Supplementary Information

Evaluation of a Focused Virtual Library of Heterobifunctional Ligands for *Clostridium difficile* Toxins

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Supplementary Figure 1. Sequence alignment of residues from the primary carbohydrate-binding site (red) and peripheral binding site (green) in the two repeats defined by crystallography (repeats vi and vii), as well as the five repeats not defined by crystallography (repeats i – v) in TcdA for C. difficile strain VPI 10463.

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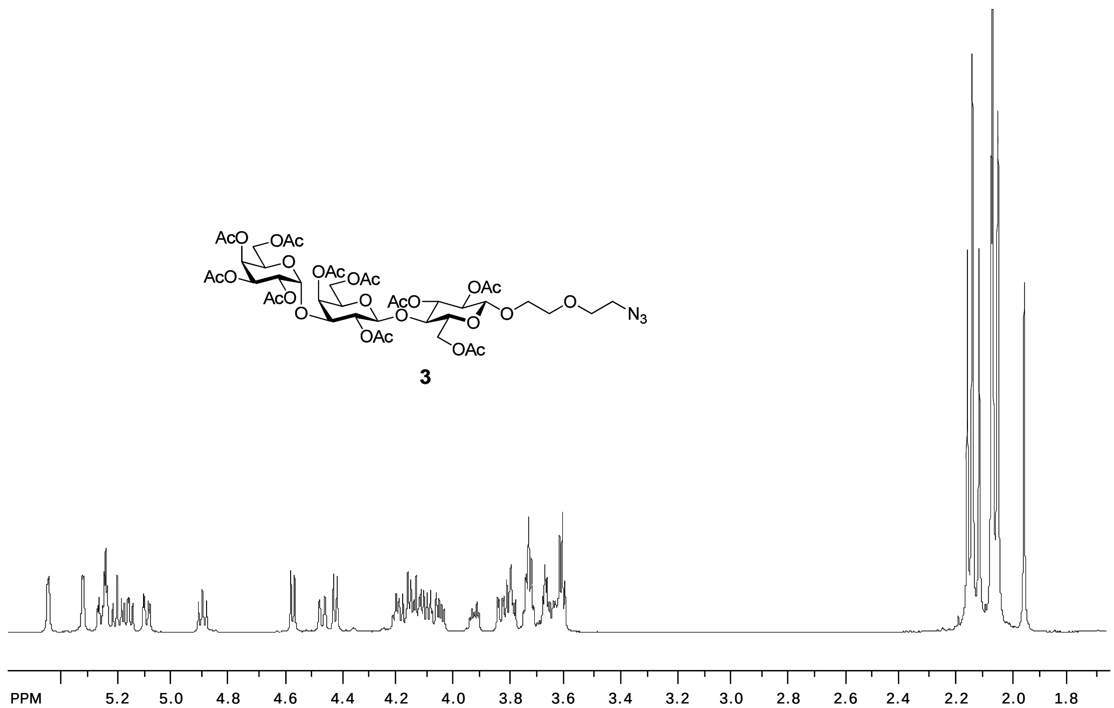
Supplementary Figure 2. Top 100 alignments obtained from BLAST search of the non-redundant NCBI database on October 15, 2014. Accession codes and residue positions are given before and after each alignment. Dots indicate identical residues and letters indicate differences from the search sequence.



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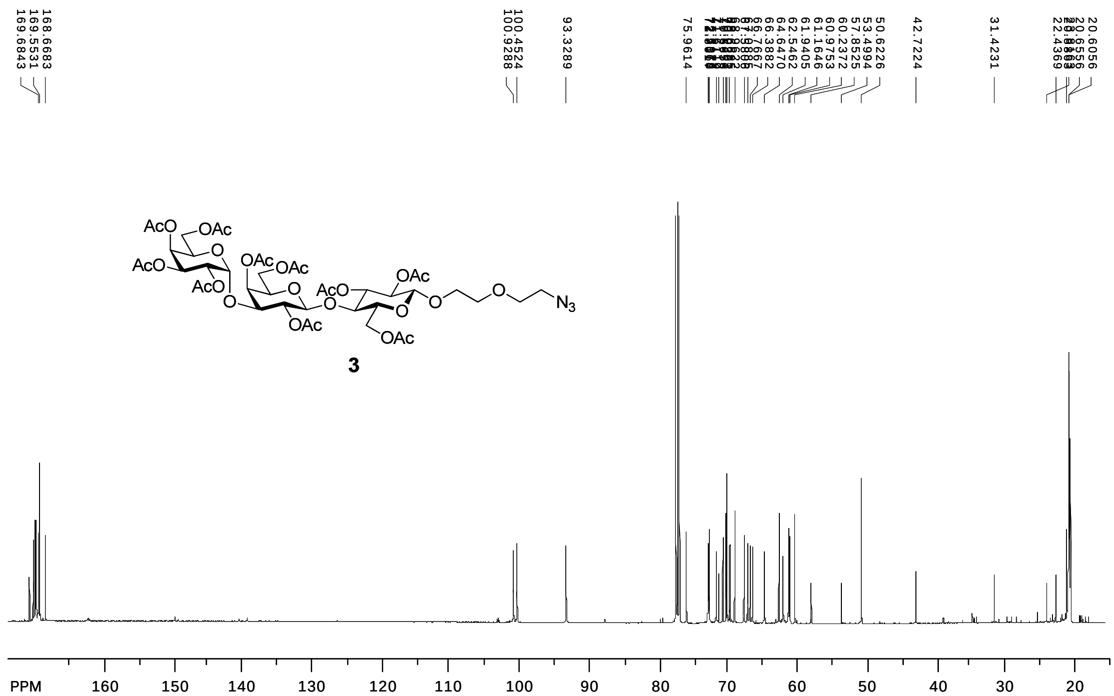

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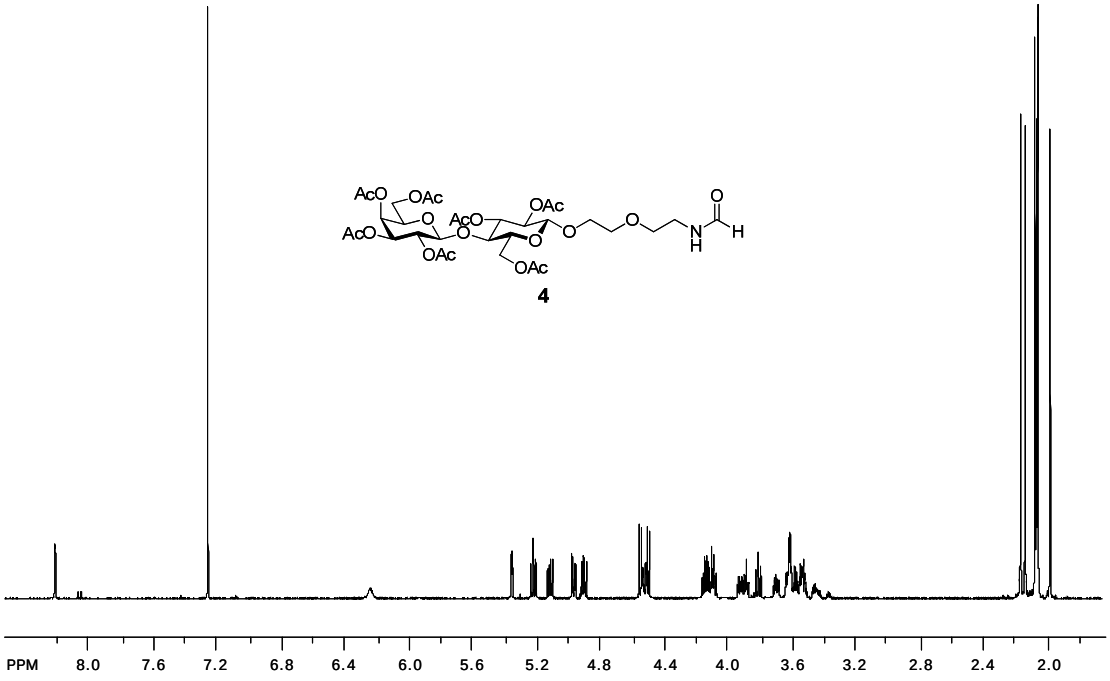
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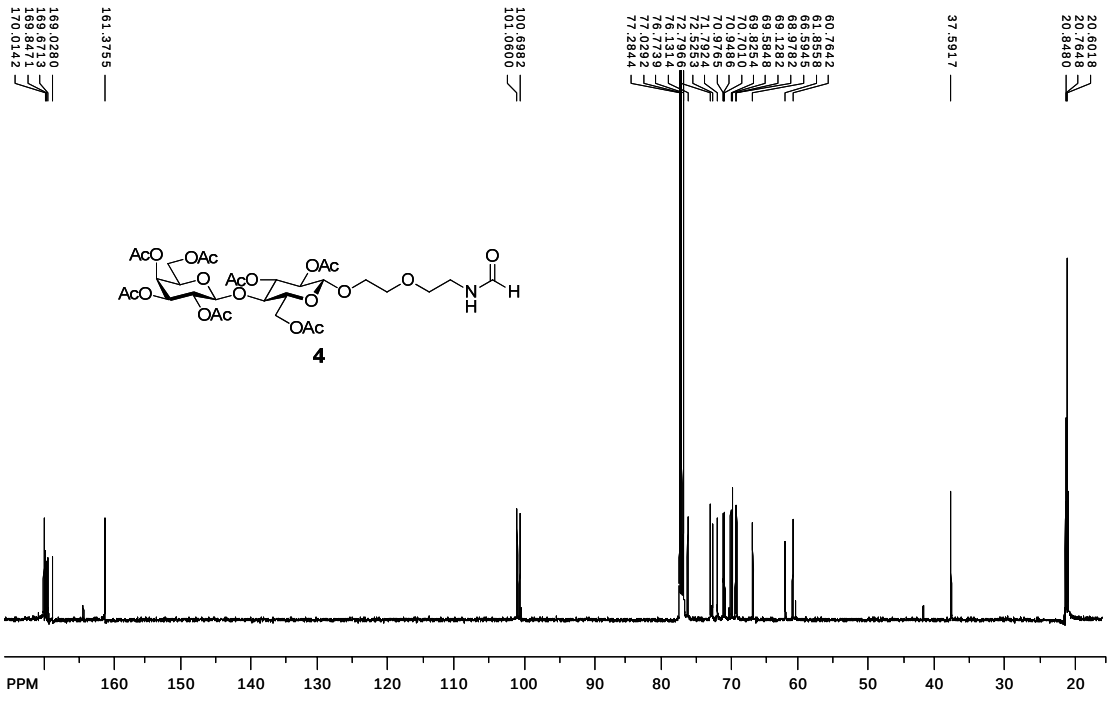
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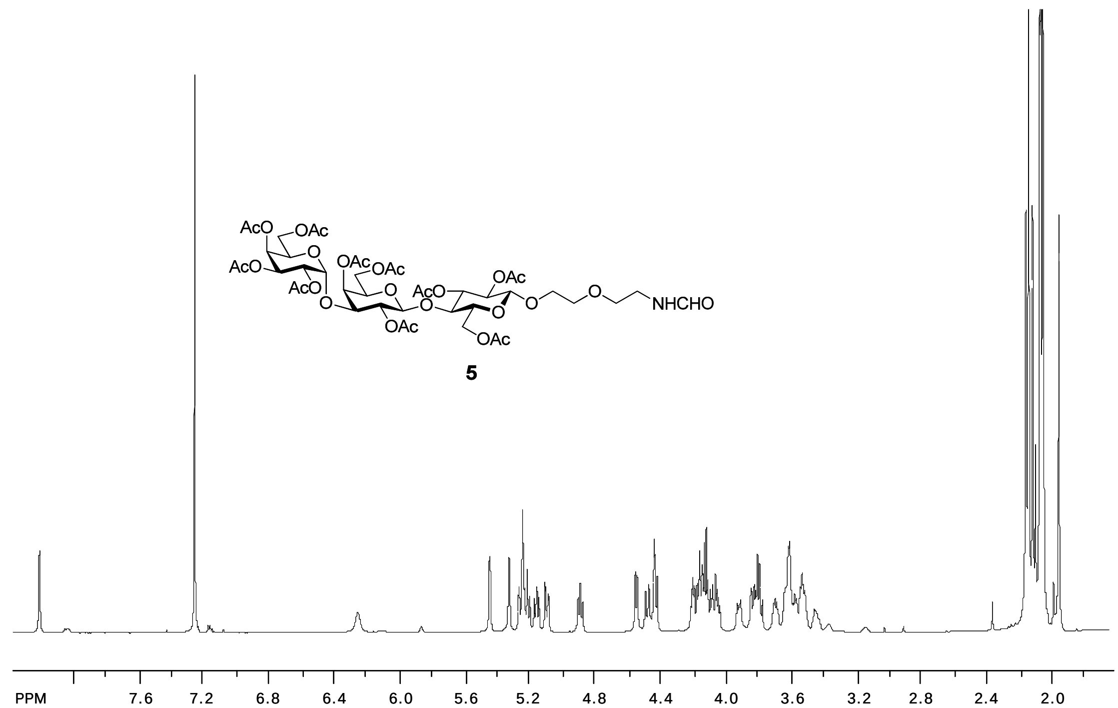
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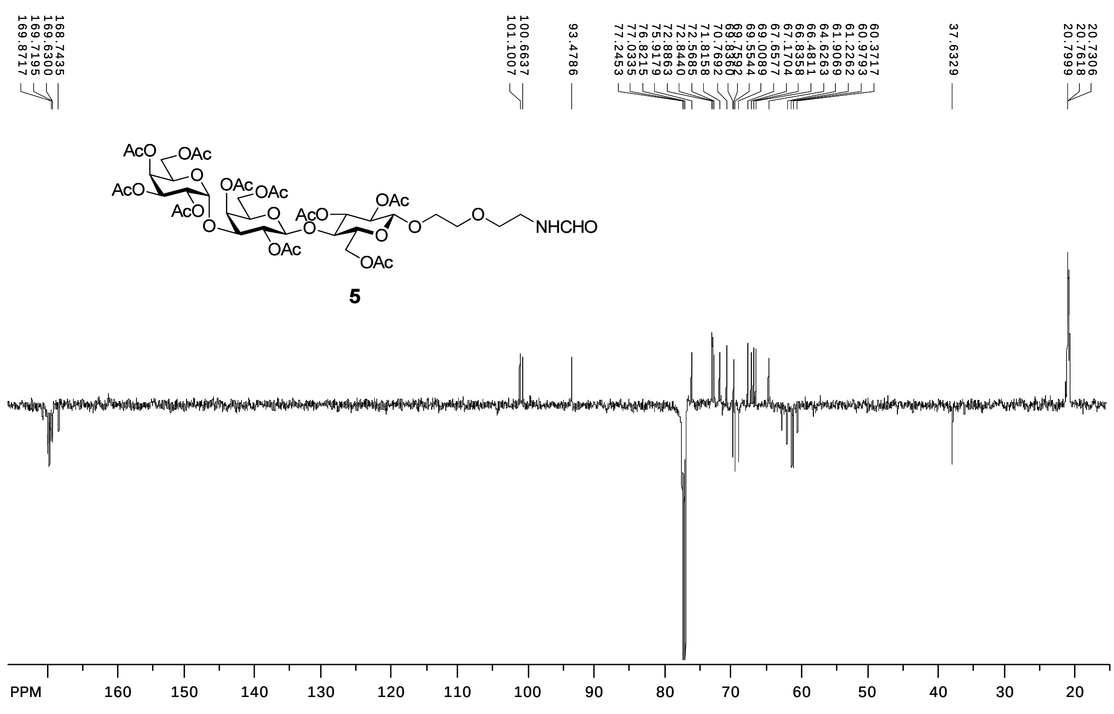
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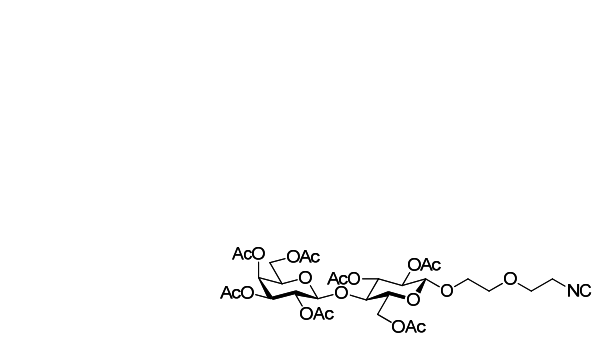

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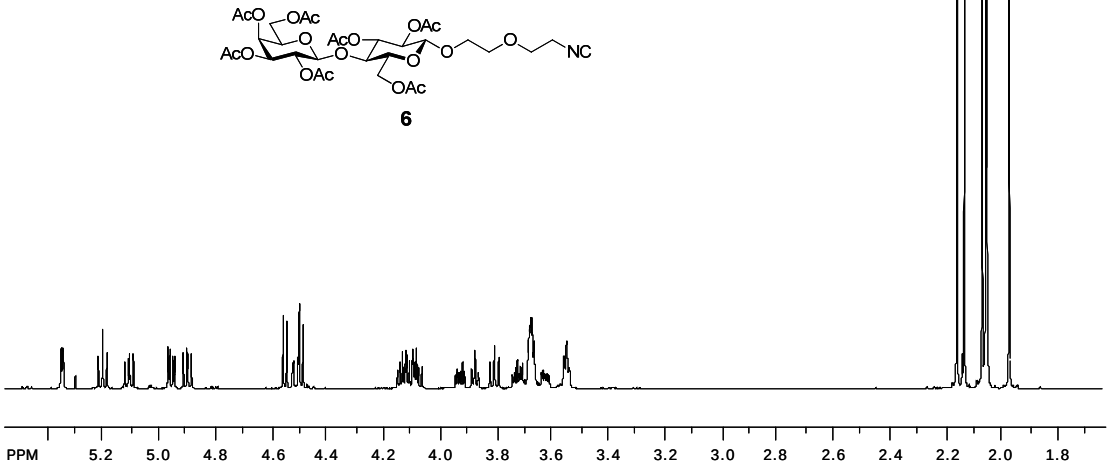

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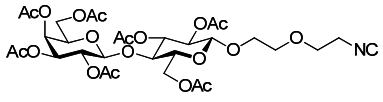

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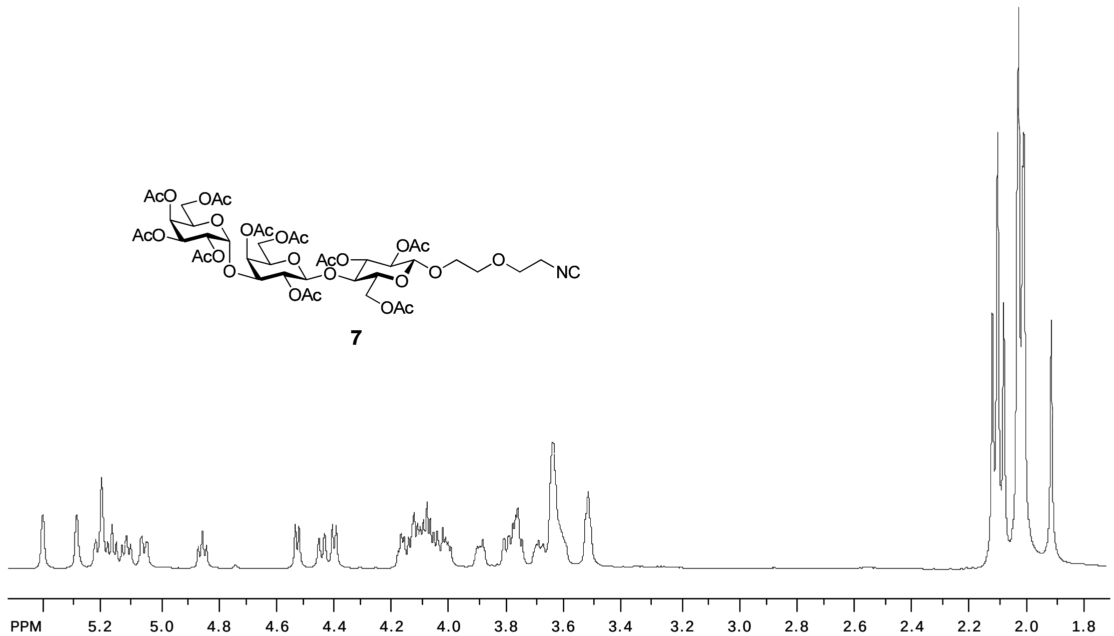
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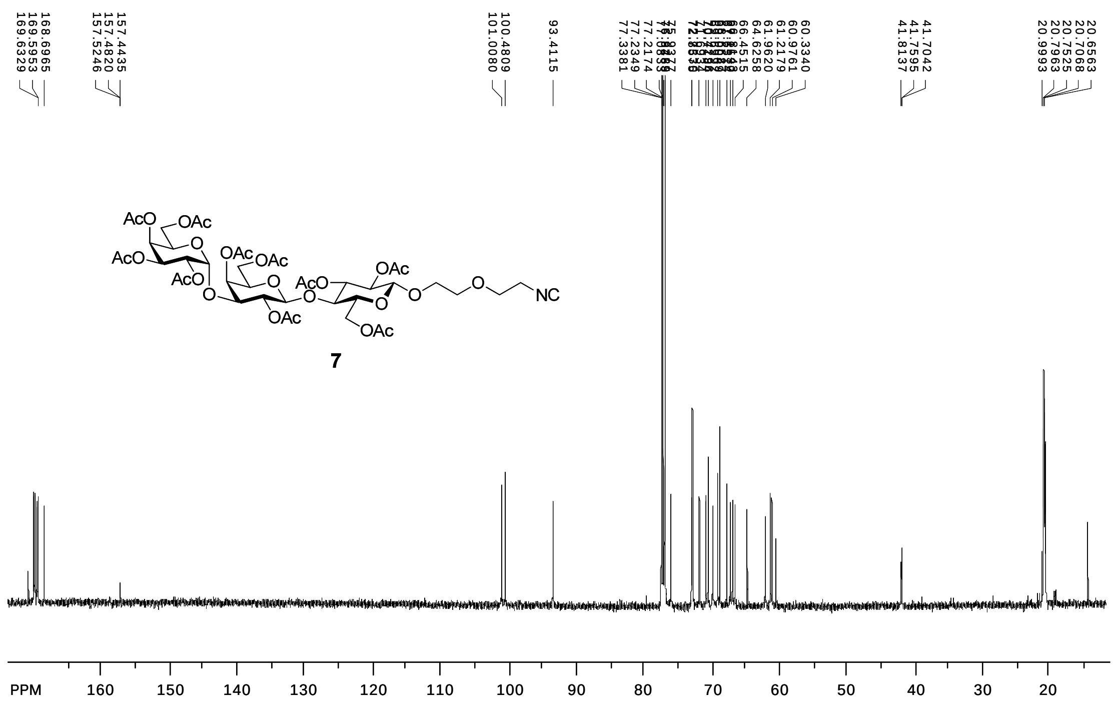
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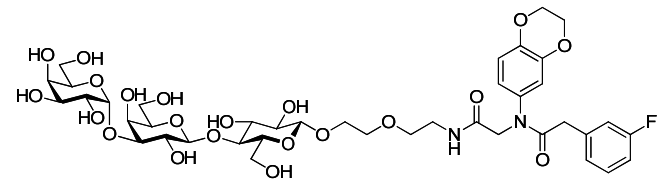

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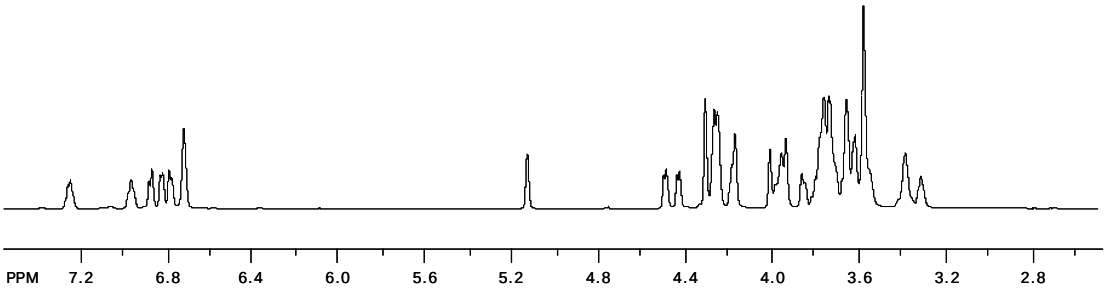
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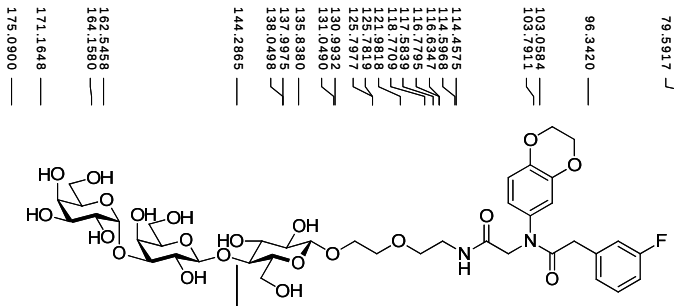

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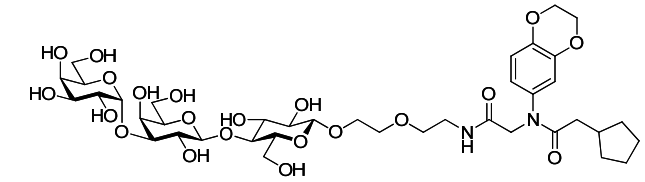

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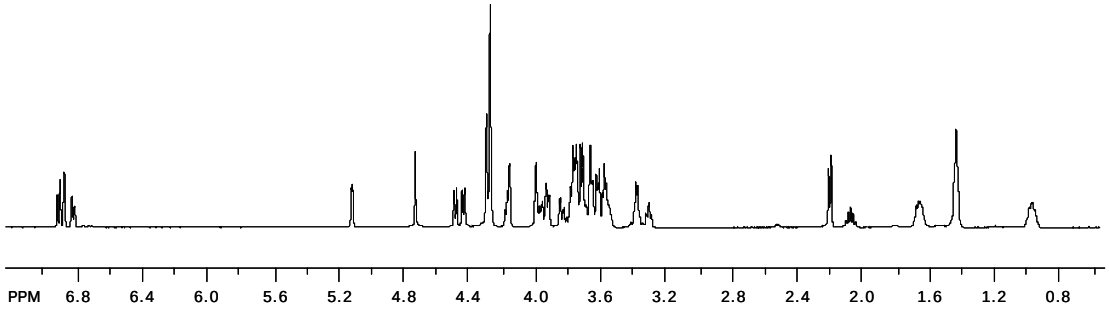
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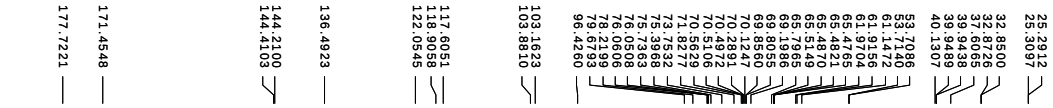
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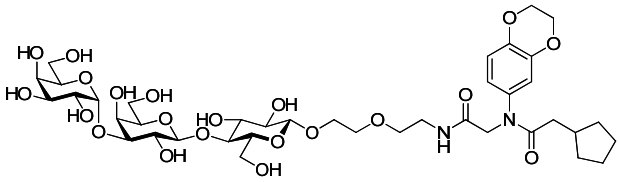

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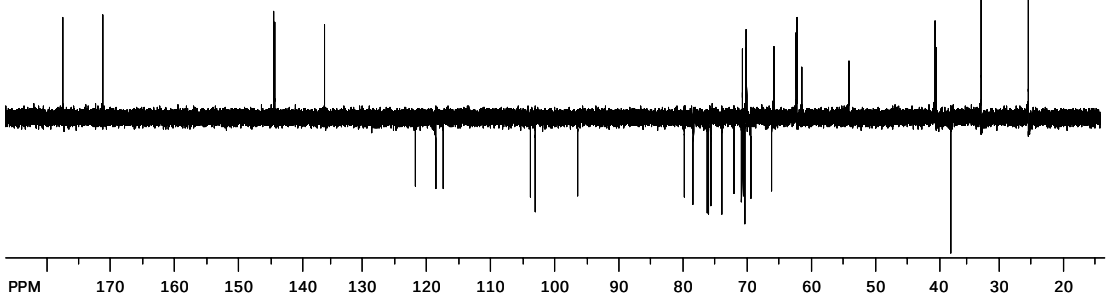
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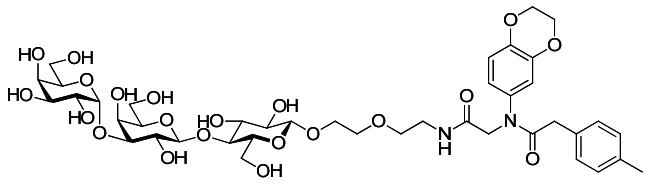

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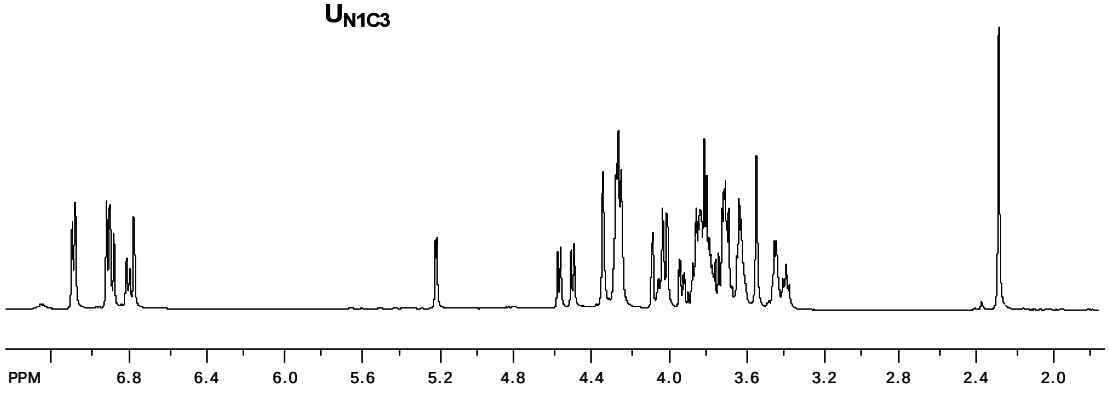
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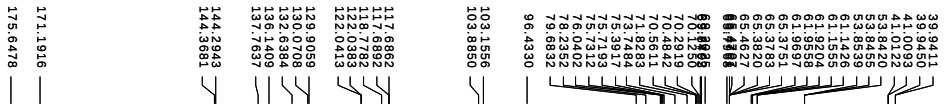
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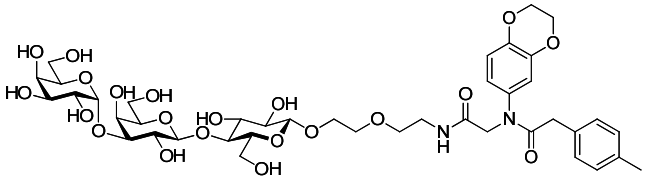
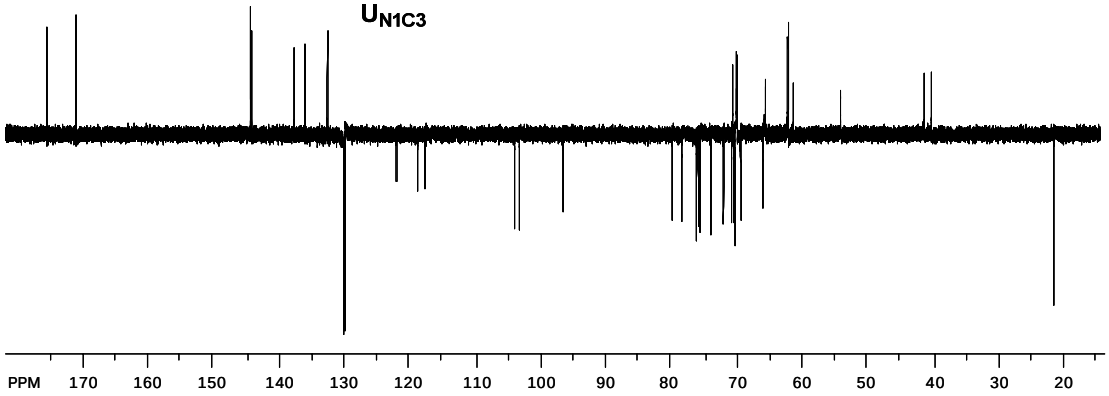


