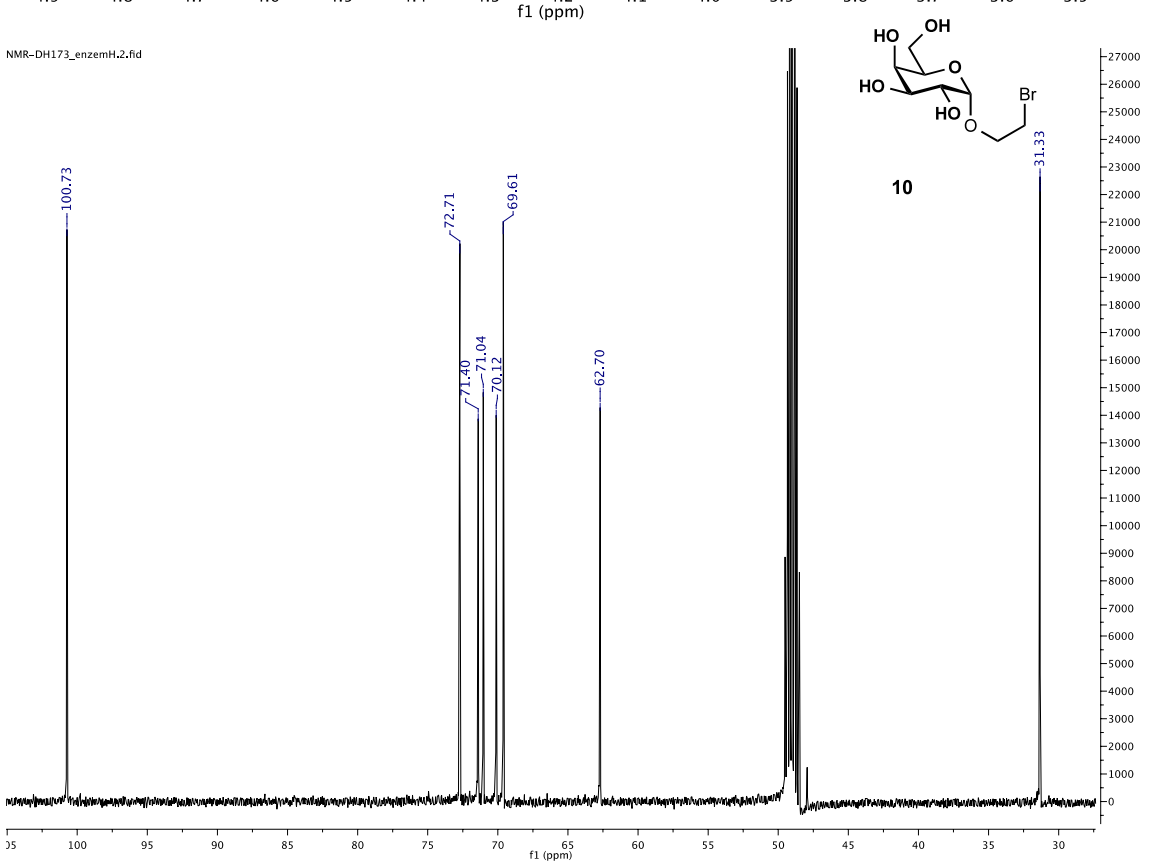
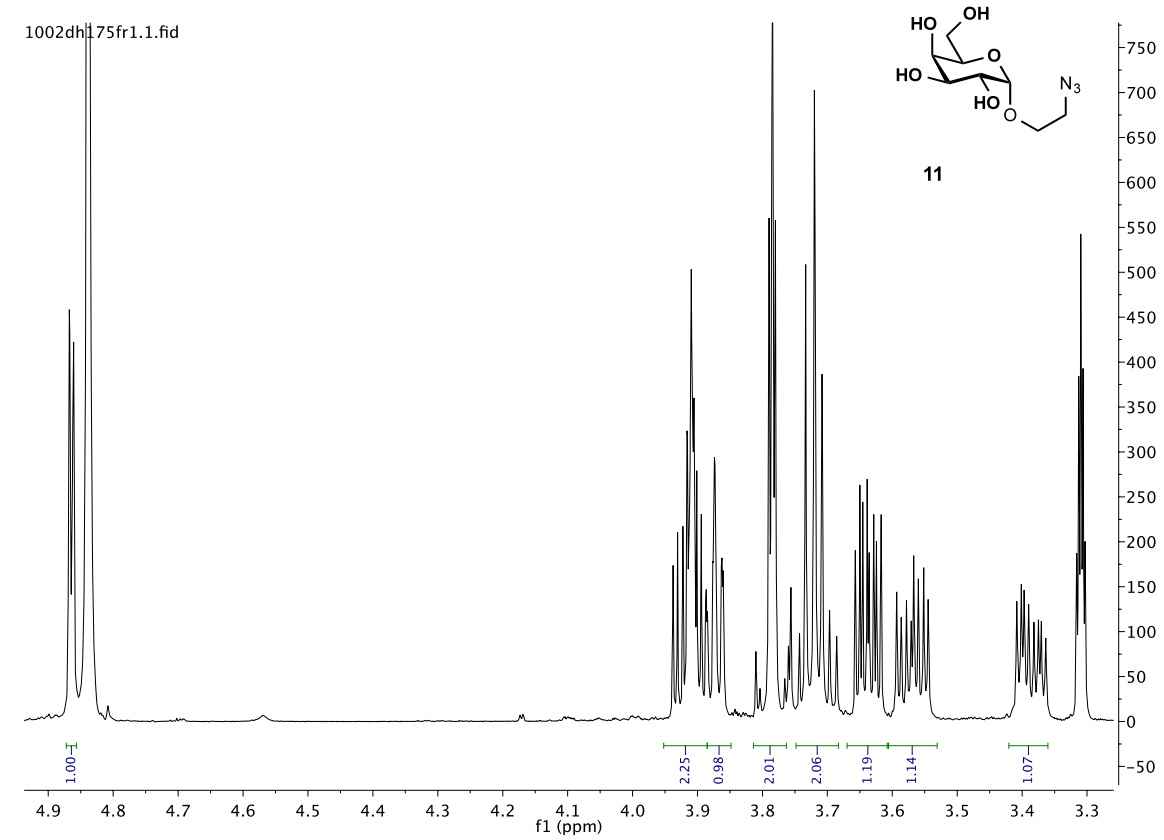
^{1}H and ^{13}C spectra of synthesized compounds



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HO
HO
O
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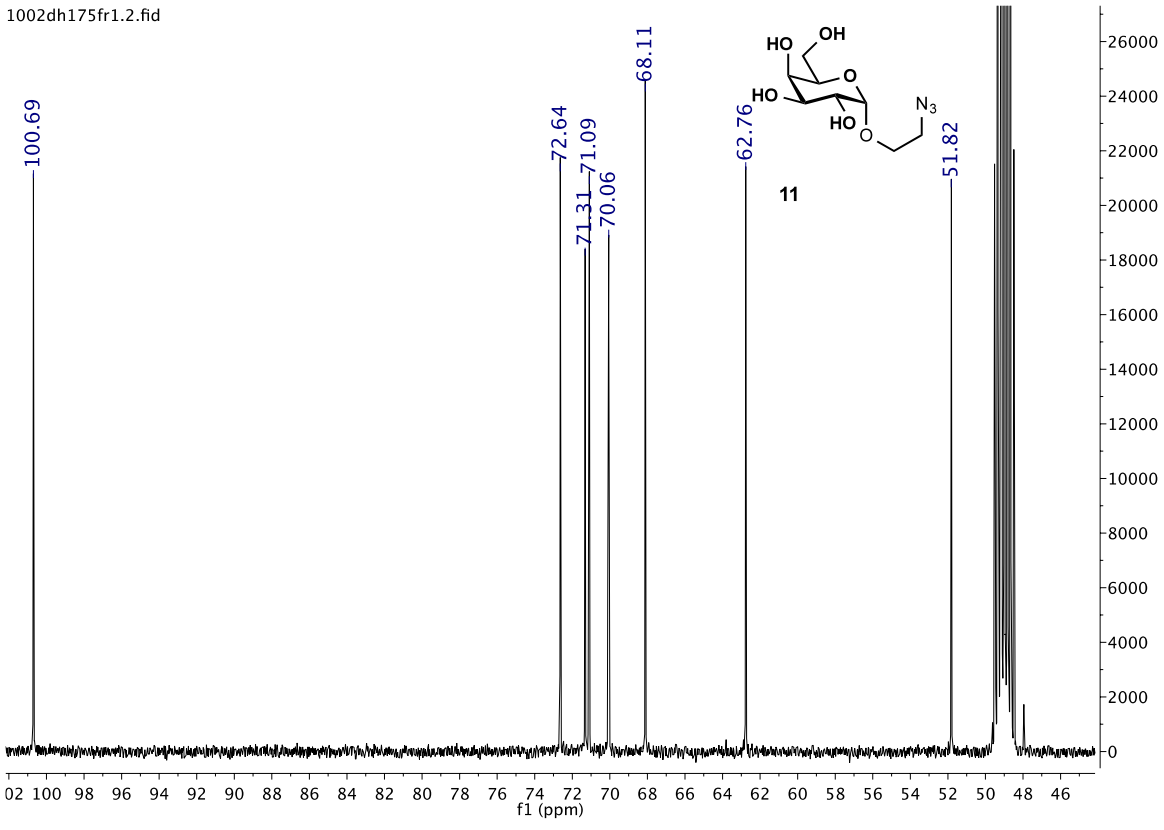
1.14
1.07
f1 (ppm)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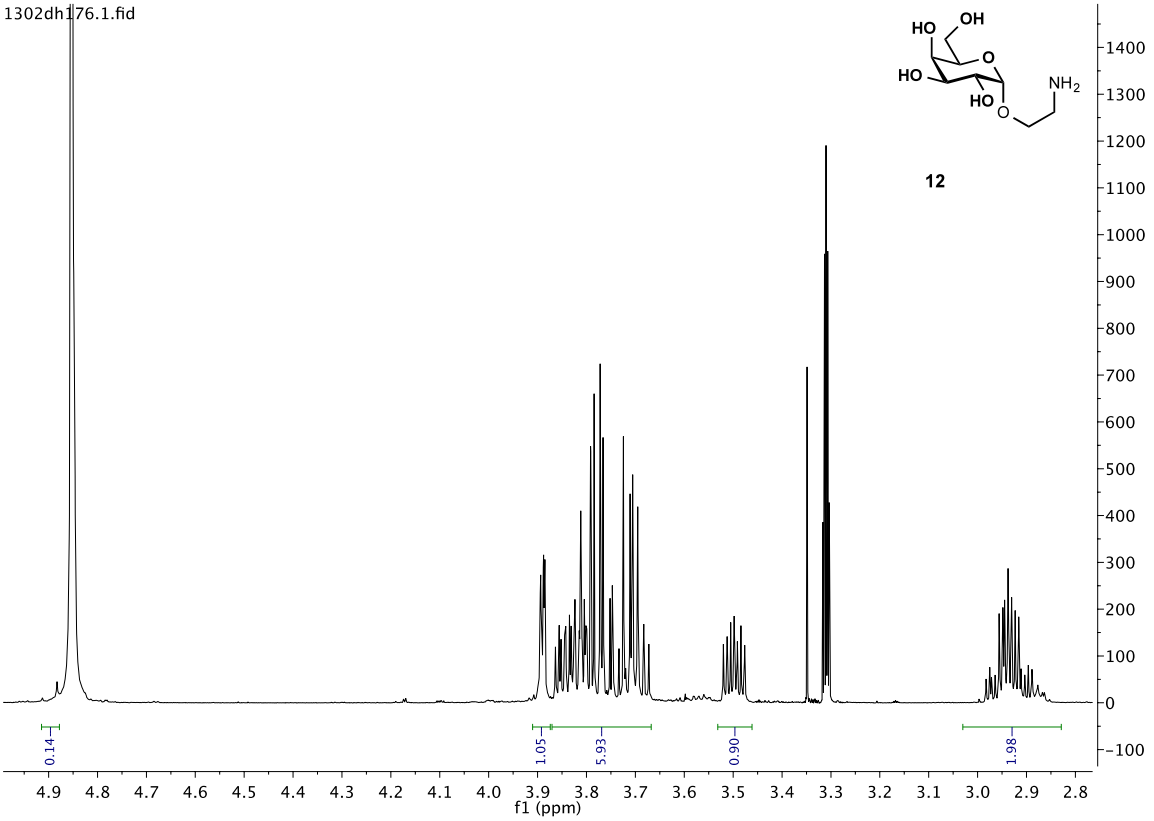
O
HO
HO
O
N3
11
f1 (ppm)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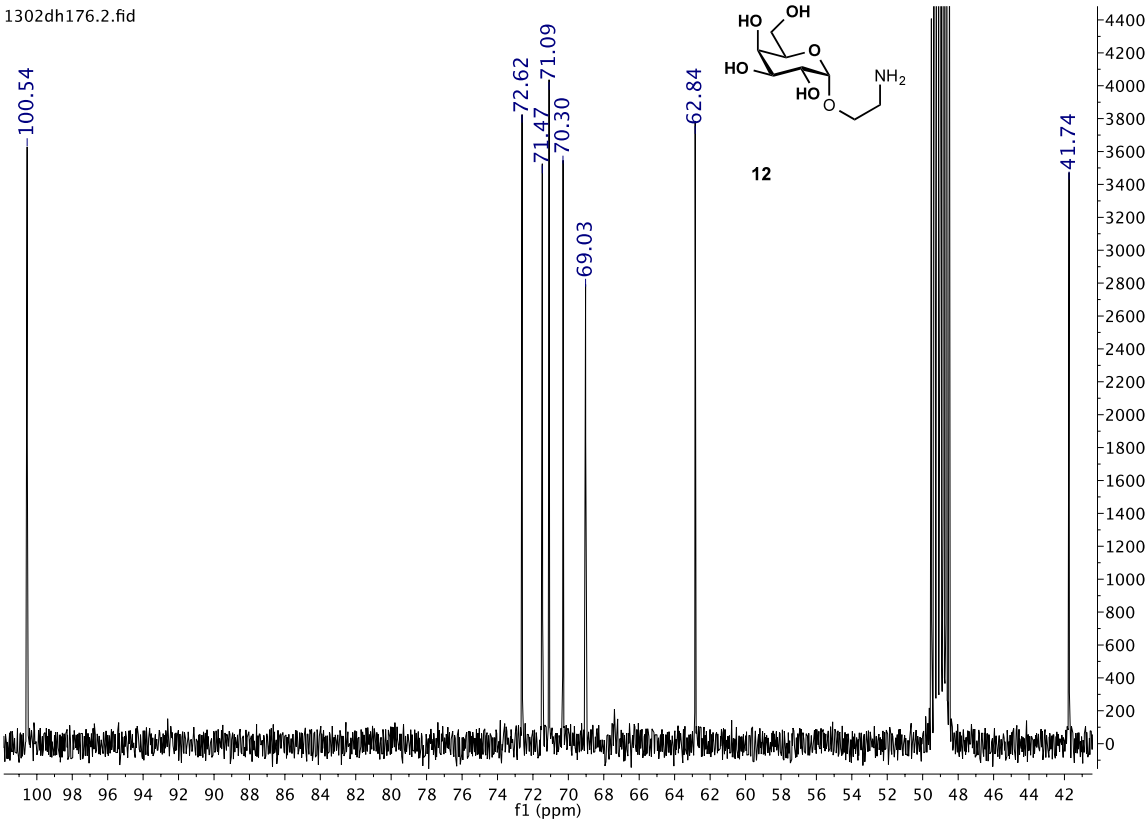
f1 (ppm)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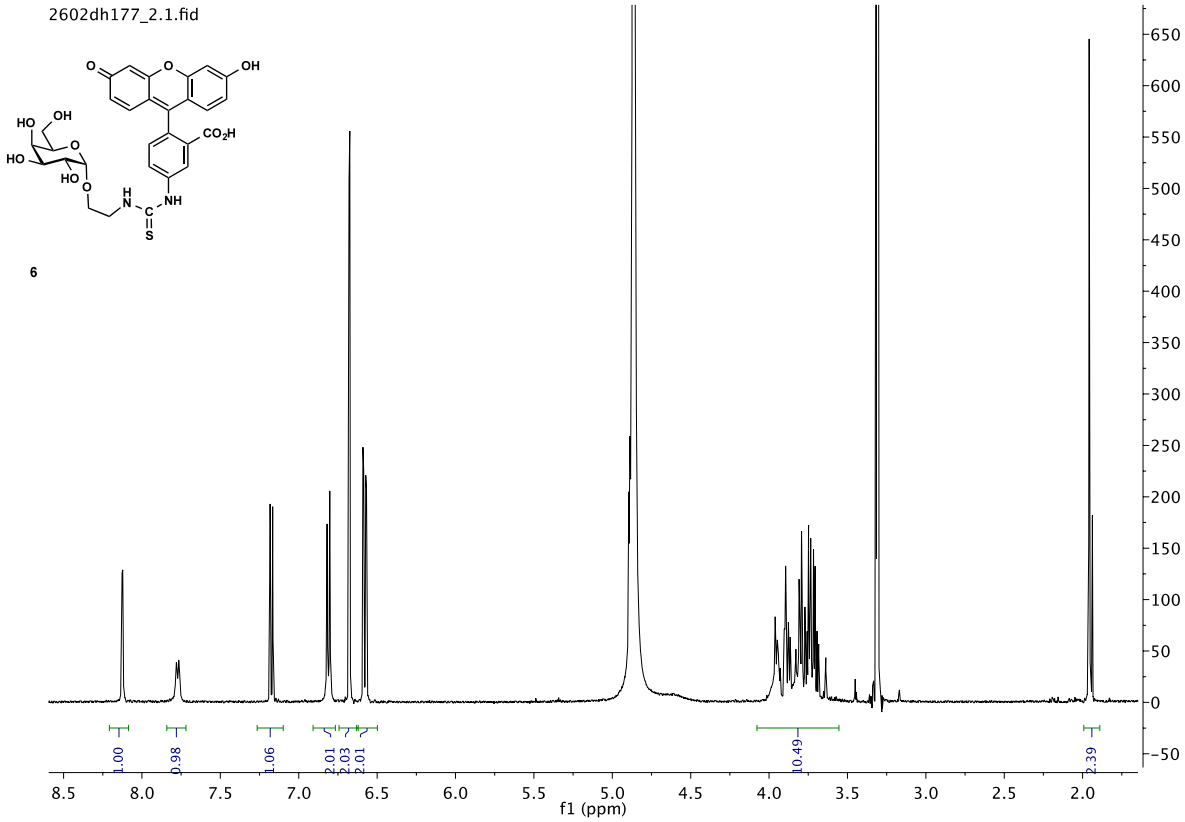
O
HO
HO
O
NH2
12
f1 (ppm)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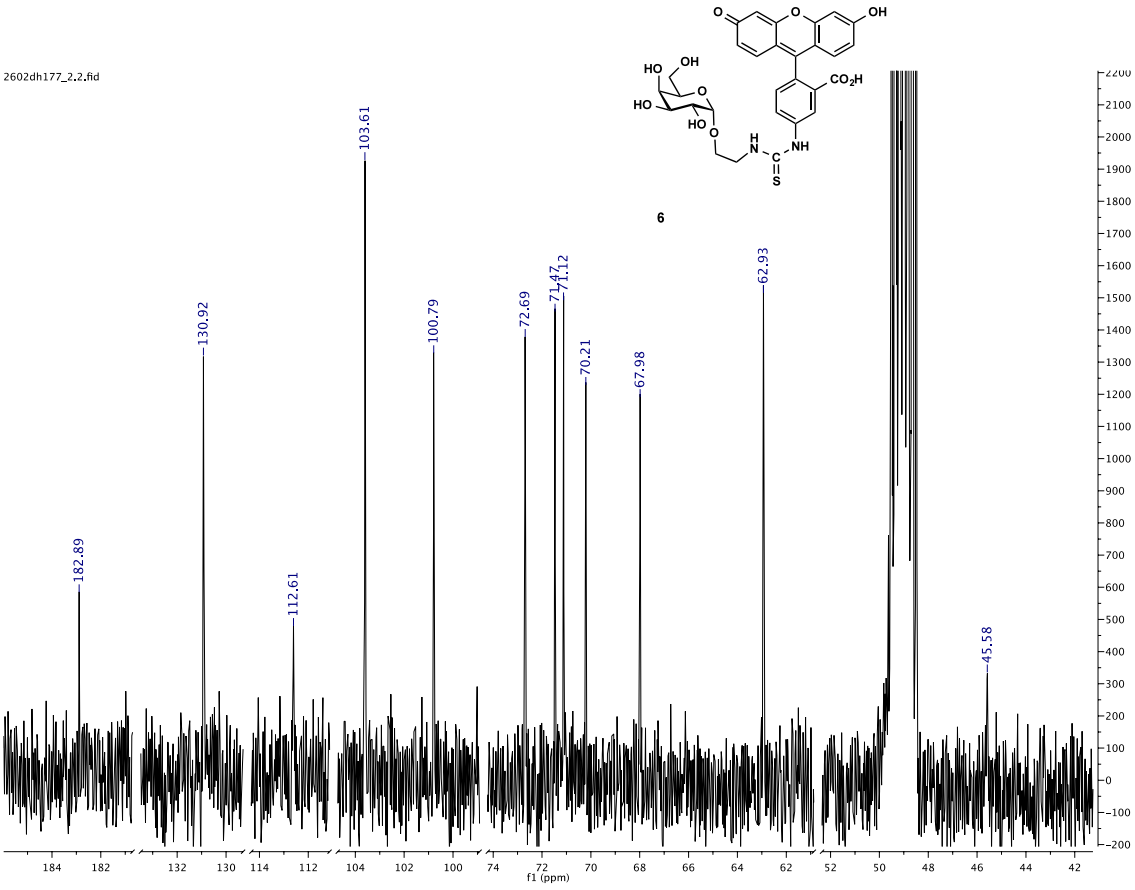
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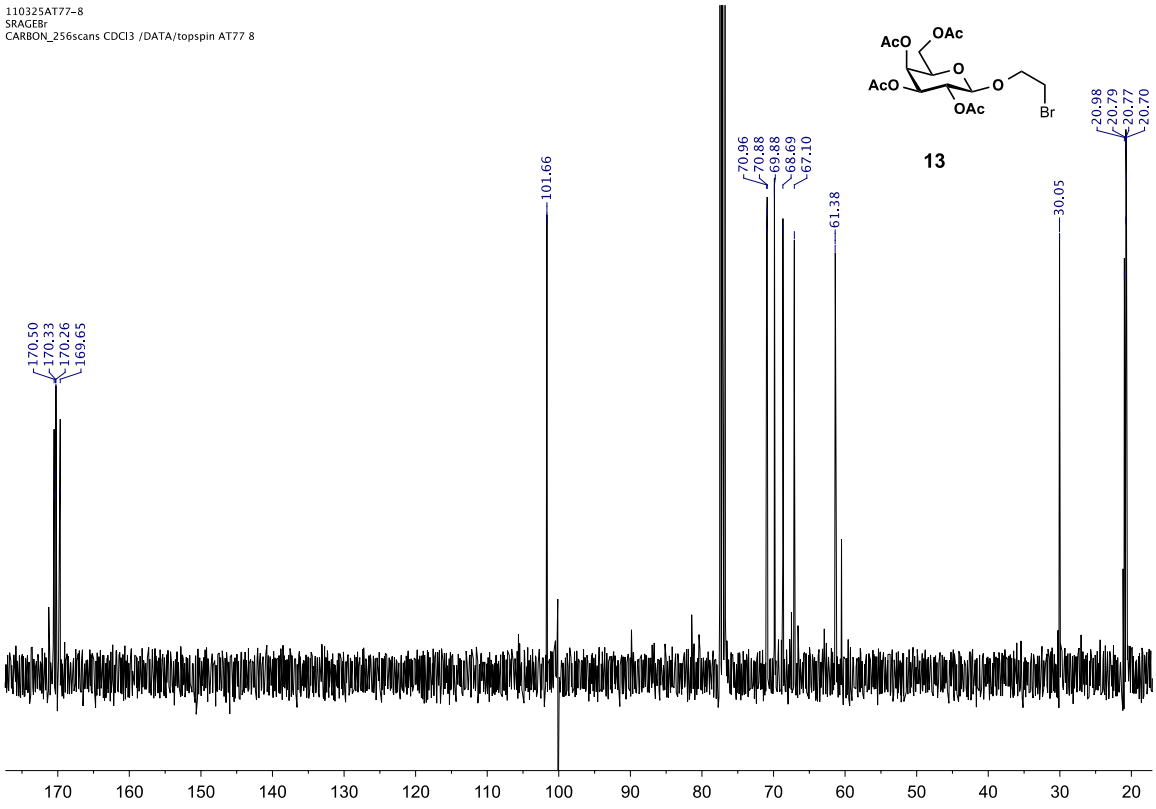
62.93
45.58
f1 (ppm)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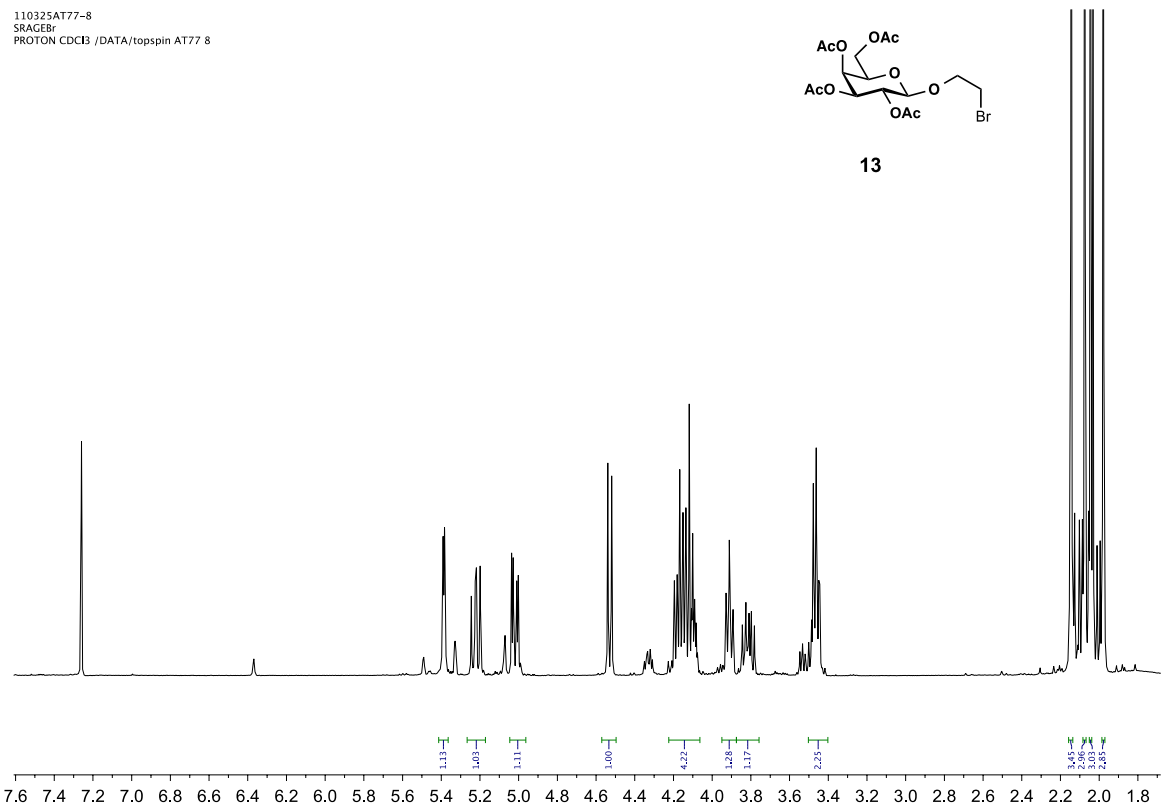
AcO
O
O
OAc
Br
13
170.50
170.33
170.26
169.65
101.66
70.96
70.88
69.88
68.69
67.10
61.38
30.05
20.98
20.79
20.77
20.70
