Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting information:

Aromatic Thioglycoside Inhibitors Against the Virulence Factor LecA from *Pseudomonas aeruginosa*

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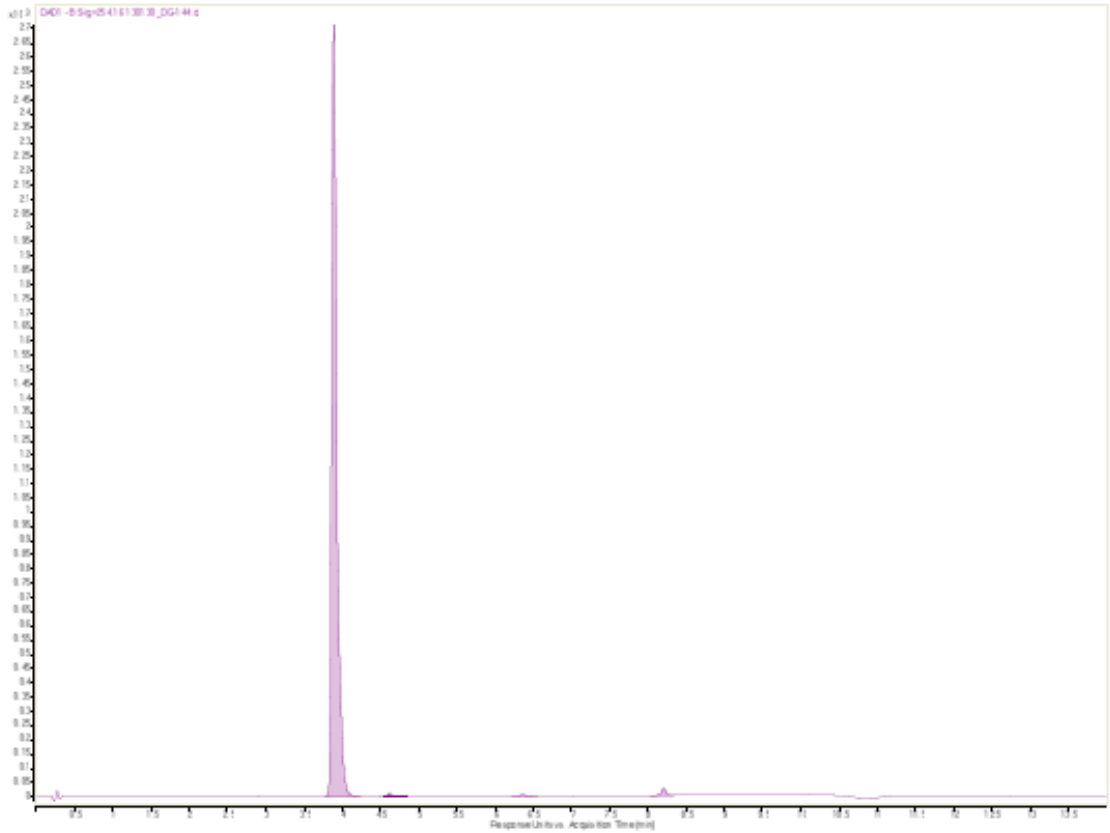
Table of content

Table . Data collection and refinement statistics. Numbers between parentheses refer to the outer shell.

	LecA-**11**
Beamline (wavelength, Å)	BM14/0.976
Spacegroup	$P3_221$
Cell dimensions *a*,*b*,*c* (Å) α, β, γ (deg.)	54.33 54.33 3 90.50 90.0 90.0 120.0
Resolution (Å)	40.00-2.15 (2.27-2.15)
Measured/ Unique reflections	132611/37963
Average multiplicity	3.5 (3.5)
R_{merge}	0.045 (0.386)
Completeness (%)	99.5 (99.9)
Mean I / σI	14.4 (2.3)
Wilson B	40.0
R_{cryst}/ R_{free}	21.4/25.9
R_{msd} bonds, Å	0.014
R_{msd} angles,°	1.66
Rmsd chiral, $Å^3$	0.102
Protein atoms /per chain Bfac $Å^2$	907/901/901/901 40.4/44.4/50.2/44.3
Water molecules Bfac, $Å^2$	235 43.7
Ligand atoms Bfac, $Å^2$	22/22/22/22 42.4/55.7/63.5/48.3
Calcium atoms Bfac, $Å^2$	1/1/1/1 39.0/51.0/64.6/47.5
PDB code	4A6S

130130 – Cpd 11-(DG144) Percent purity by LC (UV 254)



Peak	RT	Area	Area%	Height	Width	purity
1	3,89	13006,15	100	2715,27	0,48	98,77%
2	4,62	48,03	0,37	12,53	0,29	0,37%
3	6,37	22,83	0,18	5,78	0,35	0,18%
4	8,21	91,2	0,7	23,67	0,31	0,69%
			101,25			

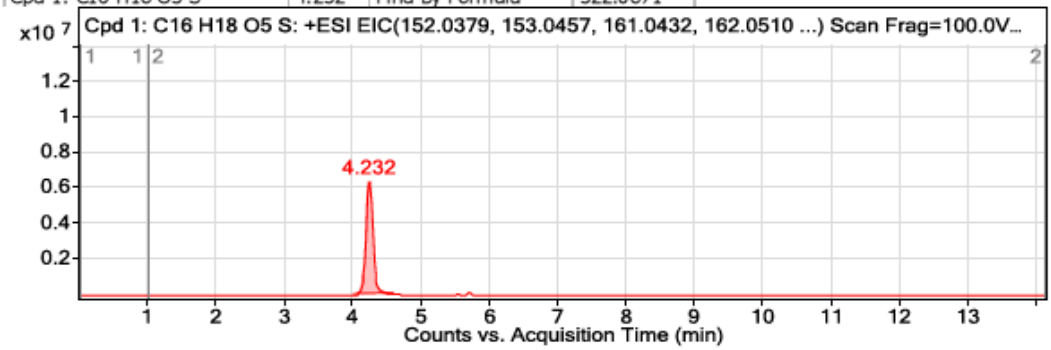
Qualitative Compound Report

Data File	Roy_Chichi_DG-144_20130129.d	**Sample Name**	Cpd 11: DG-144
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Vladimir_LC_10-95-6_pos_100a2000.m	**IRM Calibration Status**	Success
DA Method	Default.m	**Comment**	

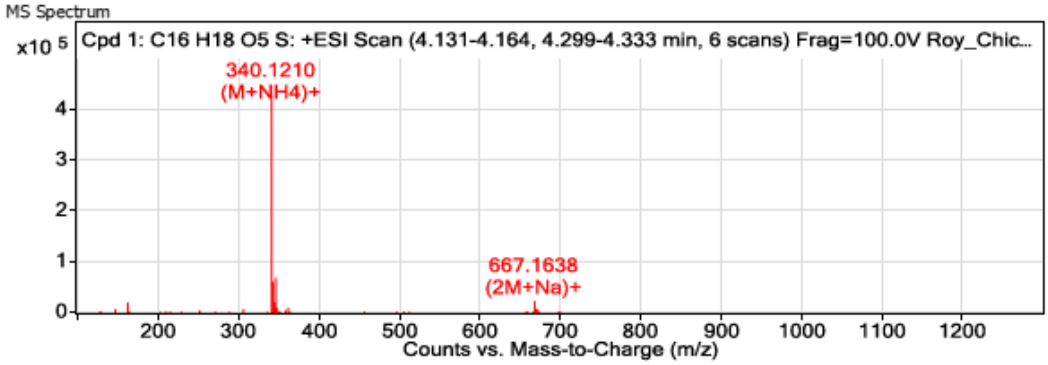
Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C16 H18 O5 S	4.232	322.0871	426982	C16 H18 O5 S	322.0875	-1.13

Compound Label	RT	Algorithm	Mass
Cpd 1: C16 H18 O5 S	4.232	Find By Formula	322.0871

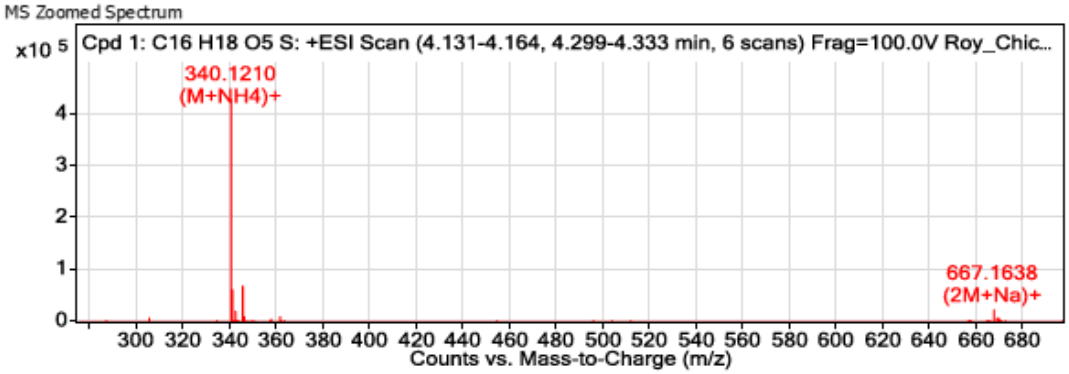


MS Spectrum



Qualitative Compound Report

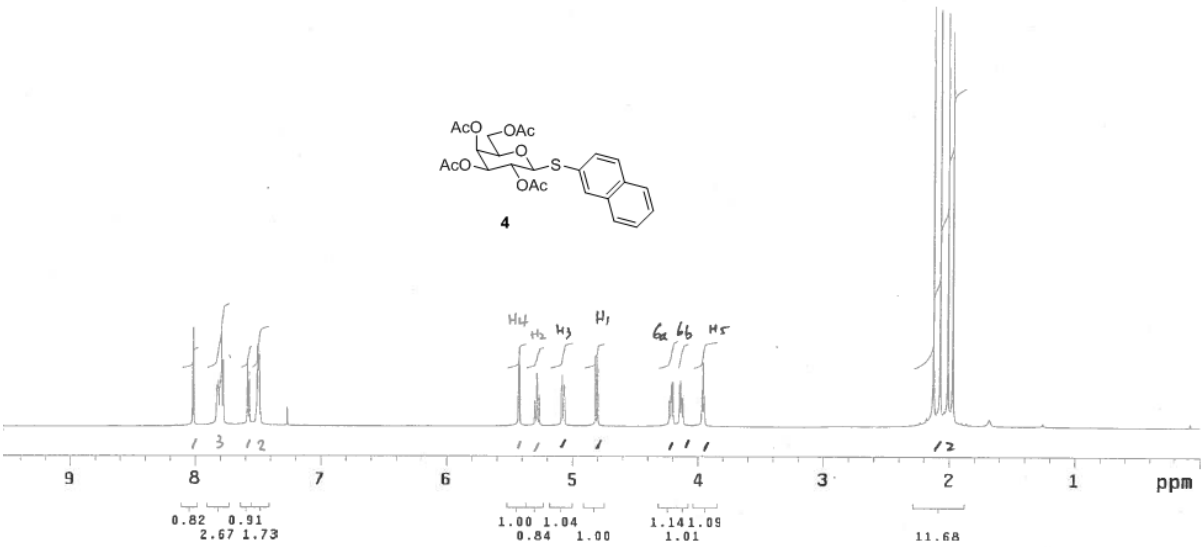
MS Zoomed Spectrum

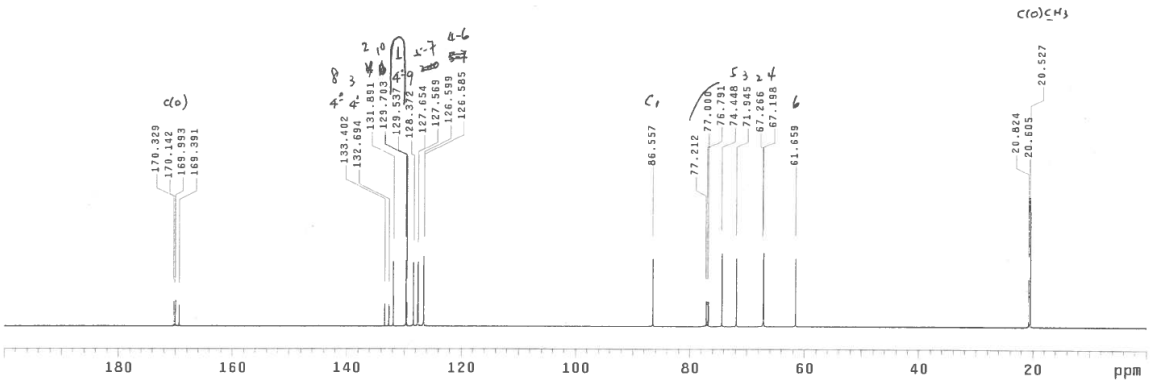


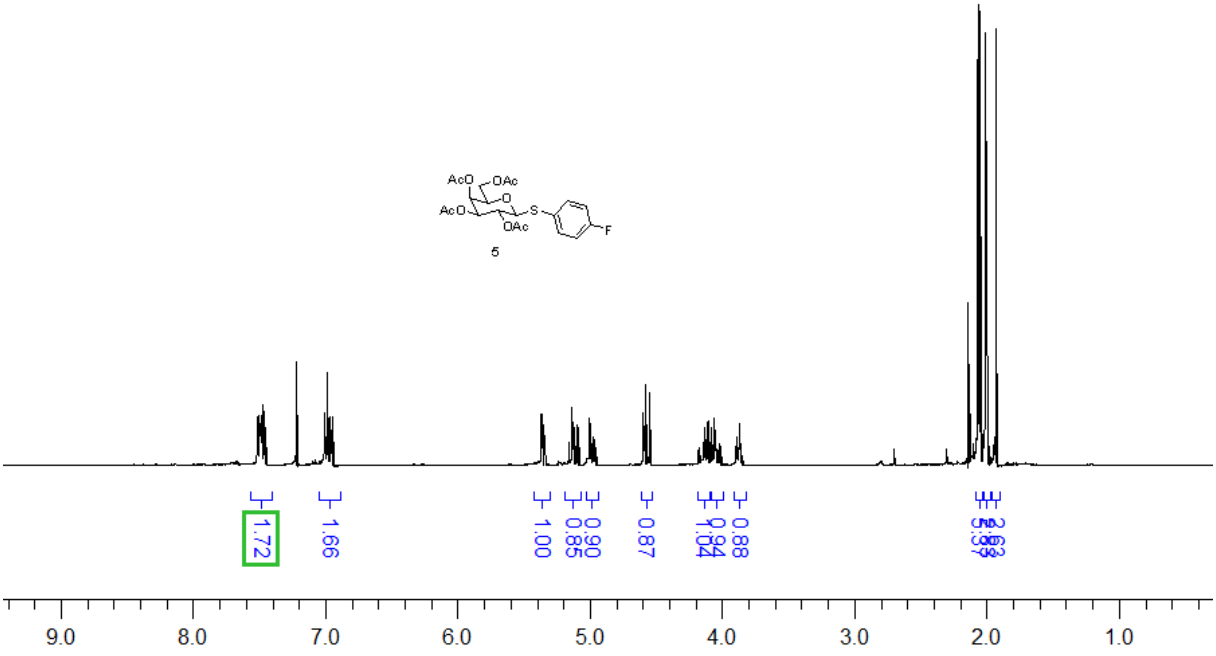
MS Spectrum Peak List

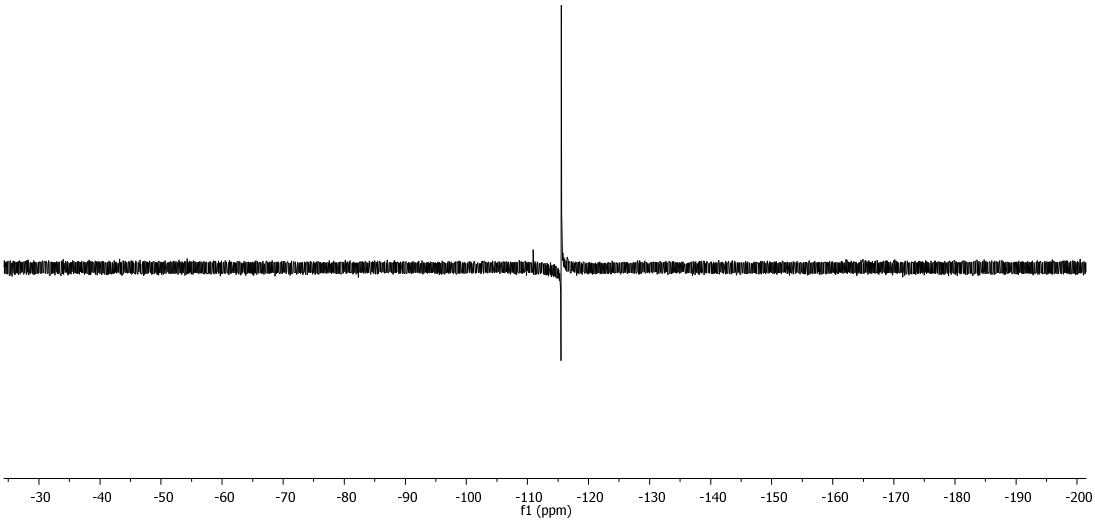
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
305.0836	305.0842	-2.06	1	7015	C16 H17 O4 S	(M+H)+[-H2O]
322.0876	322.0869	1.98	1	230	C16 H18 O5 S	M*+
323.0951	323.0948	0.99	1	257	C16 H19 O5 S	(M+H)+
340.121	340.1213	-1.07		426998	C16 H22 N O5 S	(M+NH4)+
340.3517				26881		
341.124	341.1244	-1.31		63082	C16 H22 N O5 S	(M+NH4)+
342.1199	342.1208	-2.46		21069	C16 H22 N O5 S	(M+NH4)+
345.0762	345.0767	-1.45		75654	C16 H18 Na O5 S	(M+Na)+
361.0502	361.0507	-1.14	1	9851	C16 H18 K O5 S	(M+K)+
667.1638	667.1642	-0.56	1	22886	C32 H36 Na O10 S2	(2M+Na)+