U_{N1C3}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60
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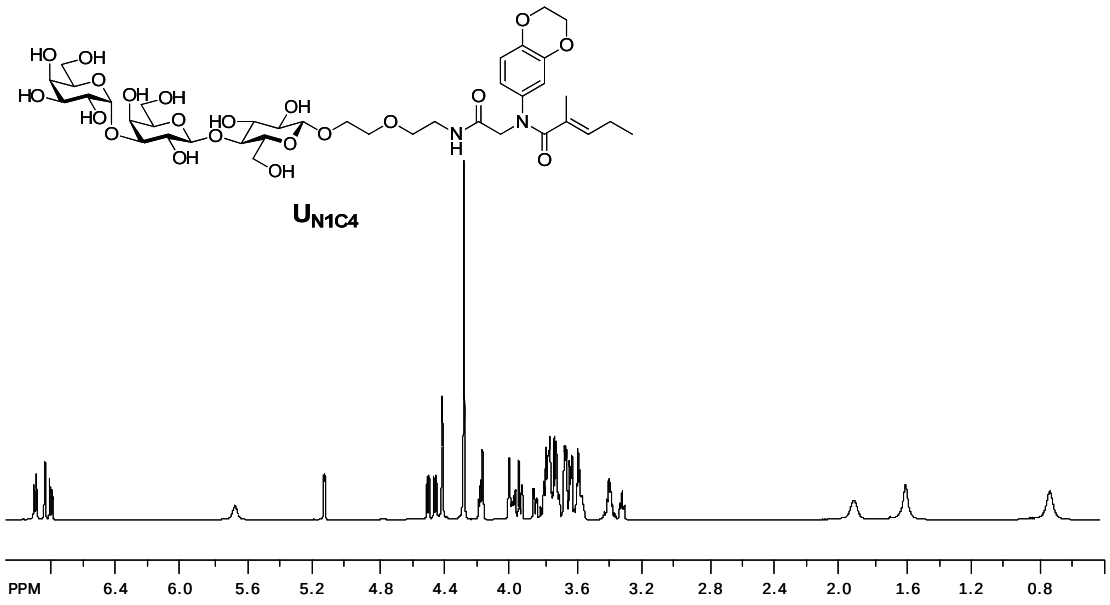
20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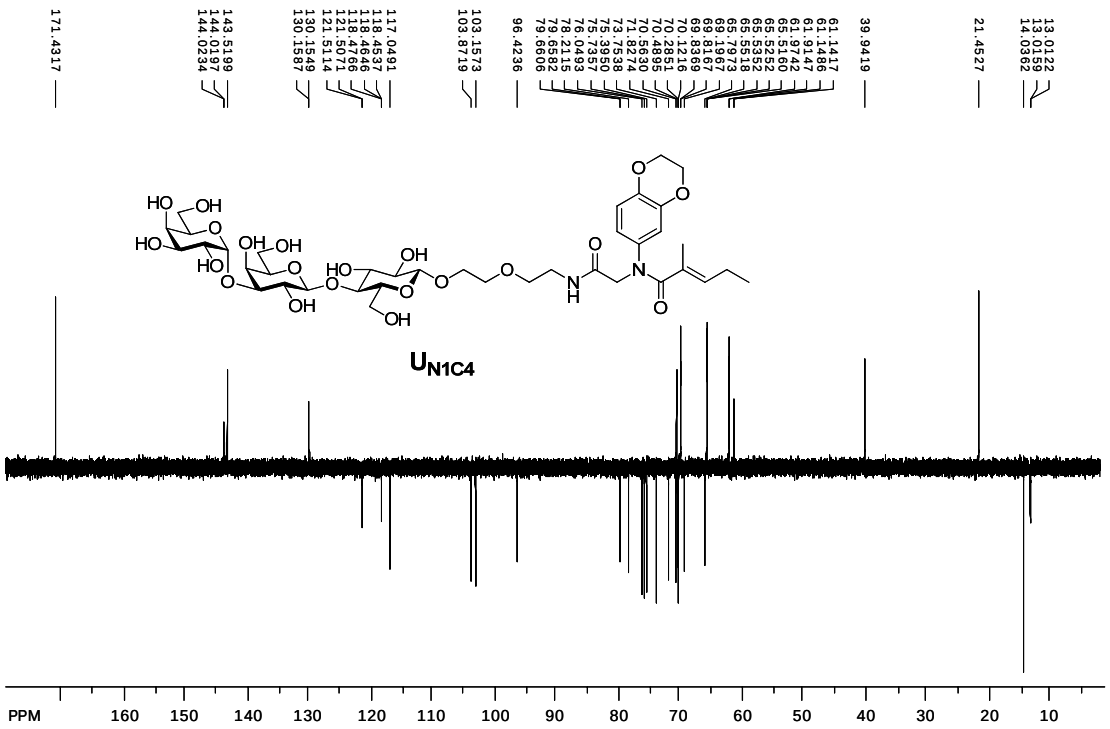
3.2
2.8
2.4
2.0
1.6
1.2
0.8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U_{N1C4}
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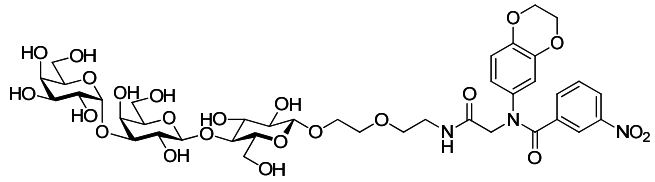

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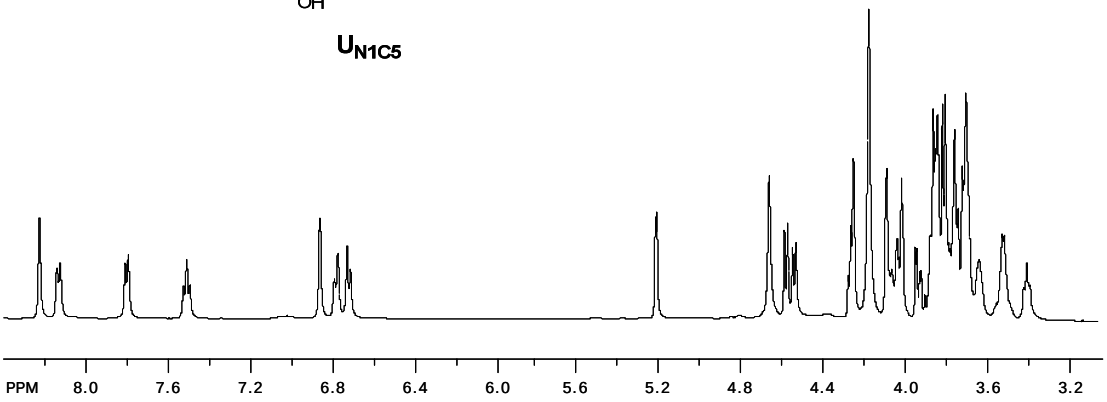
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6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2


170.9029
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136.9998
136.5109
135.4818
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124.2339
122.0888
118.5969
117.4893
117.4831
103.1728
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79.7095
78.2320
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75.7356
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73.7610
71.8292
70.5624
70.5134
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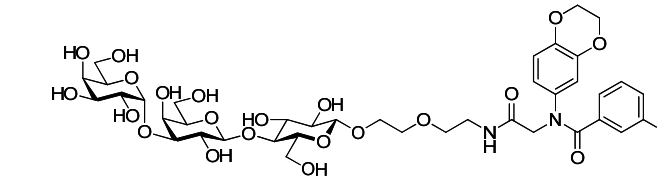

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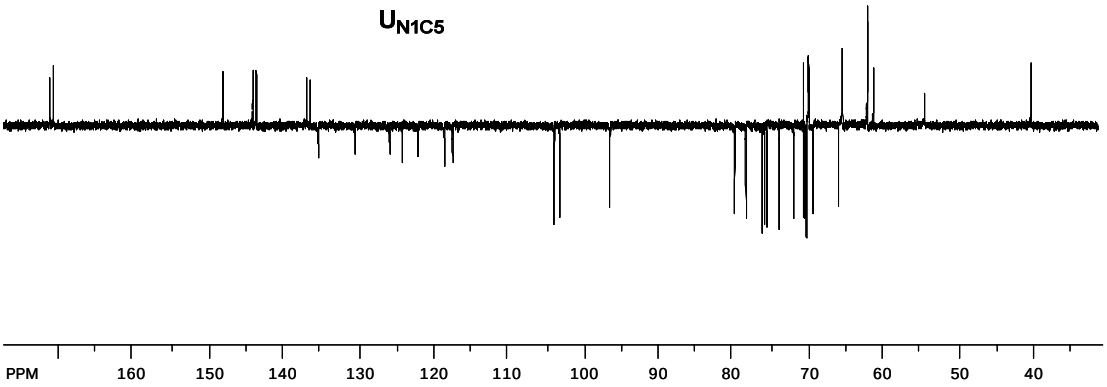
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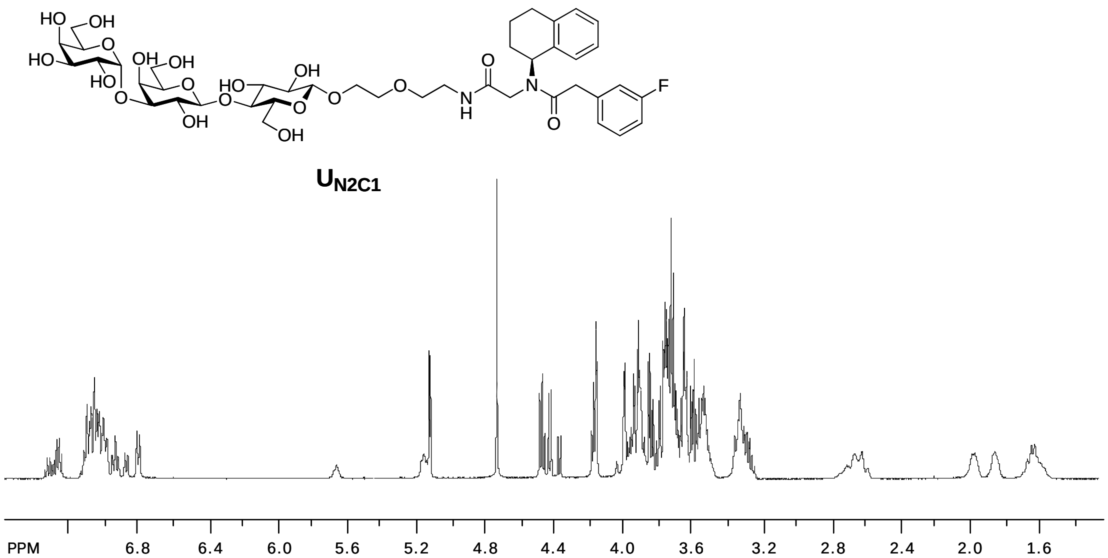
HO
OH
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OH
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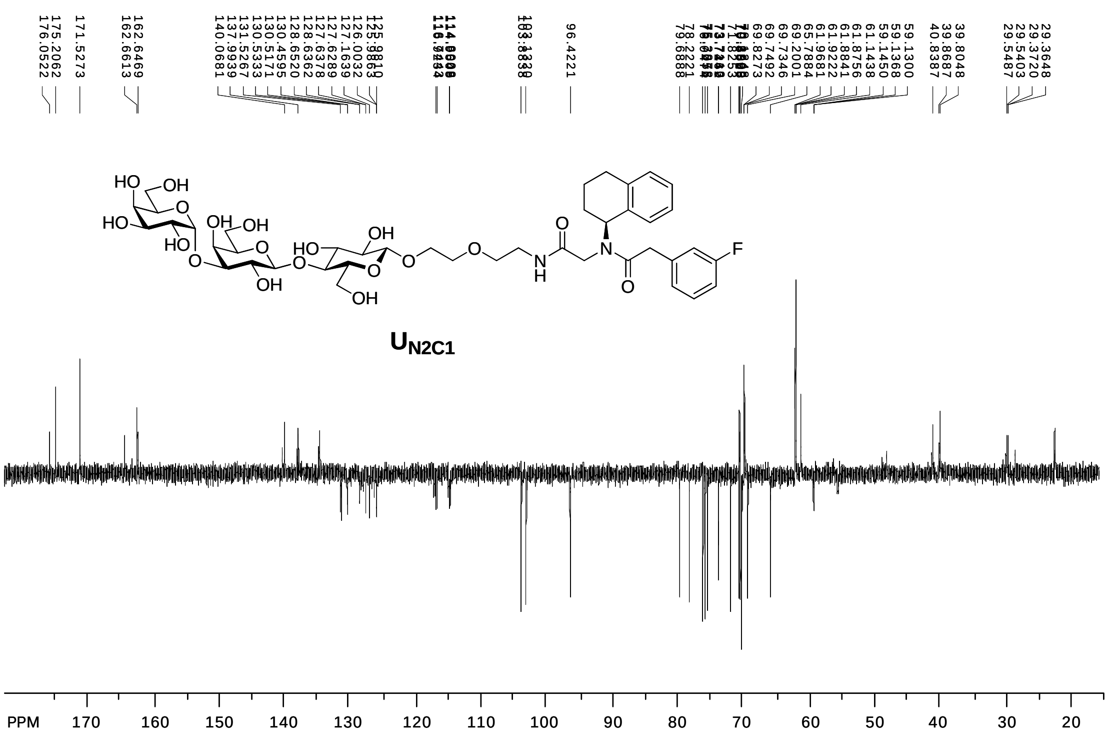
OH
O
O
O
O
O
O
N
H
N
O
O
F
U_{N2C1}
PPM
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6


U_{N2C1}
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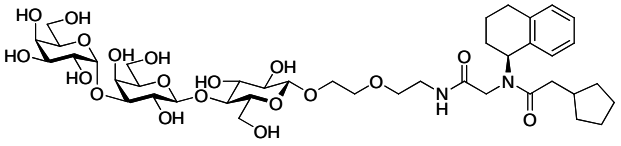
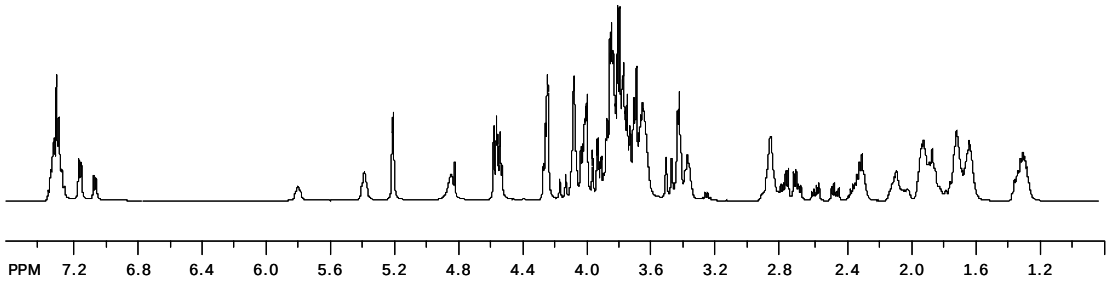


U_{N2C2}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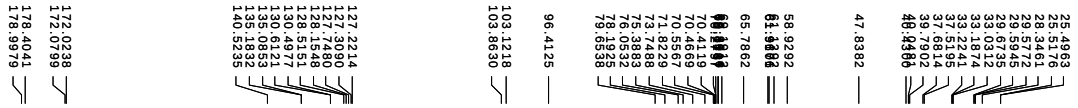
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78.1925
76.0532
75.3883
73.7488
71.8229
70.5567
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58.9292
47.8382
39.7902
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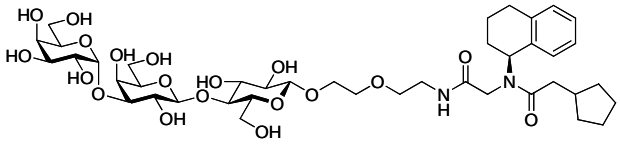
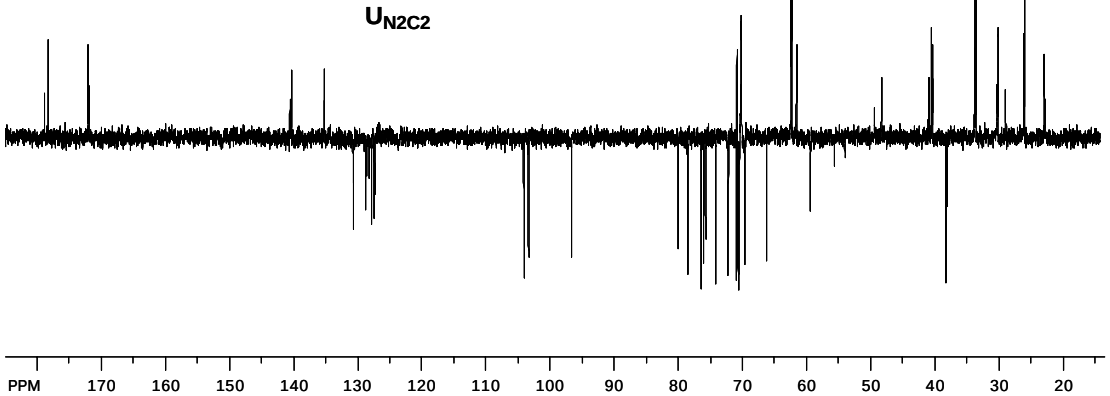
28.5772
28.3461
25.4963



U_{N2C2}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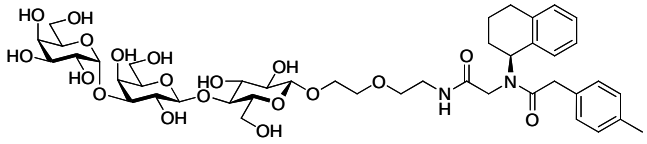
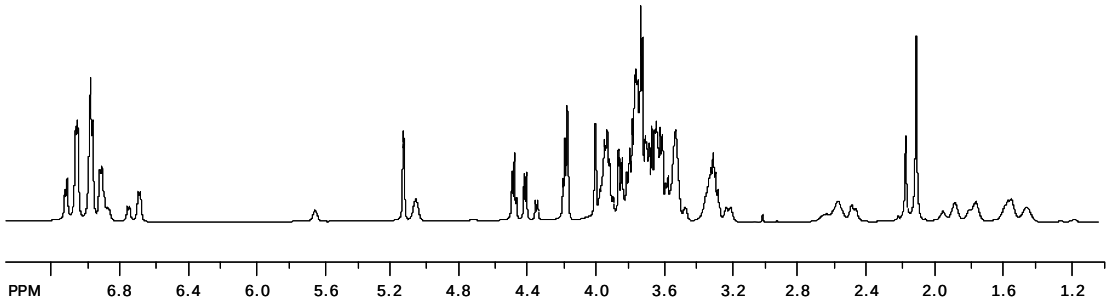


U_{N2C3}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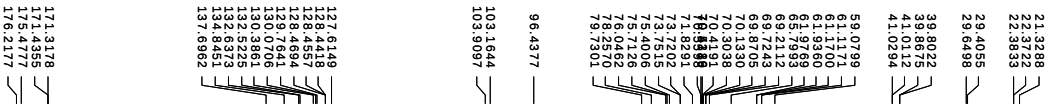
3.6
3.2
2.8
2.4
2.0
1.6
1.2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128.4418
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96.4377
79.7301
76.0462
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75.4006
73.7515
73.7202
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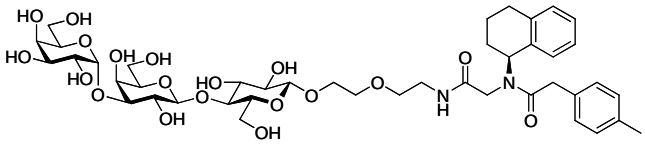
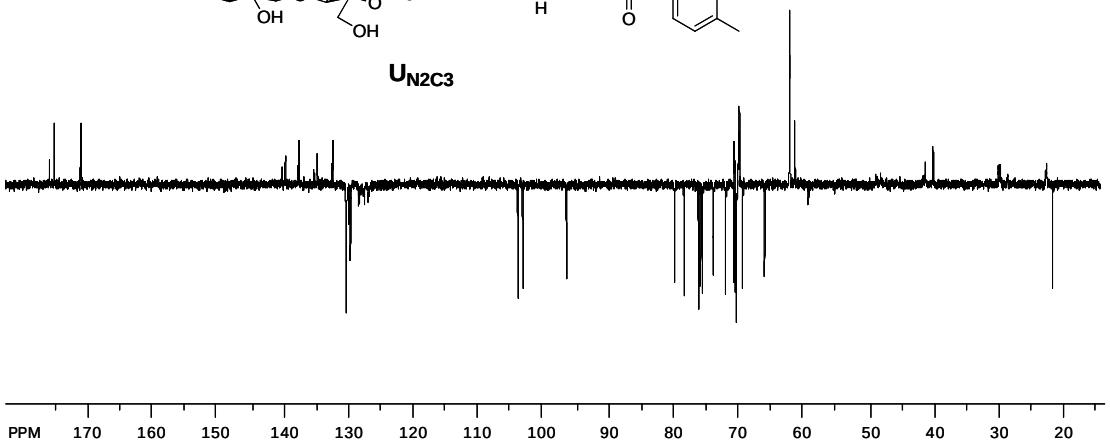
21.3288



U_{N2C3}


PPM
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50
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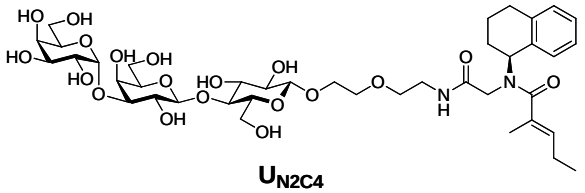
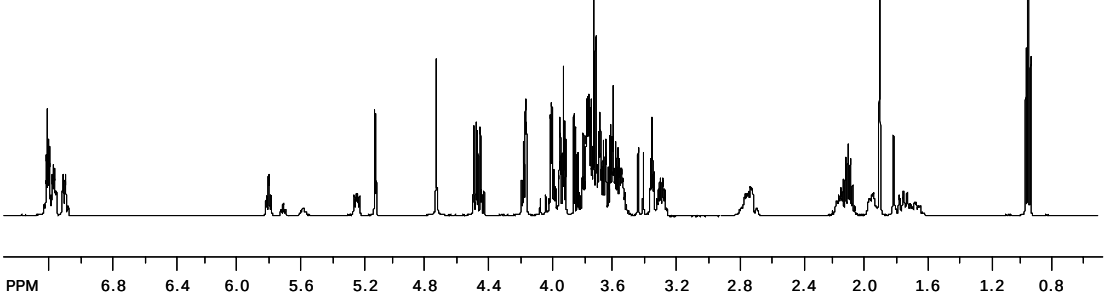
30
20



U_{N2C4}



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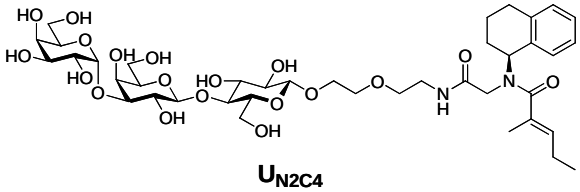
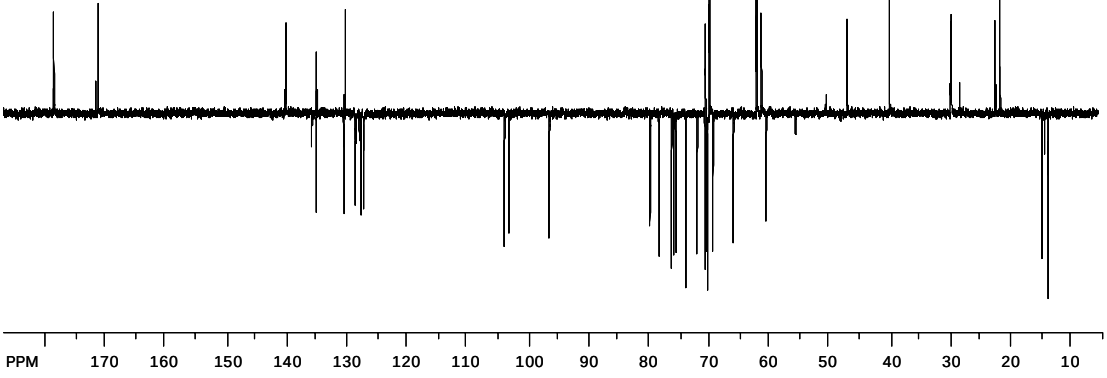
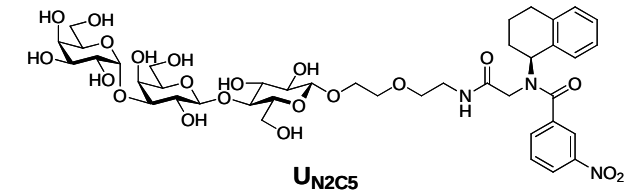
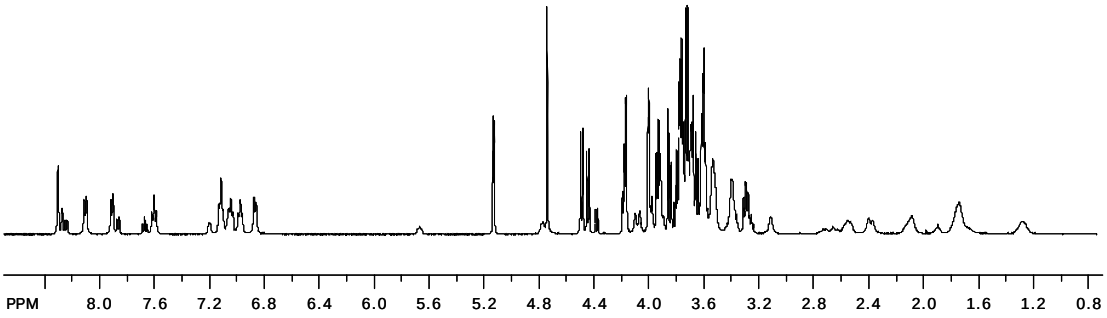


U_{N2C4}





U_{N2C5}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6.0
5.6
5.2
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4.4
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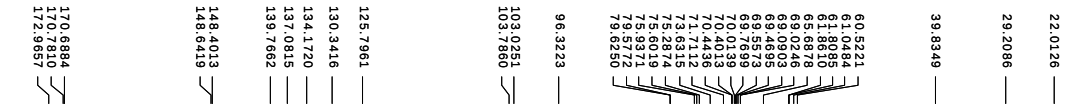
3.2
2.8
2.4
2.0
1.6
1.2
0.8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96.3223
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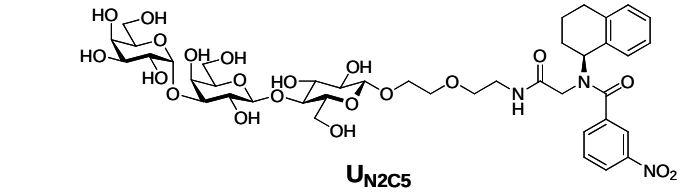
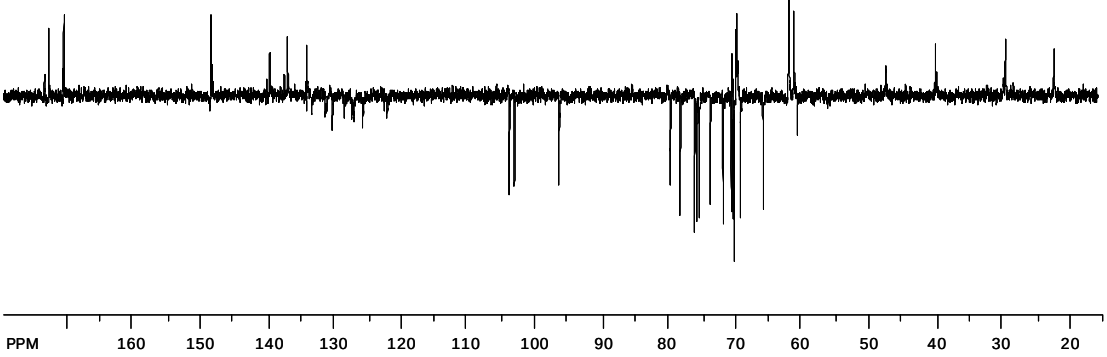
22.0126



U_{N2C5}


PPM
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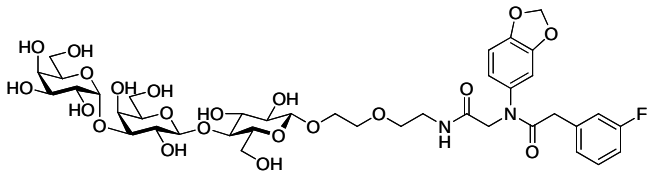
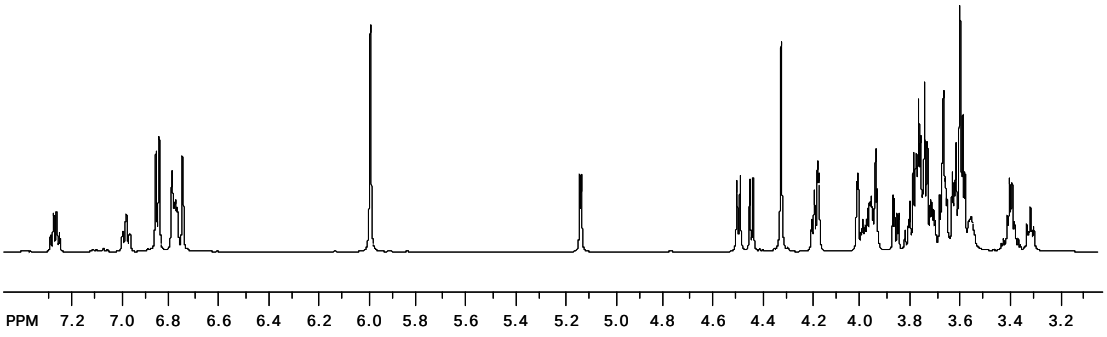


