

Stereocomplementary synthesis of casuarine and its 6-*epi*-, 7-*epi*-, and 6,7-*diepi*-diastereomers

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Fleet and Chu-Yi Yu*

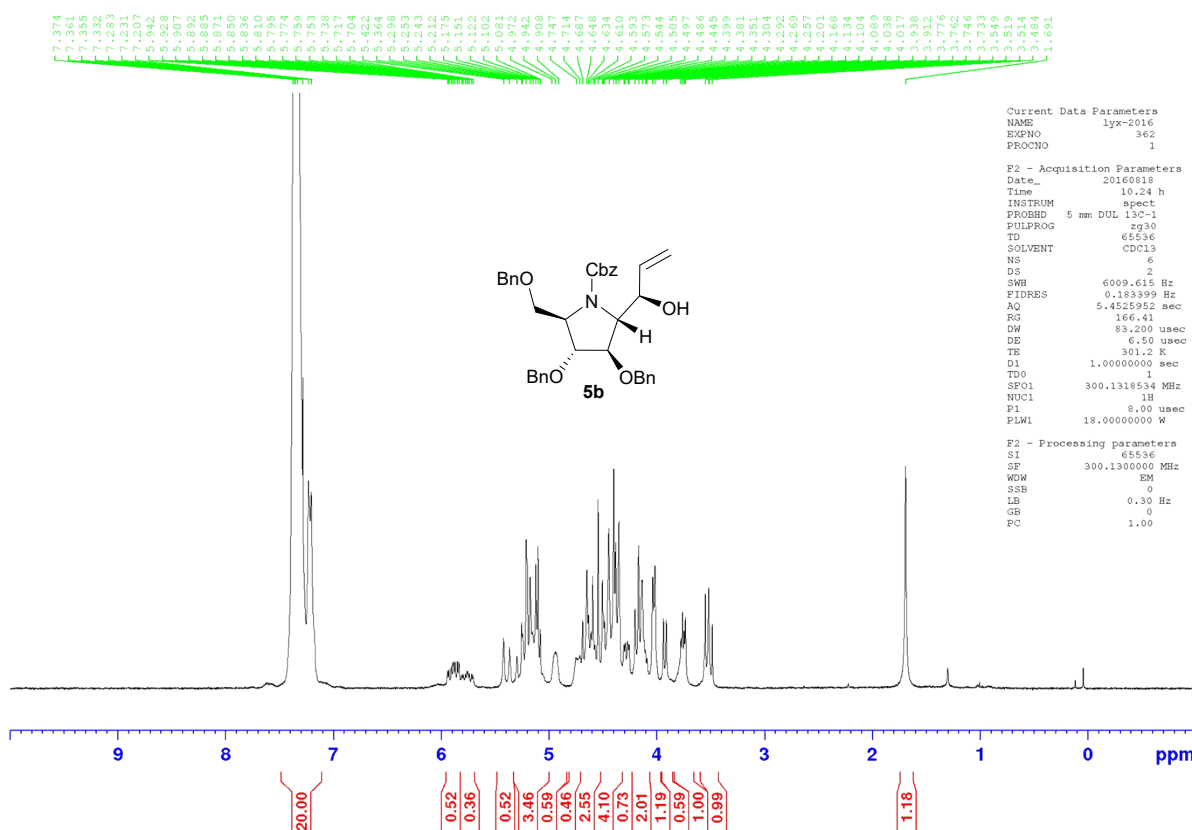
*Corresponding author: yucy@iccas.ac.cn and kato@med.u-toyama.ac.jp

Supplementary data

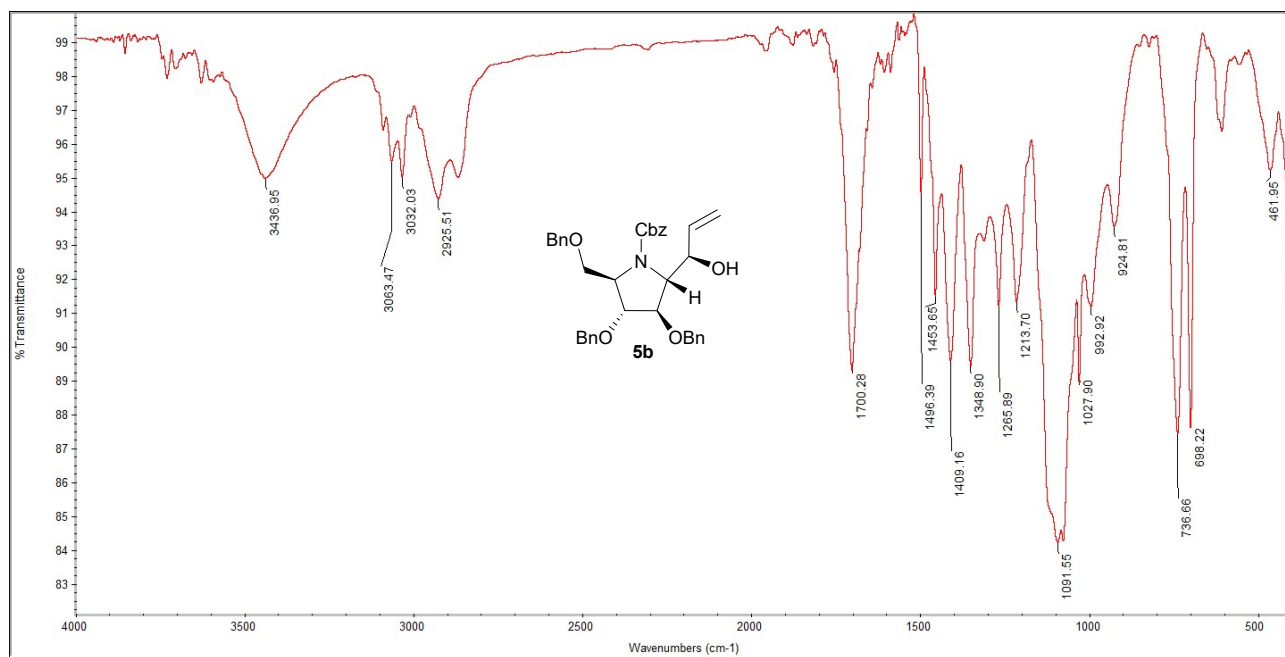
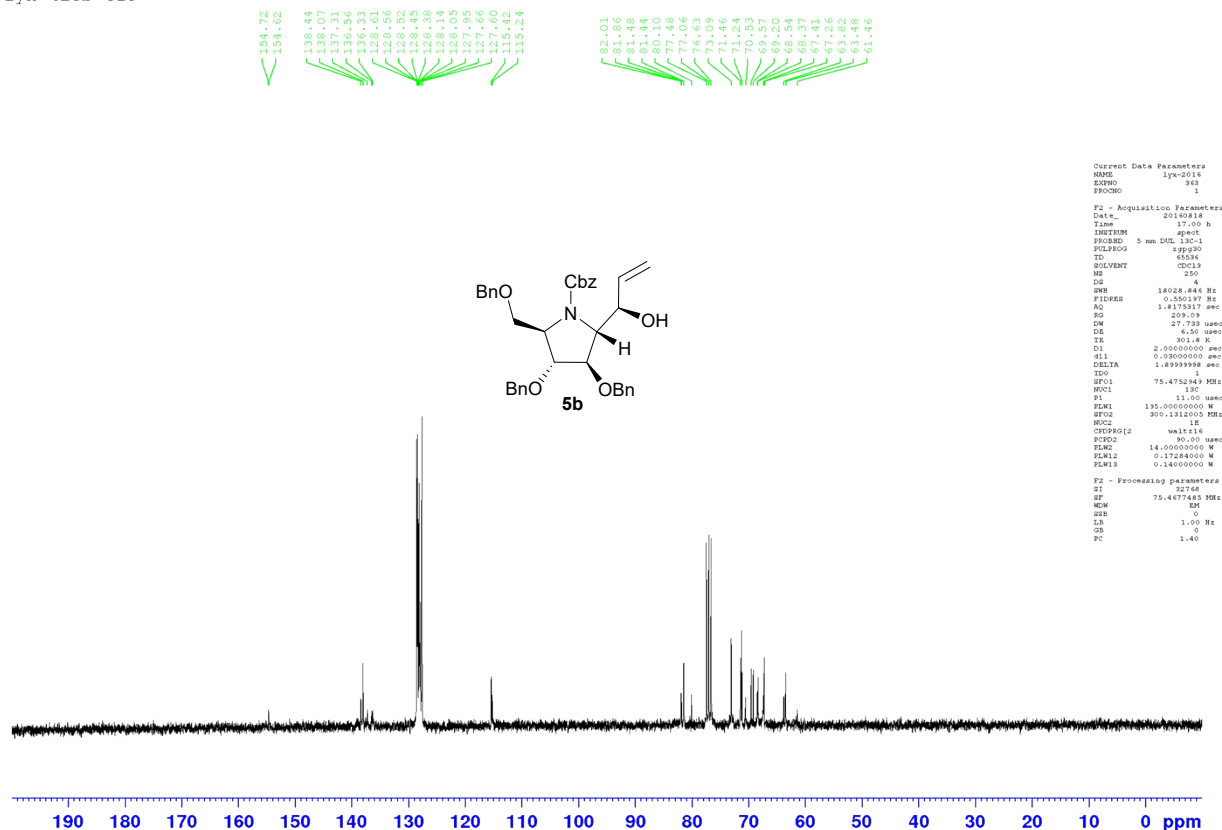
(NMR spectra and Infrared spectra)

Compound 5b:

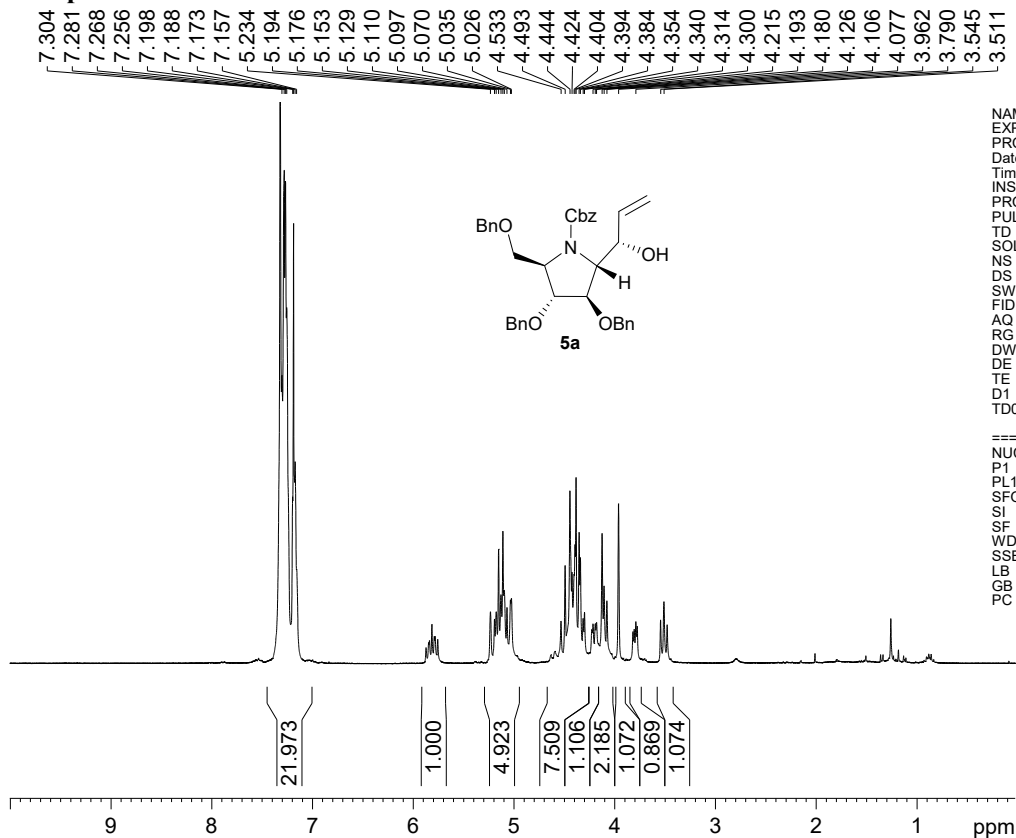
lyx-425b



lyx-425b-C13

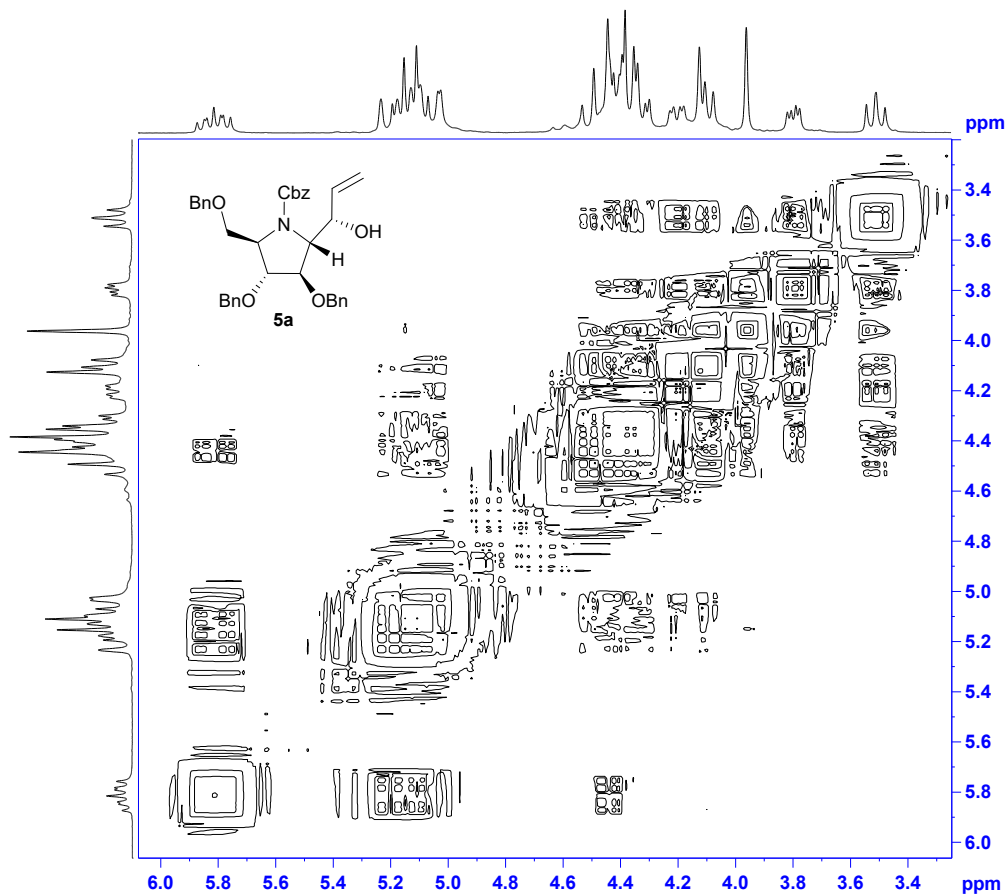


Compound 5a:



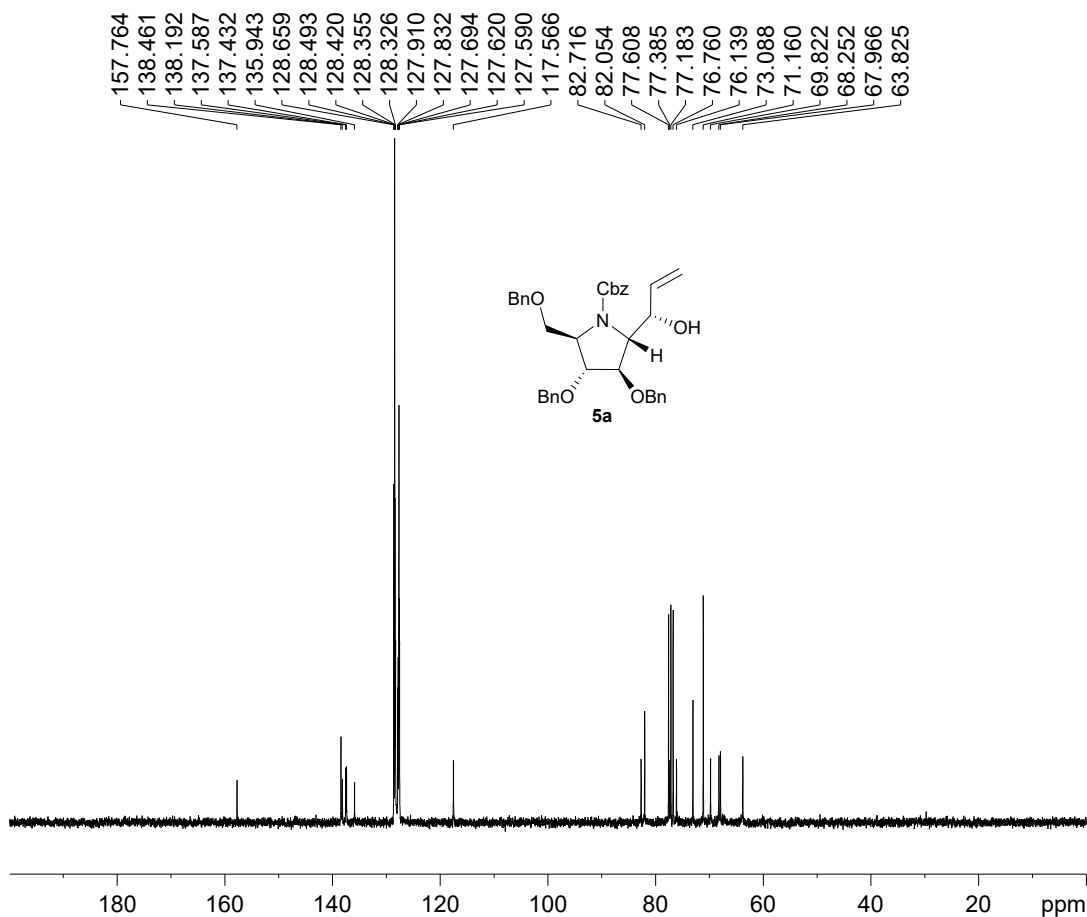
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 PROCNO 1
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 Time 17.15
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 2
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 35.9
 DW 55.600 usec
 DE 8.00 usec
 TE 299.0 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 3.00 dB
 SFO1 300.1324010 MHz
 SI 32768
 SF 300.1300273 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NAME lyx-425
 EXPNO 11
 PROCNO 1
 Date_ 20121009
 Time 17.16
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG cosygpgf
 TD 2048
 SOLVENT CDCl3
 NS 4
 DS 8
 SWH 2540.650 Hz
 FIDRES 1.240552 Hz
 AQ 0.4030964 sec
 RG 32
 DW 196.800 usec
 DE 8.00 usec
 TE 298.9 K
 D0 0.00000300 sec
 D1 1.39309299 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00039360 sec