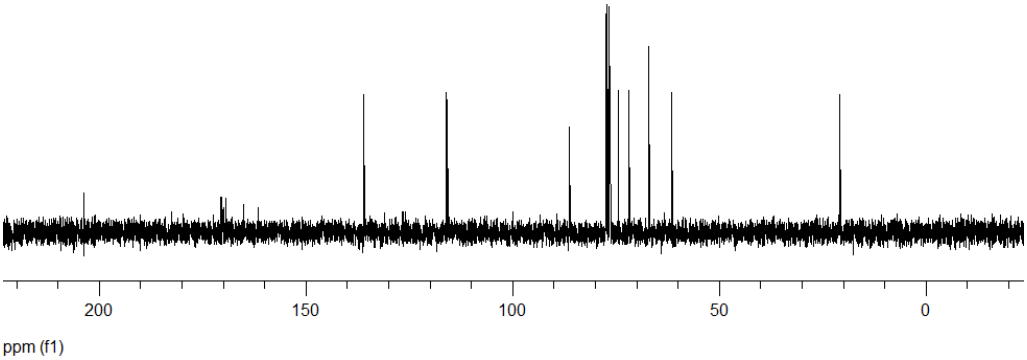
--- End Of Report ---

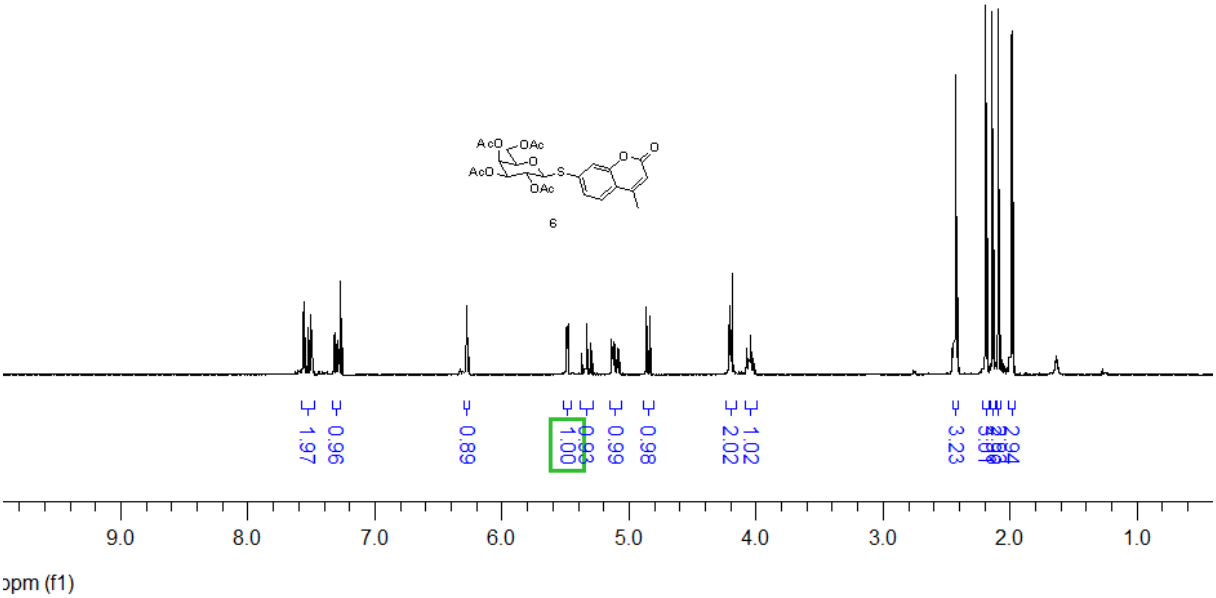








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AcO
O
S
OAc
O
O
6
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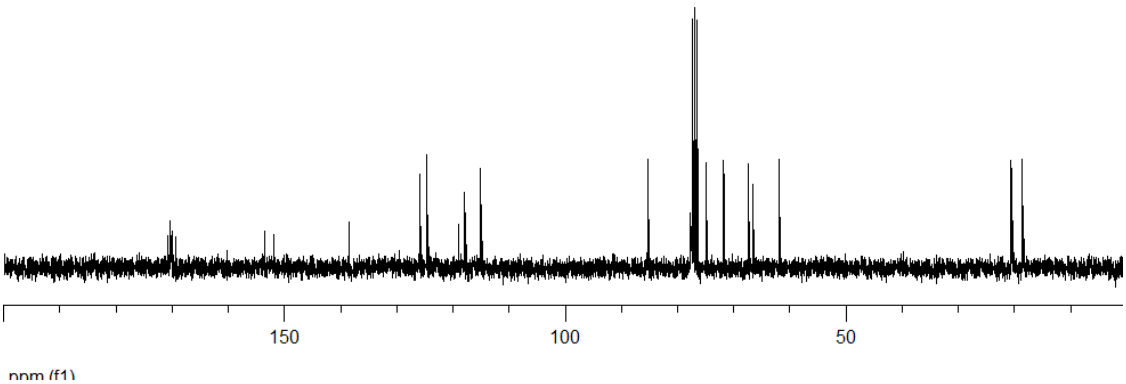
0.96
0.89
1.00
0.99
0.98
2.02
1.02
3.23
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)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100
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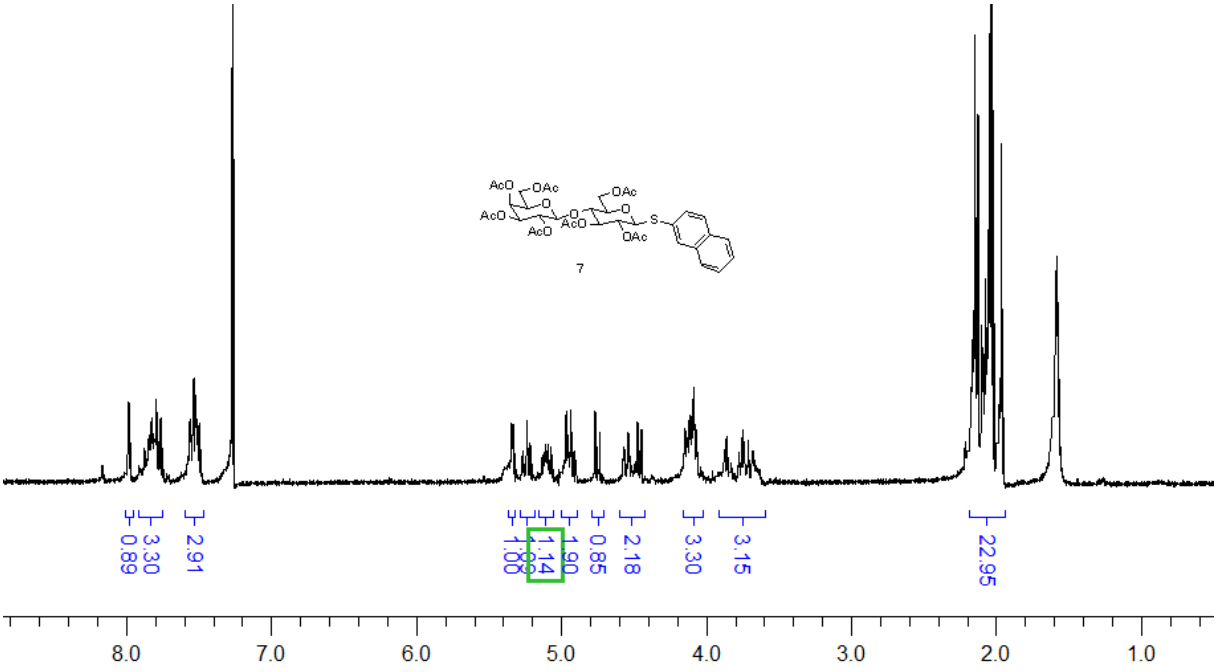

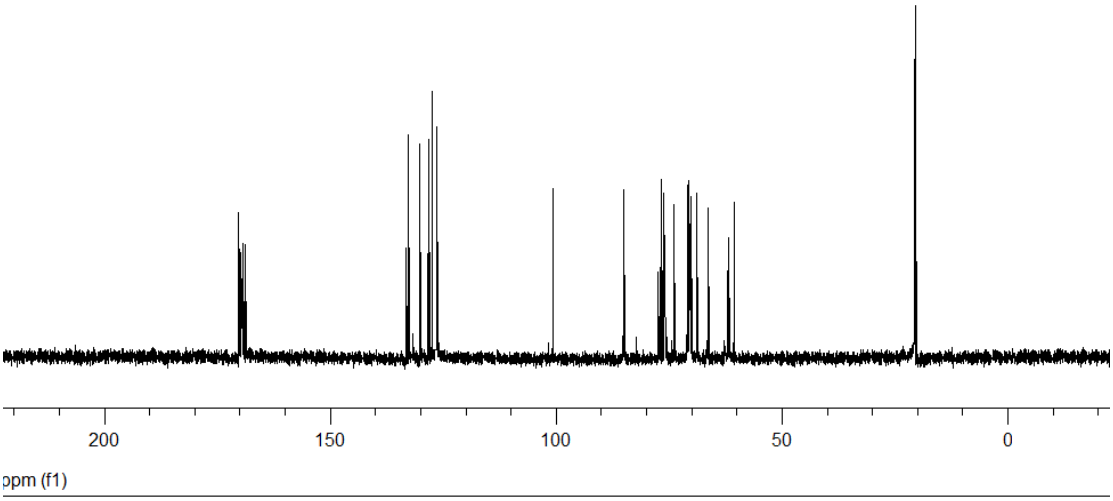

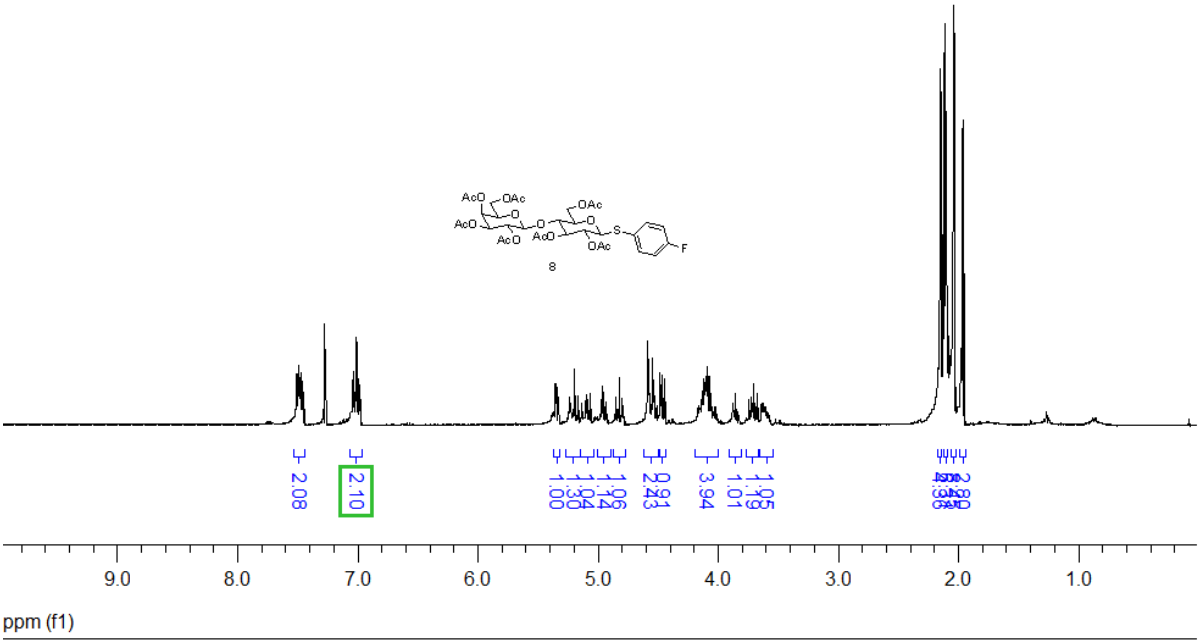
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OAc
AcO
AcO
AcO
AcO
OAc
OAc
S
F
8
2.08
2.10
1.00
1.05
1.14
1.06
1.04
1.05
2.43
0.91
3.94
1.01
1.05
1.08
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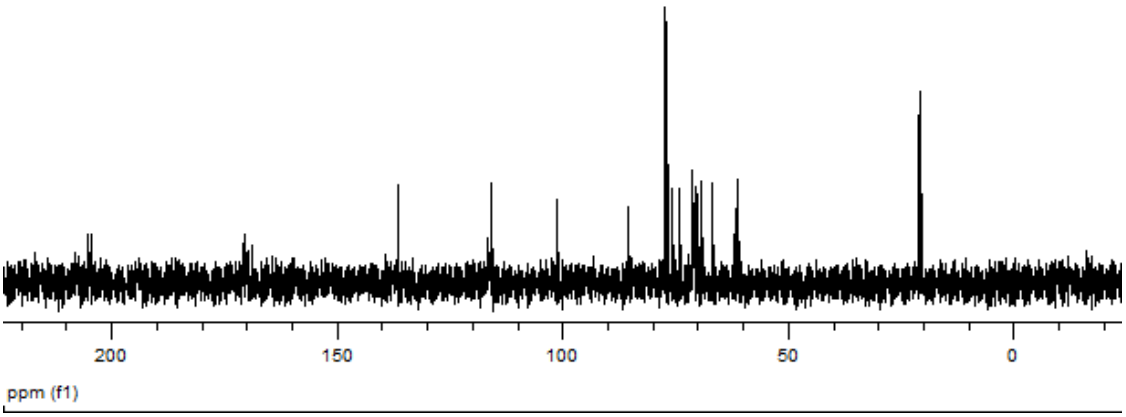
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)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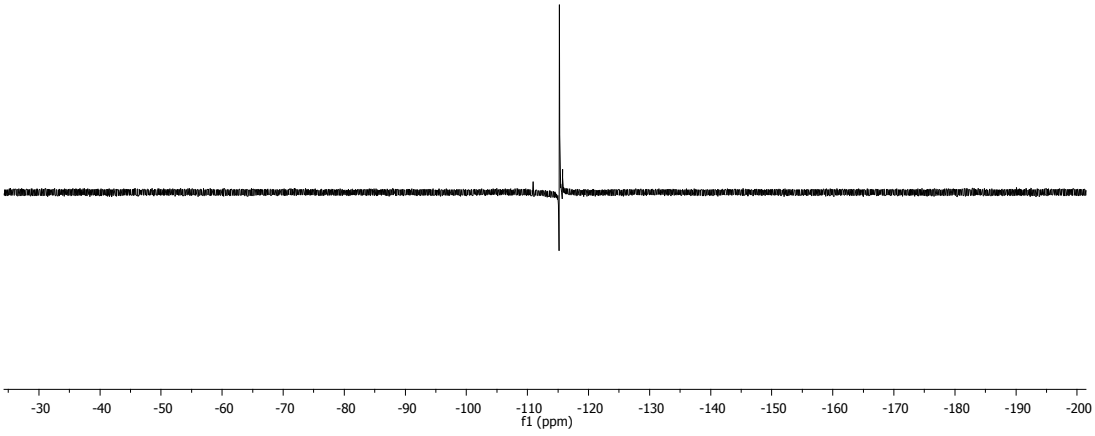
150
100
50
0
ppm (f1)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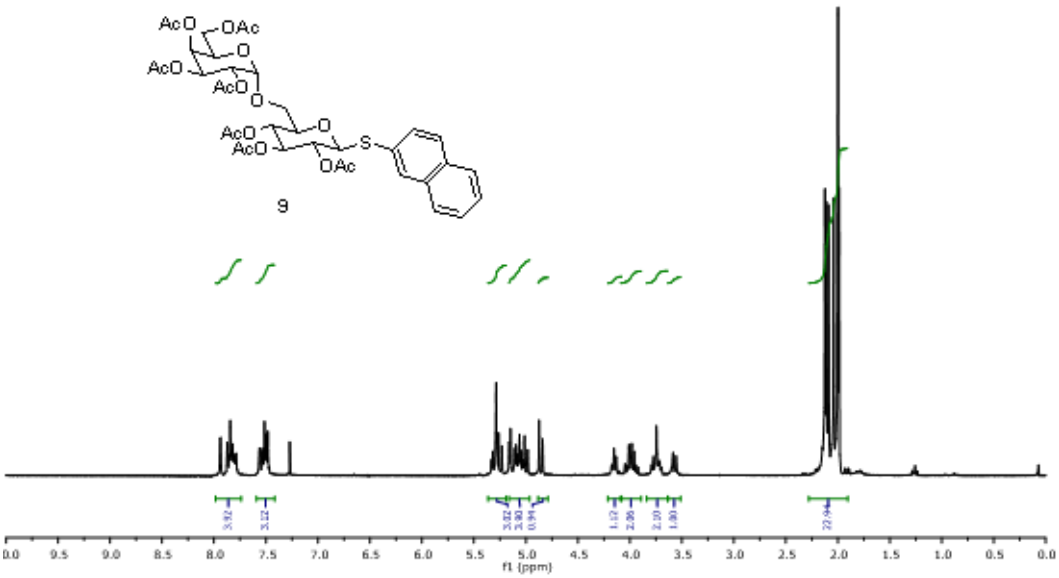
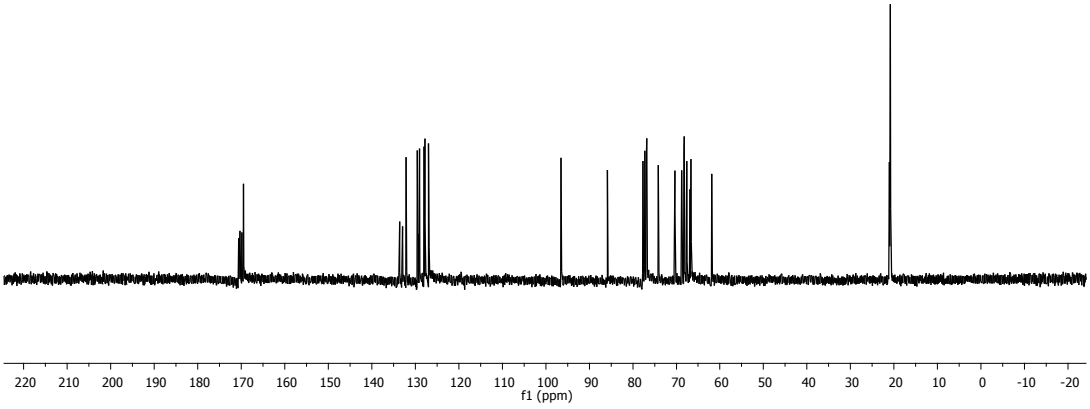
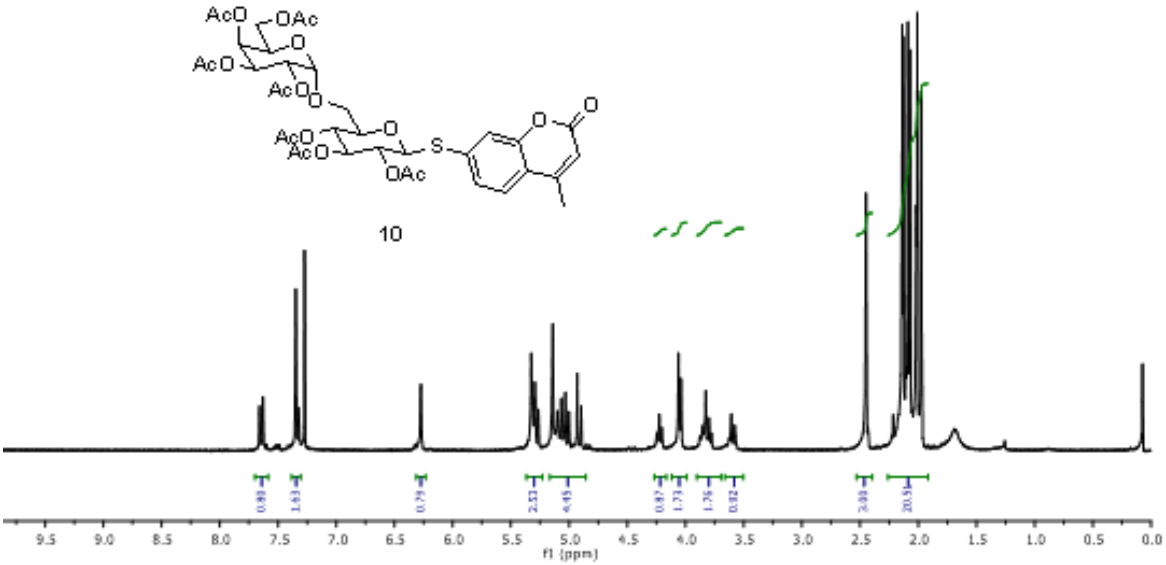
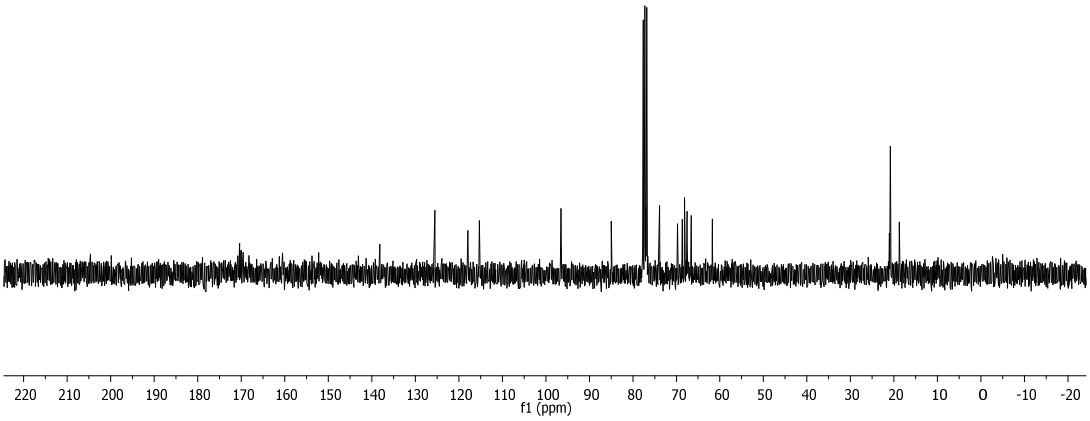
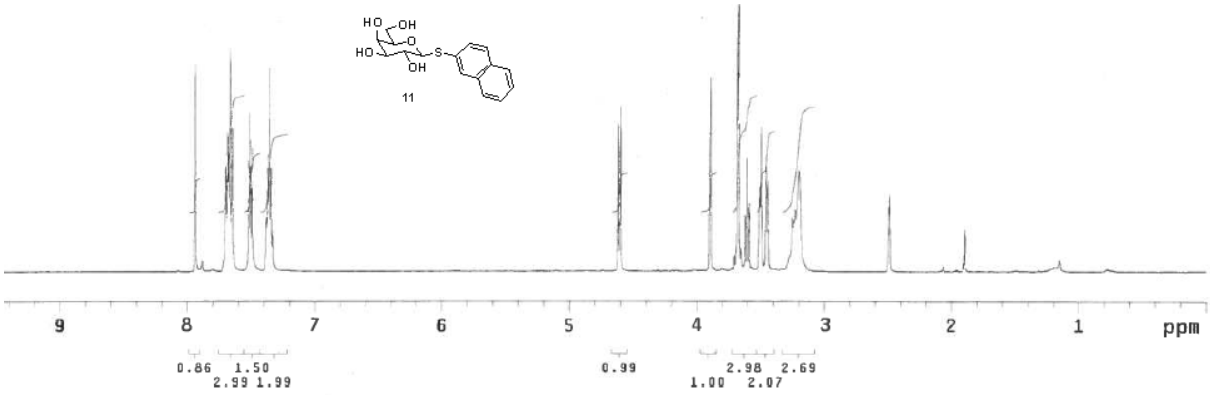
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