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20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PROTON CDCl3 /DATA/topspin AT77 8
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OAc
AcO
O
O
OAc
Br
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1.13
1.03
1.11
1.00
4.22
1.28
1.17
2.25
3.45
2.96
3.03
2.85
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
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3.4
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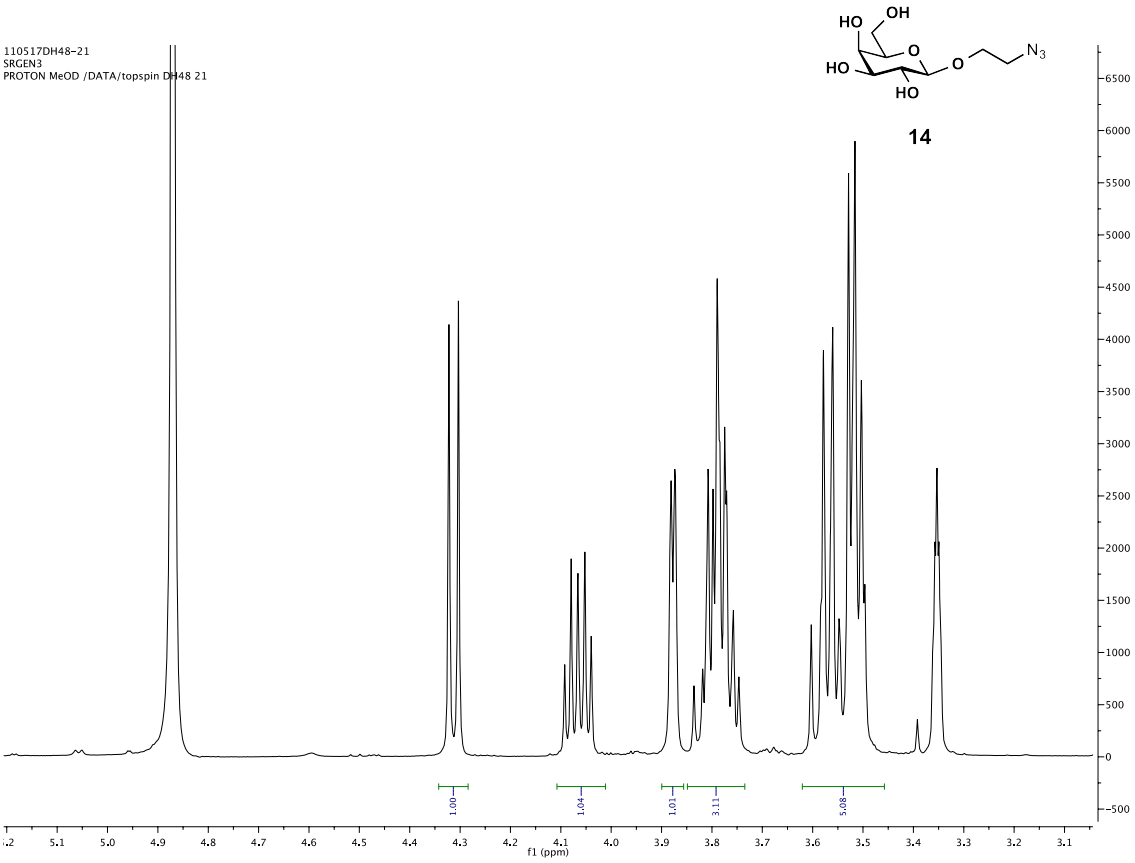
2.2
2.0
1.8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PROTON MeOD /DATA/topspin DH48 21
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HO
O
O
N3
HO
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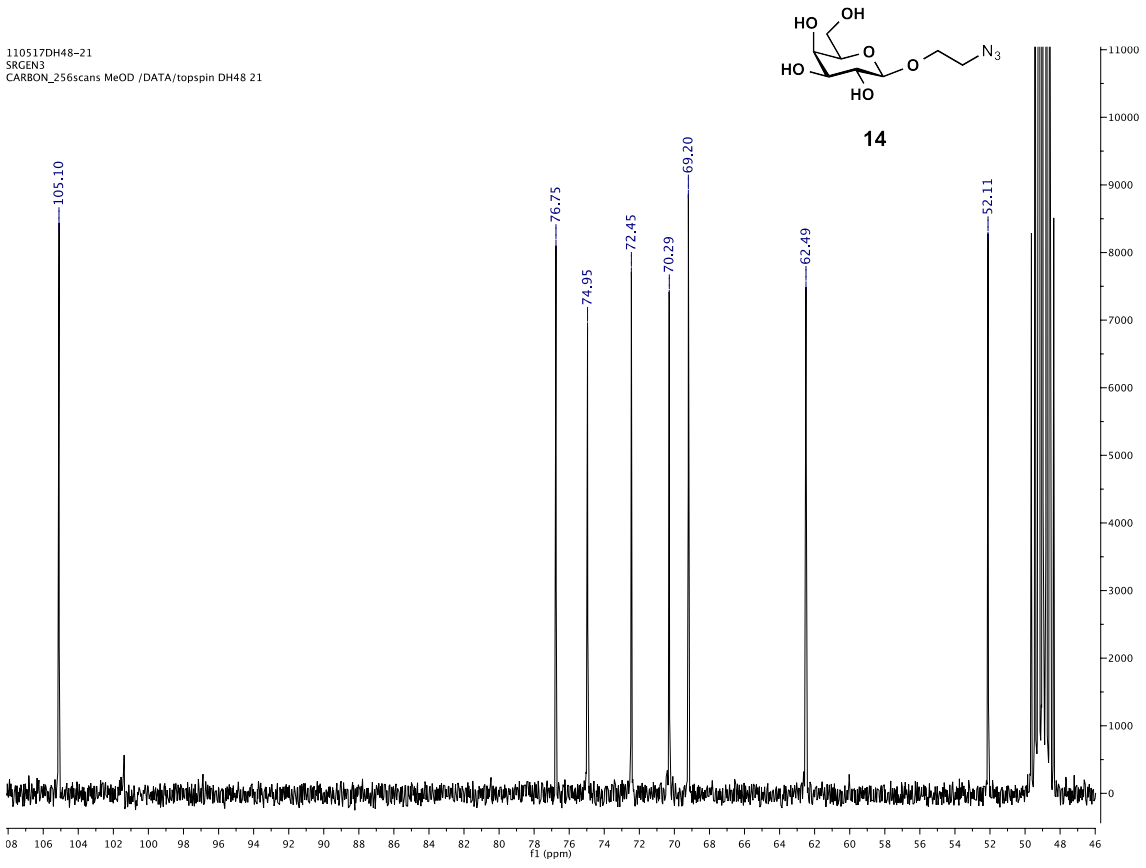
1.04
1.01
3.11
5.08
f1 (ppm)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CARBON_256scans MeOD /DATA/topspin DH48 21
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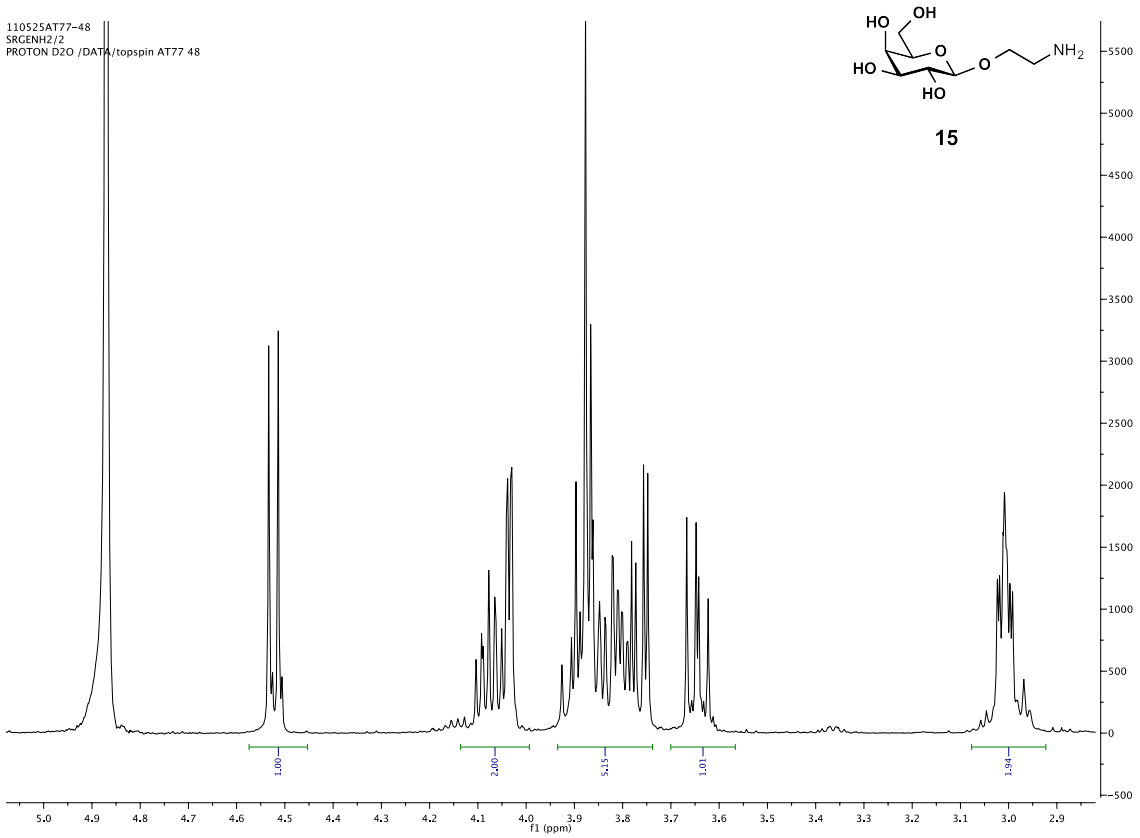
OH
HO
O
O
N3
HO
14
105.10
76.75
74.95
72.45
70.29
69.20
62.49
52.11