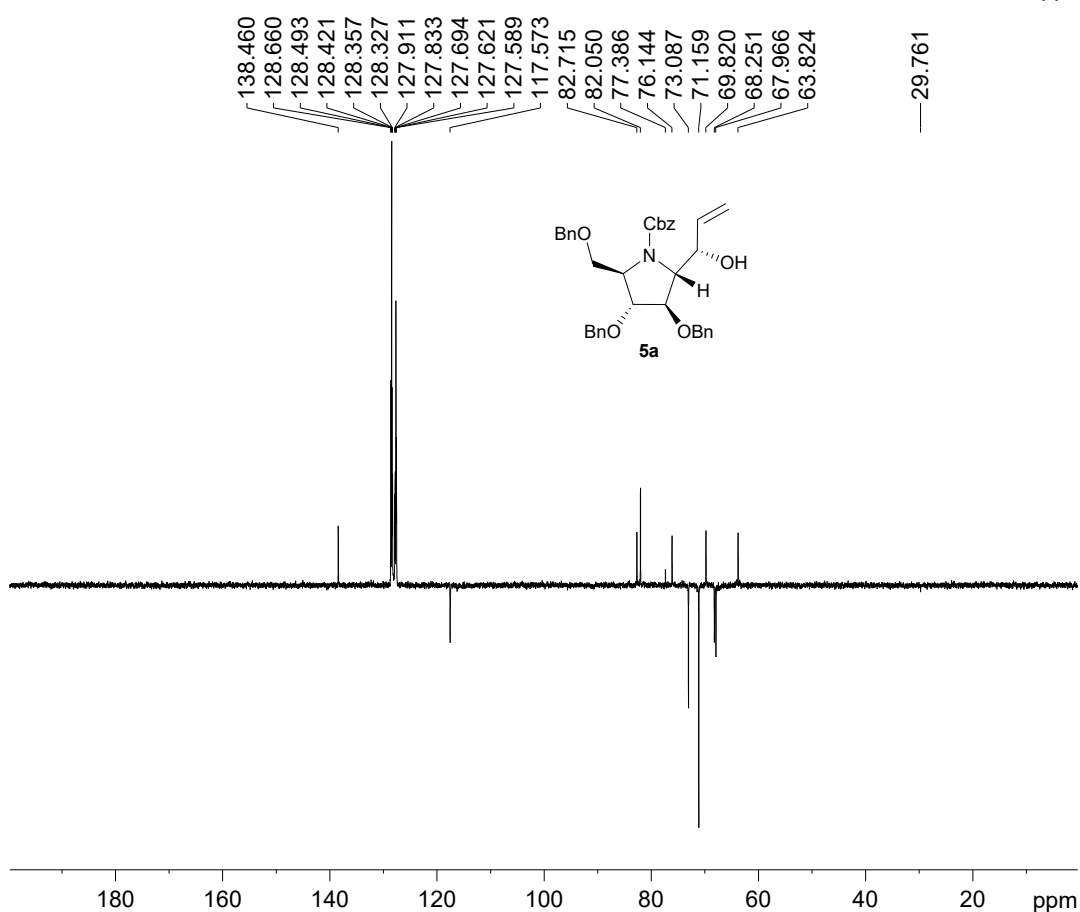
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 NUC1 1H
 P0 10.30 usec
 P1 10.30 usec
 PL1 3.00 dB
 SFO1 300.1313330 MHz
 ===== GRADIENT CHANNEL =====
 GPNAM1 SINE.100
 GP21 10.00 %
 P16 1000.00 usec
 NDO 1
 TD 21
 SFO1 300.1313 MHz
 FIDRES 120.983353 Hz
 SW 8.465 ppm
 FMODE QF
 SI 1024
 SF 300.1300273 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 300.1300273 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0



```

NAME lyx-425
EXPNO 12
PROCNO 1
Date_ 20121009
Time 17.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 71
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DE 27.800 usec
TE 299.2 K
D1 2.0000000 sec
D11 0.0300000 sec
D10 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 22.74 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

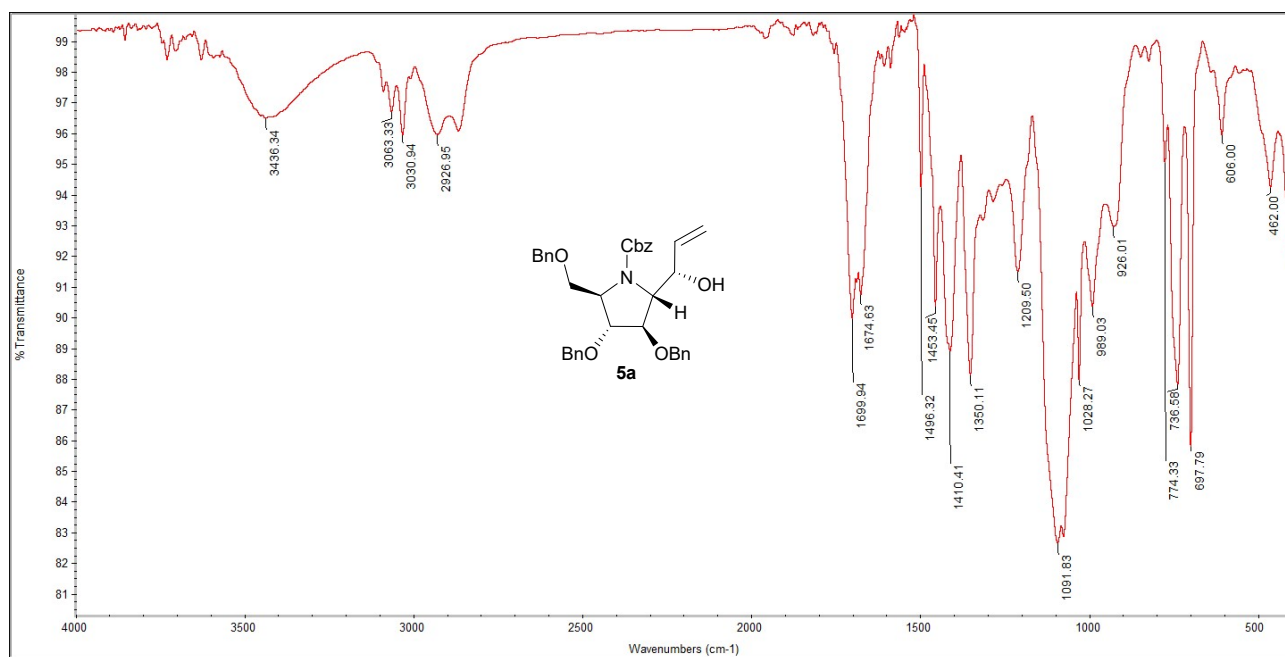
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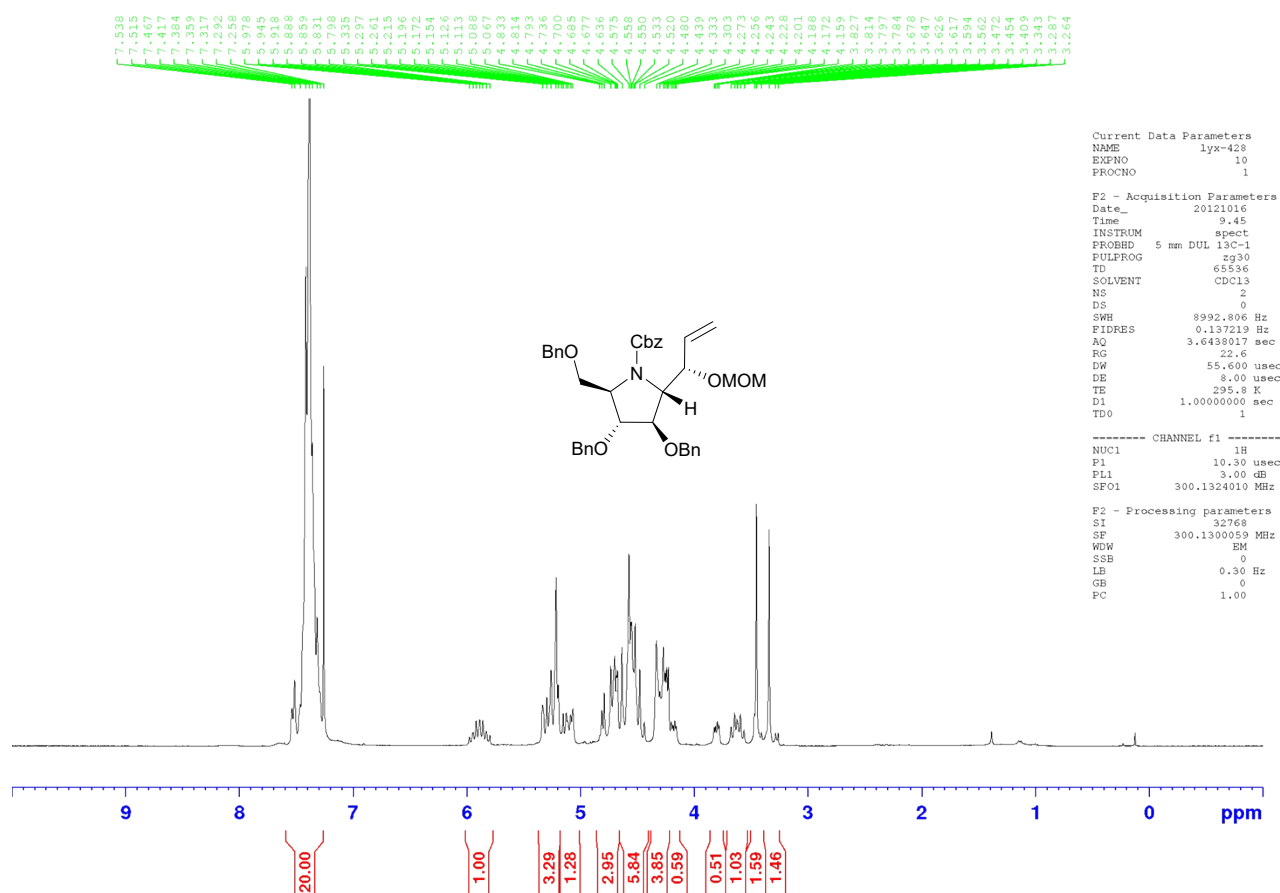
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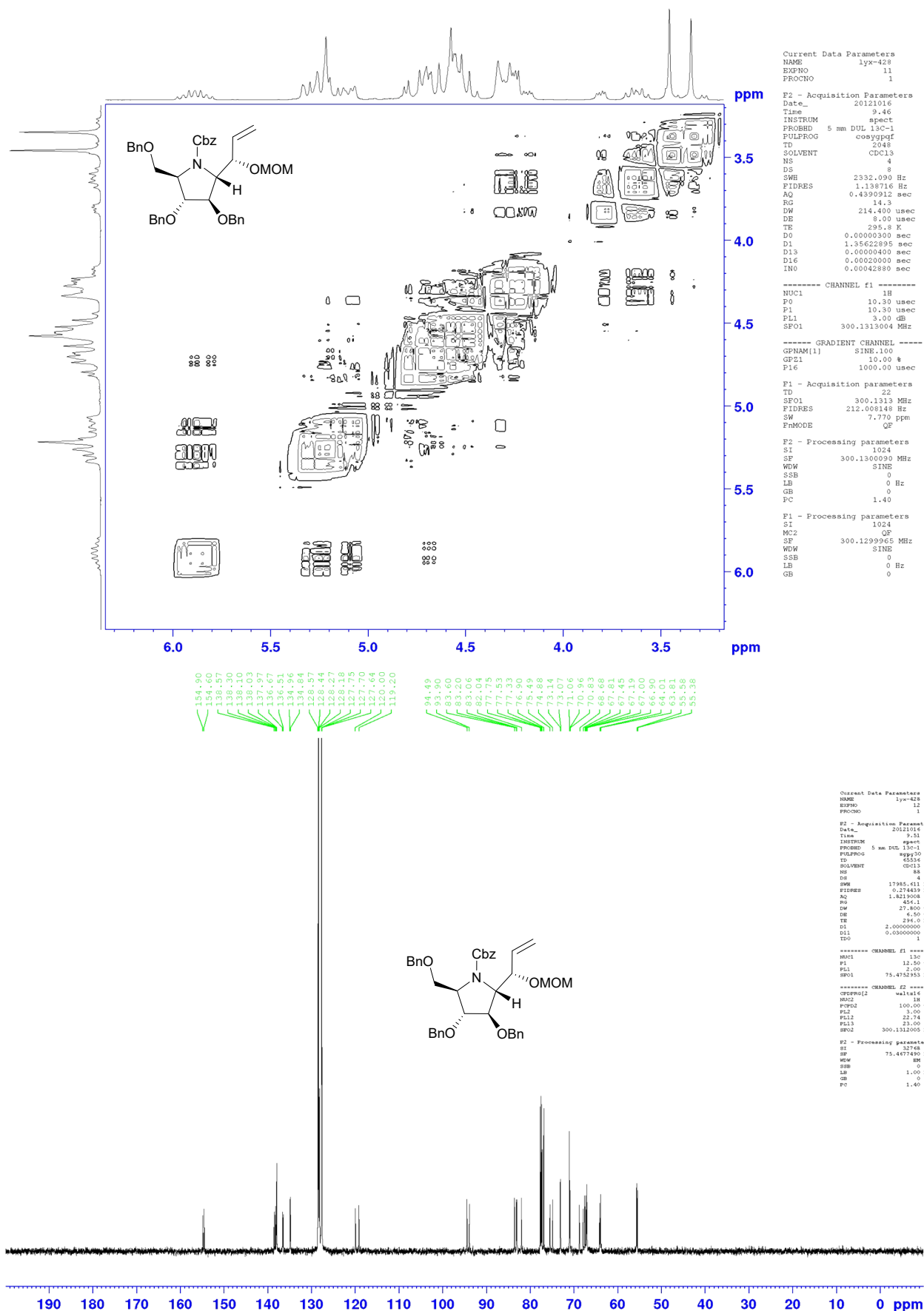
