

# Supplementary Information

## C-2 Fluorinated Castanospermines as Potent and Specific $\alpha$ -Glucosidase Inhibitors: Synthesis and Structure-Activity Relationship Study

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### Section 2 NMR and IR spectra

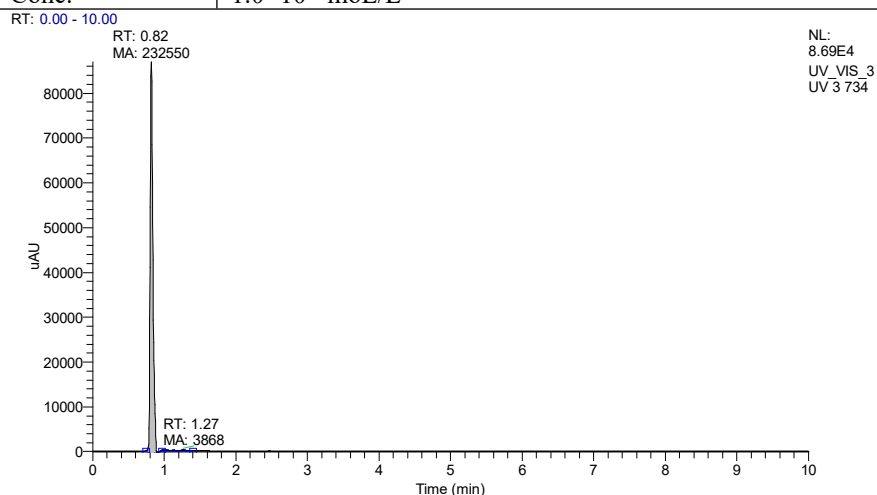
Compound 15:	S9
Compound 16:	S11
Compound 17:	S13
Compound 18a:	S15
Compound 18b:	S17
Compound 19:	S20
Compound 20:	S23
Compound 14:	S25
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Compound 25:	S39
Compound 26:	S41
Compound 28a:	S43
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Compound 29a:	S46
Compound 29b:	S48
Compound 30:	S50

Compound 31:	S52
Compound 32:	S54
Compound 34a:	S56
Compound 34b:	S58
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Compound 48:	S102
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## Section 1 HPLC data

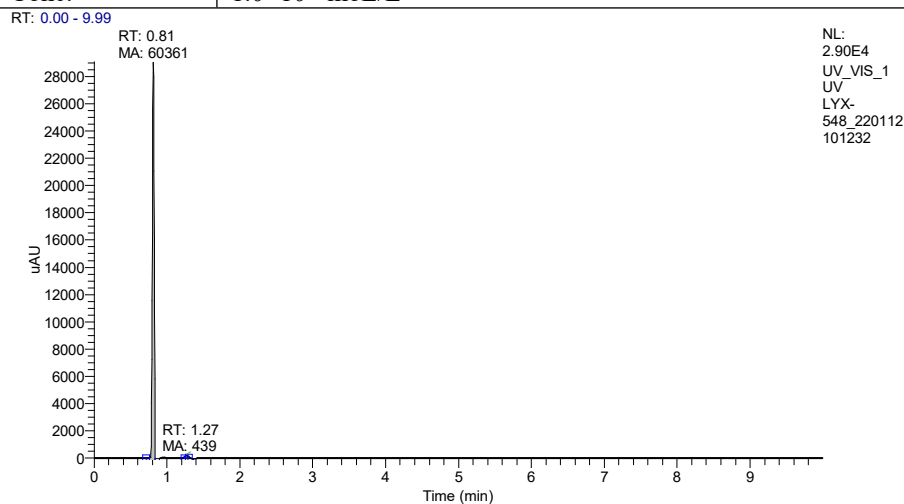
### Table S1-1. HPLC Data for compound 1

Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 μm; 2.1×100 mm Column			
Mobile Phase	Time (min)	A%: Me	Integration	Purity (%)
Gradient program:	0.82	100	232550	98.36
	1.27	100	3868	1.64
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 300 nm			
Conc.	1.0×10 <sup>-3</sup> mol/L			



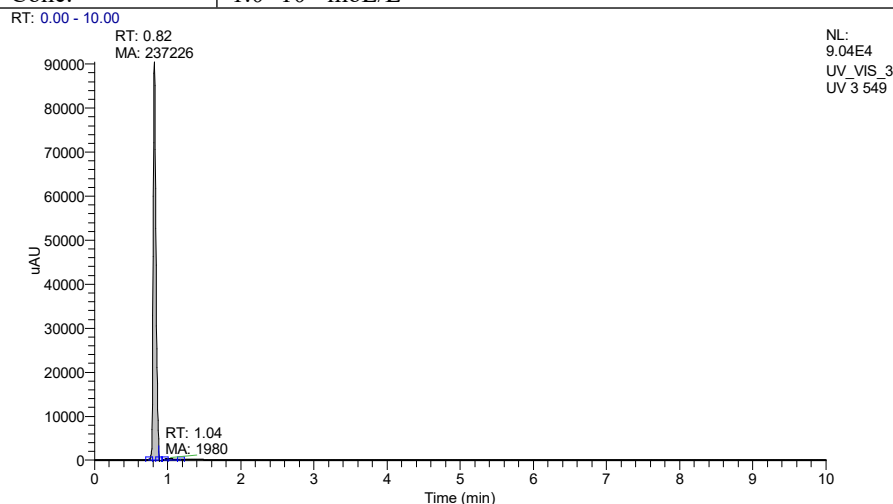
### Table S1-2. HPLC Data for compound 8

Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 μm; 2.1×100 mm Column			
Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient program:	0.81	100	60361	99.28
	1.27	100	439	0.72
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 254 nm			
Conc.	1.0×10 <sup>-3</sup> mol/L			



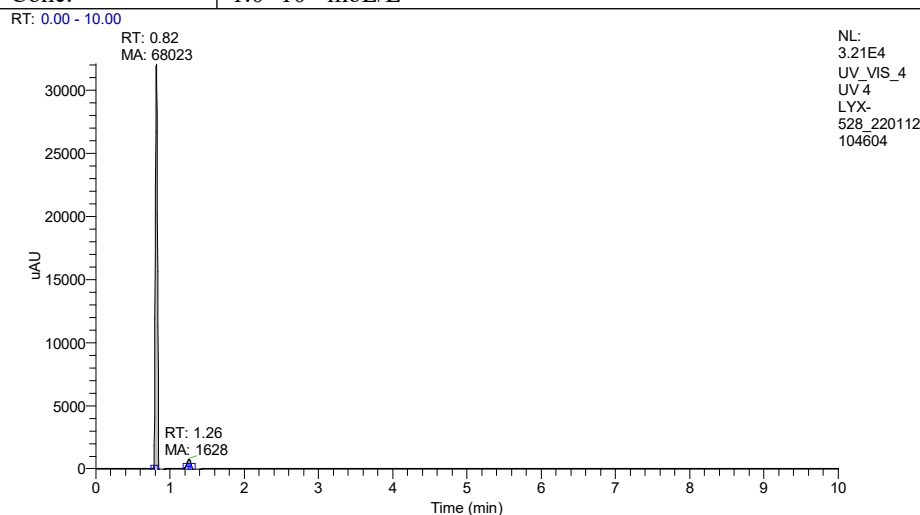
**Table S1-3. HPLC Data for compound 49**

Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 μm; 2.1×100 mm Column			
Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient	0.832	100	237226	99.17
program:	1.04	100	1980	0.83
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 300 nm			
Conc.	1.0×10 <sup>-3</sup> mol/L			



**Table S1-4. HPLC Data for compound 14**

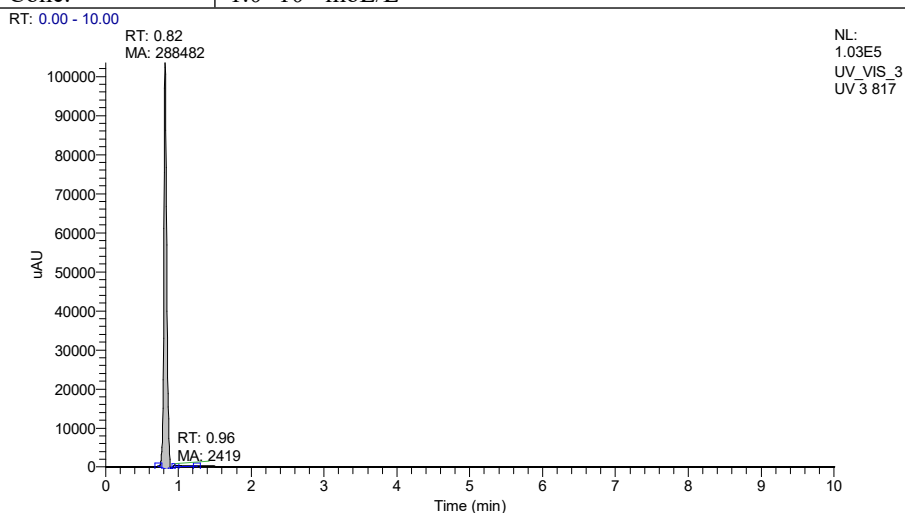
Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 μm; 2.1×100 mm Column			
Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient	0.82	100	68023	97.66
program:	1.26	100	1628	2.34
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 278 nm			
Conc.	1.0×10 <sup>-3</sup> mol/L			





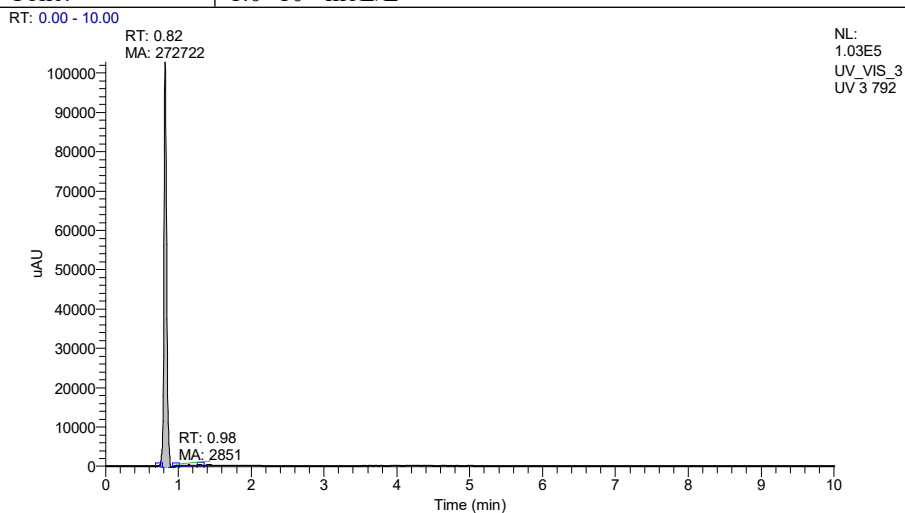
**Table S1-5. HPLC Data for compound 13b**

Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 μm; 2.1×100 mm Column			
Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient	0.82	100	288482	99.17
program:	0.96	100	2419	0.83
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 300 nm			
Conc.	1.0×10 <sup>-3</sup> mol/L			



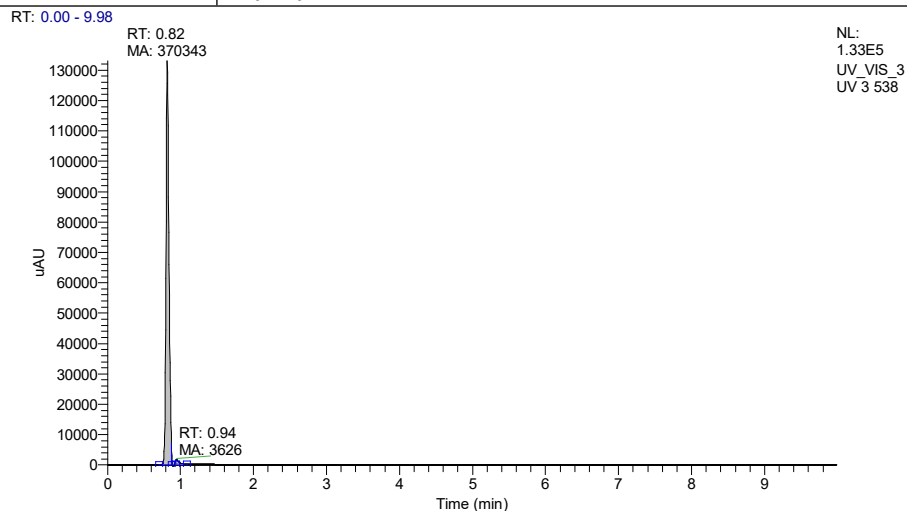
**Table S1-6. HPLC Data for compound 13a**

Instrument	Orbitrap Fusion Lumos			
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Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient	0.82	100	272722	98.97
program:	0.98	100	2851	1.03
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 300 nm			
Conc.	1.0×10 <sup>-3</sup> mol/L			



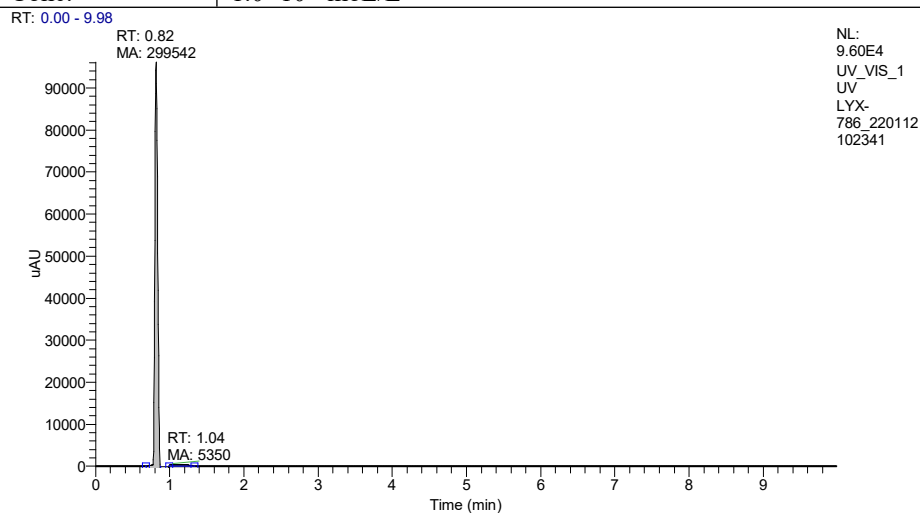
**Table S1-7. HPLC Data for compound 1-*epi*-1**

Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 μm; 2.1×100 mm Column			
Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient	0.82	100	370343	99.03
program:	0.94	100	3626	0.97
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 300 nm			
Conc.	1.0×10 <sup>-3</sup> mol/L			



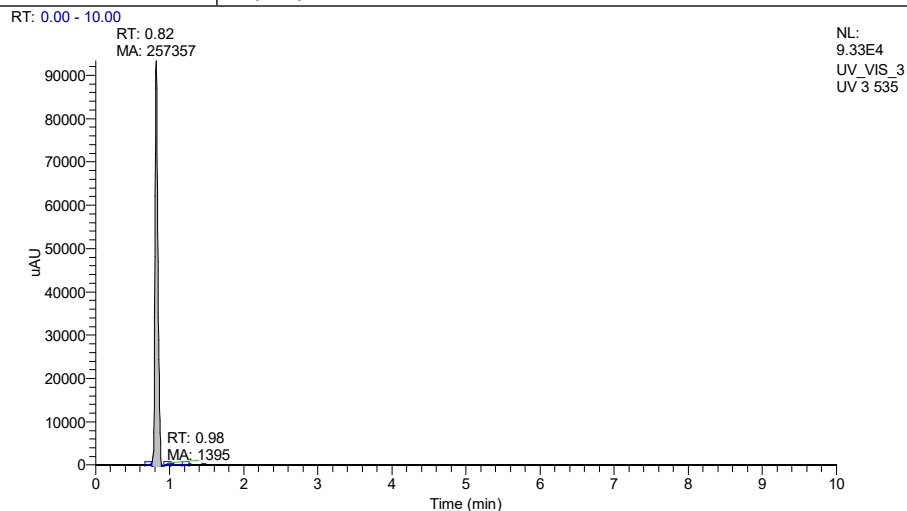
**Table S1-8. HPLC Data for compound 1-*epi*-8**

Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 μm; 2.1×100 mm Column			
Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient	0.82	100	299542	98.25
program:	1.04	100	5350	1.75
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 254 nm			
Conc.	1.0×10 <sup>-3</sup> mol/L			



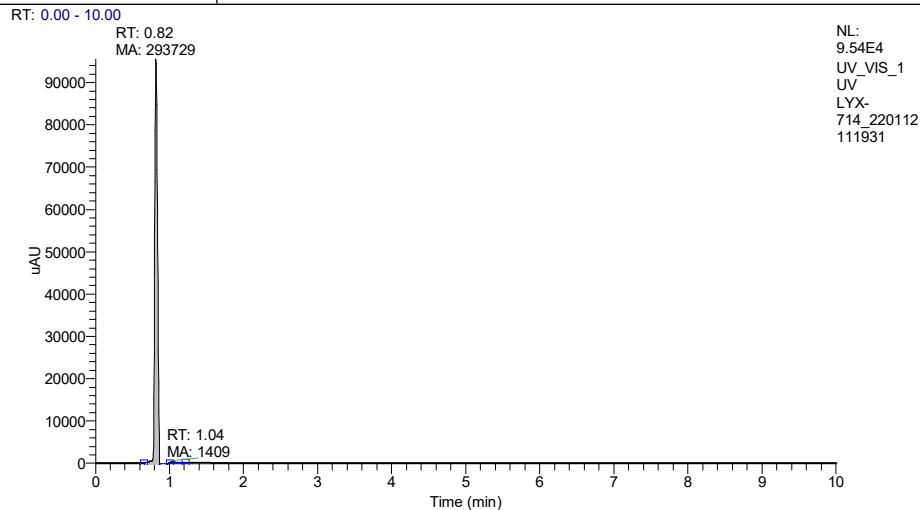
**Table S1-9. HPLC Data for compound 21**

Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 $\mu$ m; 2.1 $\times$ 100 mm Column			
Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient	0.82	100	257357	99.46
program:	0.98	100	1395	0.54
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 300 nm			
Conc.	1.0 $\times$ 10 <sup>-3</sup> mol/L			



**Table S1-10. HPLC Data for compound 37**

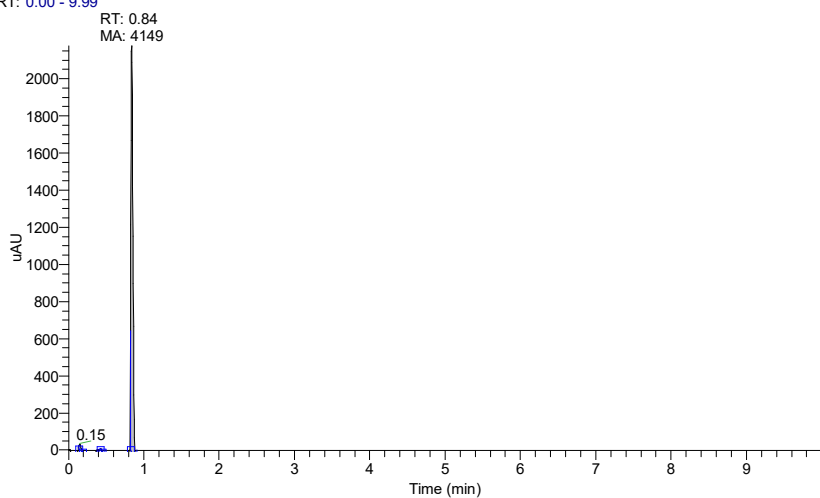
Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 $\mu$ m; 2.1 $\times$ 100 mm Column			
Mobile Phase	Time (min)	A%: MeCN	Integration	Purity (%)
Gradient	0.82	100	293729	99.52
program:	1.04	100	1409	0.48
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 254 nm			
Conc.	1.0 $\times$ 10 <sup>-3</sup> mol/L			



**Table S1-11. HPLC Data for compound 36**

Instrument	Orbitrap Fusion Lumos			
Column	ACQUITY UPLC <sup>®</sup> BEH C18 1.7 $\mu$ m; 2.1 $\times$ 100 mm Column			
Mobile Phase Gradient program:	Time (min)	A%: MeCN	Integration	Purity (%)
	0.15	100	54	1.28
	0.43	100	10	0.24
	0.84	100	4149	98.48
Stop time	10 min			
Post time	OFF			
Flow rate	0.3 mL/min			
UV detector	Detection 540 nm			
Conc.	1.0 $\times$ 10 <sup>-3</sup> mol/L			

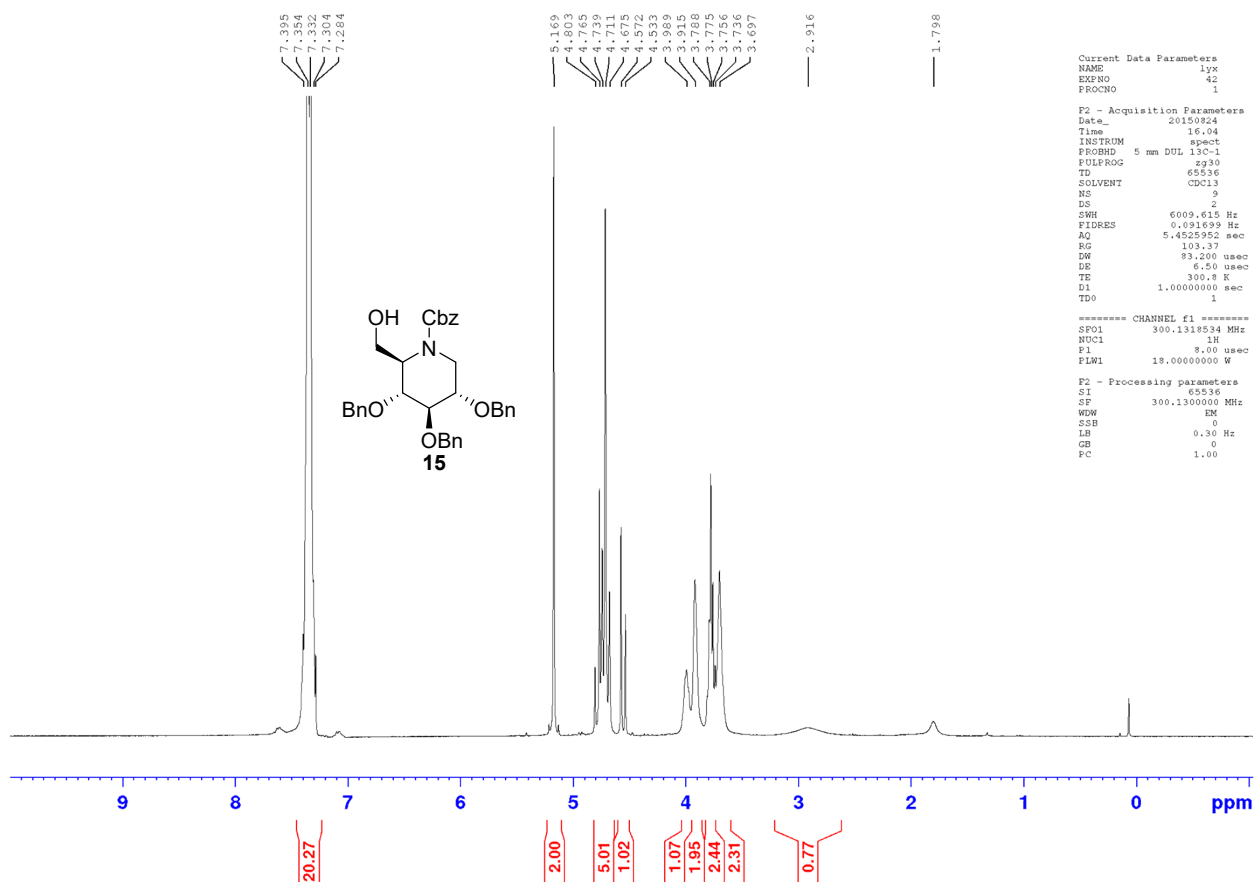
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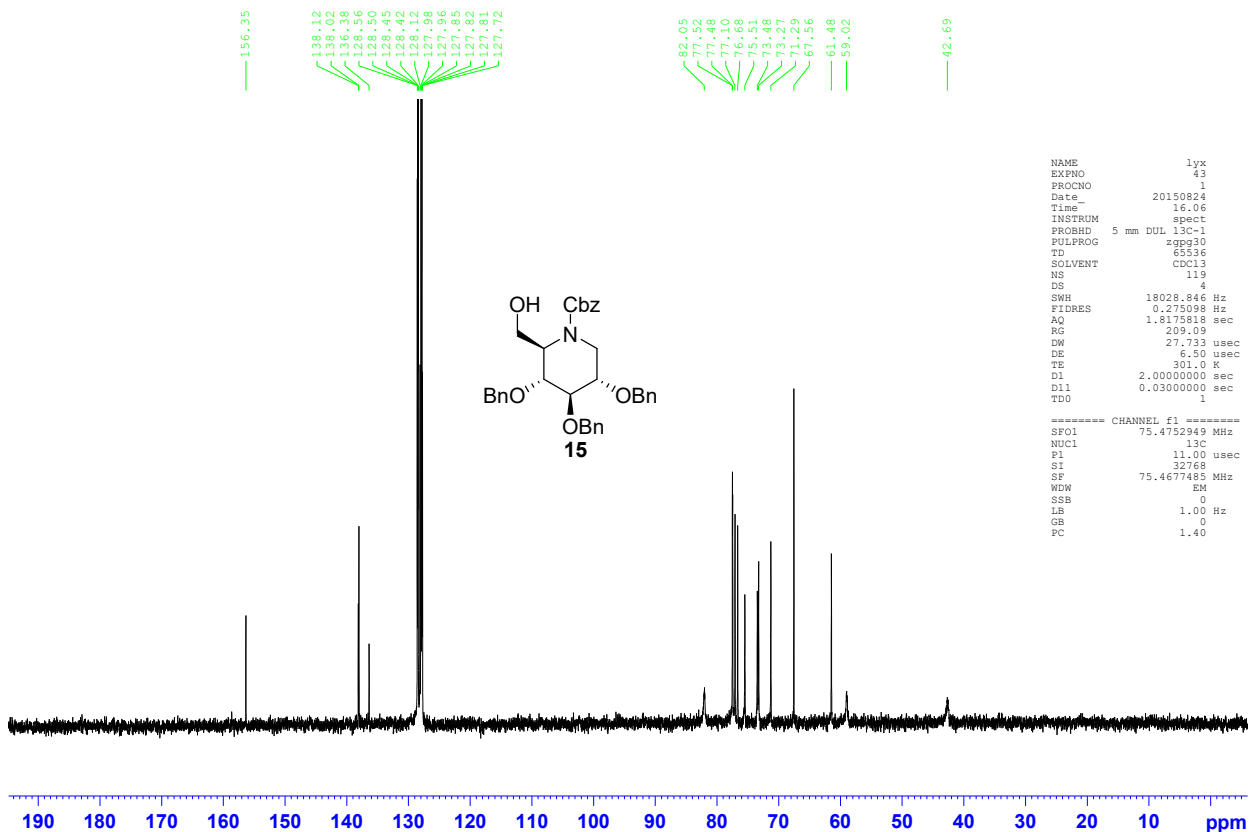
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UV\_VIS\_2  
UV 2  
LYX744\_22  
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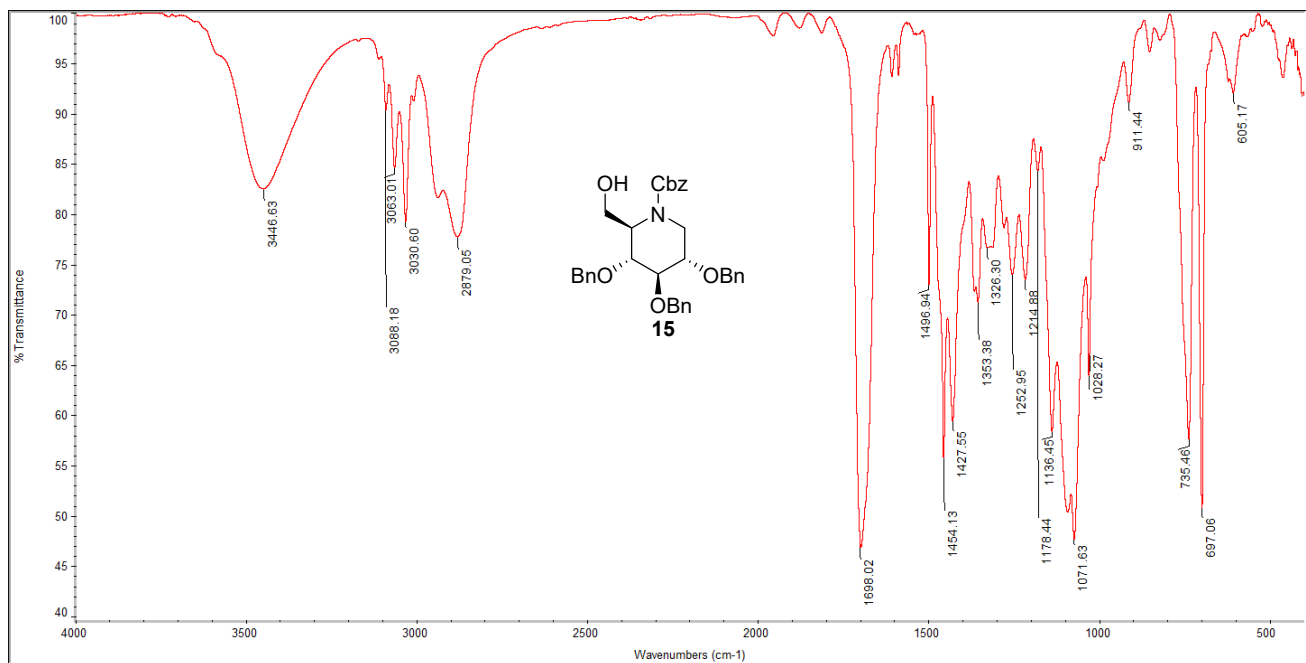
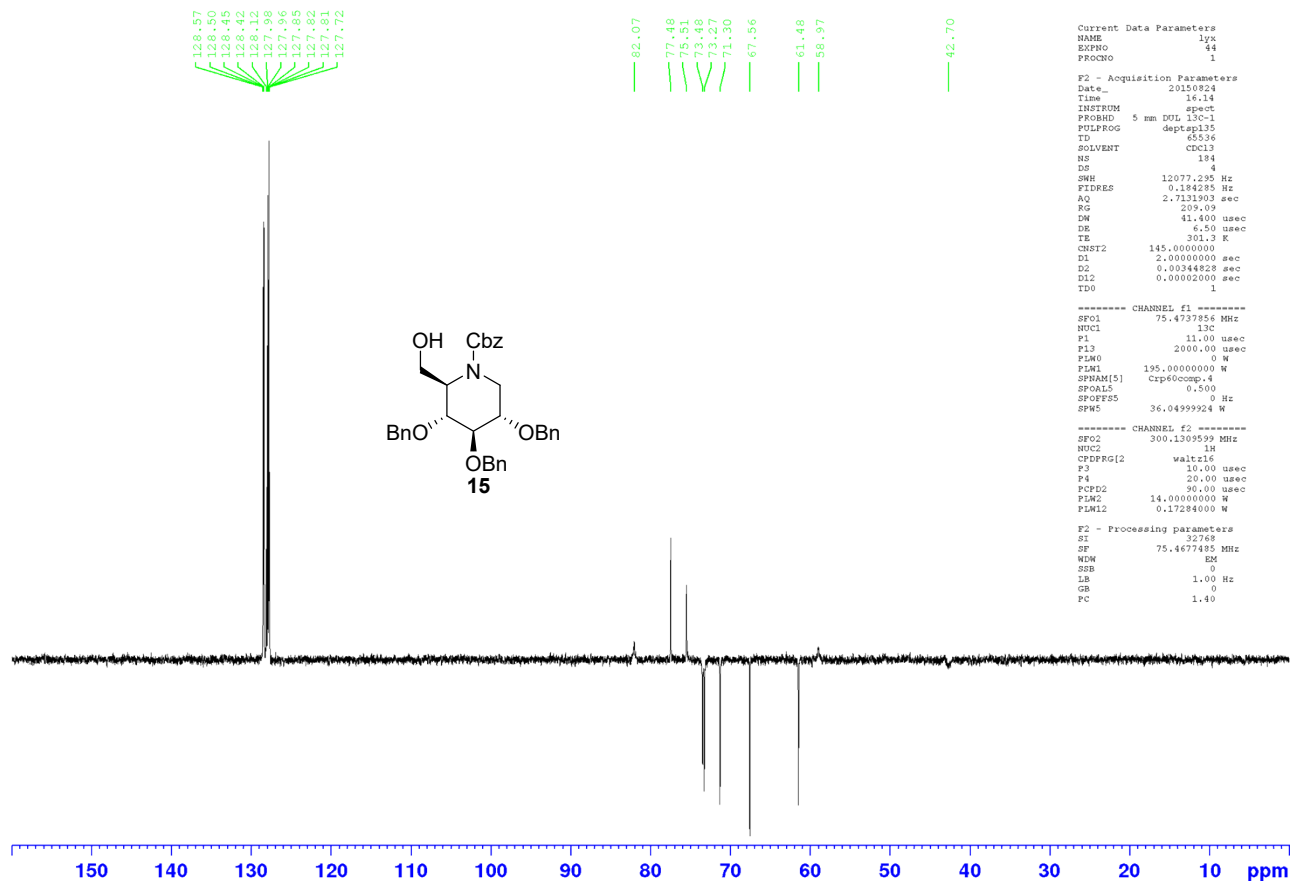
lyx-508b