U_{N3C1}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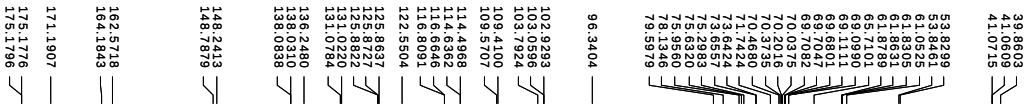
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69.1111
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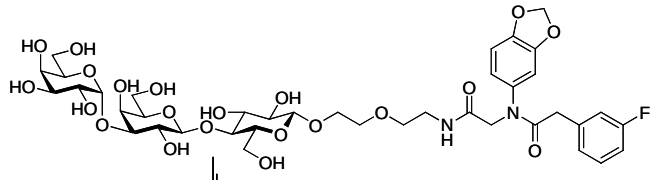
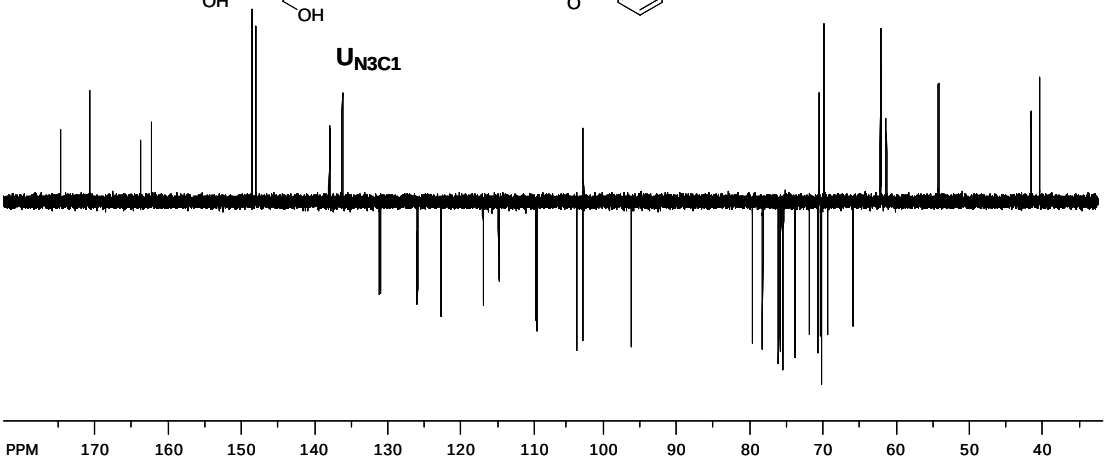
41.0715



U_{N3C1}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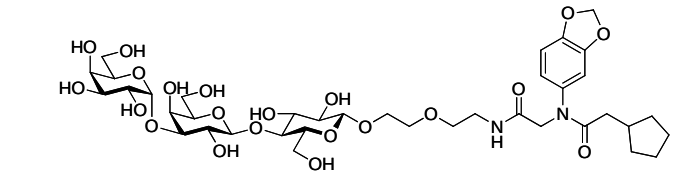
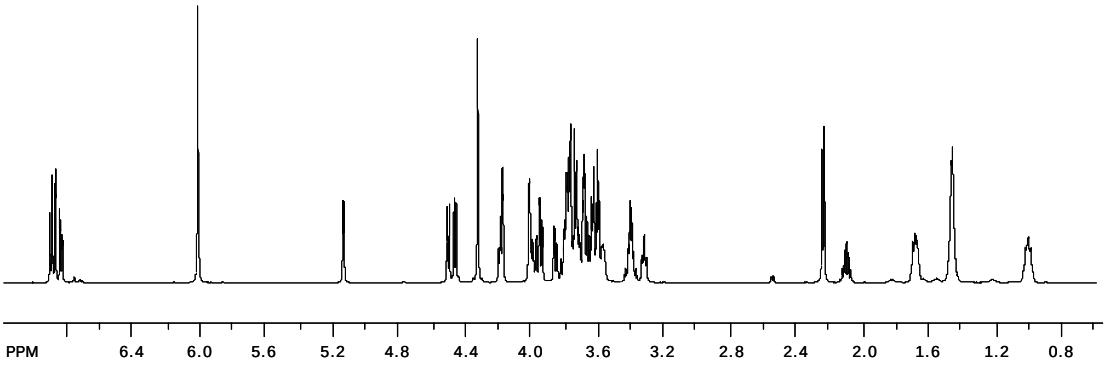


U_{N3C2}


PPM
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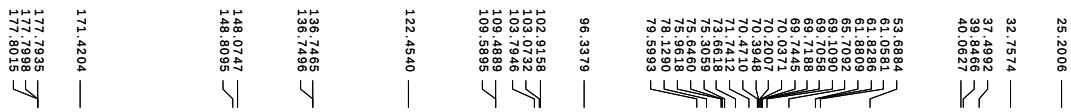
1.2
0.8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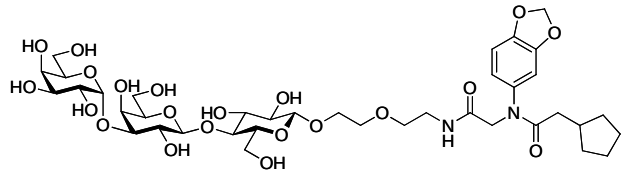
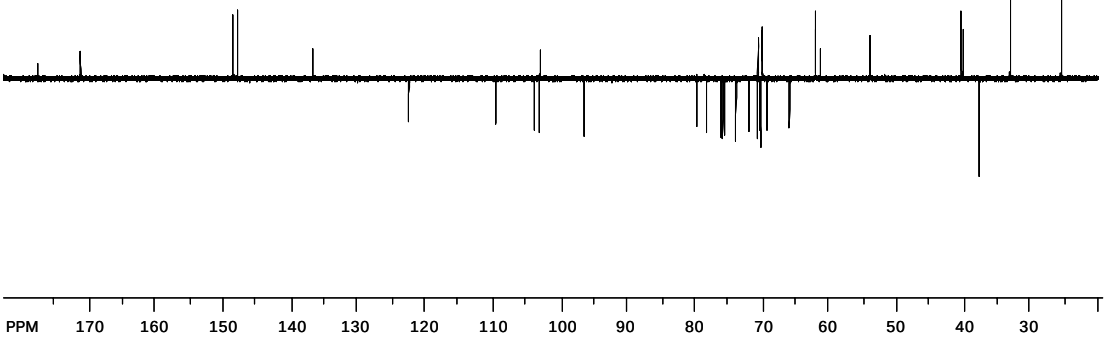


U_{N3C2}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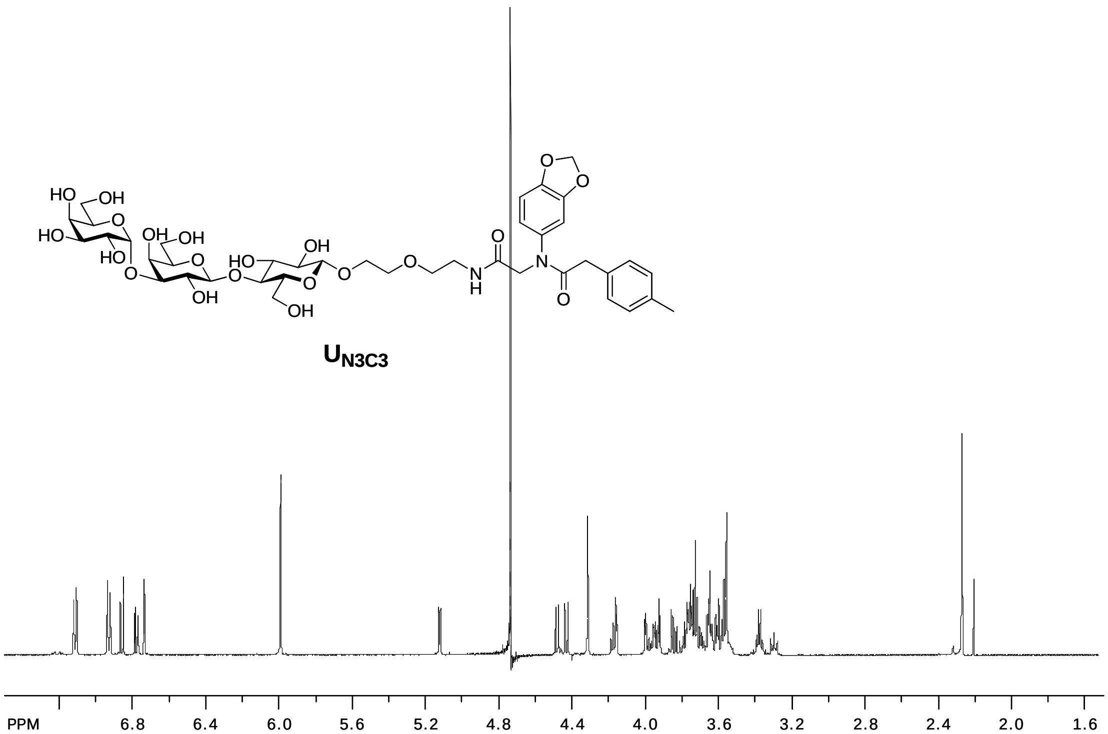
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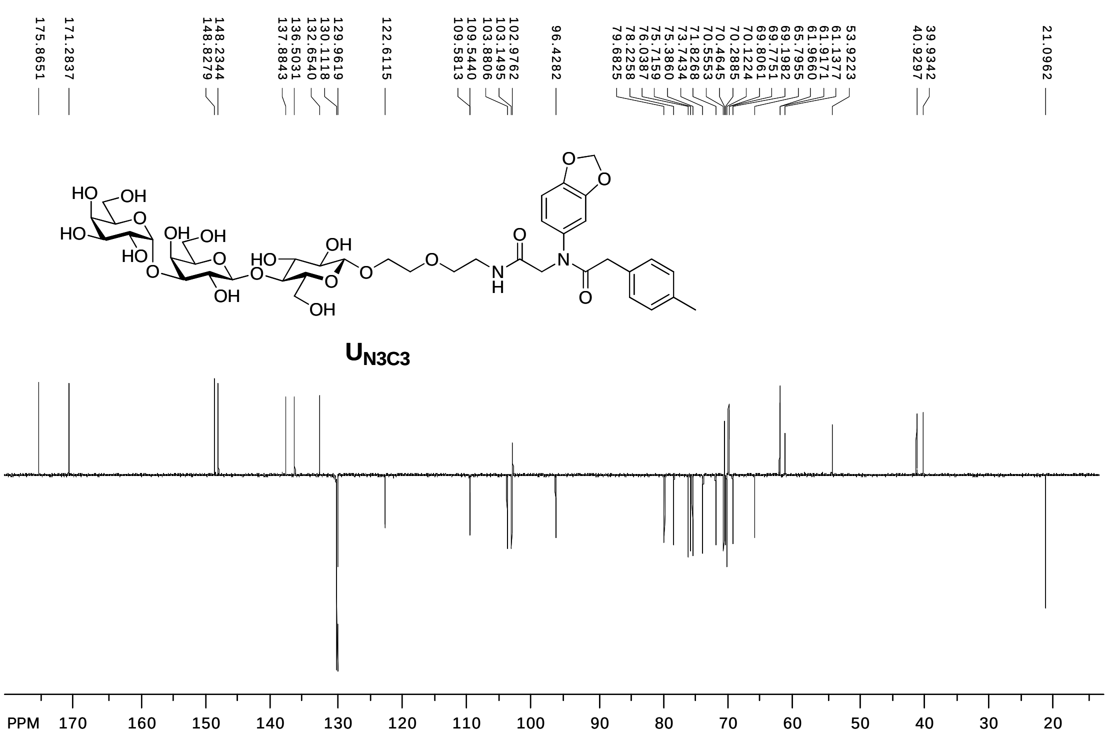
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75.3860
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69.1982
65.7955
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61.9171
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21.0962
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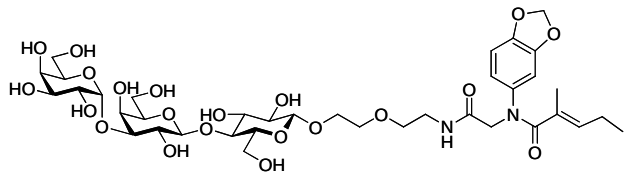

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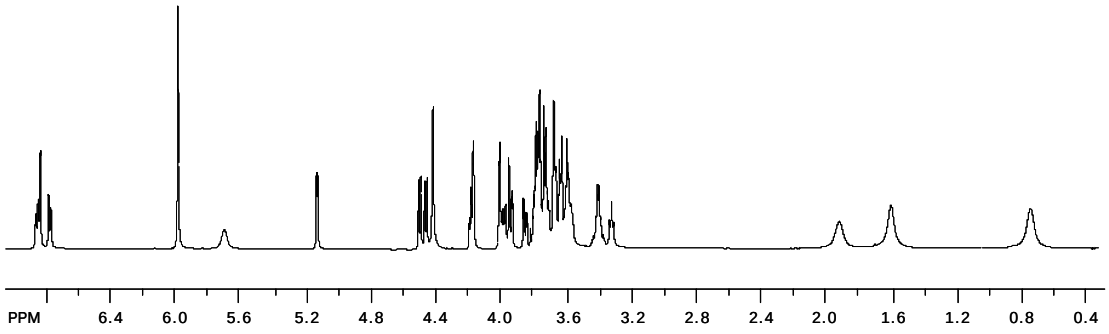
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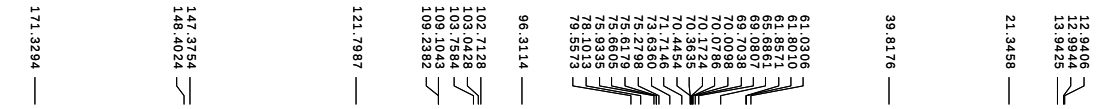
0.4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70.0098
69.7038
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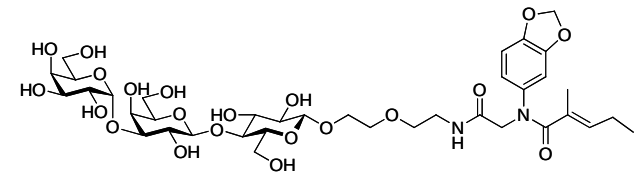

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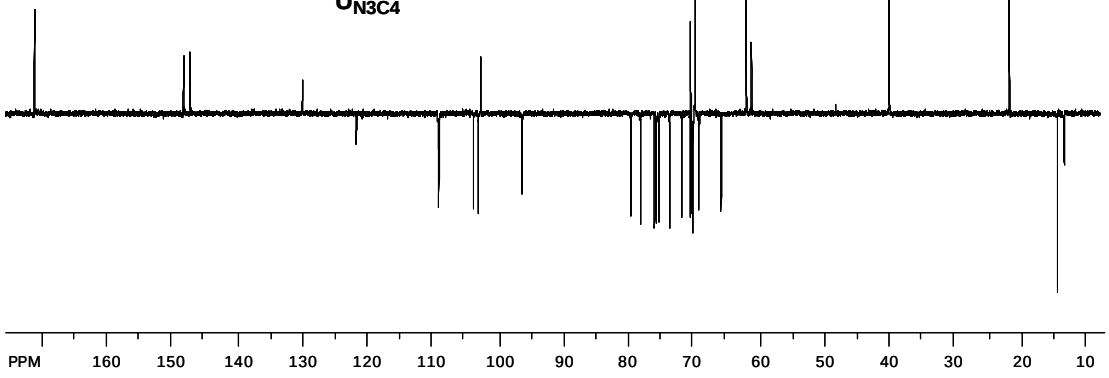
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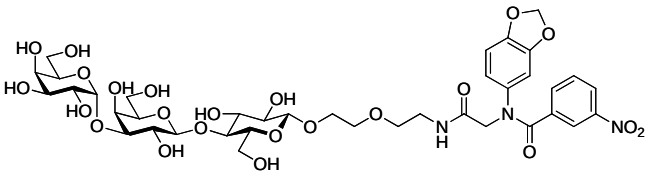

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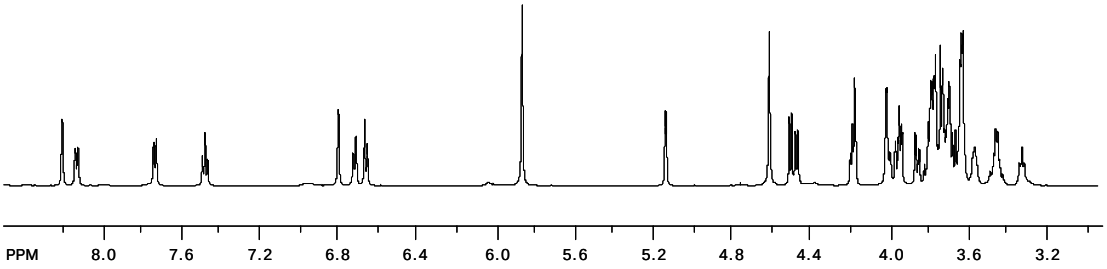
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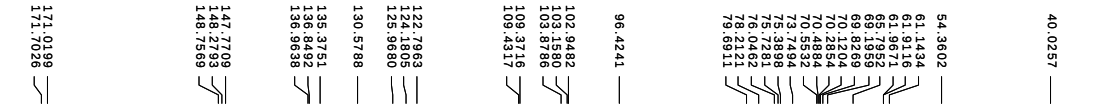
5.6
5.2
4.8
4.4
4.0
3.6
3.2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124.1805
125.9680
109.3716
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102.9482
103.1580
103.8786
96.4241
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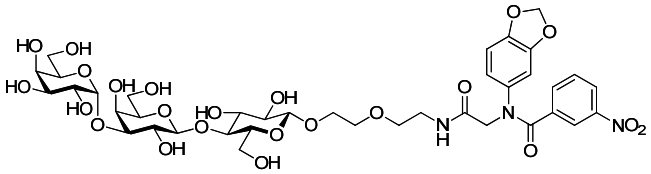

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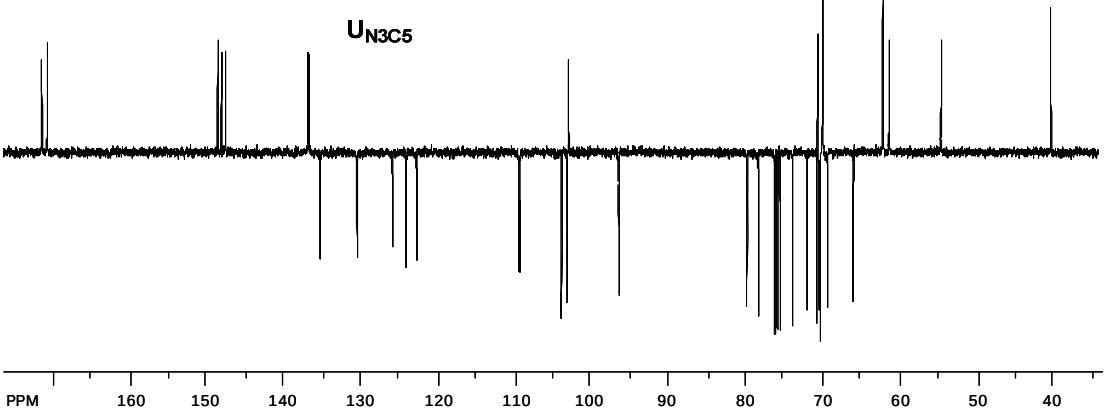
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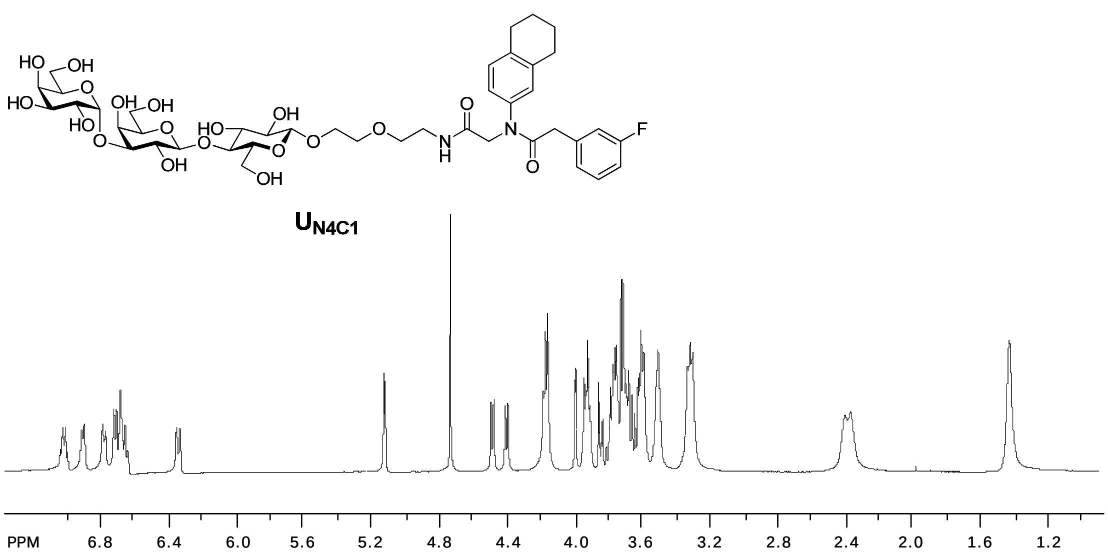

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N
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OH
U_N4C1
PPM
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6.4
6.0
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2.8
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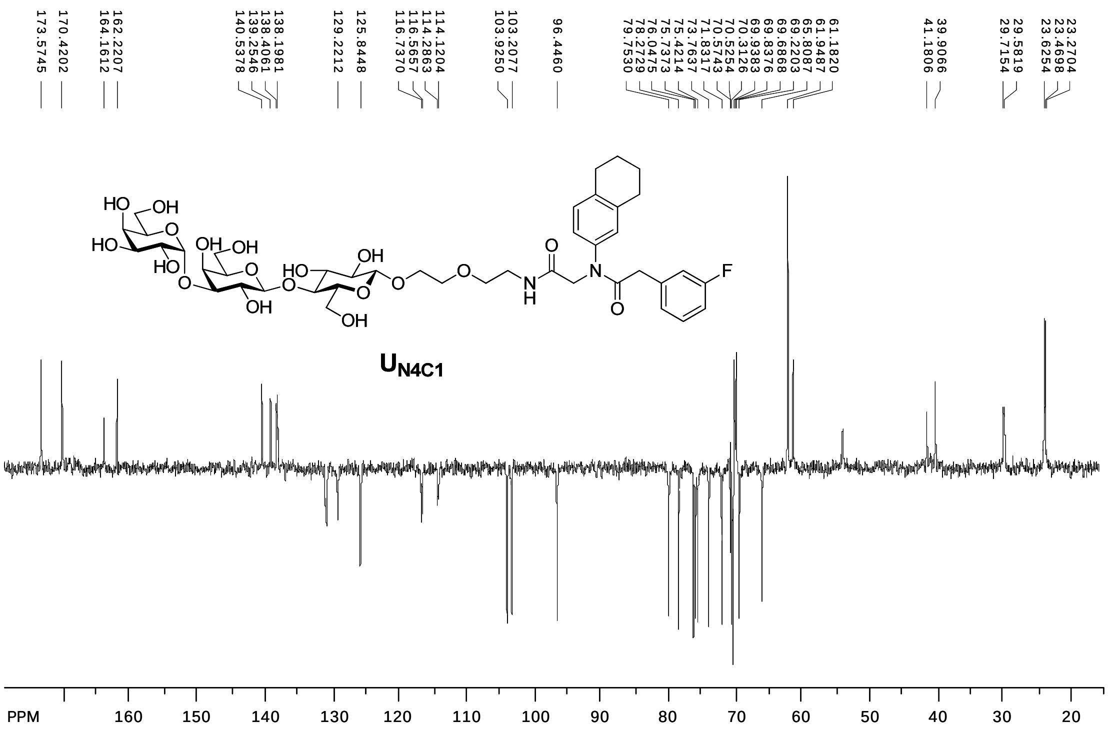
1.6
1.2



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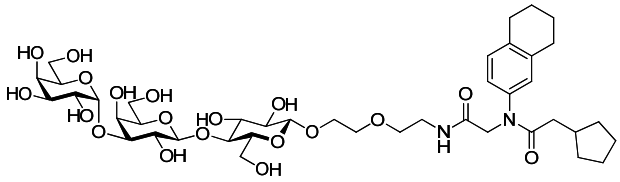

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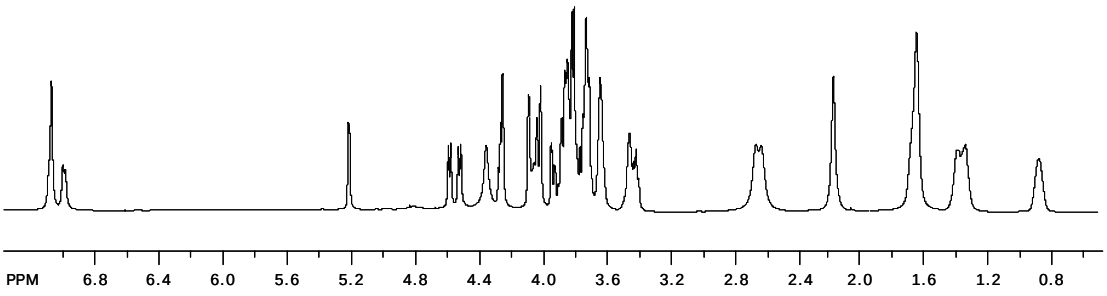
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2.4
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1.2
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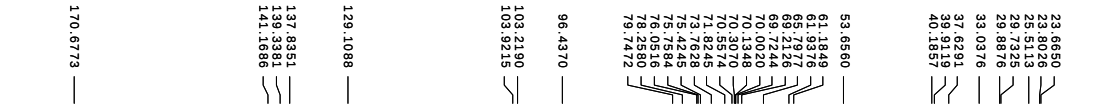
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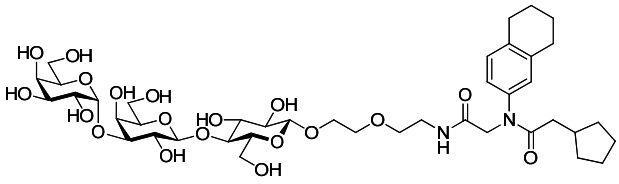

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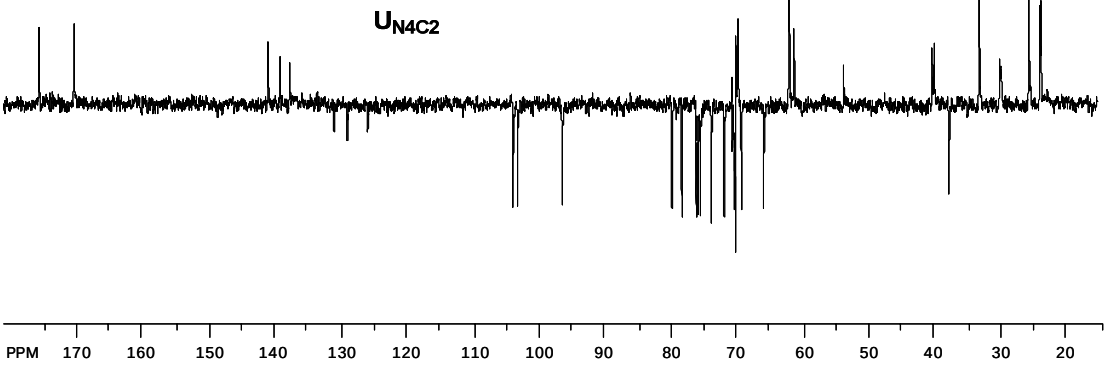
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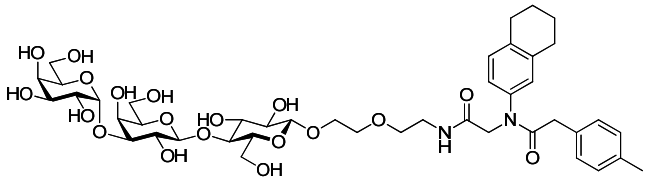

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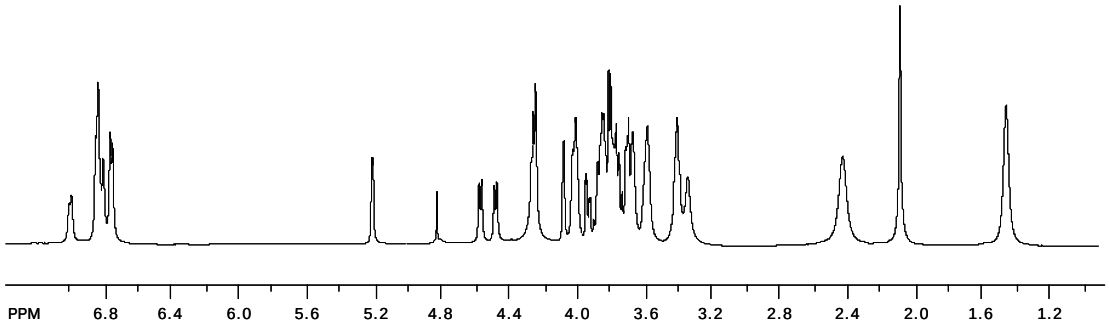
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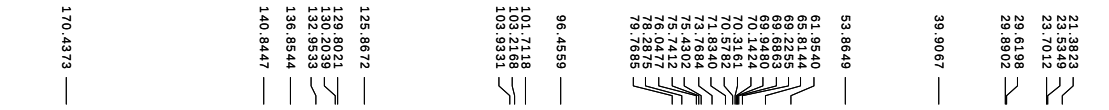
1.2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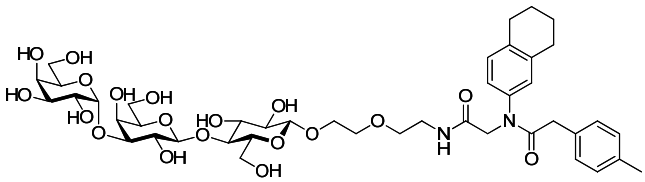