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EXPNO 13
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Time 17.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 41
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DE 27.800 usec
TE 299.3 K
CNST2 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D10 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 10.30 usec
P4 20.60 usec
PCPD2 100.00 usec
PL2 3.00 dB
PL12 22.74 dB
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SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

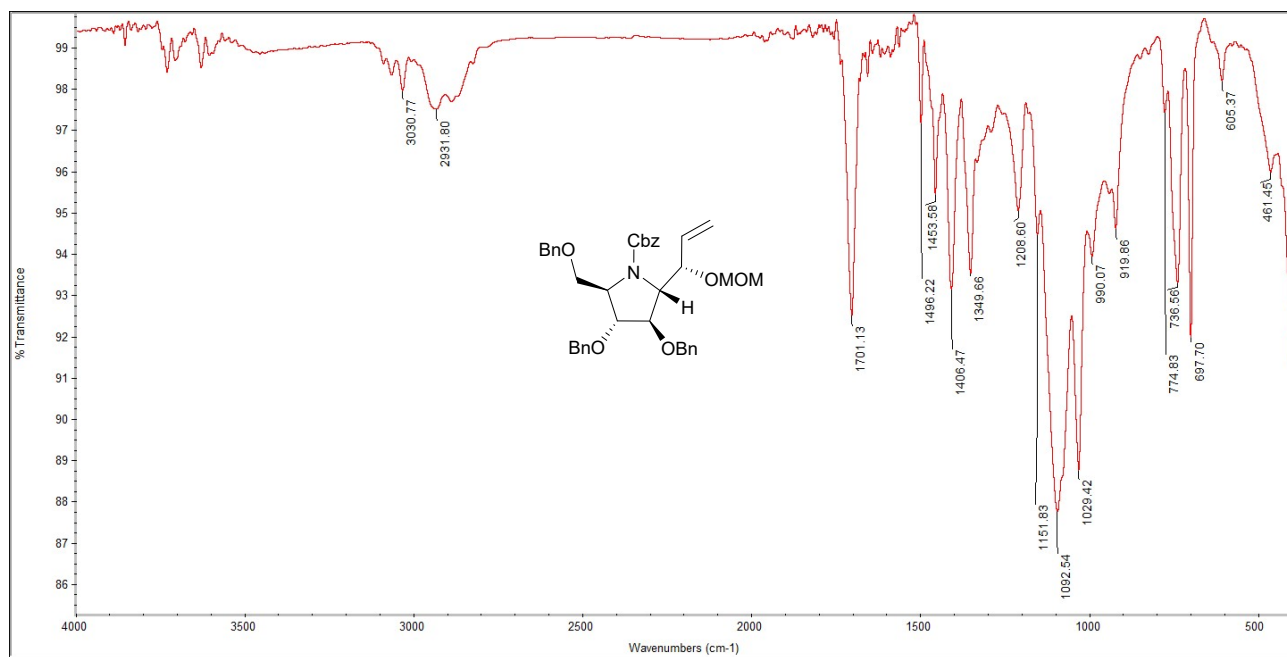
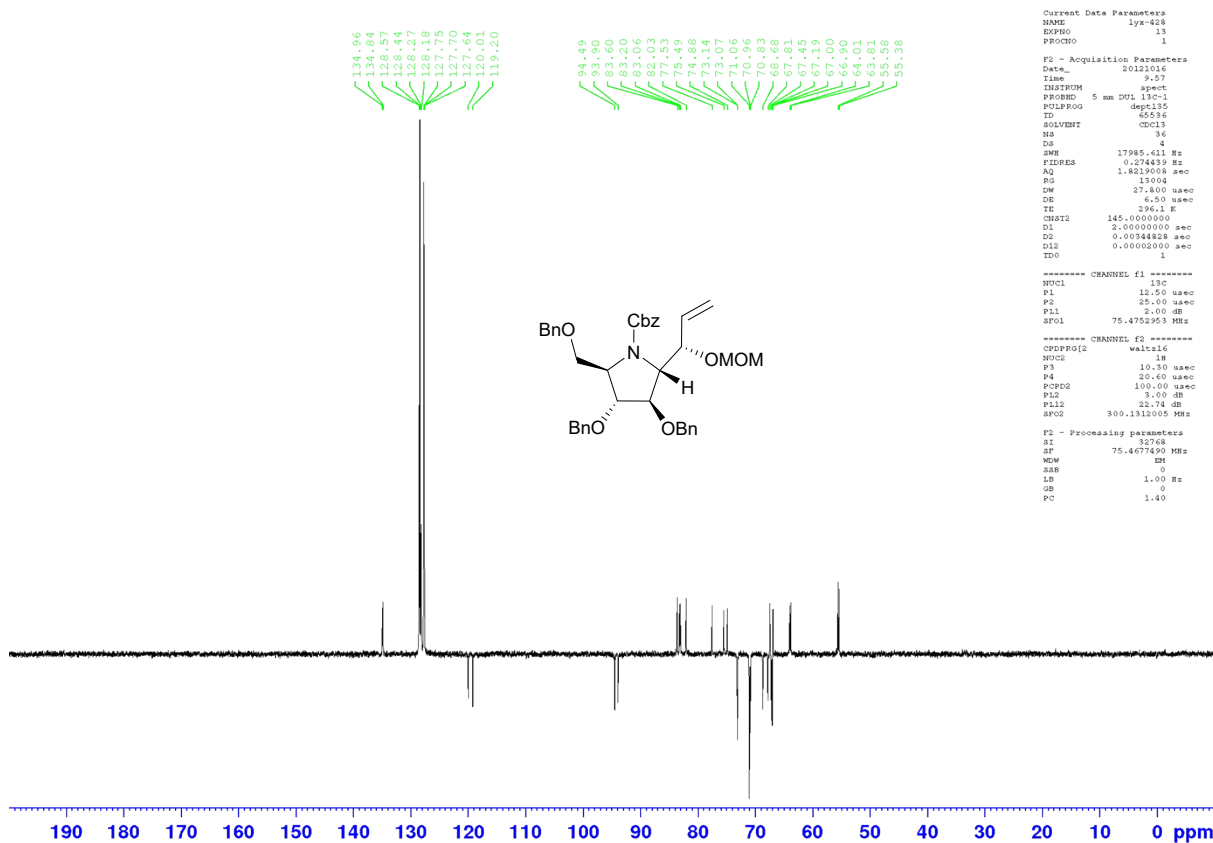
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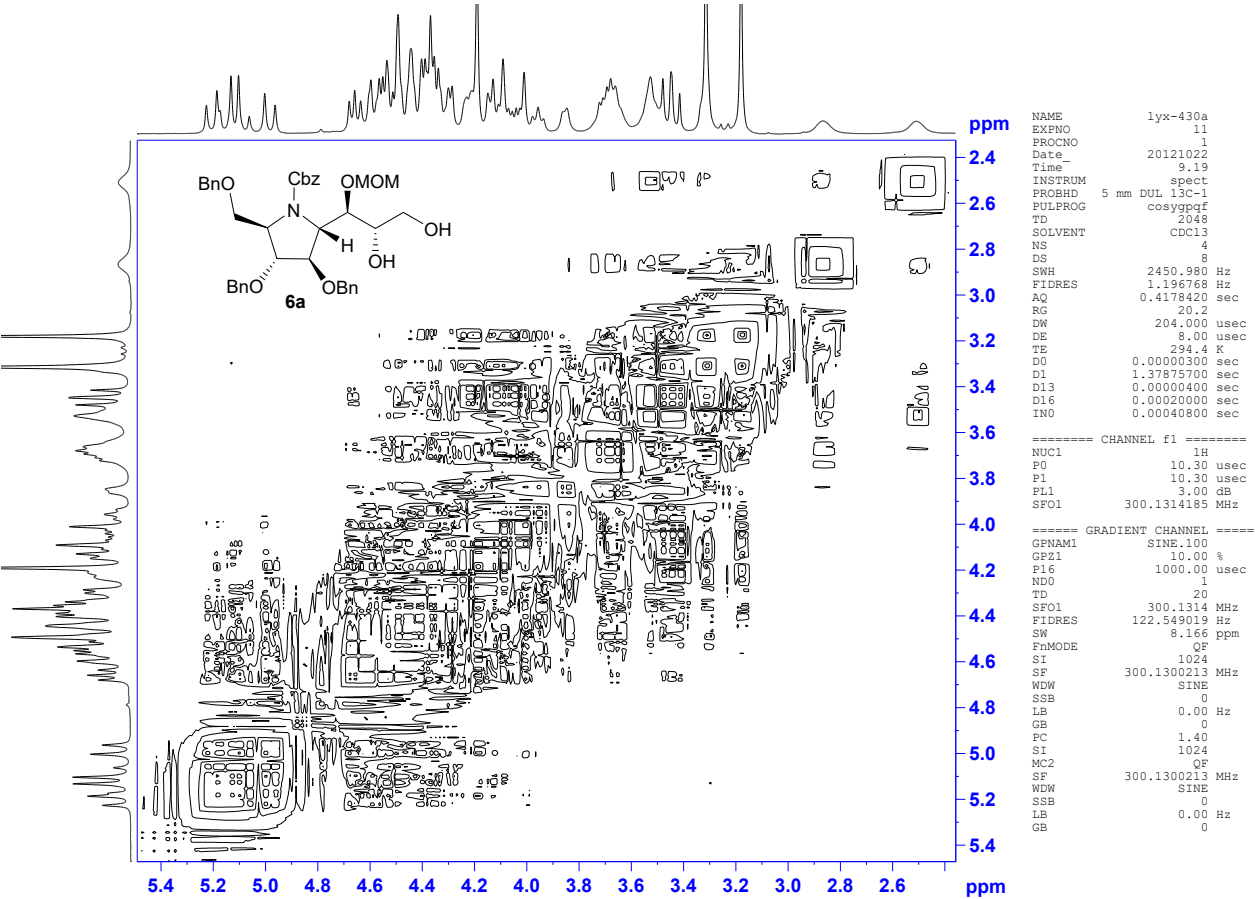
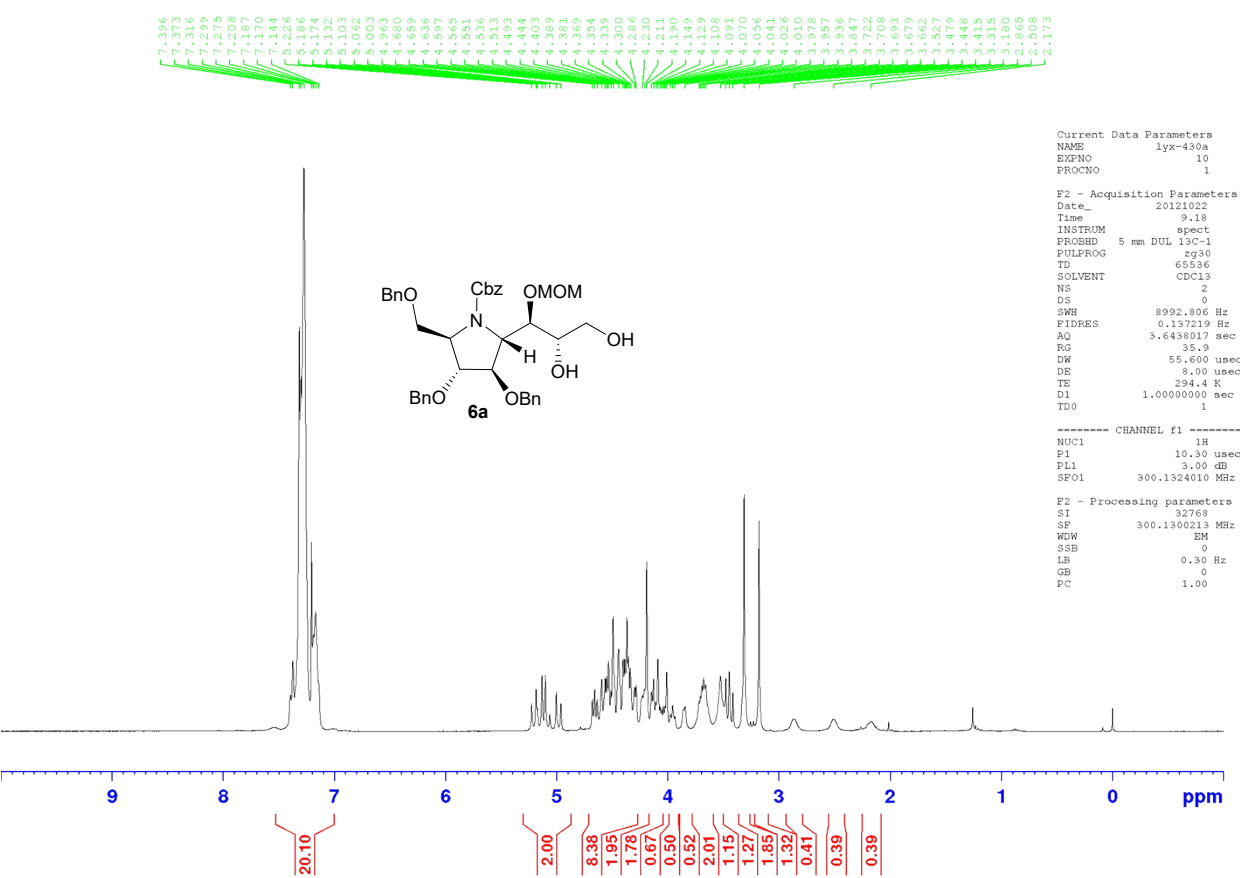
C-6 Hydroxyl MOM-protected intermediate for **6a** and **6b**:

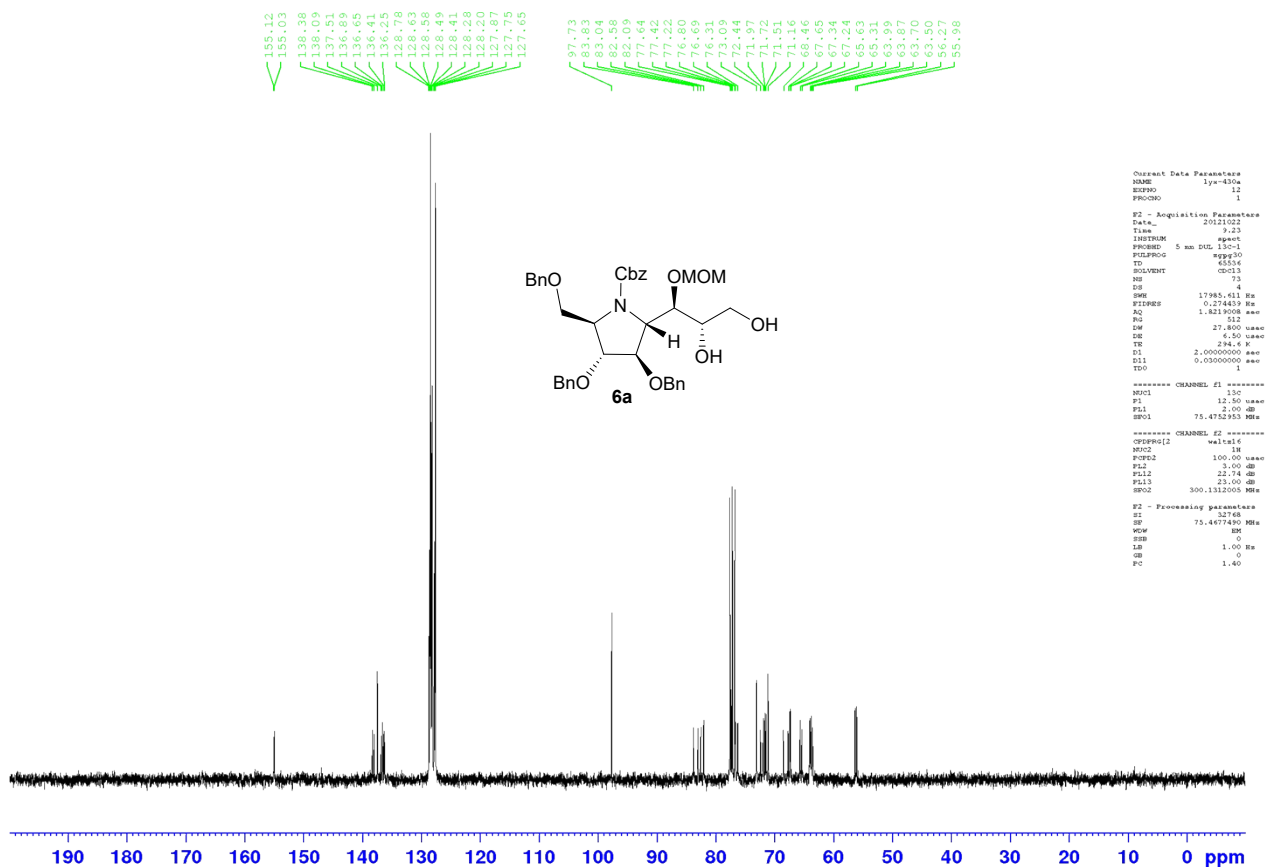


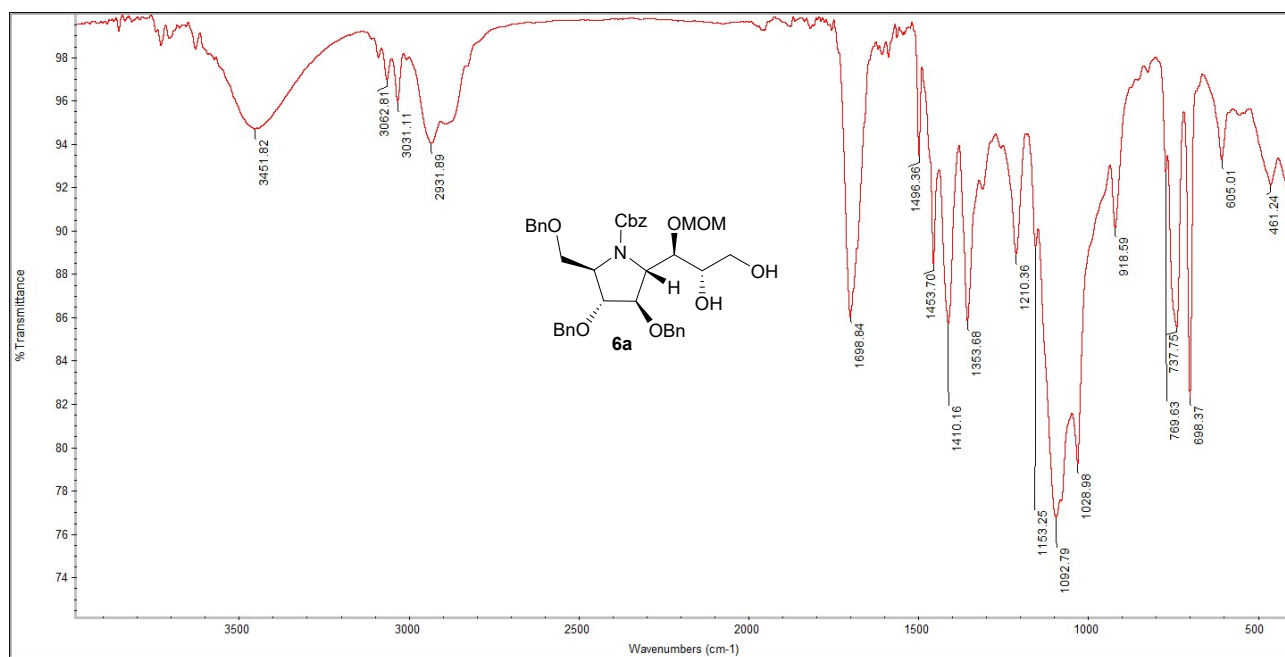




Compound 6a:

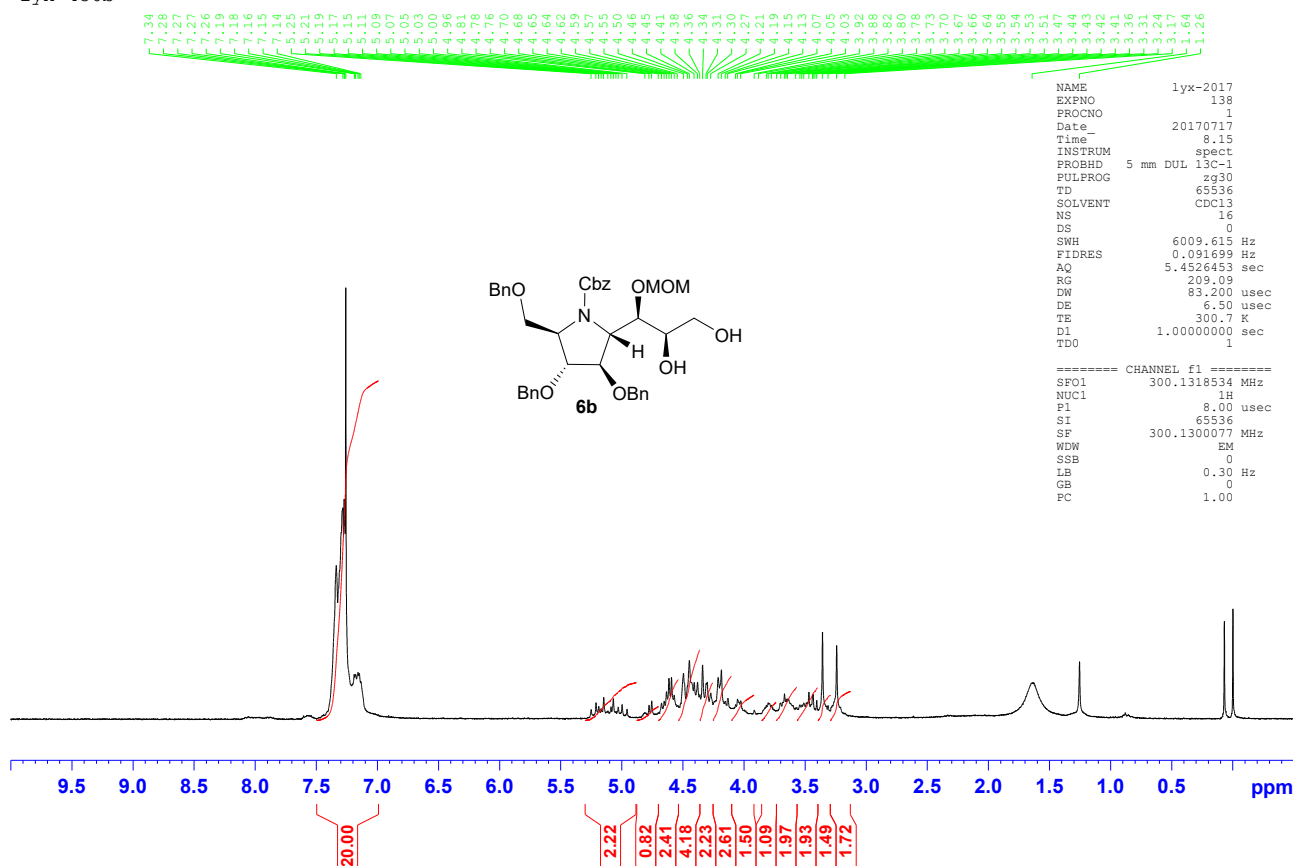




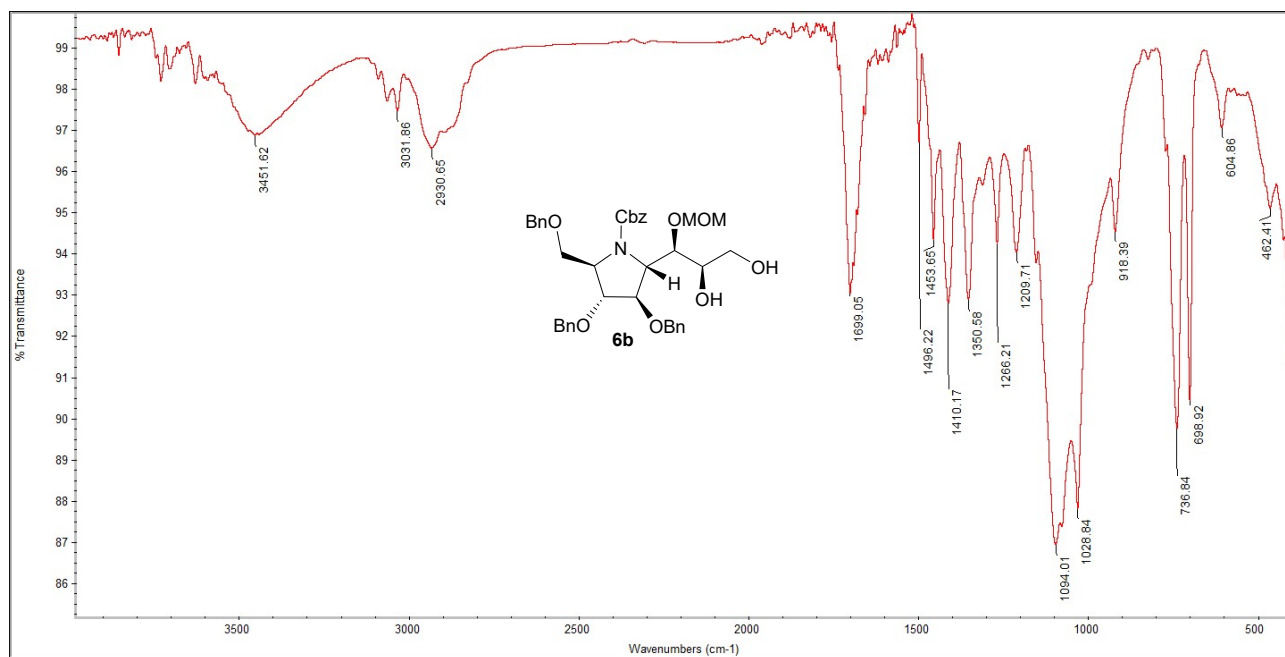
