Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

ELECTRONIC SUPPLEMENTARY INFORMATION

Protecting Group Directed Diversity During Mitsunobu Cyclization of a Carbohydrate Derived Diamino Triol. Synthesis of Bridged Bicyclic and Six-membered Iminocyclitols.

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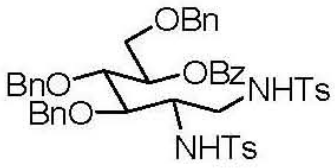
COPIES OF NMR SPECTRA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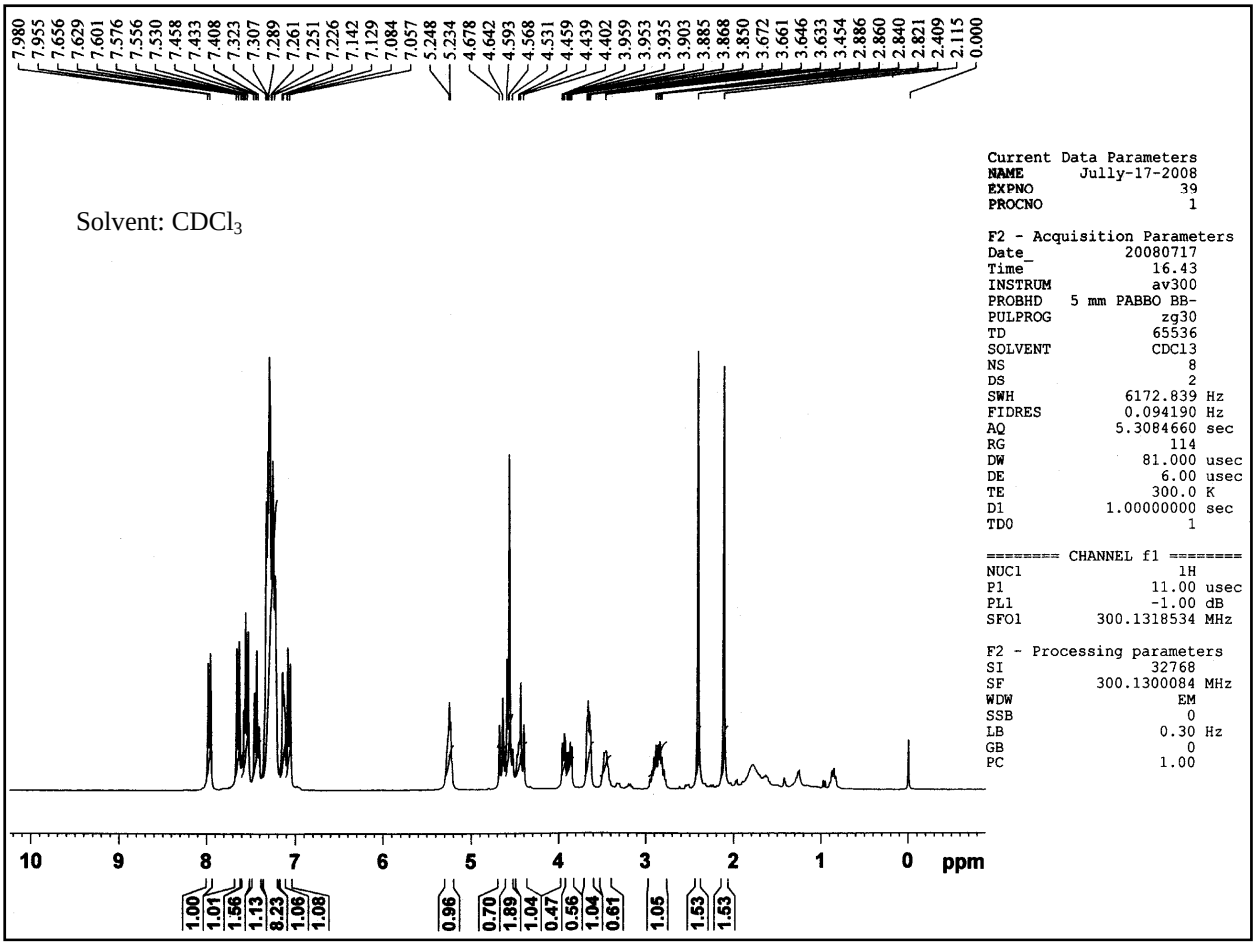
OBz
NHTs
BnO
NHTs

14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7.289
7.261
7.251
7.226
7.142
7.129
7.084
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5.248
5.234
4.678
4.642
4.593
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3.953
3.935
3.903
3.885
3.868
3.850
3.672
3.661
3.646
3.633
3.454
2.886
2.860
2.840
2.821
2.409
2.115
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PULPROG zg30
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SOLVENT CDCl3
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FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
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SF 300.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.56
1.13
8.23
1.06
1.08
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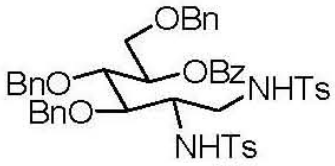
1.04
0.61
1.05
1.53
1.53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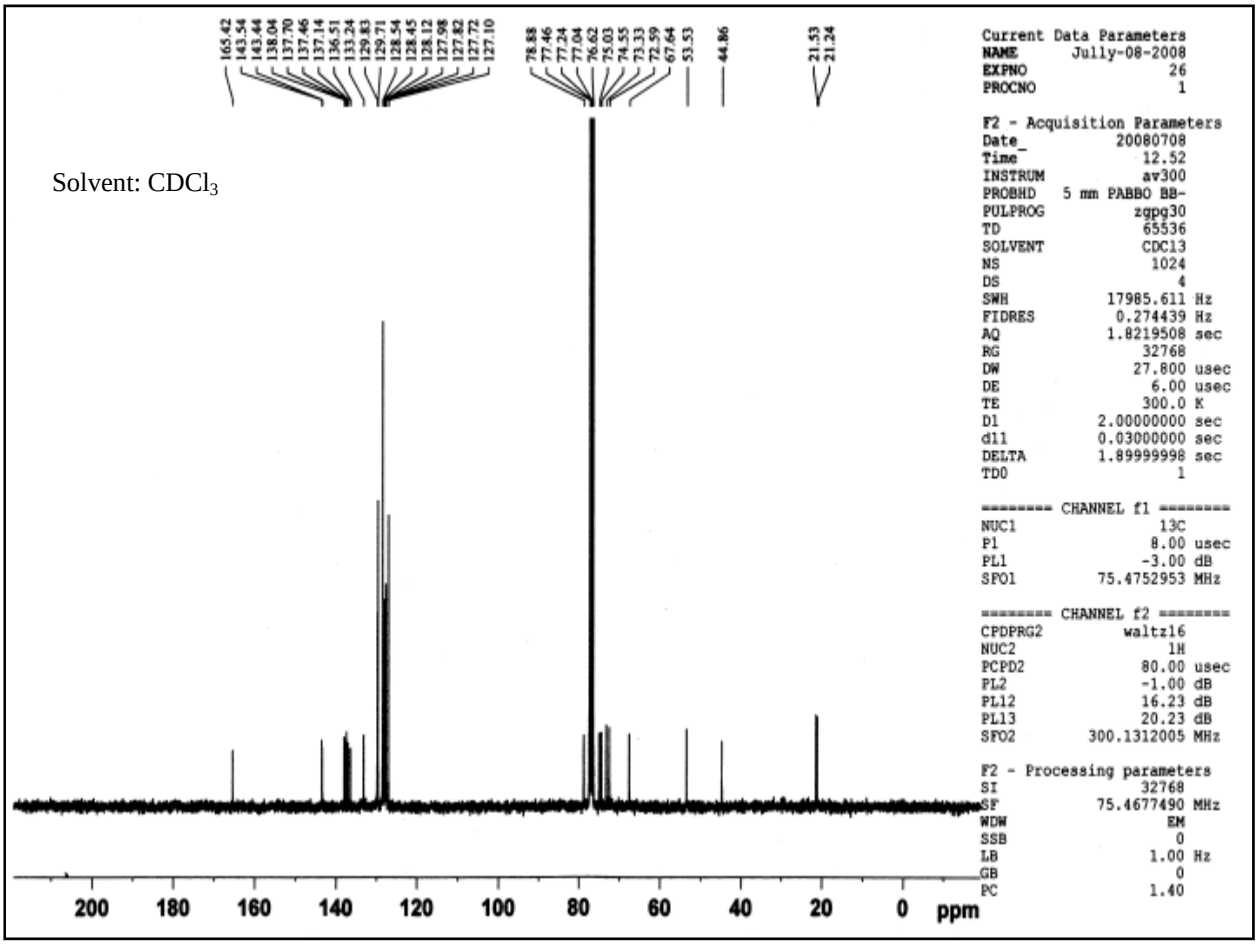
BnO
OBz
NHTs
BnO
NHTs

14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128.45
128.12
127.98
127.82
127.72
127.10
78.88
77.46
77.24
77.04
76.62
75.03
74.55
73.33
72.59
67.64
53.53
44.86
21.53
21.24
200
180
160
140
120
100
80
60
40
20
0
ppm
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EXPNO 26
PROCNO 1
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Time 12.52
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PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.23 dB
PL13 20.23 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
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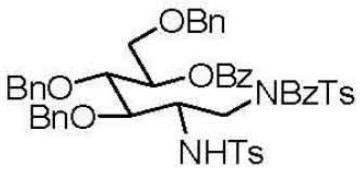
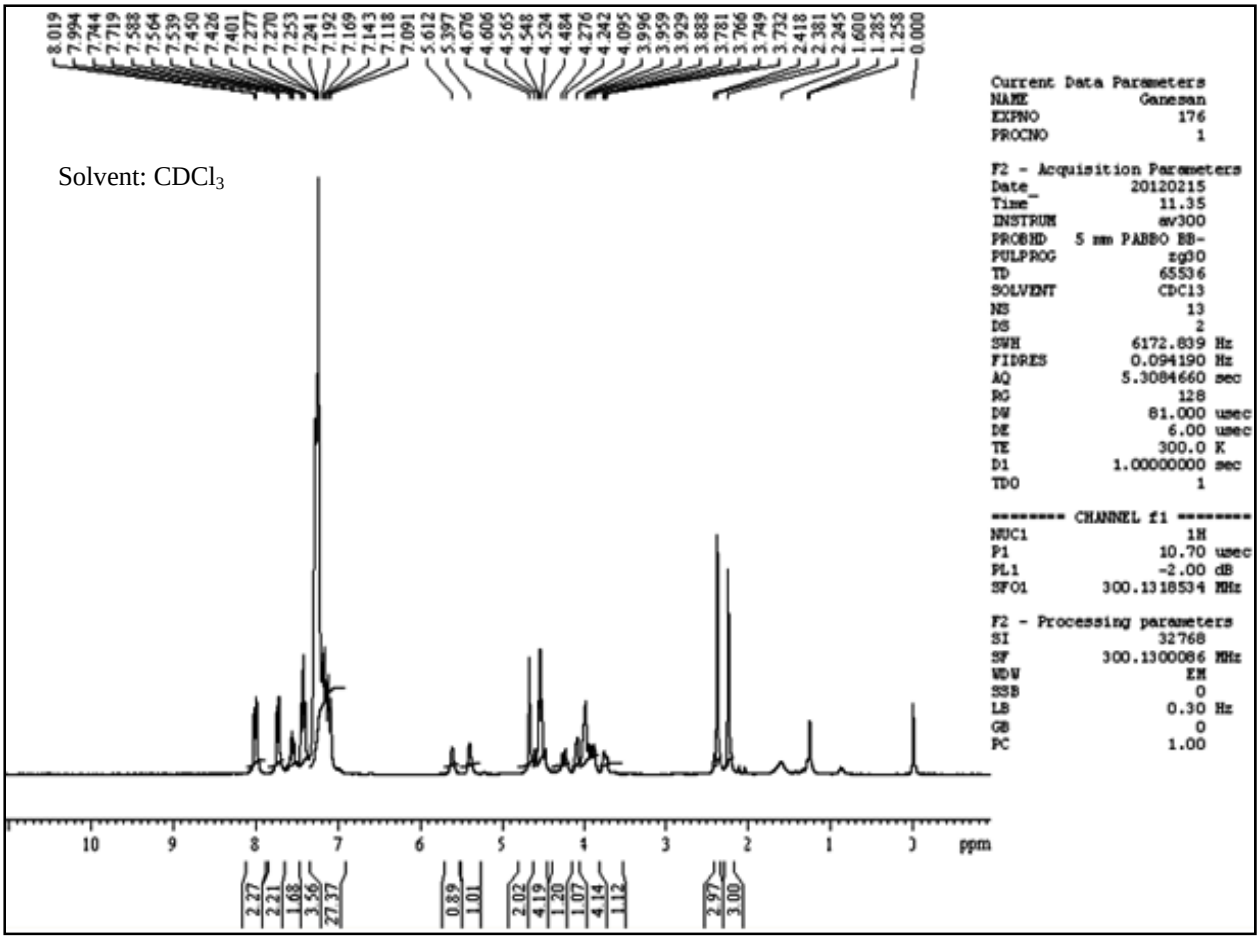
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


OBn
BnO
OBz
NBzTs
BnO
NHTs

15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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
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F2 - Processing parameters
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WDW EM
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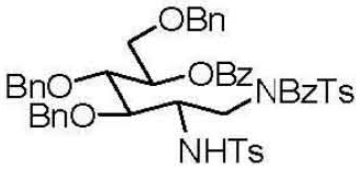
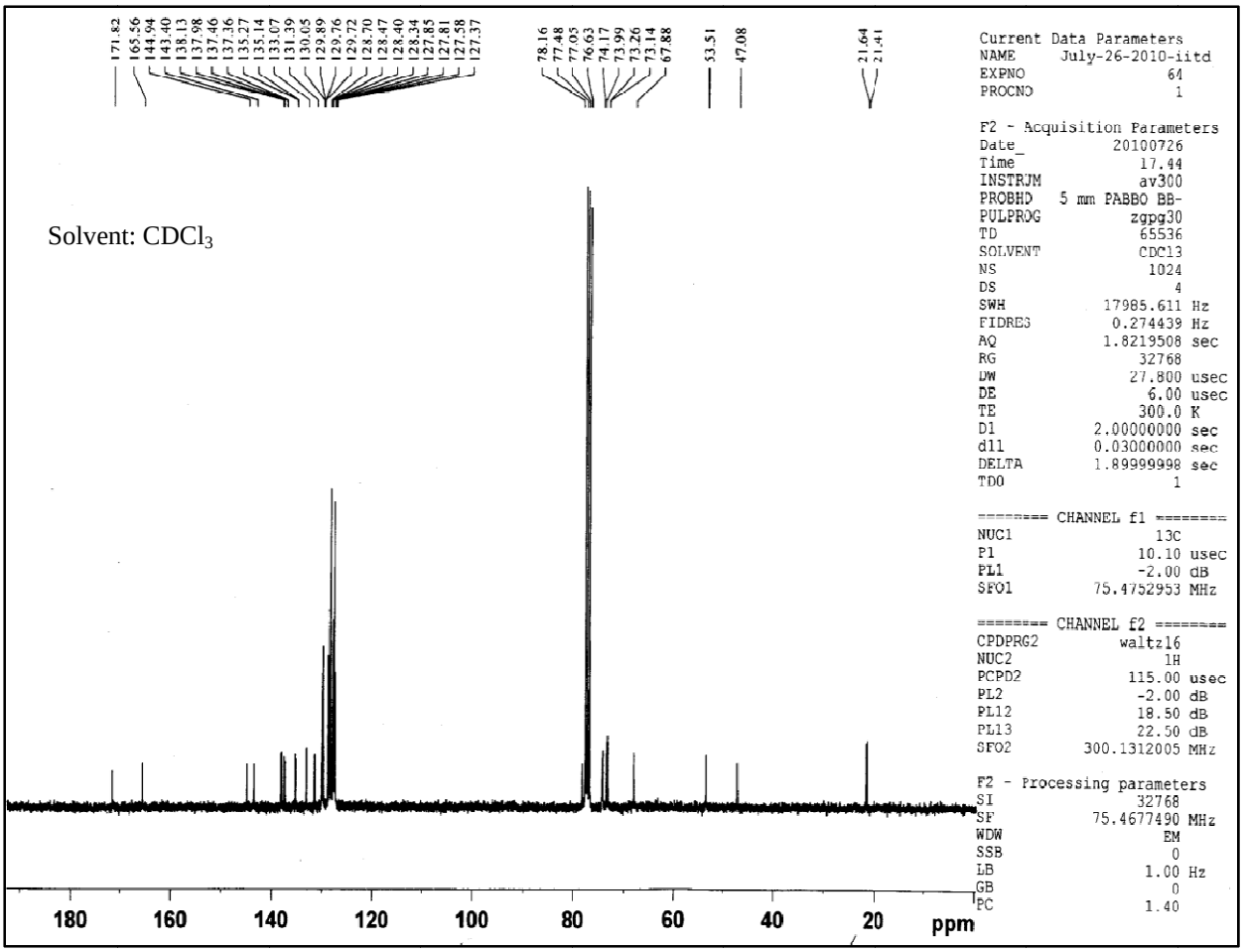
LB 0.30 Hz
GB 0
PC 1.00
ppm