lyx-508b-C13

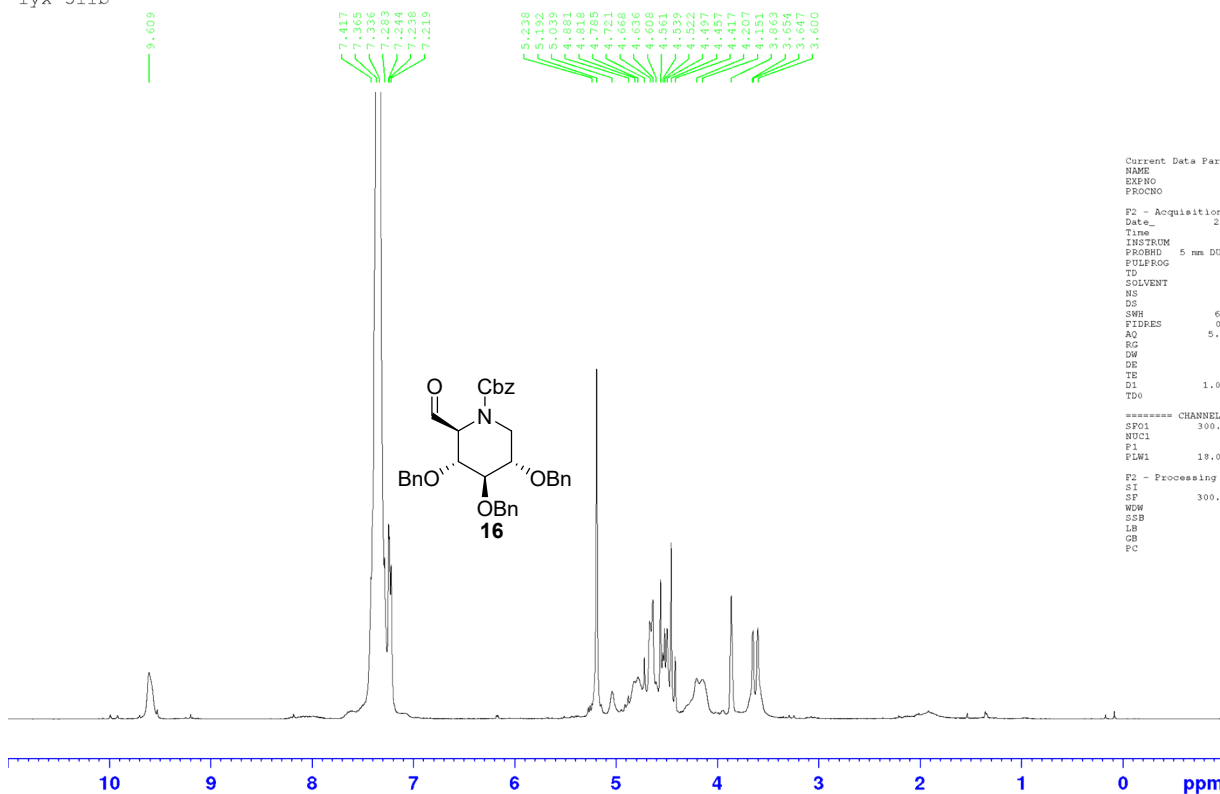


lyx-508b-dept135

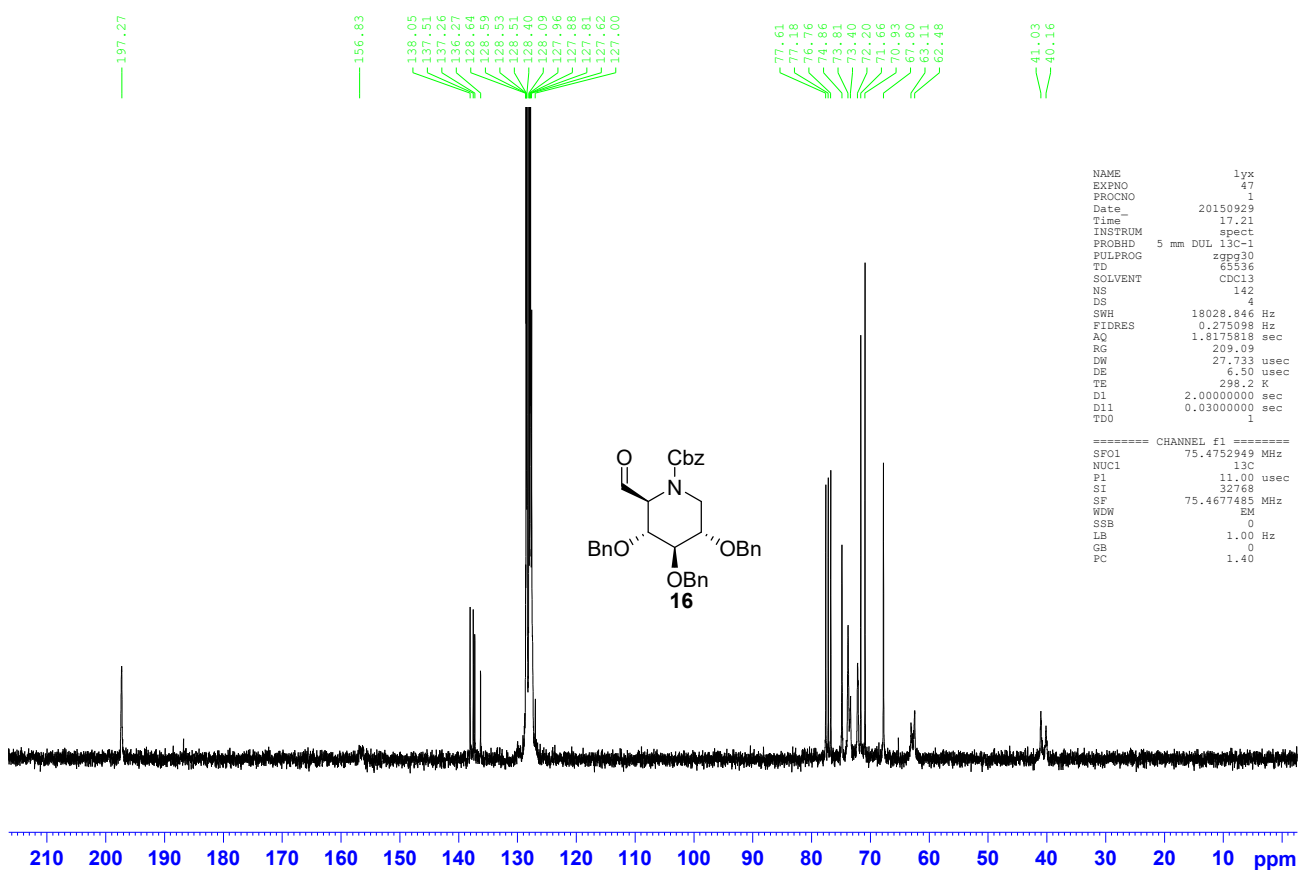


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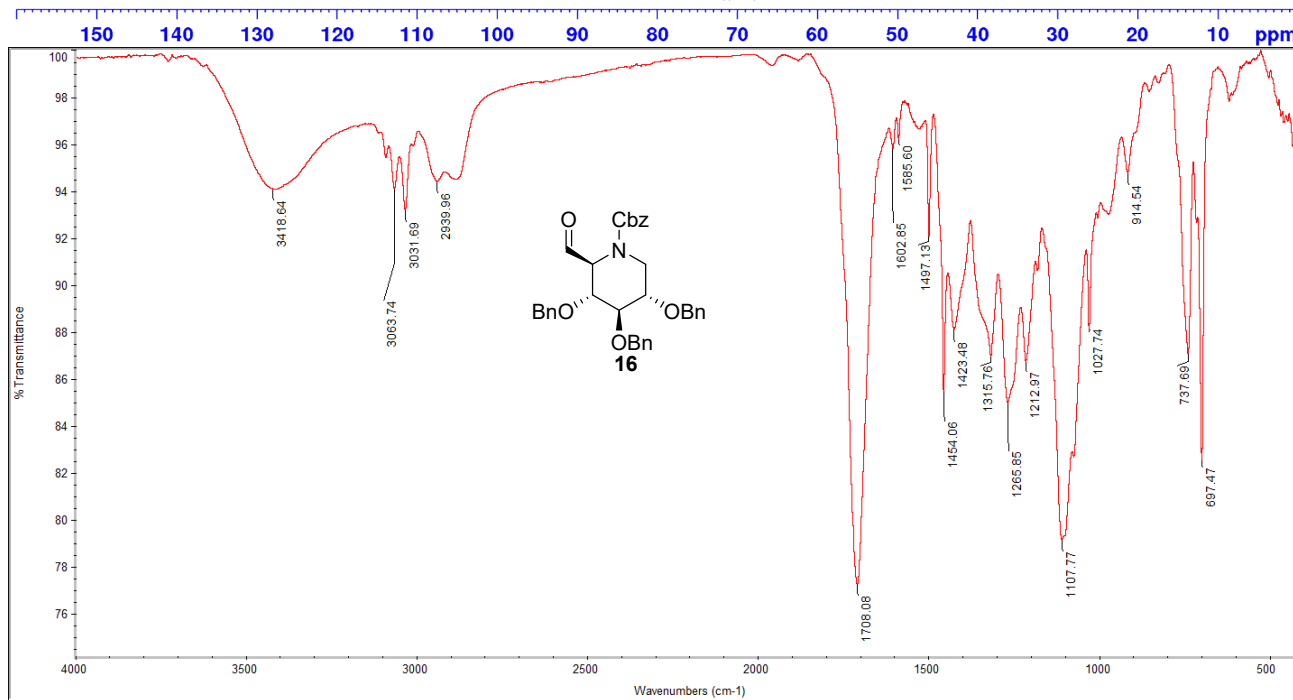
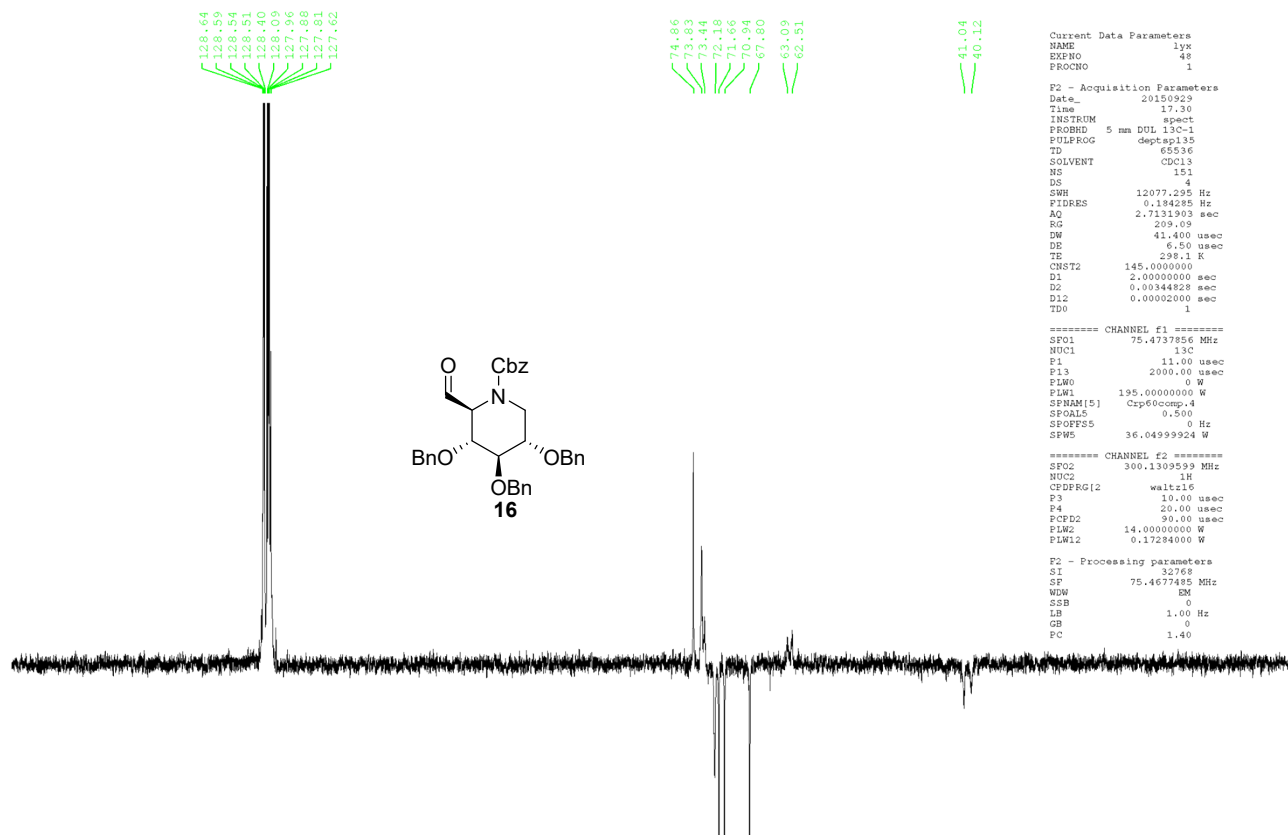
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lyx-511b-C13



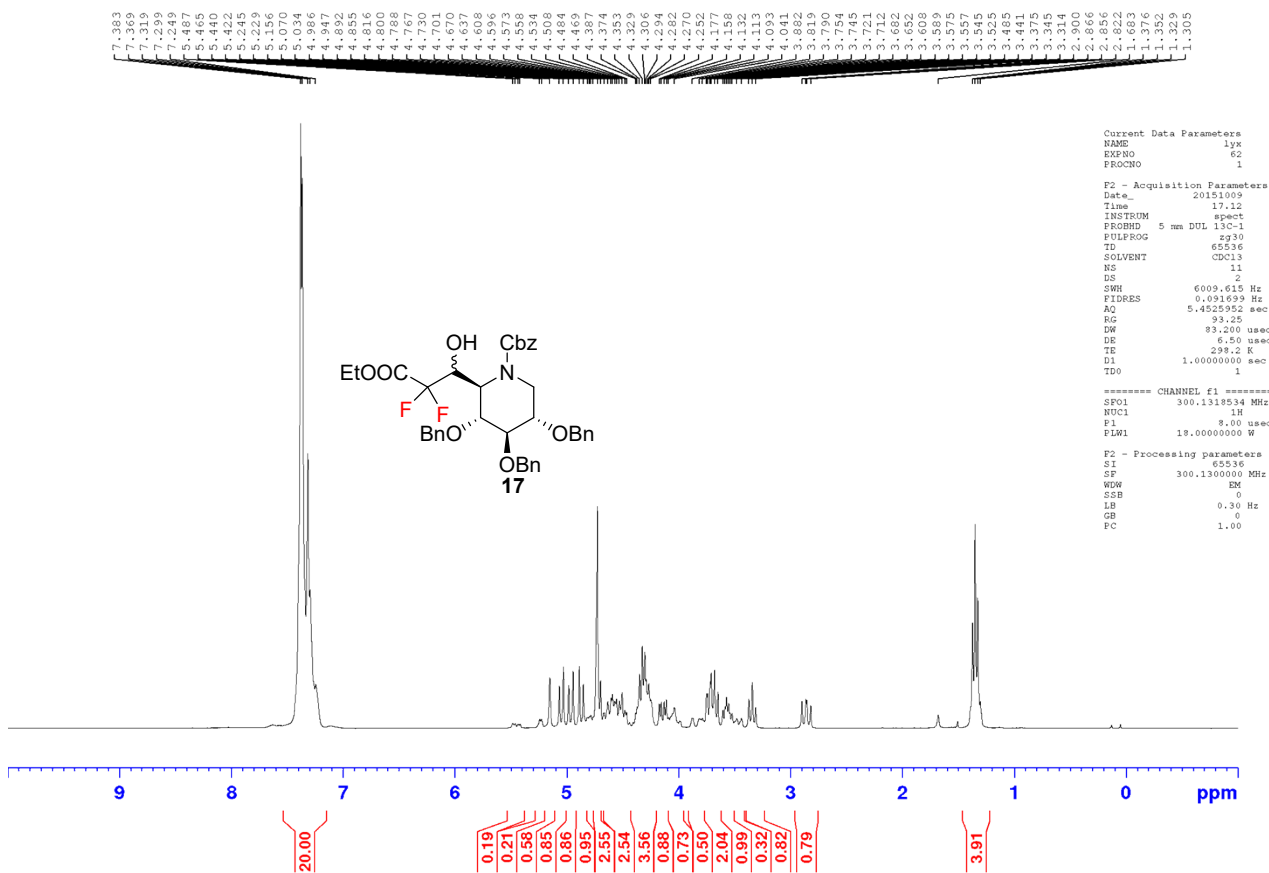
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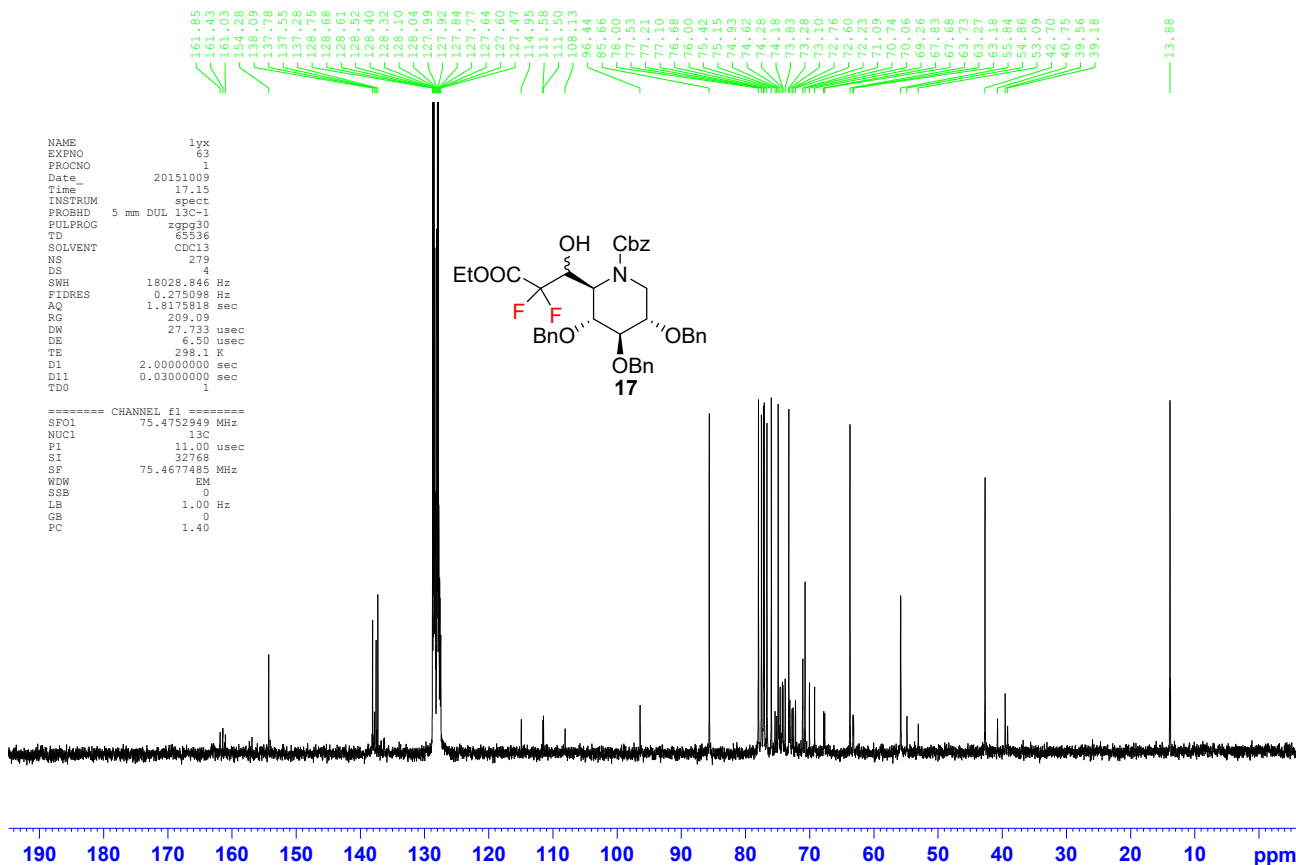