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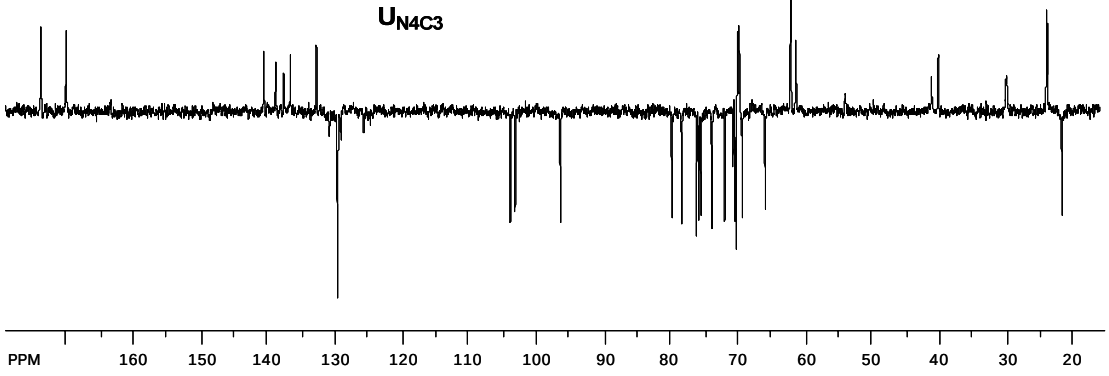
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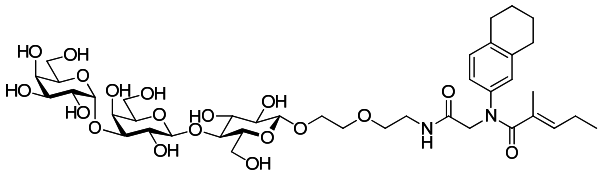

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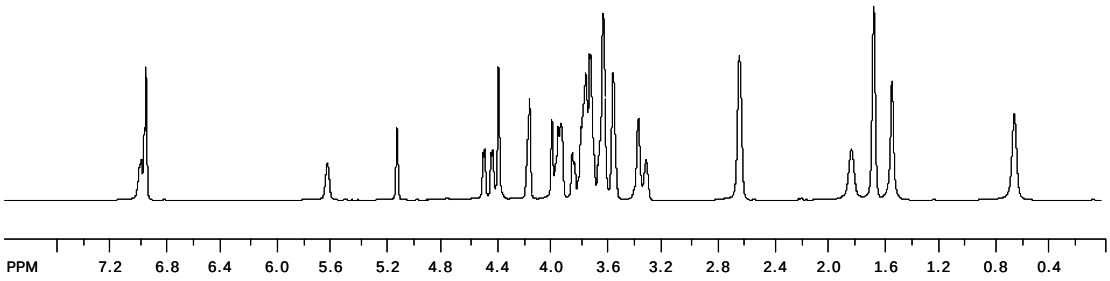
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5.2
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2.8
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1.6
1.2
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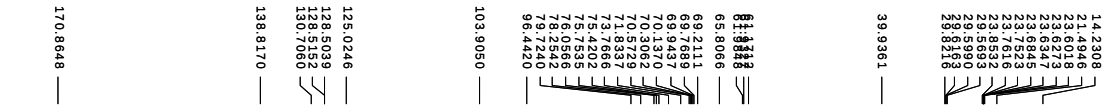
0.4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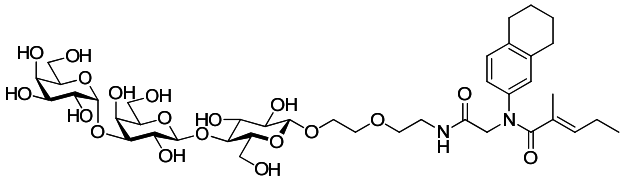
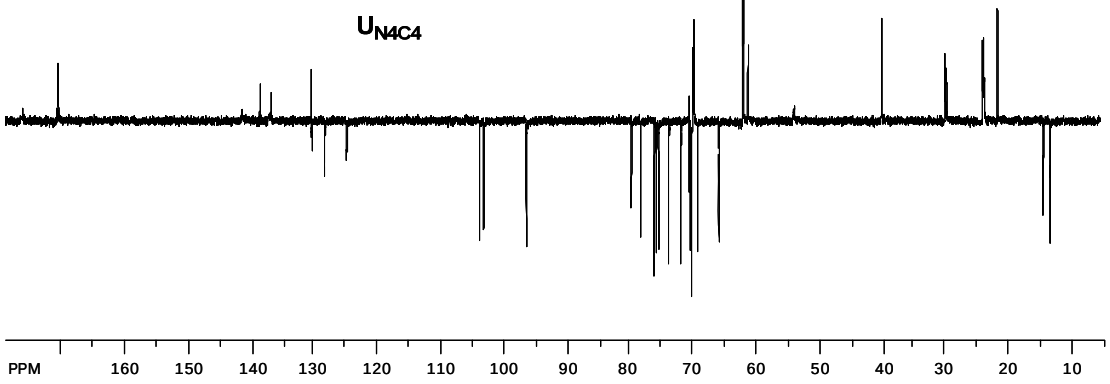


U_{N4C4}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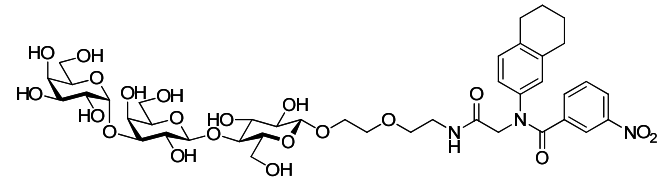
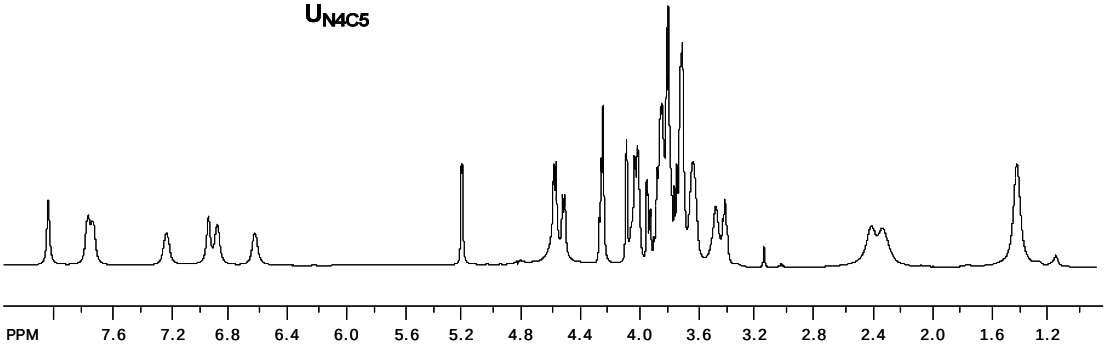
10



U_{N4C5}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3.6
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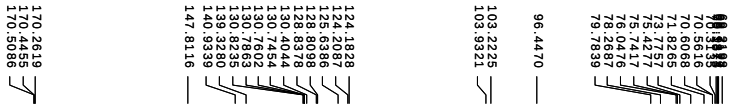
1.6
1.2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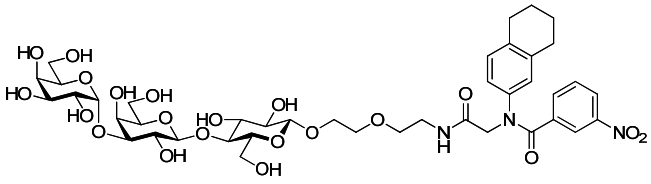
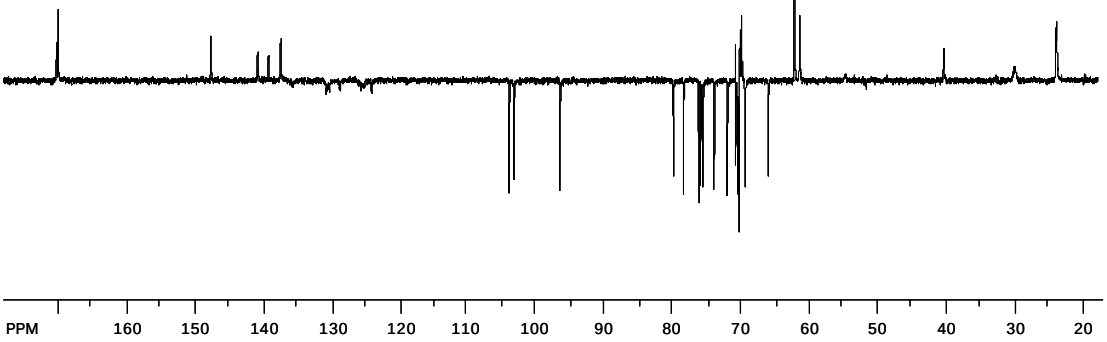


U_{N4C5}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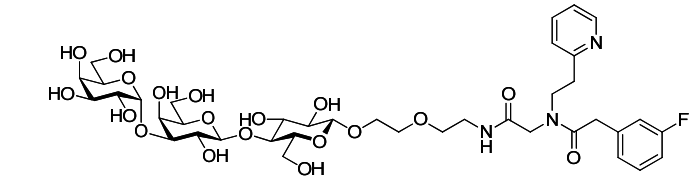

U_{N5C1}


PPM
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5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8

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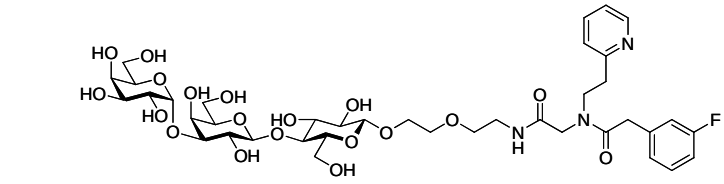
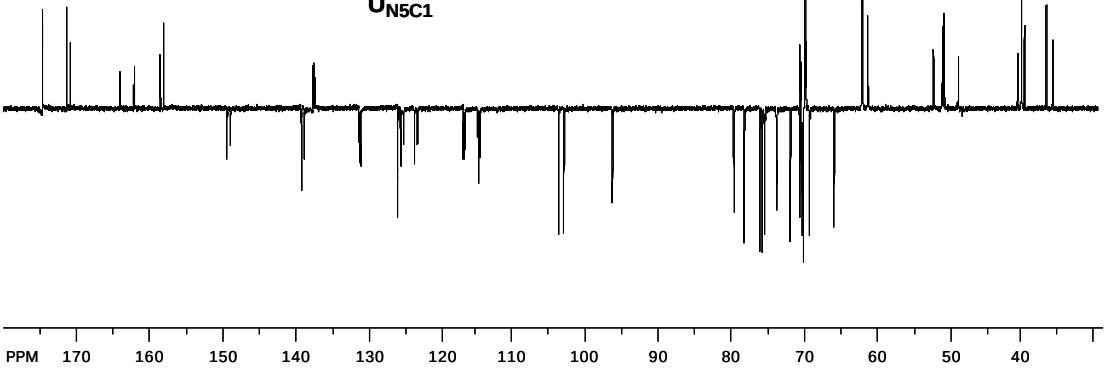
40.3430



U_{N5C1}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70
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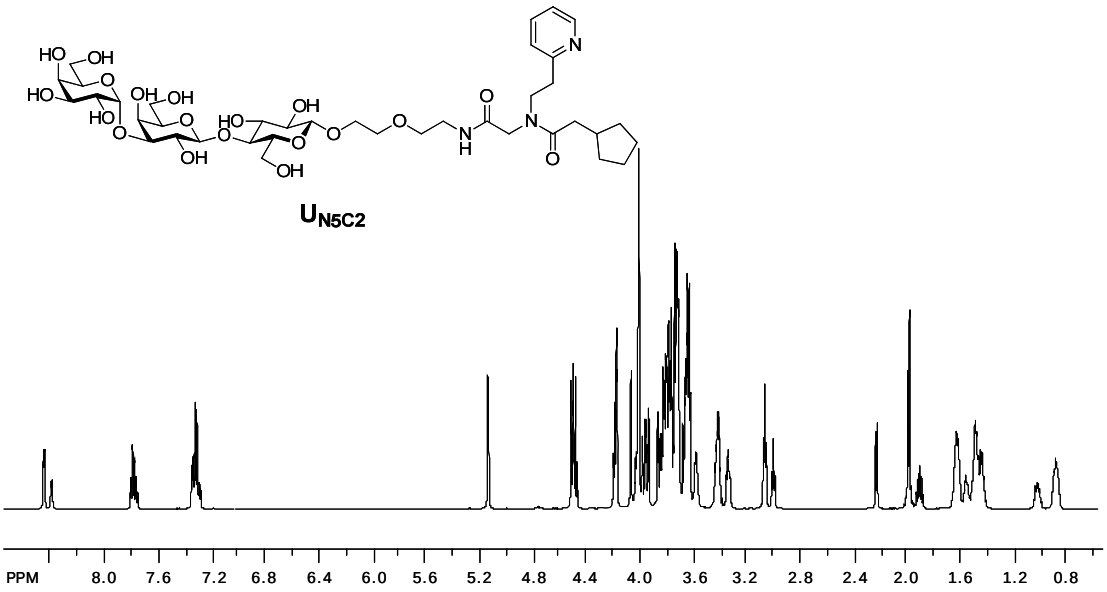
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7.2
6.8
6.4
6.0
5.6
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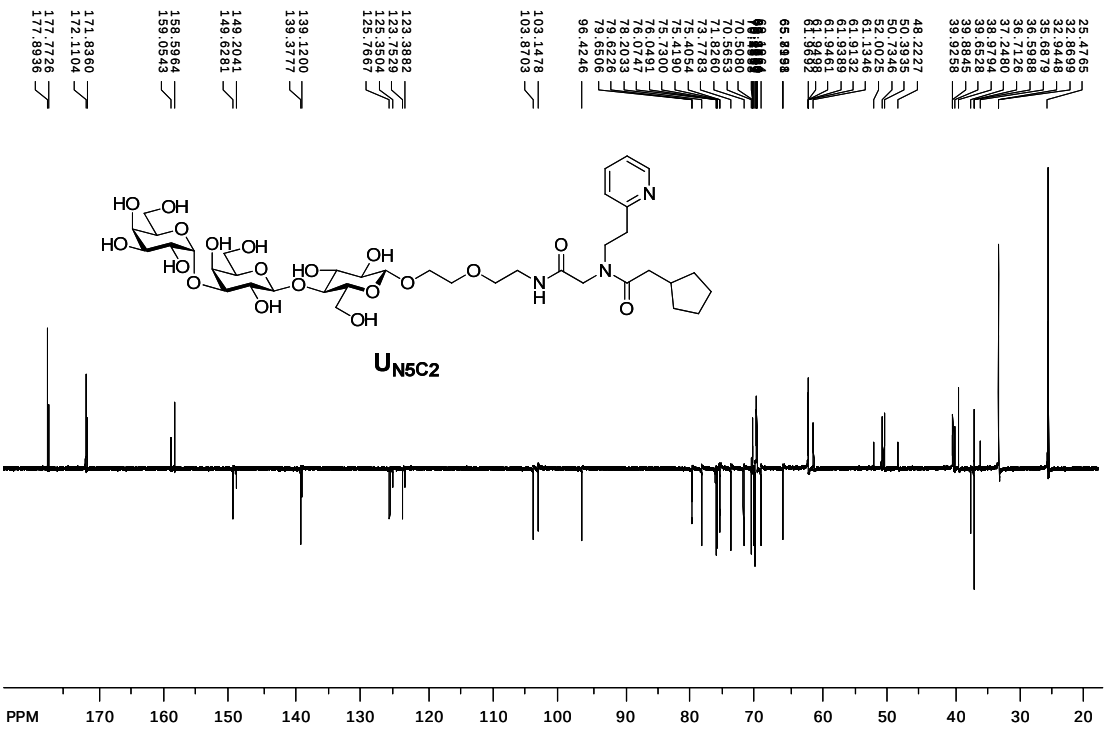
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8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172.1104
158.5964
159.0543
149.2041
149.6281
139.1200
139.3777
123.3882
123.7529
125.3504
125.7667
103.1478
103.8703
96.4246
79.6526
78.2033
76.0747
76.0491
75.7300
75.4054
75.4190
73.7783
71.8260
70.5653
65.8998
61.9692
61.9461
61.9389
61.9132
61.1346
52.0025
50.3935
48.2227
39.9258
39.8845
39.6528
39.6194
38.6794
37.2186
36.5988
35.6879
32.9448
32.8699
25.4765
U_{N5C2}
PPM
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160
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140
130
120
110
100
90
80
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60
50
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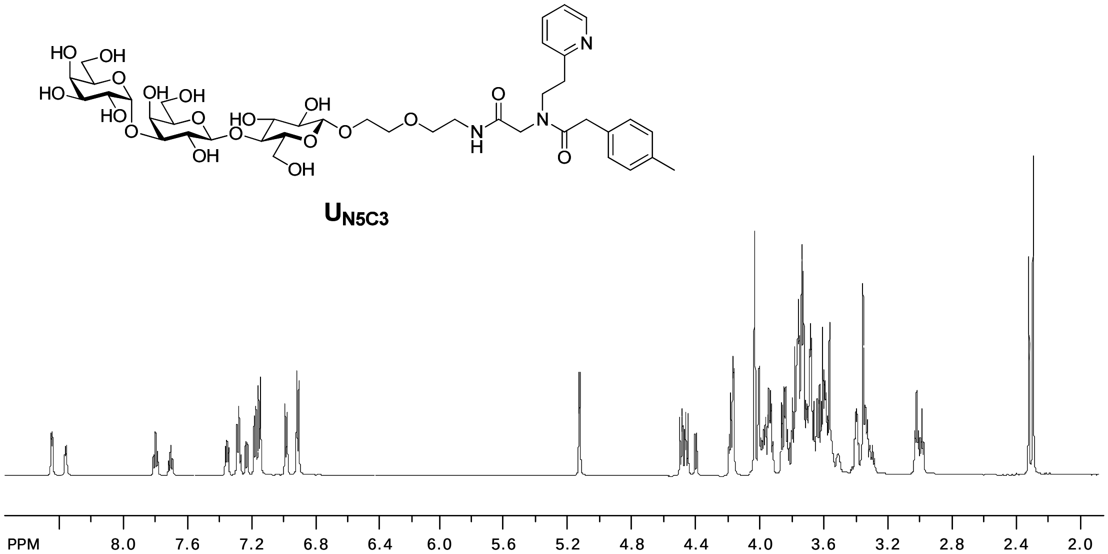
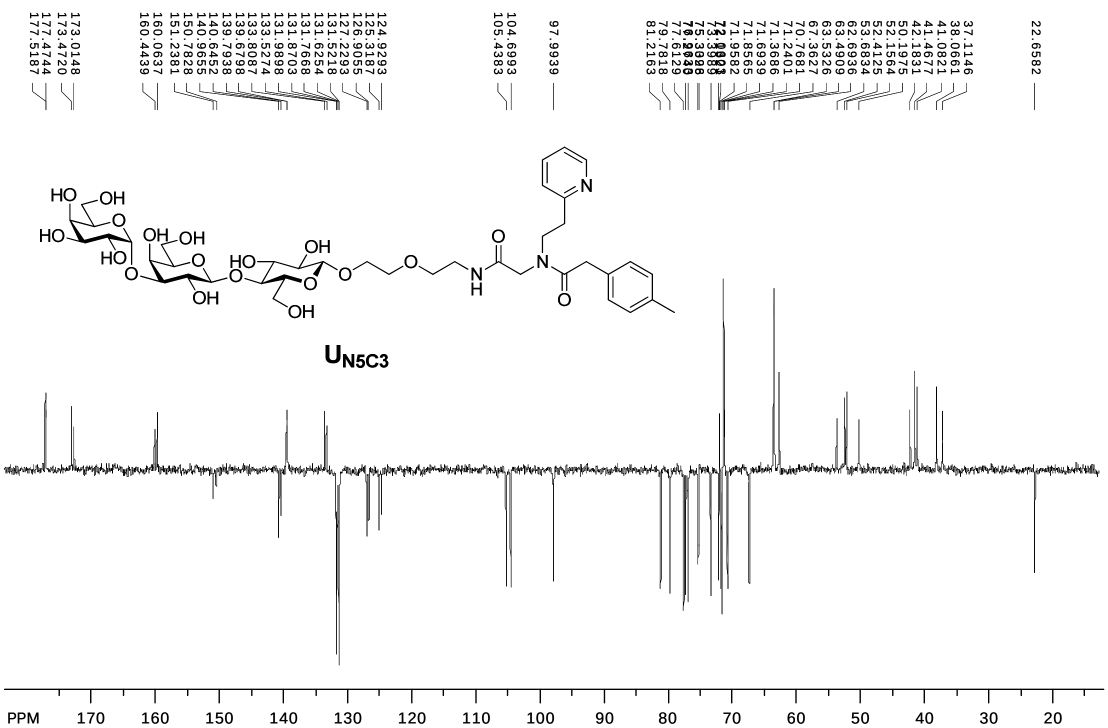
30
20



HO
OH
HO
HO
OH
OH
OH
HO
OH
OH
O
O
O
N
H
N
O
N
U_{N5C3}
PPM
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0



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160.0637
151.2381
150.7828
140.9655
140.6452
139.7938
139.6798
133.8087
133.5274
131.9898
131.8703
131.7668
131.6254
131.5218
127.2293
126.9055
125.3187
124.9293
105.4383
104.6993
97.9939
81.2163
79.7818
77.6129
71.9582
71.8565
71.6939
71.3686
71.2401
70.7681
67.3627
63.5326
63.4909
62.6936
53.6834
52.4125
52.1564
50.1975
42.1831
41.4677
41.0821
38.0661
37.1146
22.6582
HO
OH
HO
HO
OH
OH
OH
HO
OH
OH
O
O
O
N
H
N
O
N
U_{N5C3}
PPM
170
160
150
140
130
120
110
100
90
80
70
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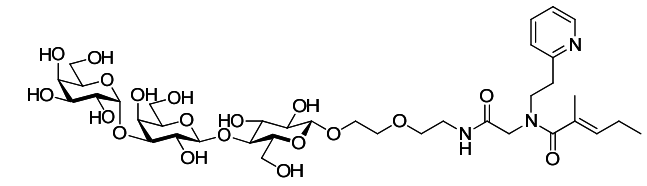
50
40
30
20



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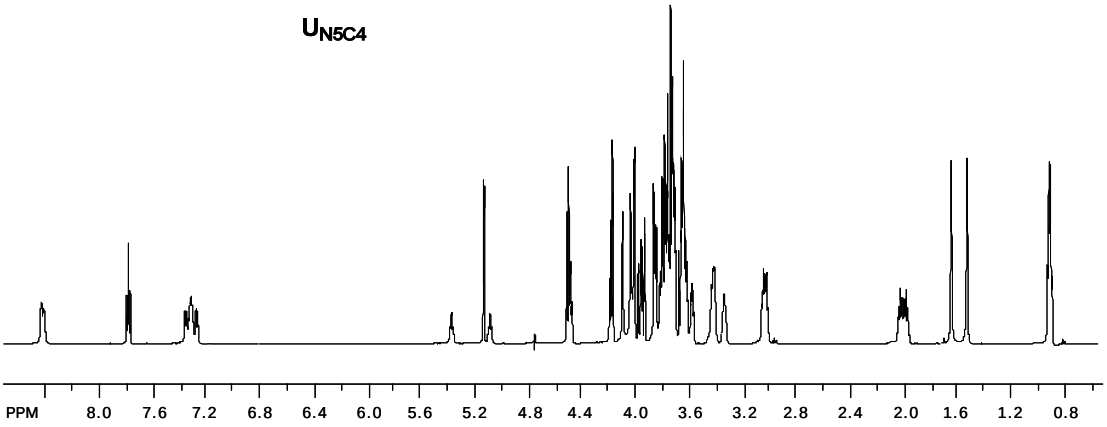
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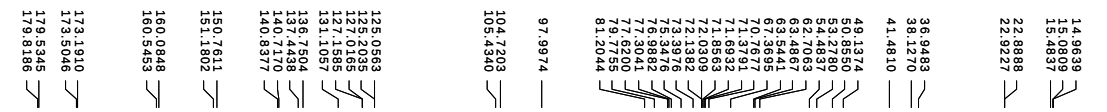
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8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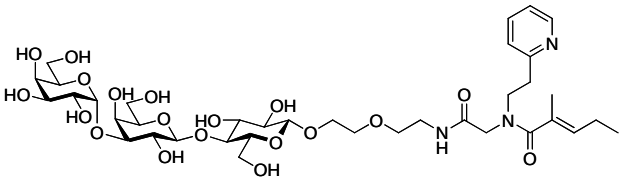
179.8186
173.1910
173.5046
160.0848
160.5453
150.7611
151.1802
140.8377
137.4484
135.7594
131.1057
127.1585
127.0165
125.2035
125.0563
105.4340
104.7203
97.9974
81.2044
79.7755
77.3041
76.9882
75.3476
73.3976
72.1382
72.0309
71.8563
71.6932
71.3791
70.7677
67.3695
63.5461
62.7063
54.4837
53.2780
50.8550
49.1374
41.4810
38.1270
36.9483
22.8888
22.9227
15.0809
15.4837
14.9639



U_{N5C4}

PPM
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160
150
140
130
120
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100
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80
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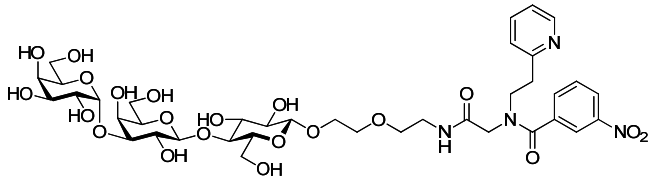
60
50
40
30
20
10



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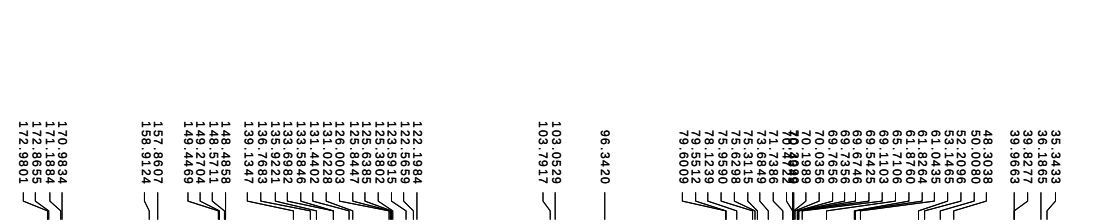
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7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8

172.9801
172.8655
171.1884
170.9834
158.9124
157.8607
149.4469
149.2704
148.5711
148.4858
139.1347
136.7621
133.6982
133.5846
131.4402
131.0228
126.0003
125.8447
125.6385
125.3802
123.5915
122.5659
122.1984
103.7917
103.0529
96.3420
79.6009
79.1239
75.9590
75.6298
75.3115
73.6849
71.7386
70.1989
70.0356
69.7656
69.7356
69.6746
69.5425
69.1103
65.7106
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61.0435
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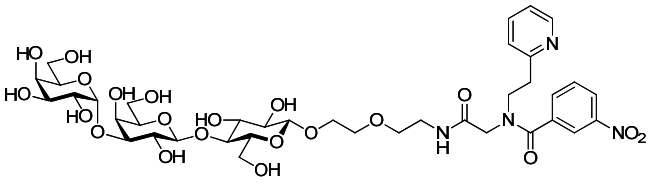
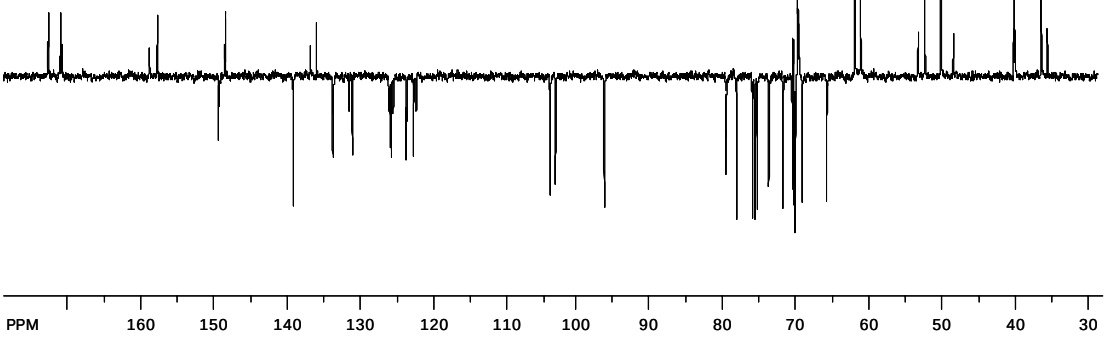
39.9663
39.8277
36.1865
35.3433



U_{N5C5}


PPM
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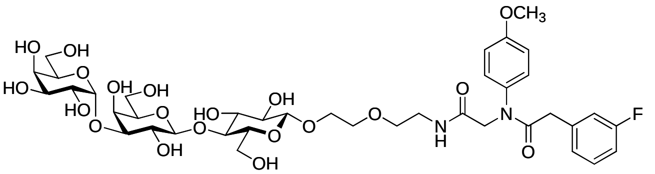
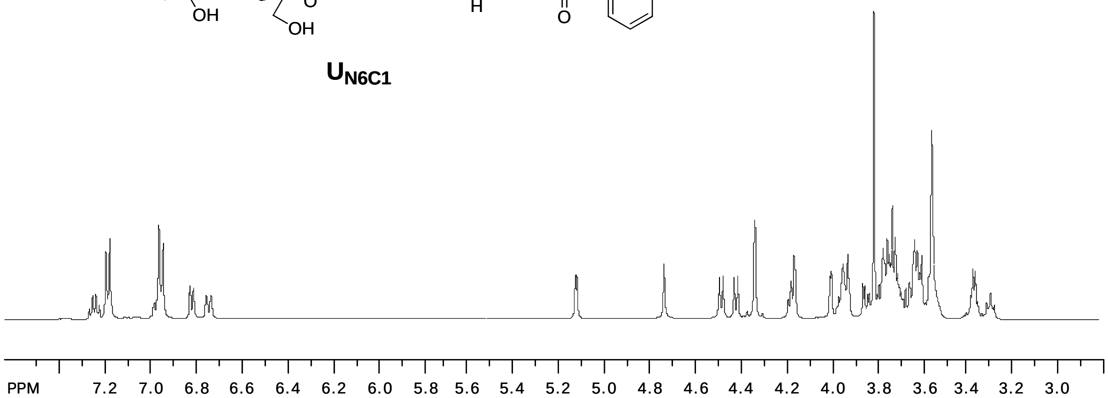
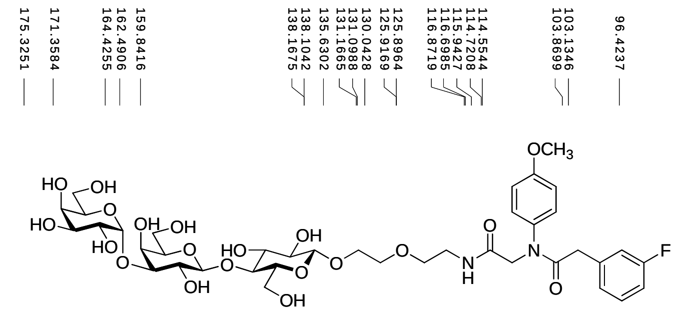
150
140
130
120
110
100
90
80
70
60
50
40
30