OBn
BnO
OBz
NBzTs
BnO
NHTs

15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138.13
137.98
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137.36
135.27
135.14
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67.88
53.51
47.08
21.64
21.41
Solvent: CDCl3
180
160
140
120
100
80
60
40
20
ppm
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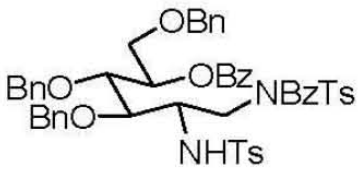
EXPNO 64
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100726
Time 17.44
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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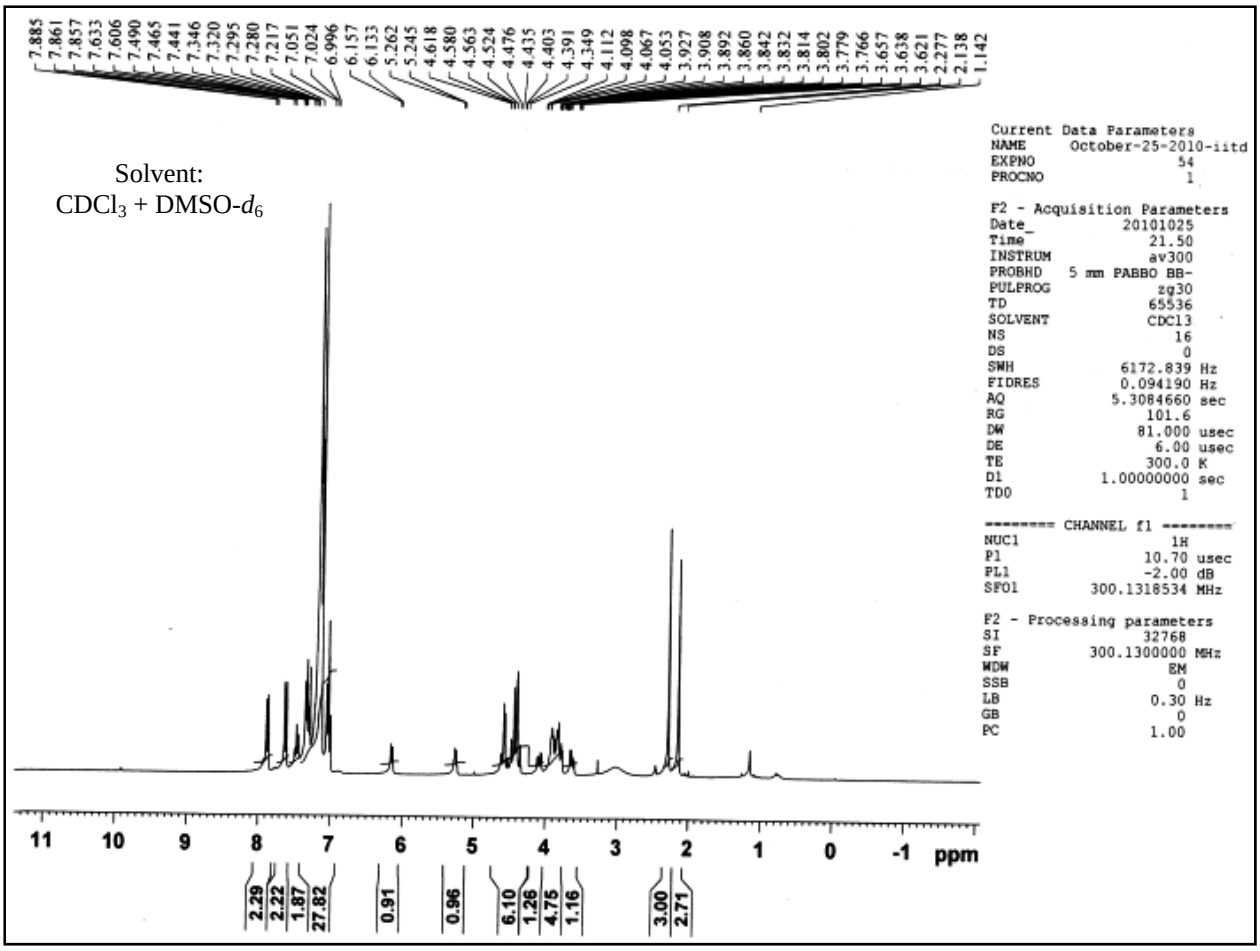
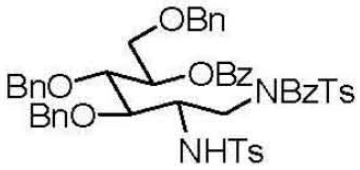
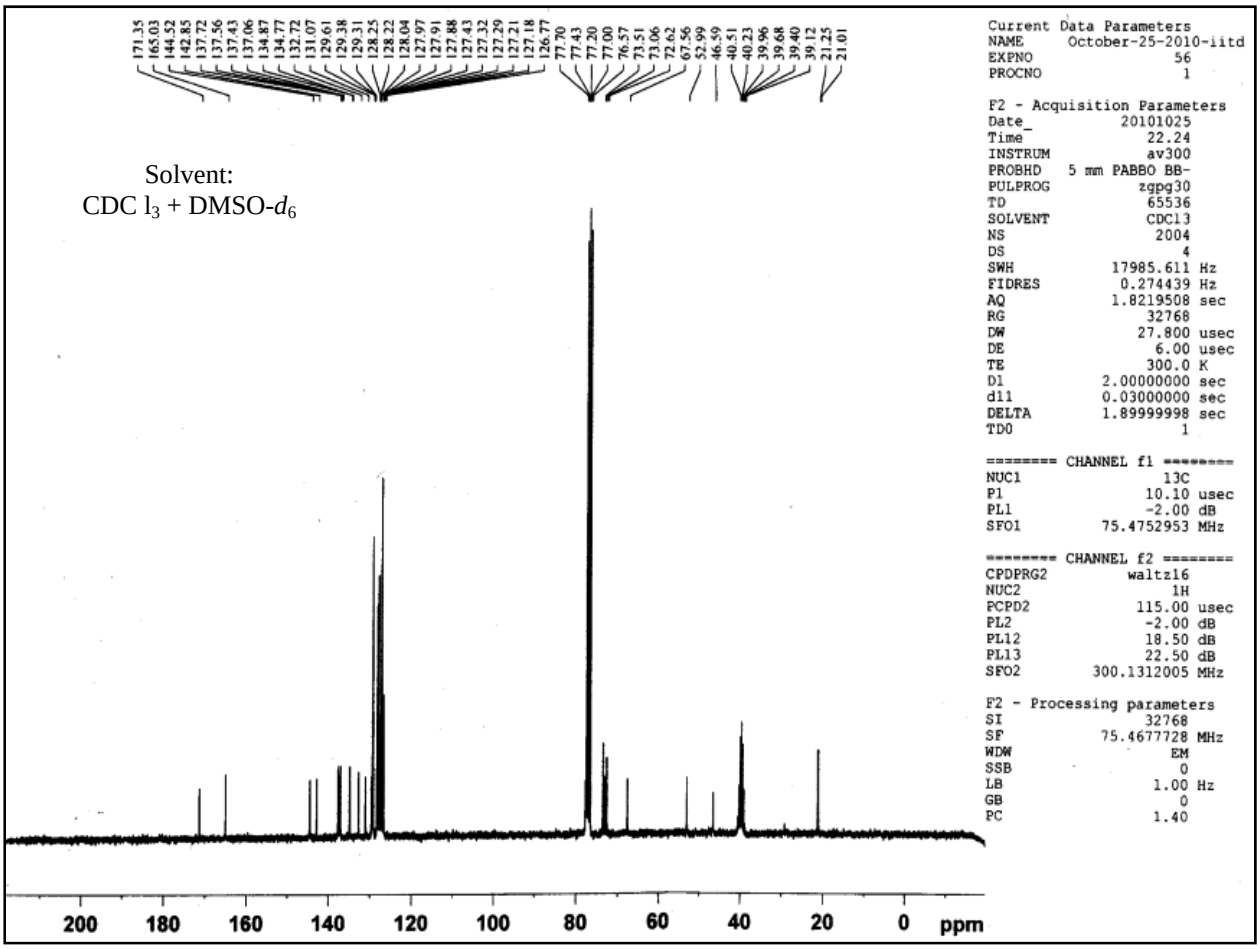



OBn
BnO
OBz
NBzTs
BnO
NHTs

15


171.35
165.03
144.52
142.85
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137.43
137.06
134.87
134.77
132.72
131.07
129.61
129.38
129.31
128.25
128.22
128.04
127.97
127.91
127.88
127.43
127.32
127.29
127.21
127.18
126.77
77.70
77.43
77.20
77.00
76.57
73.51
73.06
72.62
67.56
52.99
46.59
40.51
40.23
39.96
39.68
39.40
39.12
21.25
21.01
Solvent:
CDC l3 + DMSO-d6
200
180
160
140
120
100
80
60
40
20
0
ppm
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EXPNO 56
PROCNO 1
F2 - Acquisition Parameters
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Time 22.24
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2004
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
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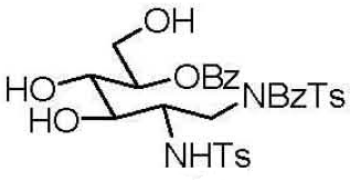
SF 75.4677728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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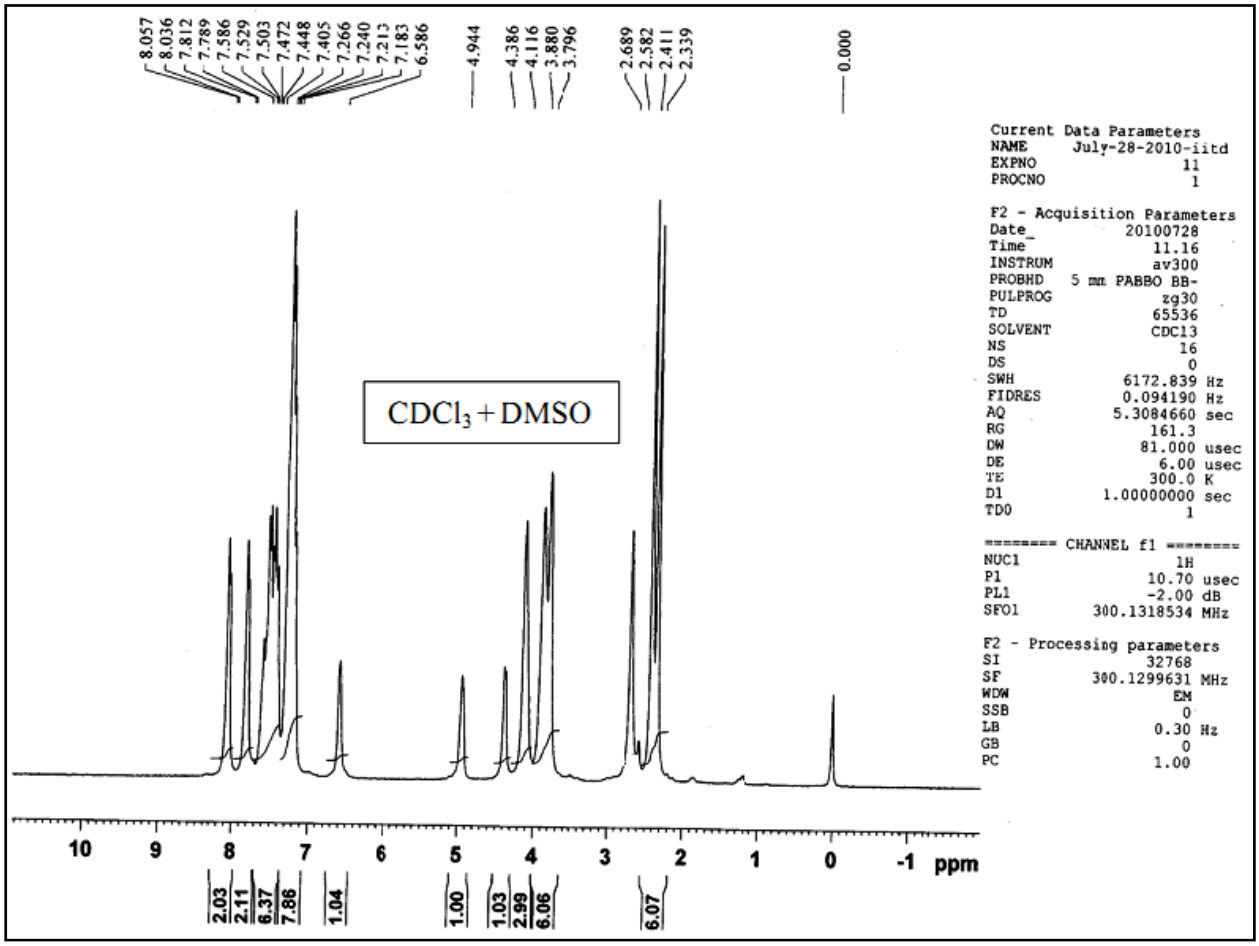
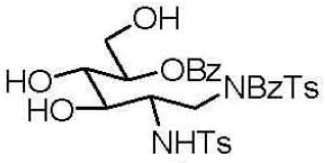
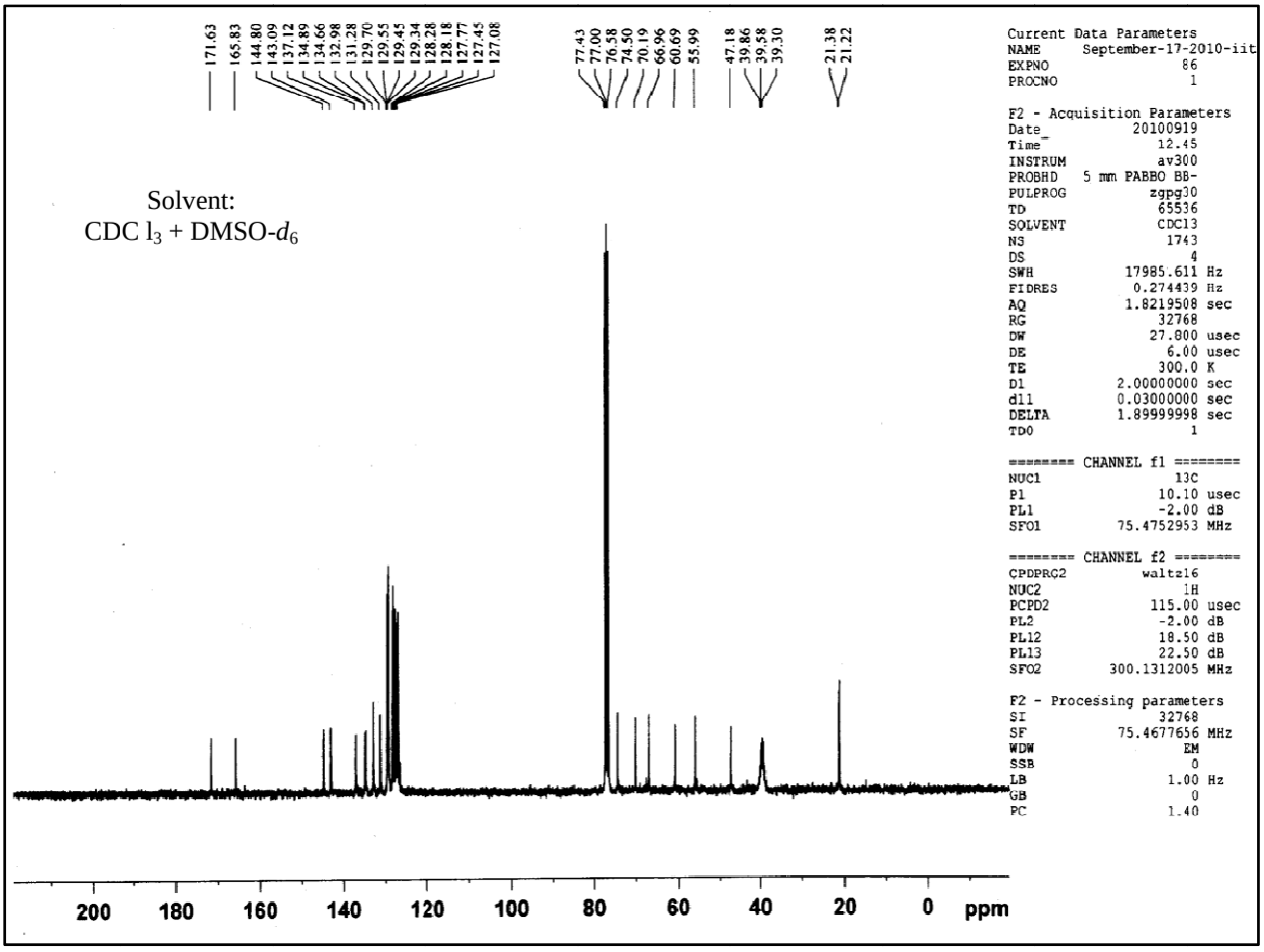



OH
HO
OBz
NBzTs
HO
NHTs

16


171.63
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132.98
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129.45
129.34
128.28
128.18
127.77
127.45
127.08
77.43
77.00
76.58
74.50
70.19
66.96
60.69
55.99
47.18
39.86
39.58
39.30
21.38
21.22
Solvent:
CDC l3 + DMSO-d6
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
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EXPNO 86
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100919
Time 12.45
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1743
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
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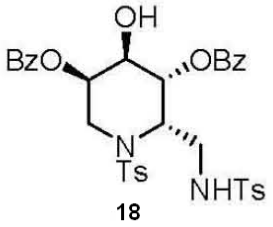
SF 75.4677656 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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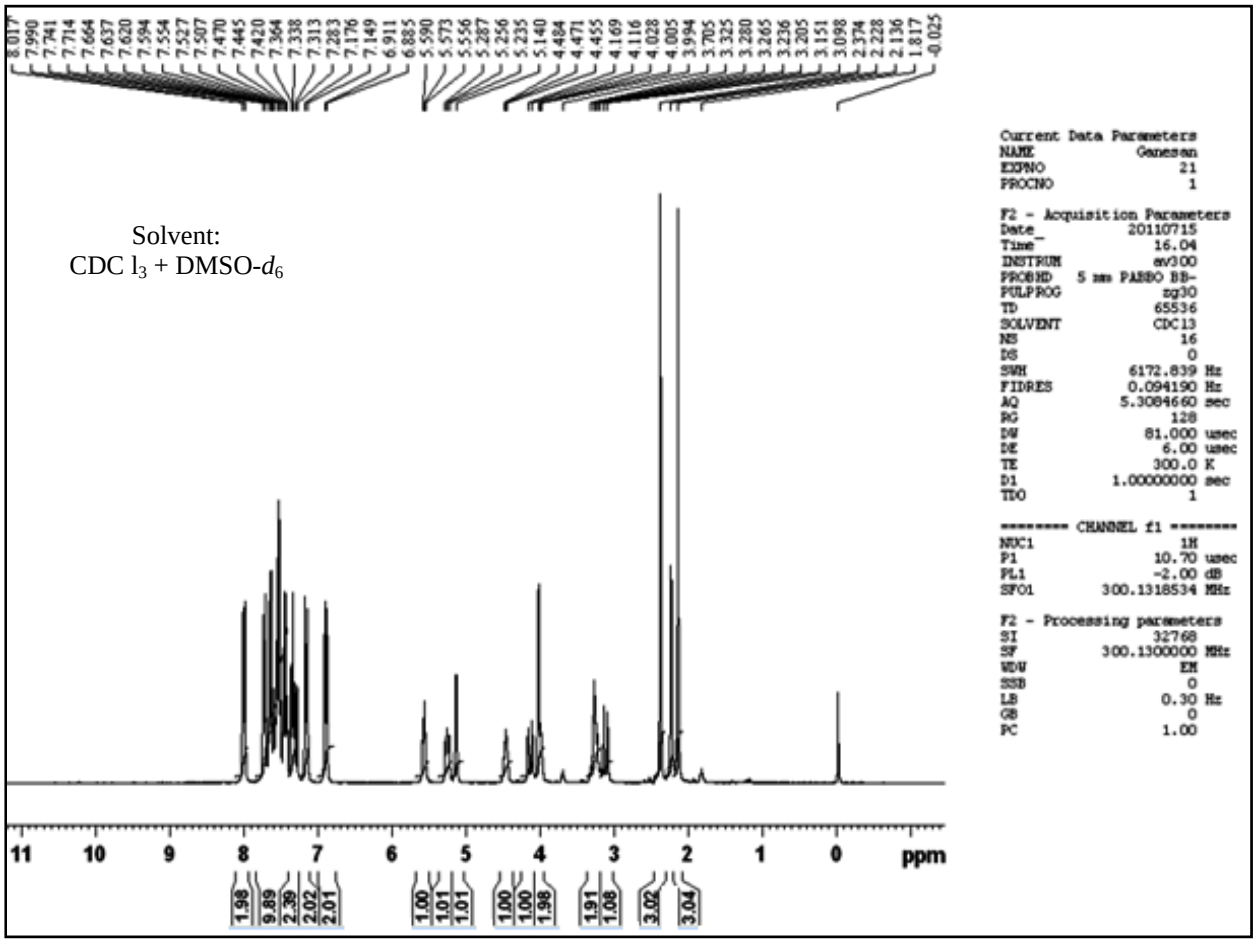