# Compound 17:

lyx-513-CF2



lyx-513-C13



lyx-513-dept135

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128.63  
128.40  
128.32  
128.10  
127.99  
127.84  
127.78  
127.64  
127.47

96.44

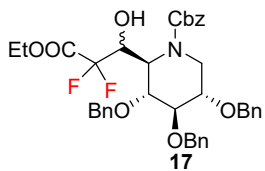
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78.00  
77.21  
76.00  
75.12  
74.93  
74.62  
74.28  
74.18  
73.84  
73.28  
73.10  
72.77  
72.60  
72.23  
70.74  
70.06  
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67.83  
67.68  
63.74  
63.27  
63.18  
55.84

42.70

39.56

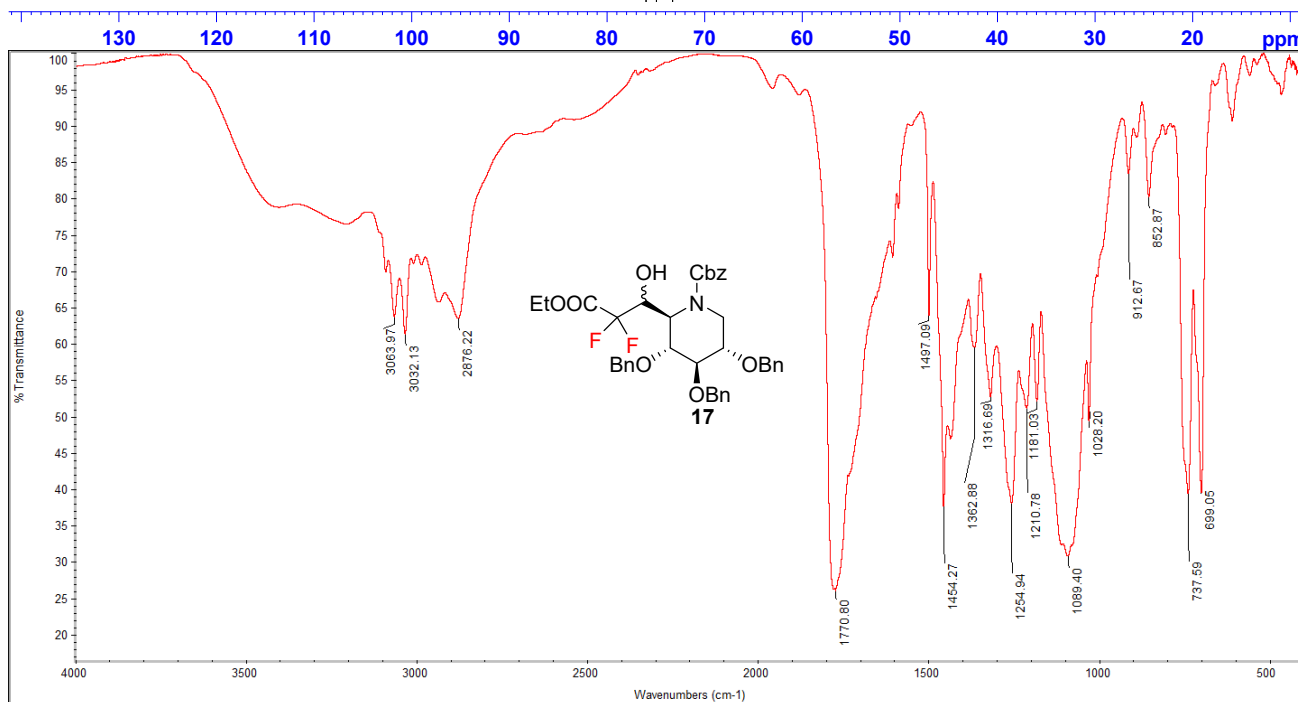
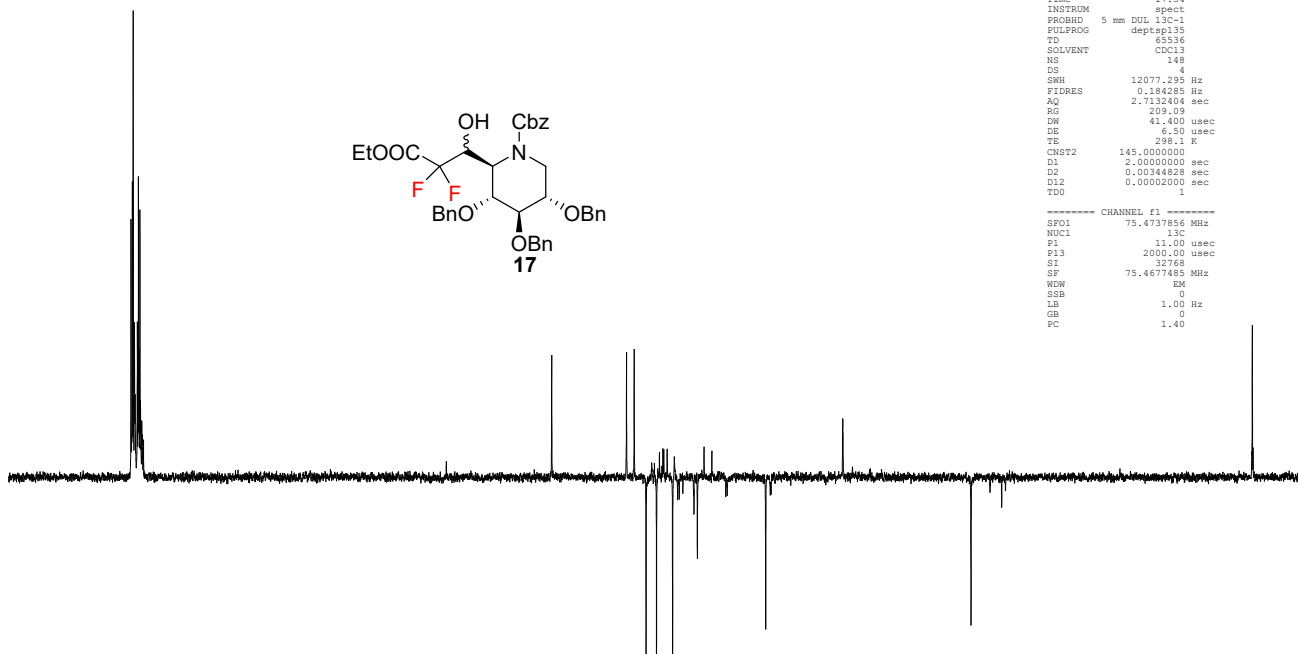
13.88

13.80



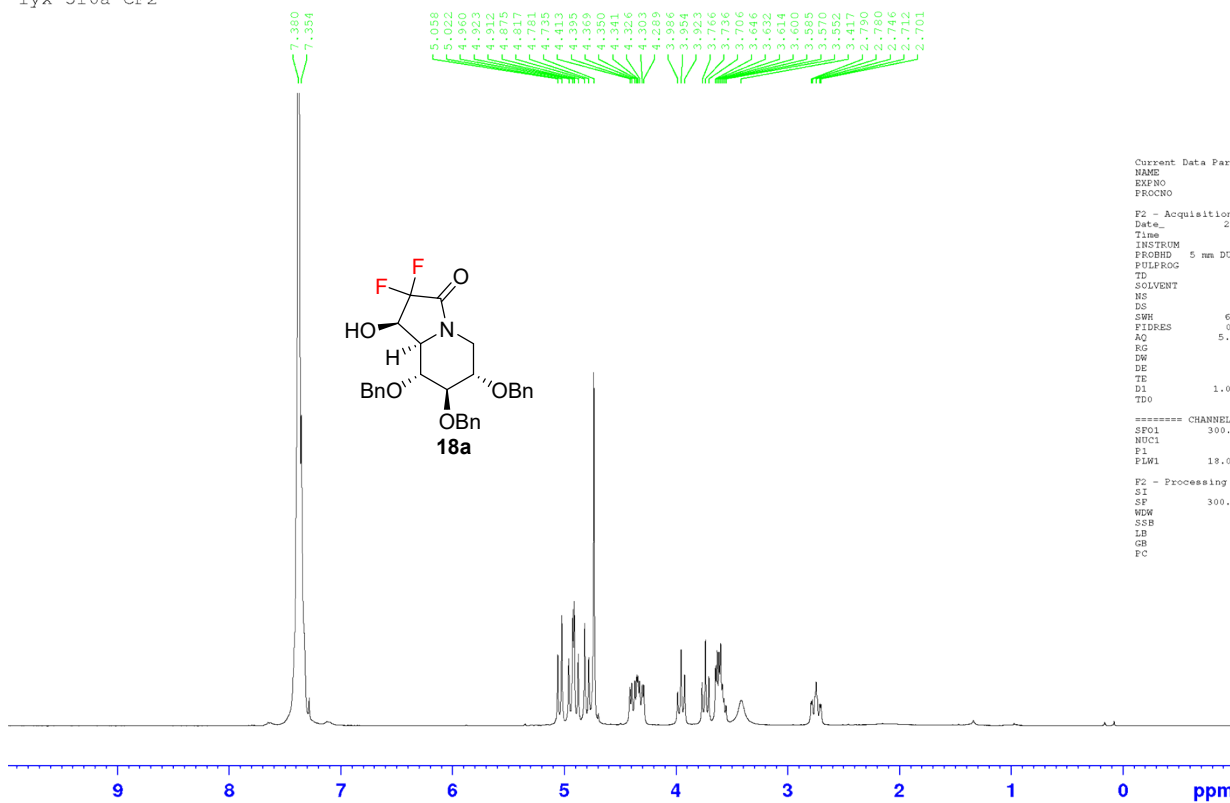
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SWH 0.184285 Hz
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AQ 209.03
RG 41.400 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.0002000 sec
TDO 1
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NUC1 13C
P1 1.00 usec
PL1 0.00 usec
SFO2 200.1313500 MHz
SI 32768
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Compound **18a**:

lyx-516a-CF2



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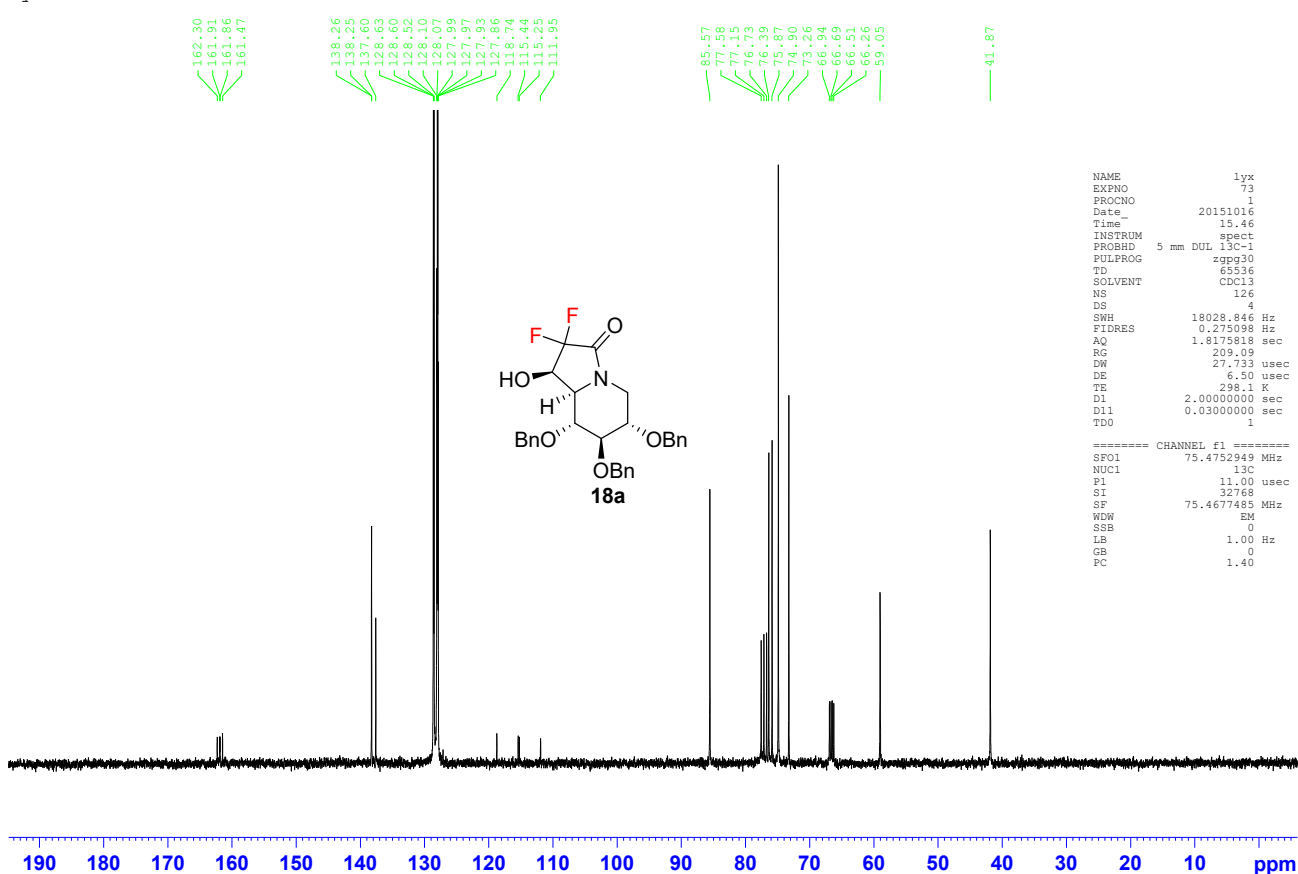
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SOLVENT  CDCl3
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lyx-516a-C13



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DE        6.50 usec
TE        298.1 K
D1        2.00000000 sec
D11      0.03000000 sec
TDO       1

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LB       1.00 Hz
GB       0
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lyx-516a-dept135

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128.60  
128.52  
128.10  
128.00  
127.97  
127.93  
127.86

85.58  
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66.51  
66.26  
59.05

