Supporting Information

Synthesis of a 35-Member Stereoisomer Library of Bistramide A: Evaluation of Effects on Actin State, Cell Cycle and Tumor Cell Growth.

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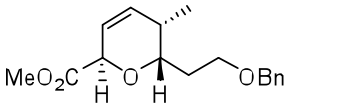
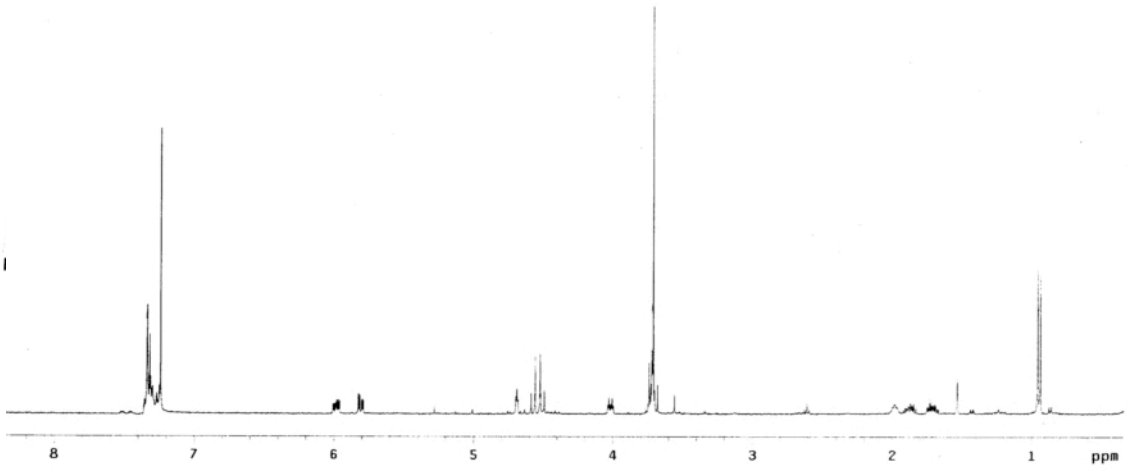
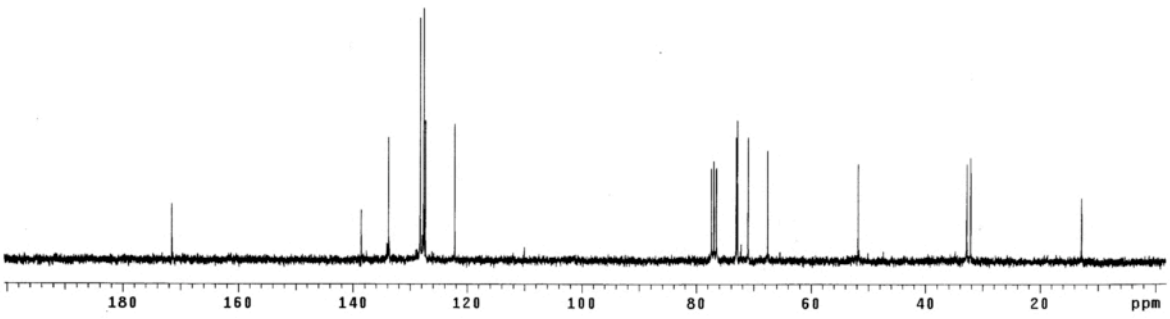
Department of Chemistry and Center for Chemical Methodology and Library Development (CMLD-BU), Boston University 590, Commonwealth Avenue, Boston, Massachusetts, 02215, and Molecular Targets Development Program National Cancer Institute at Frederick, Building 560-15, Frederick, Maryland, 21702

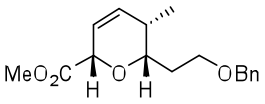
^{1}H and ^{13}C Spectra



21a (400 MHz, $CDCl_3$)







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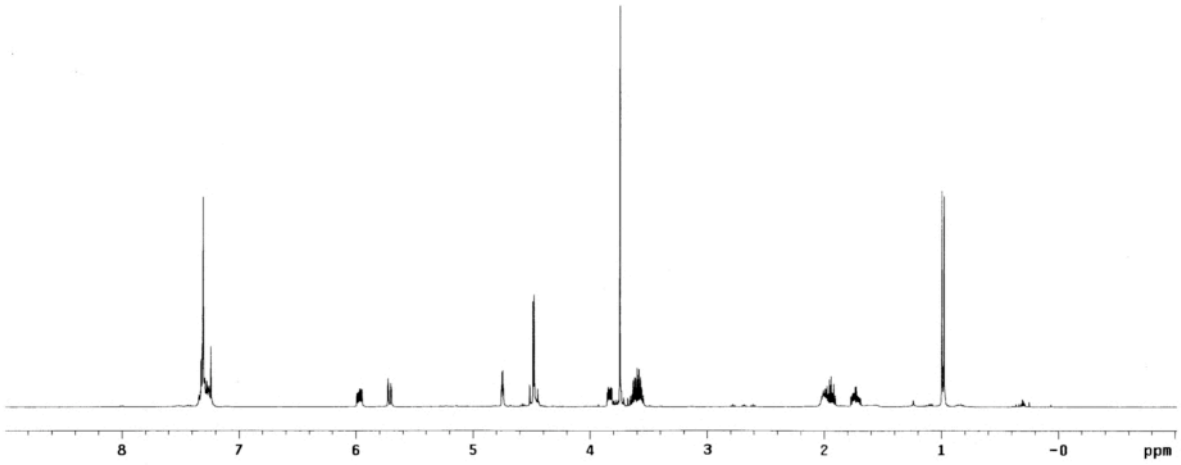

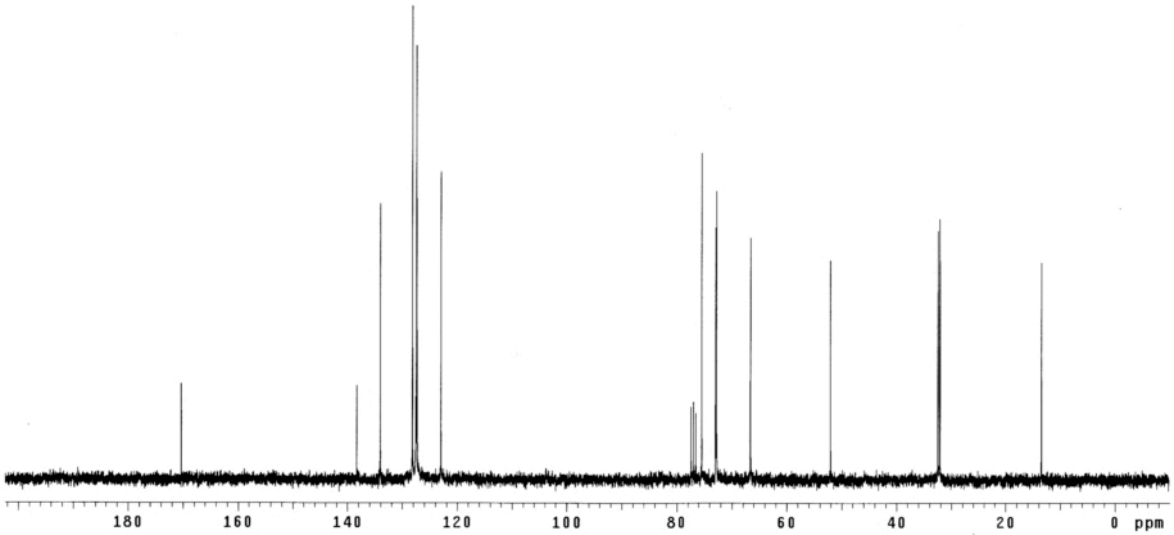

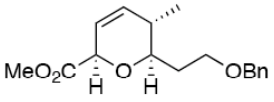
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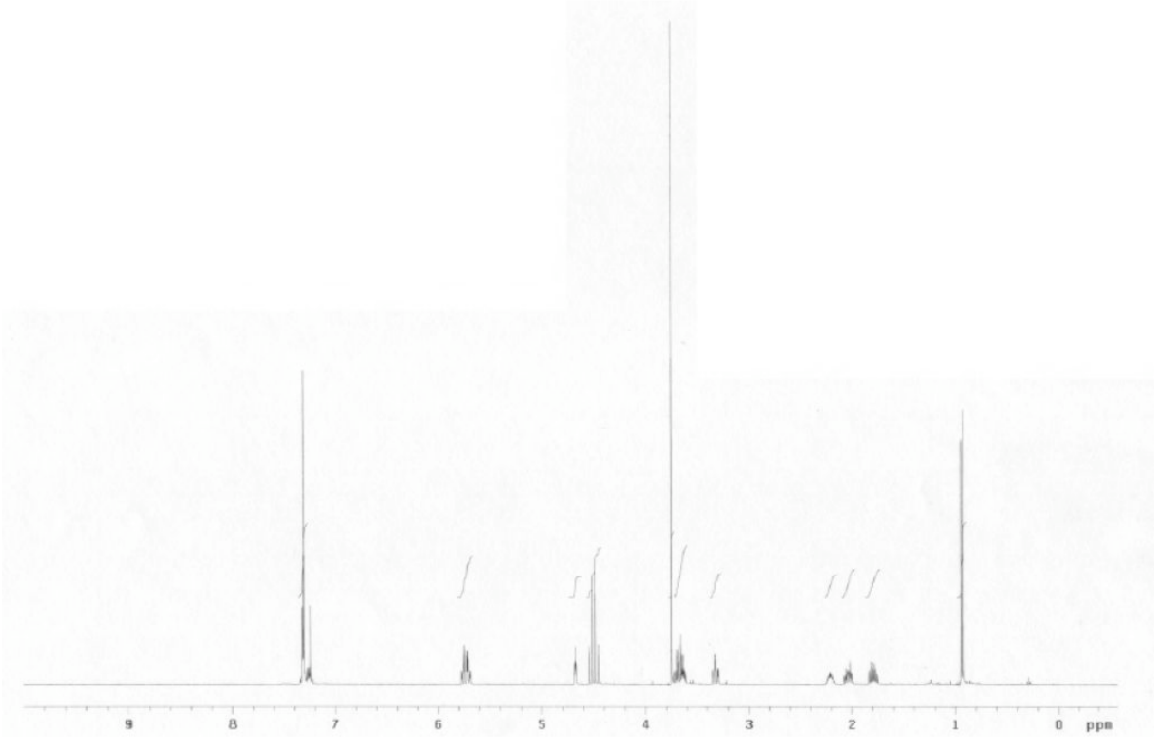
O
H
OBn

21c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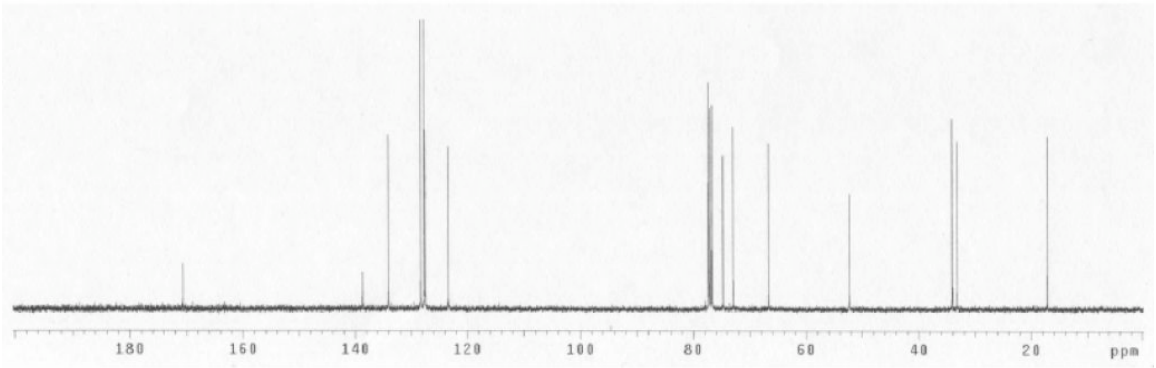
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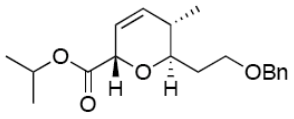

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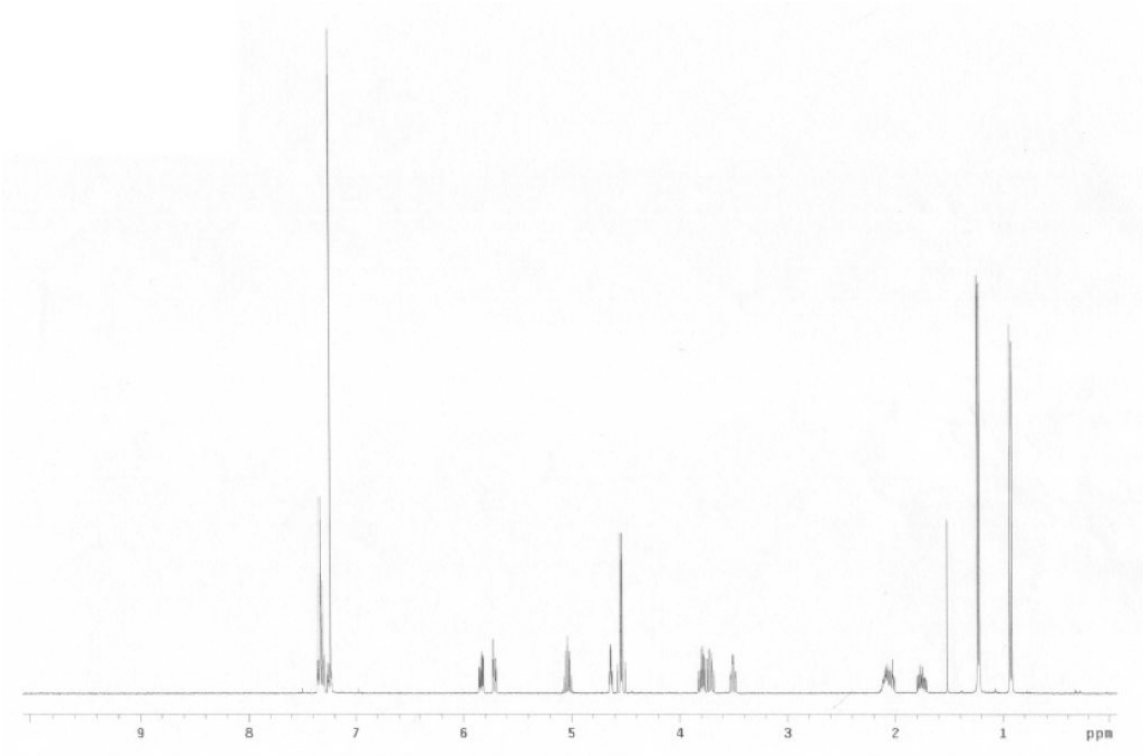

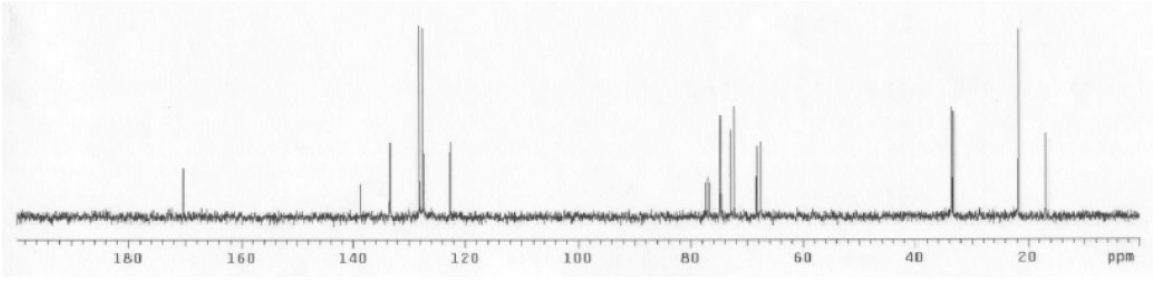

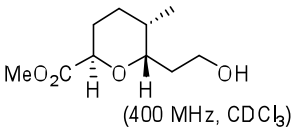

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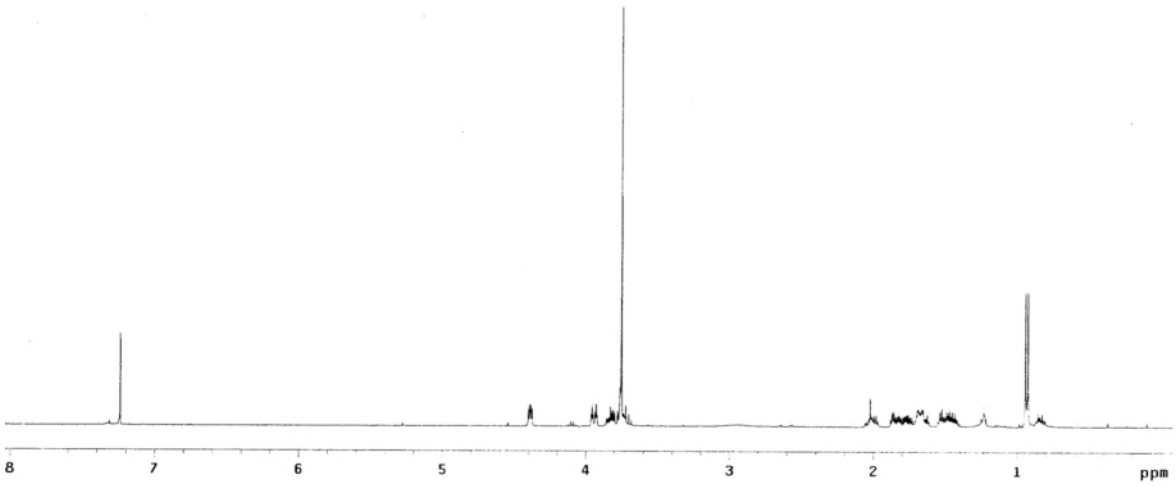

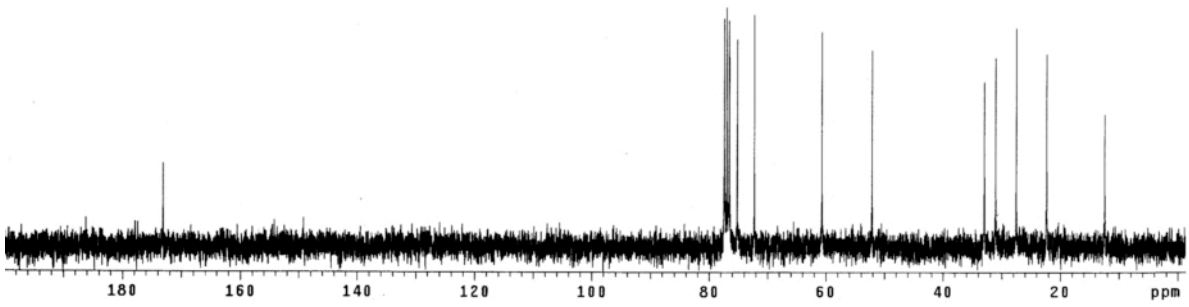

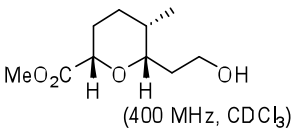

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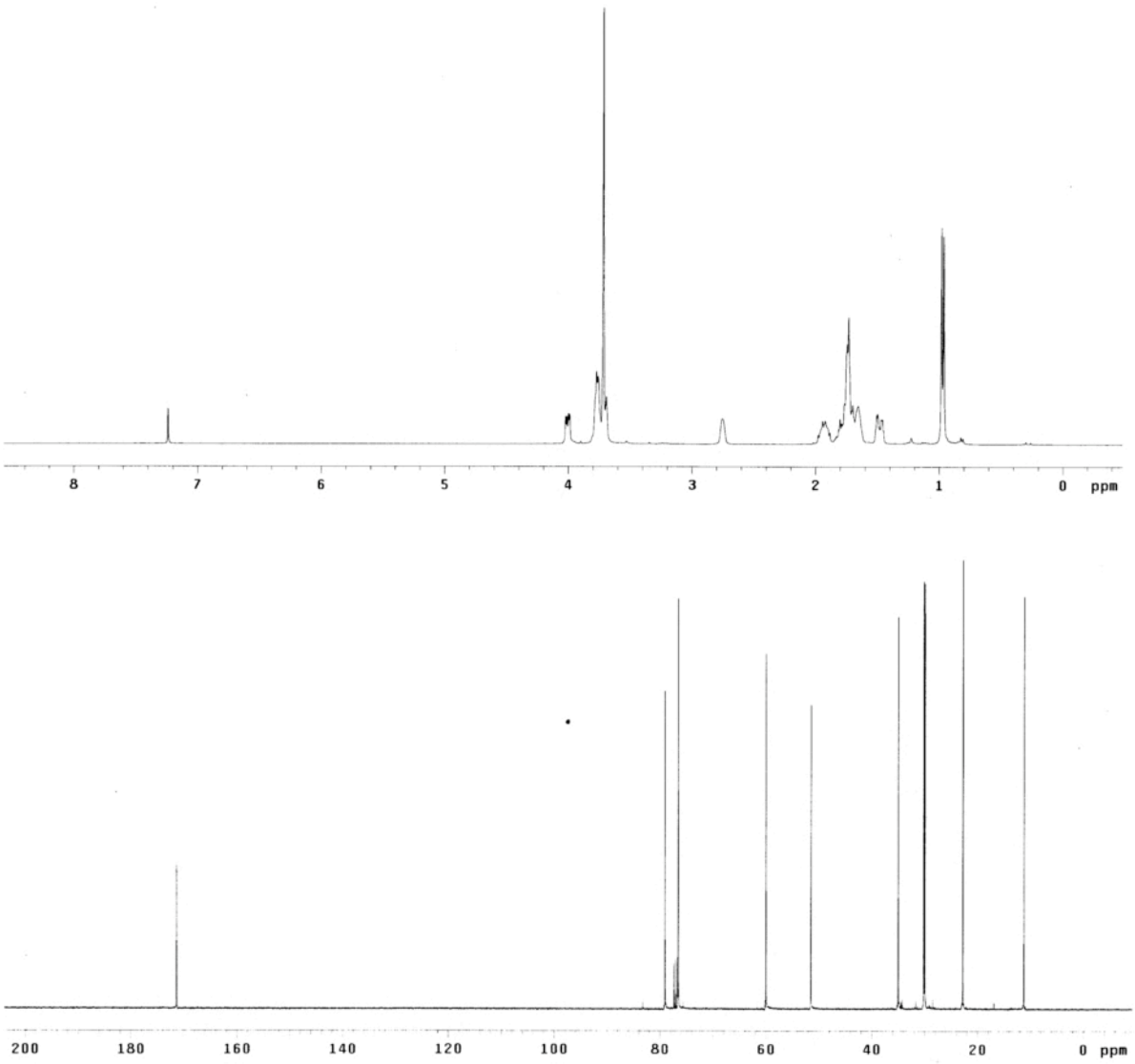
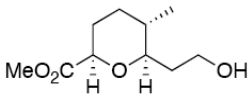
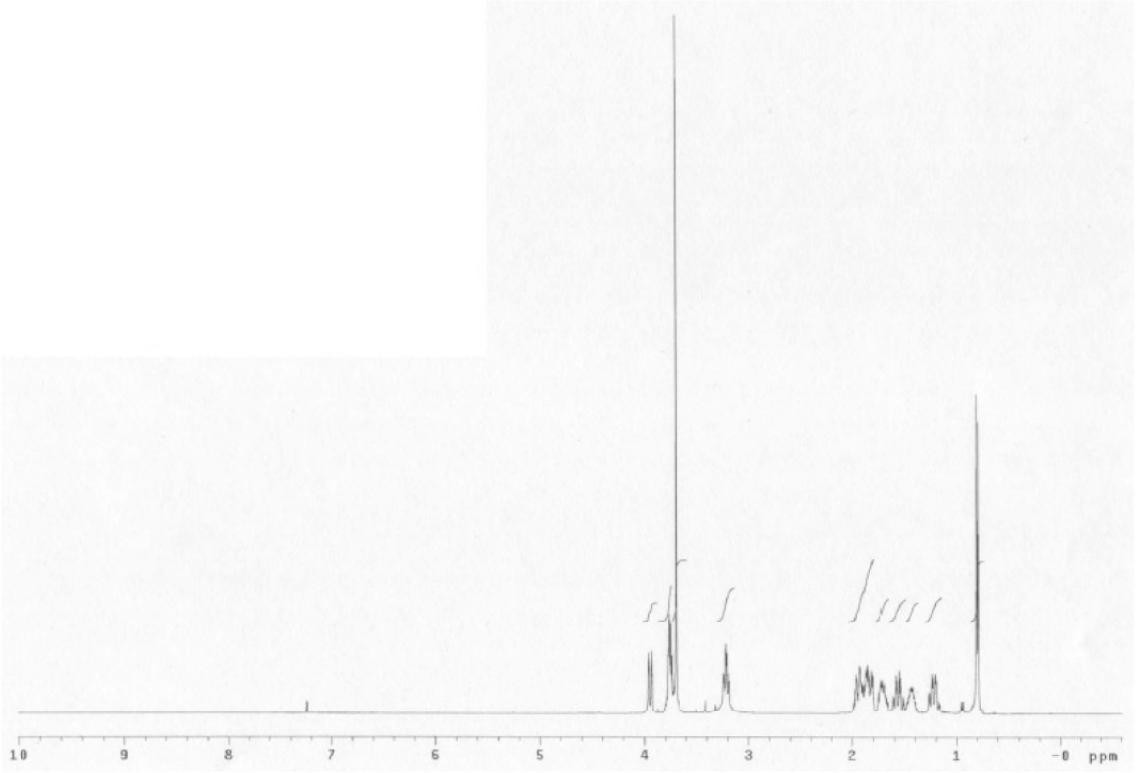



MeO2C
O
OH
H
H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7
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5
4
3
2
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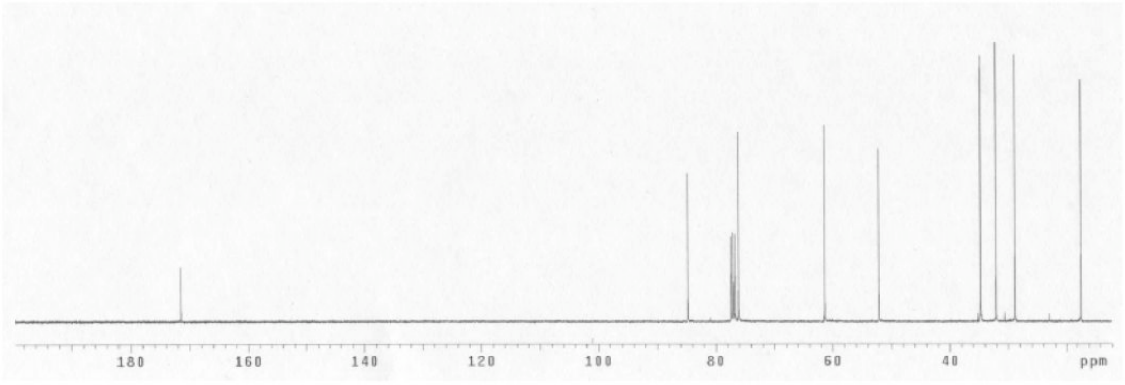
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60
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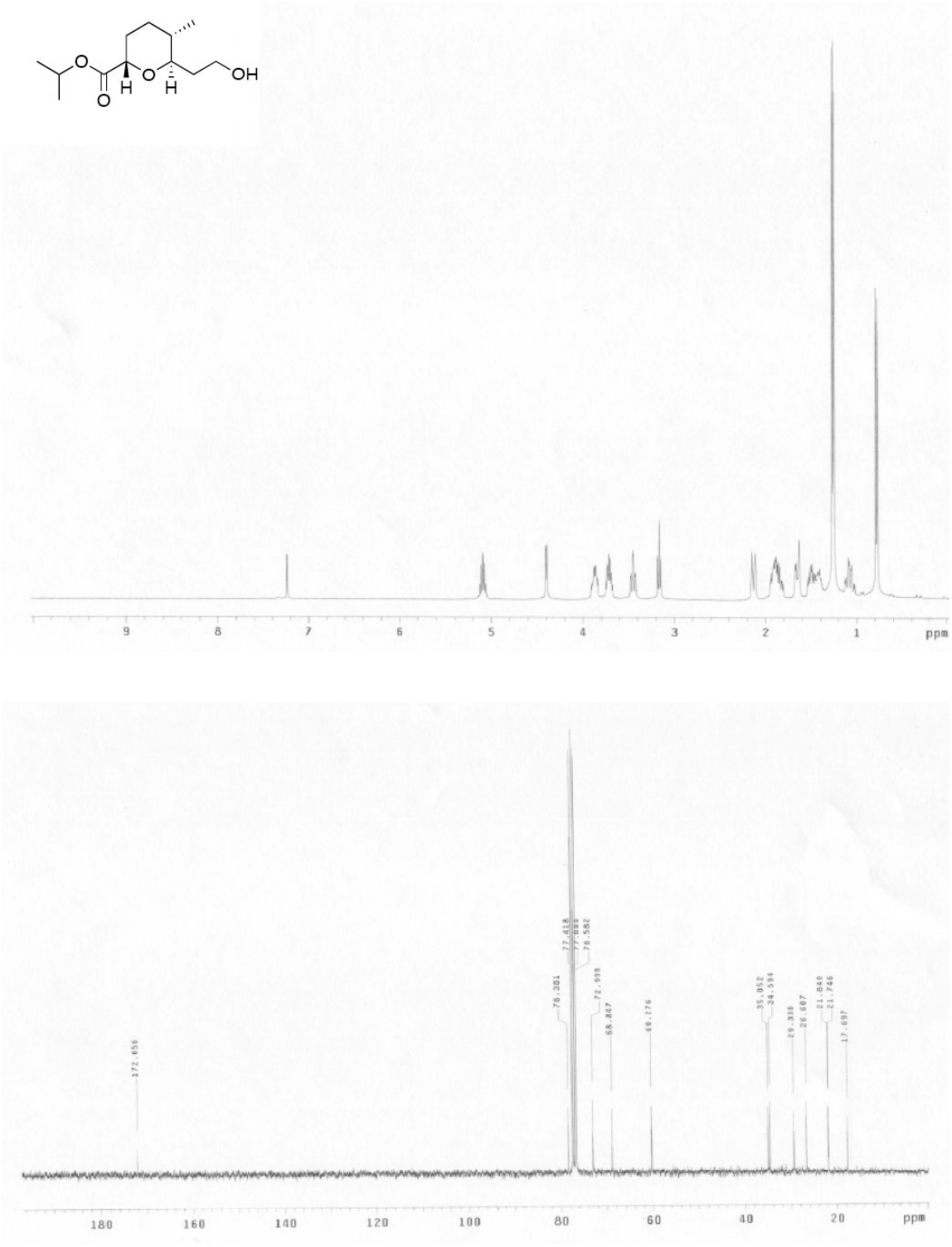
O
O
H
O
H
OH
9
8
7
6
5
4
3
2
1
ppm
172.656
77.418
76.582
70.301
72.999
68.867
69.176
35.952
34.594
29.338
26.607
21.840
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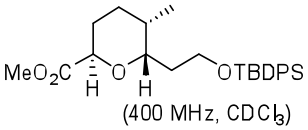
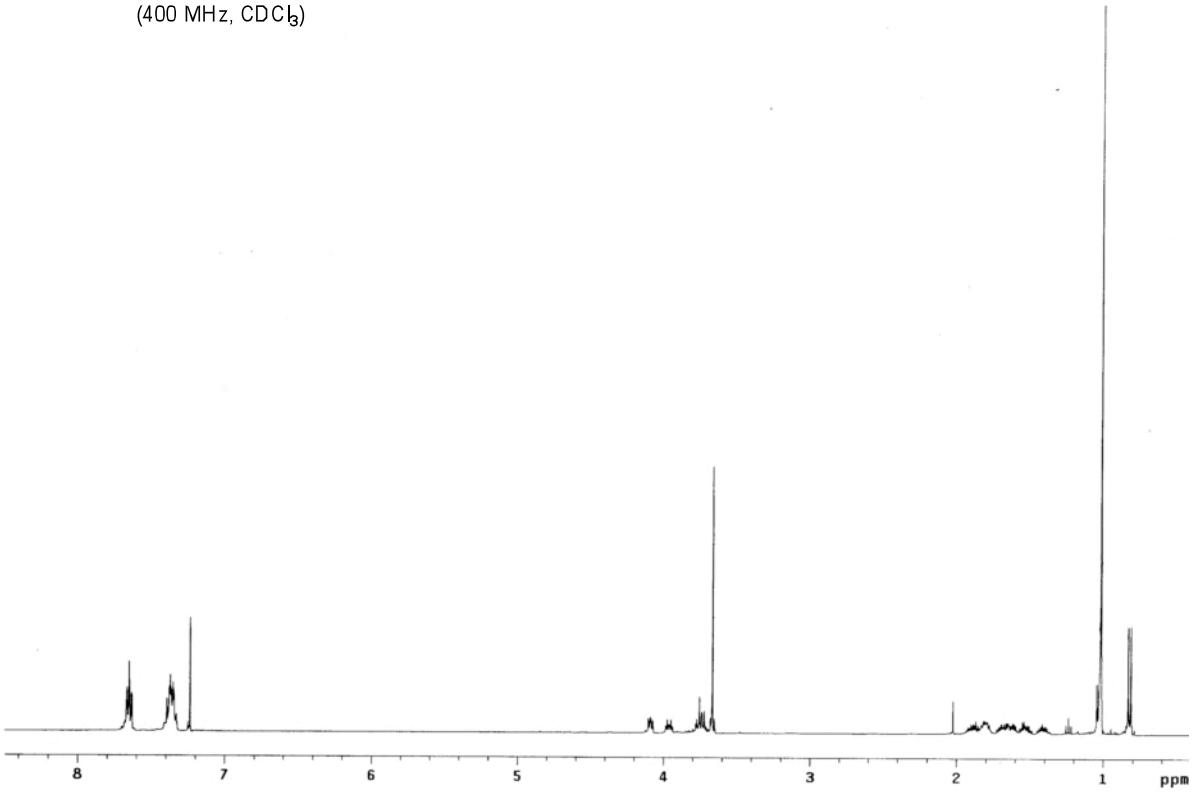
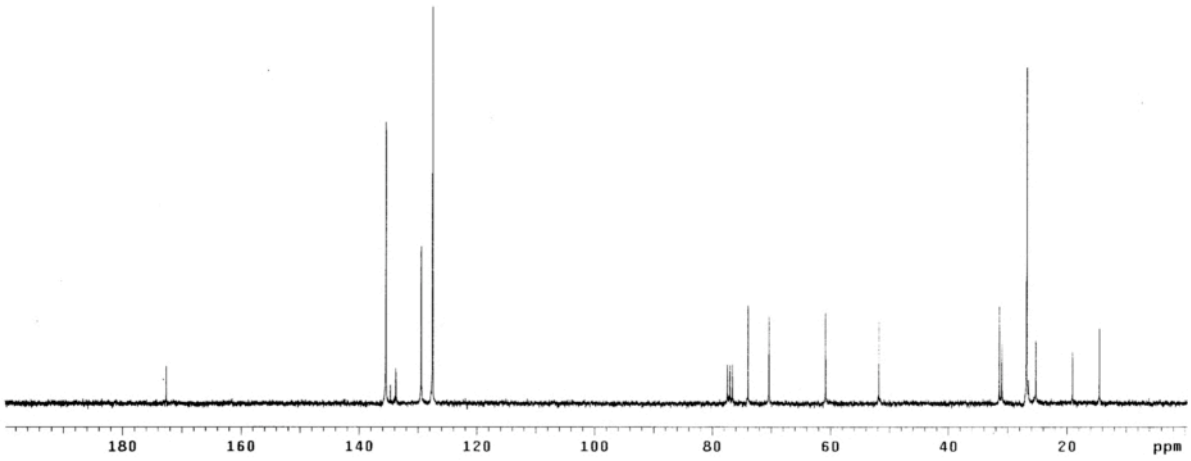
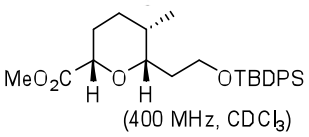
140
120
100
80
60
40
20
ppm

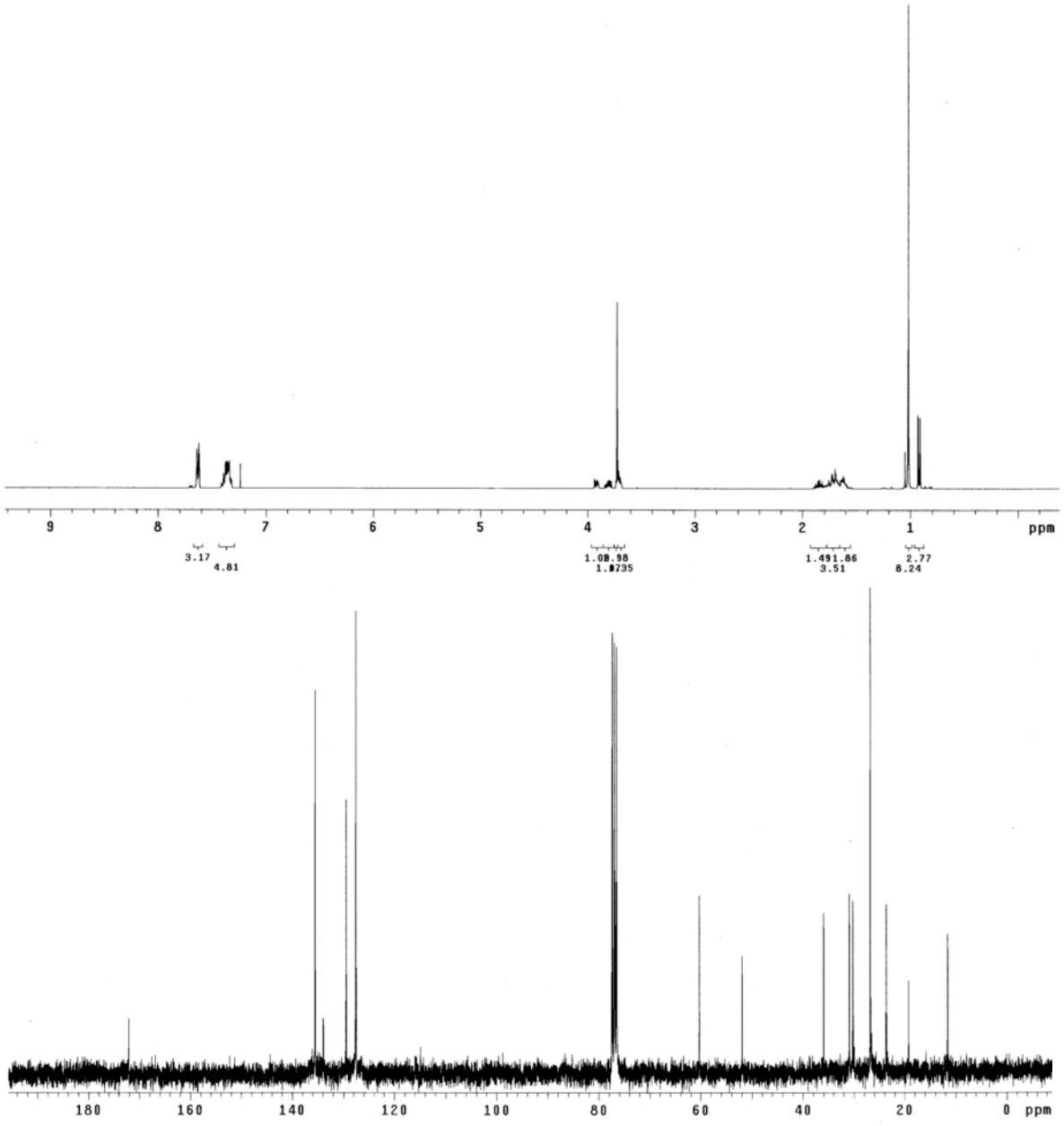


(400 MHz, $CDCl_3$)






MeO2C
H
O
H
OTBDPS
(400 MHz, CDCl3)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8.24
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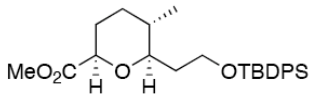
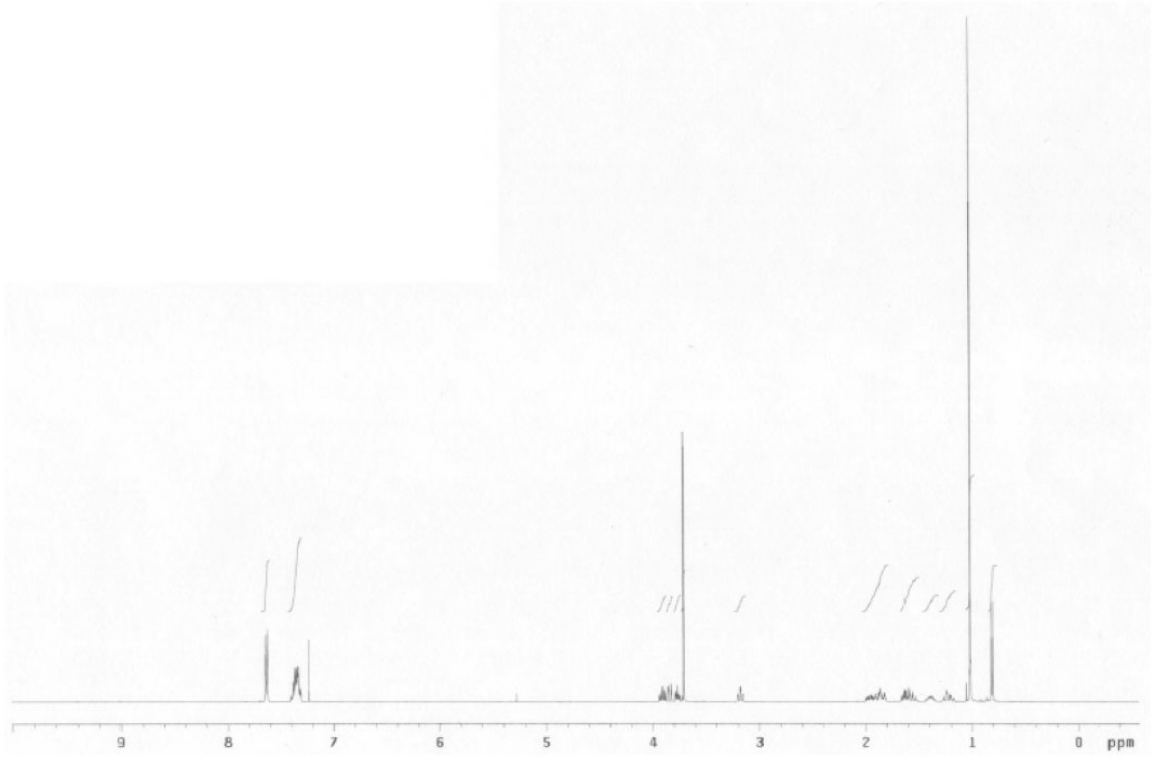
40
20
0 ppm


MeO2C
H
O
H
OTBDPS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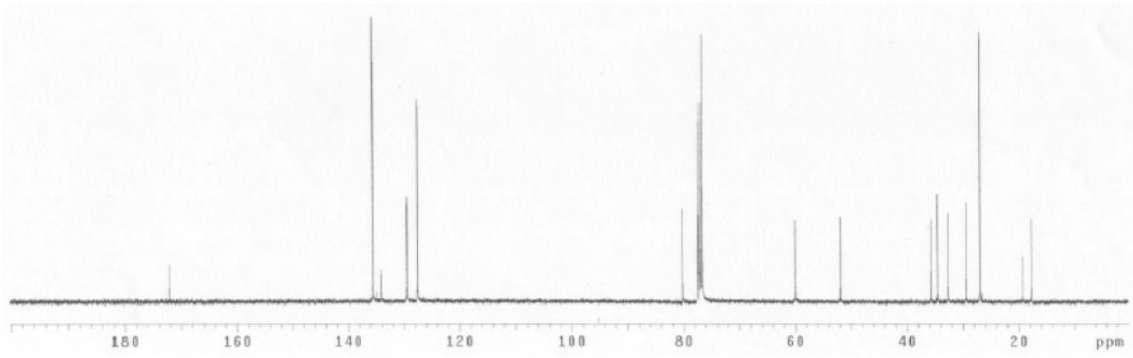
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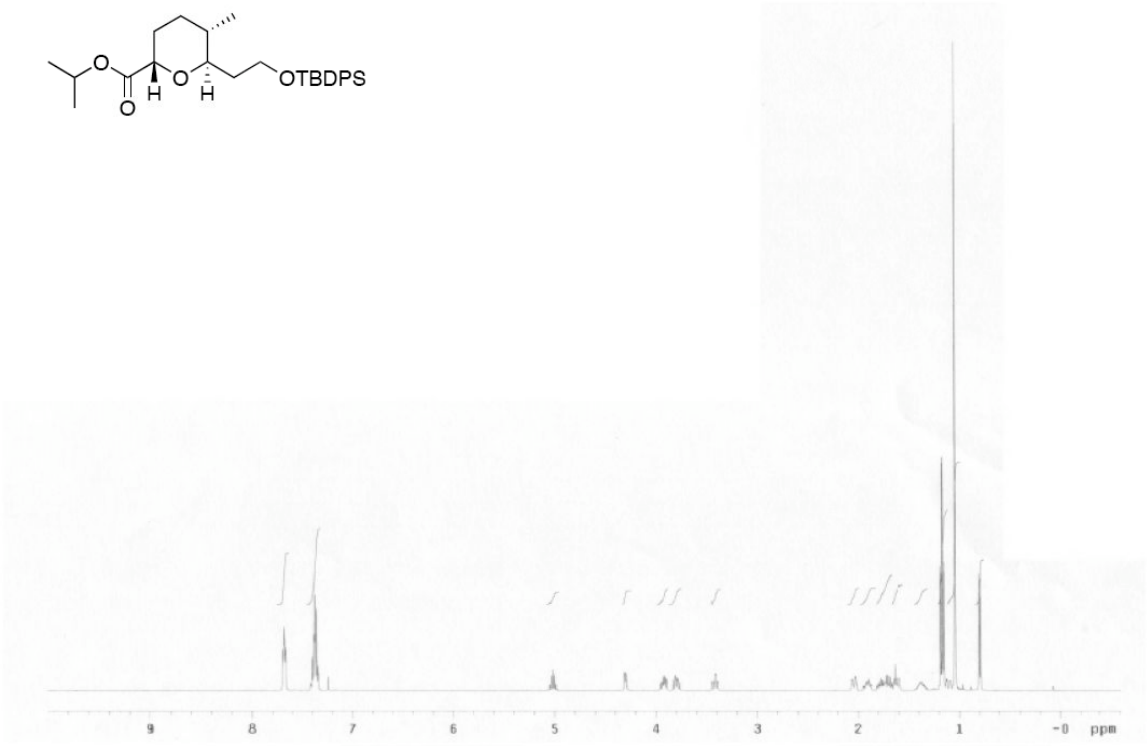
20
ppm

O
O
H
O
H
OTBDPS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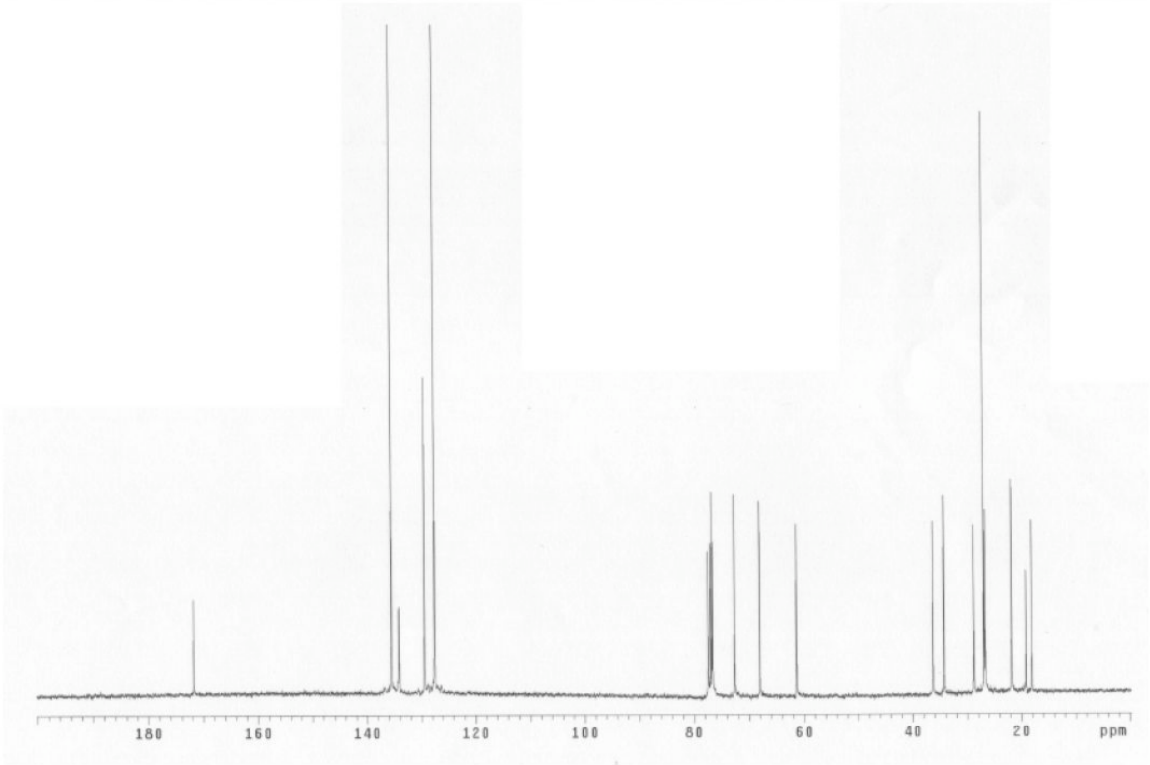
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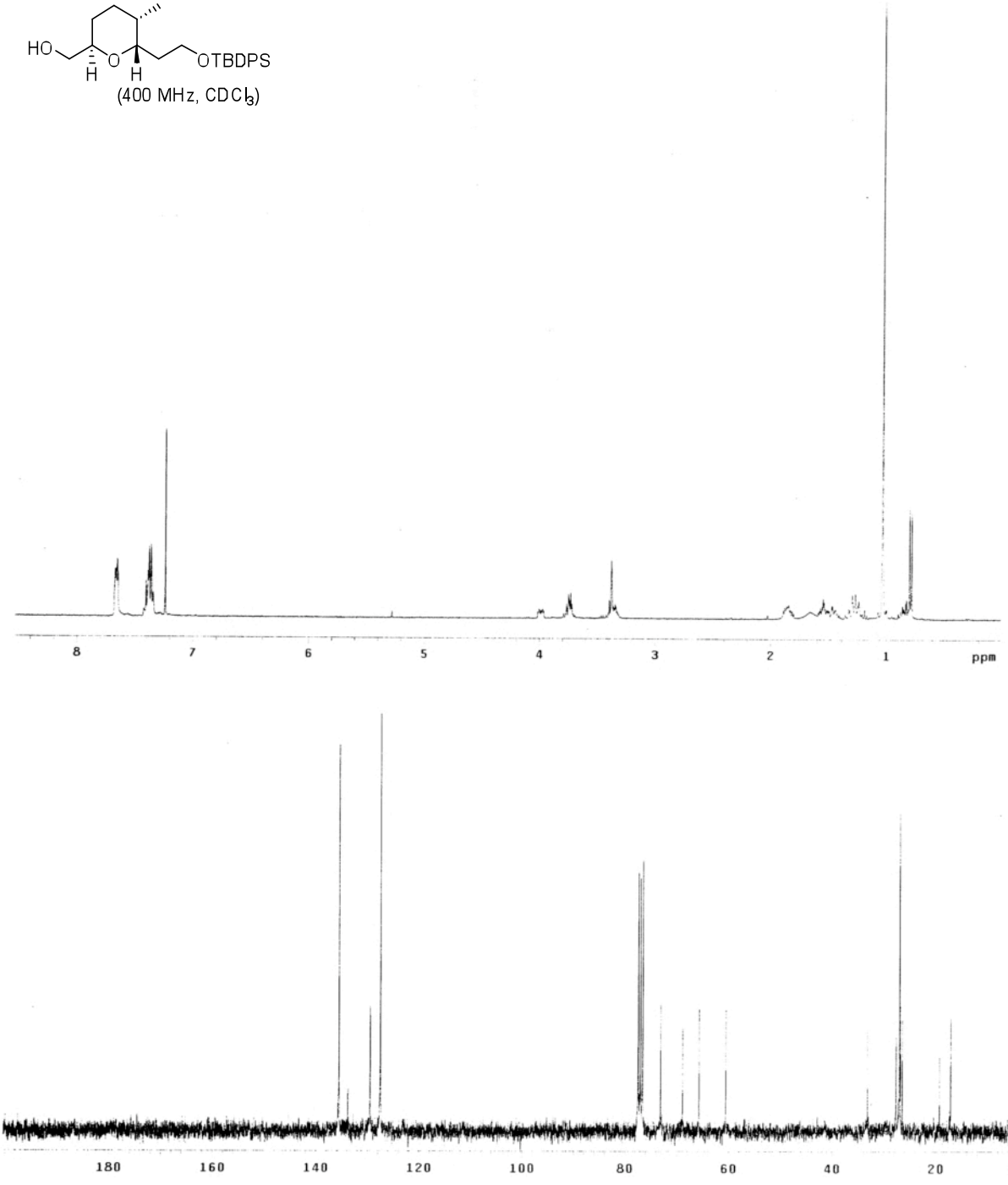
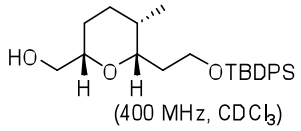
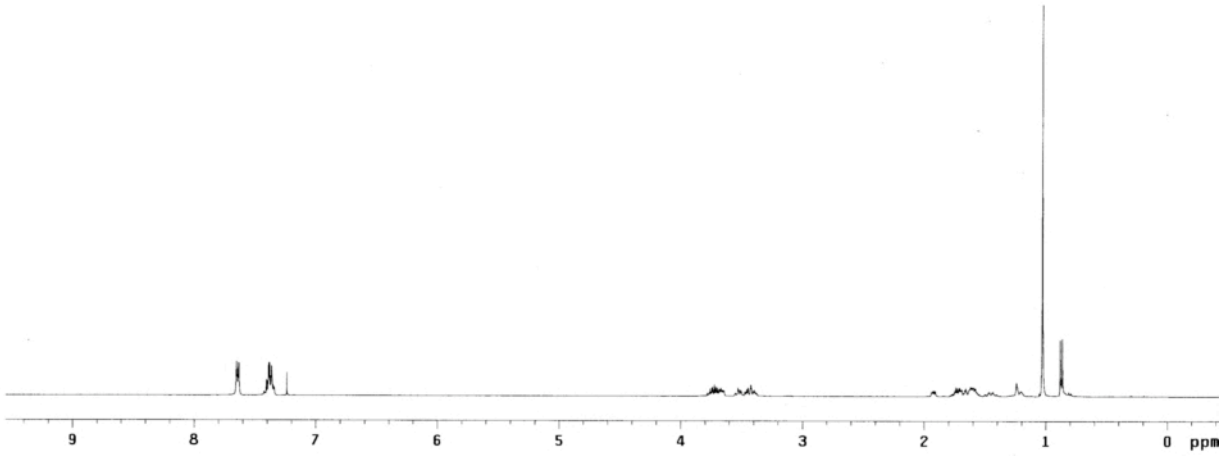
ppm

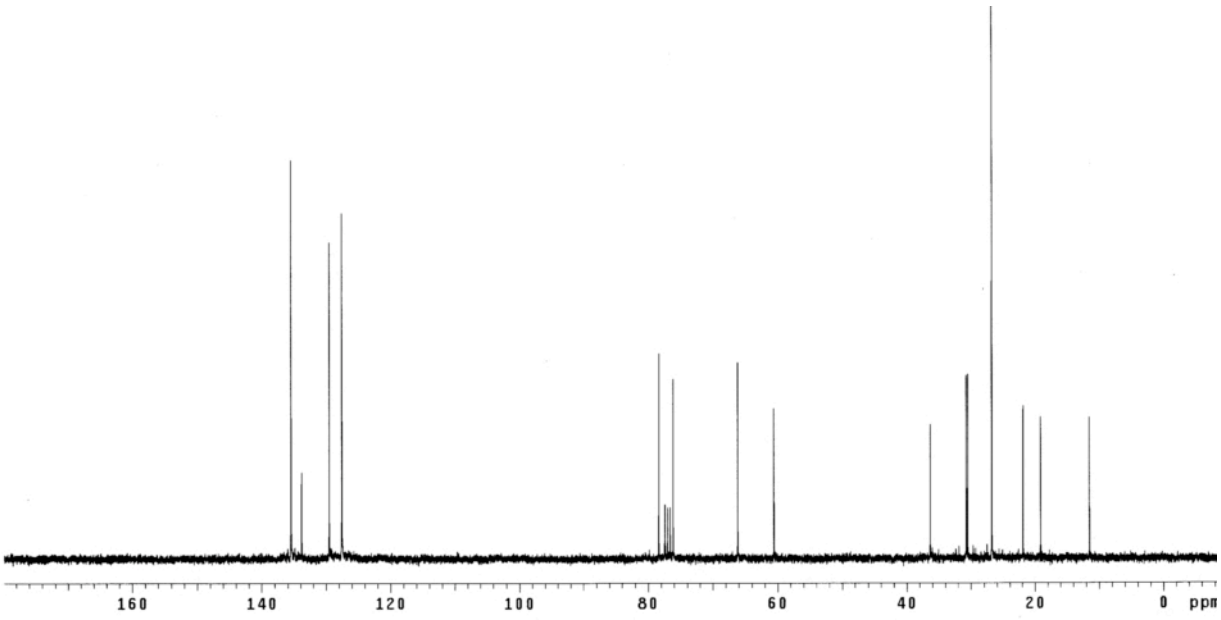
(400 MHz, $CDCl_3$)

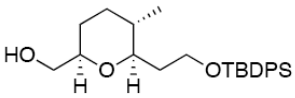


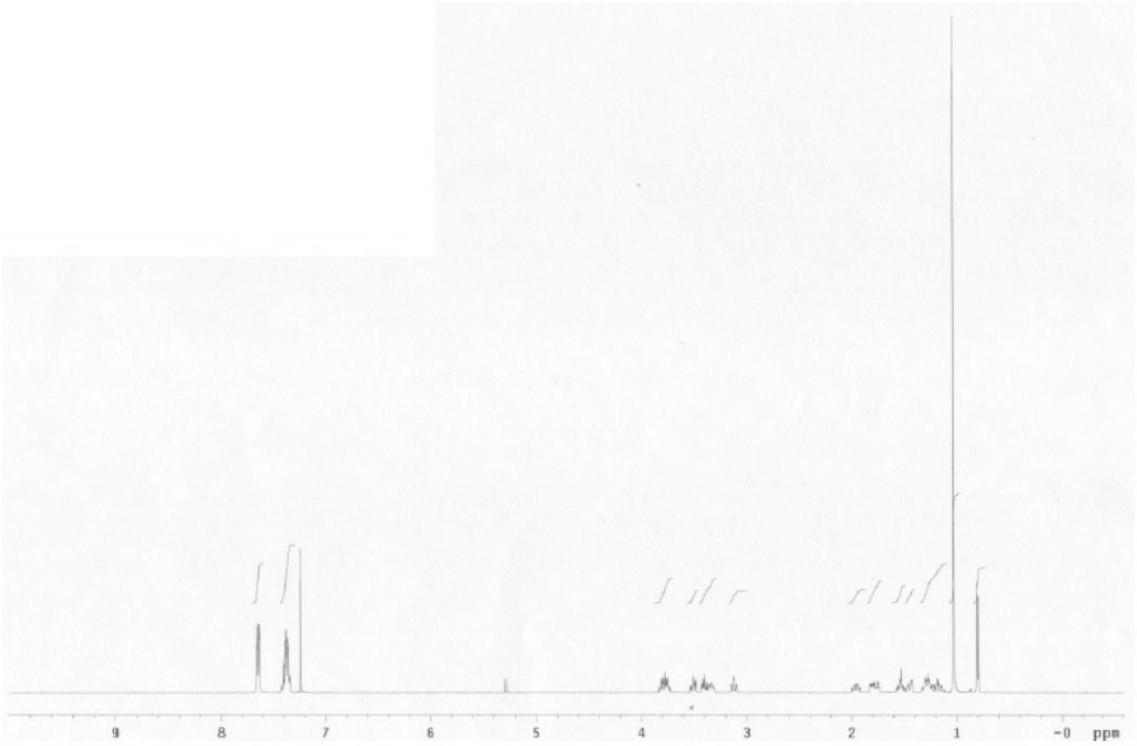


(400 MHz, $CDCl_3$)