OCH3
HO
OH
HO
HO
OH
OH
O
OH
HO
OH
O
O
N
H
N
F
OH

U$_{N6C1}$


PPM
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 3.8 3.6 3.4 3.2 3.0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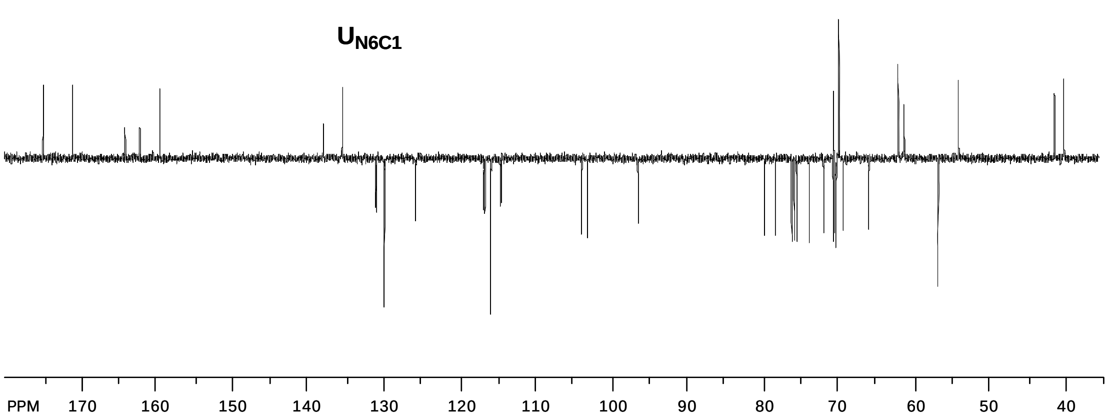
159.8416
138.1675
138.1042
135.6302
131.1665
131.0988
130.0428
125.9169
125.8964
116.8719
116.6985
115.9427
114.7208
114.5544
103.8699
103.1346
96.4237
79.6566
78.2152
76.0391
75.7105
75.3792
73.7383
71.8266
70.5589
70.4616
70.2858
70.1217
69.7866
69.1956
65.7923
61.9642
61.9152
61.1296
56.6145
53.9051
41.1872
39.9444
OCH3
HO
OH
HO
HO
OH
OH
O
OH
HO
OH
O
O
N
H
N
F
OH

U$_{N6C1}$


PPM
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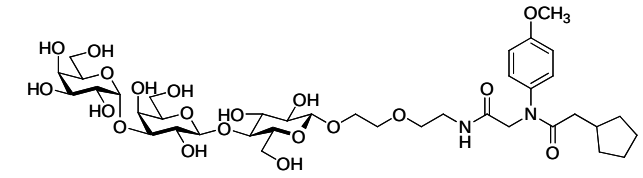
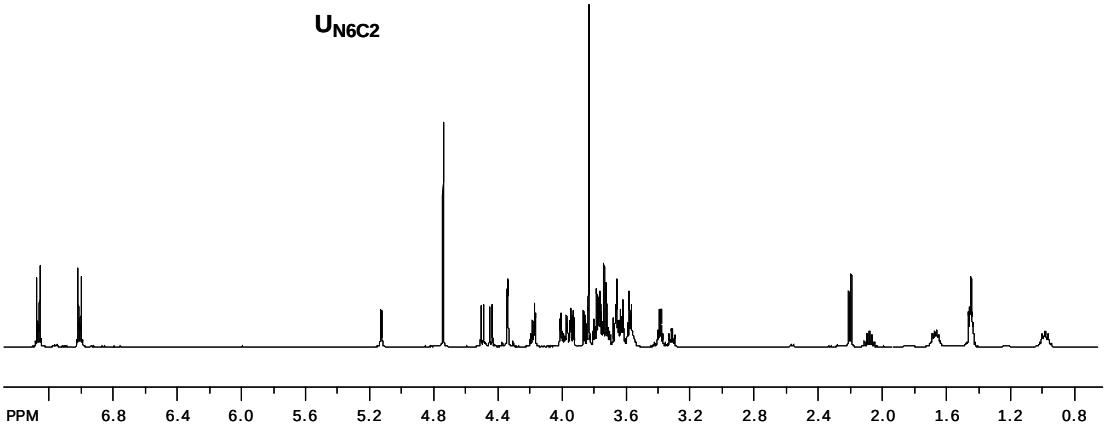
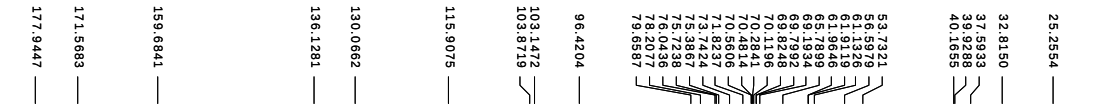


U_{N6C2}


PPM
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8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78.2077
76.0436
75.7238
75.3867
73.7424
71.8237
70.5606
70.4814
70.2841
70.1196
69.8248
69.1934
65.7899
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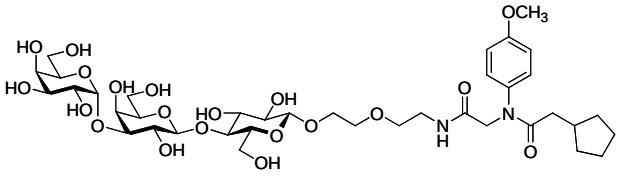
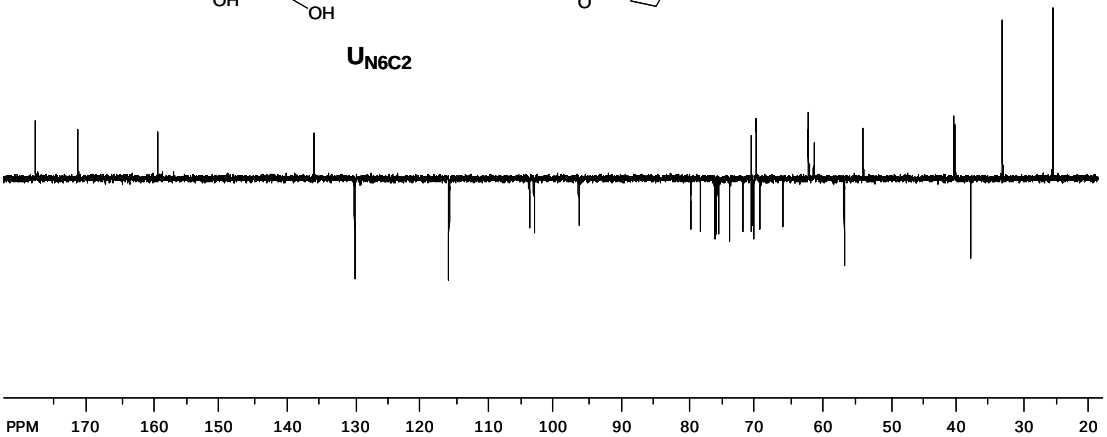
25.2554



U_{N6C2}


PPM
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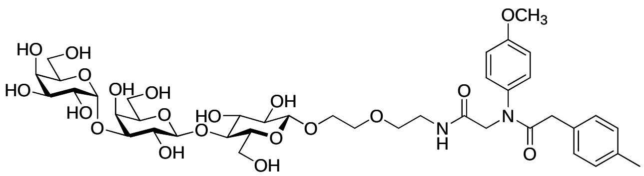
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20



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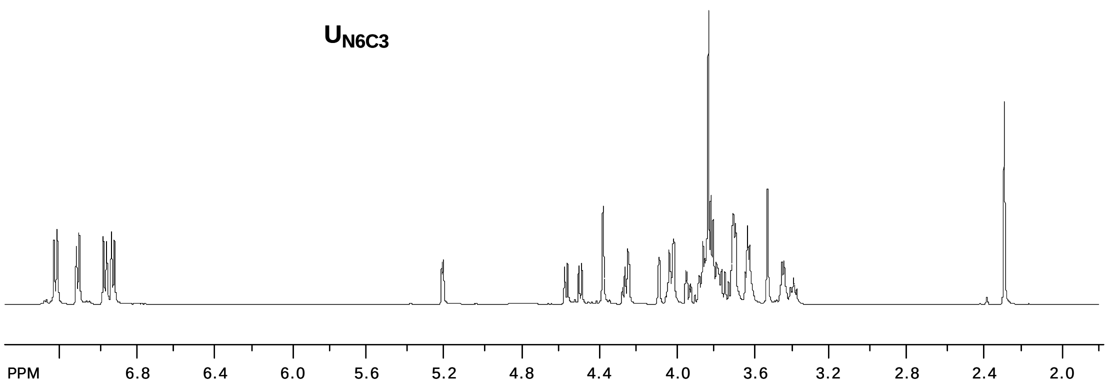

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159.7810
129.9176
130.0486
130.1057
132.6389
135.8052
115.8417
103.1484
103.8821
96.4353
79.6710
78.2370
76.0392
75.7127
75.3886
73.7451
71.8303
70.5647
70.4731
70.2942
70.1275
69.8087
69.7651
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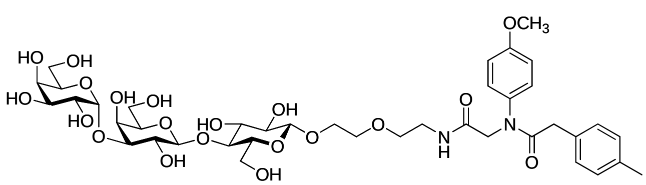
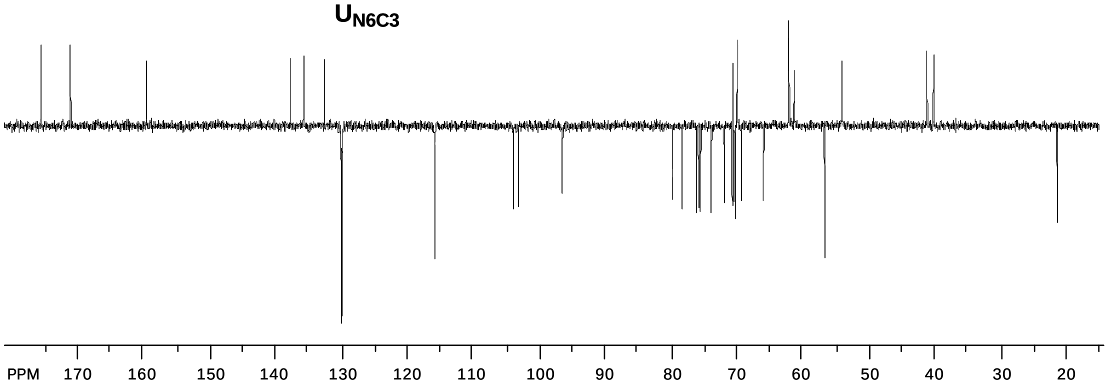
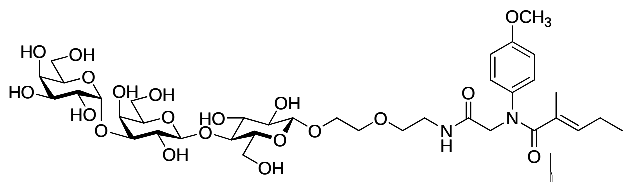
40.9002
21.1220

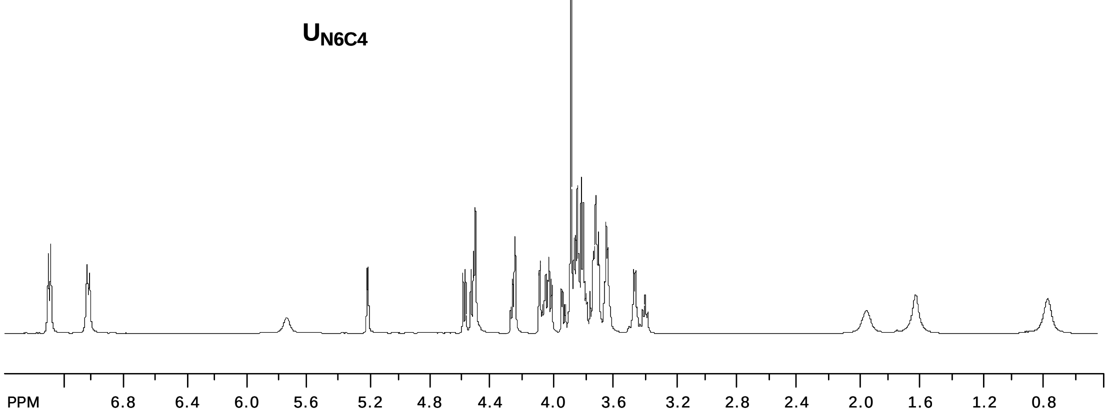


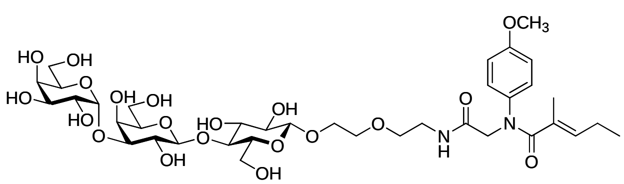
U_{N6C3}



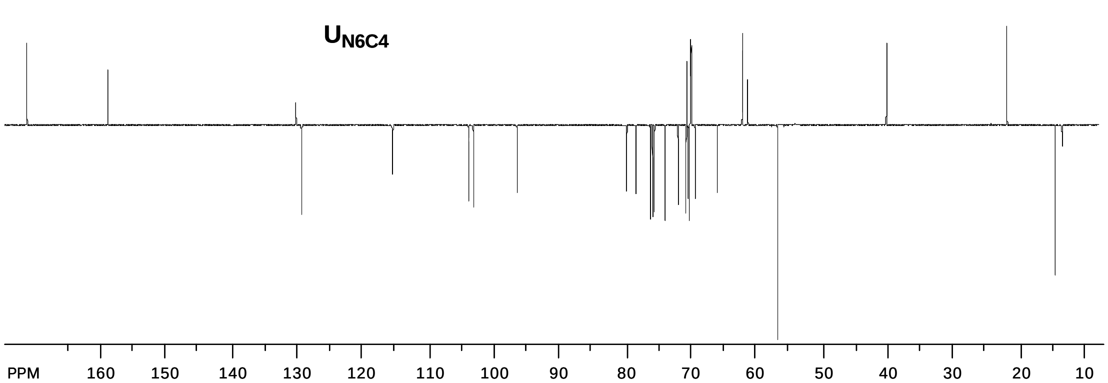


U$_{N6C4}$


PPM
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8



U$_{N6C4}$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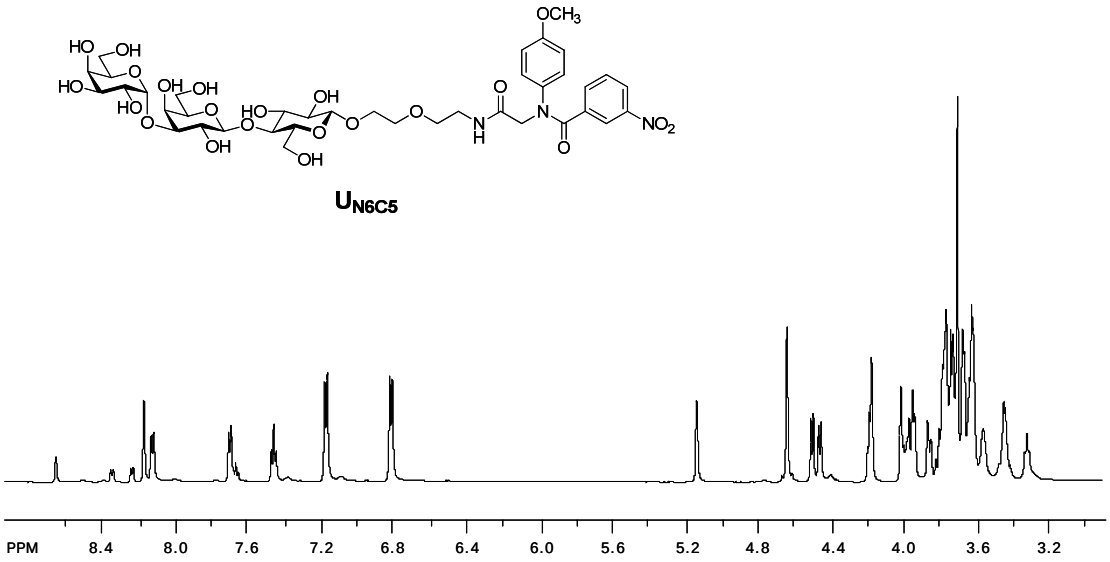
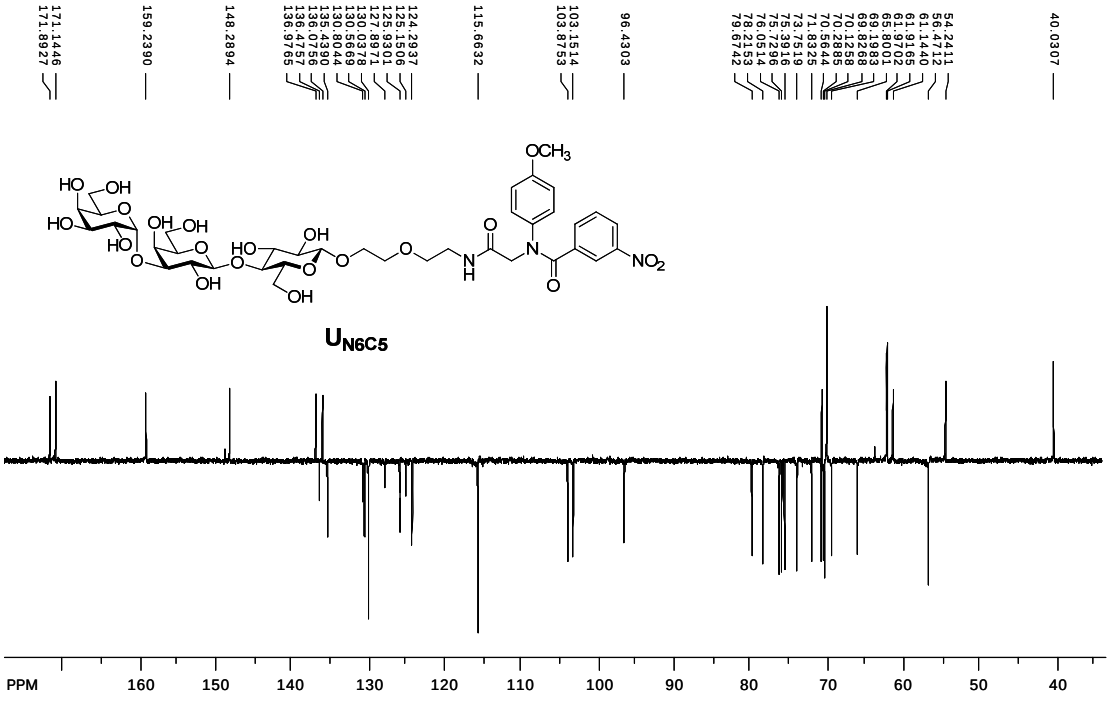
129.4289
115.4821
103.8756
103.1574
96.4287
79.6612
78.2192
76.0478
75.7294
75.3969
73.7512
71.8275
70.5659
70.4652
70.2907
70.1258
69.8282
69.8029
69.1998
65.8002
61.9769
61.9195
61.1416
56.5735
39.9284
21.4423
14.0801
PPM
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10


OCH3
HO
OH
O
HO
OH
OH
HO
O
HO
O
OH
HO
OH
O
O
O
N
H
O
N
O
NO2
OH
U N6C5
PPM
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2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159.2390
148.2894
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136.4757
136.0756
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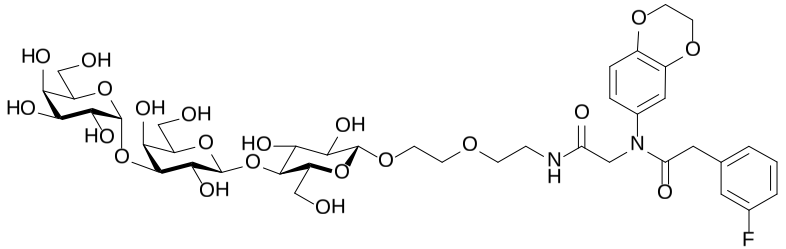
130.8044
130.5669
127.8971
125.9301
125.1506
124.2937
115.6632
103.1514
103.8753
96.4303
79.6742
78.2153
76.0514
75.7296
75.3916
73.7519
71.8325
70.5845
70.1258
69.8268
69.1983
65.8001
61.9702
61.9165
61.1440
54.2411
54.4712
40.0307
OCH3
HO
OH
O
HO
OH
OH
HO
O
HO
O
OH
HO
OH
O
O
O
N
H
O
N
O
NO2
OH
U N6C5
PPM
160
150
140
130
120
110
100
90
80
70
60
50
40

Qualitative Compound Report

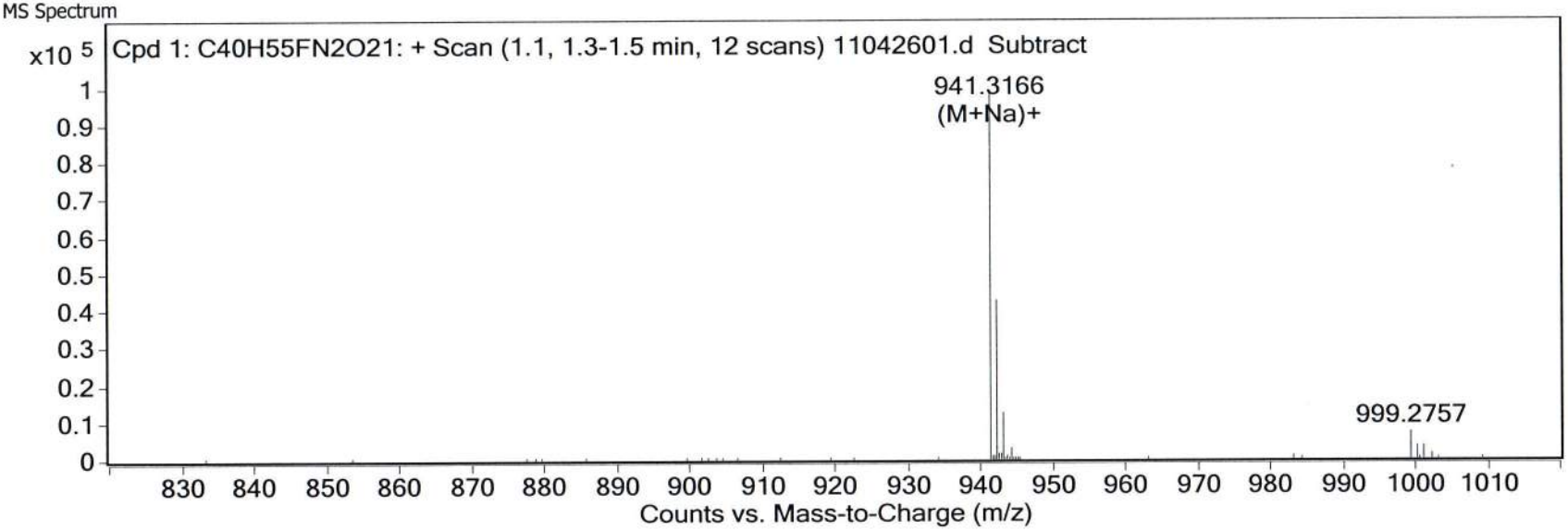
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t3.99
Data File	11042601.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N1C1

Compound Table

MS Spectrum



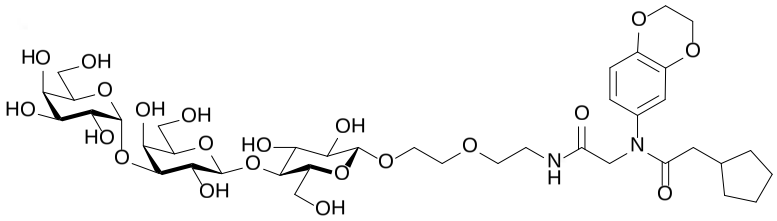
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
941.3166	941.3174	-0.85	1	99129	C40 H55 F N2 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

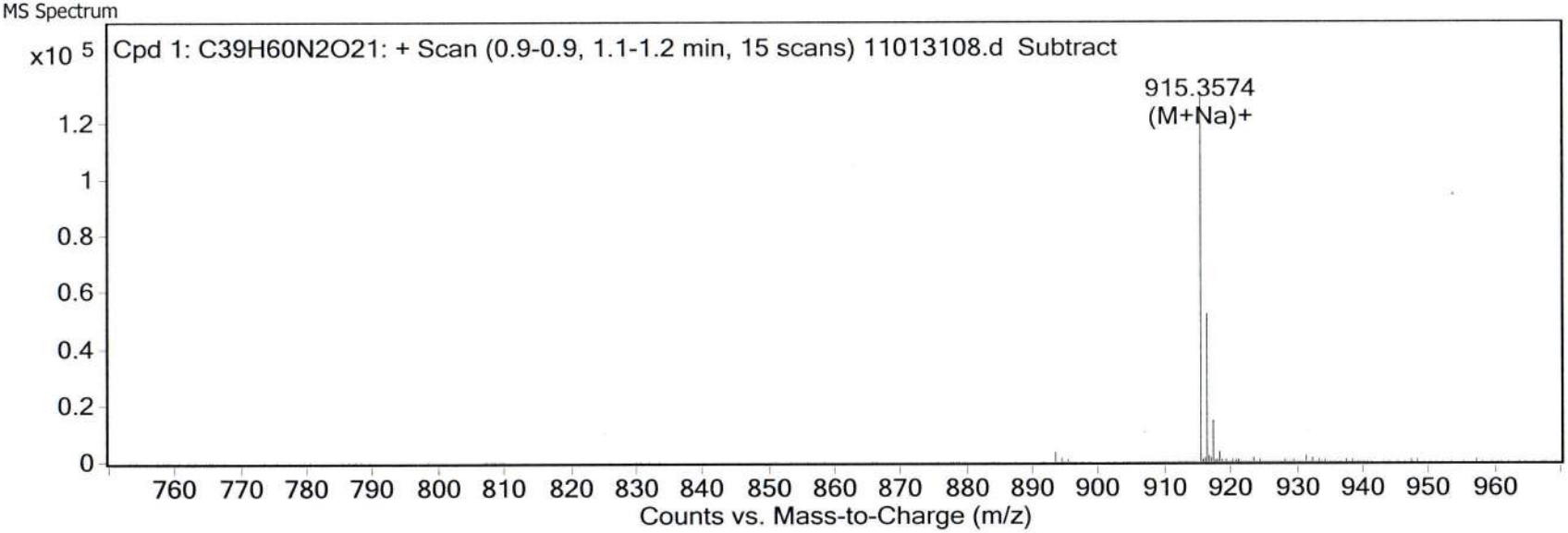
Comment	P. Kitov, Bundle	**Sample Name**	t4.33
Data File	11013108.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N1C2

Compound Table

MS Spectrum



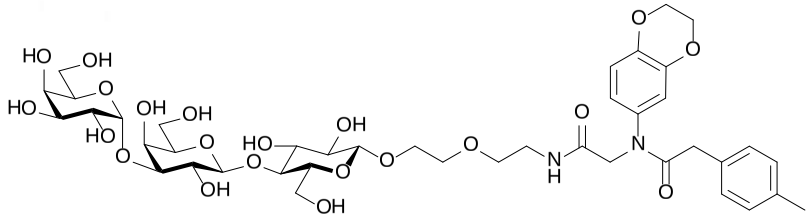
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
915.3574	915.3581	-0.7	130296	C39 H60 N2 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

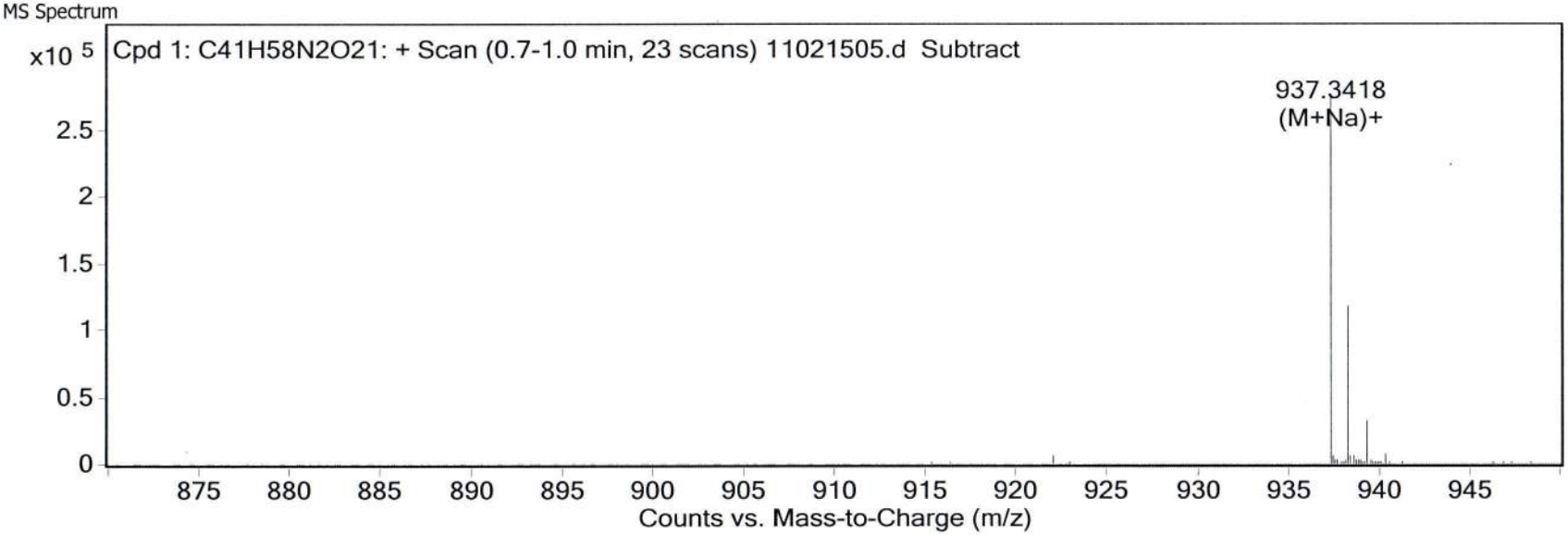
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t4.45
Data File	11021505.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N1C3