41.87

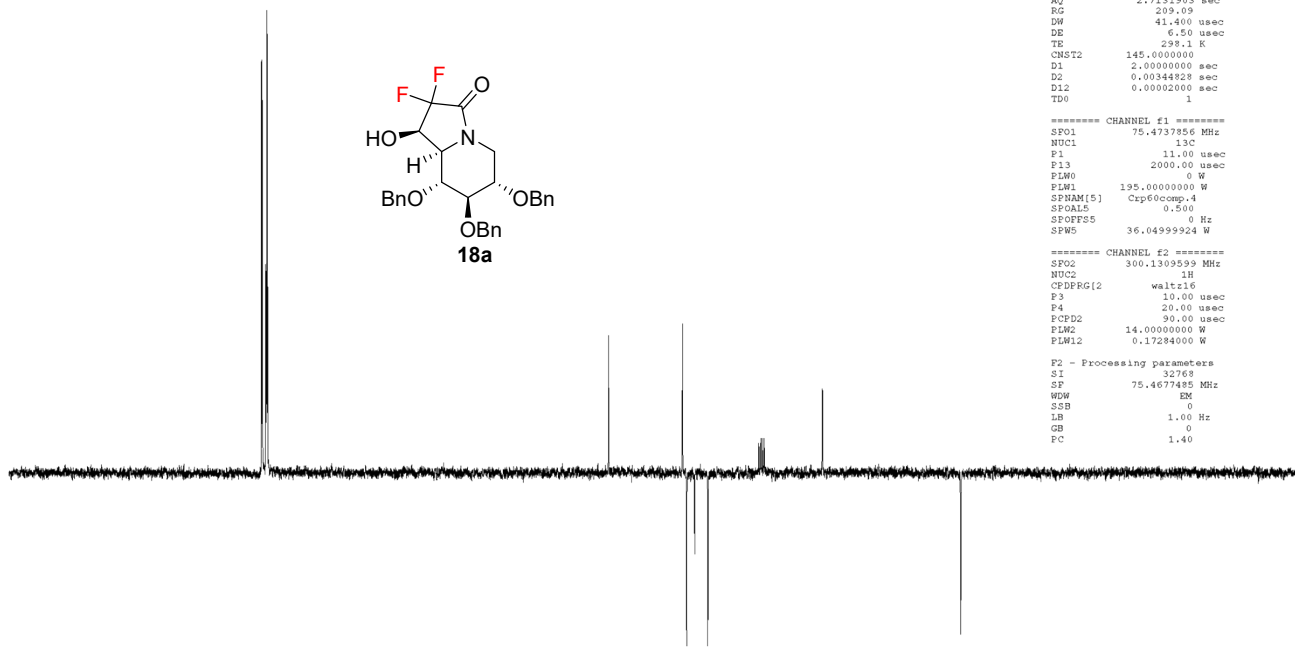
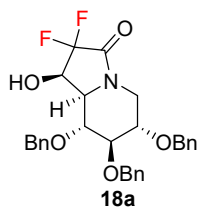
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FIDRES 0.184285 Hz  
AQ 2.7131903 sec  
RG 209.09  
DW 41.400 usec  
DE 6.50 usec  
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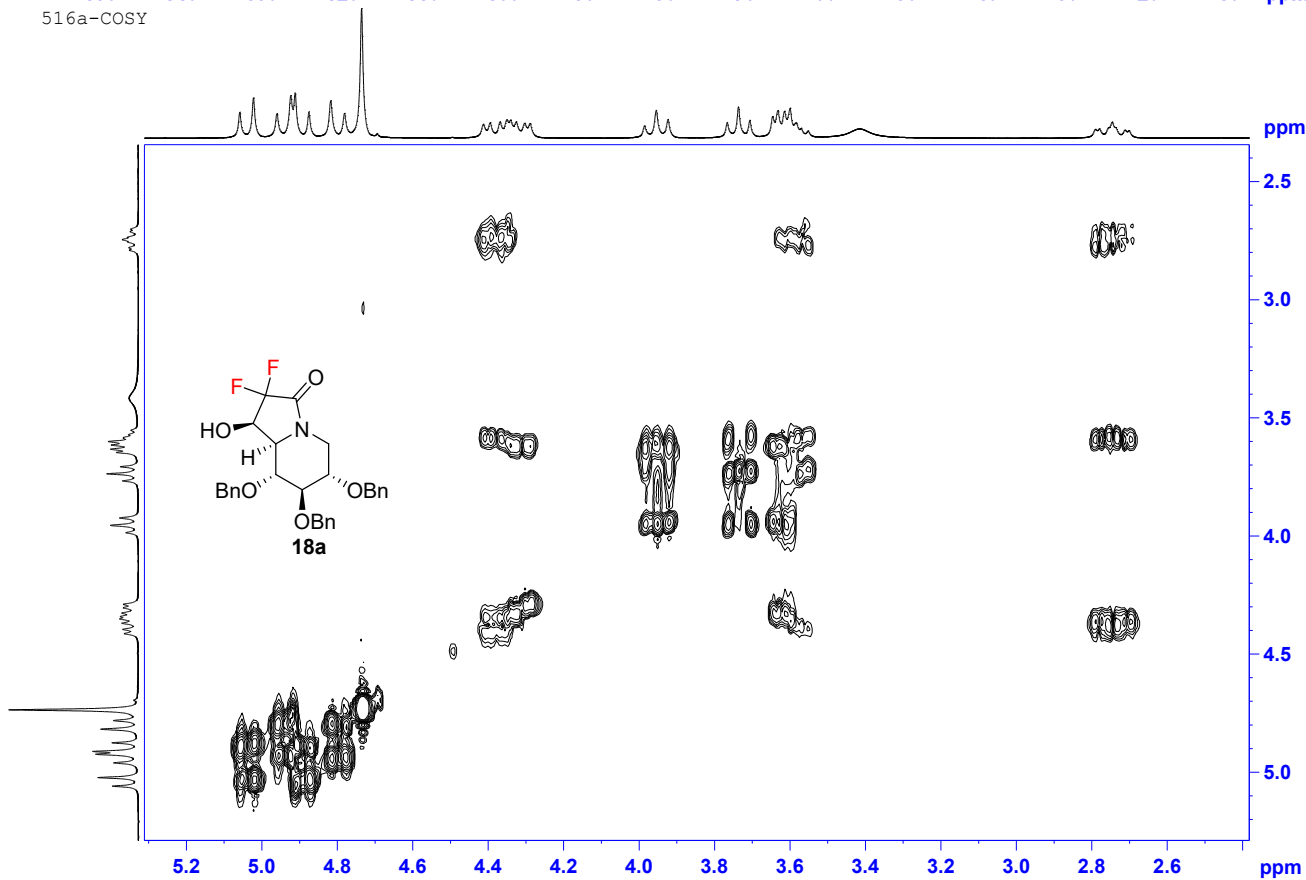
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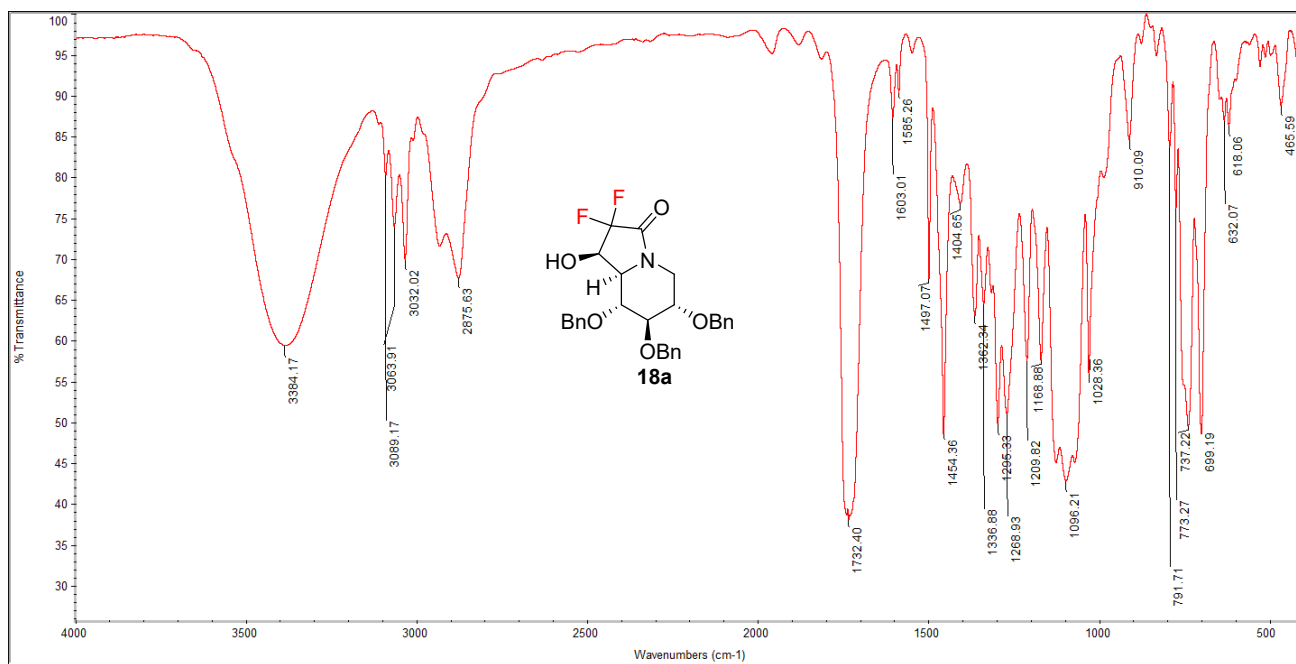
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PCED2 90.00 usec  
PLW2 14.00000000 W  
PLW12 0.17284000 W

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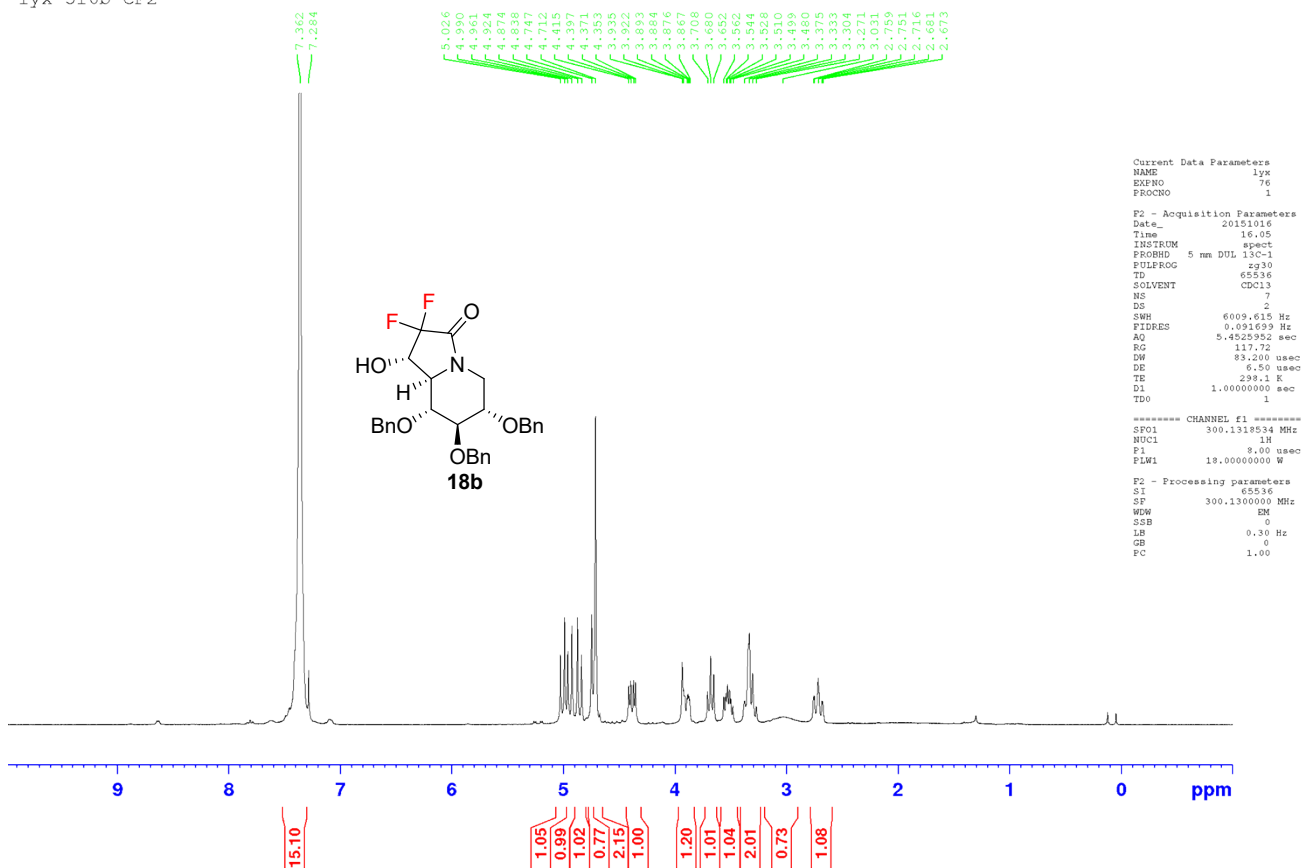
516a-COSY





Compound **18b**:

lyx-516b-CF2



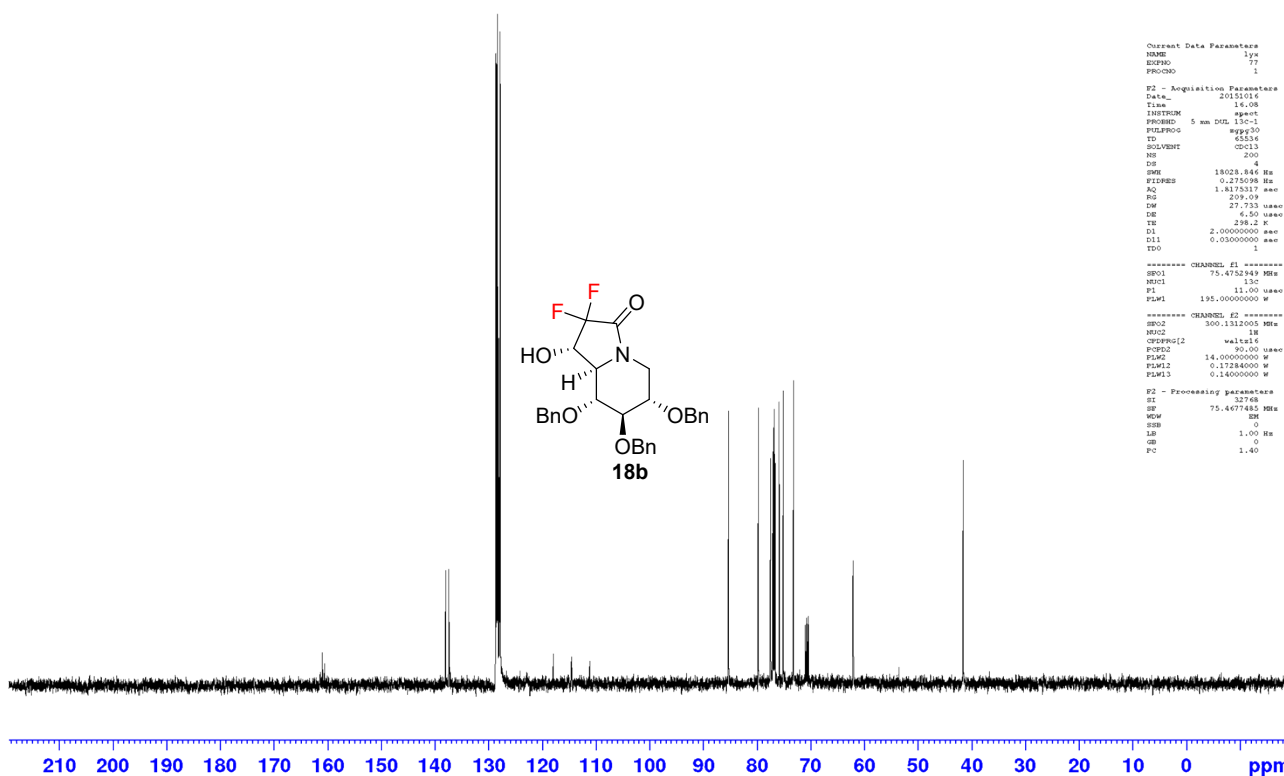
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128.40  
128.35  
128.13  
127.96  
127.91  
117.88  
117.97  
114.62  
114.56  
111.20

85.33  
79.79  
77.50  
77.08  
76.87  
76.65  
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75.25  
73.25  
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70.80  
70.66  
70.42  
62.13  
62.07

41.61



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PROCNO       1

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FIDRES     0.275098 Hz
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RG          259.09
DM          27.733 usec
DE          6.50 usec
TE          298.2 K
D1          2.0000000 sec
d11         0.0300000 sec
TD0         1

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NUC1       13C
P1         11.00 usec
PL1        195.0000000 W

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NUC2       1H
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PLM13     0.1400000 W

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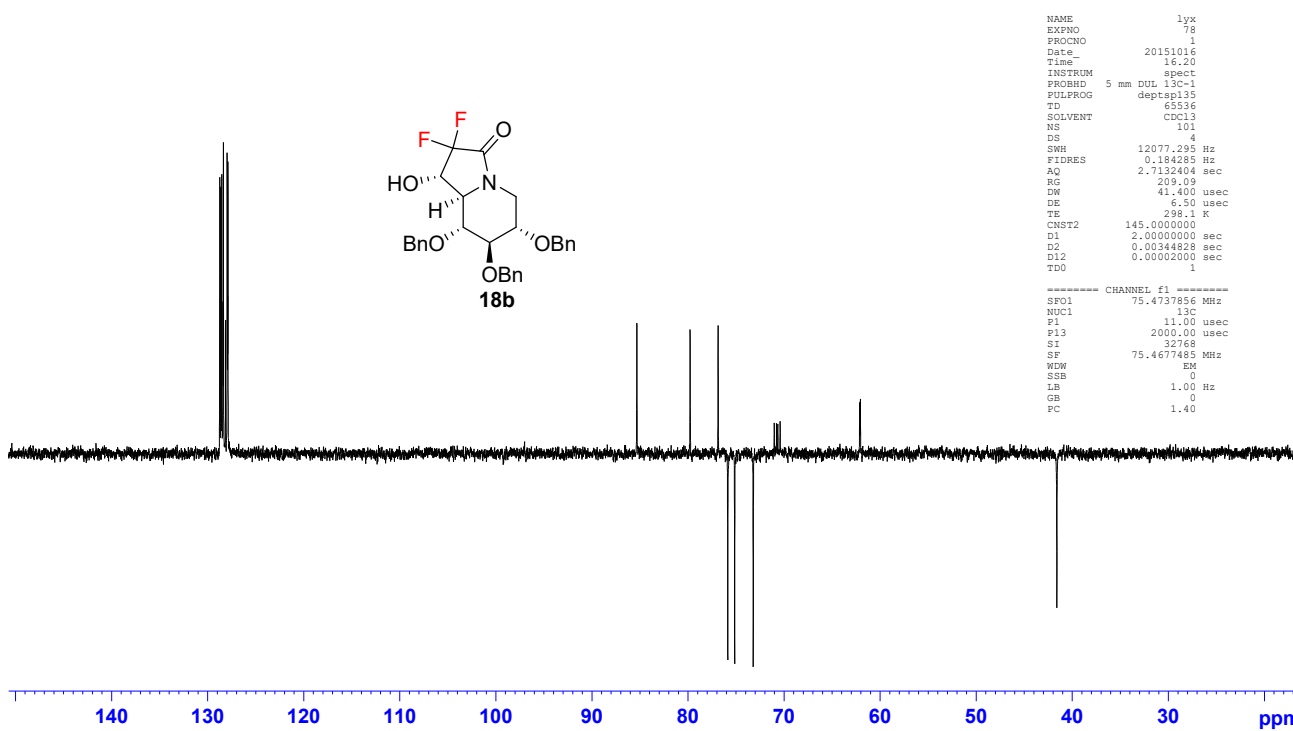
lyx-516b-dept135

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128.52  
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128.35  
128.13  
127.96  
127.91  
127.88