HO
O
H
H
OTBDPS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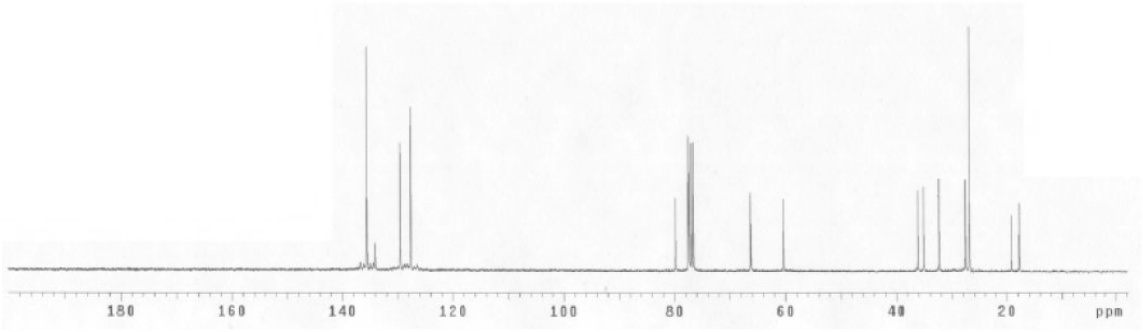
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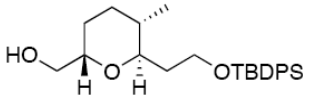
HO
O
H
H
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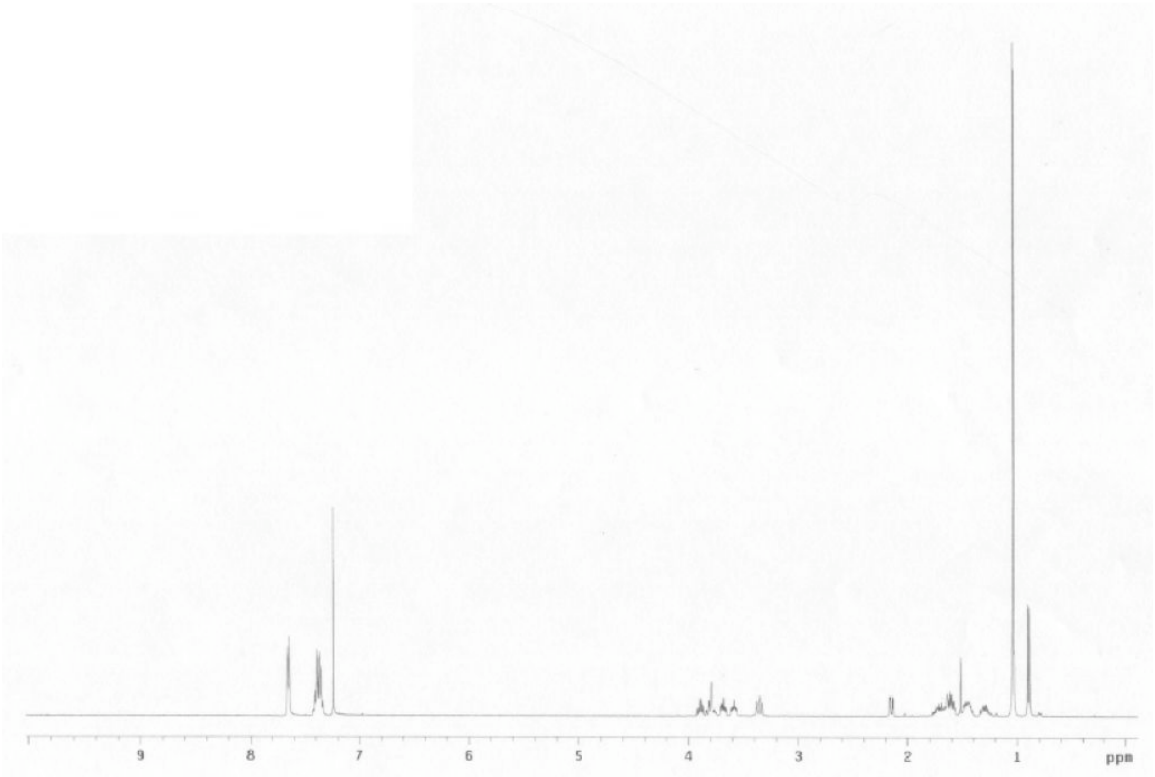
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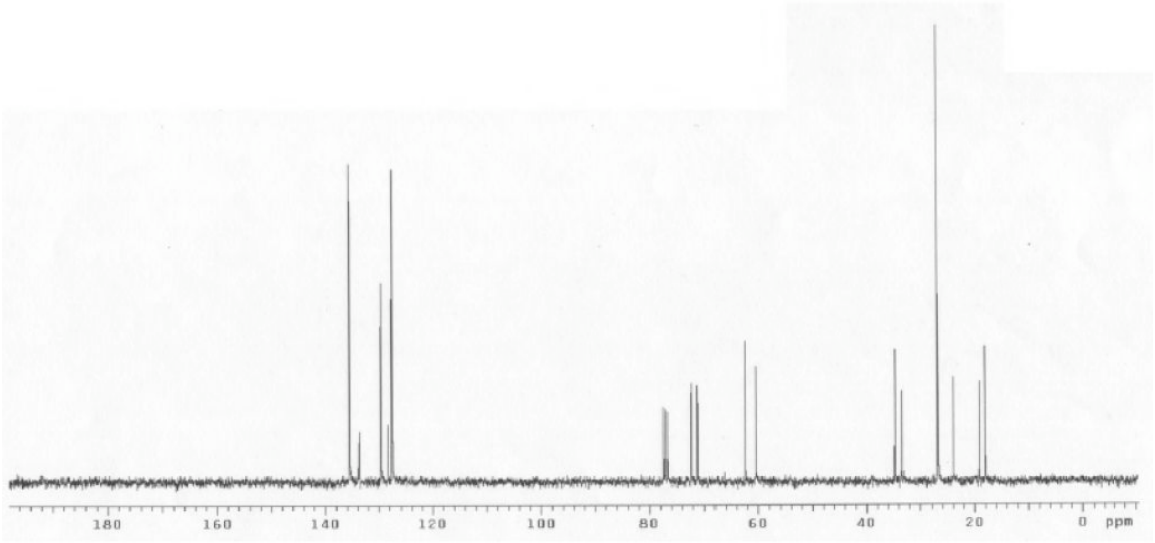
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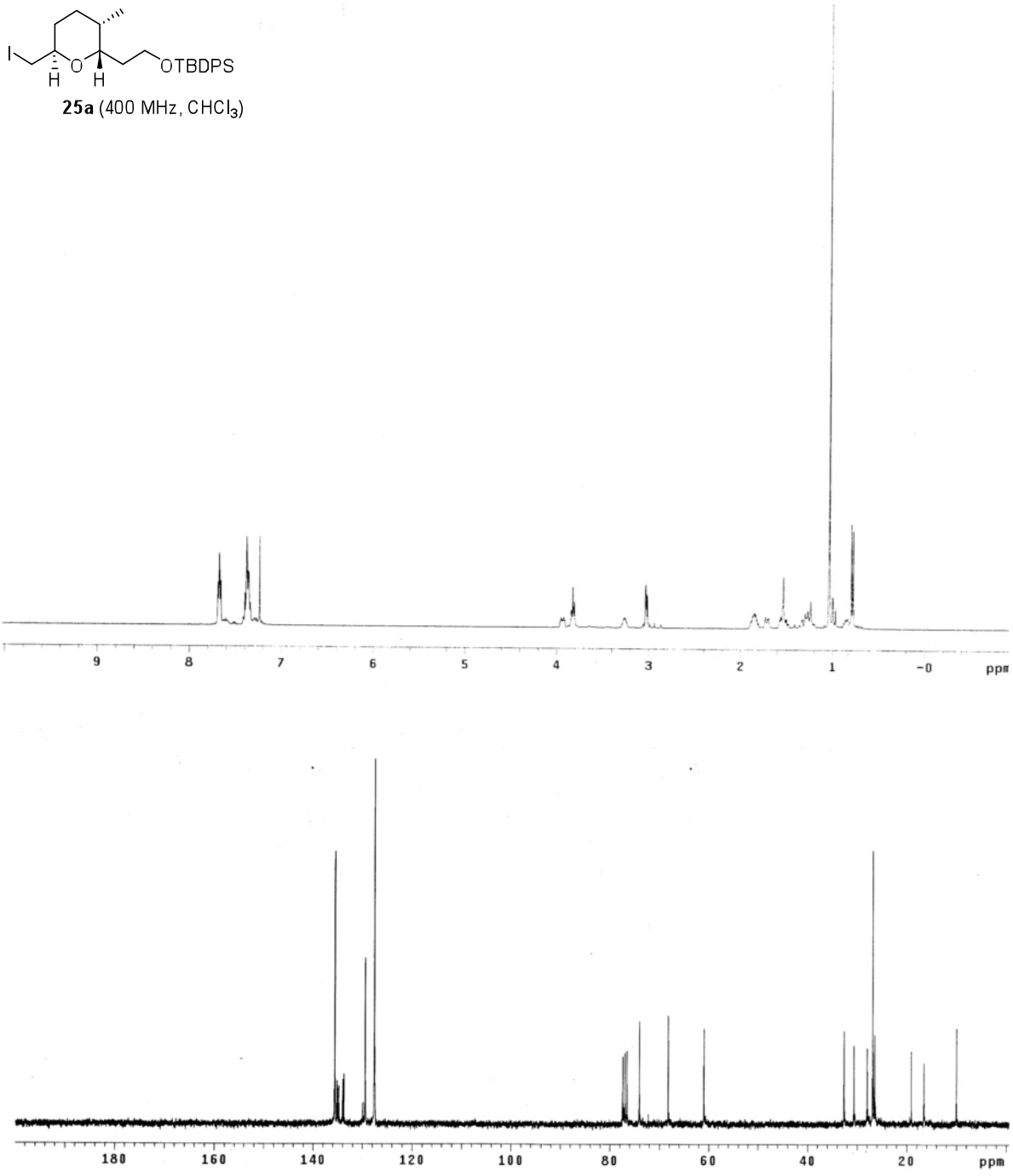
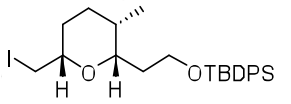


25a (400 MHz, $CHCl_3$)



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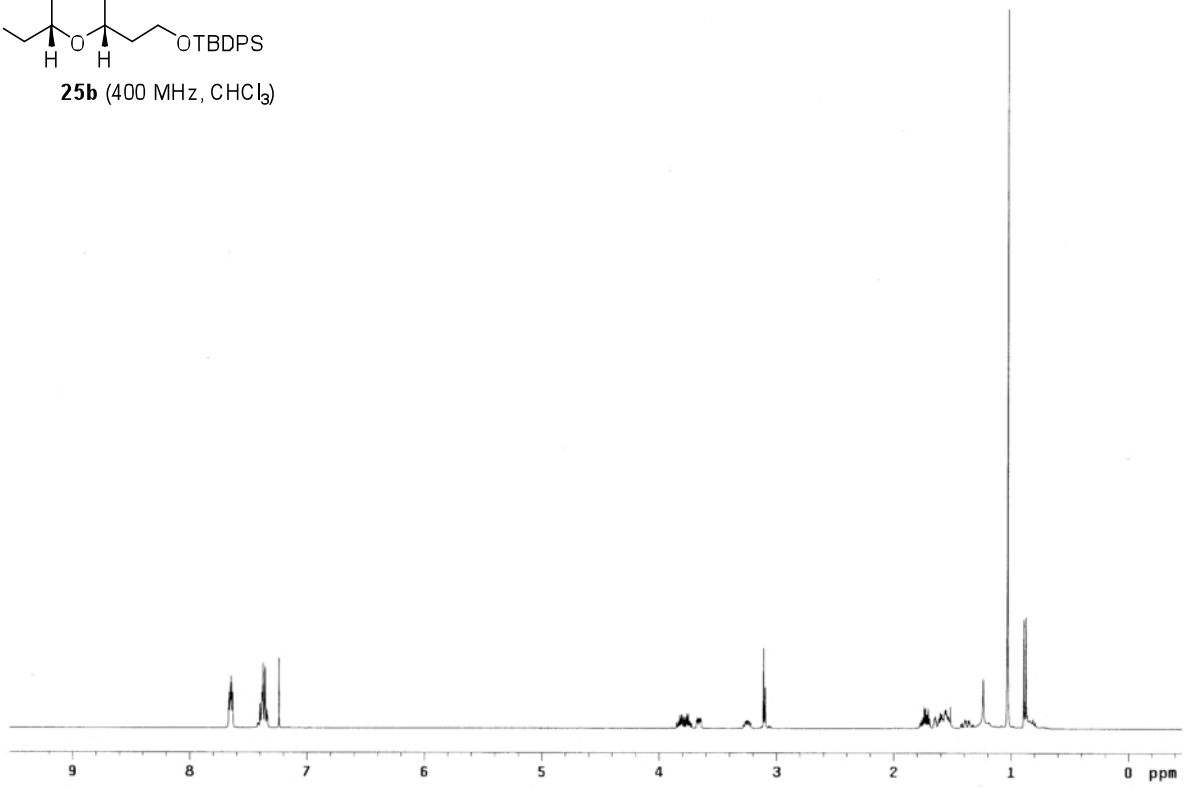
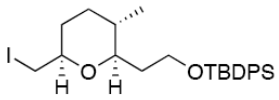
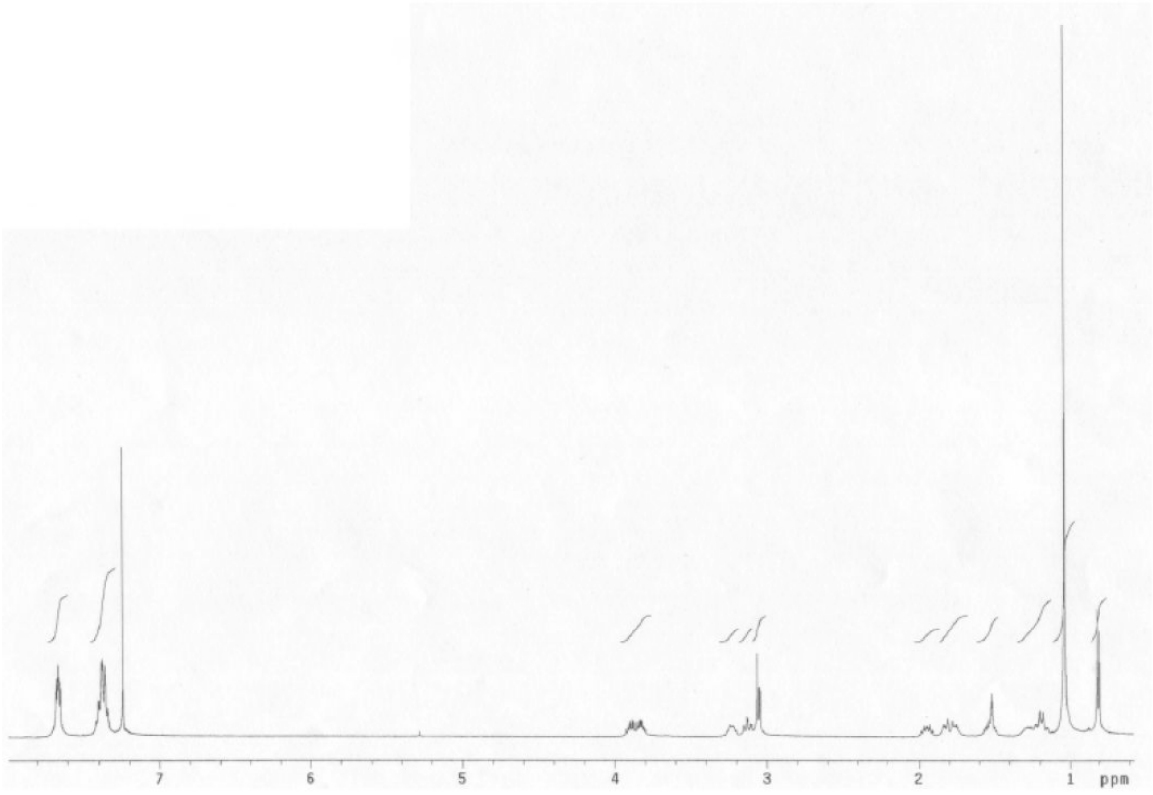
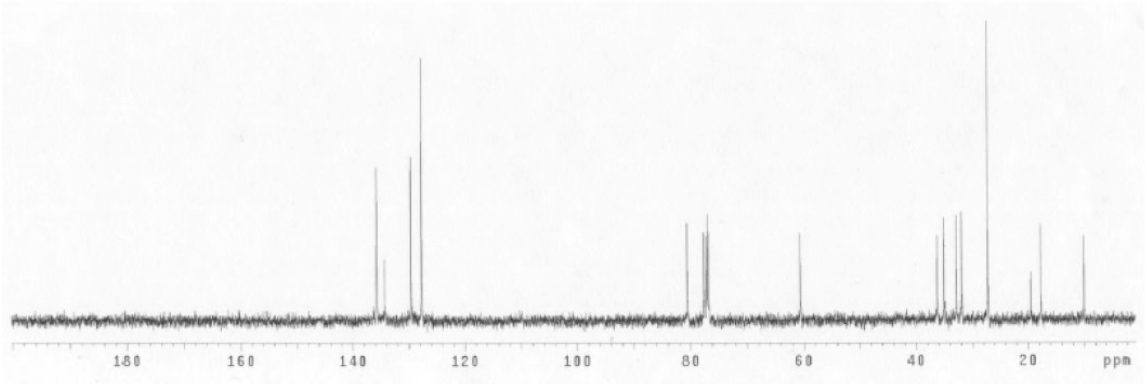
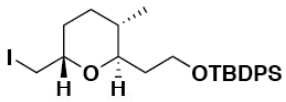




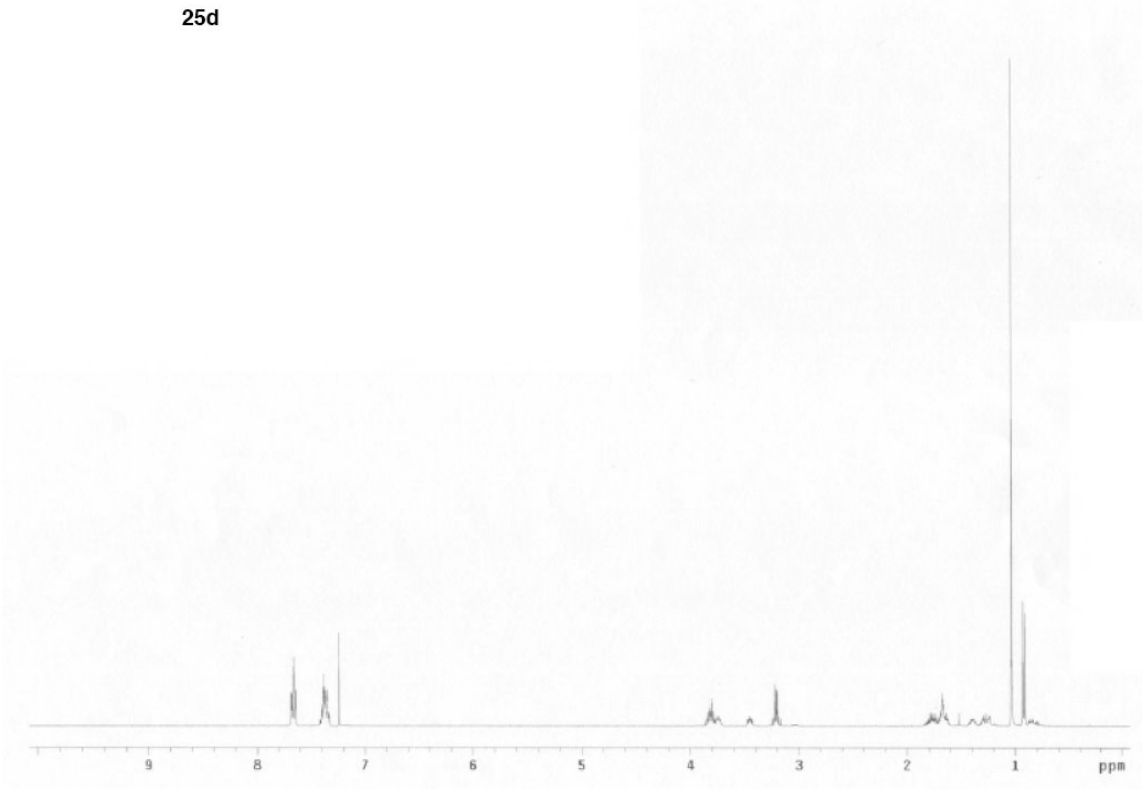
25c






I
O
H
H
OTBDPS

25d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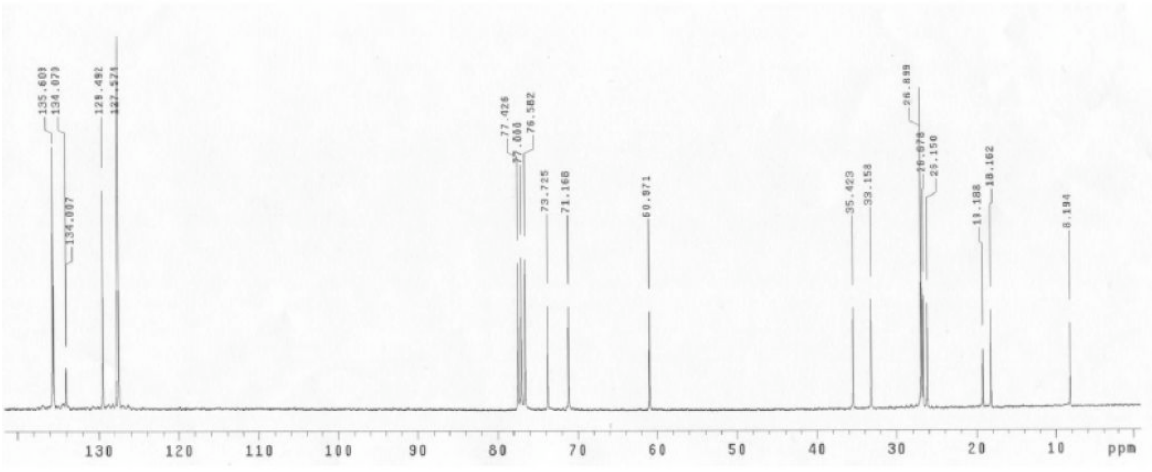
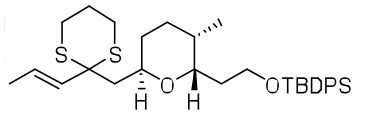
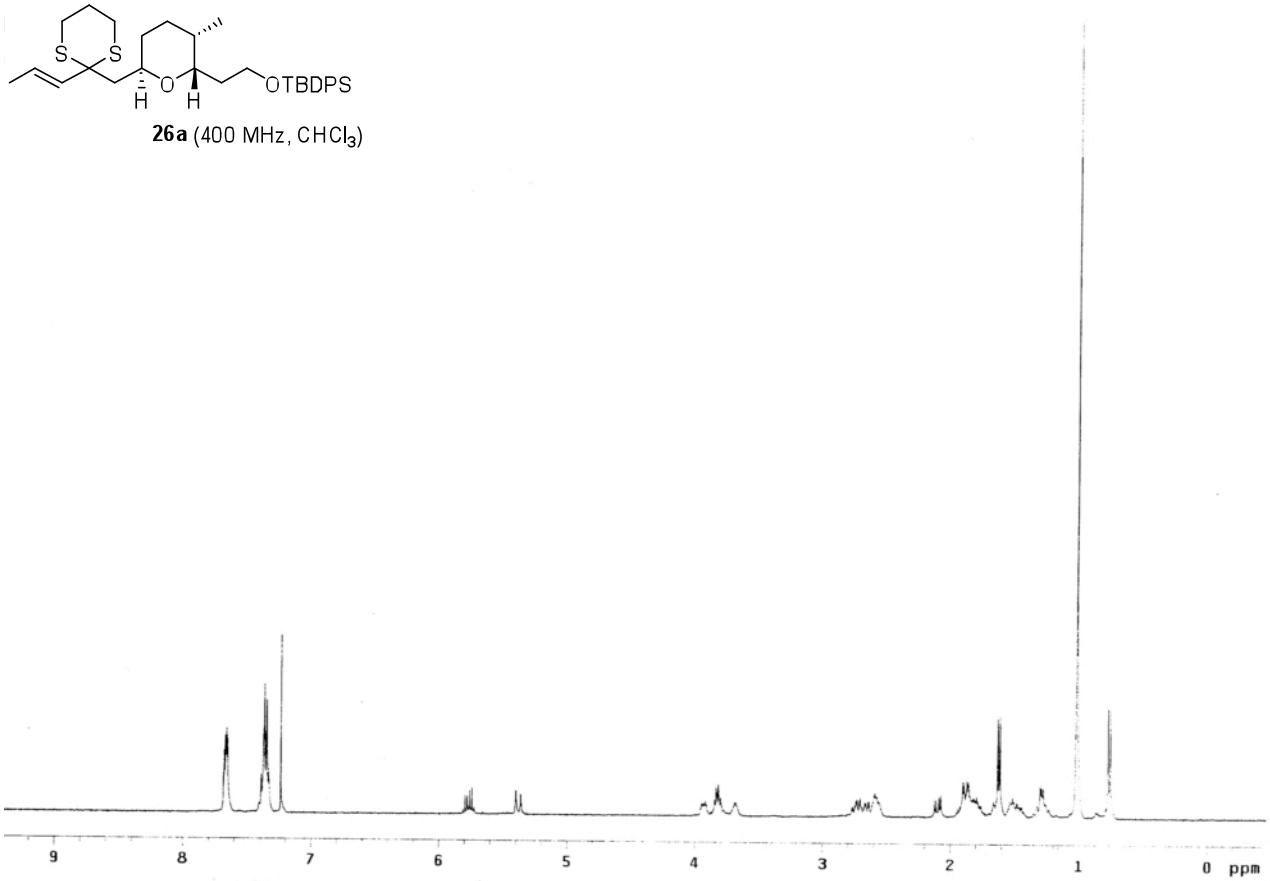
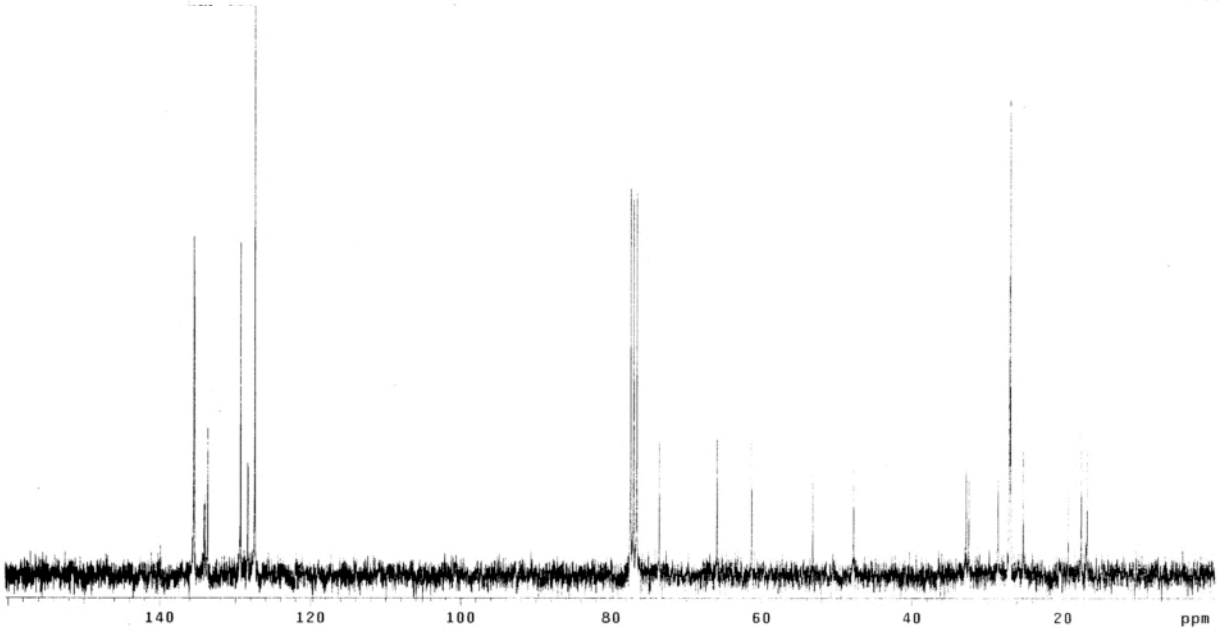

135.609
134.079
134.007
129.492
127.521
77.426
77.000
76.582
73.725
71.168
60.971
35.429
33.158
26.899
26.878
25.150
19.388
18.162
8.194
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

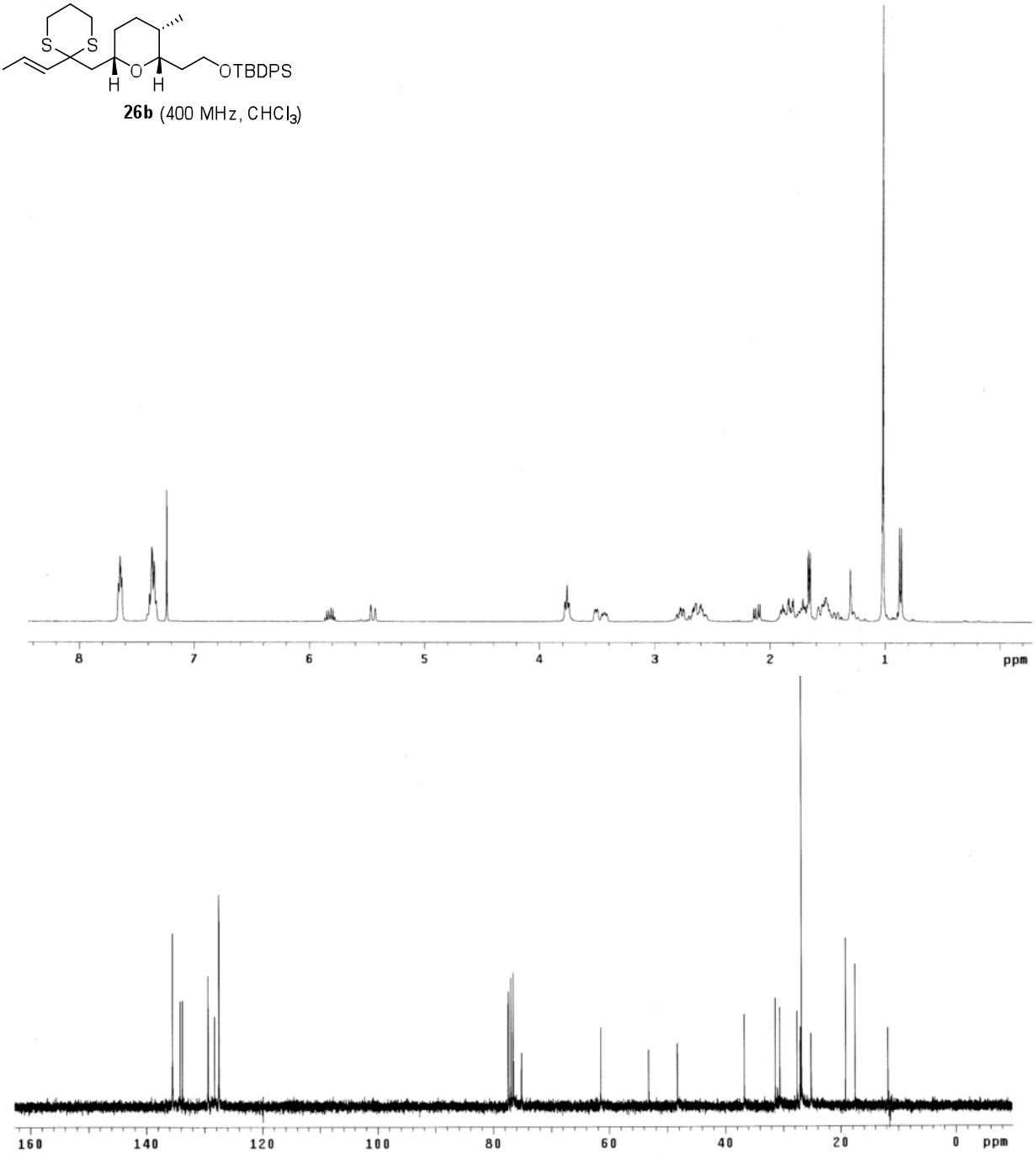


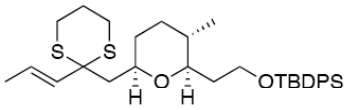
26a (400 MHz, $CHCl_3$)



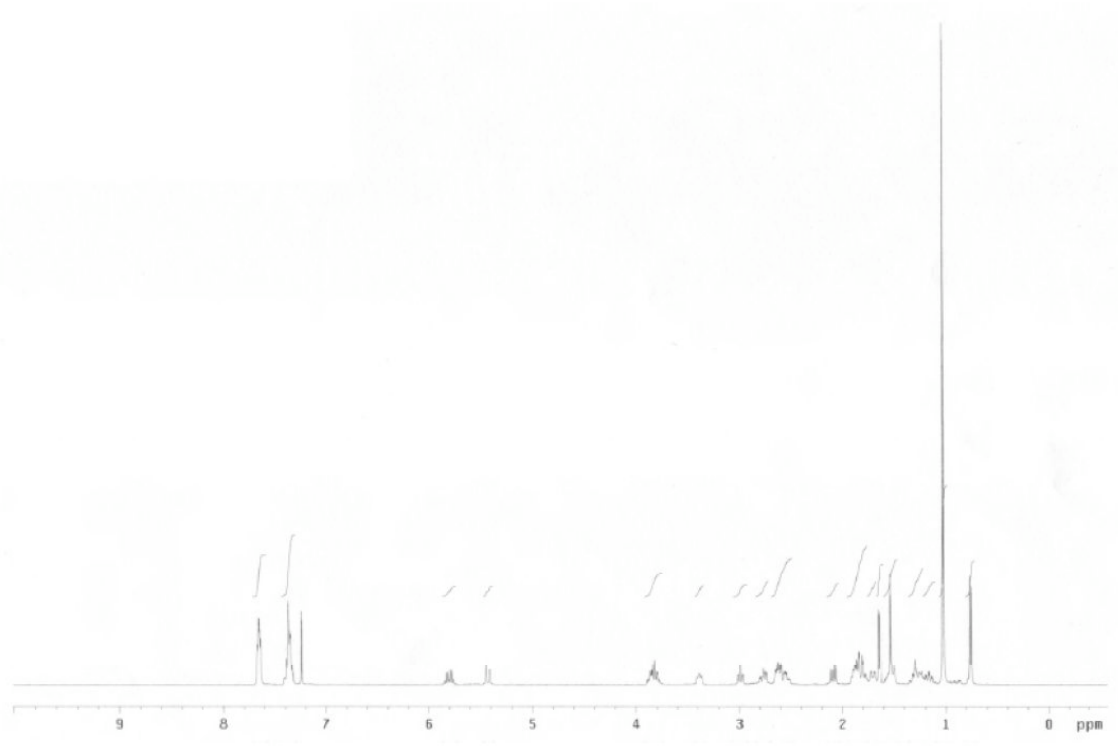


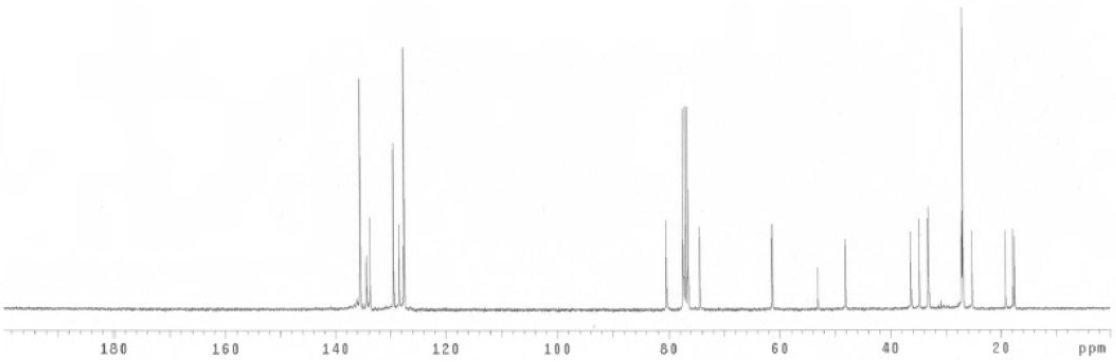
26b (400 MHz, $CHCl_3$)

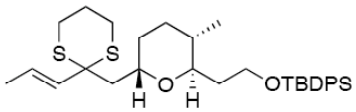



S
S
O
H
H
OTBDPS

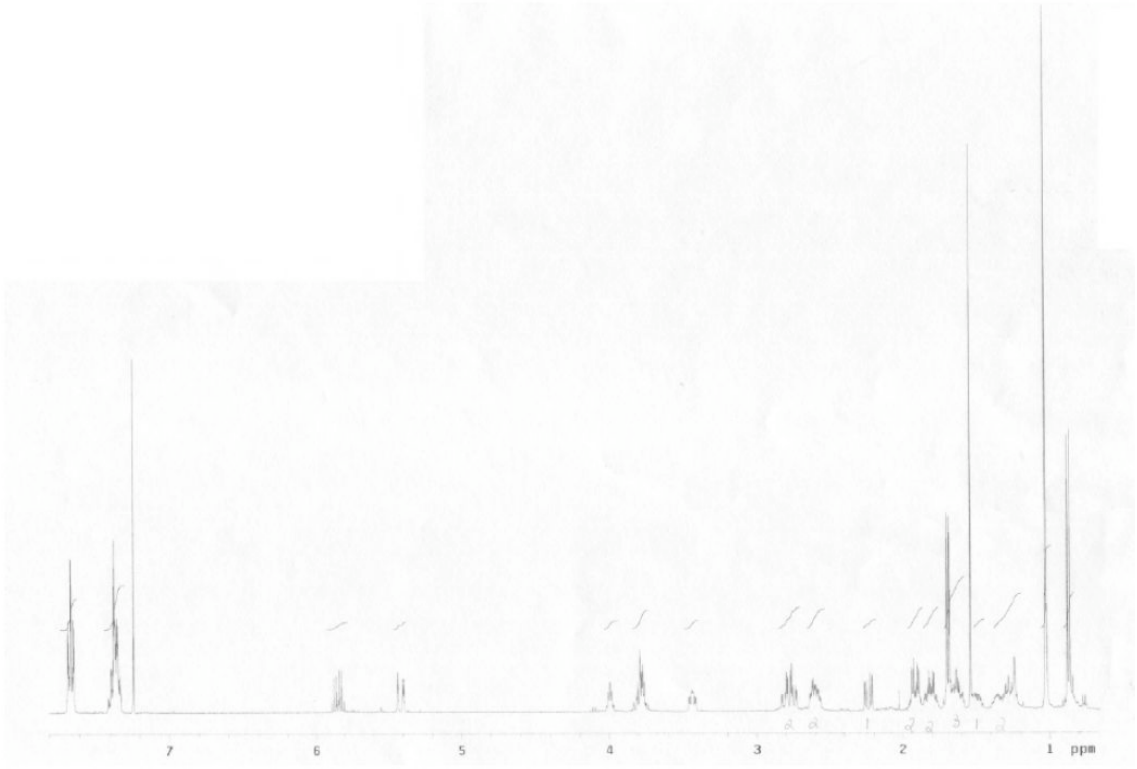
26c

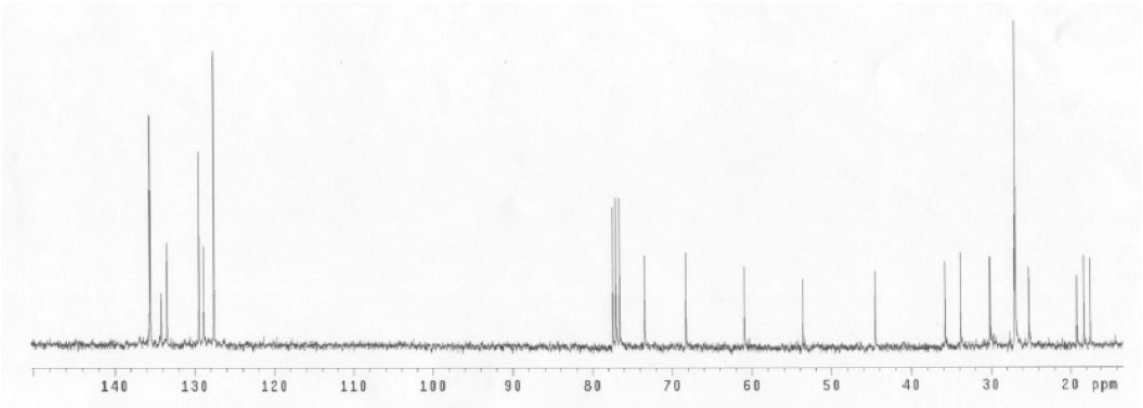

9
8
7
6
5
4
3
2
1
0
ppm

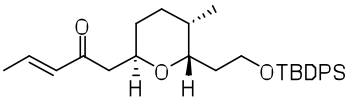

180
160
140
120
100
80
60
40
20
ppm


S
S
O
H
H
OTBDPS

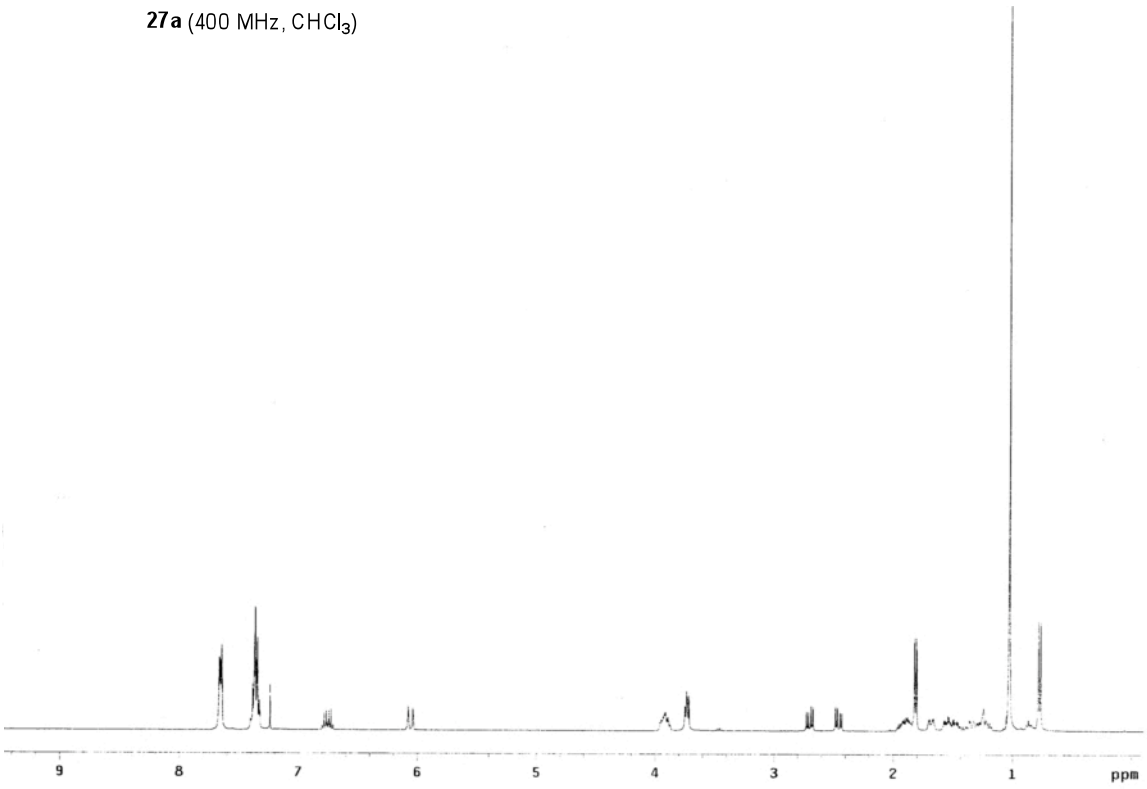
26d

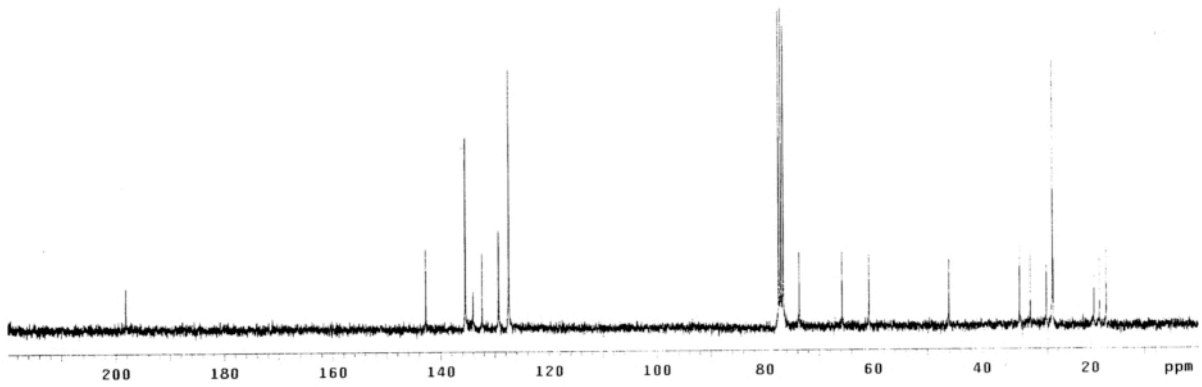

7
6
5
4
3
2
1 ppm

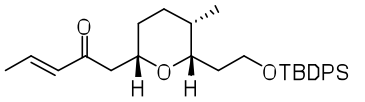

140
130
120
110
100
90
80
70
60
50
40
30
20 ppm



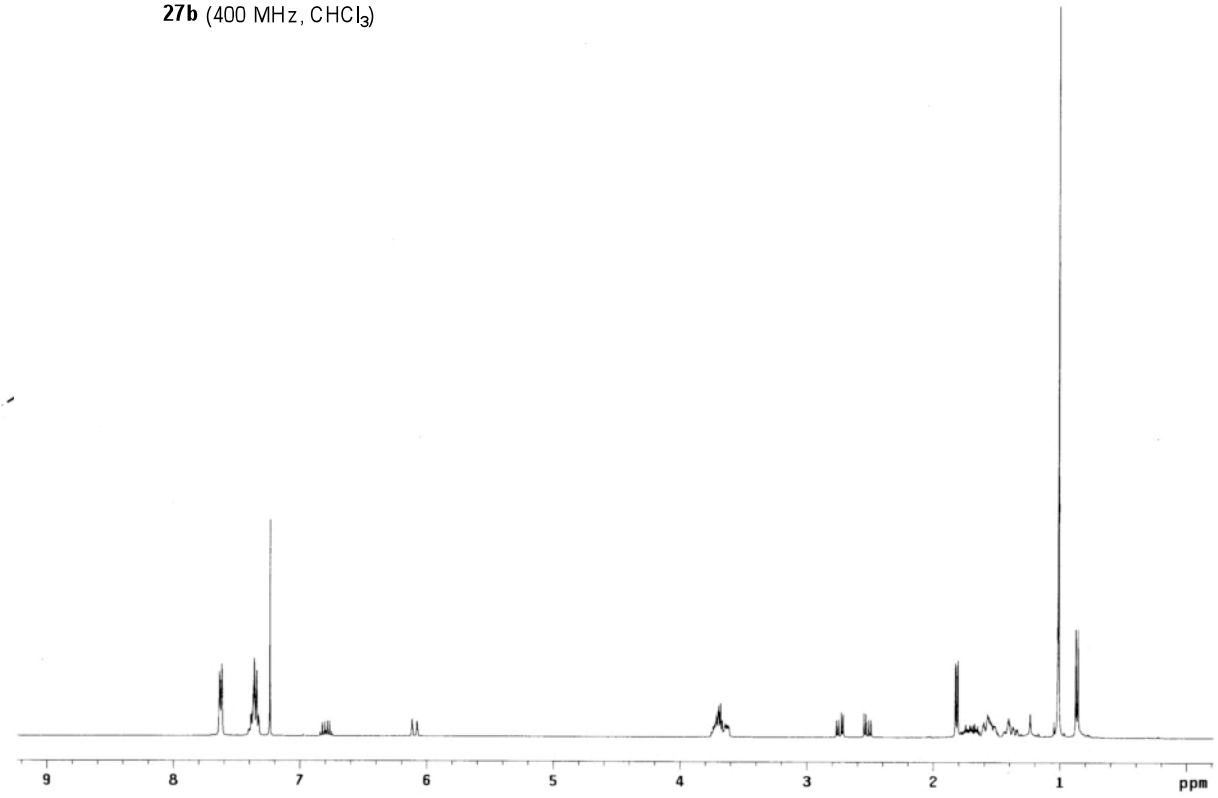
27a (400 MHz, $CHCl_3$)

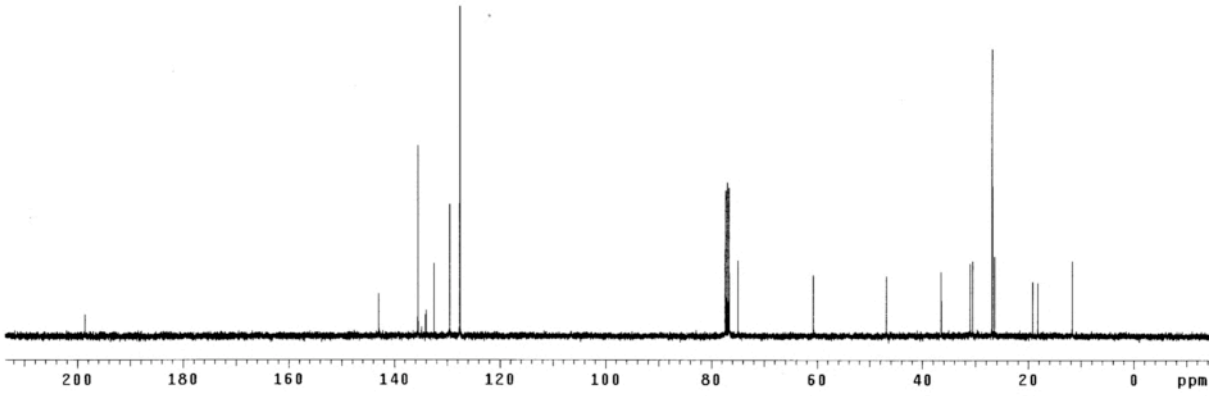


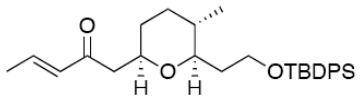




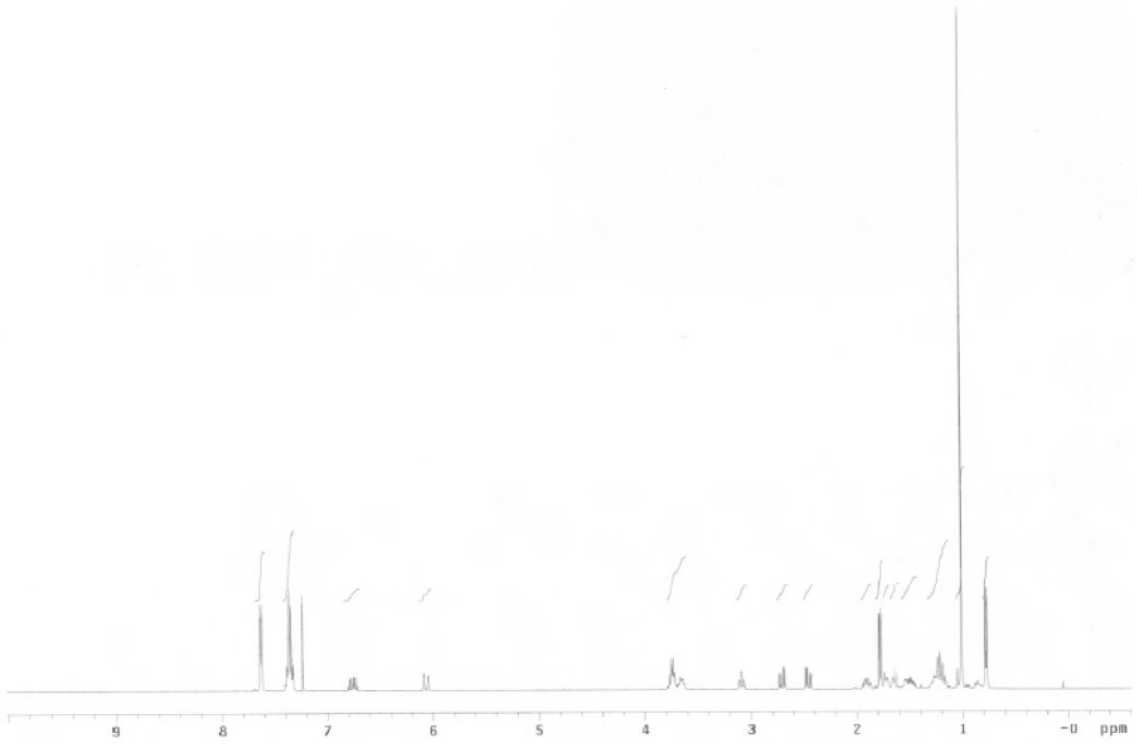
27b (400 MHz, $CHCl_3$)

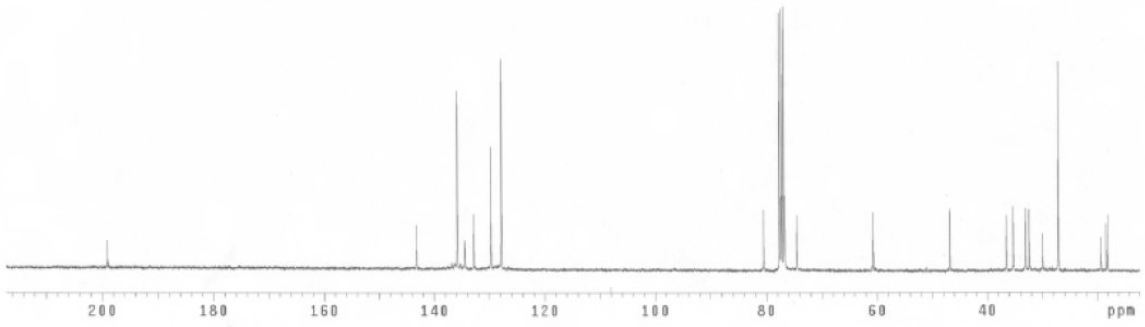


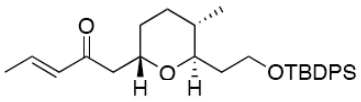



O
O
H
H
OTBDPS

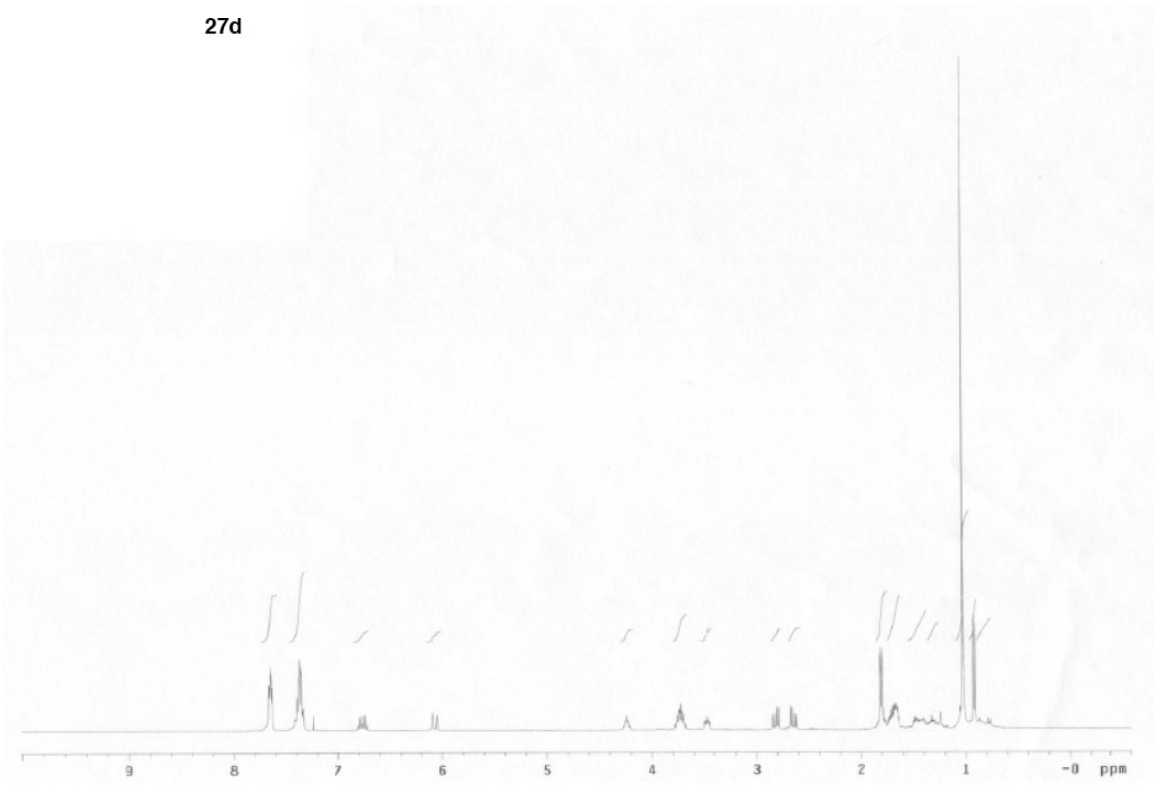
27c

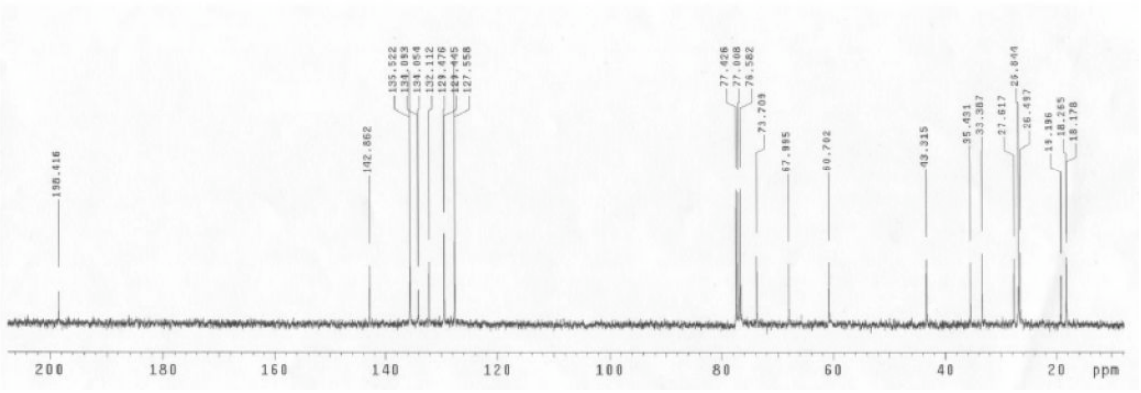

9
8
7
6
5
4
3
2
1
-0
ppm

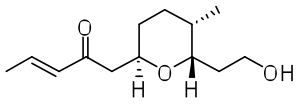

200
180
160
140
120
100
80
60
40
ppm


O
O
H
H
OTBDPS

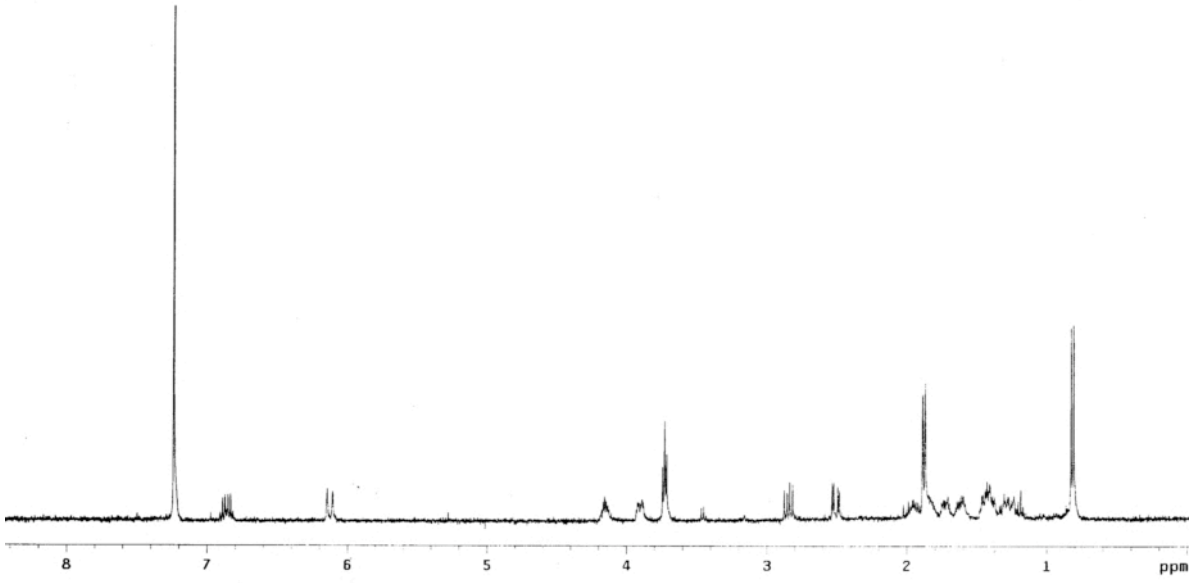
27d

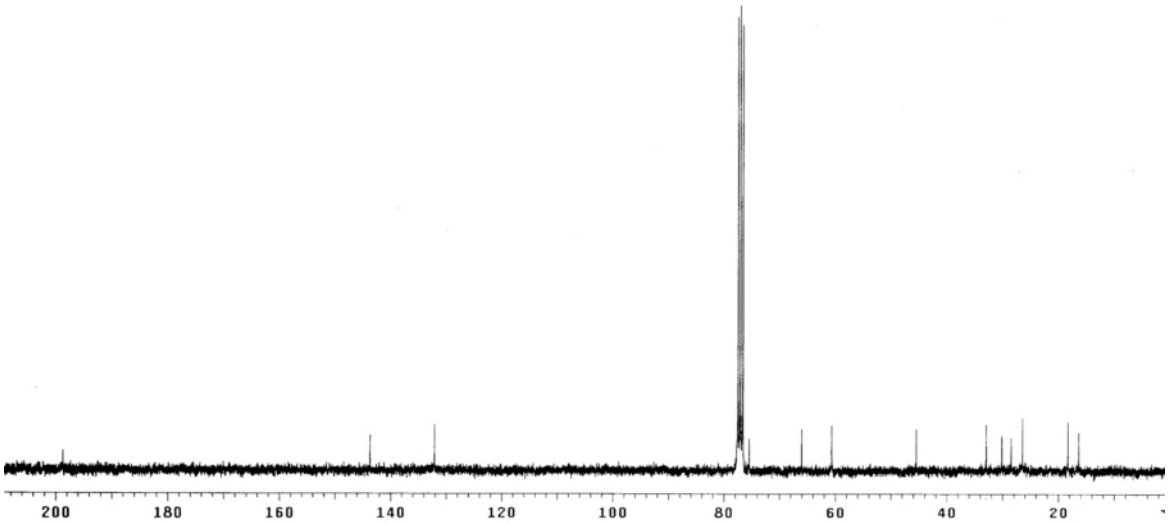

9
8
7
6
5
4
3
2
1
-0
ppm

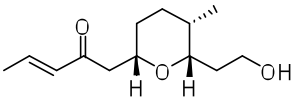

198.416
142.862
135.522
135.053
134.054
132.132
129.476
129.445
127.588
77.426
77.008
76.582
73.709
67.985
60.702
43.315
35.451
33.387
27.817
26.497
25.844
19.196
18.265
18.178
200
180
160
140
120
100
80
60
40
20
ppm