f1 (ppm)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OH
O
HO
O
NH2
HO
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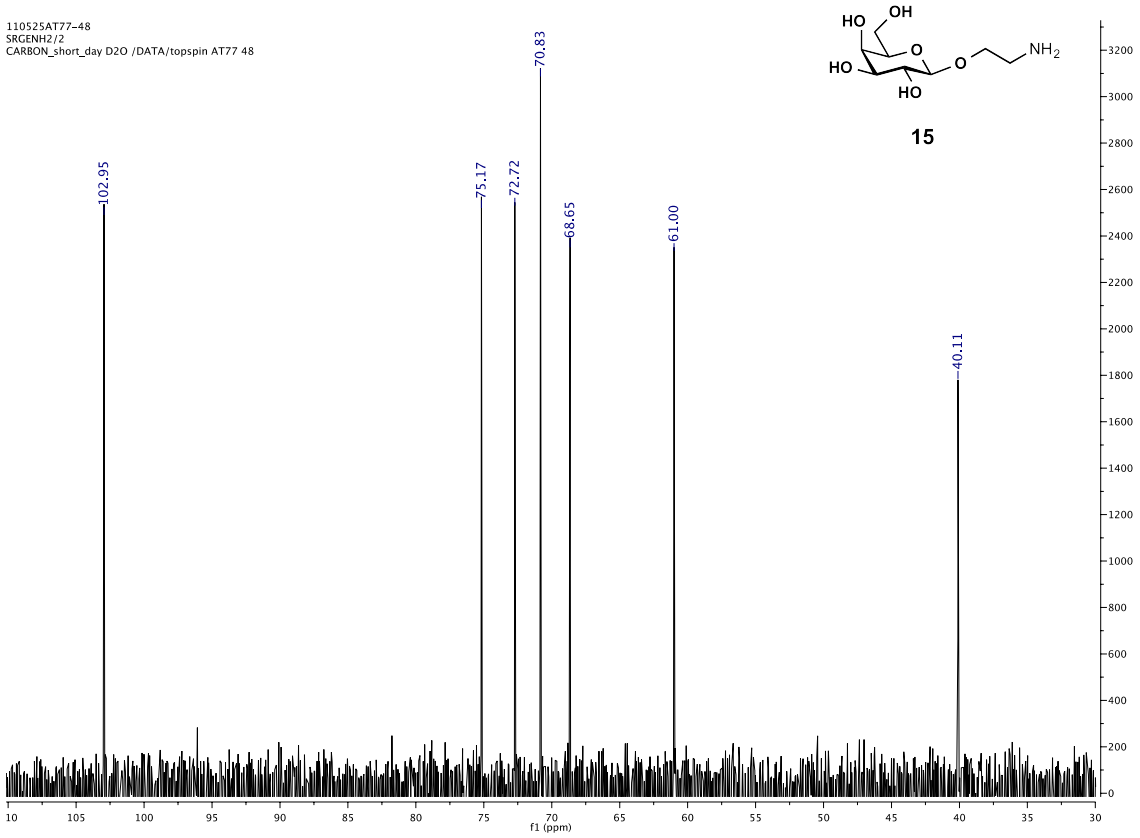
2.00
5.15
1.01
1.94
f1 (ppm)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SRGENH2/2
CARBON_short_day D2O /DATA/topspin AT77 48
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OH
O
HO
O
NH2
HO
15
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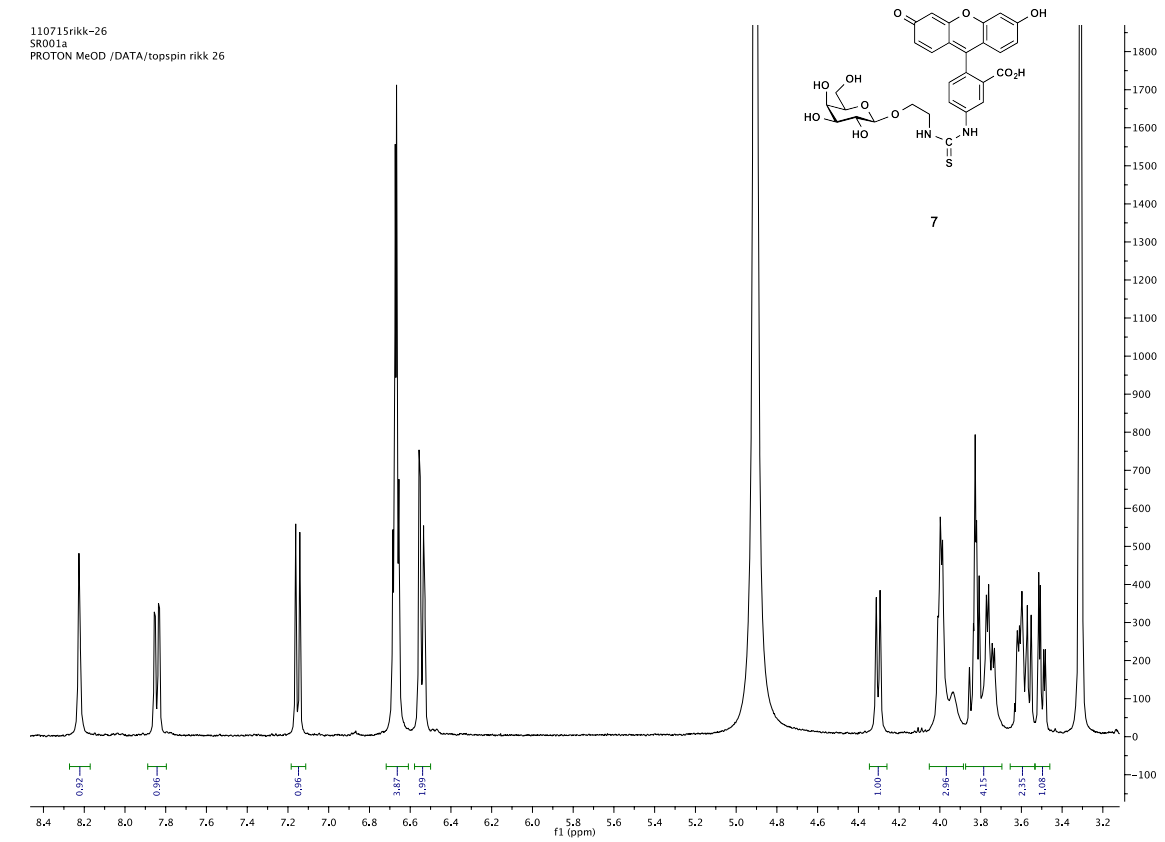
75.17
72.72
70.83
68.65
61.00
40.11
f1 (ppm)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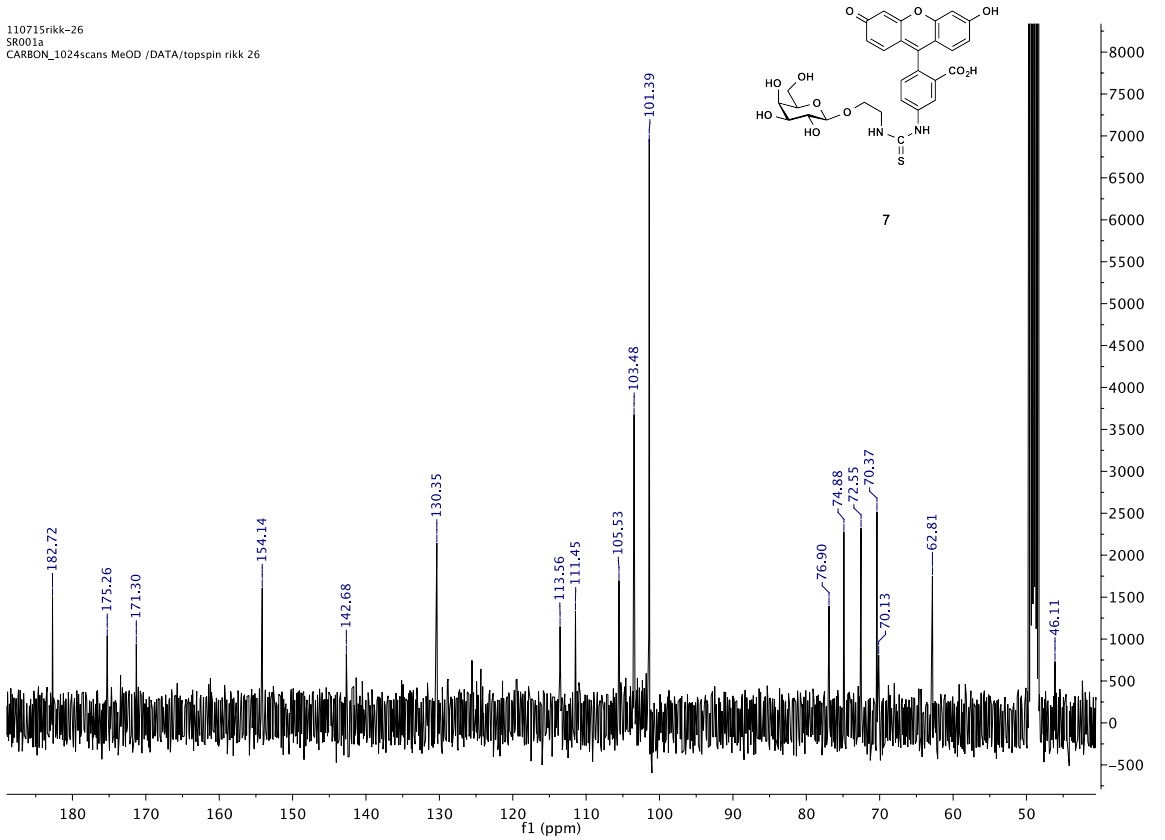
SR001a
PROTON MeOD /DATA/topspin rikk 26
7
f1 (ppm)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SR001a
CARBON_1024scans MeOD /DATA/topspin rikk 26
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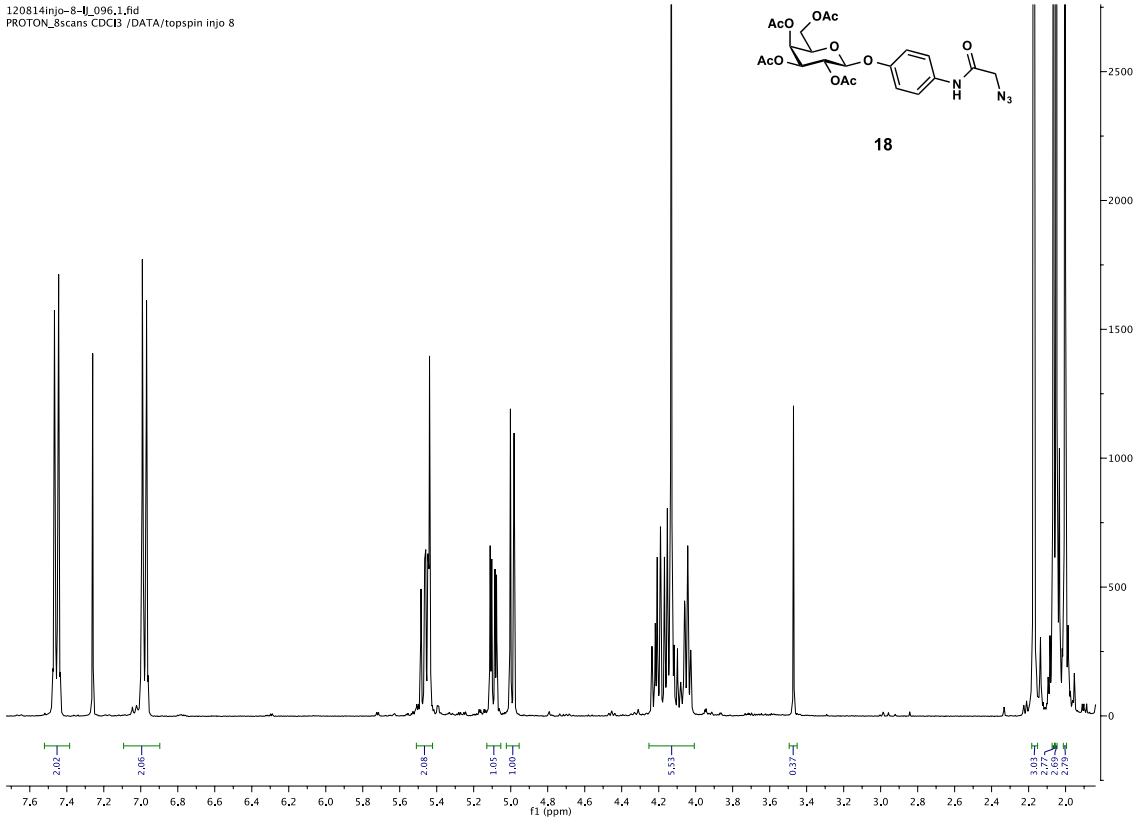
182.72
175.26
171.30
154.14
142.68
130.35
113.56
111.45
105.53
103.48
101.39
76.90
74.88
72.55
70.37
70.13
62.81
46.11
f1 (ppm)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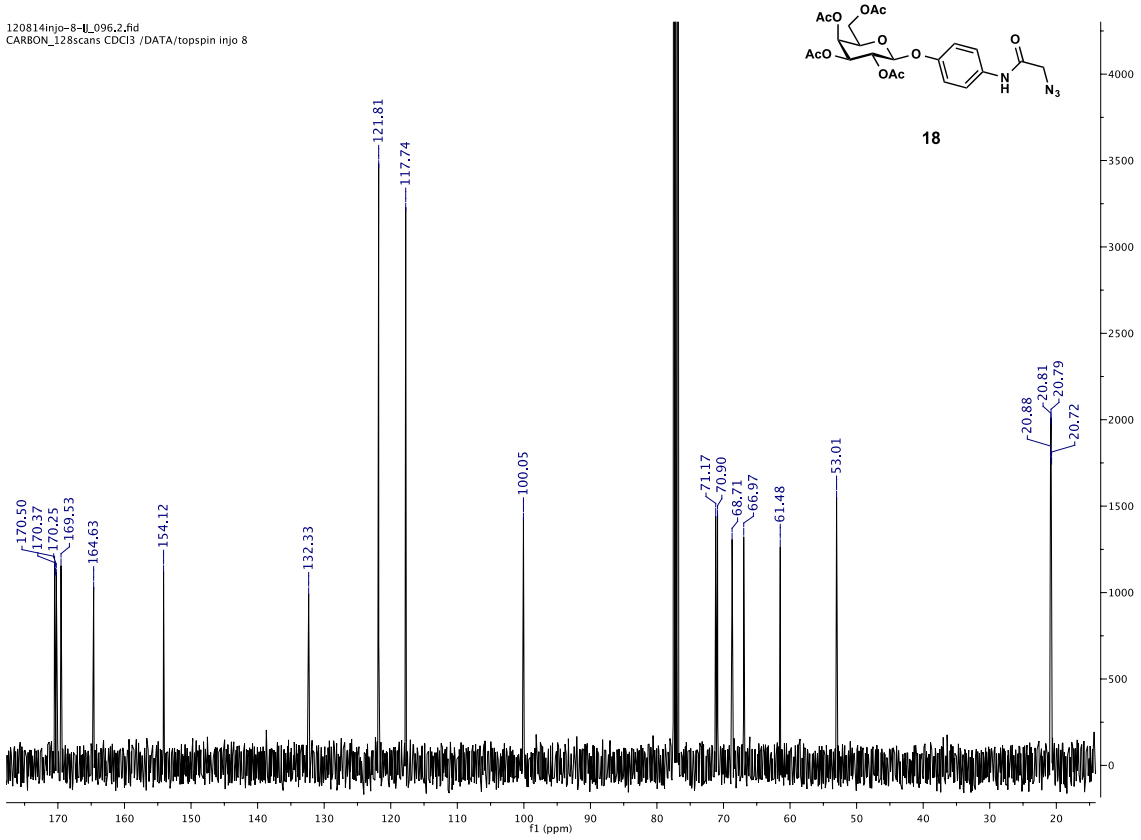
18
f1 (ppm)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170.37