85.33  
79.79  
76.88  
75.87  
75.15  
73.22  
71.04  
70.80  
70.66  
70.42

62.14  
62.07

41.62

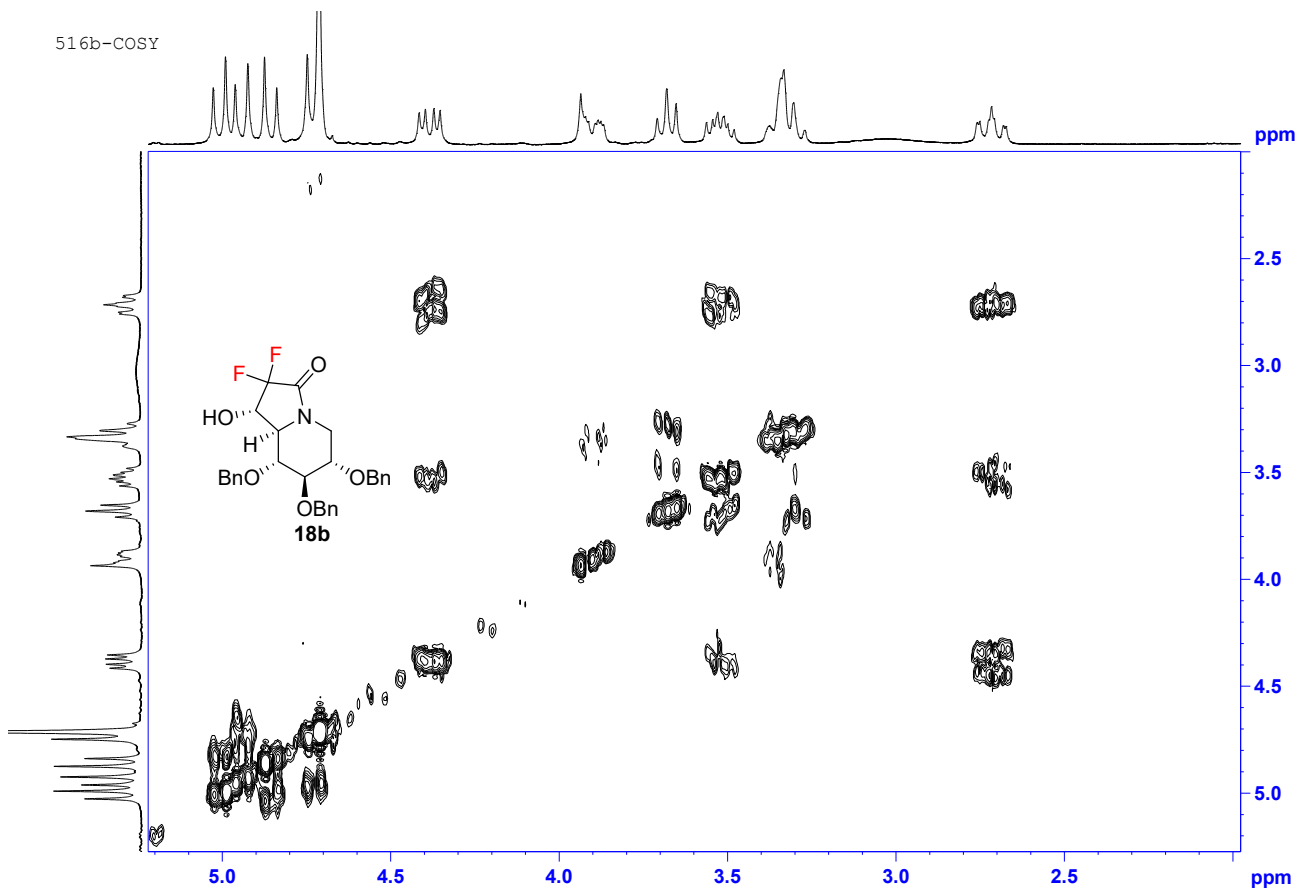


```

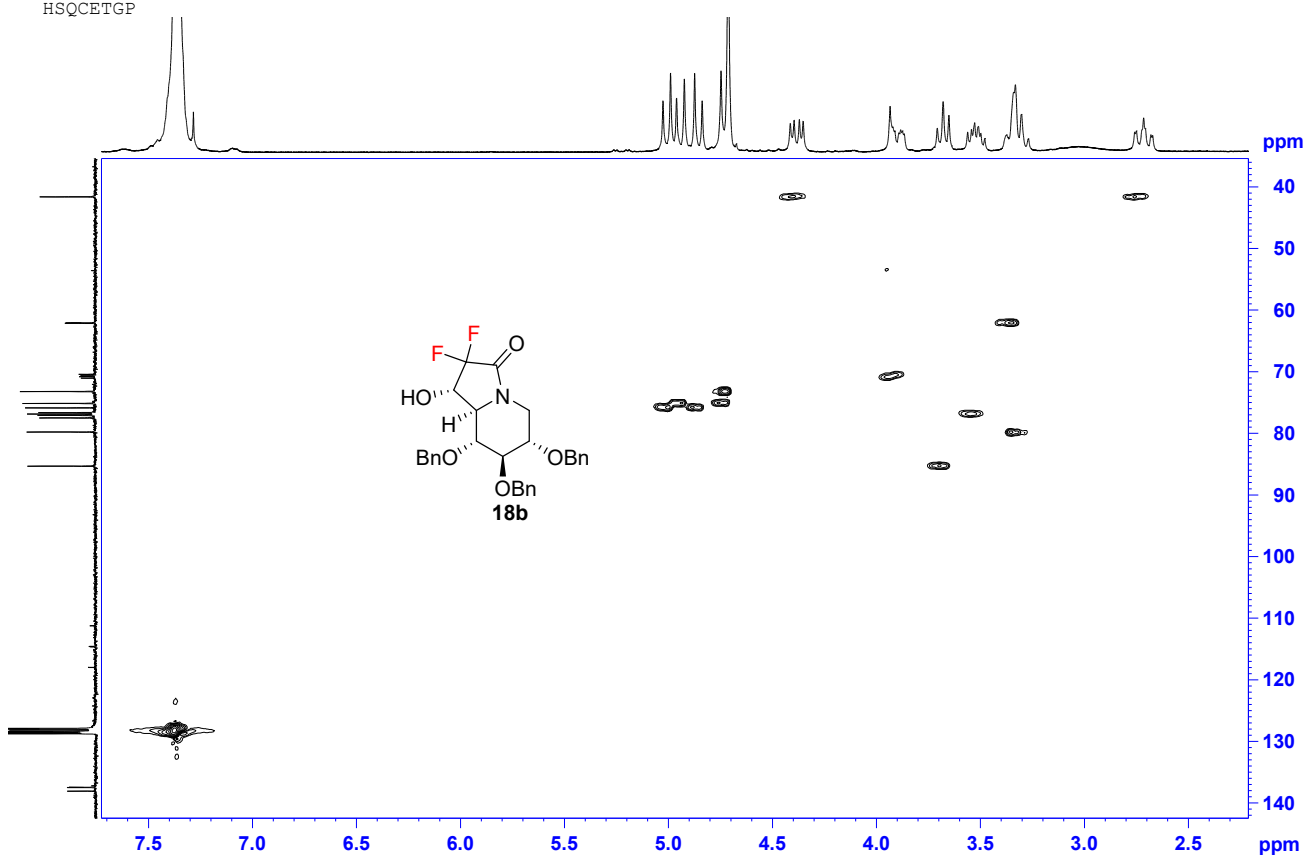
NAME          lyx
EXPNO        1
PROCNO       1
Date_        20151016
Time         16.20
INSTRUM     spect
PROBHD      5 mm DUL 13C-1
PULPROG     deptap135
TD           65536
SOLVENT     CDCl3
NS           101
DS           4
SWH         12077.295 Hz
FIDRES     0.184285 Hz
AQ          2.7132404 sec
RG          209.09
DM          41.400 usec
DE          6.50 usec
TE          298.1 K
D1          2.0000000 sec
D2          0.00344828 sec
D12         0.00002000 sec
TD0         1

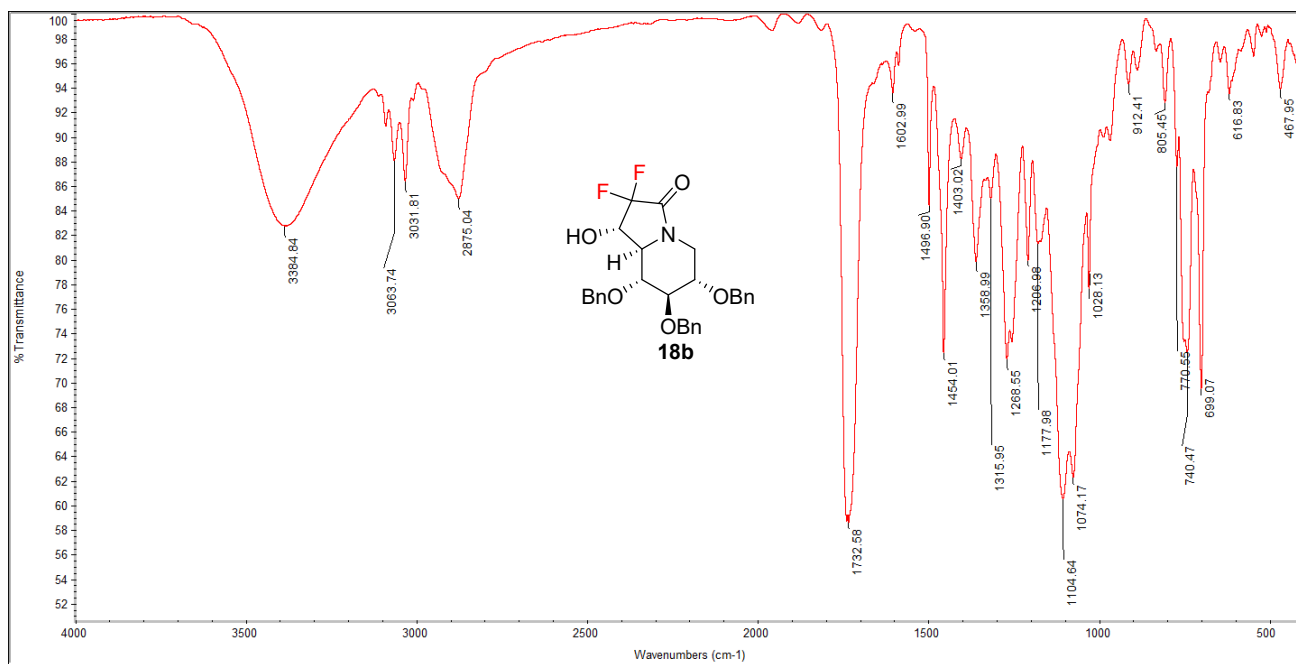
----- CHANNEL f1 -----
SFO1       75.4737856 MHz
NUC1       13C
P1         11.00 usec
PL1        2000.00 usec
SI         32768
SF         75.4677485 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