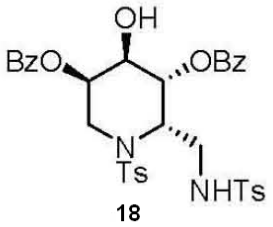

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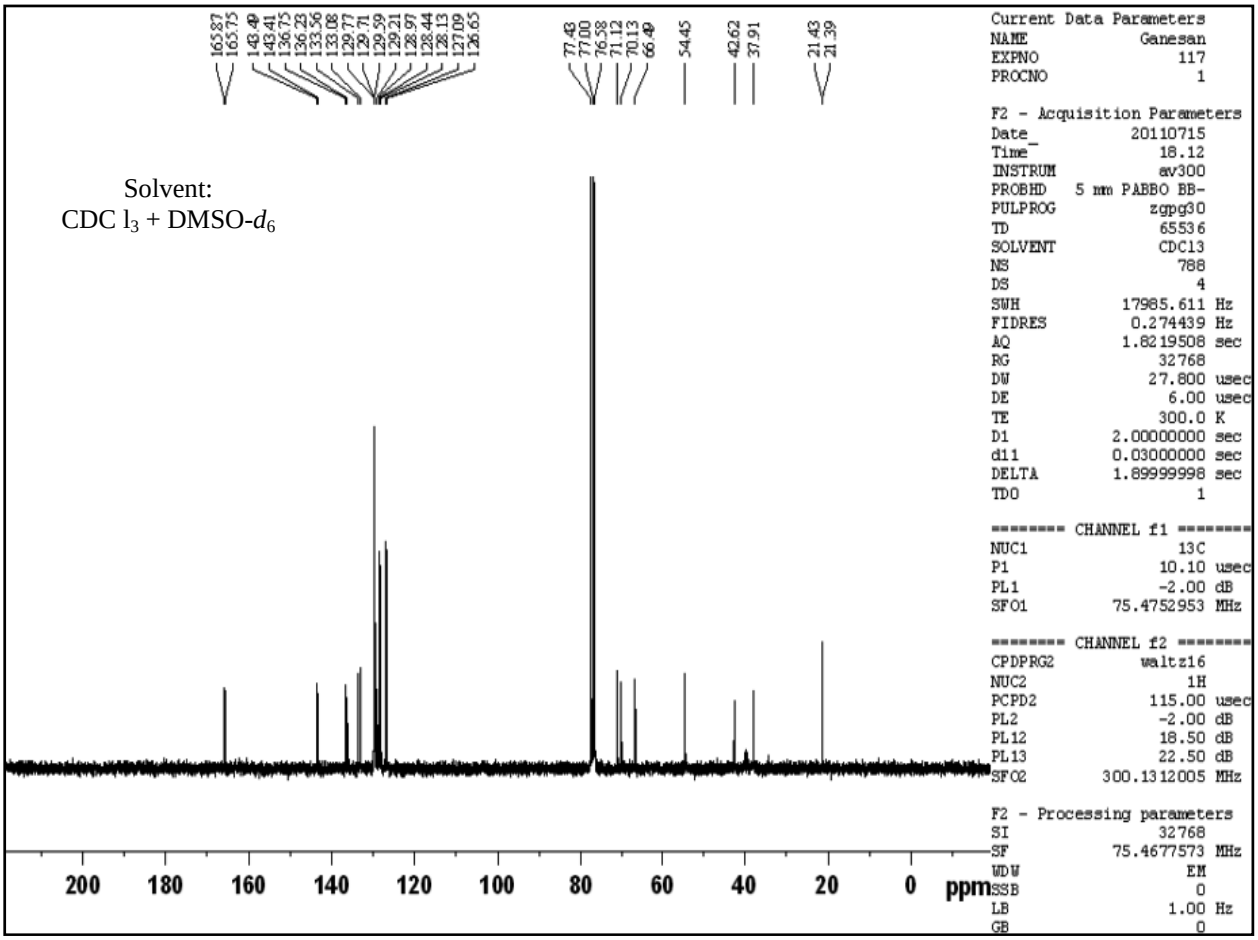

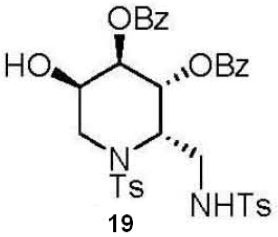

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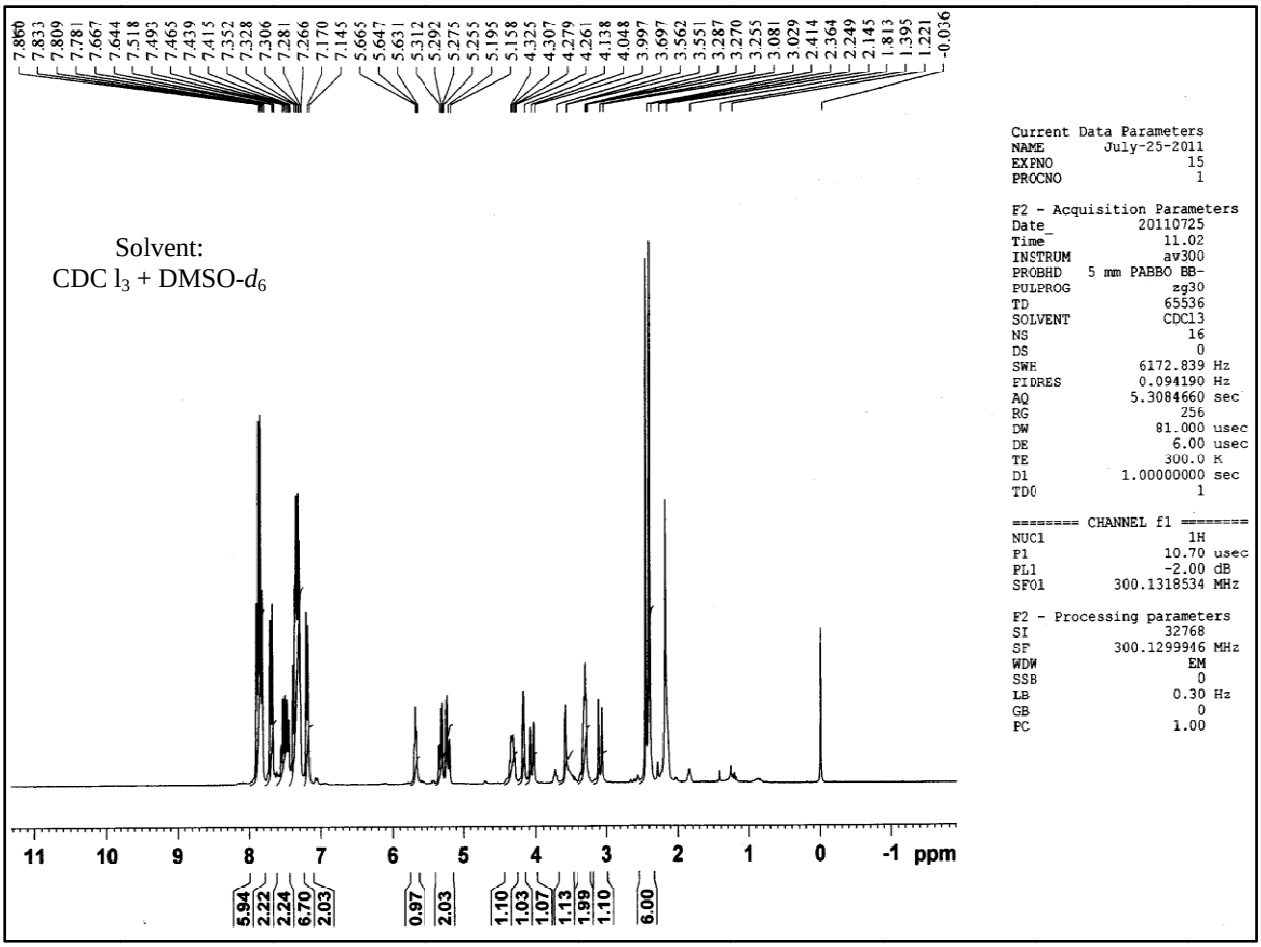
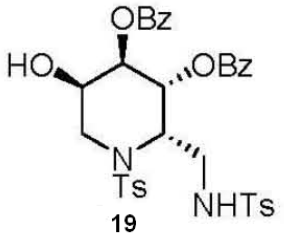
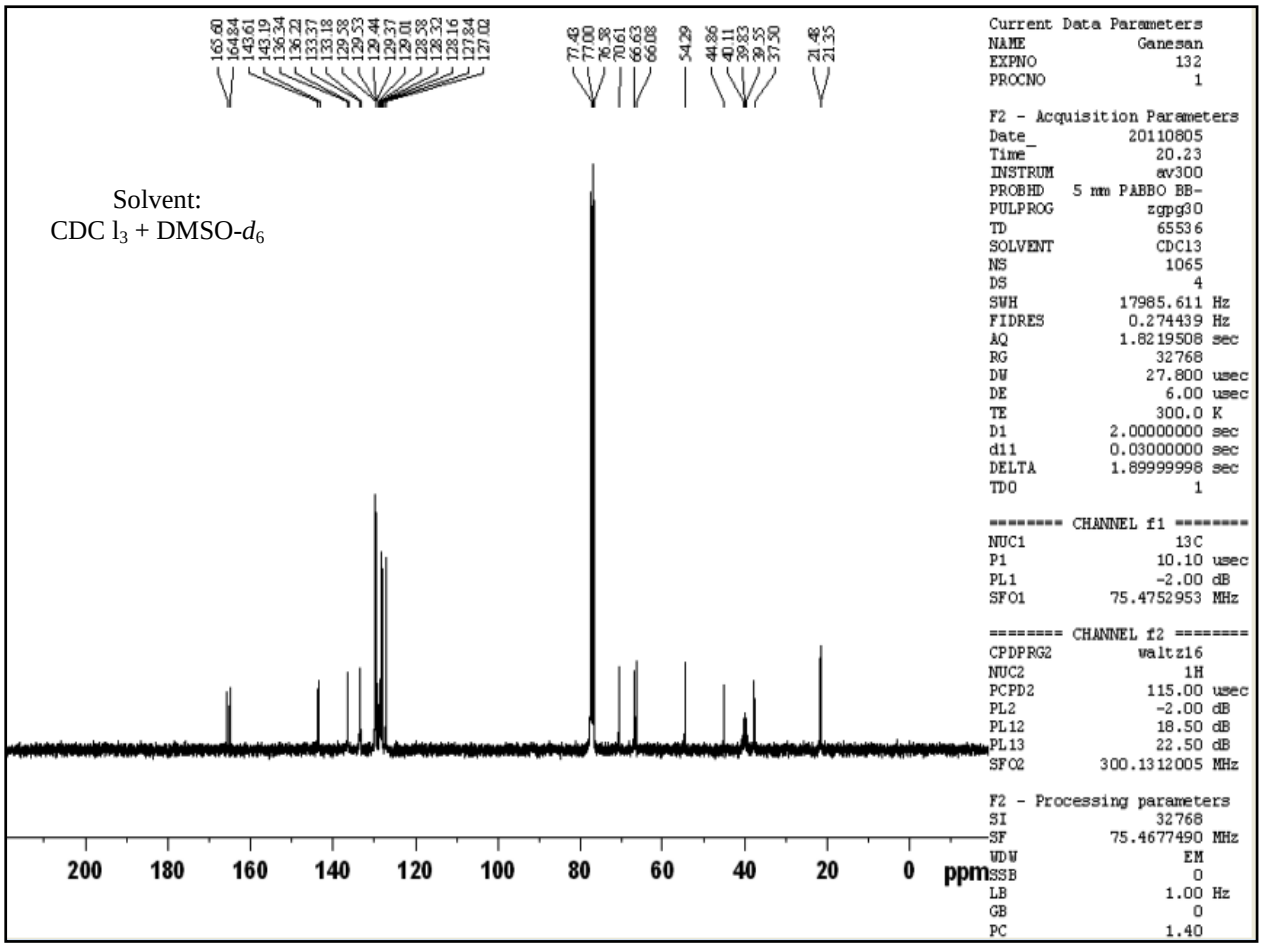



OBz
HO
OBz
N
Ts
NHTs

19


165.60
164.84
143.61
143.19
136.34
136.22
133.37
133.18
129.58
129.53
129.44
129.37
129.01
128.58
128.32
128.16
127.84
127.02
77.43
77.00
76.58
70.61
66.63
66.08
54.29
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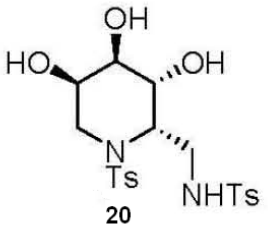
40.11
39.83
39.55
37.30
21.48
21.35
Solvent:
CDC l3 + DMSO-d6
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Ganesan
EXPNO 132
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110805
Time 20.23
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1065
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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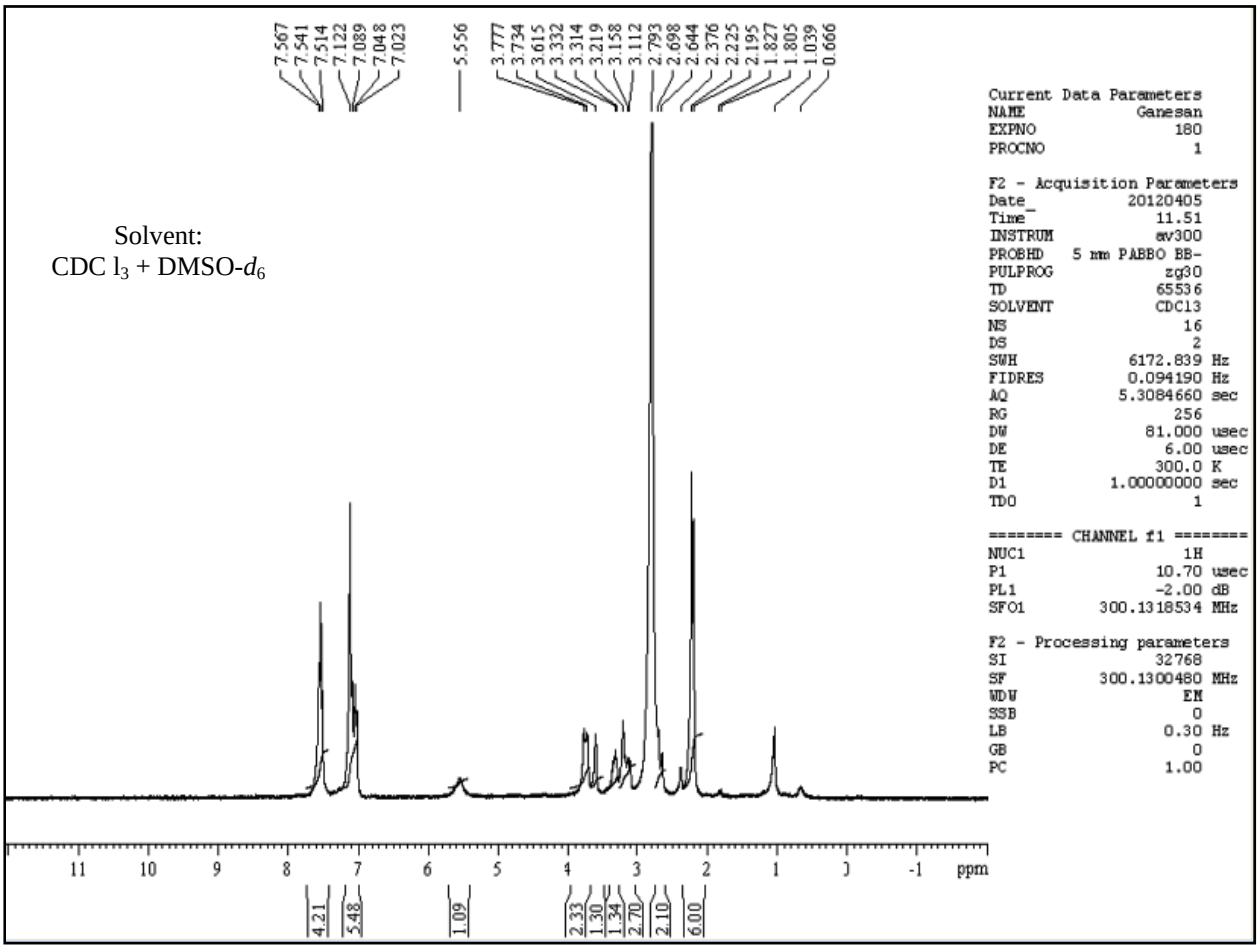