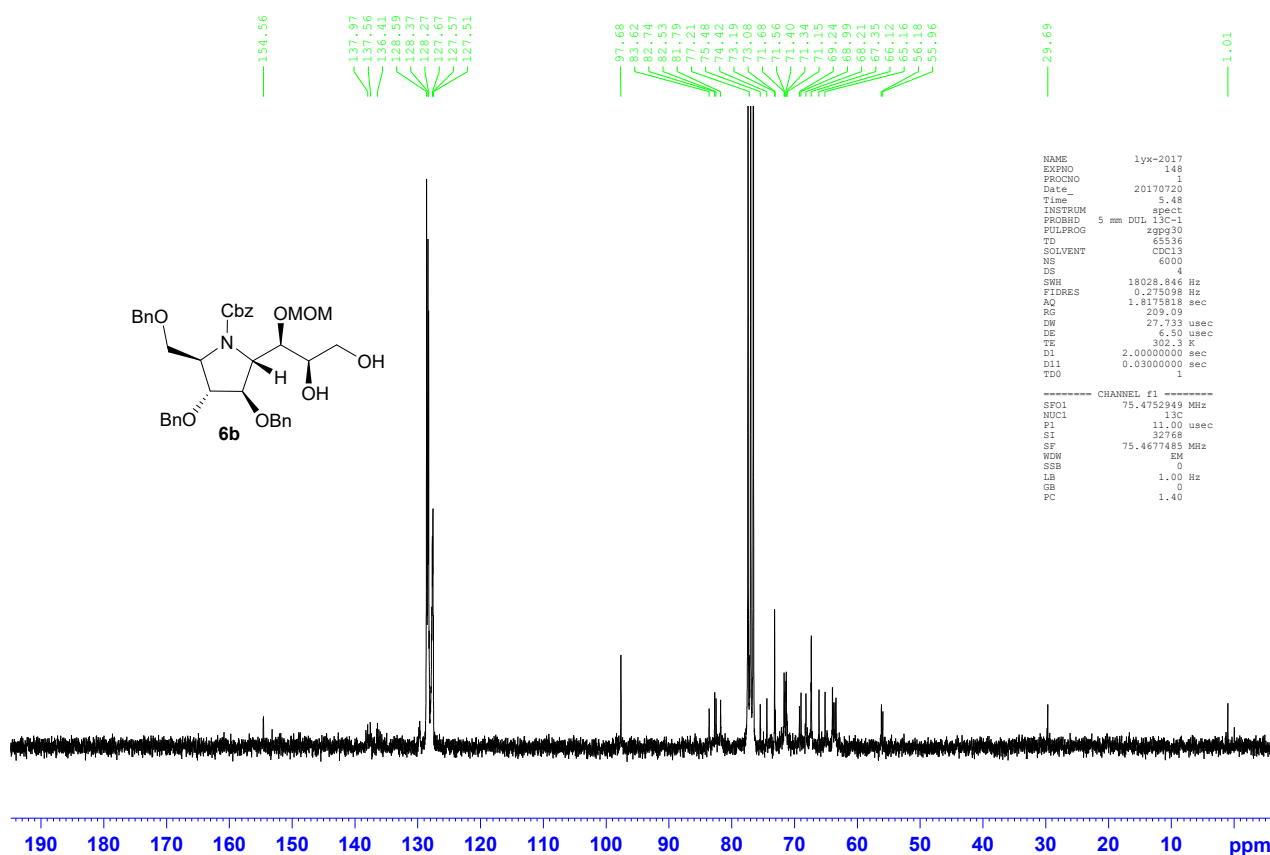


Compound 6b:

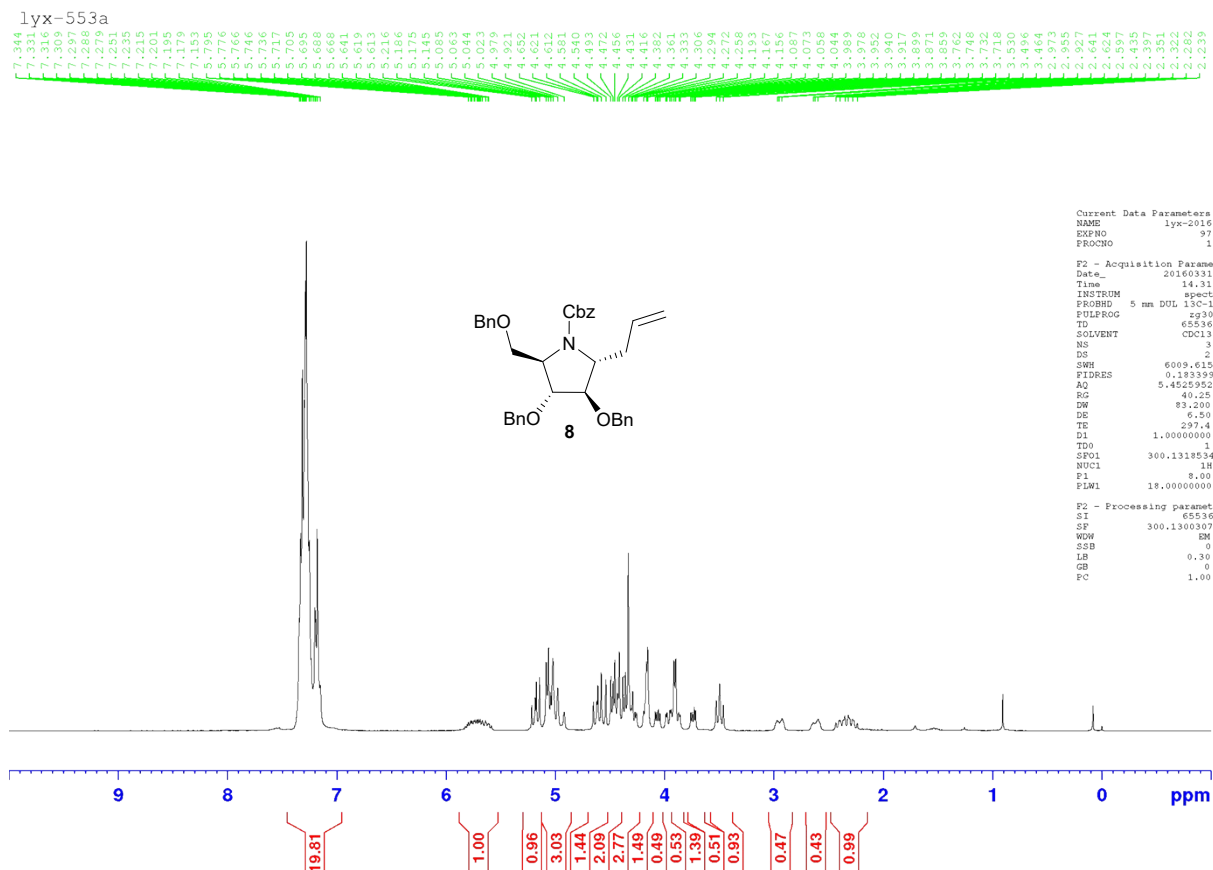
lyx-430b



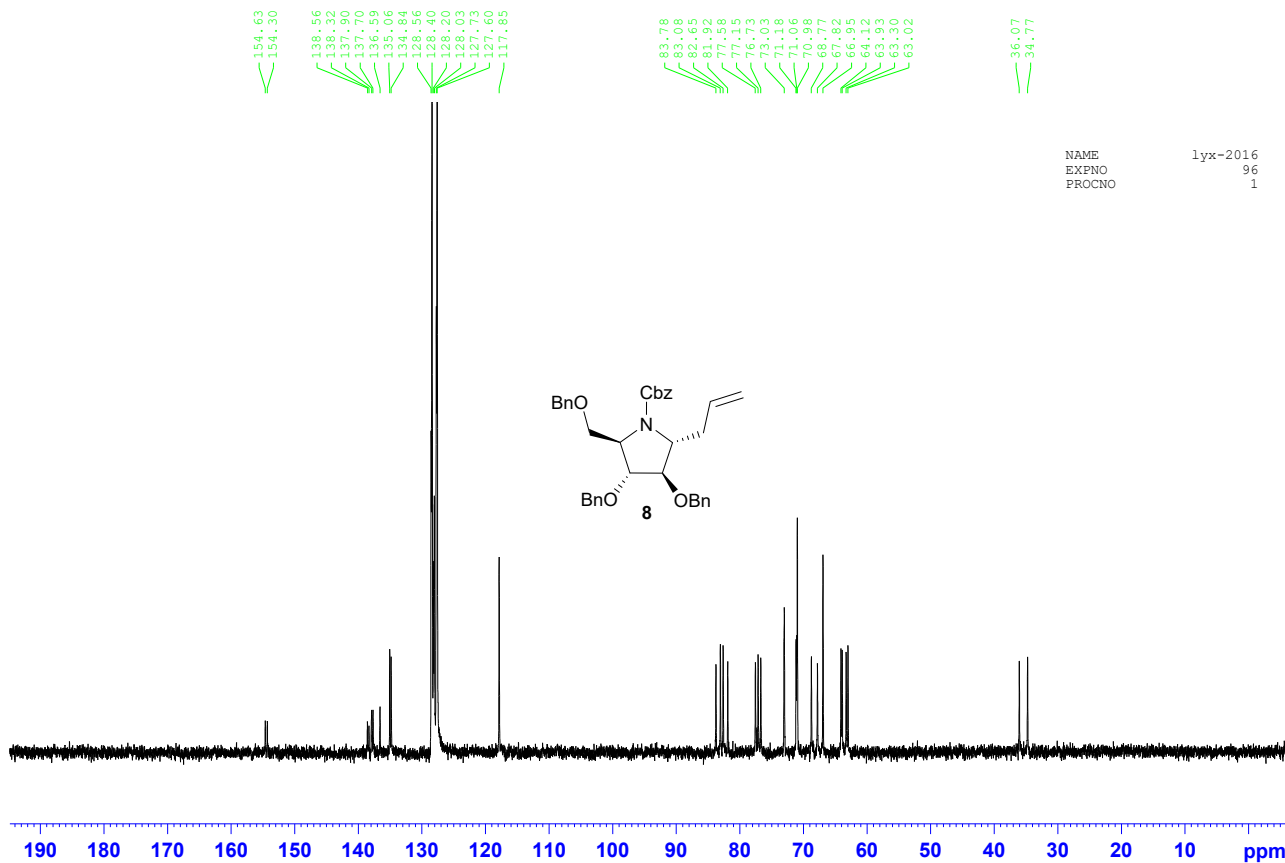
lyx-430b

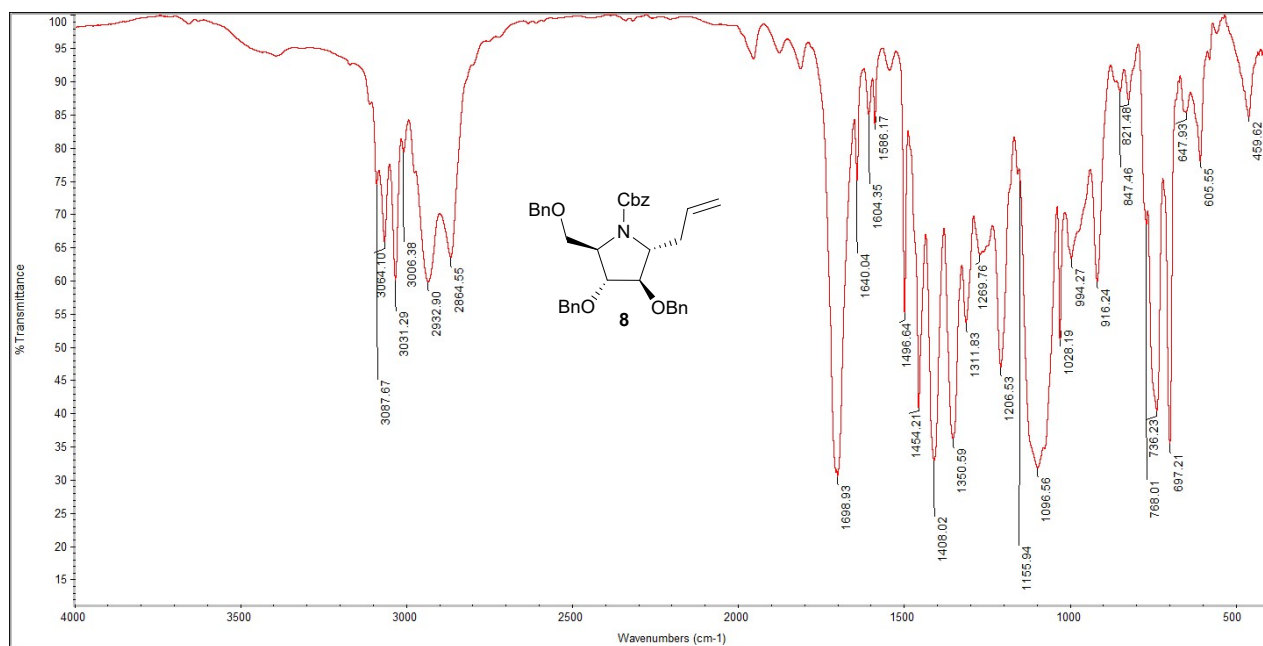


Compound 8:



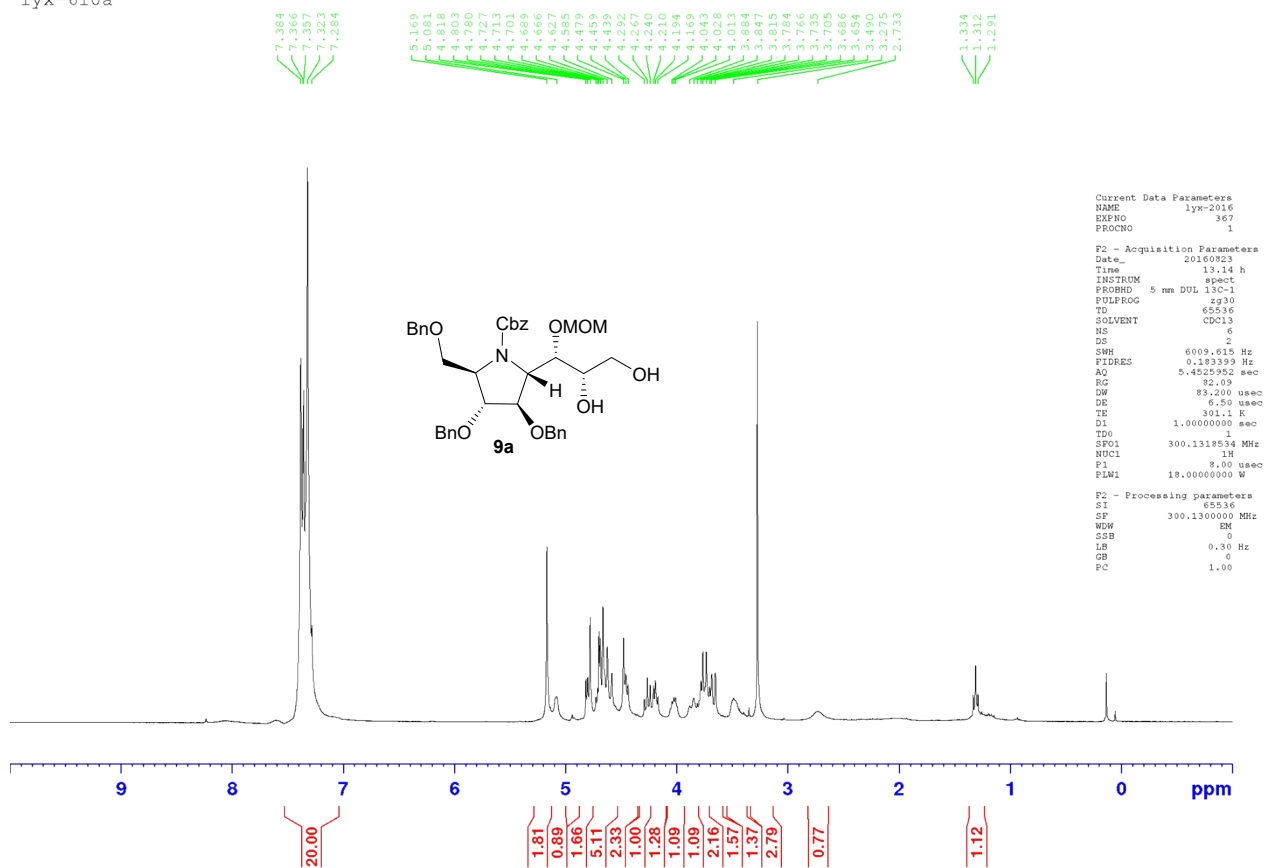
lyx-553a-C13

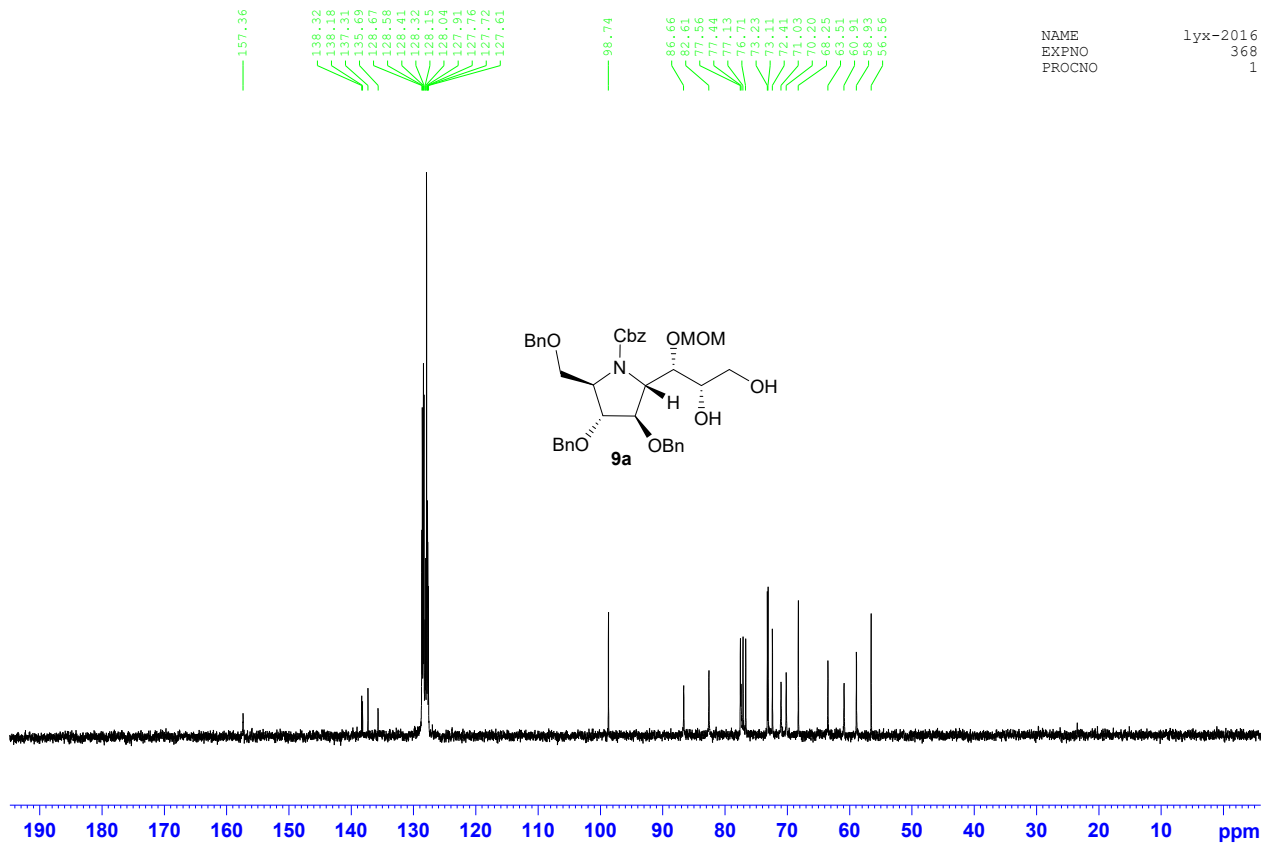
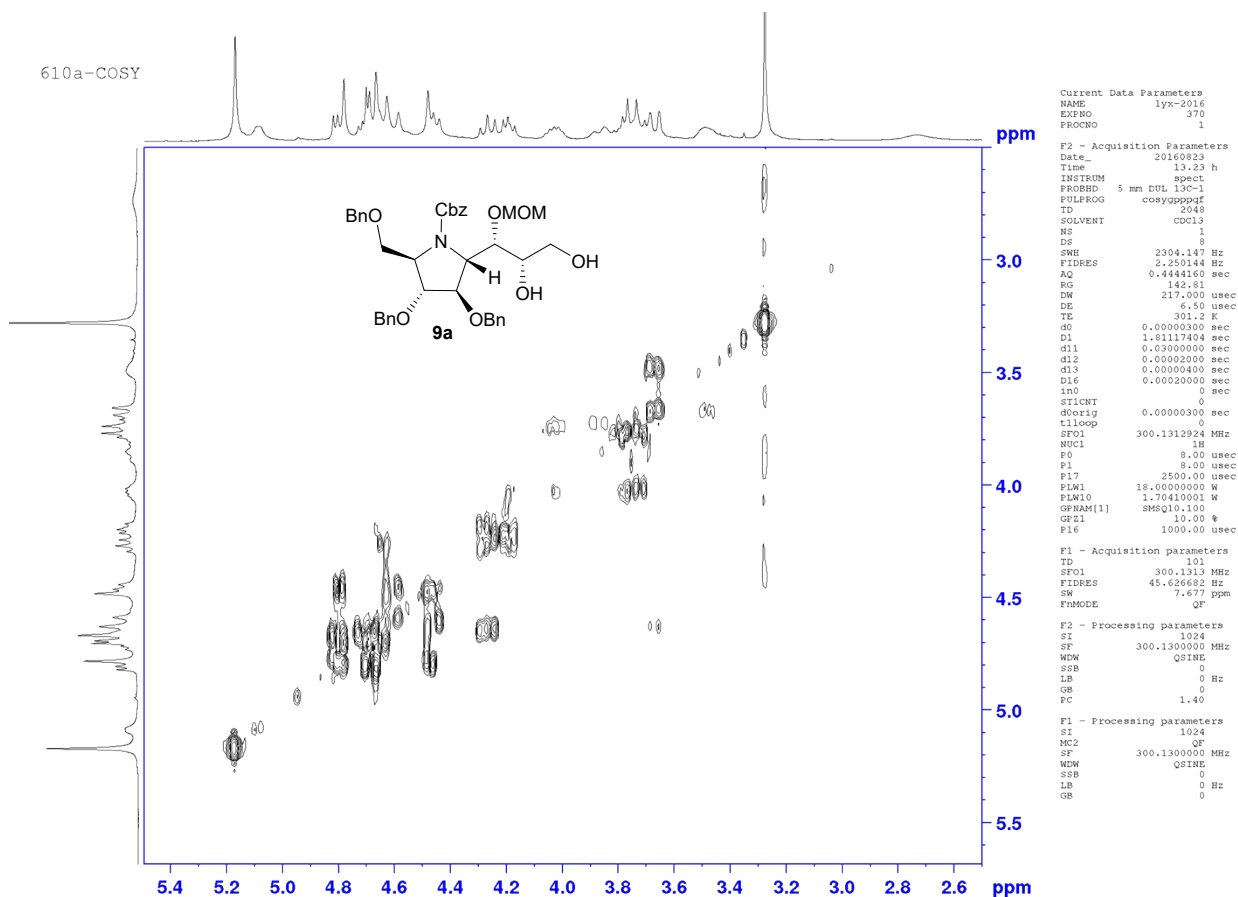




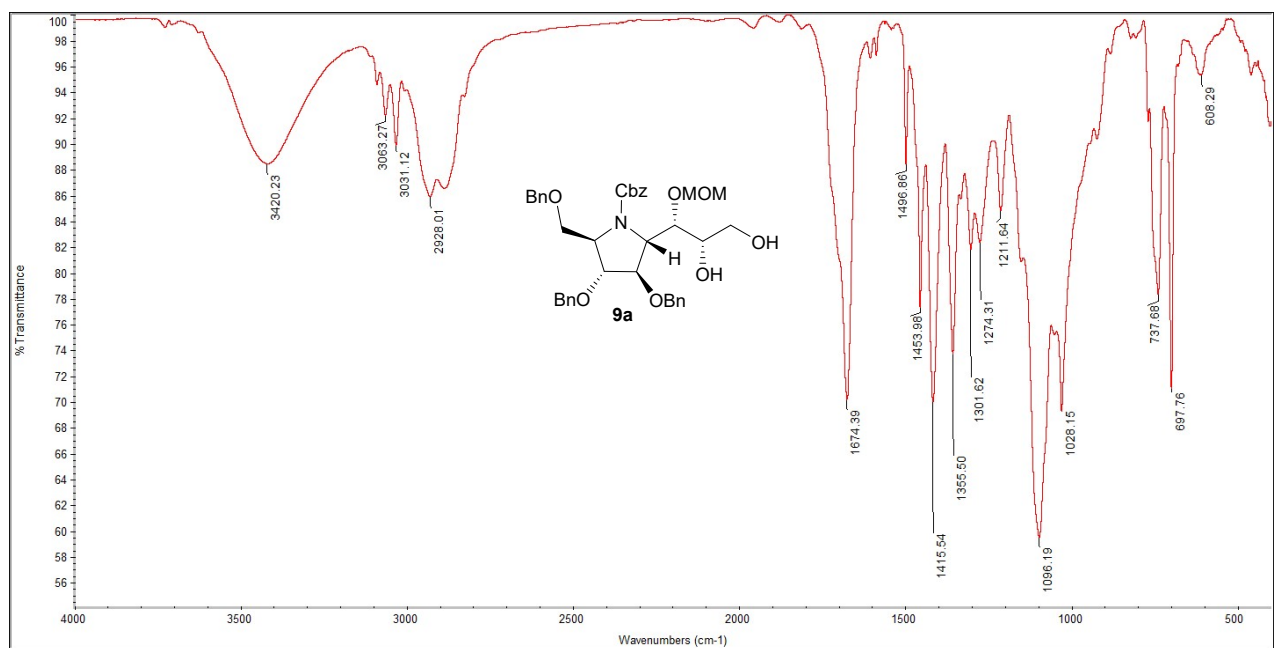
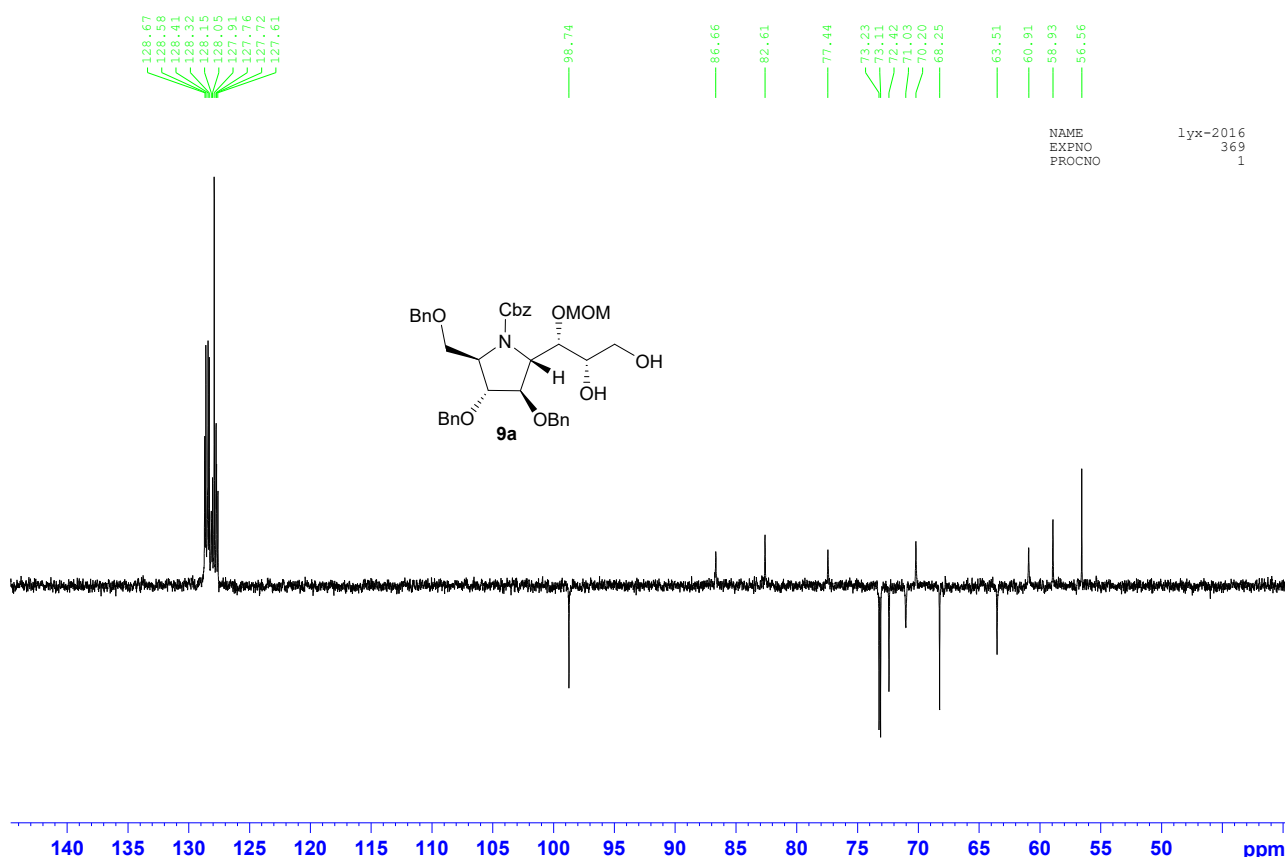
Compound 9a:

lyx-610a



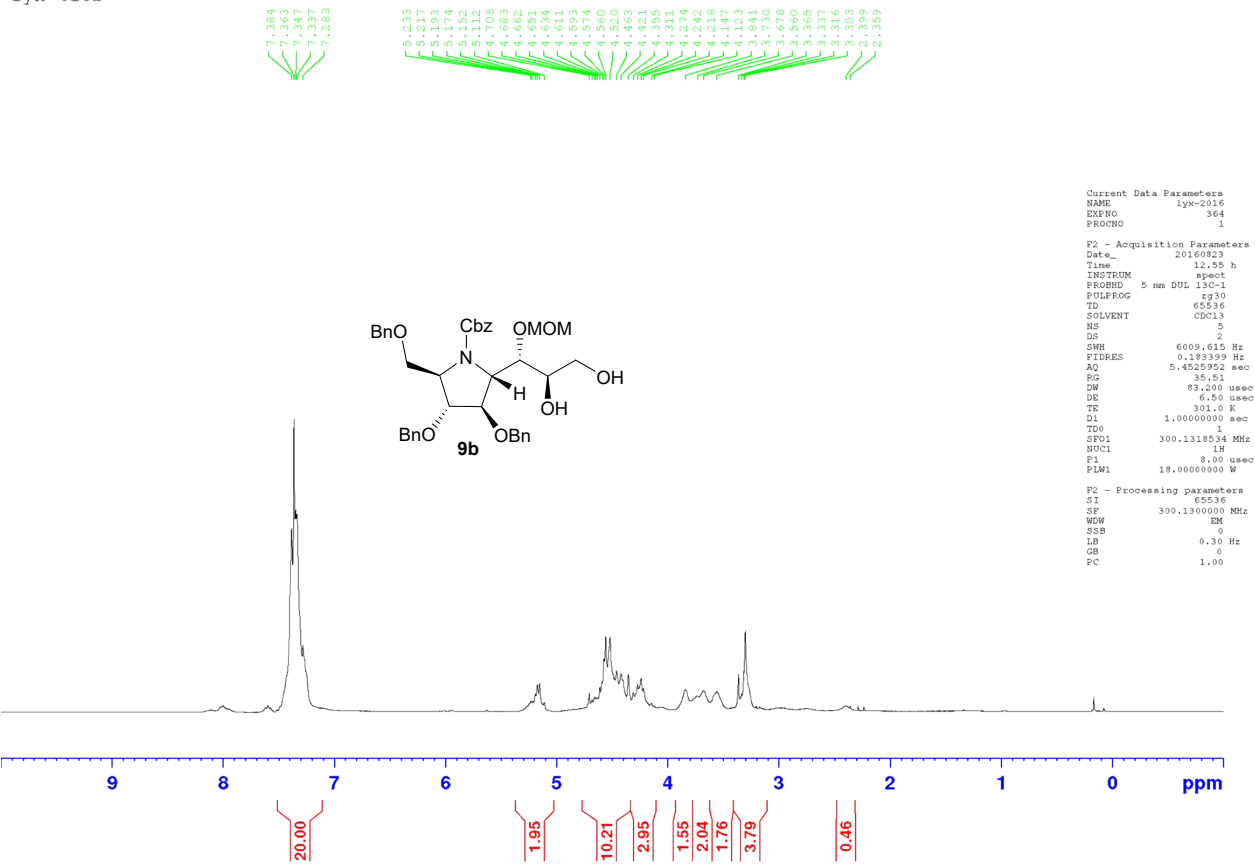


lyx-610a-dept135

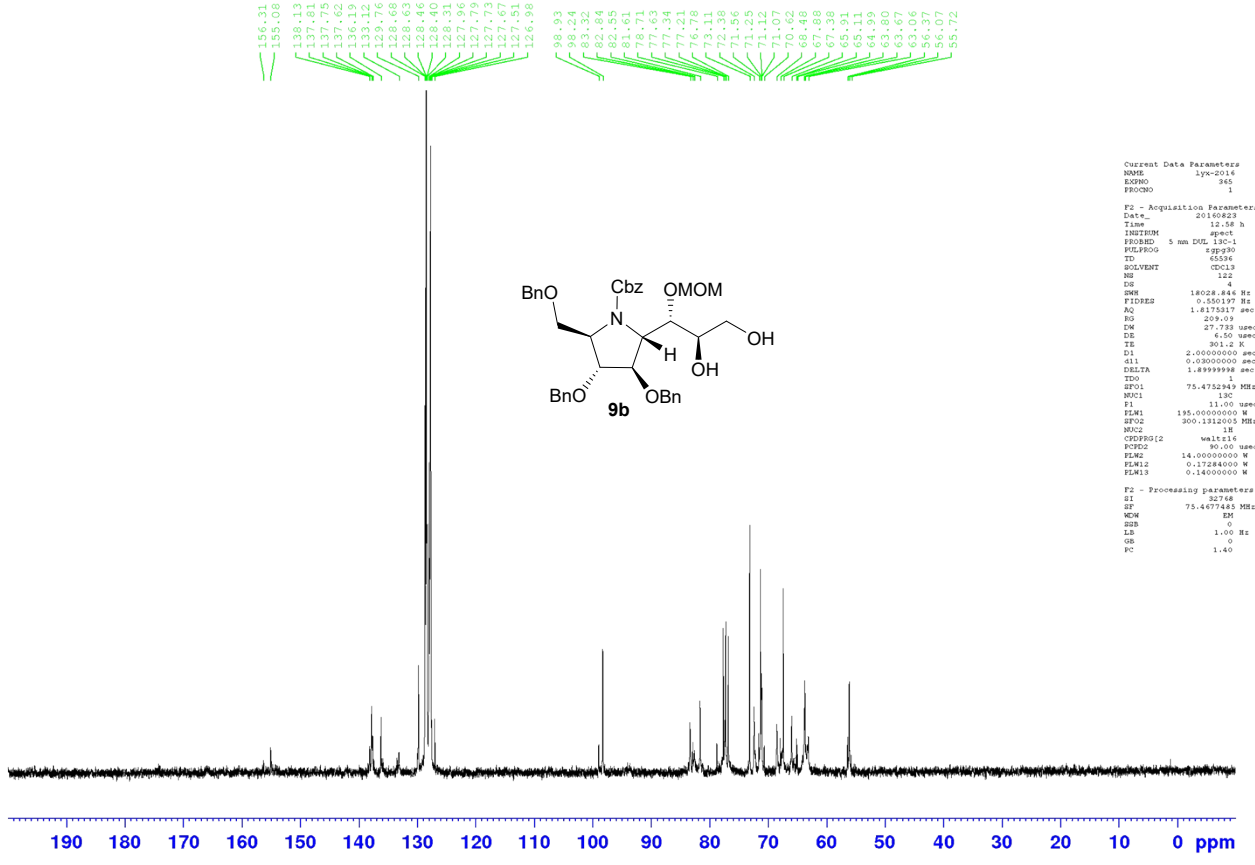


Compound 9b:

lyx-610b



lyx-610b-C13



lyx-610b-dept135

129.76
128.68
128.63
128.46
128.40
128.31
127.96
127.73
127.67
126.98

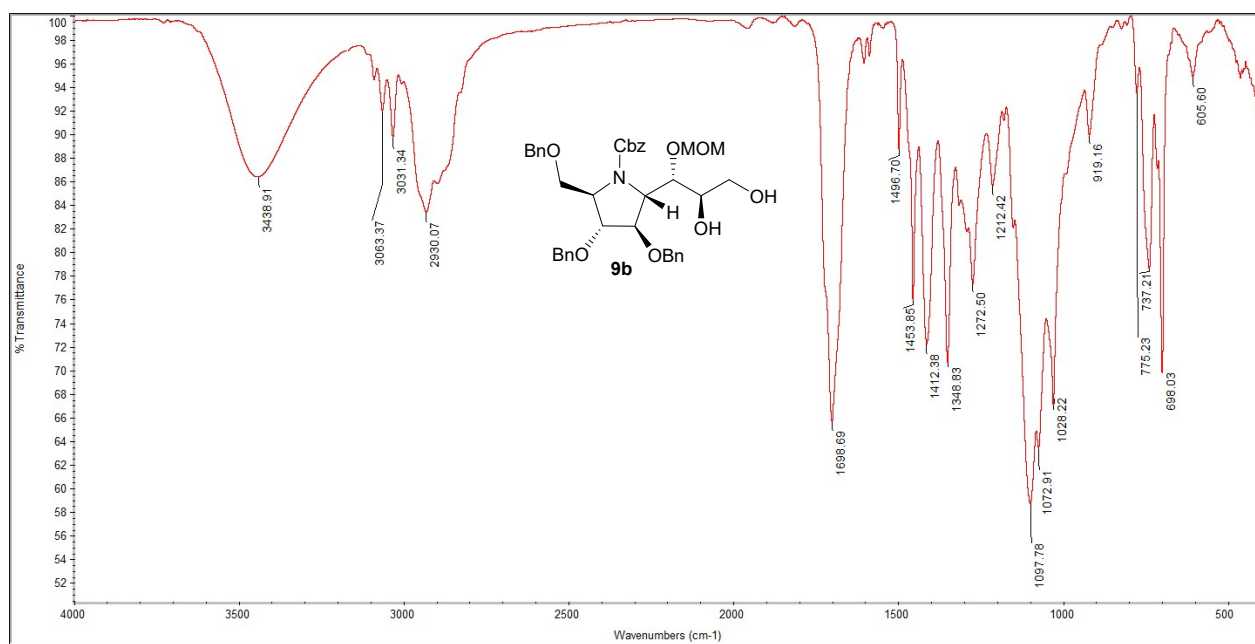
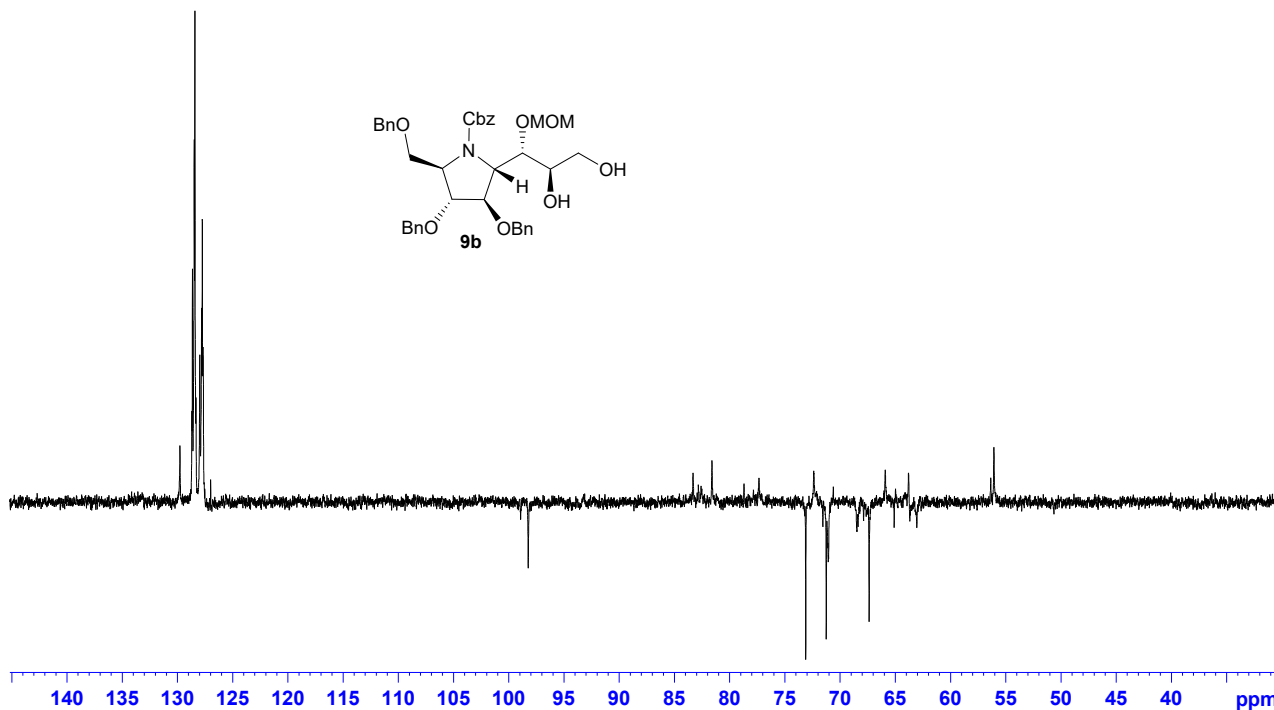
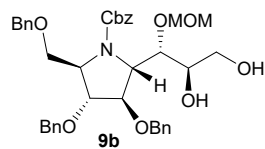
98.93
98.24

83.32
82.84
82.60
81.61
78.70
77.35
73.12
72.39
71.56
71.26
71.08
68.48
67.88
65.92
63.11
63.81
63.06

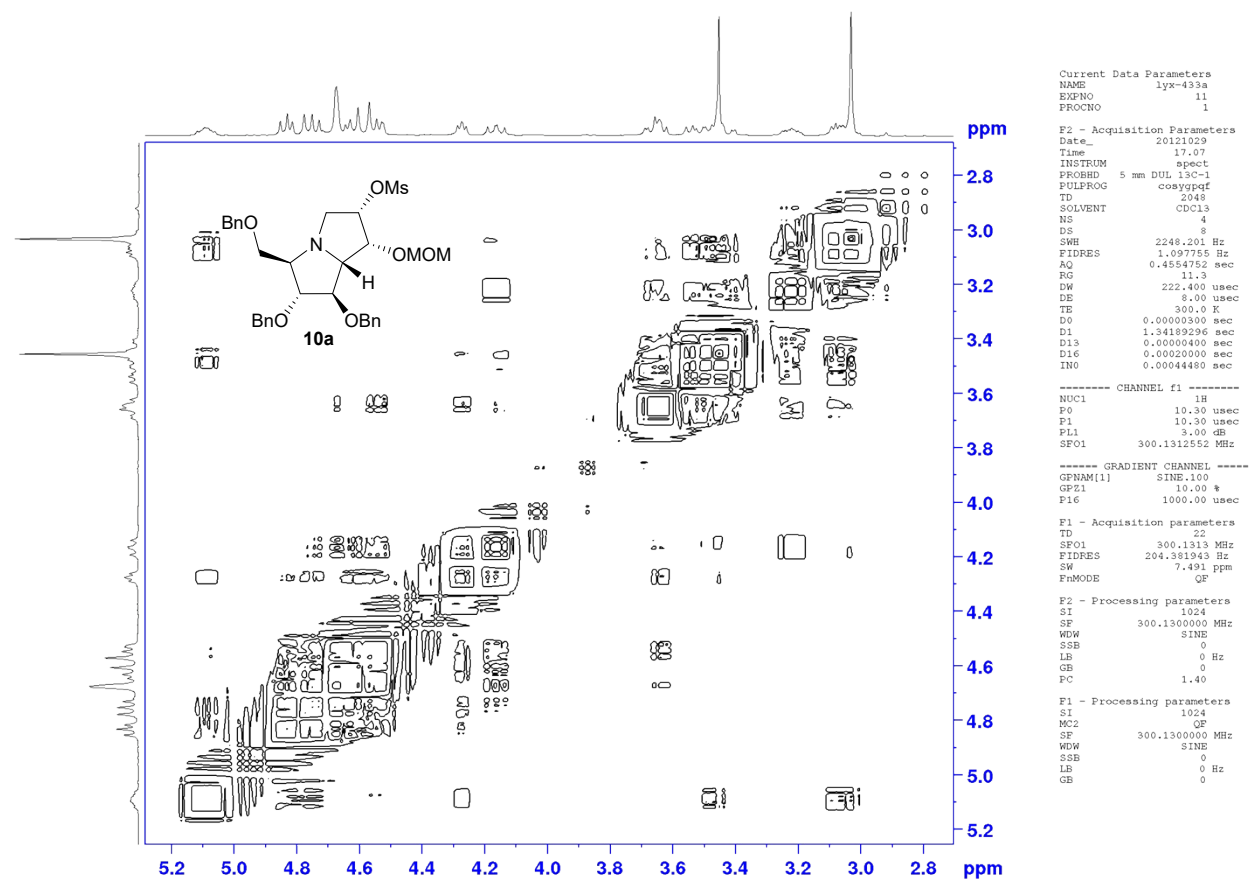
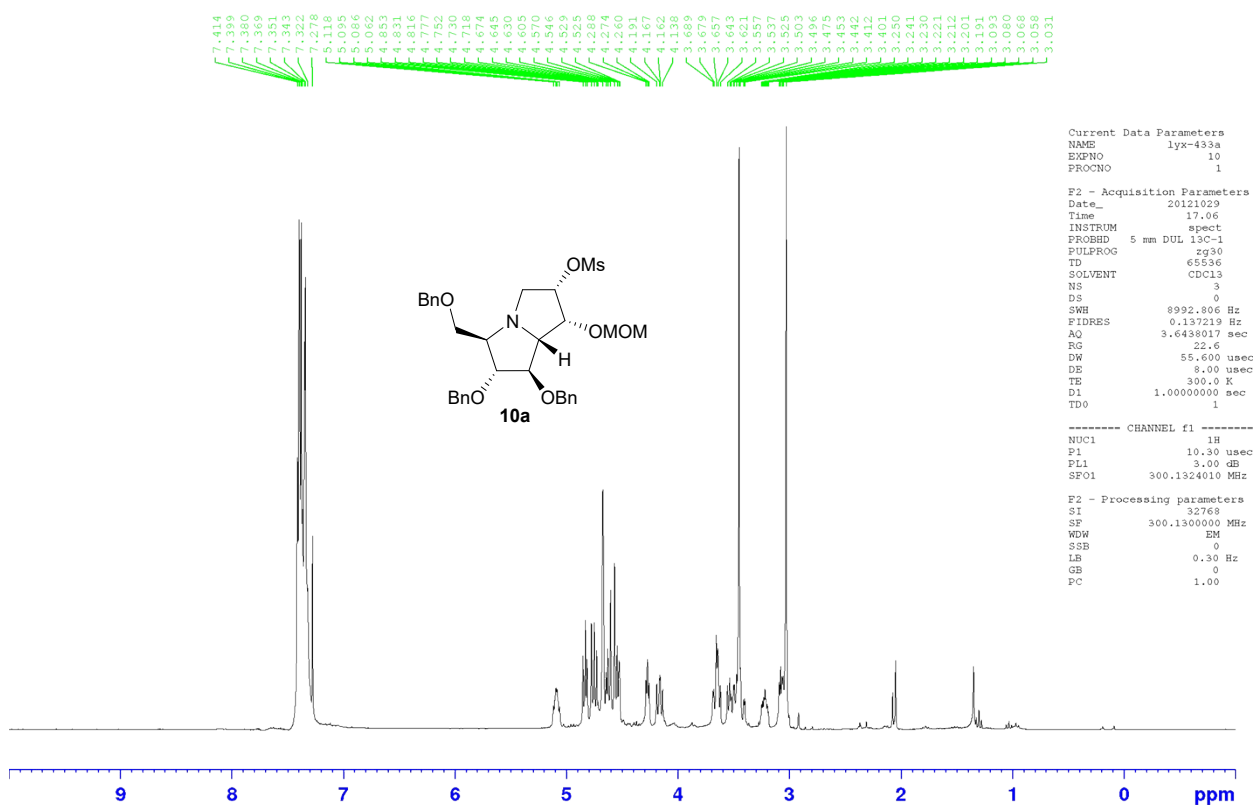
56.37
56.08