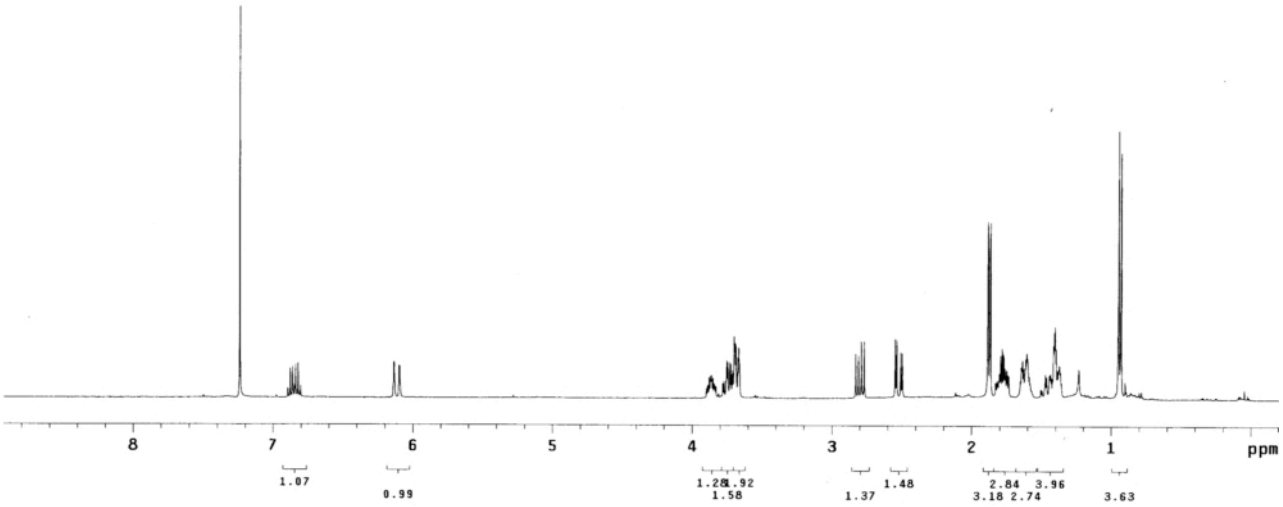
(400 MHz, $CHCl_3$)

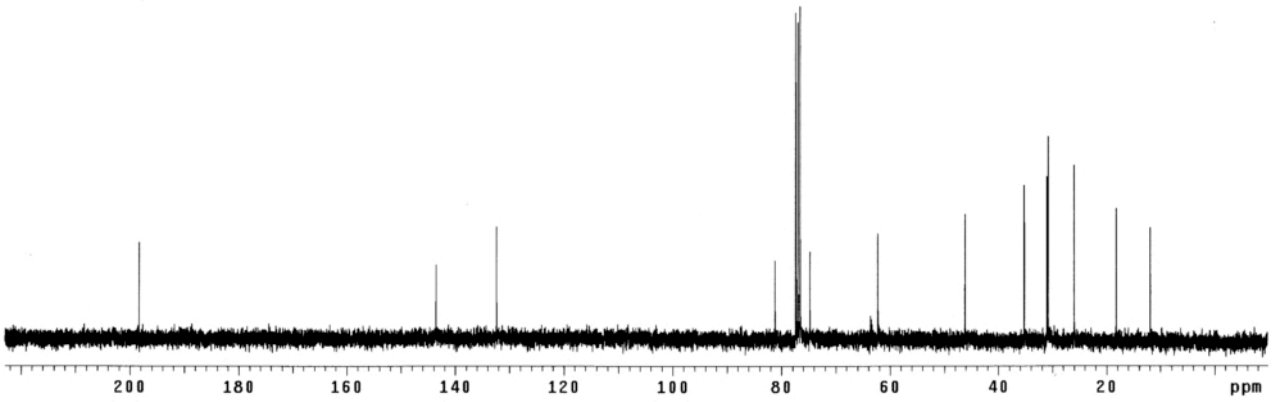


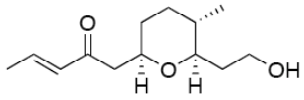


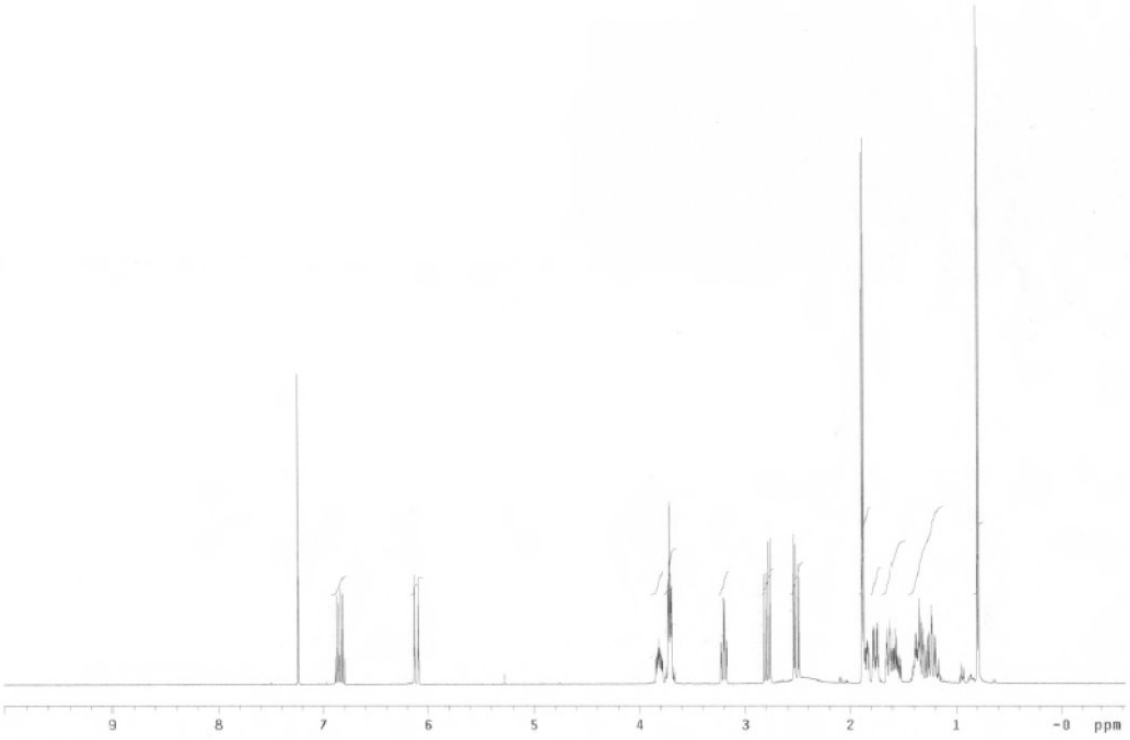


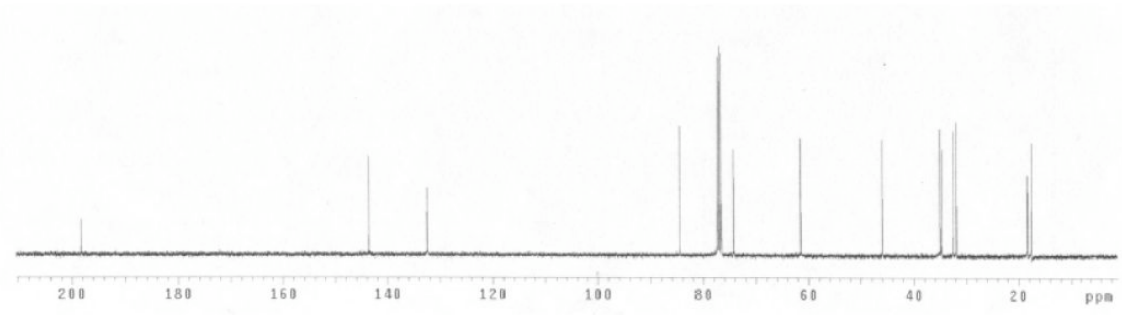
(400 MHz, $CHCl_3$)

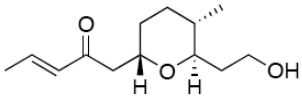


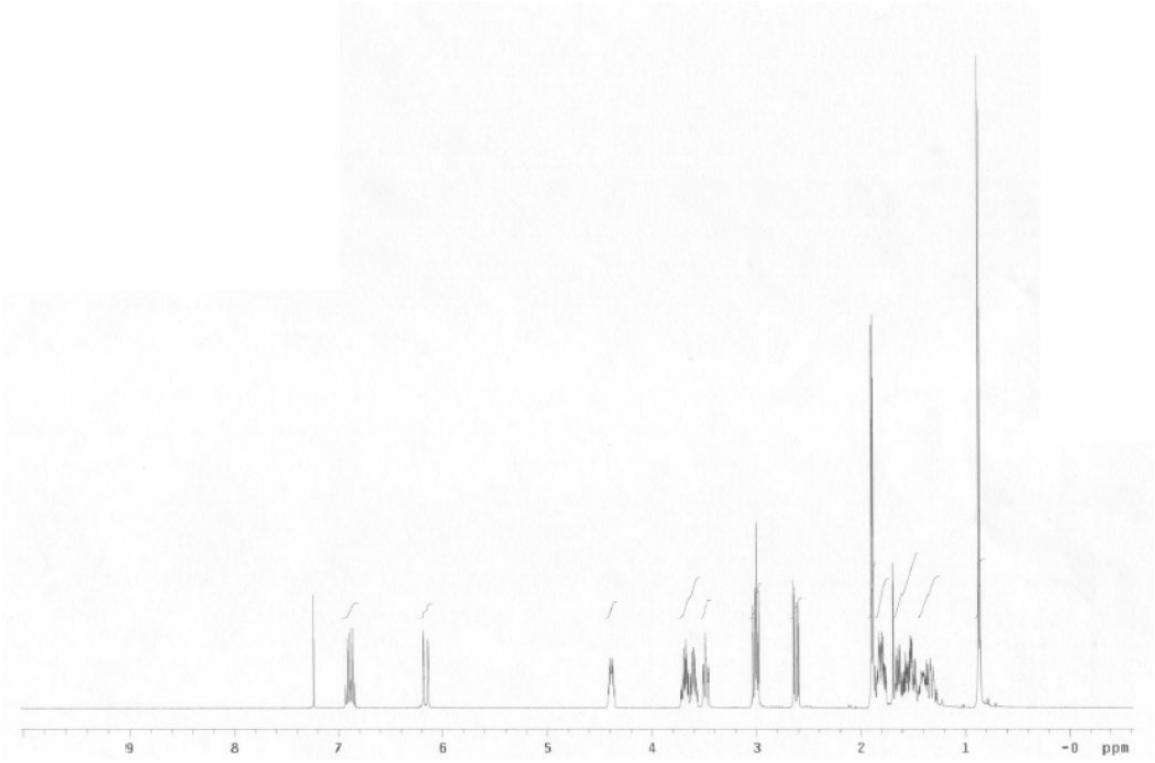


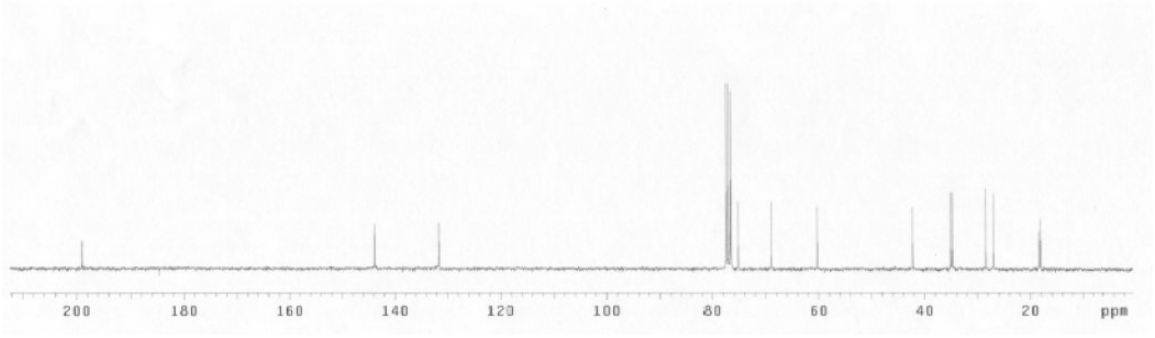

O
H
O
H
OH

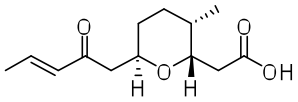

9
8
7
6
5
4
3
2
1
-0
ppm


200
180
160
140
120
100
80
60
40
20
ppm

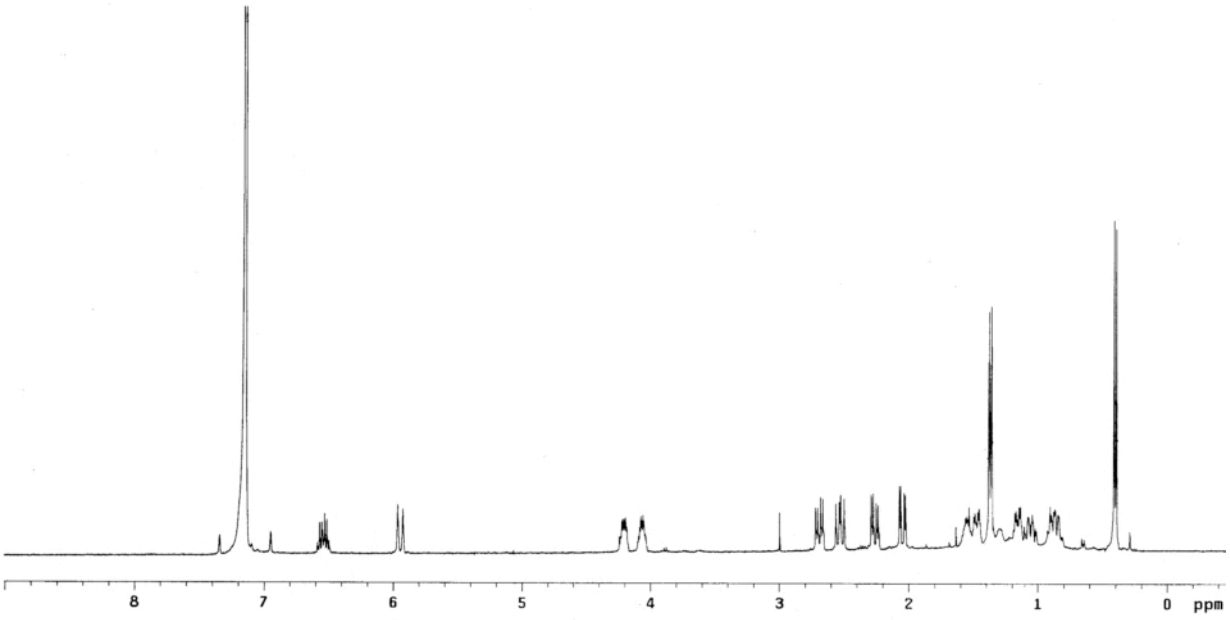

O
O
H
H
OH

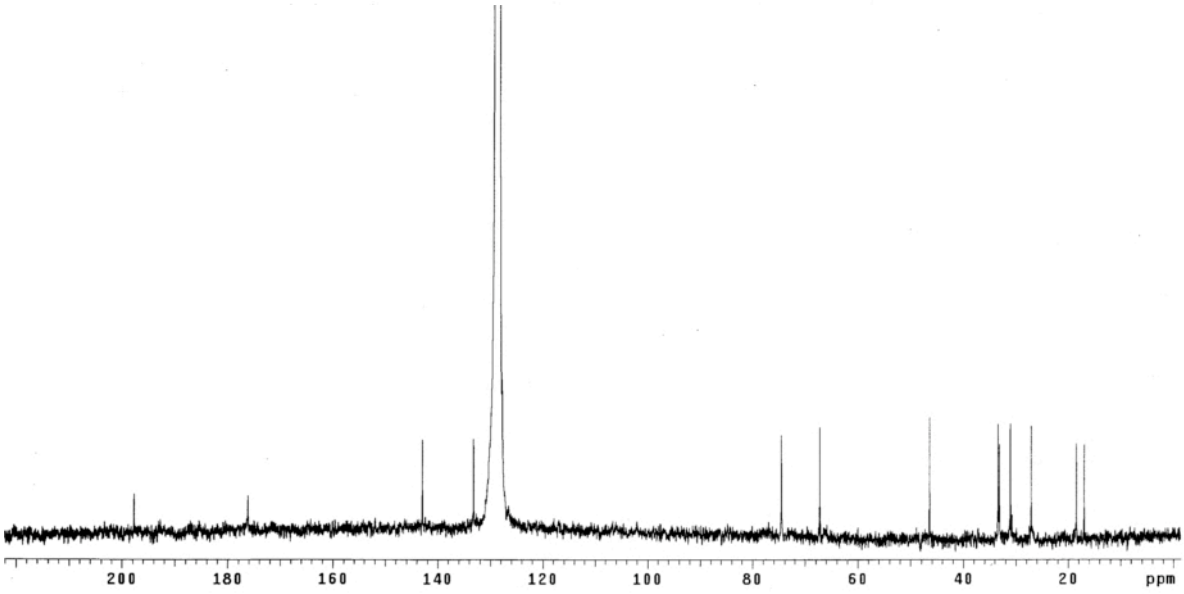

9
8
7
6
5
4
3
2
1
-0
ppm

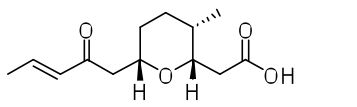

200
180
160
140
120
100
80
60
40
20
ppm



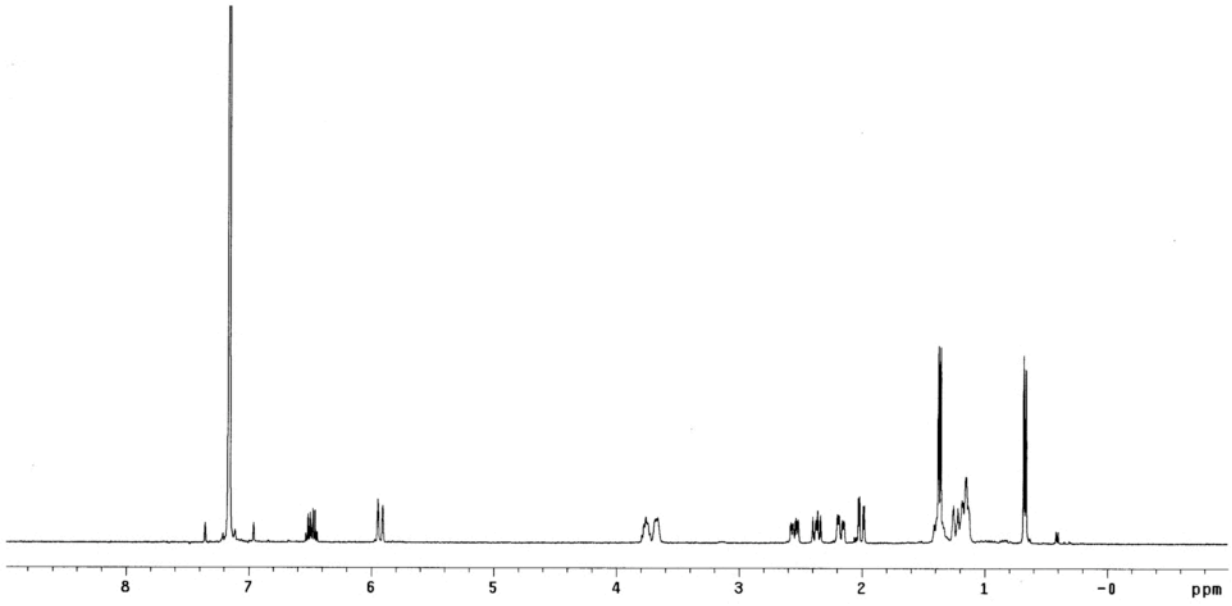
6a (400 MHz, C_6D_6)

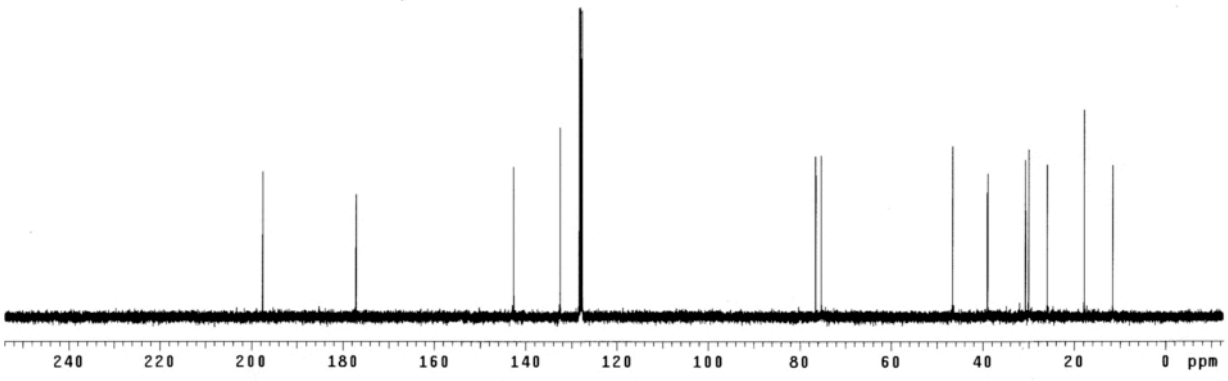


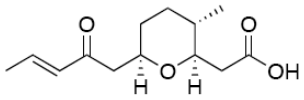




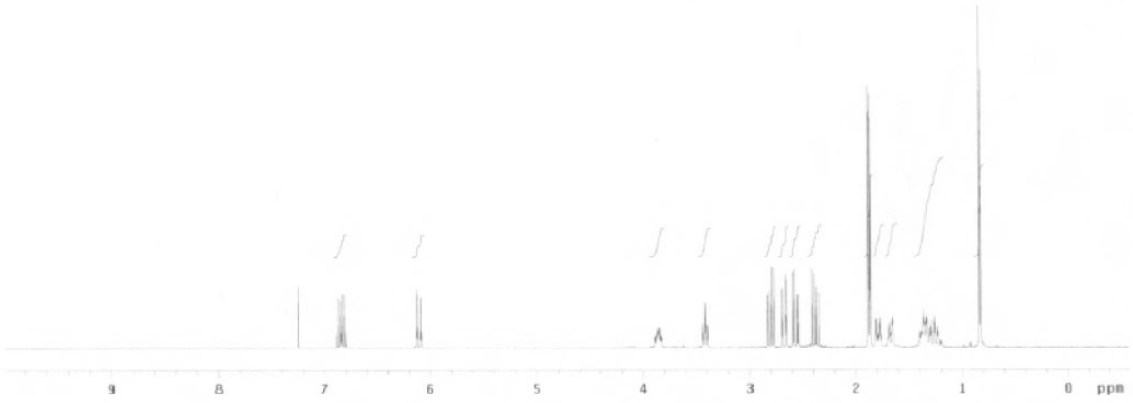
6b (400 MHz, C_6D_6)

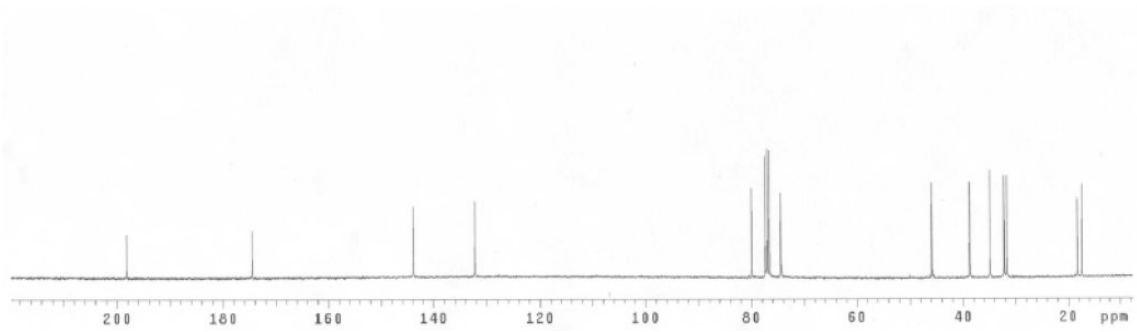


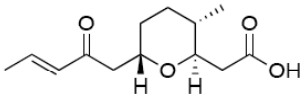




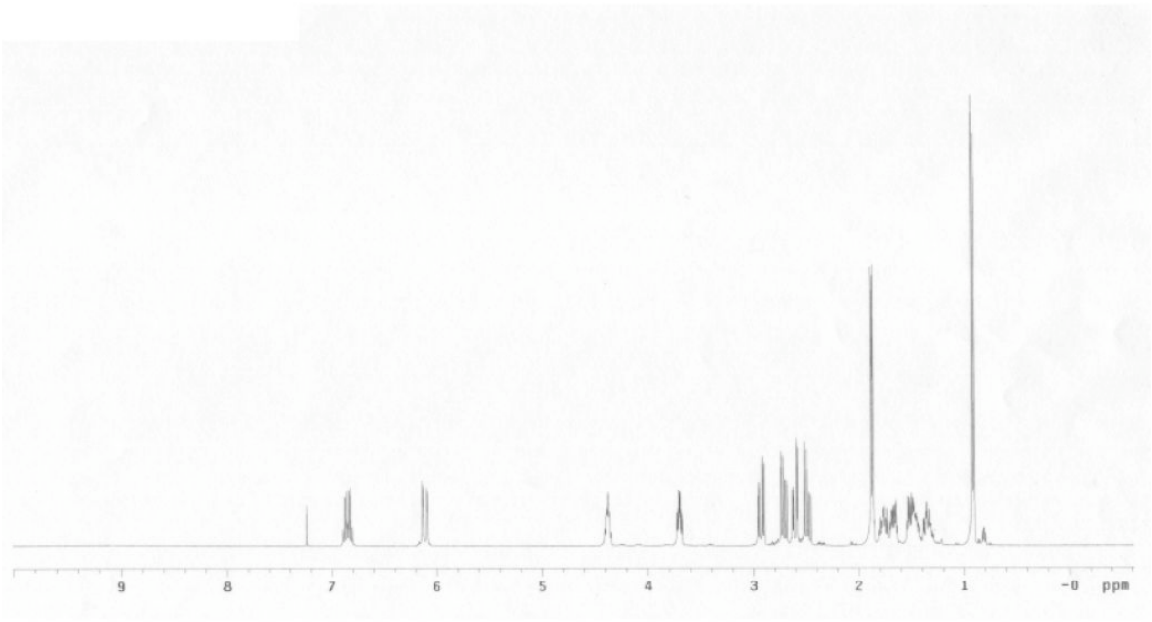
6c

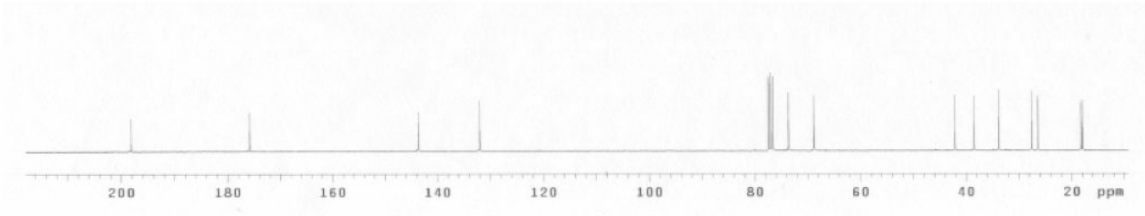


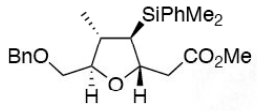




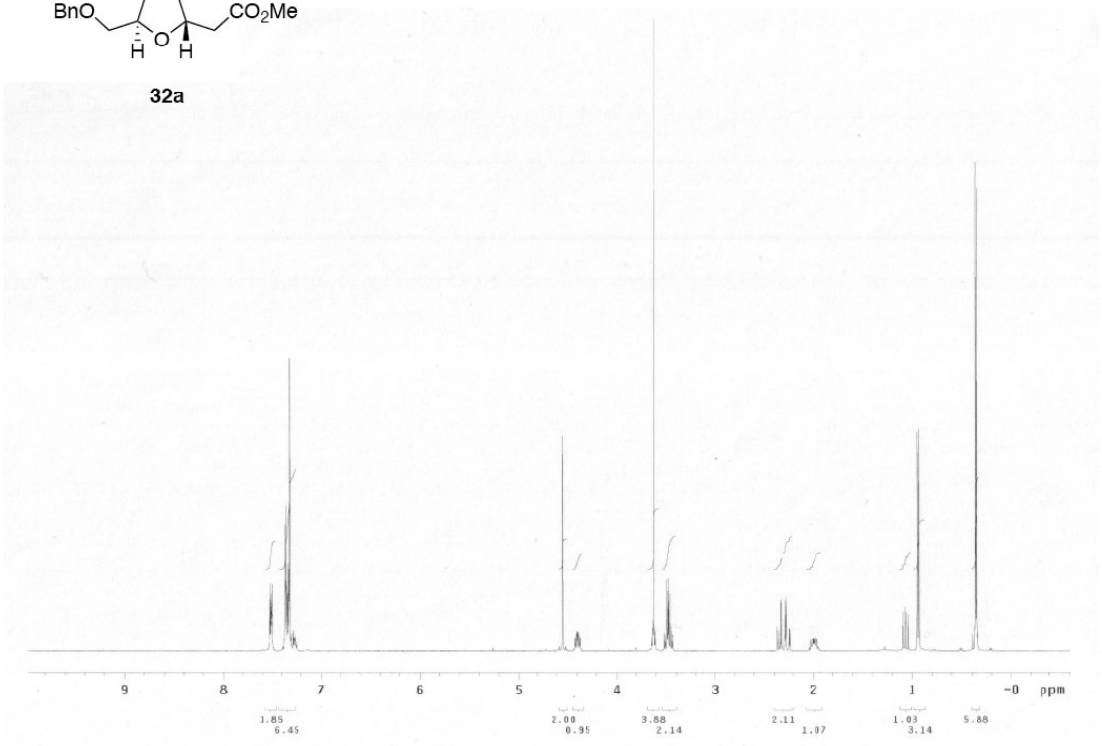
6d






SiPhMe2
BnO
CO2Me
O
H
H

32a


9
8
7
6
5
4
3
2
1
-0
ppm
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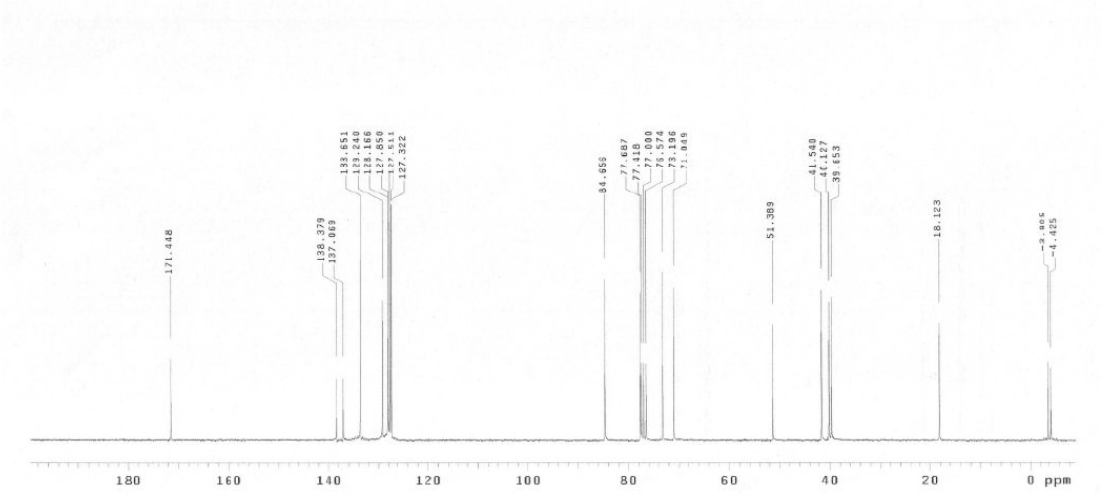
2.00
0.95
3.88
2.14
2.11
1.07
1.03
3.14
5.88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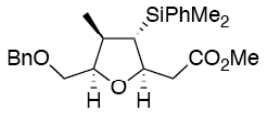
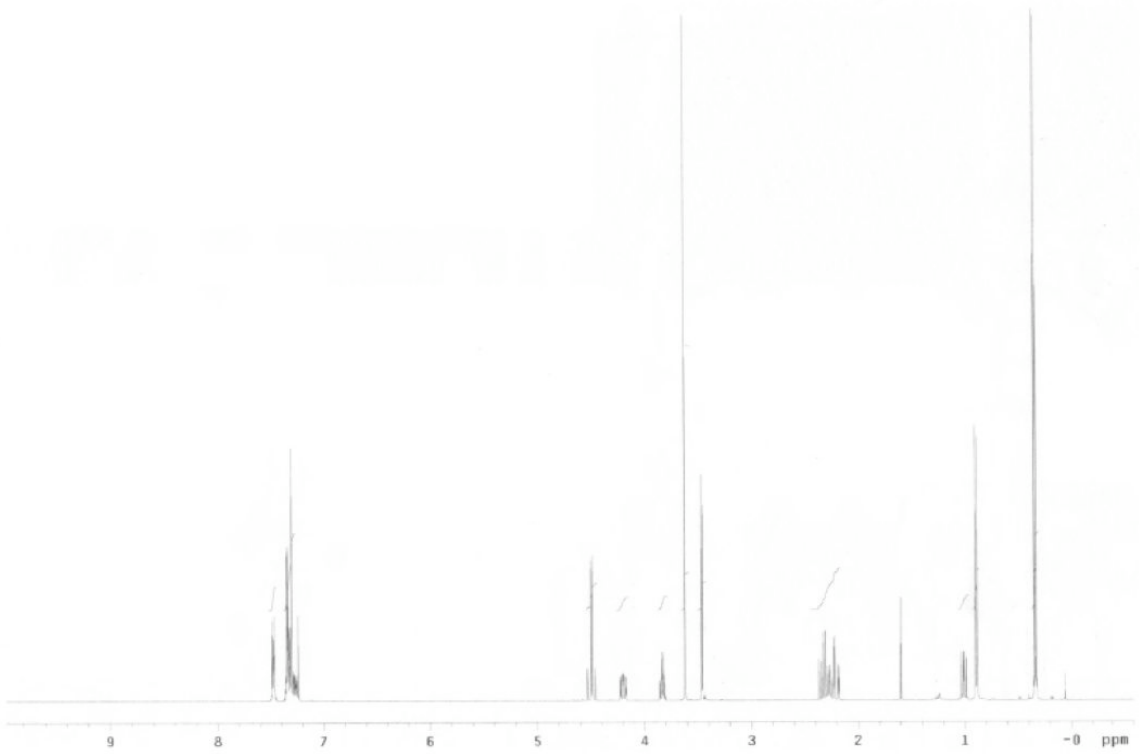
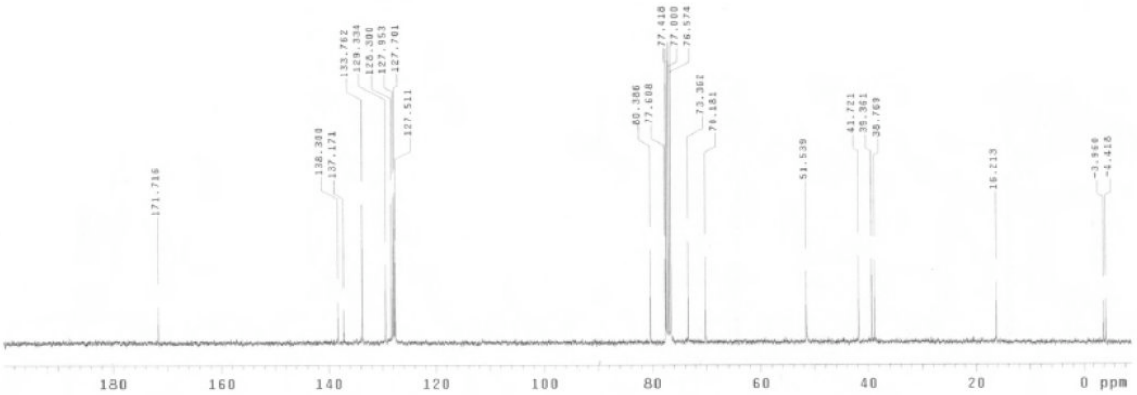
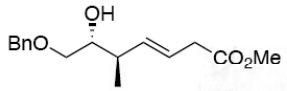
133.651
129.240
128.166
127.850
127.511
127.322
84.656
77.687
77.418
77.000
76.574
73.196
71.049
51.389
41.540
40.127
39.653
18.123
-2.005
-4.425
180
160
140
120
100
80
60
40
20
0
ppm


SiPhMe2
BnO
CO2Me
O
H
H

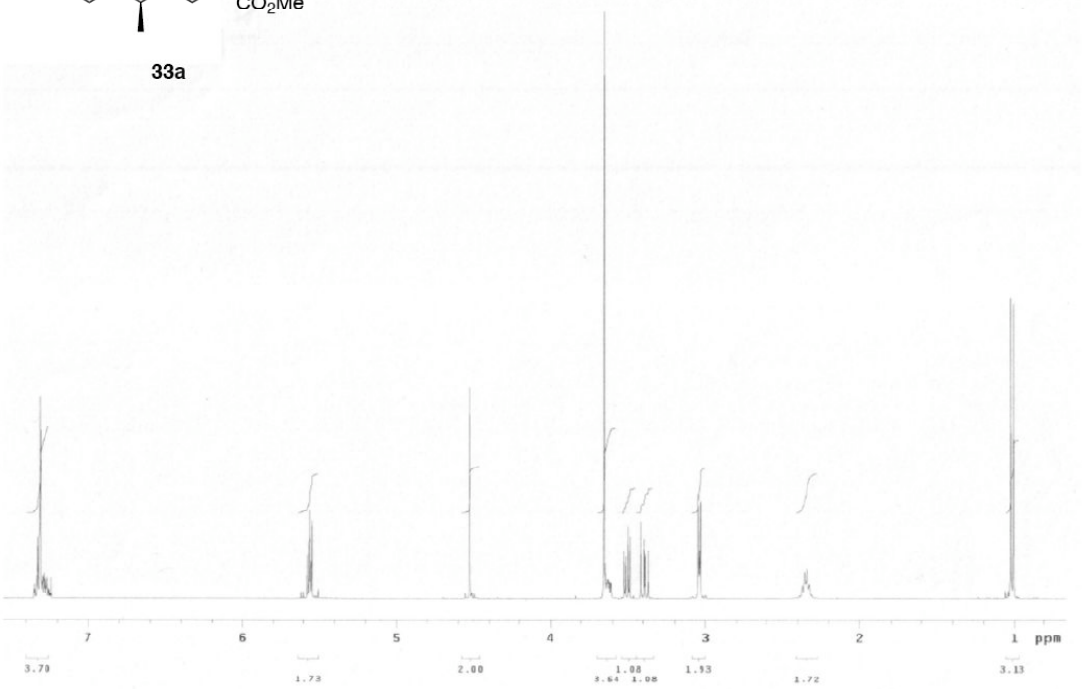
***ent*-32b**

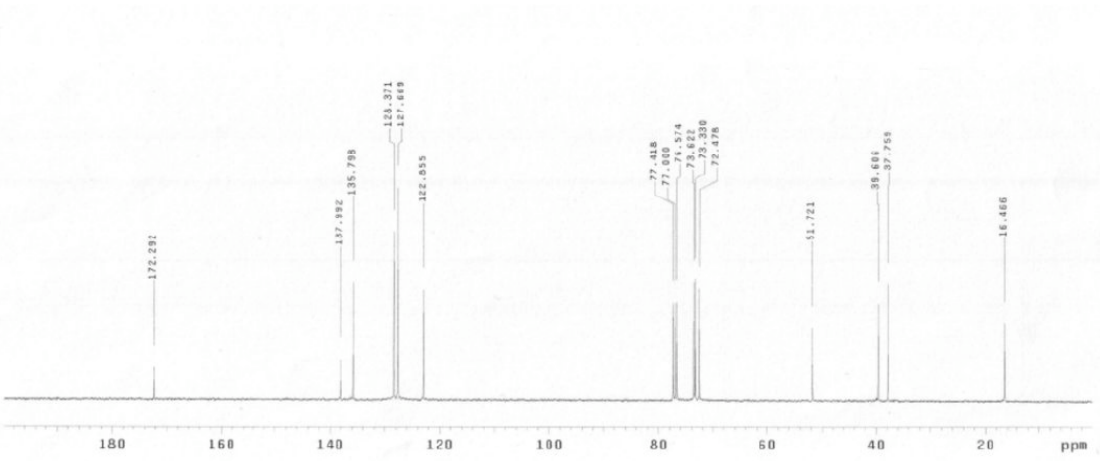

9
8
7
6
5
4
3
2
1
-0 ppm

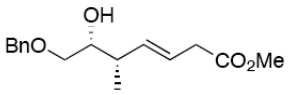

171.716
138.388
137.171
133.762
129.334
128.300
127.953
127.761
127.511
80.386
77.698
77.418
77.000
76.574
73.361
70.181
51.539
41.721
38.361
35.769
16.213
-3.966
-4.416
180
160
140
120
100
80
60
40
20
0 ppm


OH
BnO
CO2Me

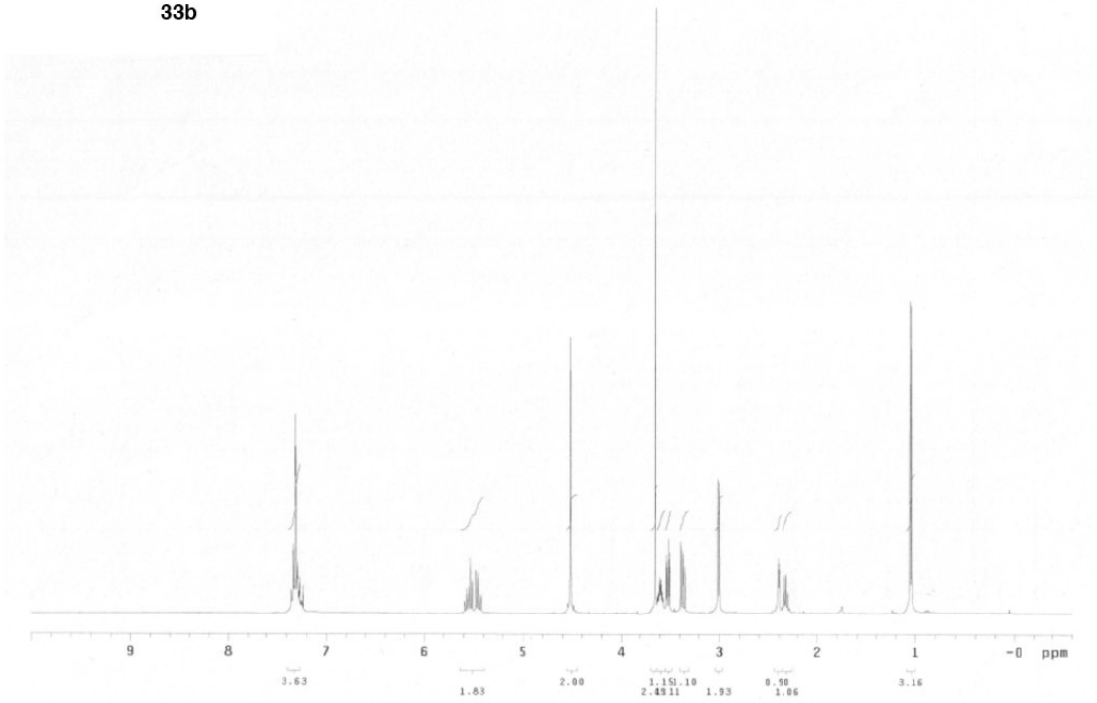
33a

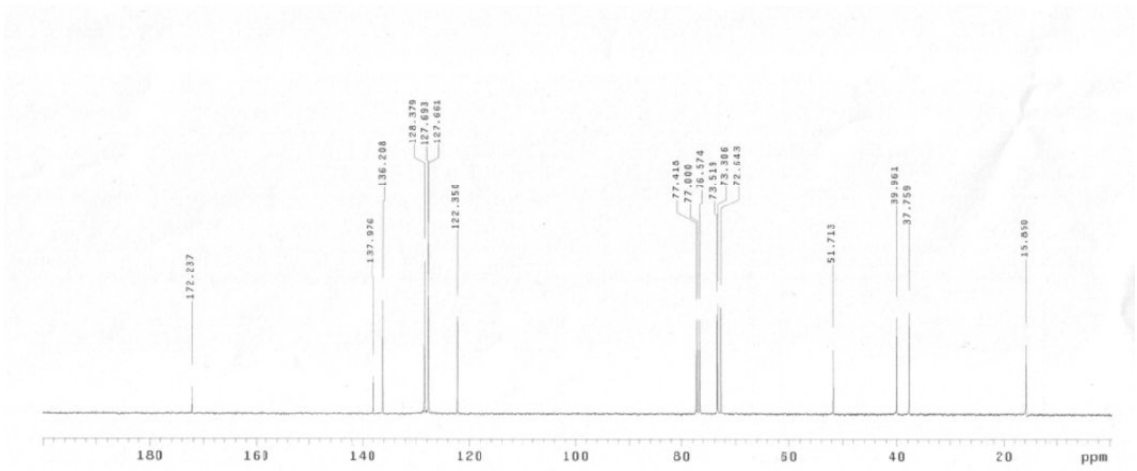

7
6
5
4
3
2
1 ppm
3.79
1.73
2.00
1.08
3.64
1.08
1.93
1.72
3.13

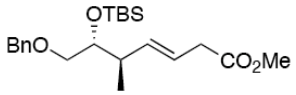

172.291
157.992
135.798
128.371
127.669
122.655
77.418
77.000
76.582
73.330
72.478
51.721
39.691
37.759
16.466
180
160
140
120
100
80
60
40
20
ppm

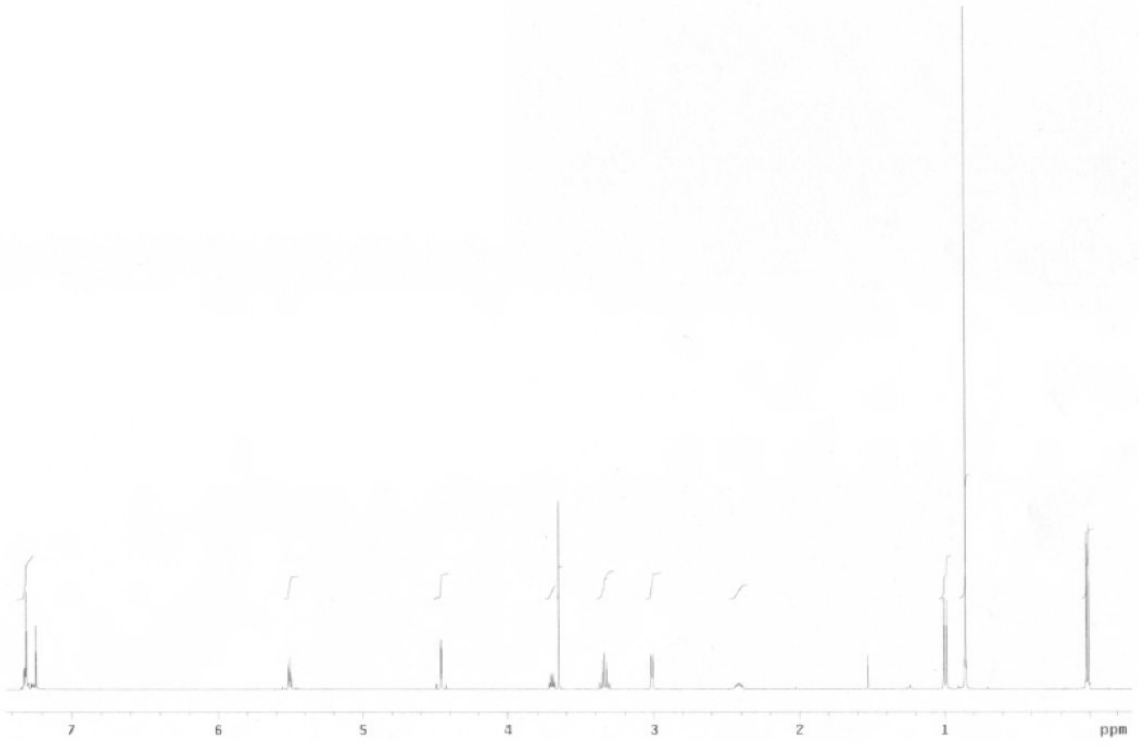

OH
BnO
CO2Me

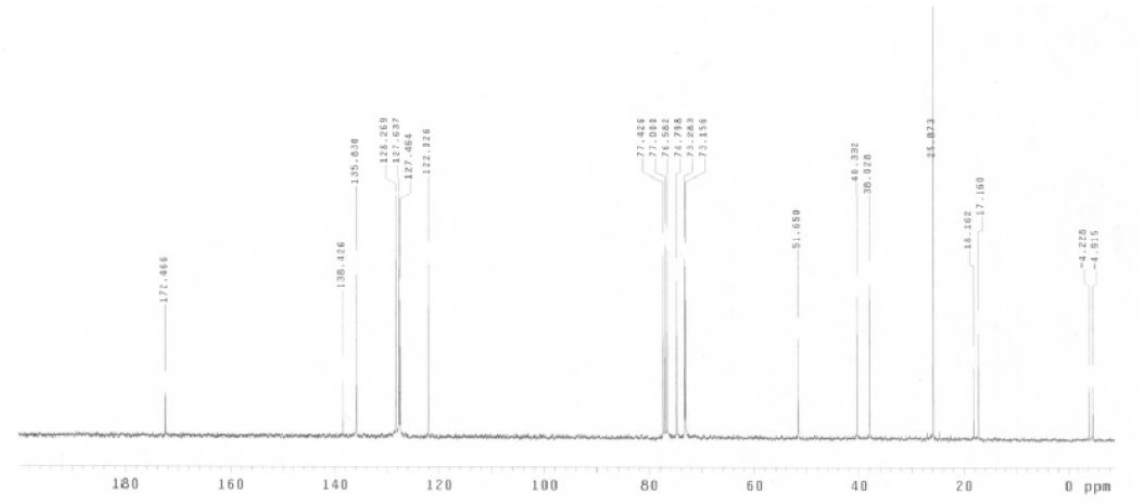
33b

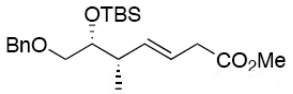

9
8
7
6
5
4
3
2
1
-0
ppm
3.63
1.83
2.00
1.93
3.16

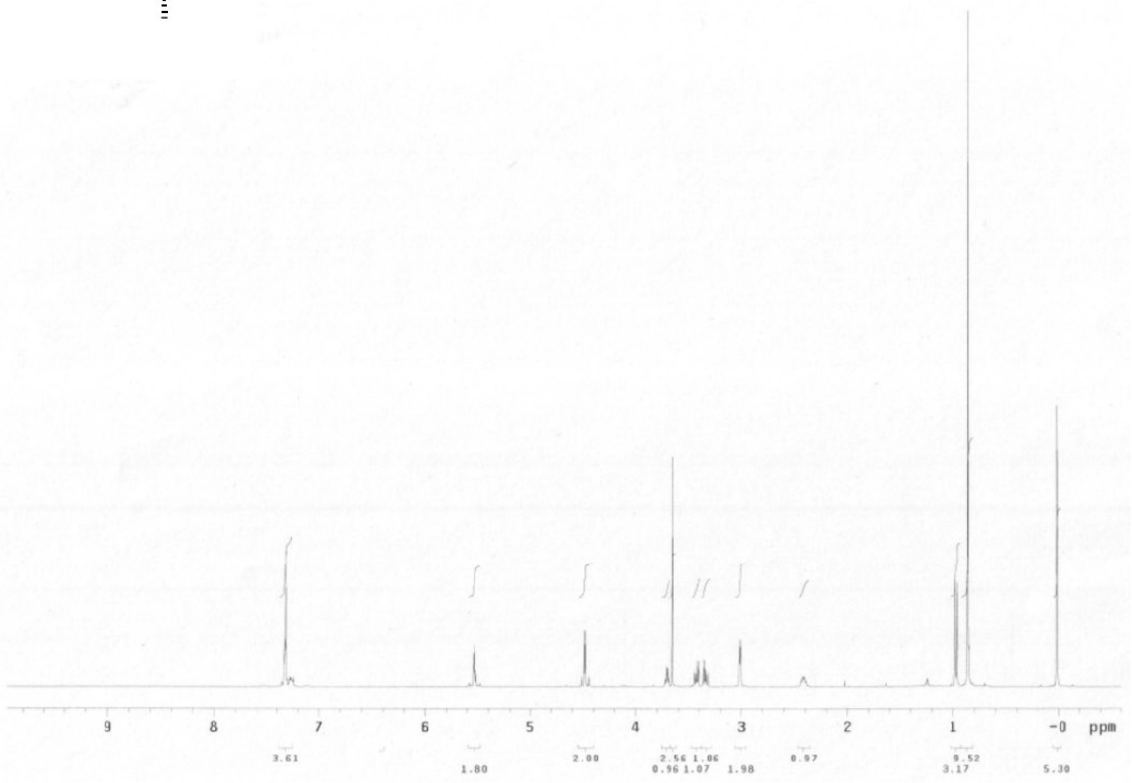

172.237
137.976
136.208
128.379
127.693
127.661
122.354
77.416
73.511
73.386
72.643
51.713
39.961
37.759
15.850
180
160
140
120
100
80
60
40
20
ppm

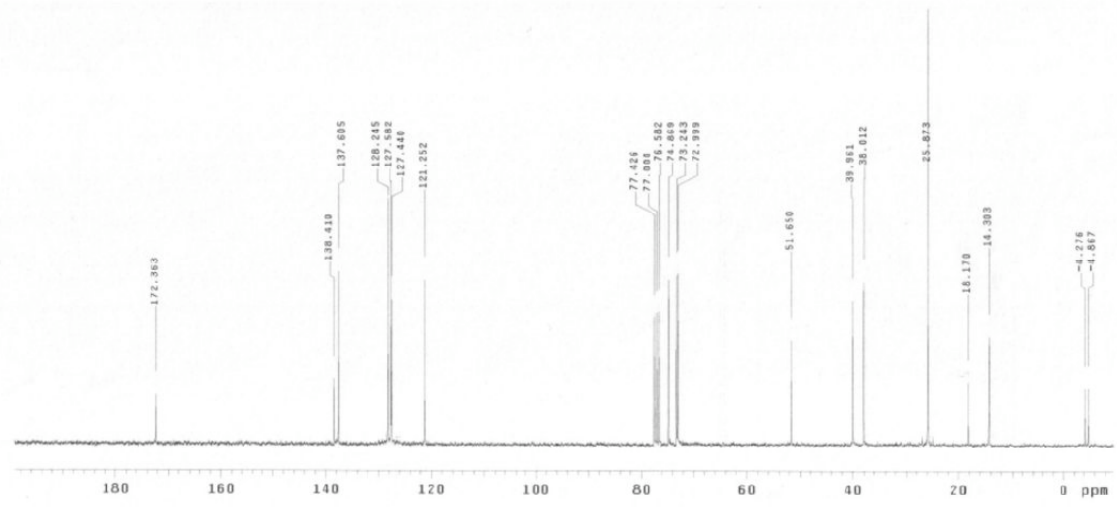

OTBS
BnO
CO2Me

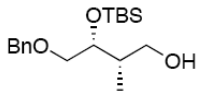

7
6
5
4
3
2
1
ppm

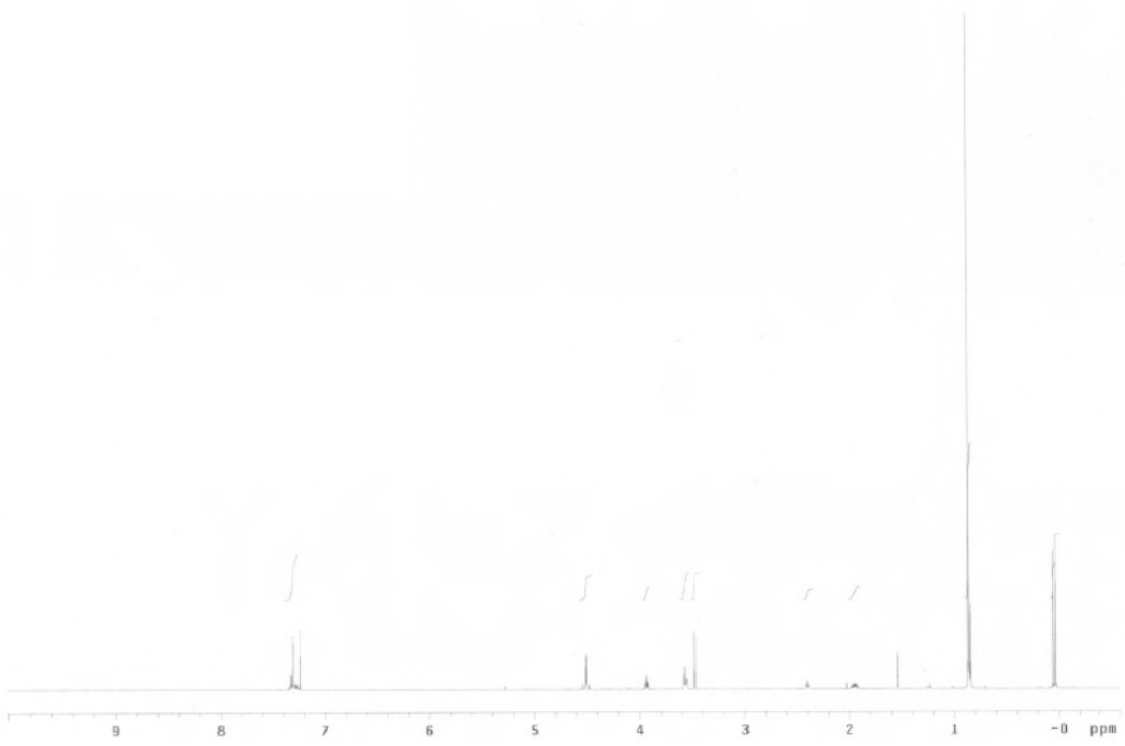

172.466
138.426
135.630
128.269
127.637
127.464
122.926
77.426
77.000
76.582
74.798
73.263
73.156
51.659
40.332
36.028
25.873
18.162
17.160
-4.228
-4.915
180
160
140
120
100
80
60
40
20
0 ppm

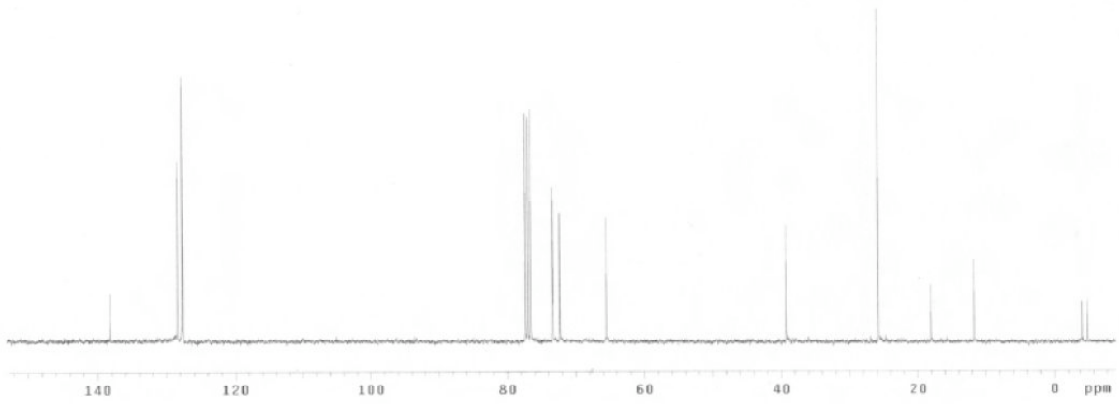

OTBS
BnO
CO2Me

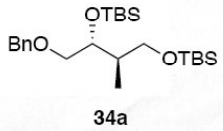

9
8
7
6
5
4
3
2
1
-0
ppm
3.61
1.80
2.00
2.56
1.06
0.96
1.07
1.98
0.97
9.52
3.17
5.30


172.363
138.410
137.605
128.245
127.582
127.440
121.252
77.486
77.061
76.582
74.869
73.243
72.999
51.650
39.961
38.012
25.873
18.170
14.303
-4.276
-4.867
180
160
140
120
100
80
60
40
20
0
ppm