170.25
169.53
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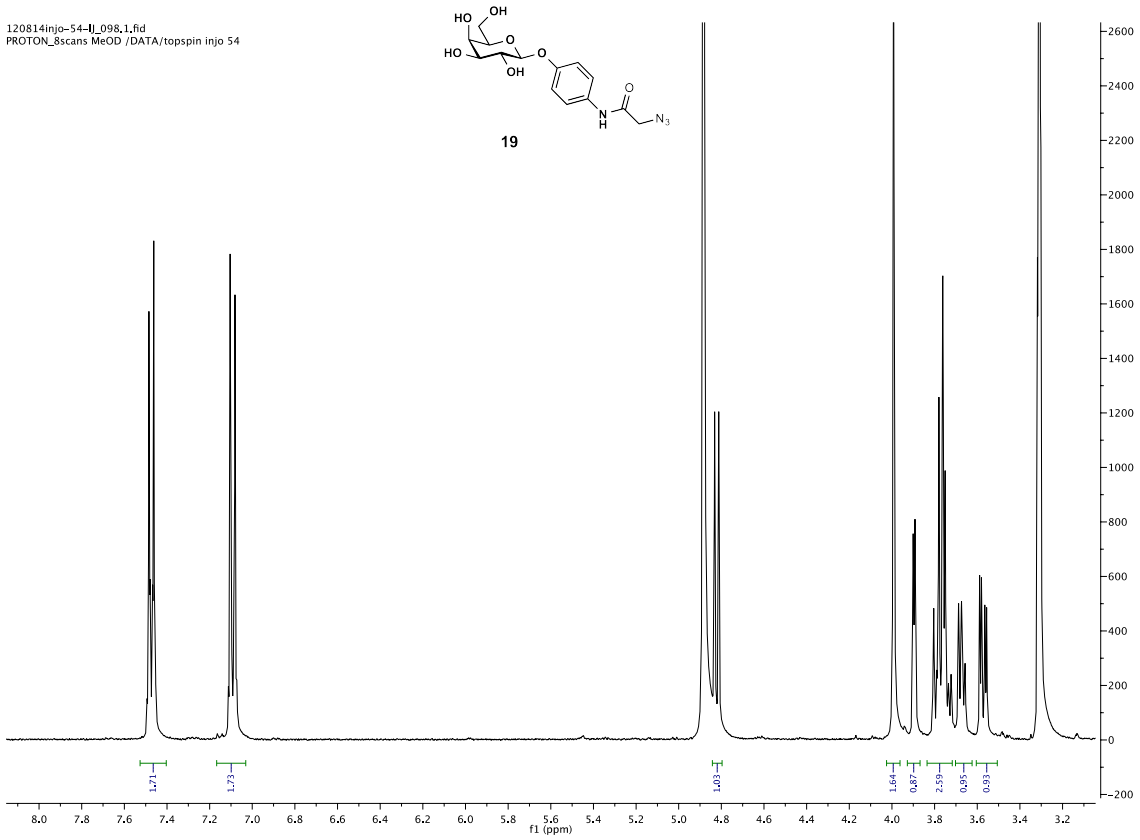
154.12
132.33
121.81
117.74
100.05
71.17
70.90
68.71
66.97
61.48
53.01
20.88
20.81
20.79
20.72
f1 (ppm)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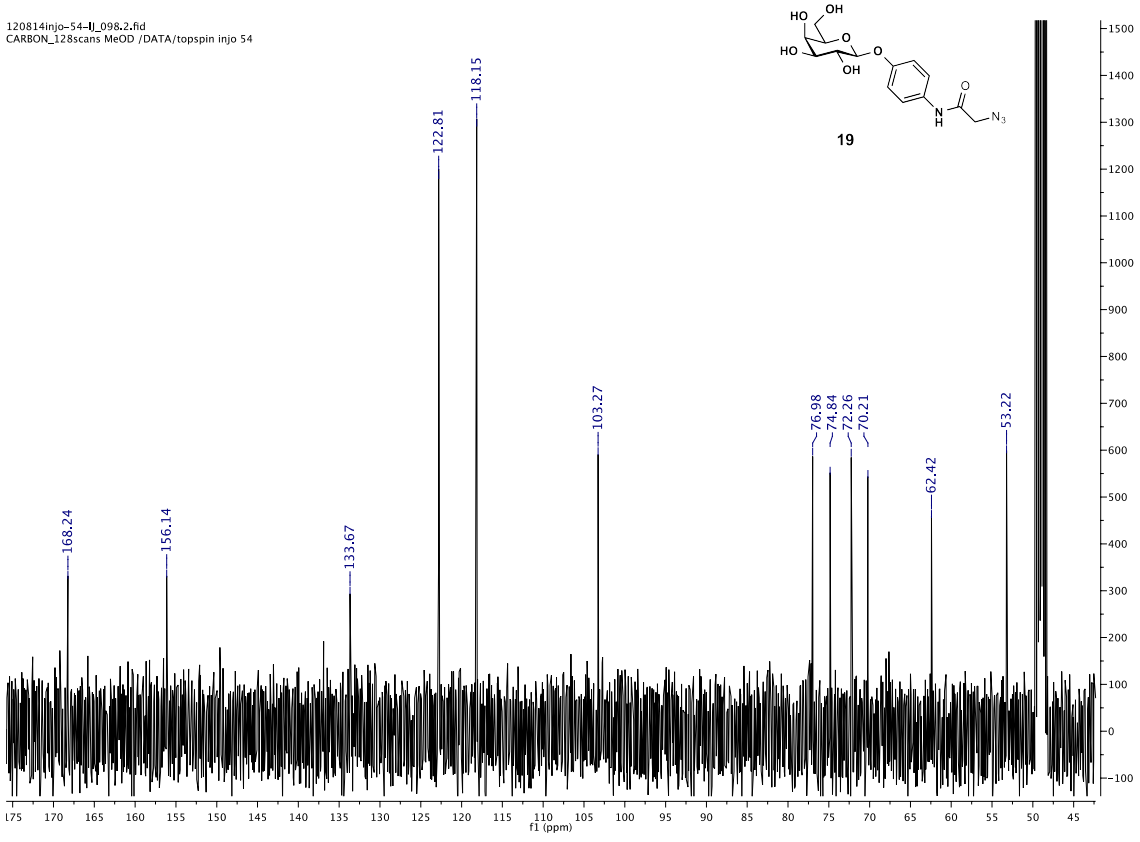
2.59
0.95
0.93
f1 (ppm)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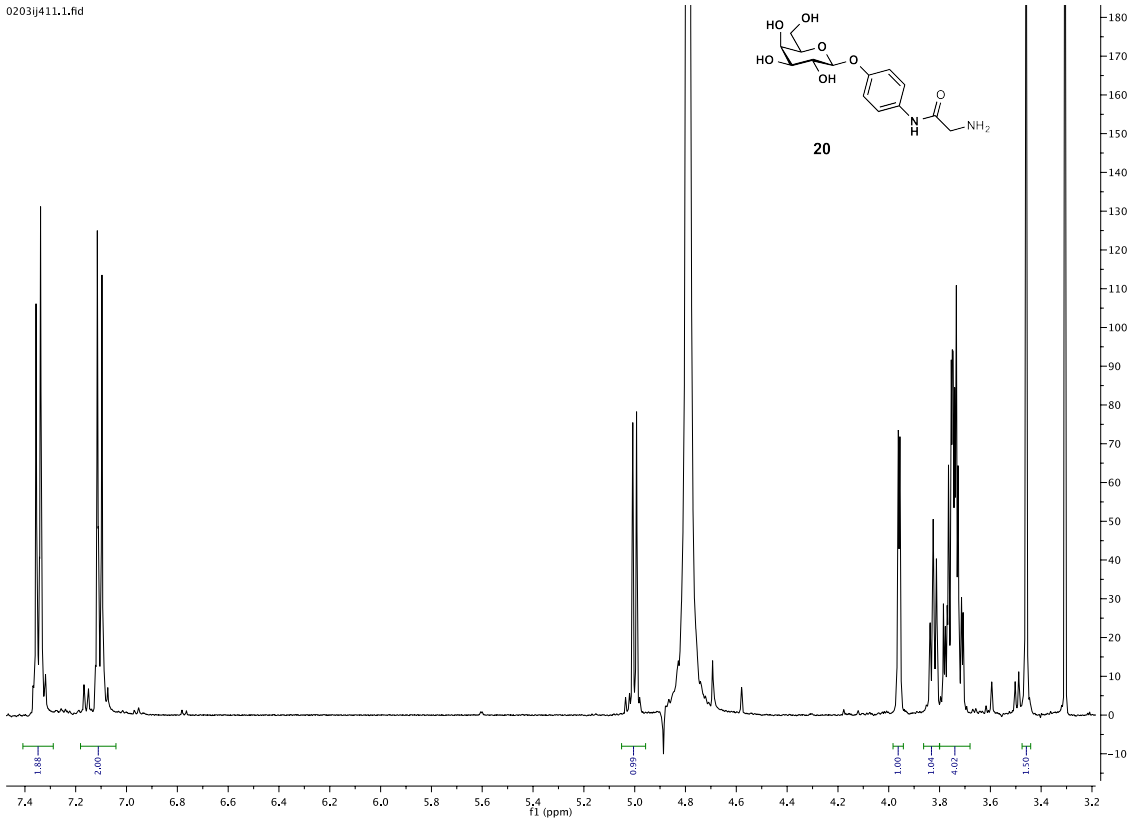
70.21
62.42
53.22
f1 (ppm)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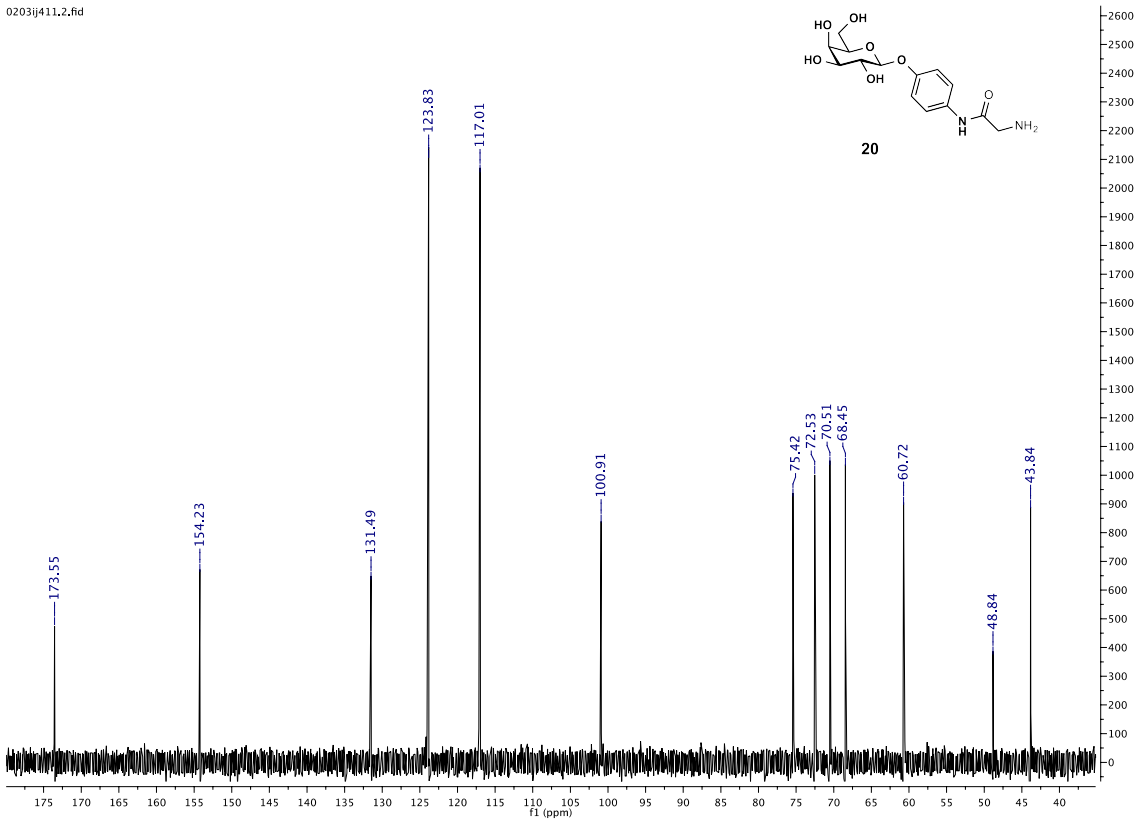
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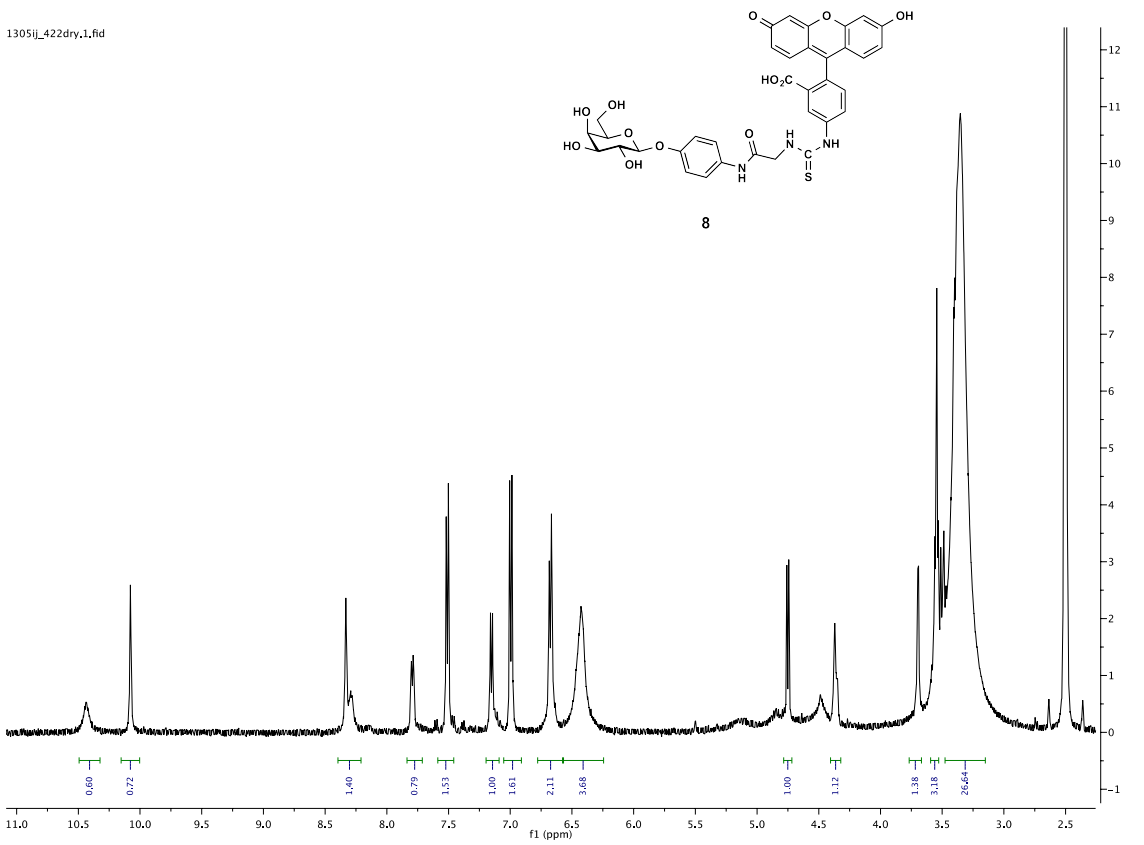
60.72
48.84
43.84
f1 (ppm)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0.72
1.40
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1.12
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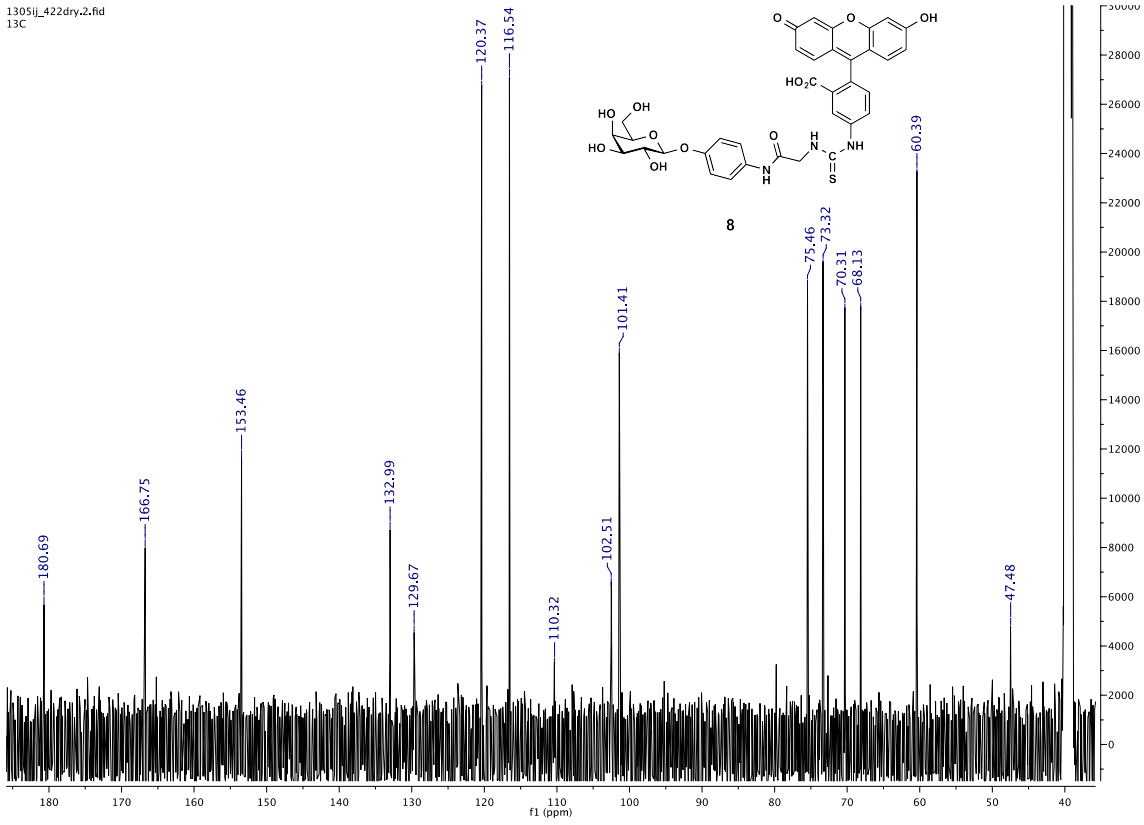
3.18
26.64
f1 (ppm)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129.67
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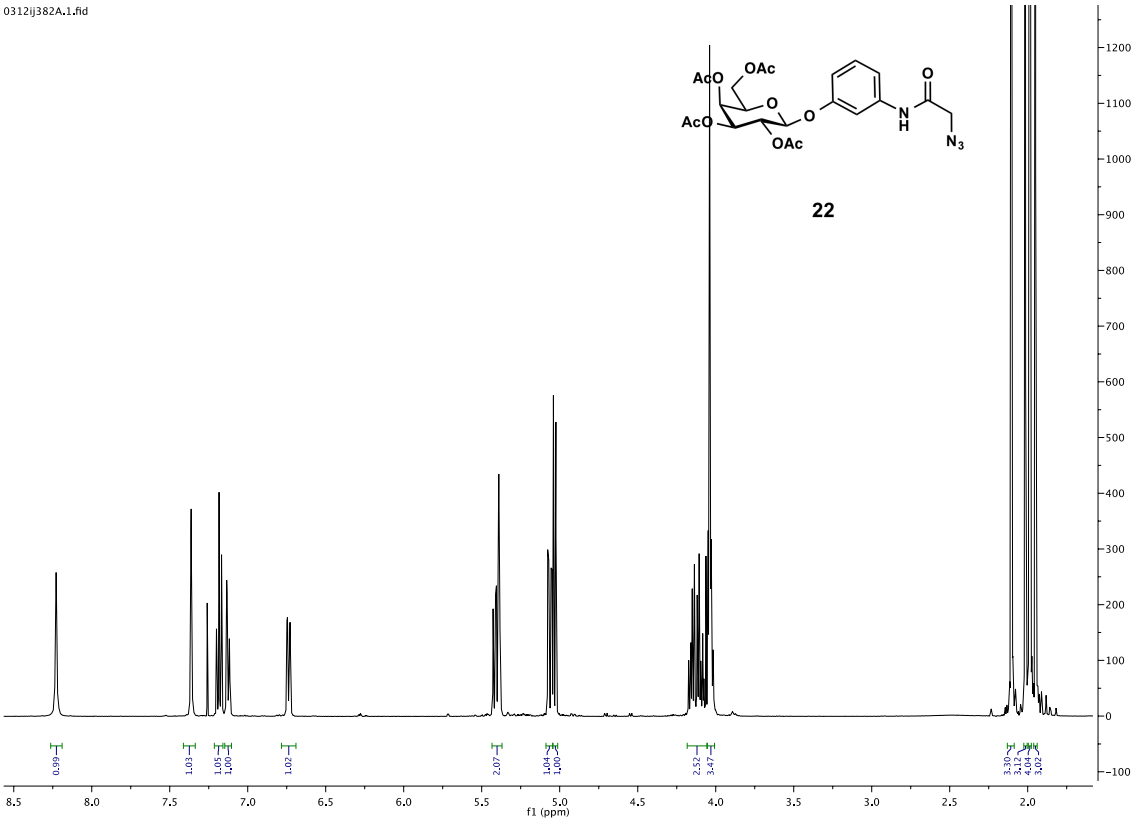