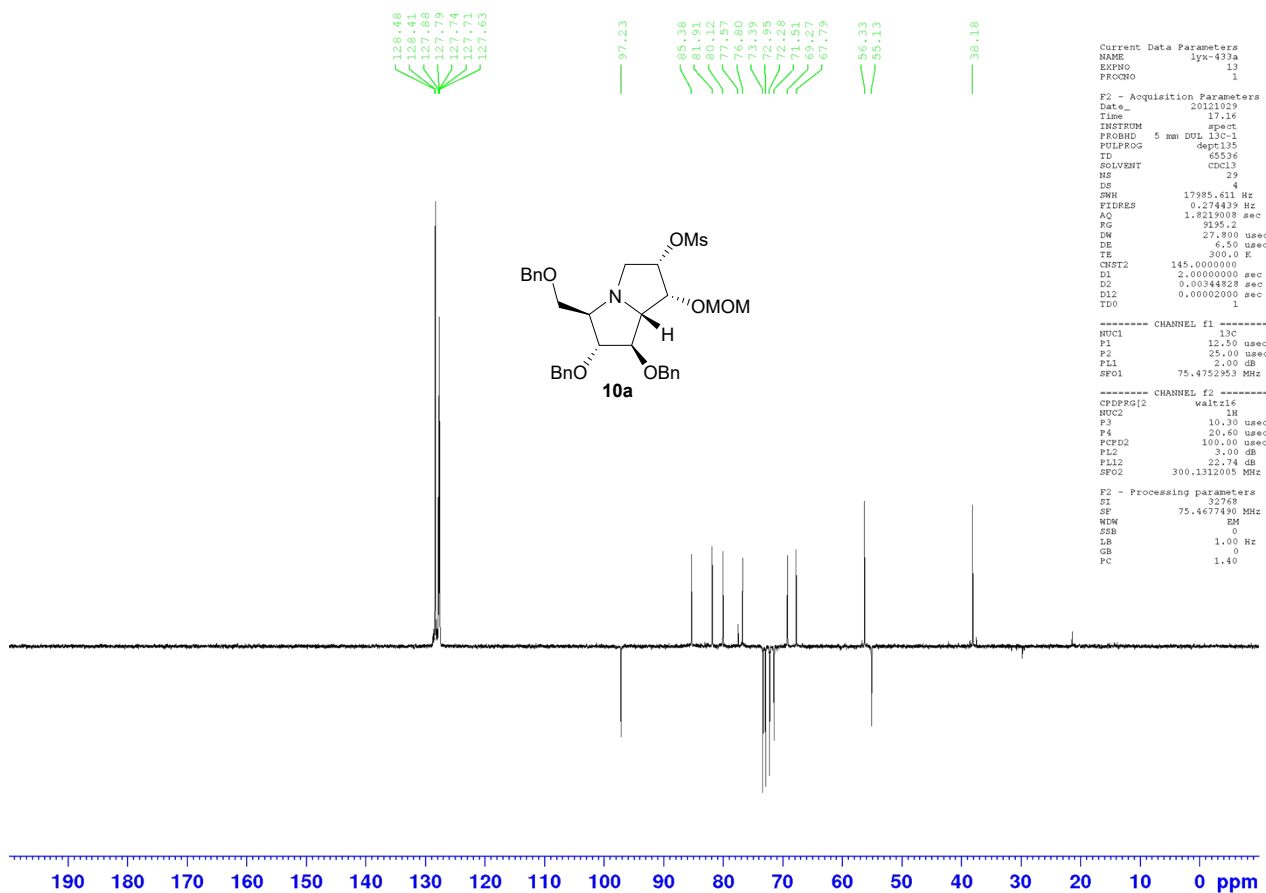
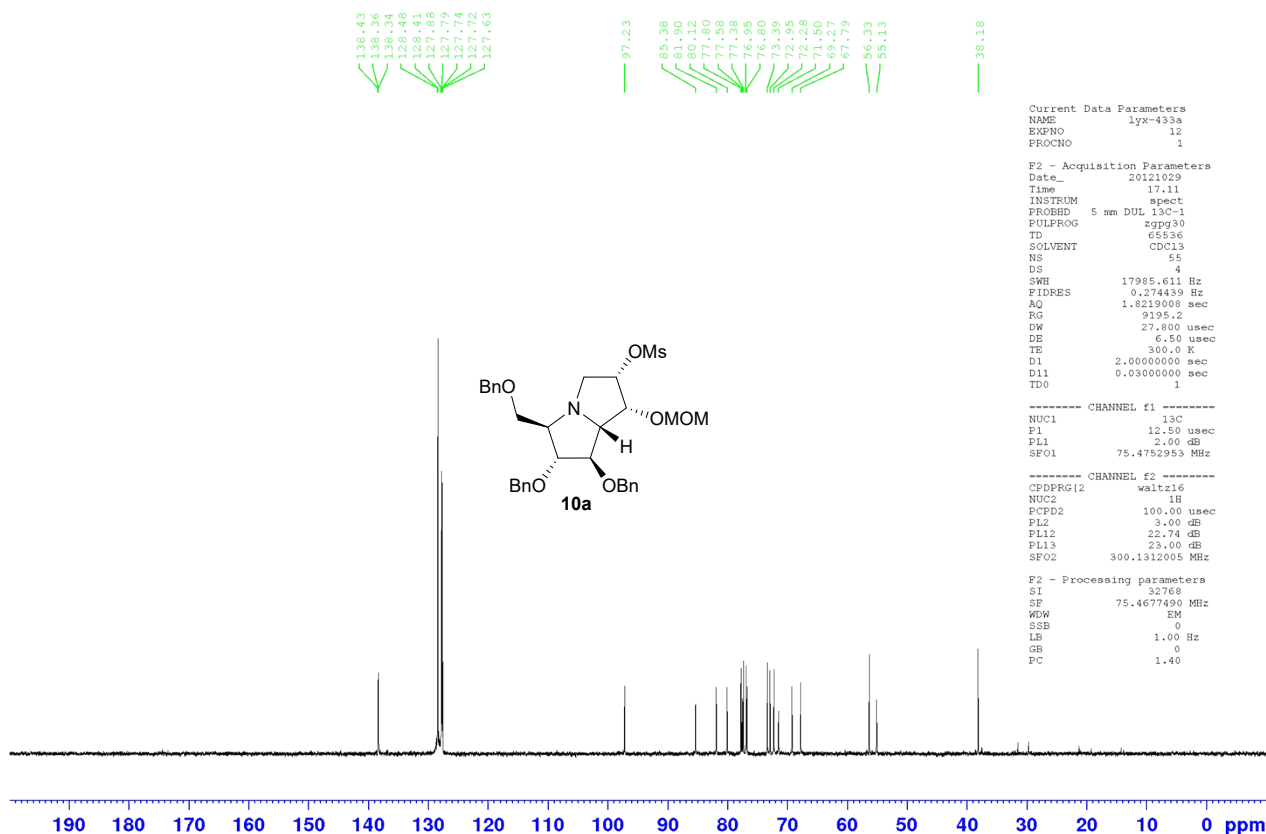
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EXPNO
PROCNO

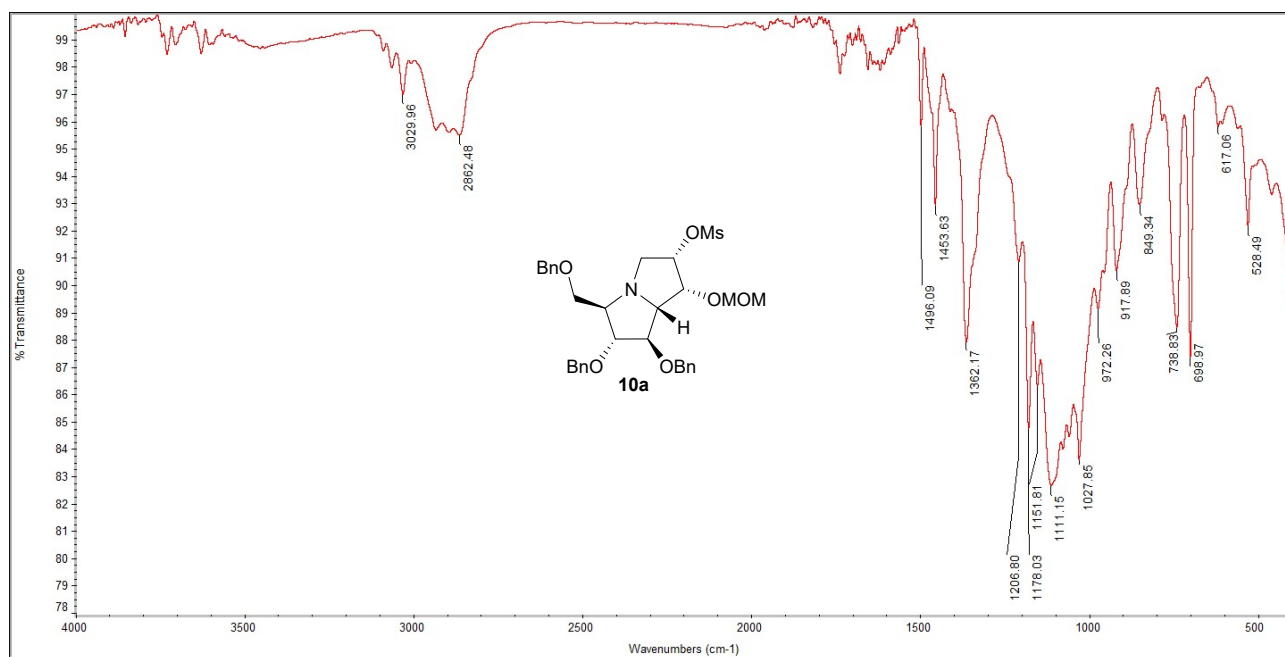
lyx-2016
366
1



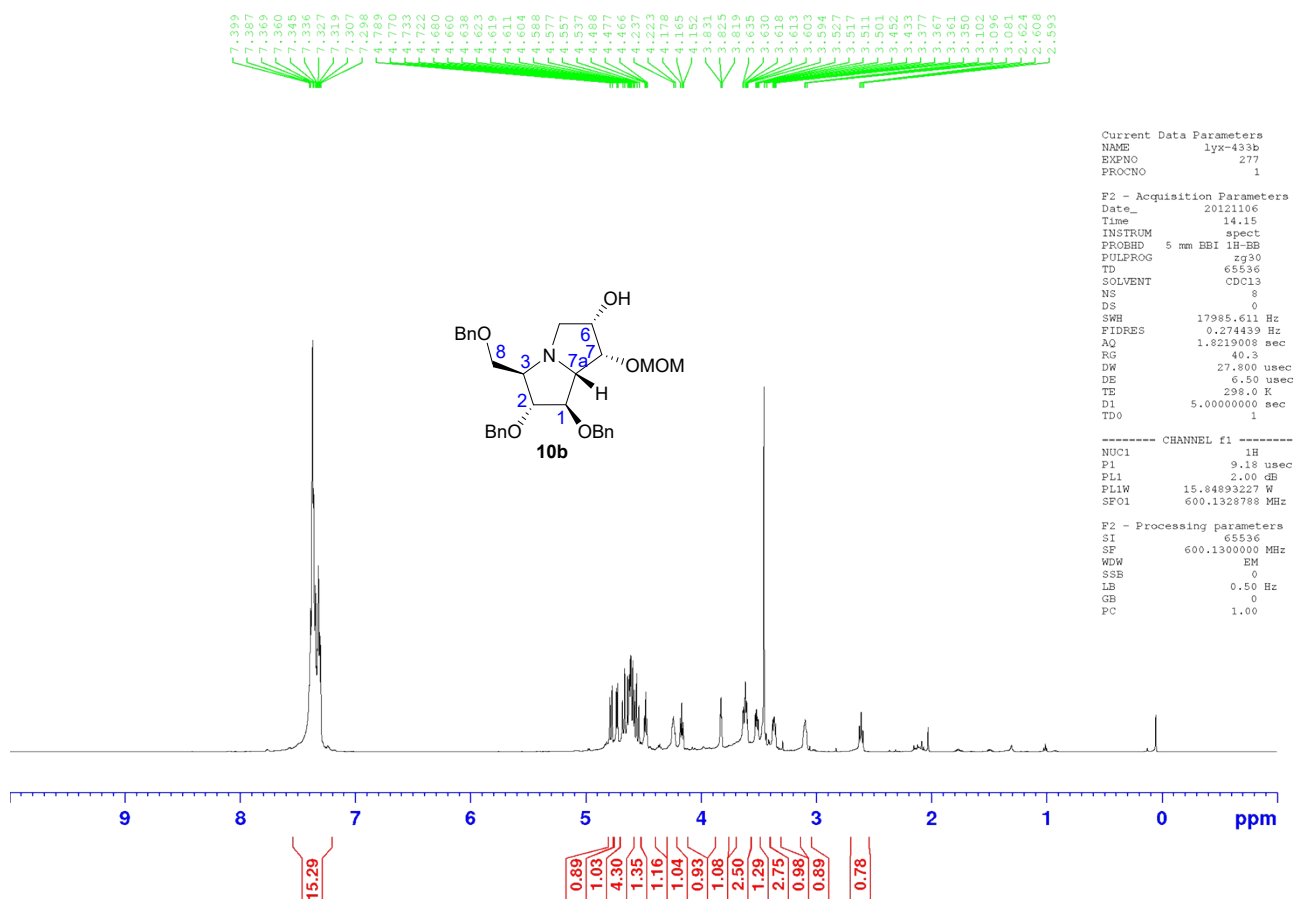
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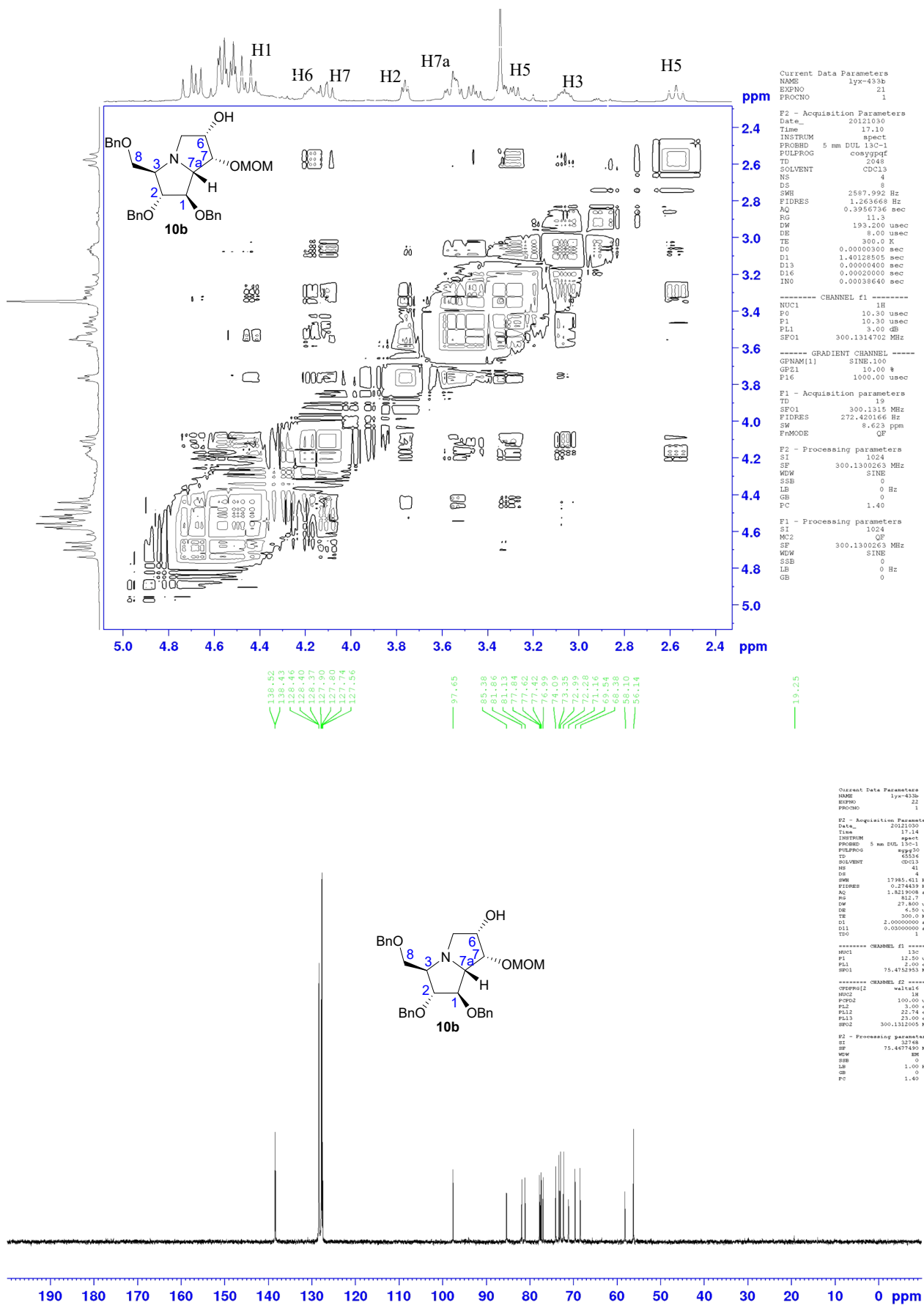


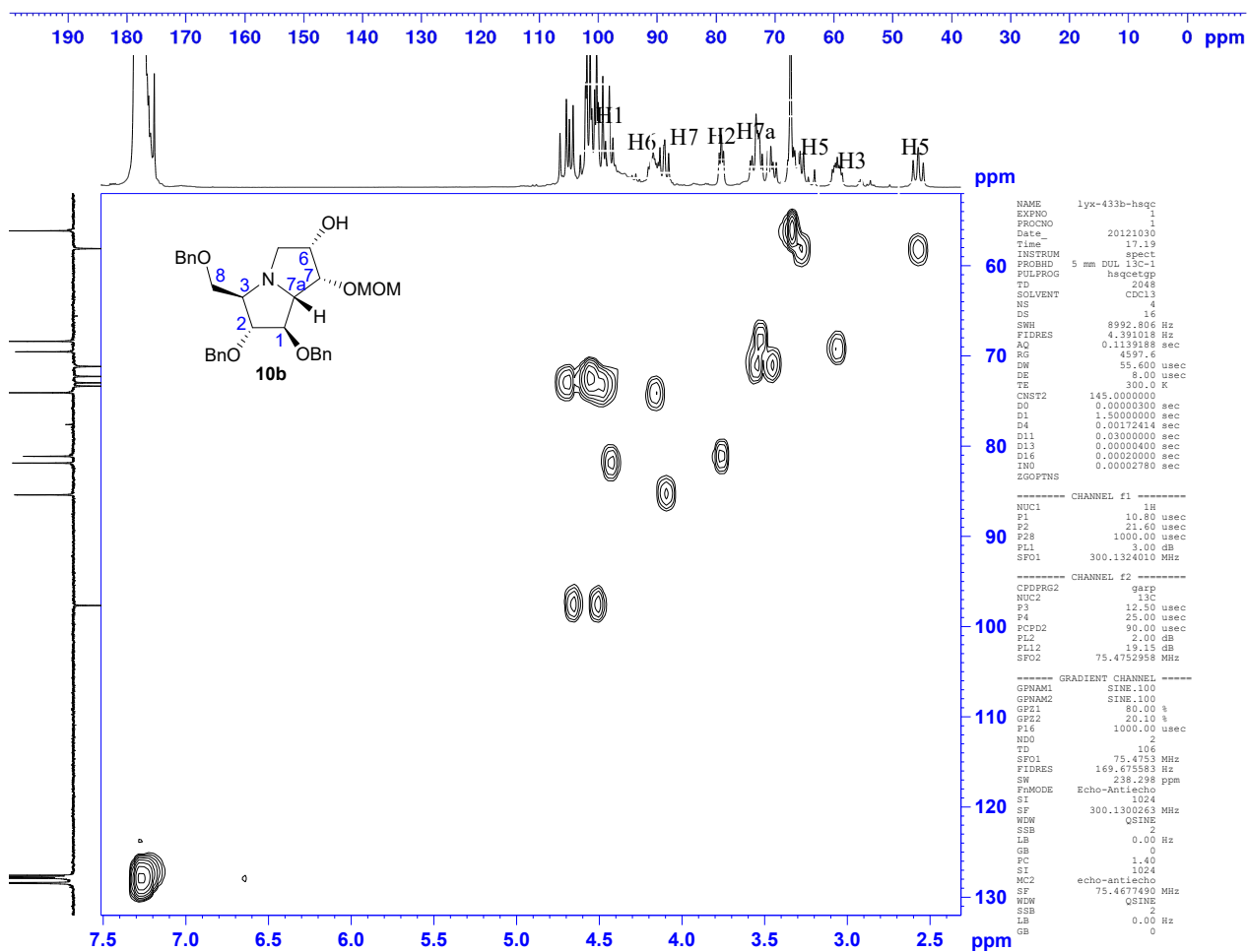
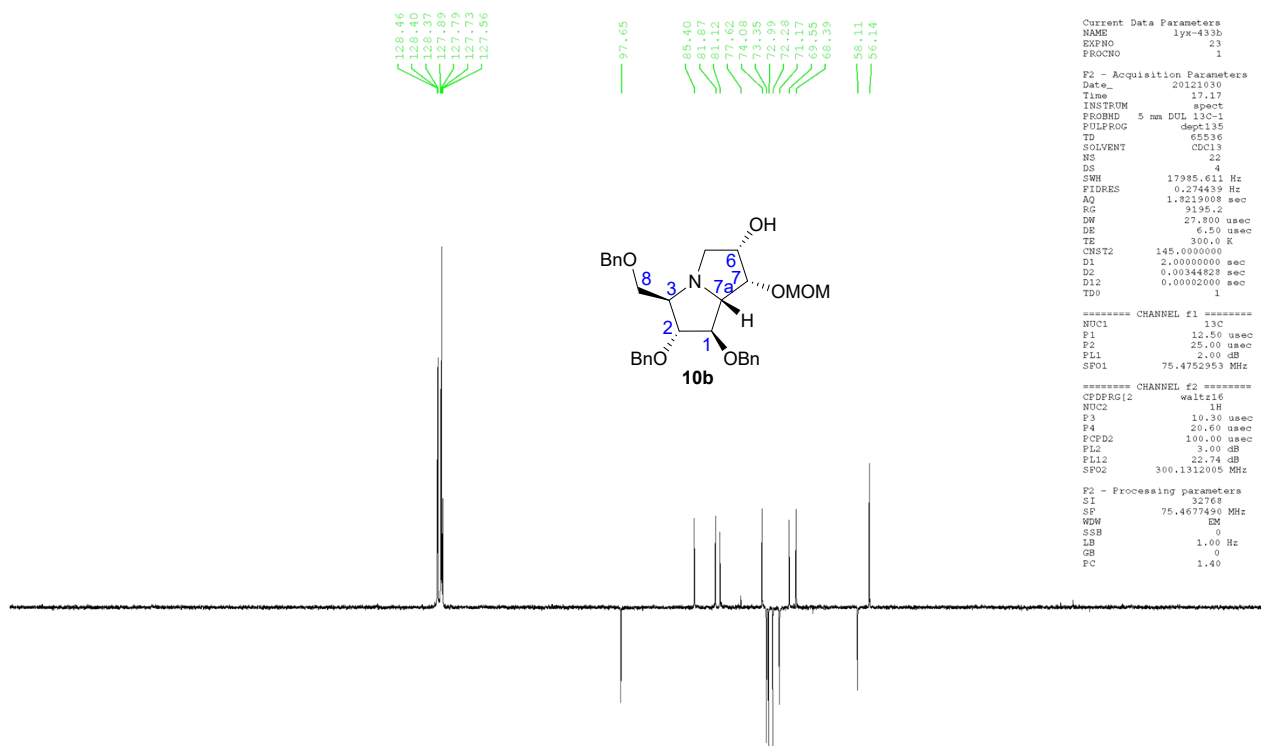


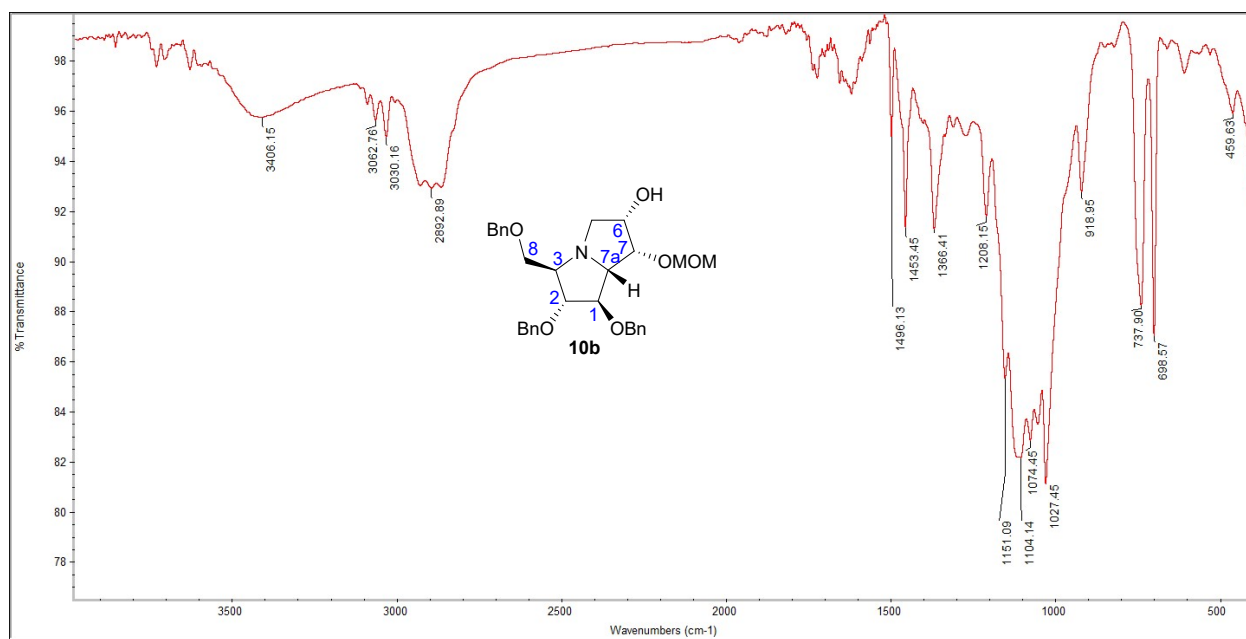
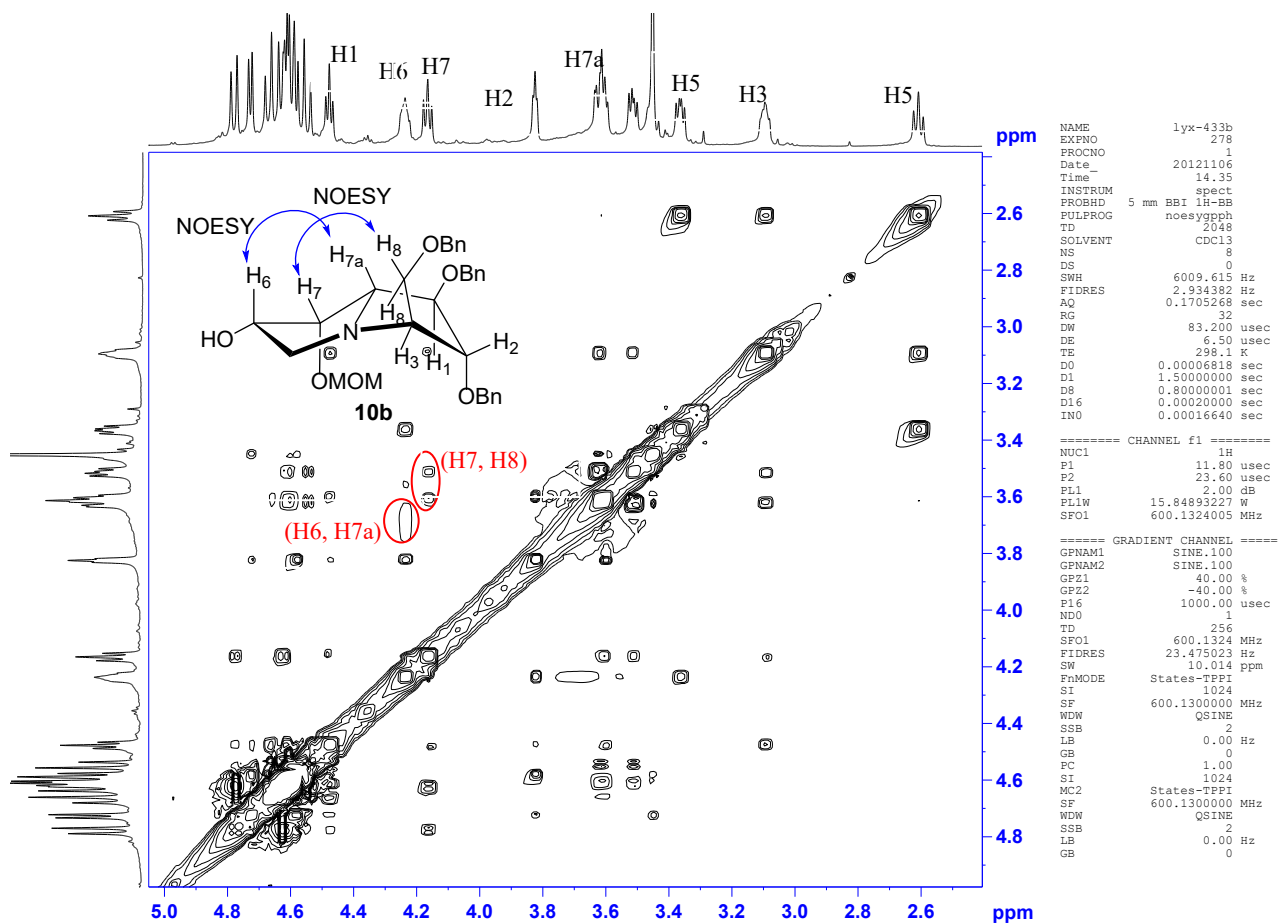


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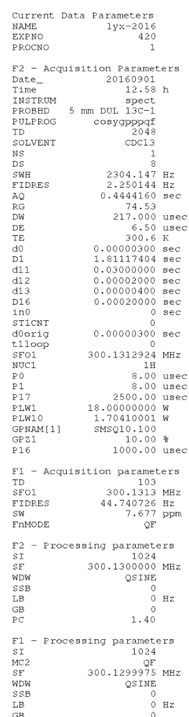
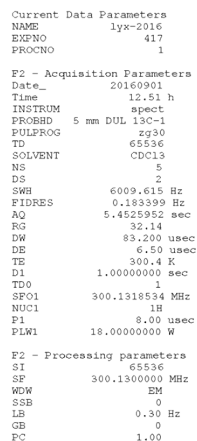




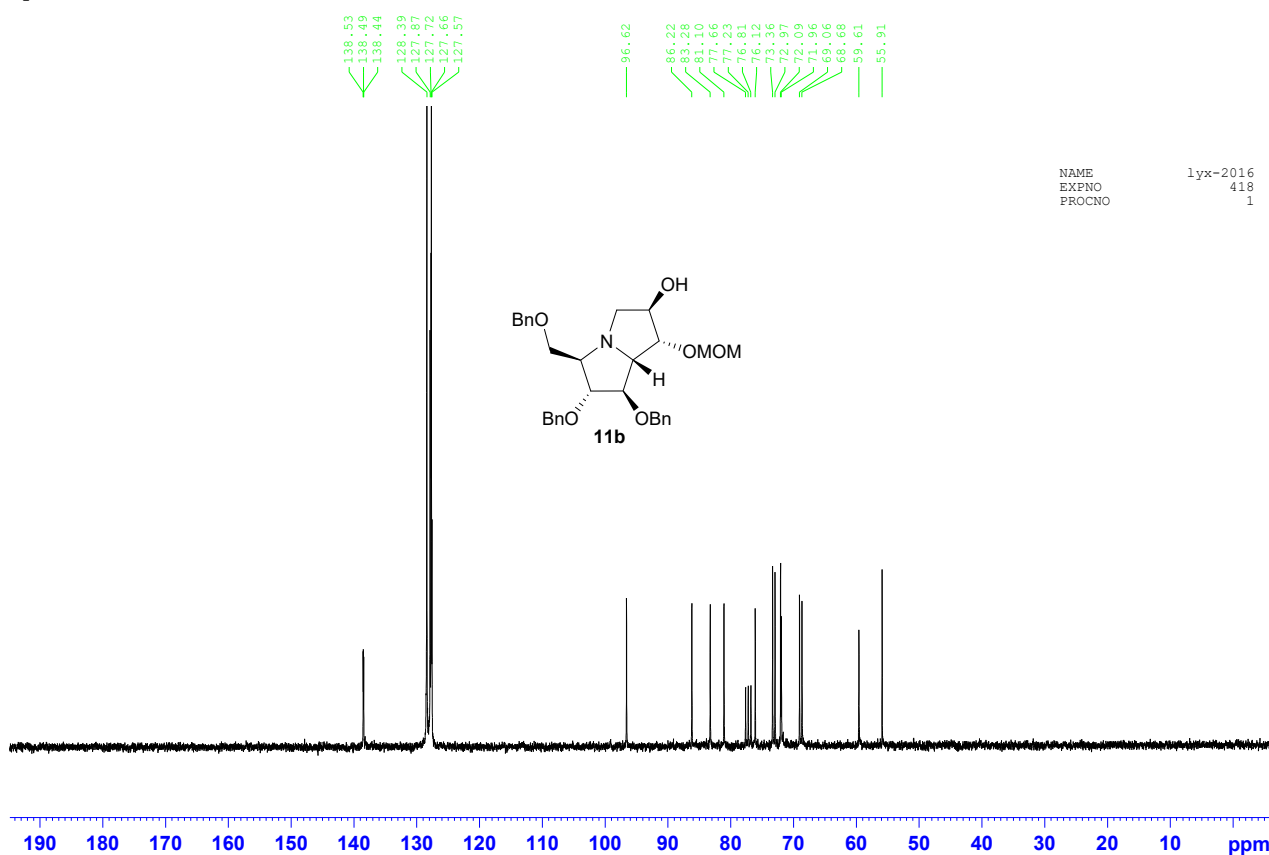




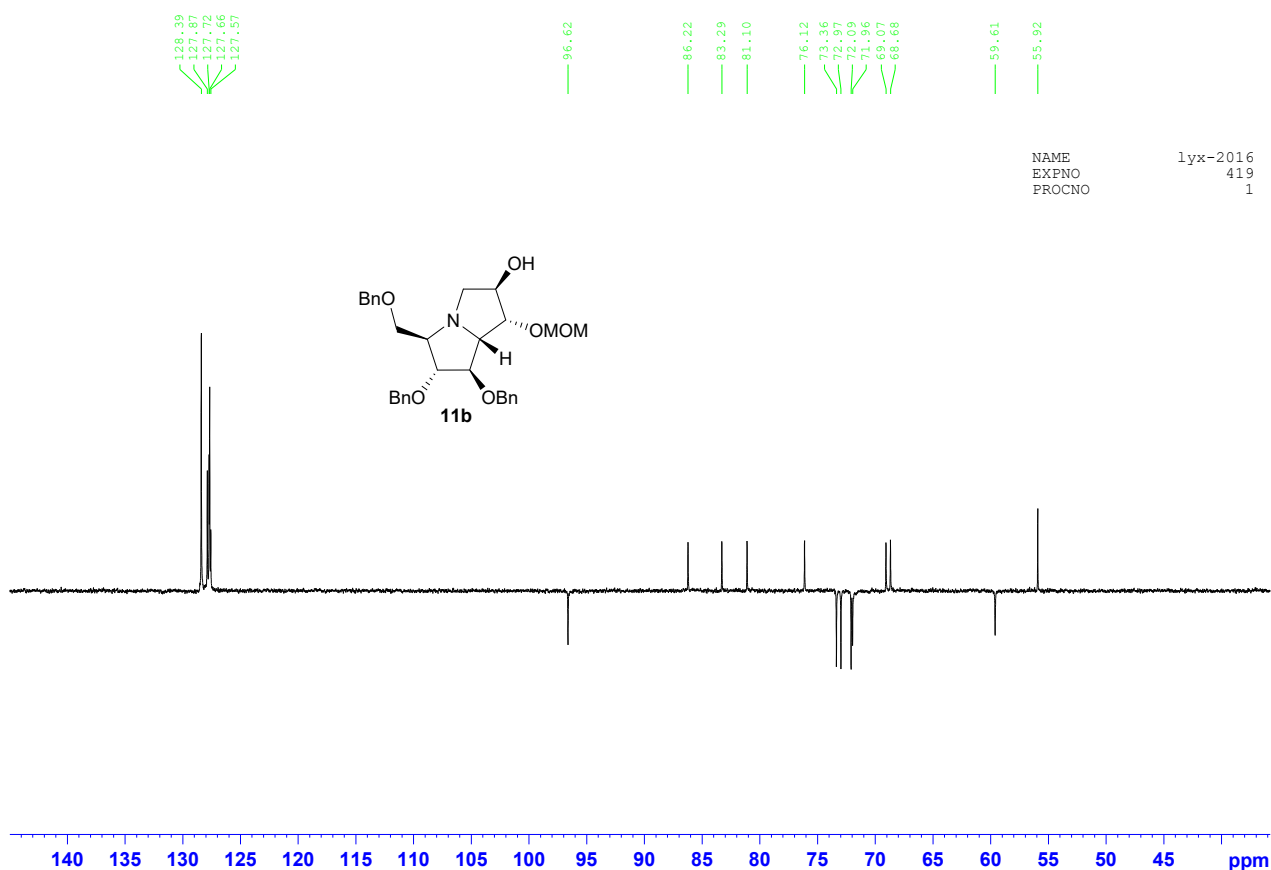
lyx-619b

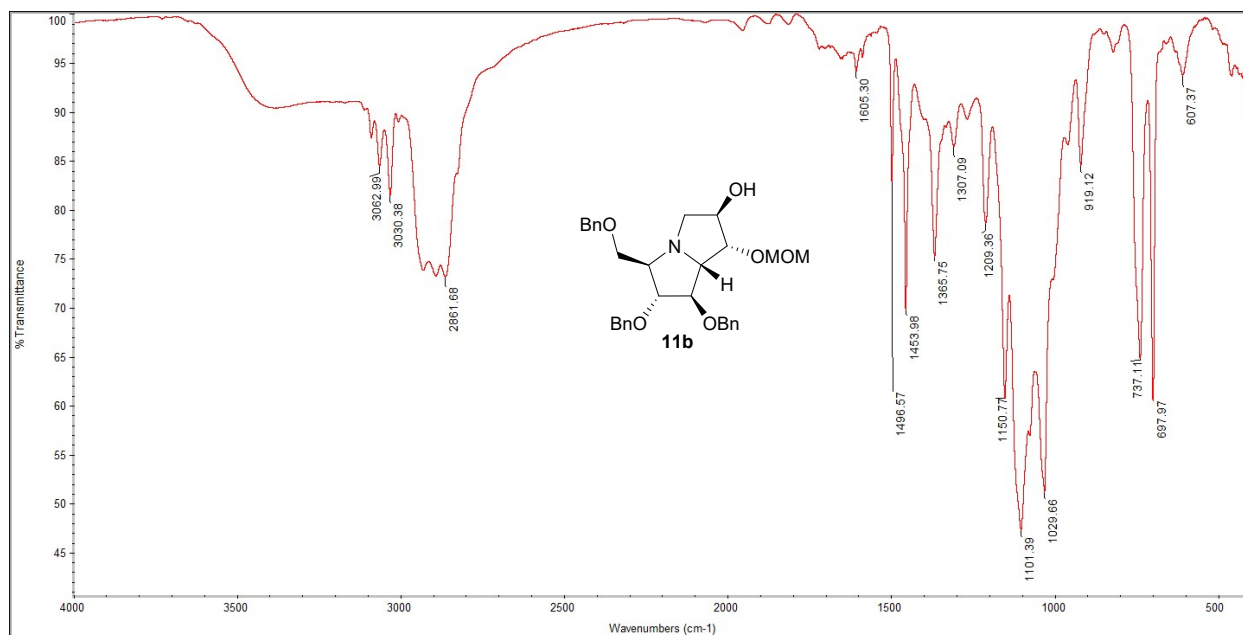


lyx-619b-C13

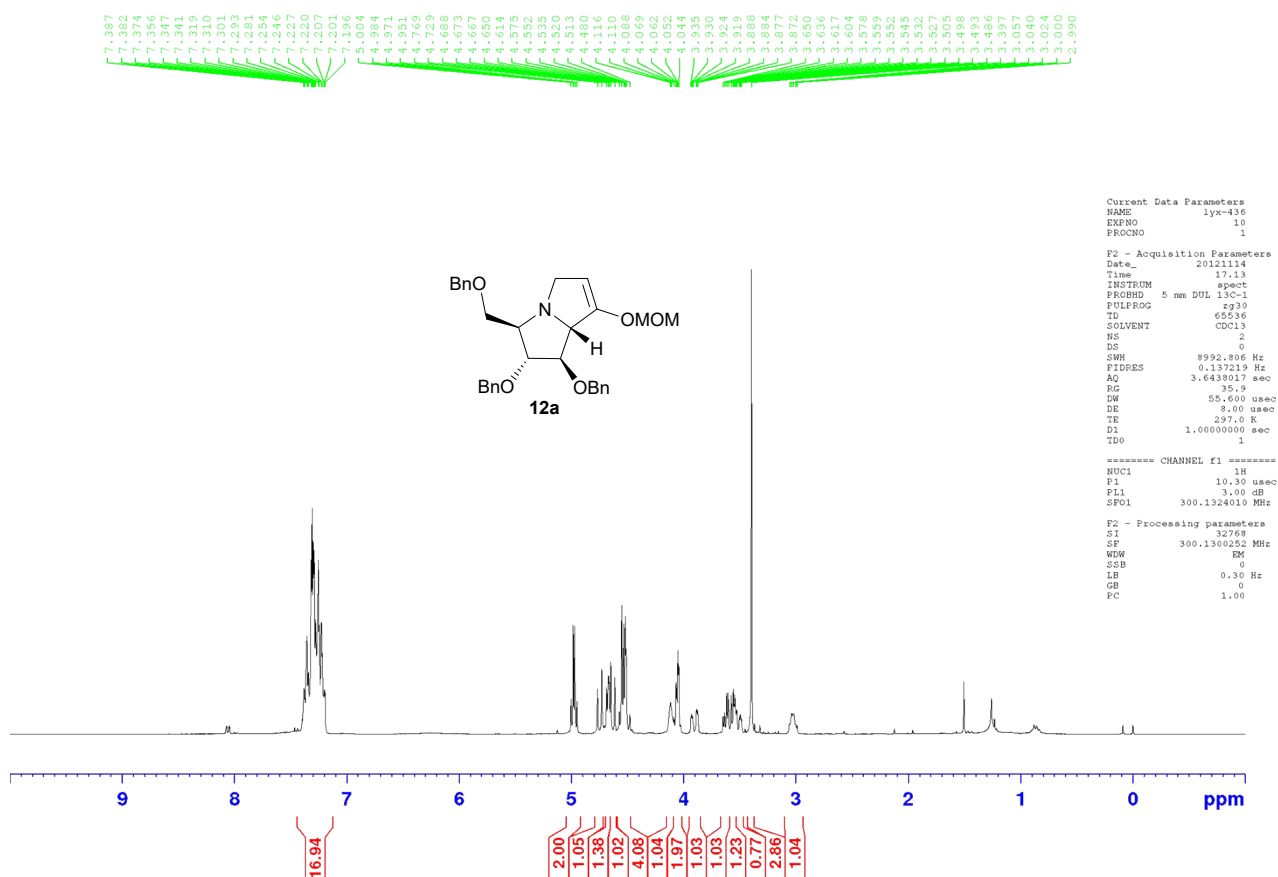


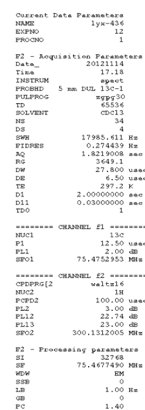
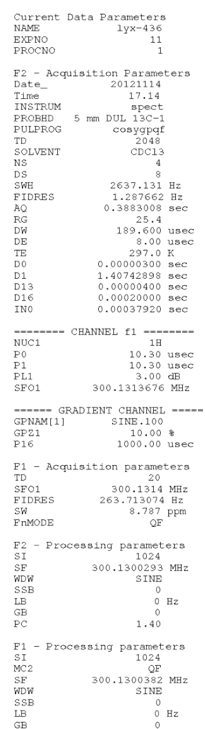
lyx-619b-dept135

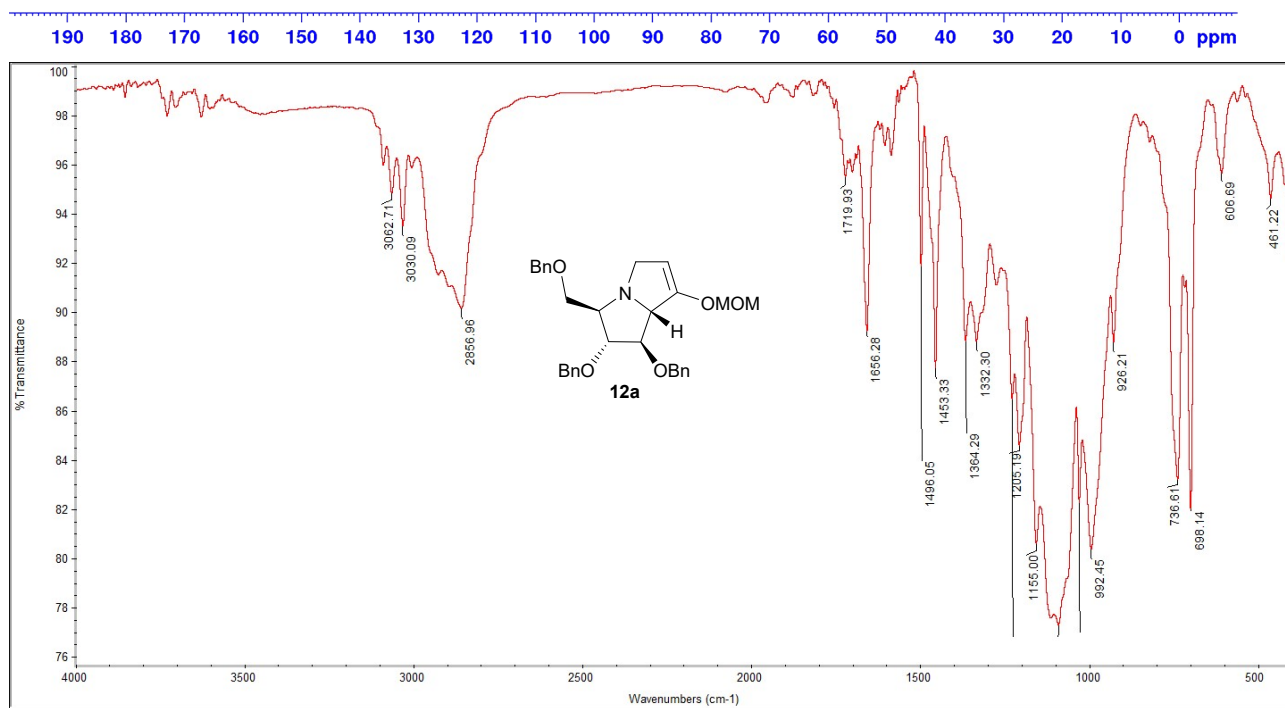
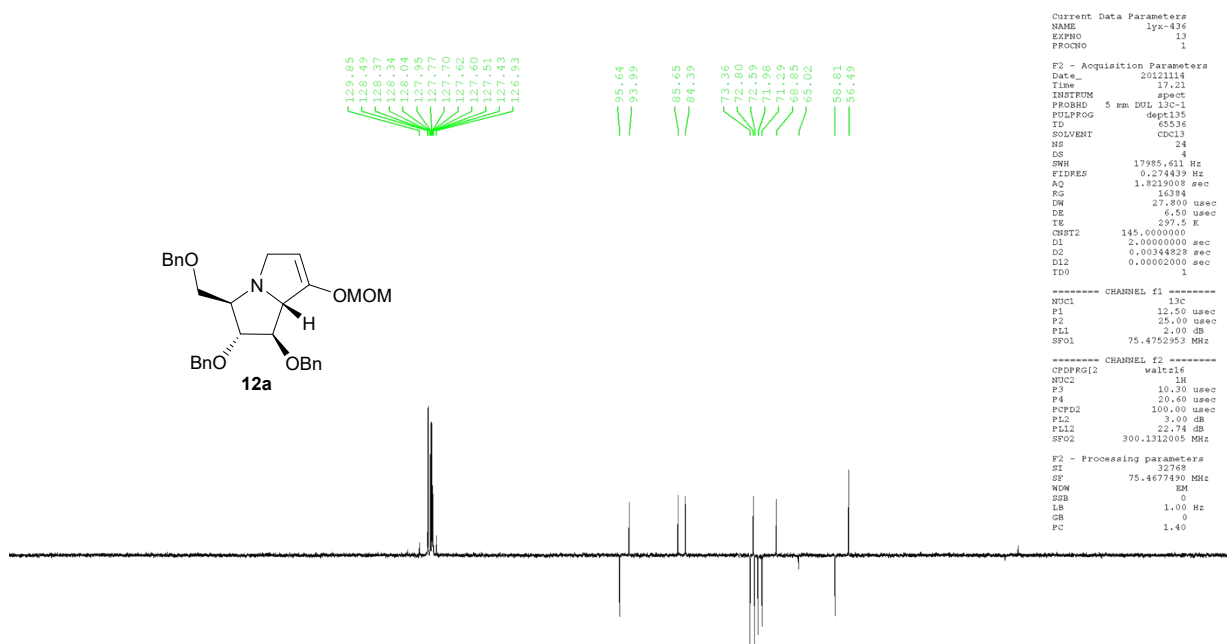