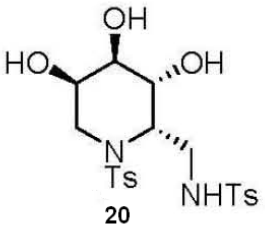

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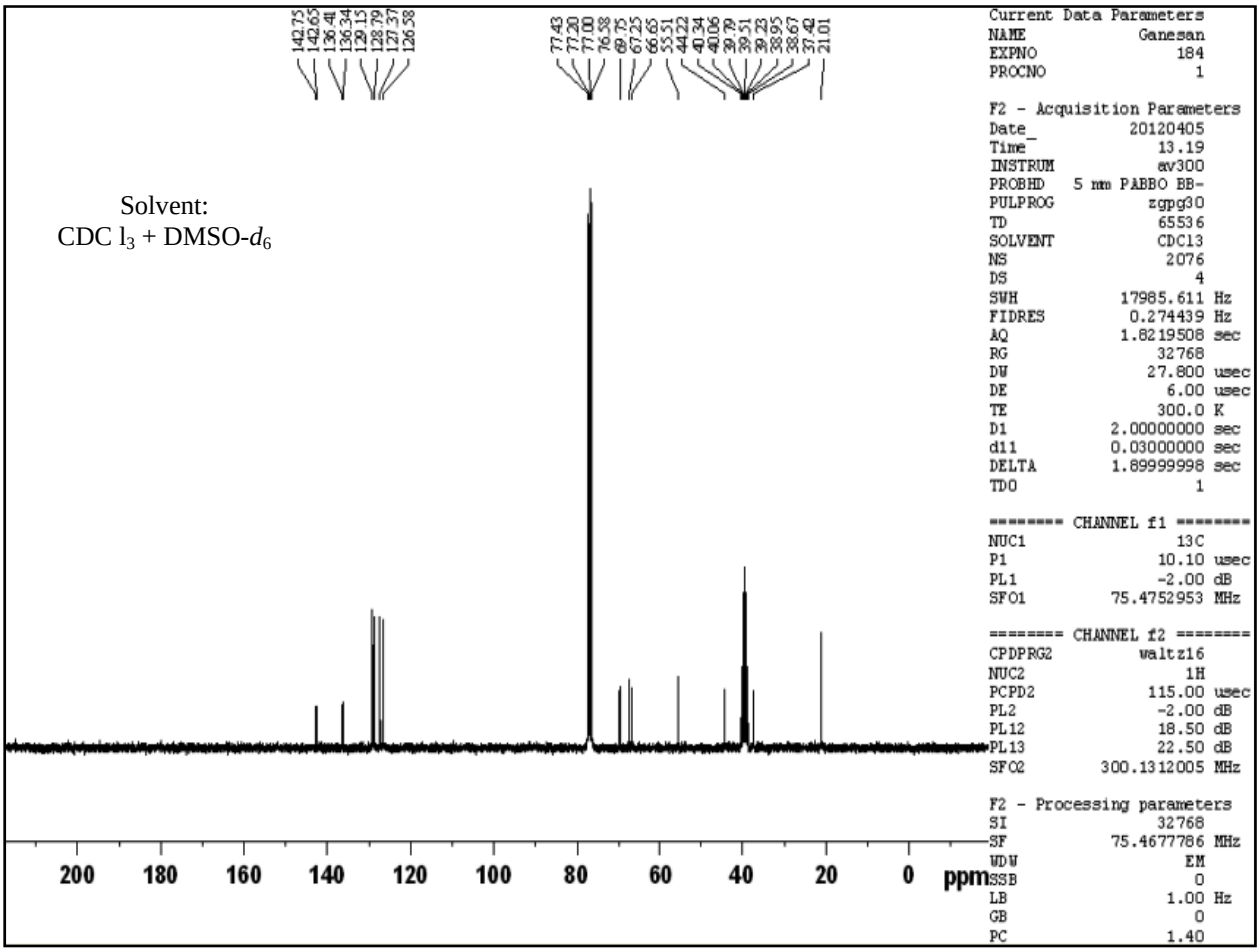
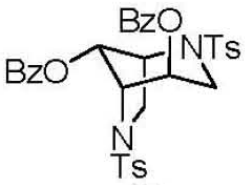
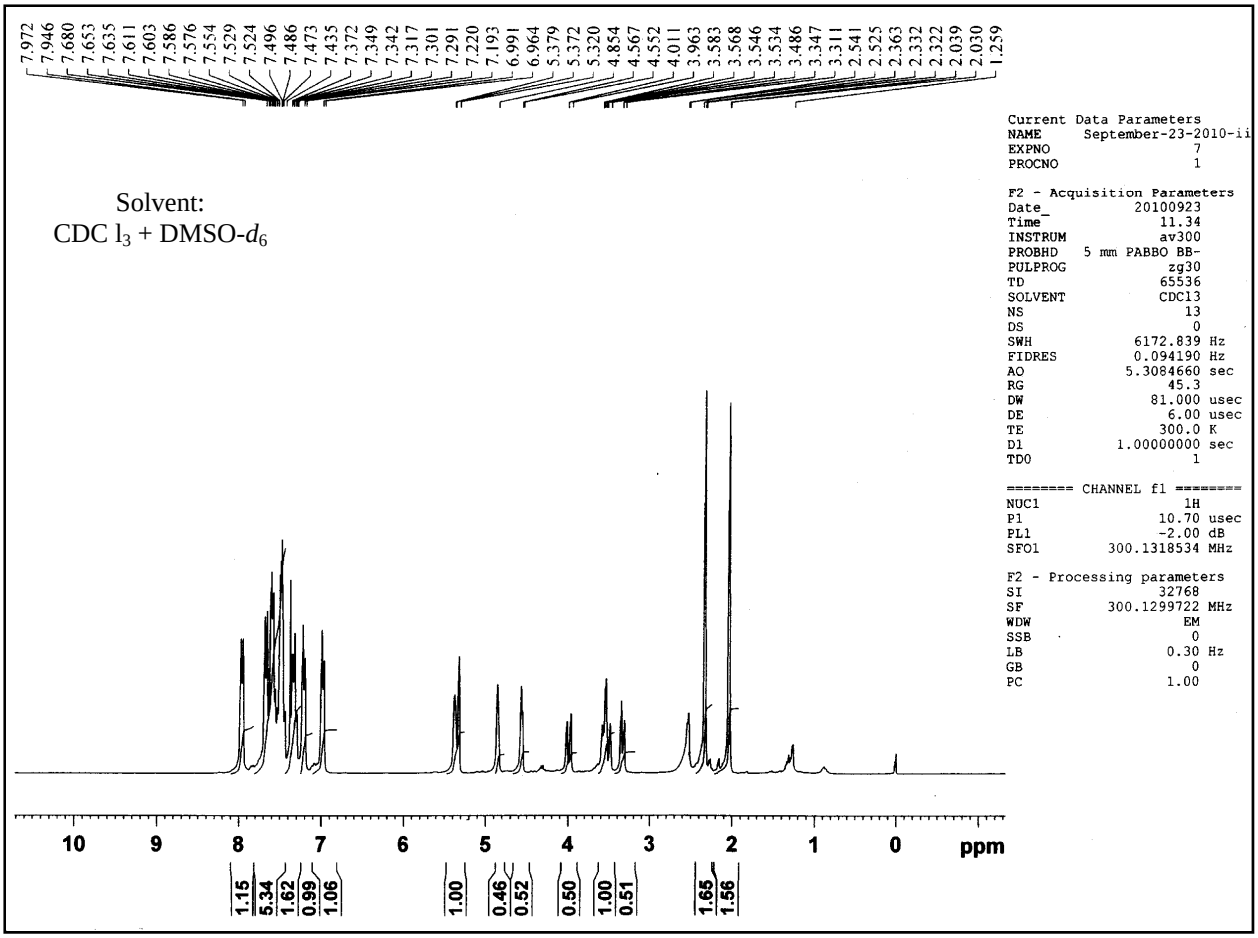
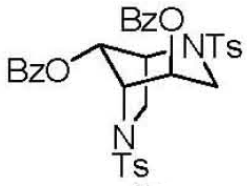


