

Gem-difluoromethylated and Trifluoromethylated Derivatives of DMDP-related Iminosugars: Synthesis and Glycosidase Inhibition

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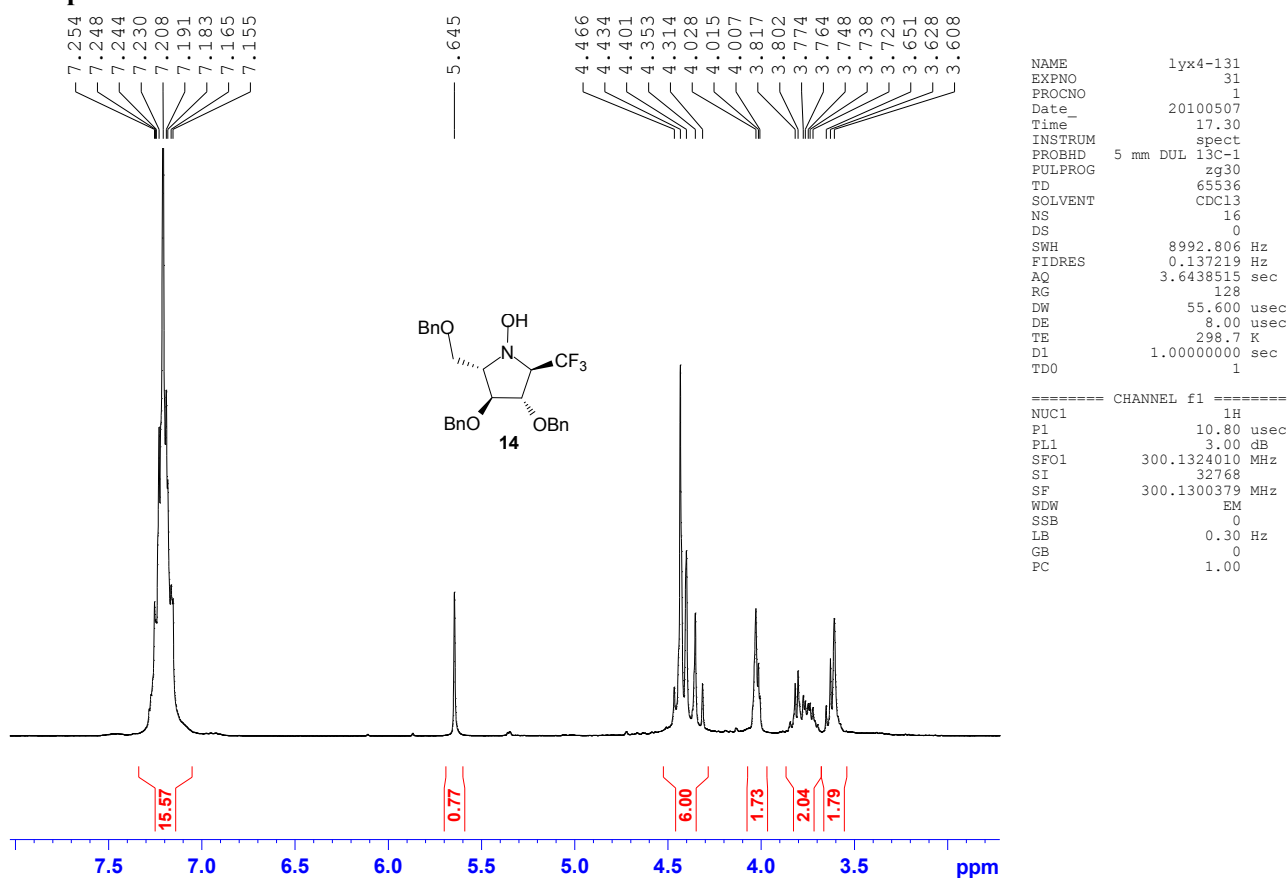
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^d National Engineering Research Center for Carbohydrate Synthesis, Jiangxi Normal University, Nanchang 330022, PR China

Supplementary Information

(NMR spectra and Infrared spectra)

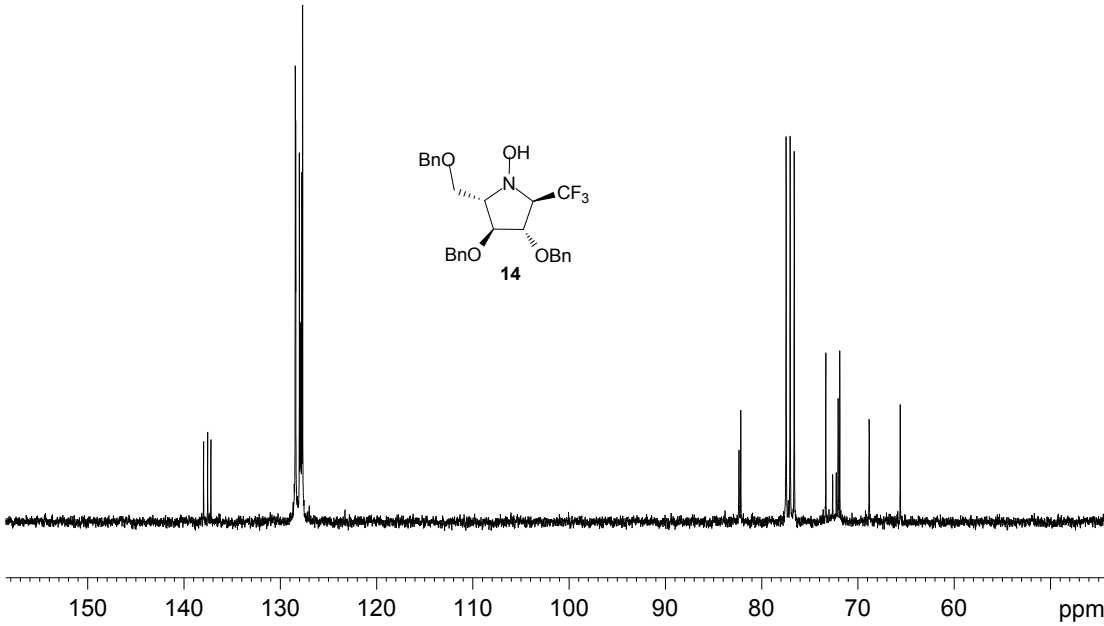
Compound 14:



137.974
137.555
137.214
128.449
128.430
128.400
128.021
127.948
127.881
127.801
127.706
127.016
82.363
82.186
77.473
77.049
76.626
73.349
72.636
72.260
72.067
71.901
68.840
65.614
130.695
123.323
73.031

NAME lyx4-131
EXPNO 30
PROCNO 1
Date_ 20100509
Time 16.50
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 231
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 8.00 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



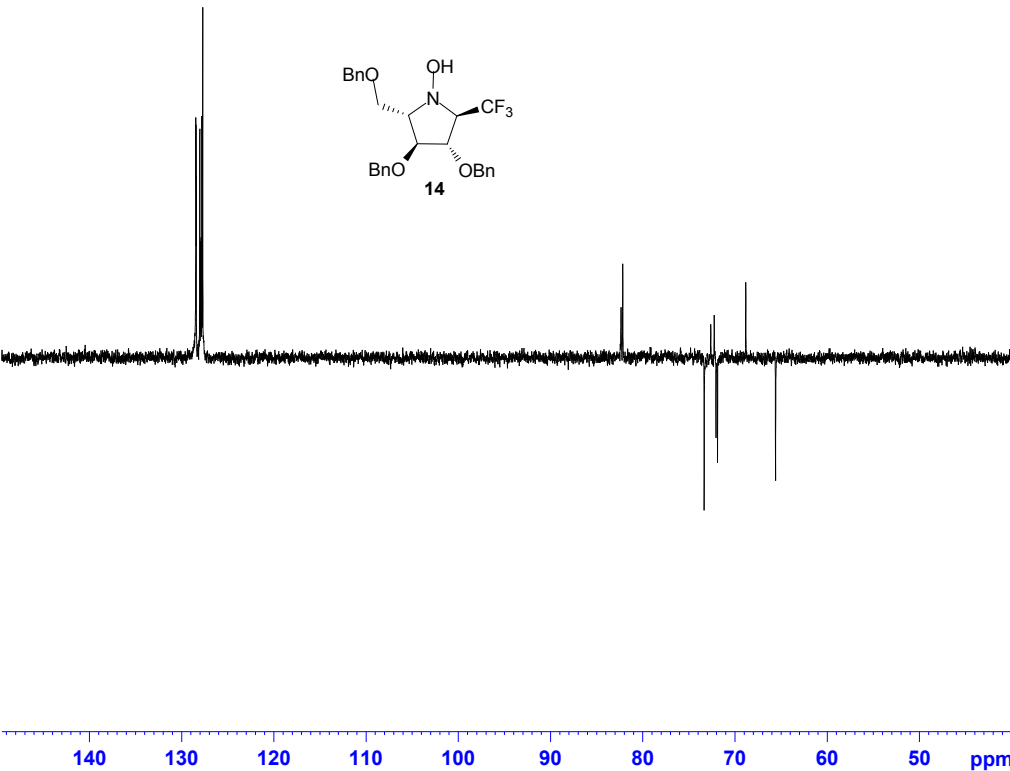
128.45
128.43
128.40
128.02
127.95
127.88
127.80
127.71

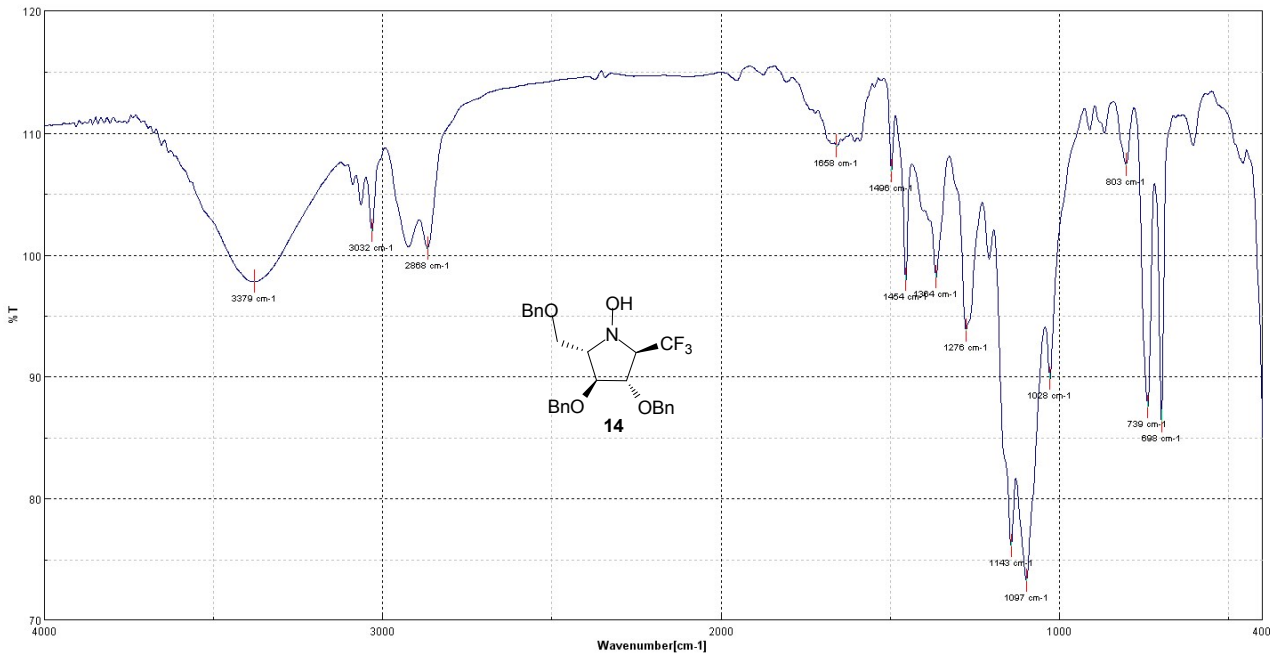
82.36
82.16
73.35
72.63
72.26
72.06
71.90
68.84
65.61

NAME lyx4-131
EXPNO 40
PROCNO 1
Date_ 20100509
Time 17.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 299.1 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

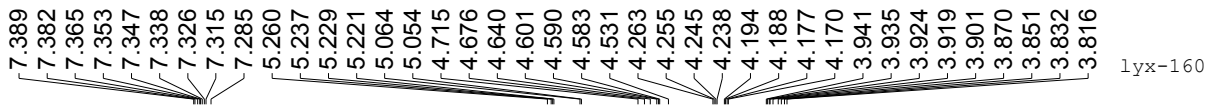
===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
P2 25.00 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.60 usec
P4 21.60 usec
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

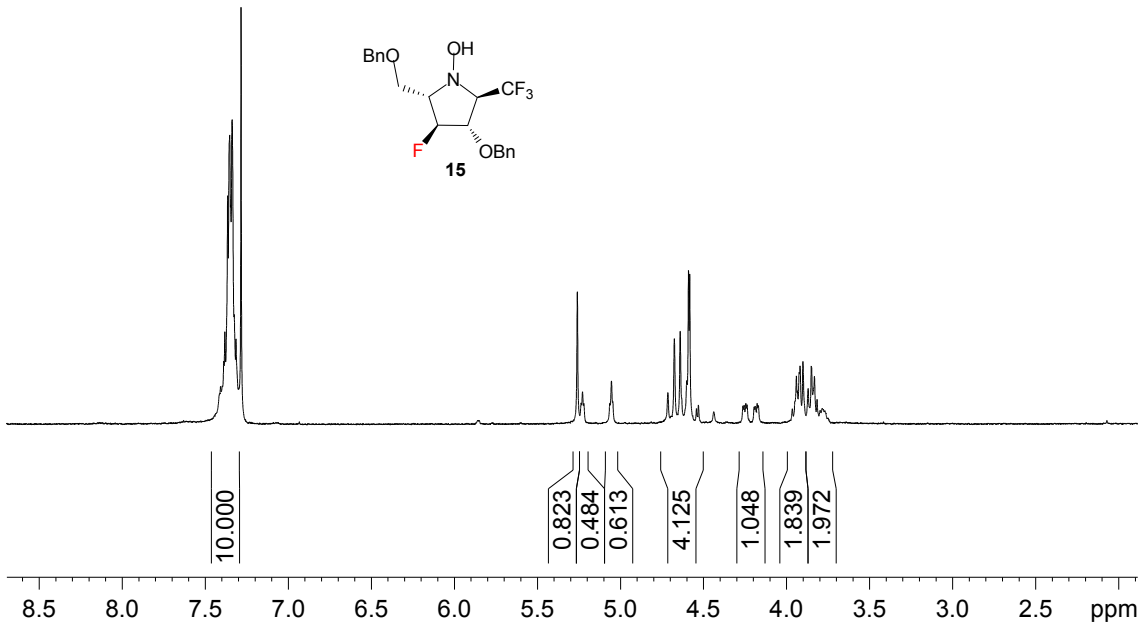


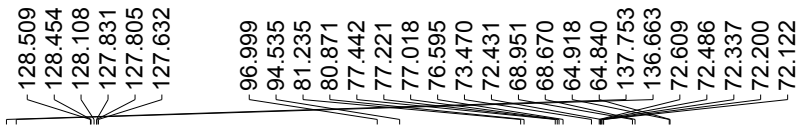


Compound 15:

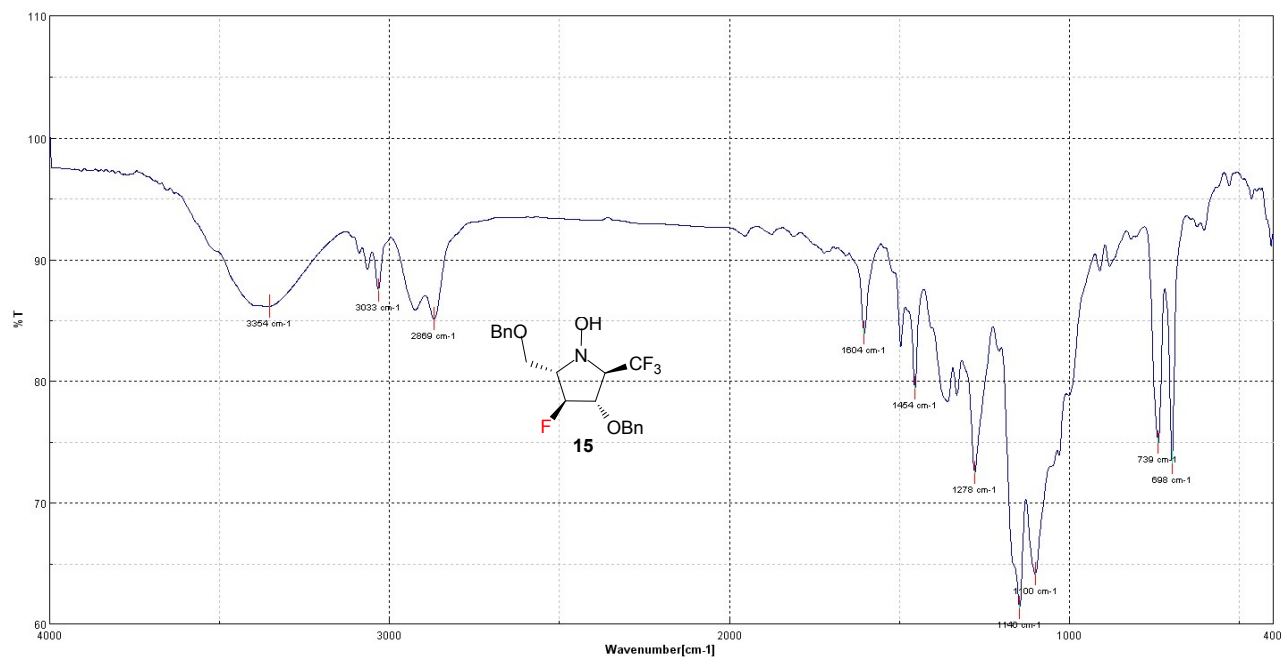
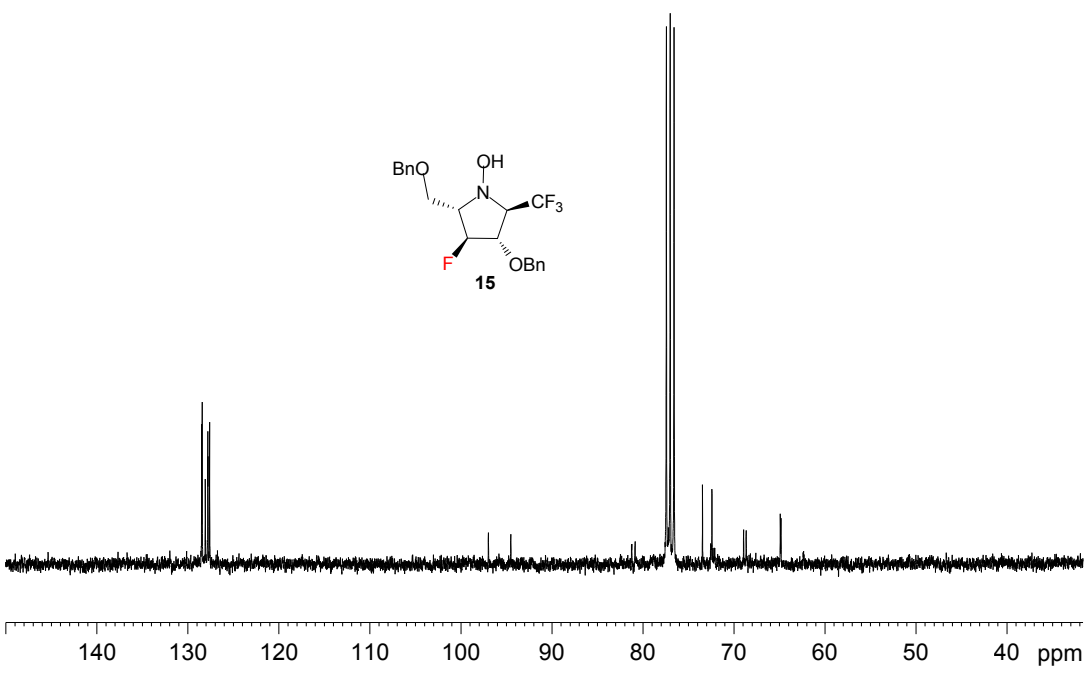


NAME lyx-2016
 EXPNO 55
 PROCNO 1

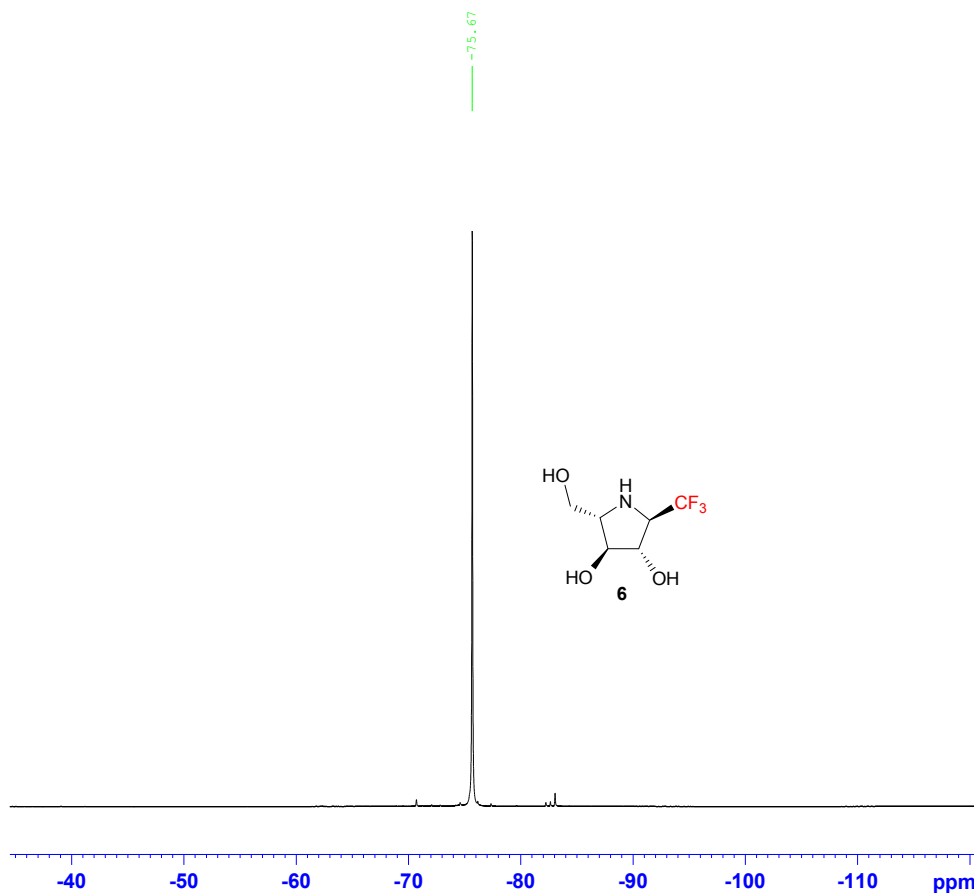




lyx-160-C13
NAME lyx-2016
EXPNO 56
PROCNO 1



Compound 6:



```

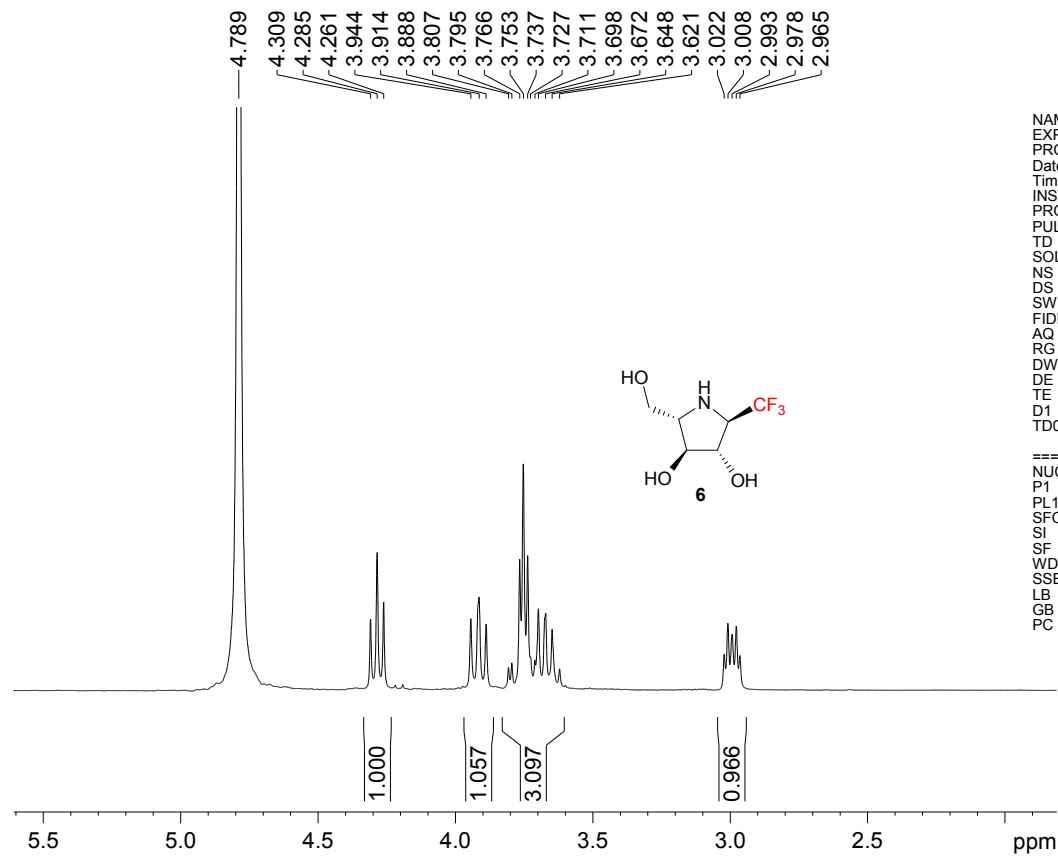
Current Data Parameters
NAME      lyx4-151
EXPNO    208
PROCNO   1

F2 - Acquisition Parameters
Date_    20100609
Time     11.54
INSTRUM  AV400
PROBHD   5 mm BBO BB-1H
PULPROG  zgfgln
TD       32768
SOLVENT  CDCl3
NS       16
DS       0
SWH      75187.969 Hz
FIDRES   2.294555 Hz
AQ       0.2179572 sec
RG       45
DW       6.650 usec
DE       6.00 usec
TE       673.2 K
D1       1.00000000 sec

===== CHANNEL f1 =====
NUC1     19F
P1       12.50 usec
PL1      0.00 dB
SFO1     376.4644691 MHz

F2 - Processing parameters
SI       65536
SF       376.4983540 MHz
WDW      EM
SSB      0
LB       20.00 Hz
GB       0
PC       0.10

1D NMR plot parameters
CX       24.00 cm
CY       8.00 cm
F1P      -51.980 ppm
F1       -19570.51 Hz
F2P      -109.410 ppm
F2       -41192.70 Hz
FPMCM    2.39290 ppm/cm
HZCM     900.92450 Hz/cm
    
```



```

NAME      lyx4-151
EXPNO    10
PROCNO   1
Date_    20100519
Time     9.44
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  zg30
TD       65536
SOLVENT  D2O
NS       6
DS       0
SWH      8992.806 Hz
FIDRES   0.137219 Hz
AQ       3.6438515 sec
RG       128
DW       55.600 usec
DE       8.00 usec
TE       299.9 K
D1       1.00000000 sec
TD0      1

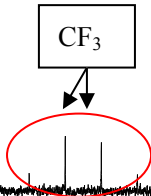
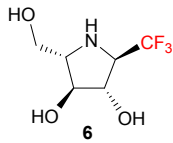
===== CHANNEL f1 =====
NUC1     1H
P1       10.80 usec
PL1      3.00 dB
SFO1     300.1324010 MHz
SI       32768
SF       300.1299726 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

131.55
127.85
124.15
120.45

76.59

61.81
61.50
61.42
61.03
60.64
59.67

NAME lyx4-151
EXPNO 12
PROCNO 1
Date_ 20100519
Time_ 9.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 816
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



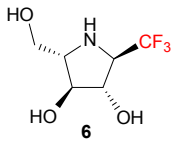
===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

140 130 120 110 100 90 80 70 60 ppm

76.57

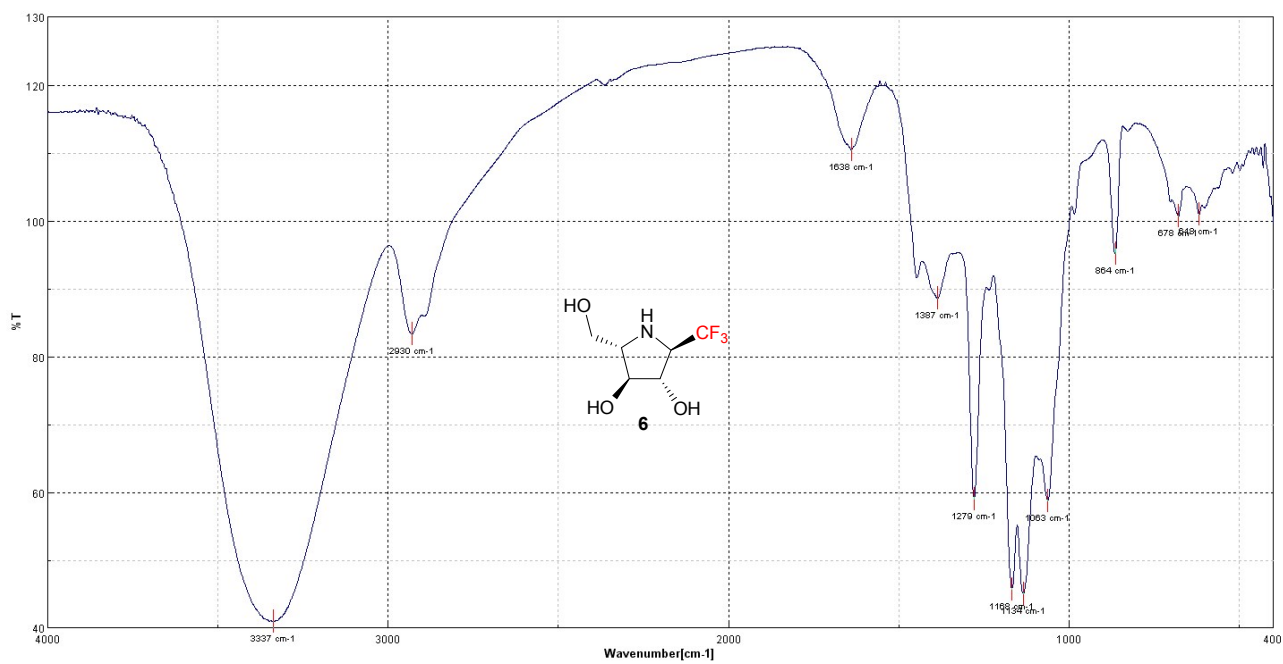
61.79
61.49
61.40
61.01
60.62
59.65

NAME lyx4-151
EXPNO 21
PROCNO 1
Date_ 20100526
Time_ 9.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT D2O
NS 79
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 300.4 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1



===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
P2 25.00 usec
PL1 2.00 dB
SFO1 75.4752953 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.80 usec
P4 21.60 usec
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

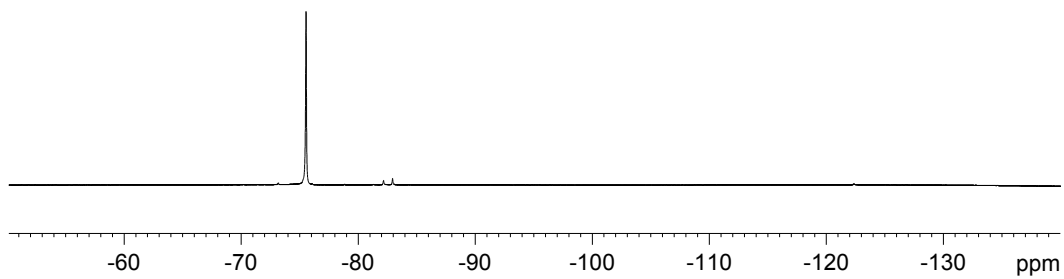
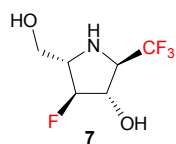
85 80 75 70 65 60 55 ppm

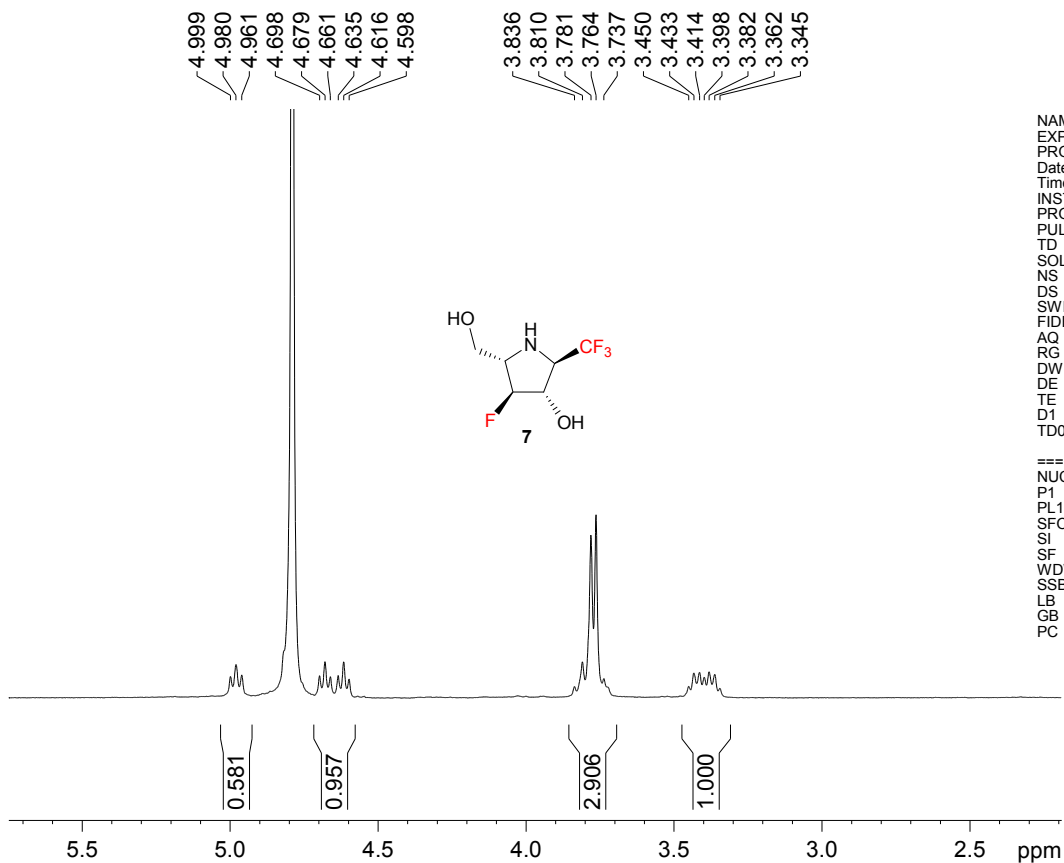


Compound 7:

— -75.535

NAME	19F
EXPNO	207
PROCNO	1





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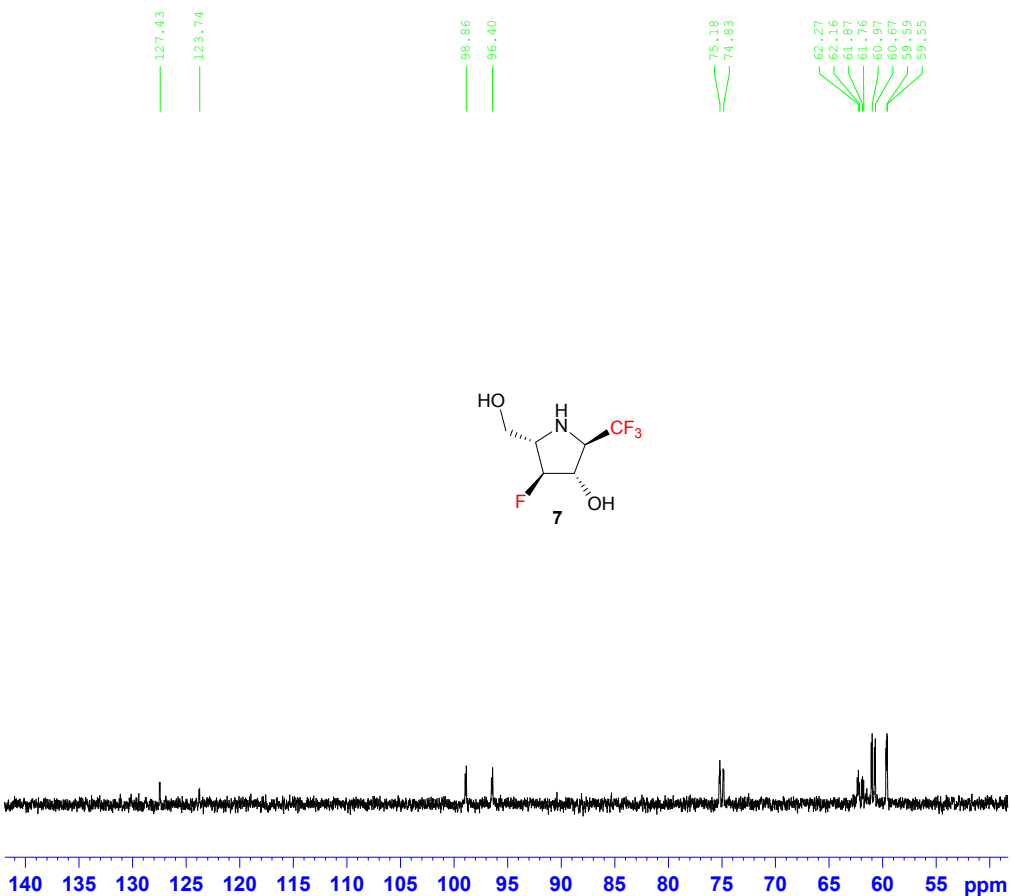
NAME lyx4-161
EXPNO 10
PROCNO 1
Date_ 20100607
Time 17.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT D2O
NS 3
DS 0
SWH 892.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 256
DW 55.600 usec
DE 8.00 usec
TE 300.6 K
D1 1.00000000 sec
TD0 1