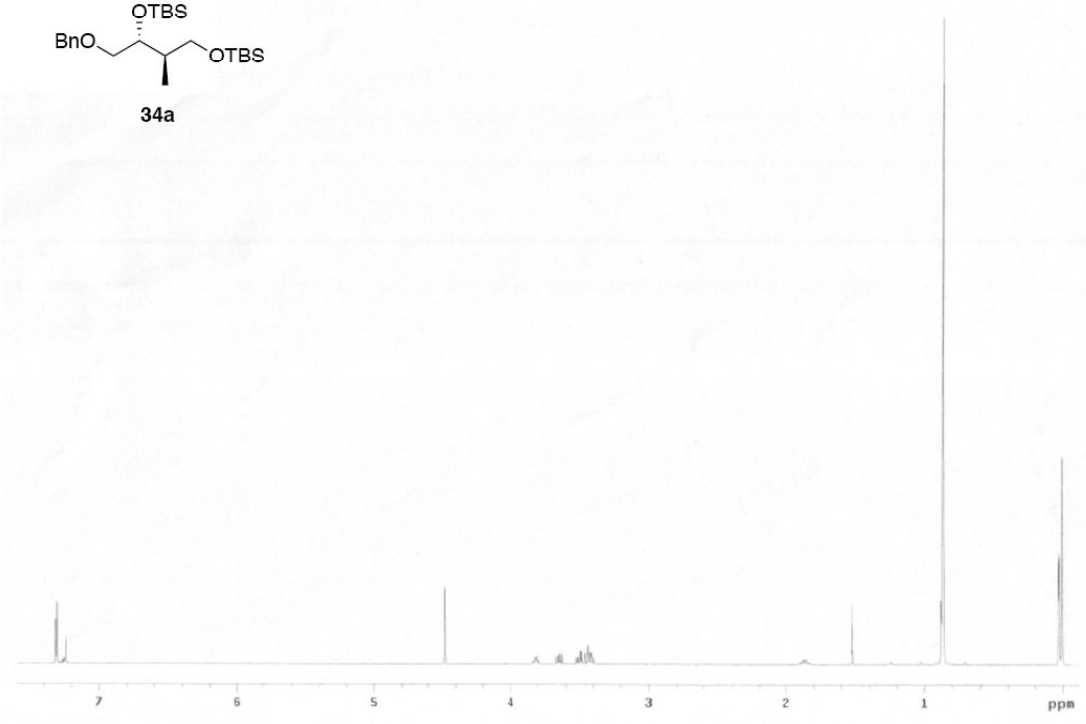

OTBS
BnO
OH

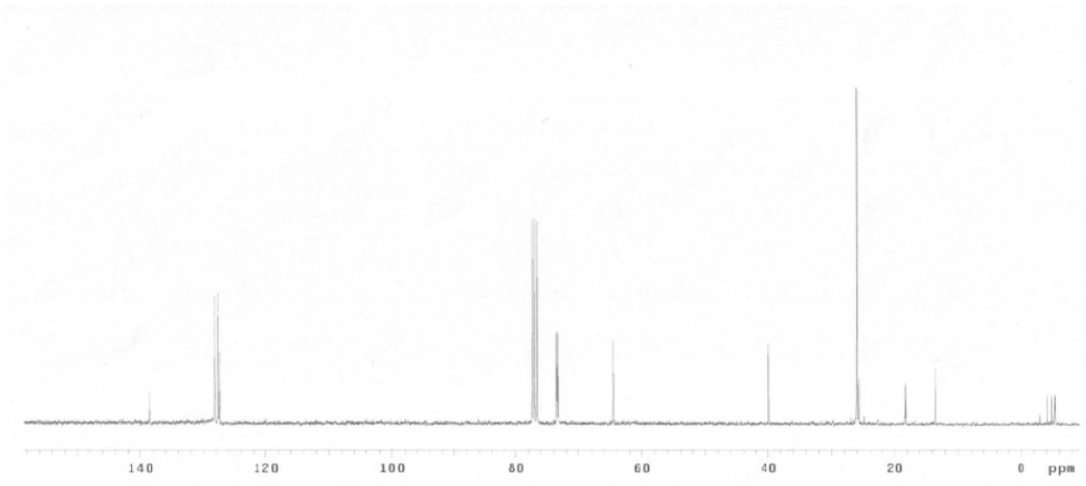

9
8
7
6
5
4
3
2
1
-0
ppm

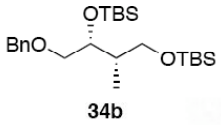

140
120
100
80
60
40
20
0
ppm



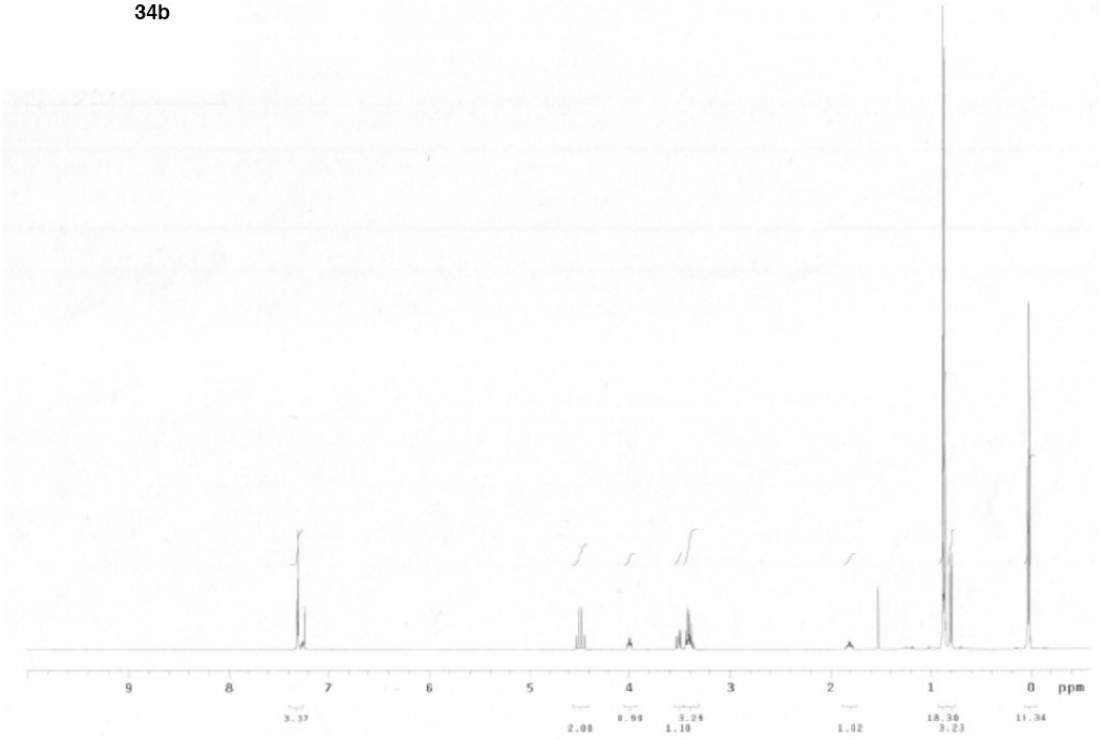
34a

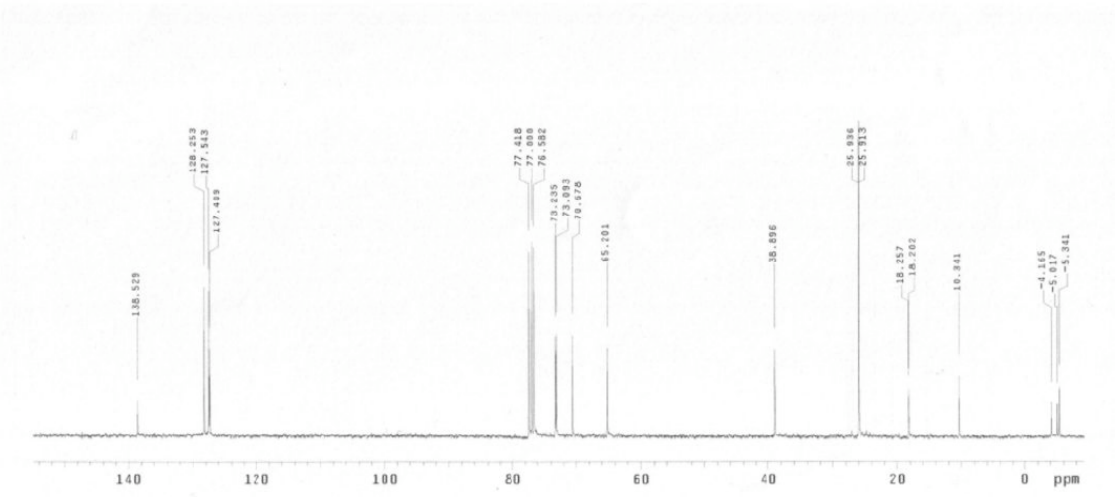


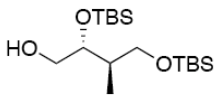


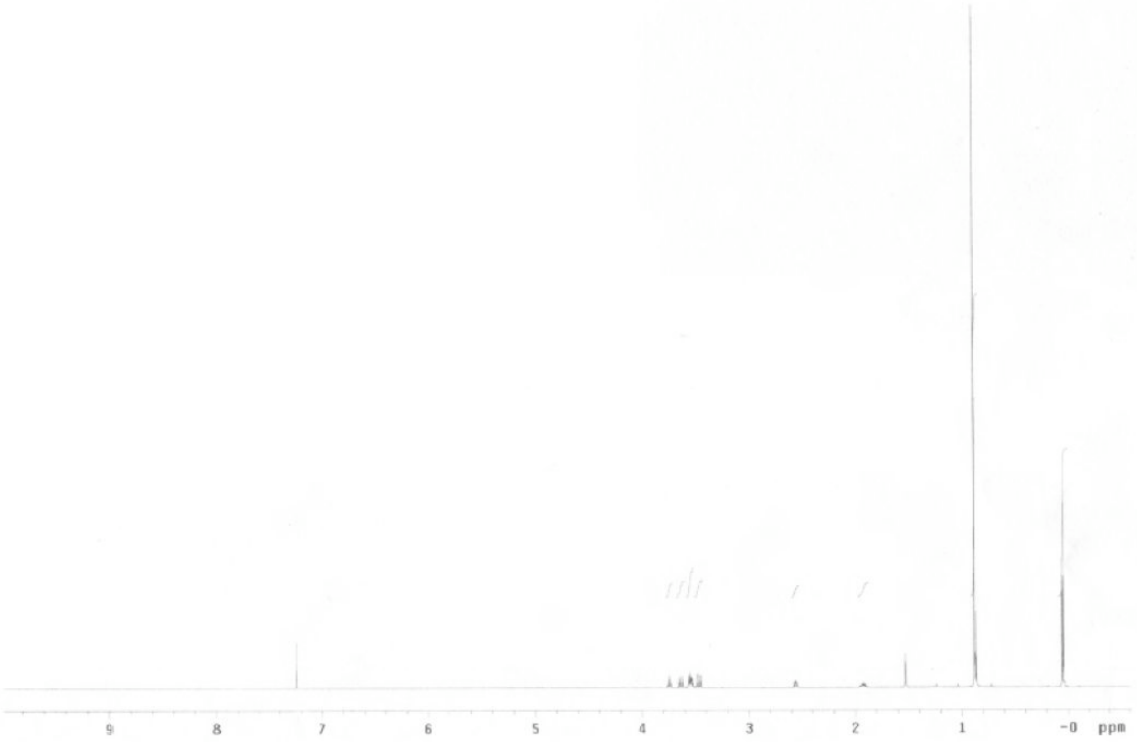

OTBS
BnO
OTBS

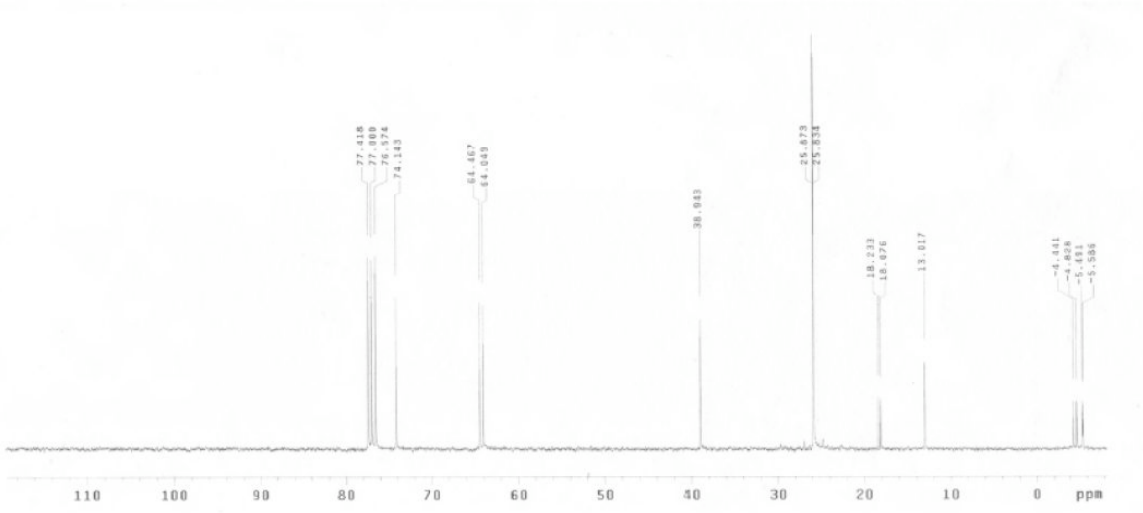
34b

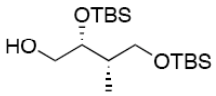

9
8
7
6
5
4
3
2
1
0
ppm
3.37
2.08
0.99
3.29
1.10
1.02
18.38
3.23
11.34

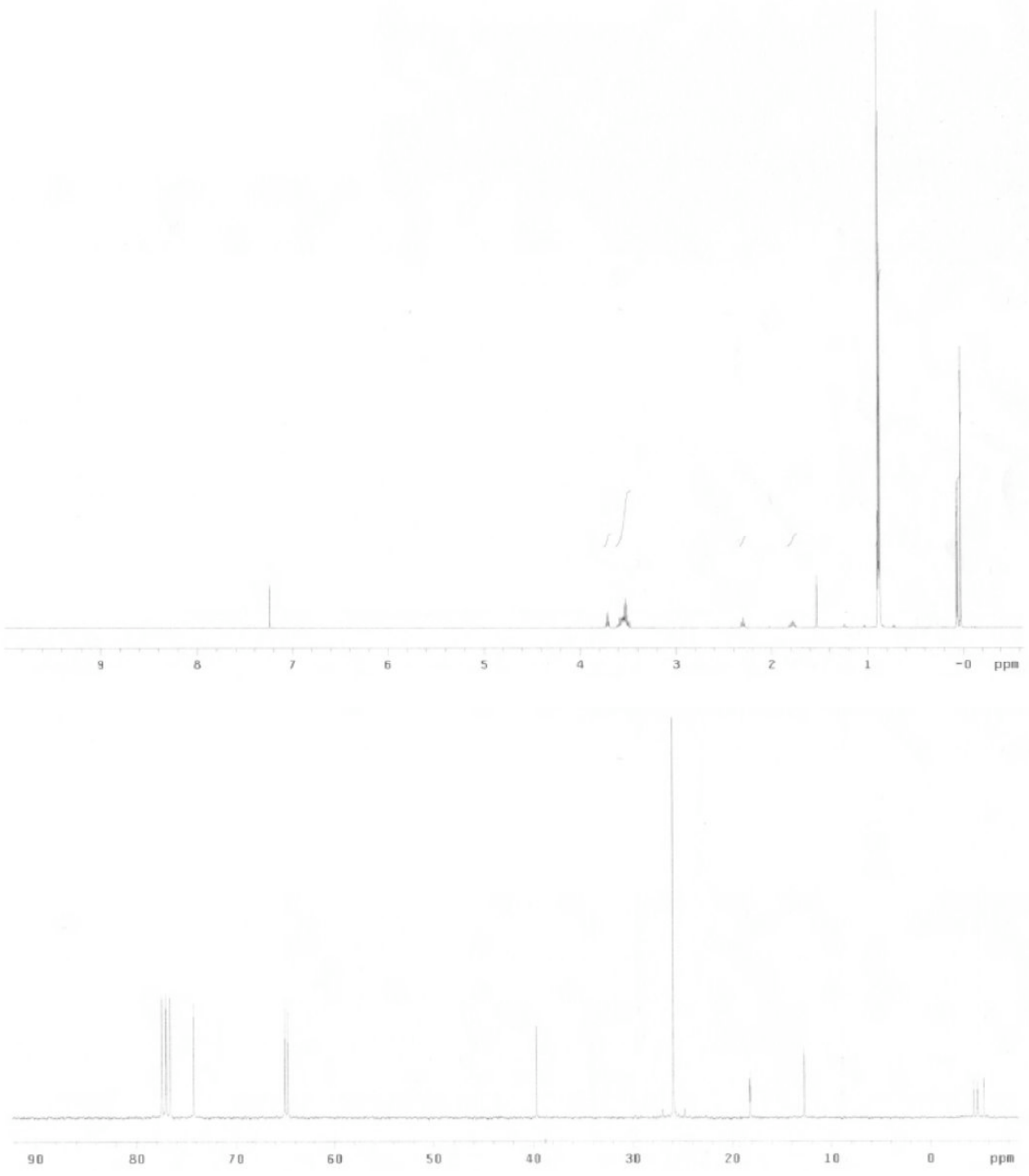

138.529
128.553
127.543
127.419
77.418
77.000
76.582
73.436
73.093
70.678
65.201
38.896
25.936
25.913
18.257
18.202
10.341
-4.165
-5.017
-5.341
140
120
100
80
60
40
20
0
ppm

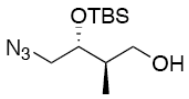

OTBS
HO
OTBS


9
8
7
6
5
4
3
2
1
-0
ppm

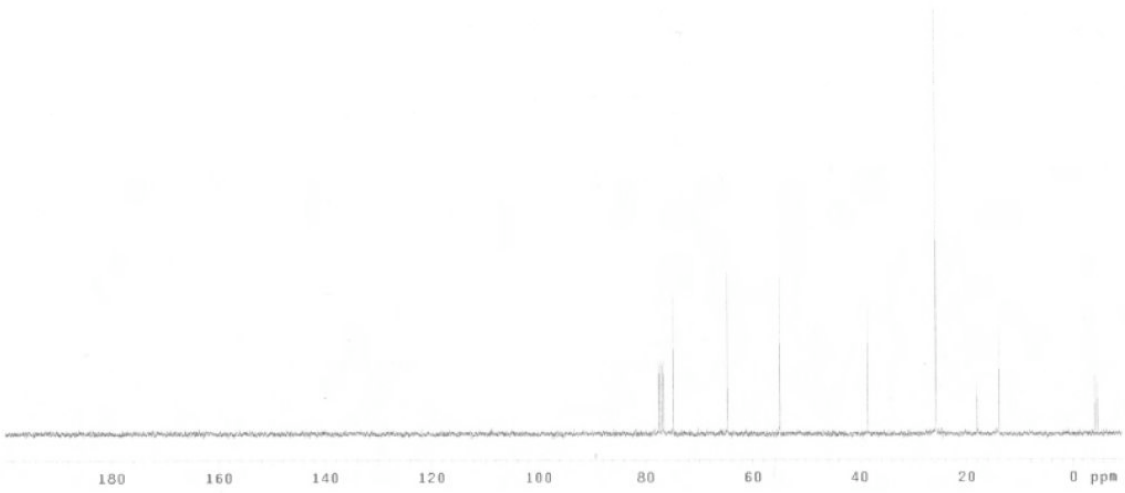

77.416
77.000
76.574
74.143
64.467
64.049
38.043
25.873
25.834
18.233
18.076
13.017
-4.441
-4.626
-5.161
-5.586
110
100
90
80
70
60
50
40
30
20
10
0
ppm

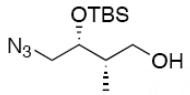

OTBS
HO
OTBS


9
8
7
6
5
4
3
2
1
-0
ppm
90
80
70
60
50
40
30
20
10
0
ppm

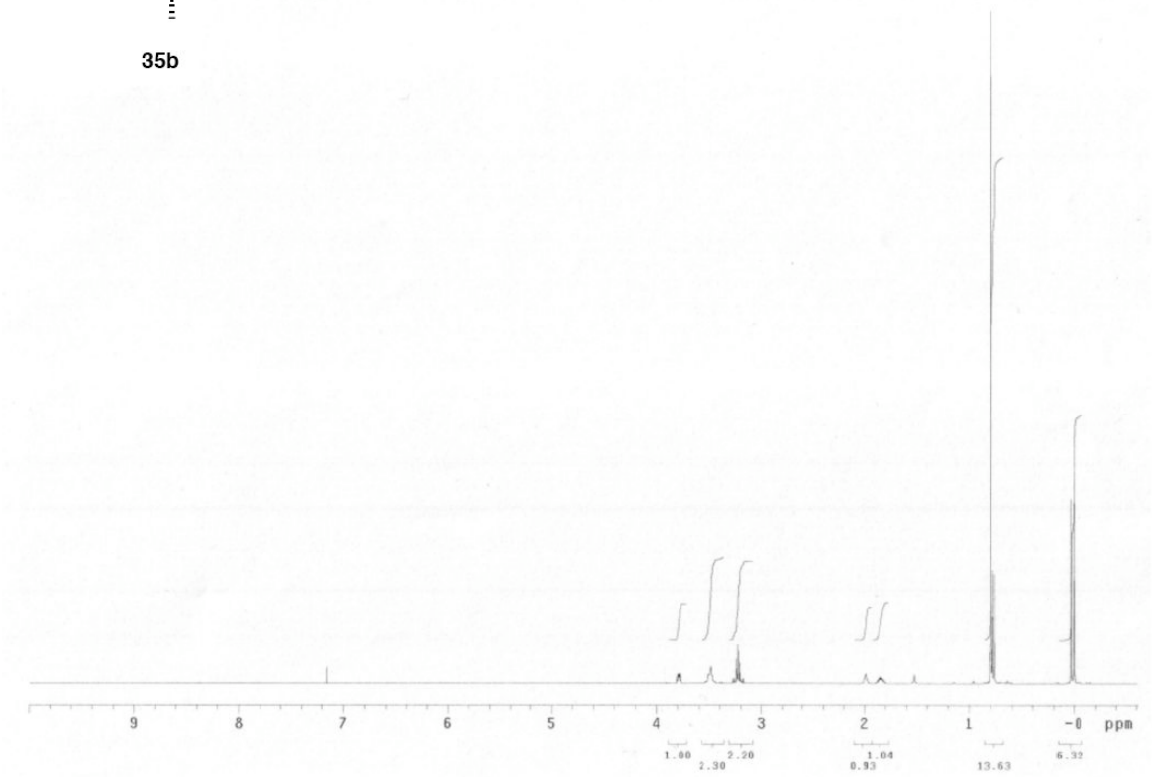


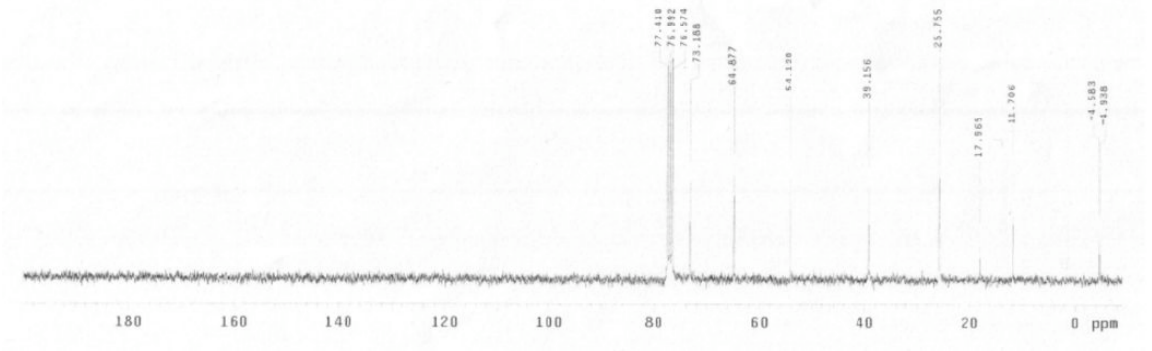
35a

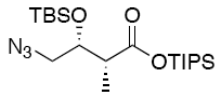


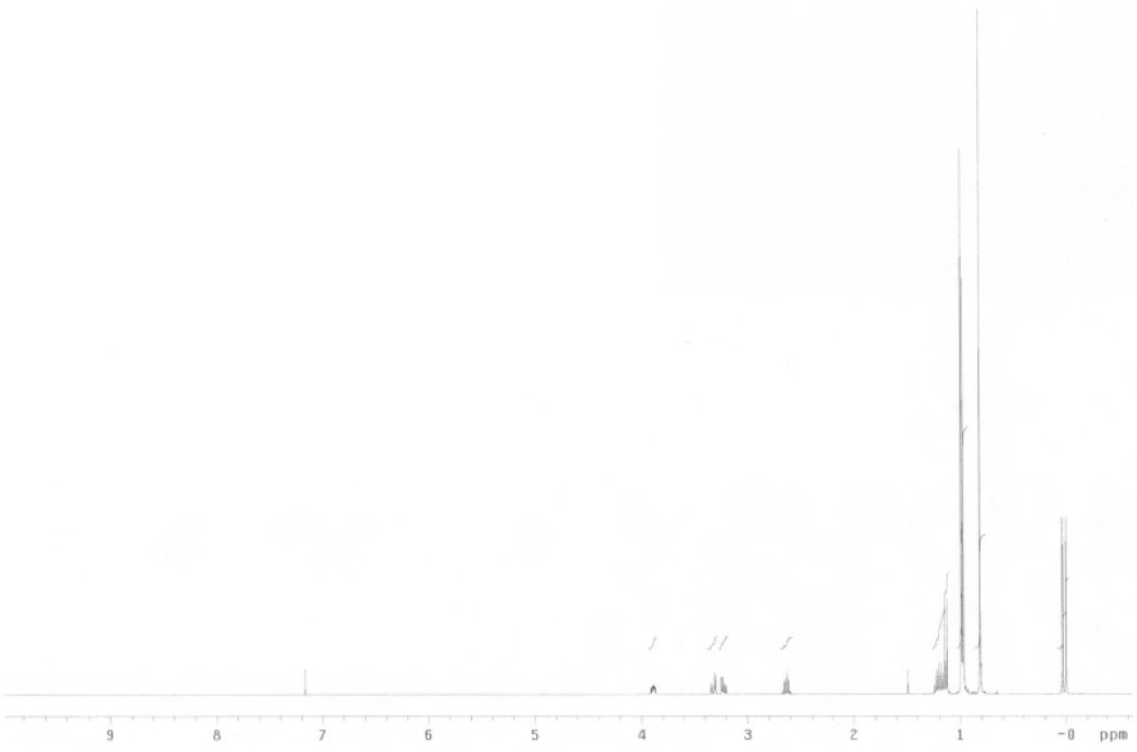

OTBS
N3
OH

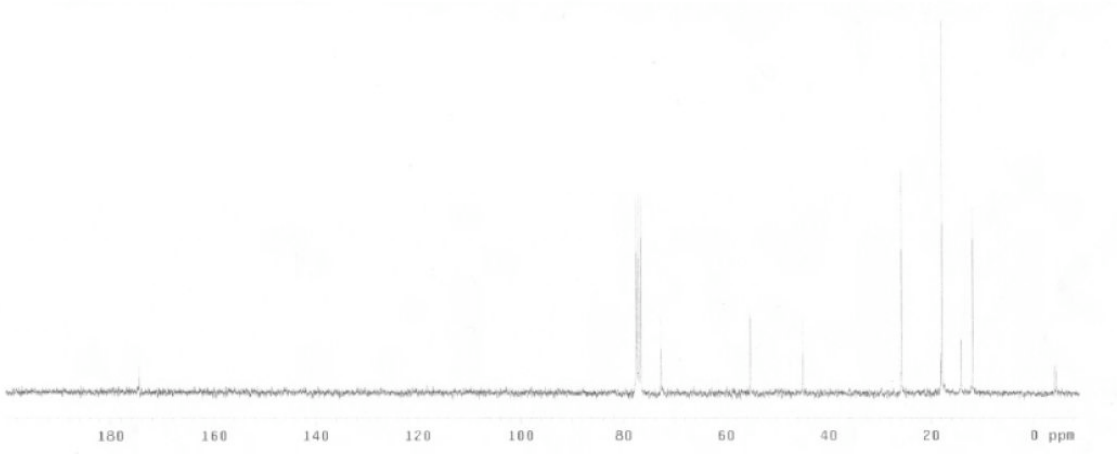
35b

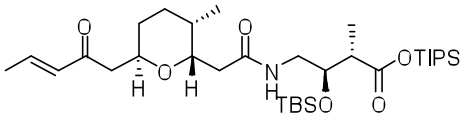

9
8
7
6
5
4
3
2
1
-0
ppm
1.00
2.30
2.20
1.04
0.93
13.63
6.32


77.410
76.992
76.574
73.188
64.877
54.130
39.156
25.755
17.965
11.706
-4.583
-4.938
180
160
140
120
100
80
60
40
20
0 ppm

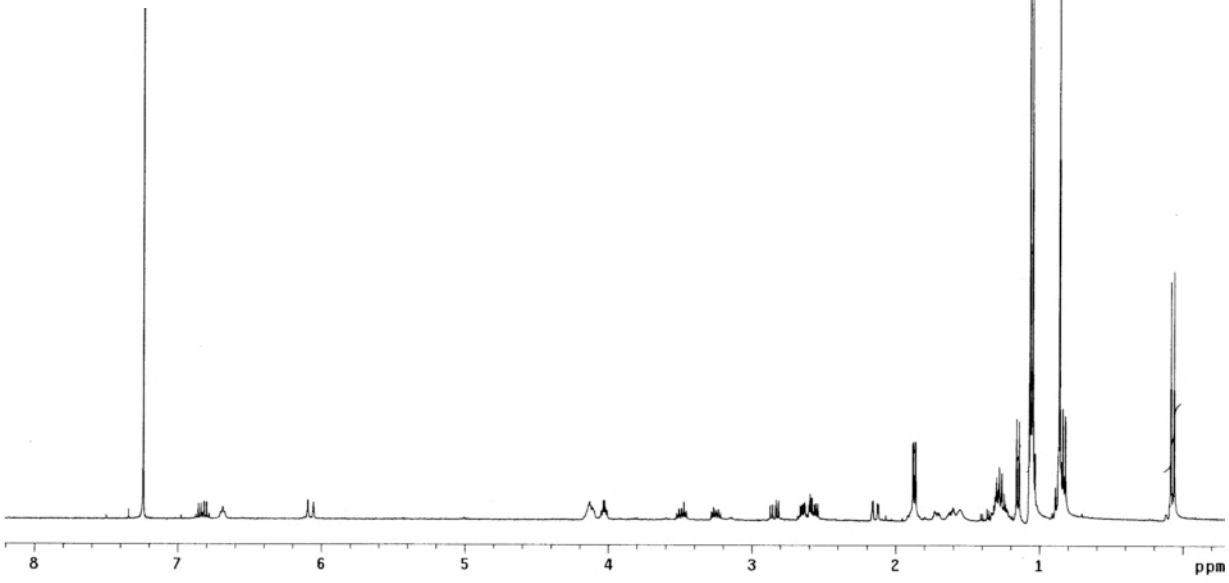

TBSO
O
N3
OTIPS

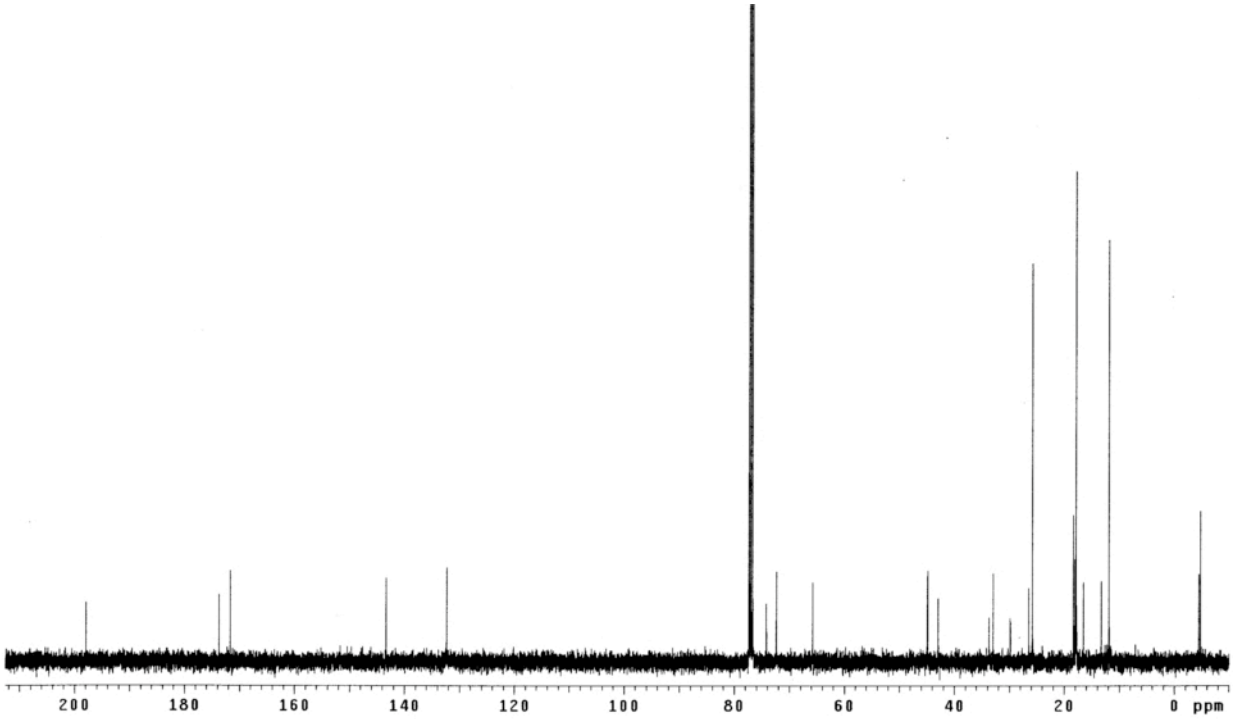

9
8
7
6
5
4
3
2
1
-0
ppm


180
160
140
120
100
80
60
40
20
0 ppm

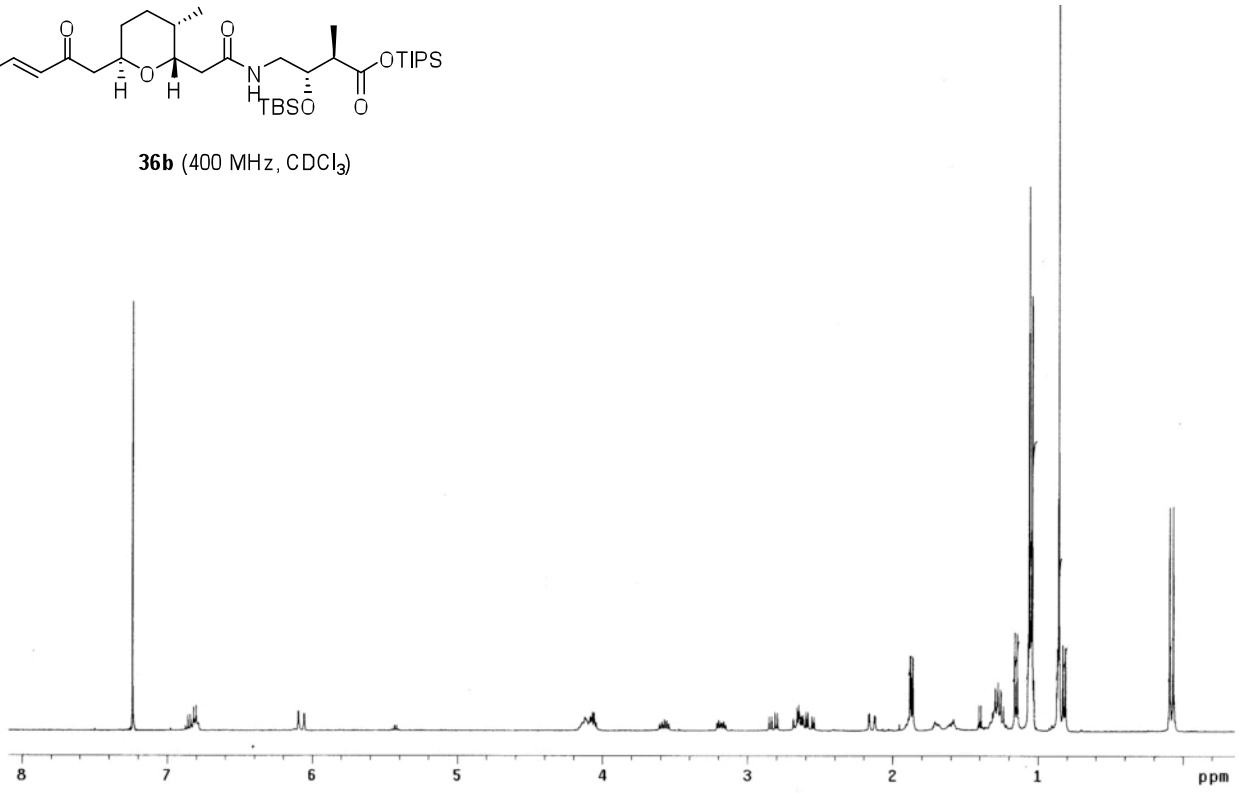


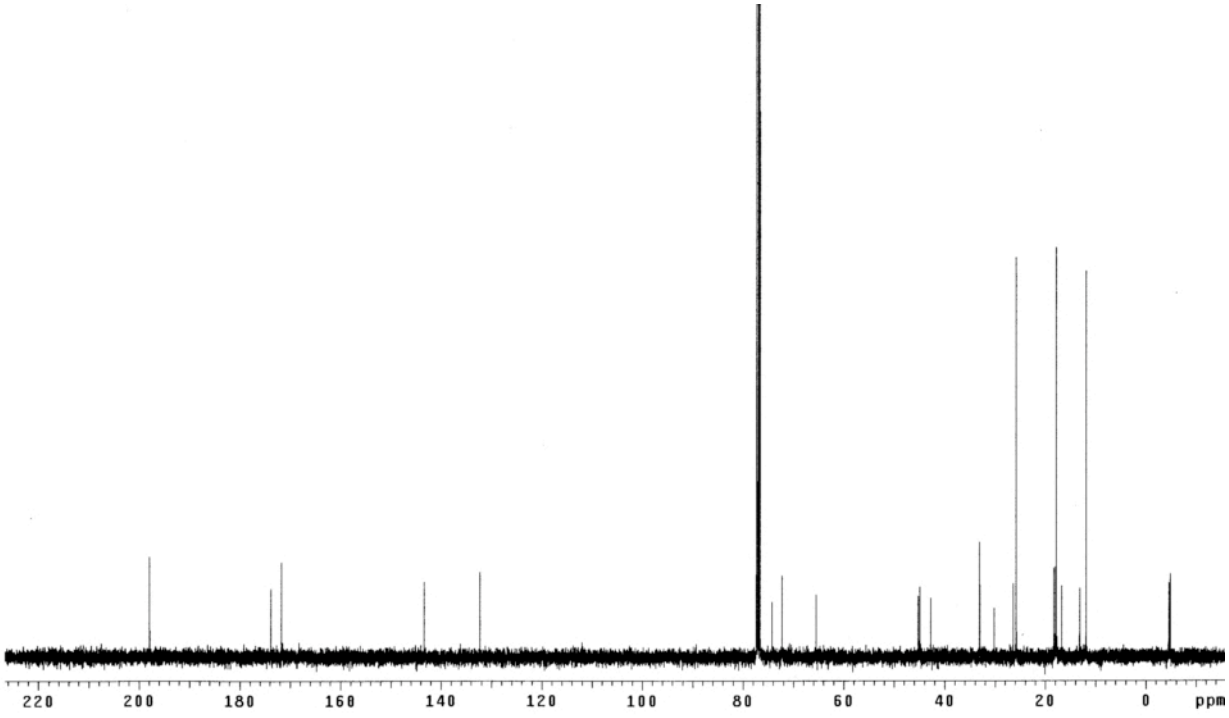
36a (400 MHz, $CDCl_3$)



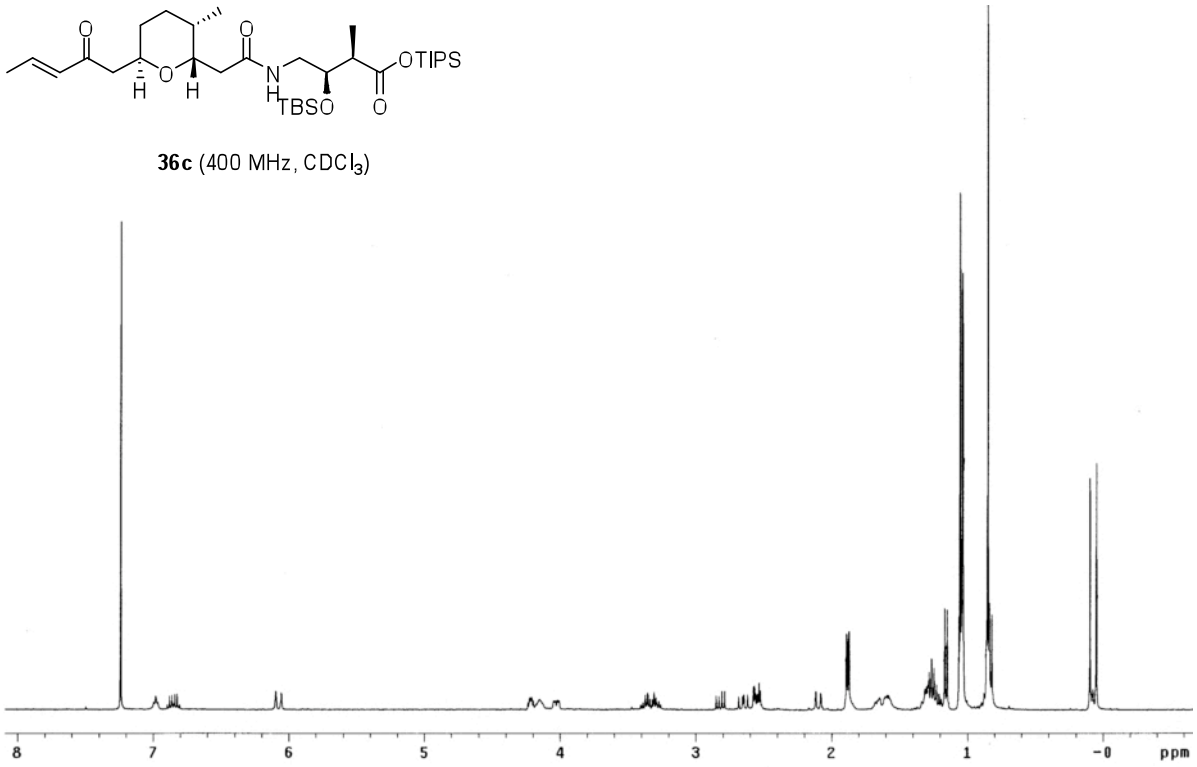


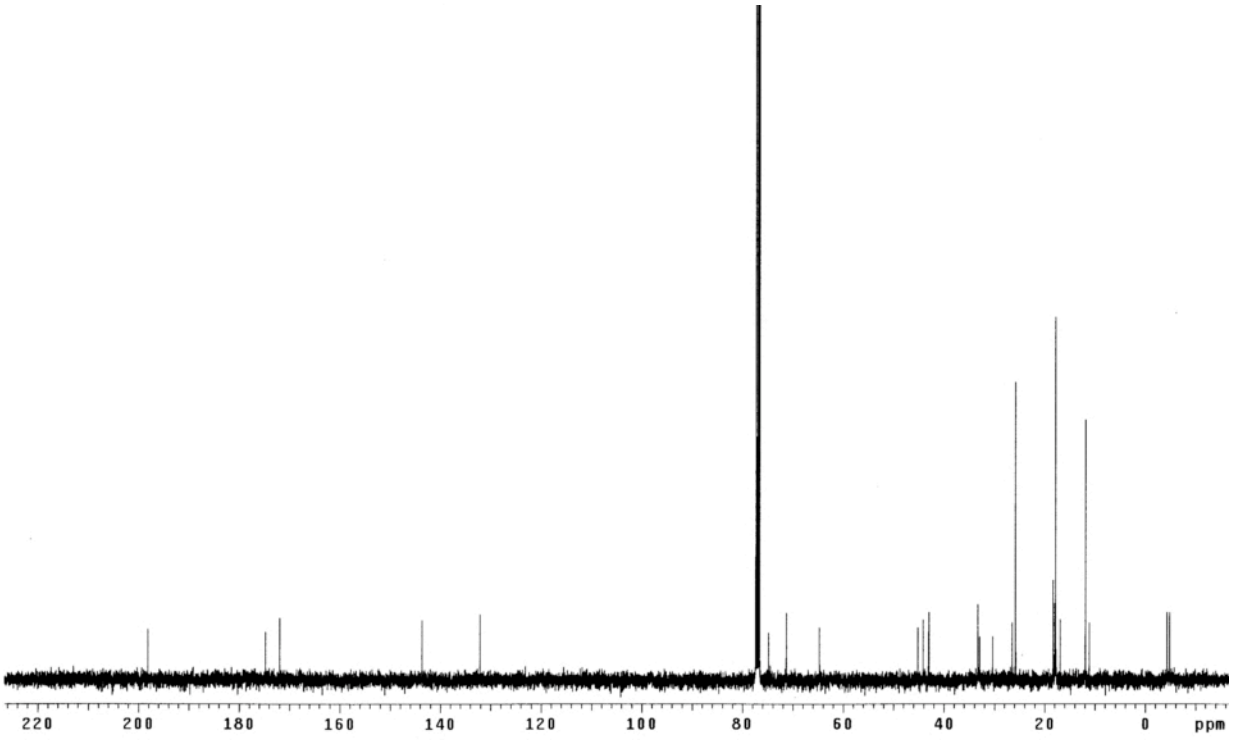
36b (400 MHz, $CDCl_3$)

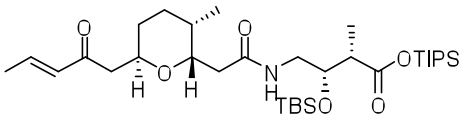




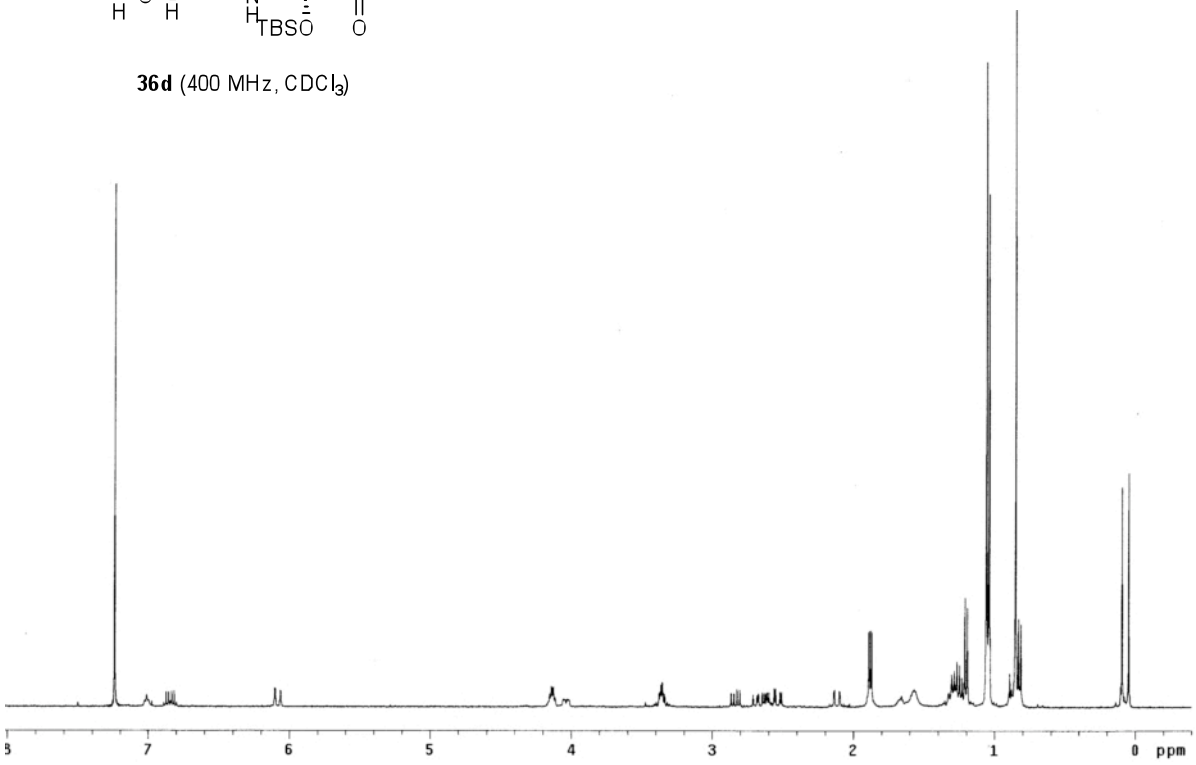
36c (400 MHz, $CDCl_3$)

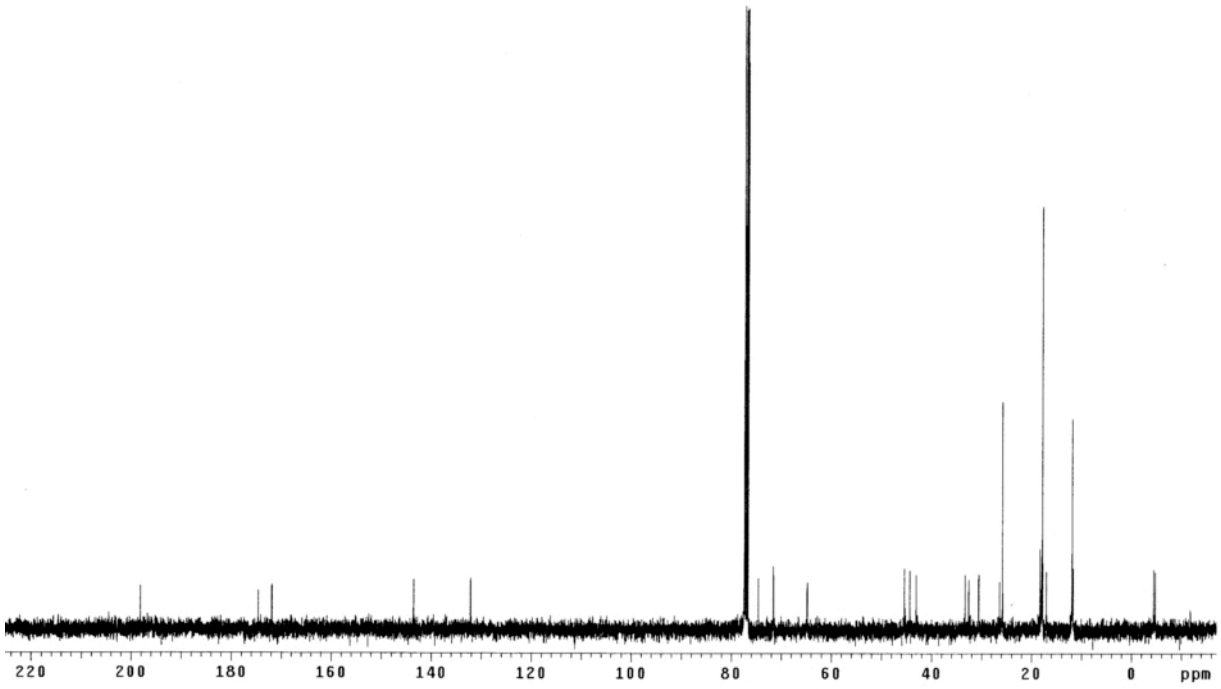


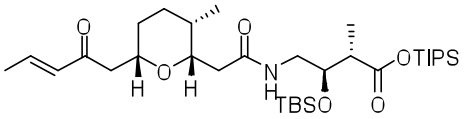




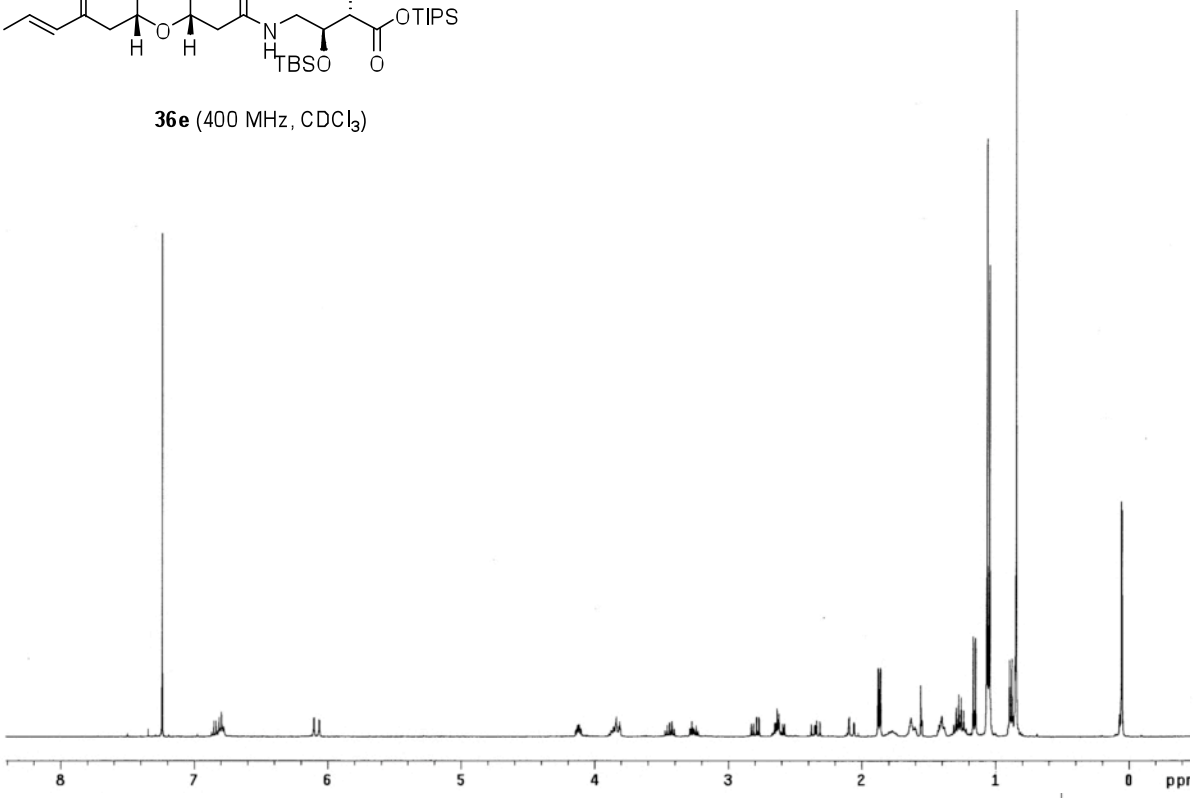
36d (400 MHz, $CDCl_3$)

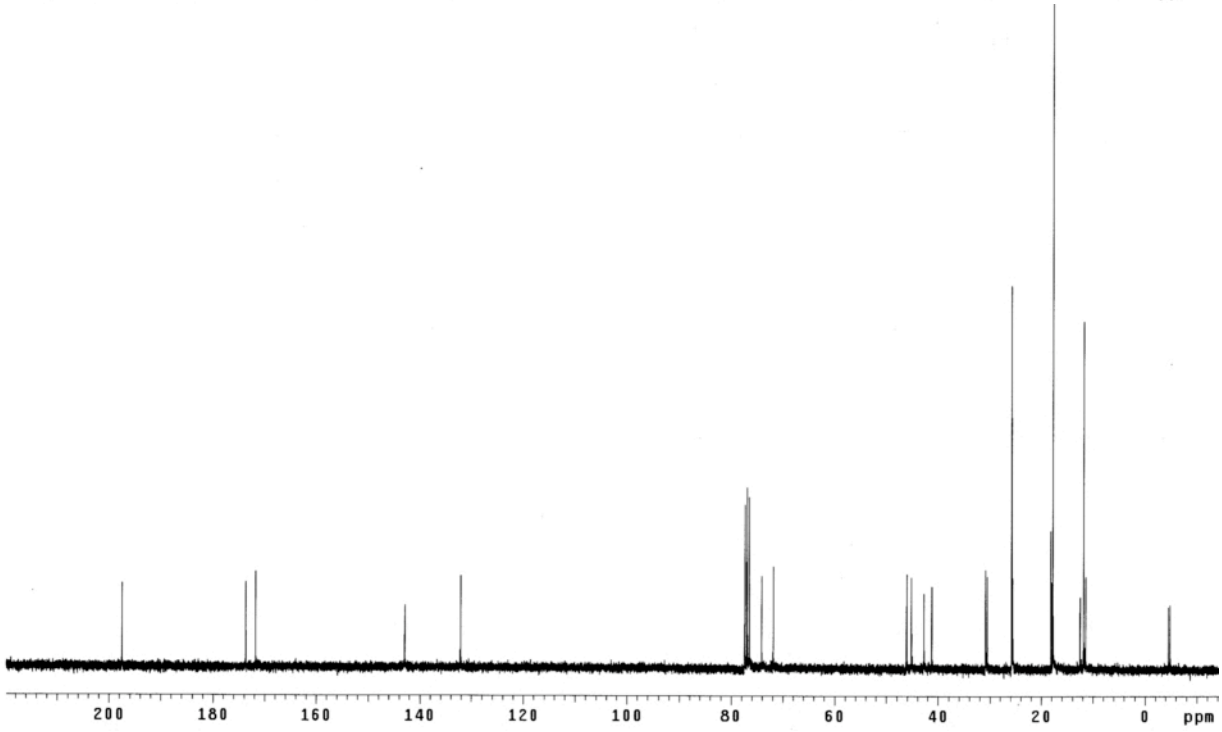


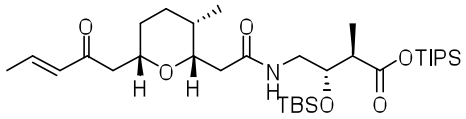




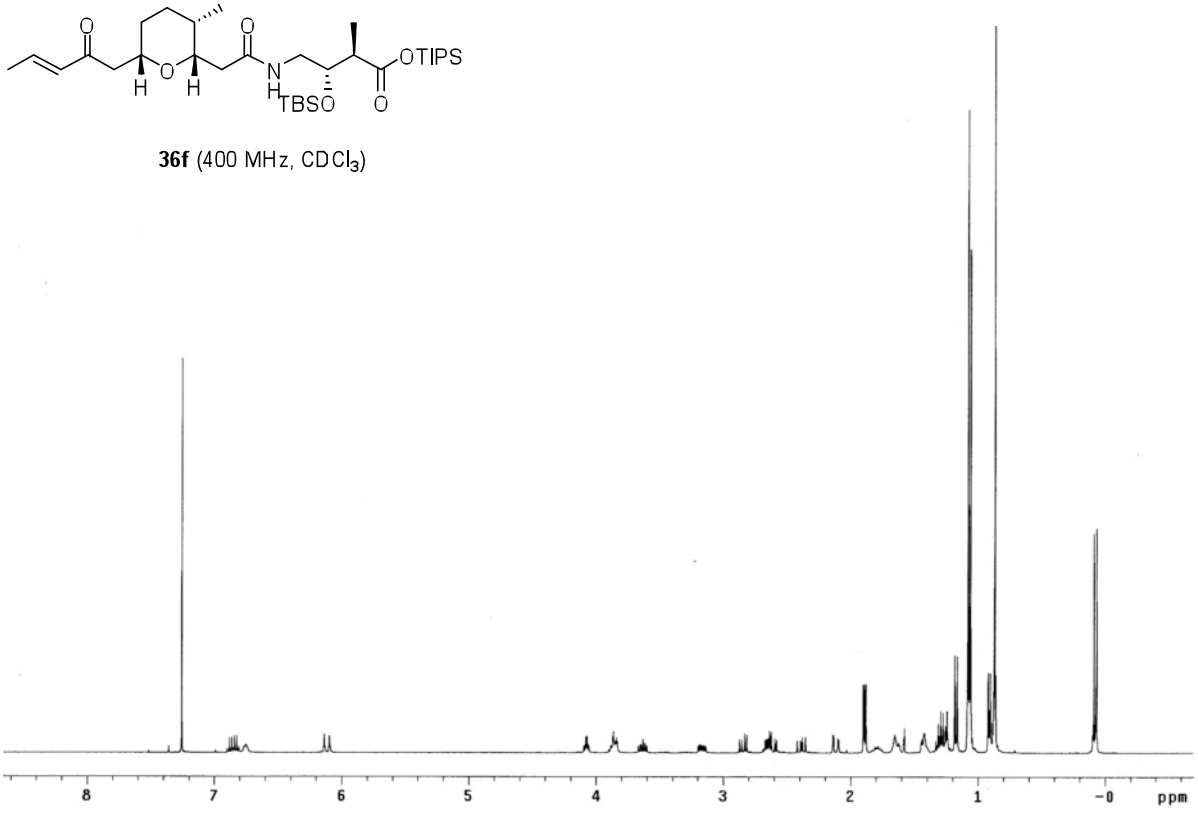
36e (400 MHz, $CDCl_3$)