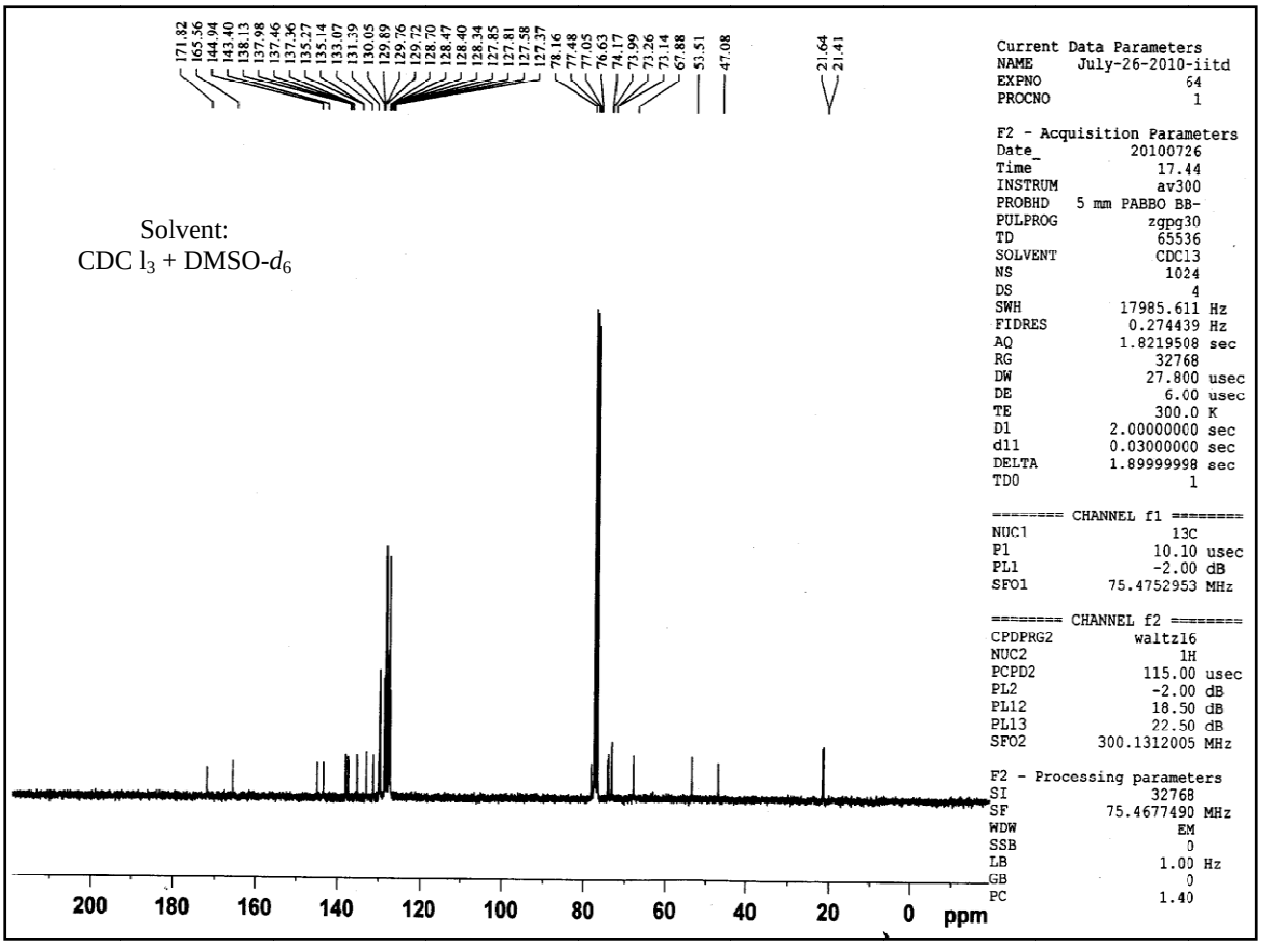


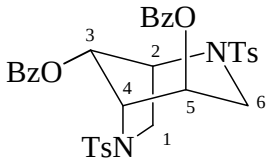
21



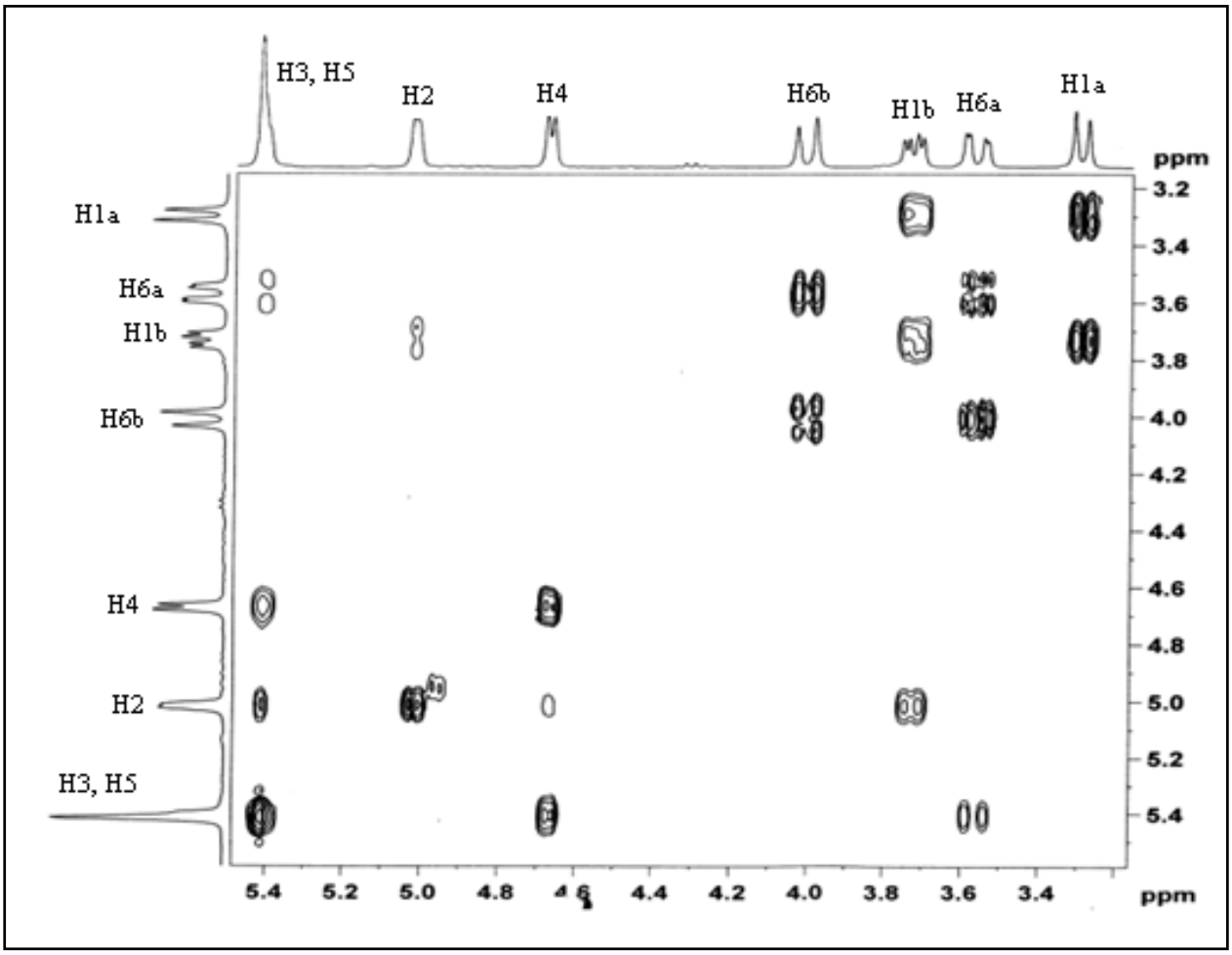


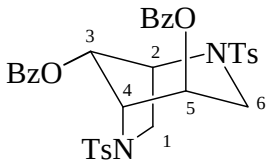
21



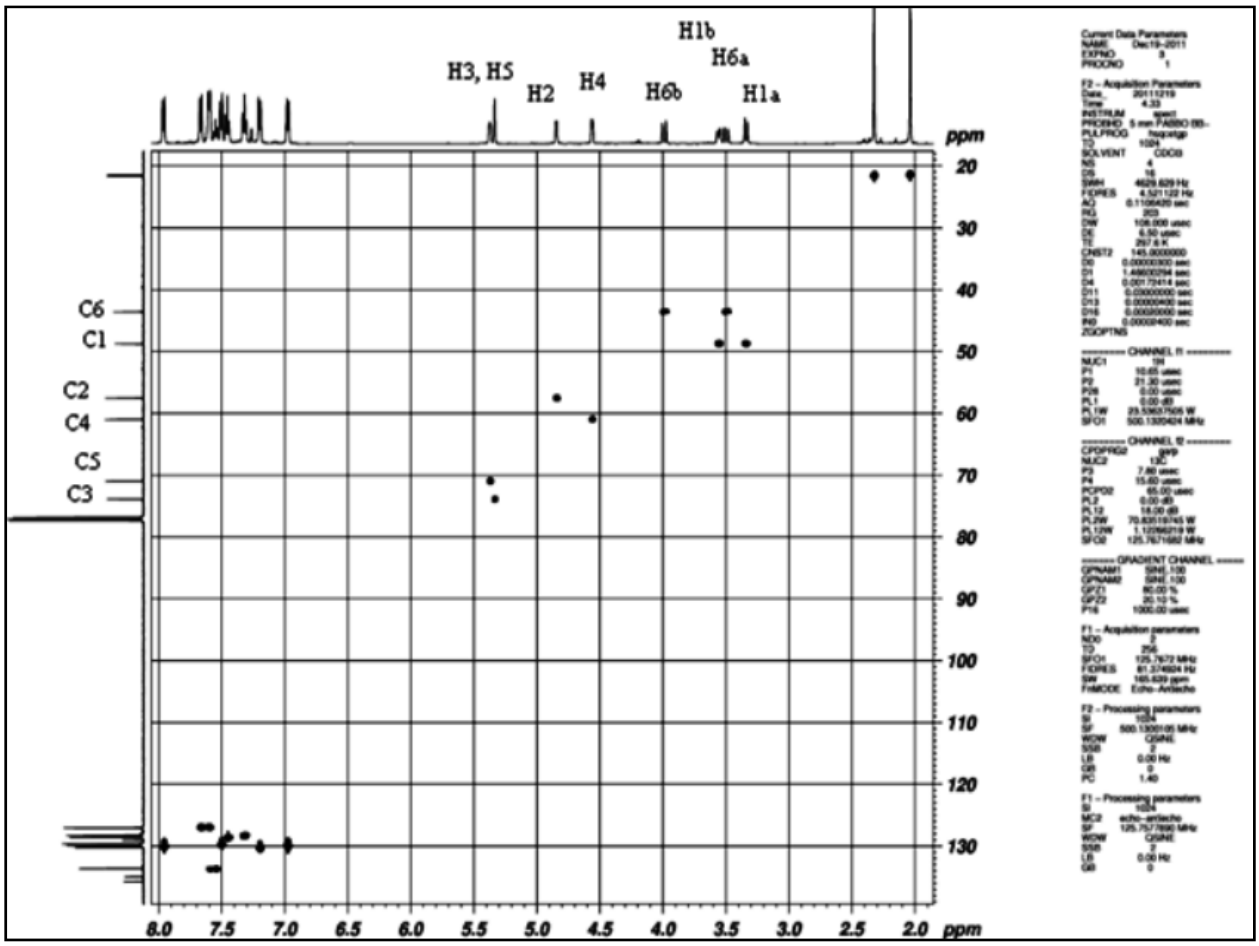


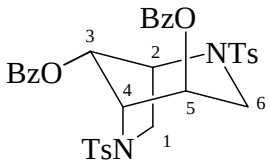
21 Solvent: $CDCl_3$



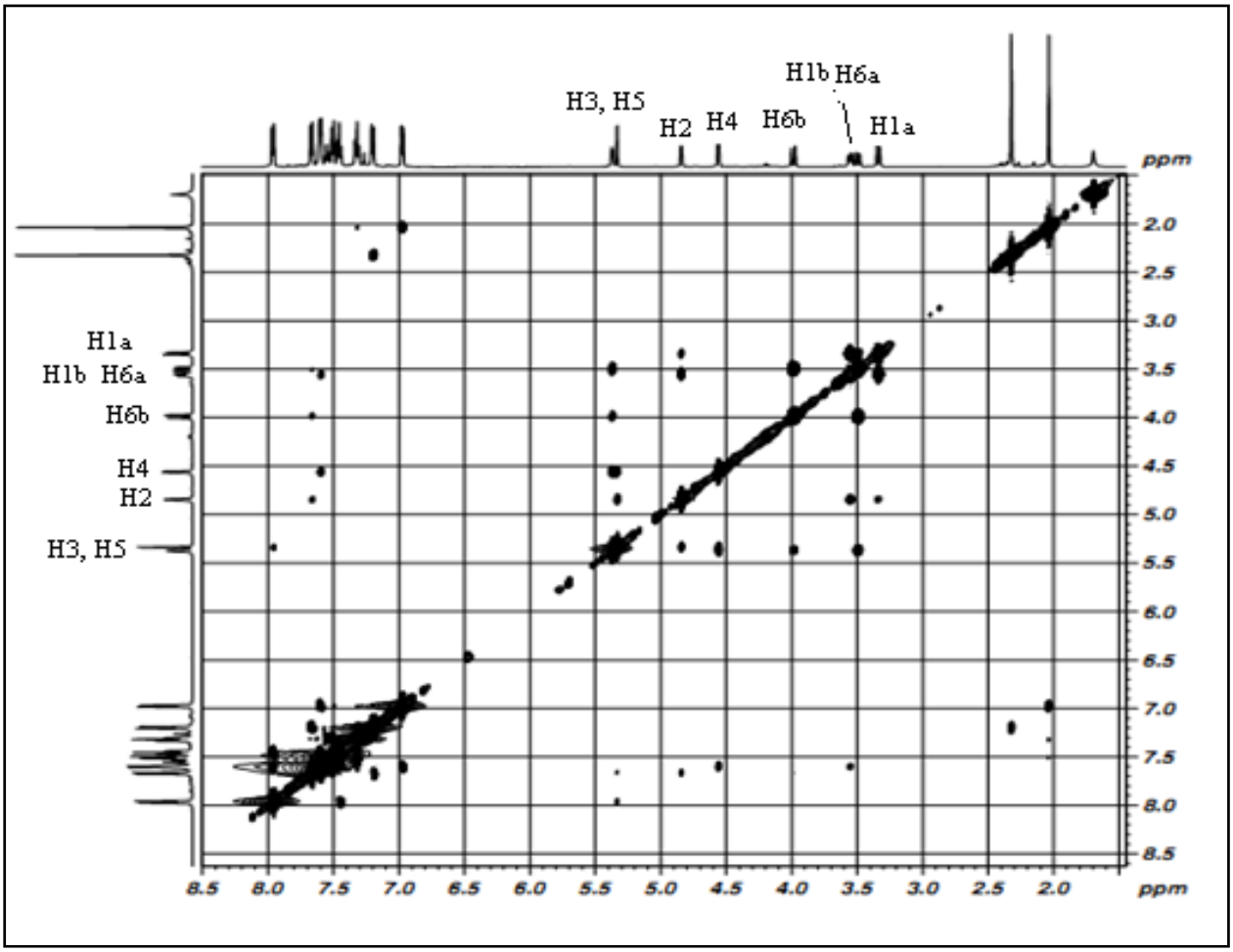


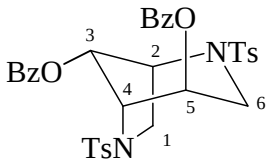
21 Solvent: CDC l_3



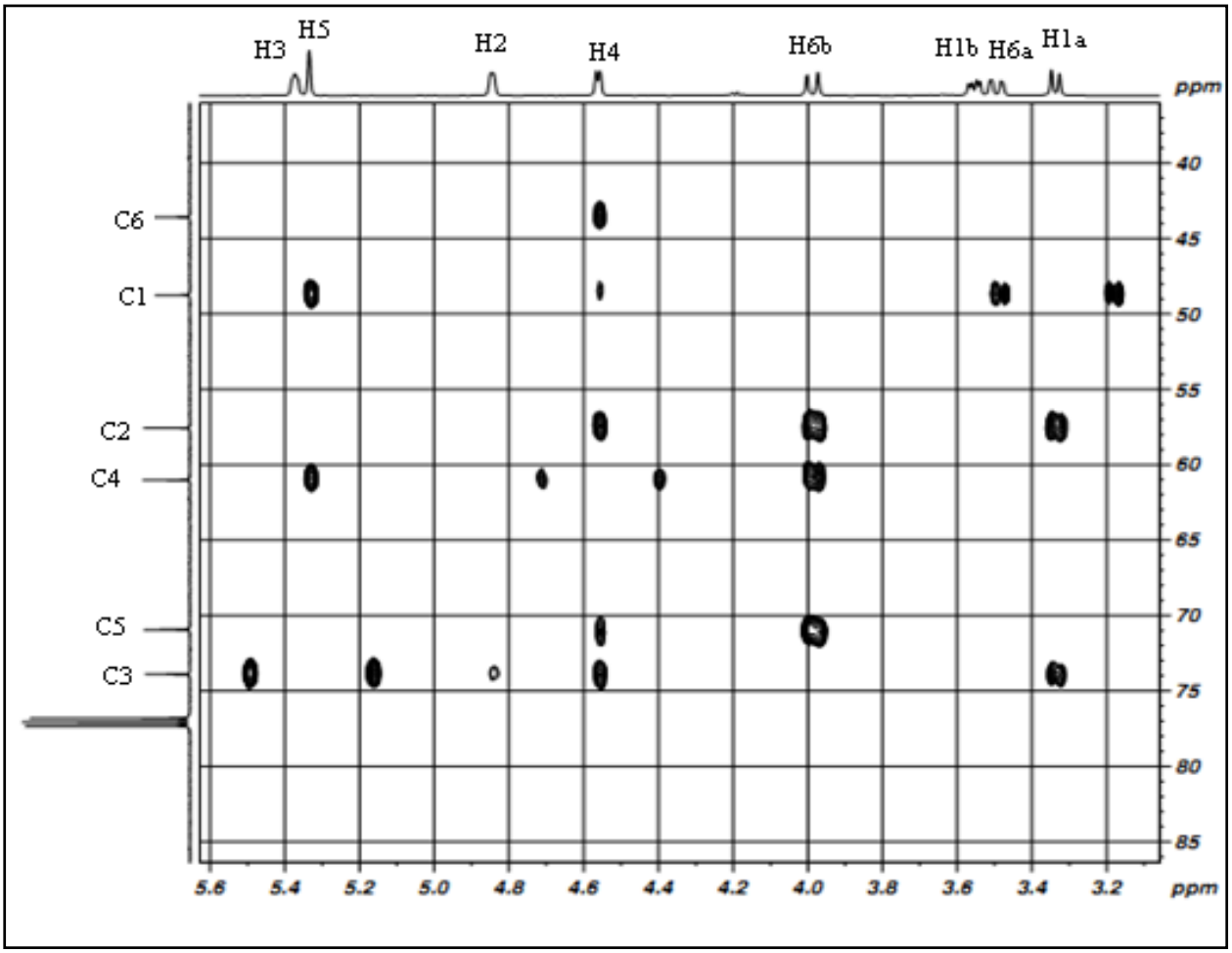


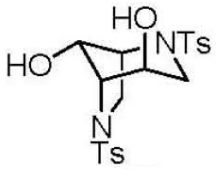
21 Solvent: $CDCl_3$



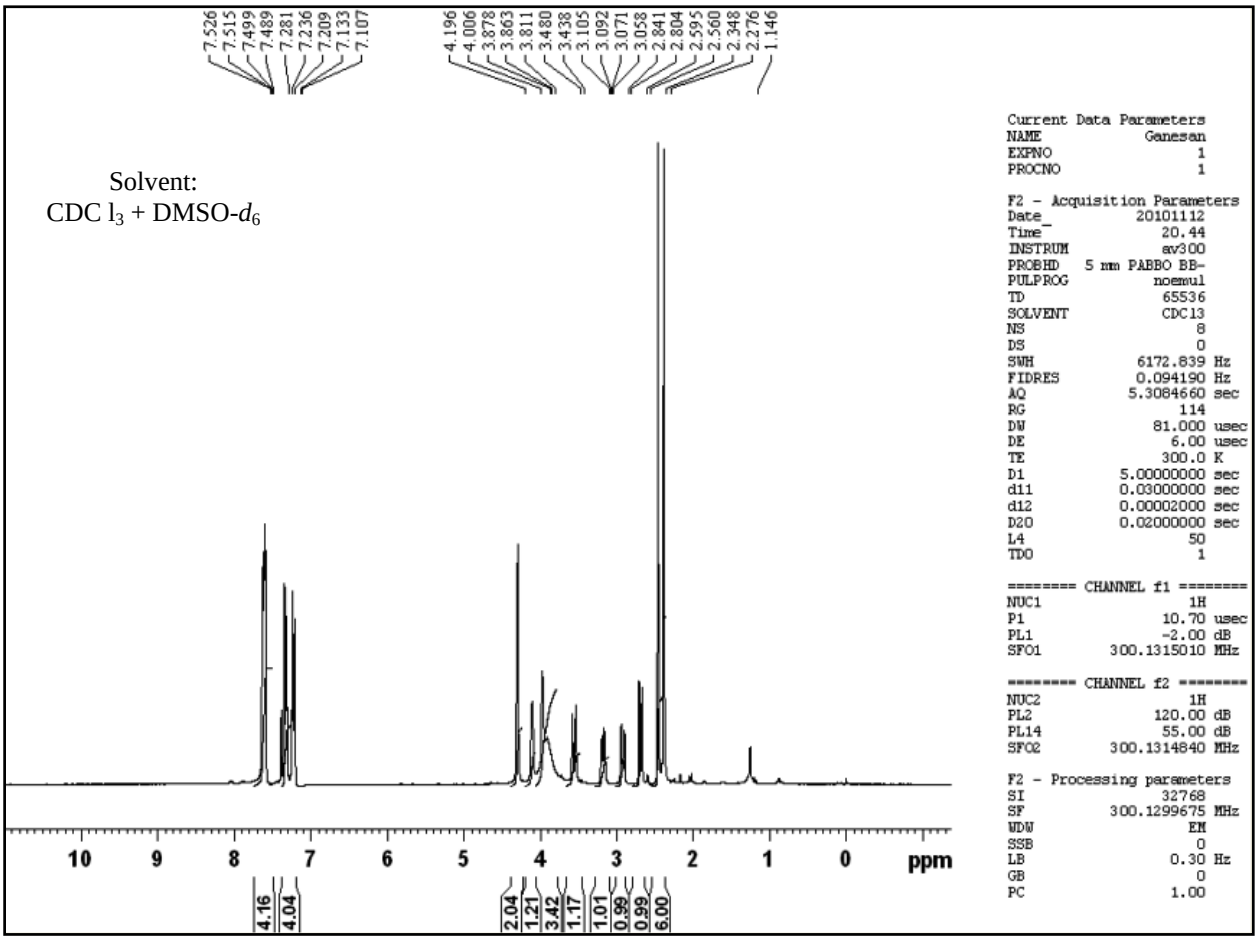


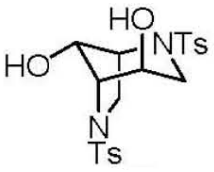
21 Solvent: CDC l_3



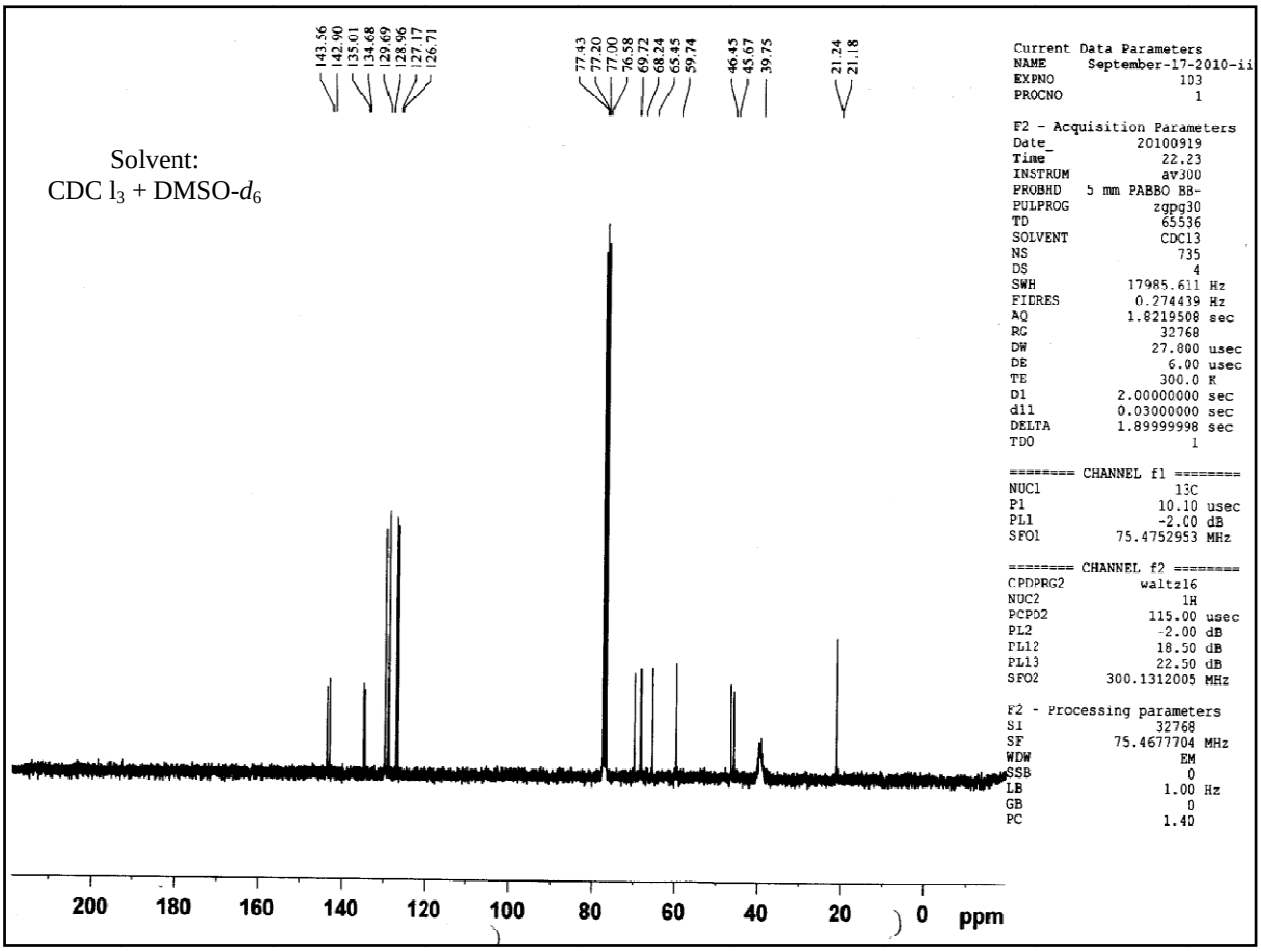


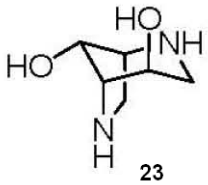
22



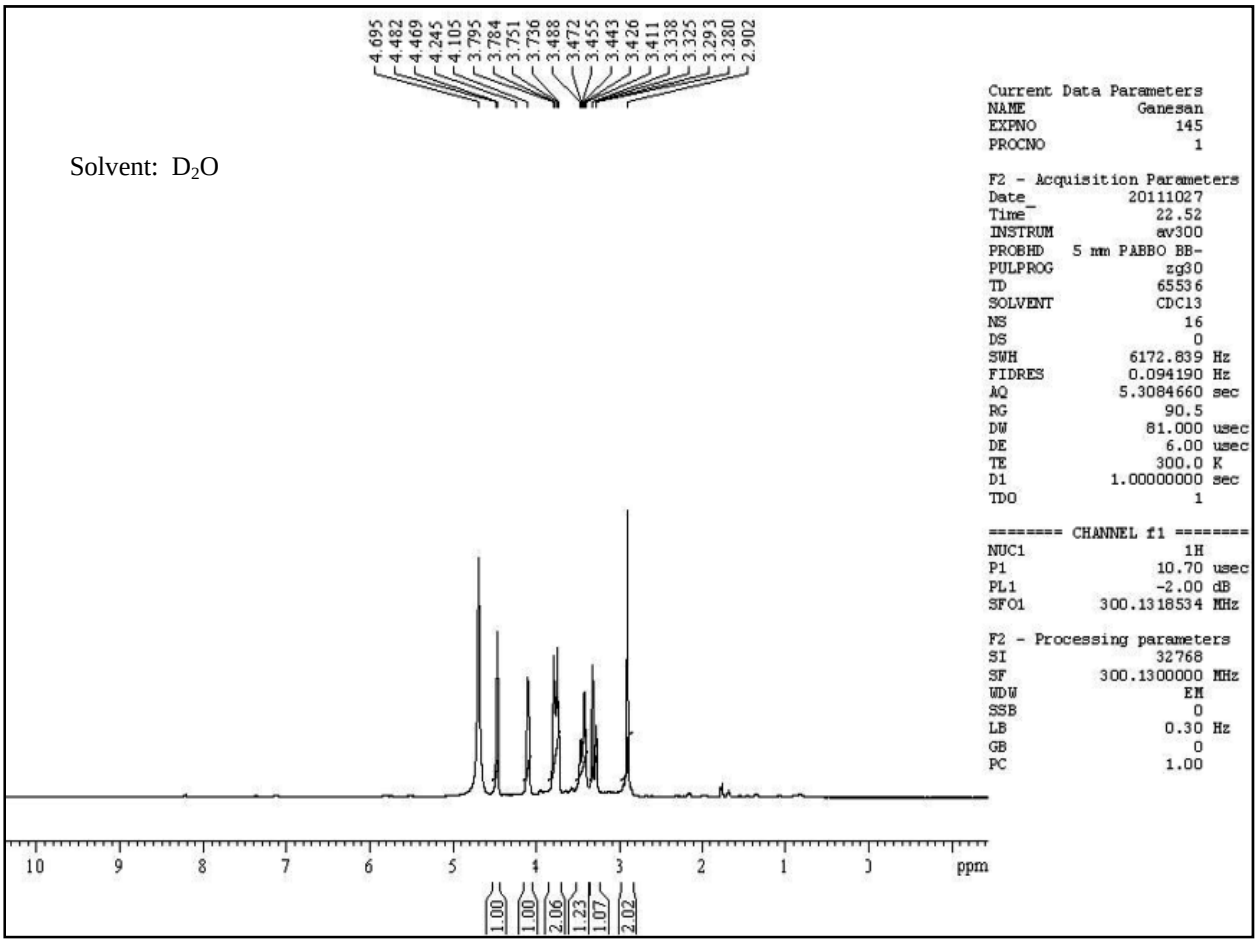

HO
NTs
HO
N
Ts

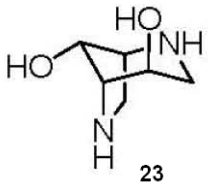
22


143.56
142.90
135.01
134.68
129.69
128.96
127.17
126.71
77.43
77.20
77.00
76.58
69.72
68.24
65.45
59.74
46.45
45.67
39.75
21.24
21.18
Solvent:
CDC l3 + DMSO-d6
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME September-17-2010-ii
EXPNO 103
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100919
Time 22.23
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 735
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677704 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

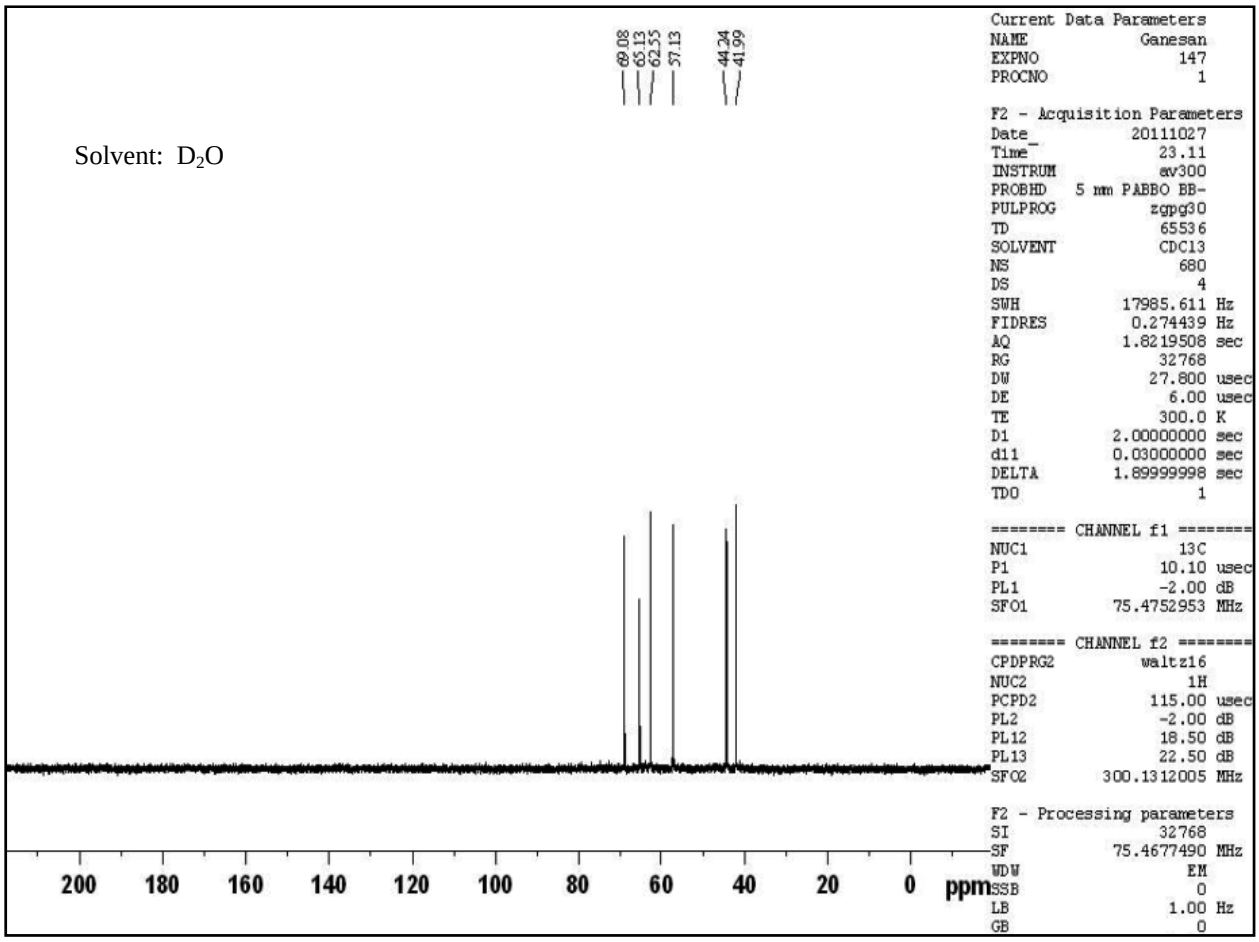

HO
NH
HO
N
H

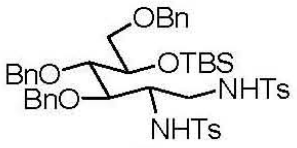
23


4.695
4.482
4.469
4.245