```

```

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.1324010 MHz
SI 32768
SF 300.1299722 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```



```

NAME lyx4-161
EXPNO 12
PROCNO 1
Date_ 20100607
Time 17.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 686
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 18390.4
DW 27.800 usec
DE 8.00 usec
TE 300.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

```

```

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```


96.85
96.39

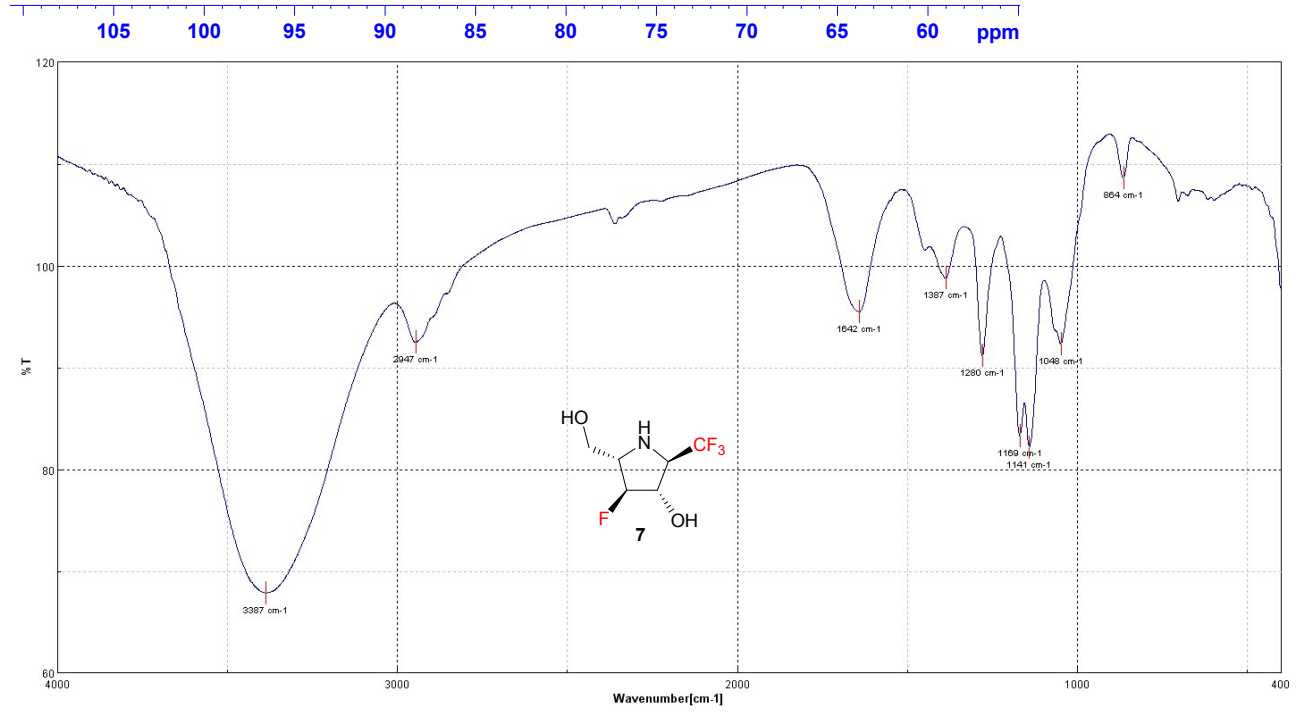
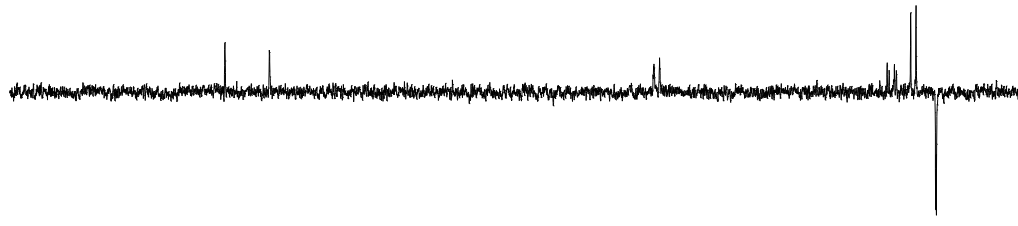
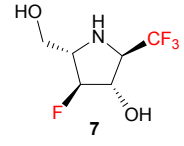
75.15
74.84

62.96
62.15
61.86
61.75
60.86
60.66
59.58
59.54

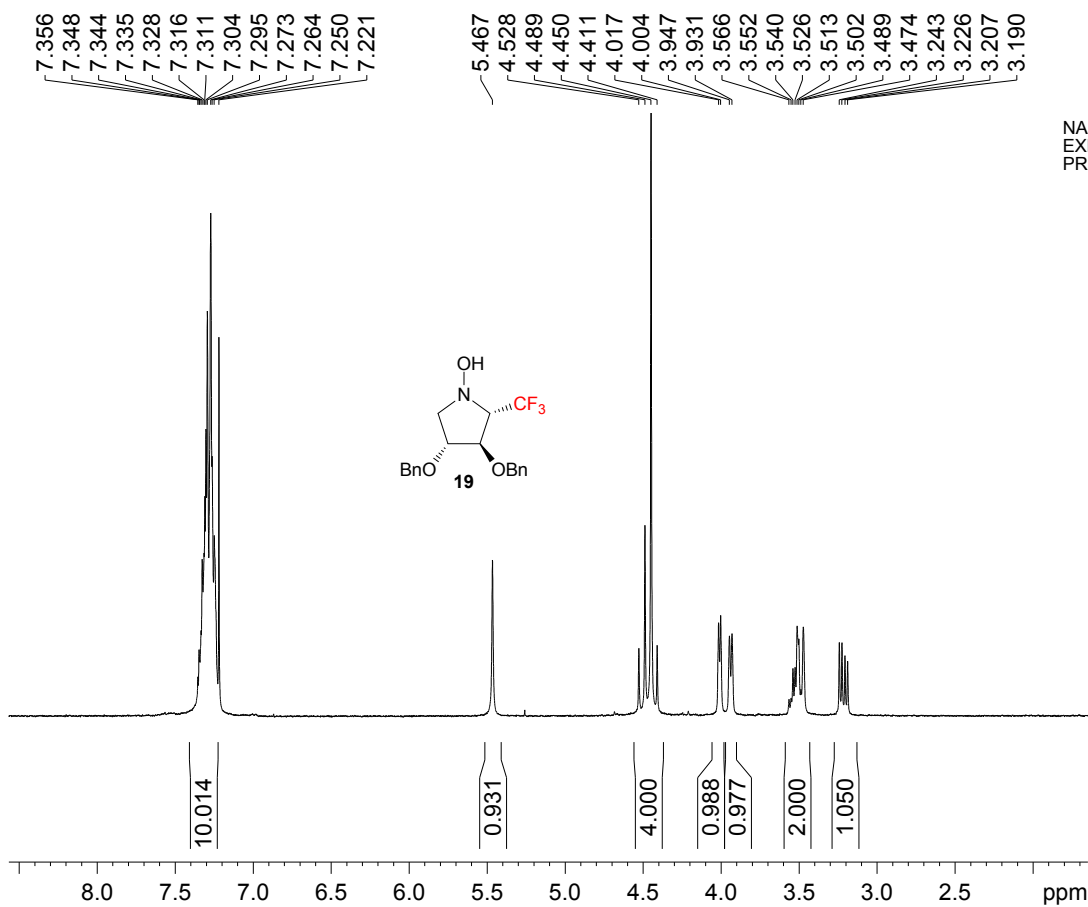
```
NAME lyx4-161
EXPNO 20
PROCNO 1
Date_ 20100609
Time 9.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT D2O
NS 111
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 299.9 K
CNST2 145.000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
P2 25.00 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.80 usec
P4 21.60 usec
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

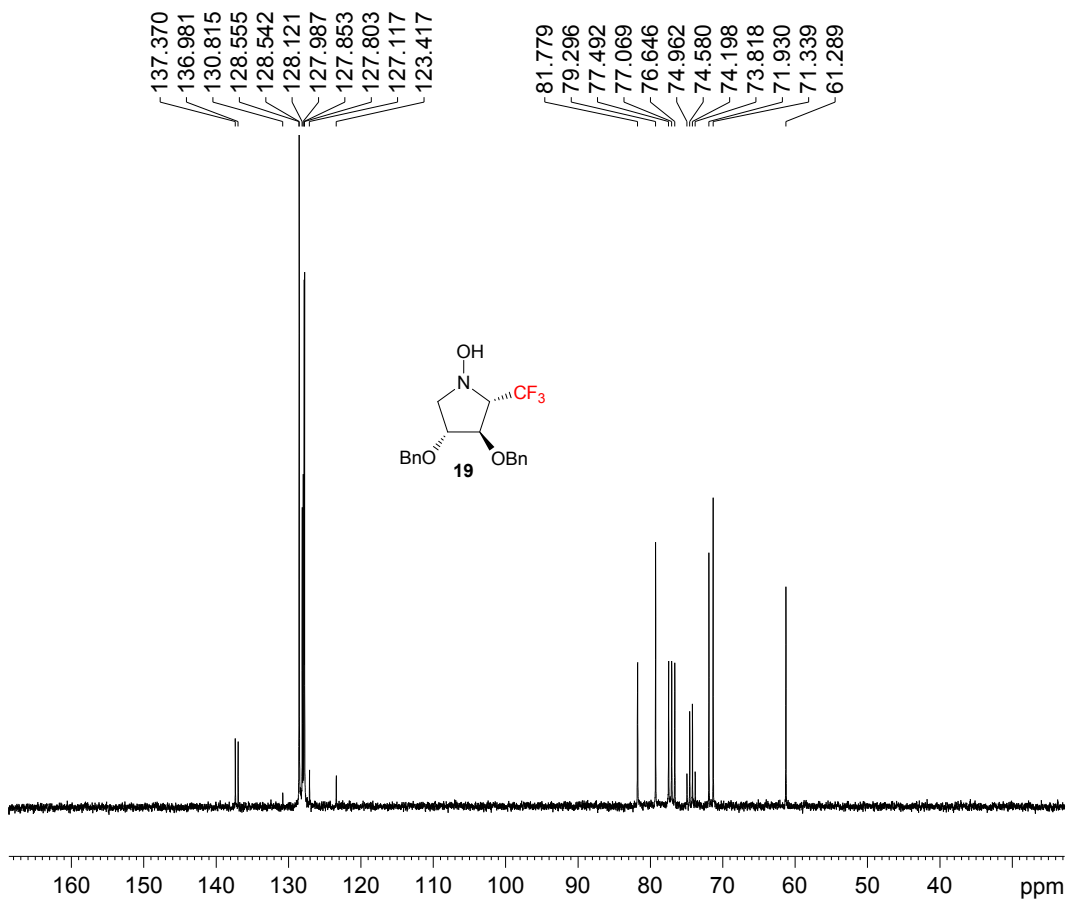


Compound 19:



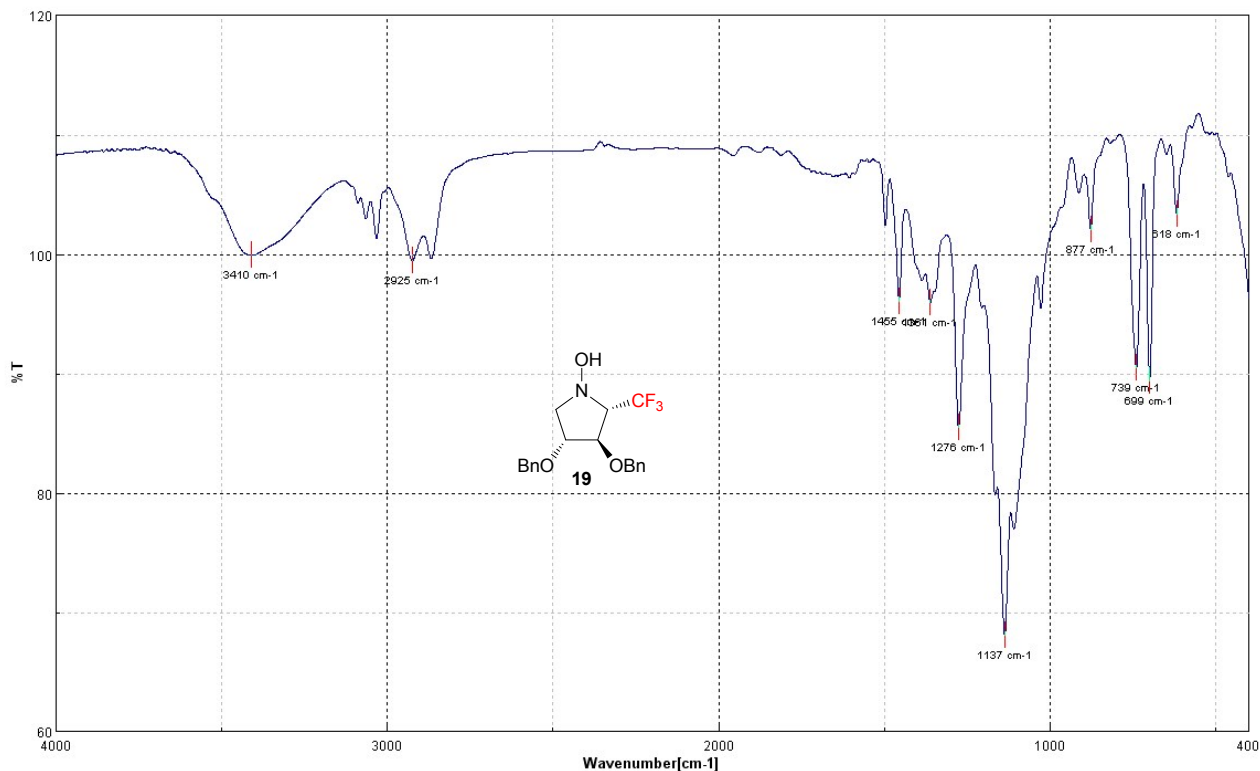
lyx-221

NAME lyx-2016
EXPNO 35
PROCNO 1

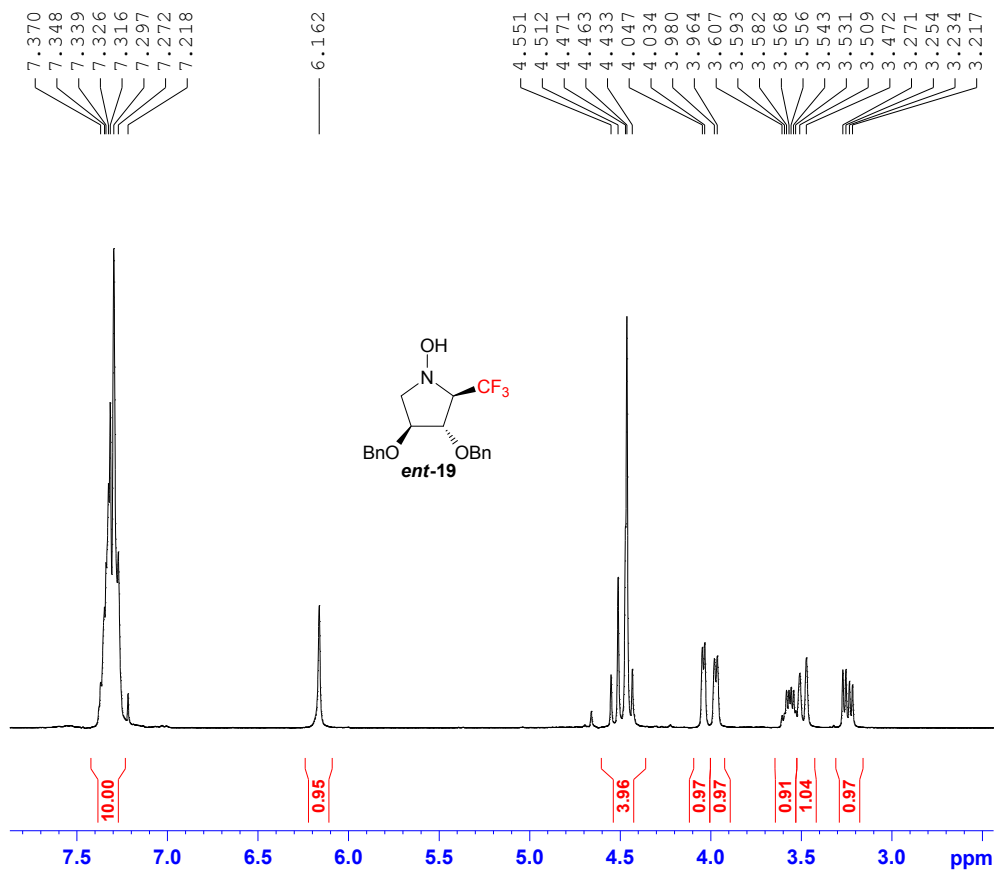


lyx-221-C13

NAME lyx-2016
EXPNO 37
PROCNO 1



Compound *ent*-19:

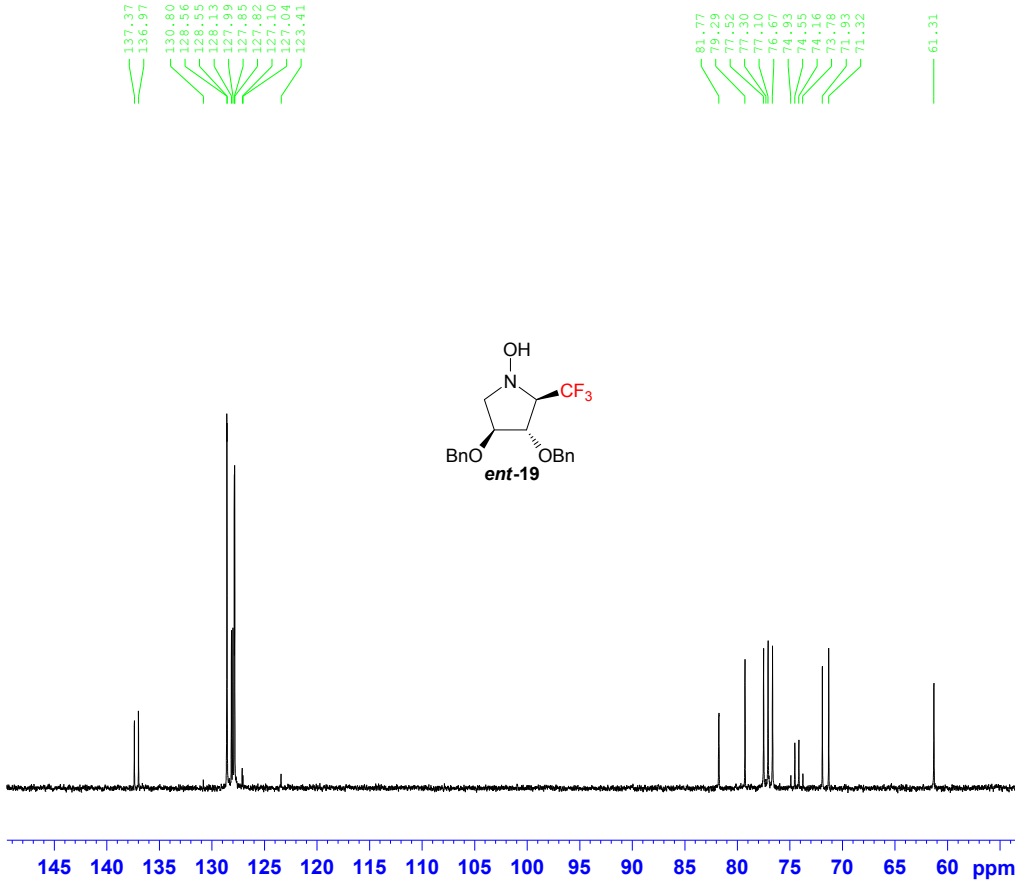


```

NAME lyx4-219a
EXPNO 10
PROCNO 1
Date_ 20101214
Time 9.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 64
DW 55.600 usec
DE 8.00 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz
SI 32768
SF 300.1300184 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```



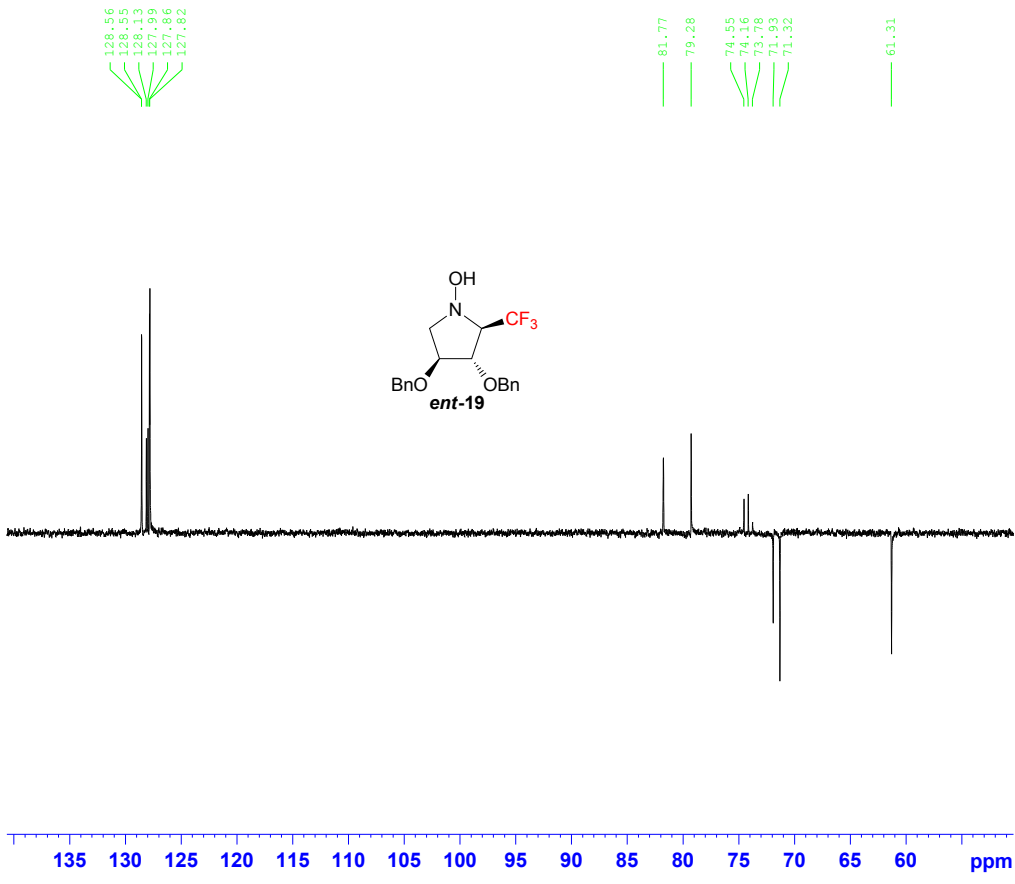
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NAME lyx4-219a
EXPNO 12
PROCNO 1
Date_ 20101214
Time 9.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 96
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 8.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



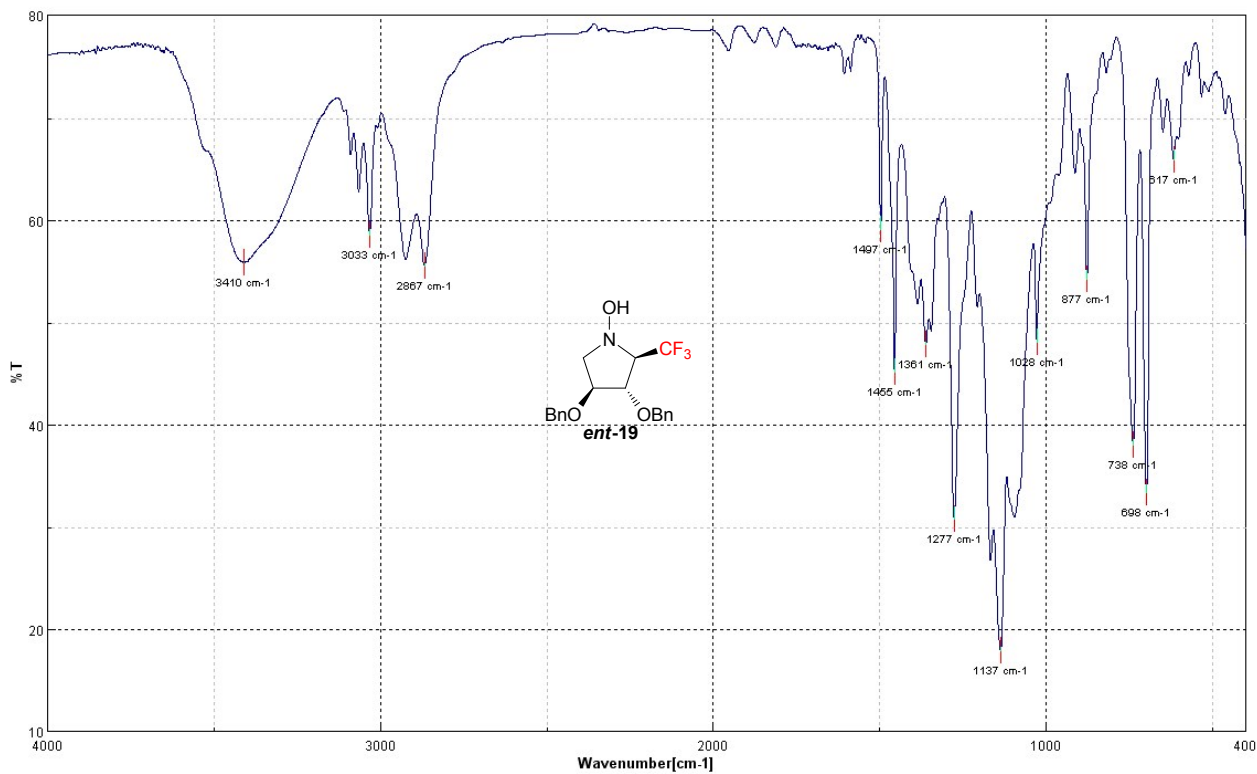
```

NAME lyx4-219a
EXPNO 13
PROCNO 1
Date_ 20101214
Time 9.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 36
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 295.8 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
P2 25.00 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

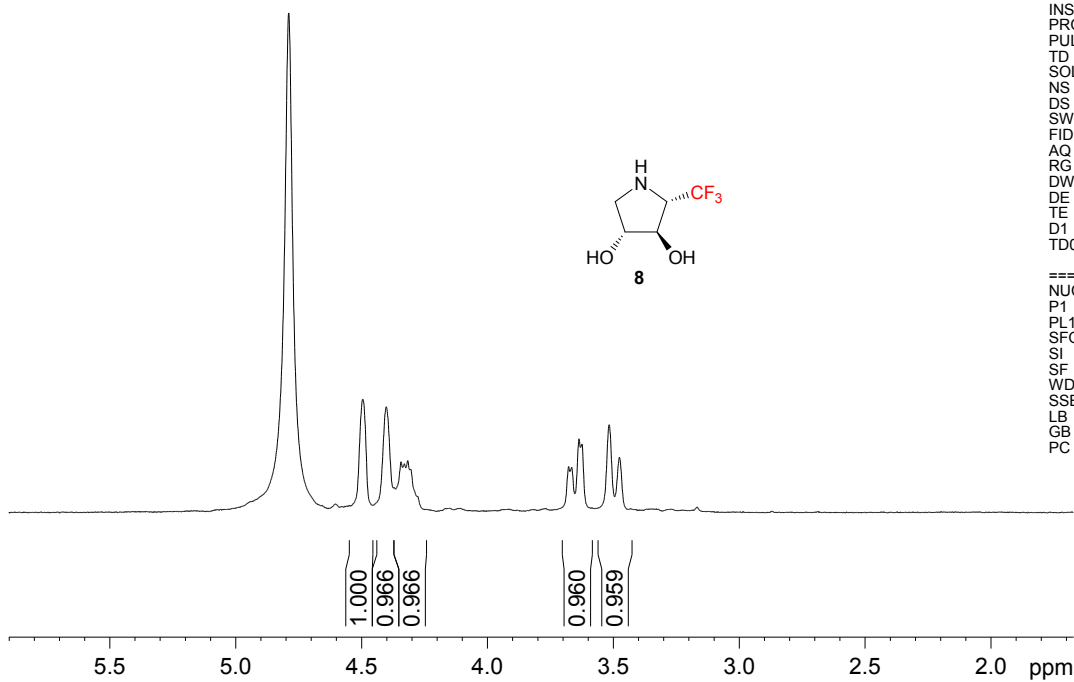
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.80 usec
P4 21.60 usec
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



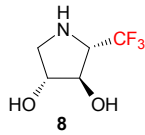
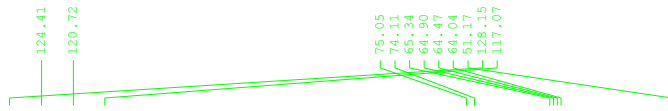
Compound 8:

4.789
 4.495
 4.402
 4.343
 4.330
 4.317
 3.677
 3.665
 3.636
 3.624
 3.517
 3.476



NAME lyx4-222
 EXPNO 10
 PROCNO 1
 Date_ 20101221
 Time 9.20
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 1
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 228.1
 DW 55.600 usec
 DE 8.00 usec
 TE 297.6 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 3.00 dB
 SFO1 300.1324010 MHz
 SI 32768
 SF 300.1299684 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