Compound Table

MS Spectrum



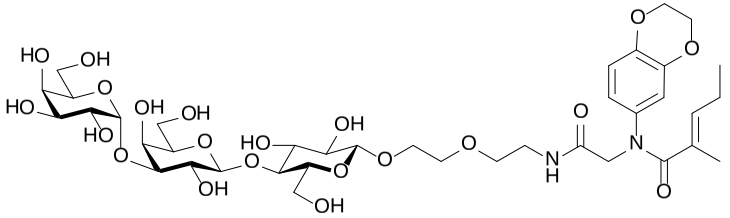
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
937.3418	937.3424	-0.7	276404	C41 H58 N2 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

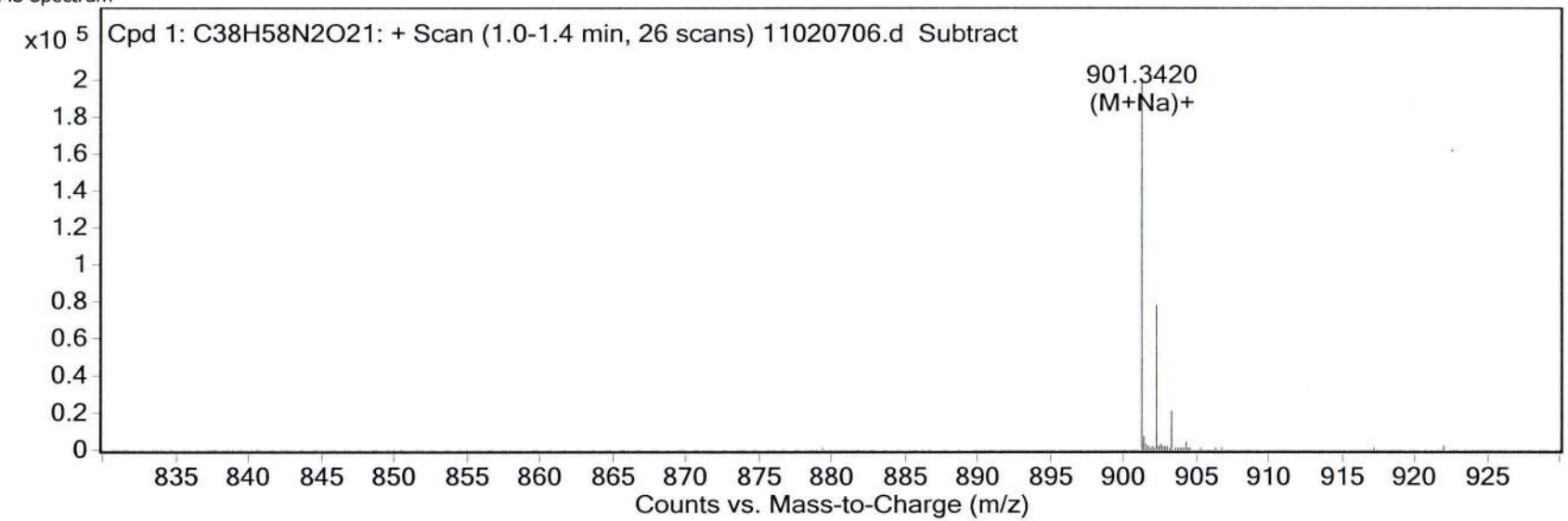
Comment	C. A. Sanhueza, Bundle	**Sample Name**	T 4.60
Data File	11020706.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N1C4

Compound Table

MS Spectrum



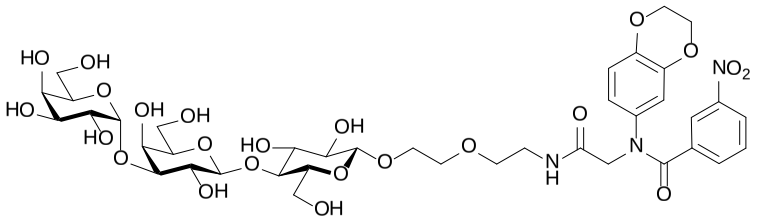
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
901.342	901.3424	-0.43	200943	C38 H58 N2 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

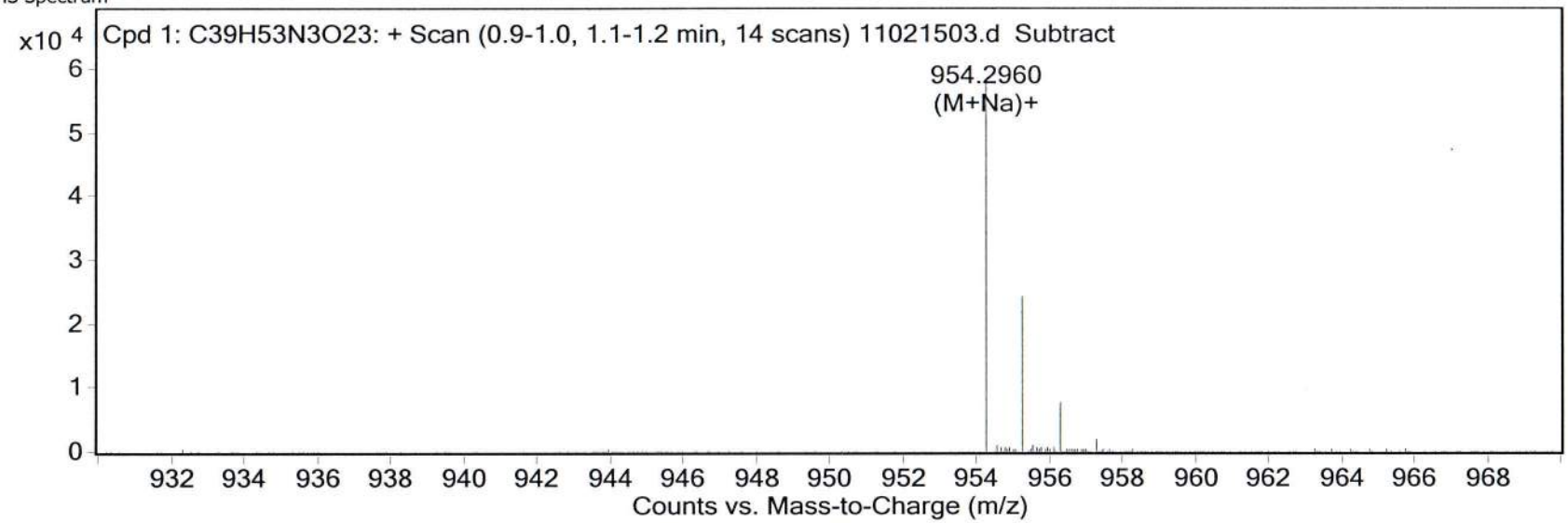
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t4.46
Data File	11021503.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N1C5

Compound Table

MS Spectrum



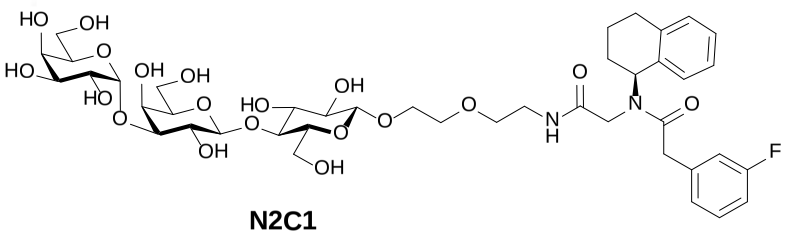
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
954.296	954.2962	-0.26	1	58344	C39 H53 N3 Na O23	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

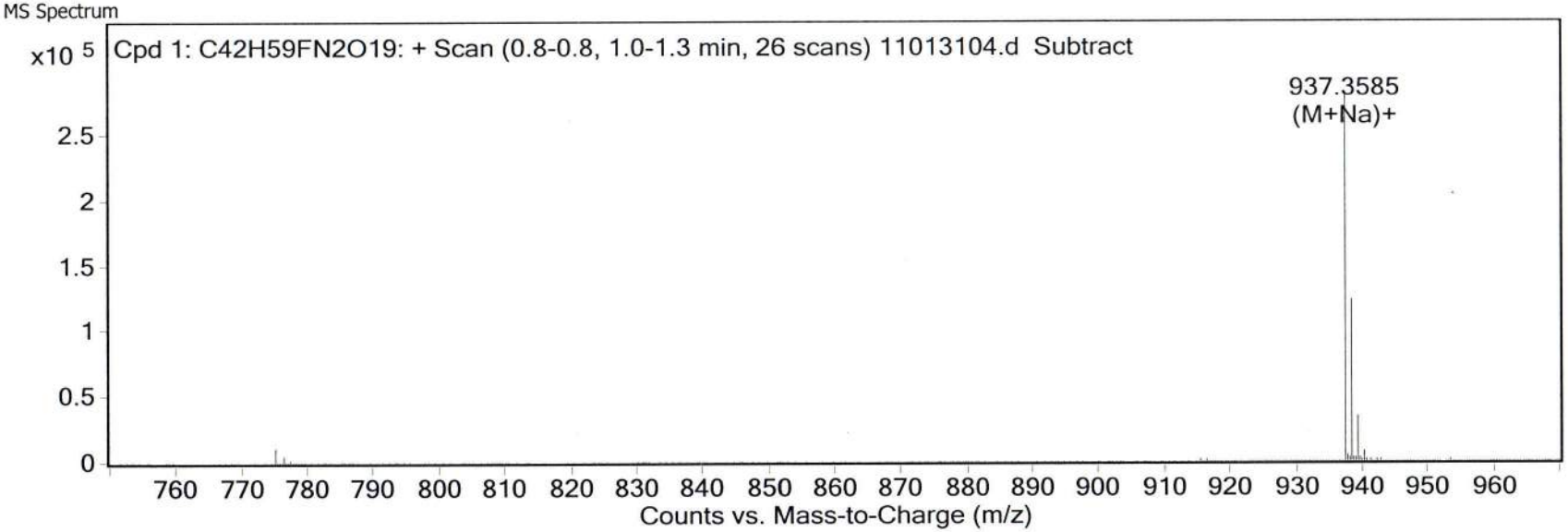
Comment	P. Kitov, Bundle	**Sample Name**	t4.12
Data File	11013104.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N2C1

Compound Table

MS Spectrum



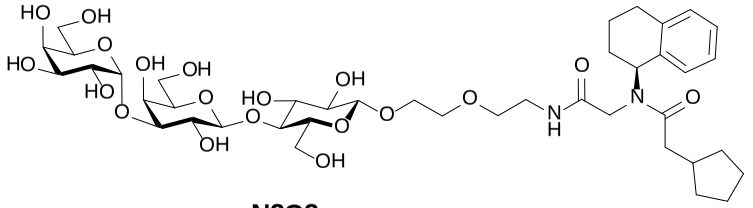
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
937.3585	937.3588	-0.33	281824	C42 H59 F N2 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

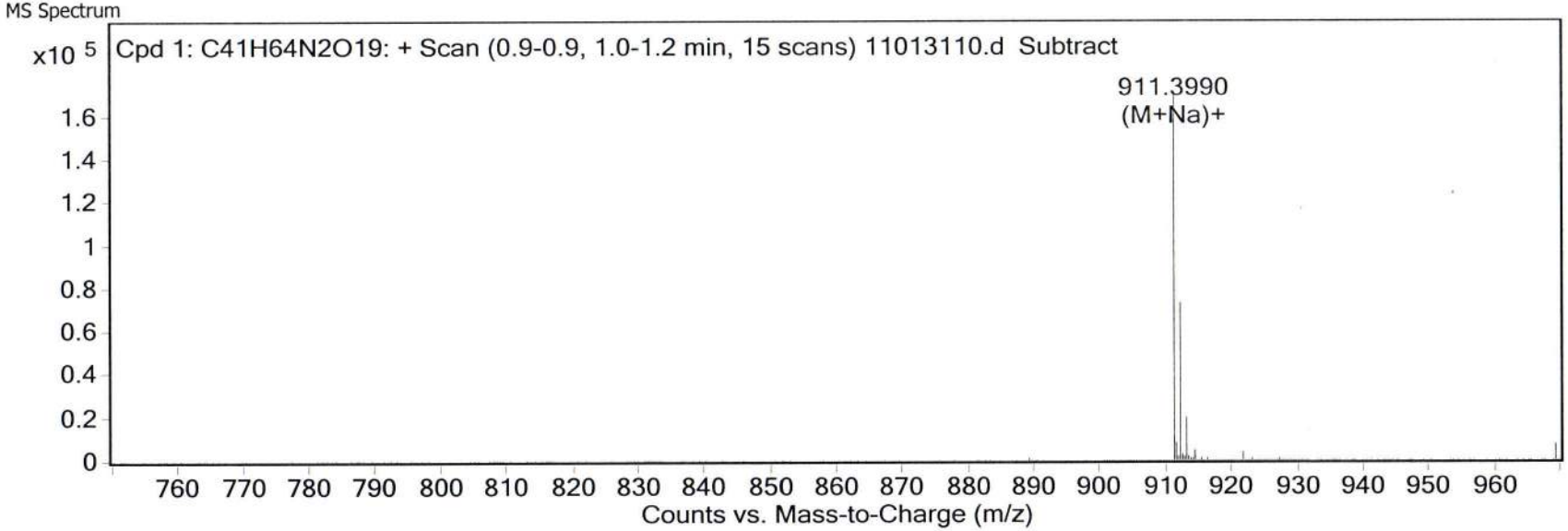
Comment	P. Kitov, Bundle	**Sample Name**	t4.8
Data File	11013110.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N2C2

Compound Table

MS Spectrum



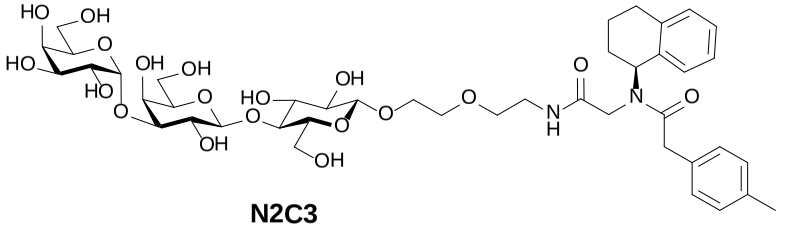
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
911.399	911.3995	-0.59	171065	C41 H64 N2 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

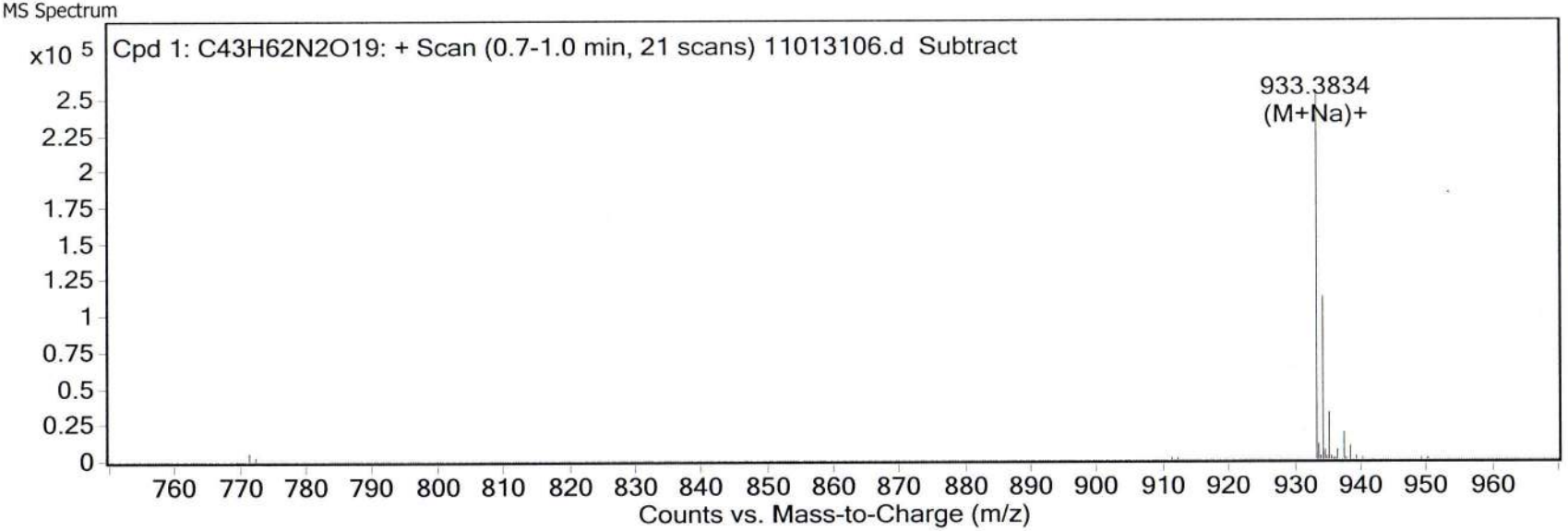
Comment	P. Kitov, Bundle	**Sample Name**	t4.13
Data File	11013106.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N2C3

Compound Table

MS Spectrum



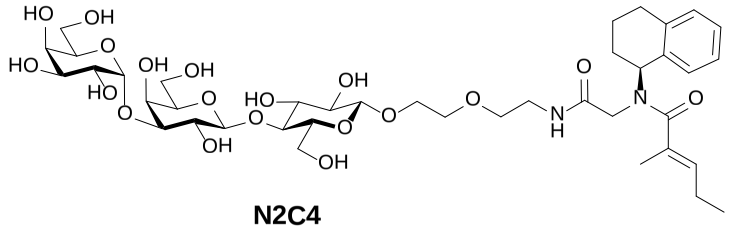
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
933.3834	933.3839	-0.58	254540	C43 H62 N2 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

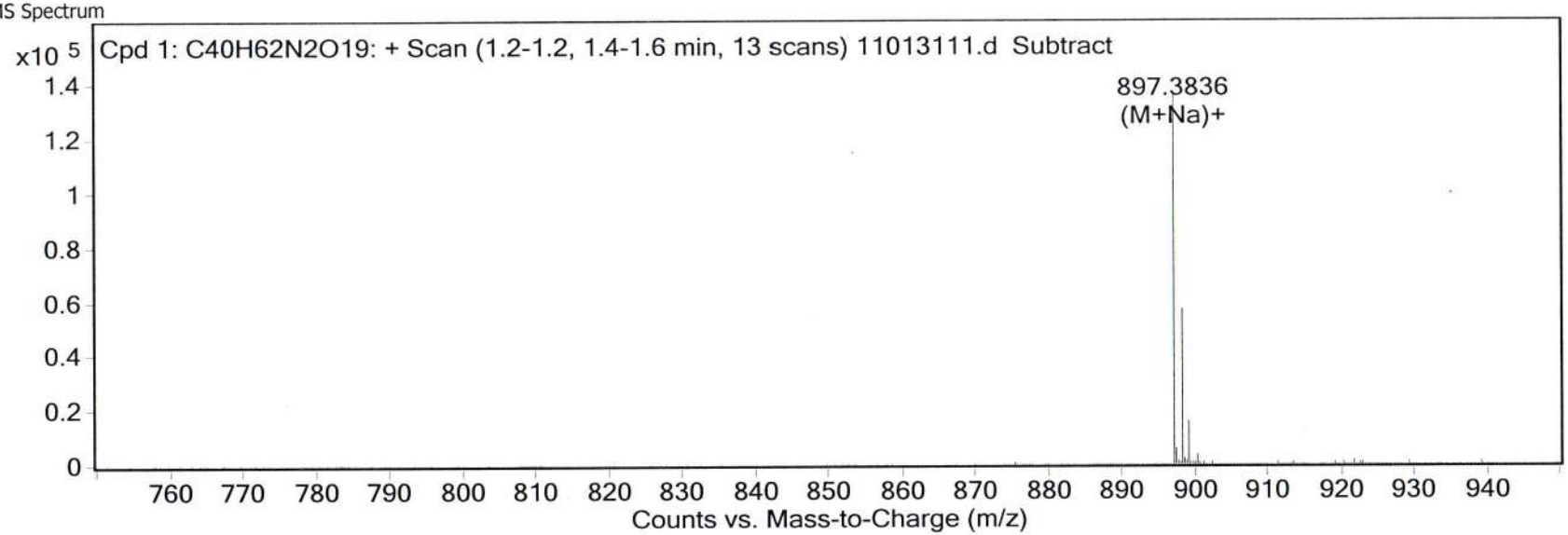
Comment	P. Kitov, Bundle	**Sample Name**	t4.14
Data File	11013111.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N2C4

Compound Table

MS Spectrum



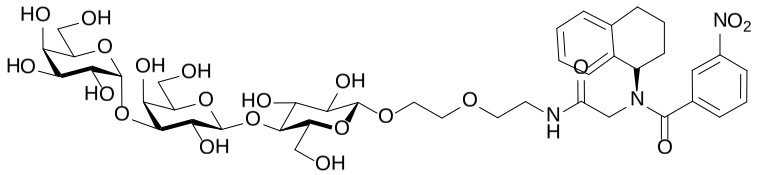
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
897.3836	897.3839	-0.35	137019	C40 H62 N2 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

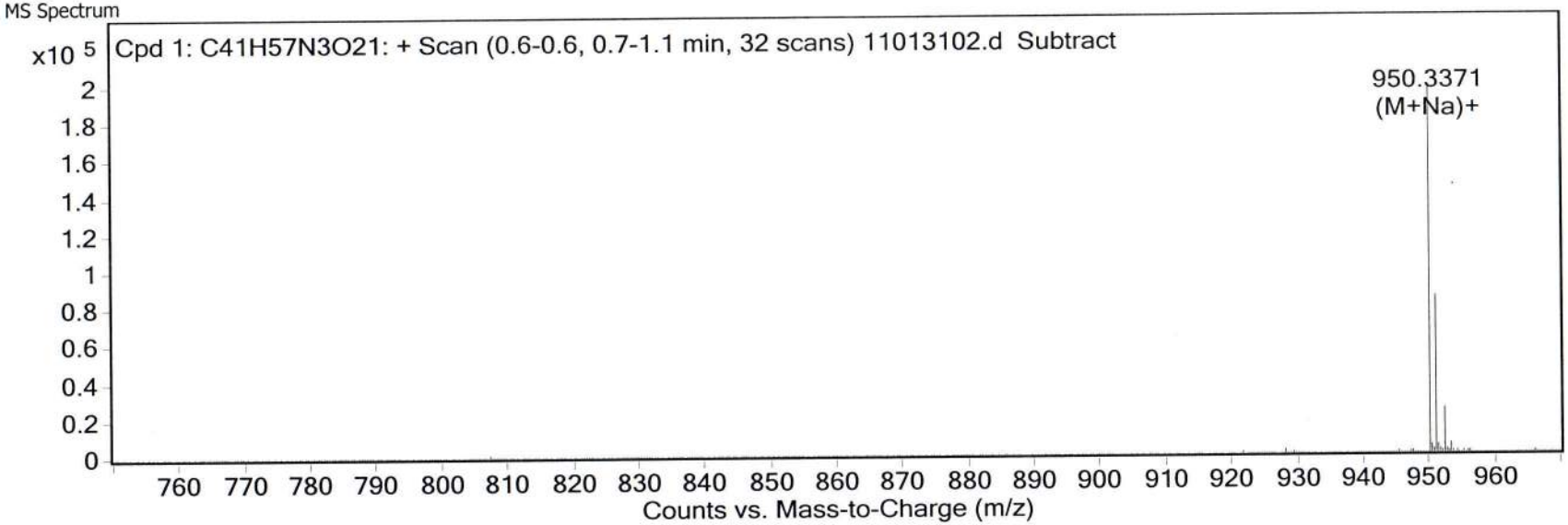
Comment	P. Kitov, Bundle	**Sample Name**	t4.30
Data File	11013102.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N2C5

Compound Table

MS Spectrum



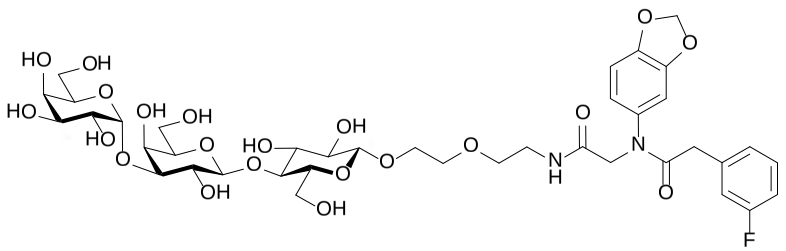
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
950.3371	950.3377	-0.6	198531	C41 H57 N3 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

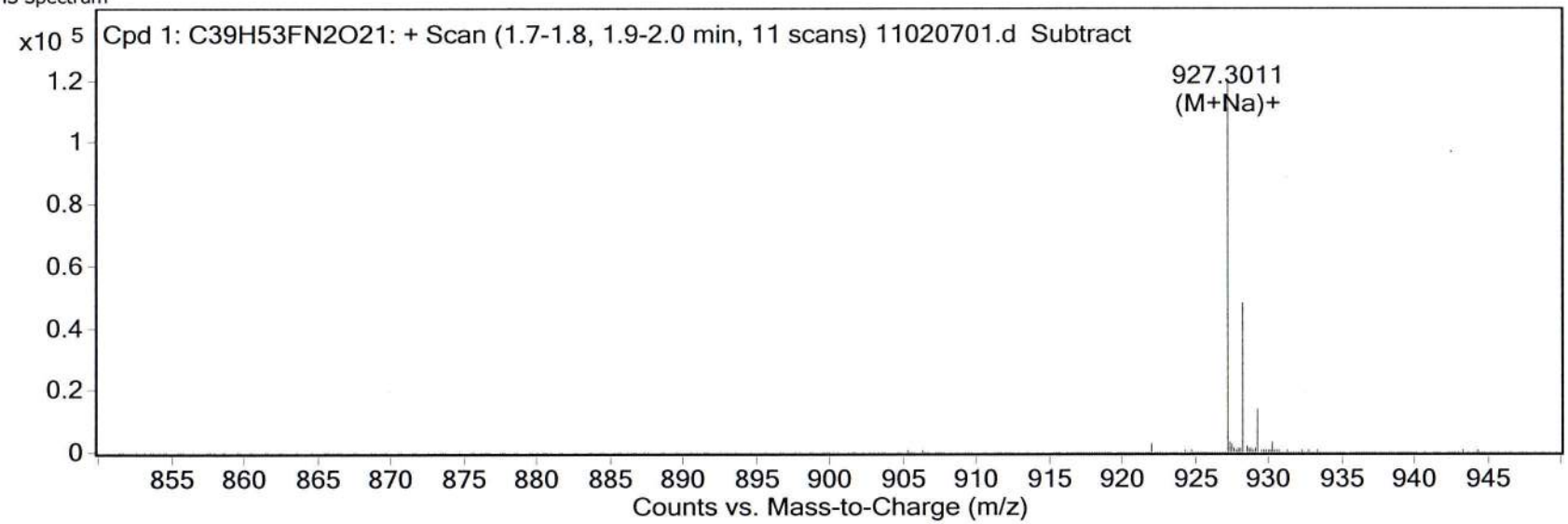
Comment	C. A. Sanhueza, Bundle	**Sample Name**	T 4.48
Data File	11020701.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N3C1

Compound Table

MS Spectrum



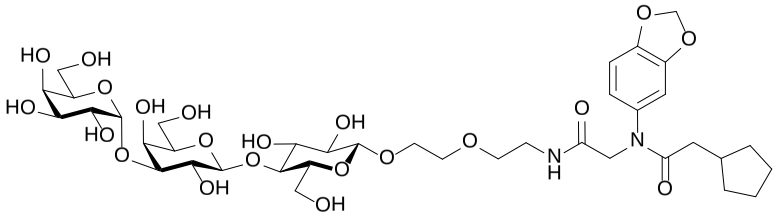
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
927.3011	927.3017	-0.69	120072	C39 H53 F N2 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

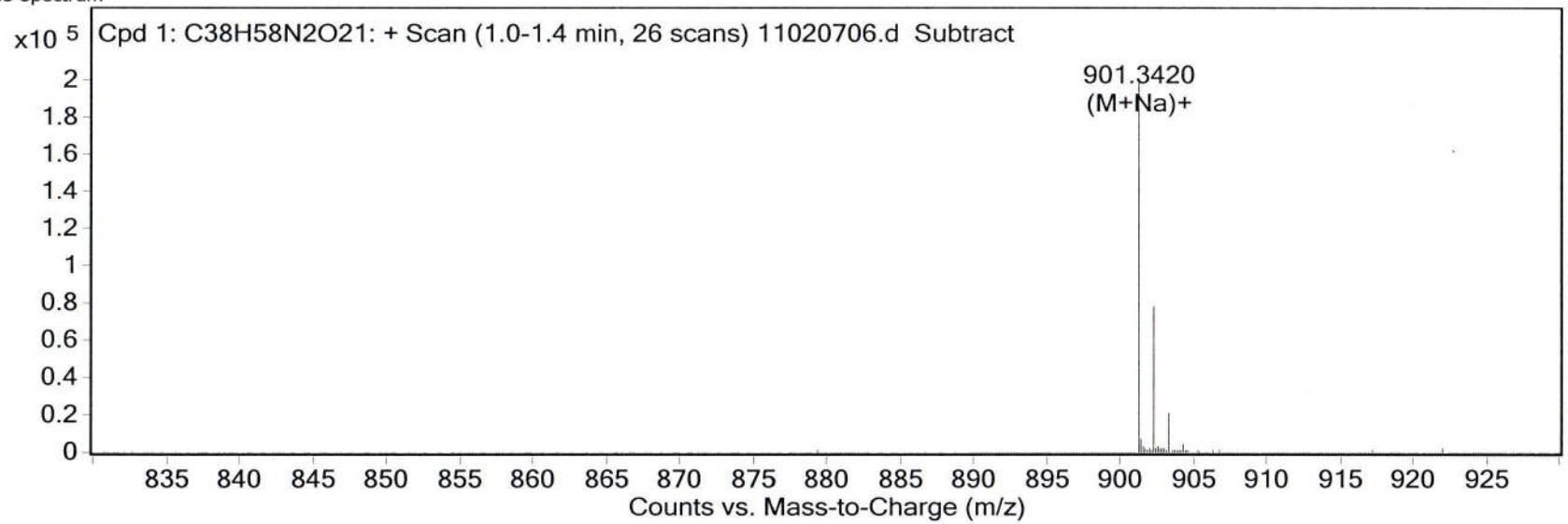
Comment	C. A. Sanhueza, Bundle	**Sample Name**	T 4.60
Data File	11020706.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N3C2

Compound Table

MS Spectrum



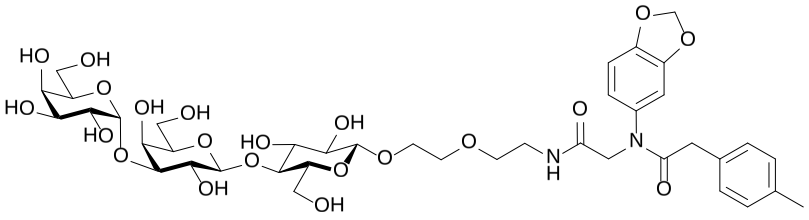
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
901.342	901.3424	-0.43	200943	C38 H58 N2 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