f1 (ppm)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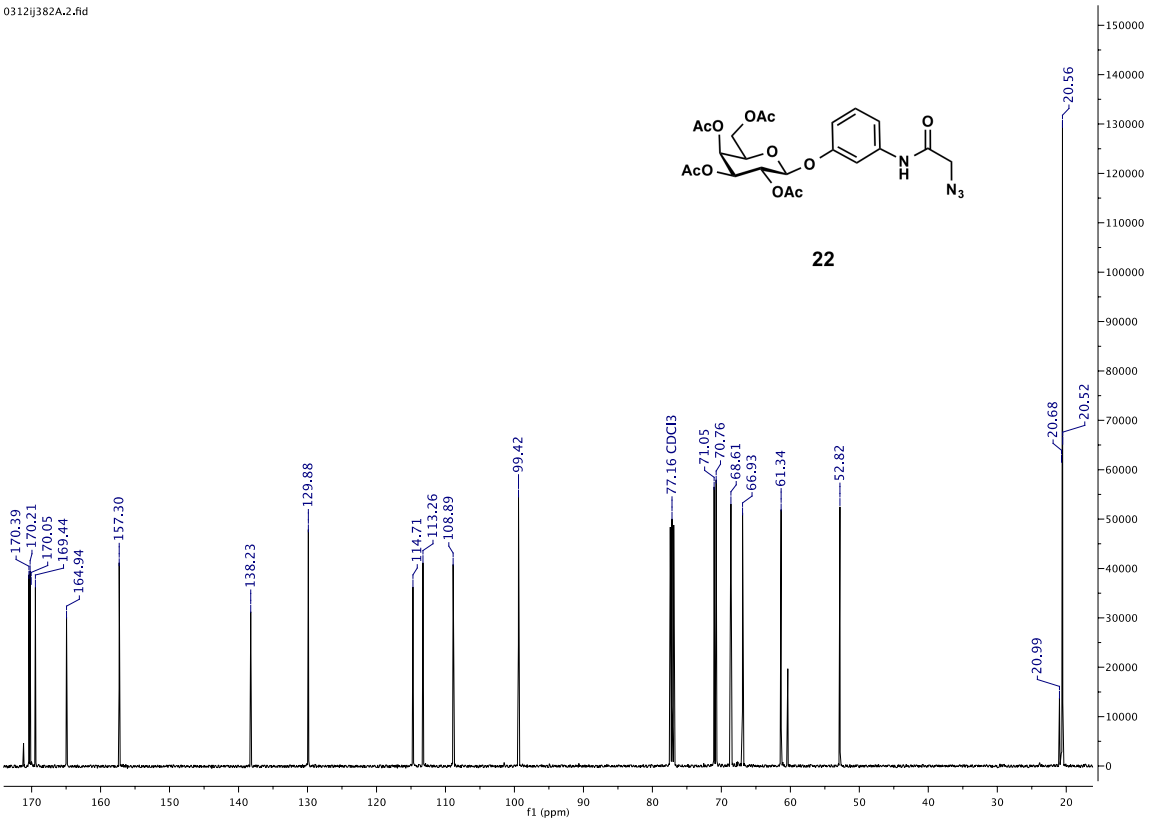
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113.26
108.89
99.42
77.16 CDCl3
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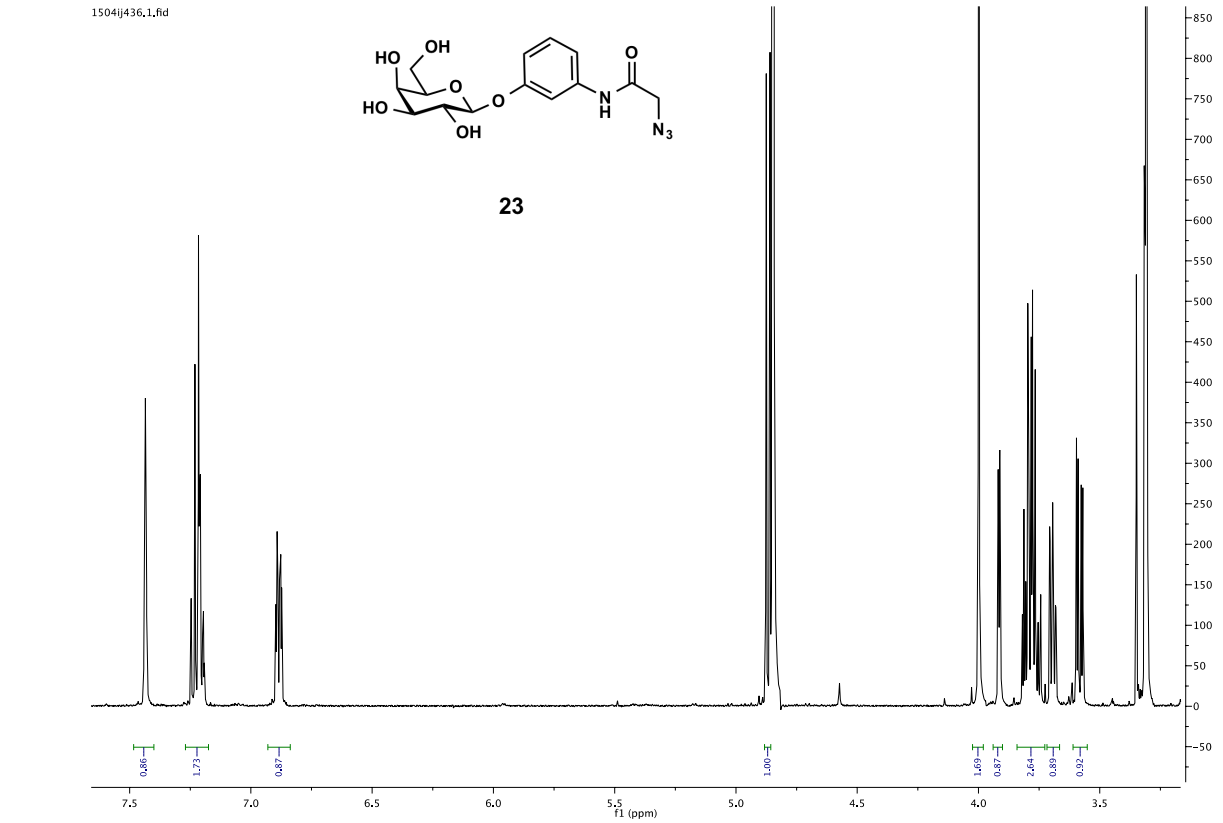
61.34
52.82
20.99
20.68
20.56
20.52
f1 (ppm)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HO
O
OH
N
H
O
N3
23
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1.73
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1.00
1.69
0.87
2.64
0.89
0.92
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7.0
6.5
6.0
5.5
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4.5
4.0
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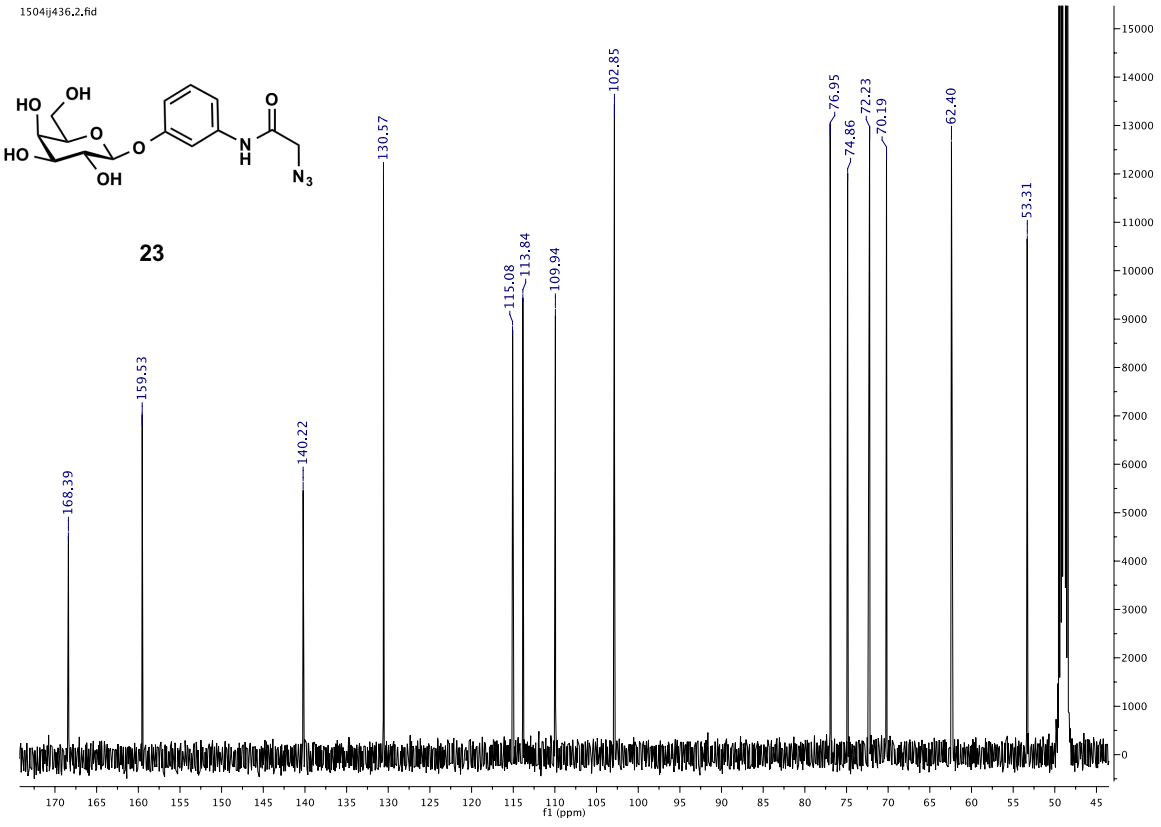
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HO
O
OH
N
H
O
N3
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159.53
140.22
130.57
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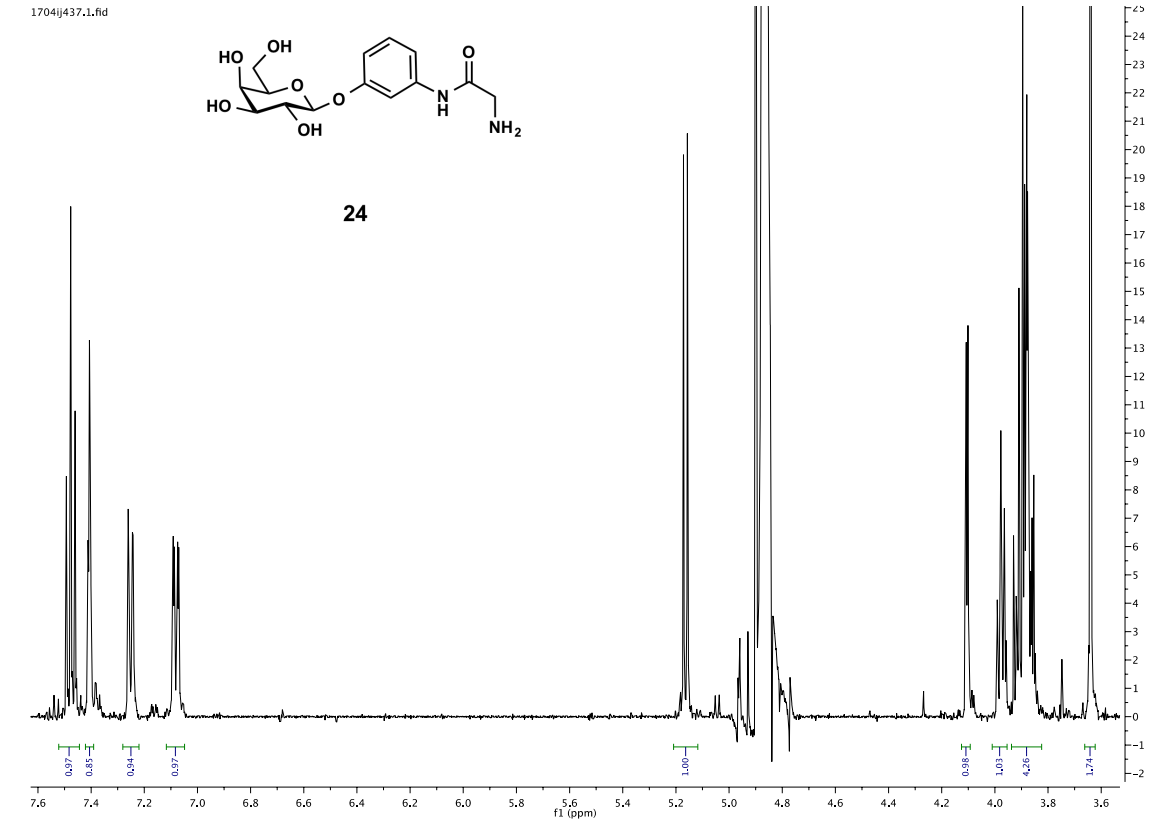
72.23
70.19
62.40
53.31
f1 (ppm)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O
OH
N