```

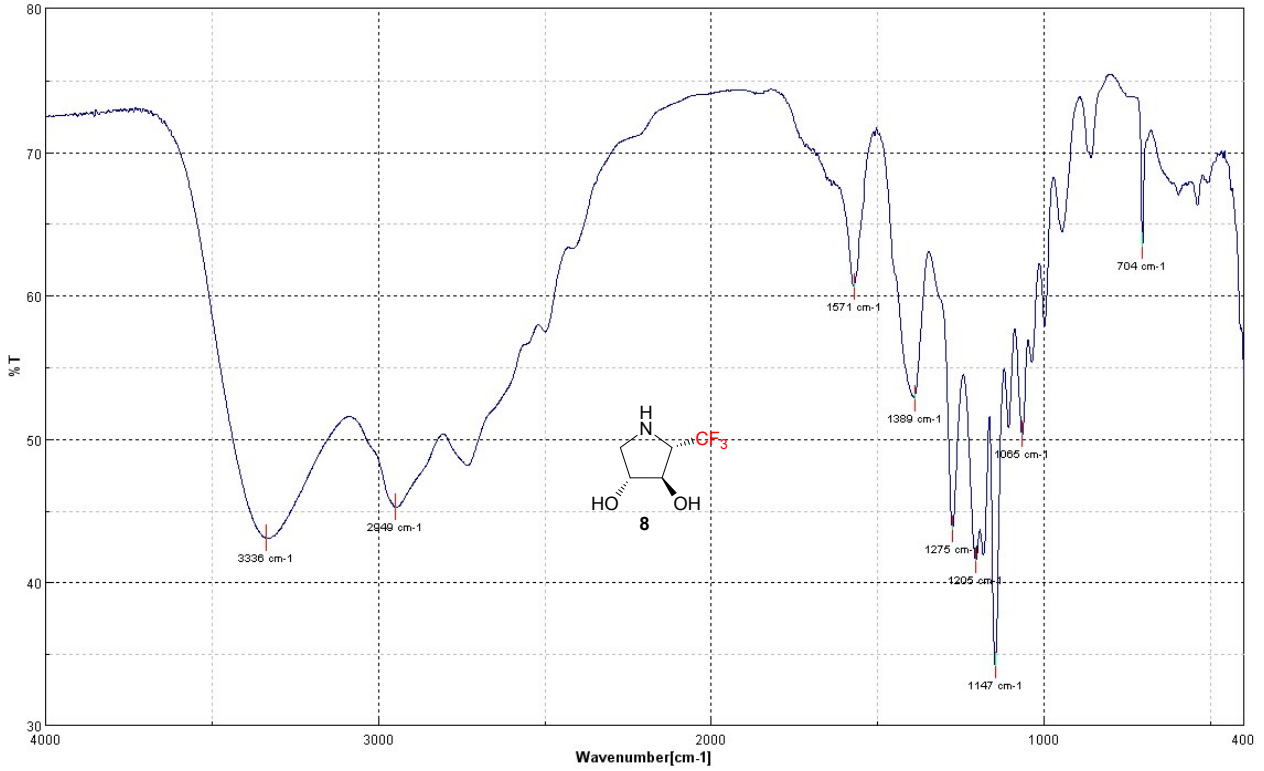
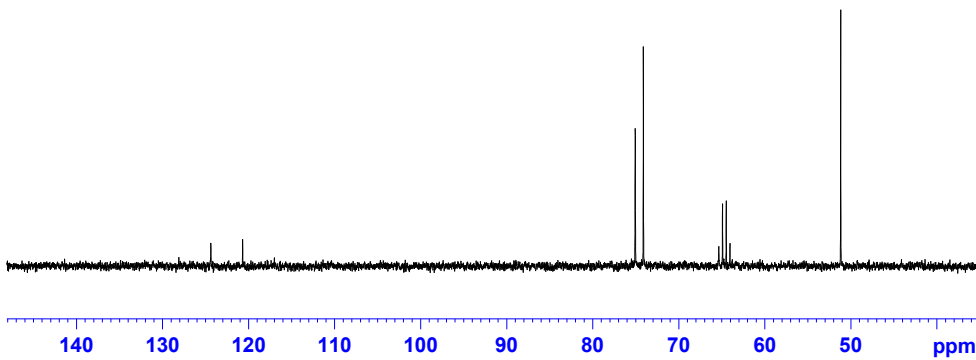
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EXPNO     11
PROCNO    1
Date_     20101221
Time      9.23
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT   D2O
NS         591
DS         4
SWH        17985.611 Hz
FIDRES     0.274439 Hz
AQ         1.8219508 sec
RG         14596.5
DW         27.800 usec
DE         8.00 usec
TE         297.9 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

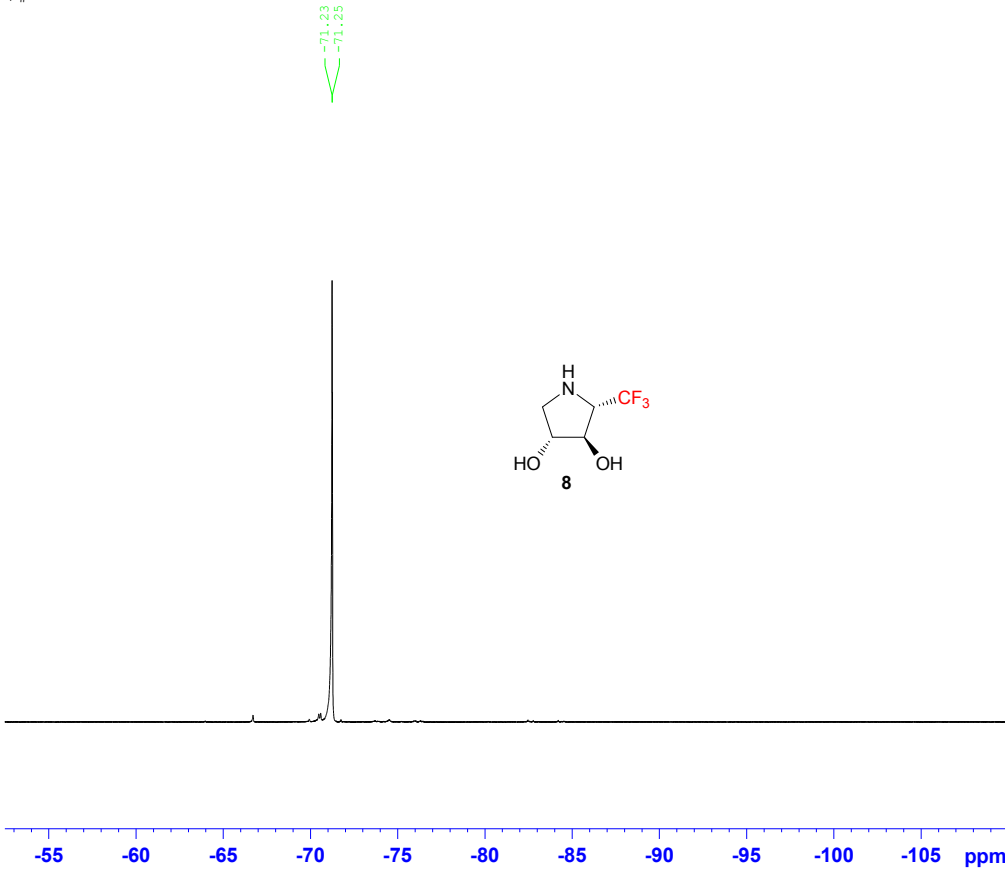
===== CHANNEL f1 =====
NUC1       13C
P1         12.50 usec
PL1        2.00 dB
SFO1       75.4752953 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       100.00 usec
PL2         3.00 dB
PLI2        22.33 dB
PLI3        23.00 dB
SFO2       300.1312005 MHz
SI          32768
SF         75.4677490 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```



7#



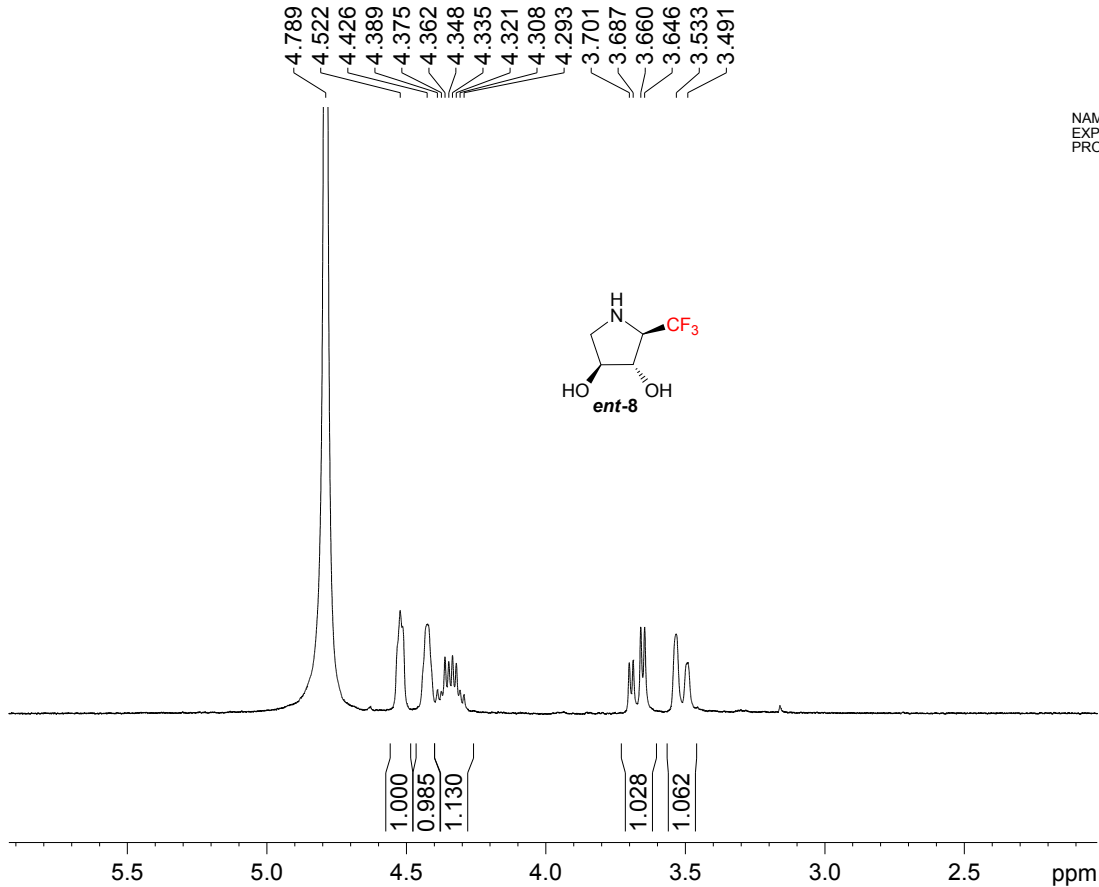
```
Current Data Parameters
NAME      19F
EXPNO    7
PROCNO   1

F2 - Acquisition Parameters
Date_    20110128
Time     8.26
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgfgln
TD       32768
SOLVENT  CDCl3
NS       16
DS       0
SWH      75187.969 Hz
FIDRES   2.294555 Hz
AQ       0.2179572 sec
RG       32
DW       6.650 usec
DE       6.00 usec
TE       673.2 K
D1       1.00000000 sec

===== CHANNEL f1 =====
NUC1     19F
P1       12.50 usec
PL1      0.00 dB
SFO1     376.4418792 MHz

F2 - Processing parameters
SI       65536
SF       376.4983540 MHz
WDW      EM
SSB      0
LB       5.00 Hz
GB       0
PC       0.10
```

Compound *ent*-8:



lyx-220

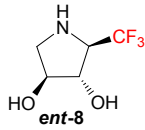
```
NAME      lyx-2016
EXPNO    39
PROCNO   1
```

124.16
120.47

74.82
73.87
65.07
64.64
64.20
63.77

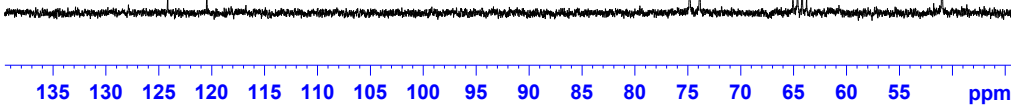
50.99

NAME lyx4-220
EXPNO 12
PROCNO 1
Date_ 20101220
Time 17.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 66
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1



===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

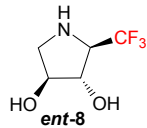


74.82
73.87

65.07
64.64
64.20
63.77

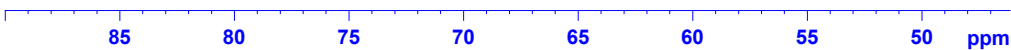
50.98

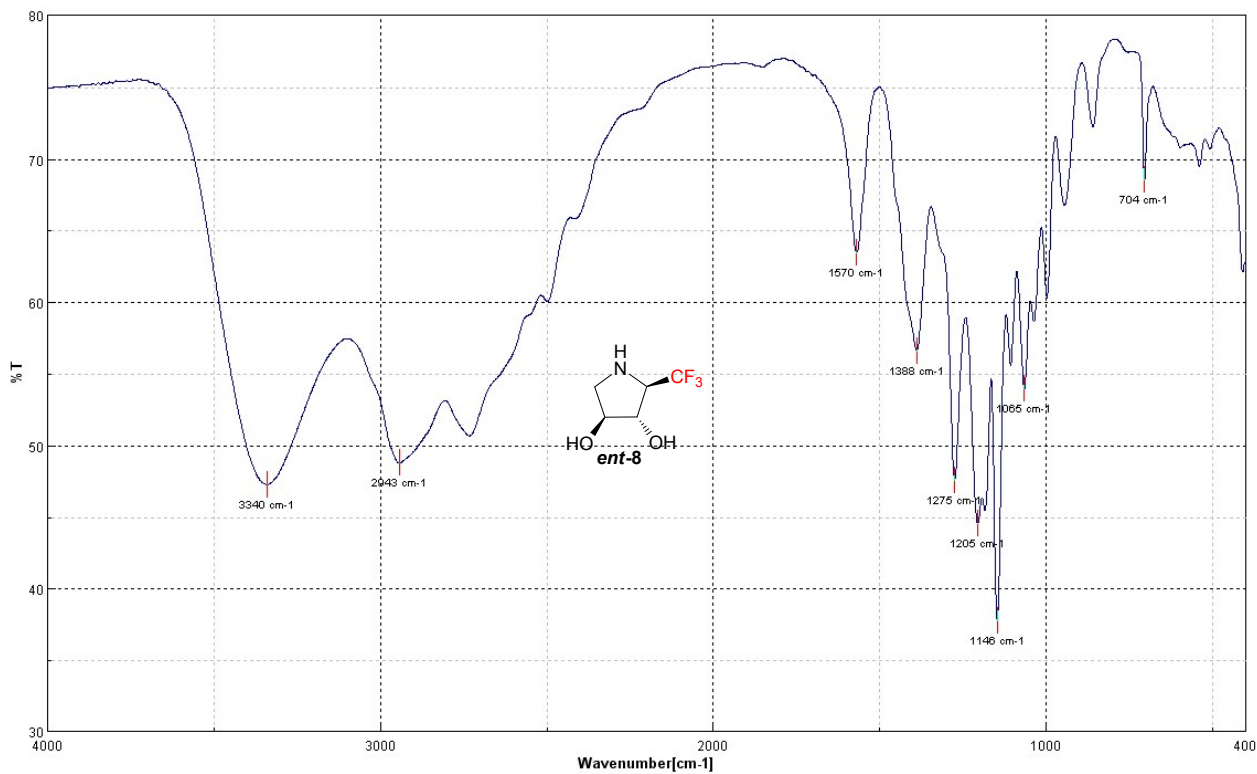
NAME lyx4-220
EXPNO 13
PROCNO 1
Date_ 20101220
Time 17.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT D2O
NS 22
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.2 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1



===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
P2 25.00 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

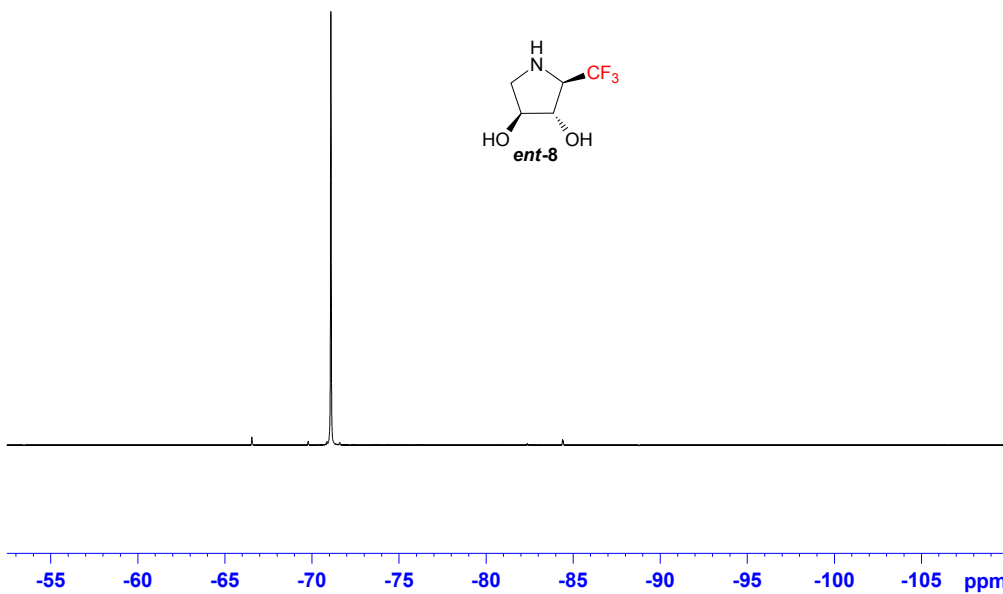
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.80 usec
P4 21.60 usec
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





6#

--71.08
--71.09



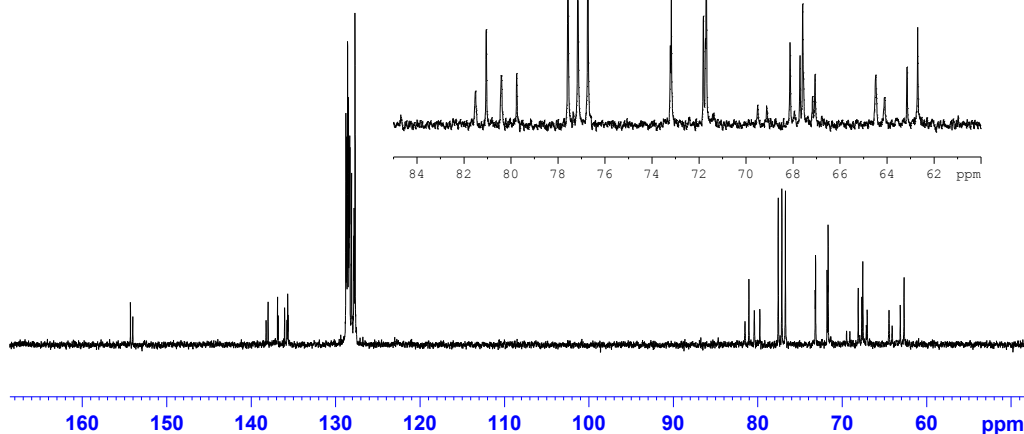
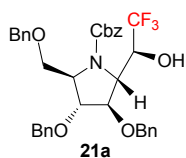
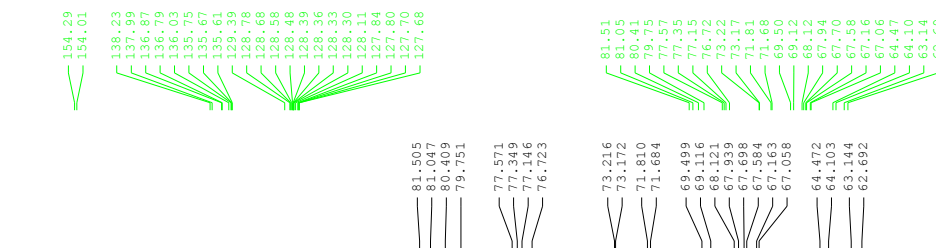
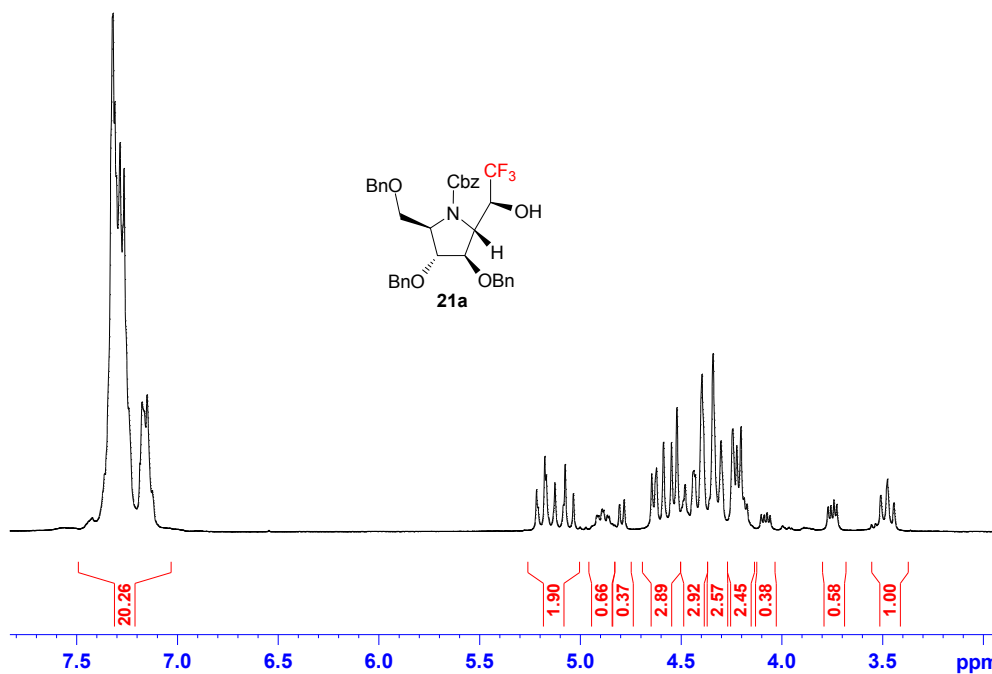
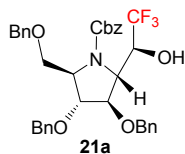
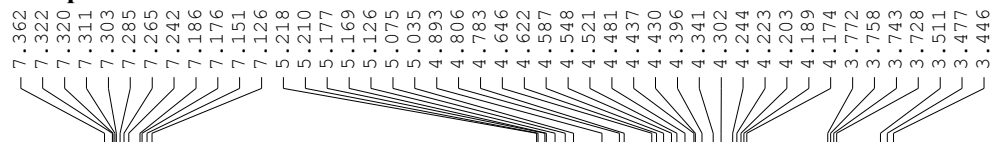
Current Data Parameters
NAME 19F
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110128
Time 8.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgflgn
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 75187.969 Hz
FIDRES 2.294555 Hz
AQ 0.2179572 sec
RG 32
DW 6.650 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 19F
P1 12.50 usec
PL1 0.00 dB
SFO1 376.4418792 MHz

F2 - Processing parameters
SI 65536
SF 376.4983540 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 0.10

Compound 21a:



```

NAME lyx4-237a
EXPNO 10
PROCNO 1
Date_ 20110224
Time 22.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 45.3
DW 55.600 usec
DE 8.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
    
```

```

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.1324010 MHz
SI 32768
SF 300.1300276 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```

```

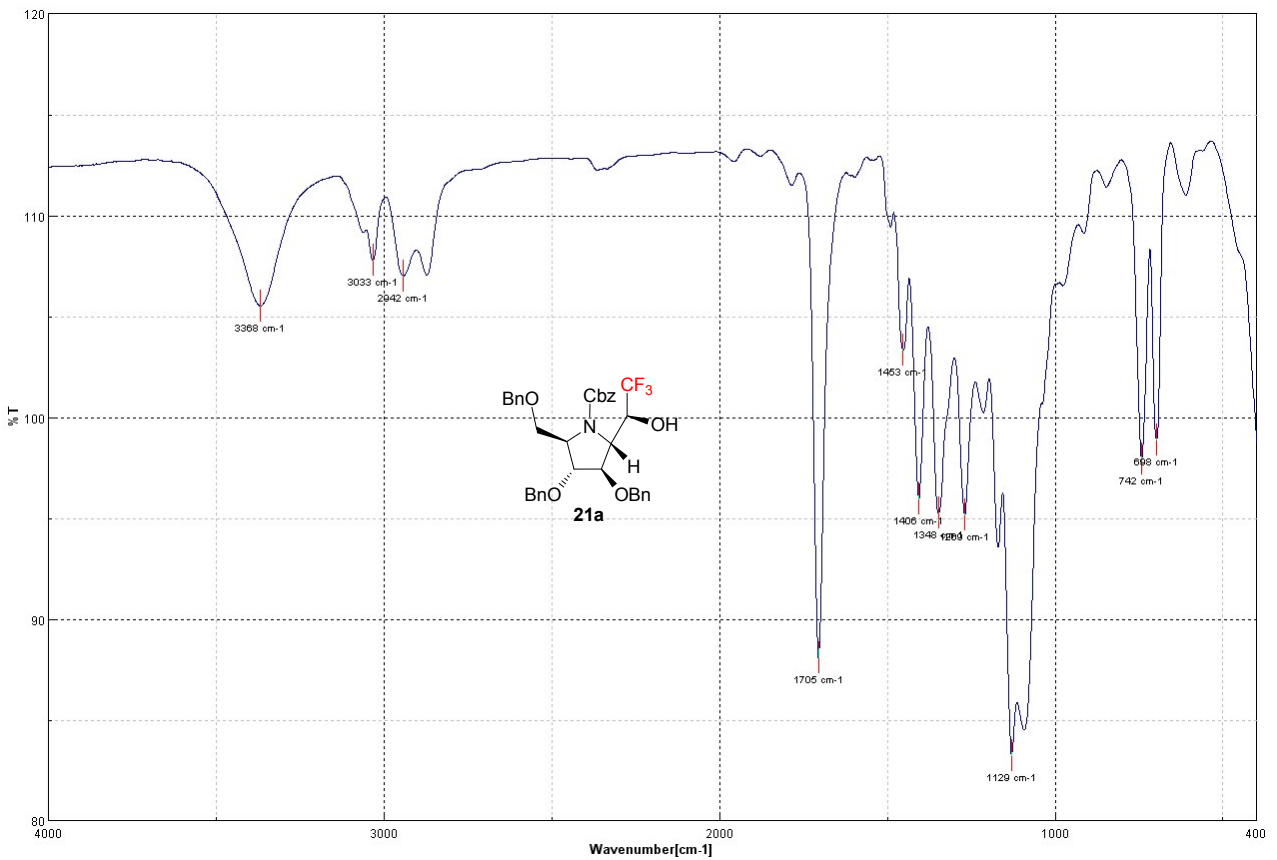
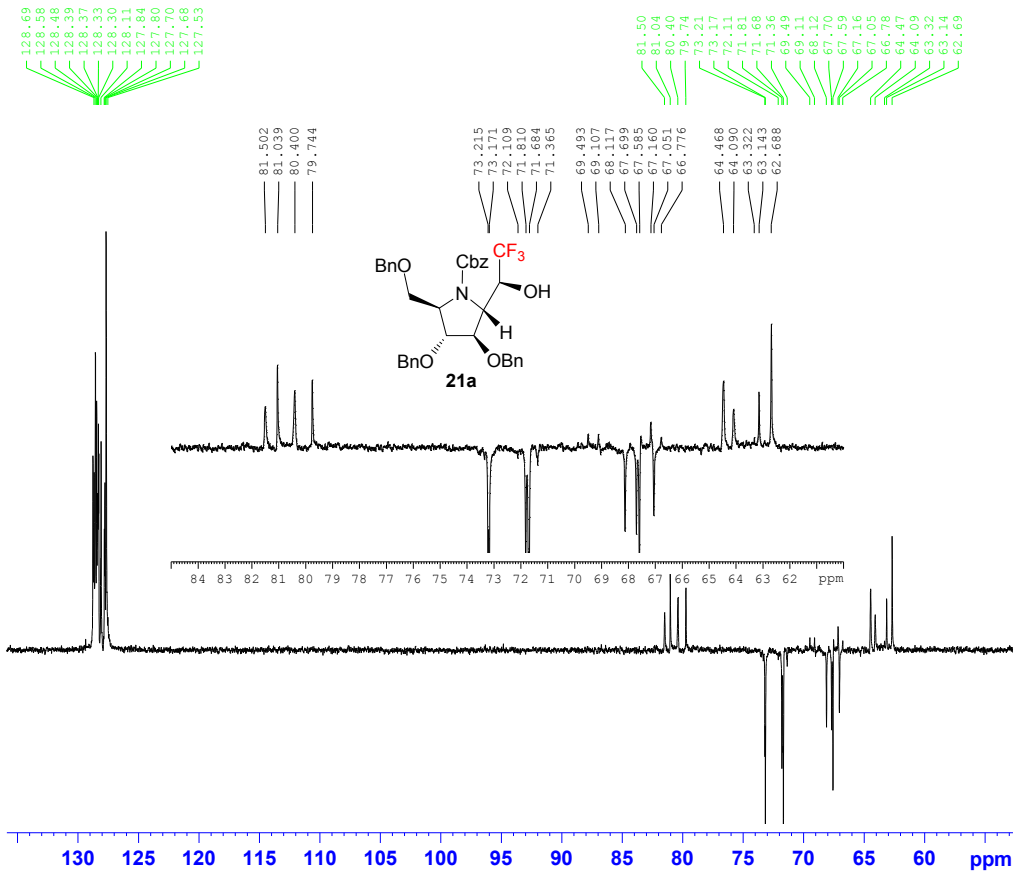
NAME lyx4-237a
EXPNO 20
PROCNO 1
Date_ 20110225
Time 13.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 104
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 8.00 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
    
```

```

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz
    
```

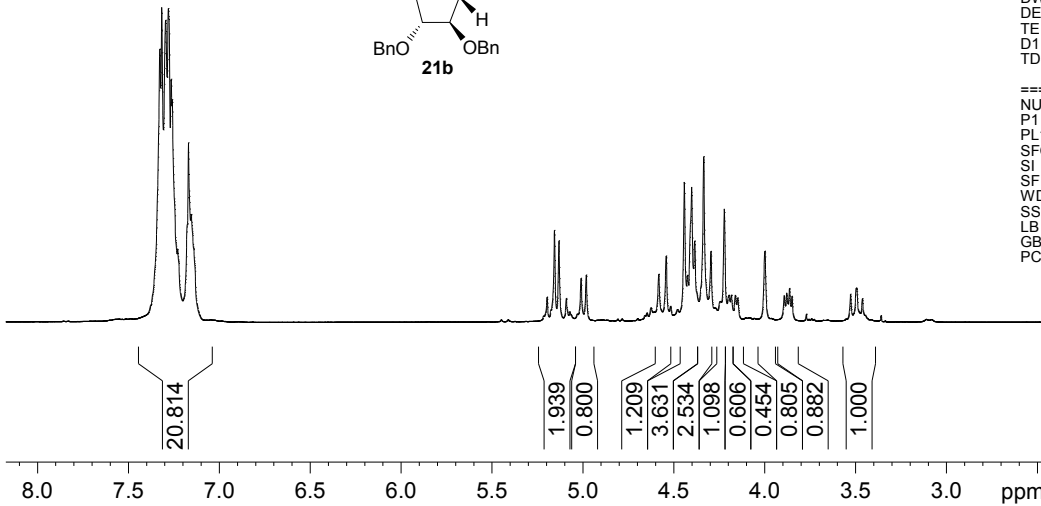
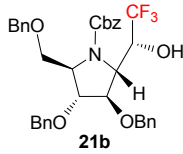
```

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```



Compound 21b:

7.317
7.296
7.281
7.266
7.260
7.230
7.170
7.155
5.197
5.157
5.132
5.092
5.010
4.982
4.627
4.583
4.542
4.519
4.442
4.425
4.402
4.385
4.335
4.296
4.276
4.246
4.222
4.197
4.184
4.162
4.149
3.999
3.893
3.879
3.863
3.850
3.527
3.463

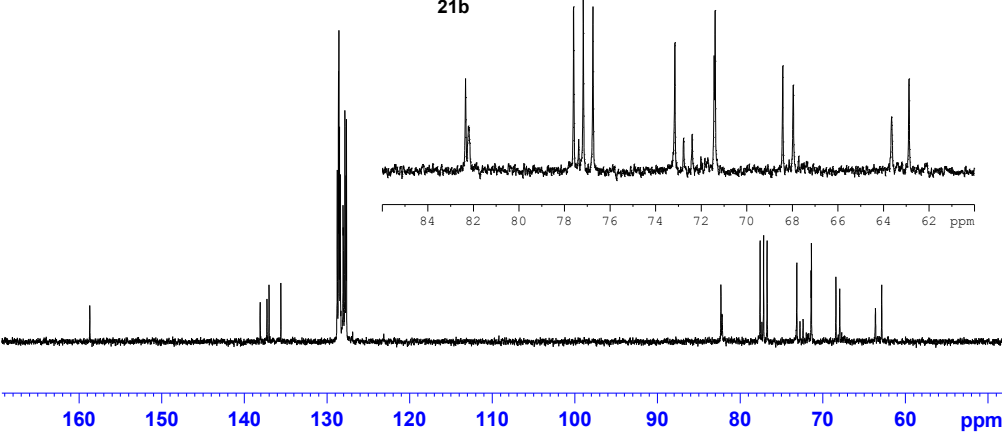
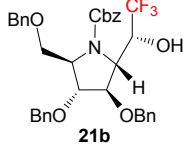


NAME lyx4-237b
EXPNO 10
PROCNO 1
Date_ 20110224
Time 22.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 3
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 40.3
DW 55.800 usec
DE 8.00 usec
TE 296.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.132410 MHz
SI 32768
SF 300.1300324 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

156.70
138.08
137.26
137.00
135.58
128.75
128.60
128.55
128.48
128.04
128.02
127.82
127.68
127.63