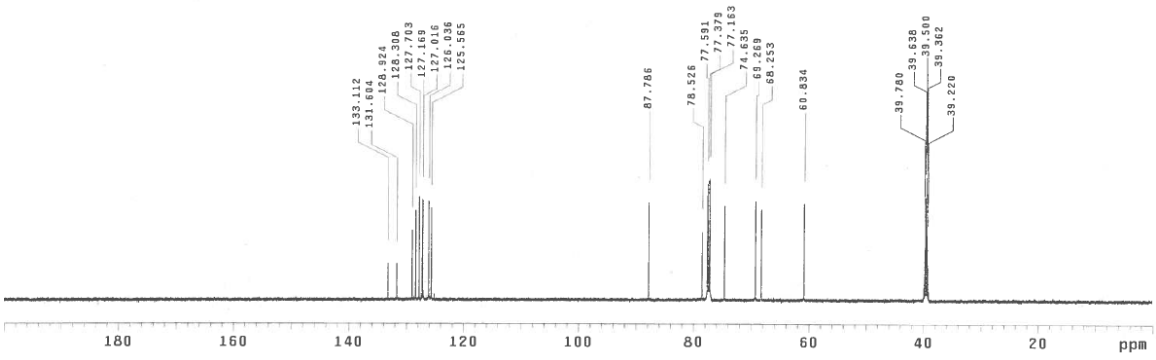









HO
OH
HO
O
S
OH
11
9
8
7
6
5
4
3
2
1
ppm
0.86
1.50
2.99
1.99
0.99
2.98
2.69
1.00
2.07


133.112
131.684
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128.308
127.703
127.169
127.016
126.036
125.565
87.786
78.526
77.591
77.379
77.163
74.635
69.269
68.253
60.834
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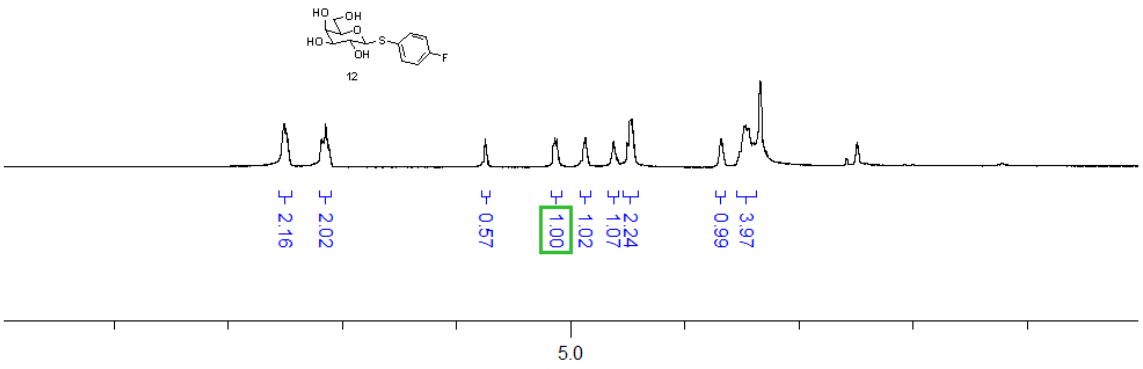
39.638
39.500
39.362
39.220
180
160
140
120
100
80
60
40
20
ppm


HO
OH
O
HO
S
OH
F
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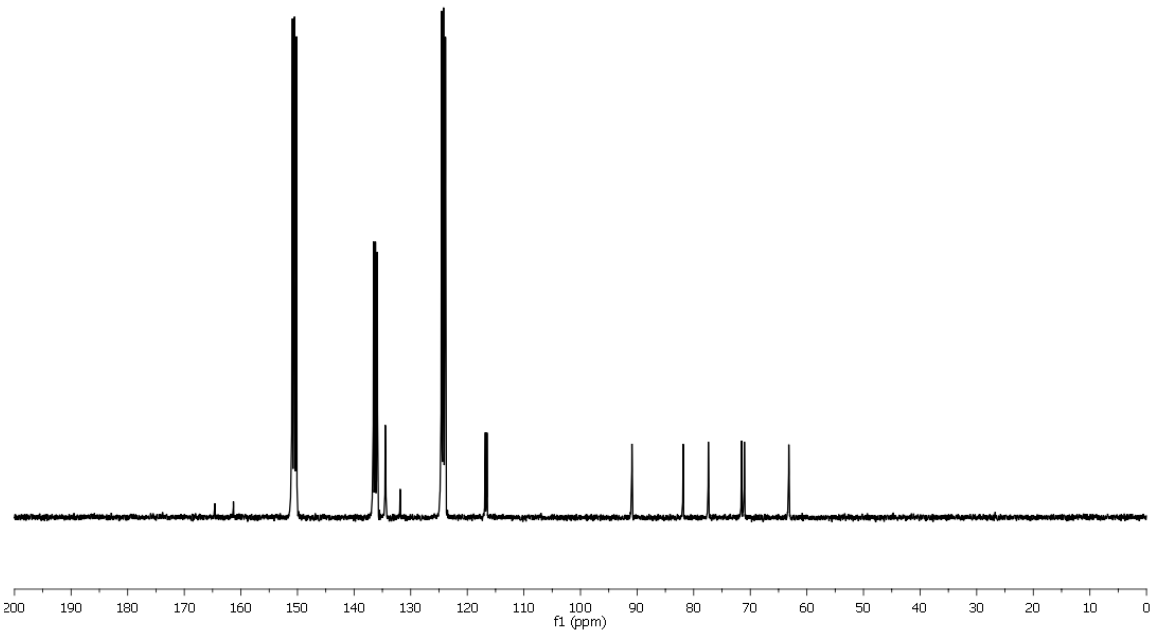
1.02
2.24
1.07
0.99
3.97
5.0
ppm (f1)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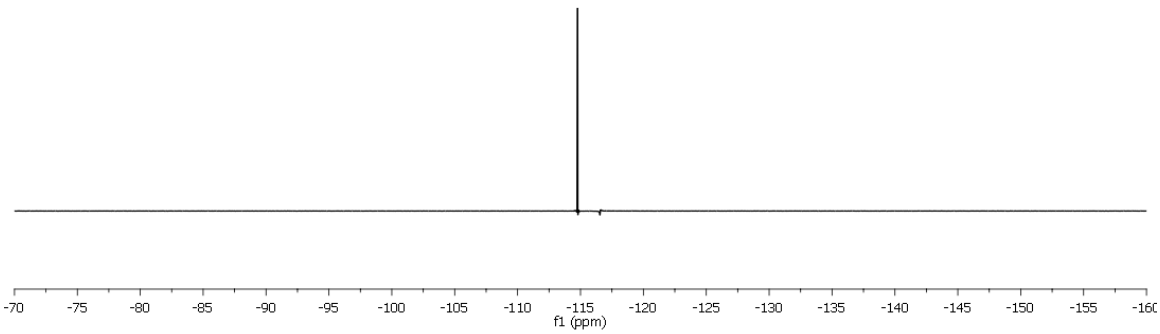
f1 (ppm)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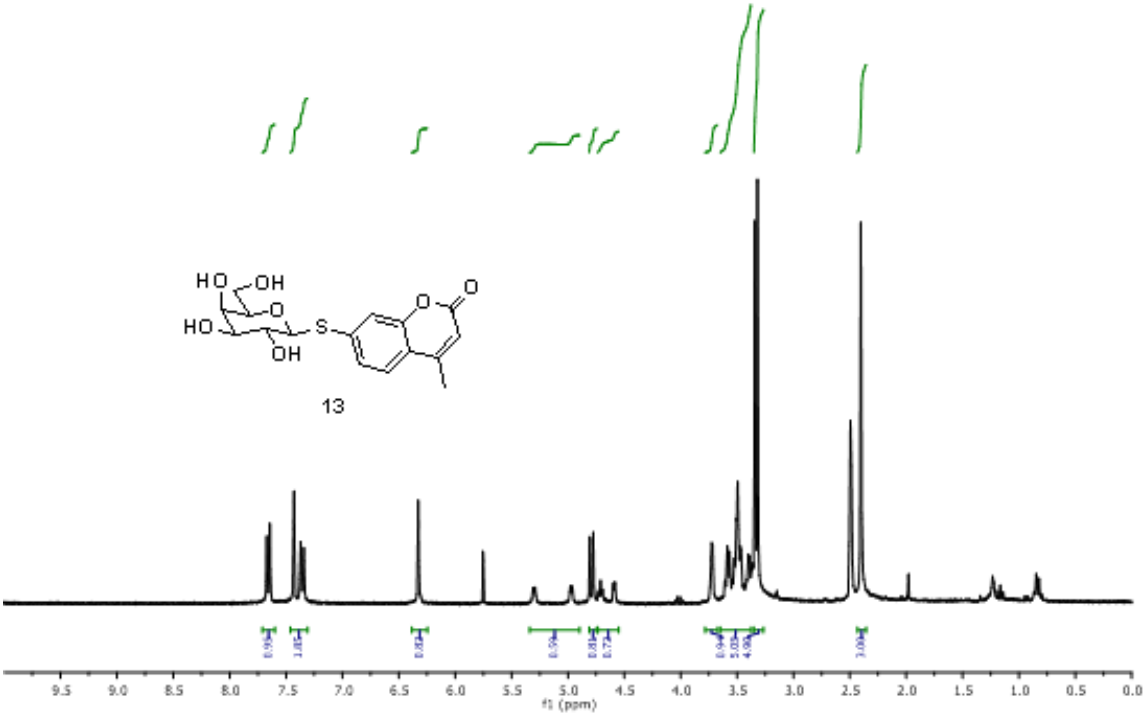
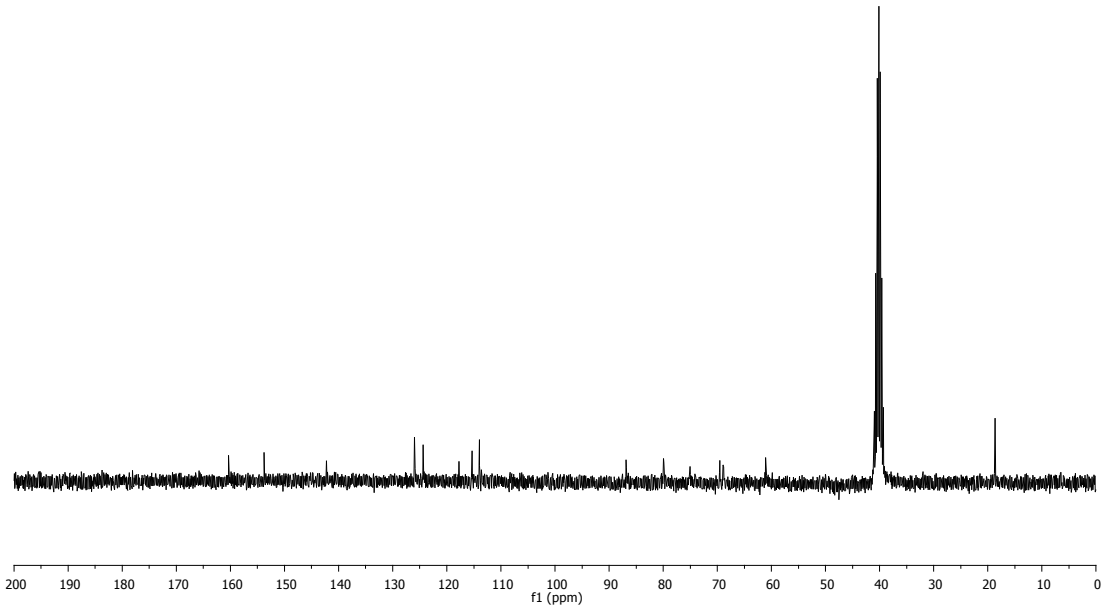
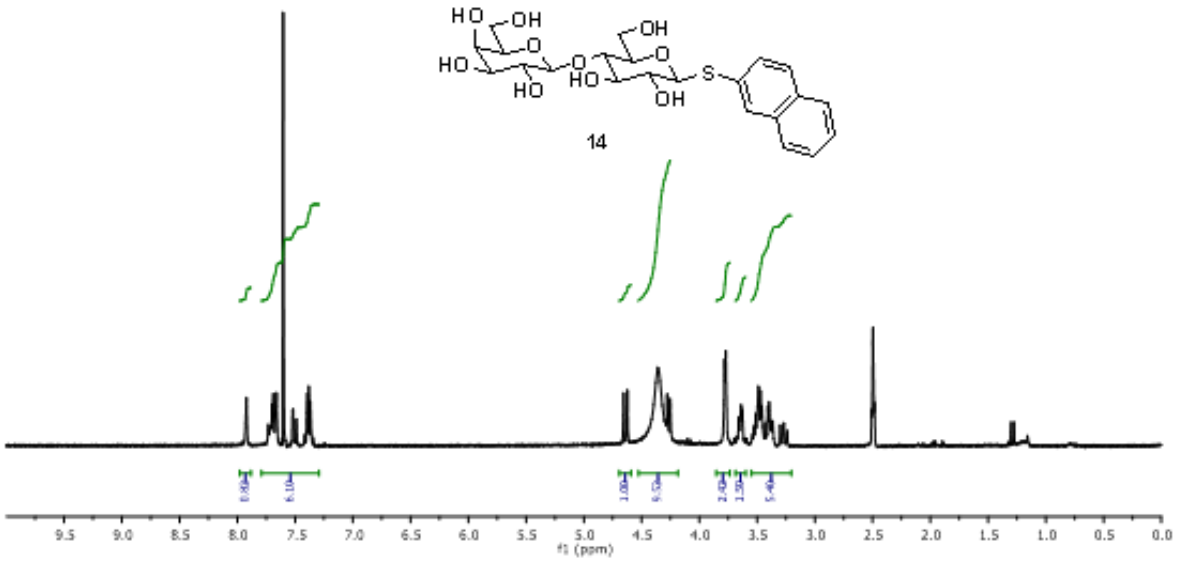
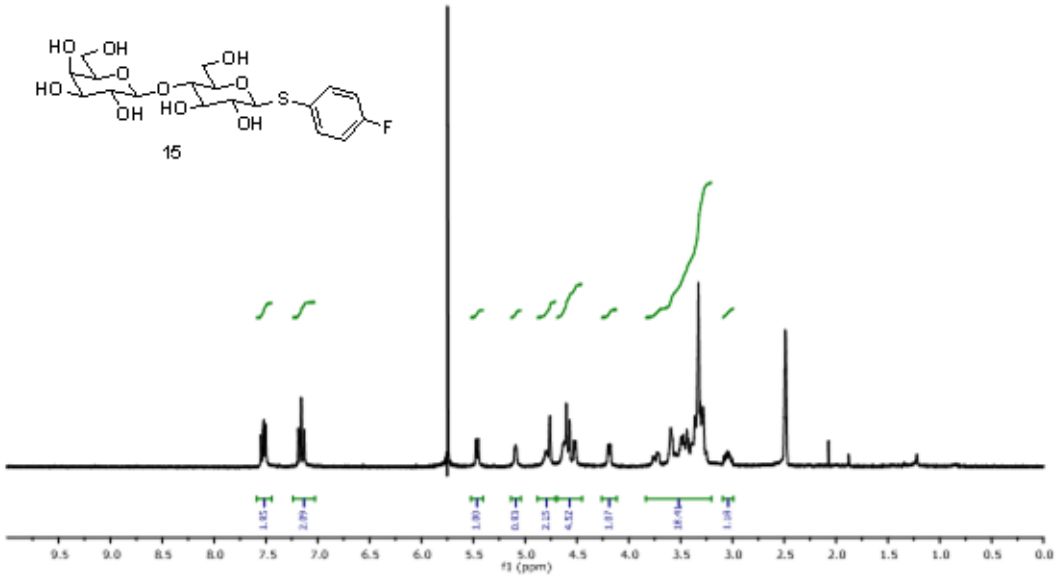
f1 (ppm)