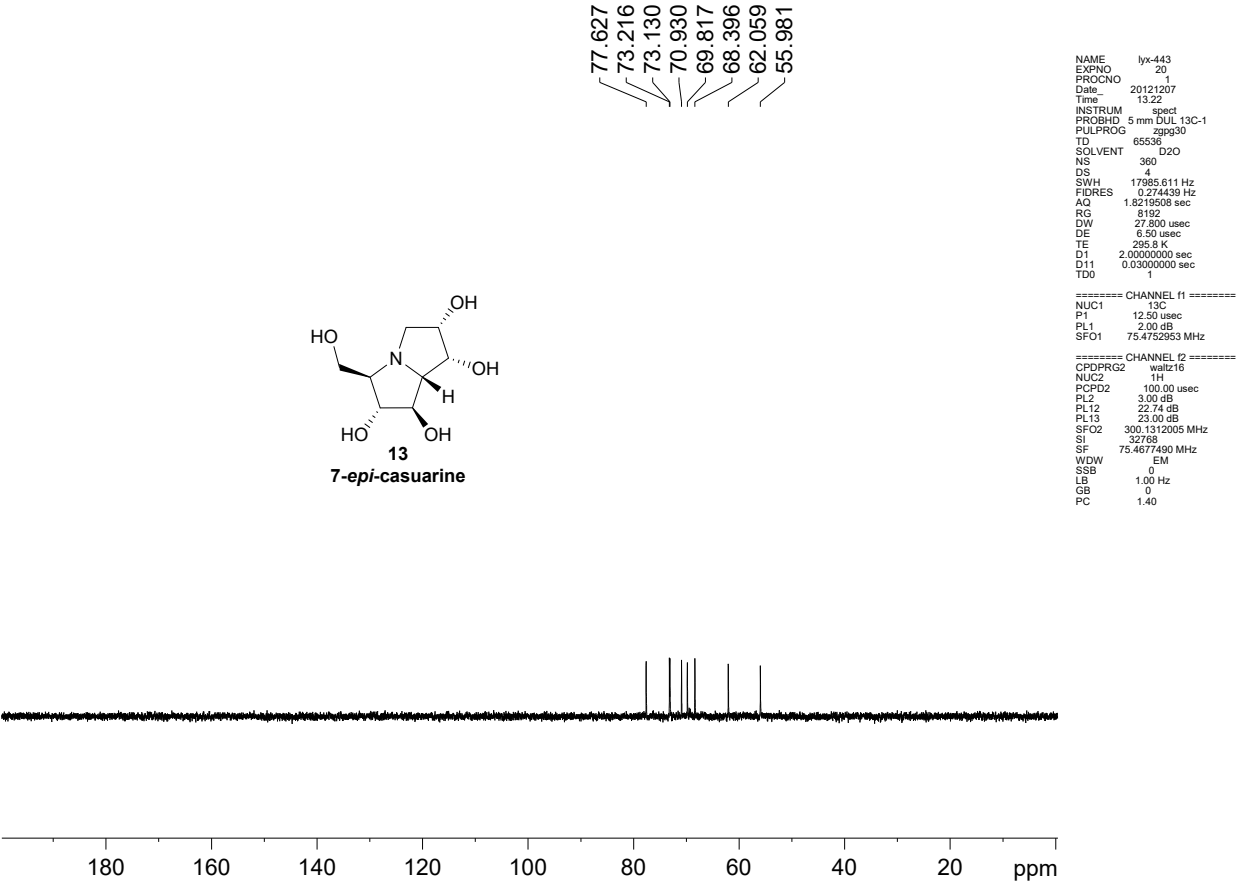
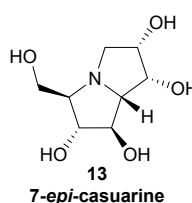
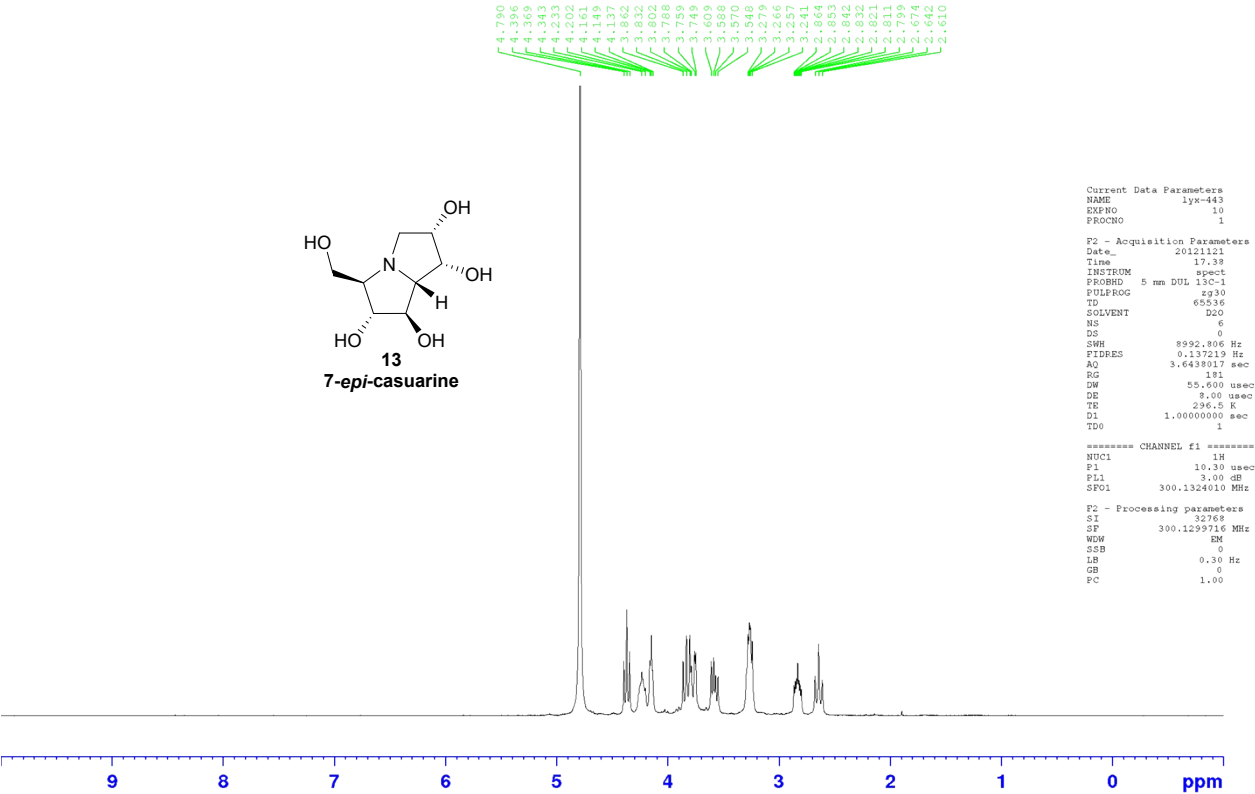
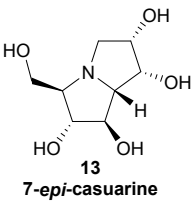
Compound 12a:





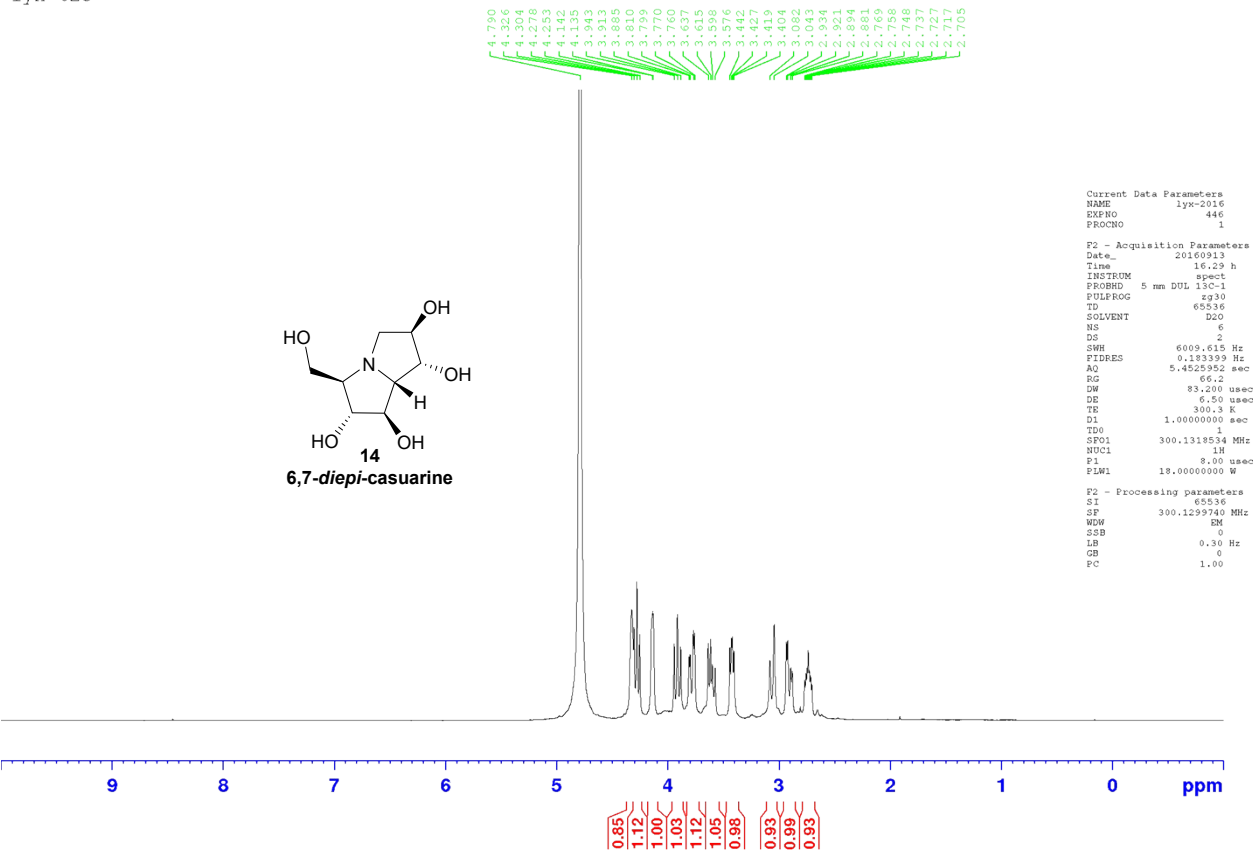
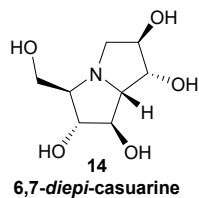


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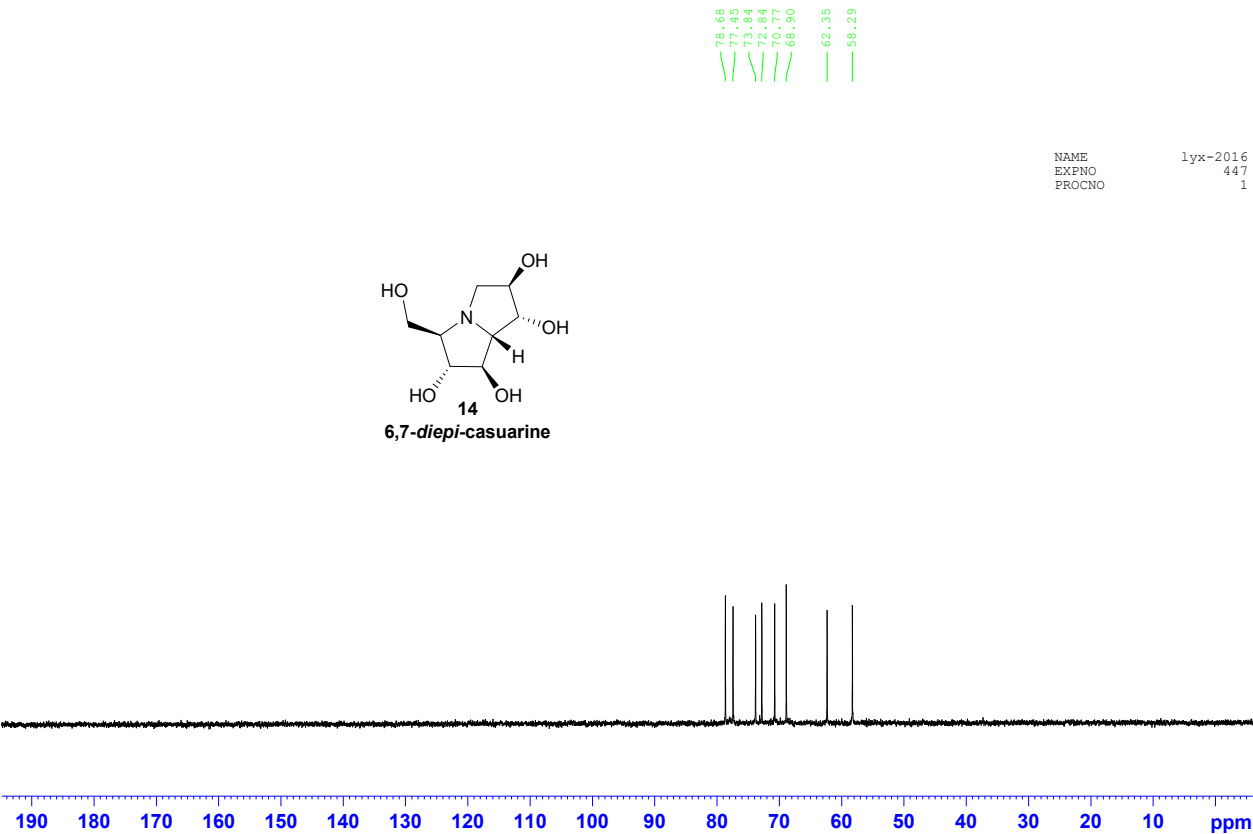
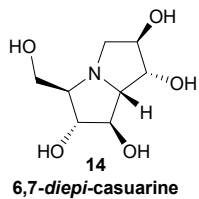


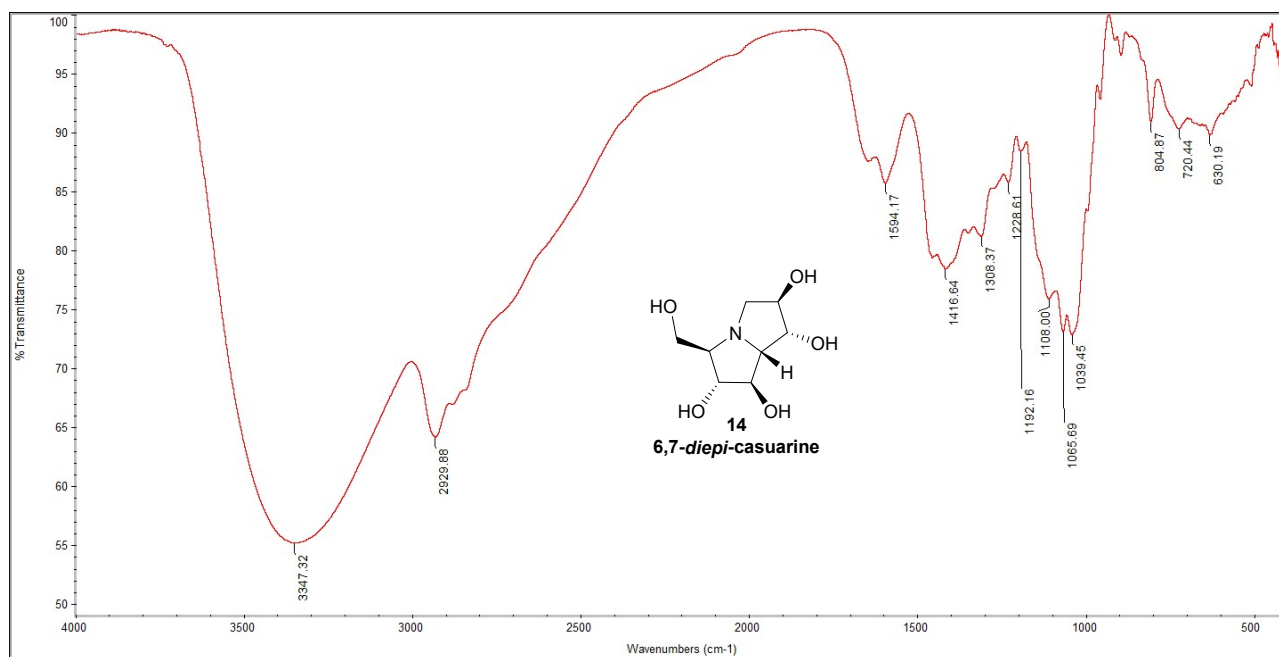
Compound 14:

lyx-623



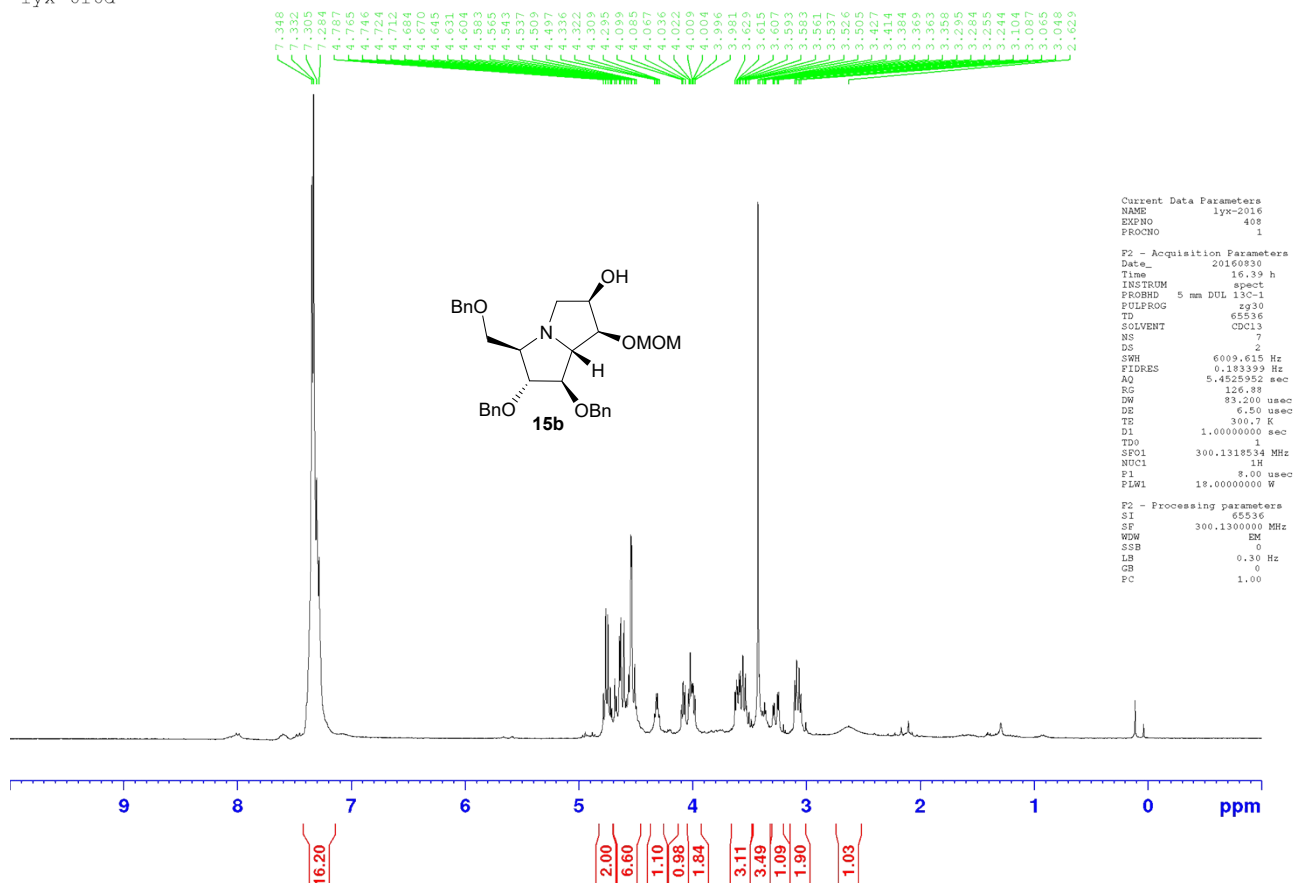
lyx-623-C13





Compound 15b:

lyx-616d



lyx-616d-dept135

128.40
128.32
127.74
127.69
127.66
127.49

96.54

86.27

85.73

82.18

73.27

72.25

71.69

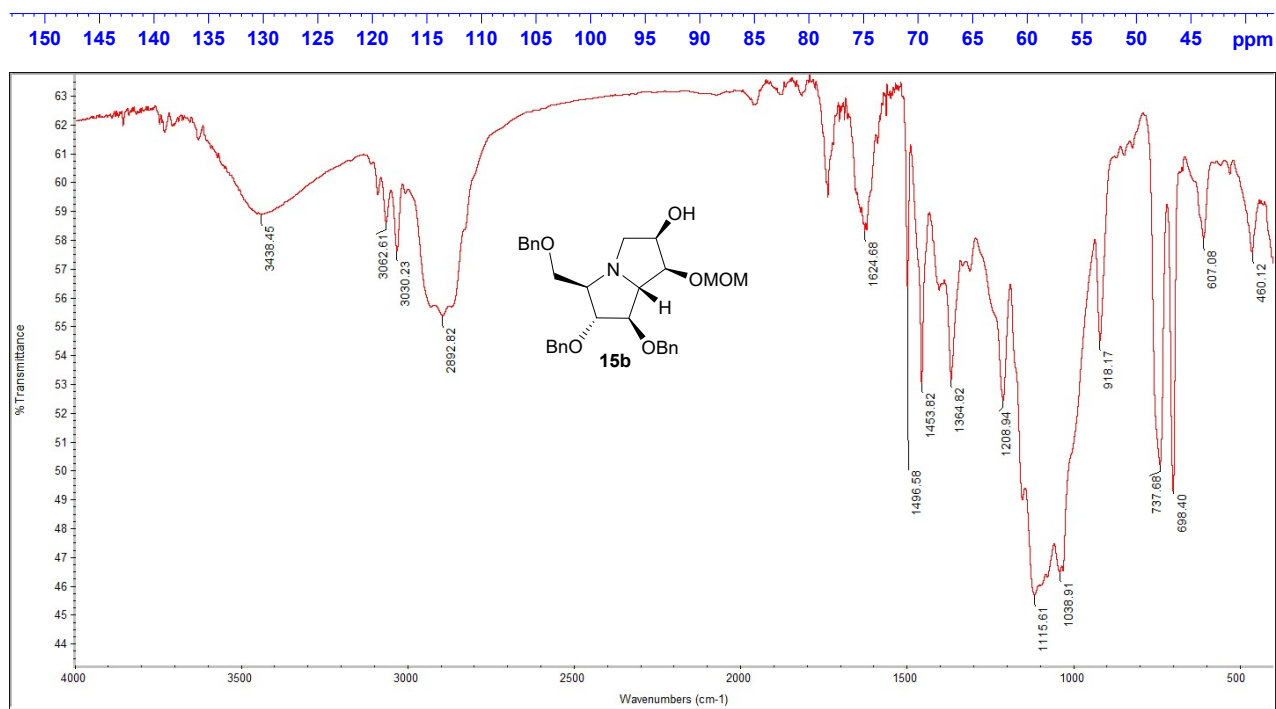
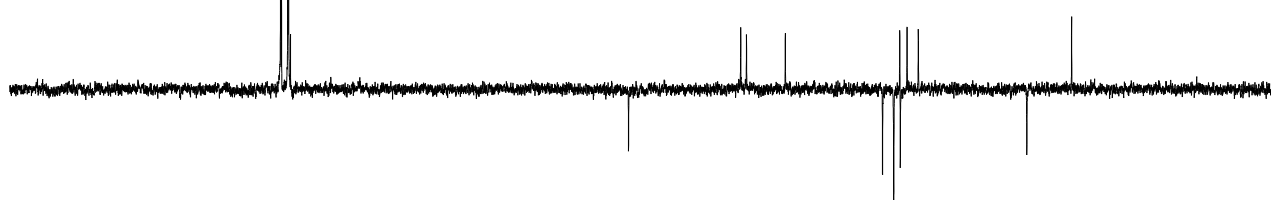
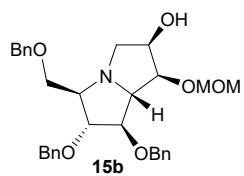
71.64

71.02

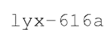
69.99

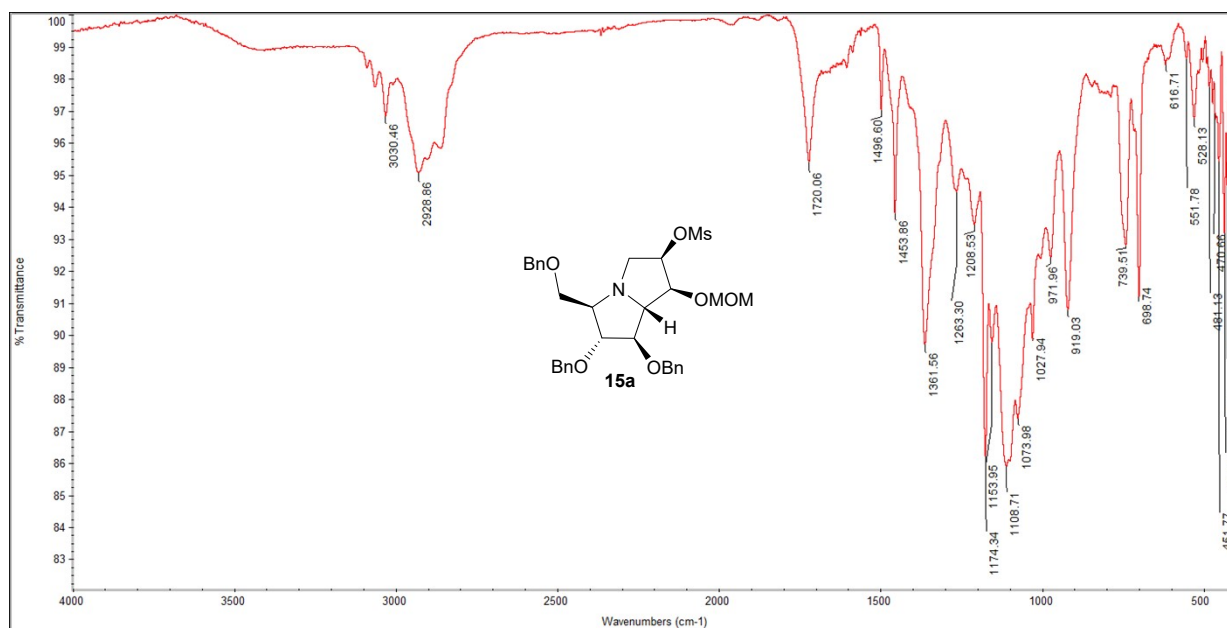
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lyx-2016
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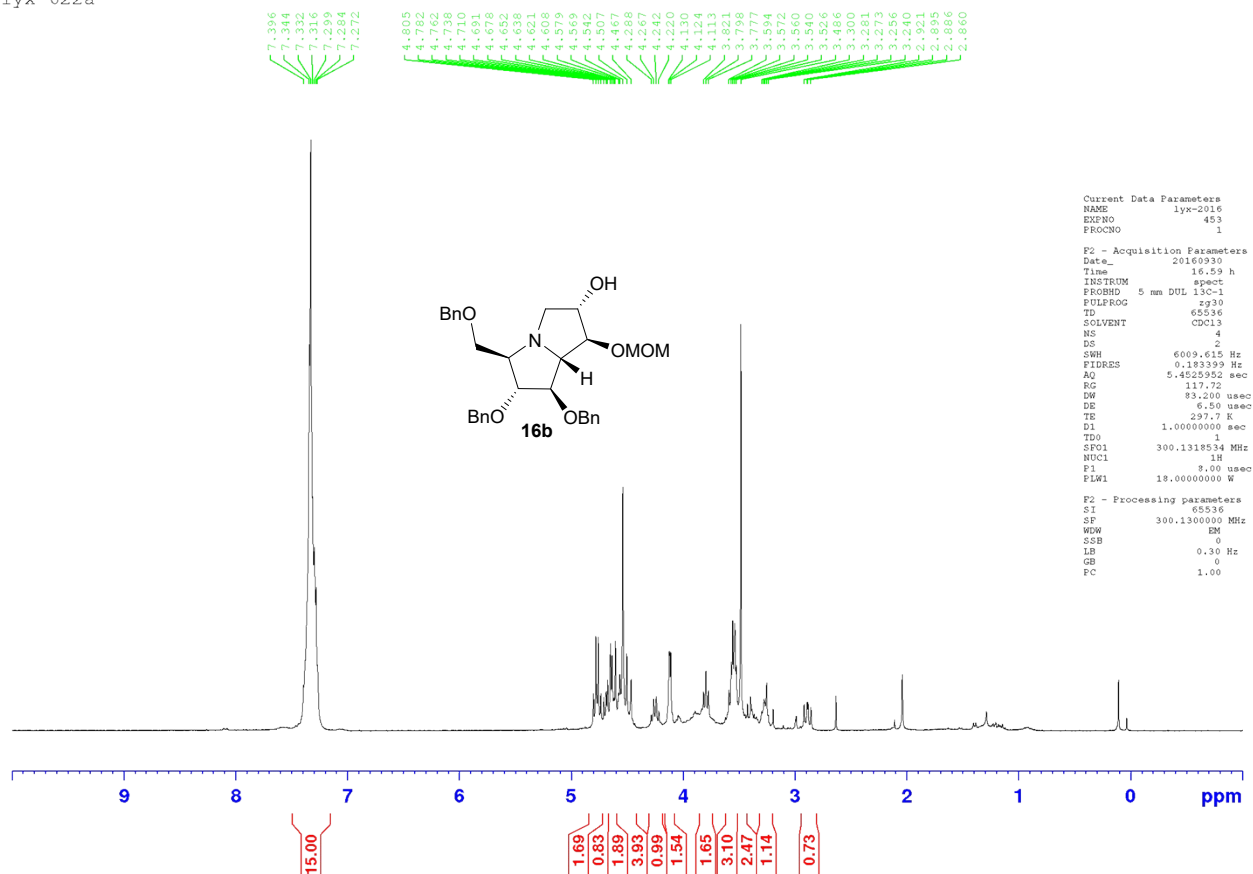