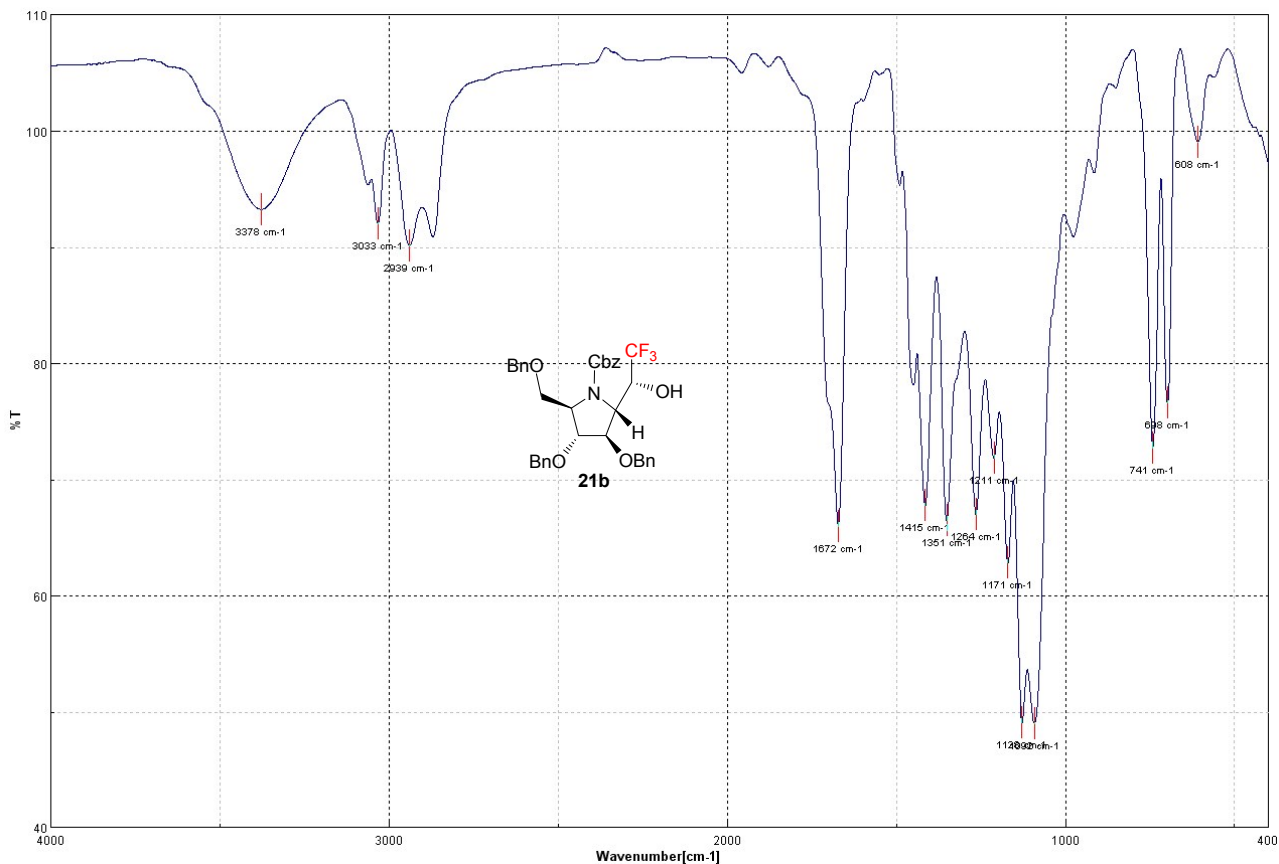
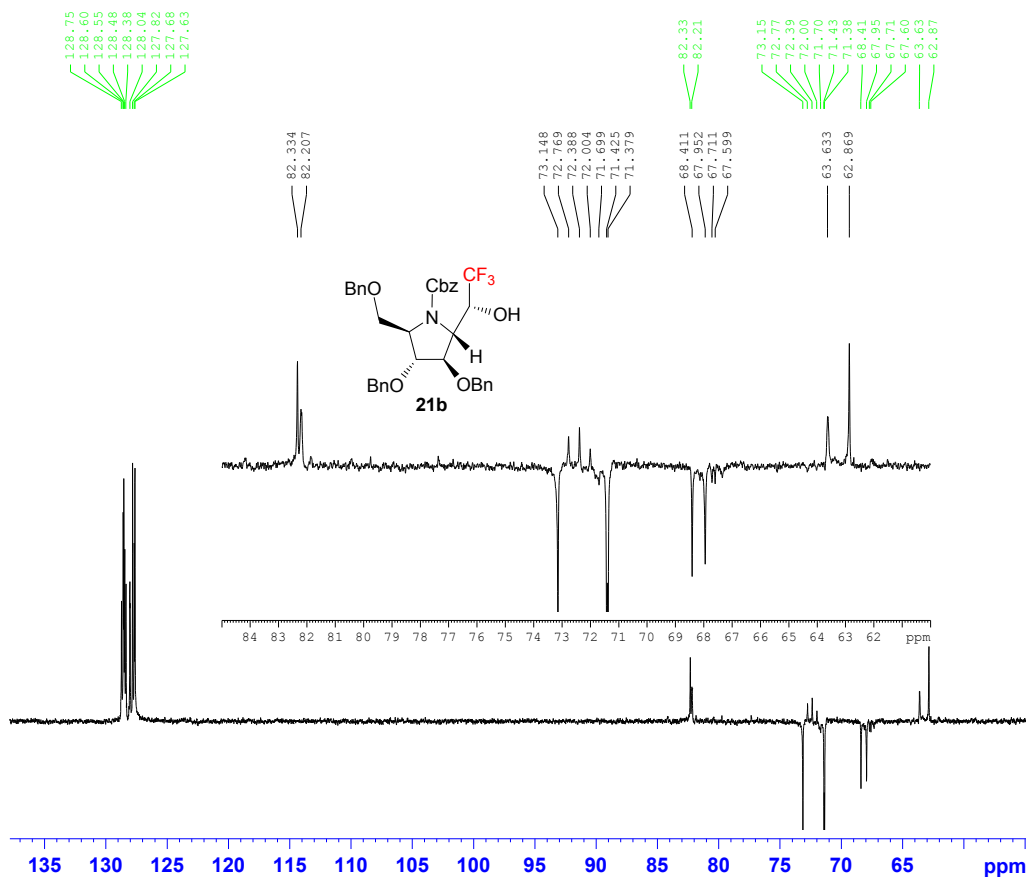
82.335
82.209
77.592
77.368
77.168
76.744
73.149
72.767
72.389
72.006
71.701
71.425
71.379
71.170
71.01
71.43
71.38
68.41
67.85
62.87



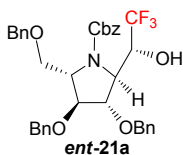
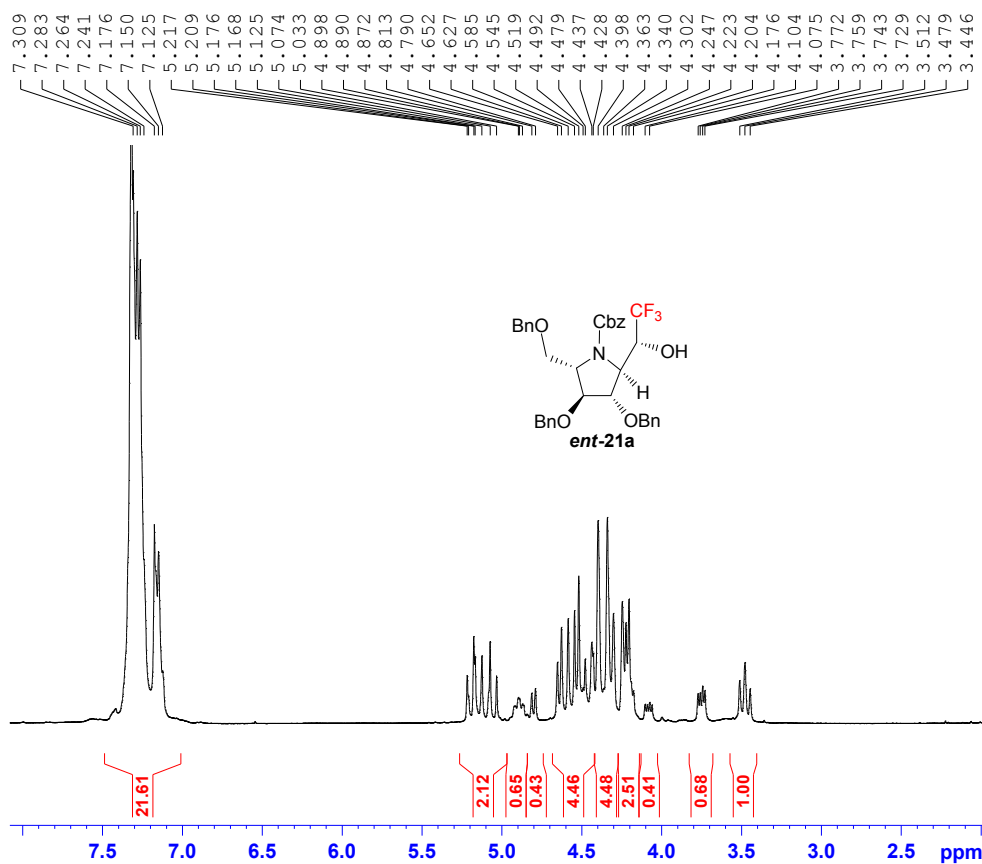
NAME lyx4-237b
EXPNO 22
PROCNO 1
Date_ 20110224
Time 12.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 49
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5792.6
DW 27.800 usec
DE 8.00 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Compound ent-21a:

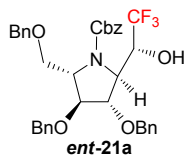
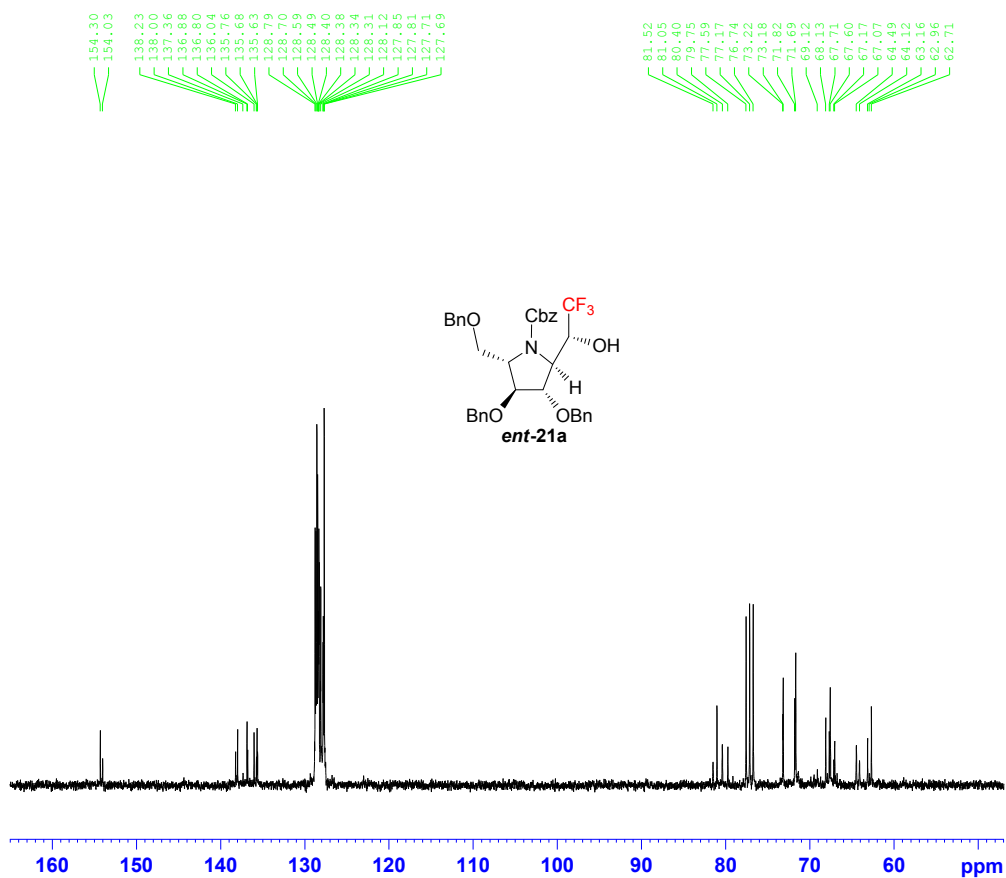


```

NAME      lyx4-224a
EXPNO    10
PROCNO   1
Date_    20110228
Time     12.34
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       4
DS       0
SWH      8992.806 Hz
FIDRES   0.137219 Hz
AQ       3.6438515 sec
RG       40.3
DW       55.600 usec
DE       8.00 usec
TE       295.8 K
D1       1.00000000 sec
TD0      1
    
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       10.80 usec
PL1      3.00 dB
SFO1     300.1324010 MHz
SI       32768
SF       300.1300310 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```



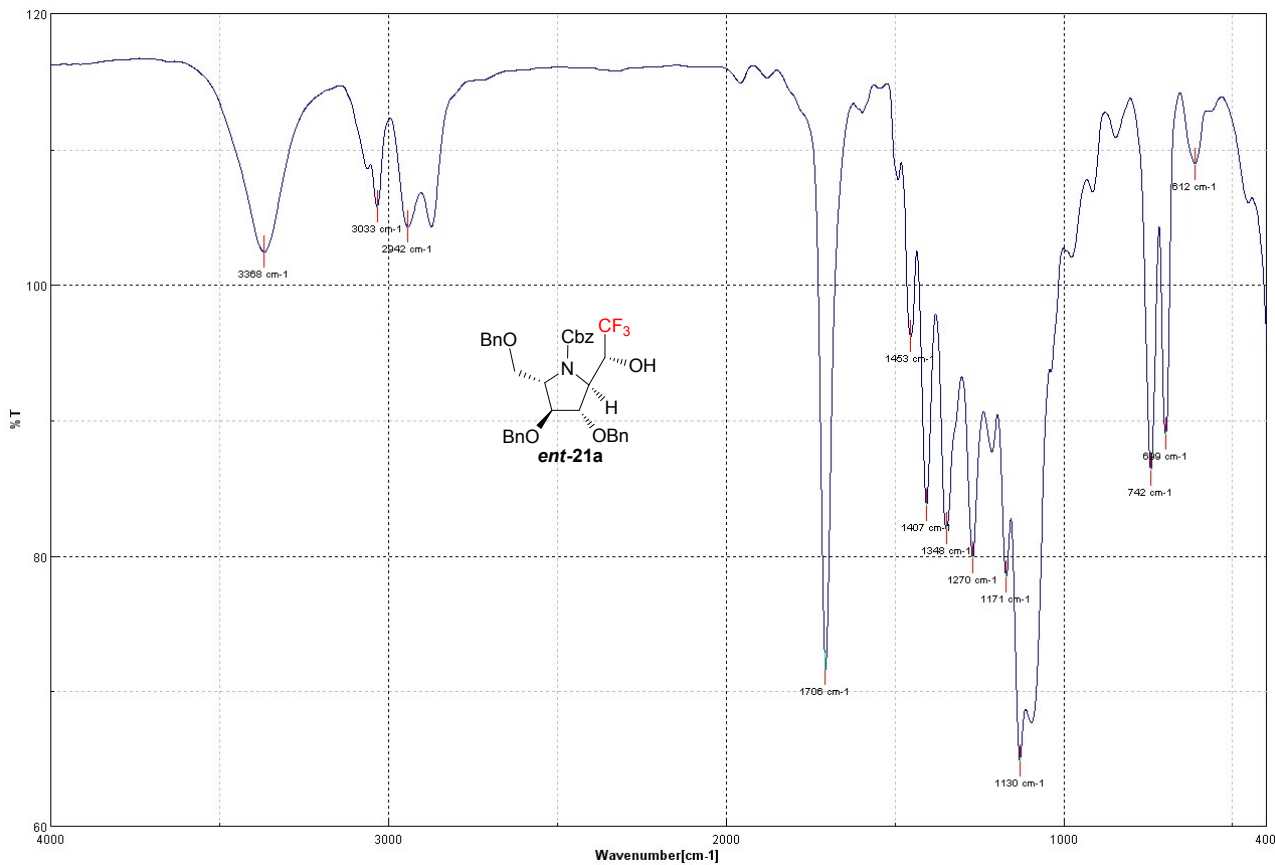
```

NAME      lyx4-224a
EXPNO    11
PROCNO   1
Date_    20110228
Time     12.37
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       65
DS       4
SWH      17985.611 Hz
FIDRES   0.274439 Hz
AQ       1.8219508 sec
RG       5160.6
DW       27.800 usec
DE       8.00 usec
TE       296.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
    
```

```

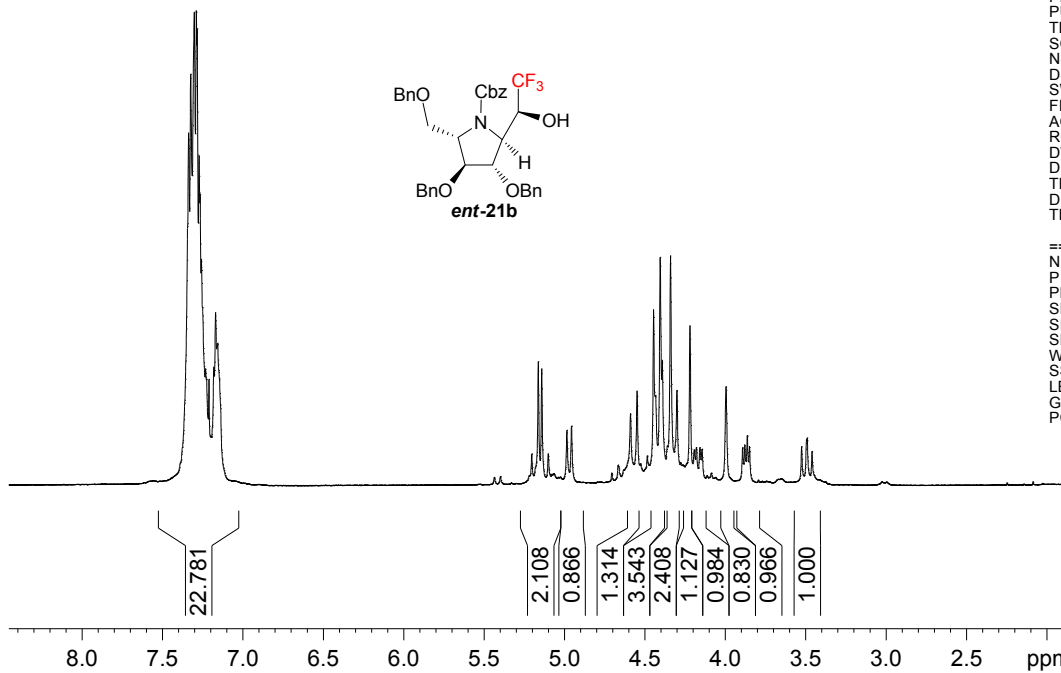
===== CHANNEL f1 =====
NUC1     13C
P1       12.50 usec
PL1      2.00 dB
SFO1     75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    100.00 usec
PL2      3.00 dB
PL12     22.33 dB
PL13     23.00 dB
SFO2     300.1312005 MHz
SI       32768
SF       75.4677490 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
    