516b-COSY



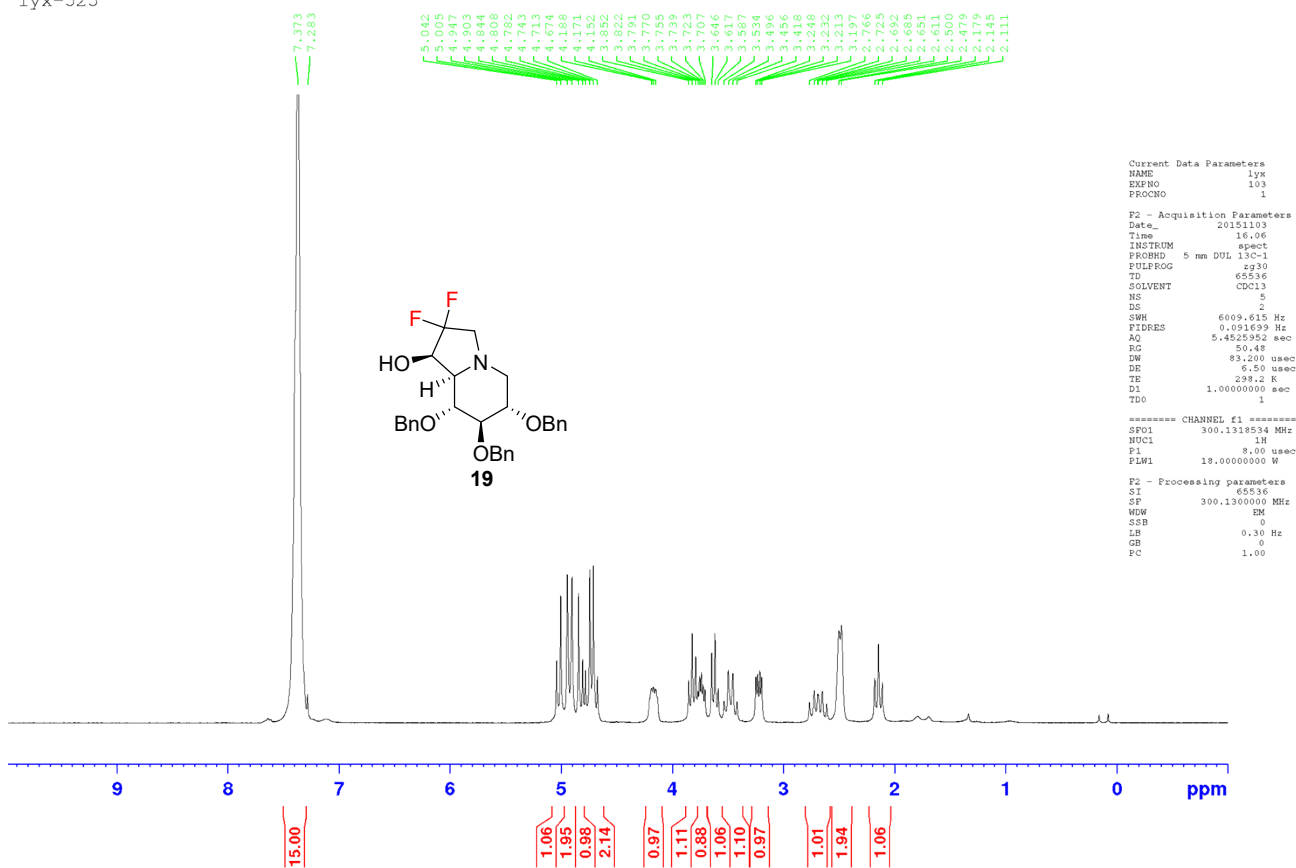
HSQCETGP





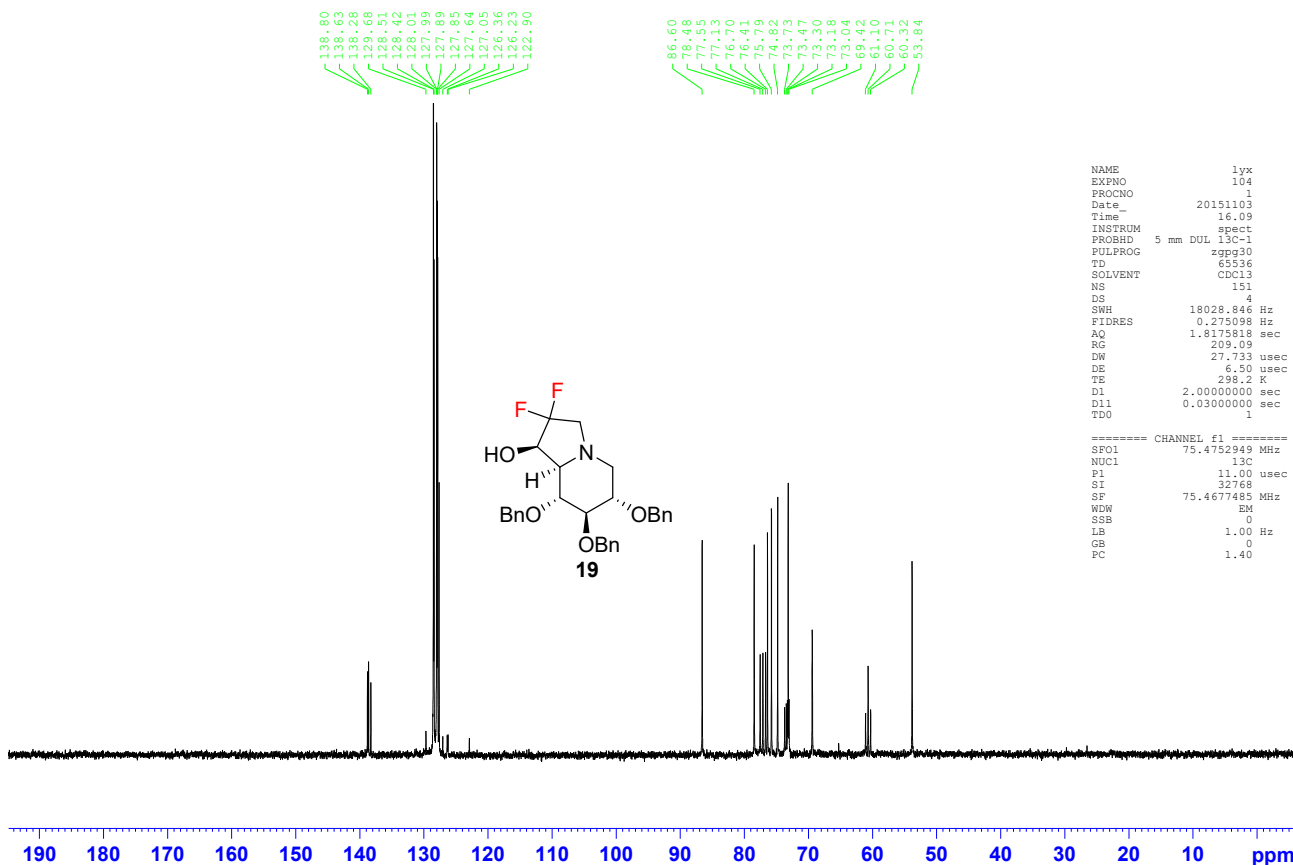
Compound 19:

lyx-525

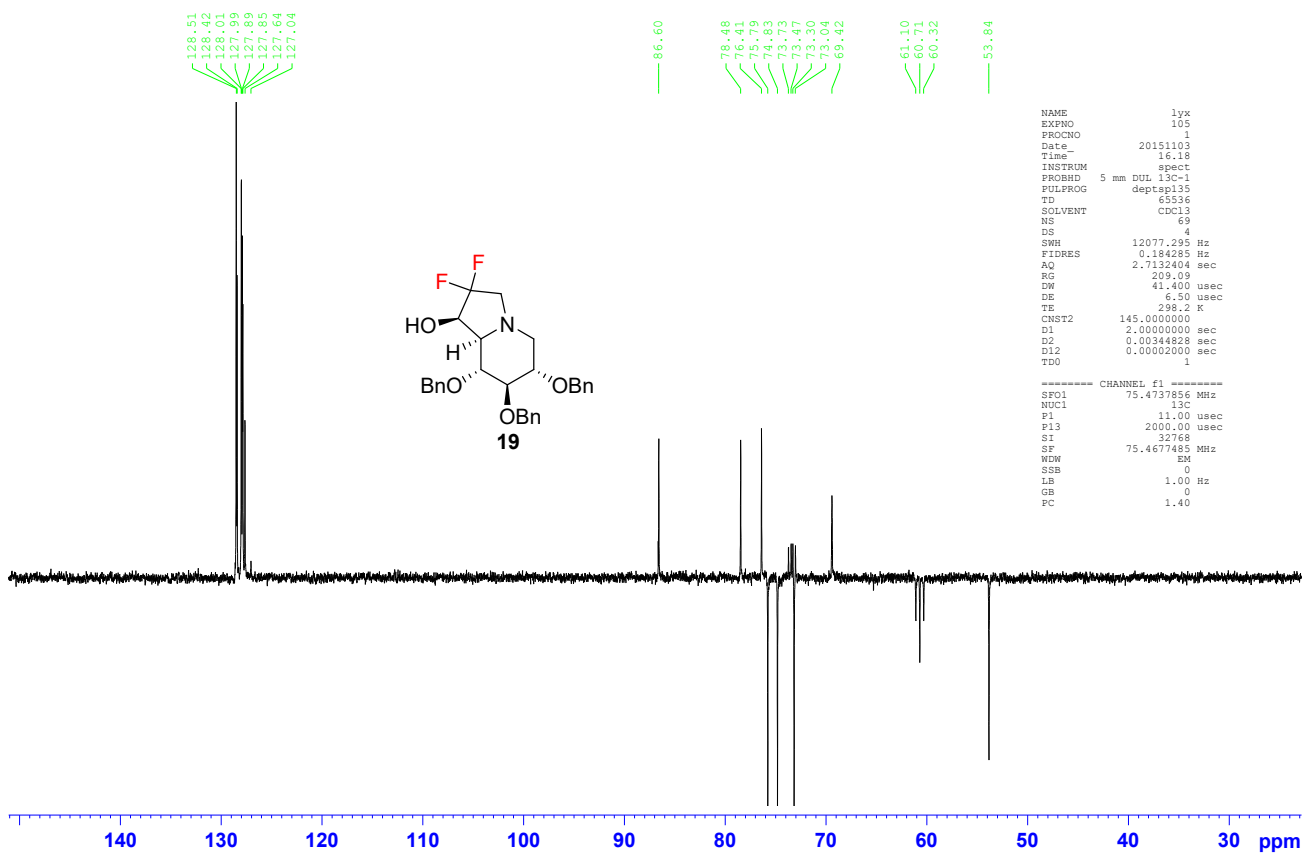




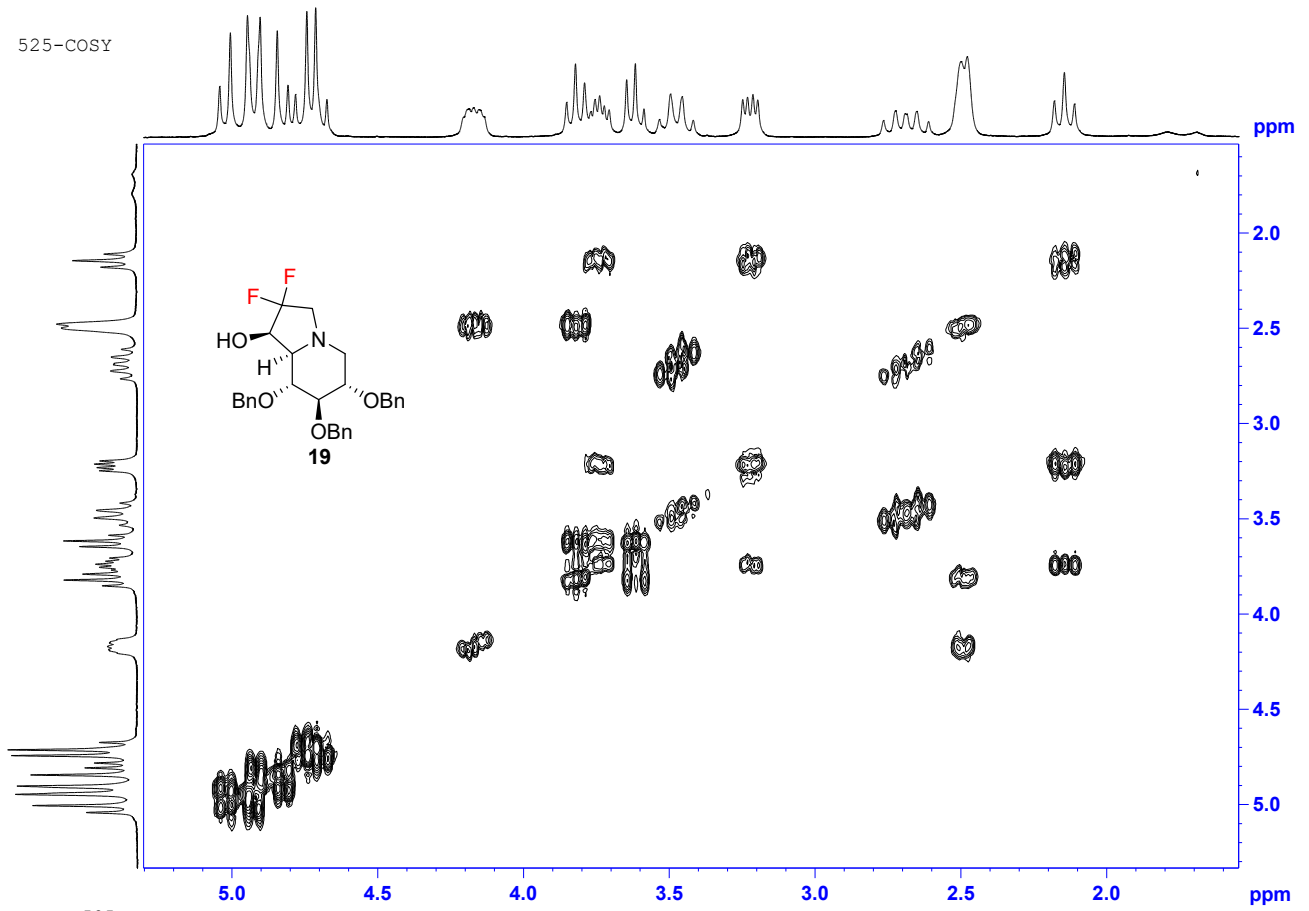
lyx-525-C13



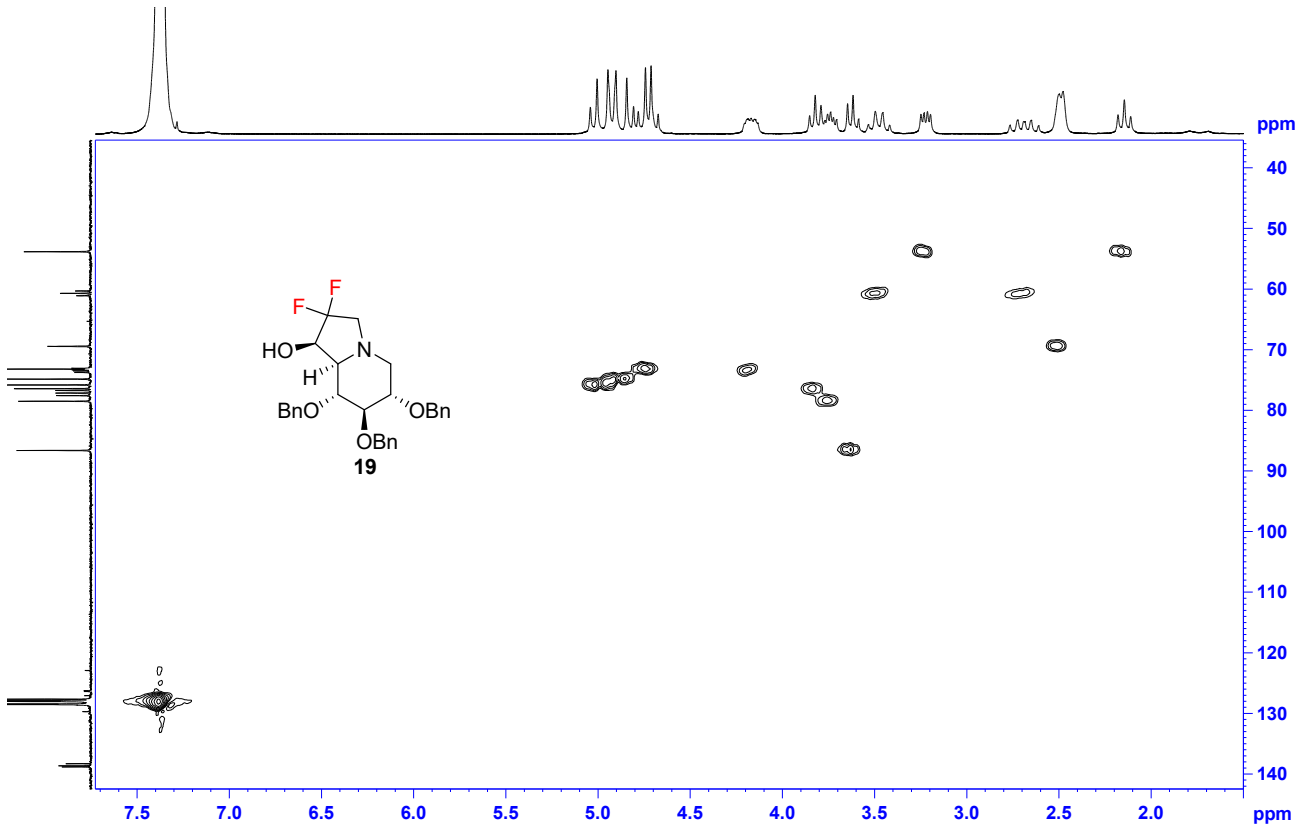
lyx-525-dept135

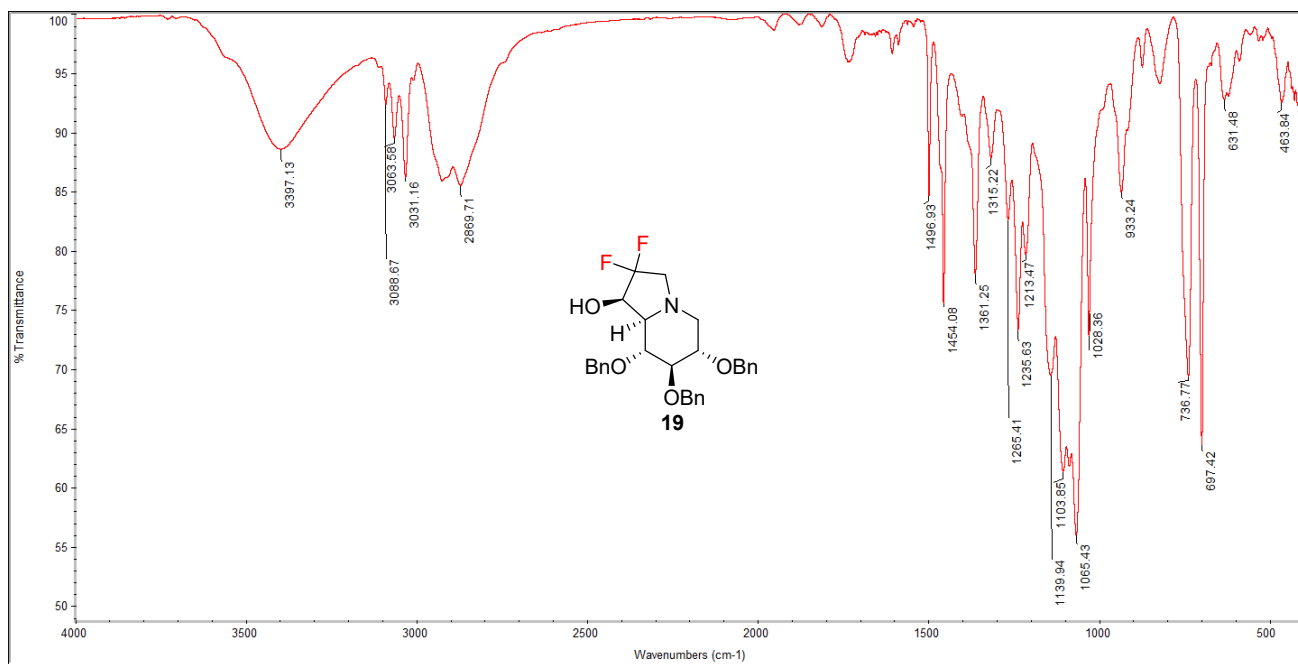


525-COSY



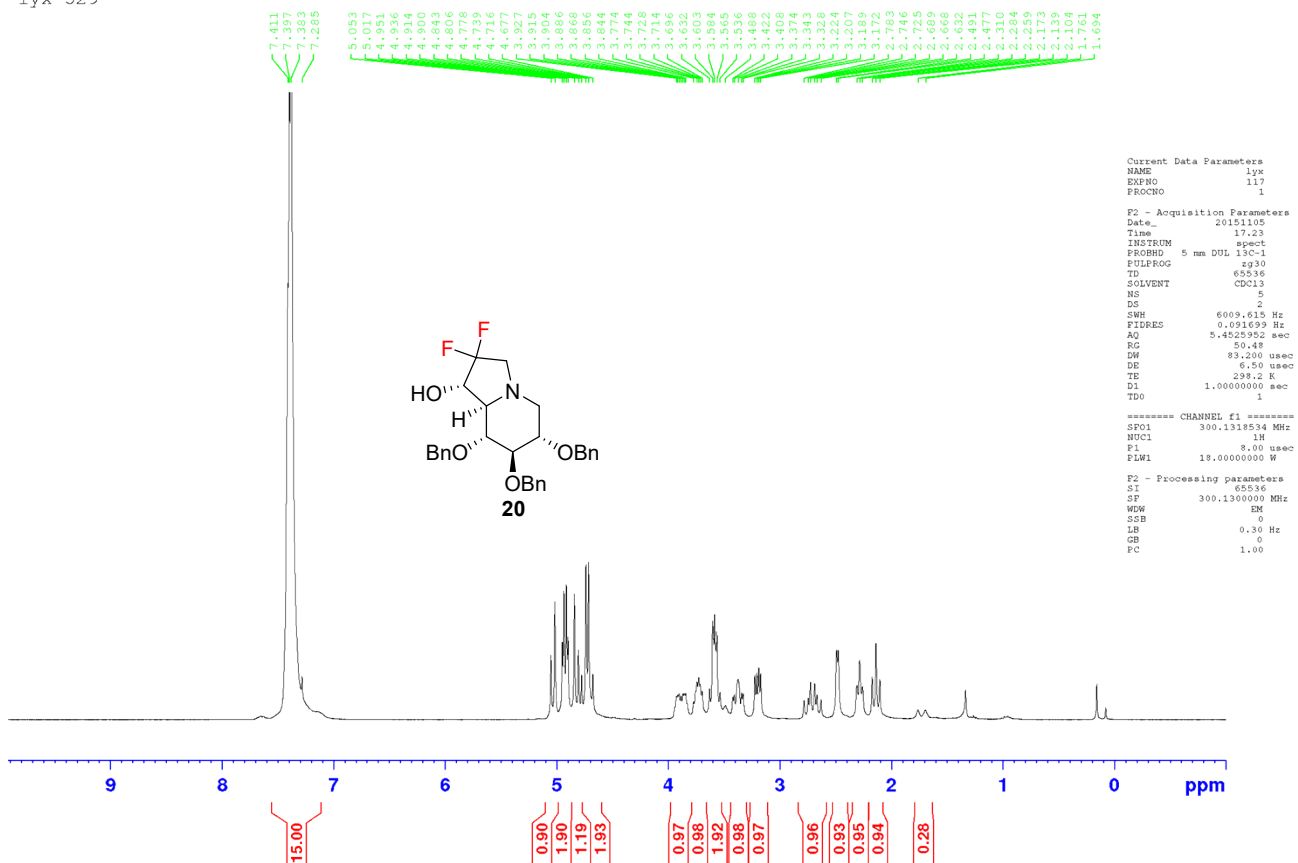
525-HSQCETGP



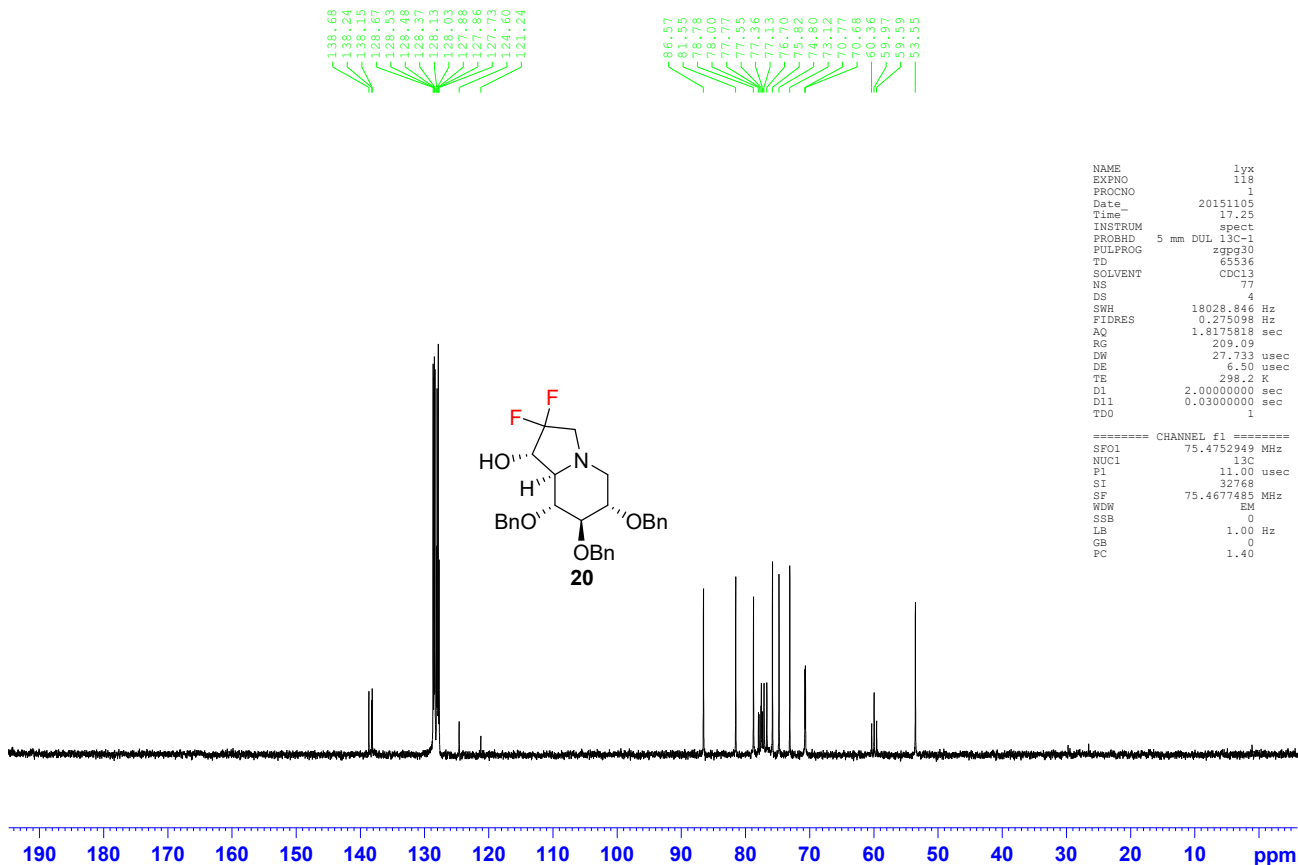


Compound 20:

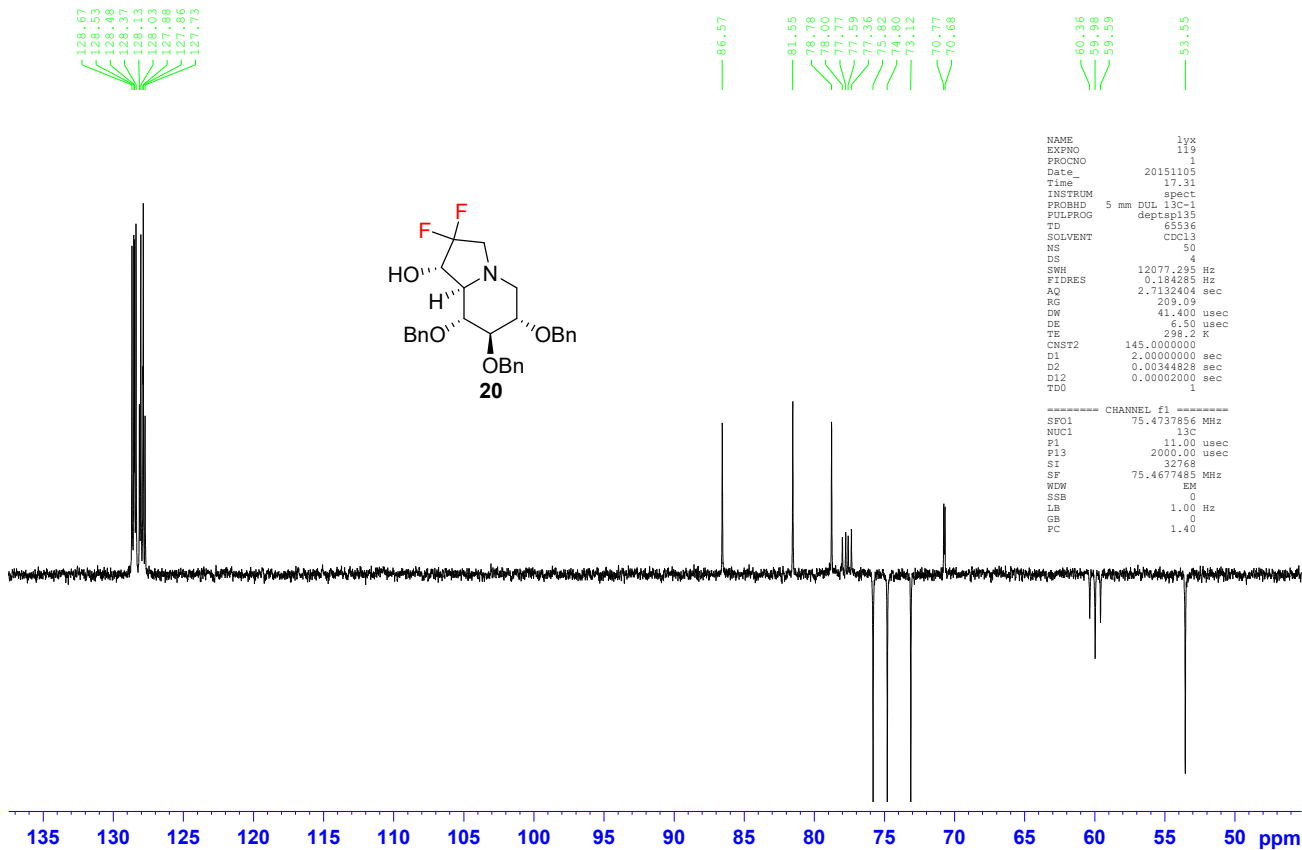
lyx-529

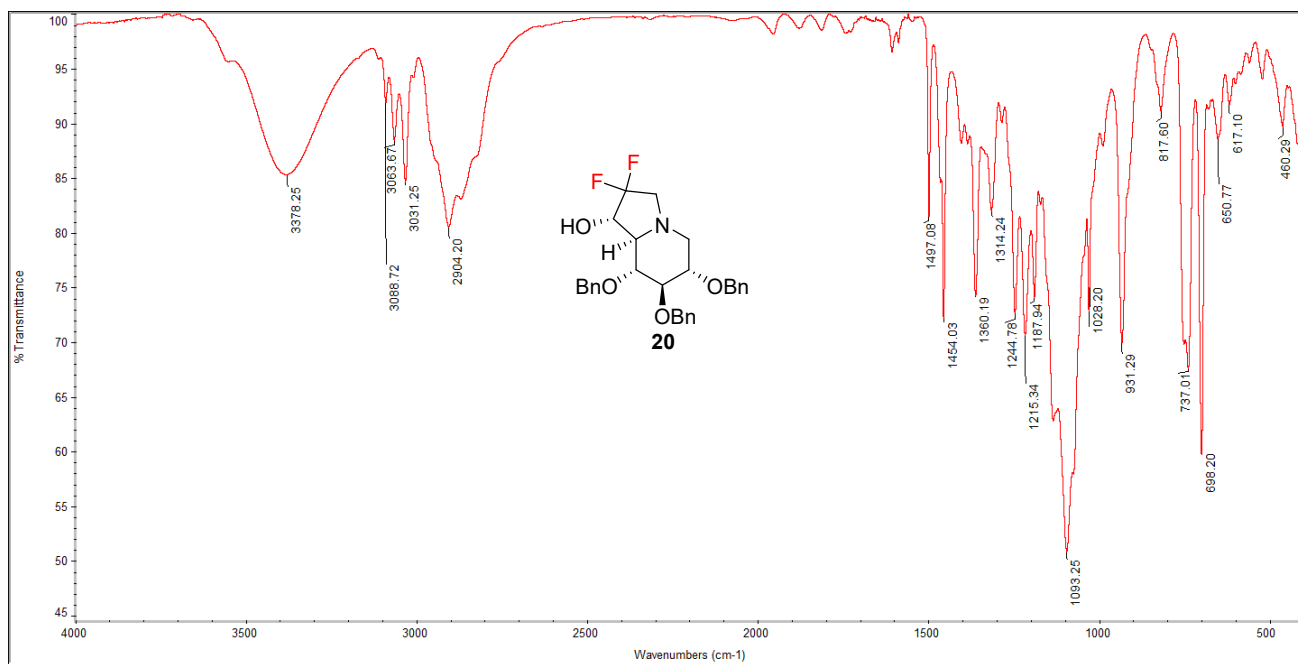


lyx-529-C13



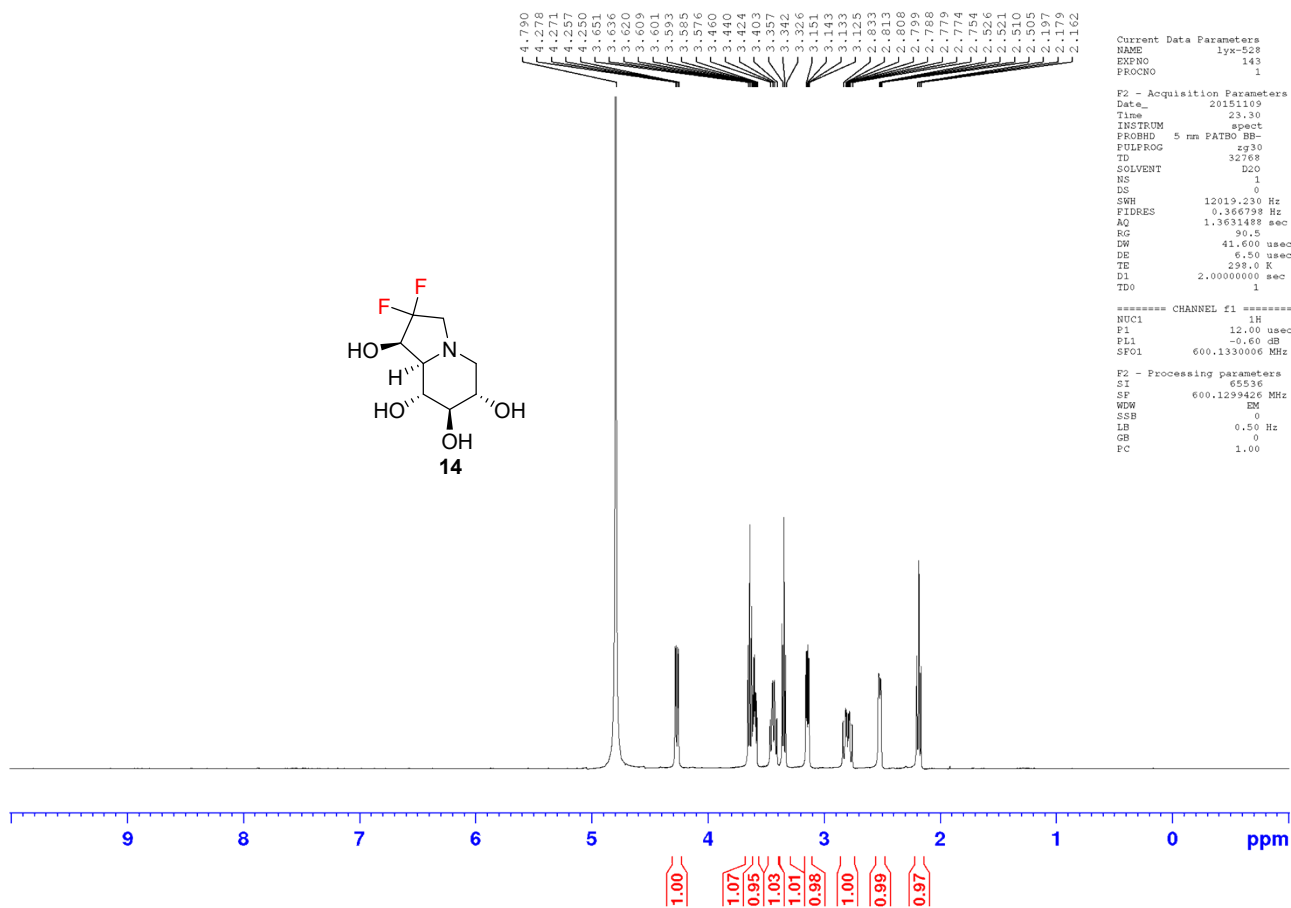
lyx-529-dept135





Compound 14:

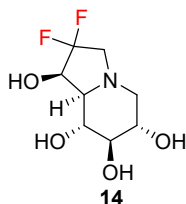
<sup>1</sup>H NMR  
lyx-528



lyx-528-C13

129.69  
126.39  
126.25  
122.94

78.21  
72.44  
72.19  
72.01  
71.76  
69.51  
68.77  
68.04  
59.64  
59.25  
54.66

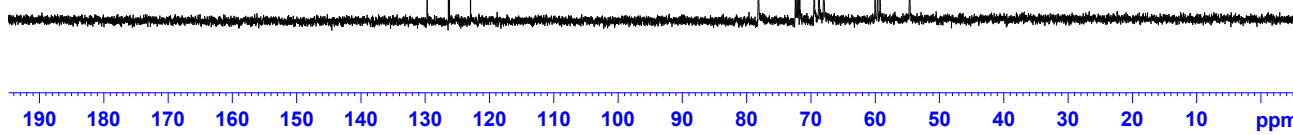