4.105
3.795
3.784
3.751
3.736
3.488
3.472
3.455
3.443
3.426
3.411
3.338
3.325
3.293
3.280
2.902
Solvent: D2O
Current Data Parameters
NAME Ganesan
EXPNO 145
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111027
Time 22.52
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 90.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
2.06
1.23
1.07
2.02

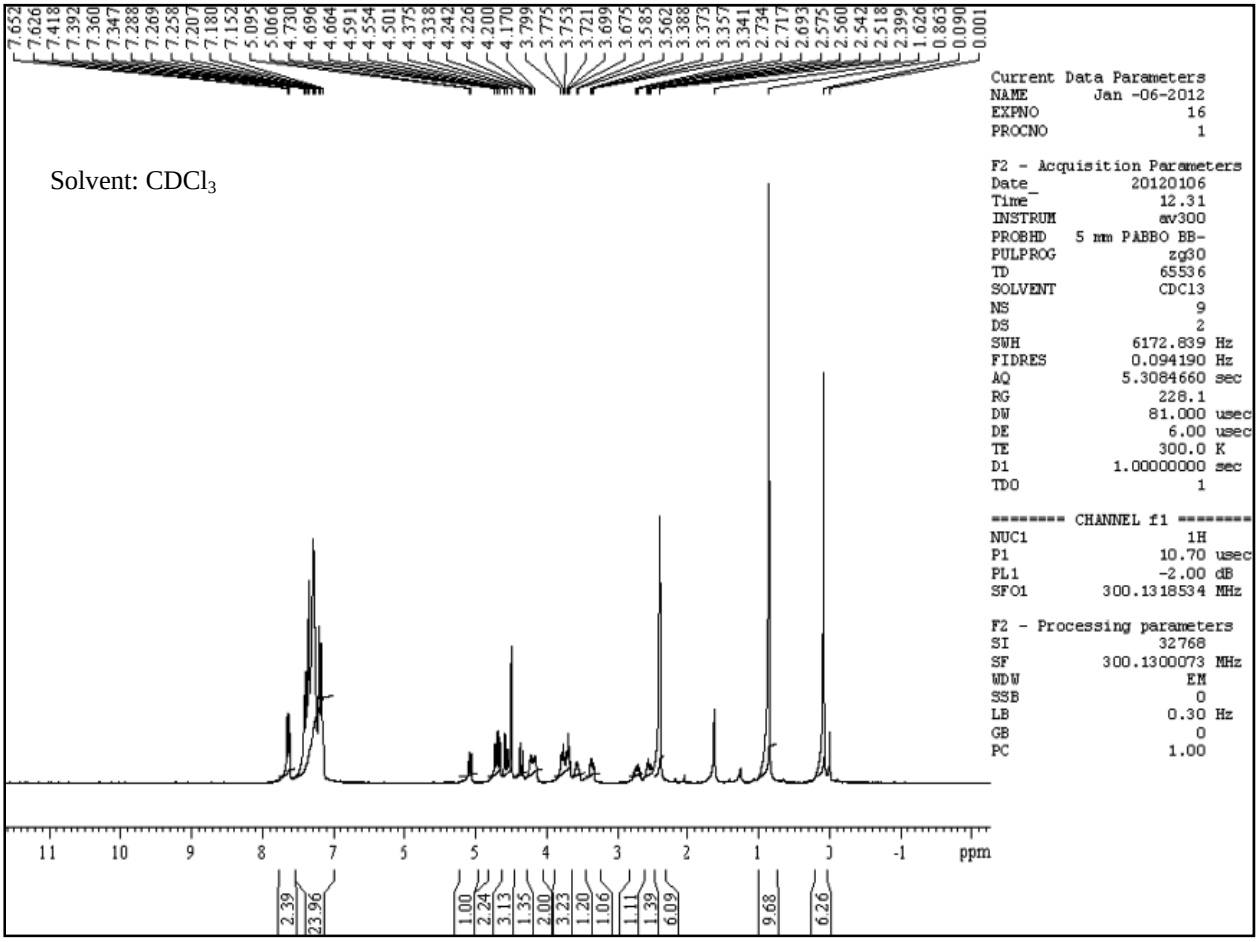


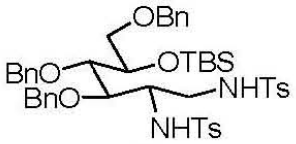
23



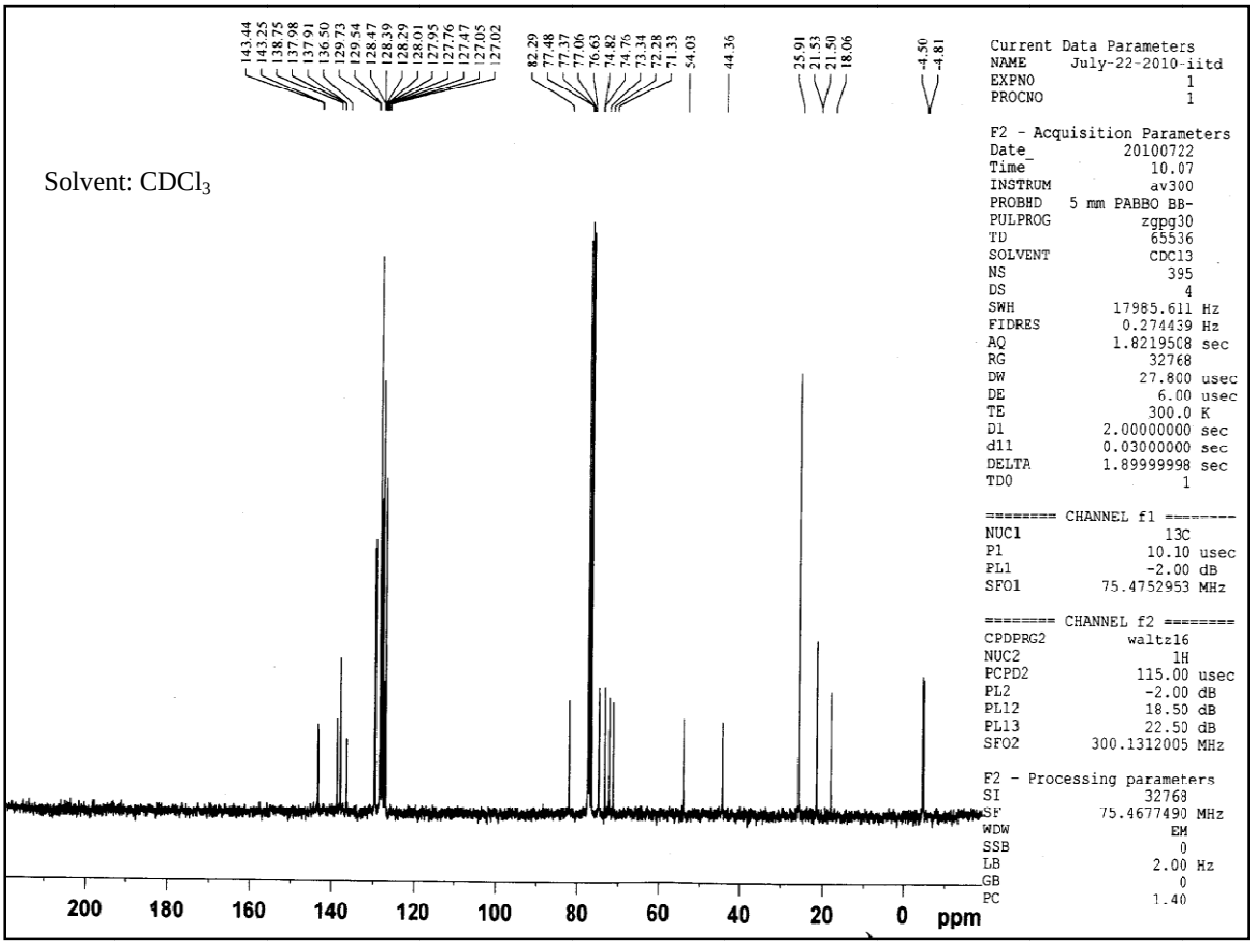

OBn
OTBS
BnO
BnO
NHTs
NHTs

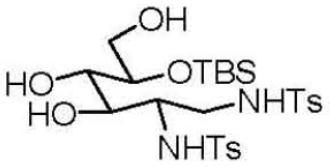
30


Solvent: CDCl3
Current Data Parameters
NAME Jan -06-2012
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120106
Time 12.31
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 228.1
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm

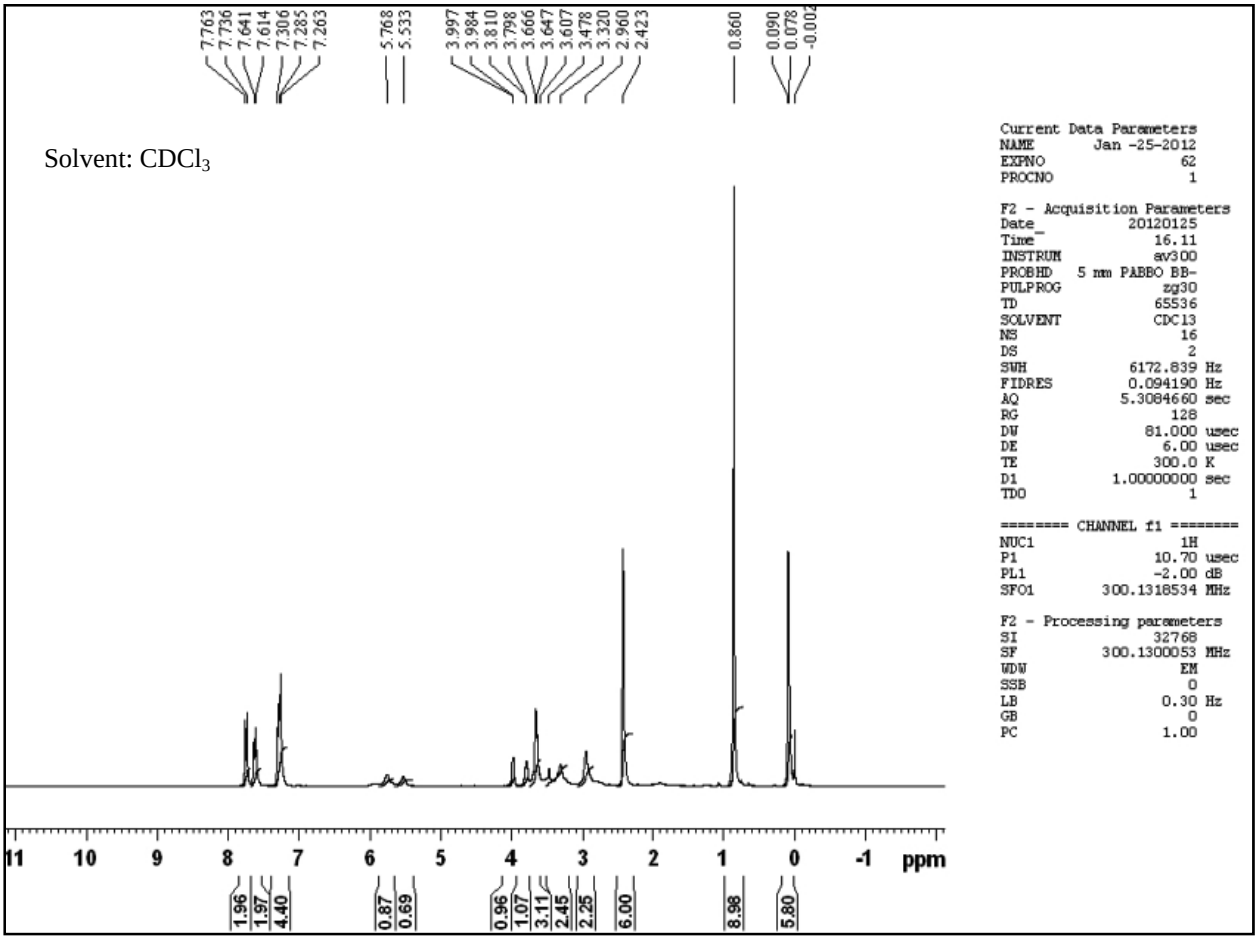

OBn
OTBS
BnO
BnO
NHTs
NHTs

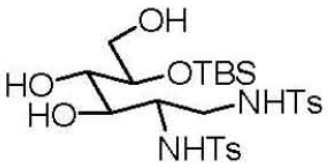
30


143.44
143.25
138.75
137.98
137.91
136.50
129.73
129.54
128.47
128.39
128.29
128.01
127.95
127.76
127.47
127.05
127.02
82.29
77.48
77.37
77.06
76.63
74.82
74.75
73.34
72.28
71.33
54.03
44.36
25.91
21.53
21.50
18.06
-4.50
-4.81
Solvent: CDCl3
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME July-22-2010-iitd
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100722
Time 10.07
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 395
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