```



Compound ent-21b:

7.325
7.303
7.290
7.285
7.273
7.267
7.259
7.233
7.228
7.212
7.200
7.182
7.171
7.159
5.164
5.142
4.985
4.957
4.590
4.549
4.446
4.435
4.405
4.392
4.341
4.301
4.220
4.193
4.180
4.158
4.145
3.996
3.893
3.879
3.863
3.850
3.526
3.495
3.491



NAME lyx4-224b
EXPNO 10
PROCNO 1
Date_ 20110228
Time 12.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 2
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 71.8
DW 55.600 usec
DE 8.00 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1

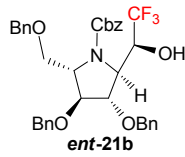
===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SF01 300.1324010 MHz
SI 32768
SF 300.1300204 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

158.66

138.04
137.21
136.96
135.53
128.71
128.57
128.44
128.34
128.01
127.78
127.64
127.59

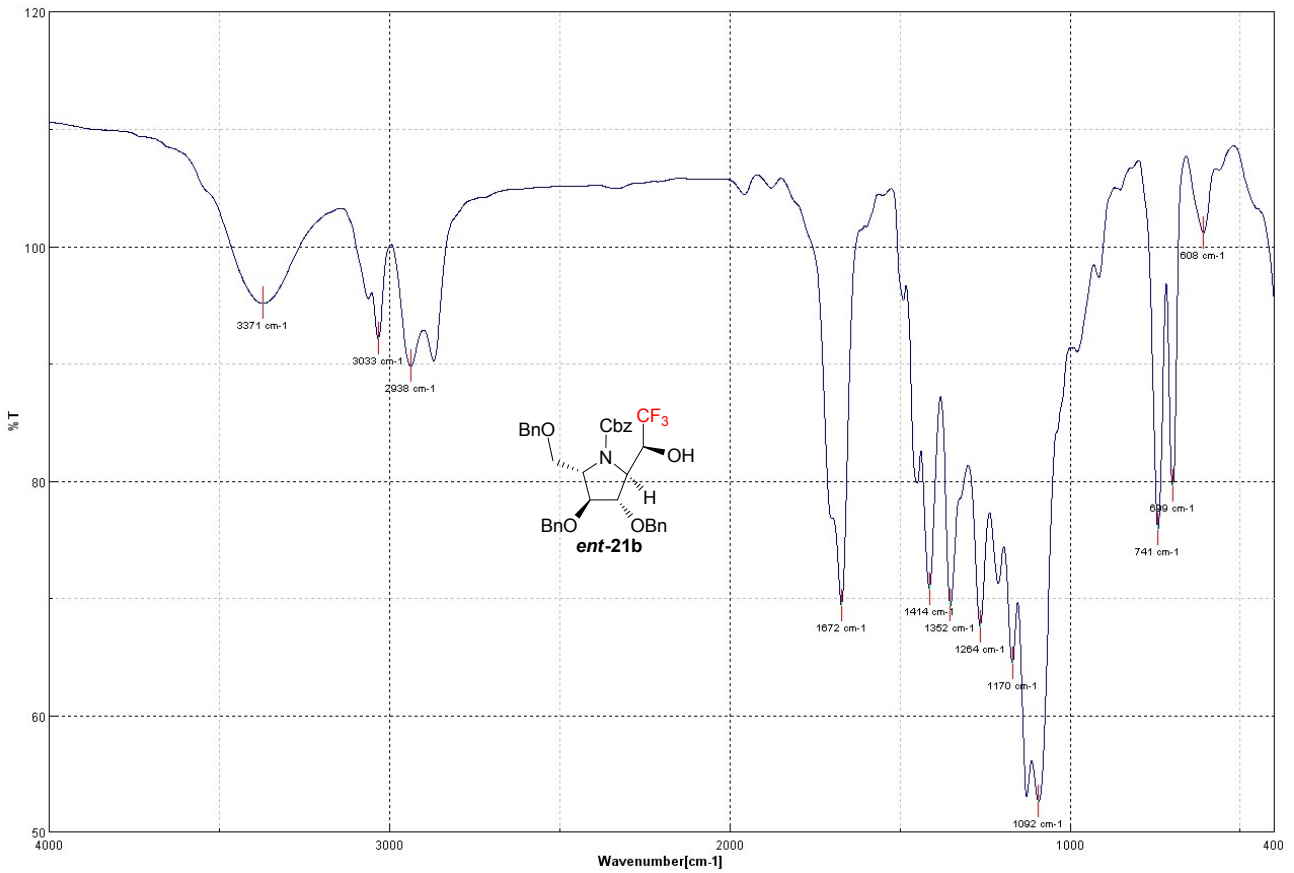
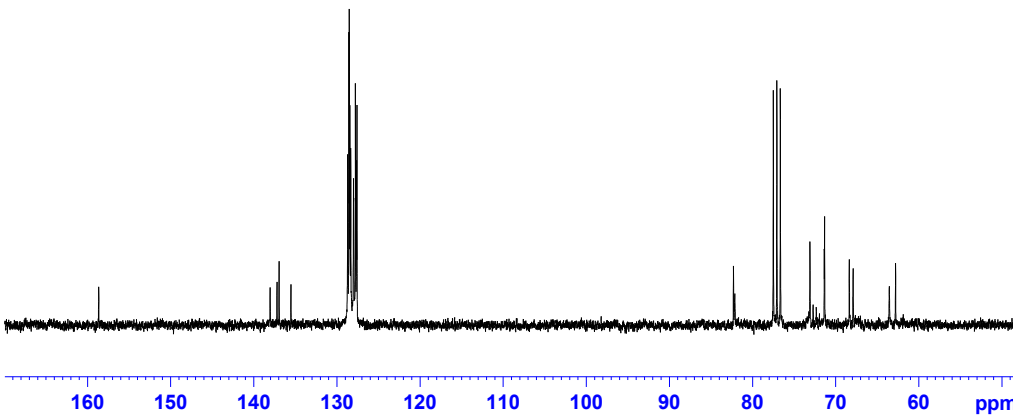
82.32
82.15
77.52
77.10
76.67
72.73
72.35
71.39
71.35
68.38
67.91
63.56
62.81

NAME lyx4-224b
EXPNO 11
PROCNO 1
Date_ 20110228
Time_ 12.46
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 94
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 8.00 usec
TE 295.9 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1



===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

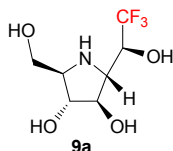
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



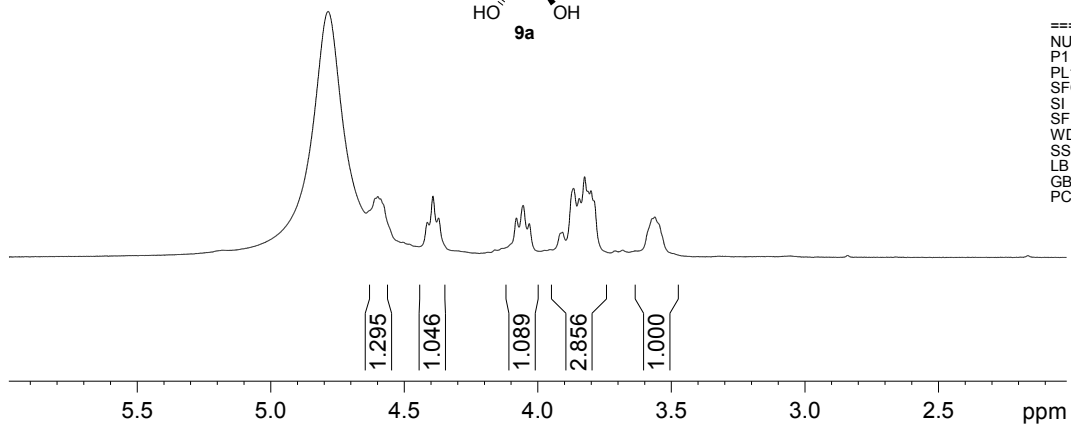
Compound 9a:

4.785
4.600
4.414
4.394
4.372
4.081
4.056
4.033
3.909
3.867
3.846
3.825
3.813
3.802
3.572
3.563

NAME lyx4-240a
EXPNO 20
PROCNO 1
Date_ 20110301
Time 17.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT D2O
NS 3
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 8.00 usec
TE 295.6 K
D1 1.0000000 sec
TD0 1



===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.1324010 MHz
SI 32768
SF 300.1299535 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

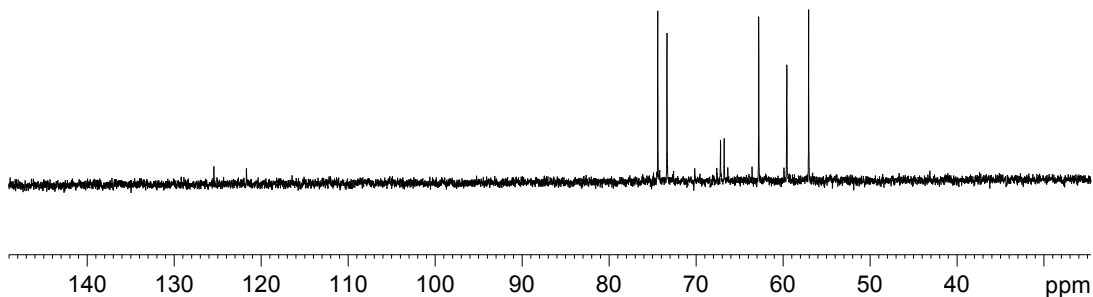
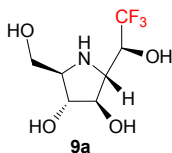


125.440
121.695

74.421
73.360
67.635
67.209
66.784
66.366
62.812
59.582
57.072

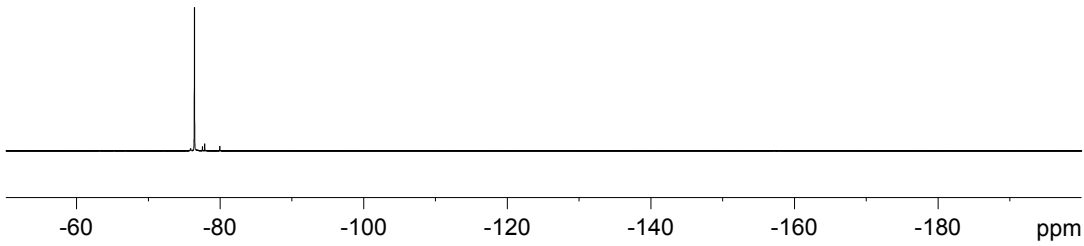
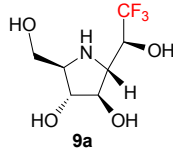
lyx-240a-C13

NAME lyx-2016
EXPNO 46
PROCNO 1



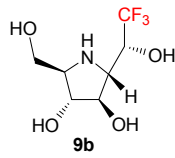
-76.403
-76.413

NAME 19F
EXPNO 110318
PROCNO 1



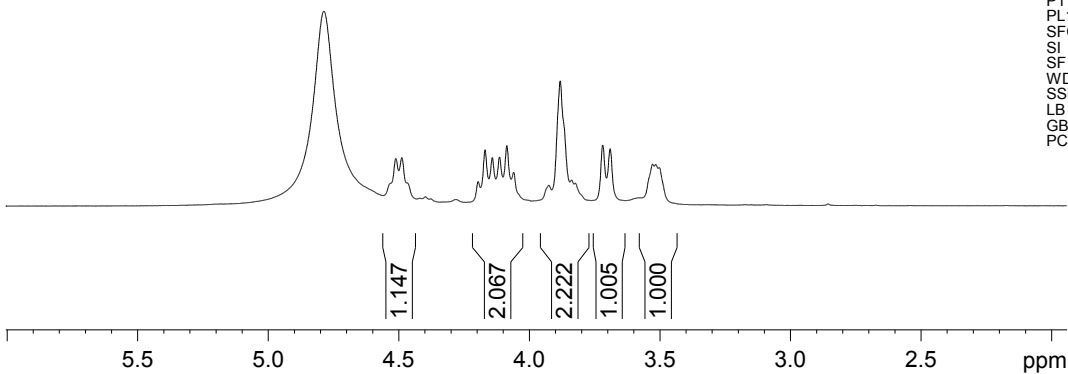
Compound 9b:

4.787
4.511
4.489
4.196
4.170
4.142
4.114
4.086
4.060
3.925
3.882
3.838
3.824
3.719
3.691
3.528
3.516
3.502



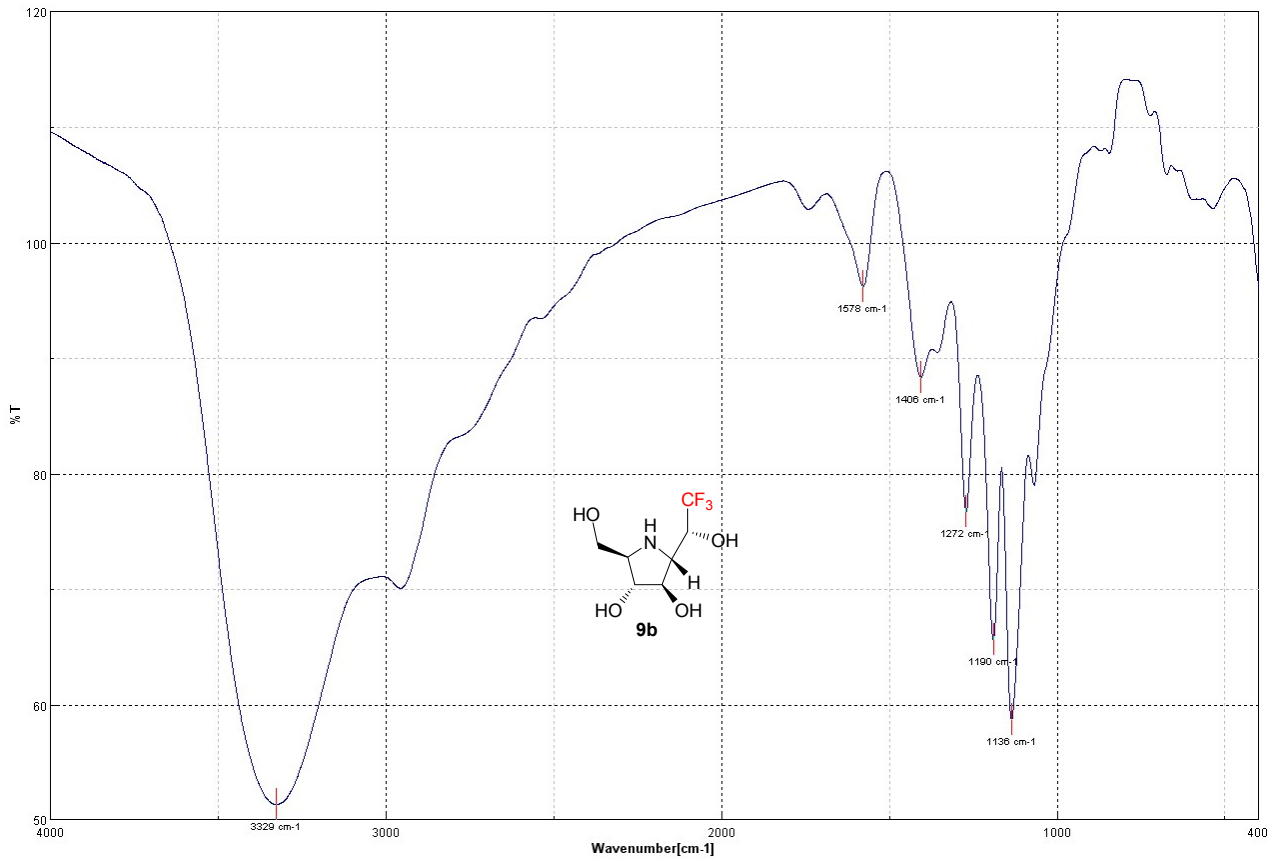
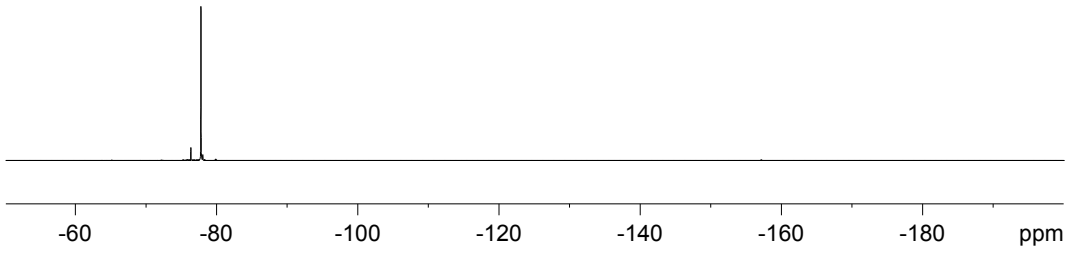
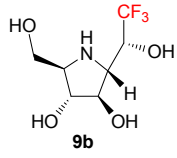
NAME lyx4-240b
EXPNO 10
PROCNO 1
Date_ 20110301
Time 9.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT D2O
NS 5
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 8.00 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.1324010 MHz
SI 32768
SF 300.1299574 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



-77.765
-77.781

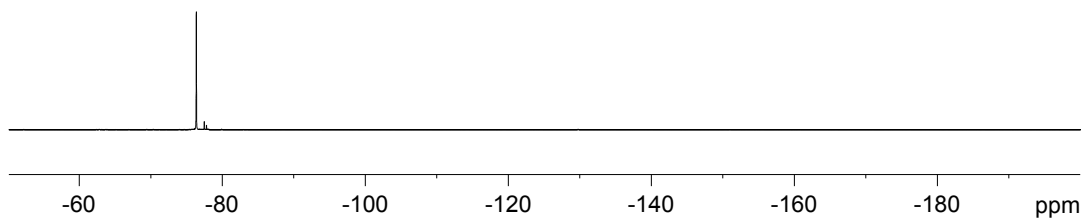
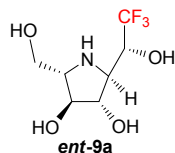
NAME
EXPNO 19F
PROCNO 90318
1



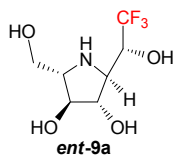
Compound *ent-9a*:

—76.359

NAME 19F
EXPNO 100318
PROCNO 1

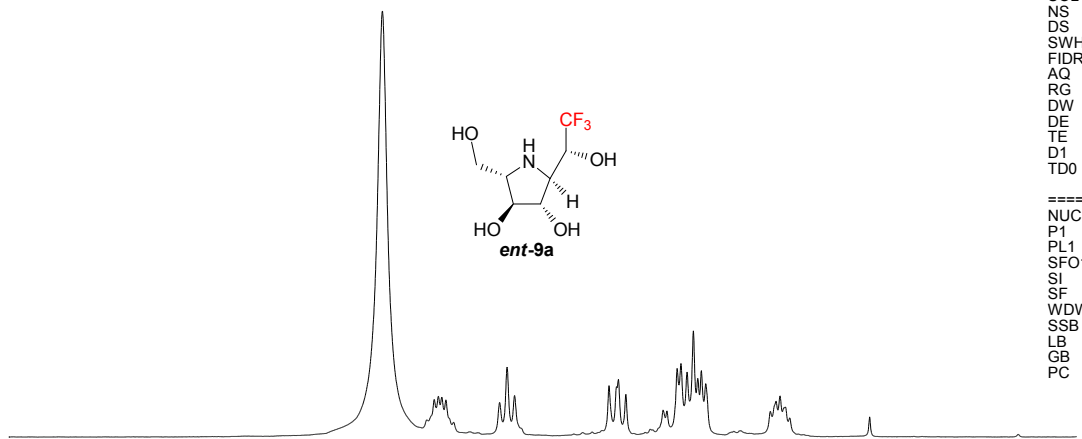


4.789
4.654
4.632
4.619
4.609
4.596
4.573
4.433
4.410
4.388
4.101
4.078
4.072
4.049
3.936
3.925
3.893
3.882
3.863
3.844
3.831
3.820
3.807
3.610
3.593
3.581
3.564
3.551



NAME lyx4-242a
EXPNO 10
PROCNO 1
Date_ 20110302
Time 15.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT D2O
NS 2
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 8.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

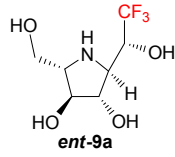
==== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.1324010 MHz
SI 32768
SF 300.1299666 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.190
1.027
1.044
3.074
1.000

125.37
121.63

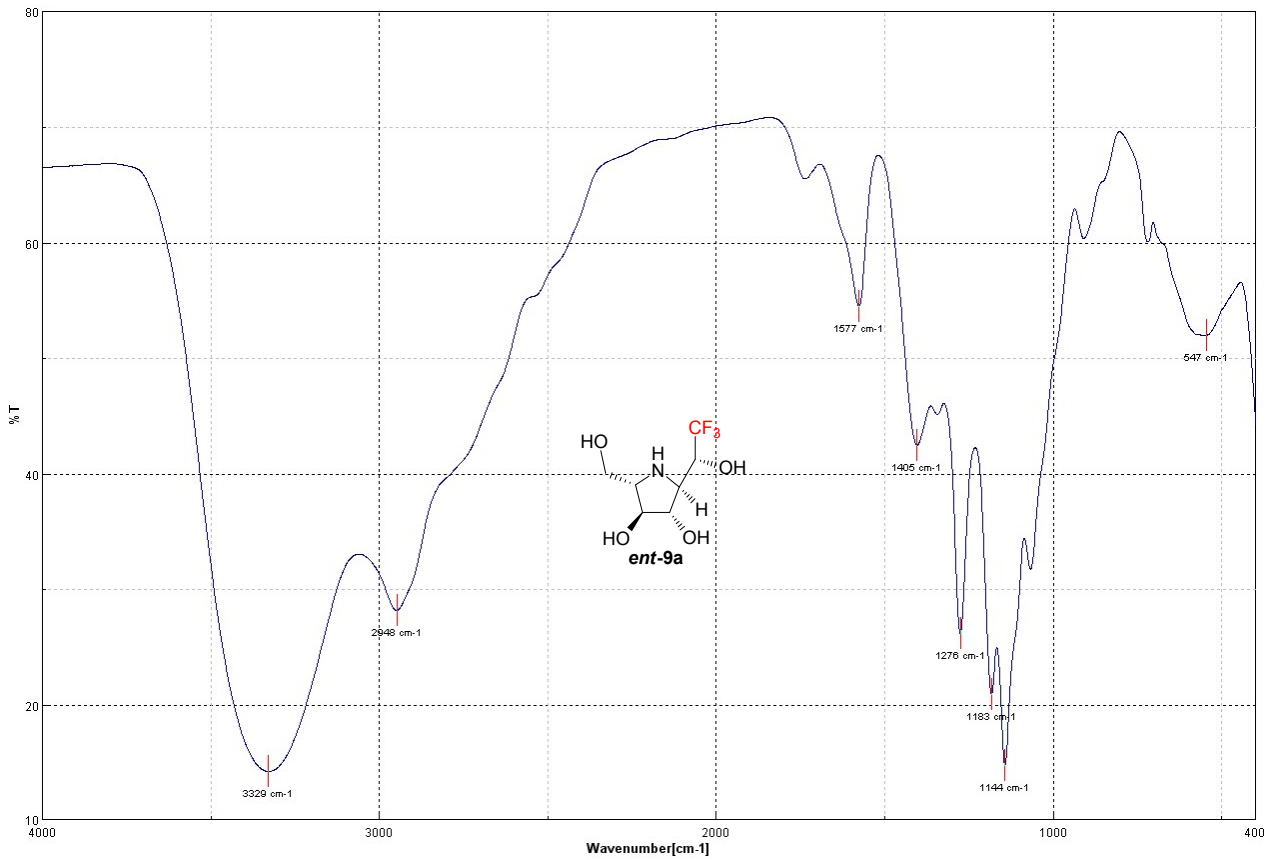
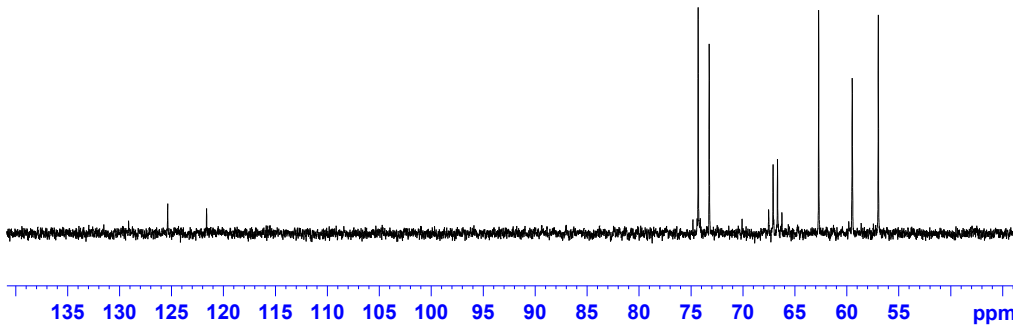
74.33
73.27
70.10
67.54
67.12
66.69
66.26
62.73
59.50
56.99



NAME lyx4-242a
EXPNO 11
PROCNO 1
Date_ 20110302
Time_ 15.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 177
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 14596.5
DW 27.800 usec
DE 8.00 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

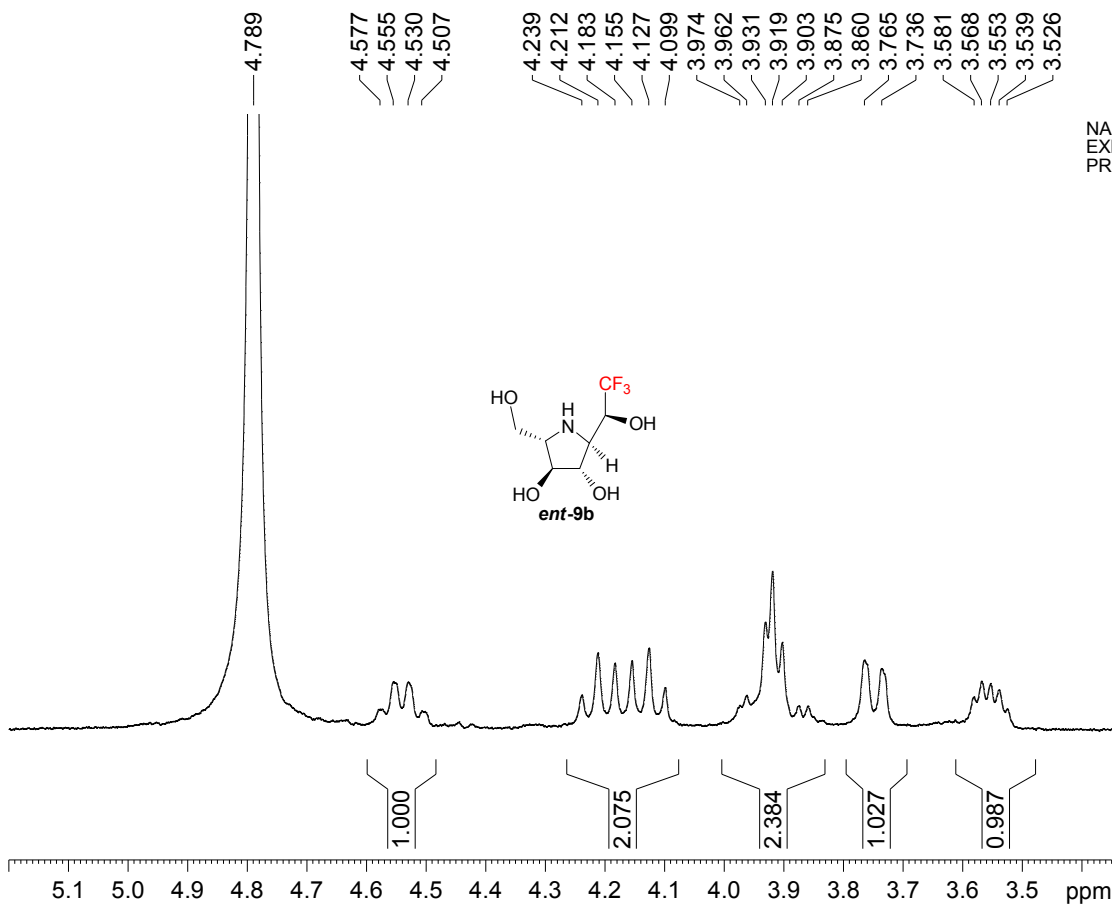
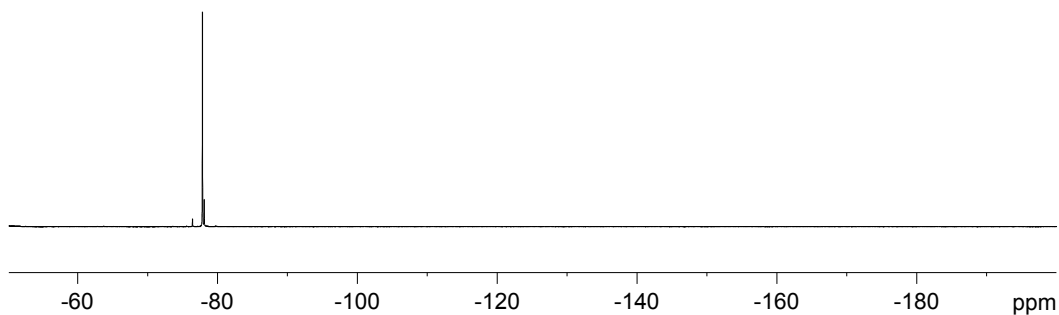
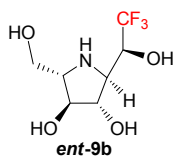
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Compound *ent-9b*:

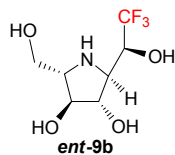
-77.822
-77.837

NAME 19F
EXPNO 40318
PROCNO 1



lyx-242b

NAME lyx-2016
EXPNO 44
PROCNO 1

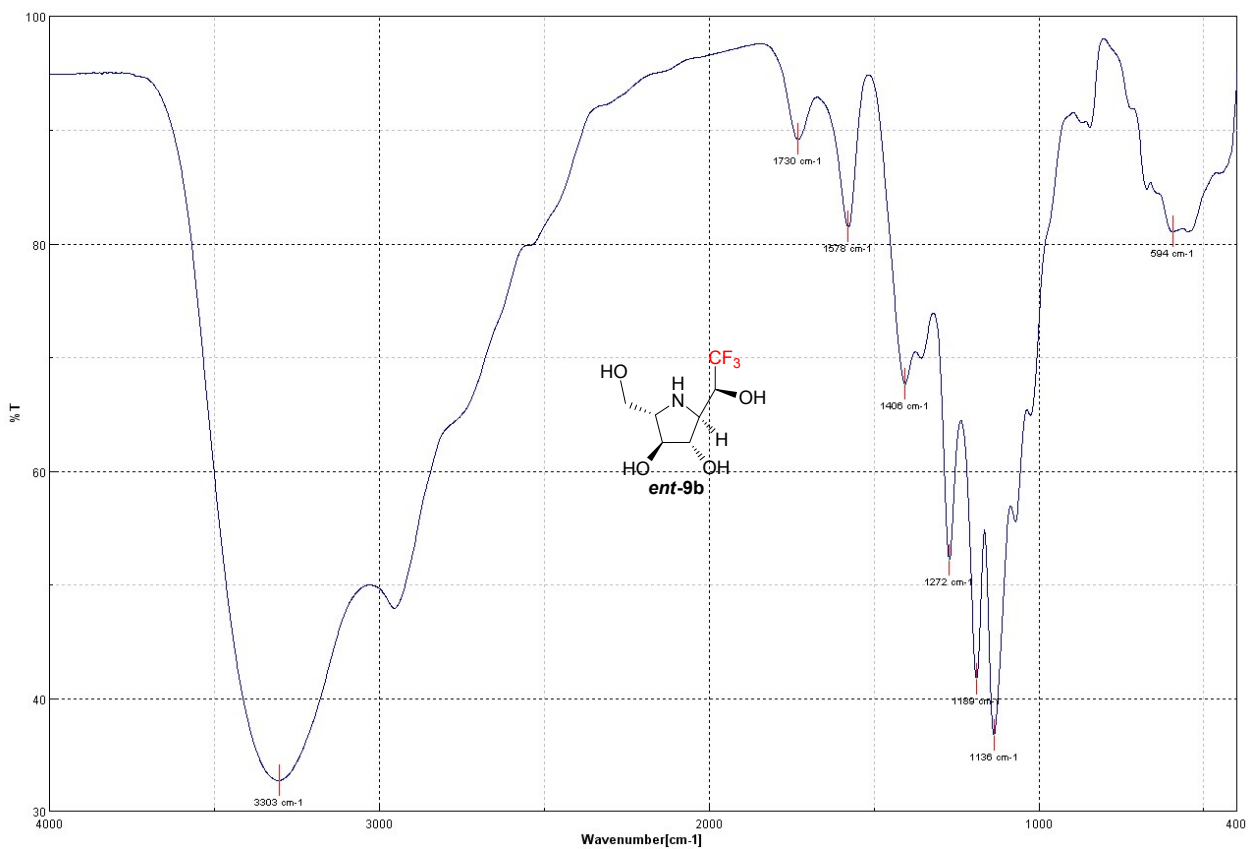
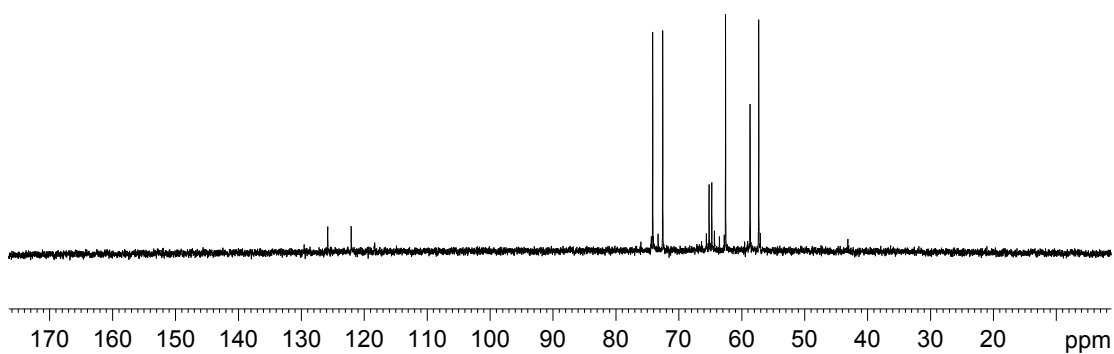
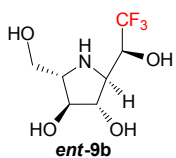


129.578
125.842
122.106
118.370

74.187
72.591
65.646
65.216
64.791
64.365
62.604
58.702
57.331

lyx-242b-C13

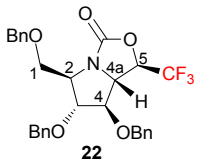
NAME lyx-2016
EXPNO 42
PROCNO 1



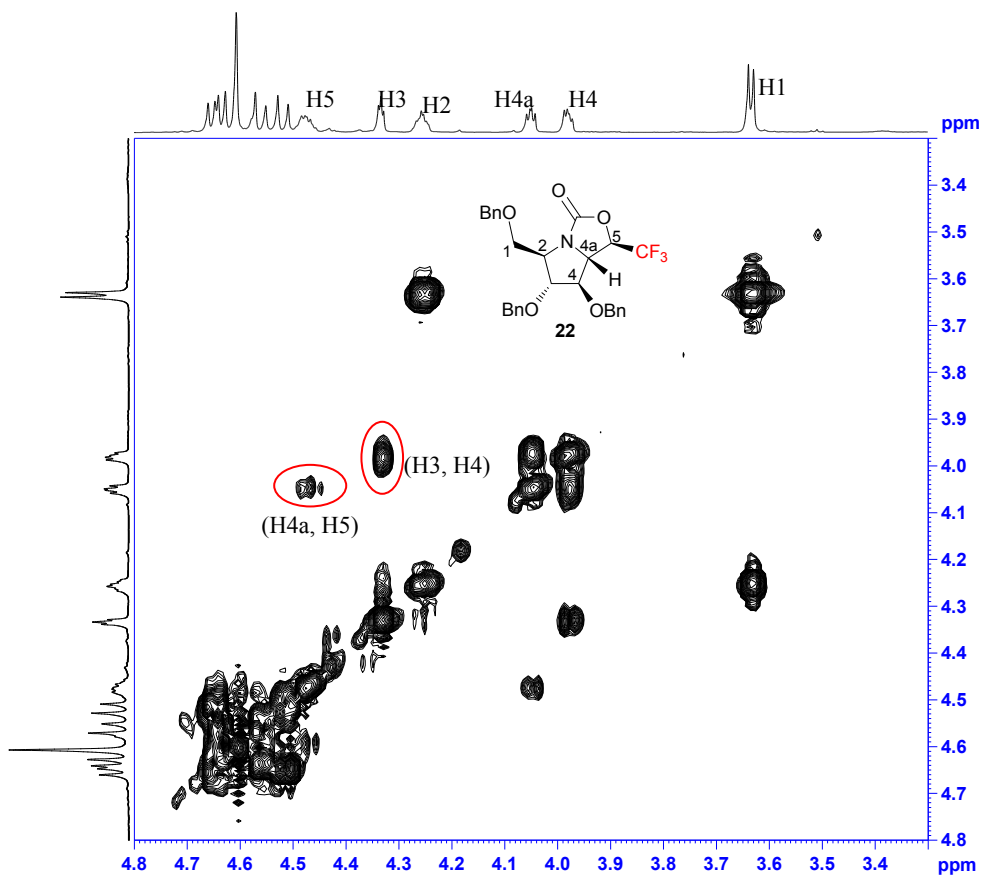
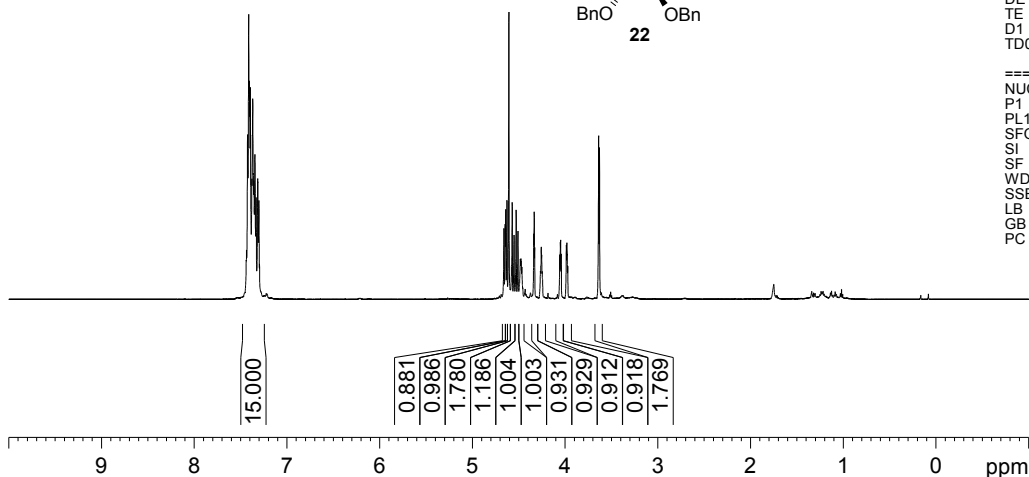
Compound 22:

7.426
7.414
7.410
7.407
7.401
7.396
7.379
7.374
7.370
7.364
7.358
7.347
7.334
7.317
7.315
7.304
4.660
4.648
4.641
4.628
4.607
4.571
4.551
4.529
4.509
4.339
4.334
4.329
4.258
4.254
4.059
4.052
4.049
4.043
3.987
3.982
3.978
3.639
3.630

NAME lyx-243b
EXPNO 117
PROCNO 1
Date_ 20150820
Time 21.51
INSTRUM spect
PROBHD 5 mm PATBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 15015.015 Hz
FIDRES 0.229111 Hz
AQ 2.1824322 sec
RG 57
DW 33.300 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
TD0 1



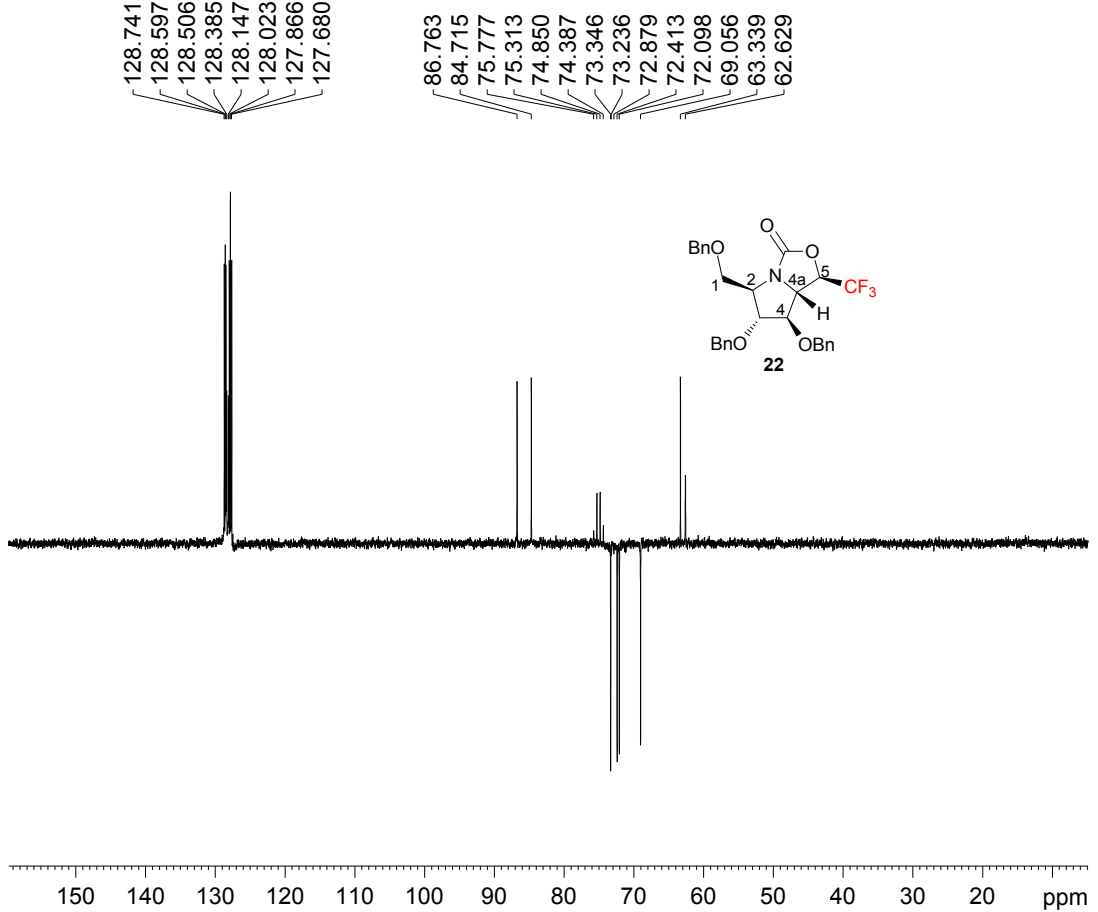
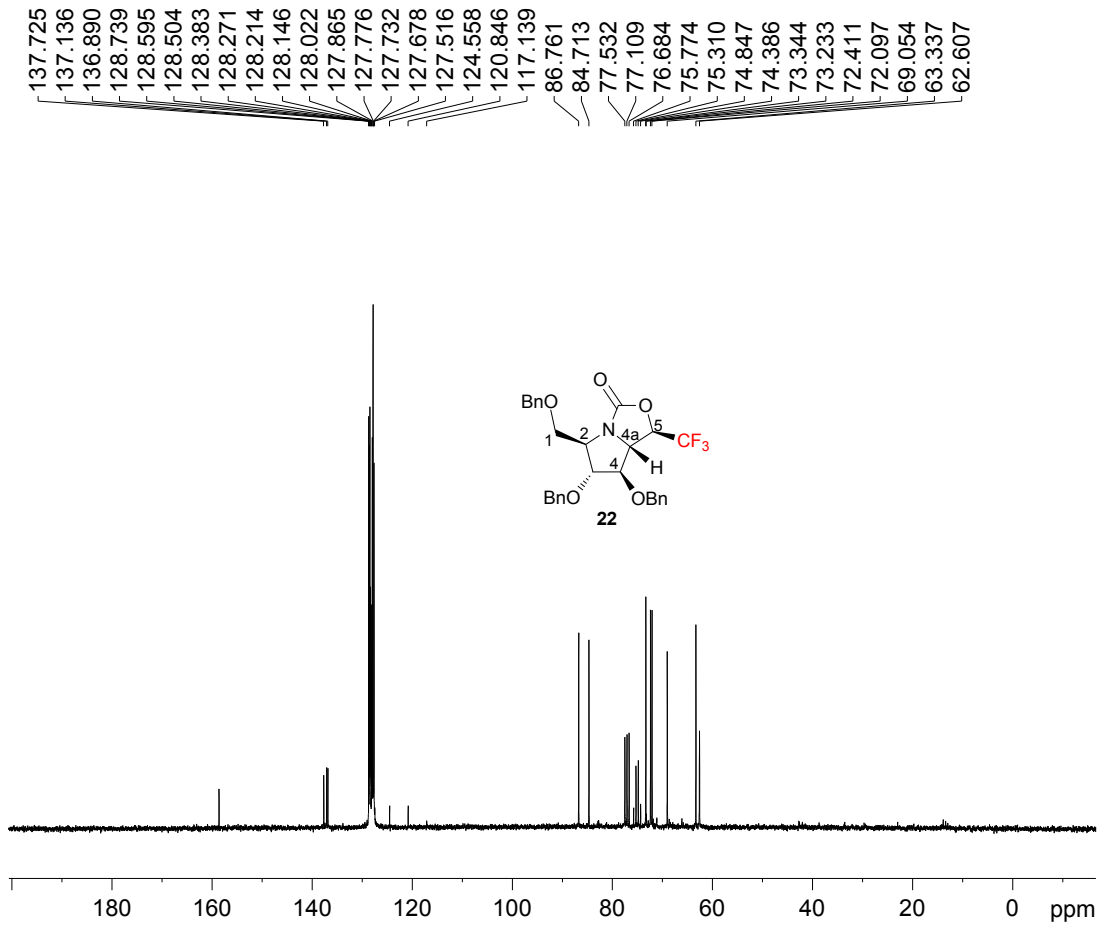
===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -0.60 dB
SFO1 600.1330006 MHz
SI 65536
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

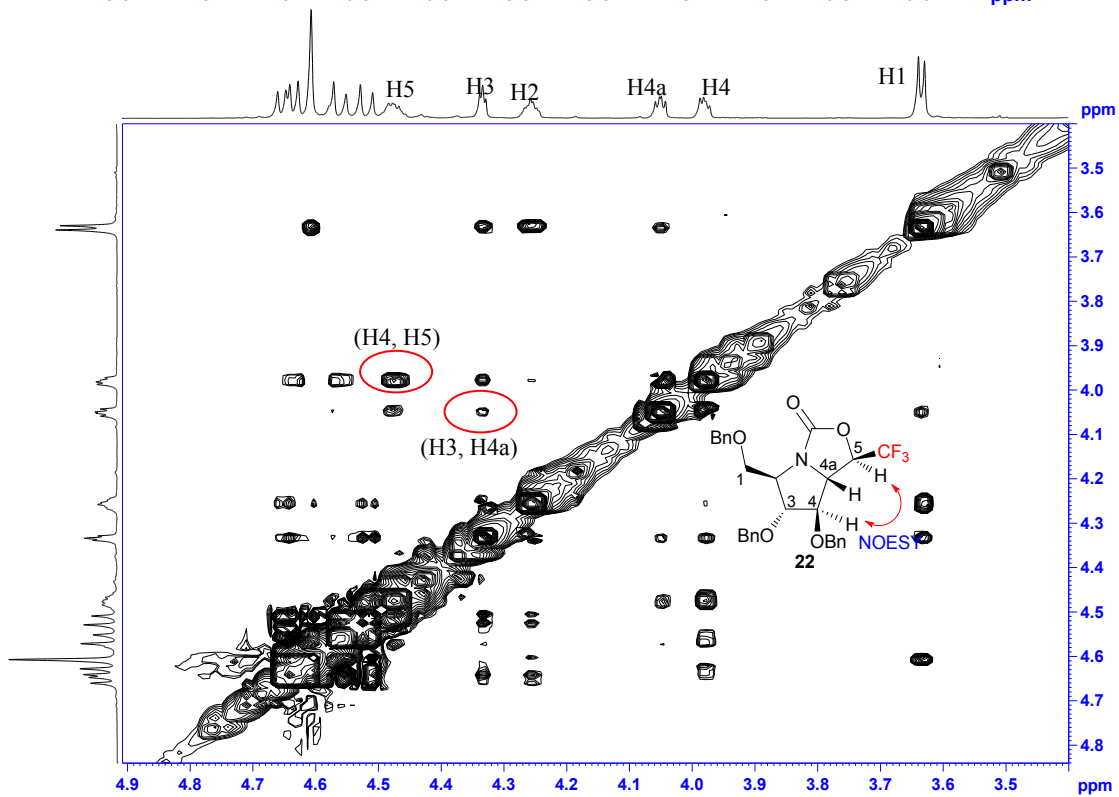
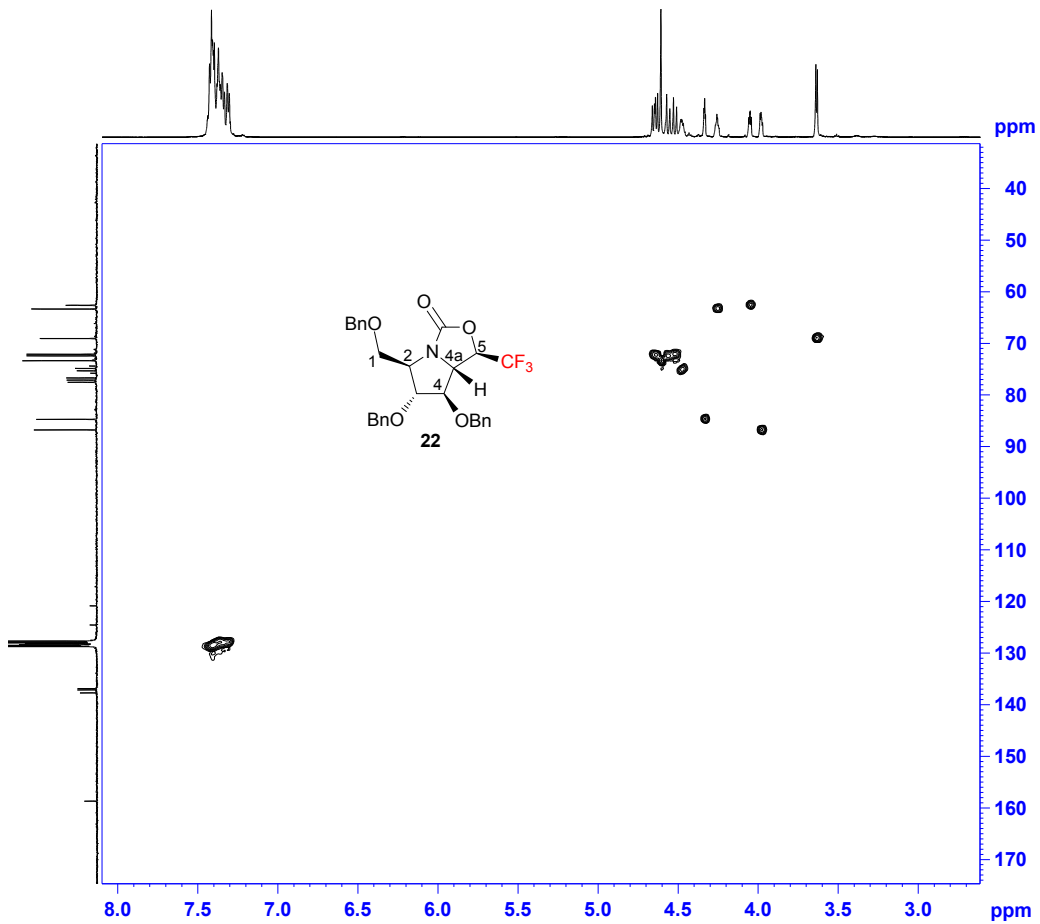


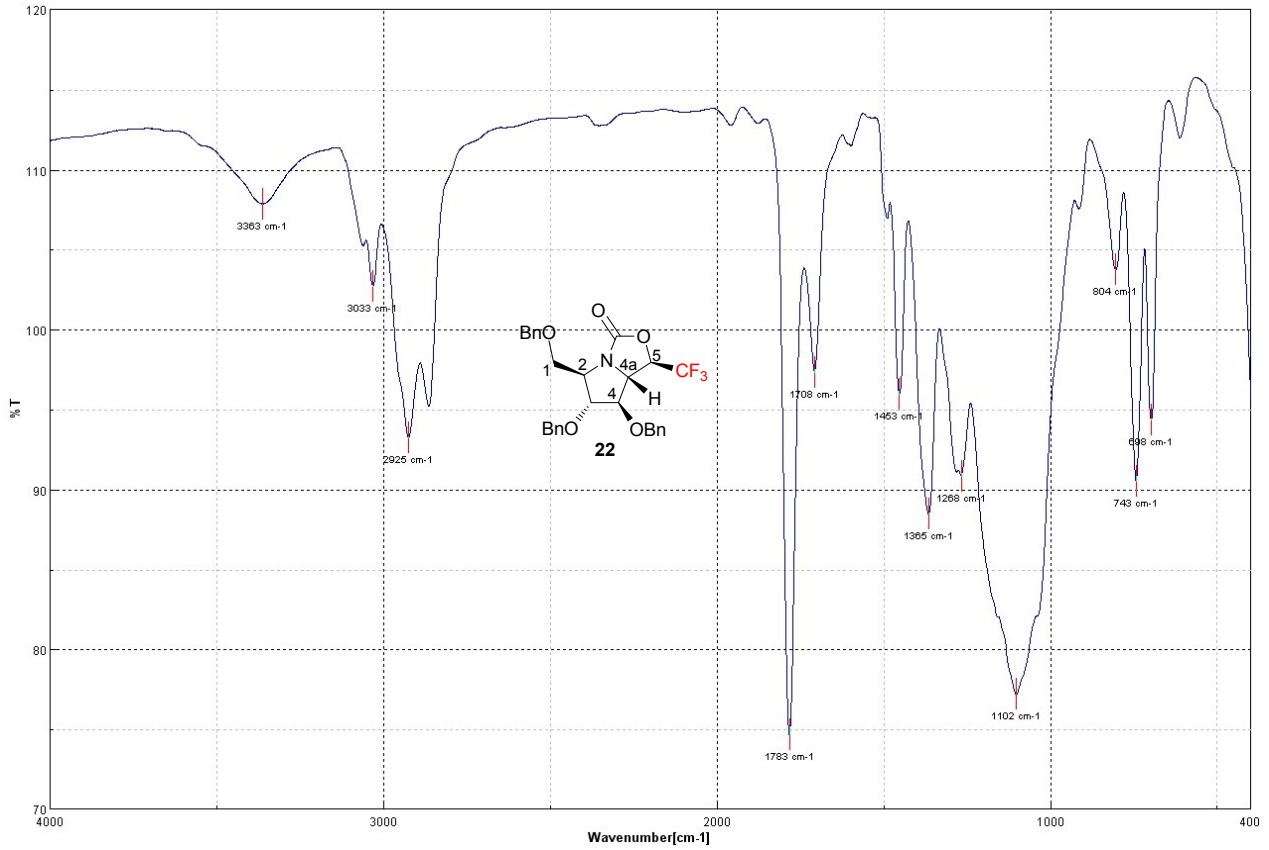
NAME lyx-243b
EXPNO 118
PROCNO 1
Date_ 20150820
Time 21.53
INSTRUM spect
PROBHD 5 mm PATBO BB-
PULPROG cosyppgf
TD 2048
SOLVENT CDCl3
NS 16
DS 8
SWH 6009.615 Hz
FIDRES 2.934382 Hz
AQ 0.1705268 sec
RG 35.9
DW 83.200 usec
DE 6.50 usec
TE 298.1 K
D0 0.00000300 sec
D1 1.48689198 sec
D13 0.00000400 sec
D16 0.00020000 sec
IND 0.00016640 sec

===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -0.60 dB
SFO1 600.1327006 MHz

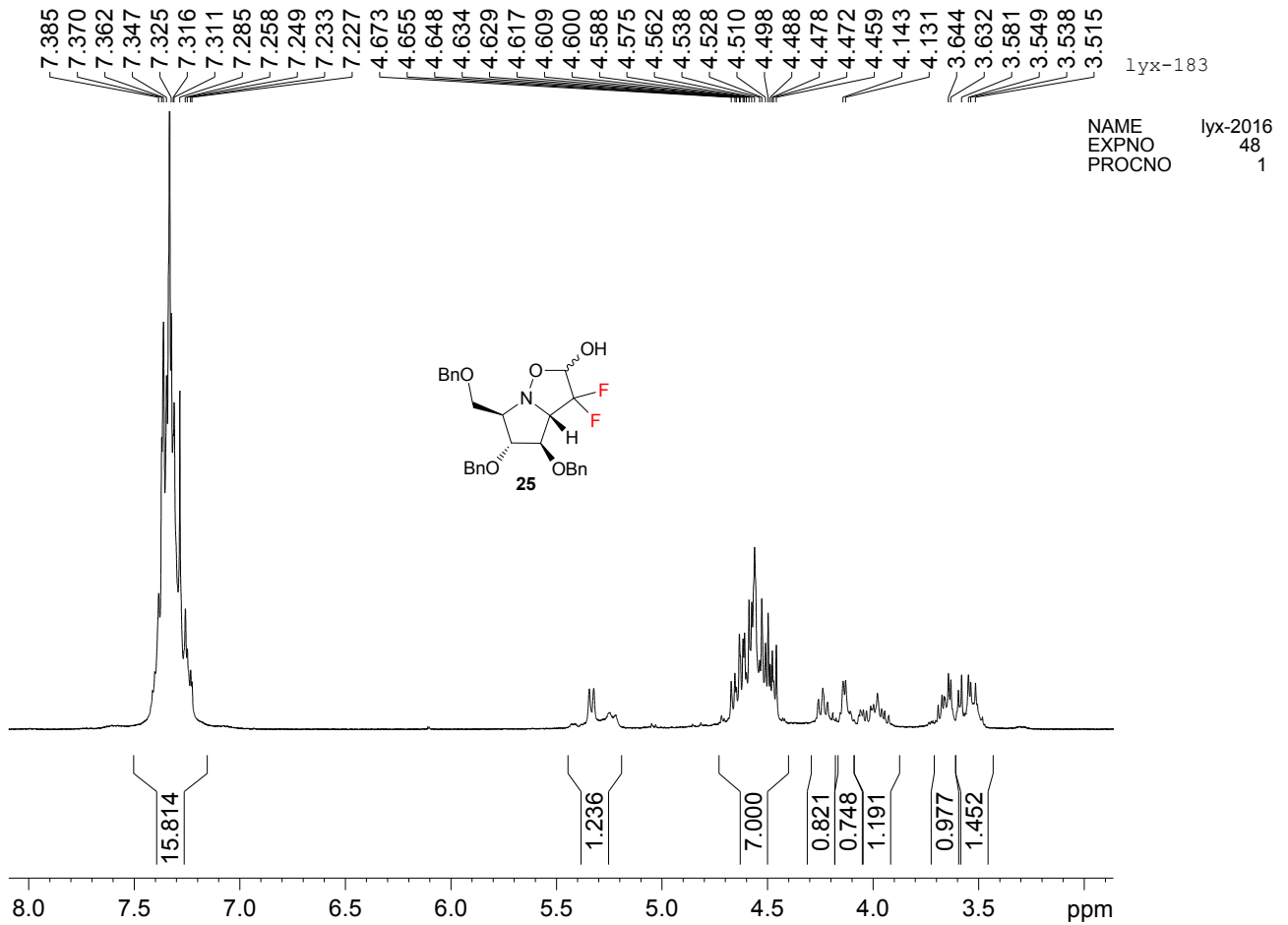
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec
NDO 1
TD 256
SFO1 600.1327 MHz
FIDRES 23.475035 Hz
SW 10.014 ppm
FMODE QF
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 QF
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0





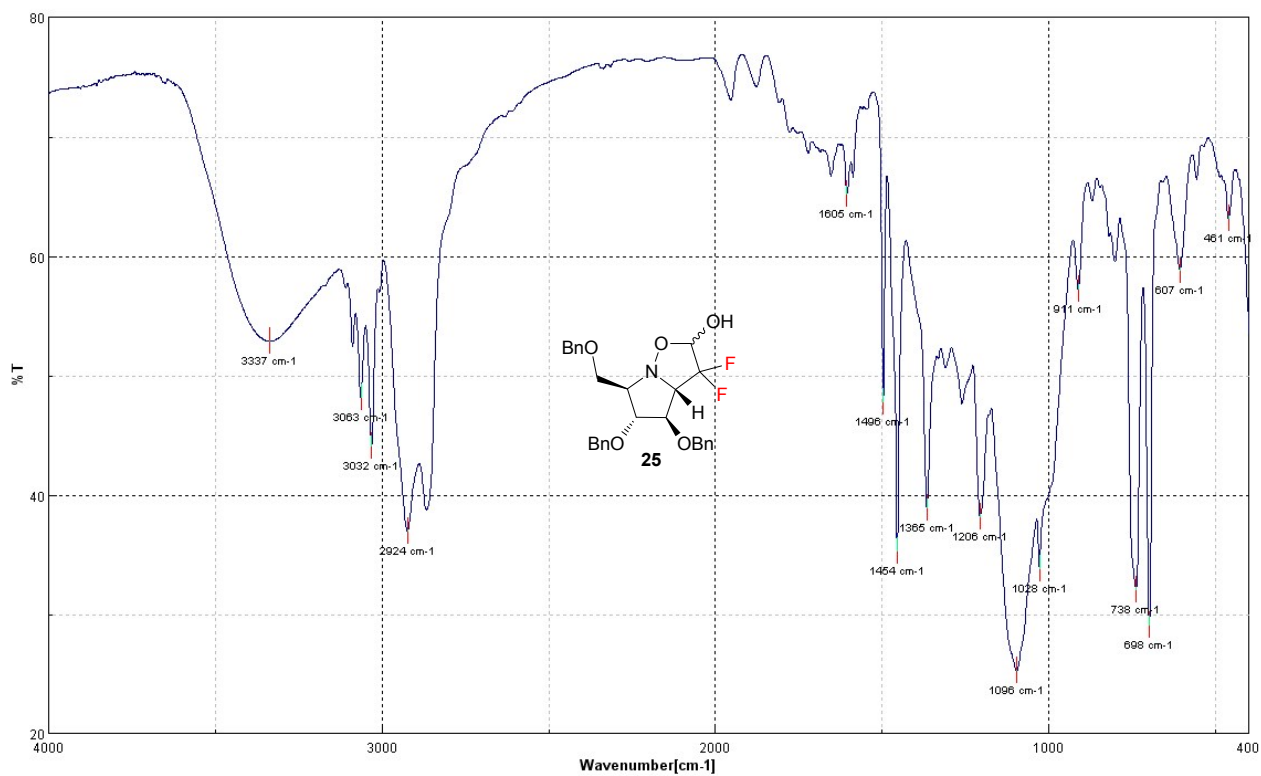
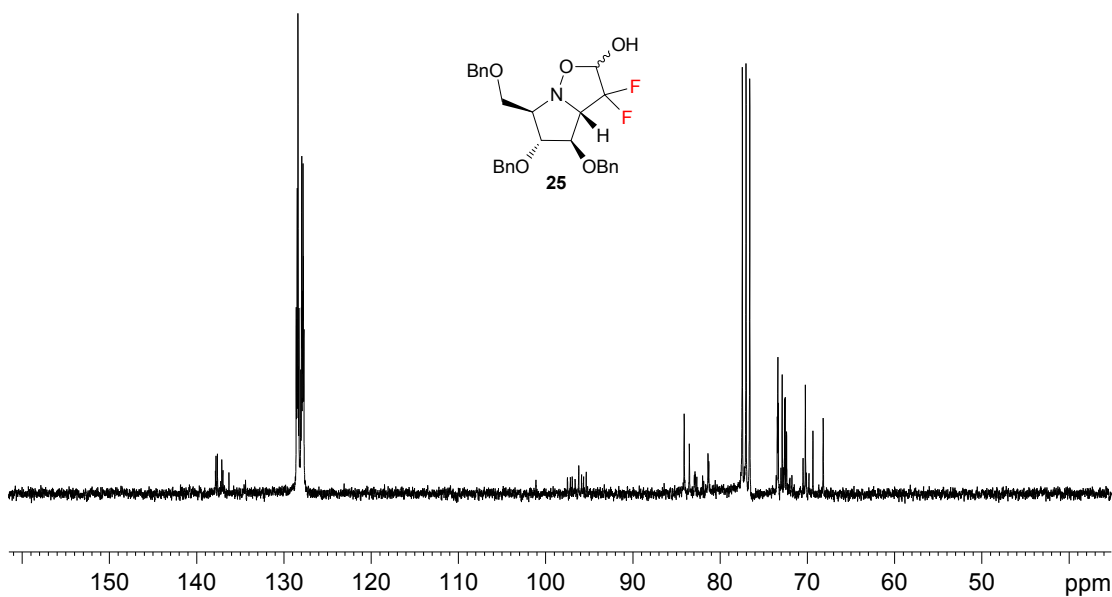


Compound 25:



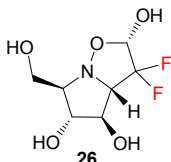
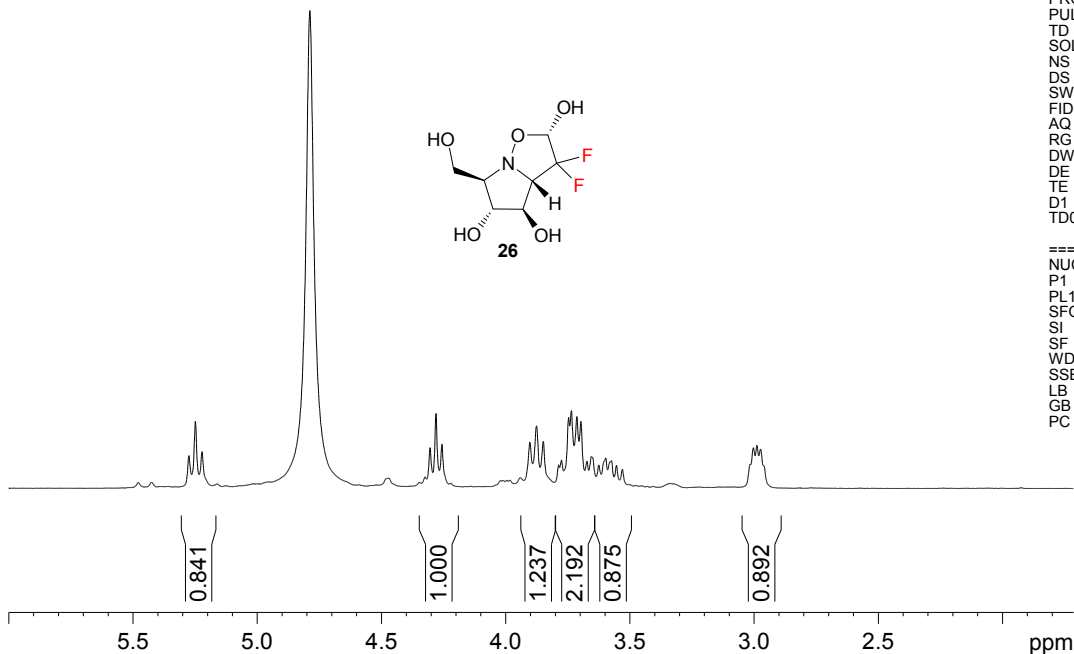
137.871
 137.809
 137.647
 137.141
 137.013
 128.608
 128.566
 128.497
 128.409
 128.358
 128.293
 128.085
 128.015
 127.977
 127.885
 127.831
 127.790
 127.727
 96.219
 84.130
 83.546
 81.399
 81.319
 77.463
 77.040
 76.617
 73.451
 73.396
 73.340
 73.036
 72.895
 72.738
 72.624
 72.549
 72.390
 70.502
 70.239
 69.371
 68.192

lyx-183-C13
 NAME lyx-2016
 EXPNO 49
 PROCNO 1



Compound 26:

5.275
5.249
5.222
4.788
4.304
4.280
4.256
3.903
3.876
3.849
3.787
3.775
3.747
3.735
3.713
3.697
3.673
3.655
3.625
3.597
3.574
3.554
3.530
3.016
3.003
2.989
2.974



NAME lyx4-193
EXPNO 10
PROCNO 1
Date_ 20101009
Time_ 15.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT D2O
NS 1
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 64
DW 55.600 usec
DE 8.00 usec
TE 300.3 K
D1 1.00000000 sec
TD0 1

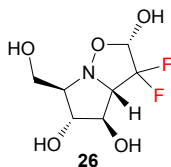
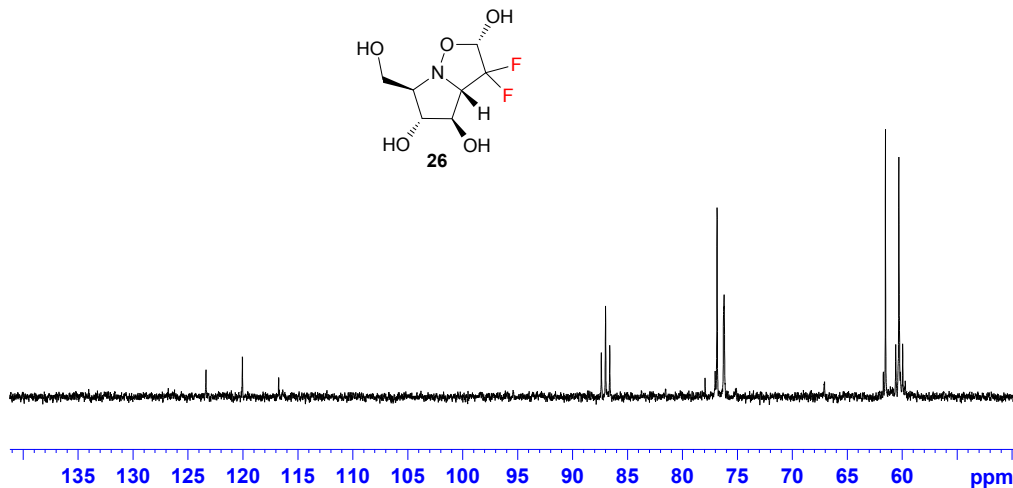
===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.1324010 MHz
SI 32768
SF 300.1299692 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

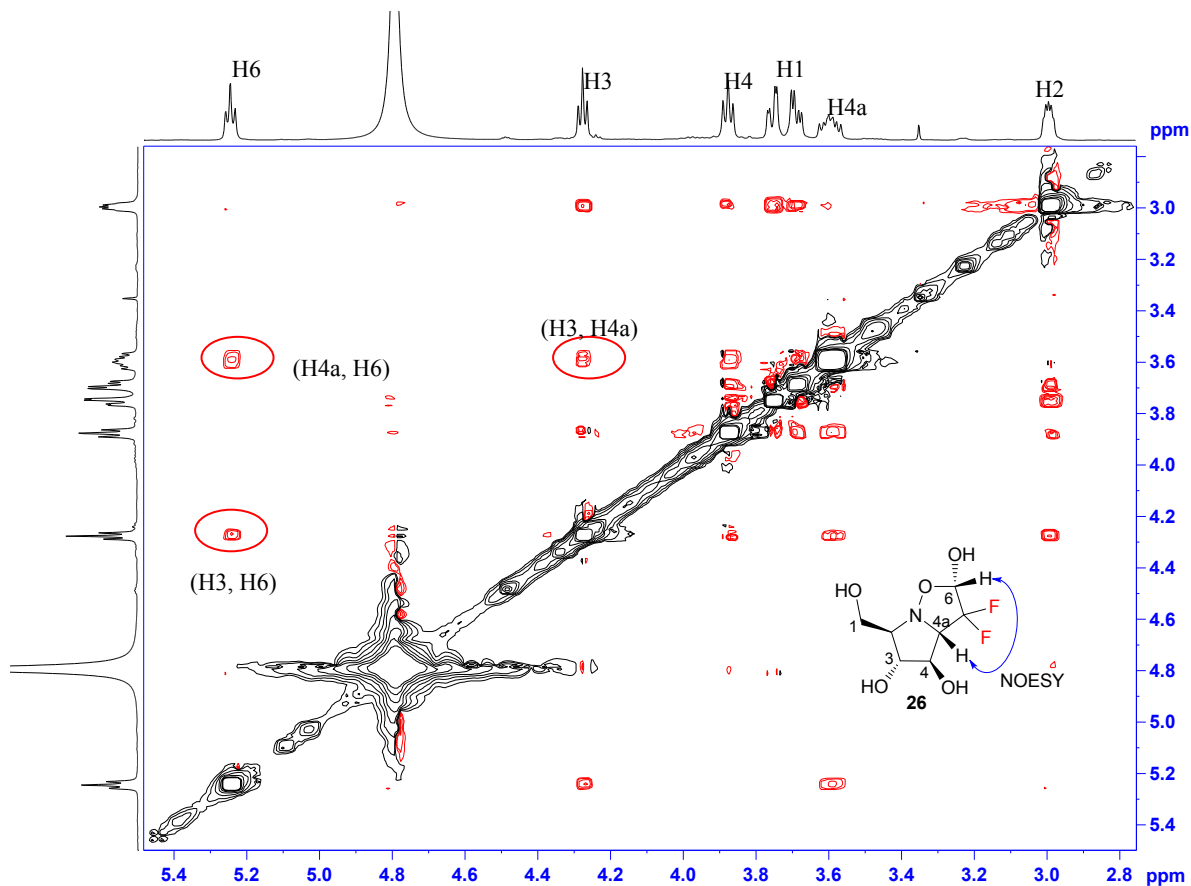
123.37
120.07
116.77
87.40
86.03
86.03
76.84
76.21
61.71
61.51
60.58
60.30
59.95
59.71

NAME lyx4-193
EXPNO 11
PROCNO 1
Date_ 20101009
Time_ 15.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 156
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 14596.5
DW 27.800 usec
DE 8.00 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

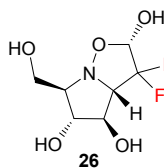
===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





2#



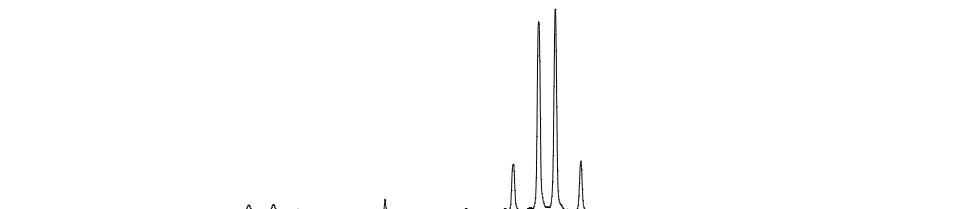
```