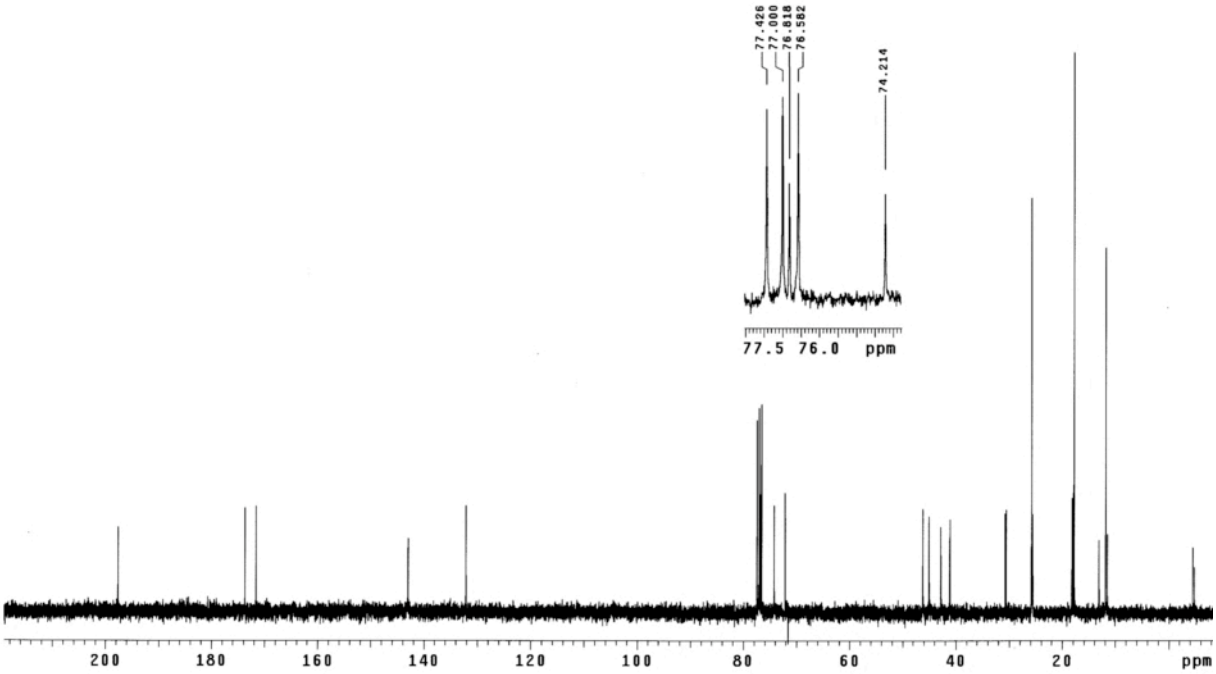




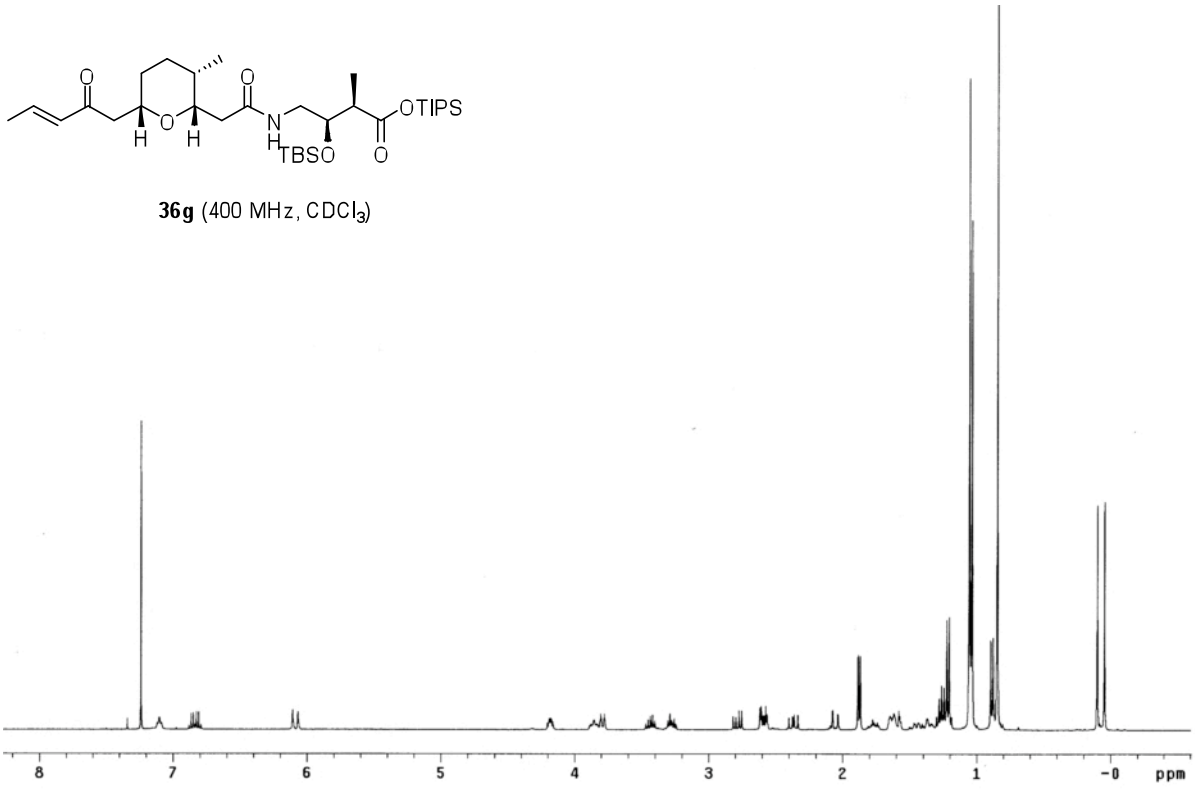


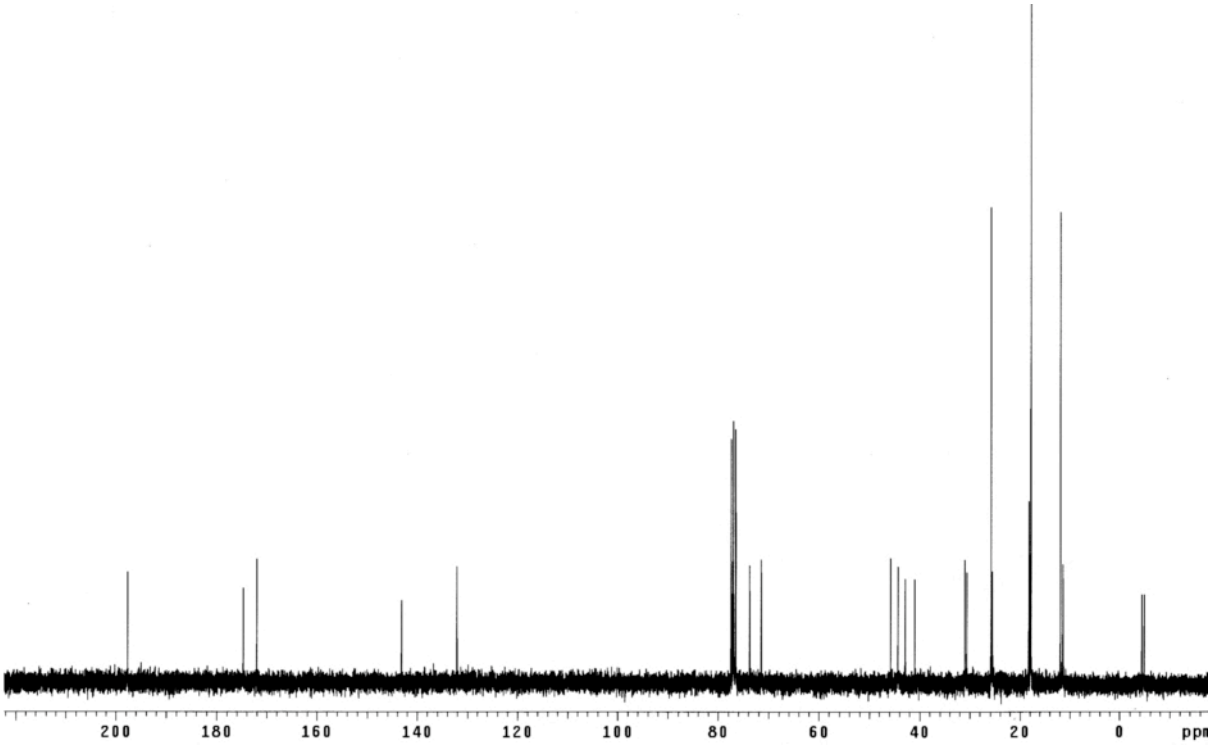
36f (400 MHz, $CDCl_3$)

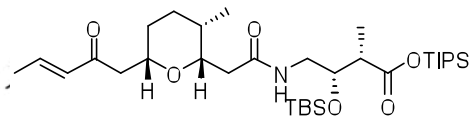




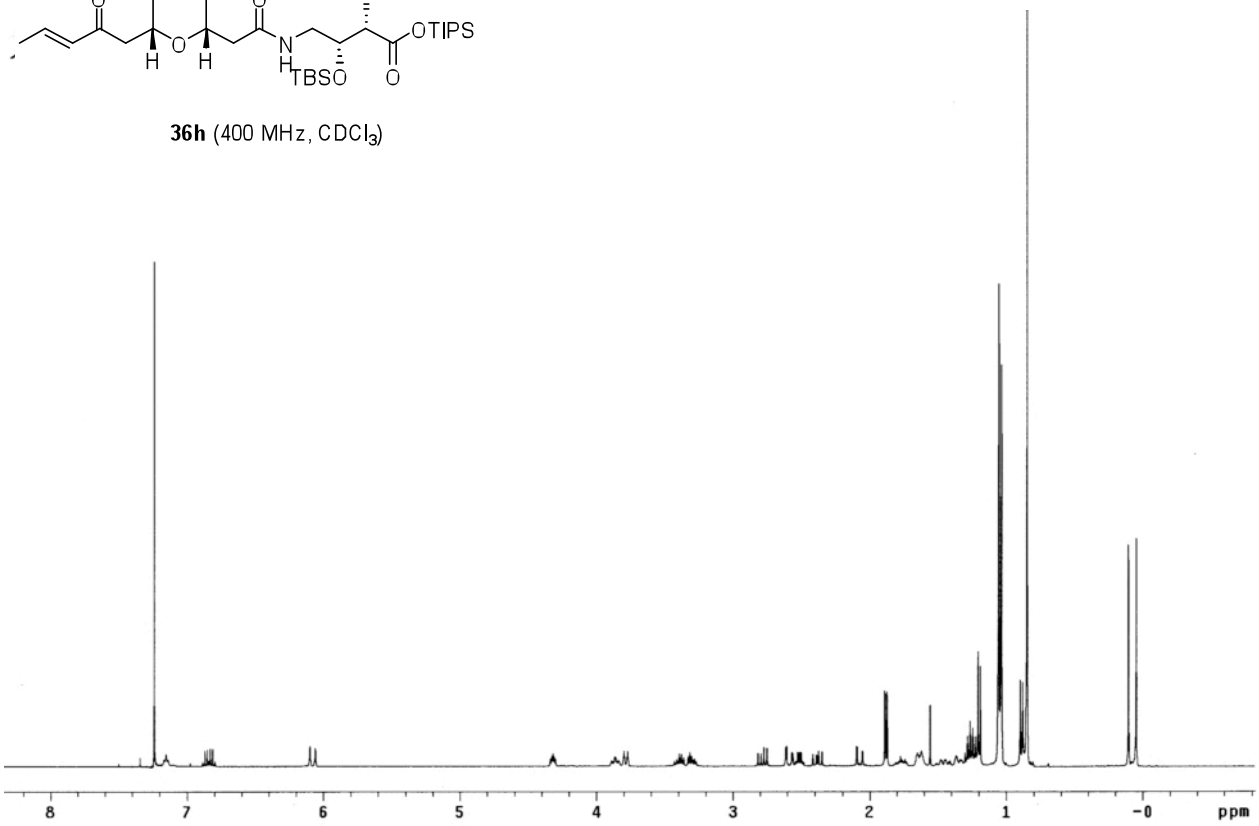
36g (400 MHz, $CDCl_3$)

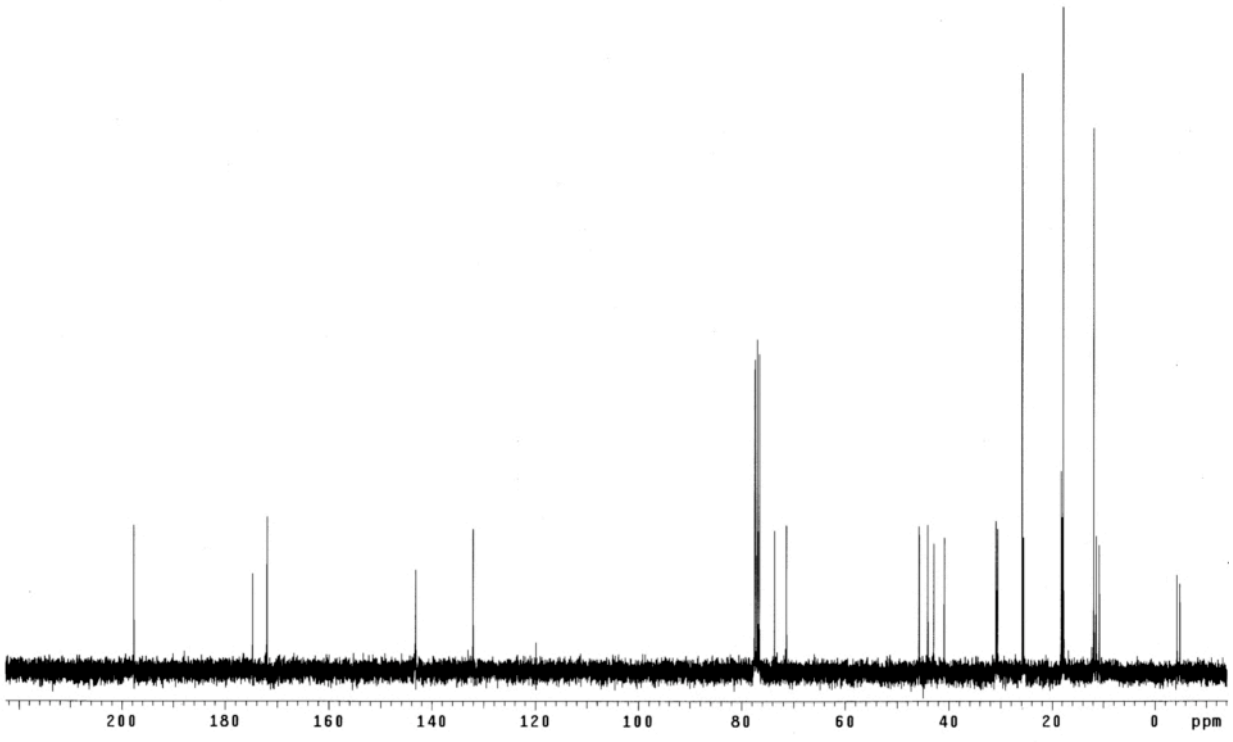


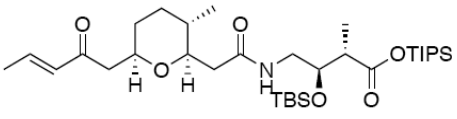




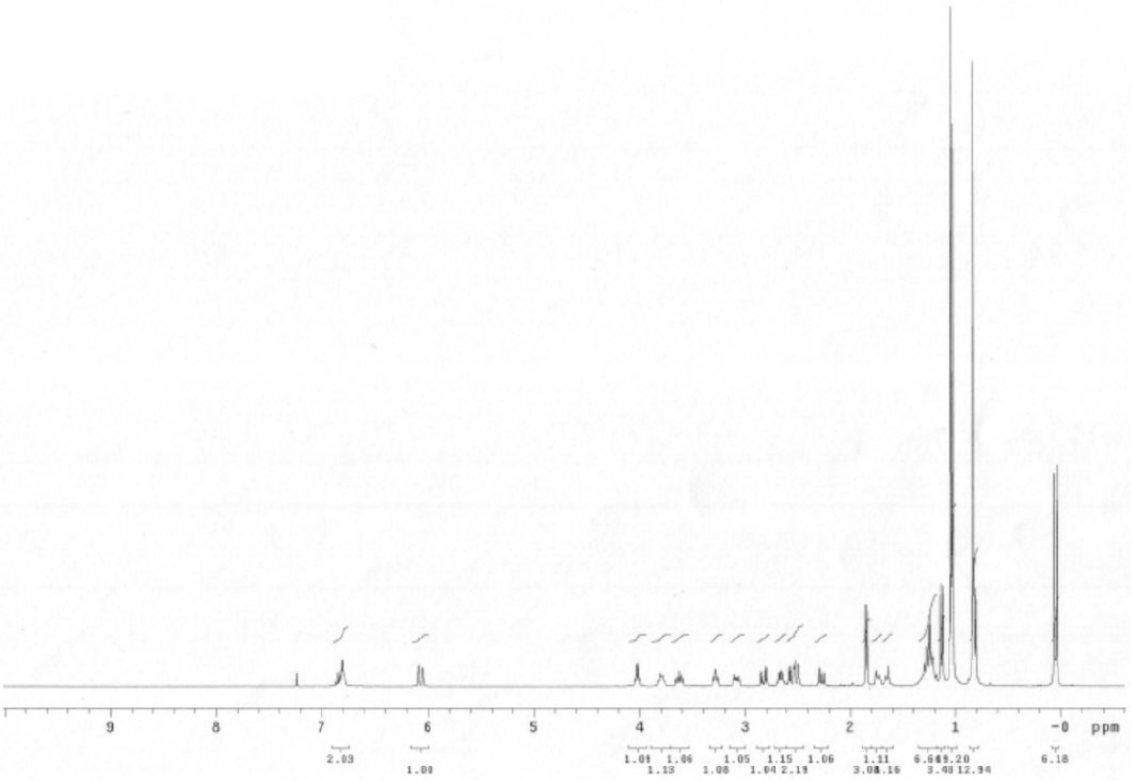
36h (400 MHz, $CDCl_3$)

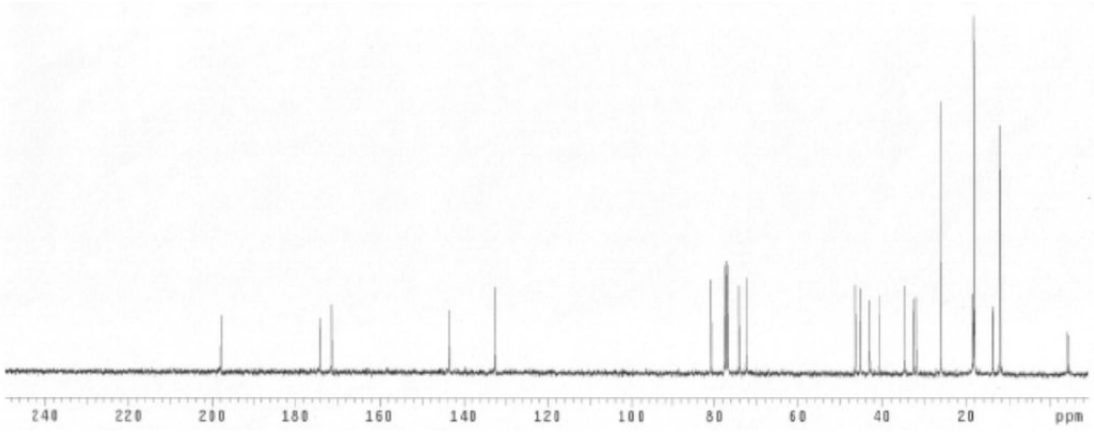





O
O
OTIPS
H
O
H
N
H
TBSO
O

36i


9
8
7
6
5
4
3
2
1
0
ppm
2.03
1.00
1.09
1.06
1.13
1.05
1.08
1.15
1.04
1.06
2.19
1.11
3.08
6.64
9.20
3.48
12.94
6.18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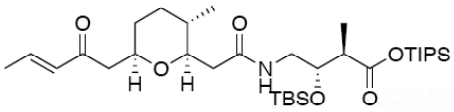
80
60
40
20
ppm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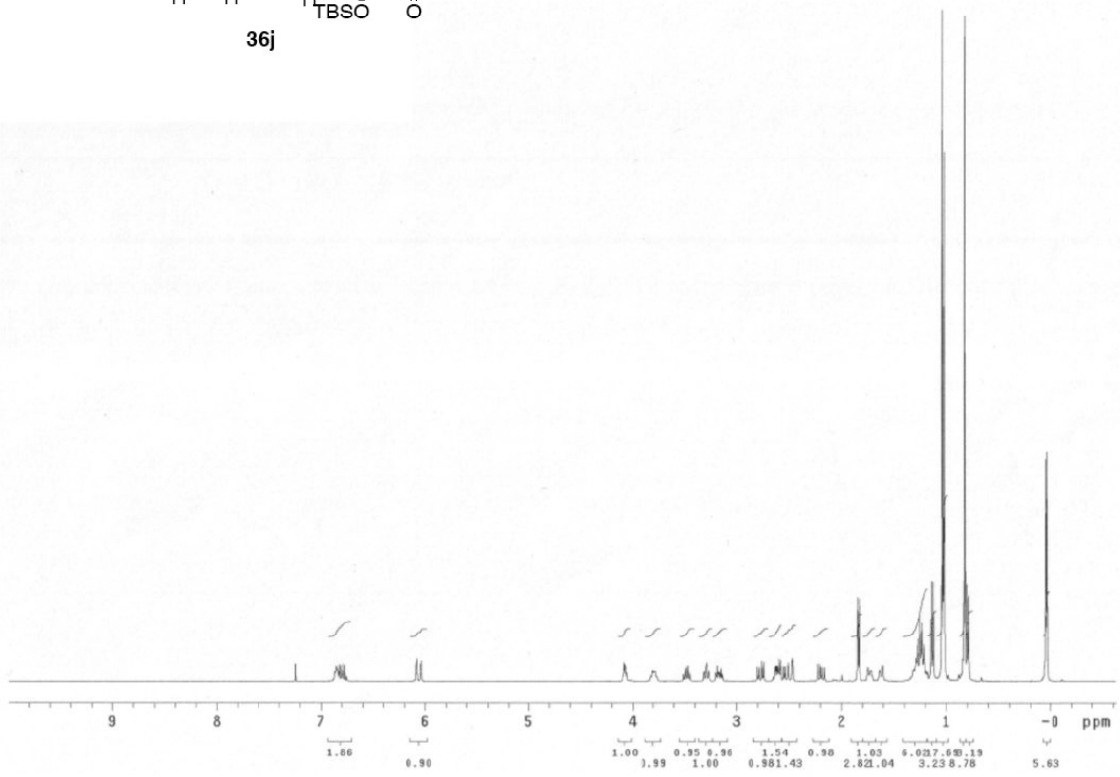
O
O
H
H
N
H
TBSO
OTIPS
O

36j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1
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ppm
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0.90
1.00
0.99
0.95
0.96
1.00
1.54
0.98
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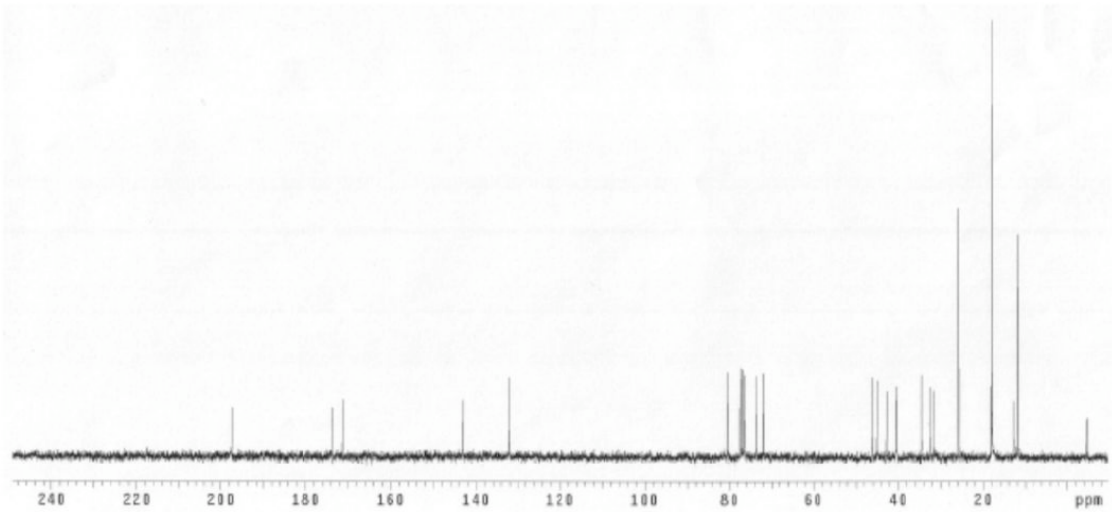
0.98
1.03
2.82
1.04
6.02
17.69
3.23
8.19
8.78
5.63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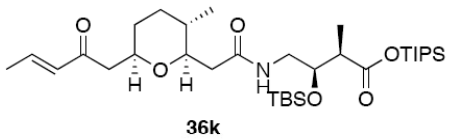
80
60
40
20
ppm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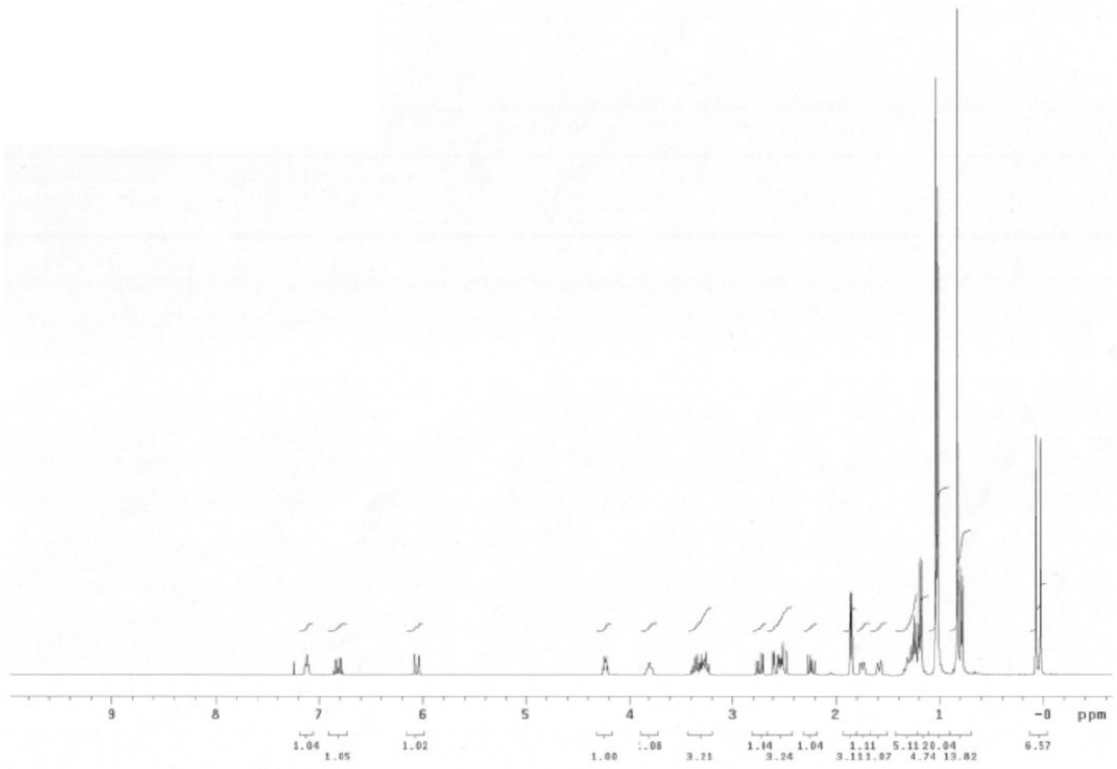
O
O
H
O
H
N
H
TBSO
OTIPS
O

36k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5
4
3
2
1
-0
ppm
1.04
1.05
1.02
1.00
1.08
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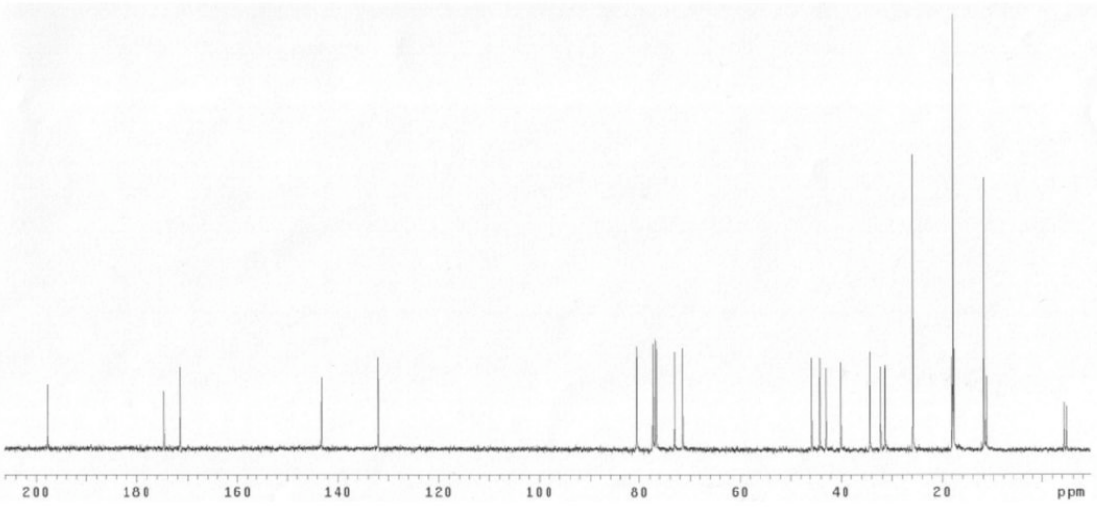
1.04
1.11
3.11
1.07
5.11
4.74
20.04
13.82
6.57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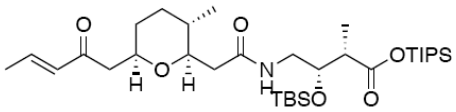
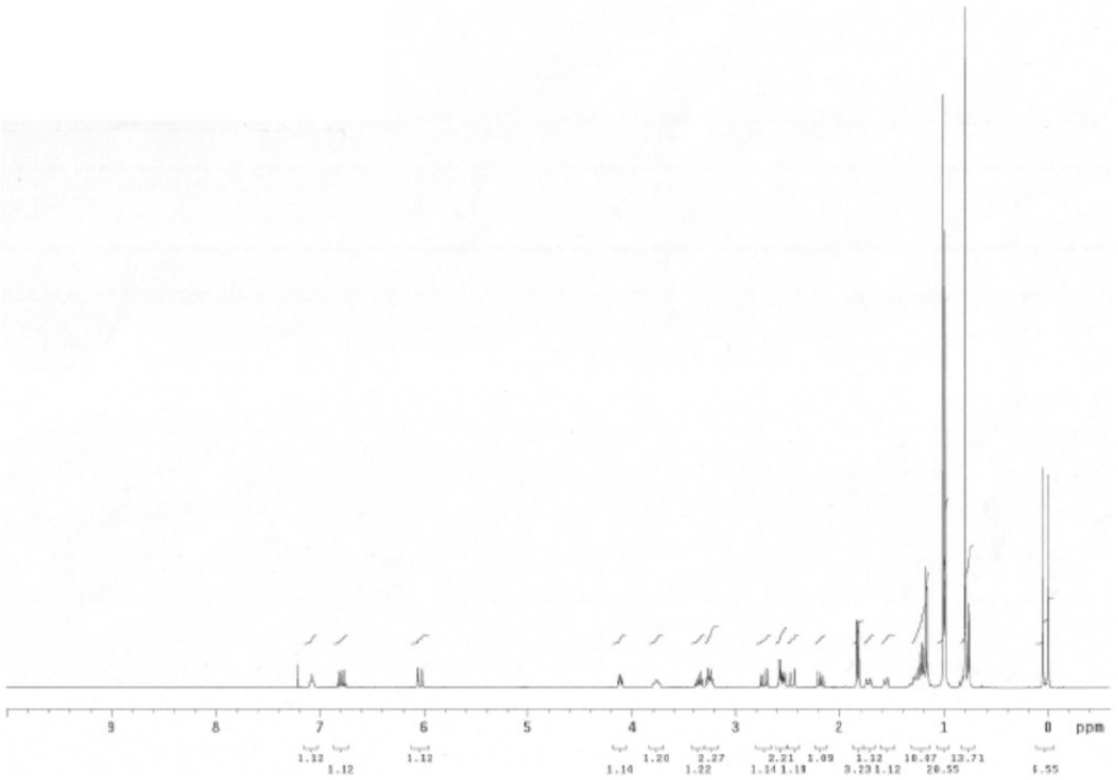
80
60
40
20
ppm


O
O
O
H
H
N
H
TBSO
OTIPS
O

36l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4
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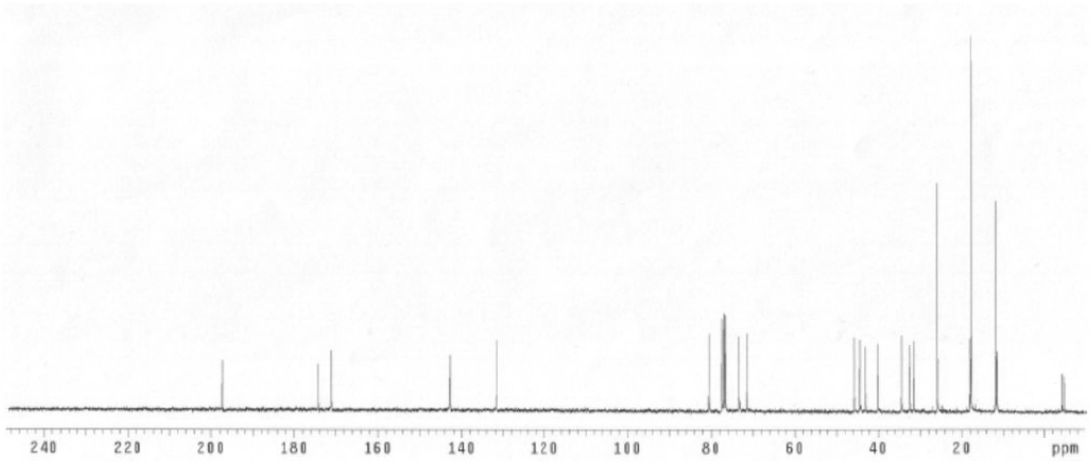
ppm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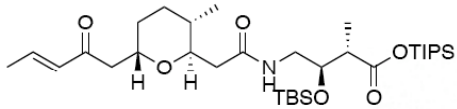
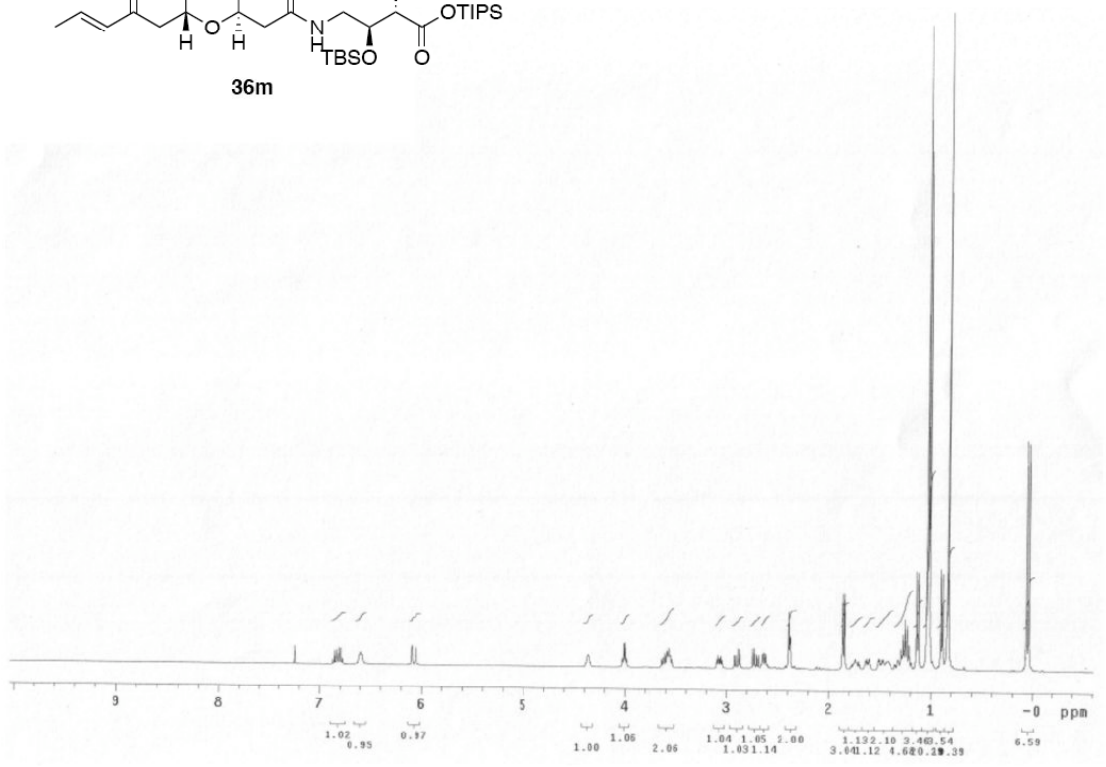

OTIPS
TBSO

36m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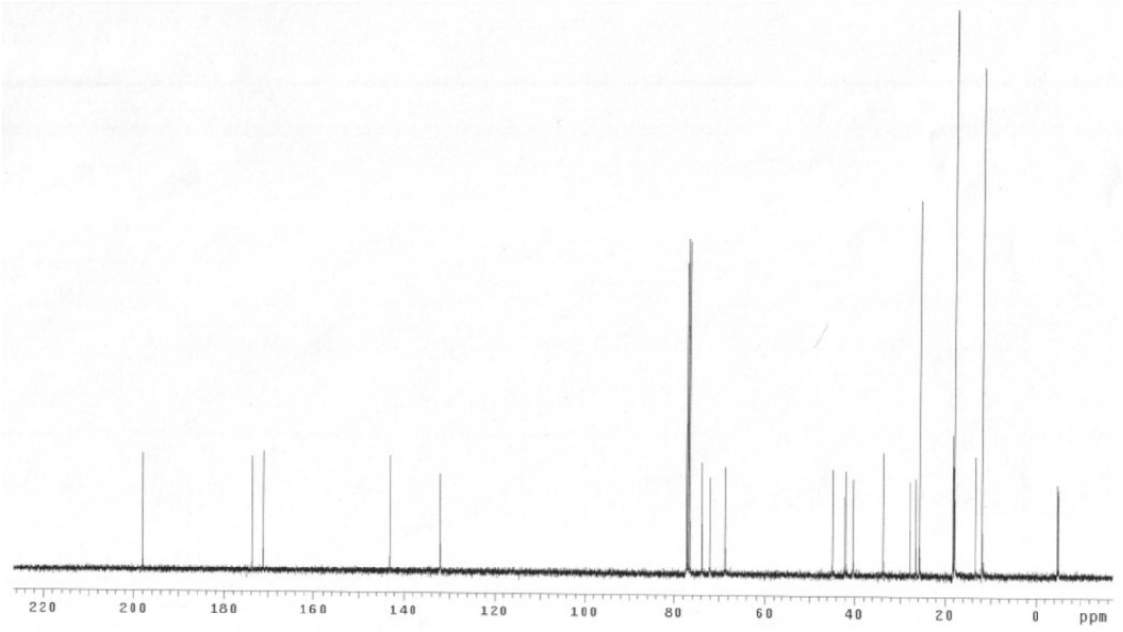
ppm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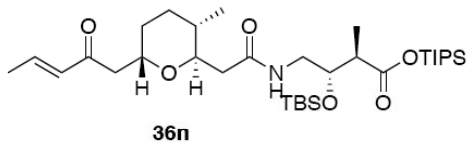
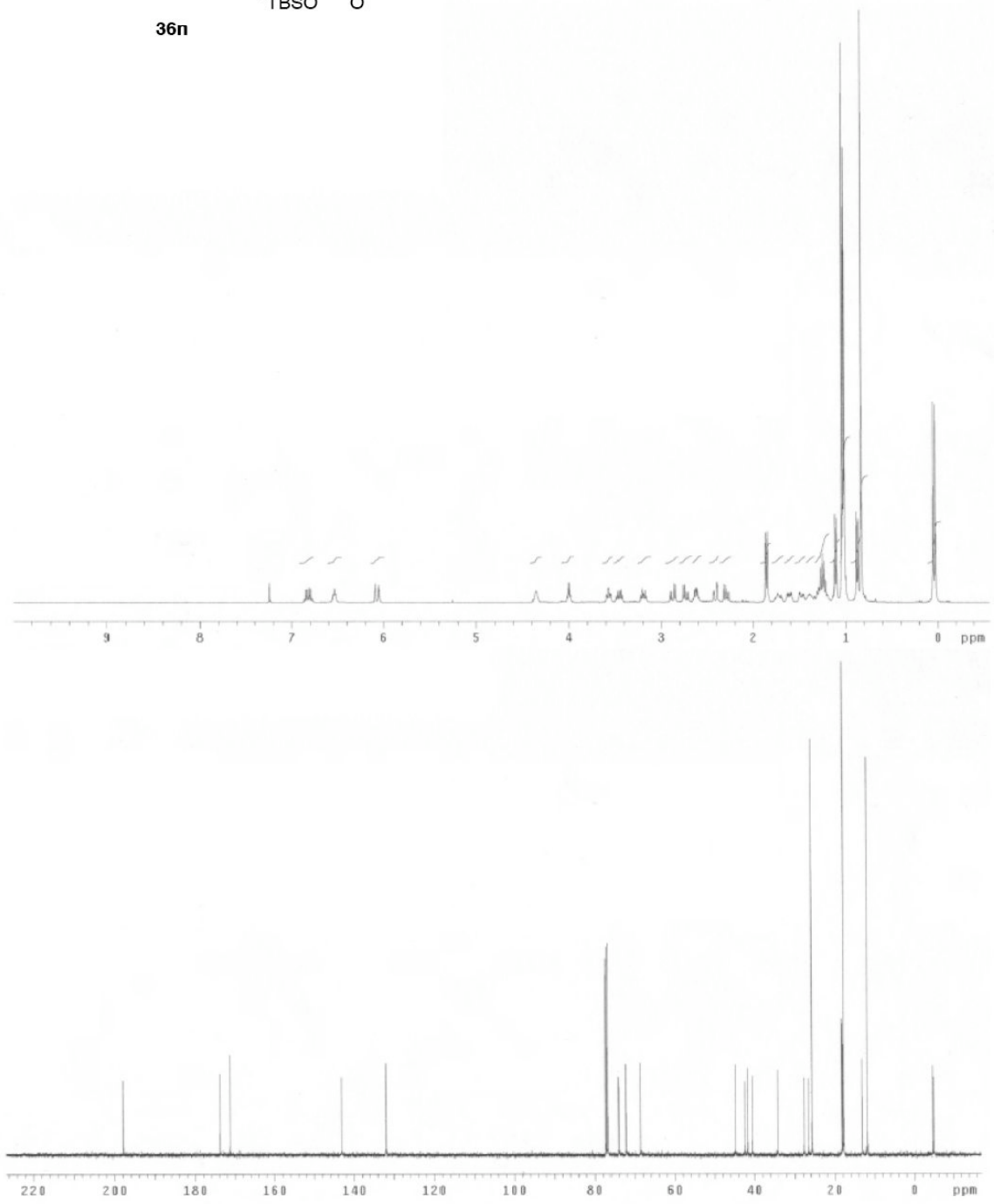

O
O
O
H
H
N
H
TBSO
OTIPS
O

36n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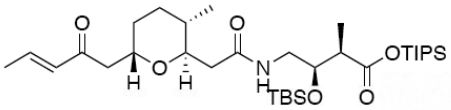
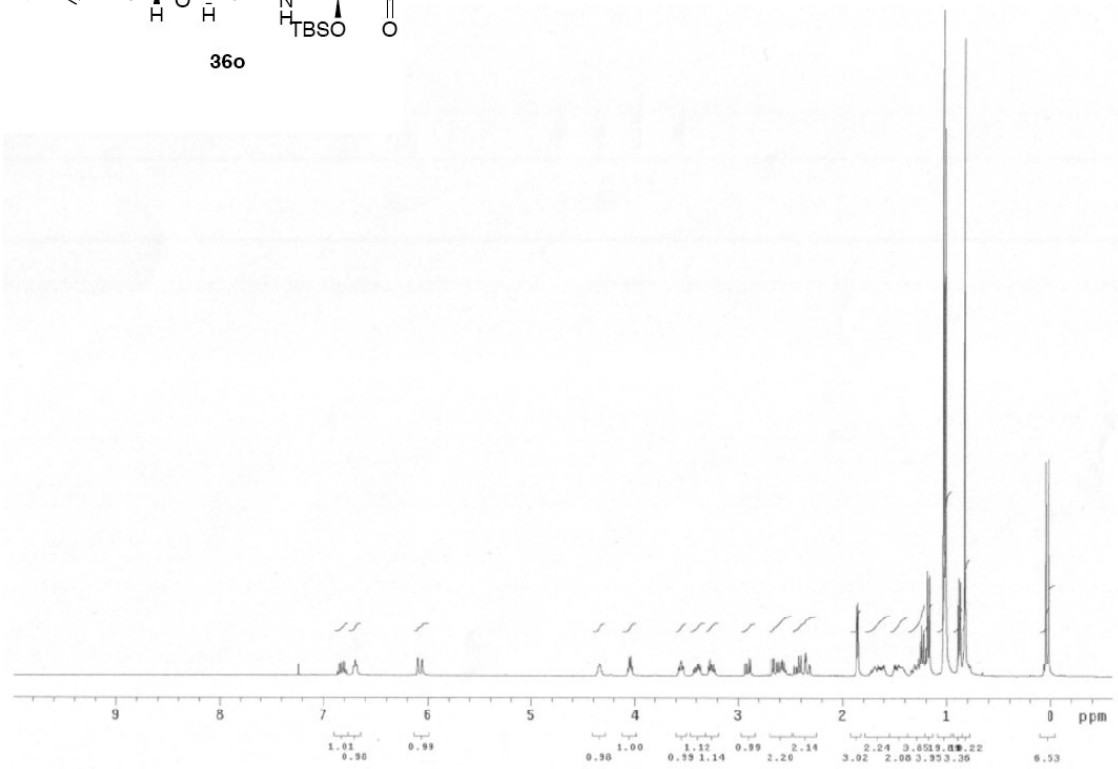

O
O
OTIPS
O
H
O
H
N
H
TBSO
O

36o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4
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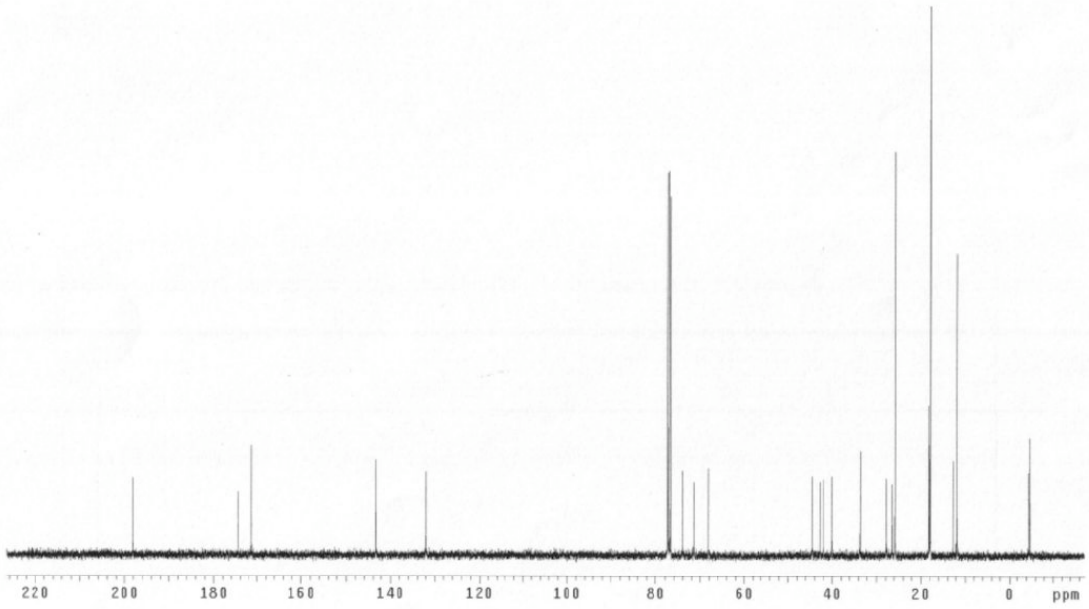
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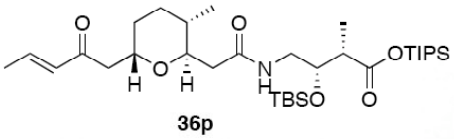
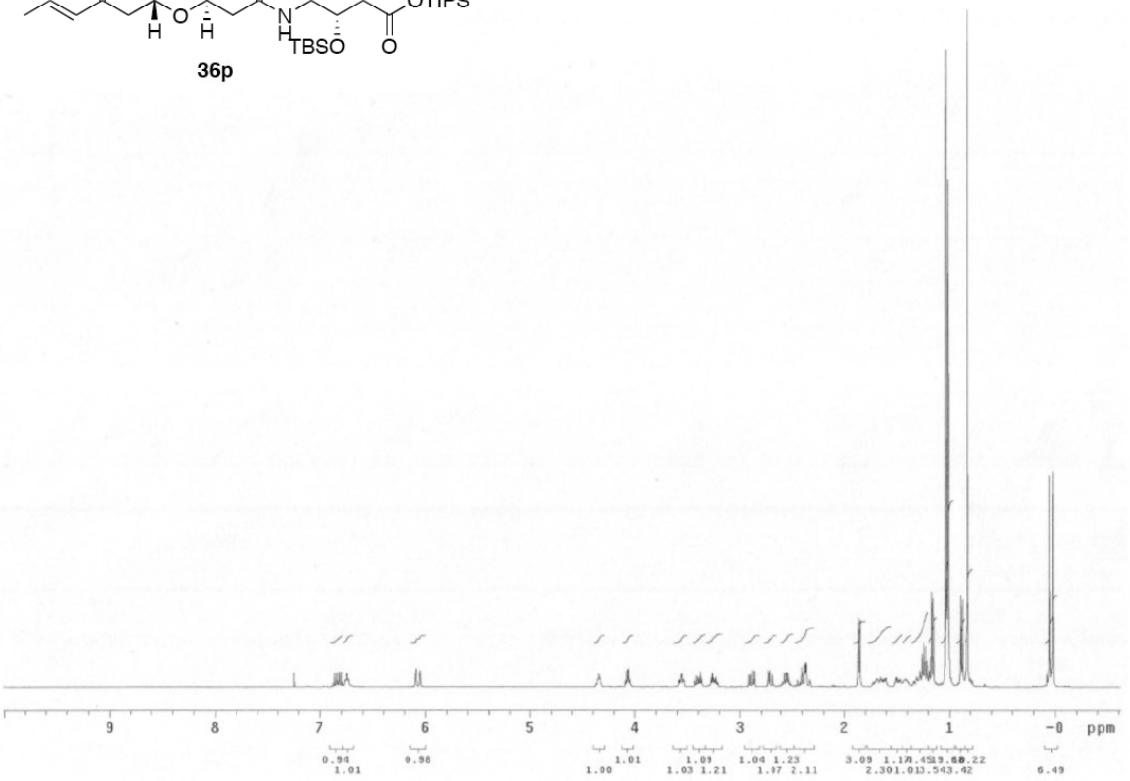
ppm


O
O
O
H
H
N
H
TBSO
OTIPS
O

36p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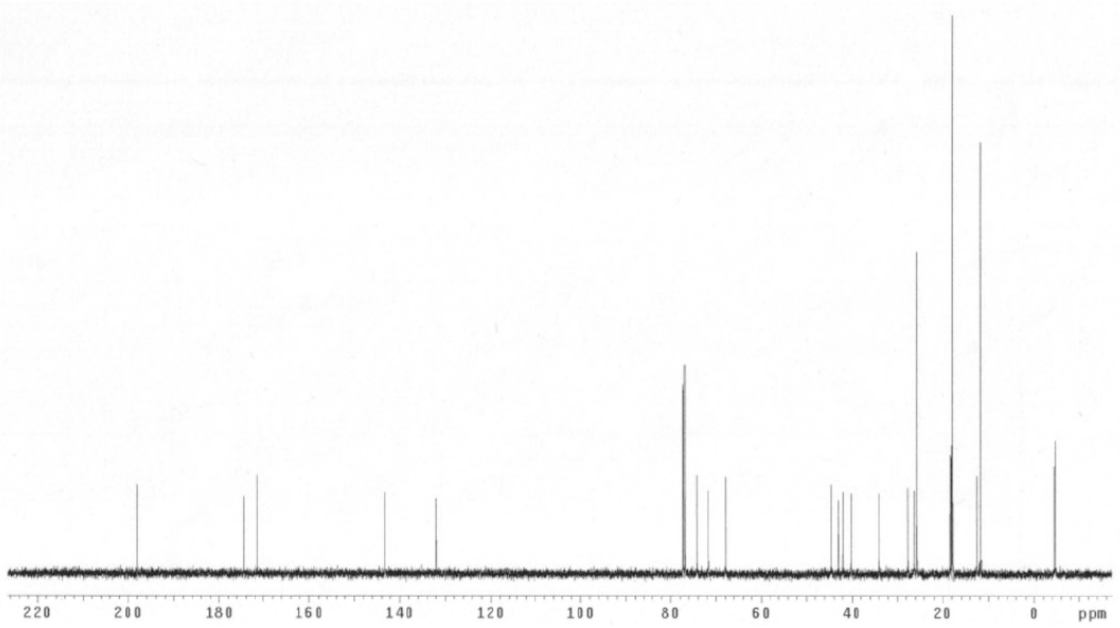
ppm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120
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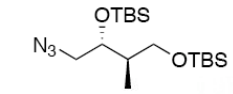
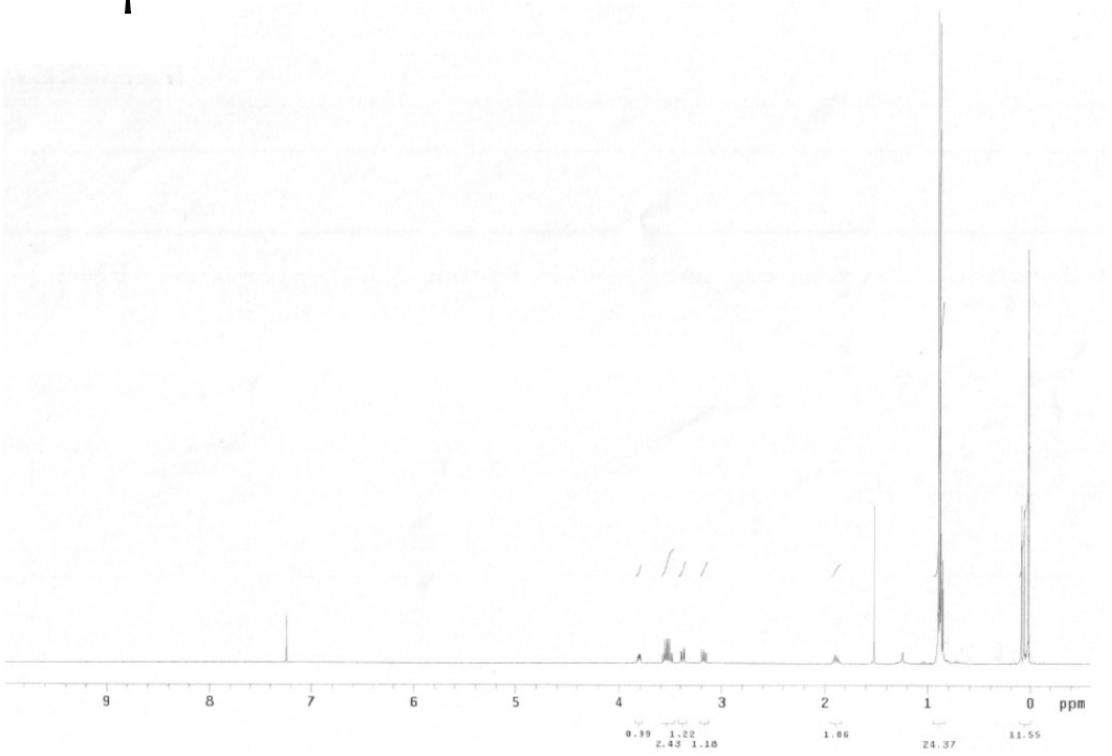

OTBS
N3
OTBS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8
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5
4
3
2
1
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ppm
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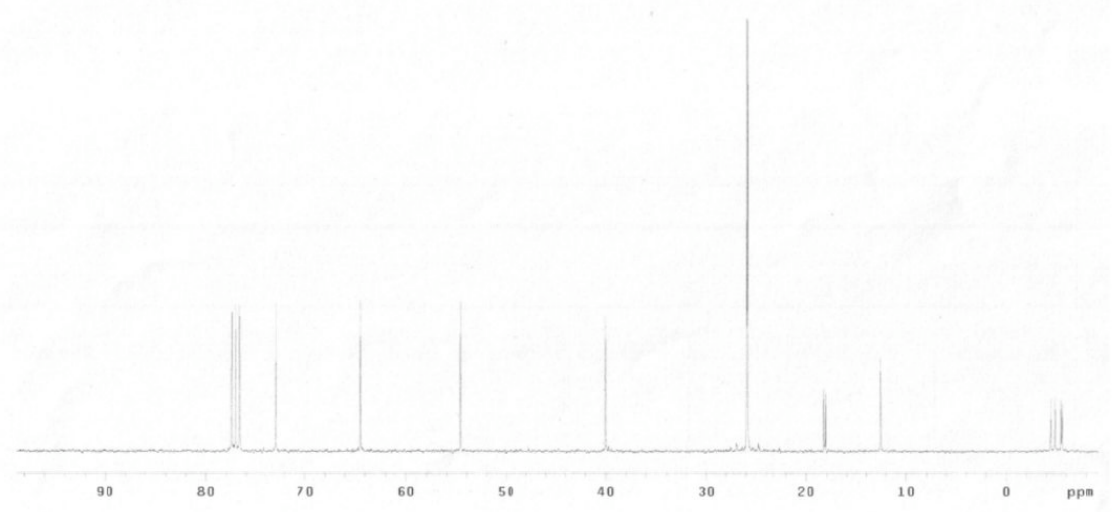
1.22
2.43
1.18
1.86
24.37
11.55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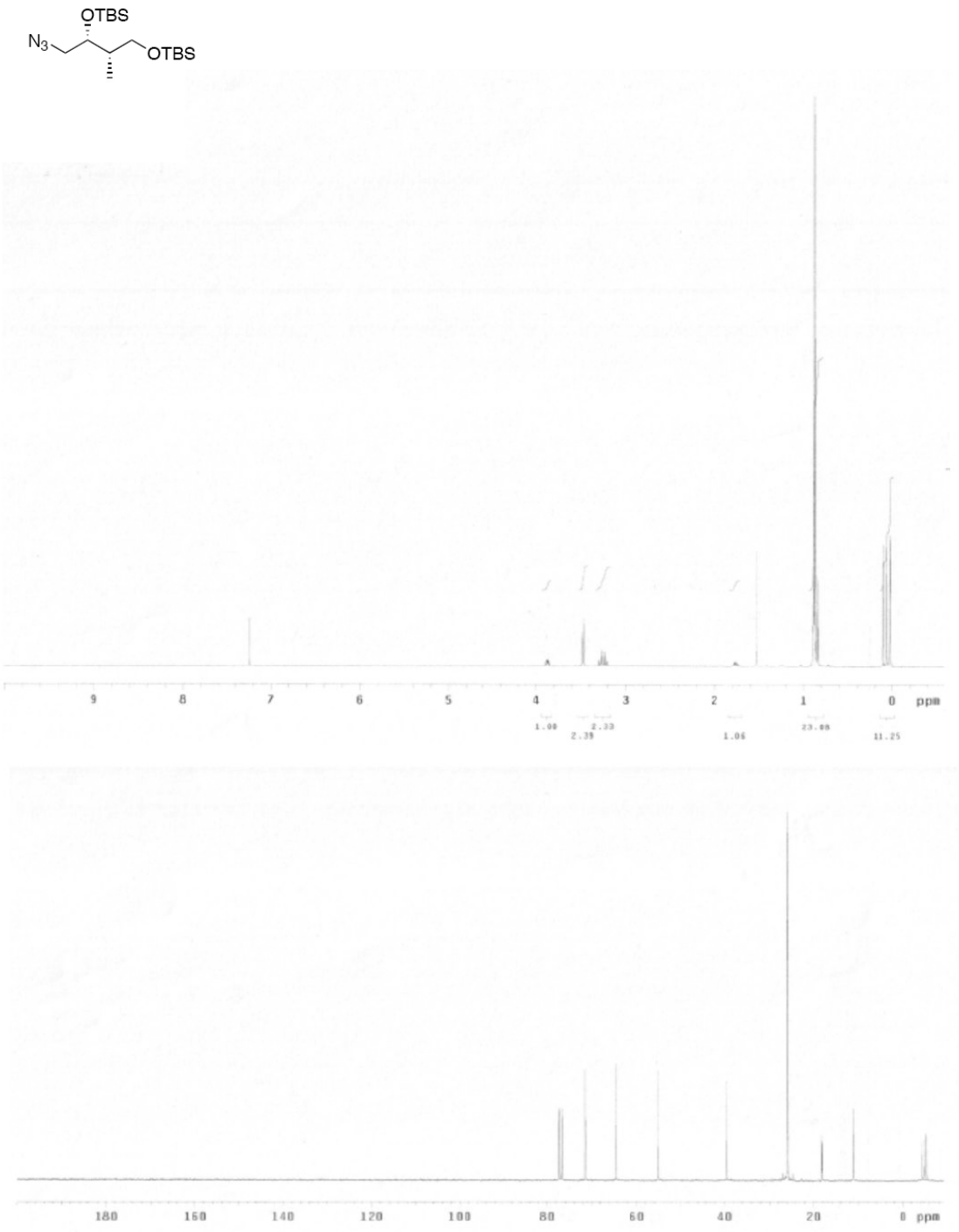
60
50
40
30
20
10
0
ppm