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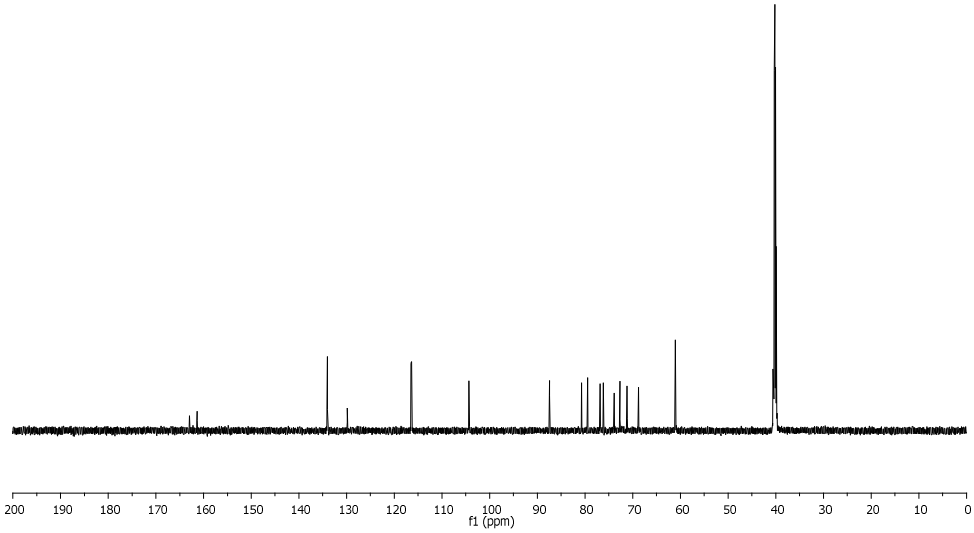
HO
O
OH
HO
OH
O
S
F
OH
15
f1 (ppm)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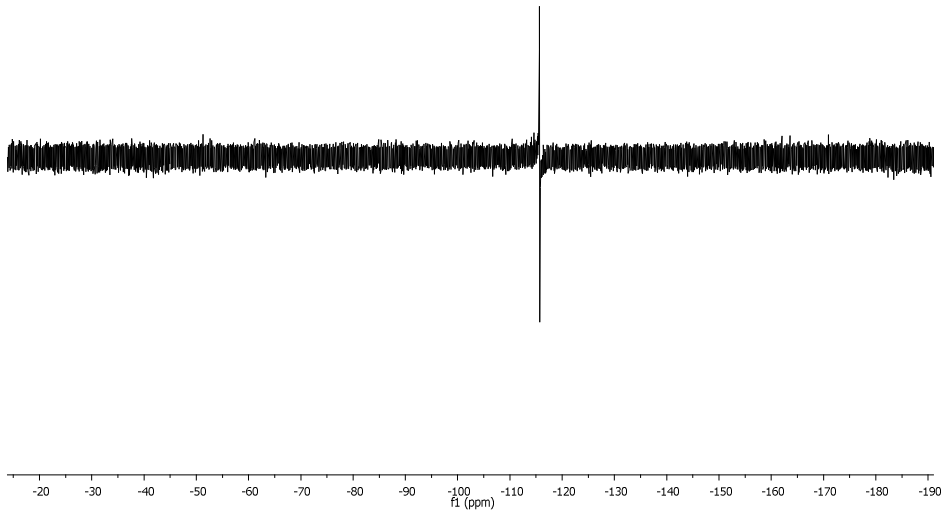
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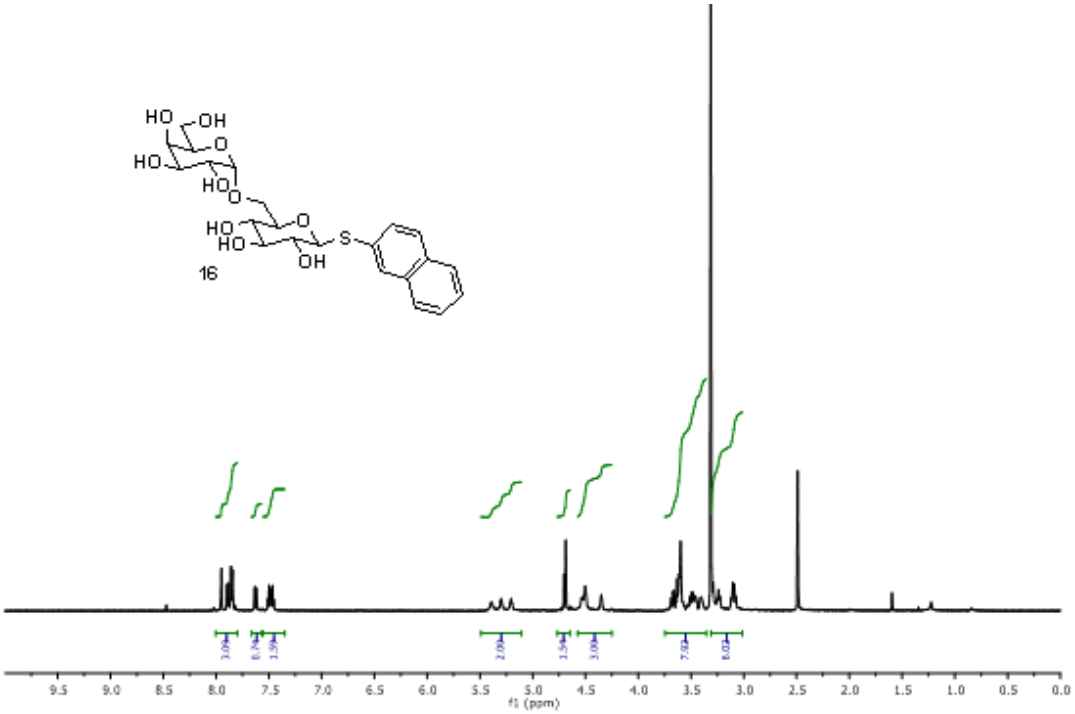