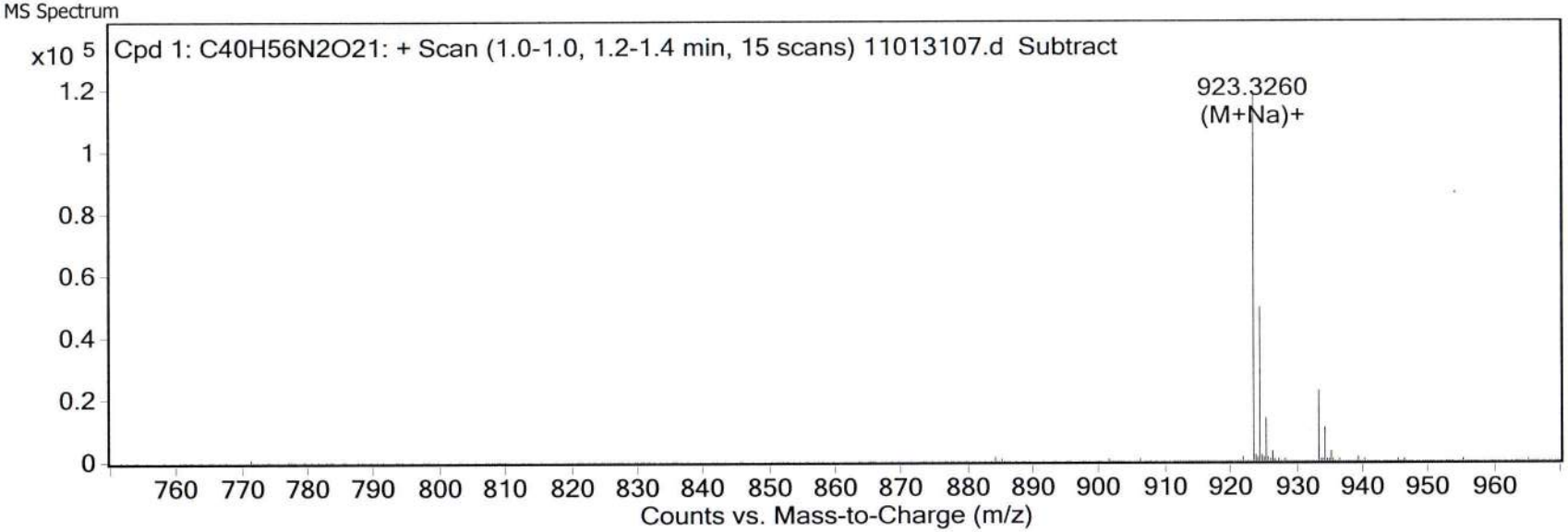
Comment	P. Kitov, Bundle	**Sample Name**	t4.11
Data File	11013107.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N3C3

Compound Table

MS Spectrum



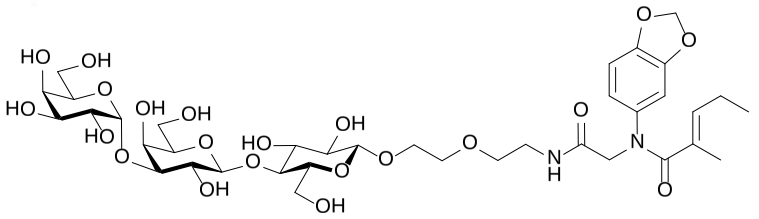
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
923.326	923.3268	-0.86	1	118902	C40 H56 N2 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

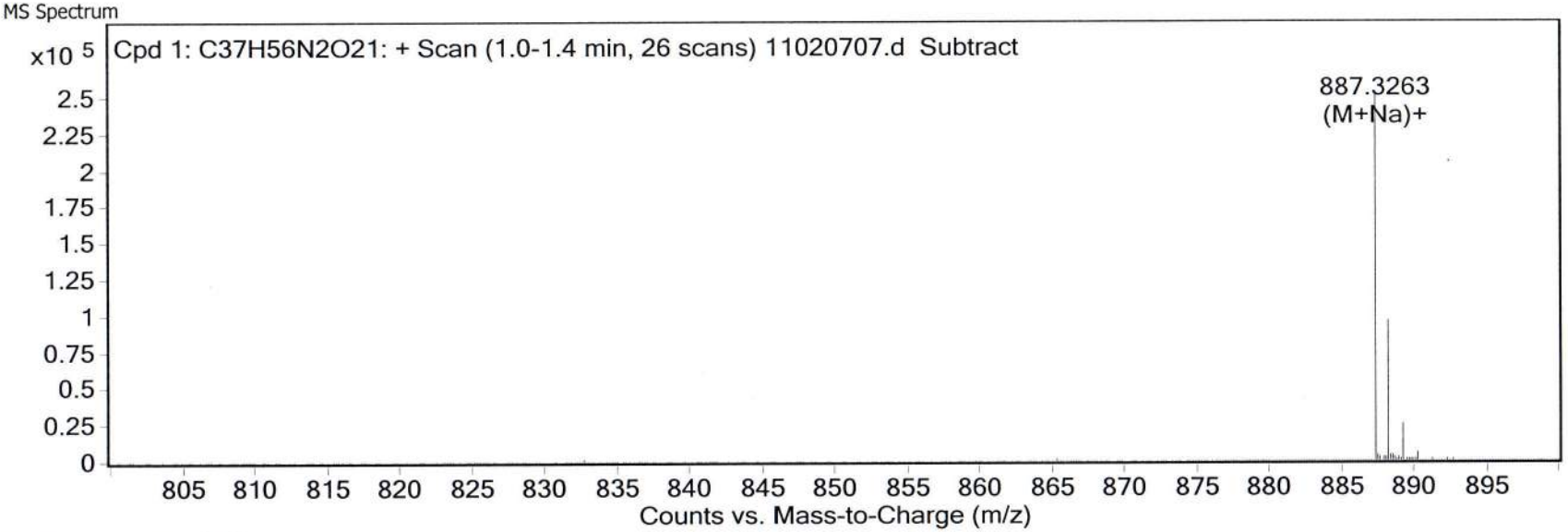
Comment	C. A. Sanhueza, Bundle	**Sample Name**	4.61
Data File	11020707.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N3C4

Compound Table

MS Spectrum



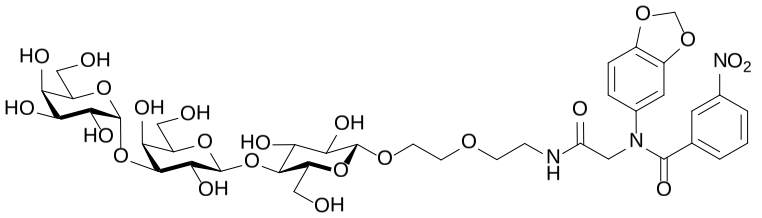
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
887.3263	887.3268	-0.54	253431	C37 H56 N2 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

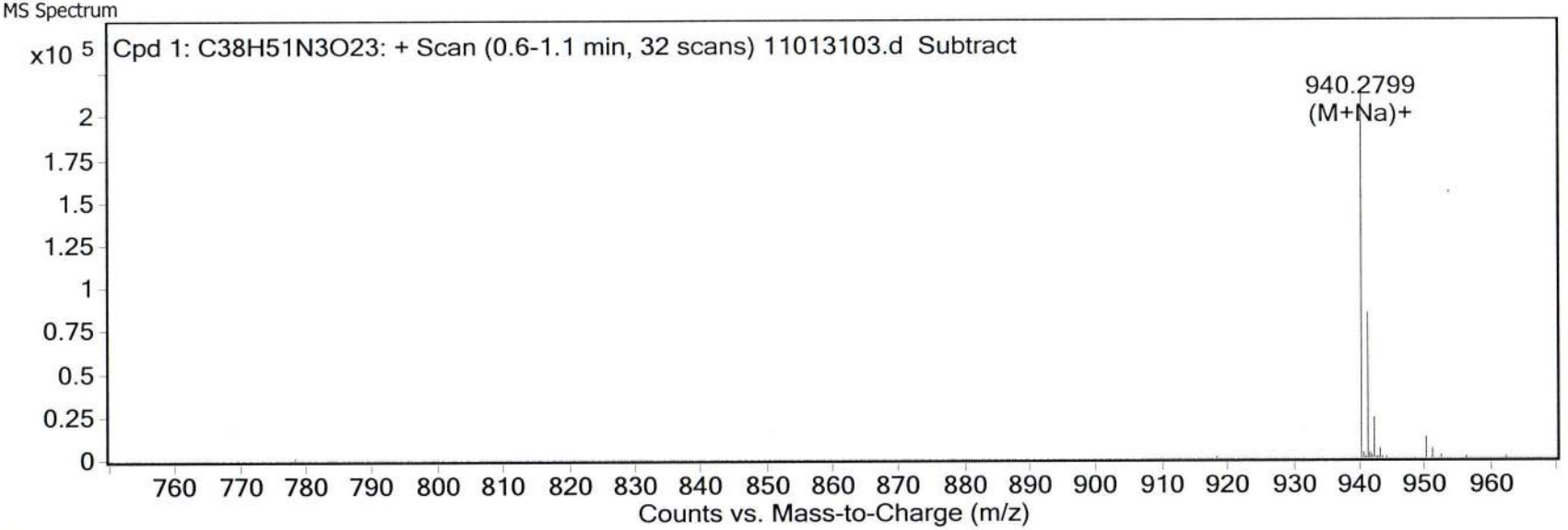
Comment	P. Kitov, Bundle	**Sample Name**	t4.37
Data File	11013103.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N3C5

Compound Table

MS Spectrum



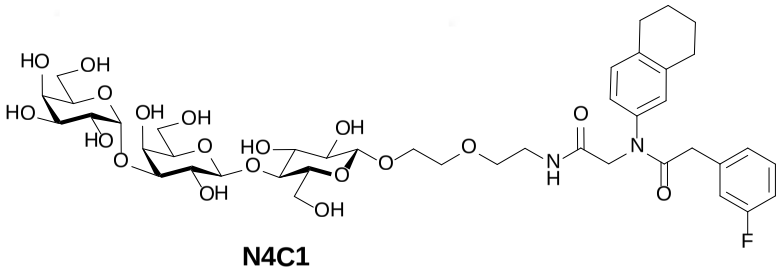
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
940.2799	940.2806	-0.75	214561	C38 H51 N3 Na O23	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

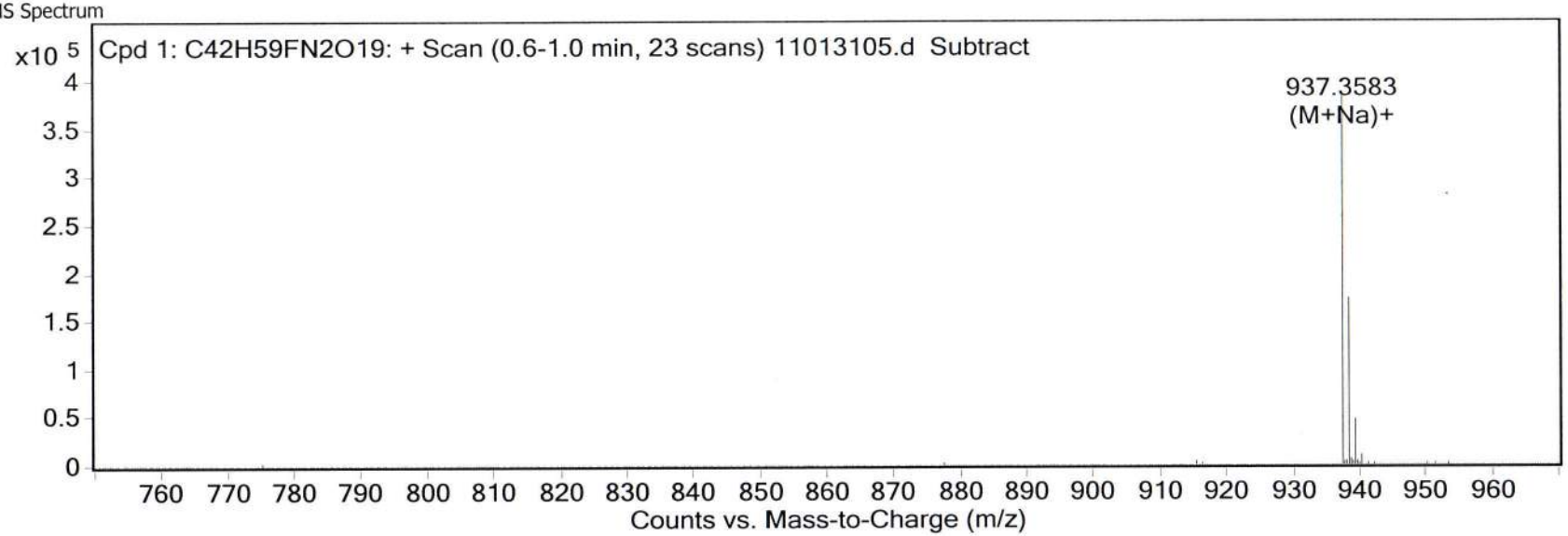
Comment	P. Kitov, Bundle	**Sample Name**	t4.36
Data File	11013105.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N4C1

Compound Table

MS Spectrum



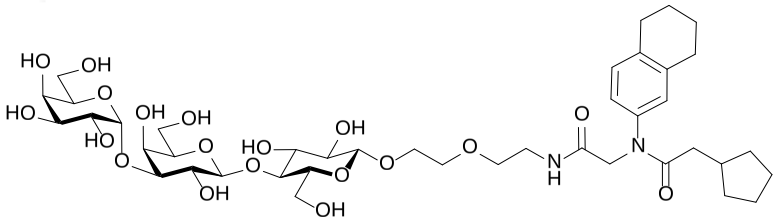
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
937.3583	937.3588	-0.57	387262	C42 H59 F N2 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

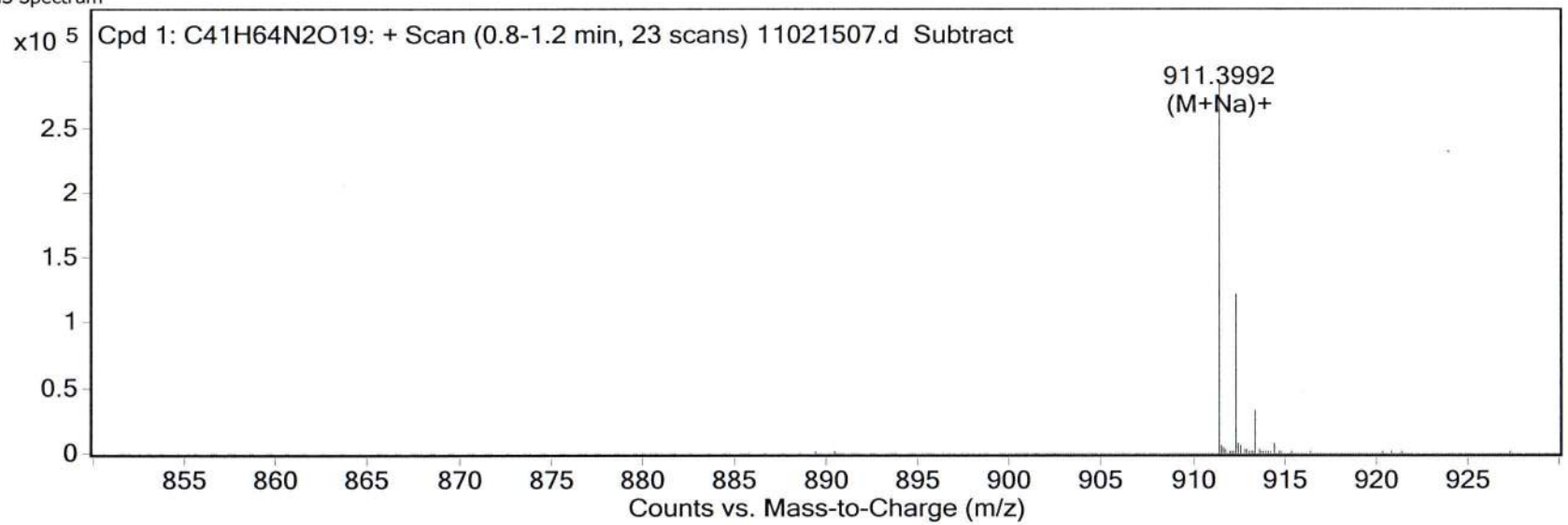
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t4.41
Data File	11021507.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N4C2

Compound Table

MS Spectrum



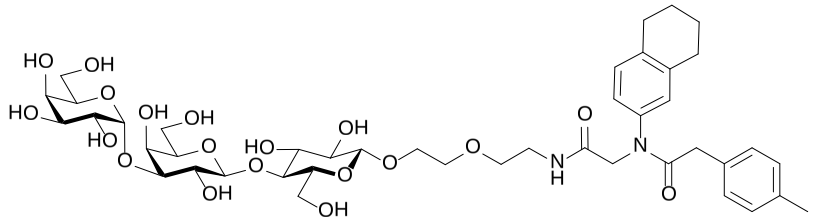
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
911.3992	911.3995	-0.38	286011	C41 H64 N2 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

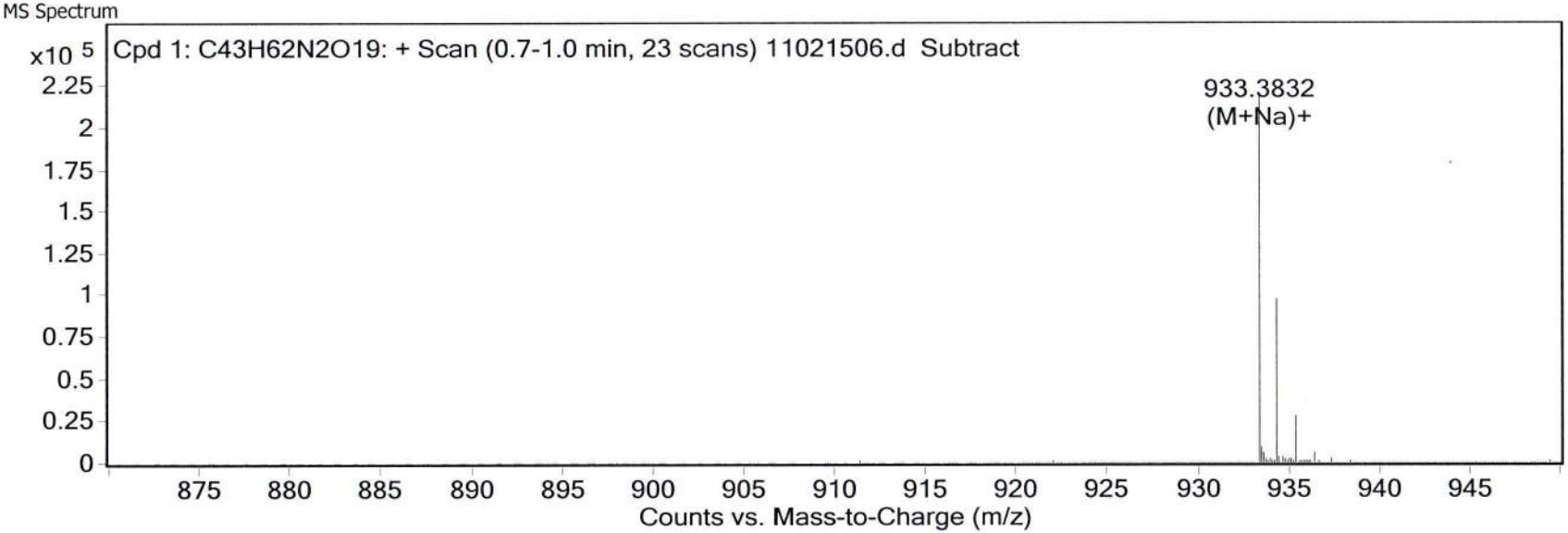
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t4.42
Data File	11021506.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N4C3

Compound Table

MS Spectrum



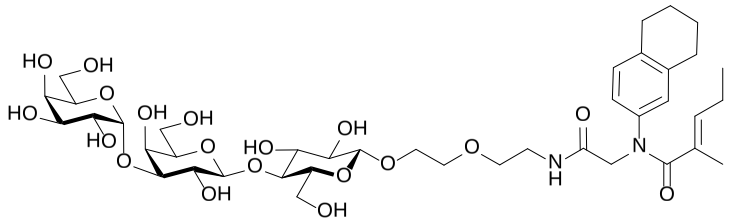
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
933.3832	933.3839	-0.79	1	220140	C43 H62 N2 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

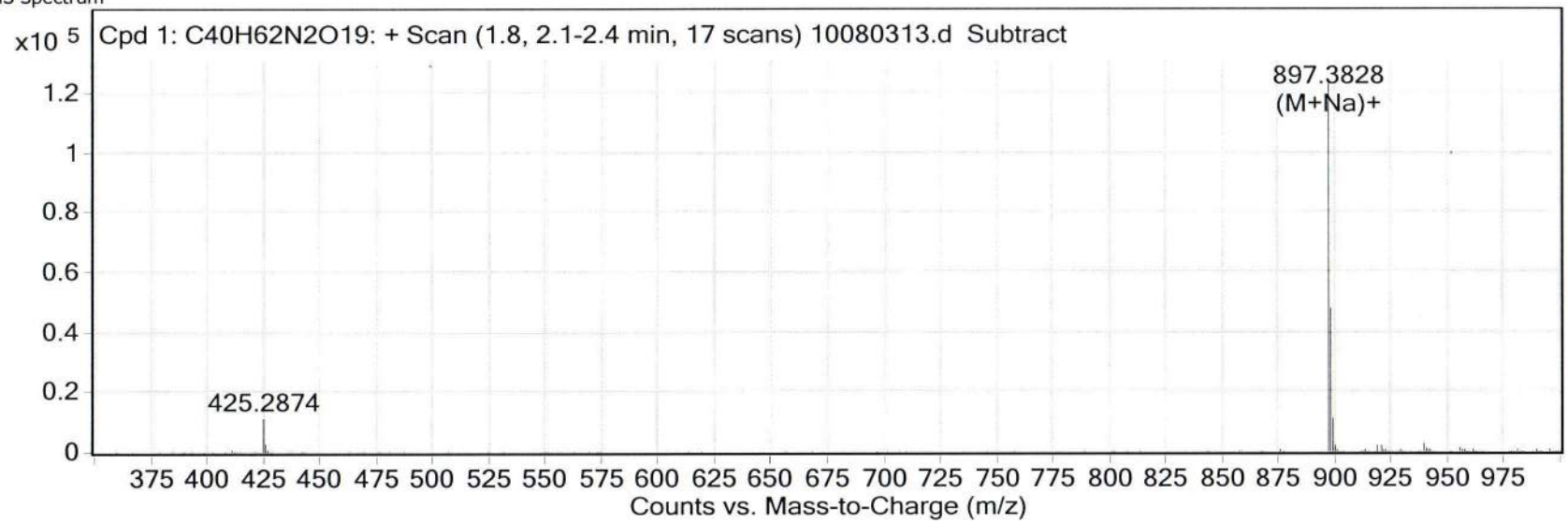
Comment	C. A. Sanhueza, Bundle	**Sample Name**	3.90
Data File	10080313.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N4C4

Compound Table

MS Spectrum



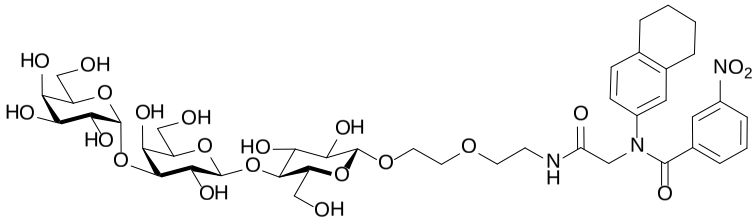
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
897.3828	897.3839	-1.19	1	124191	C40 H62 N2 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

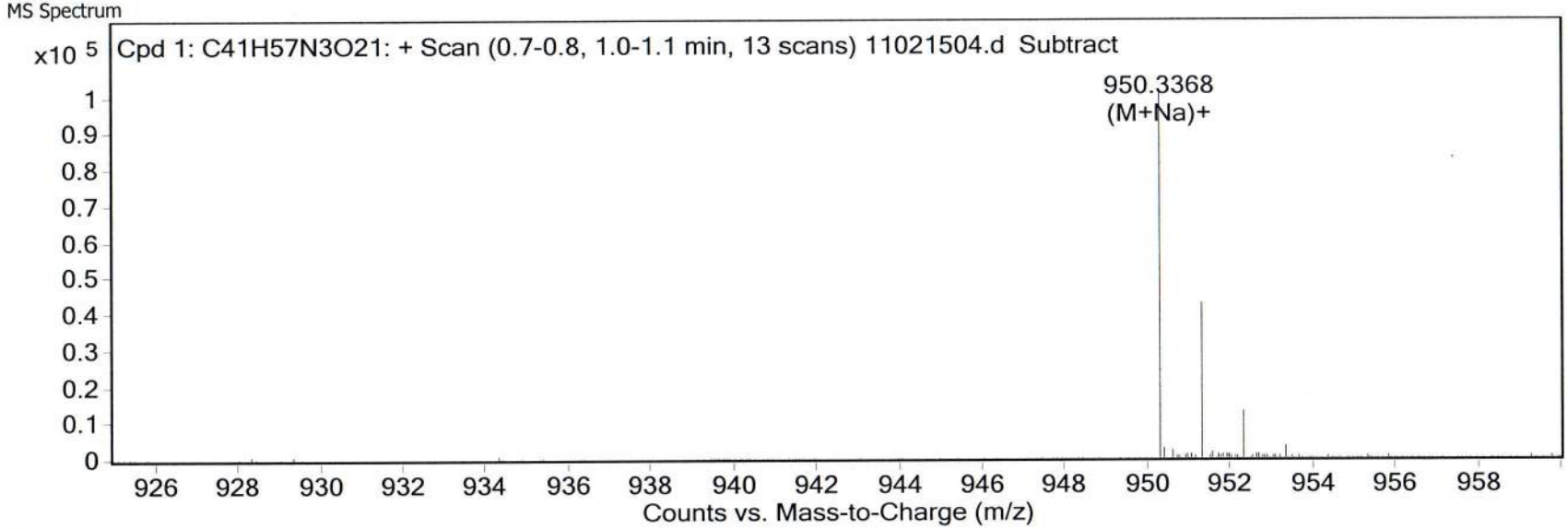
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t4.44
Data File	11021504.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N4C5

Compound Table

MS Spectrum



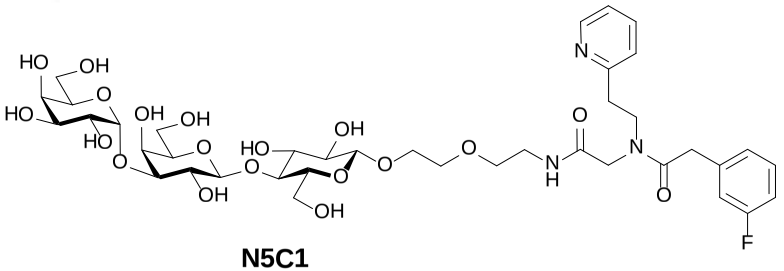
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
950.3368	950.3377	-0.91	1	101614	C41 H57 N3 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

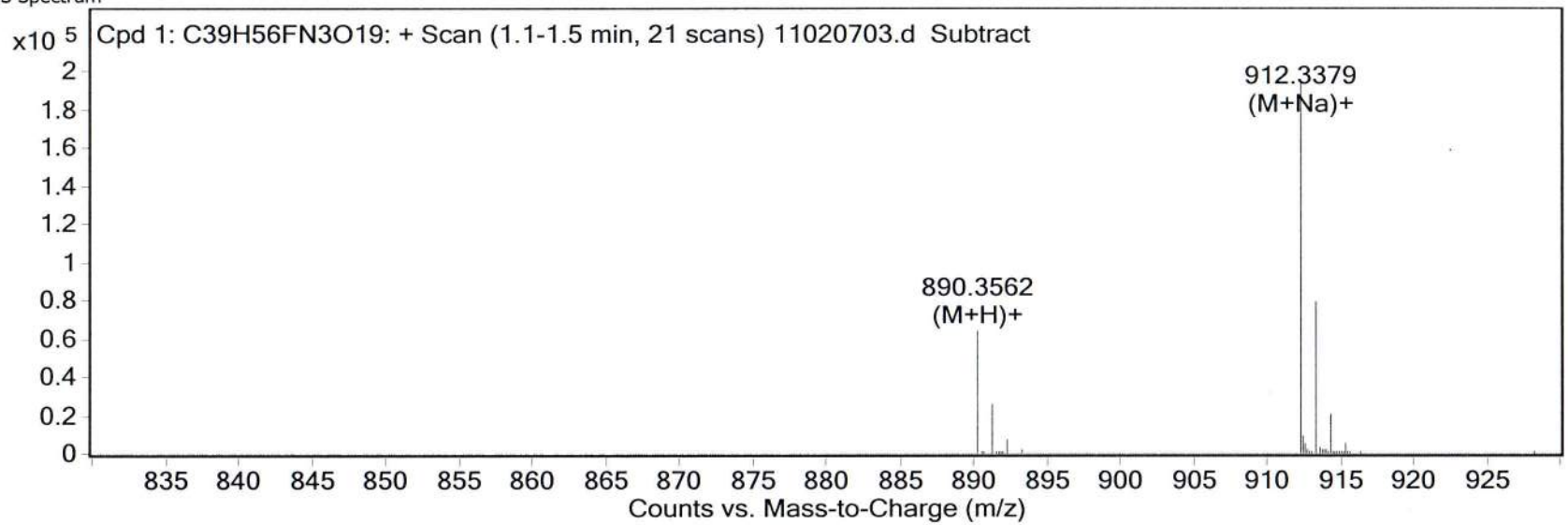
Comment	C. A. Sanhueza, Bundle	**Sample Name**	T 4.62
Data File	11020703.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N5C1

Compound Table

MS Spectrum



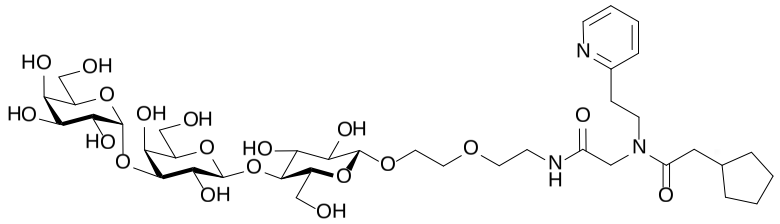
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
890.3562	890.3565	-0.31	1	63943	C39 H57 F N3 O19	(M+H)+
912.3379	912.3384	-0.59		195806	C39 H56 F N3 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