OTBS
N3
OTBS
9
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5
4
3
2
1
0
ppm
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2.39
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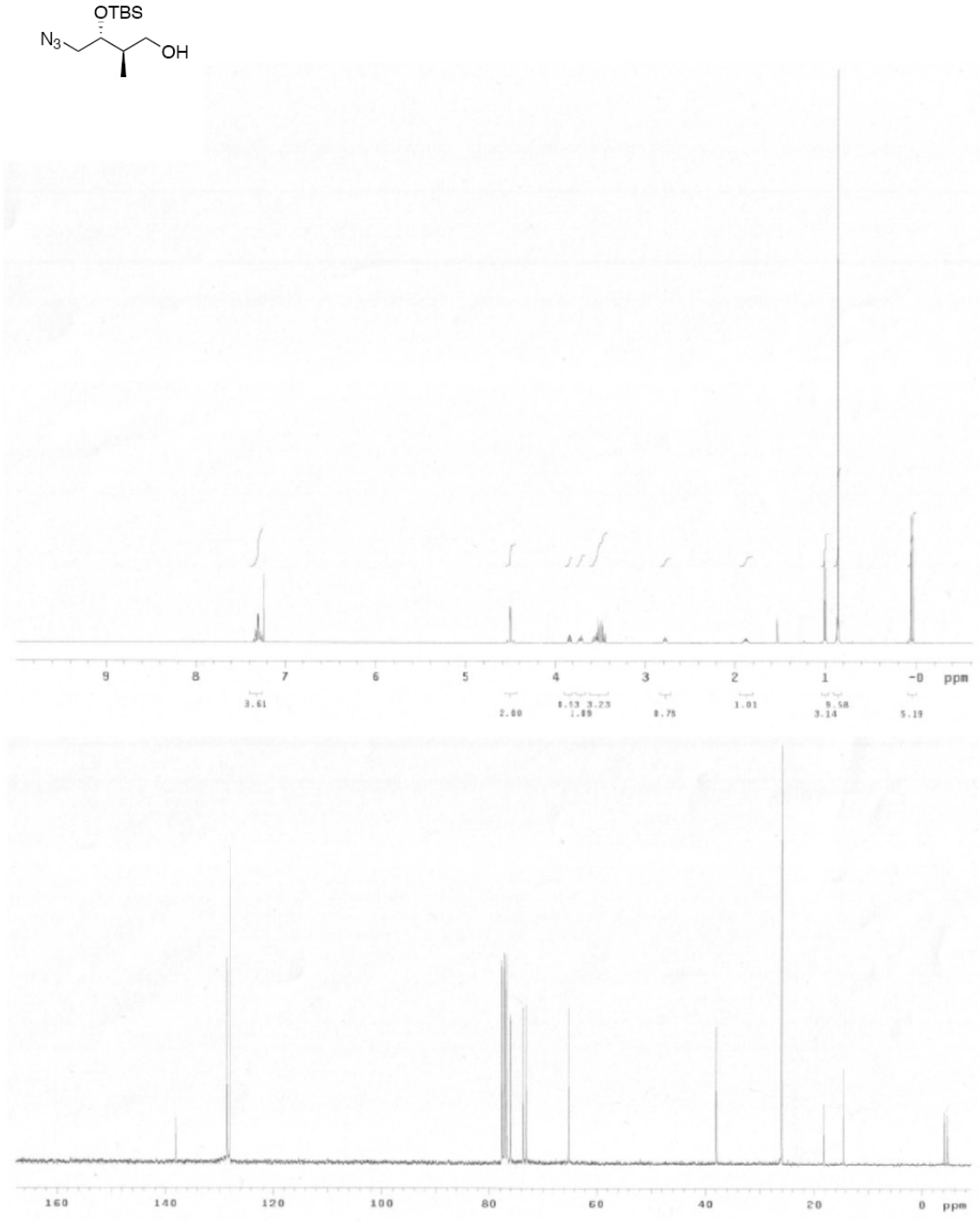
1.06
23.00
11.25
180
160
140
120
100
80
60
40
20
0
ppm


OTBS
N3
OH
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8
7
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5
4
3
2
1
-0
ppm
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1.89
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120
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40
20
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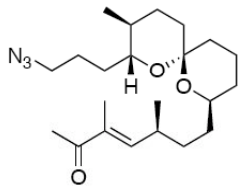
ppm


N3
H
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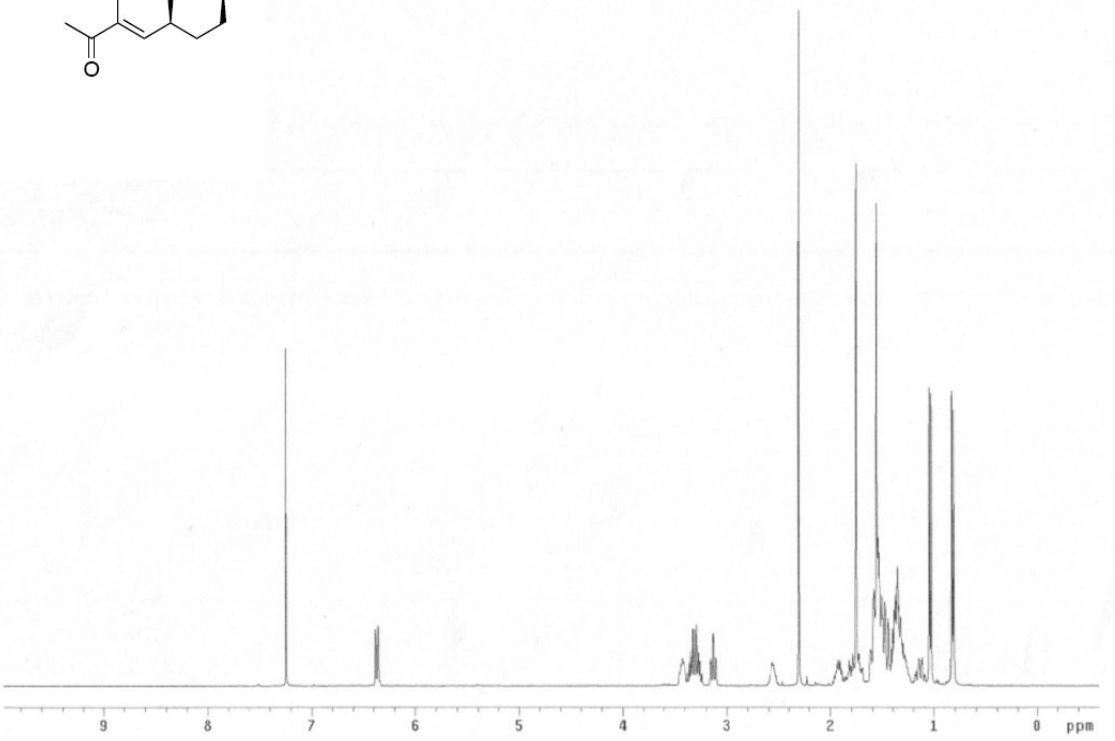
O
O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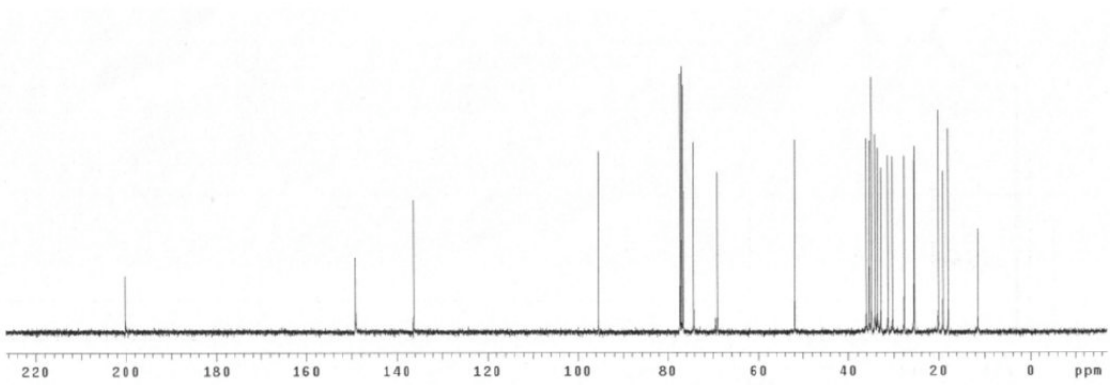
0
ppm


220
200
180
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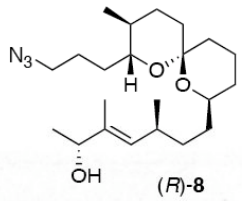
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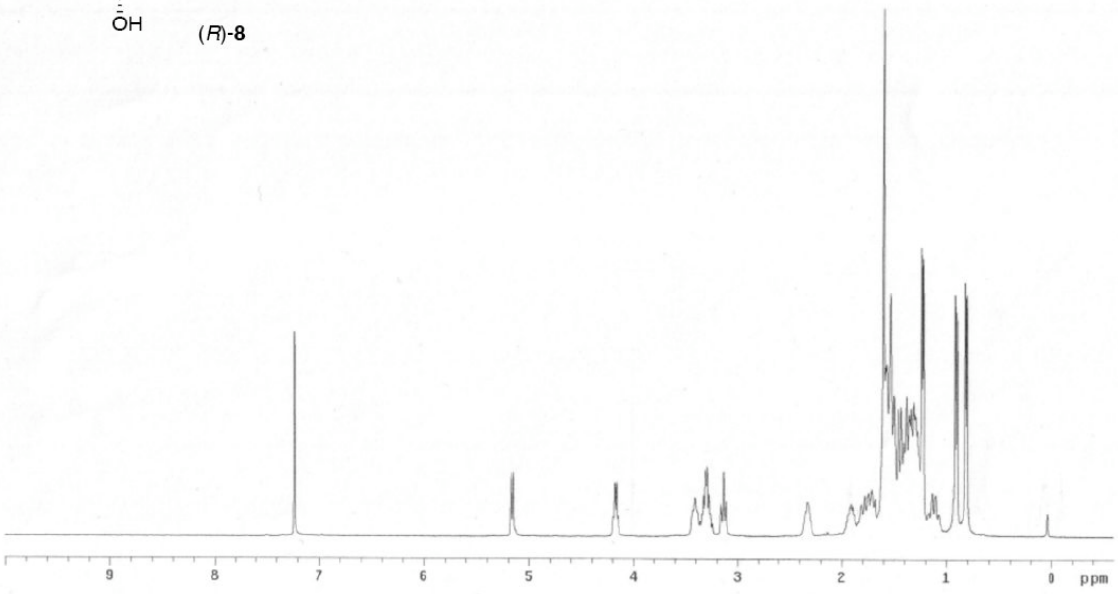
(*R*)-**8**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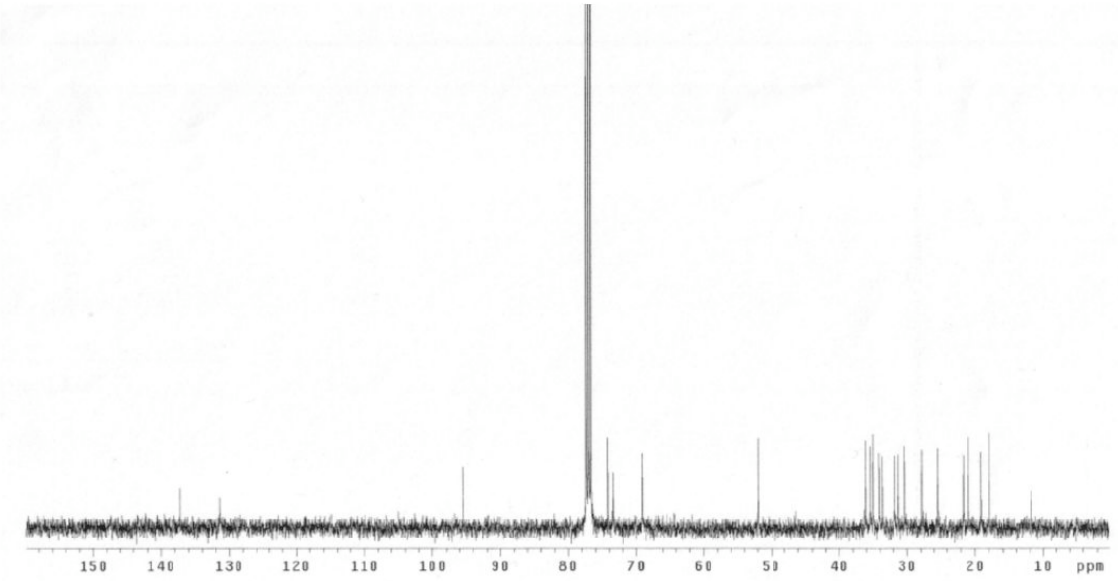
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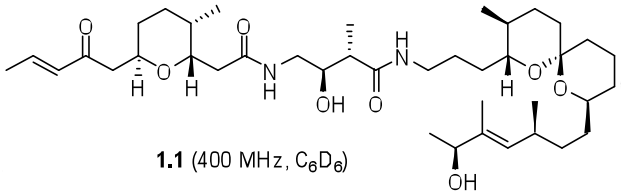
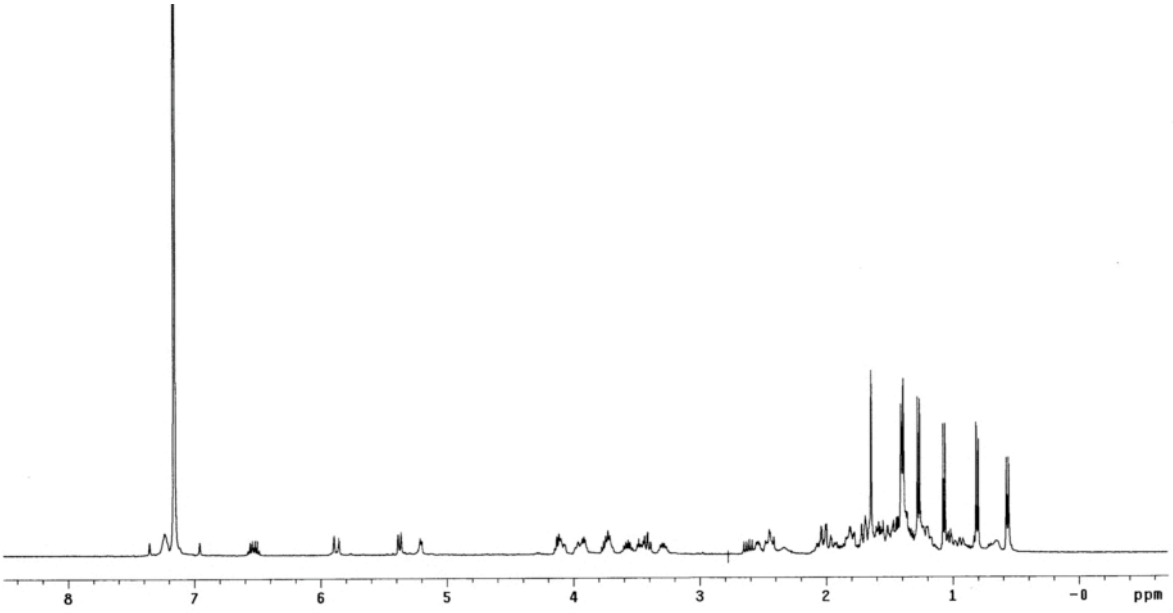
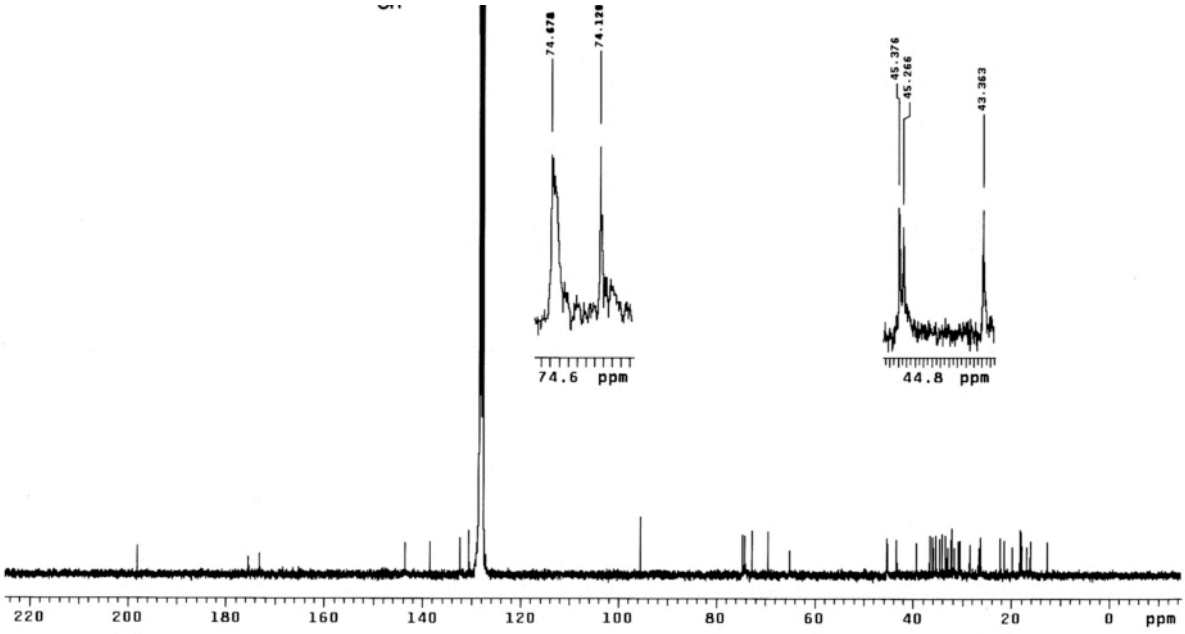
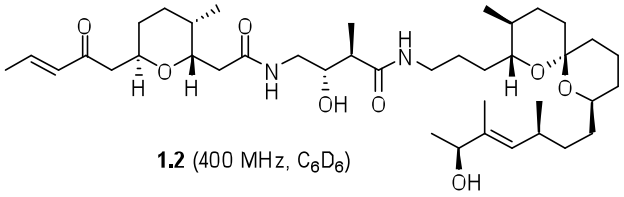


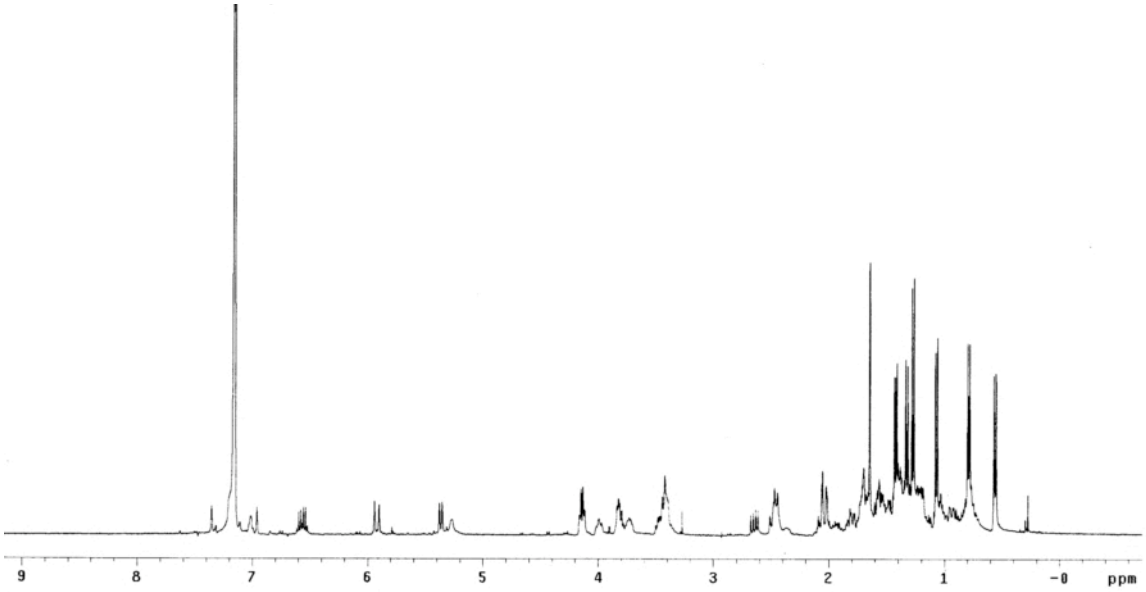
1.1 (400 MHz, C_6D_6)

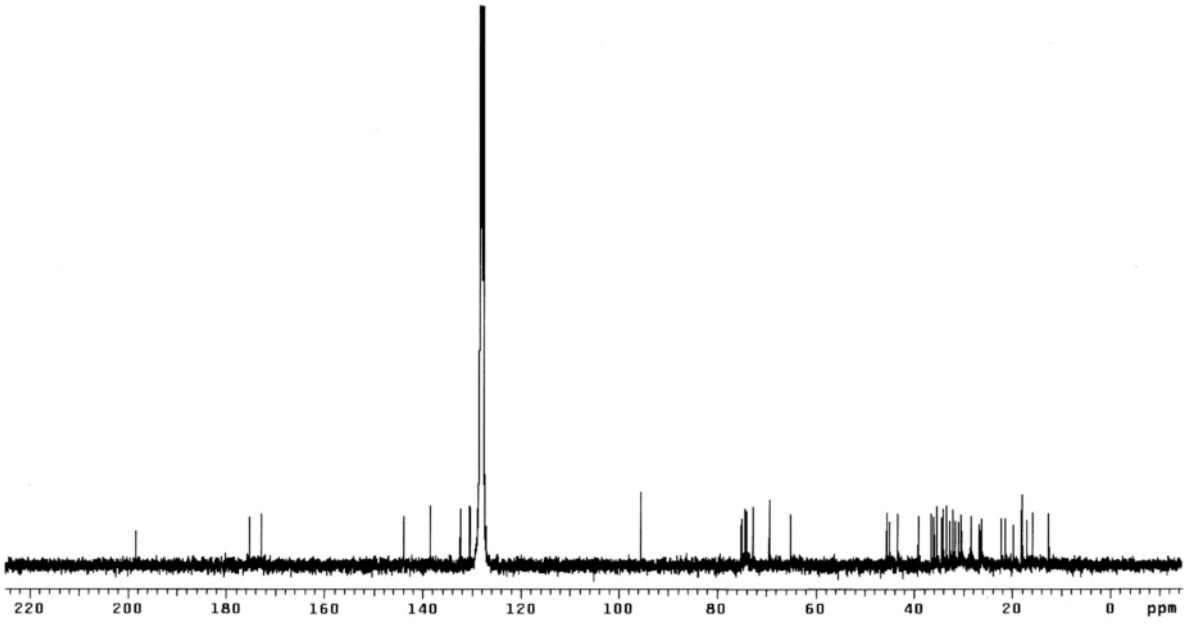


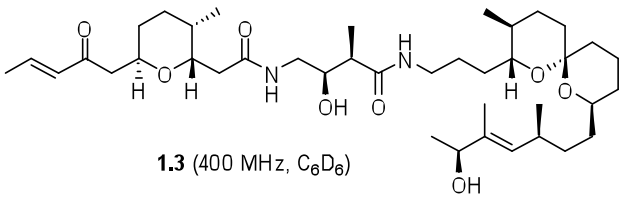




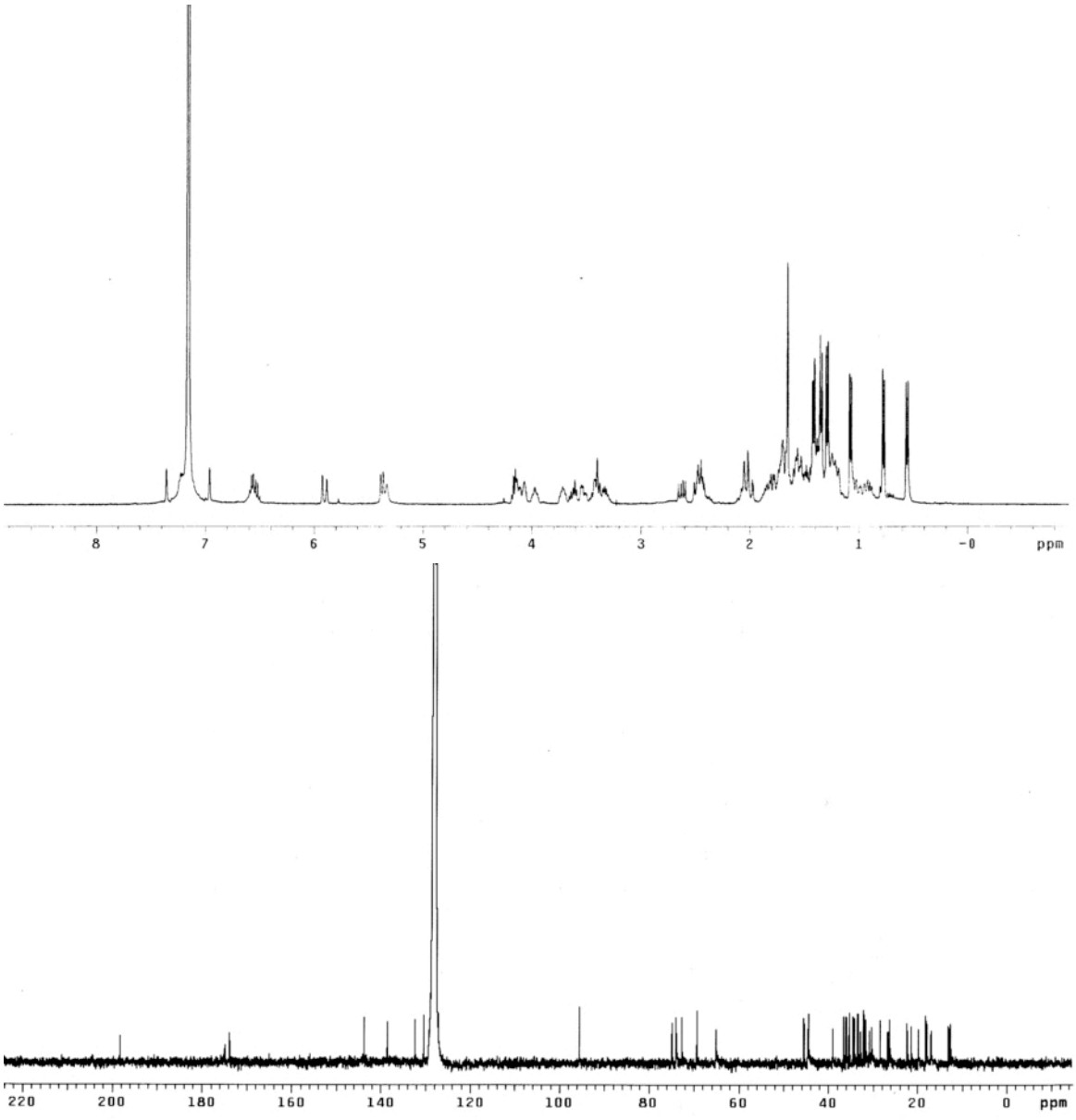
1.2 (400 MHz, C_6D_6)

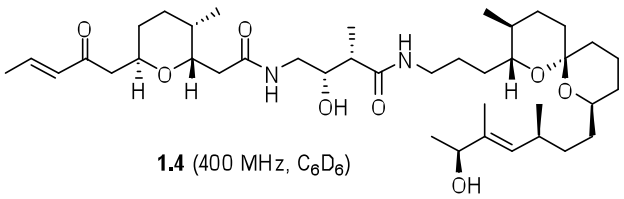




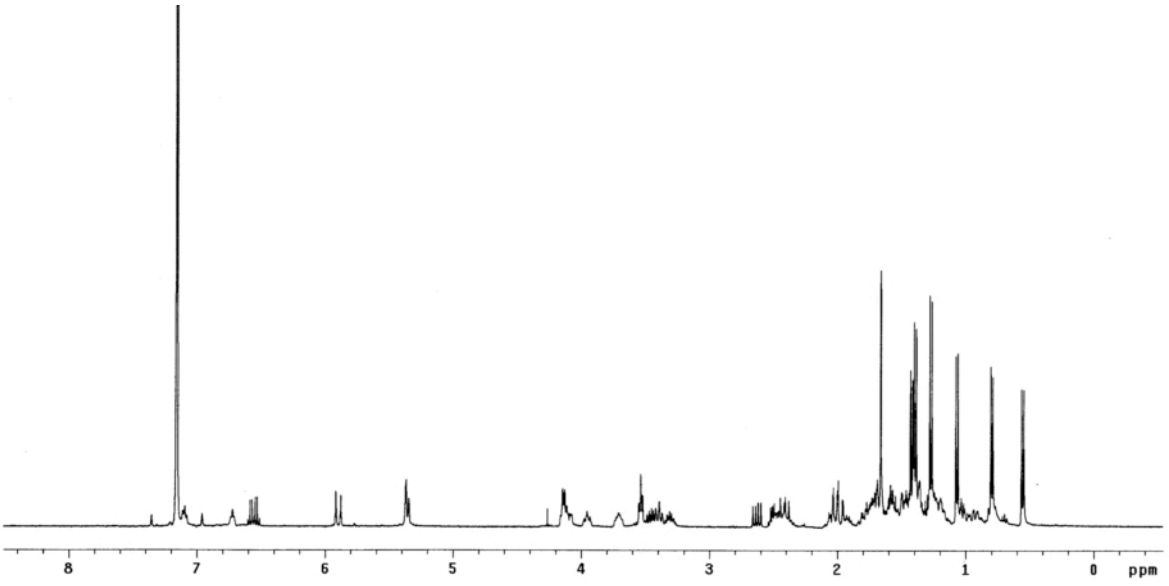


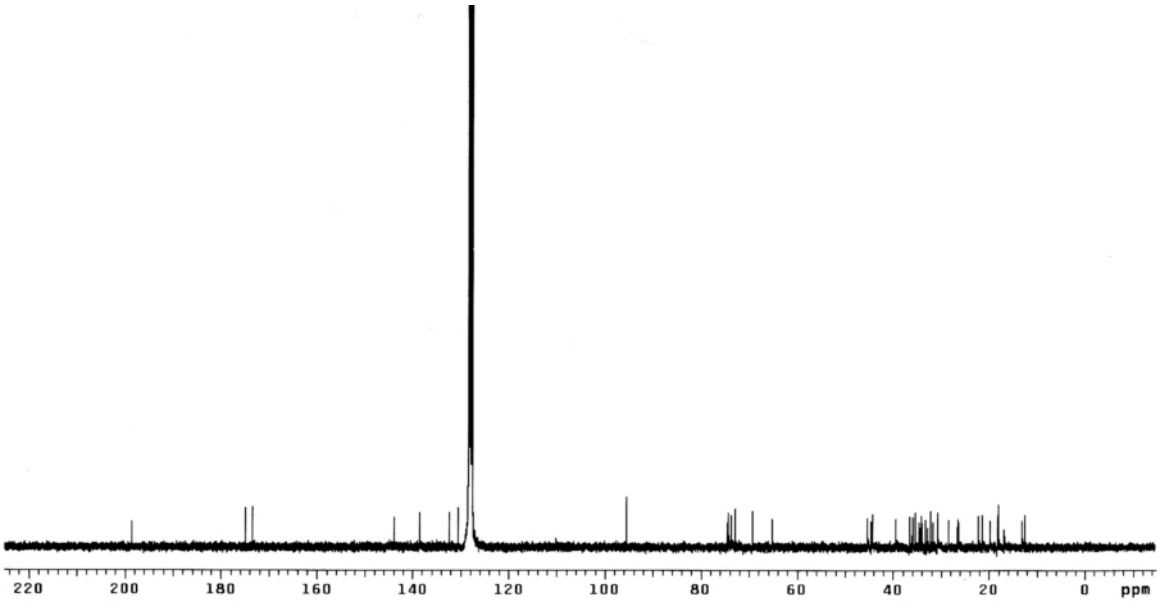
1.3 (400 MHz, C_6D_6)

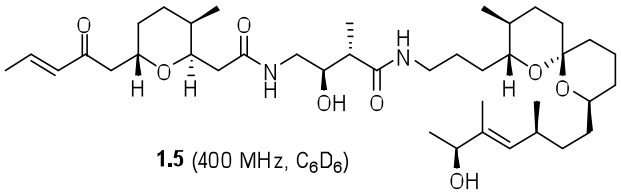




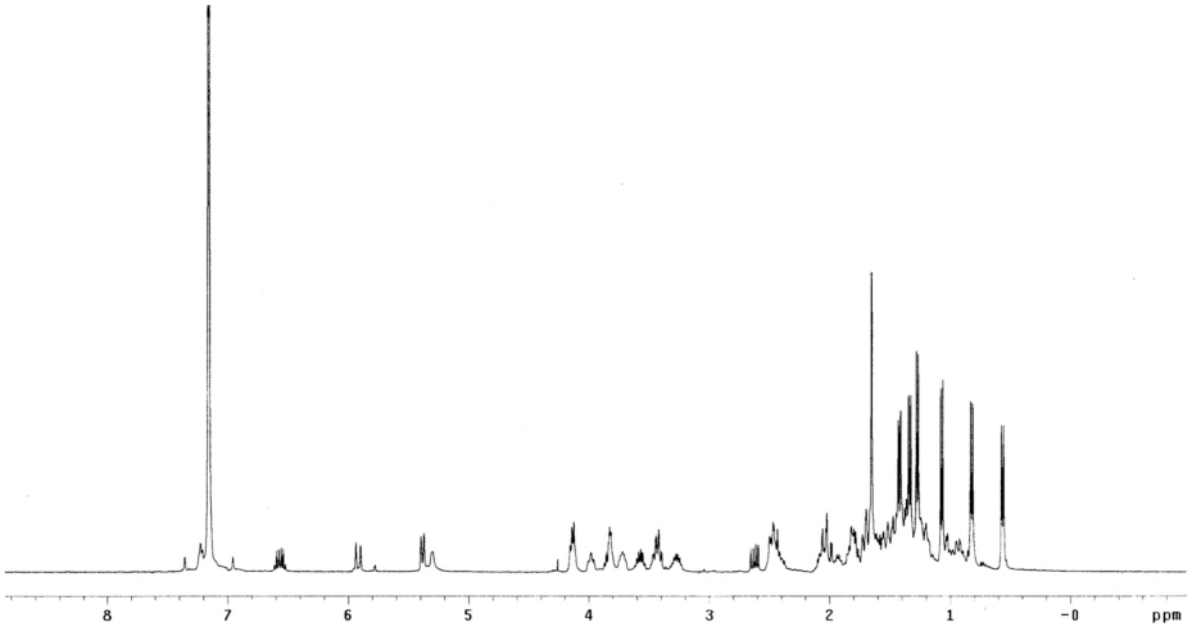
1.4 (400 MHz, C_6D_6)

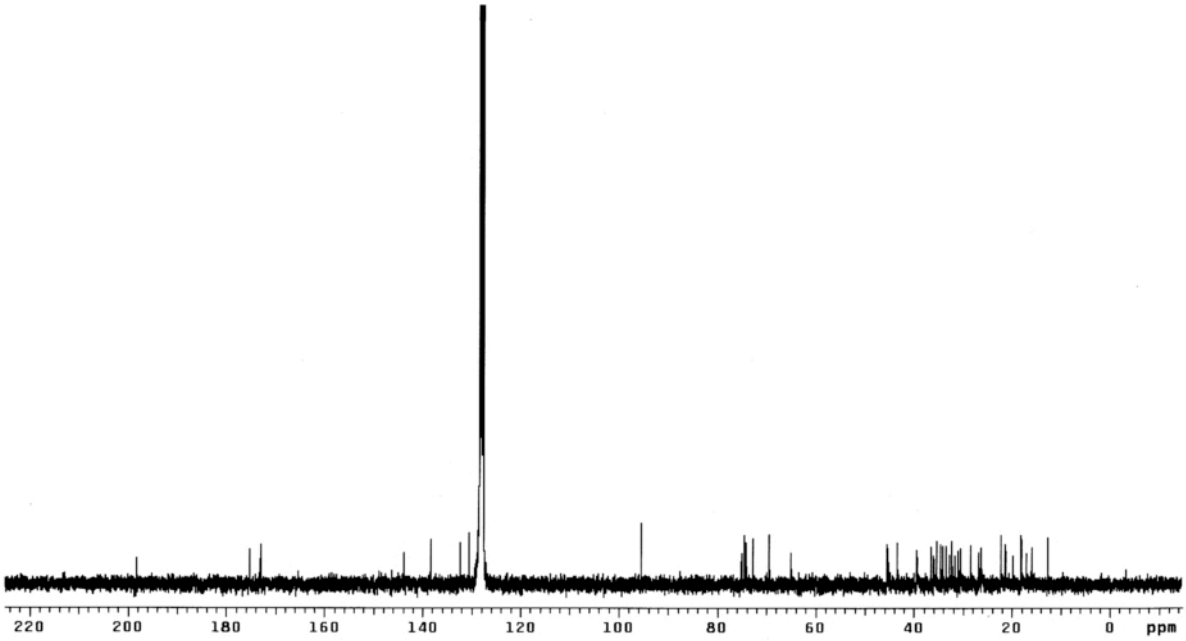


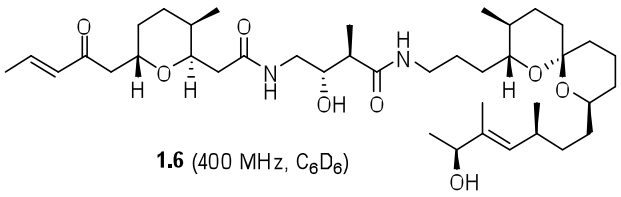




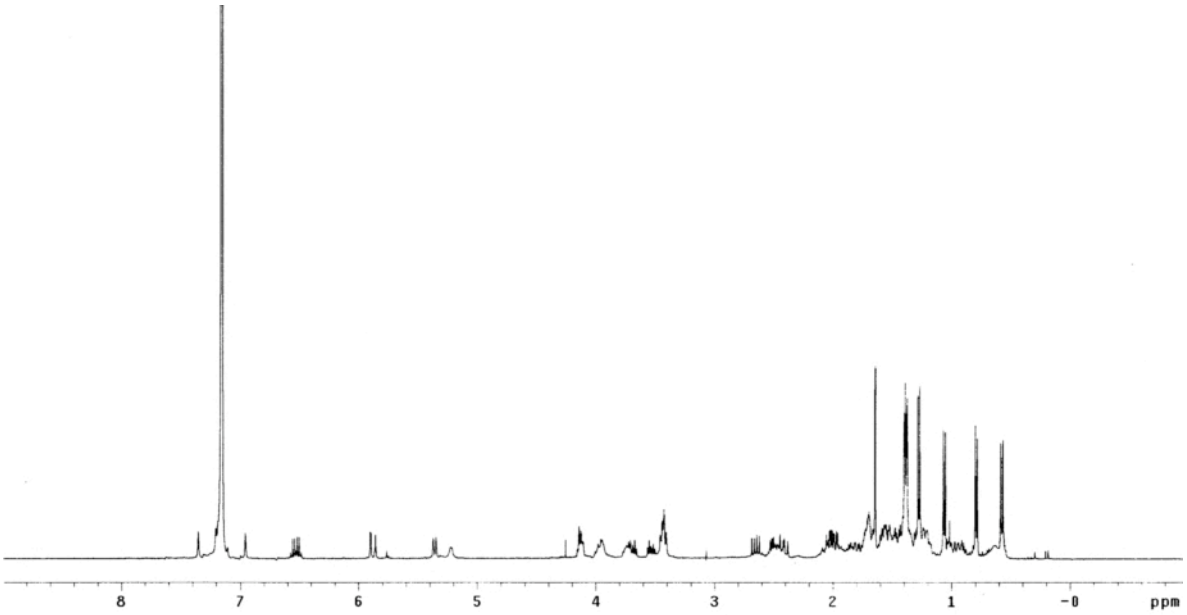
1.5 (400 MHz, C_6D_6)

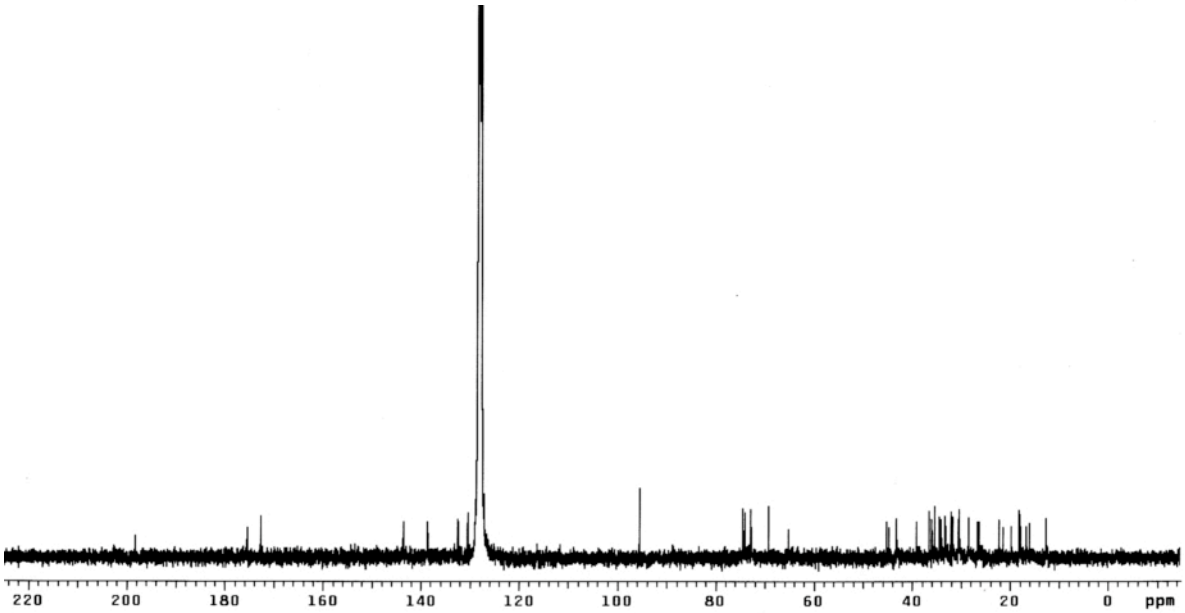


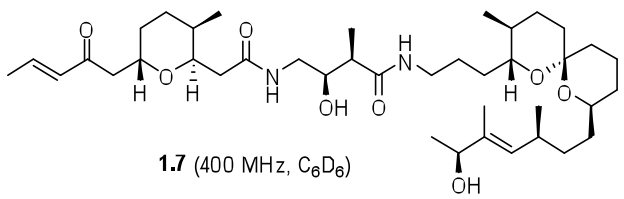




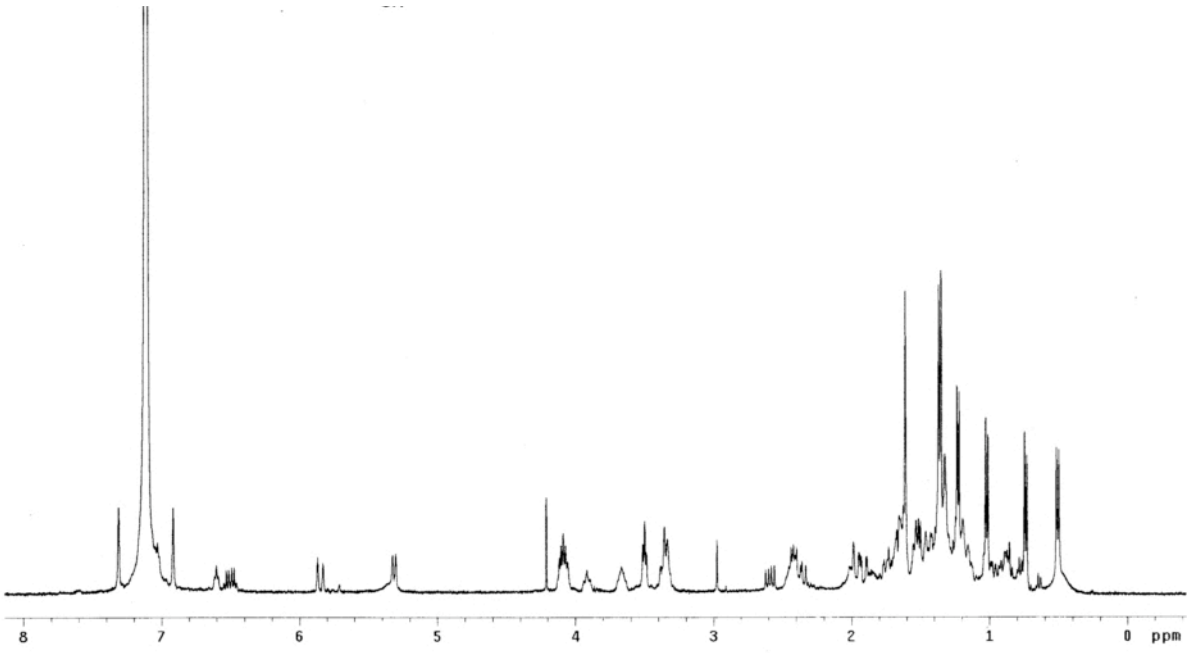
1.6 (400 MHz, C_6D_6)

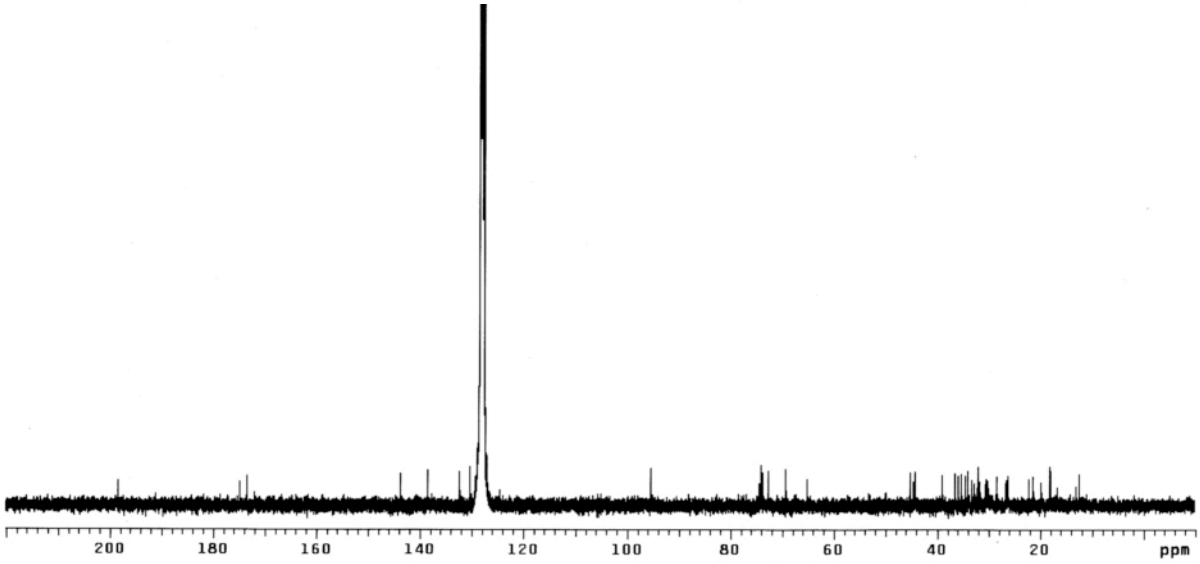


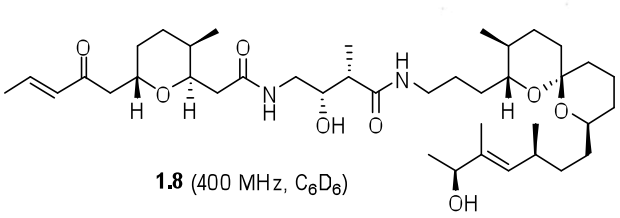




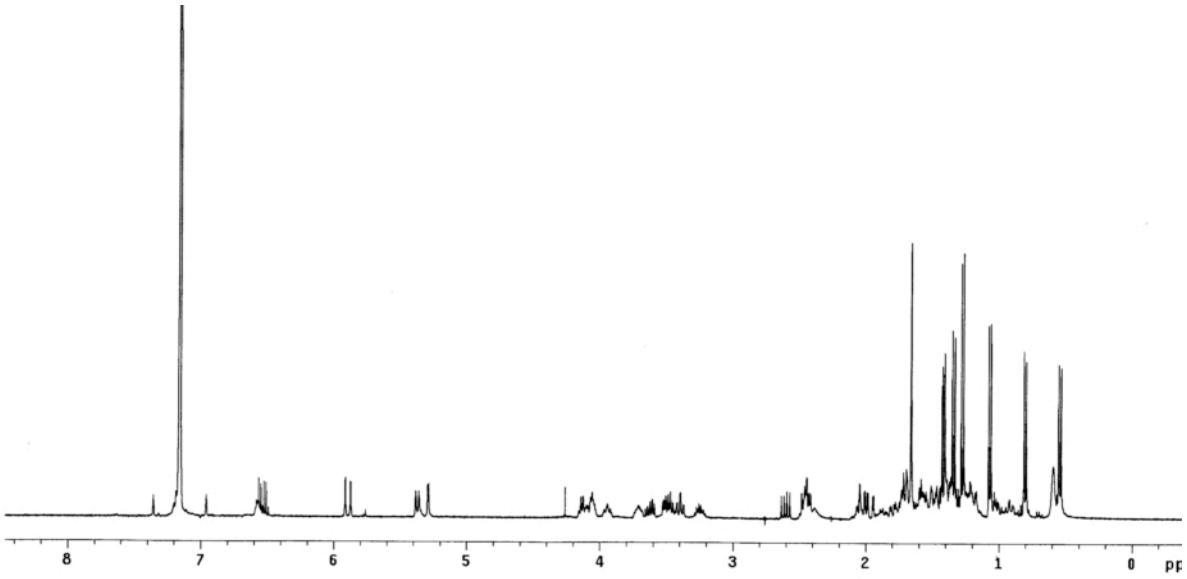
1.7 (400 MHz, C_6D_6)

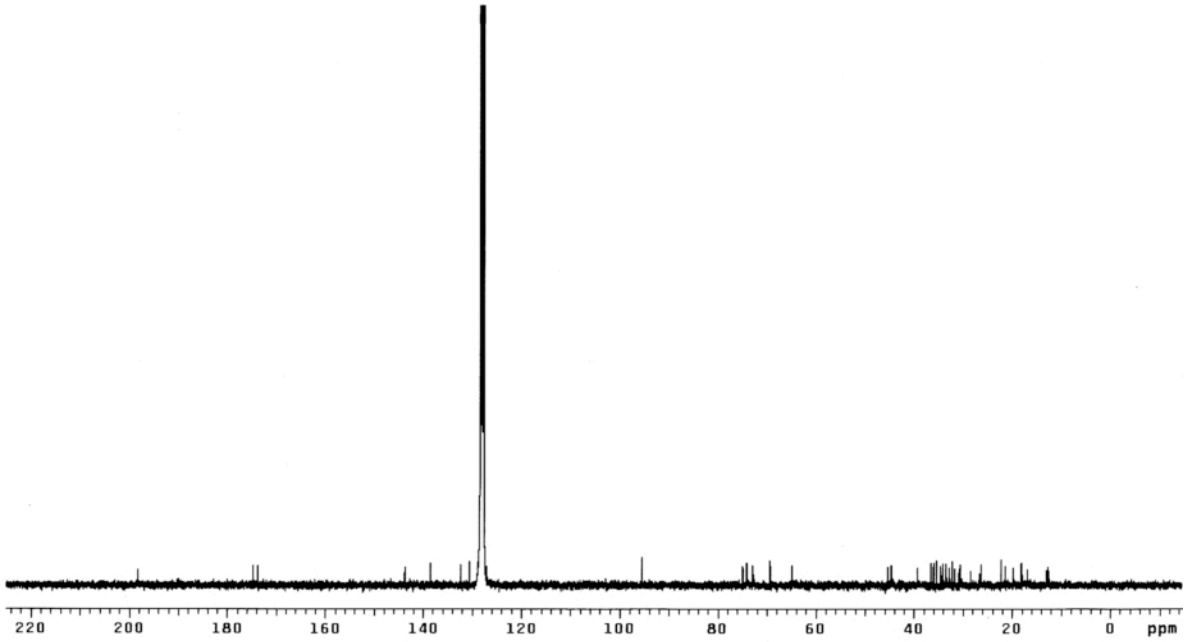


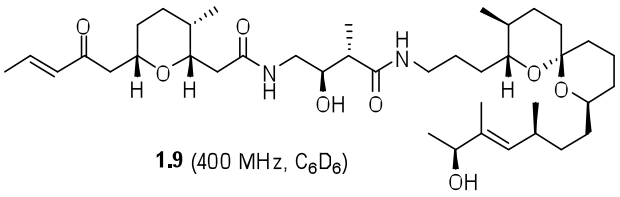




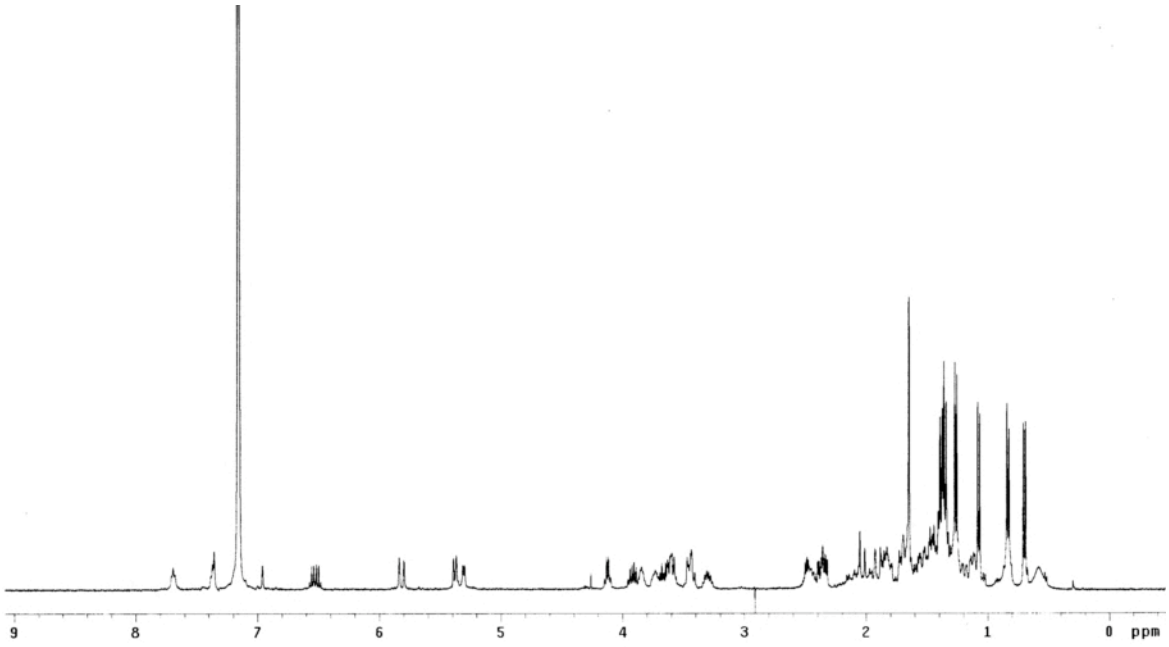
1.8 (400 MHz, C_6D_6)

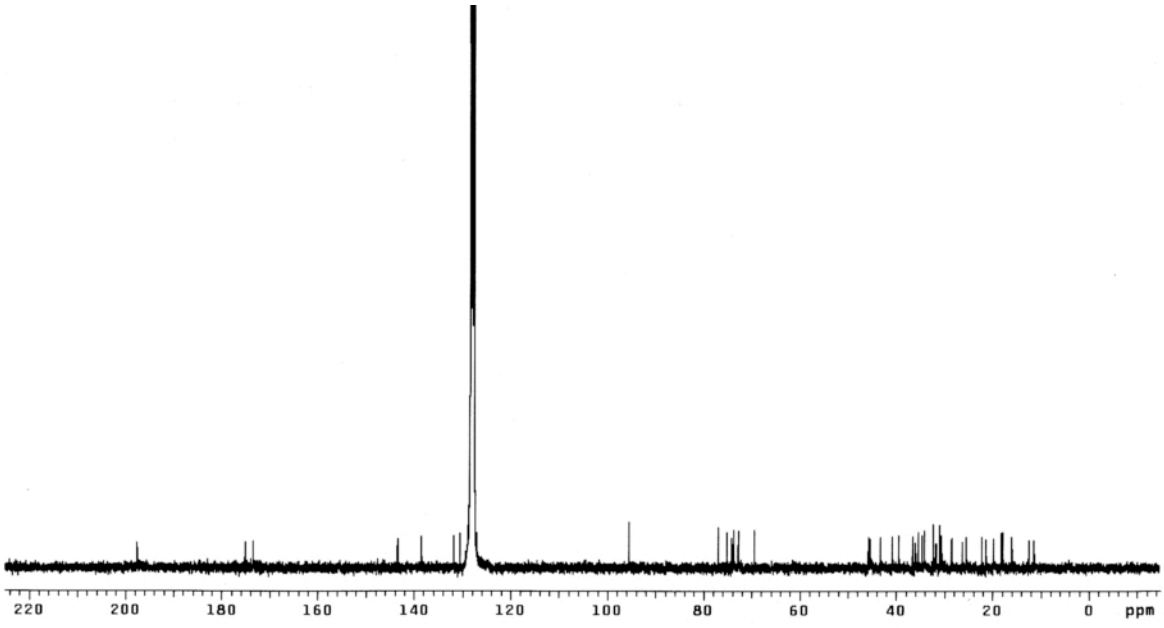


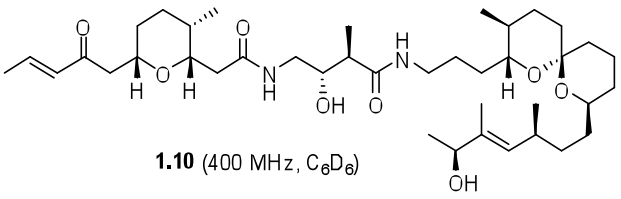




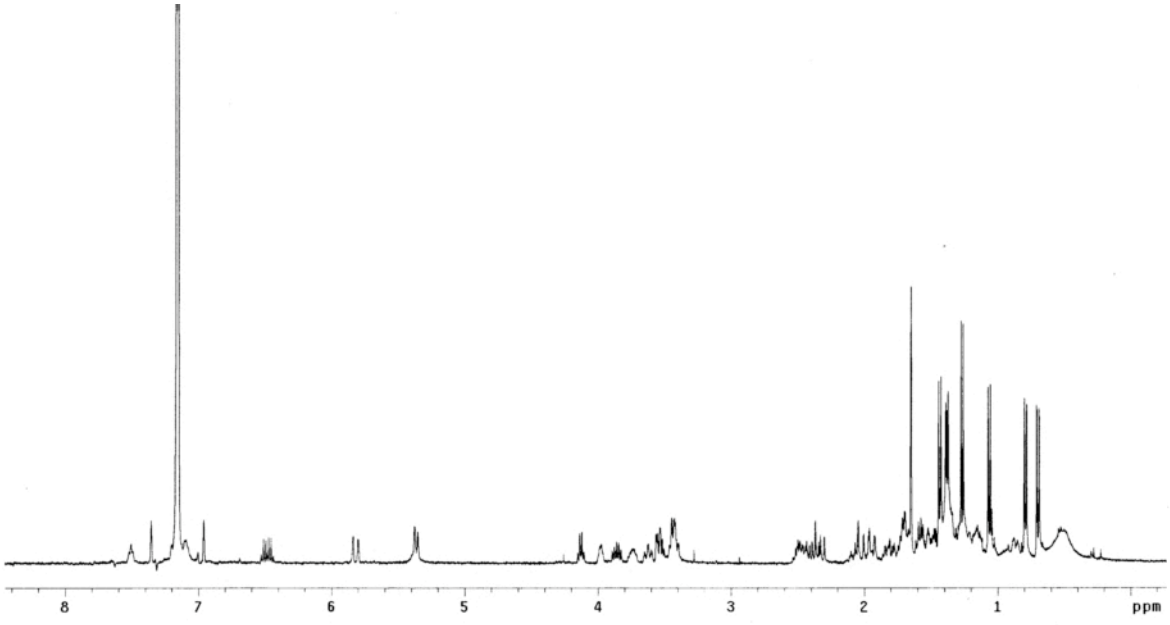
1.9 (400 MHz, C_6D_6)

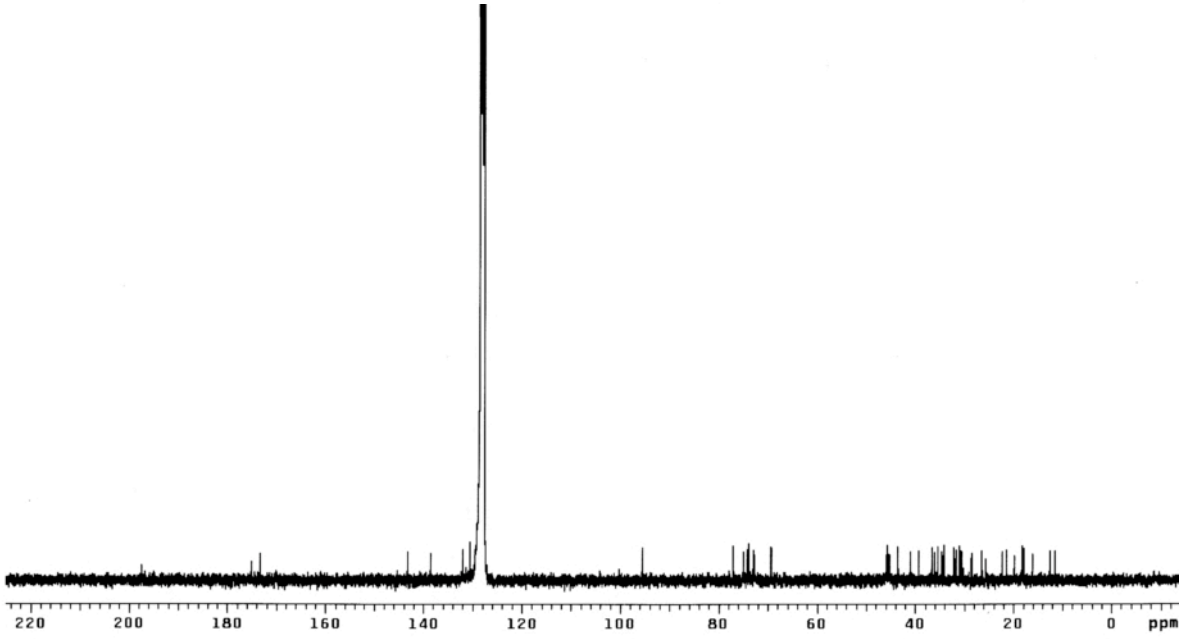


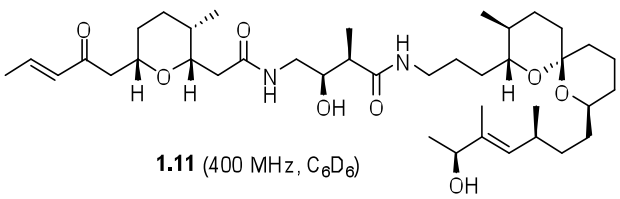




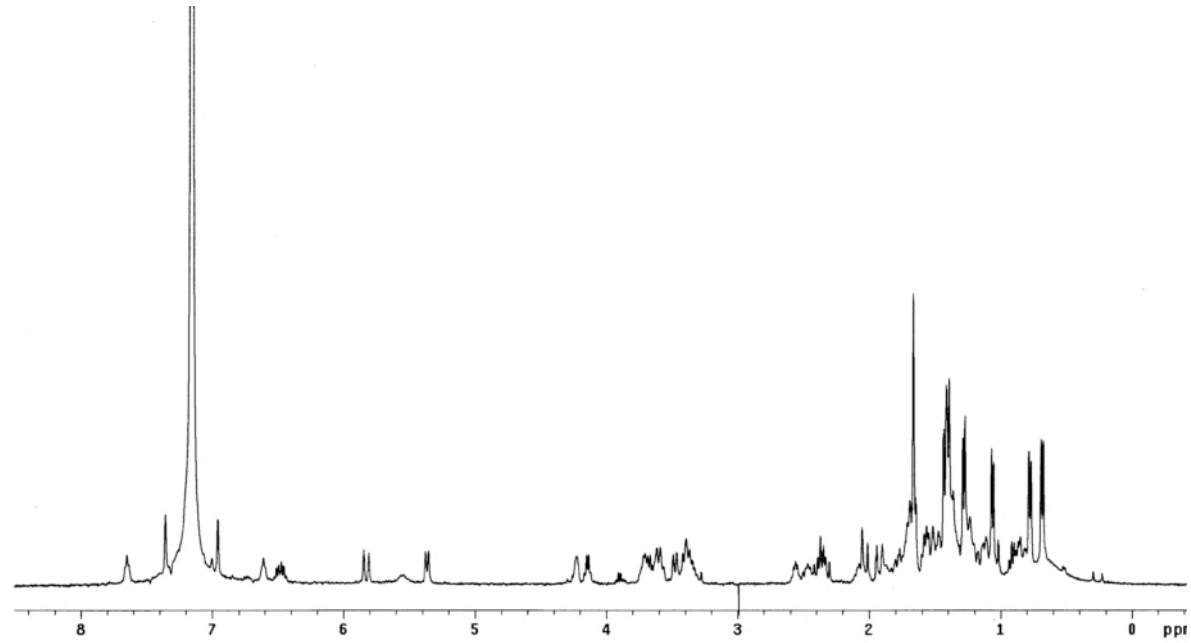
1.10 (400 MHz, C_6D_6)