Current Data Parameters
NAME          19F
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20110128
Time          8.19
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zgflgn
TD           32768
SOLVENT      CDC13
NS           16
DS           0
SWH          75187.969 Hz
FIDRES       2.294555 Hz
AQ           0.2179572 sec
RG           32
DW           6.650 usec
DE           6.00 usec
TE           673.2 K
D1           1.00000000 sec

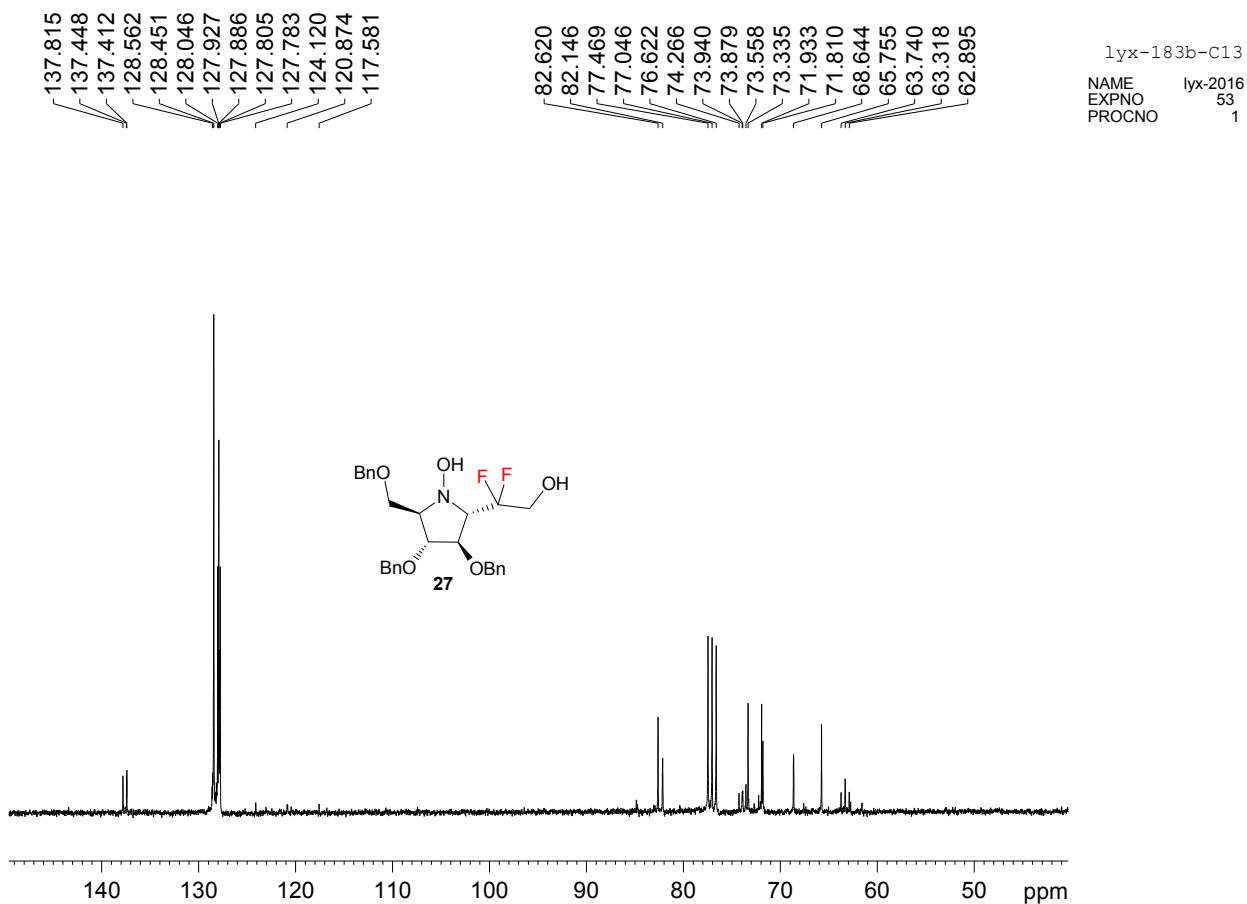
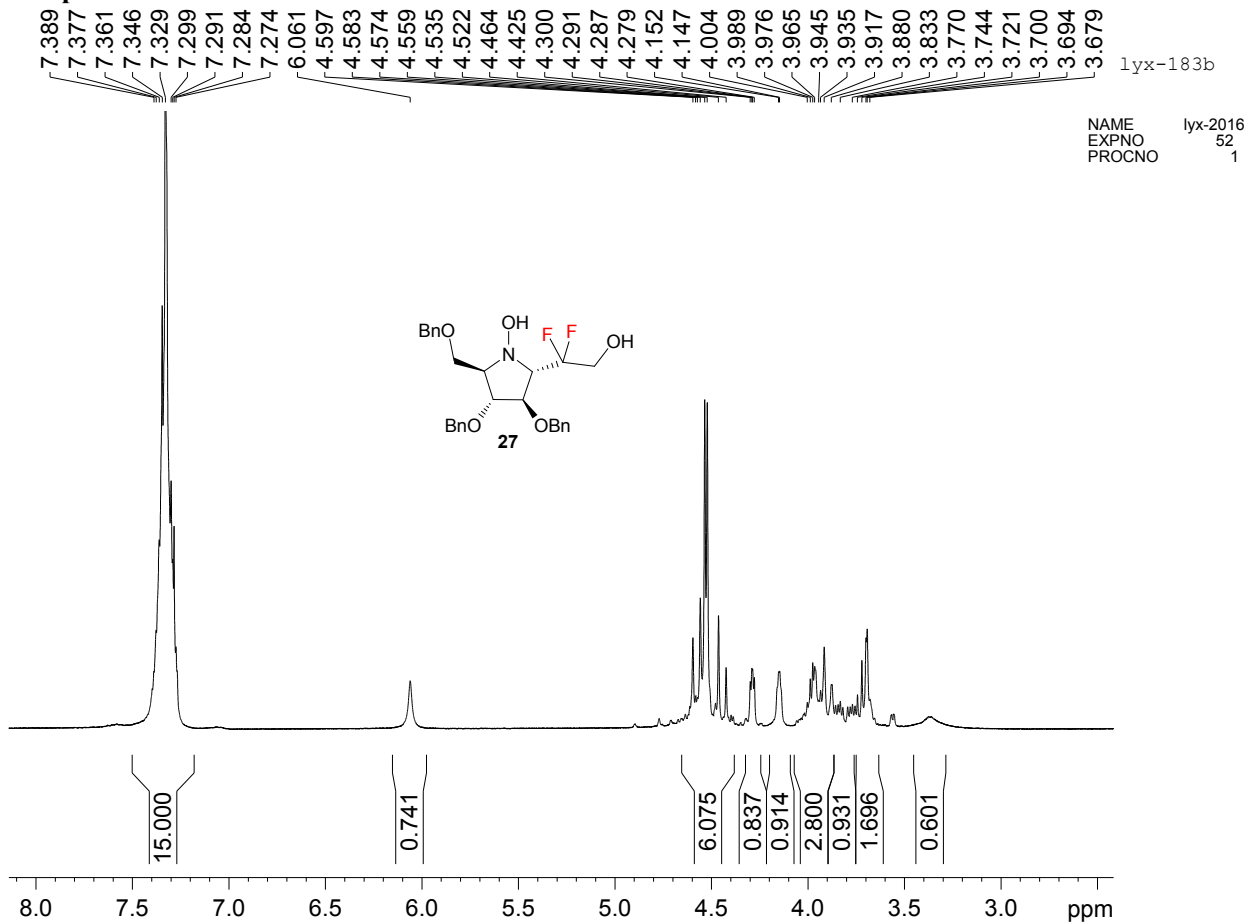
===== CHANNEL f1 =====
NUC1          19F
P1            12.50 usec
PL1           0.00 dB
SFO1          376.4418792 MHz