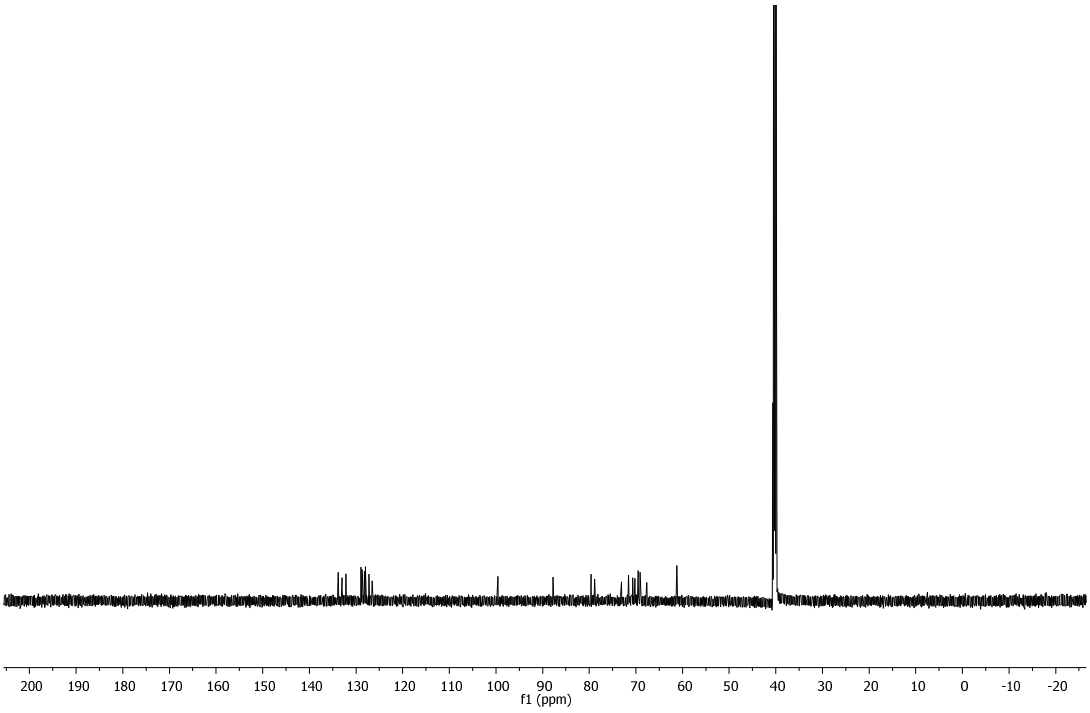

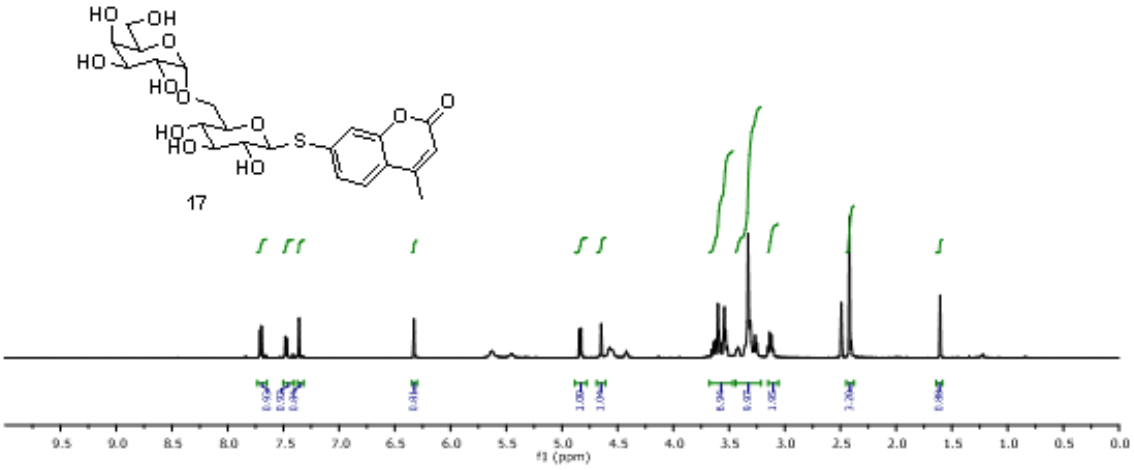

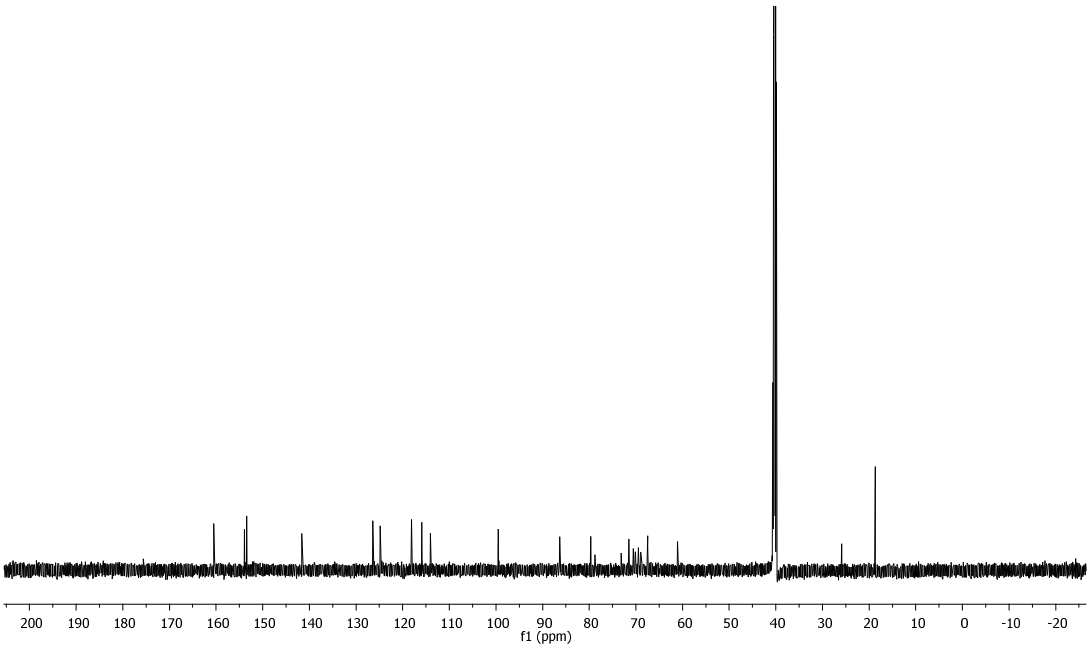

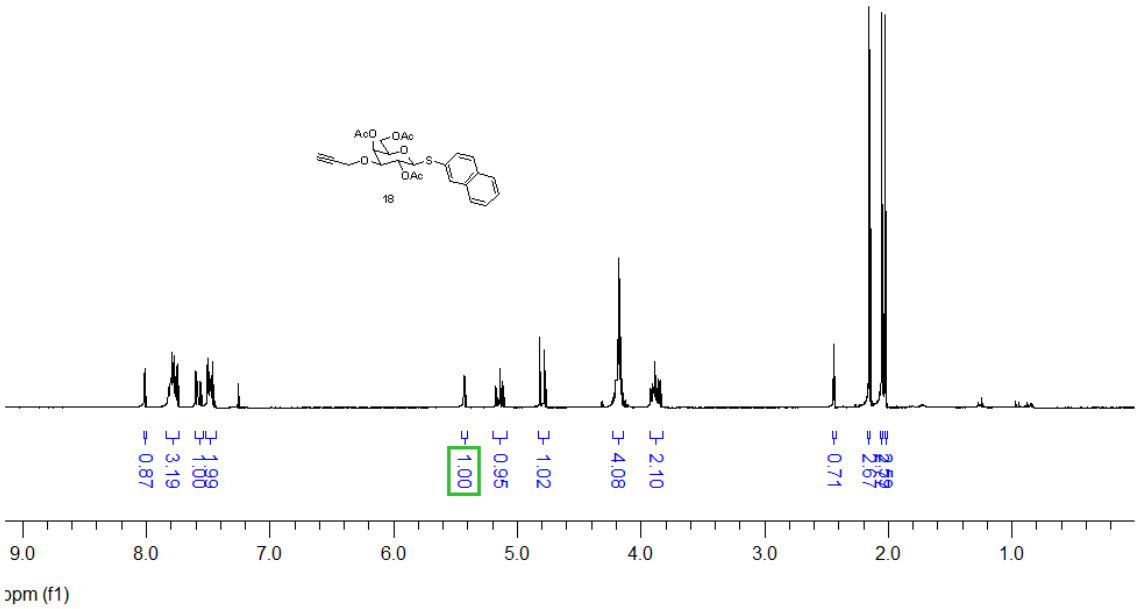
AcO
OAc
O
S
OAc
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1.00
0.95
1.02
4.08
2.10
0.71
2.67
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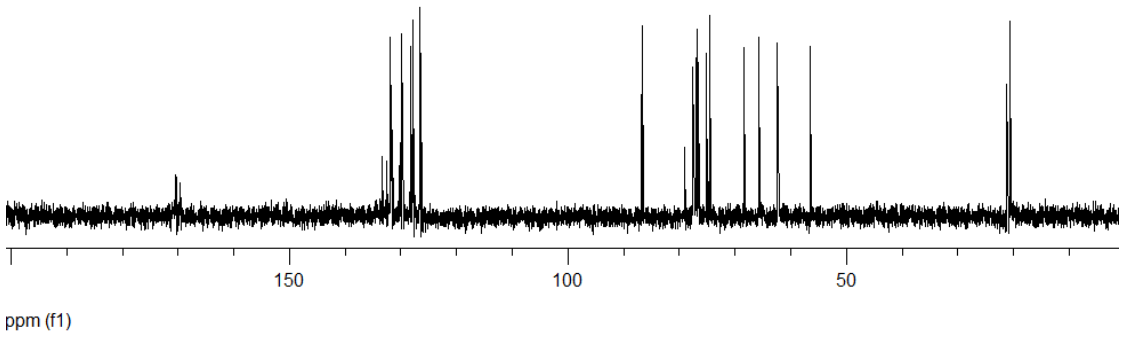
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)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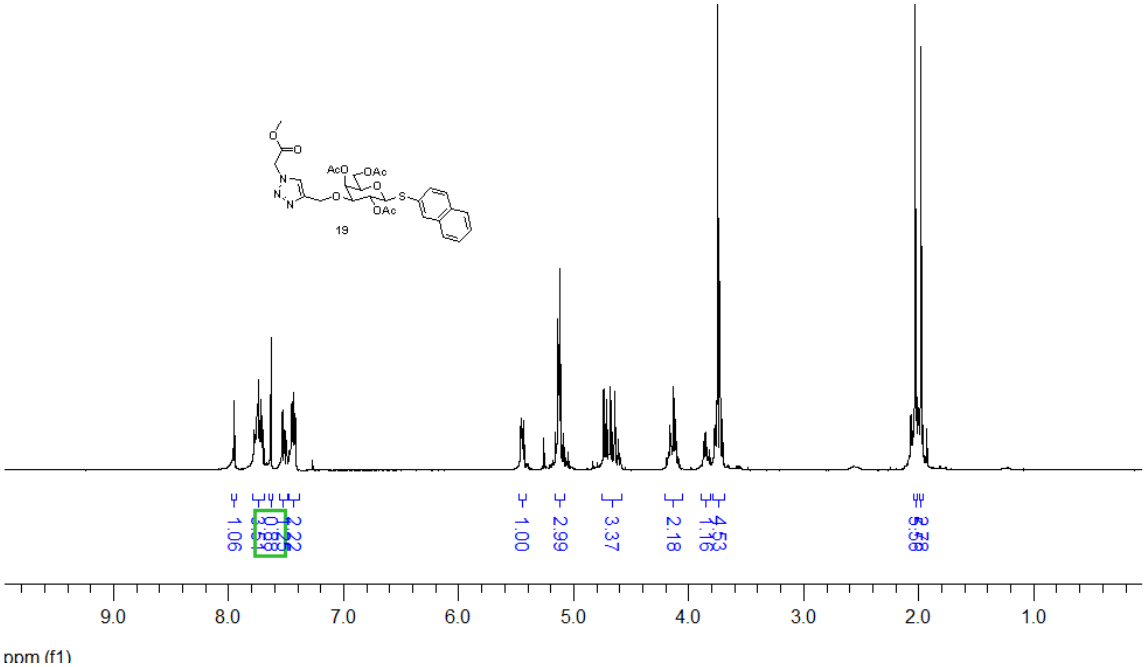
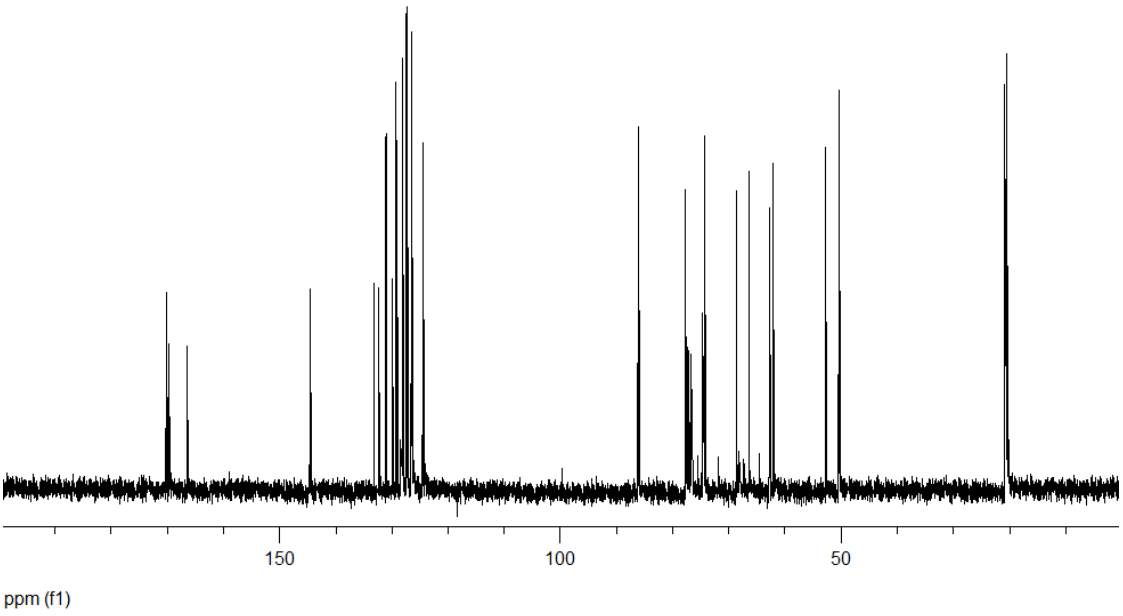
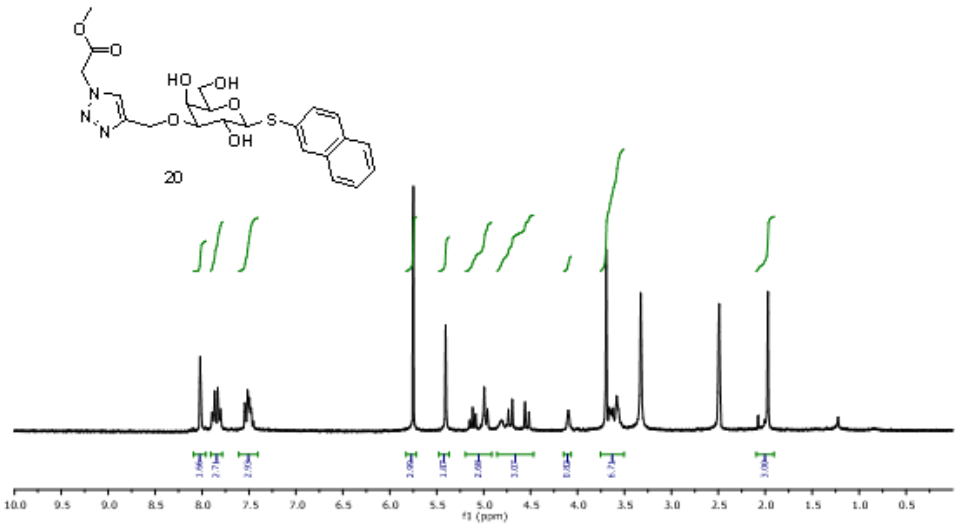
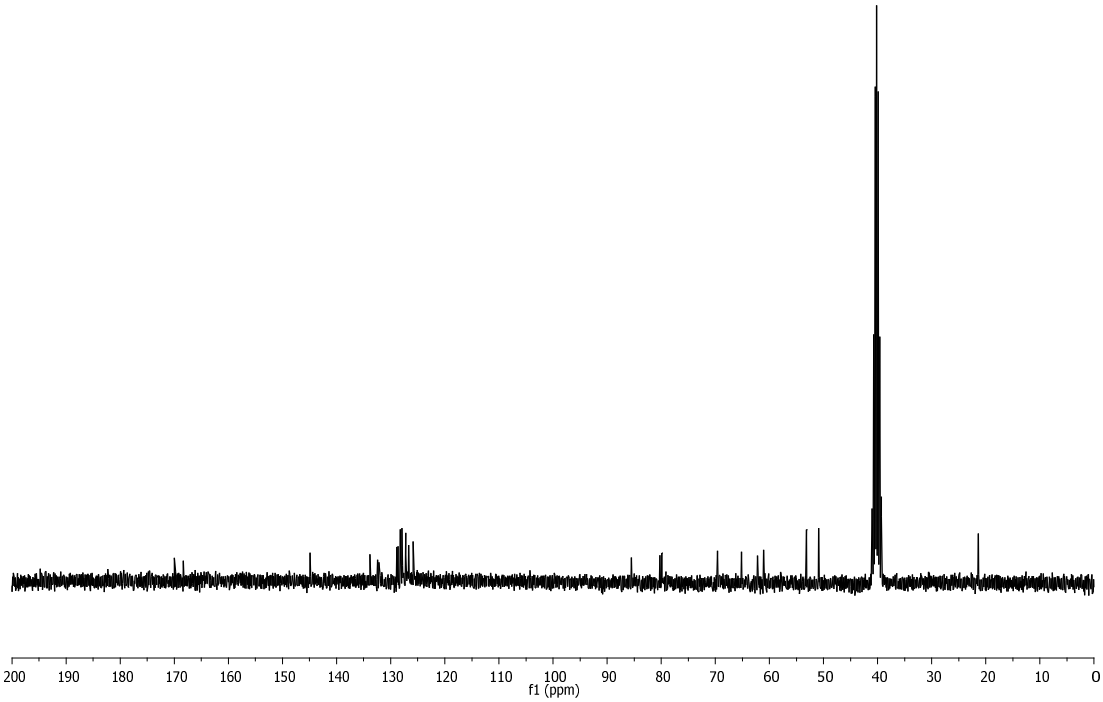
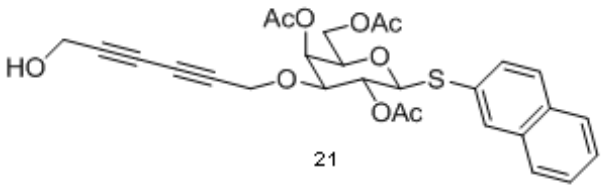
100
50
ppm (f1)