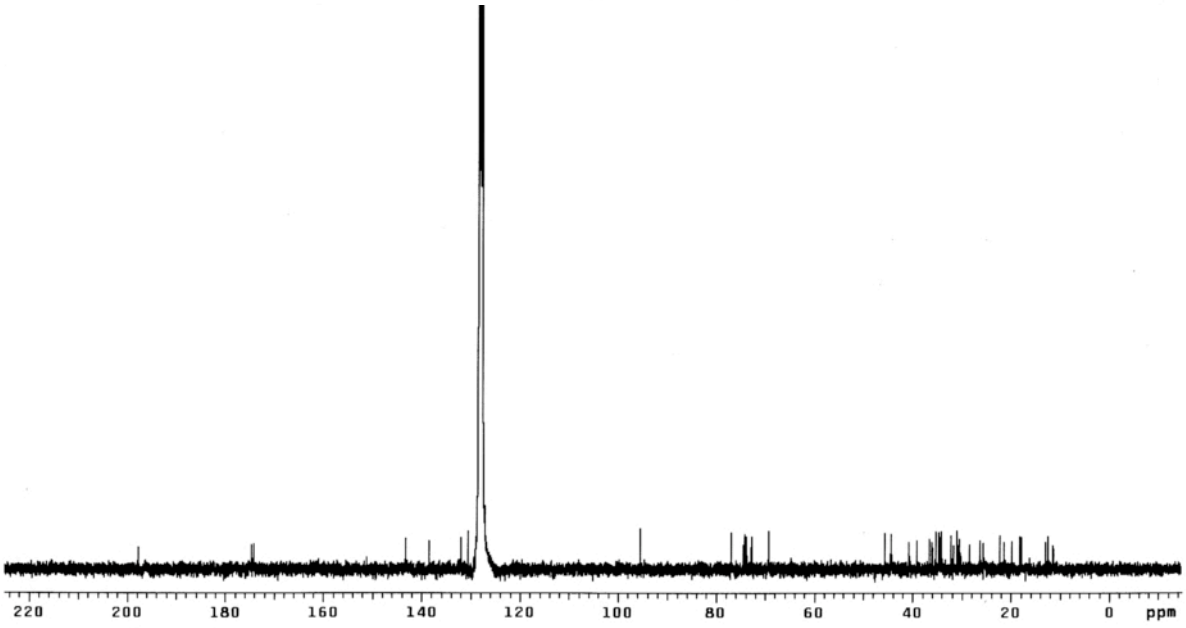


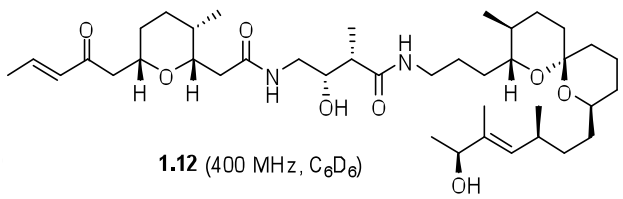




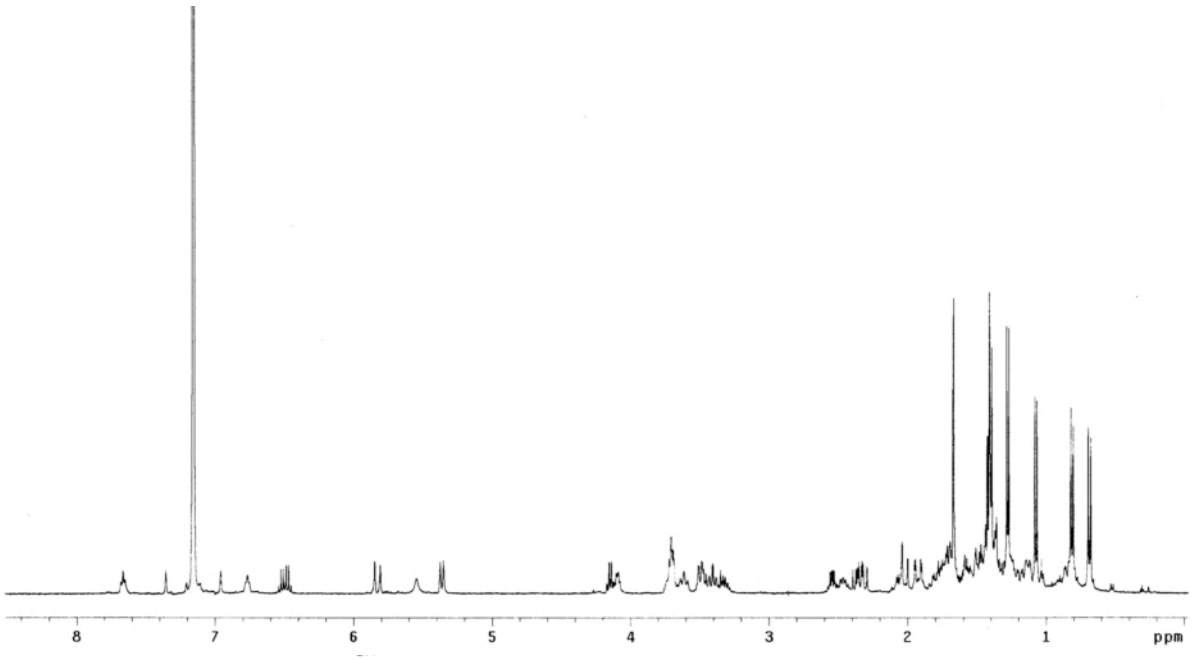
1.11 (400 MHz, C_6D_6)

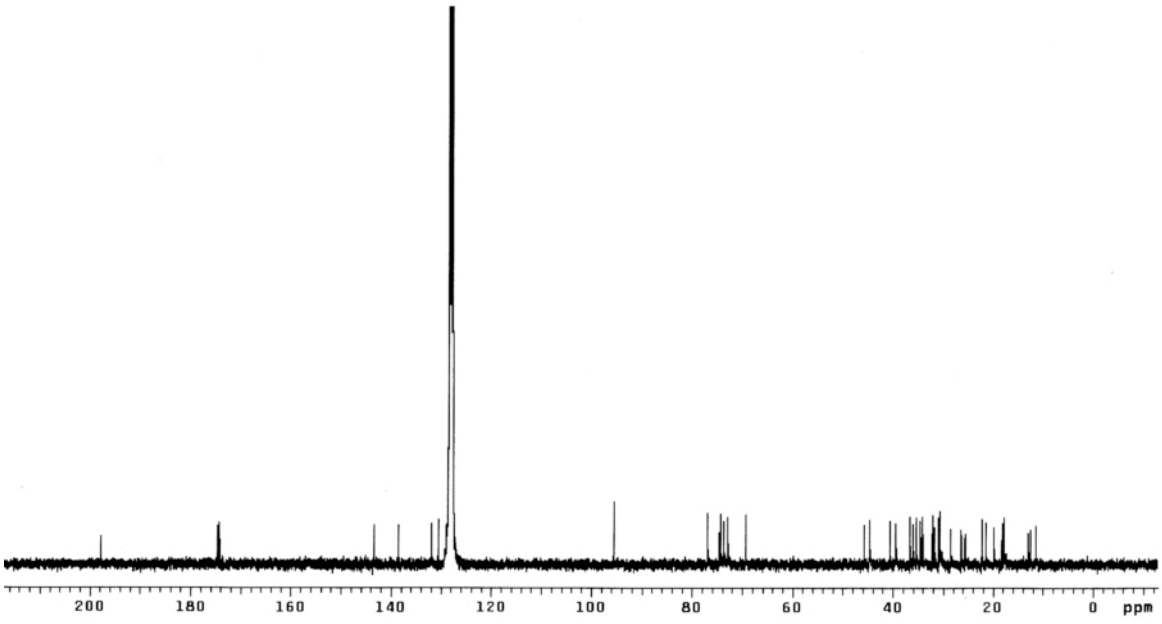


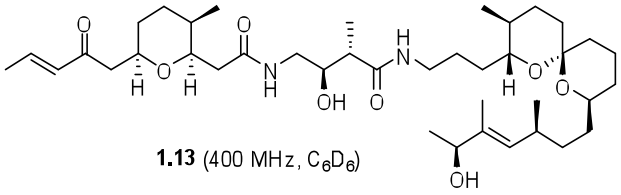




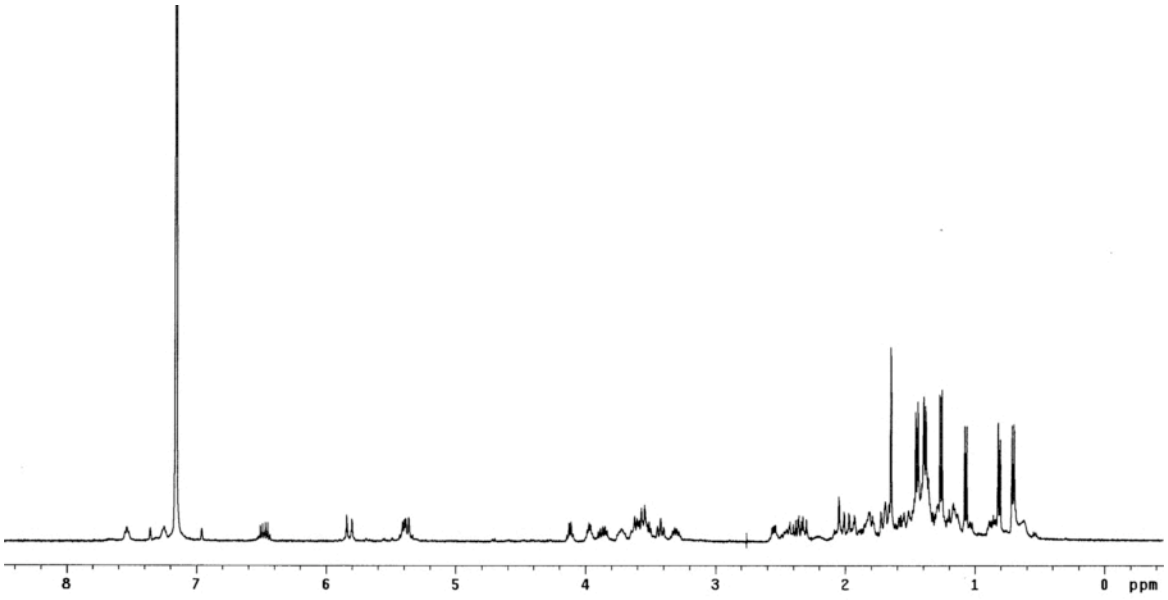
1.12 (400 MHz, C_6D_6)

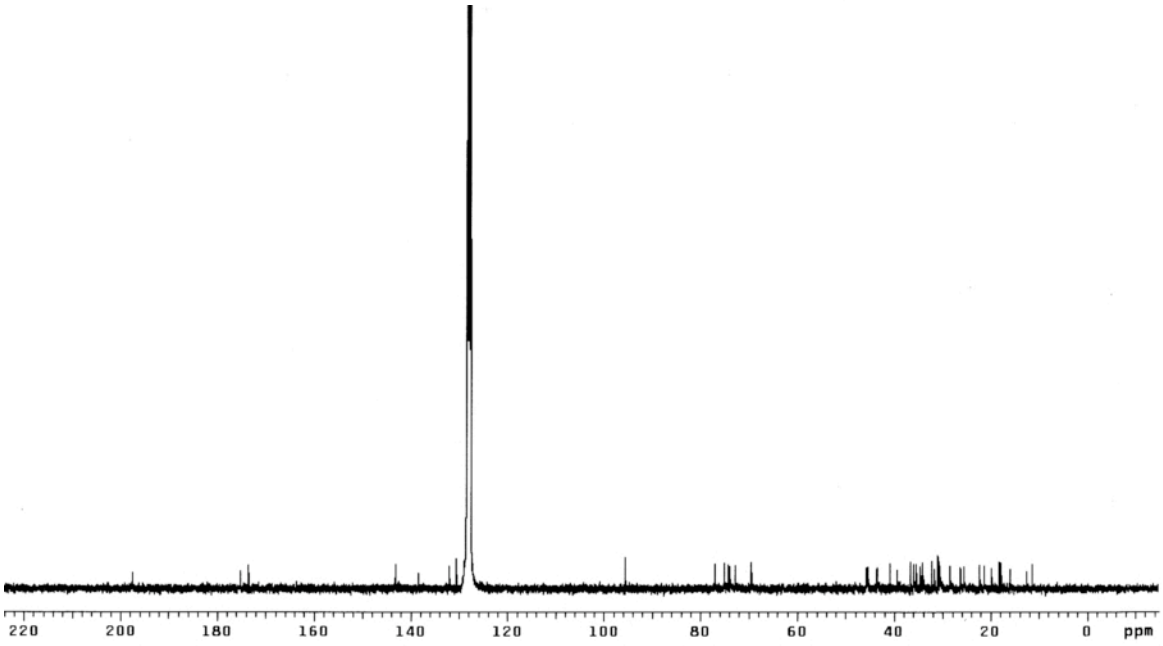


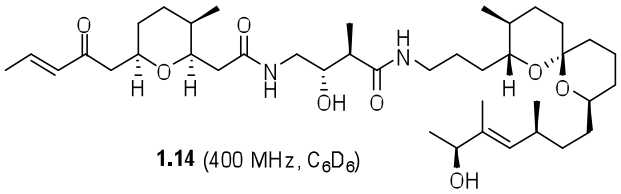




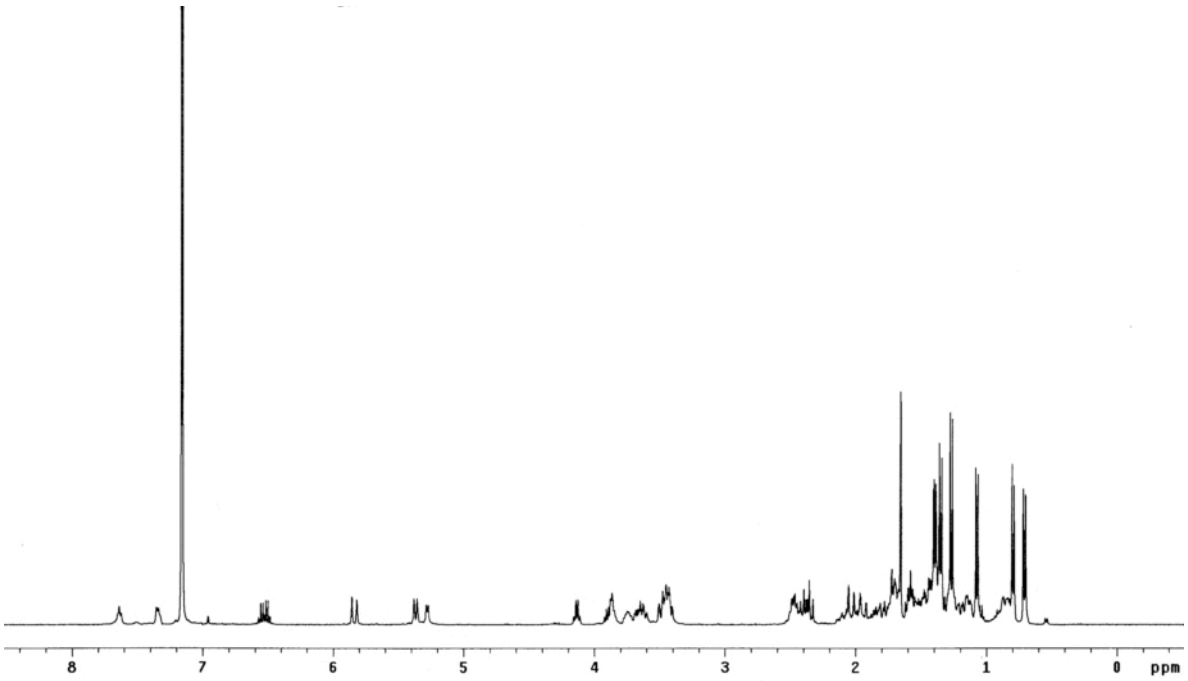
1.13 (400 MHz, C_6D_6)

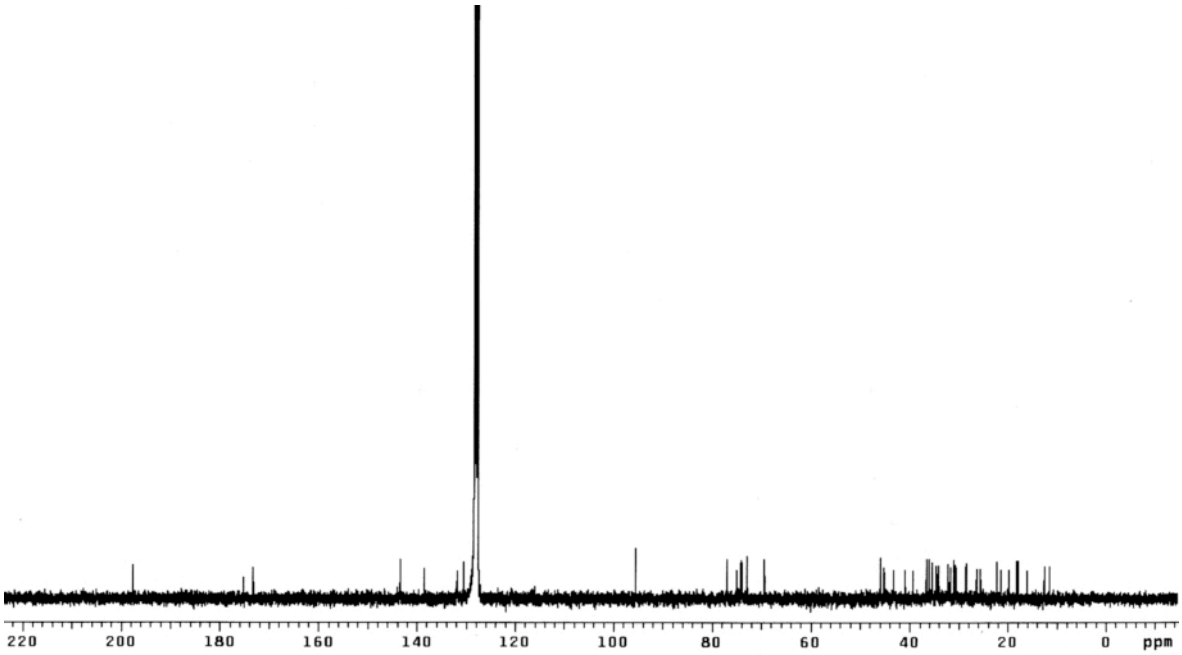


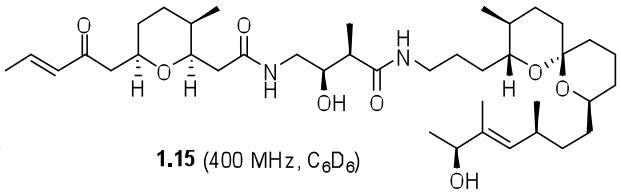




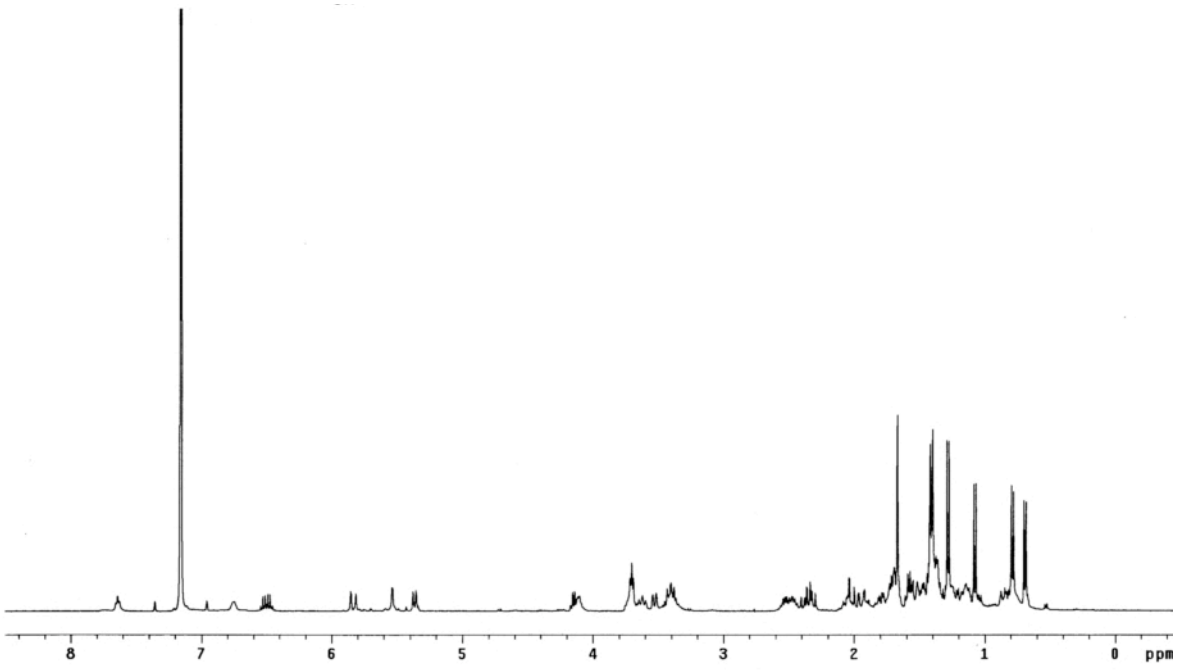
1.14 (400 MHz, C_6D_6)

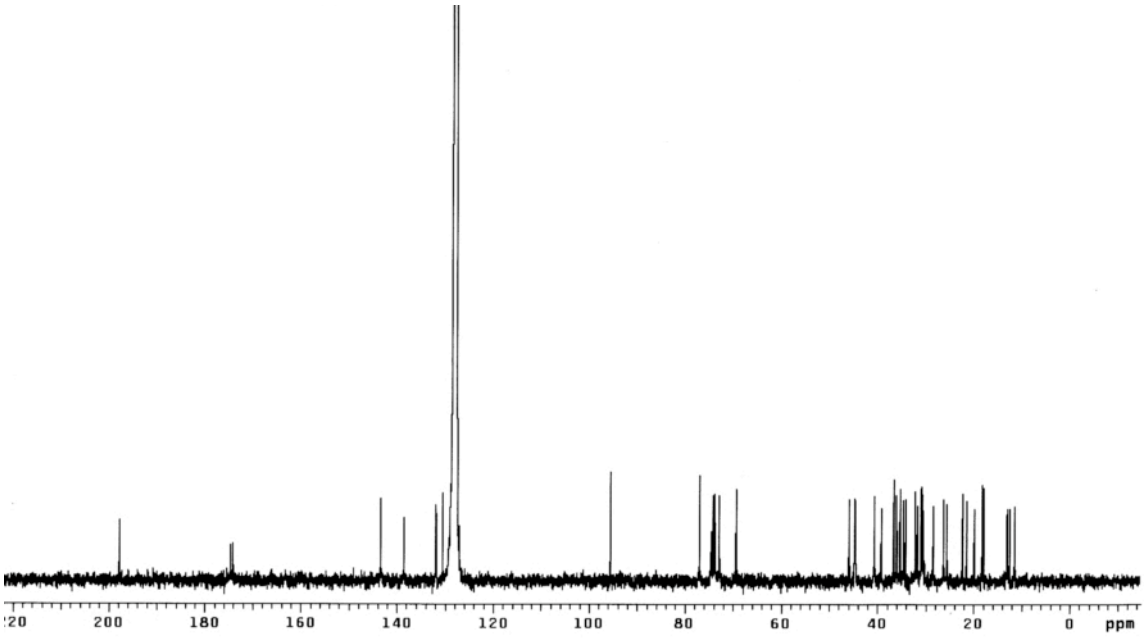


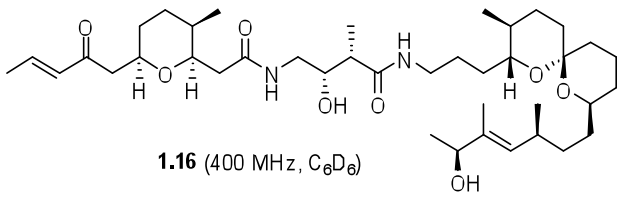




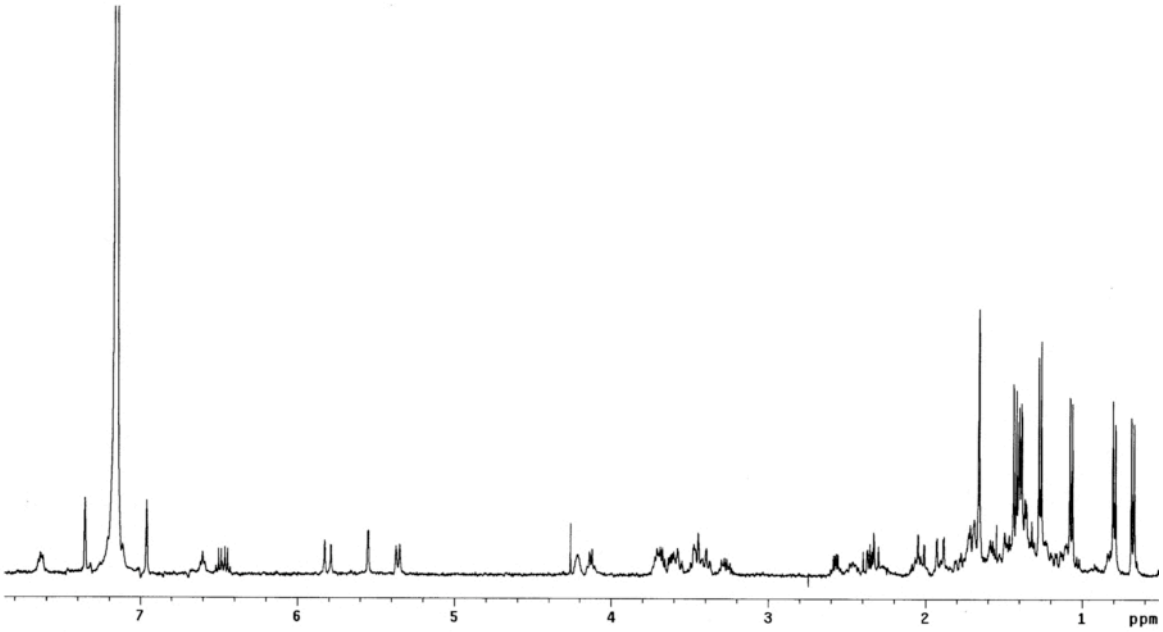
1.15 (400 MHz, C_6D_6)

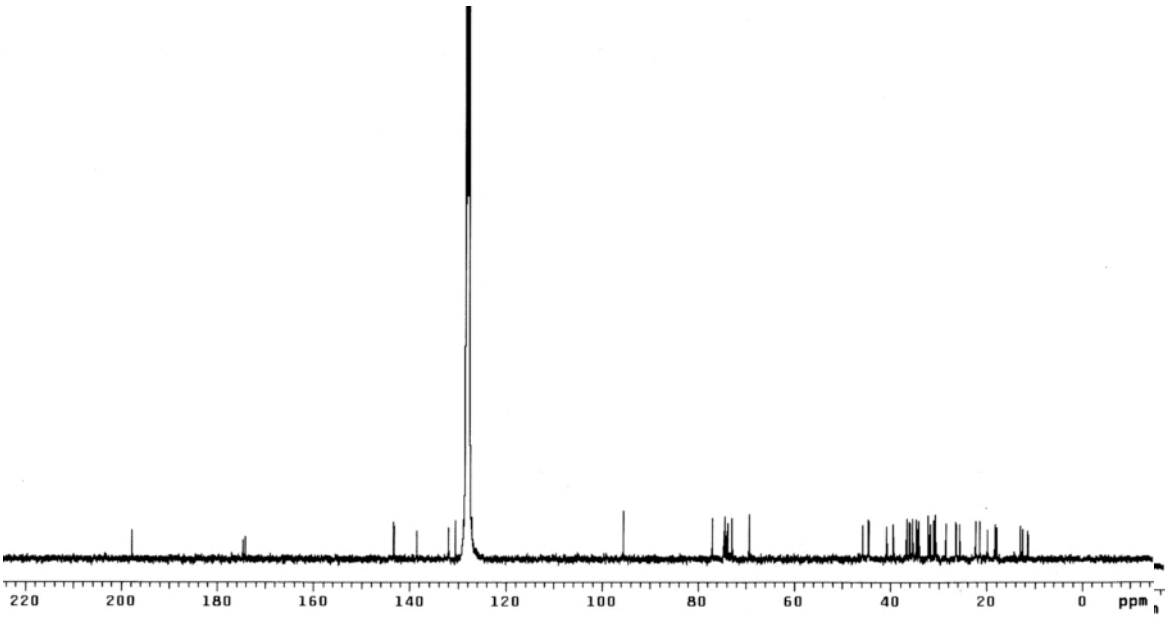


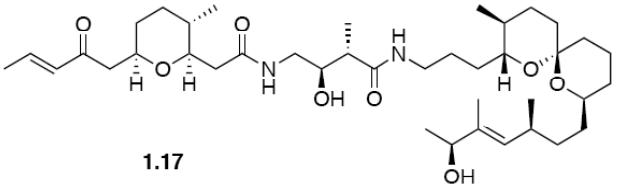




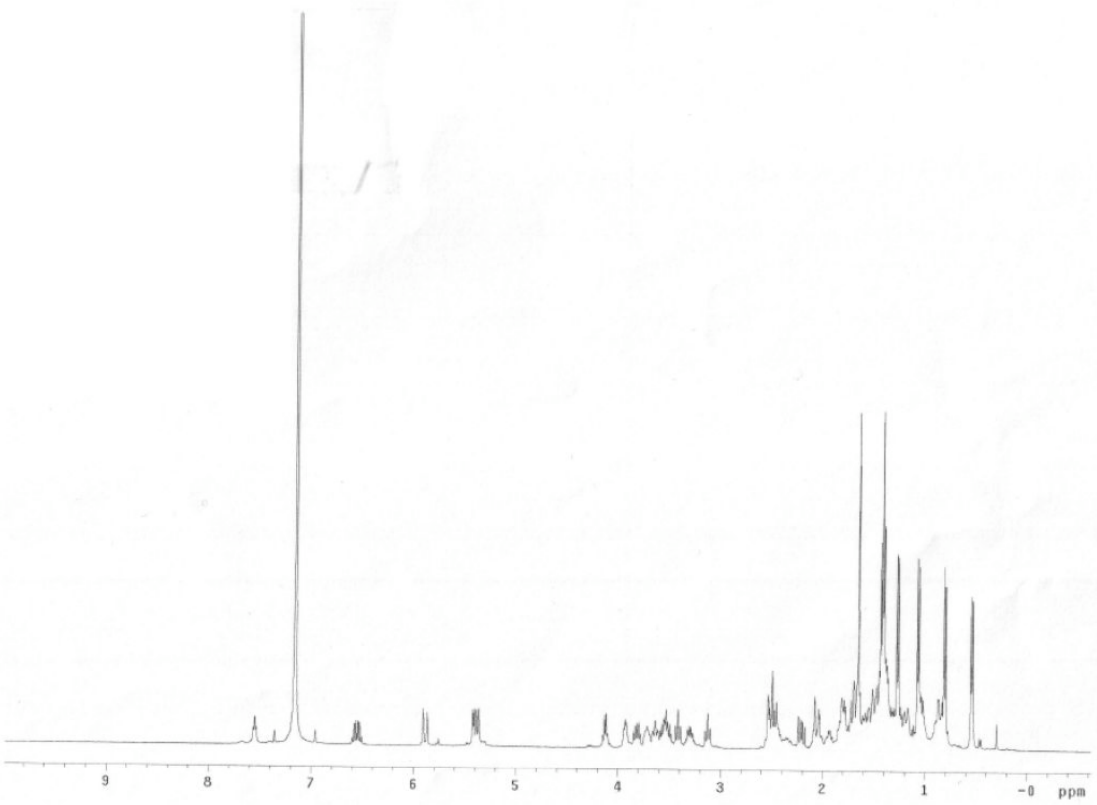
1.16 (400 MHz, C_6D_6)

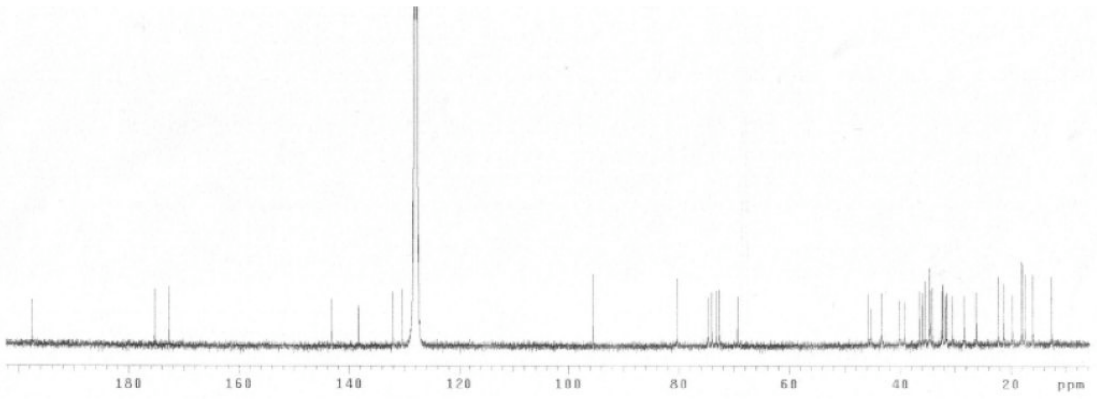


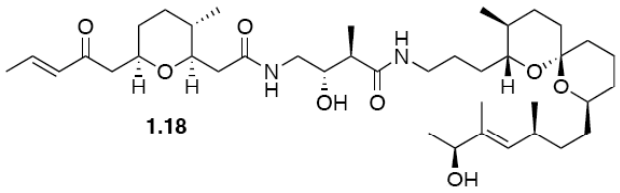




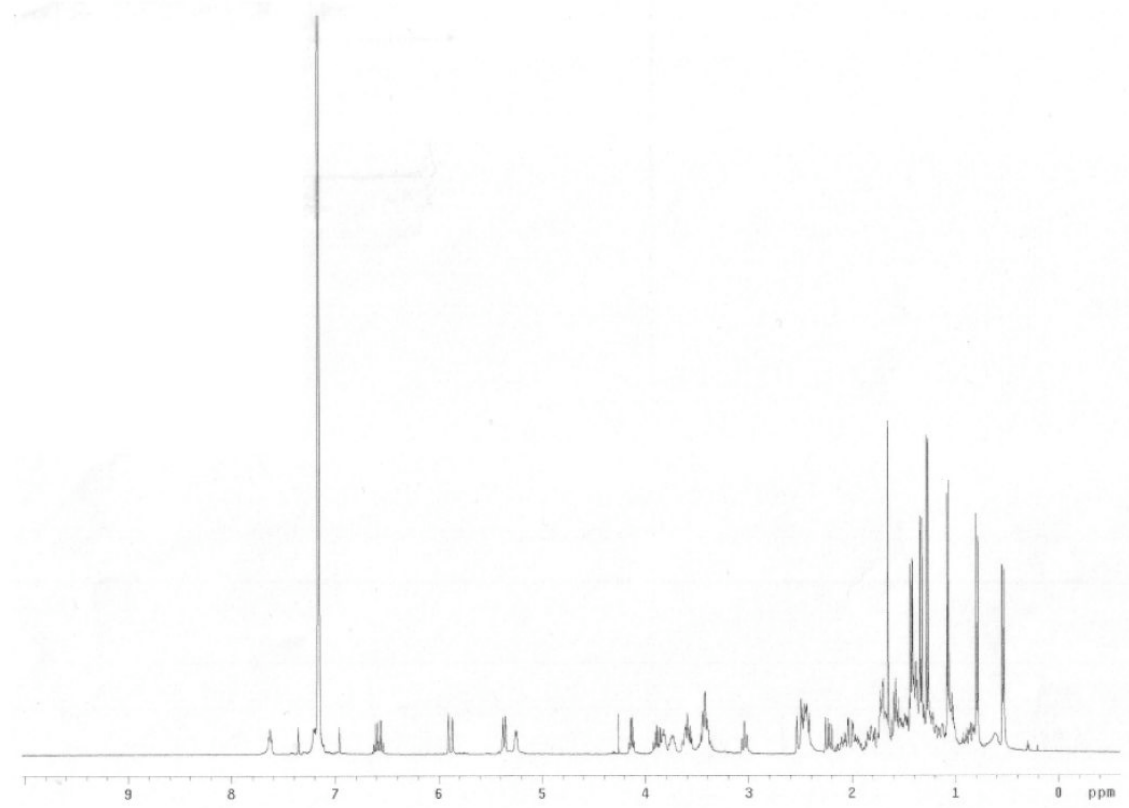
1.17






O
O
H
O
H
N
H
OH
O
H
N
H
O
O
OH

1.18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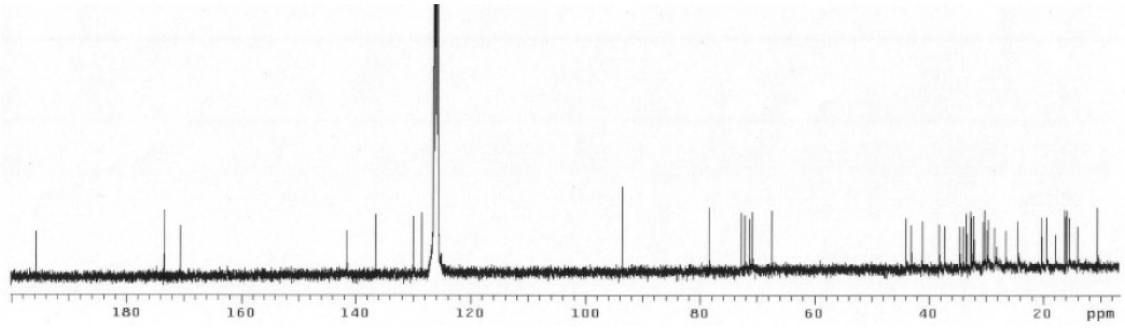
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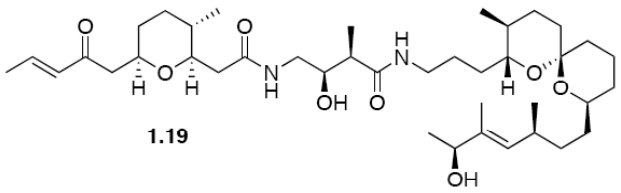
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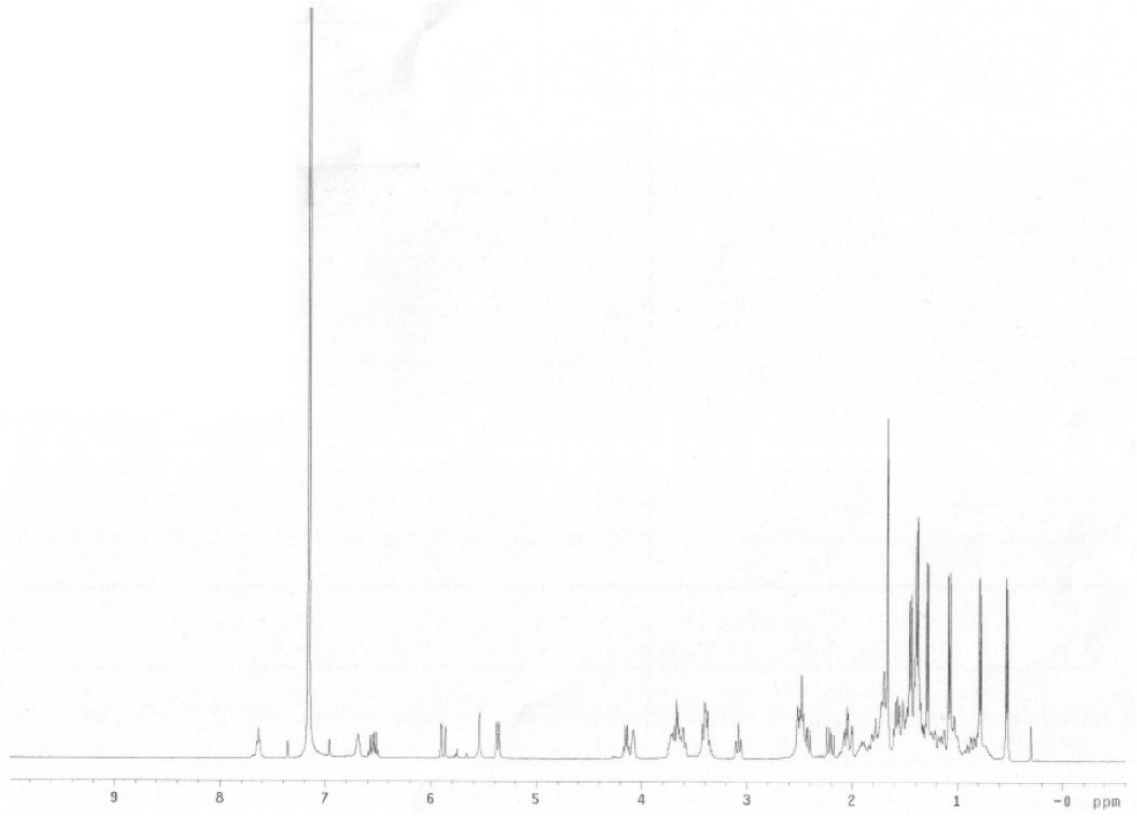
OH

1.19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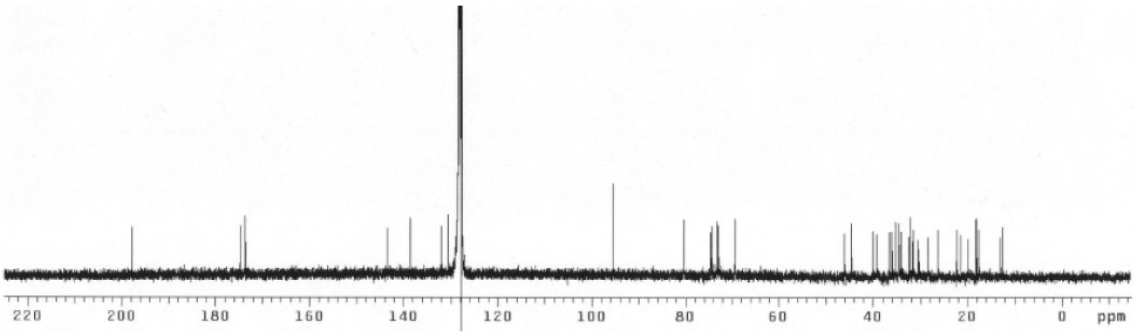
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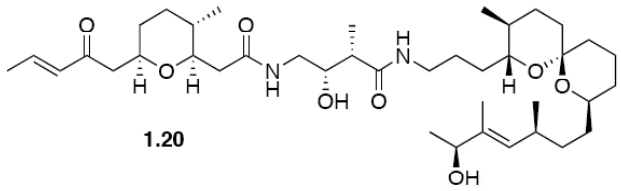

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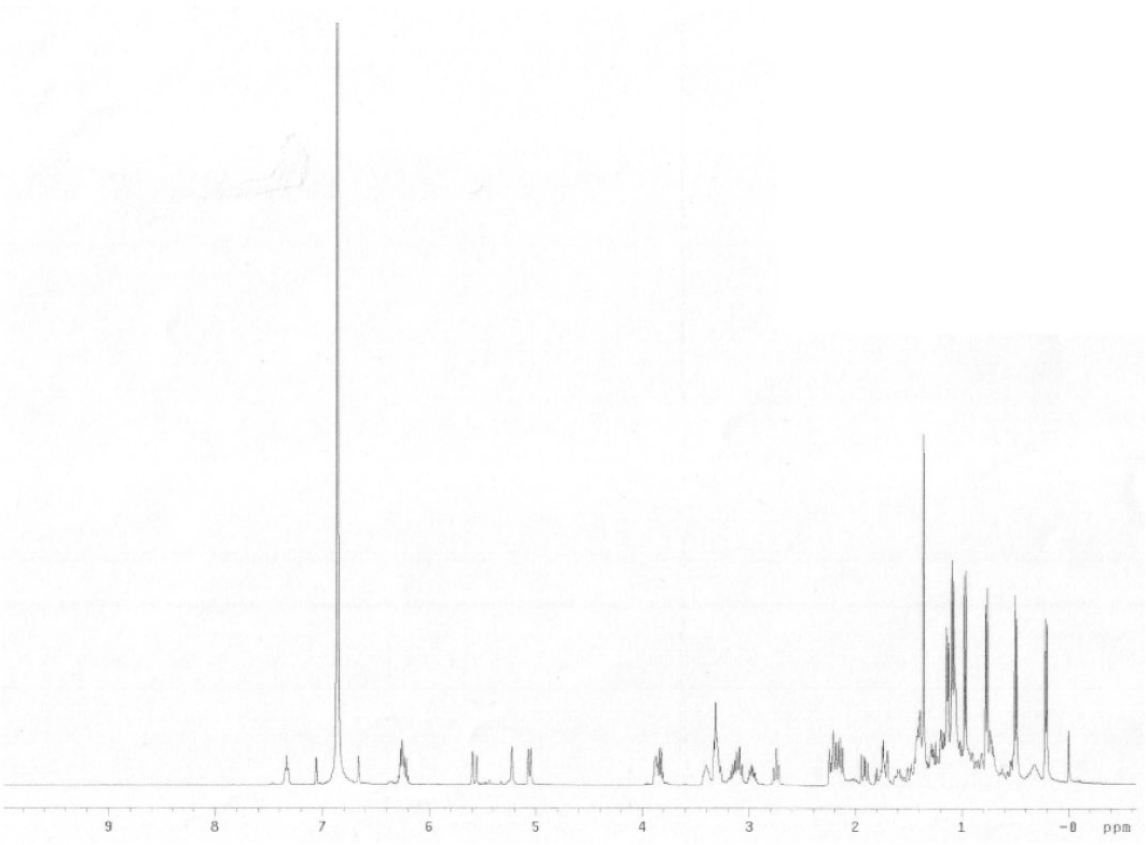

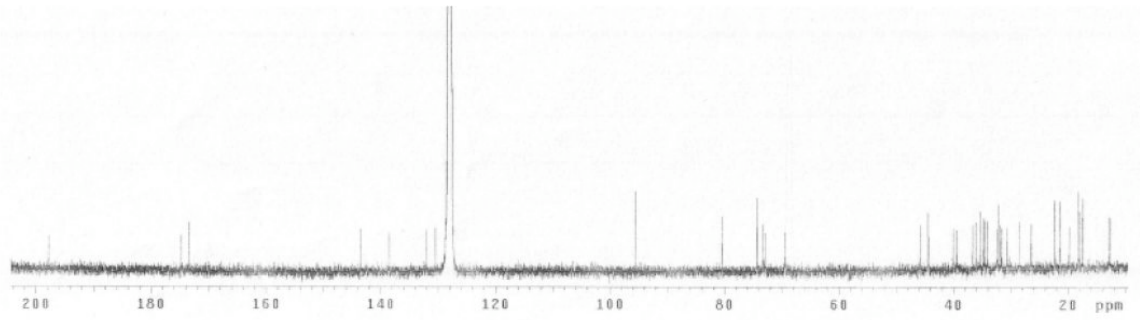

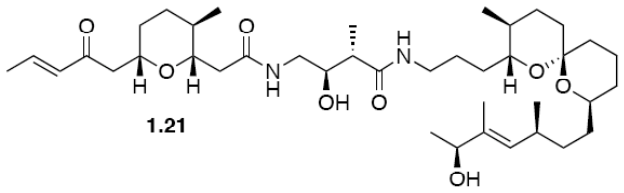
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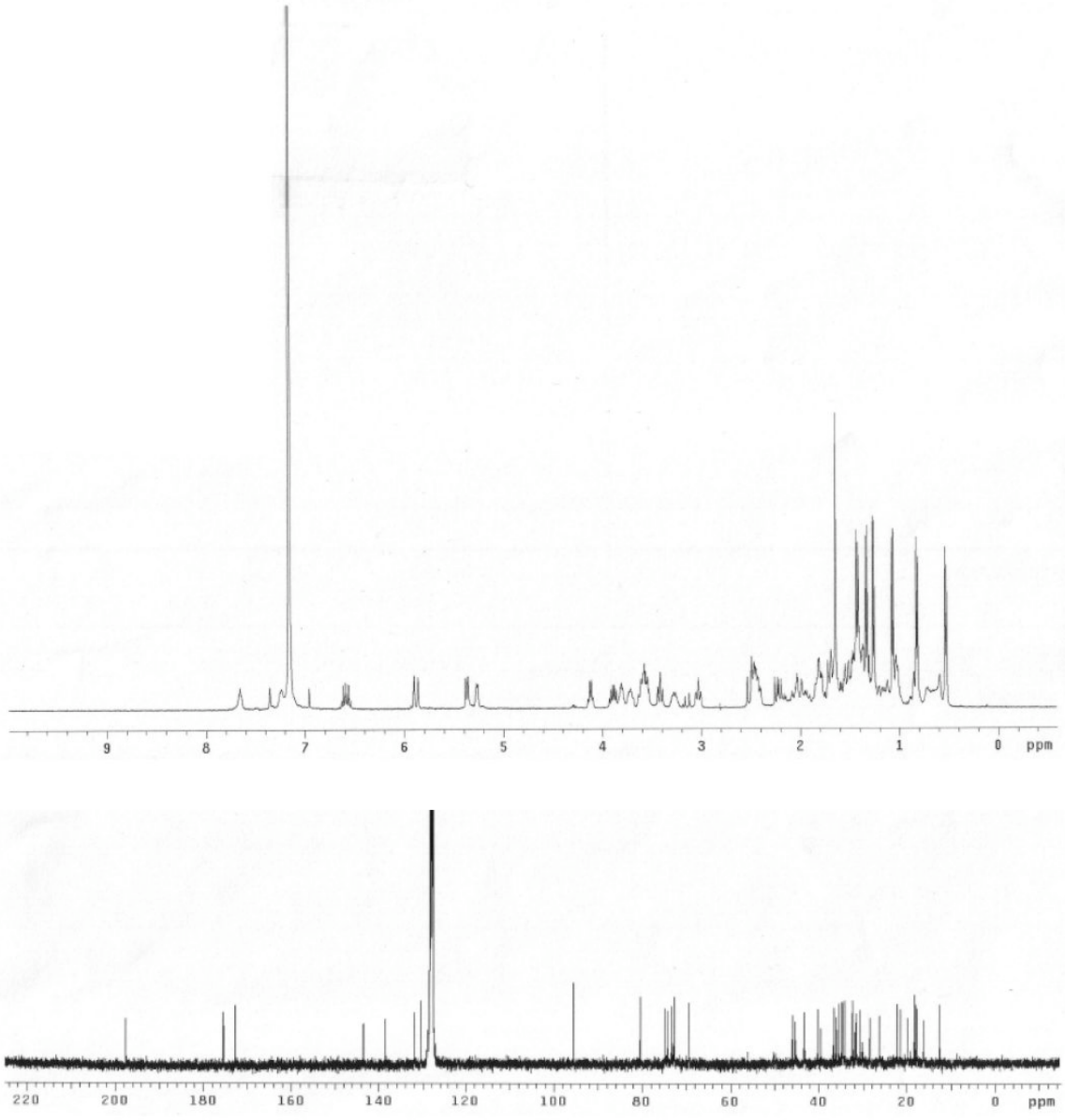
OH

1.21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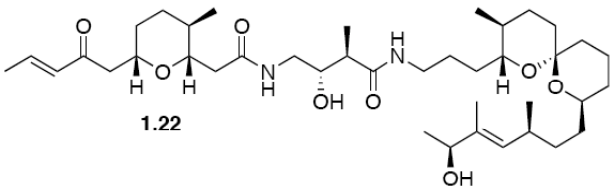
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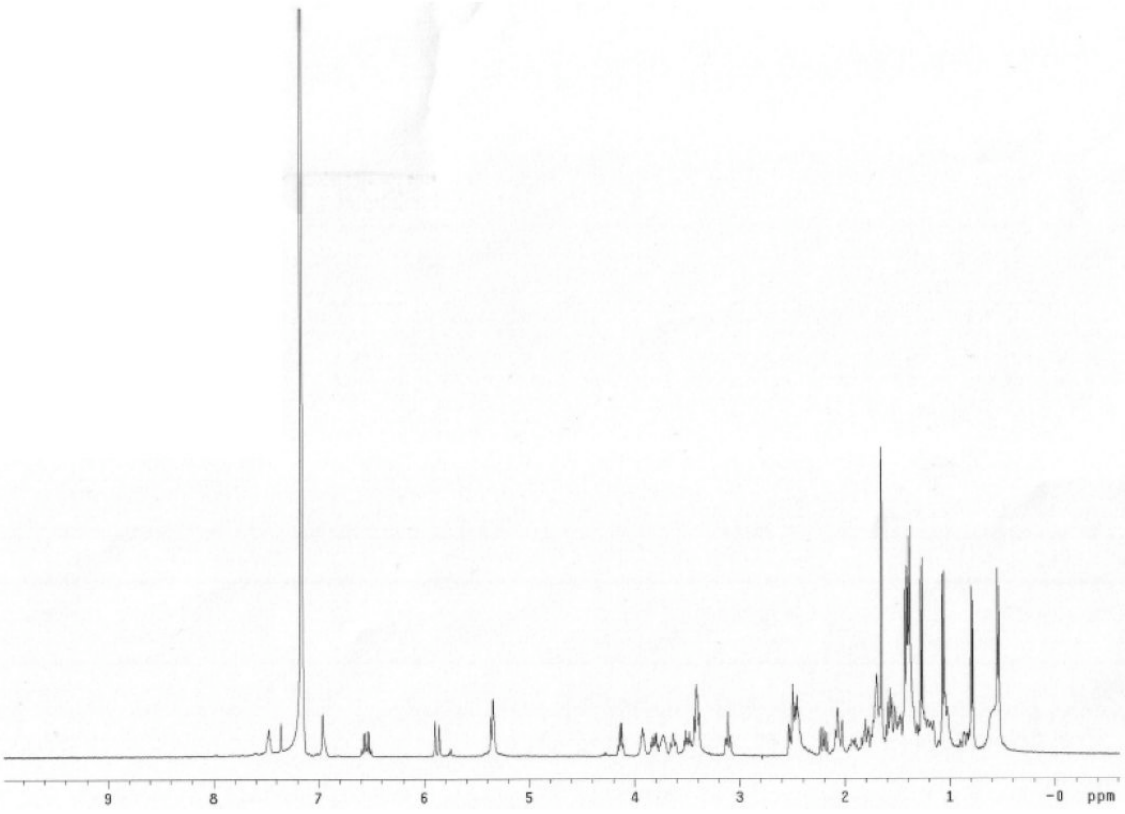
OH

1.22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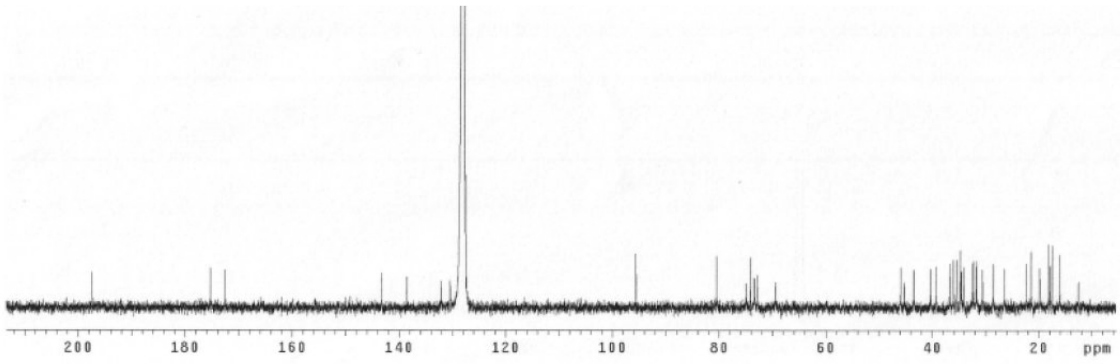
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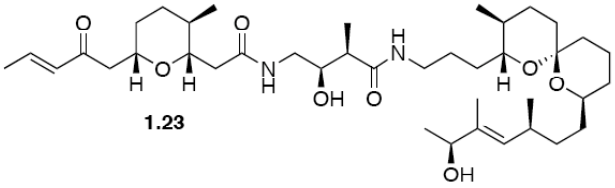

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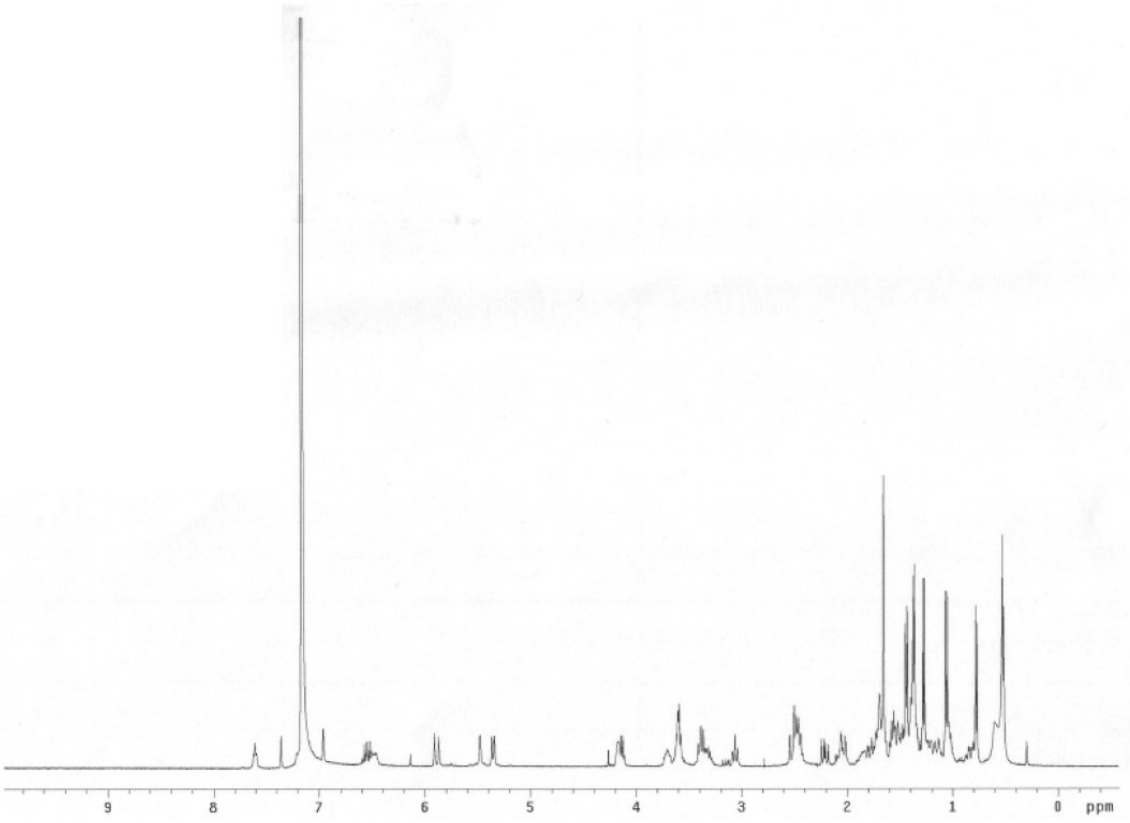