1yx-616a



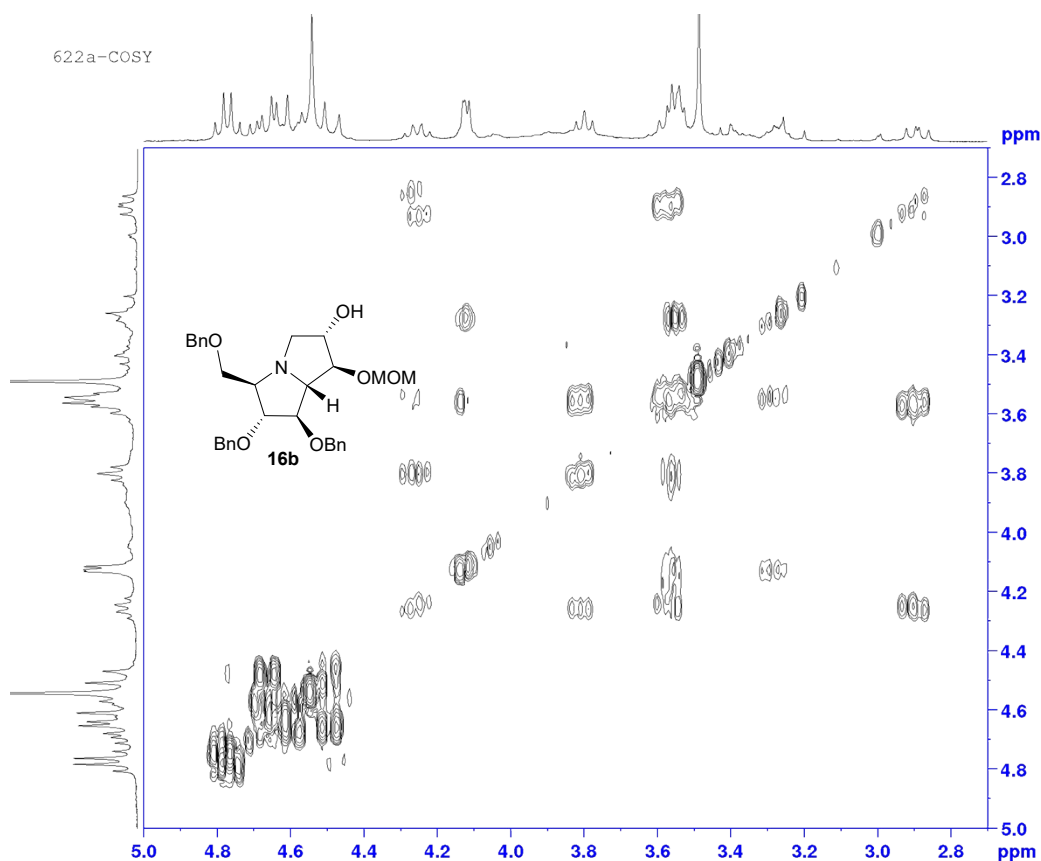


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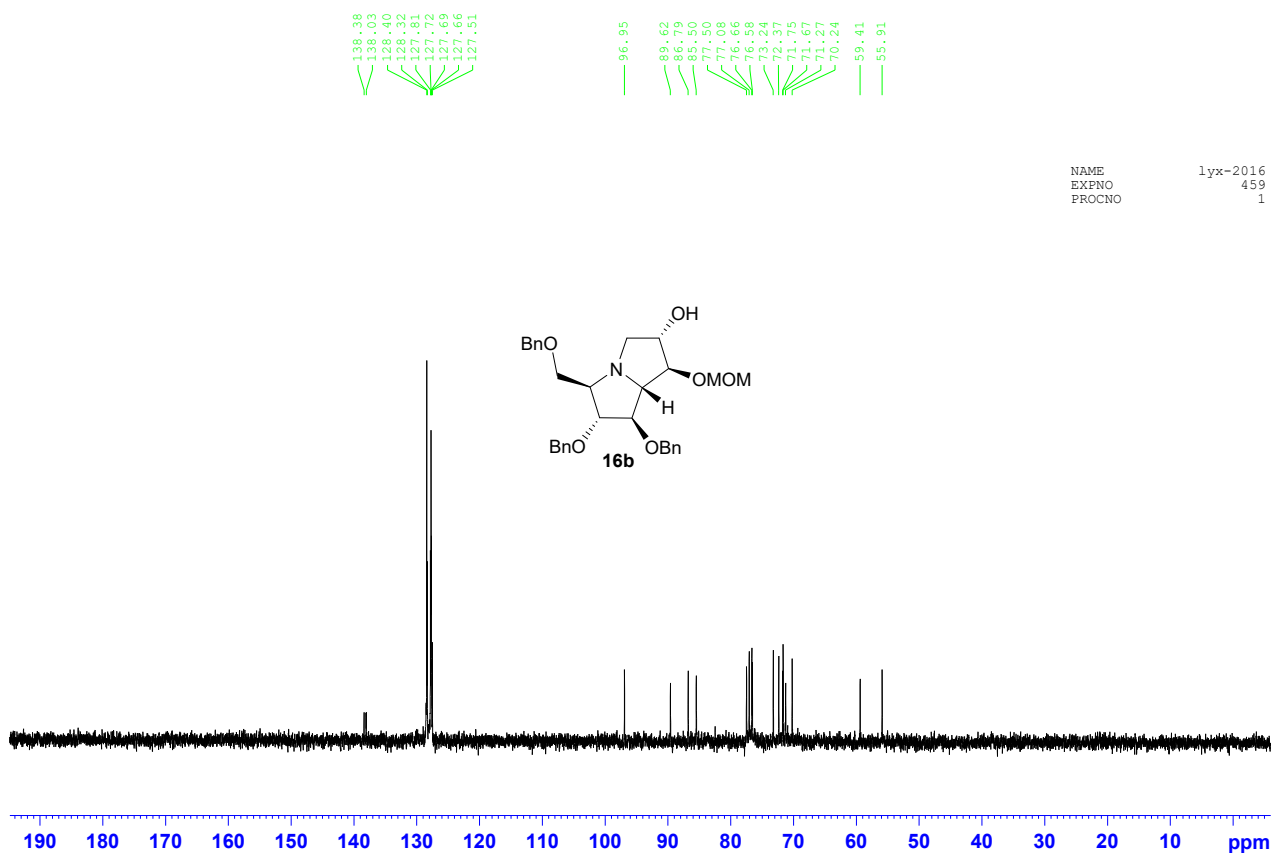
lyx-622a



622a-COSY



lyx-622a-C13



lyx-622a-dept135

128.40
128.32
127.72
127.66
127.50

96.95

89.62

86.80

85.52

76.59

73.24

72.37

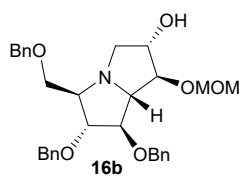
71.68

71.29

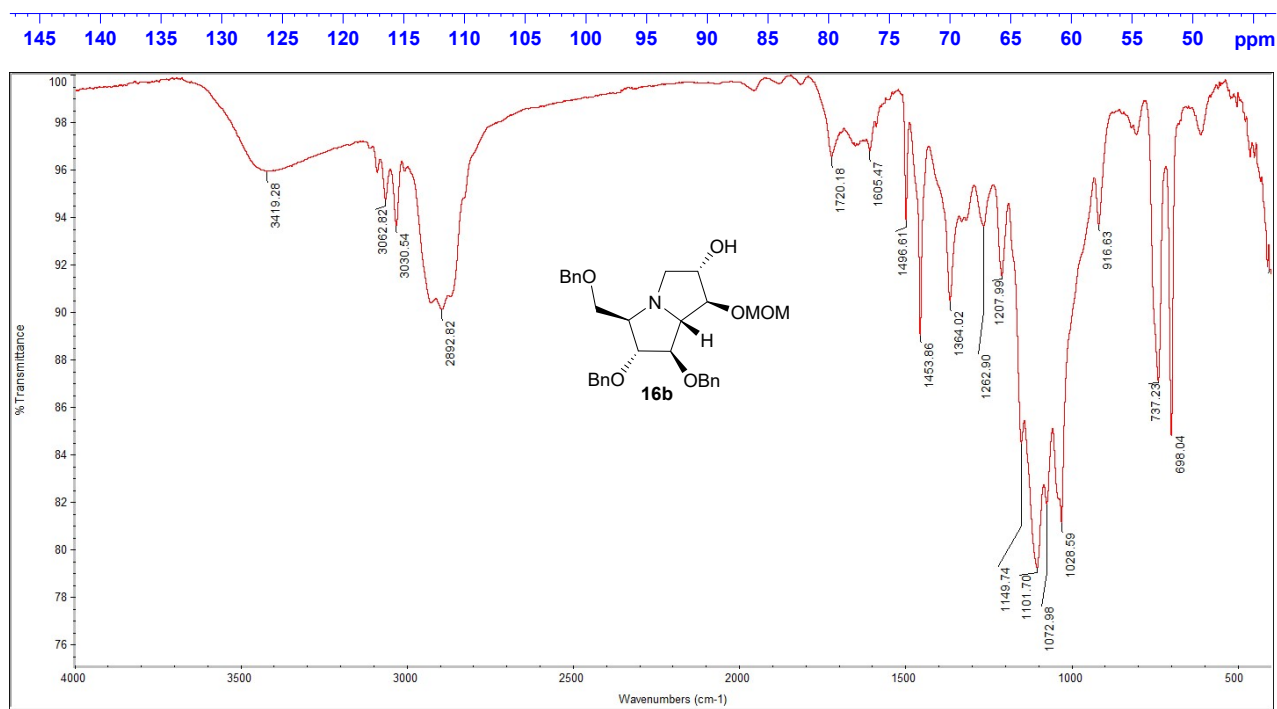
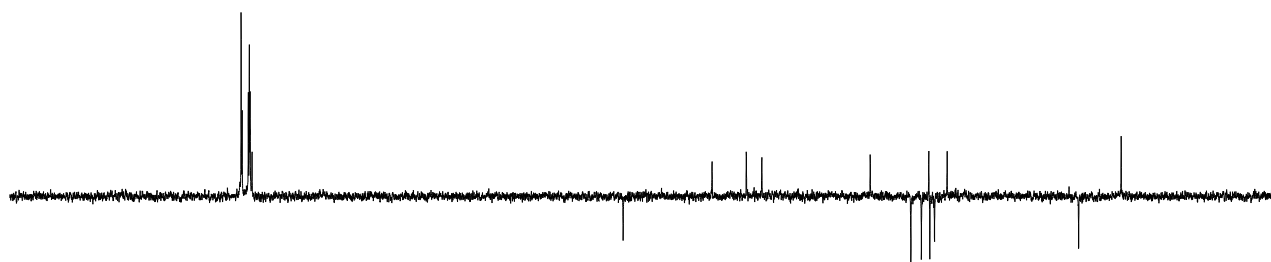
70.25

59.42

55.91

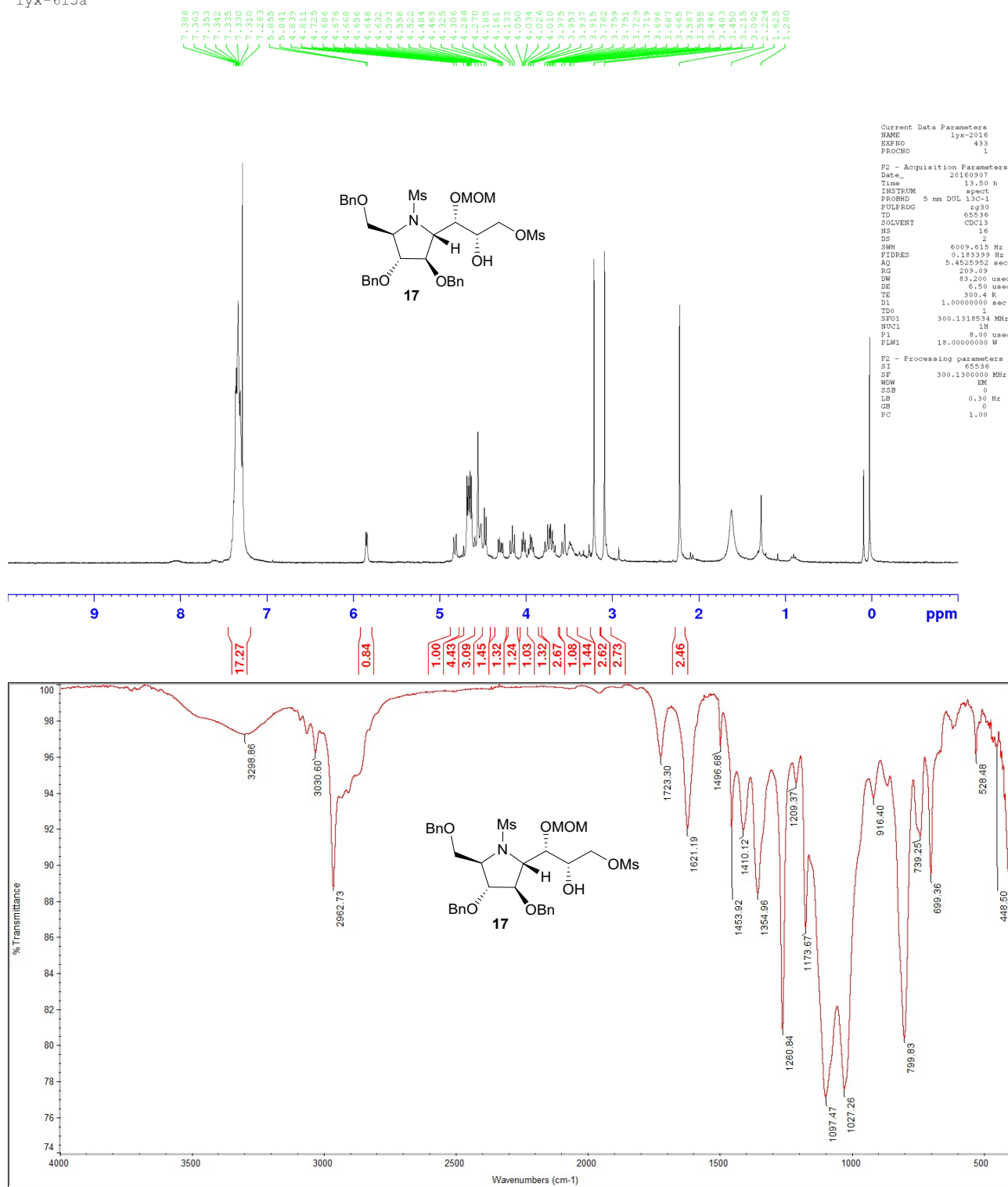


NAME lyx-2016
EXPNO 460
PROCNO 1



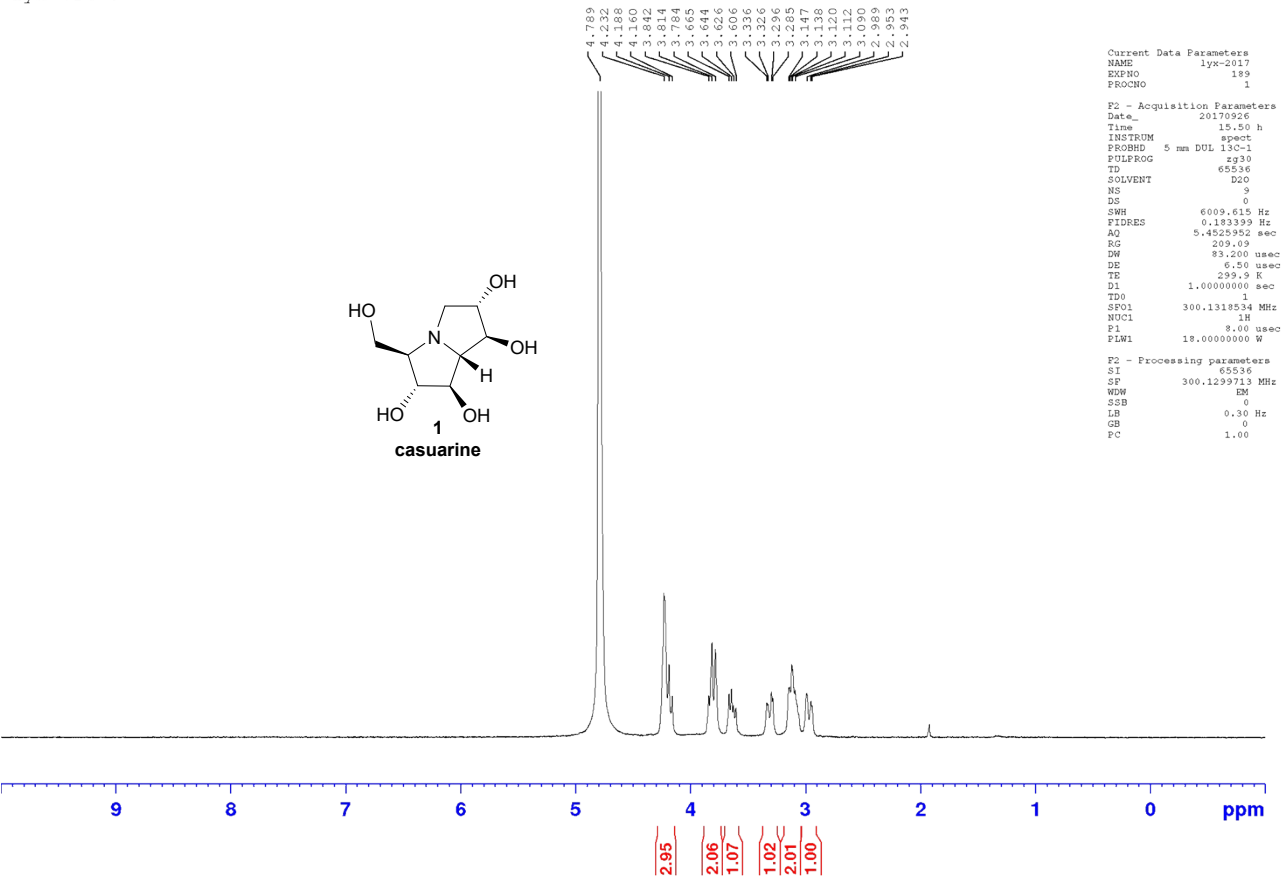
Compound 17:

lyx-615a

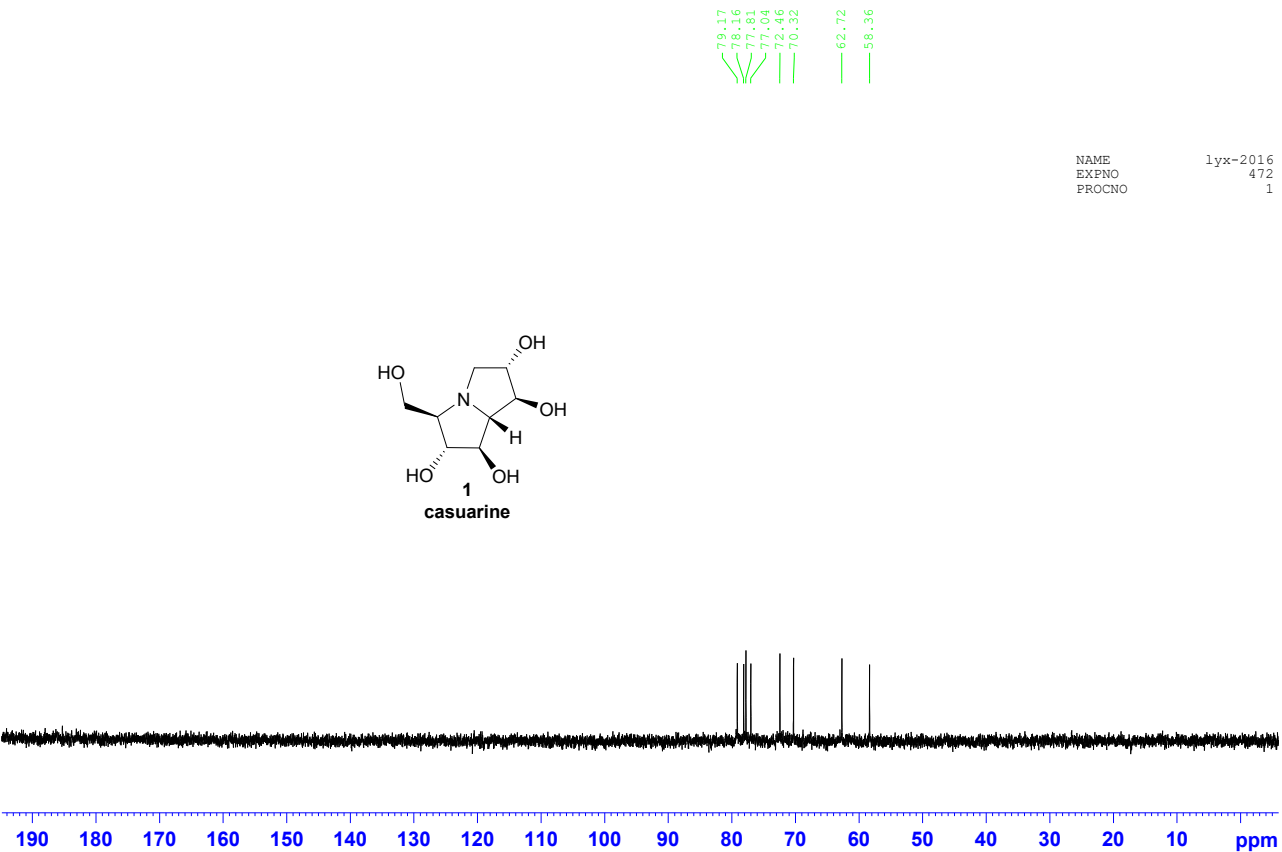


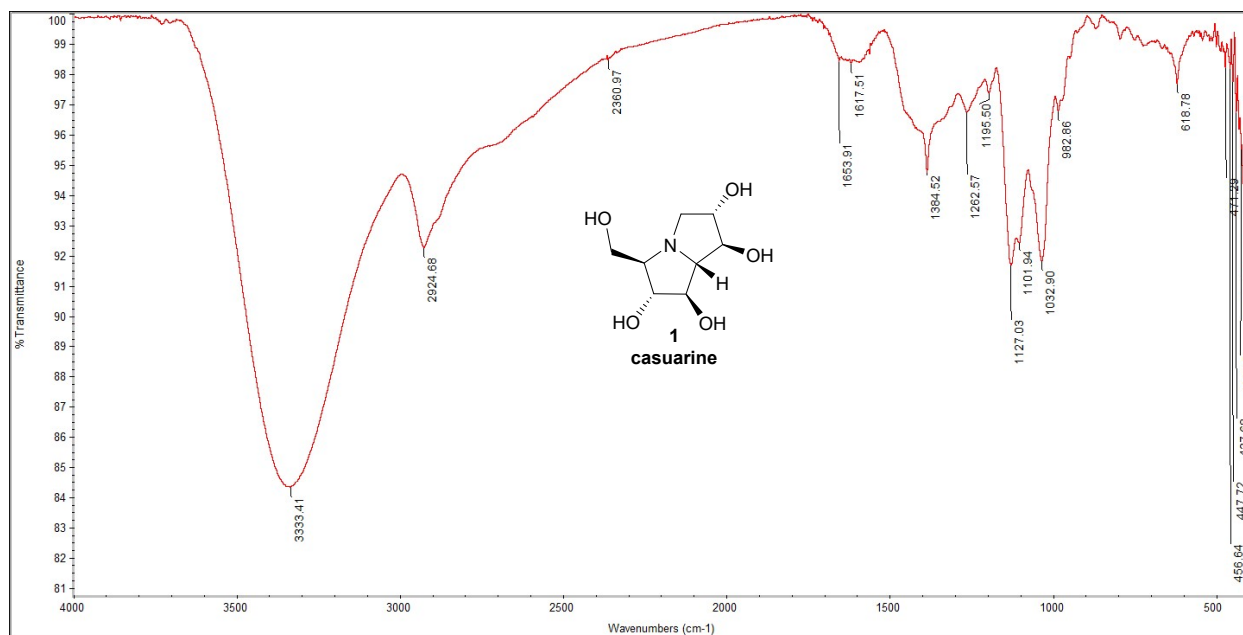
Compound 1:

lyx-624-3

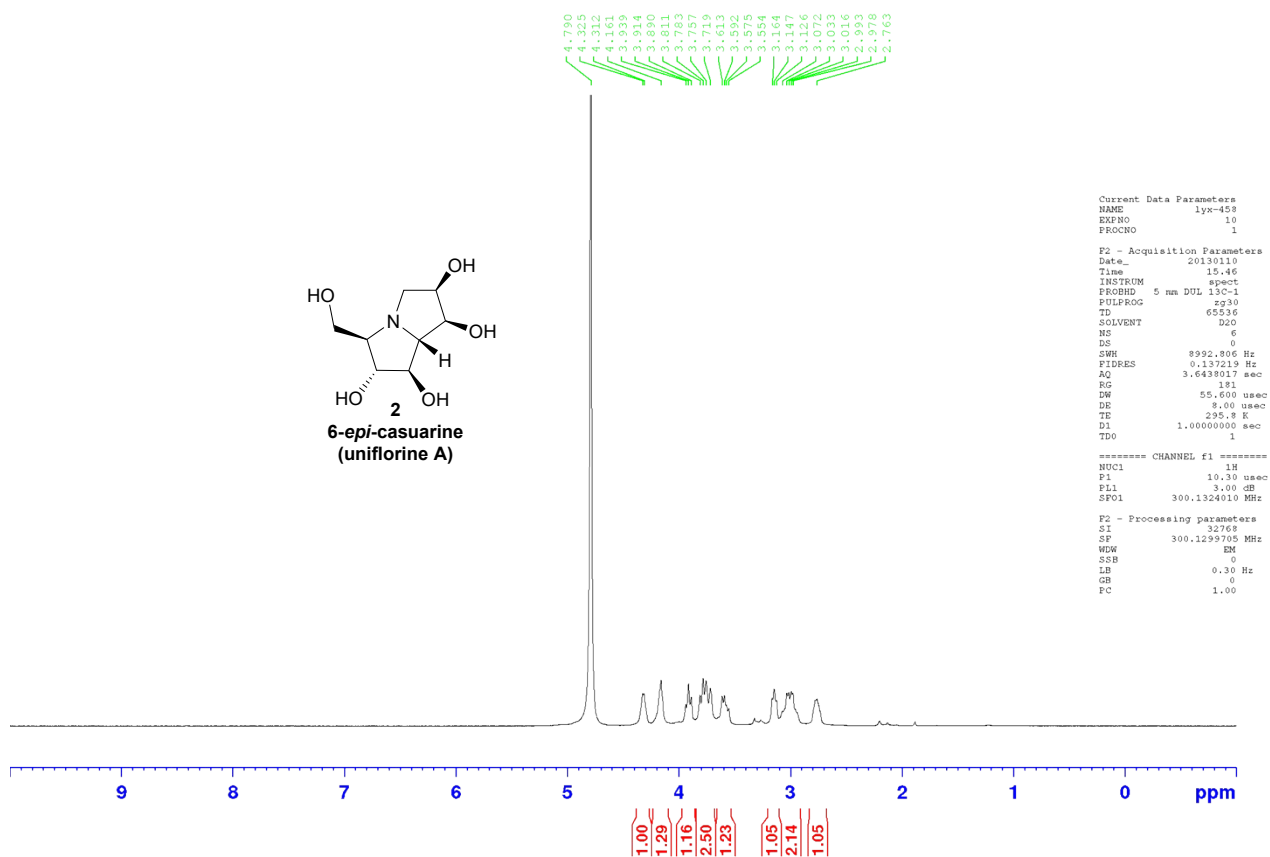


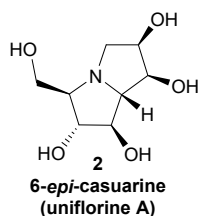
lyx-624-2-C13





Compound 2:





78.23
76.99
75.17
73.38
71.59
69.94
62.10
57.27

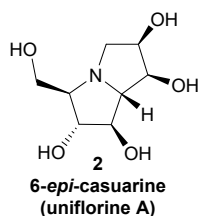
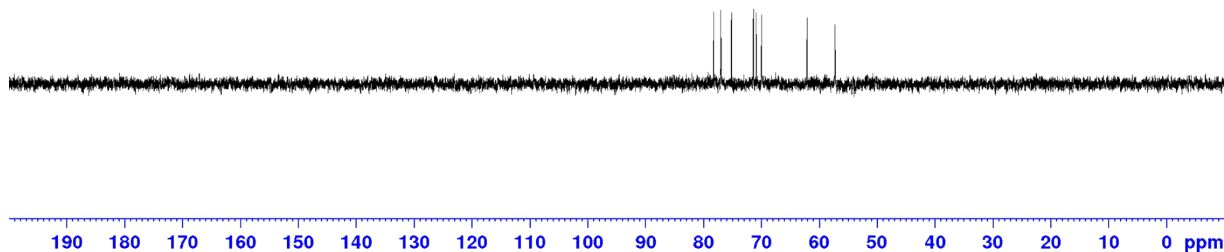
```
Current Data Parameters
NAME      lya-458
EXPNO     12
PROCNO    1