F2 - Processing parameters
SI            65536
SF            376.4983540 MHz
WDW           EM
SSB           0
LB            5.00 Hz
GB            0
PC            0.10
  
```



-114 -116 -118 -120 -122 -124 -126 -128 -130 -132 -134 -136 ppm

Compound 27:

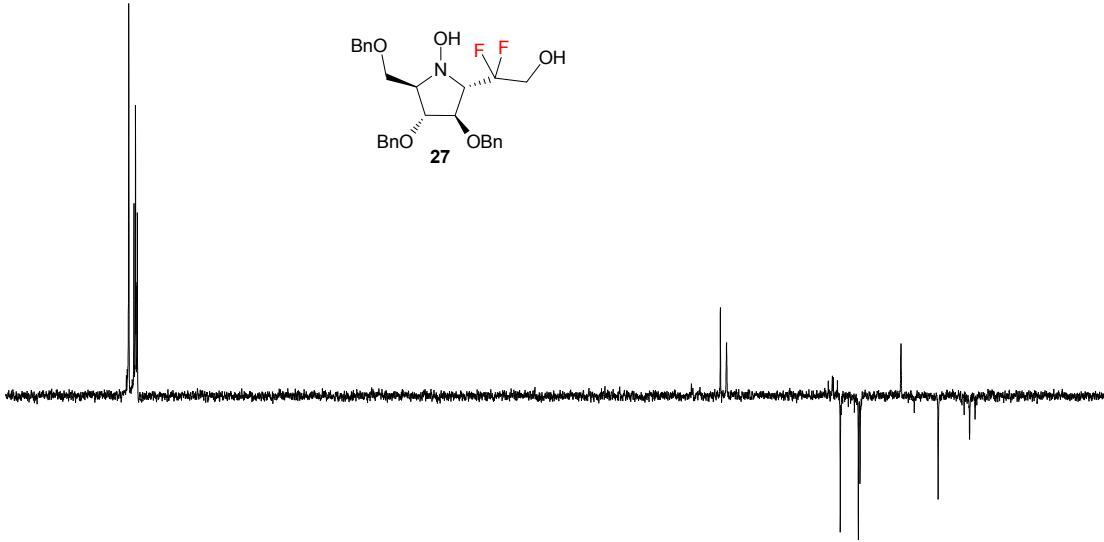


128.452
128.049
127.929
127.888
127.808
127.784

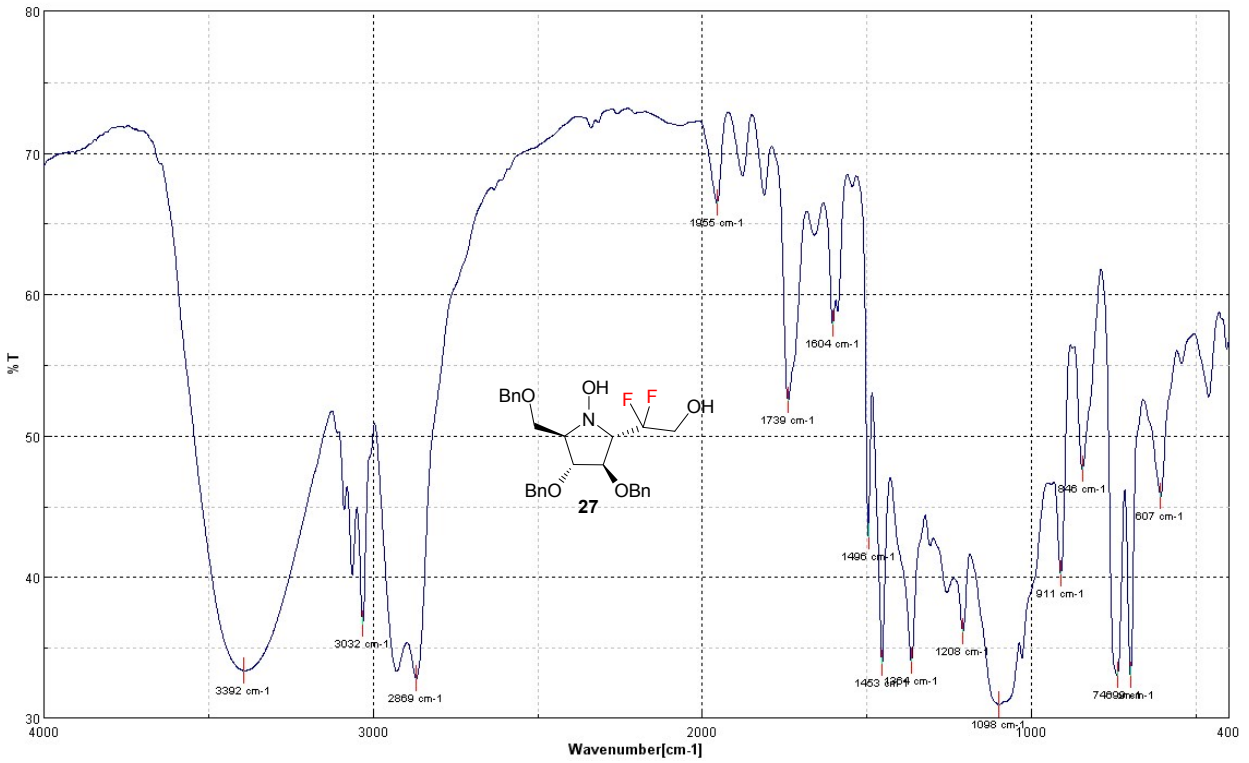
82.621
82.145
74.265
73.944
73.879
73.335
71.934
71.811
68.631
65.755
63.740
63.320
62.897

x-183b-dept1

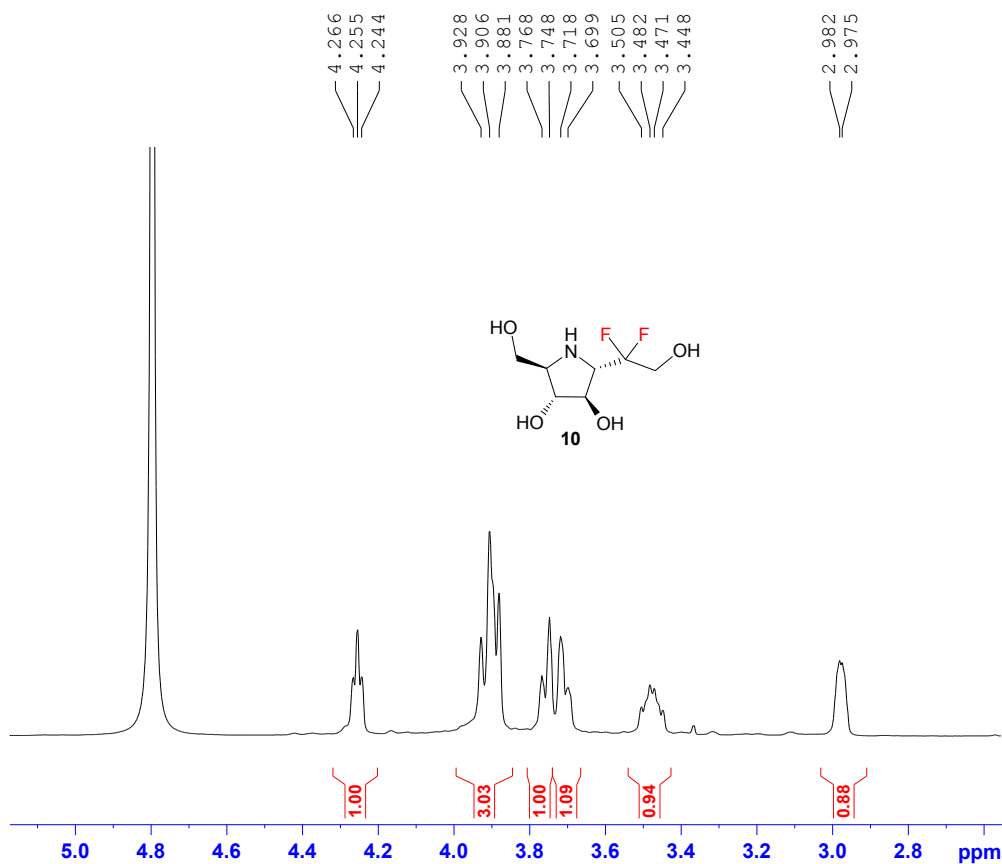
NAME lyx-2016
EXPNO 54
PROCNO 1



135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 ppm



Compound 10:

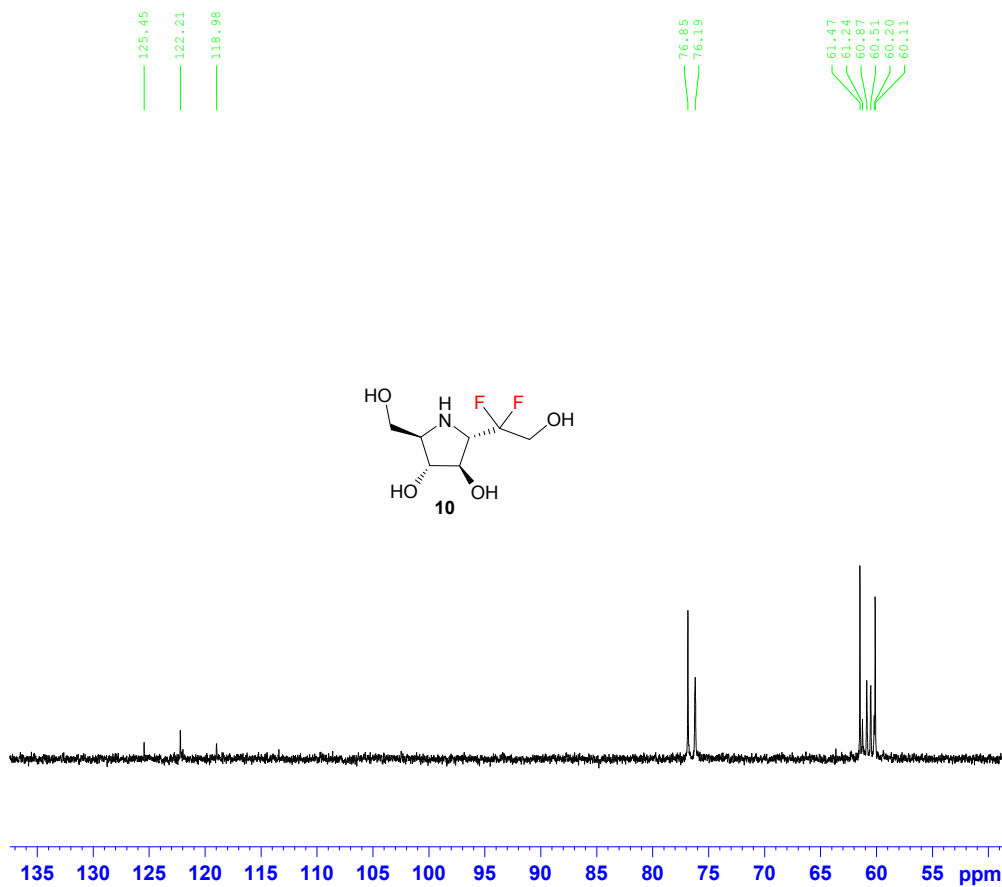


Current Data Parameters
 NAME lyx-noe
 EXPNO 50
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110114
 Time_ 9.17
 INSTRUM spect
 PROBHD 5 mm BBI 1H-BB
 PULPROG zg30
 TD 32768
 SOLVENT D2O
 NS 8
 DS 0
 SWH 17985.611 Hz
 FIDRES 0.548877 Hz
 AQ 0.9110004 sec
 RG 90.5
 DW 27.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.80 usec
 PL1 2.00 dB
 PL1W 15.84893227 W
 SFO1 600.1330006 MHz

F2 - Processing parameters
 SI 16384
 SF 600.1300000 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



NAME lyx4-193b
 EXPNO 11
 PROCNO 1
 Date_ 20101027
 Time_ 17.09
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 40
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 13004
 DW 27.800 usec
 DE 8.00 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

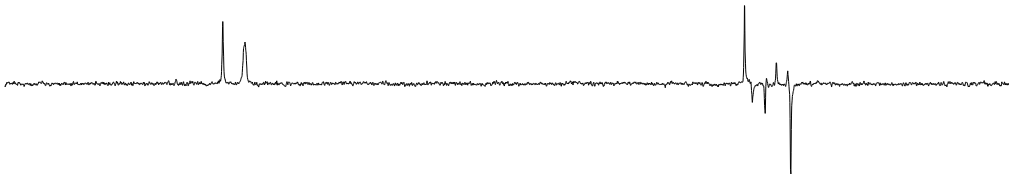
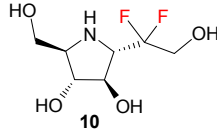
===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 usec
 PL1 2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 3.00 dB
 PL12 22.33 dB
 PL13 23.00 dB
 SFO2 300.1312005 MHz
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

76.85
76.20

61.48
61.25
60.87
60.54
60.20
60.11

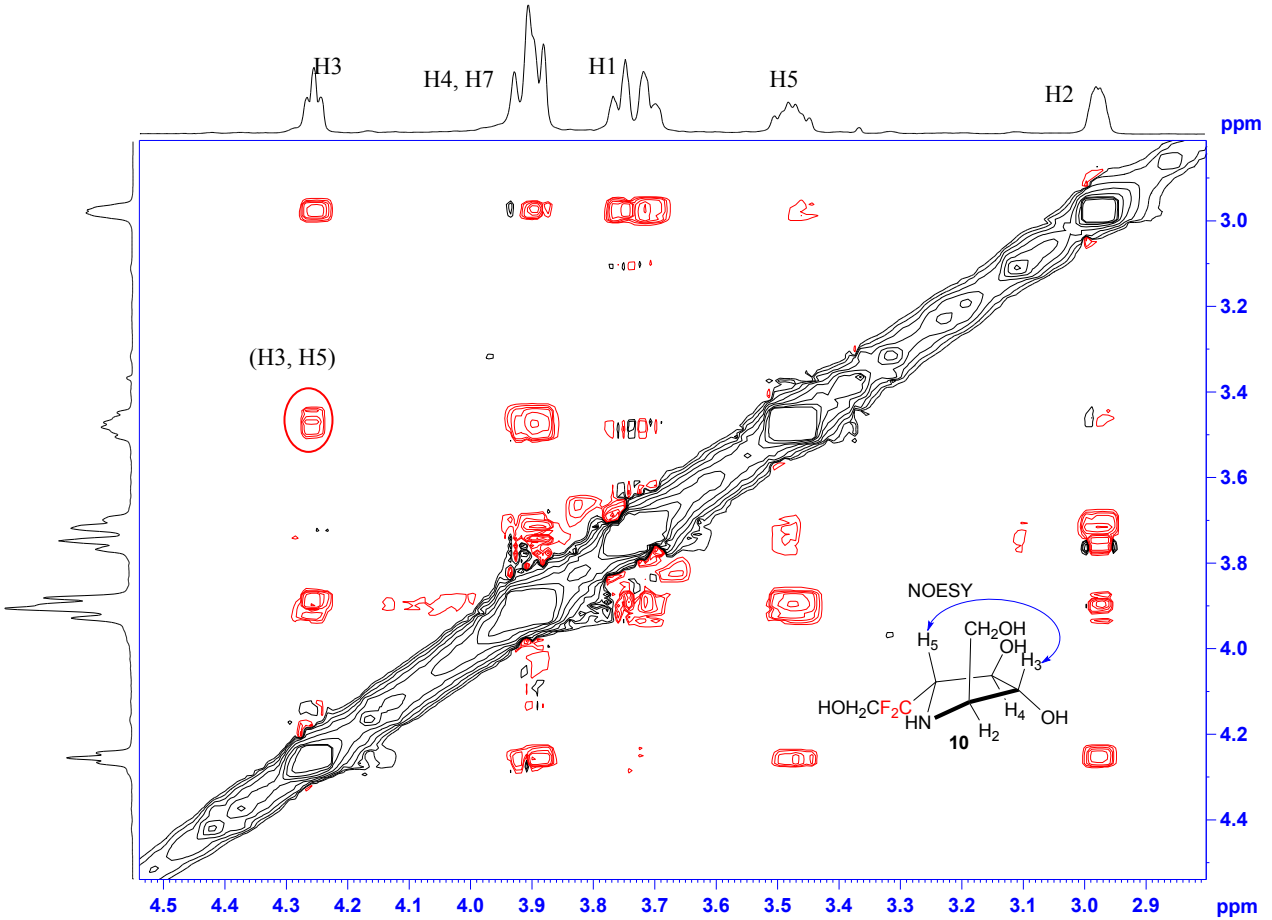
NAME lyx4-193b
EXPNO 12
PROCNO 1
Date_ 20101027
Time_ 17.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT D2O
NS 17
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 298.5 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1



===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
P2 25.00 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.80 usec
P4 21.60 usec
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
RDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

82 80 78 76 74 72 70 68 66 64 62 60 58 56 ppm



10#

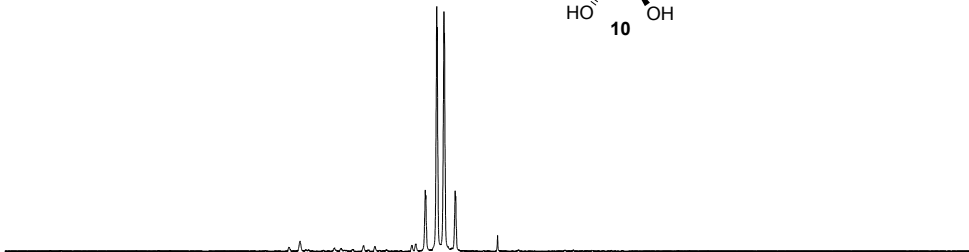
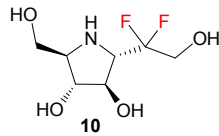
-118.22
-118.25
-118.88
-118.91
-119.31
-119.34
-119.98
-120.01

Current Data Parameters
NAME 19F
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110128
Time_ 8.29
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgflgn
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 75187.969 Hz
FIDRES 2.294555 Hz
AQ 0.2179572 sec
RG 32
DW 6.650 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 19F
P1 12.50 usec
PL1 0.00 dB
SF01 376.4418792 MHz

F2 - Processing parameters
SI 65536
SF 376.4983540 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 0.10

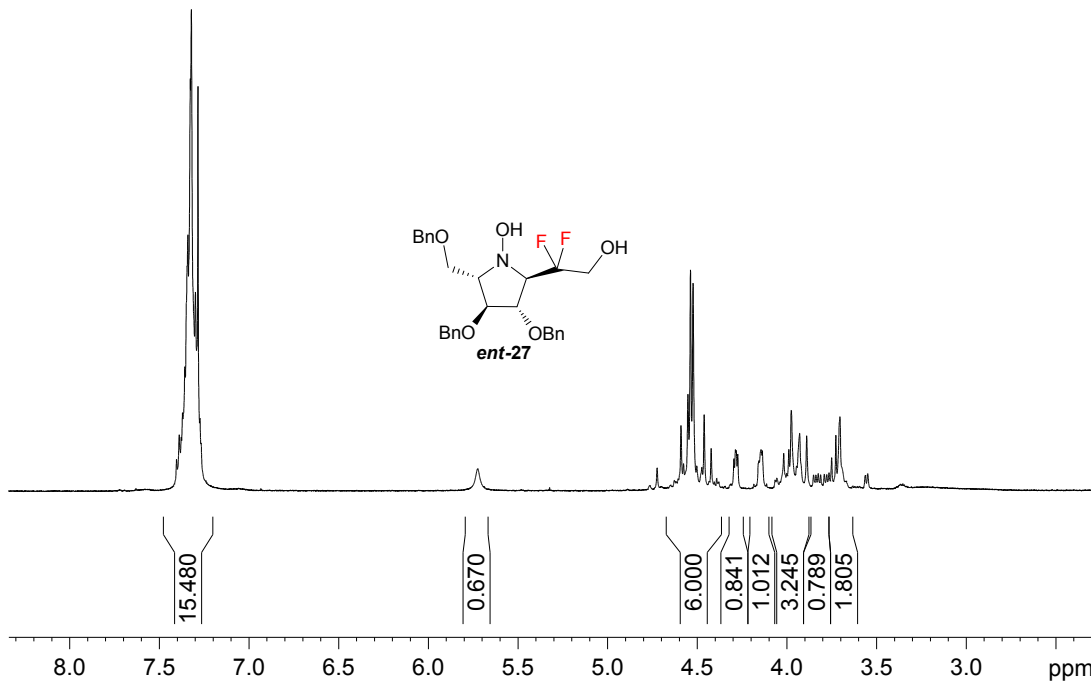
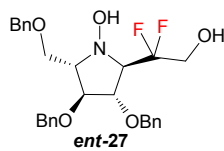


-95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 ppm

Compound ent-27:

7.388
7.377
7.370
7.357
7.340
7.327
7.321
7.298
7.284
7.273
7.266
5.725
4.591
4.552
4.538
4.524
4.462
4.423
4.296
4.287
4.283
4.274
4.157
4.145
4.137
4.018
3.990
3.976
3.946
3.929
3.890
3.825
3.812
3.792
3.778
3.766
3.751
3.727
3.704 lyx-197

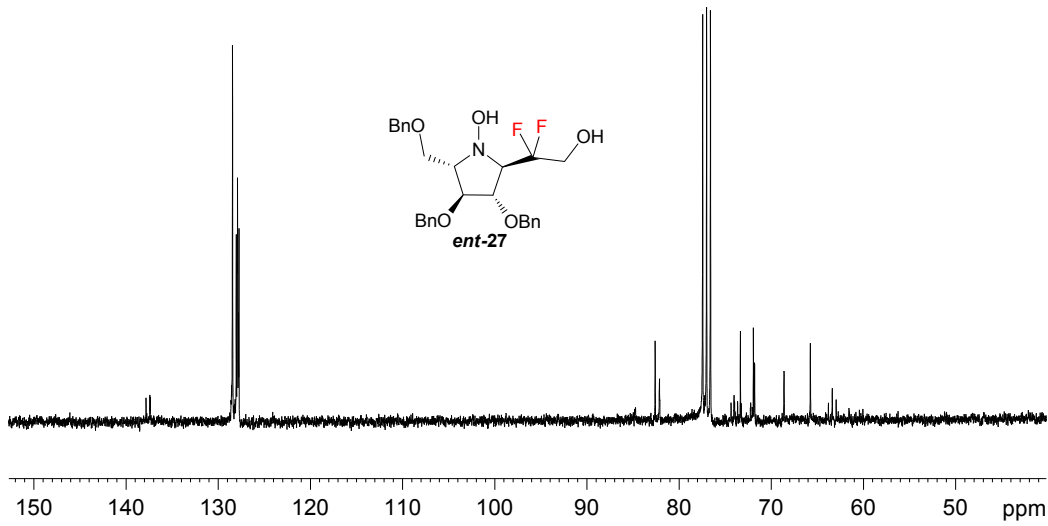
NAME lyx-2016
EXPNO 50
PROCNO 1



137.838
137.417
137.378
128.449
128.041
127.911
127.800
127.753

82.606
82.135
77.451
77.028
76.605
74.376
74.051
73.663
73.357
71.948
71.820
68.627
65.764
63.808
63.386
62.963

lyx-197-C13
NAME lyx-2016
EXPNO 51
PROCNO 1

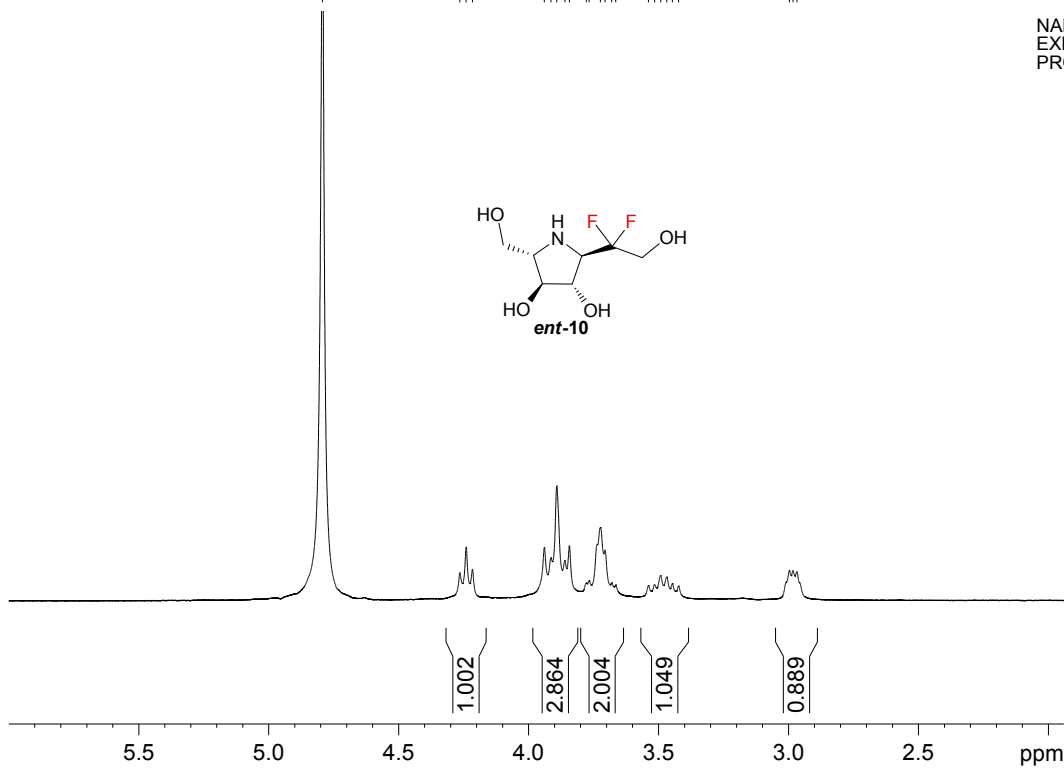


Compound *ent-10*:

4.794
4.265
4.240
4.216
3.940
3.914
3.892
3.861
3.843
3.778
3.767
3.724
3.706
3.680
3.665
3.539
3.515
3.492
3.468
3.447
3.423
2.997
2.983
2.968

lyx-169

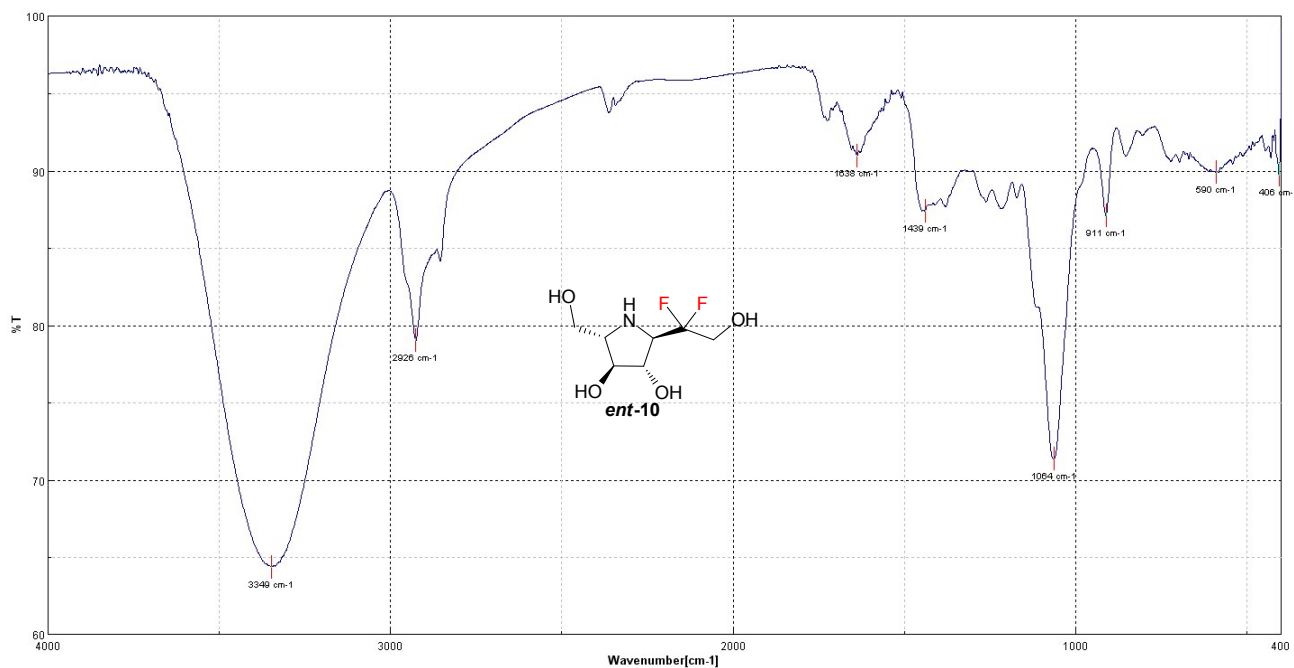
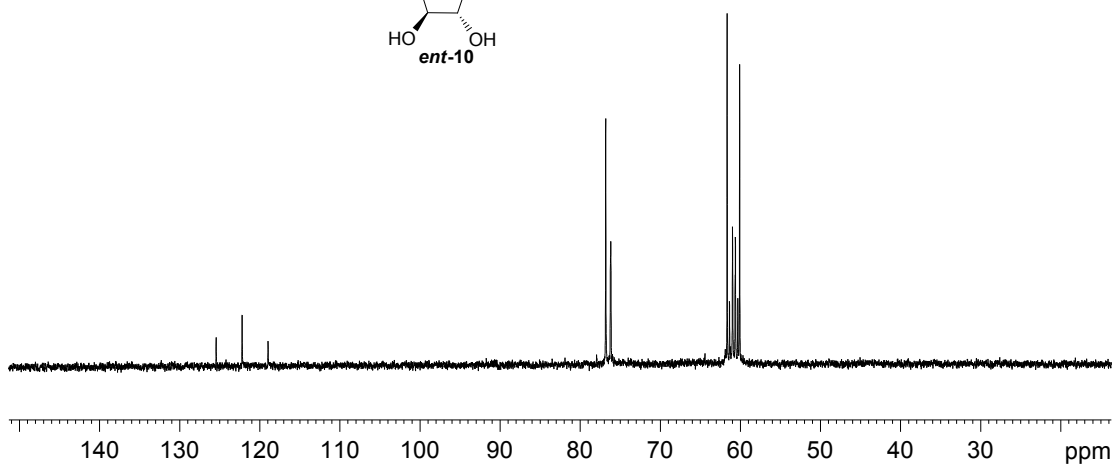
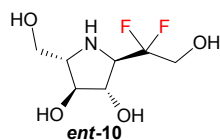
NAME lyx-2016
EXPNO 41
PROCNO 1



125.473
122.234
118.993

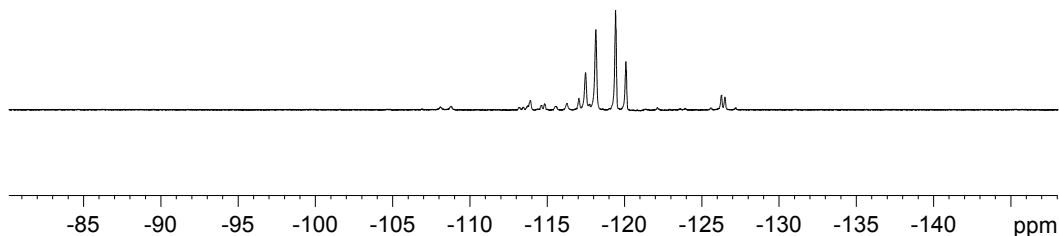
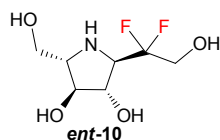
76.833
76.203
61.670
61.375
60.998
60.633
60.336
60.108

lyx-169-C13
NAME lyx-2016
EXPNO 43
PROCNO 1

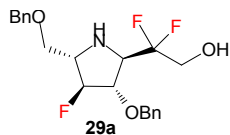
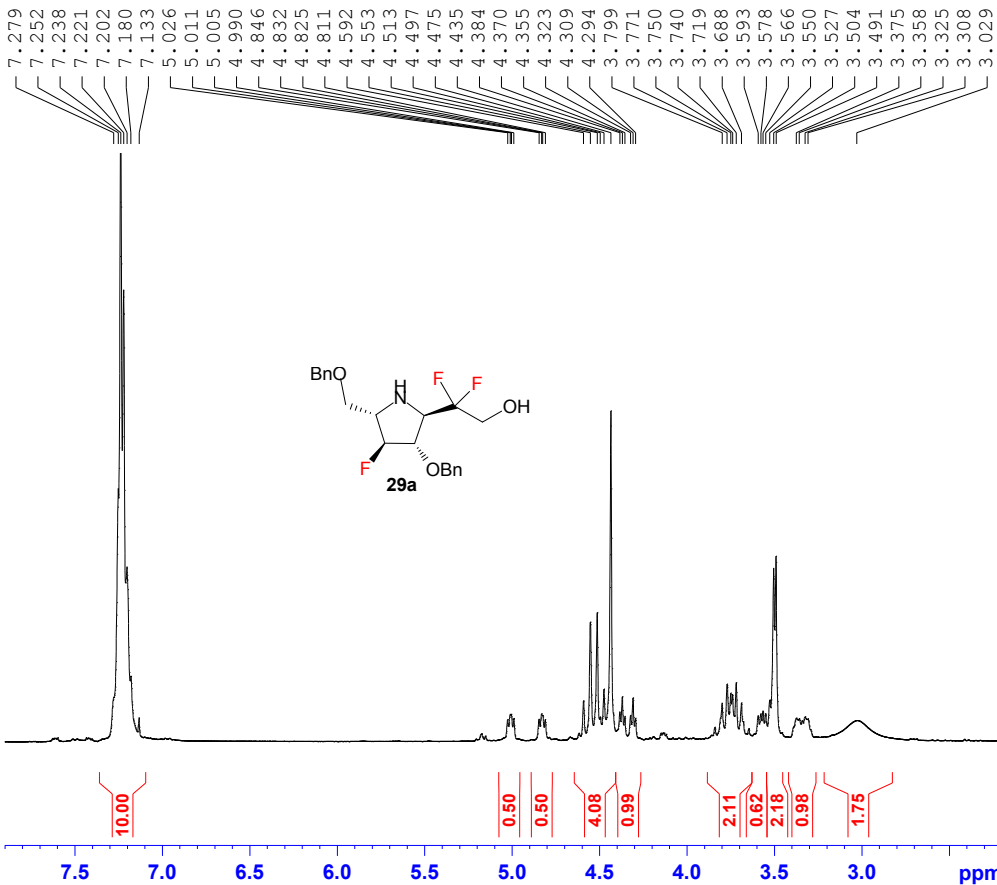


-117.471
 -118.134
 -119.413
 -119.445
 -120.079
 -120.112

NAME
 EXPNO 19F
 PROCNO 30128
 1

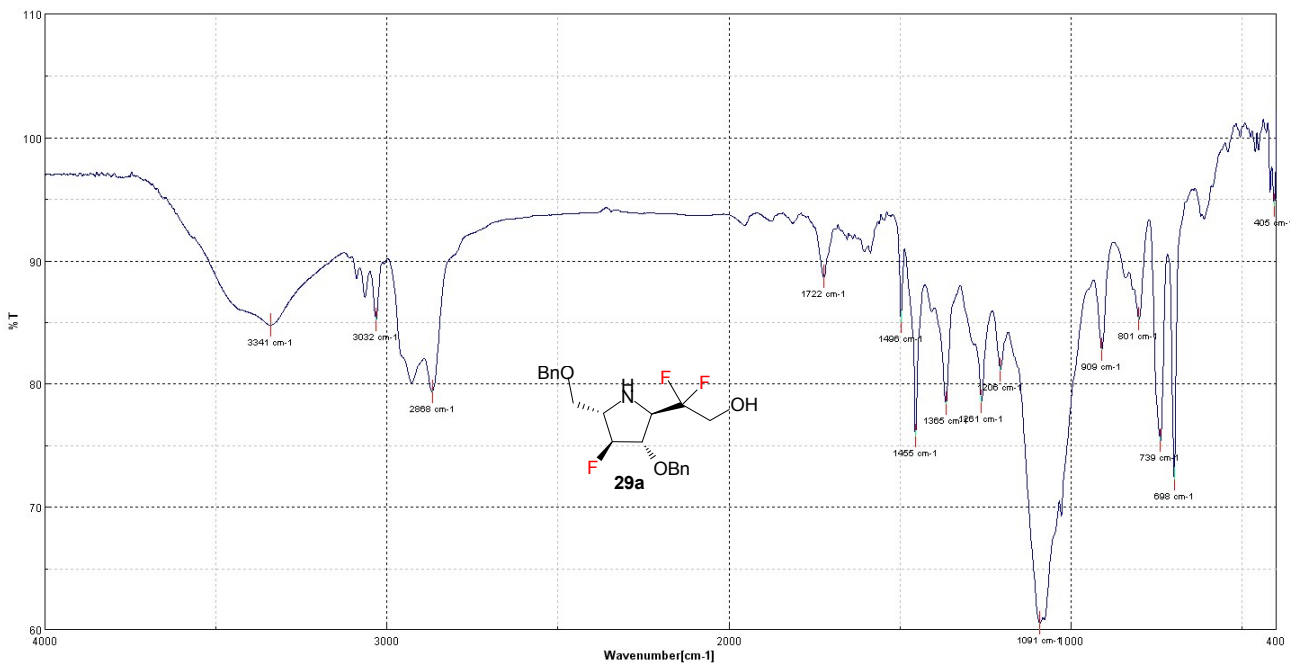
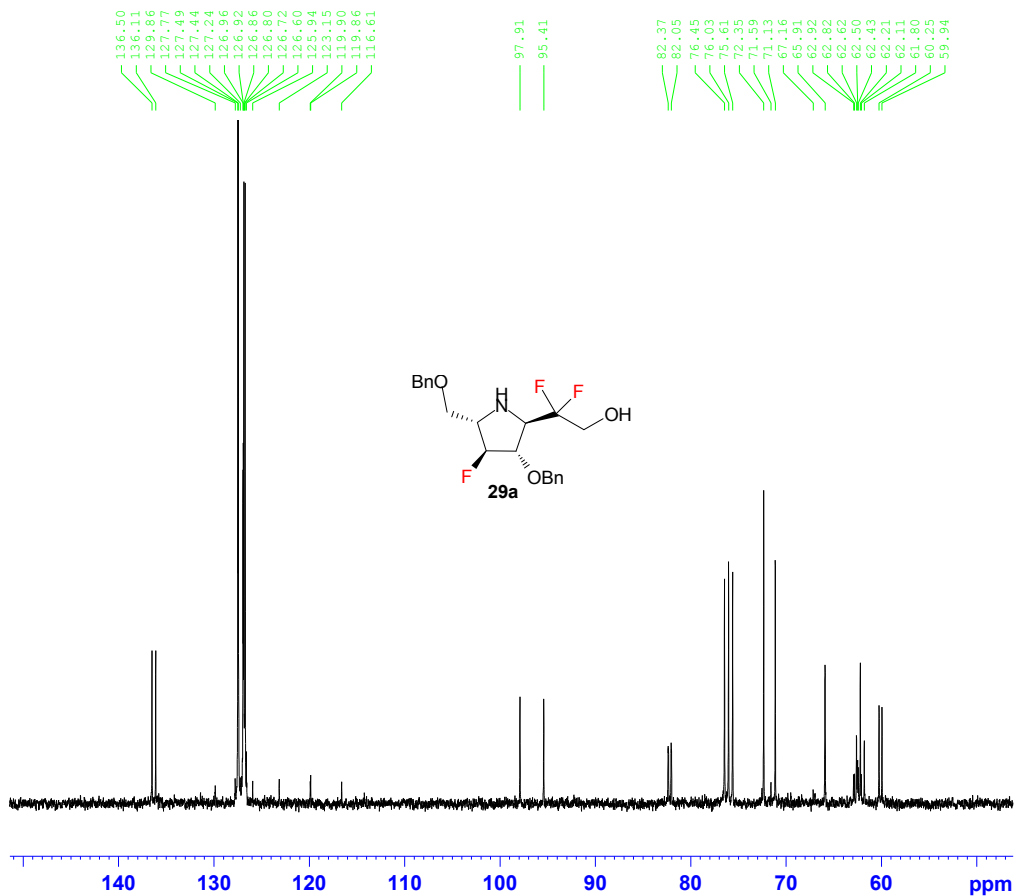


Compound 29a:

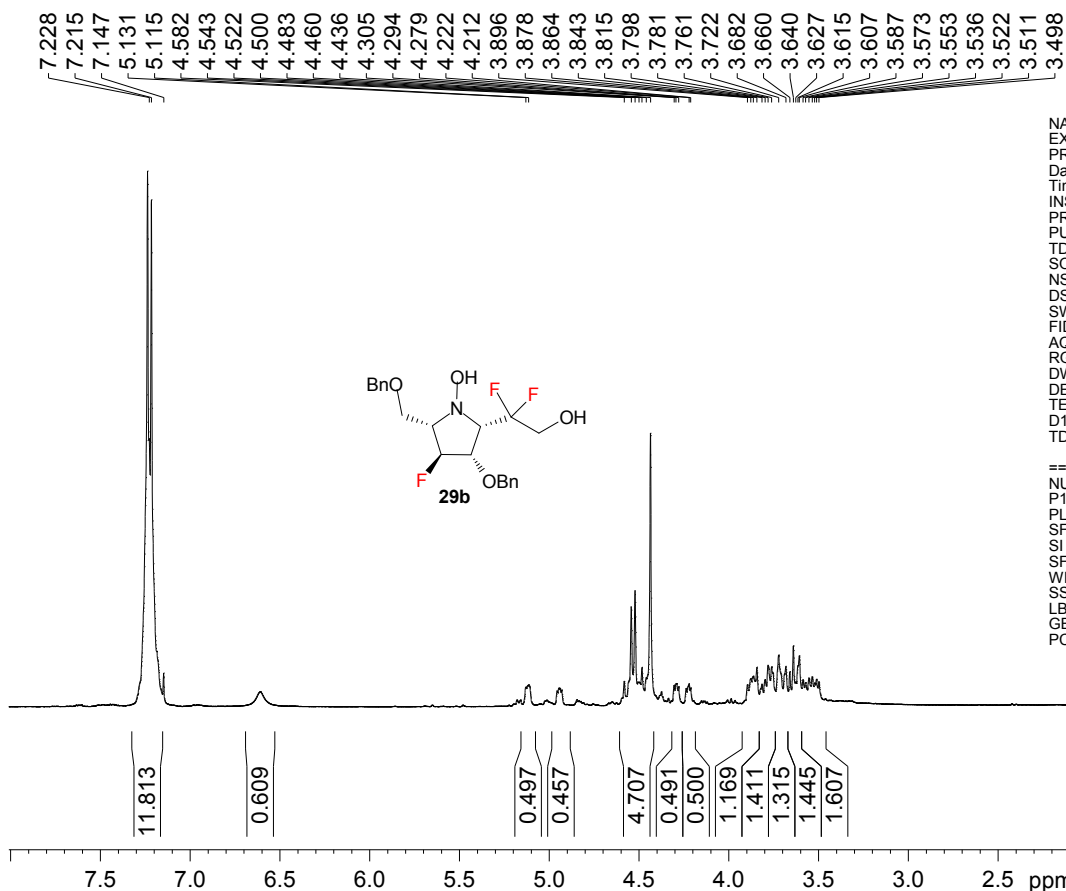


NAME lyx4-157b
 EXPNO 20
 PROCNO 1
 Date_ 20100522
 Time_ 14.46
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 2
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 45.3
 DW 55.600 usec
 DE 8.00 usec
 TE 299.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 3.00 dB
 SF01 300.1324010 MHz
 SI 32768
 SF 300.1300436 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

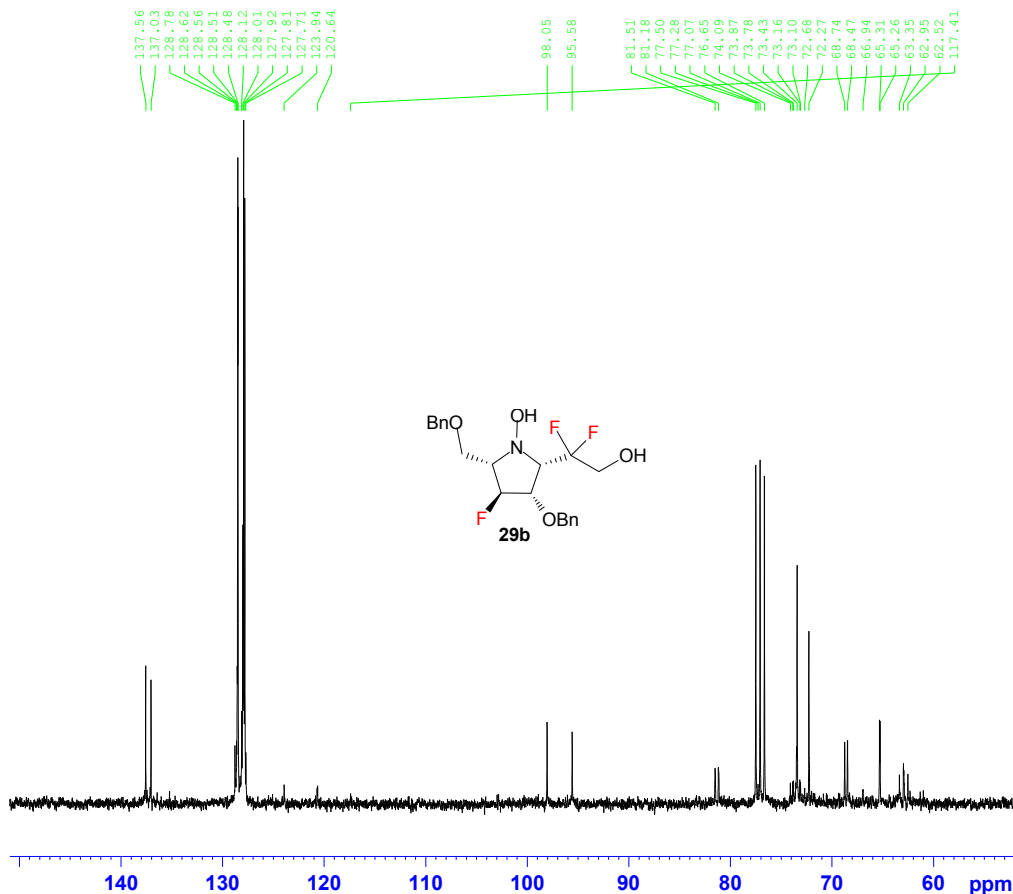


Compound 29b:



NAME lyx4-157c
EXPNO 10
PROCNO 1
Date_ 20100522
Time 15.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 3
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 71.8
DW 55.600 usec
DE 8.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

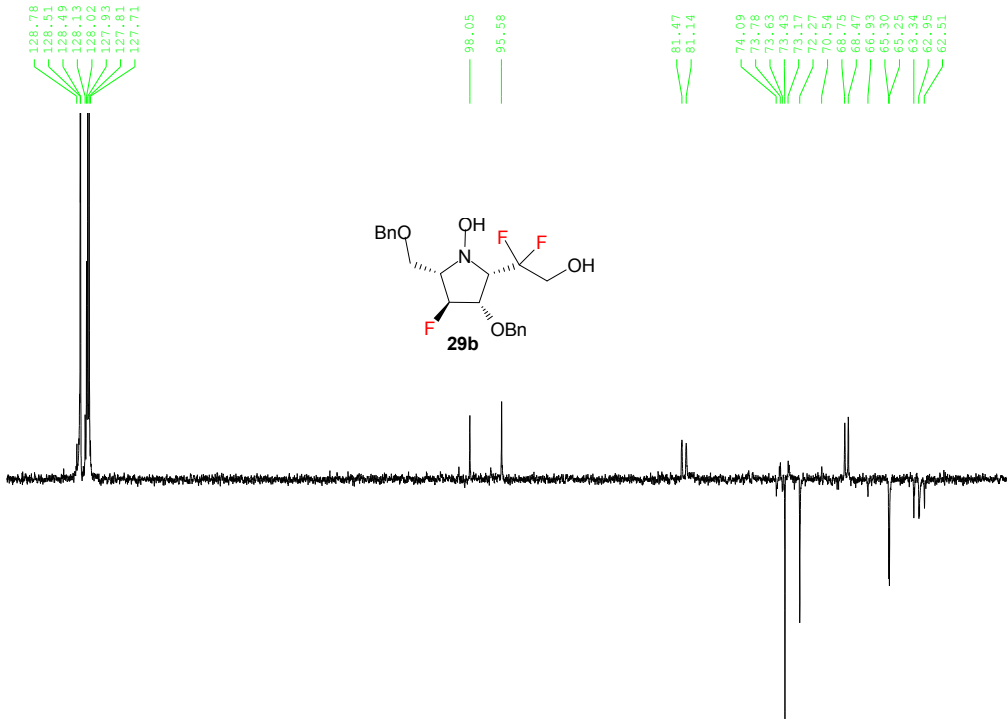
===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.1324010 MHz
SI 32768
SF 300.1300395 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME lyx4-157c
EXPNO 12
PROCNO 1
Date_ 20100522
Time 15.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 251
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 8.00 usec
TE 300.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

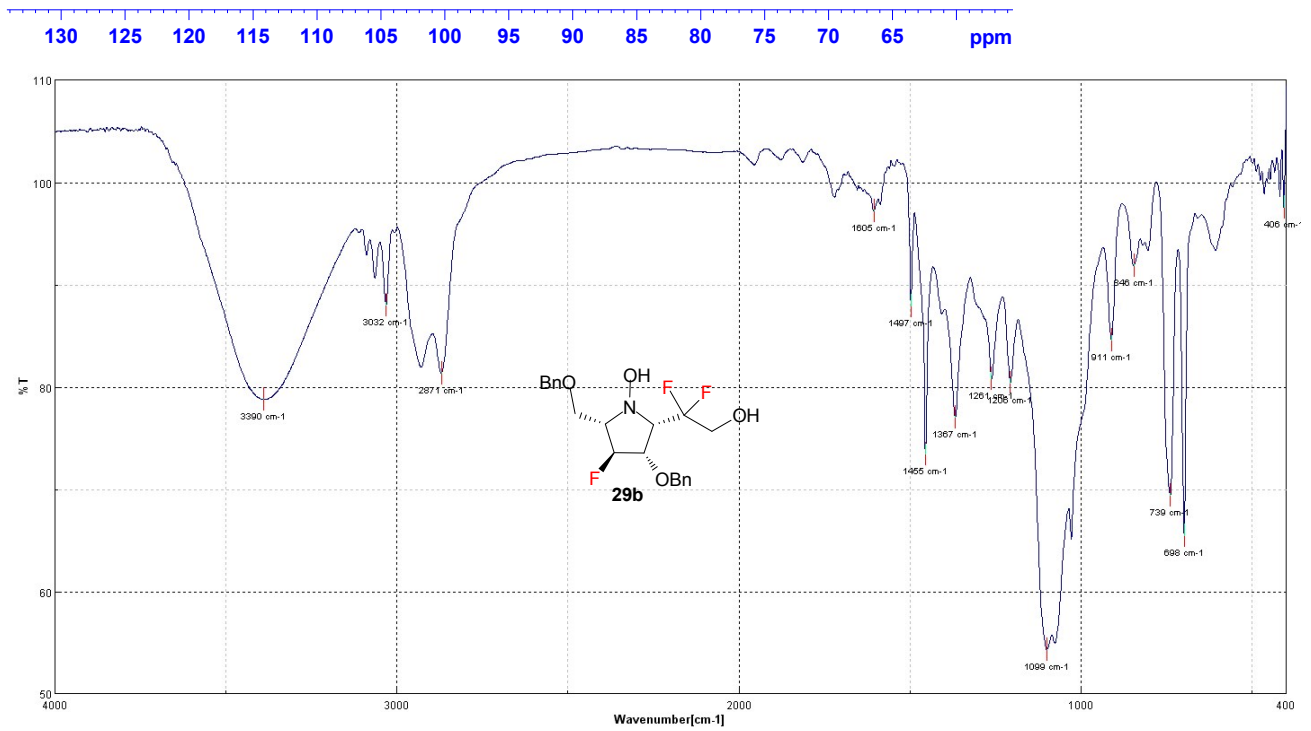