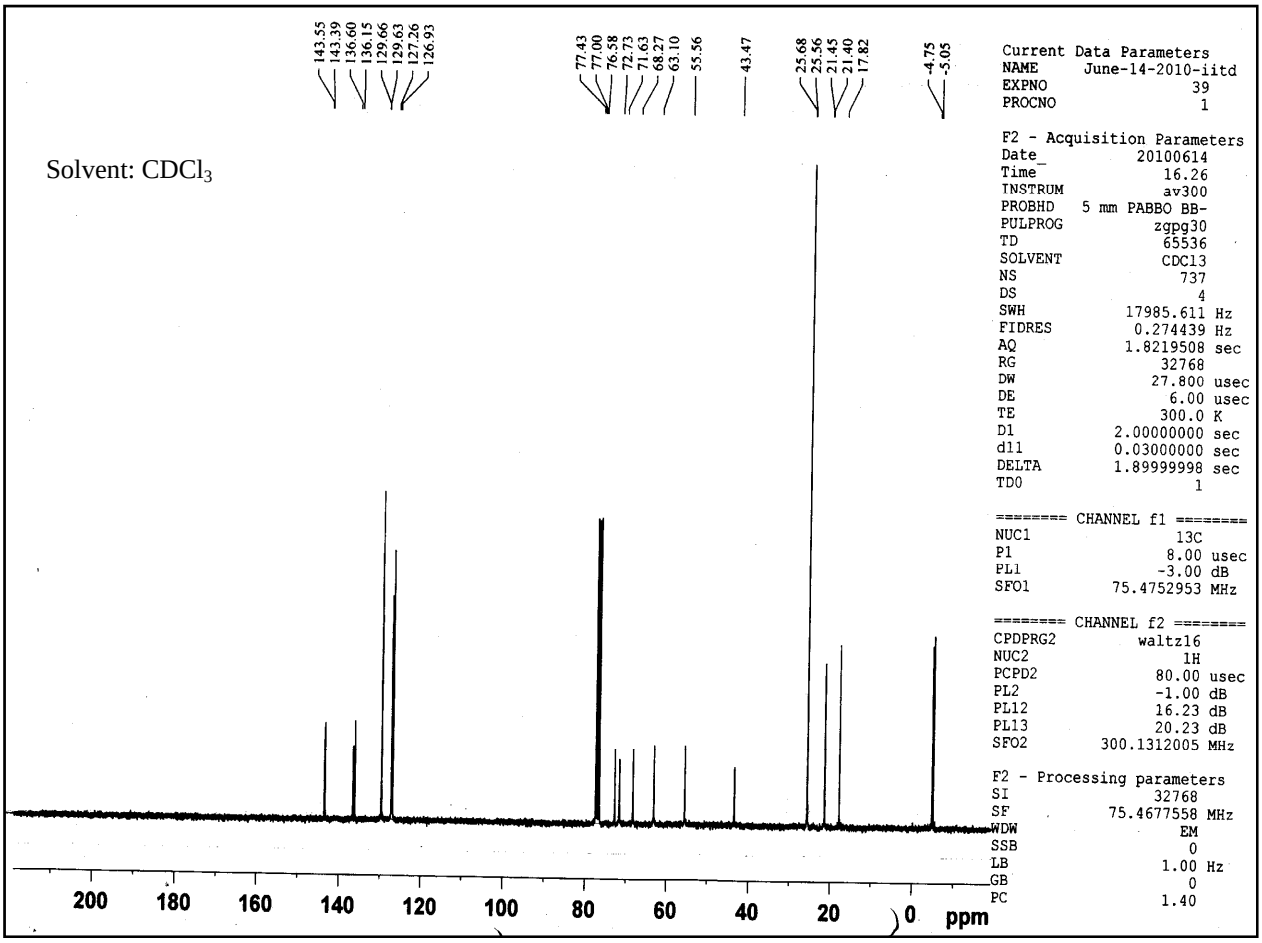

OH
HO
OTBS
HO
NHTs
NHTs

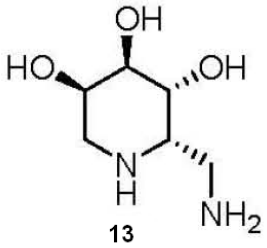
31


7.763
7.736
7.641
7.614
7.306
7.285
7.263
5.768
5.533
3.997
3.984
3.810
3.798
3.666
3.647
3.607
3.478
3.320
2.960
2.423
0.860
0.090
0.078
-0.002
Solvent: CDCl3
Current Data Parameters
NAME Jan -25-2012
EXPNO 62
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120125
Time 16.11
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.96
1.97
4.40
0.87
0.69
0.96
1.07
3.11
2.45
2.25
6.00
8.98
5.80

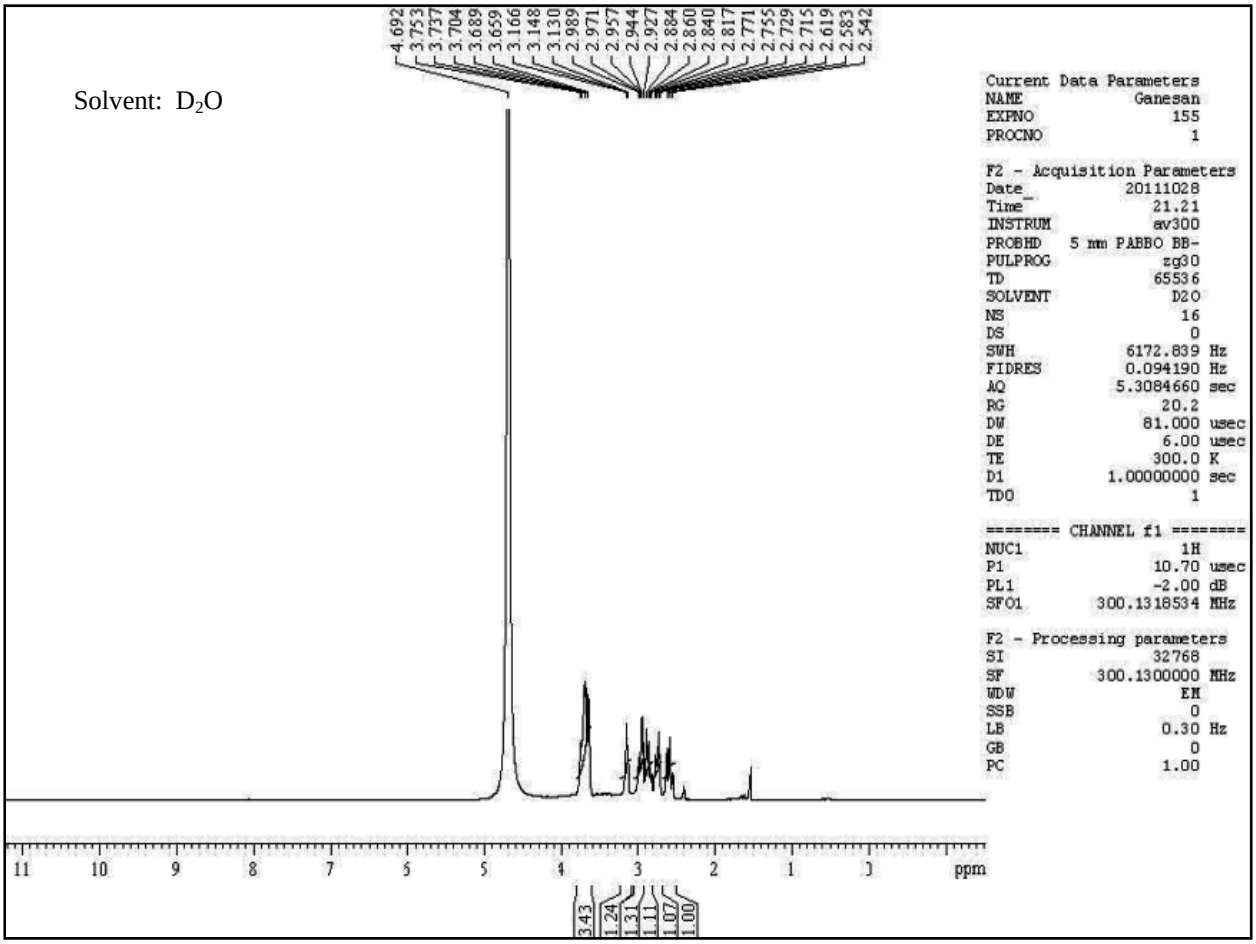

OH
HO
OTBS
HO
NHTs
NHTs

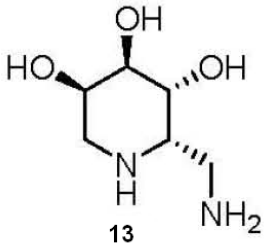
31


143.55
143.39
136.60
136.15
129.66
129.63
127.26
126.93
77.43
77.00
76.58
72.73
71.63
68.27
63.10
55.56
43.47
25.68
25.56
21.45
21.40
17.82
-4.75
-5.05
Solvent: CDCl3
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME June-14-2010-iitd
EXPNO 39
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100614
Time 16.26
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 737
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.00 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.23 dB
PL13 20.23 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677558 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



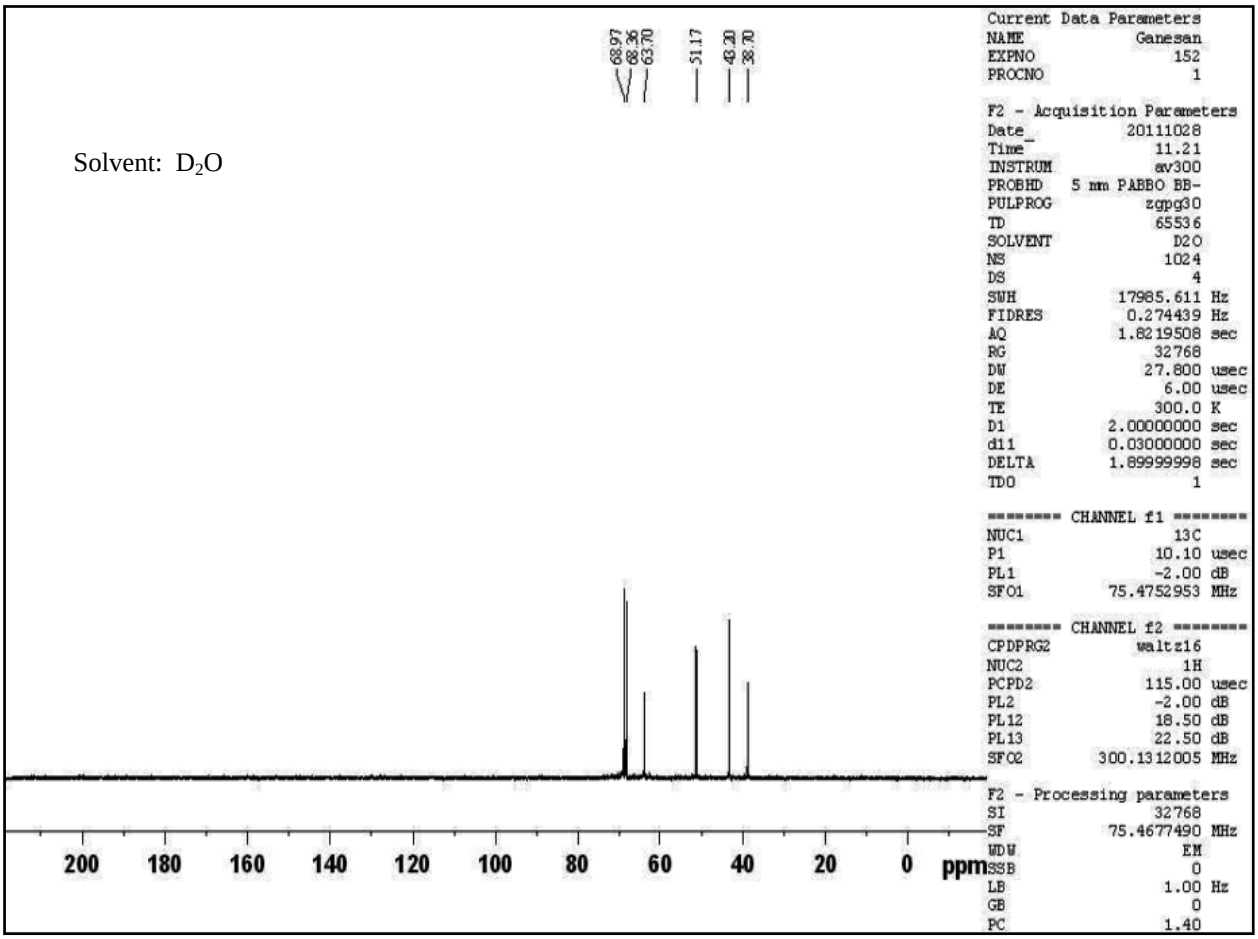
13



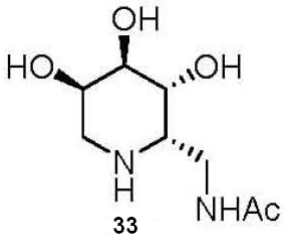


13

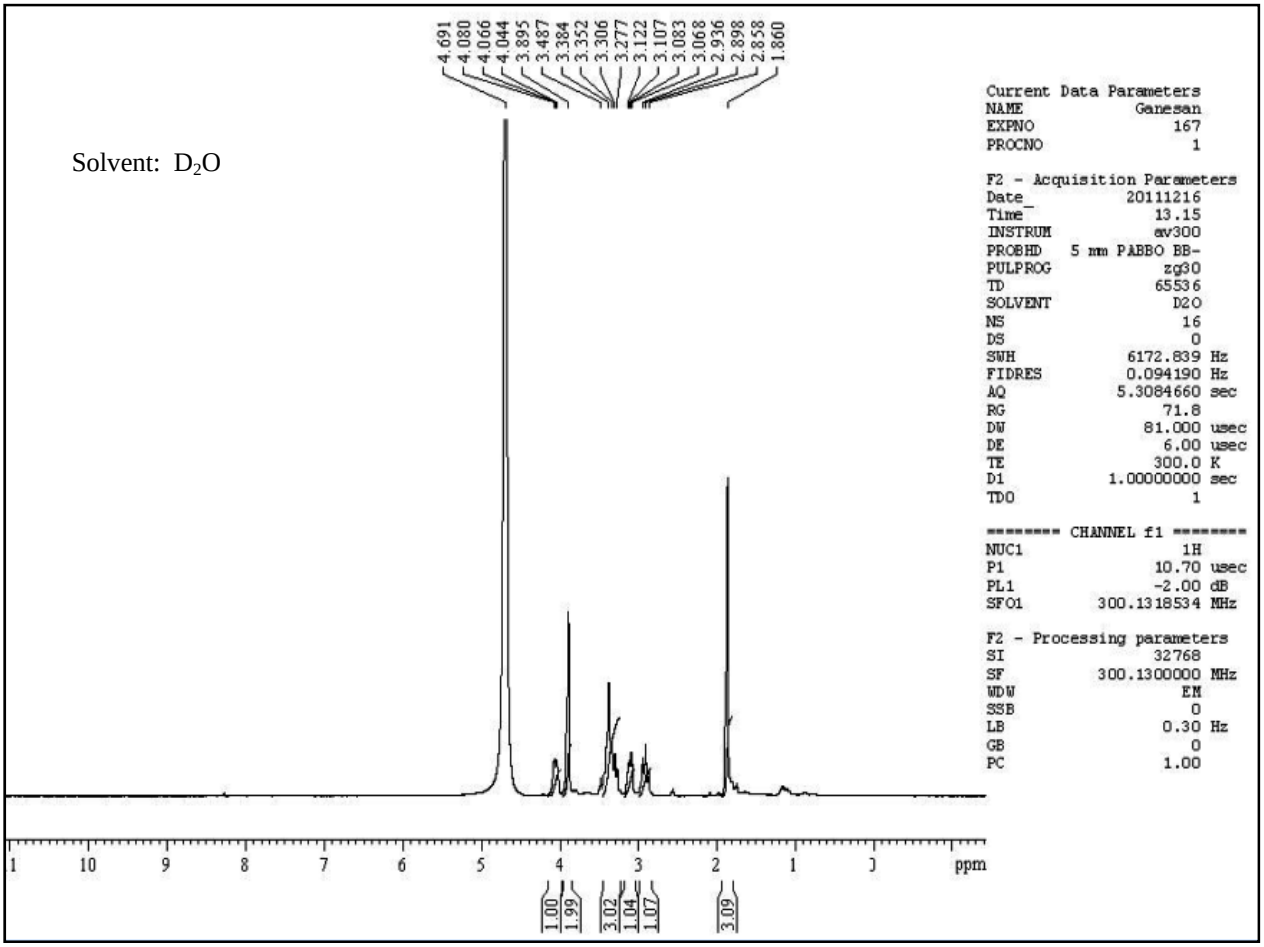
Solvent: D_2O

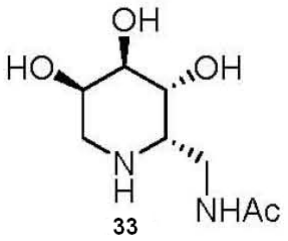



```
Current Data Parameters
NAME                  Ganesan
EXPNO                     152
PROCNO                      1

F2 - Acquisition Parameters
Date_                20111028
Time                    11.21
INSTRUM                 av300
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                   D2O
NS                       1024
DS                          4
SWH                17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                      32768
DW                   27.800 usec
DE                    6.00 usec
TE                    300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                   10.10 usec
PL1                   -2.00 dB
SFO1              75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                115.00 usec
PL2                   -2.00 dB
PL12                  18.50 dB
PL13                  22.50 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
SI                      32768
SF                75.4677490 MHz
WDW                        EM
SSB                         0
LB                    1.00 Hz
GB                          0
PC                       1.40
```