H
O
NH2
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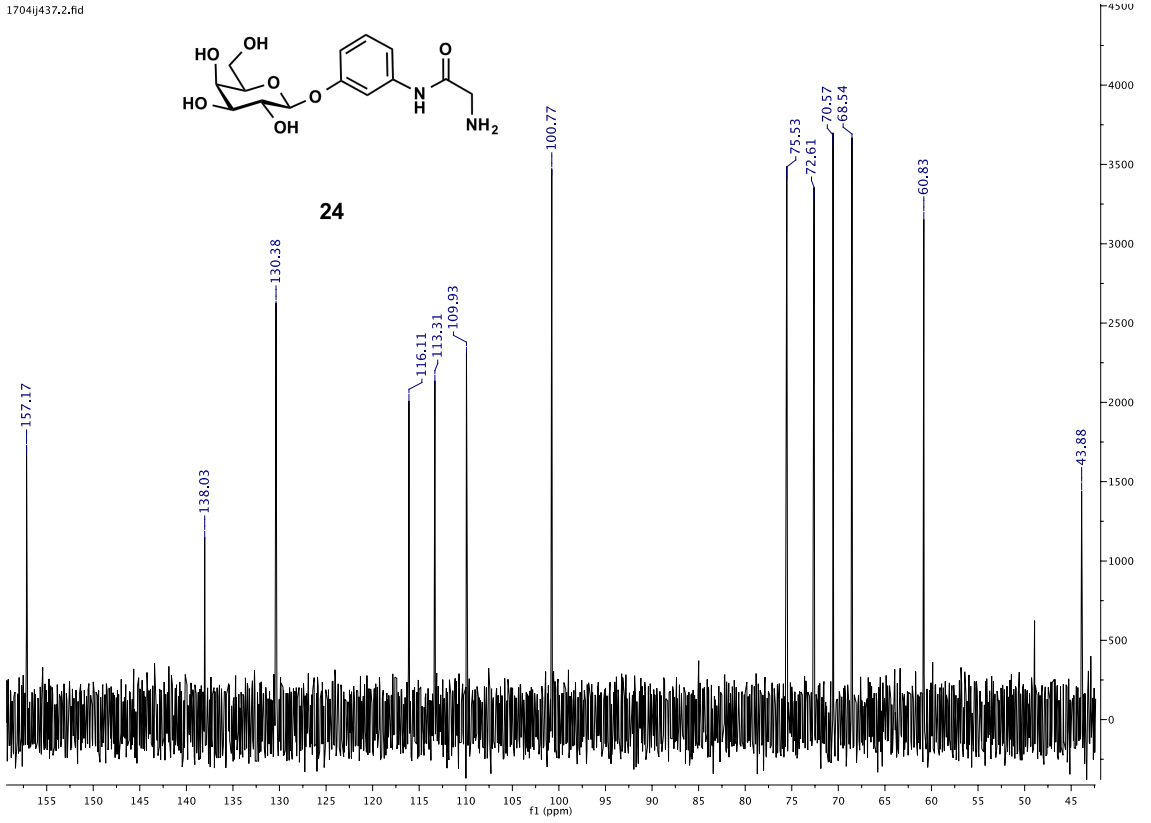
0.97
1.00
0.98
1.03
4.26
1.74
f1 (ppm)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HO
O
OH
N
H
O
NH2
24
157.17
138.03
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116.11
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109.93
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75.53
72.61
70.57
68.54
60.83
43.88
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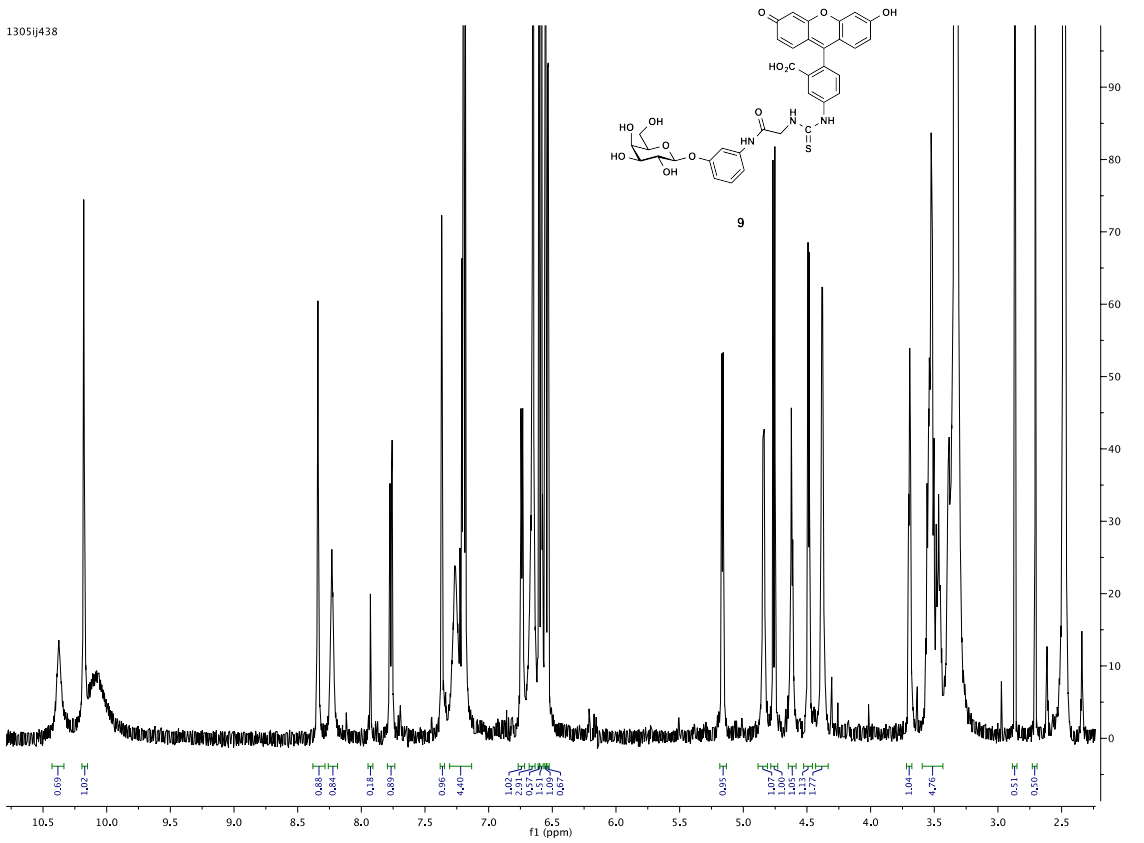
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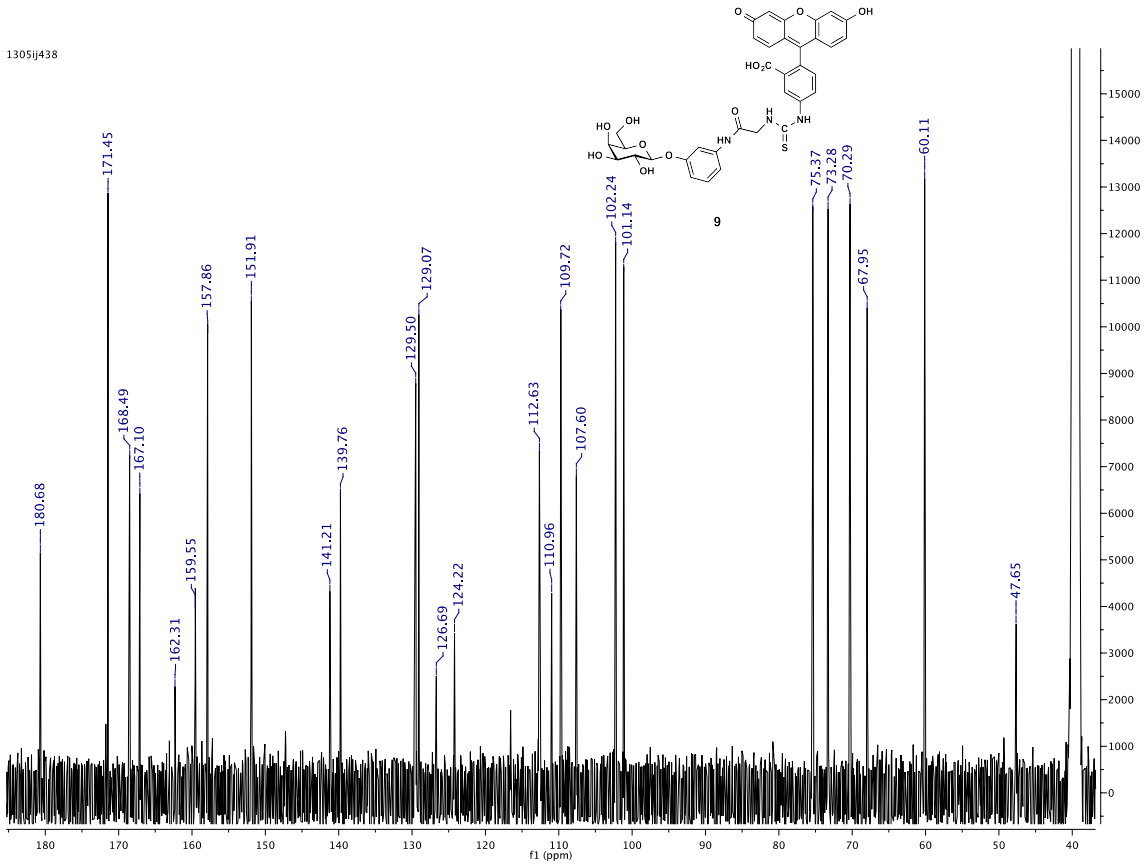
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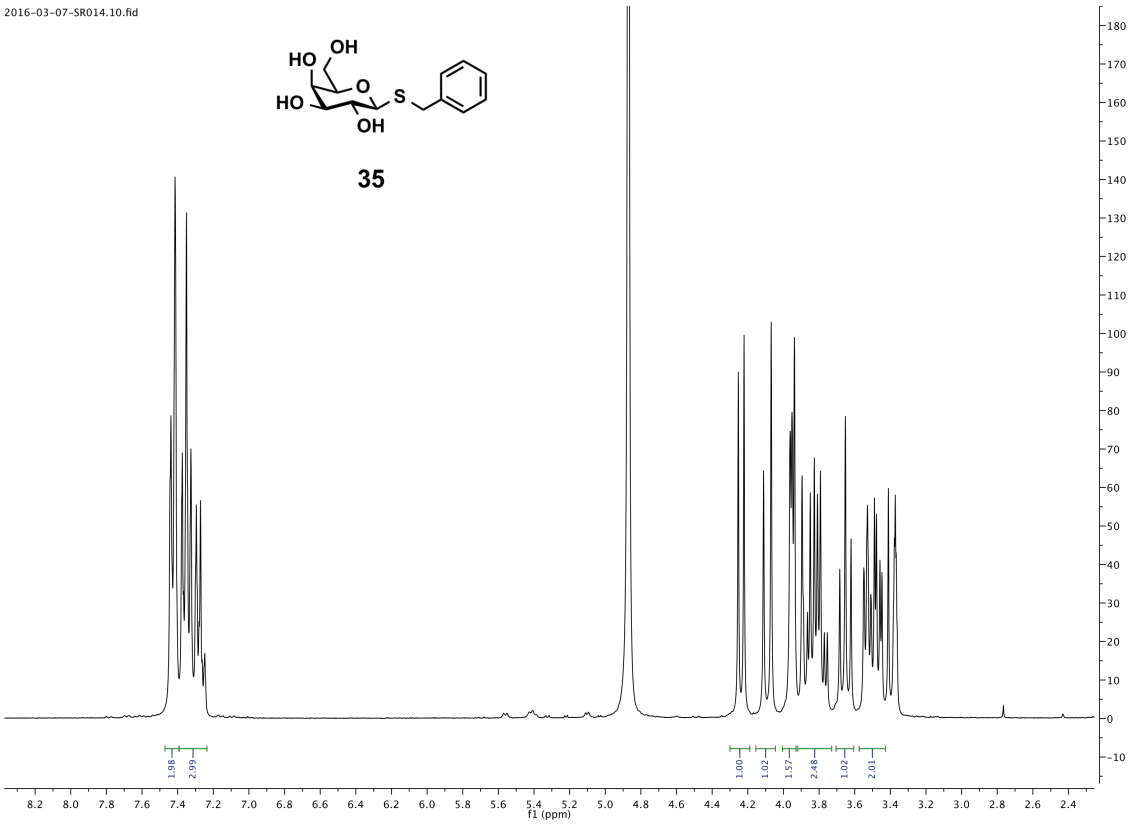
9
180.68
171.45
168.49
167.10
162.31
159.55
157.86
151.91
141.21
139.76
129.50
129.07
126.69
124.22
112.63
110.96
109.72
107.60
102.24
101.14
75.37
73.28
70.29
67.95
60.11
47.65
f1 (ppm)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OH
HO
O
S
OH
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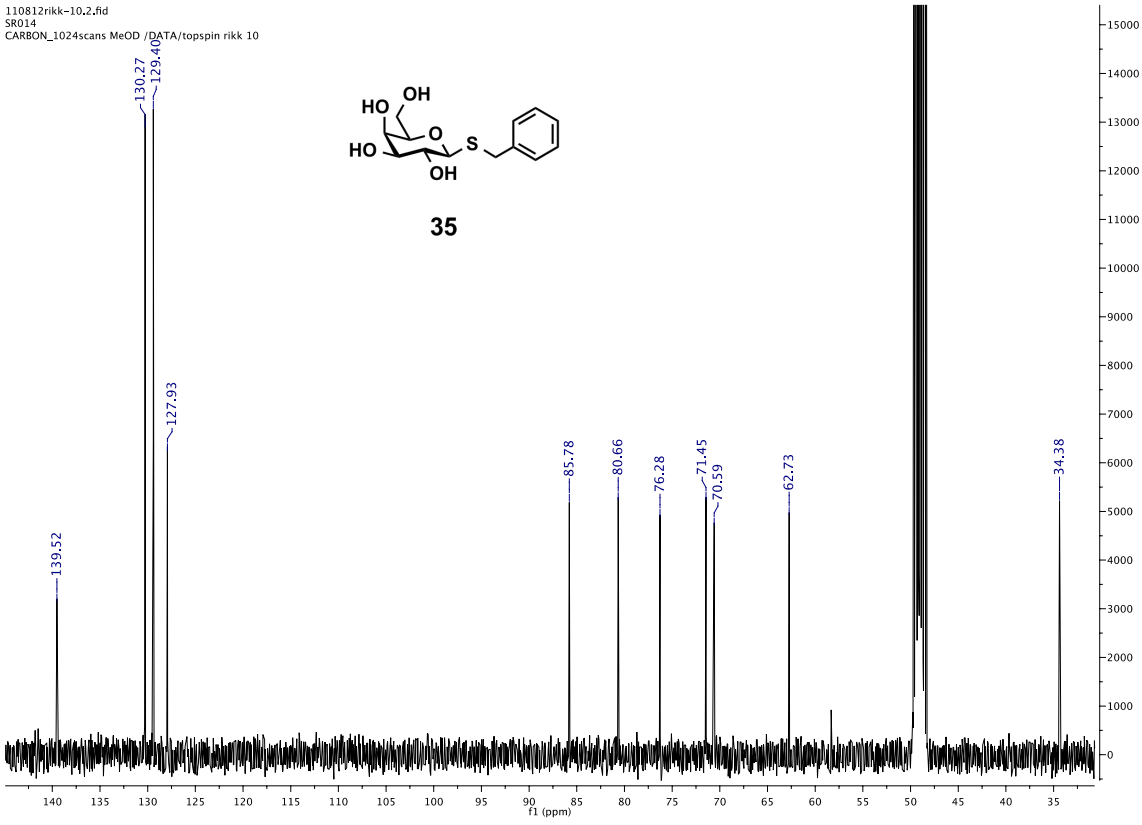
2.99
1.00
1.02
1.57