F2 - Acquisition Parameters
Date_     20150110
Time      15.51
INSTRUM   agnost
PROBHD    5 mm DOL 15C-1
PULPROG   zgpg30
TD         65536
SOLVENT   D2O
NS         40
DS         4
SWH        17985.411 Hz
FIDRES     0.274439 Hz
AQ         1.8219098 sec
RG         8192
RW         27.800 usec
DE         6.50 usec
TE         296.1 K
D1         2.00000000 sec
D11        0.00000000 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
P2         100.00 usec
PL2        3.00 dB
PL12       22.74 dB
PL13       23.00 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
```



78.23
76.99
75.17
73.38
71.59
69.94
62.10
57.27

```
Current Data Parameters
NAME      lya-458
EXPNO     13
PROCNO    1

F2 - Acquisition Parameters
Date_     20150110
Time      15.57
INSTRUM   agnost
PROBHD    5 mm DOL 15C-1
PULPROG   zgpg115
TD         65536
SOLVENT   D2O
NS         40
DS         4
SWH        17985.411 Hz
FIDRES     0.274439 Hz
AQ         1.8219098 sec
RG         16384
RW         27.800 usec
DE         6.50 usec
TE         296.1 K
D1         2.00000000 sec
D2         0.00044428 sec
D12        0.00000000 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
P2         10.50 usec
P4         20.60 usec
PCPDG      100.00 usec
PL2        3.00 dB
PL12       22.74 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
```