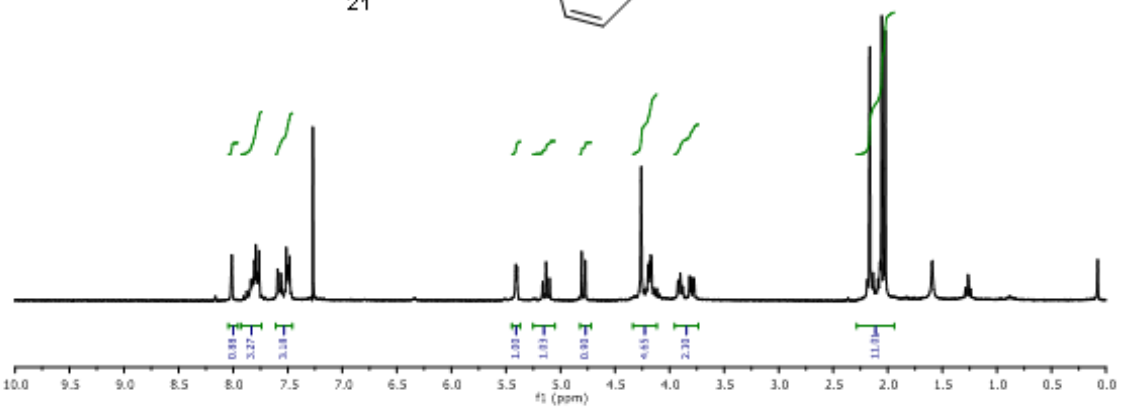


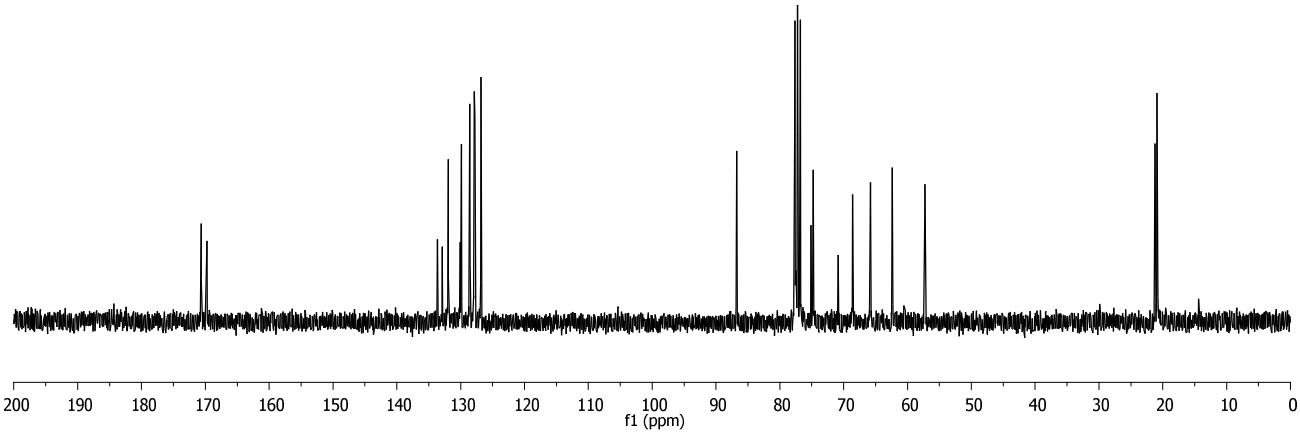


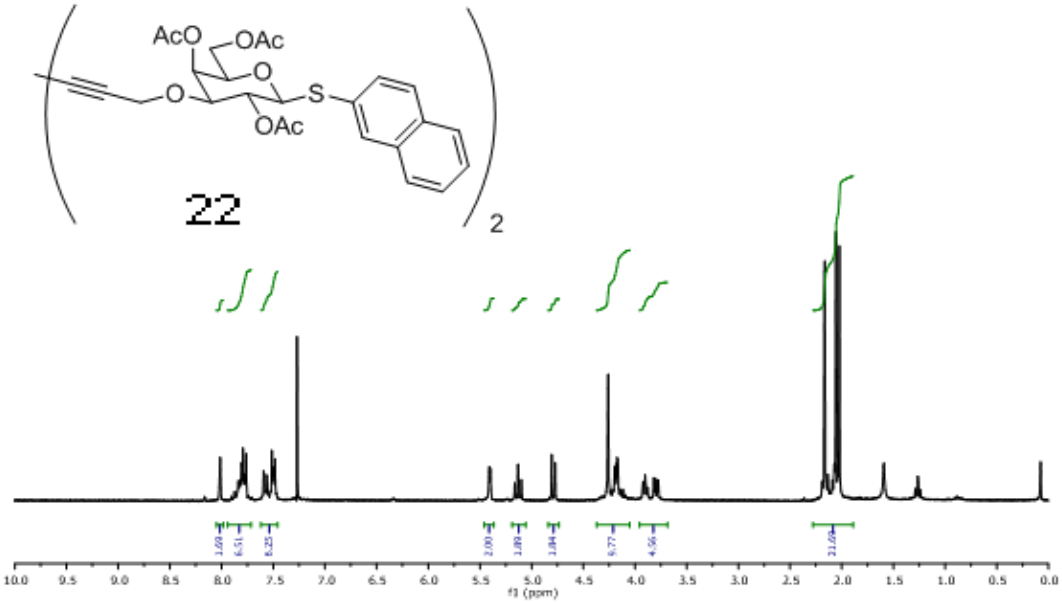


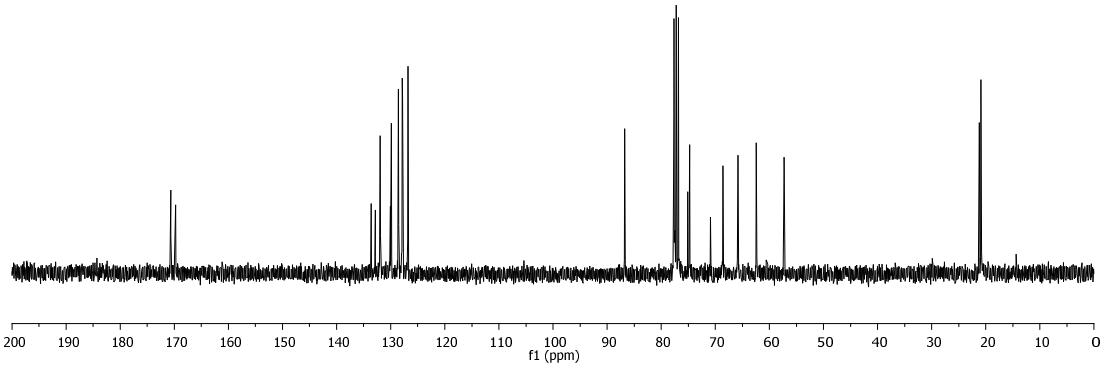


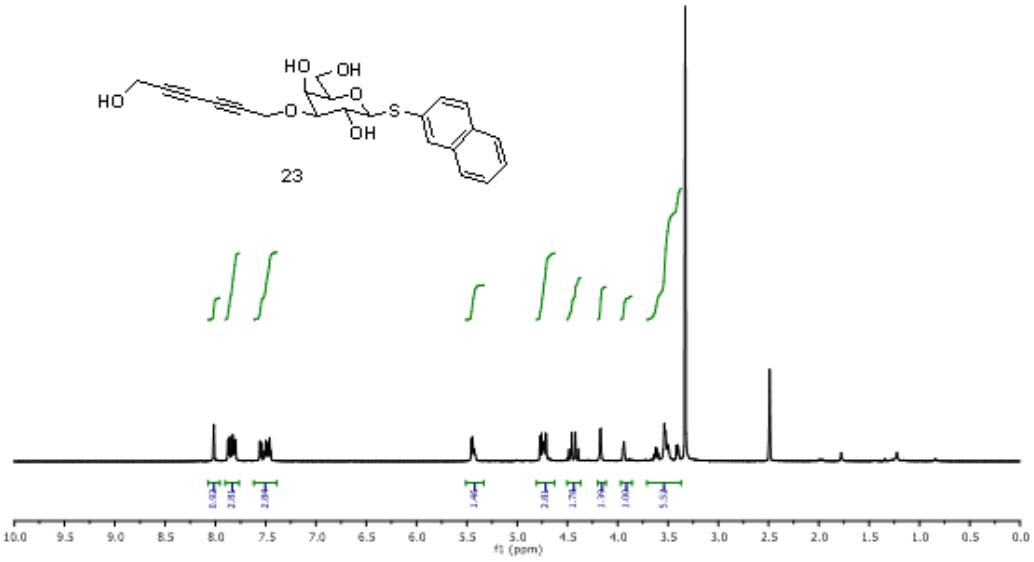
21

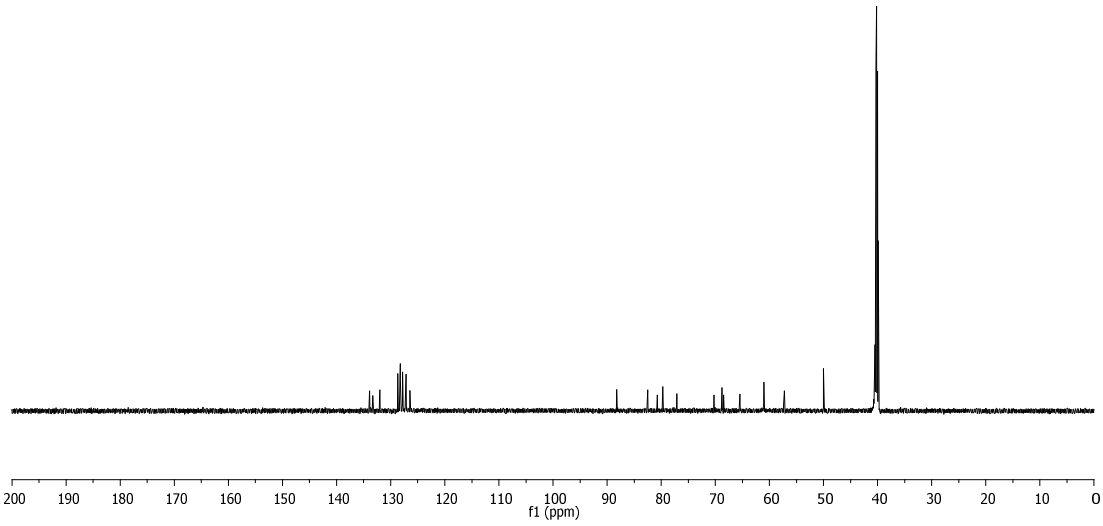


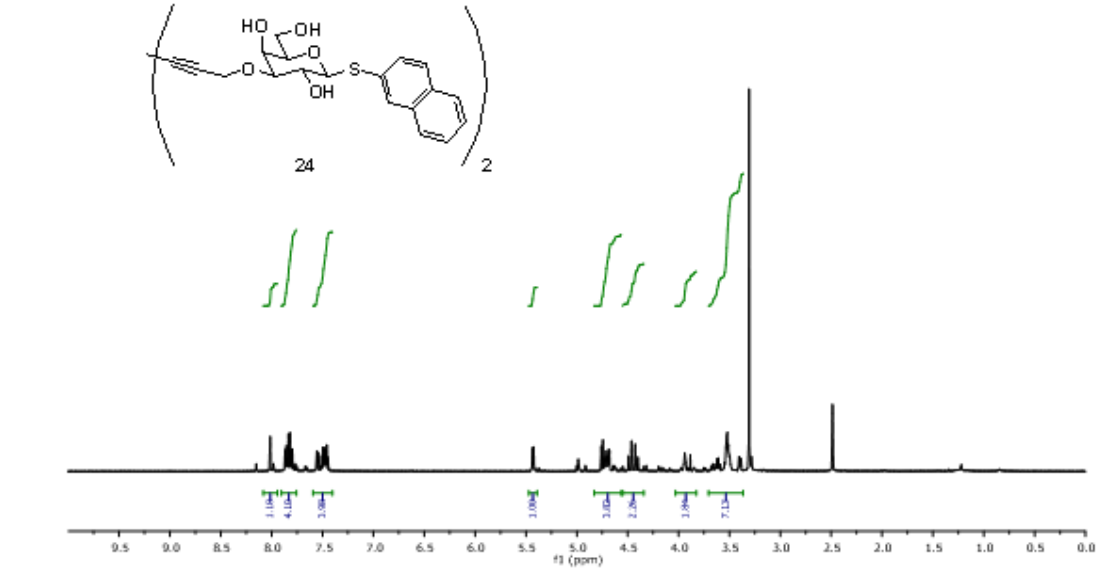


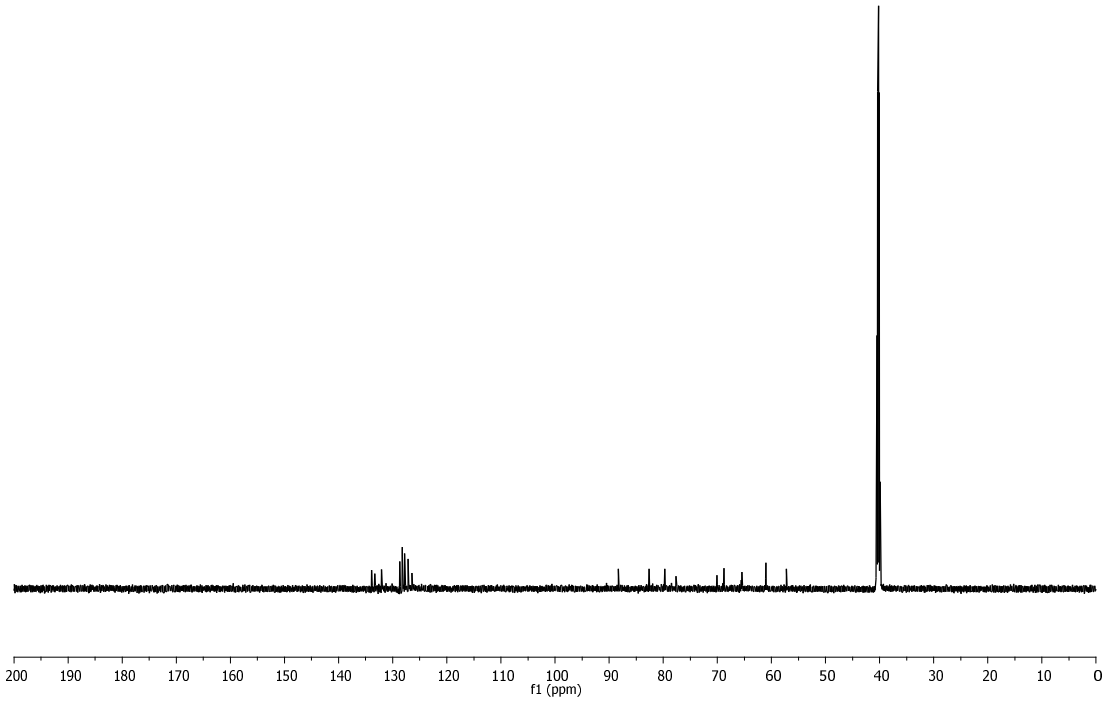


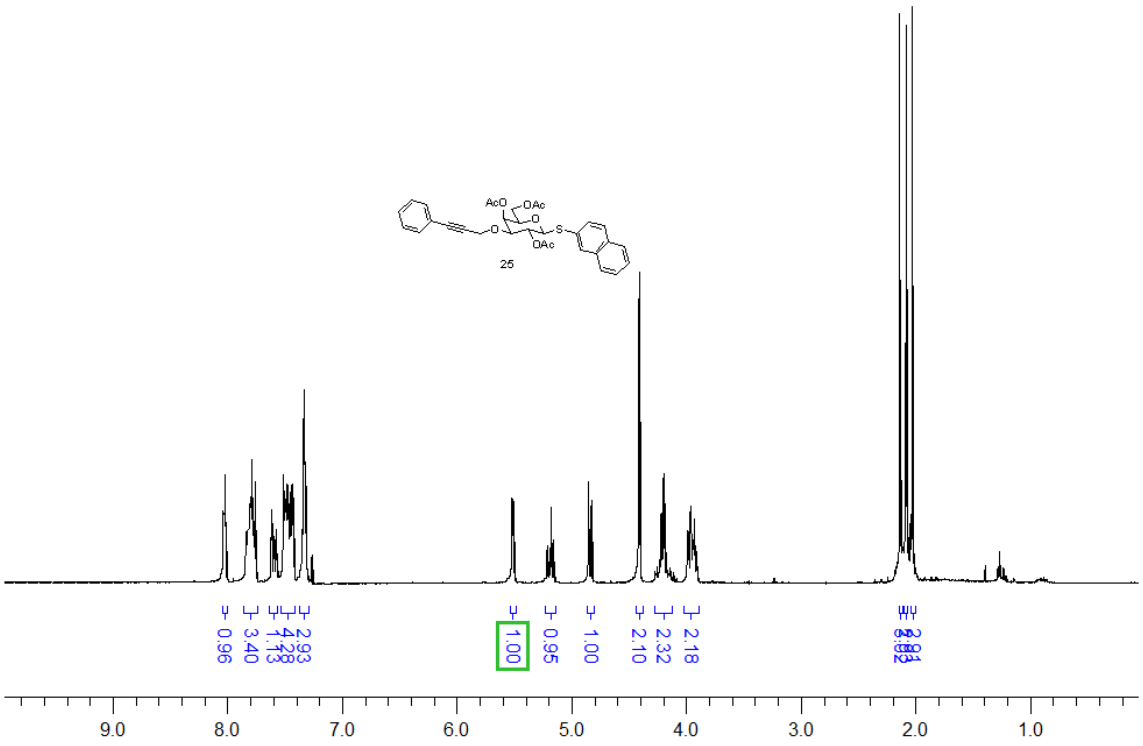


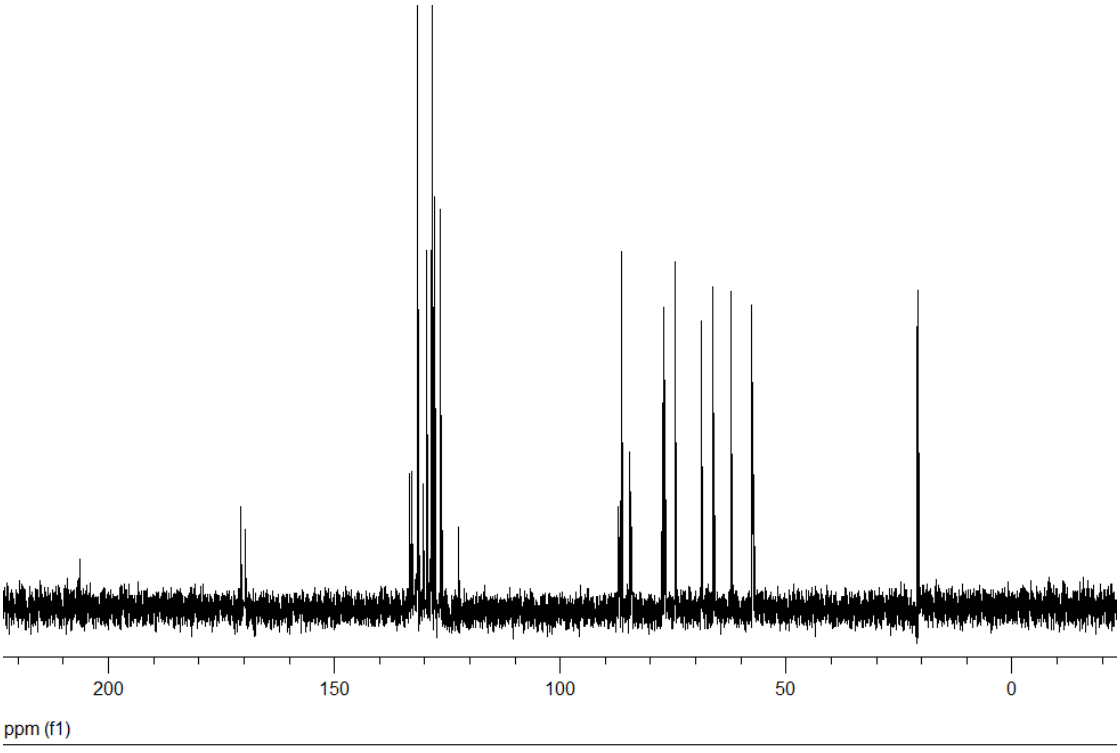


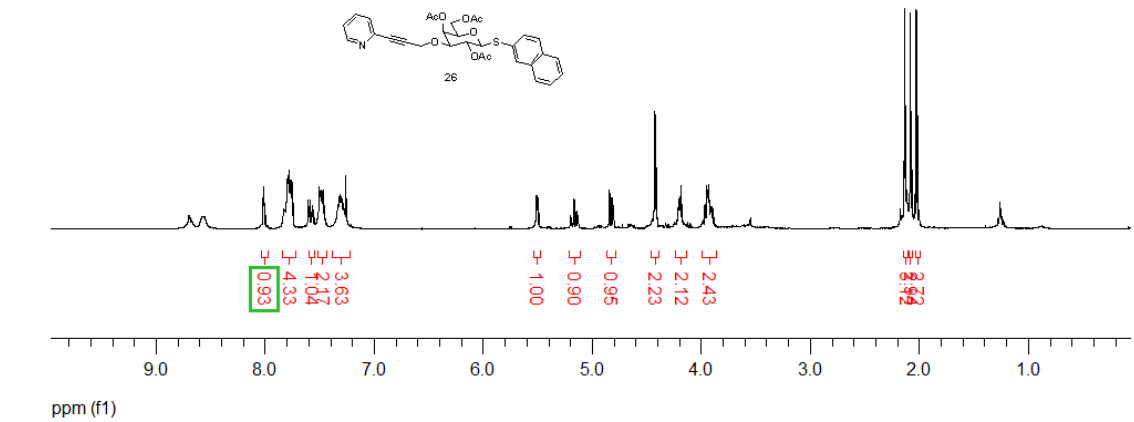


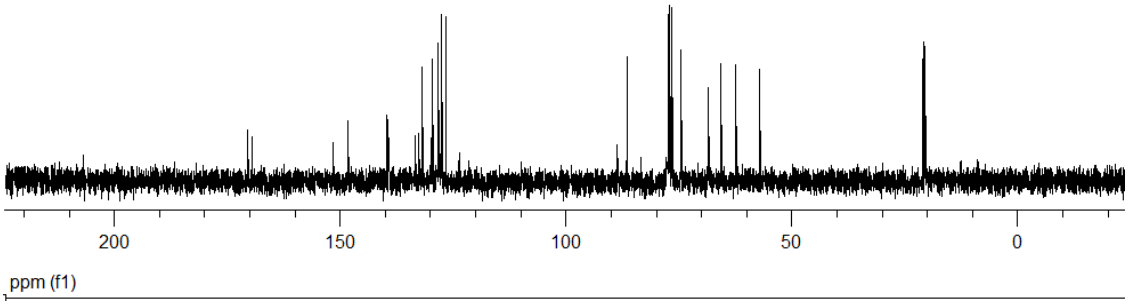


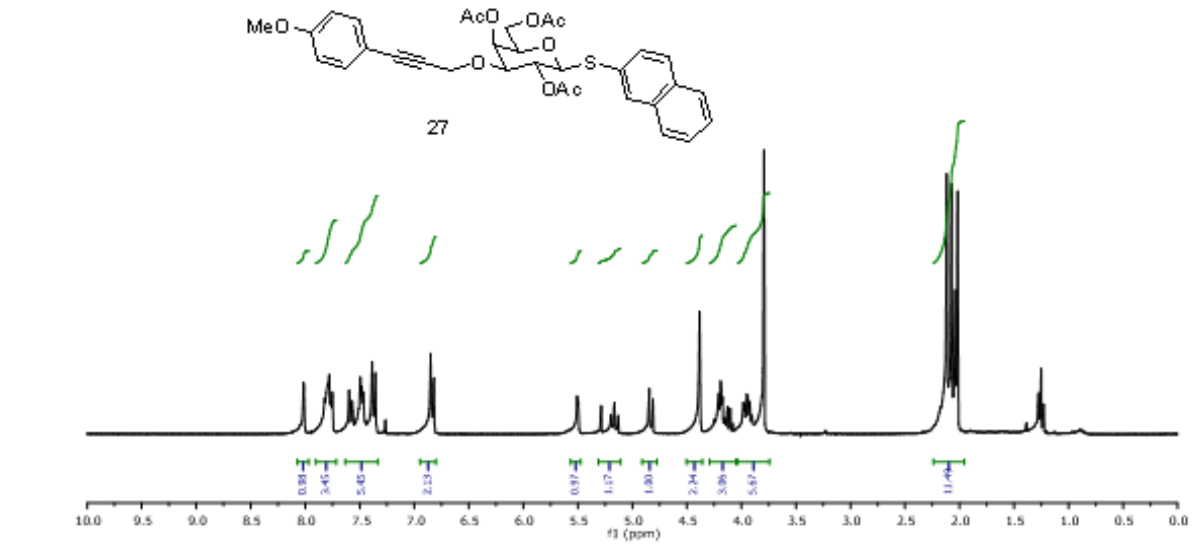


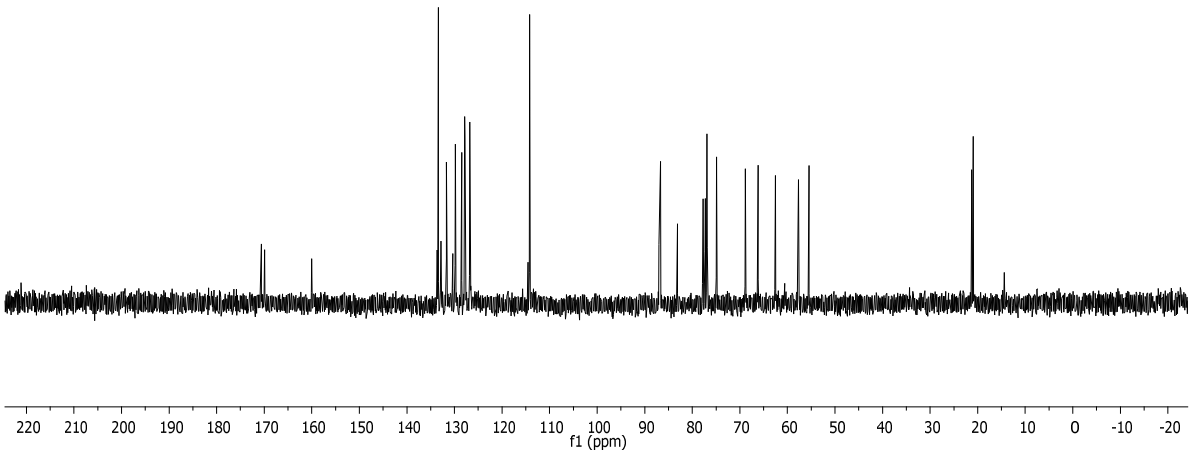

AcO
OAc
O
O
S
OAc
25
0.96
3.40
1.13
2.93
1.00
0.95
1.00
2.10
2.32
2.18
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0

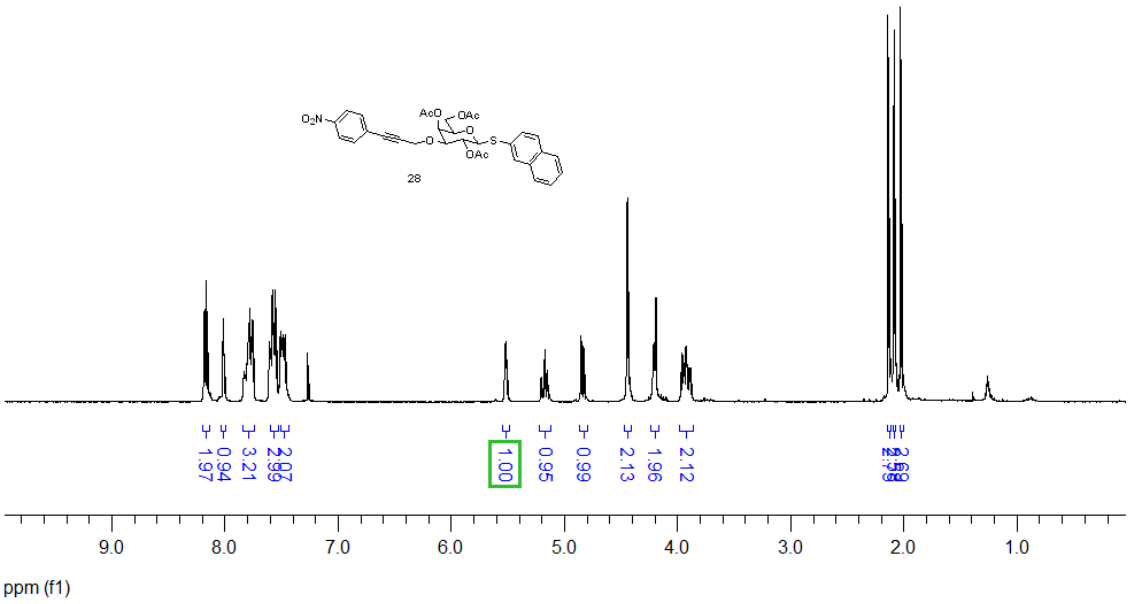

200
150
100
50
0
ppm (f1)