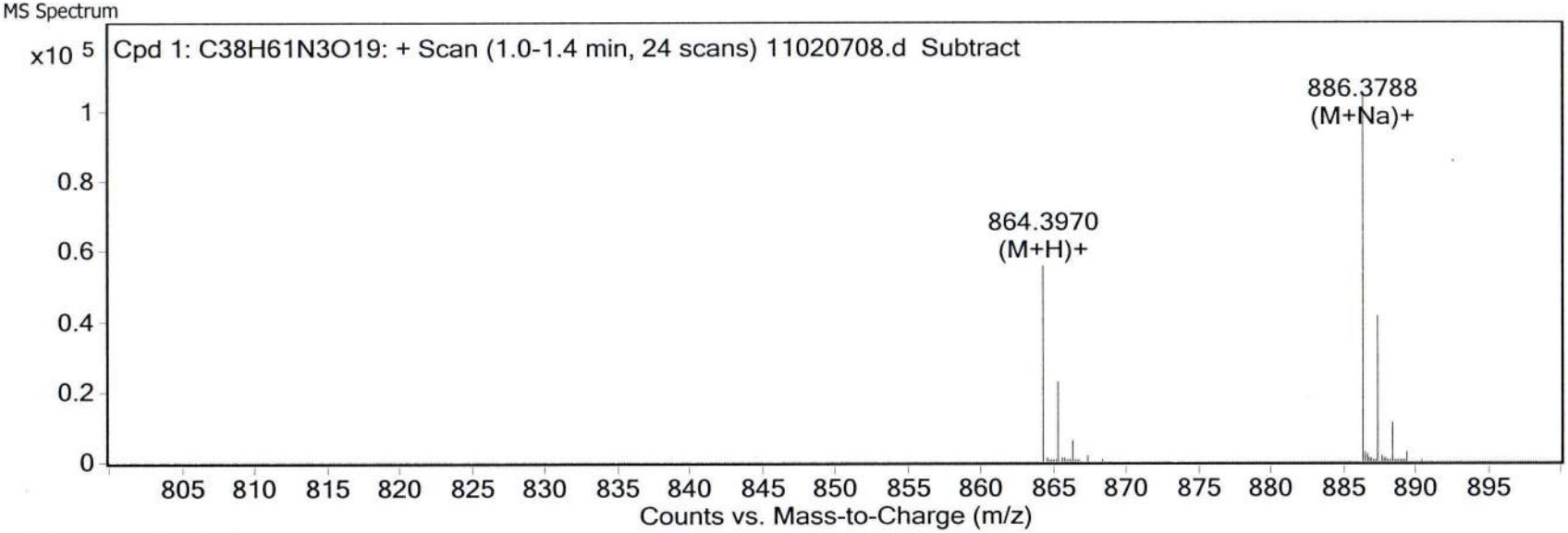
Comment	C. A. Sanhueza, Bundle	**Sample Name**	4.63
Data File	11020708.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N5C2

Compound Table

MS Spectrum



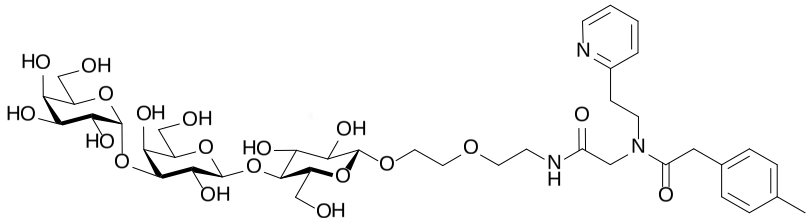
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
864.397	864.3972	-0.2	1	55610	C38 H62 N3 O19	(M+H)+
886.3788	886.3791	-0.43		105192	C38 H61 N3 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

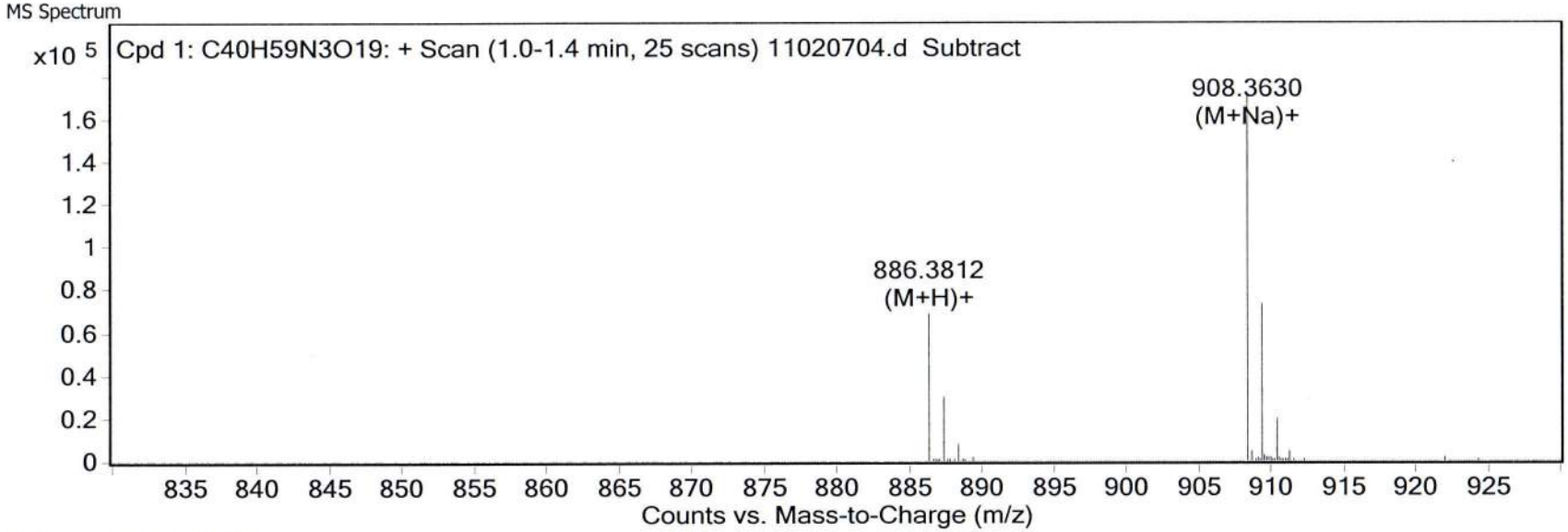
Comment	C. A. Sanhueza, Bundle	**Sample Name**	T 4.64
Data File	11020704.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N5C3

Compound Table

MS Spectrum



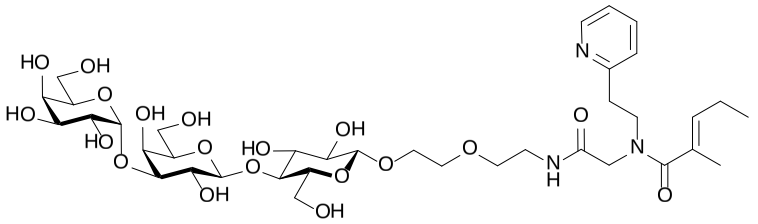
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
886.3812	886.3816	-0.45	1	68600	C40 H60 N3 O19	(M+H)+
908.363	908.3635	-0.54		172100	C40 H59 N3 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

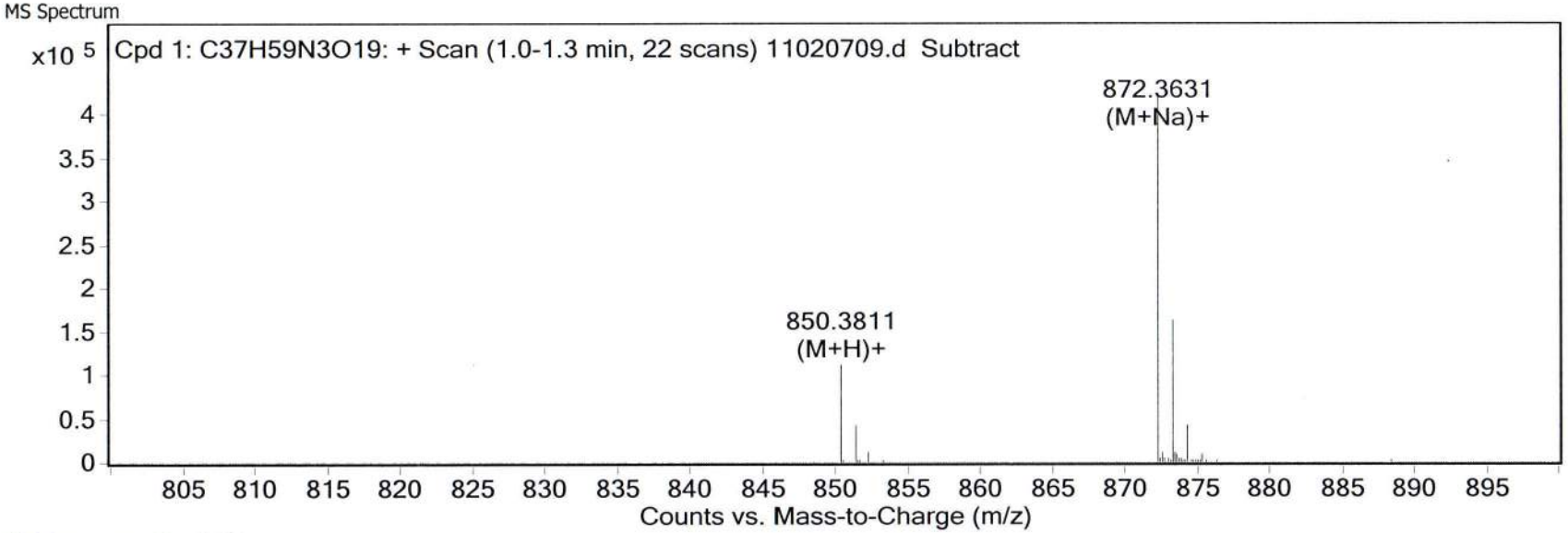
Comment	C. A. Sanhueza, Bundle	**Sample Name**	T 4.65
Data File	11020709.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N5C4

Compound Table

MS Spectrum



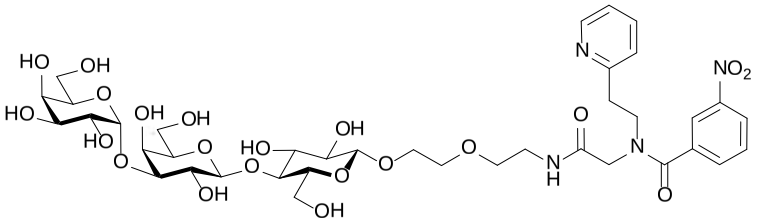
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
850.3811	850.3816	-0.5	1	110971	C37 H60 N3 O19	(M+H)+
872.3631	872.3635	-0.44		423611	C37 H59 N3 Na O19	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

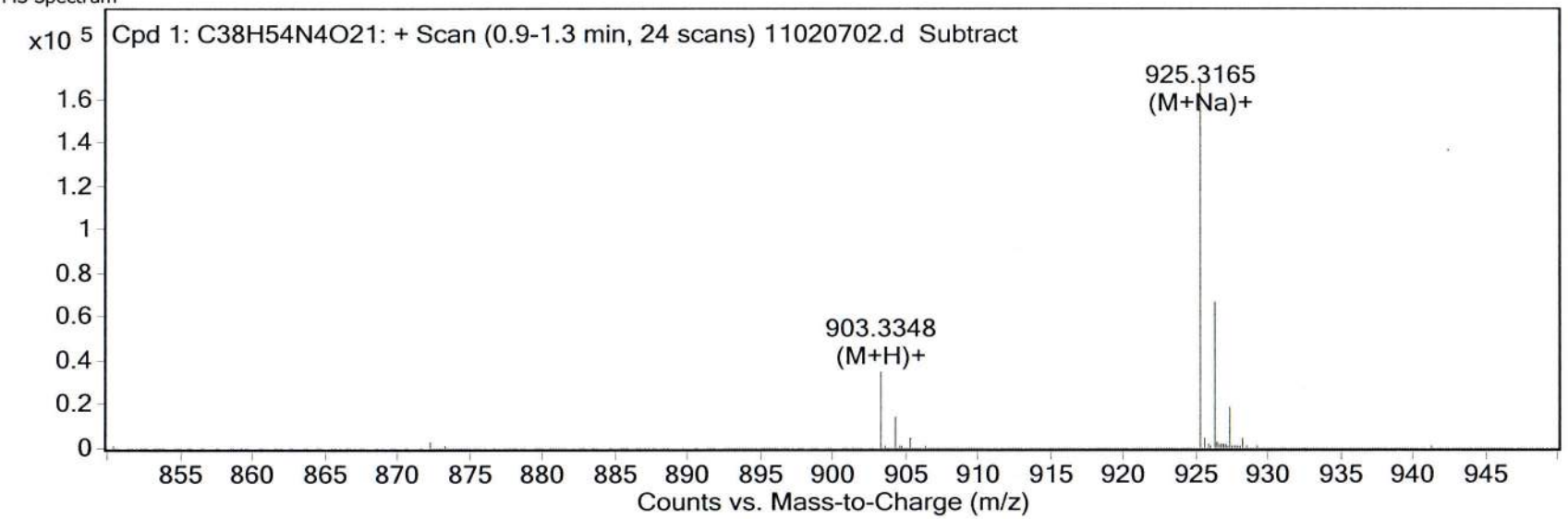
Comment	C. A. Sanhueza, Bundle	**Sample Name**	T4.66
Data File	11020702.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N5C5

Compound Table

MS Spectrum



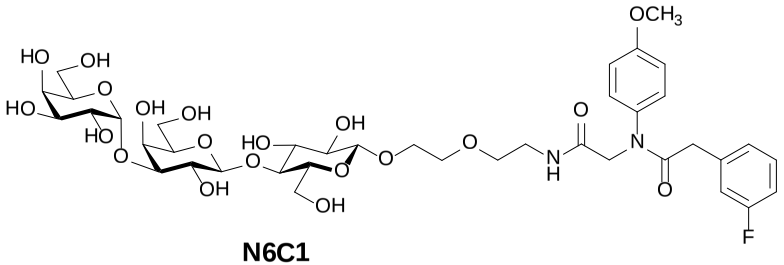
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
903.3348	903.3353	-0.56	1	34884	C38 H55 N4 O21	(M+H)+
925.3165	925.3173	-0.89		168850	C38 H54 N4 Na O21	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

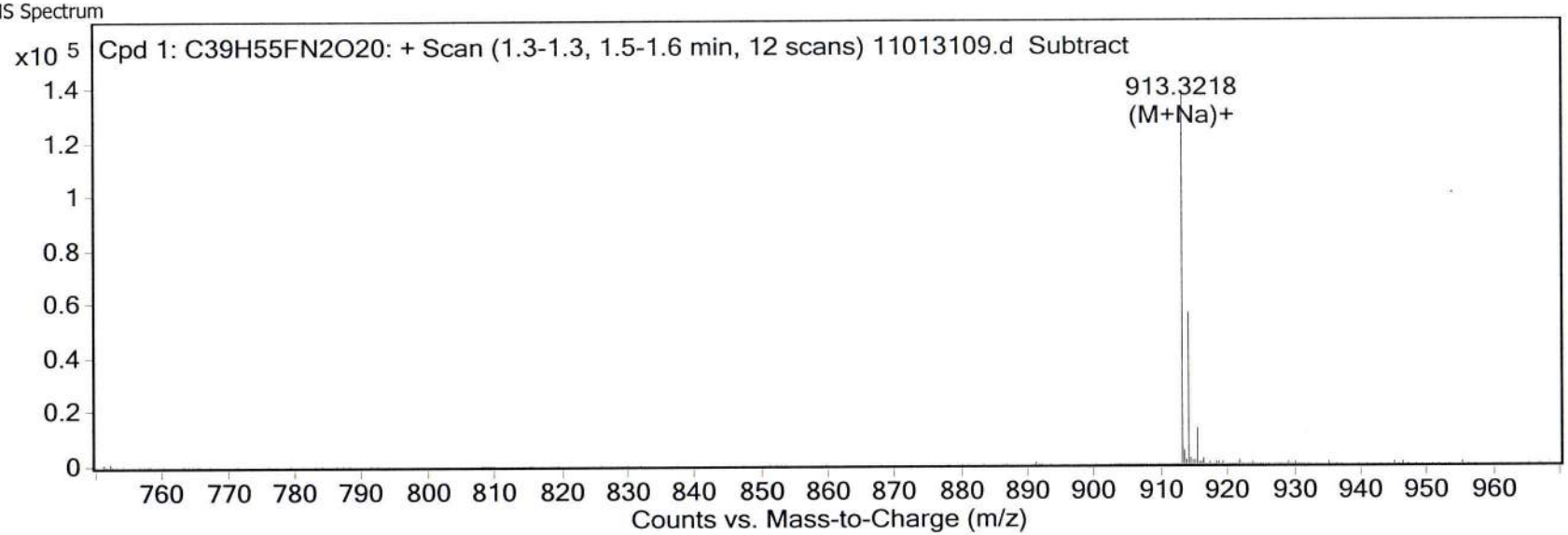
Comment	P. Kitov, Bundle	**Sample Name**	t4.31
Data File	11013109.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N6C1

Compound Table

MS Spectrum



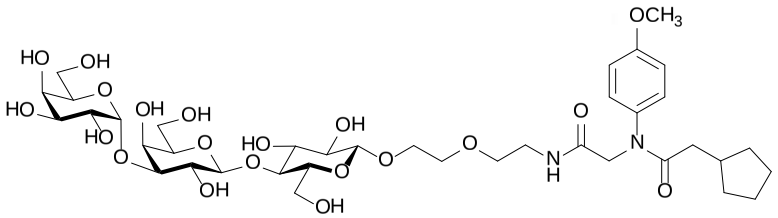
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
913.3218	913.3224	-0.73	138514	C39 H55 F N2 Na O20	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

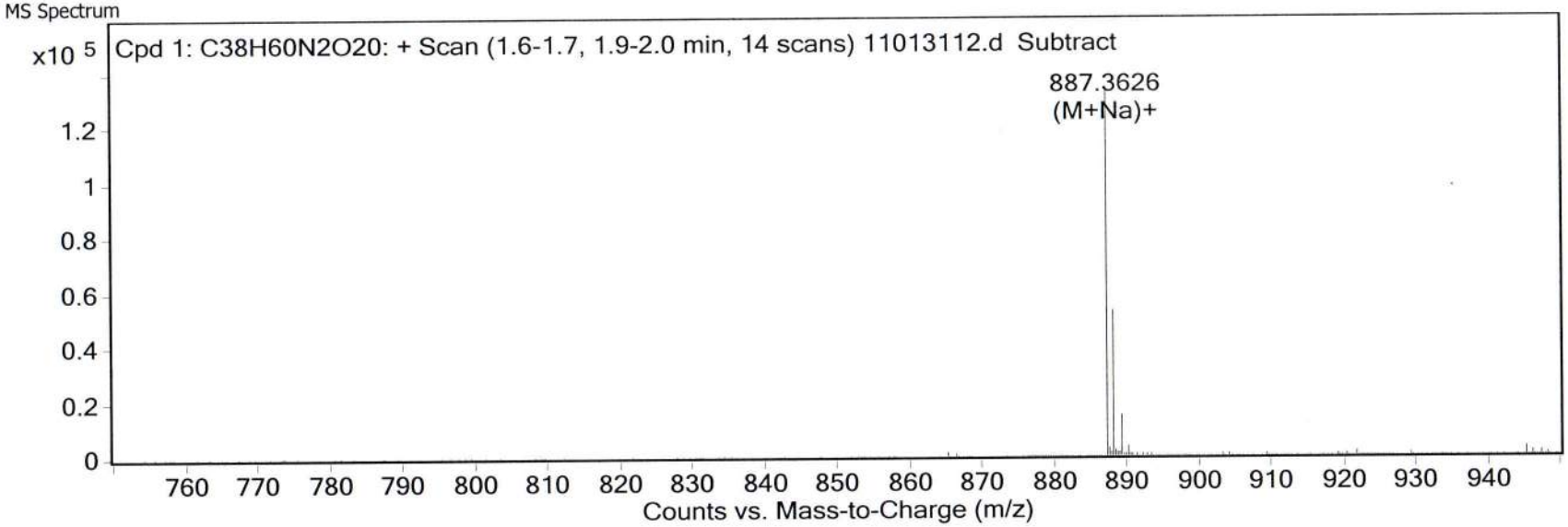
Comment	P. Kitov, Bundle	**Sample Name**	t4.32
Data File	11013112.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N6C2

Compound Table

MS Spectrum



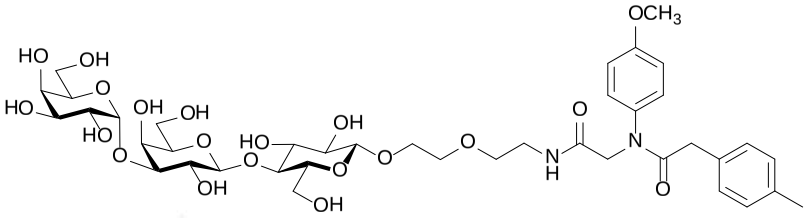
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
887.3626	887.3632	-0.6	133946	C38 H60 N2 Na O20	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

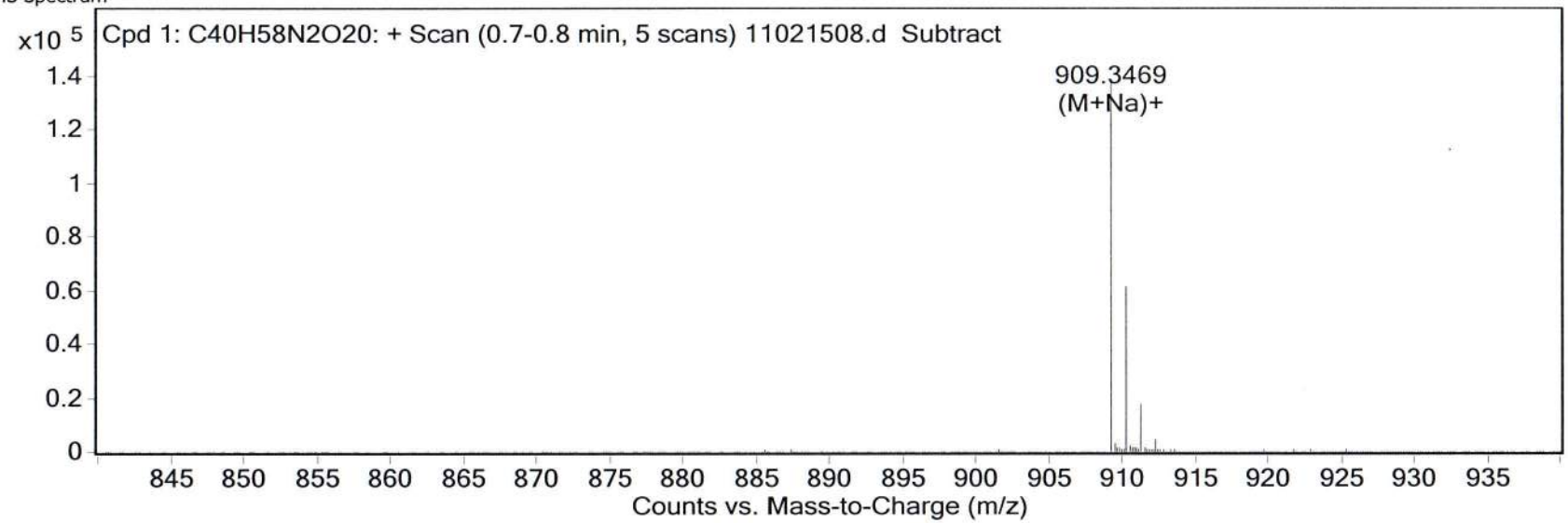
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t4.67
Data File	11021508.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N6C3

Compound Table

MS Spectrum



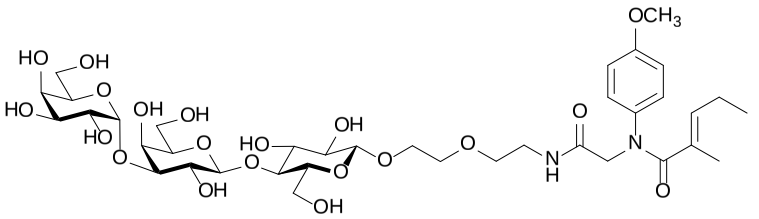
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
909.3469	909.3475	-0.7	138766	C40 H58 N2 Na O20	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

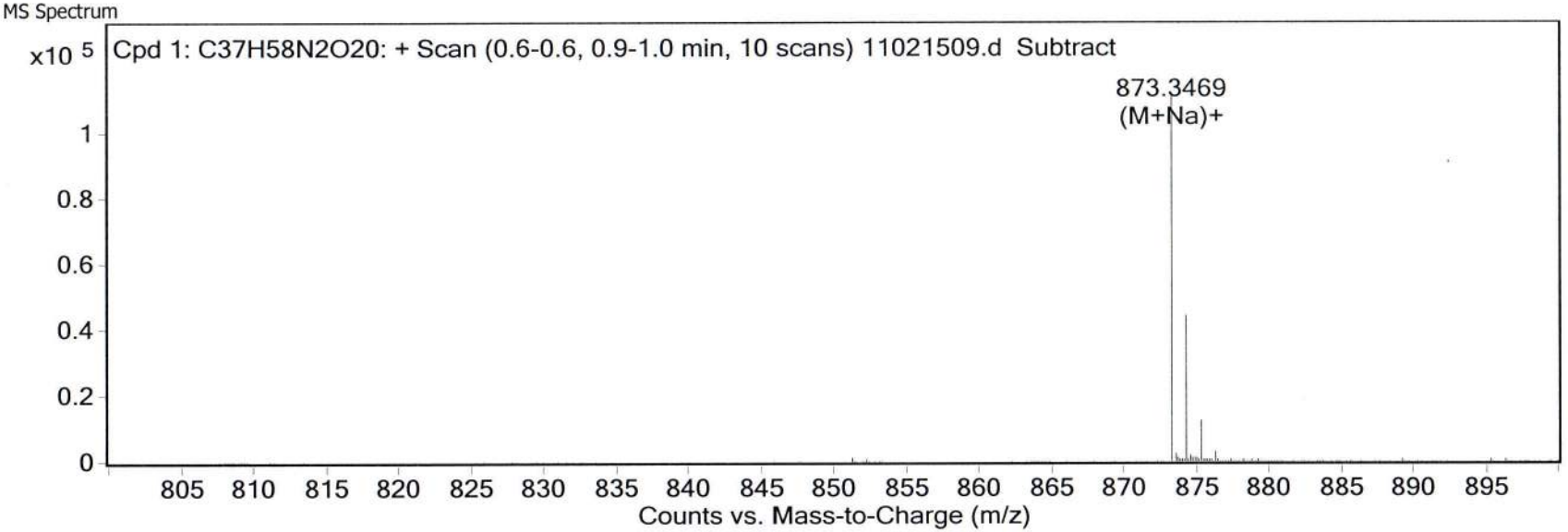
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t4.68
Data File	11021509.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N6C4

Compound Table

MS Spectrum



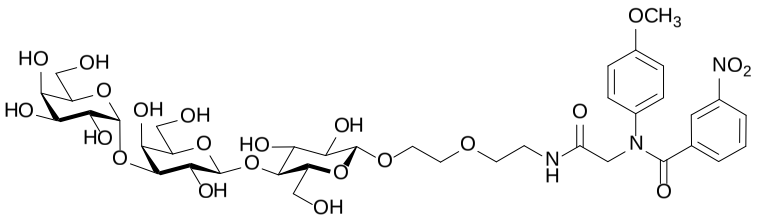
MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	Abund	Formula	Ion
873.3469	873.3475	-0.72	111772	C37 H58 N2 Na O20	(M+Na)+

--- End Of Report ---

Qualitative Compound Report

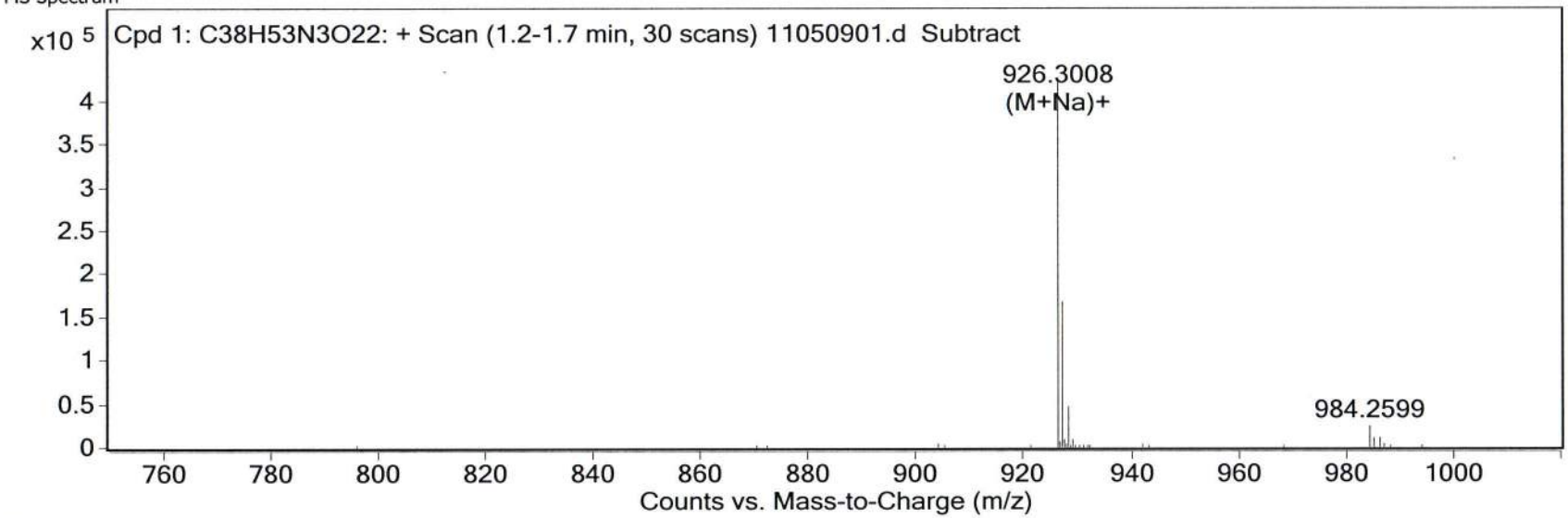
Comment	C. A. Sanhueza, Bundle	**Sample Name**	t 3.89
Data File	11050901.d	**Instrument Name**	6220 oaTOF
Position	-1	**Operator**	ami
Acq Method		**DA Method**	da ami low mass.m



N6C5

Compound Table

MS Spectrum



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
926.3008	926.3013	-0.56	1	425301	C38 H53 N3 Na O22	(M+Na)+

--- End Of Report ---