2.48
1.02
2.01
f1 (ppm)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SR014
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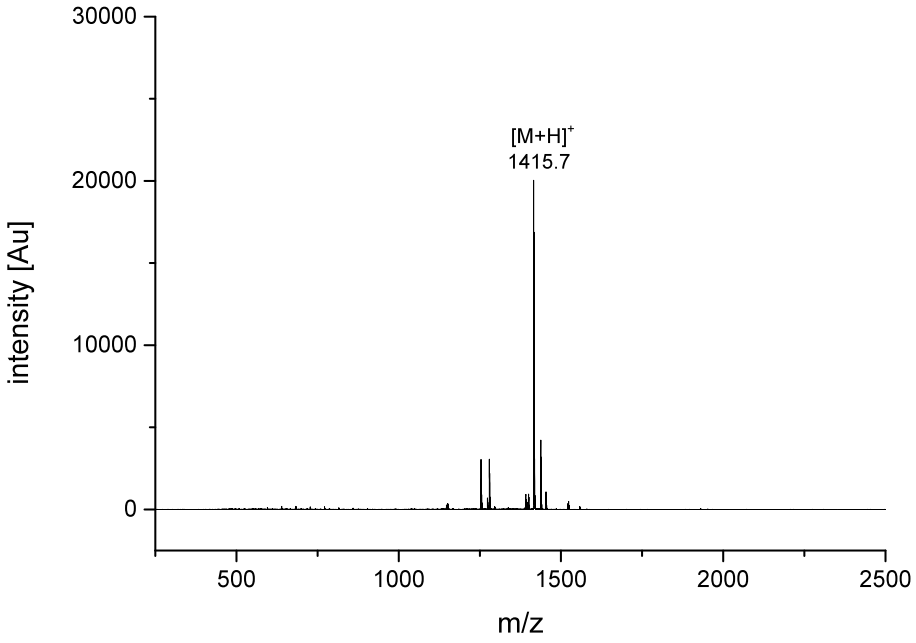
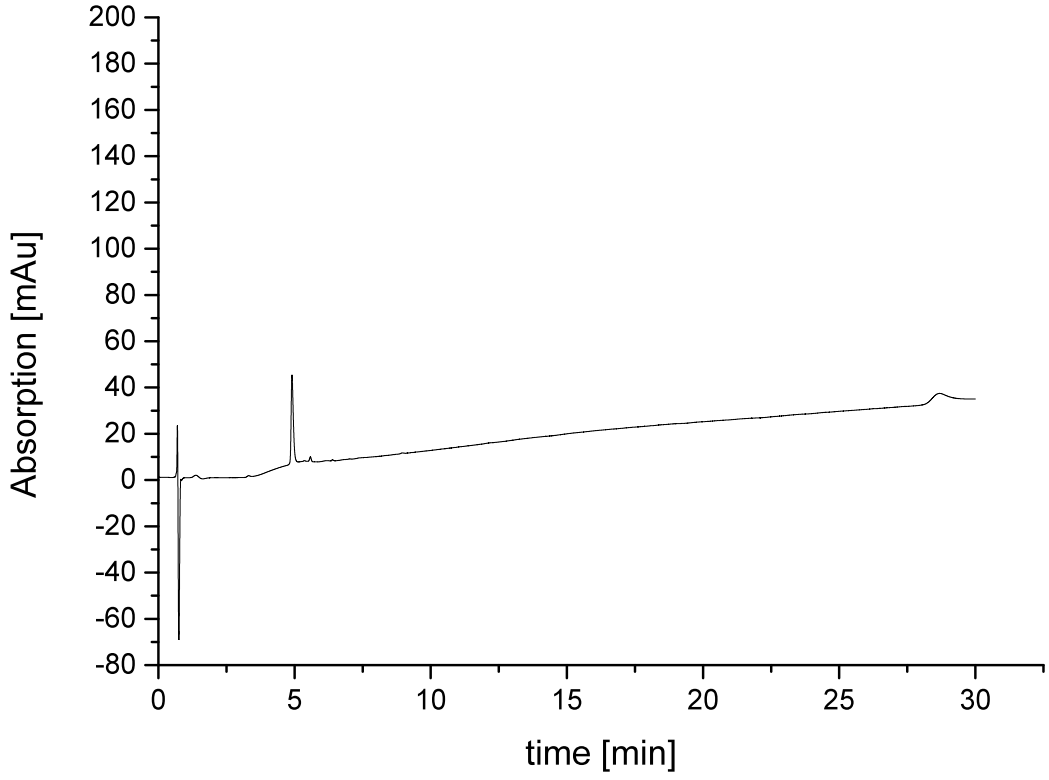
127.93
139.52
85.78
80.66
76.28
71.45
70.59
62.73
34.38
HO
OH
HO
O
S
OH
35
f1 (ppm)

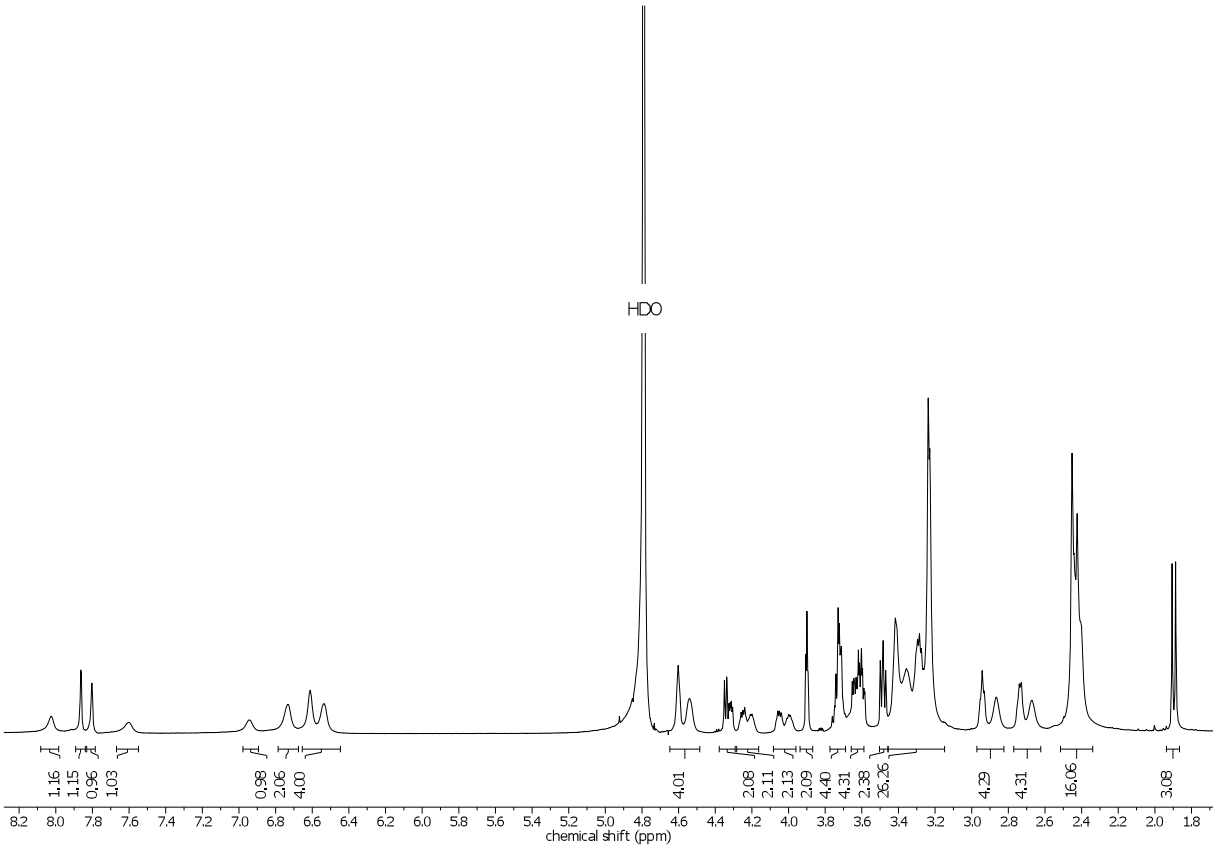
MALDI-TOF-MS spectrum of β-D-Gal(1,4)-4-SDS (**49**)



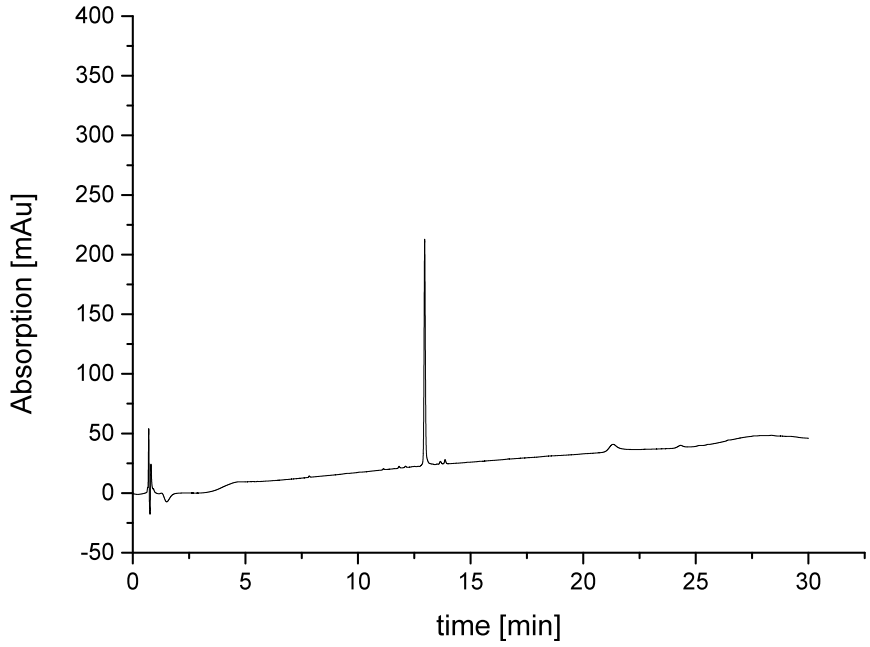
RP-HPLC chromatogram (5/95 MeCN/H_2O → 95/5 MeCN/H_2O in 30 minutes) of β-D-Gal(1,4)-4-SDS (**49**) after purification by preparative HPLC. Signals were determined at 214 nm.



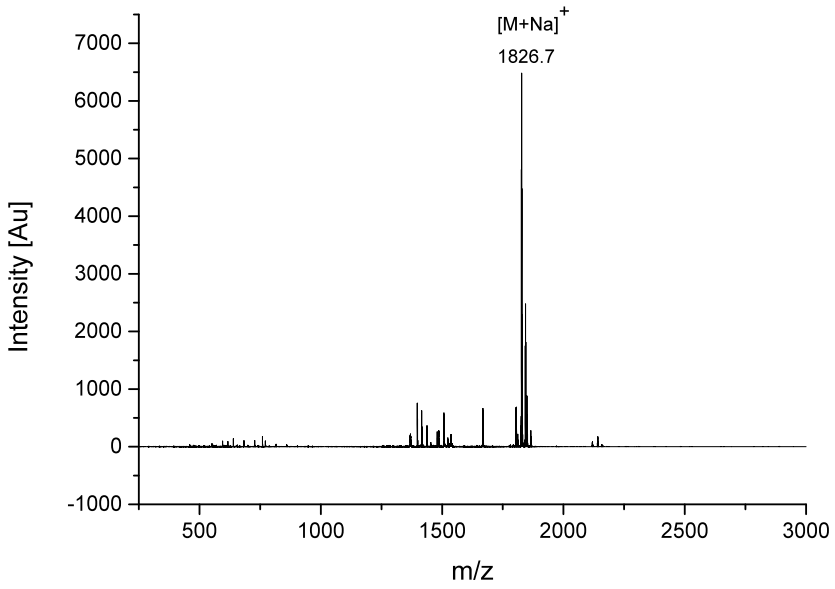
^{1}H NMR trace of fluorescent divalent LecA ligand **50** (600 MHz, D_2O).



RP-HPLC chromatogram (5/95 MeCN/H_2O → 95/5 MeCN/H_2O in 30 minutes) of β-D-Gal(1,4)-4-SDS-FITC (**50**) after purification by preparative HPLC. Signals were determined at 214 nm.



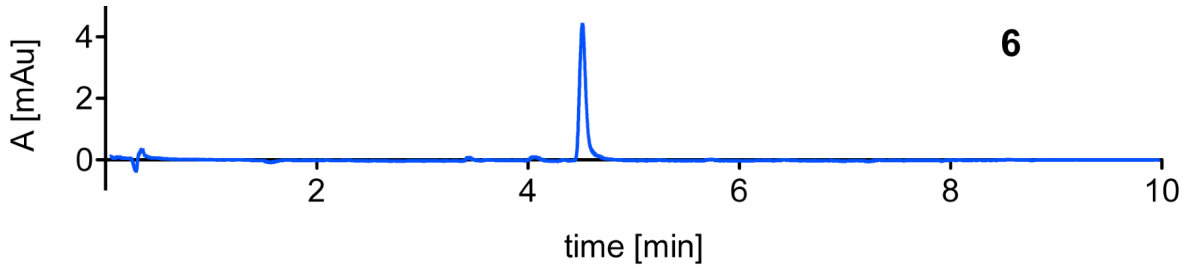
MALDI-TOF-MS spectrum of β-D-Gal(1,4)-4-SDS-FITC (**50**)

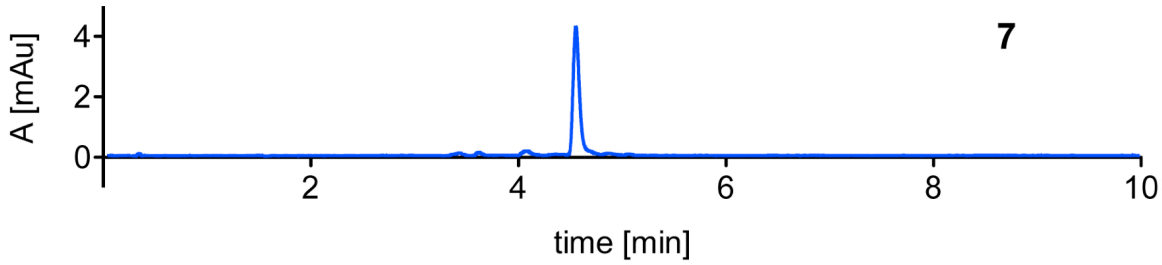