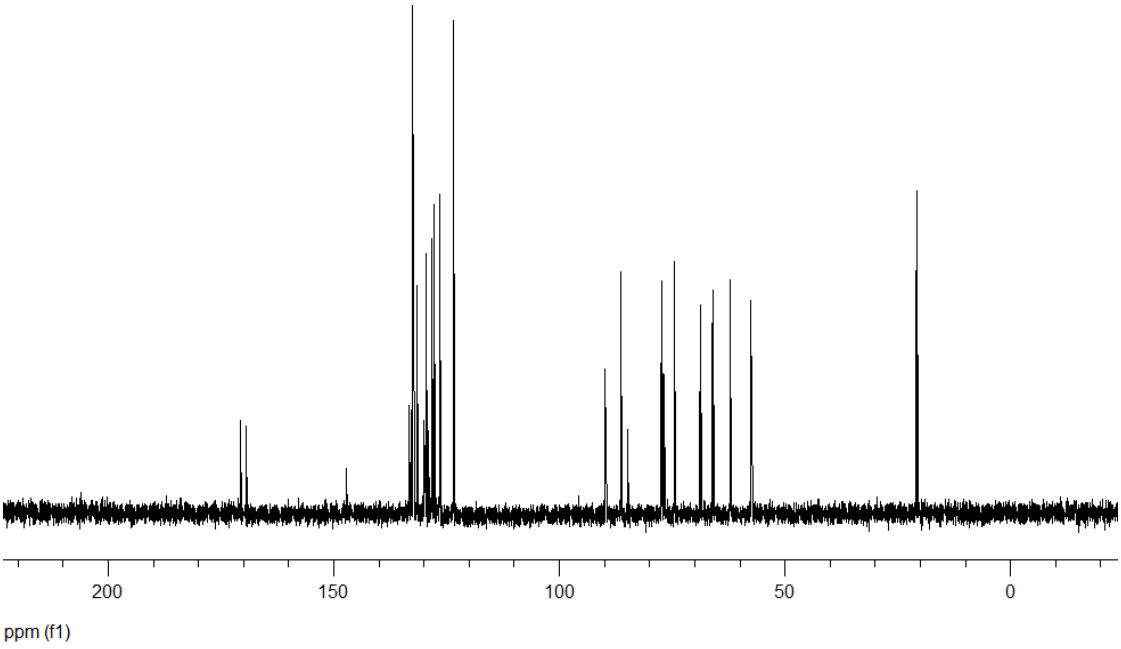

AcO
OAc
O
OAc
S
N
26
0.93
4.33
2.17
1.04
3.63
1.00
0.90
0.95
2.23
2.12
2.43
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)

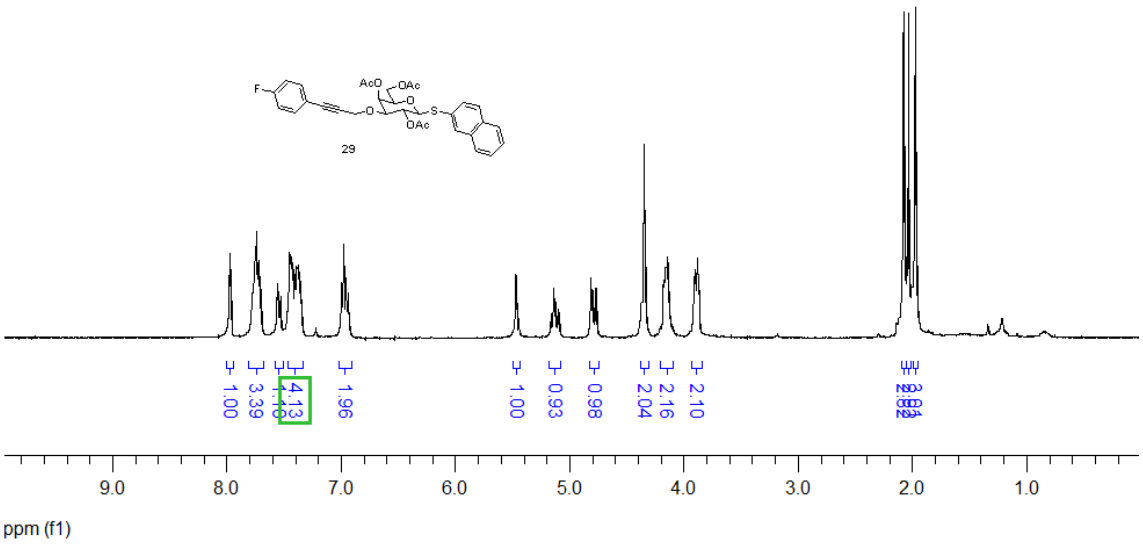

200
150
100
50
0
ppm (f1)

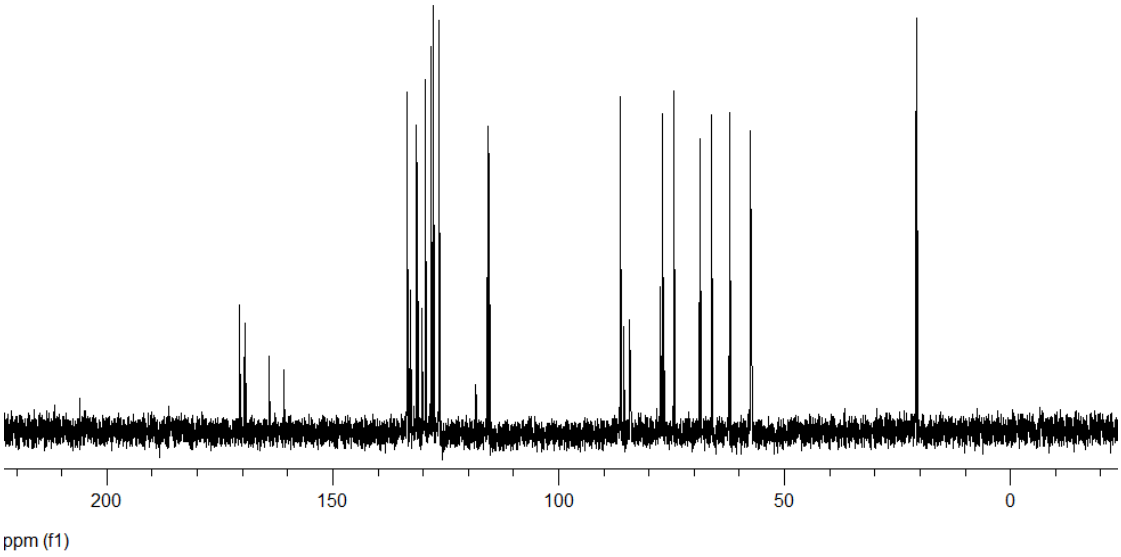


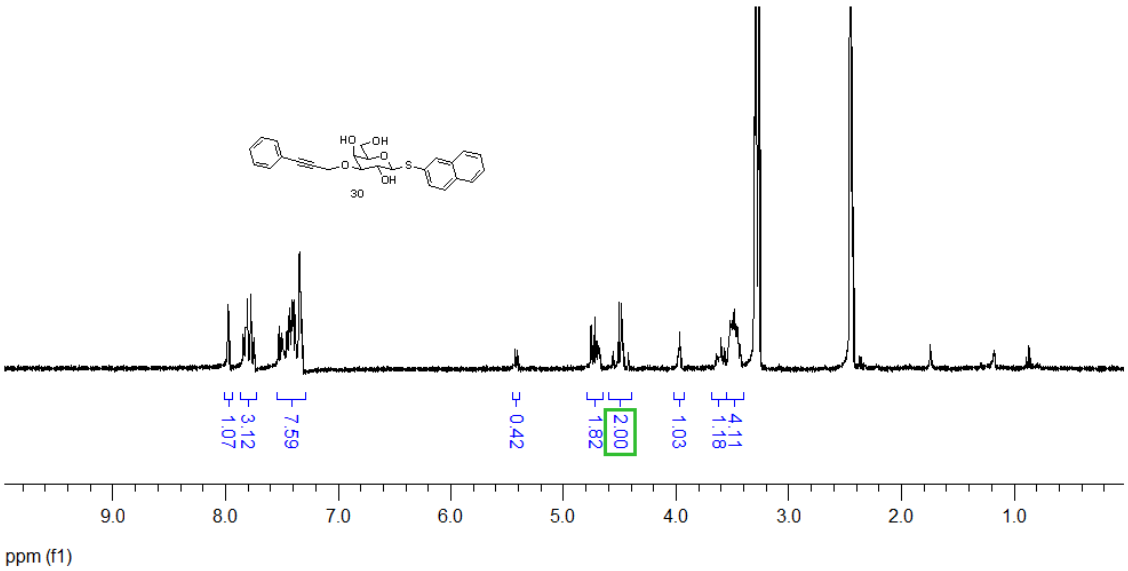


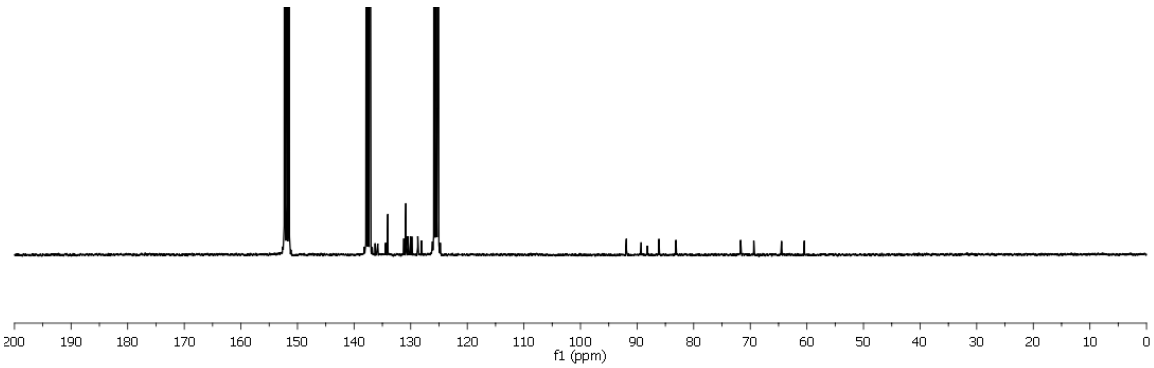

28
1.97
0.94
3.21
2.07
2.99
1.00
0.95
0.99
2.13
1.96
2.12
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)

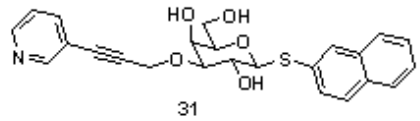

200
150
100
50
0
ppm (f1)


F
AcO
OAc
O
O
S
OAc
29
1.00
3.39
4.13
1.96
1.00
0.93
0.98
2.04
2.16
2.10
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)

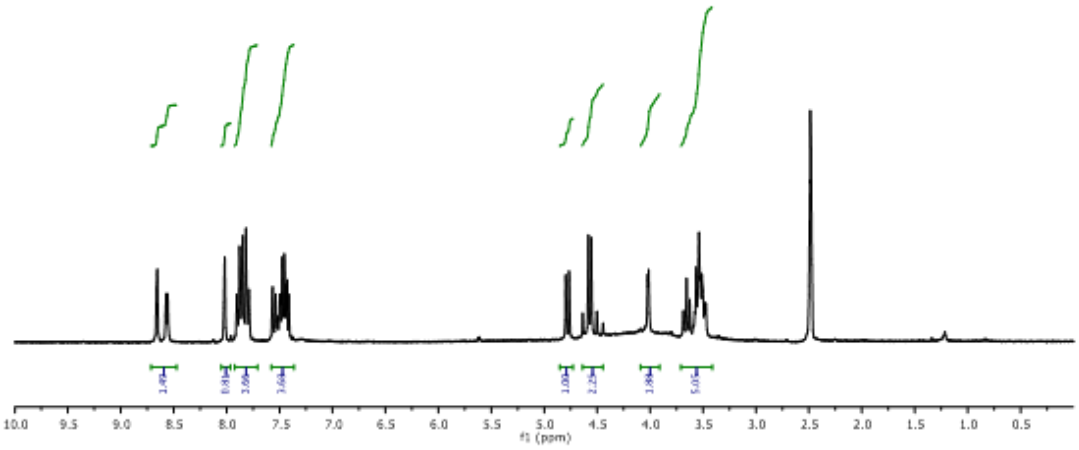

200
150
100
50
0
ppm (f1)

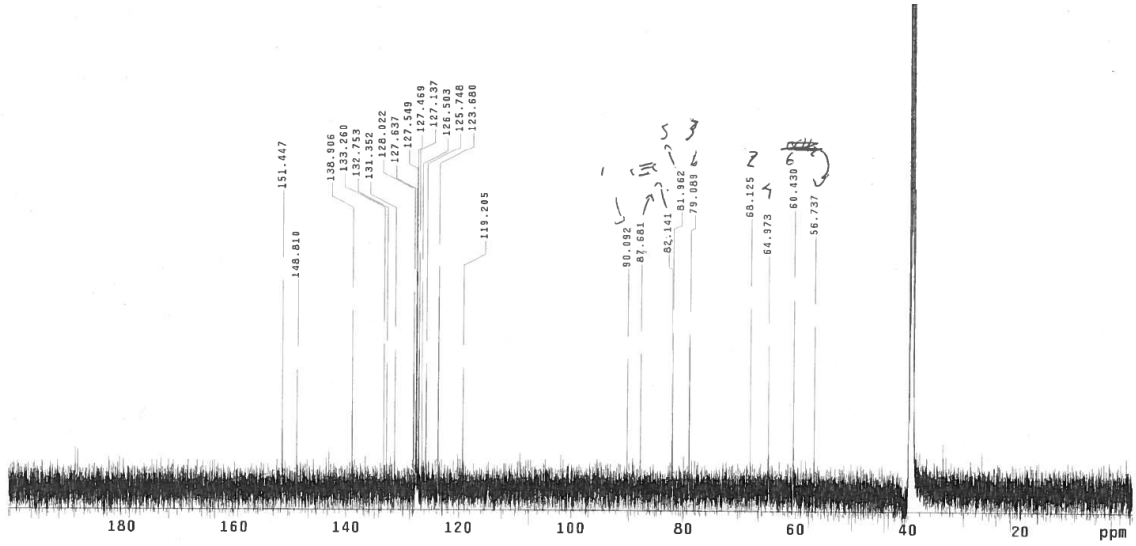

HO
OH
O
O
S
OH
30
1.07
3.12
7.59
0.42
1.82
2.00
1.03
1.18
4.11
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)