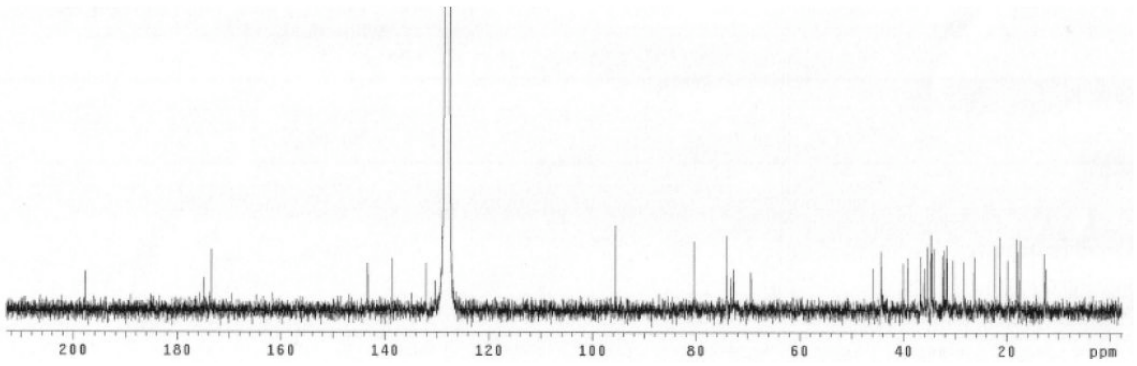

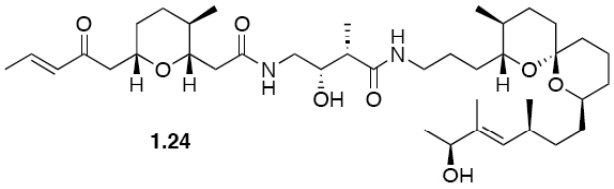

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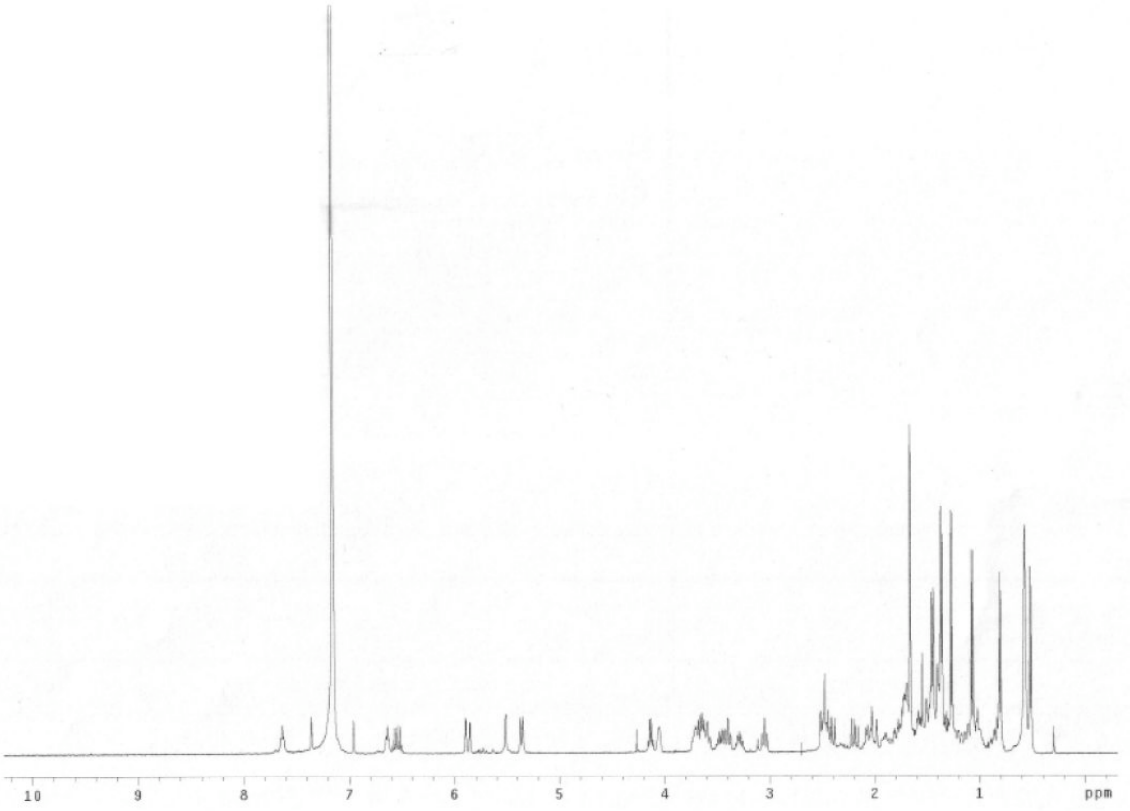

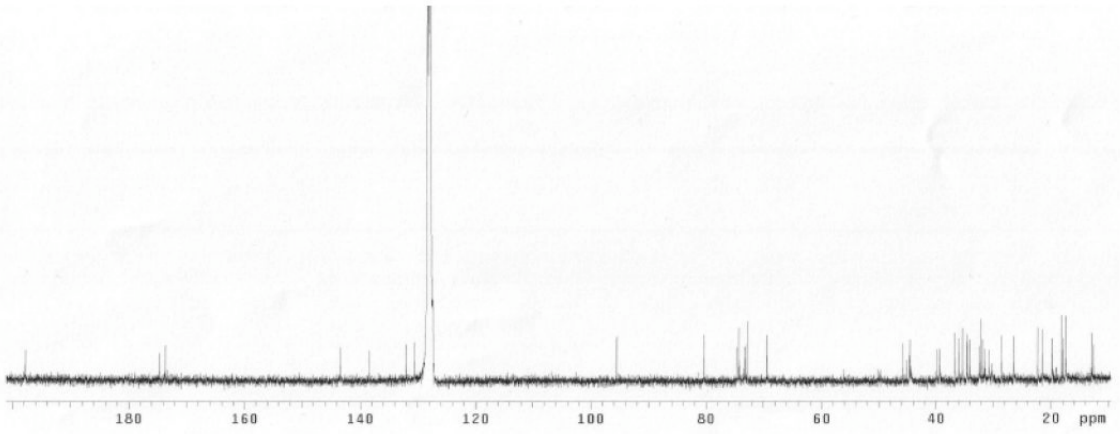

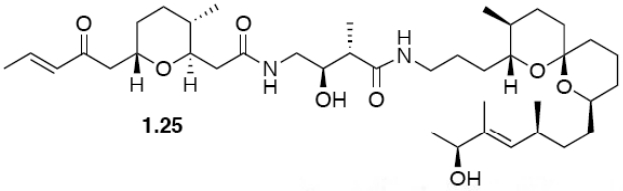
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OH
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N
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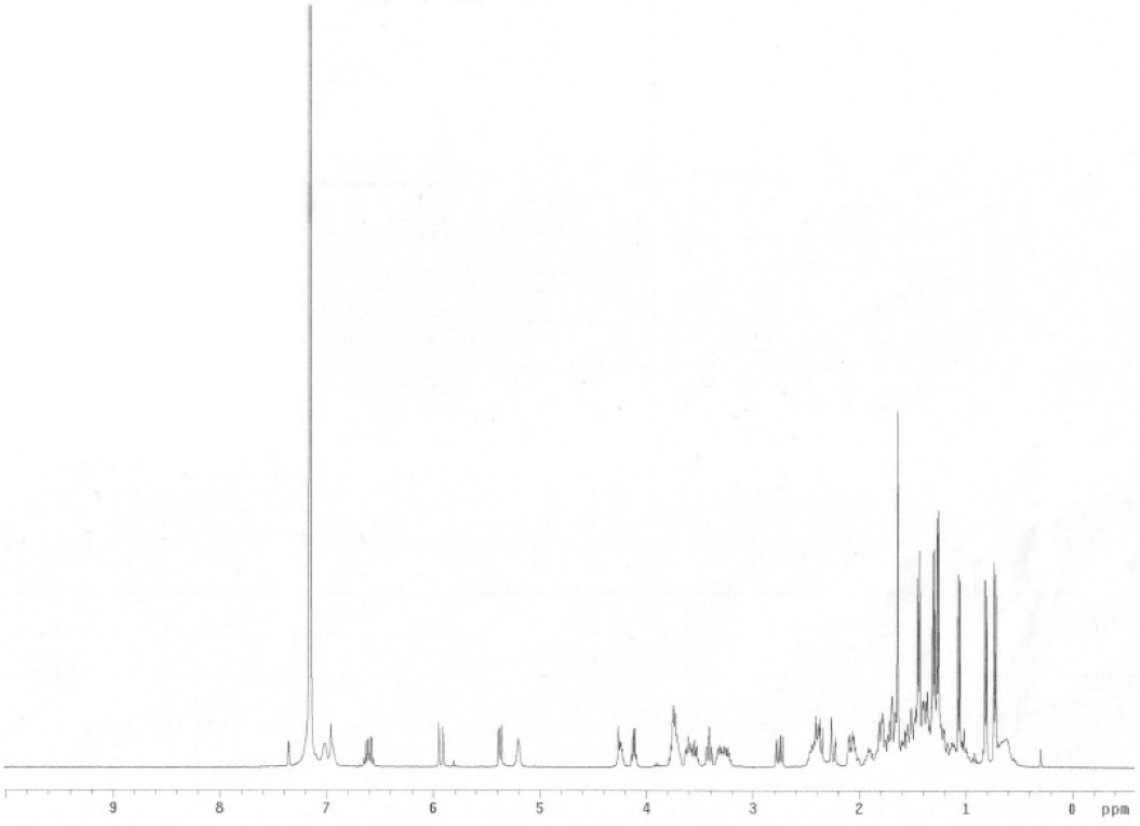
OH

1.25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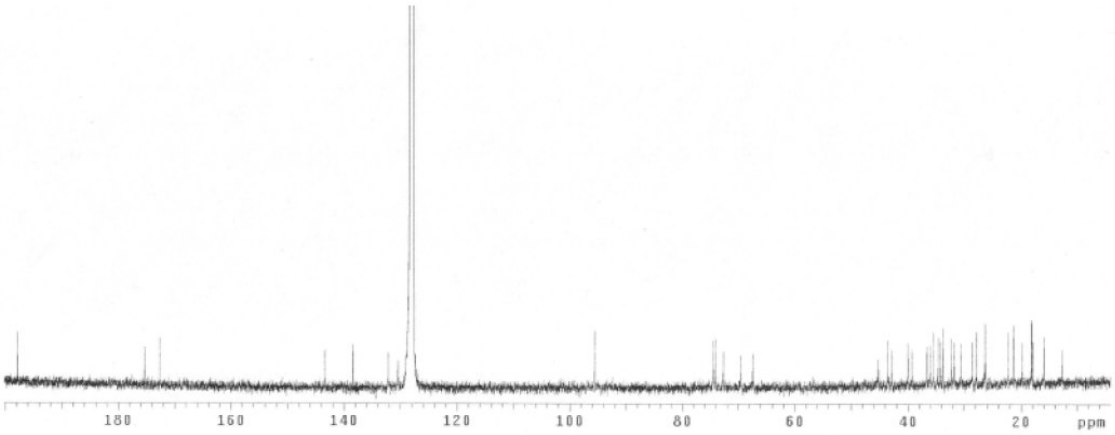
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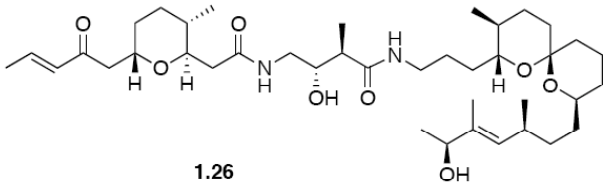

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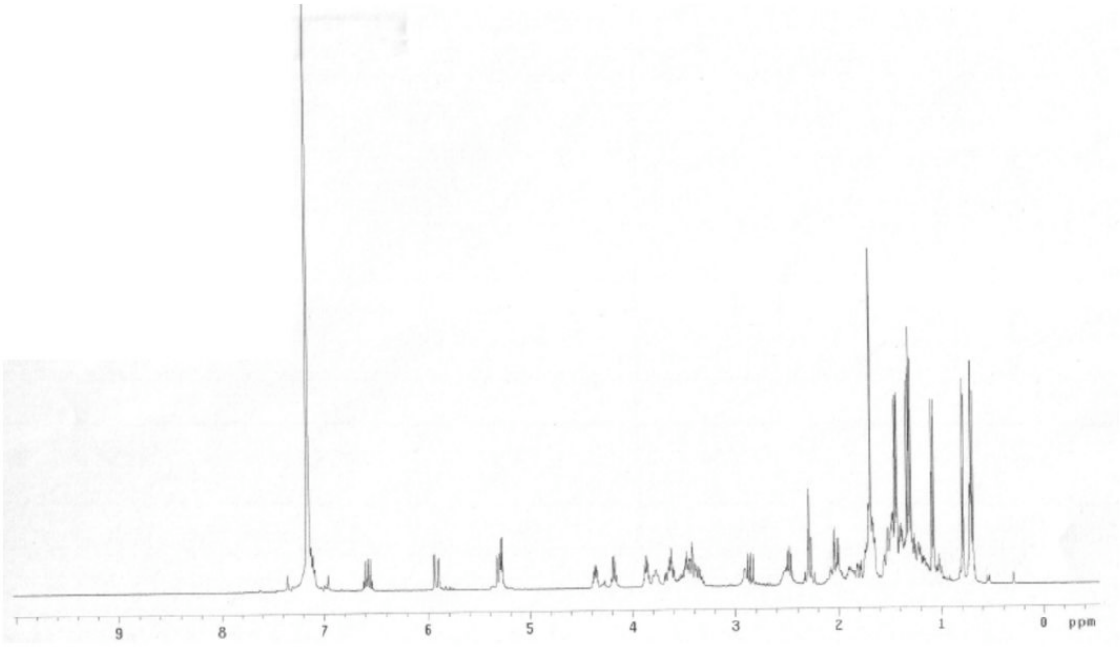

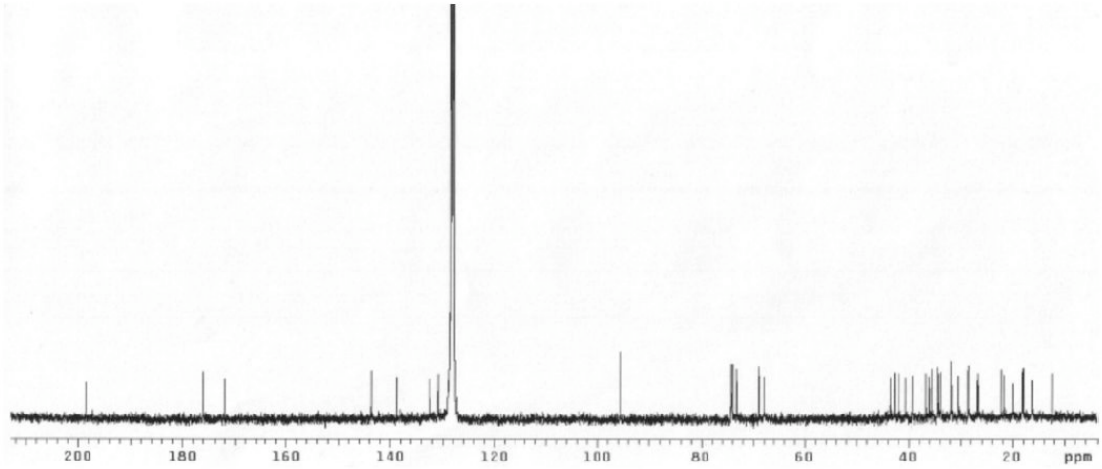

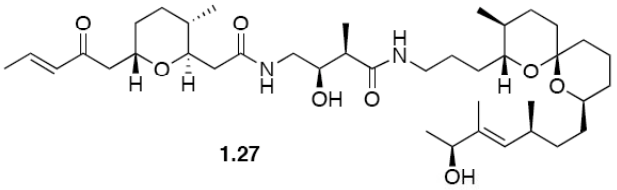
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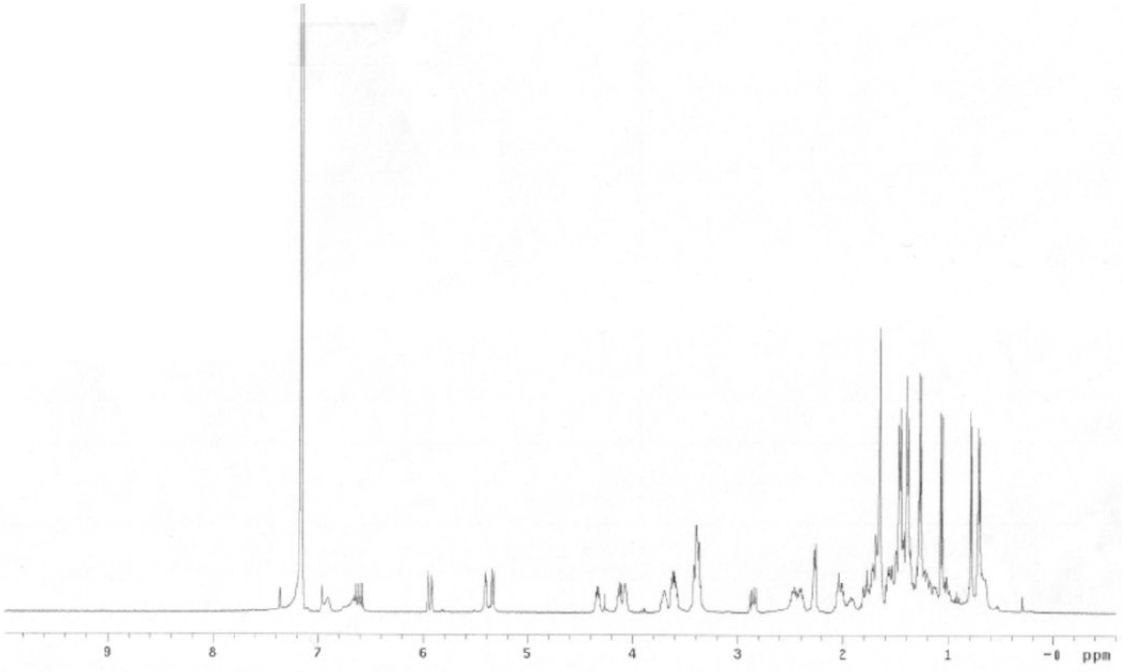
OH

1.27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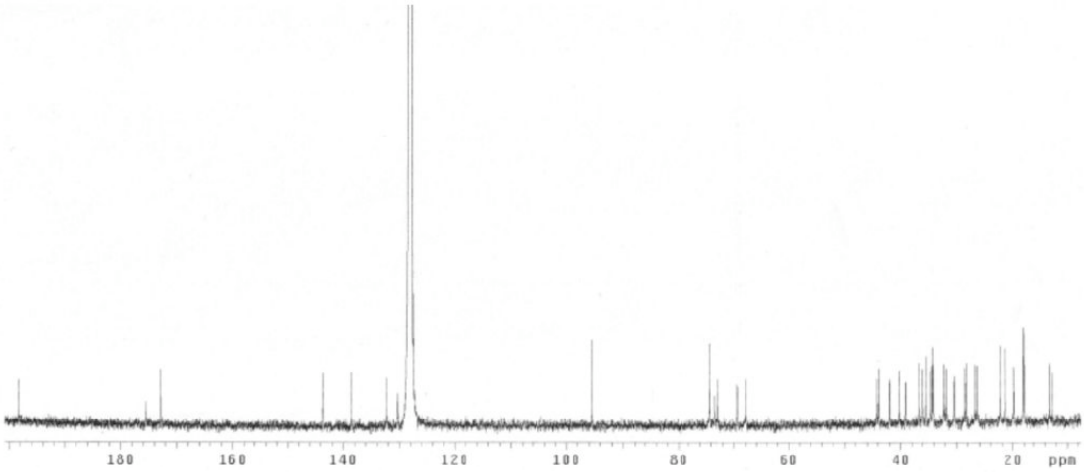
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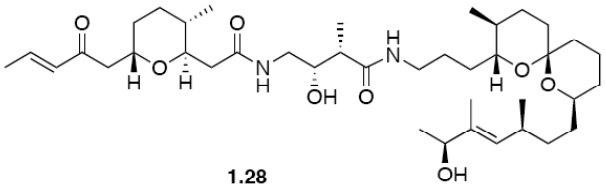

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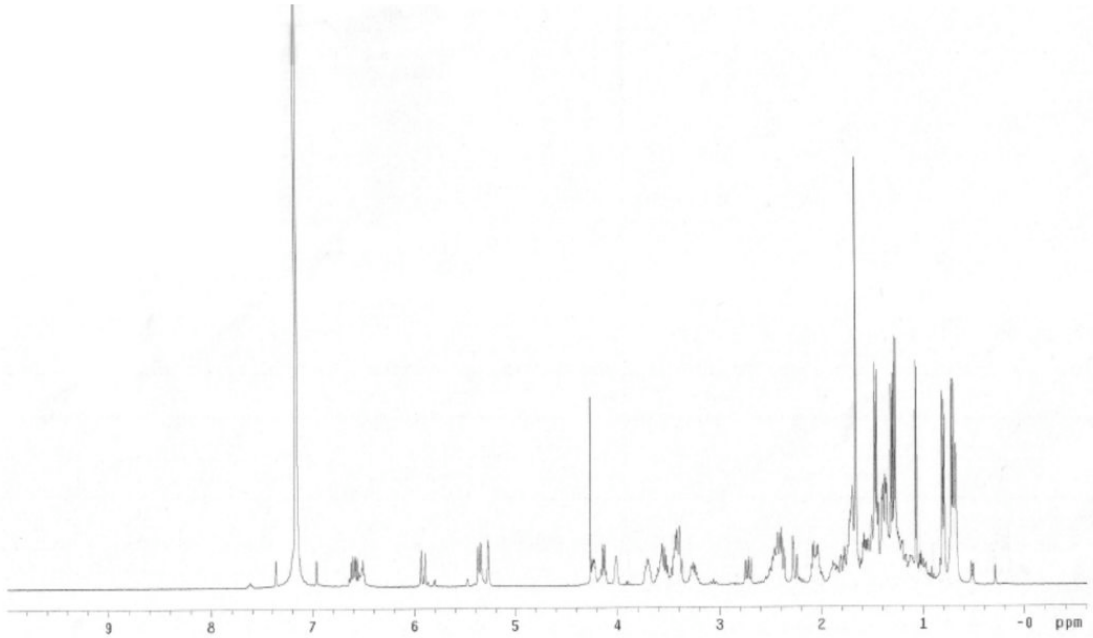

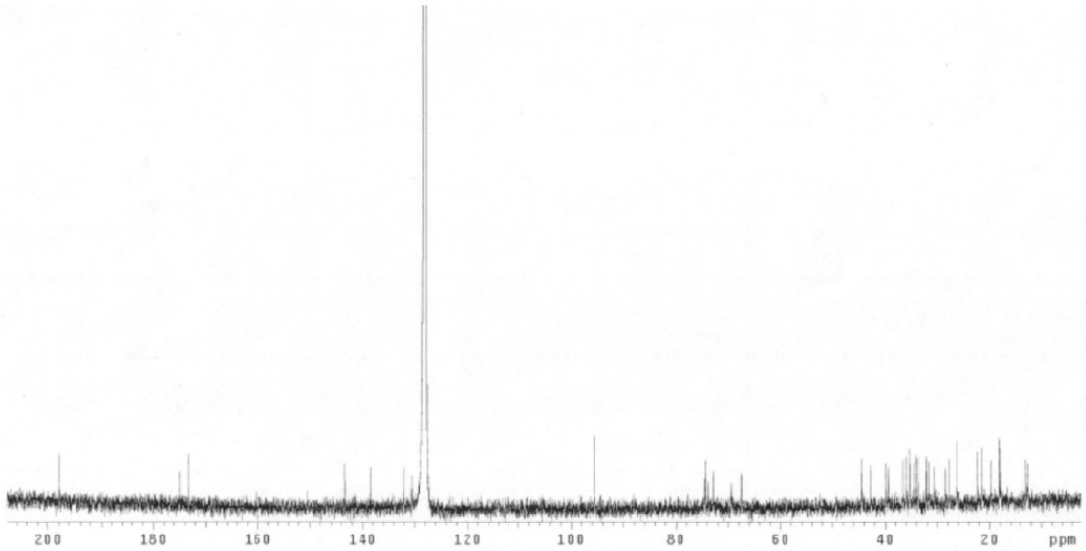

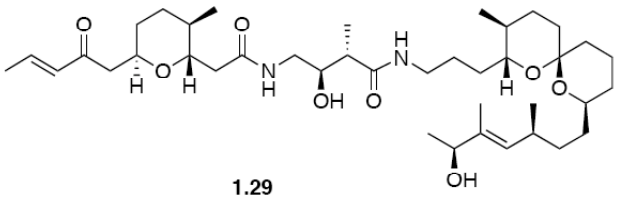

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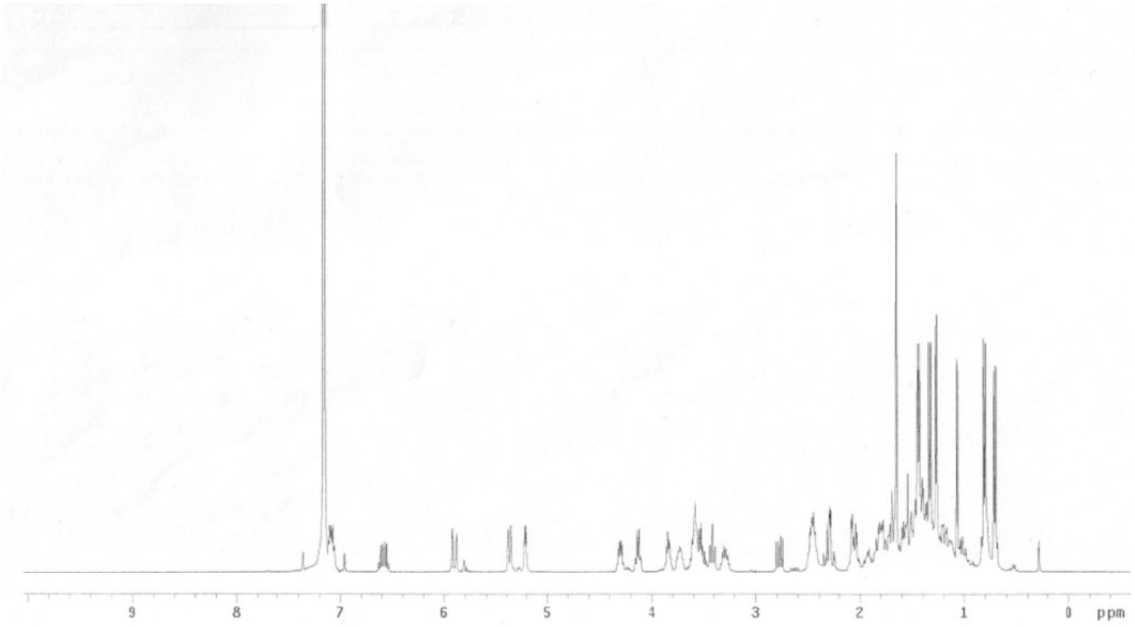

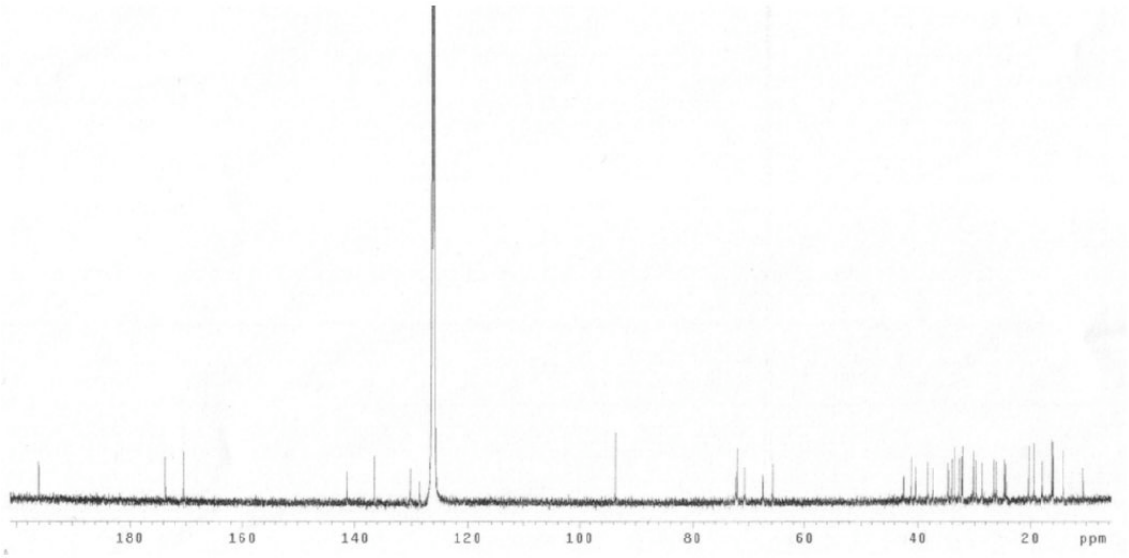

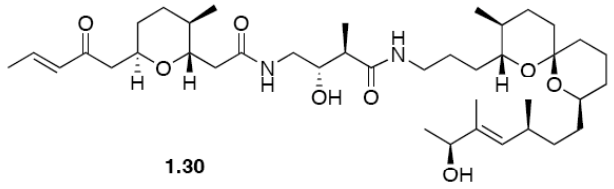

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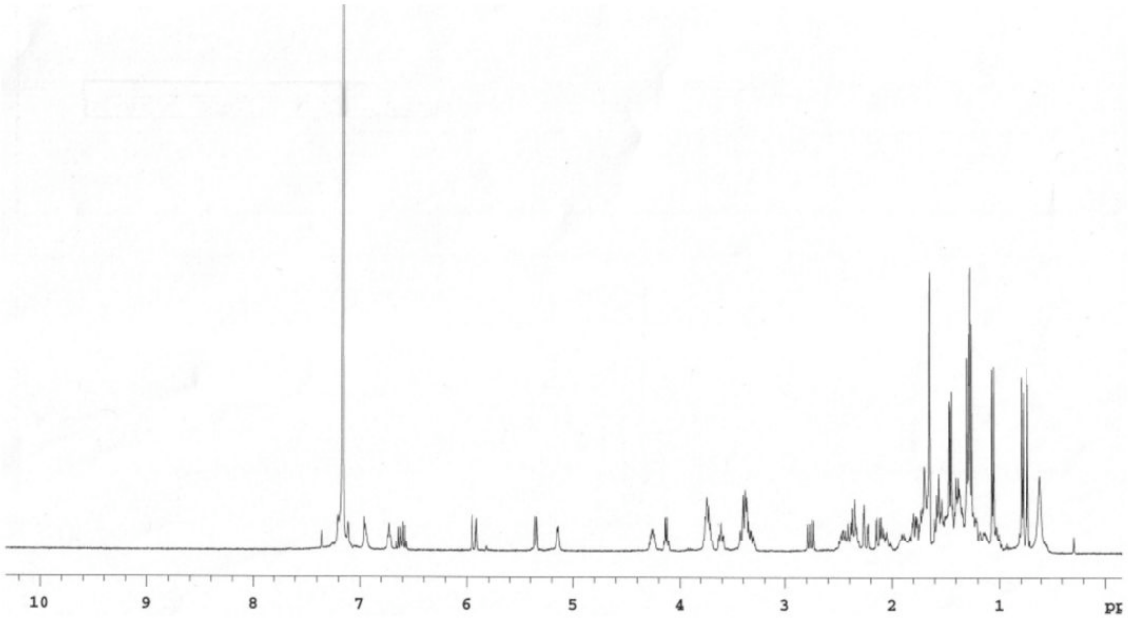

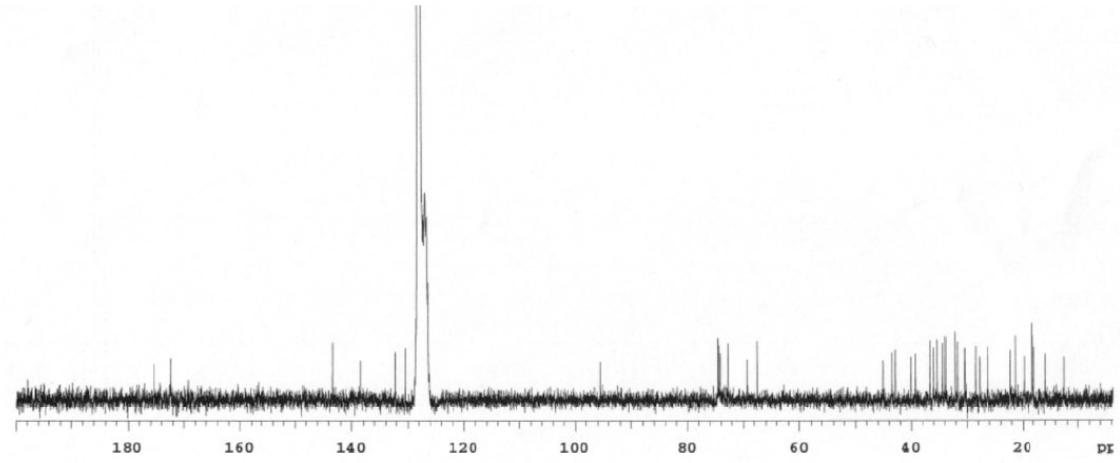

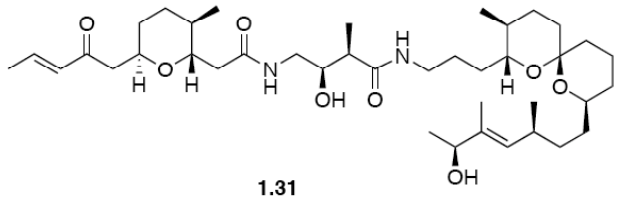

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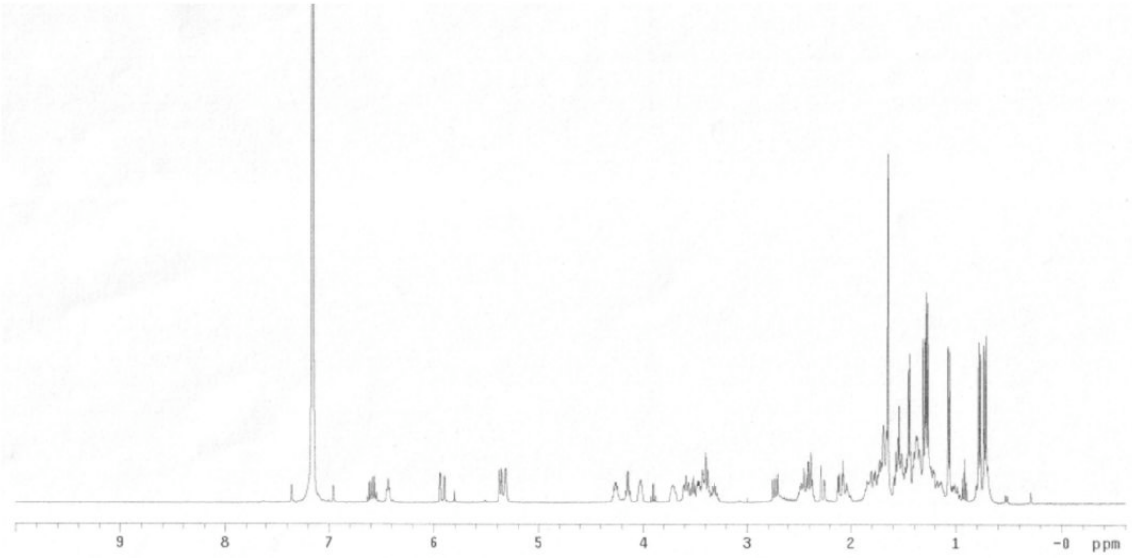

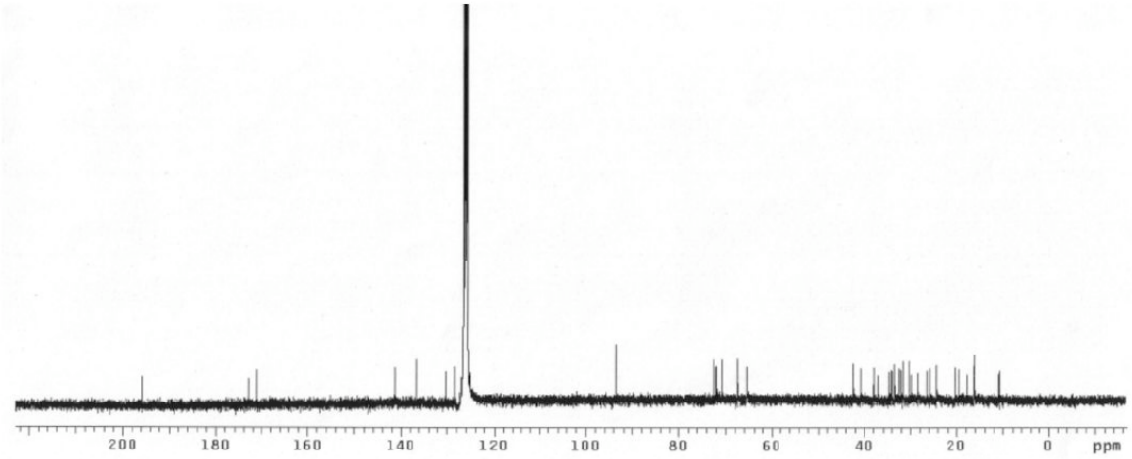

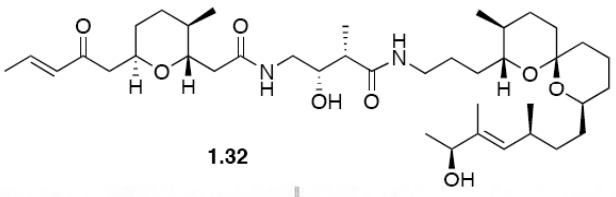

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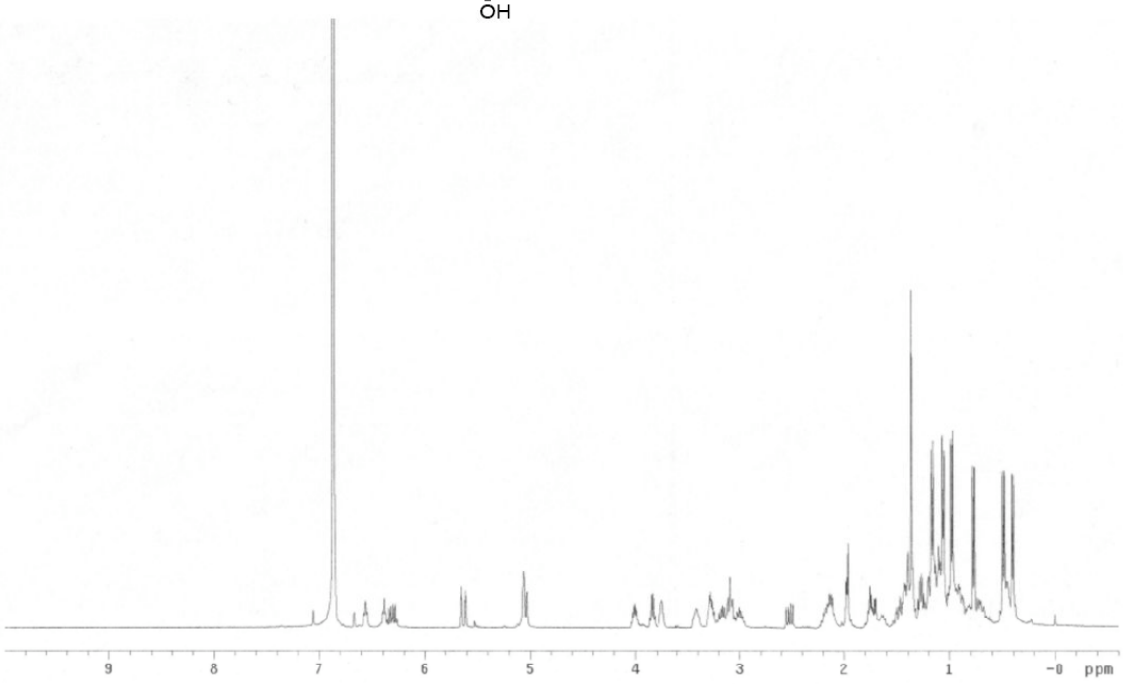
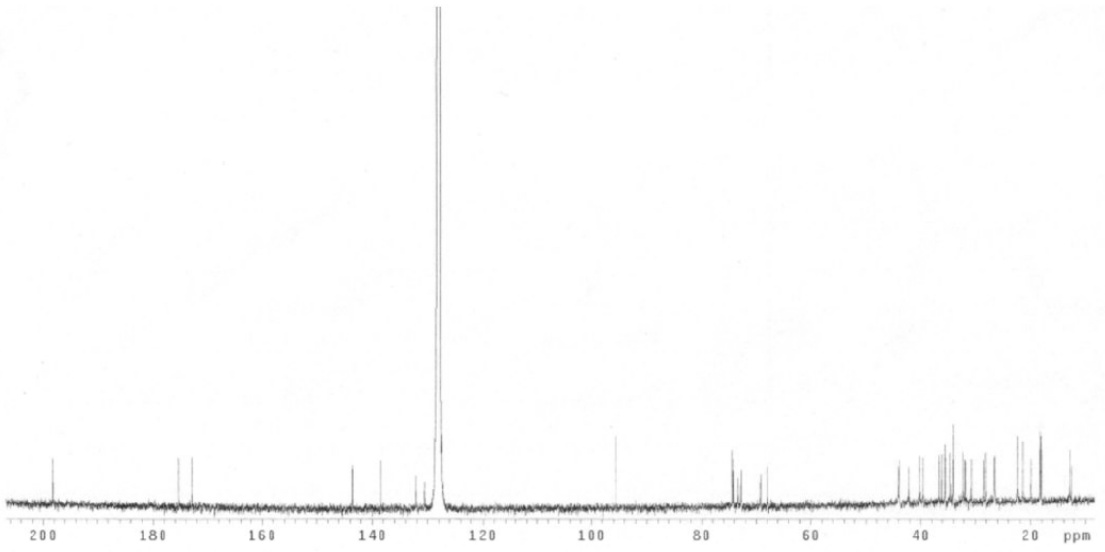
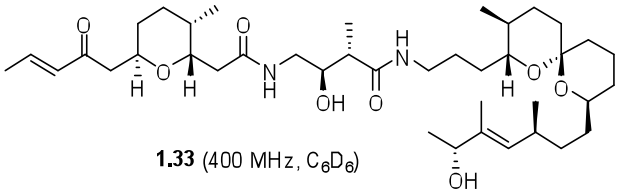
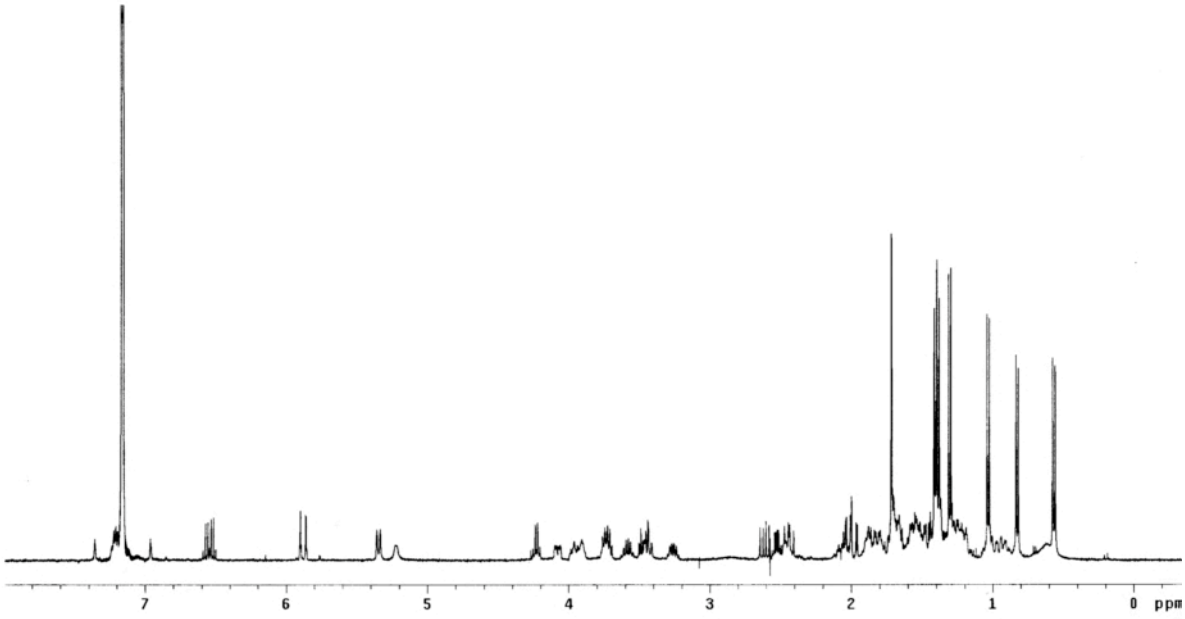
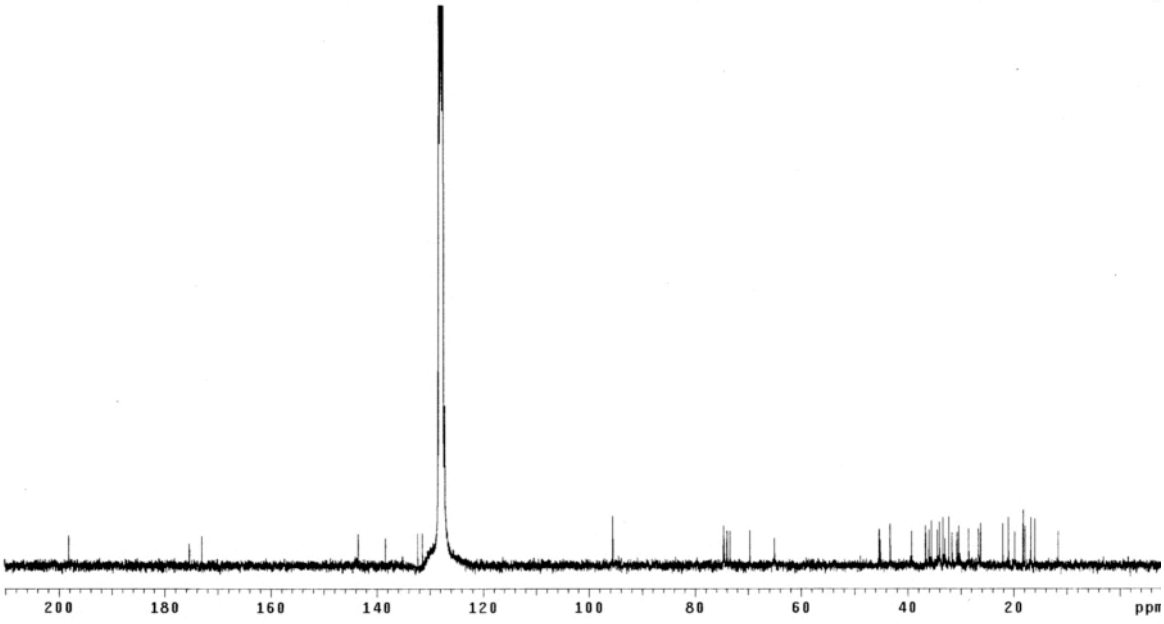


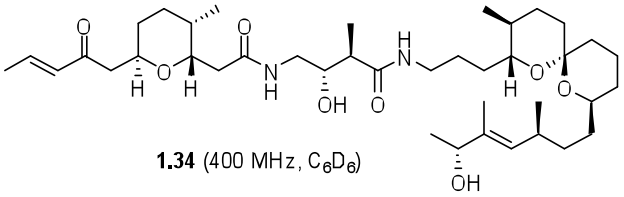




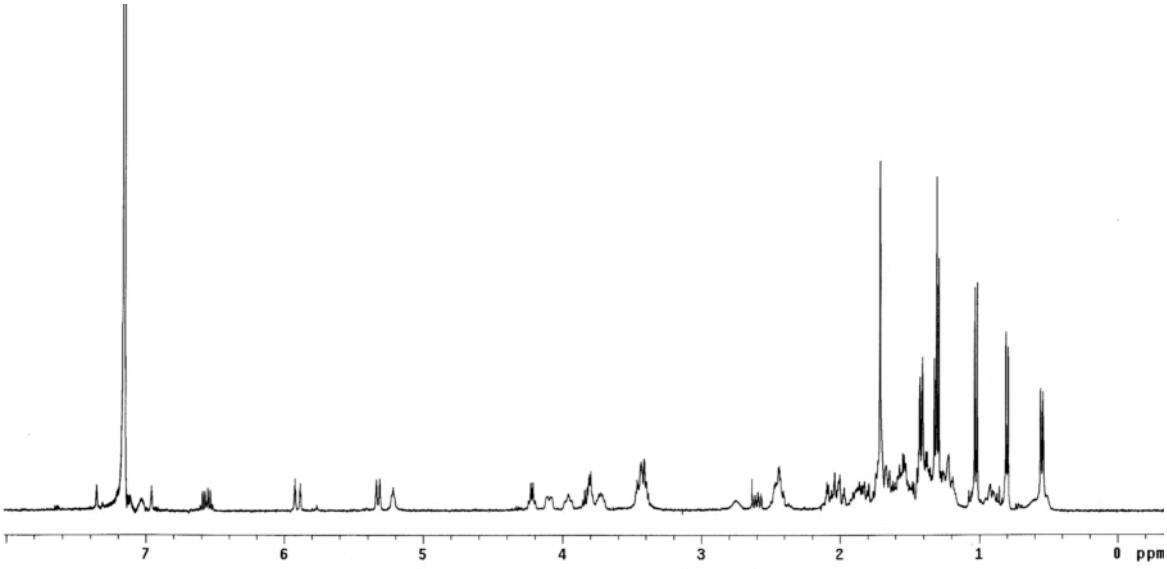
1.33 (400 MHz, C_6D_6)

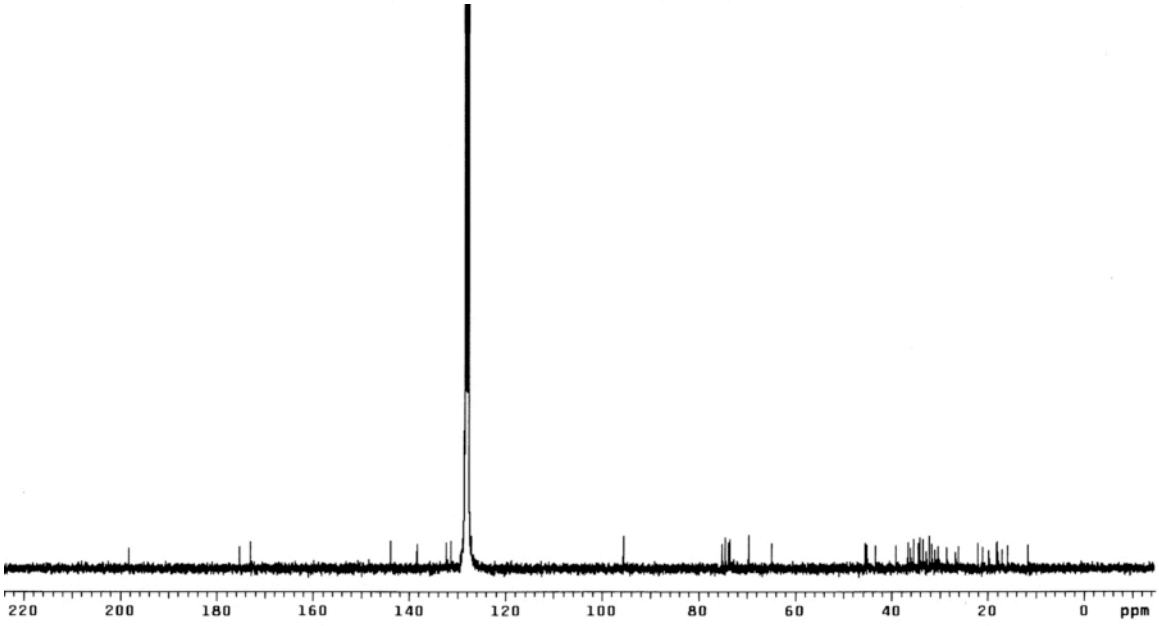


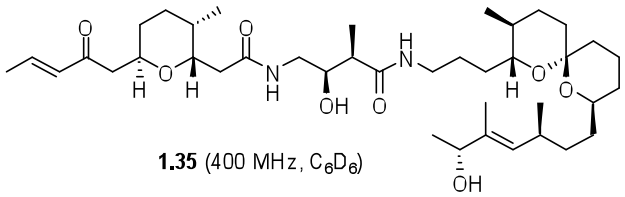




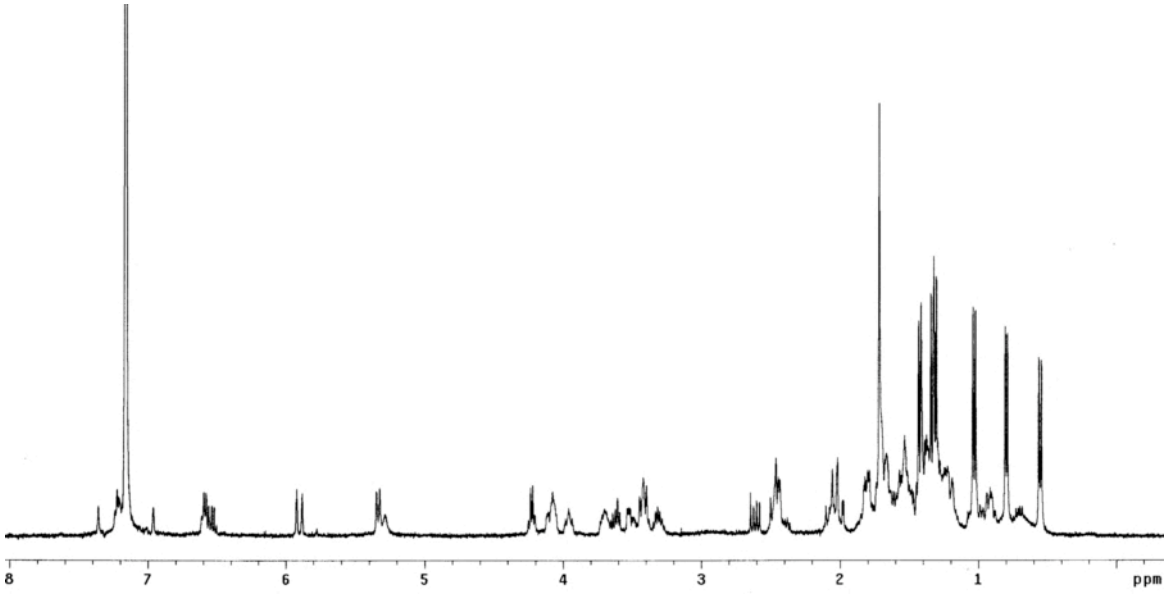
1.34 (400 MHz, C_6D_6)

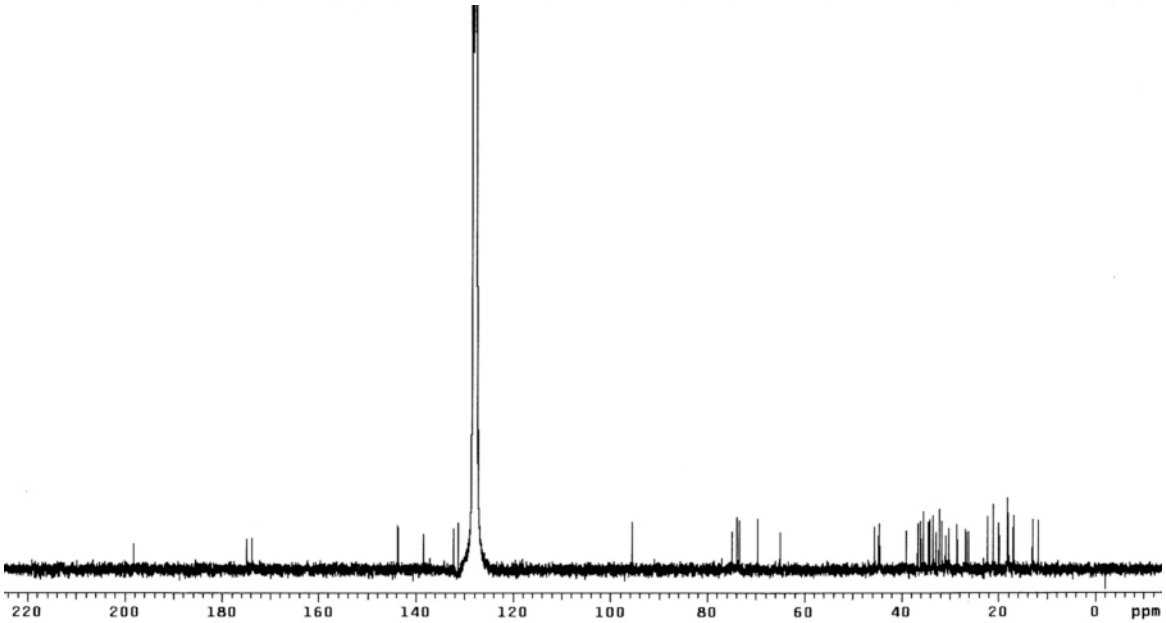


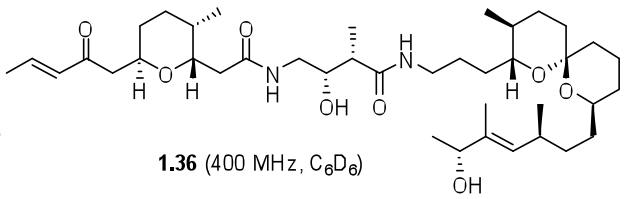
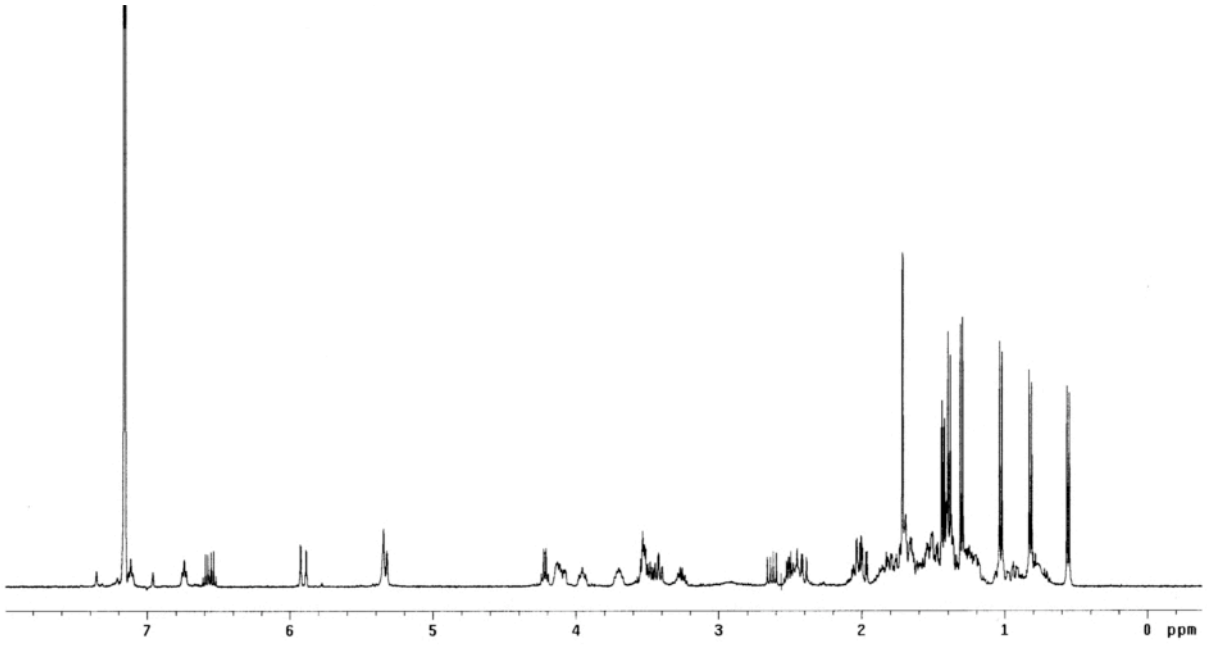
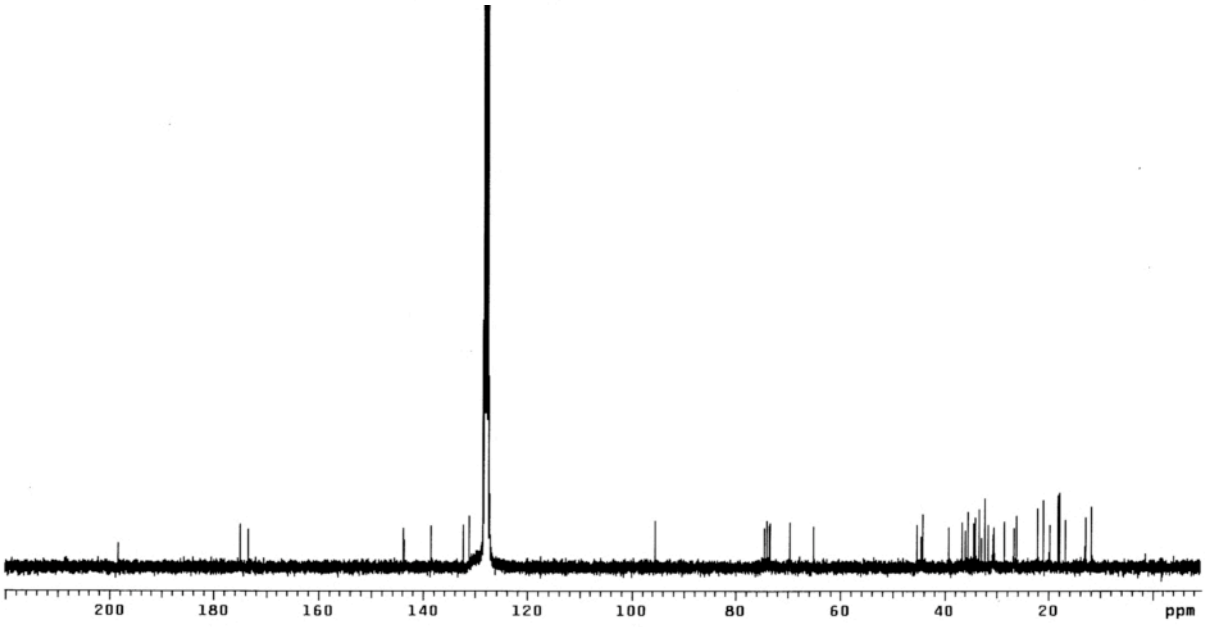




1.35 (400 MHz, C_6D_6)







1.36 (400 MHz, C_6D_6)