HPLC analysis of all fluorescent ligands (**6**-**9** and **50**)

Chromatographic separation was performed on a Dionex Ultimate 3000 HPLC (Thermo Scientific, Germany) with UV detection at 254 nm using a RP-18 column (100/2 Nucleoshell RP18plus, 2.7 μM from Machery Nagel, Germany) as stationary phase.

LCMS grade distilled MeCN and double distilled H_2O were used as mobile phases supplemented with 0.1% HCO_2H (MS grade). In a gradient run, an initial concentration of 5% MeCN in H_2O was increased to 65% during 10 min at a flow rate 800 μL/min. The injection volume was 10 μL of 1 μM compound in H_2O/TBS buffer = 10:1. Chromatograms are blank run corrected.


A [mAu]
4
2
0
2
4
6
8
10
time [min]
6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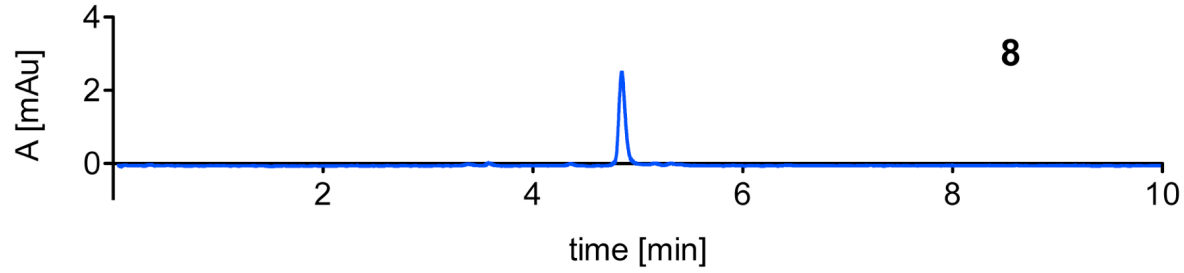
4
2
0
2
4
6
8
10
time [min]
7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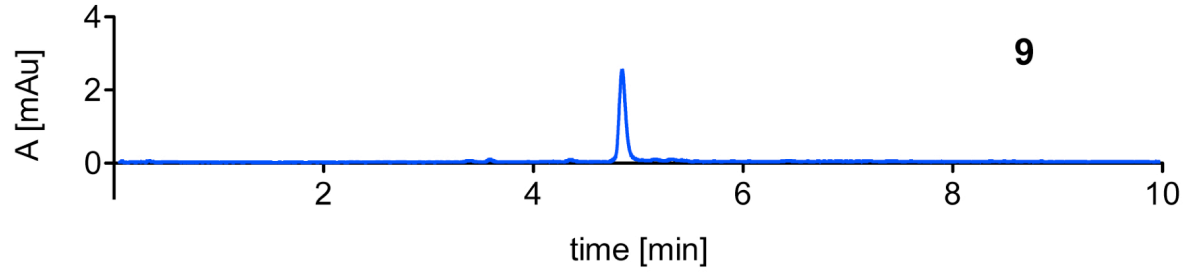
4
2
0
2
4
6
8
10
time [min]
8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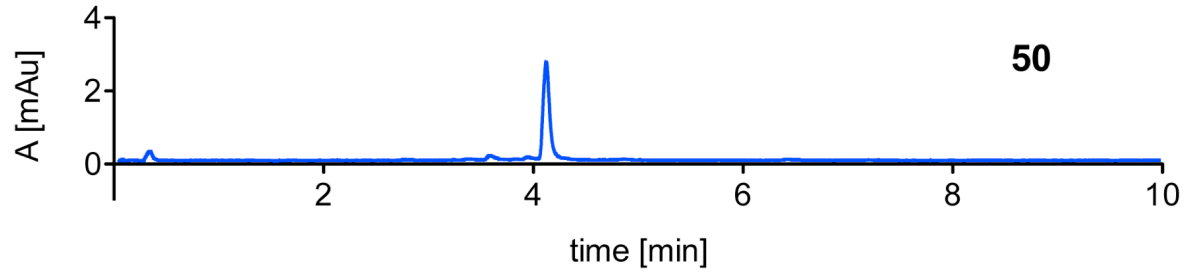
4
2
0
2
4
6
8
10
time [min]
9


A [mAu]
4
2
0
2
4
6
8
10
time [min]
50