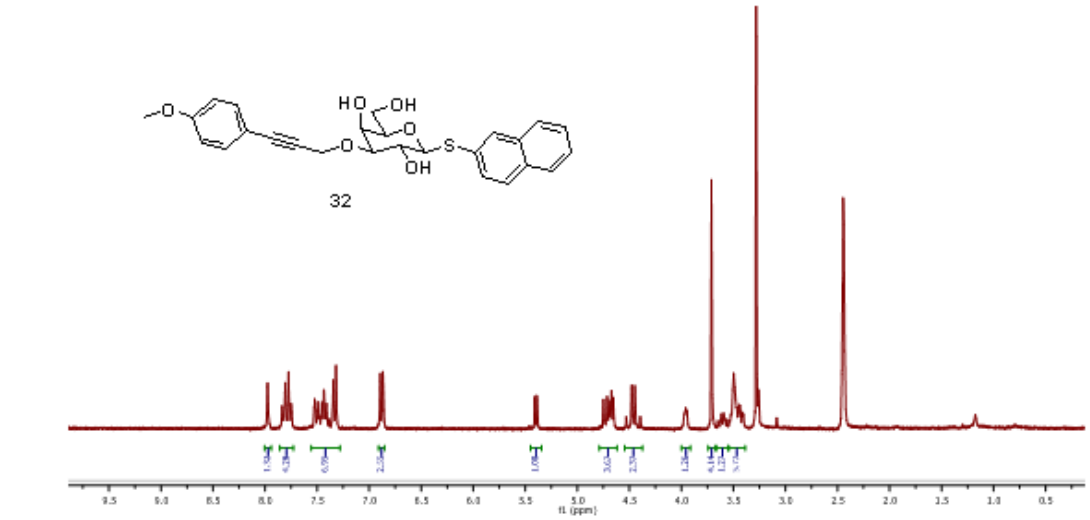

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

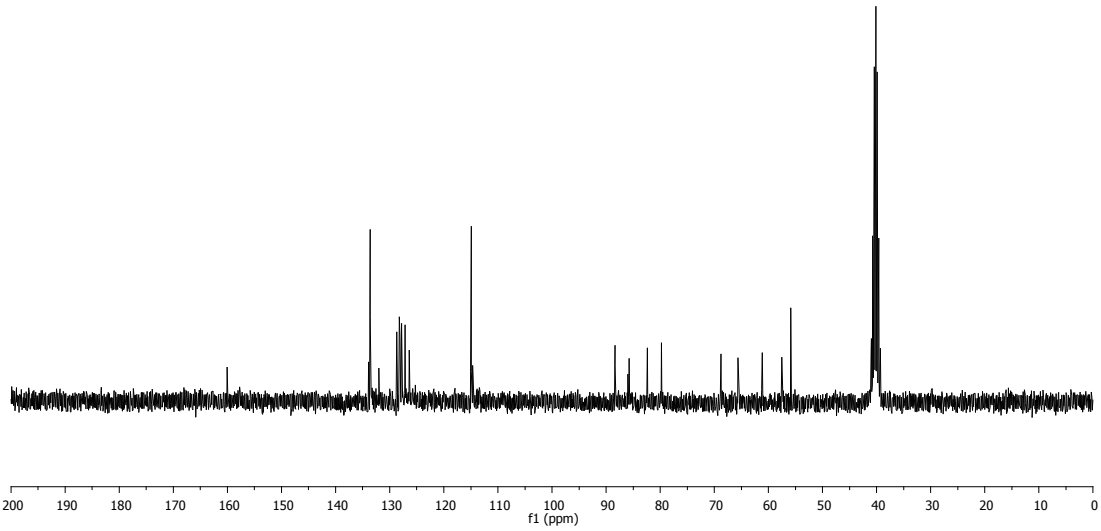


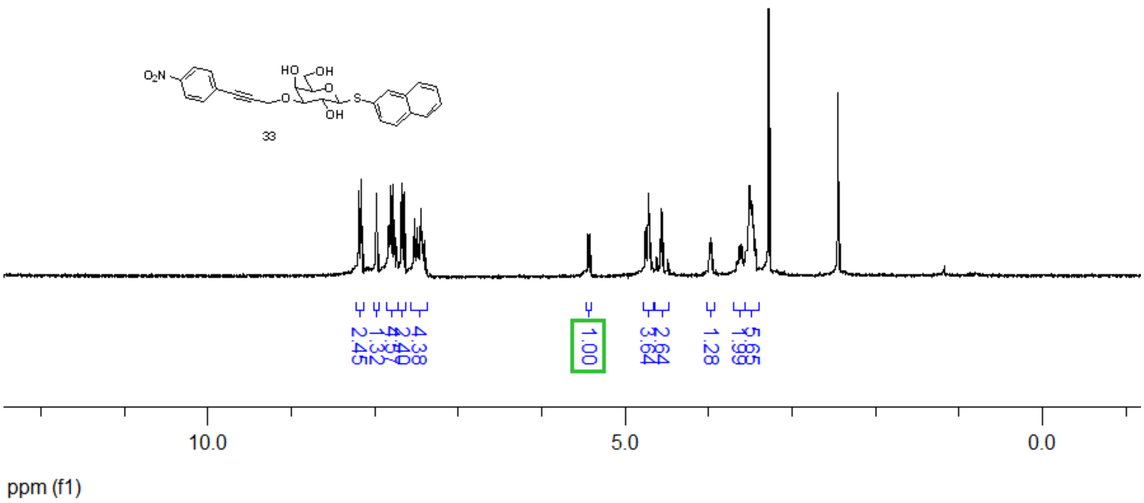
31

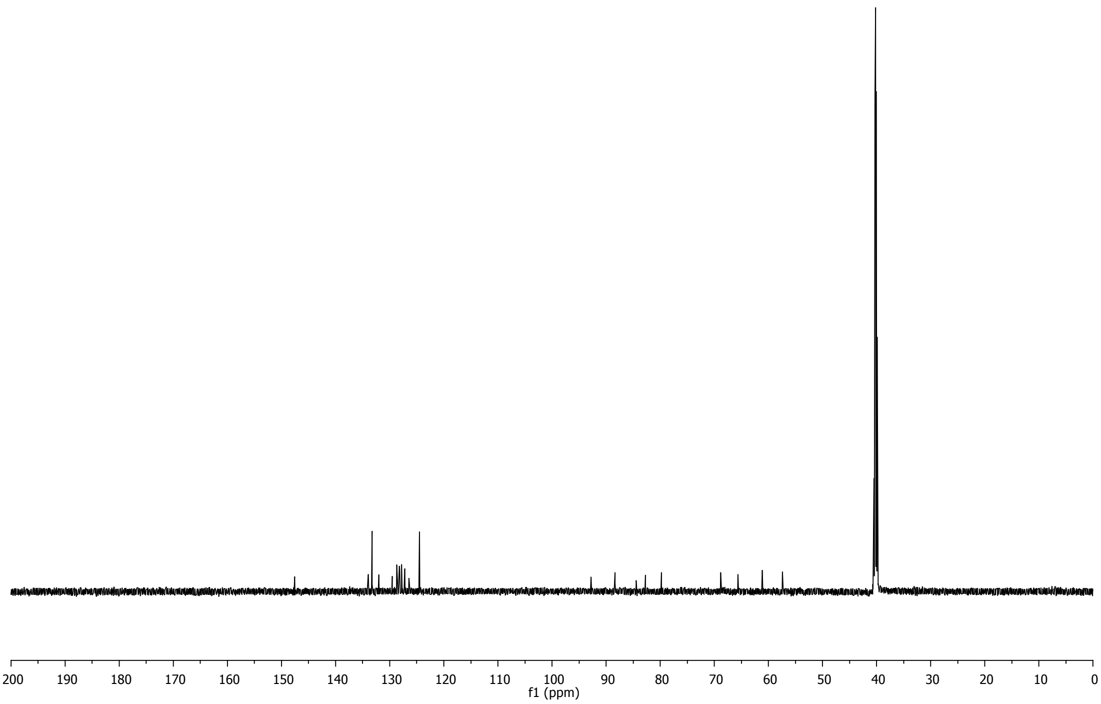


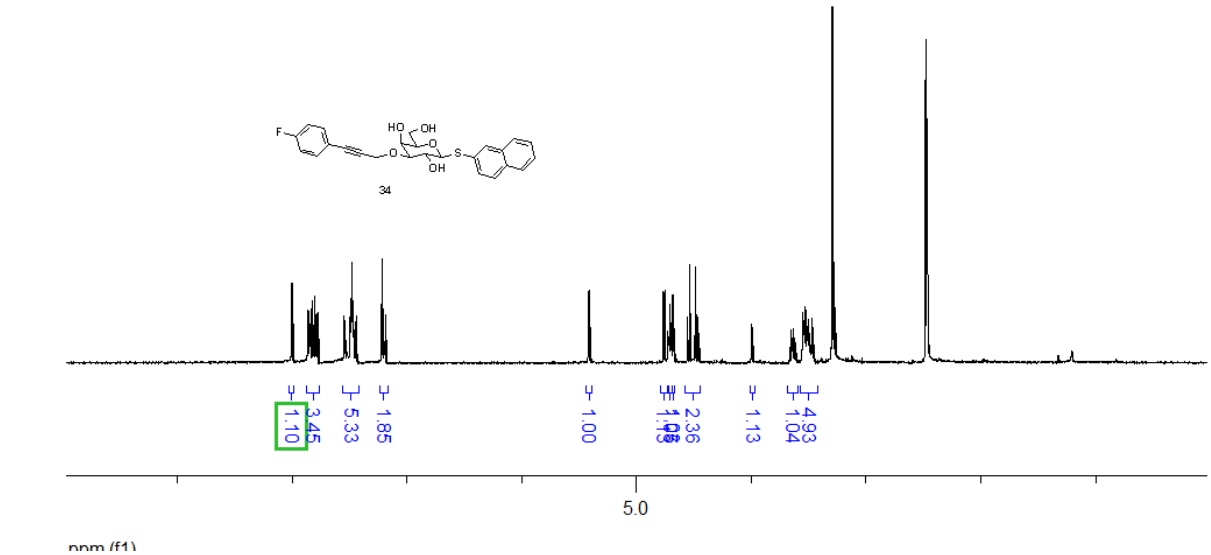


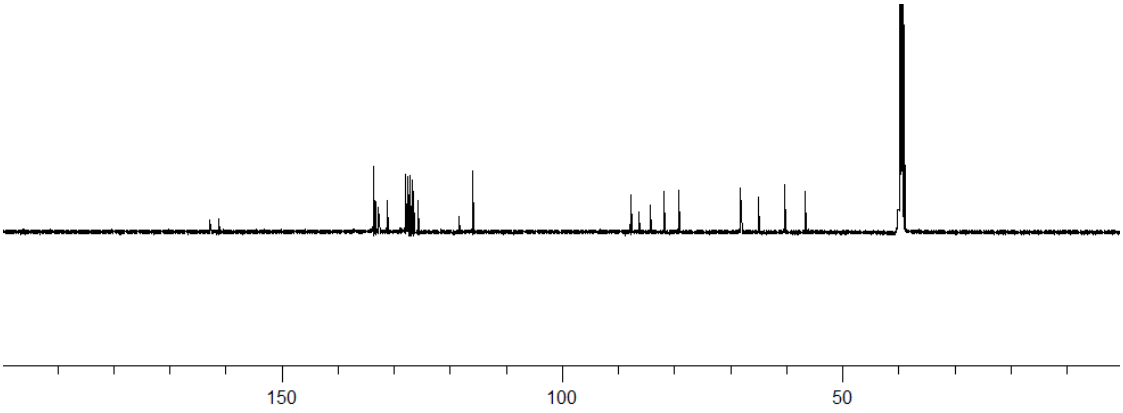


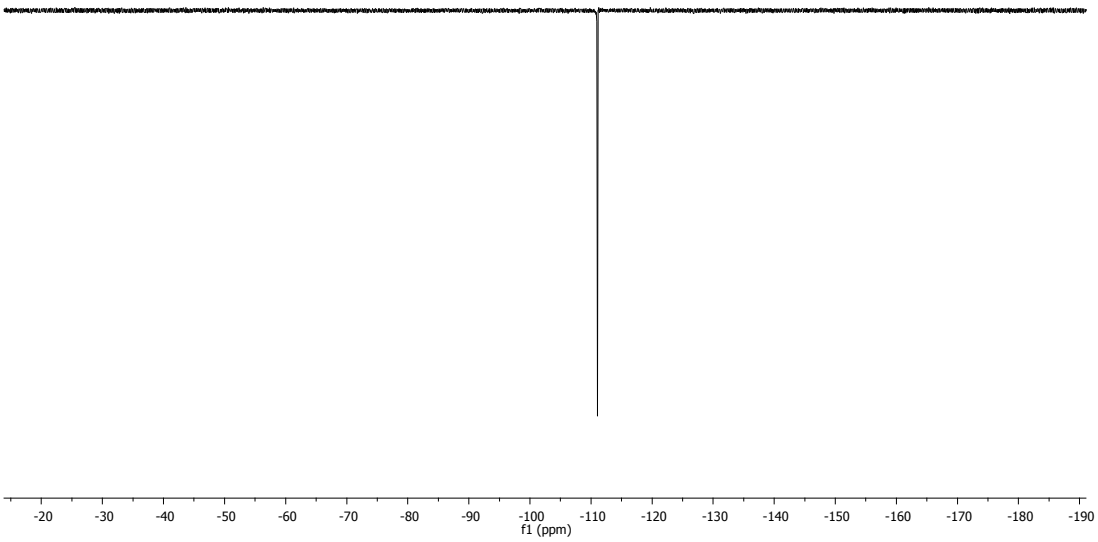


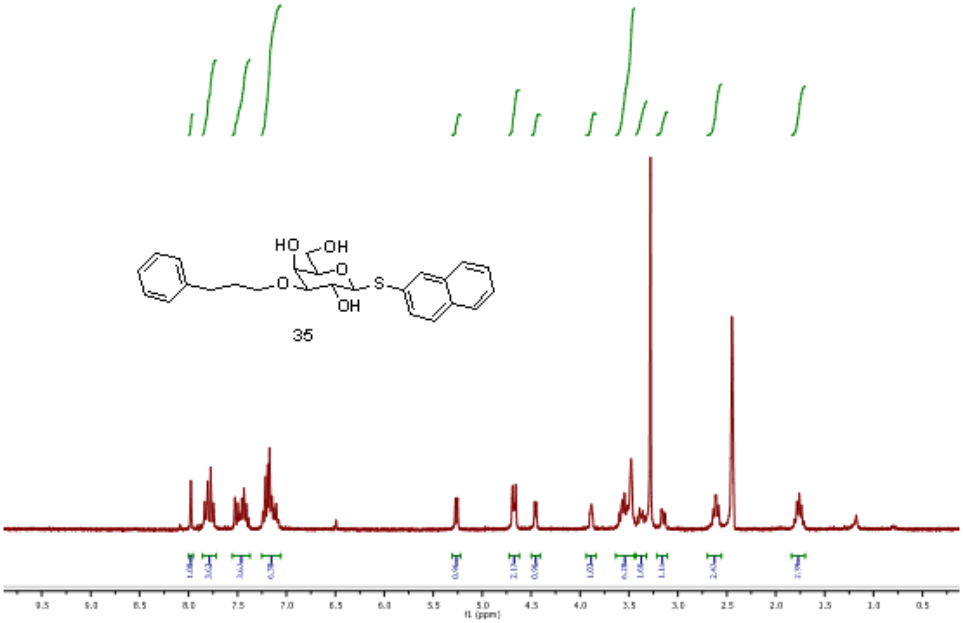

33
2.45
1.32
4.57
2.40
4.38
1.00
3.64
2.64
1.28
1.99
5.85
10.0
5.0
0.0
ppm (f1)


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

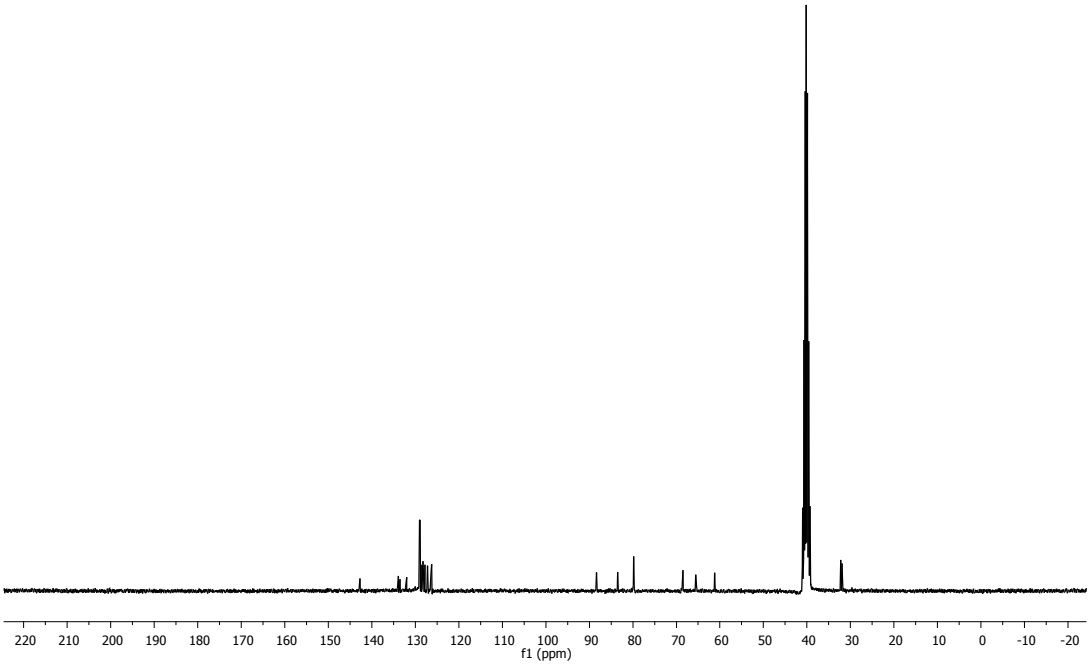


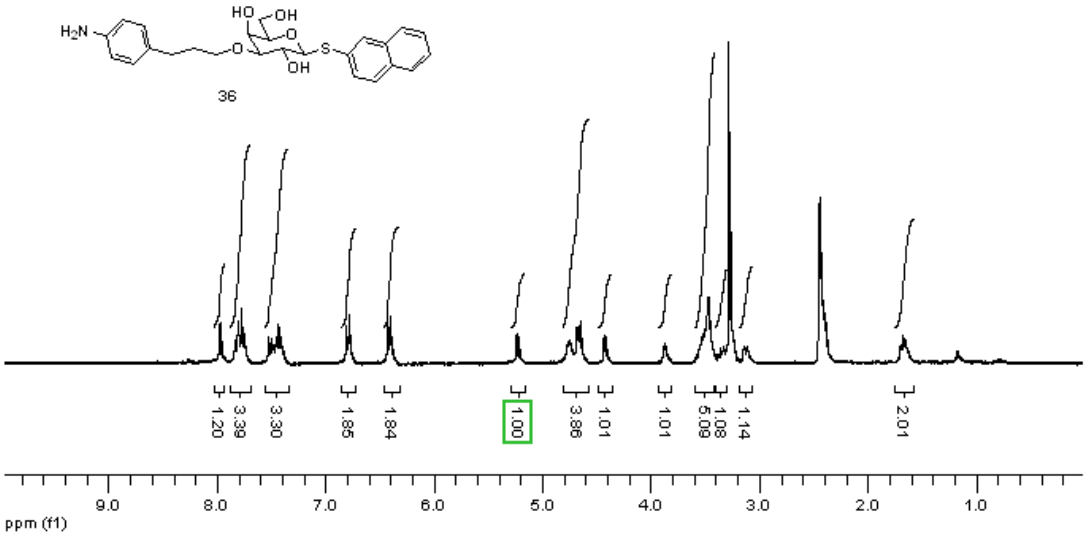


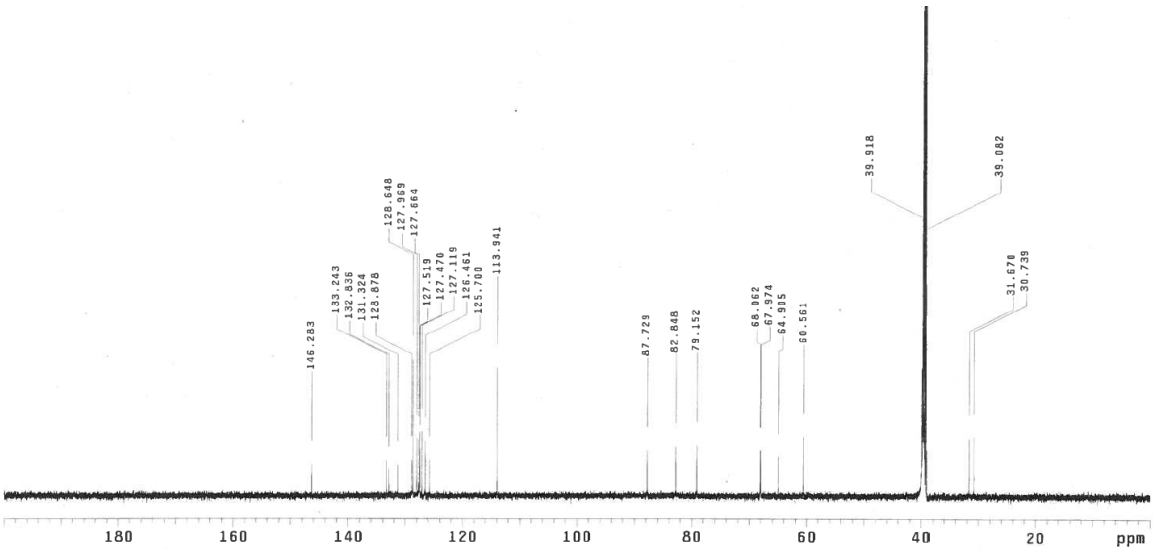




35




H2N
HO
OH
O
O
S
OH
36
1.20
3.39
3.30
1.85
1.84
1.00
3.86
1.01
1.01
5.09
1.08
1.14
2.01
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)


146.283
133.243
132.836
131.324
128.878
128.648
127.969
127.664
127.519
127.470
127.119
126.461
125.700
113.841
87.729
82.848
79.152
68.062
67.974
64.915
60.561
39.918
39.082
31.670
30.739
180
160
140
120
100
80
60
40
20
ppm