```

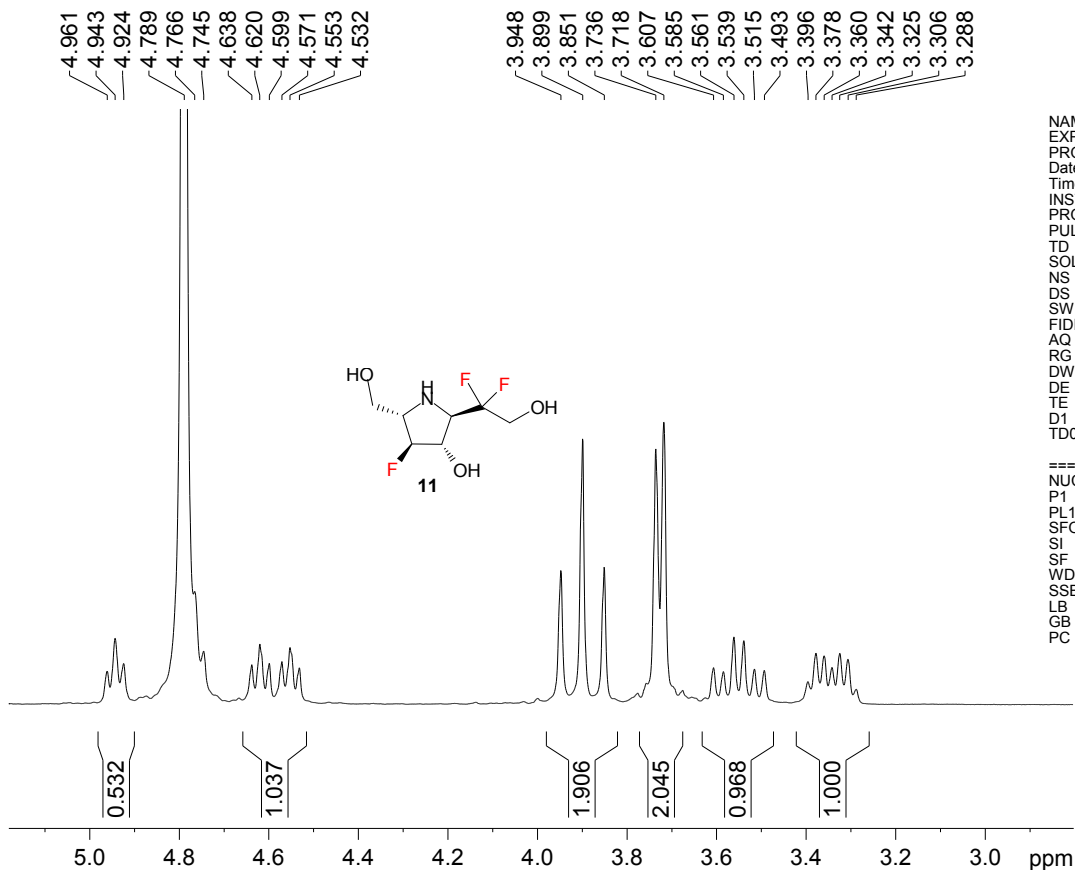
NAME          lyx4-157c
EXPNO         13
PROCNO        1
Date_         20100522
Time          15.51
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       dept135
TD            65536
SOLVENT       CDCl3
NS            173
DS            4
SWH           17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG            16384
DW            27.800 usec
DE            8.00 usec
TE            300.7 K
CNST2         145.0000000
D1            2.0000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            12.50 usec
P2            25.00 usec
PL1           2.00 dB
SFO1          75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
P3            10.80 usec
P4            21.60 usec
PCPD2         100.00 usec
PL2           3.00 dB
PL12          22.33 dB
SFO2          300.1312005 MHz
SI            32768
SF            75.4677490 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



Compound 11:

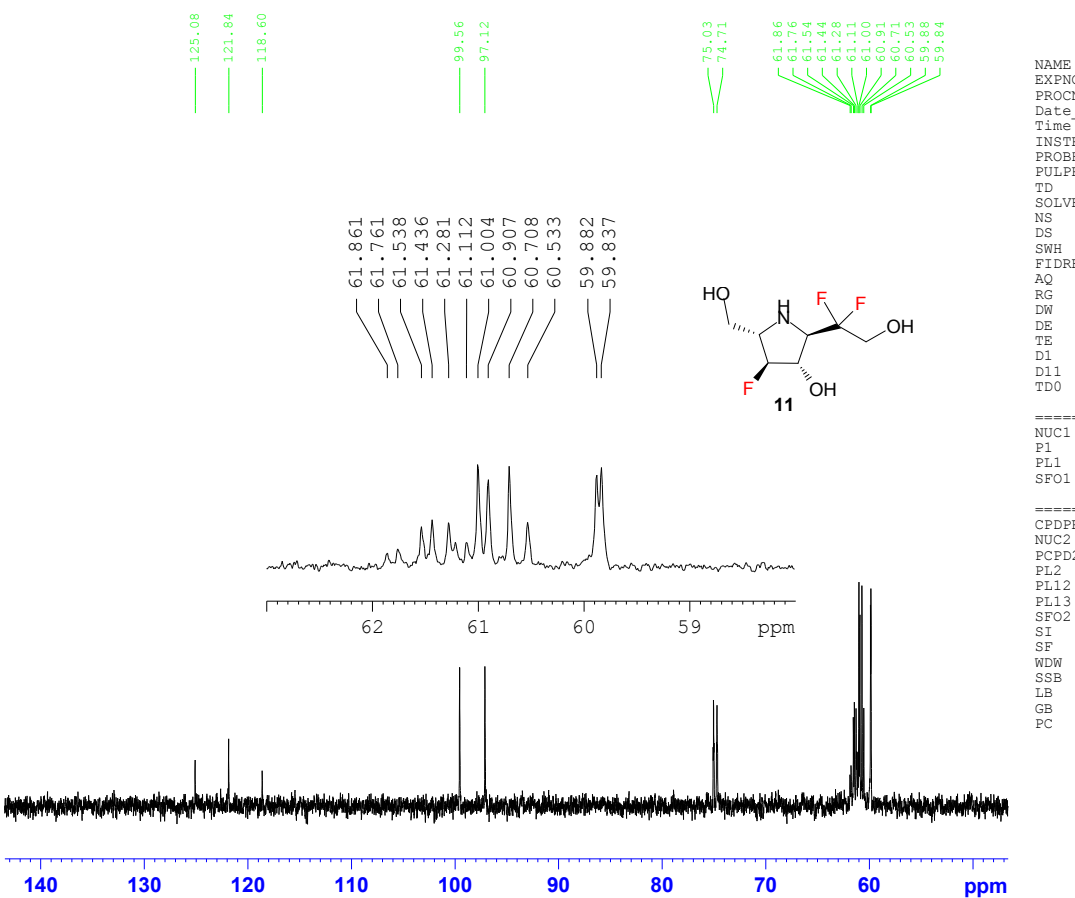


```

NAME lyx4-159a
EXPNO 10
PROCNO 1
Date_ 20100602
Time 9.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT D2O
NS 3
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 55.600 usec
DE 8.00 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1
    
```

```

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 3.00 dB
SFO1 300.1324010 MHz
SI 32768
SF 300.1299717 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```



```

NAME lyx4-159a
EXPNO 12
PROCNO 1
Date_ 20100602
Time 9.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 203
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 14596.5
DW 27.800 usec
DE 8.00 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
    
```

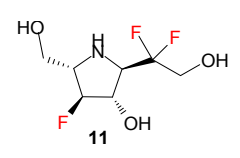
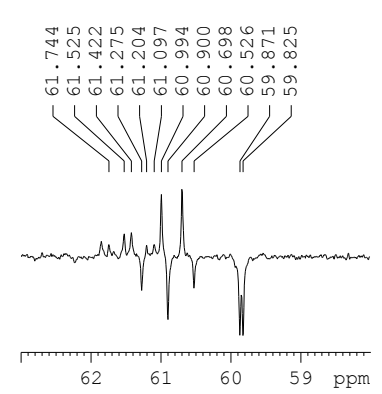
```

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 2.00 dB
SFO1 75.4752953 MHz
    
```

```

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
PL13 23.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

99.55 97.10 75.03 74.70 61.85 61.84 61.83 61.82 61.81 61.80 61.20 61.10 60.99 60.90 60.70 60.53 59.87 59.83



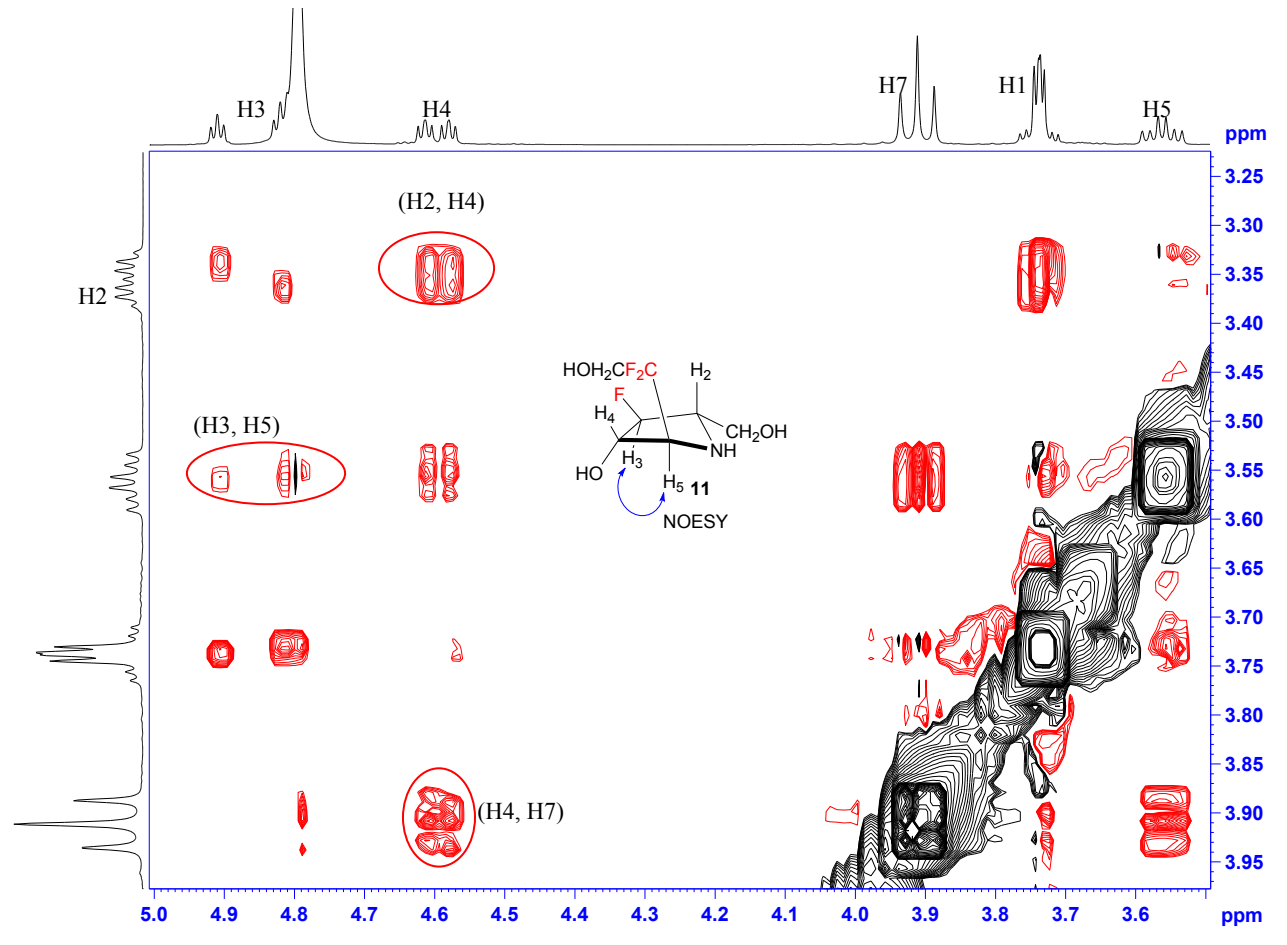
```

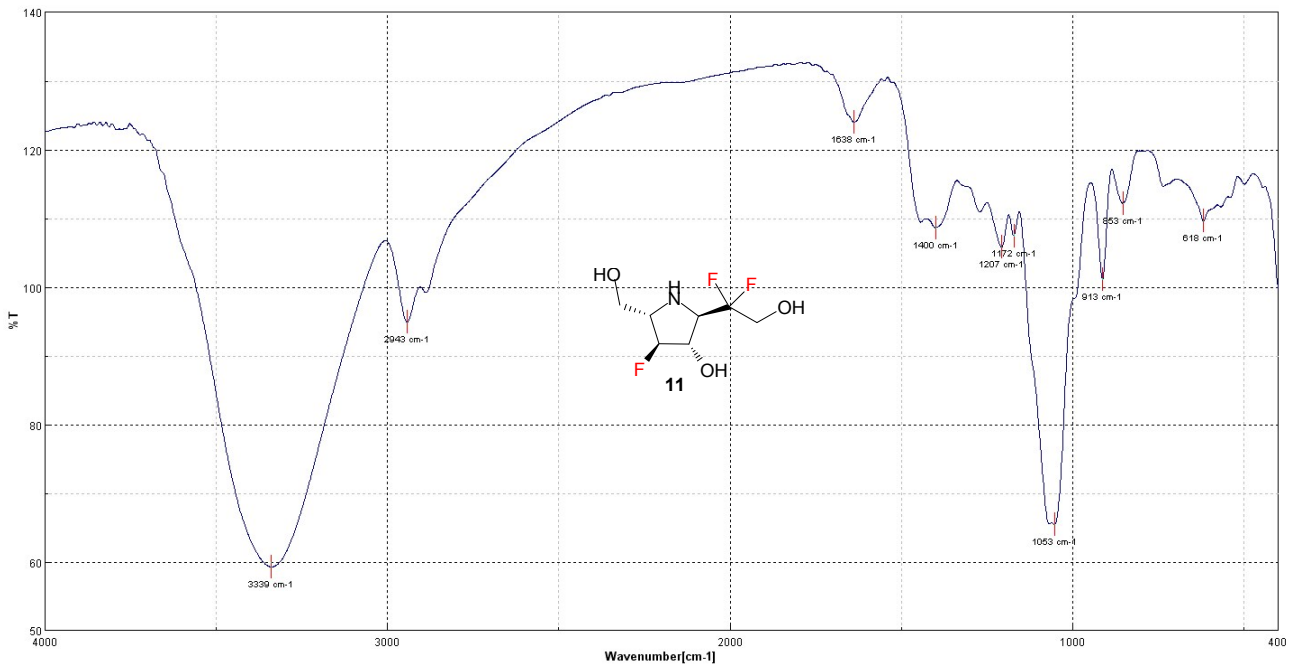
NAME lyx4-159a
EXPNO 13
PROCNO 1
Date_ 20100602
Time 9.25
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT D2O
NS 75
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 8.00 usec
TE 299.2 K
CNST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
P2 25.00 usec
PL1 2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.80 usec
P4 21.60 usec
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.33 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

105 100 95 90 85 80 75 70 65 60 ppm





-118.655
-118.688
-118.721

-192.544
-192.588
-192.638
-192.685
-192.730
-192.778

NAME 19F
EXPNO 14
PROCNO 1