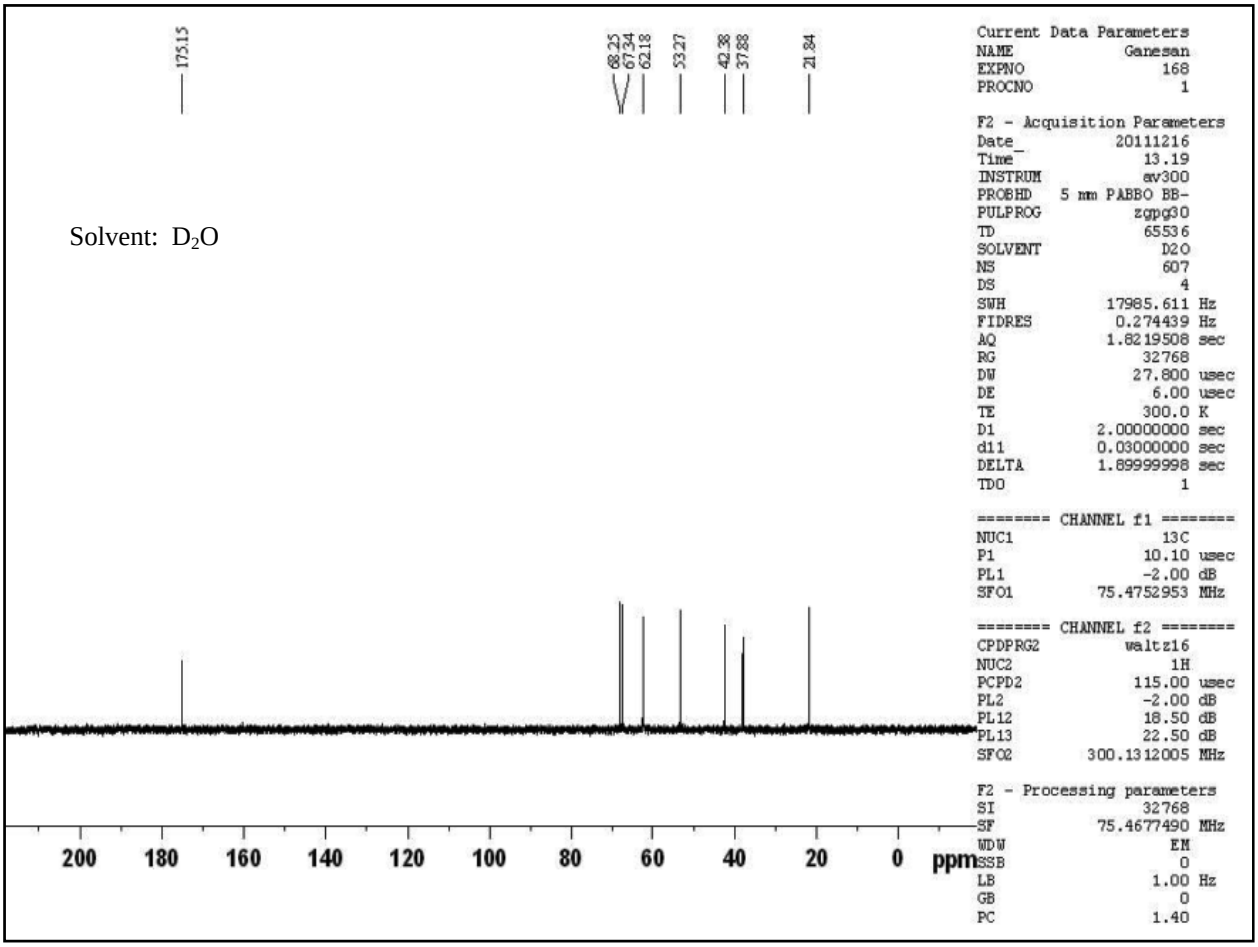


33



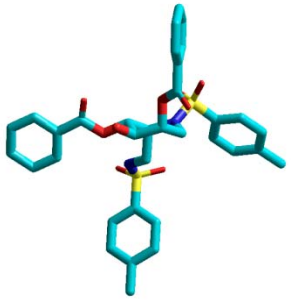

OH
HO
OH
N
H
NHAc

33


175.15
68.25
67.34
62.18
53.27
42.38
37.88
21.84
Solvent: D2O
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME Ganesan
EXPNO 168
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111216
Time 13.19
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 607
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Energy values obtained from AM1 calculations for compound **18**.

$^4C_1$ conformation



HyperChem
Single Point, SemiEmpirical, molecule = compound 18 4C1 conformation
AM1
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
RHF Calculation:

Singlet state calculation
Number of electrons = 246
Number of Double Occupied Levels = 123
Charge on the System = 0
Total Orbitals = 222

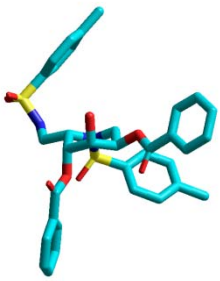
Starting AM1 calculation with 222 orbitals

Iteration = 1 Difference = 43026.92948
Iteration = 2 Difference = 835.24005
Iteration = 3 Difference = 311.20153
Iteration = 4 Difference = 60.77617
Iteration = 5 Difference = 5.77144
Iteration = 6 Difference = 0.94989
Iteration = 7 Difference = 0.36973
Iteration = 8 Difference = 0.15674
Iteration = 9 Difference = 0.01750
Iteration = 10 Difference = 0.00211
Energy=-8715.174040 kcal/mol Gradient=0.010078 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -196163.9297082 (kcal/mol)
Total Energy = -312.607081781 (a.u.)
Binding Energy = -8715.1740402 (kcal/mol)
Isolated Atomic Energy = -187448.7556680 (kcal/mol)
Electronic Energy = -2048766.1025866 (kcal/mol)
Core-Core Interaction = 1852602.1728784 (kcal/mol)
Heat of Formation = -238.6150402 (kcal/mol)
Gradient = 0.0100781 (kcal/mol/Ang)

Energy values obtained from AM1 calculations for compound **18**.

$^1C_4$ conformation



HyperChem
Single Point, SemiEmpirical, molecule = Compound 18 1C4conformation
AM1
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
RHF Calculation:

Singlet state calculation
Number of electrons = 246
Number of Double Occupied Levels = 123
Charge on the System = 0
Total Orbitals = 222

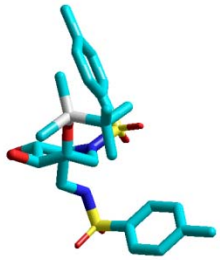
Starting AM1 calculation with 222 orbitals

Iteration = 1 Difference = 42965.74988
Iteration = 2 Difference = 739.56074
Iteration = 3 Difference = 483.93724
Iteration = 4 Difference = 37.20935
Iteration = 5 Difference = 31.04263
Iteration = 6 Difference = 12.07024
Iteration = 7 Difference = 0.49754
Iteration = 8 Difference = 0.10846
Iteration = 9 Difference = 0.03581
Iteration = 10 Difference = 0.00509
Energy=-8710.354647 kcal/mol Gradient=0.011840 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -196159.1103152 (kcal/mol)
Total Energy = -312.599401590 (a.u.)
Binding Energy = -8710.3546472 (kcal/mol)
Isolated Atomic Energy = -187448.7556680 (kcal/mol)
Electronic Energy = -2075762.5924566 (kcal/mol)
Core-Core Interaction = 1879603.4821414 (kcal/mol)
Heat of Formation = -233.7956472 (kcal/mol)
Gradient = 0.0118404 (kcal/mol/Ang)

Energy values obtained from AM1 calculations for compound **32**.

$^4C_1$ conformation



Single Point, SemiEmpirical, molecule = Compound 32 4C1 conformation
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
RHF Calculation:

Singlet state calculation
Number of electrons = 212
Number of Double Occupied Levels = 106
Charge on the System = 0
Total Orbitals = 192

Starting AM1 calculation with 192 orbitals

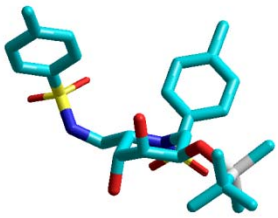
Iteration = 1 Difference = 36057.82216
Iteration = 2 Difference = 16180.24218
Iteration = 3 Difference = 233468.93302
Iteration = 4 Difference = 29013.66024
Iteration = 5 Difference = 22409.35142
Iteration = 6 Difference = 20729.57217
Iteration = 7 Difference = 18638.80718
Iteration = 8 Difference = 17267.76299
Iteration = 9 Difference = 17629.67606
Iteration = 10 Difference = 13519.35793
Iteration = 11 Difference = 13210.18953
Iteration = 12 Difference = 14745.32072
Iteration = 13 Difference = 10454.82766
Iteration = 14 Difference = 10506.87059
Iteration = 15 Difference = 10499.39503
Iteration = 16 Difference = 7818.42915
Iteration = 17 Difference = 7640.62574
Iteration = 18 Difference = 9127.54071
Iteration = 19 Difference = 1875.64288
Iteration = 20 Difference = 3848.72792
Iteration = 21 Difference = 3831.27258
Iteration = 22 Difference = 764.00322
Iteration = 23 Difference = 9557.30537

Iteration = 24 Difference = 7872.61831
Iteration = 25 Difference = 3515.24517
Iteration = 26 Difference = 716.52752
Iteration = 27 Difference = 2488.58444
Iteration = 28 Difference = 763.24803
Iteration = 29 Difference = 523.72090
Iteration = 30 Difference = 697.58419
Iteration = 31 Difference = 300.77296
Iteration = 32 Difference = 315.70935
Iteration = 33 Difference = 280.81333
Iteration = 34 Difference = 25.36051
Iteration = 35 Difference = 63.24076
Iteration = 36 Difference = 59.32193
Iteration = 37 Difference = 63.56930
Iteration = 38 Difference = 51.28497
Iteration = 39 Difference = 46.34042
Iteration = 40 Difference = 46.32716
Iteration = 41 Difference = 24.47290
Iteration = 42 Difference = 0.25808
Iteration = 43 Difference = 0.03340
Iteration = 44 Difference = 0.01278
Iteration = 45 Difference = 0.00102
Energy=-7706.619235 kcal/mol Gradient=0.010289 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -161685.7925528 (kcal/mol)
Total Energy = -257.662679630 (a.u.)
Binding Energy = -7706.6192348 (kcal/mol)
Isolated Atomic Energy = -153979.1733180 (kcal/mol)
Electronic Energy = -1669983.9726826 (kcal/mol)
Core-Core Interaction = 1508298.1801298 (kcal/mol)
Heat of Formation = -295.2962348 (kcal/mol)
Gradient = 0.0102894 (kcal/mol/Ang)

Energy values obtained from AM1 calculations for compound **32**.

$^1C_4$ conformation



HyperChem
Single Point, SemiEmpirical, molecule = Compound 32 1C4 conformation
AM1
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
RHF Calculation:

Singlet state calculation
Number of electrons = 212
Number of Double Occupied Levels = 106
Charge on the System = 0
Total Orbitals = 192

Starting AM1 calculation with 192 orbitals

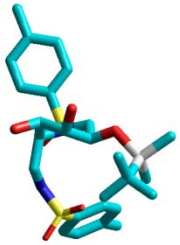
Iteration = 1 Difference = 35882.05626
Iteration = 2 Difference = 47896.12031
Iteration = 3 Difference = 246674.74739
Iteration = 4 Difference = 39465.29020
Iteration = 5 Difference = 24757.16130
Iteration = 6 Difference = 23356.55910
Iteration = 7 Difference = 21230.43919
Iteration = 8 Difference = 20233.28452
Iteration = 9 Difference = 19015.86260
Iteration = 10 Difference = 17722.81406
Iteration = 11 Difference = 15976.78819
Iteration = 12 Difference = 15122.48442
Iteration = 13 Difference = 13740.20199
Iteration = 14 Difference = 12094.50406
Iteration = 15 Difference = 11561.74809
Iteration = 16 Difference = 8861.09109
Iteration = 17 Difference = 8733.14379
Iteration = 18 Difference = 11577.03369
Iteration = 19 Difference = 835.28683
Iteration = 20 Difference = 3373.33826

Iteration = 21 Difference = 3708.87434
Iteration = 22 Difference = 81.68277
Iteration = 23 Difference = 11249.76007
Iteration = 24 Difference = 6180.56858
Iteration = 25 Difference = 862.55992
Iteration = 26 Difference = 1596.83757
Iteration = 27 Difference = 1080.21784
Iteration = 28 Difference = 1190.50429
Iteration = 29 Difference = 1356.58515
Iteration = 30 Difference = 1157.46406
Iteration = 31 Difference = 409.89978
Iteration = 32 Difference = 379.20132
Iteration = 33 Difference = 274.51429
Iteration = 34 Difference = 86.31133
Iteration = 35 Difference = 116.91906
Iteration = 36 Difference = 124.88352
Iteration = 37 Difference = 54.36405
Iteration = 38 Difference = 31.71172
Iteration = 39 Difference = 33.62510
Iteration = 40 Difference = 35.59051
Iteration = 41 Difference = 10.33701
Iteration = 42 Difference = 0.03794
Iteration = 43 Difference = 0.00527
Energy=-7704.457007 kcal/mol Gradient=0.009610 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -161683.6303251 (kcal/mol)
Total Energy = -257.659233901 (a.u.)
Binding Energy = -7704.4570071 (kcal/mol)
Isolated Atomic Energy = -153979.1733180 (kcal/mol)
Electronic Energy = -1618148.0199115 (kcal/mol)
Core-Core Interaction = 1456464.3895864 (kcal/mol)
Heat of Formation = -293.1340071 (kcal/mol)
Gradient = 0.0096105 (kcal/mol/Ang)

Energy values obtained from AM1 calculations for compound **32**.

$^{1}C_4$ conformation



HyperChem
Single Point, SemiEmpirical, molecule = Compound 32 1S5 conformation
AM1
Convergence limit = 0.0100000 Iteration limit = 50
Accelerate convergence = YES
RHF Calculation:

Singlet state calculation
Number of electrons = 212
Number of Double Occupied Levels = 106
Charge on the System = 0
Total Orbitals = 192

Starting AM1 calculation with 192 orbitals

Iteration = 1 Difference = 36036.24087
Iteration = 2 Difference = 15196.74687
Iteration = 3 Difference = 228154.36856
Iteration = 4 Difference = 31195.69228
Iteration = 5 Difference = 21004.10664
Iteration = 6 Difference = 20305.40910
Iteration = 7 Difference = 17397.18187
Iteration = 8 Difference = 17217.51135
Iteration = 9 Difference = 15731.90189
Iteration = 10 Difference = 13930.39957
Iteration = 11 Difference = 13765.70601
Iteration = 12 Difference = 12991.99102
Iteration = 13 Difference = 12058.45547
Iteration = 14 Difference = 9964.73229
Iteration = 15 Difference = 11701.03463
Iteration = 16 Difference = 5801.40067
Iteration = 17 Difference = 6427.89381
Iteration = 18 Difference = 5363.22110
Iteration = 19 Difference = 3179.34864
Iteration = 20 Difference = 2146.67160
Iteration = 21 Difference = 5262.96960

Iteration = 22 Difference = 1276.17816
Iteration = 23 Difference = 9562.13163
Iteration = 24 Difference = 5946.92328
Iteration = 25 Difference = 1812.61608
Iteration = 26 Difference = 999.28003
Iteration = 27 Difference = 726.59633
Iteration = 28 Difference = 233.16549
Iteration = 29 Difference = 535.17397
Iteration = 30 Difference = 525.38228
Iteration = 31 Difference = 136.27437
Iteration = 32 Difference = 241.47407
Iteration = 33 Difference = 246.71677
Iteration = 34 Difference = 88.53233
Iteration = 35 Difference = 112.14821
Iteration = 36 Difference = 96.98164
Iteration = 37 Difference = 62.83556
Iteration = 38 Difference = 62.03685
Iteration = 39 Difference = 81.80112
Iteration = 40 Difference = 13.57128
Iteration = 41 Difference = 3.02493
Iteration = 42 Difference = 0.02673
Iteration = 43 Difference = 0.00615
Energy=-7709.077550 kcal/mol Gradient=0.011053 Symmetry=C1

ENERGIES AND GRADIENT
Total Energy = -161688.2508683 (kcal/mol)
Total Energy = -257.666597205 (a.u.)
Binding Energy = -7709.0775503 (kcal/mol)
Isolated Atomic Energy = -153979.1733180 (kcal/mol)
Electronic Energy = -1670049.1733703 (kcal/mol)
Core-Core Interaction = 1508360.9225020 (kcal/mol)
Heat of Formation = -297.7545503 (kcal/mol)
Gradient = 0.0110525 (kcal/mol/Ang)