```

NAME lyx
EXPNO 109
PROCNO 1
Date_ 20151105
Time 10.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 166
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 209.09
DW 27.733 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

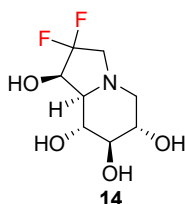
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 11.00 usec
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



lyx-528-dept135

78.21  
72.44  
72.19  
72.01  
71.76  
69.51  
68.77  
68.04  
59.64  
59.25  
54.66



```

Current Data Parameters
NAME lyx
EXPNO 110
PROCNO 1

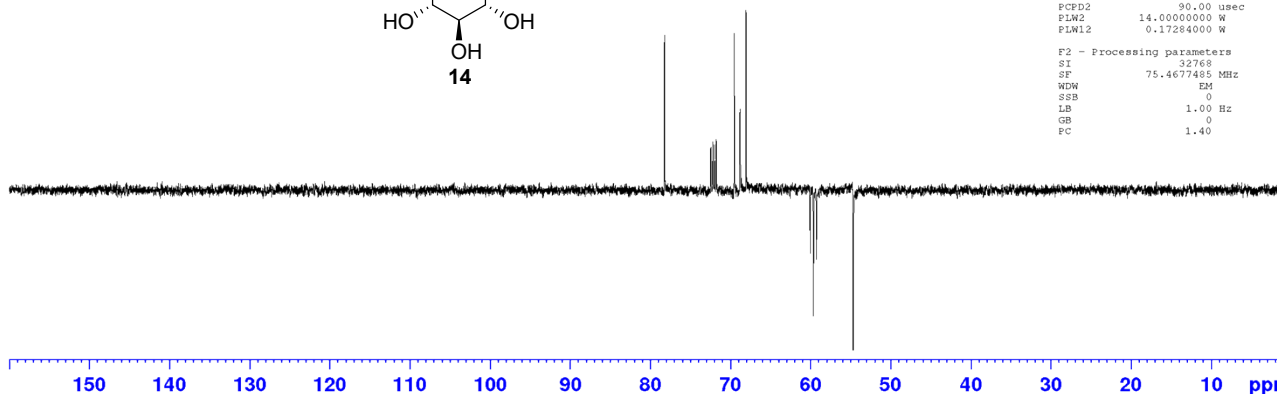
F2 - Acquisition Parameters
Date_ 20151105
Time 10.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG deptsp135
TD 65536
SOLVENT D2O
NS 101
DS 4
SWH 12077.295 Hz
FIDRES 0.194285 Hz
AQ 2.7131903 sec
RG 209.09
DW 41.400 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.0034828 sec
D12 0.00002000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 75.4737856 MHz
NUC1 13C
P1 11.00 usec
P13 2000.00 usec
ELW0 0 W
ELW1 195.0000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SFOFF5 0 Hz
SPW5 36.04999924 W

===== CHANNEL f2 =====
SFO2 300.1309599 MHz
NUC2 1H
CPDPRG2 waltz16
P3 10.00 usec
P4 20.00 usec
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.17284000 W

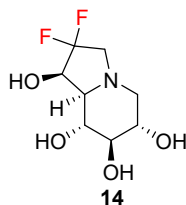
F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



-97.773  
-98.198

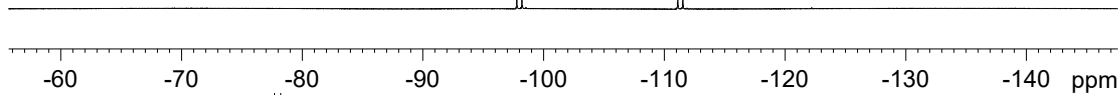
-111.112  
-111.537



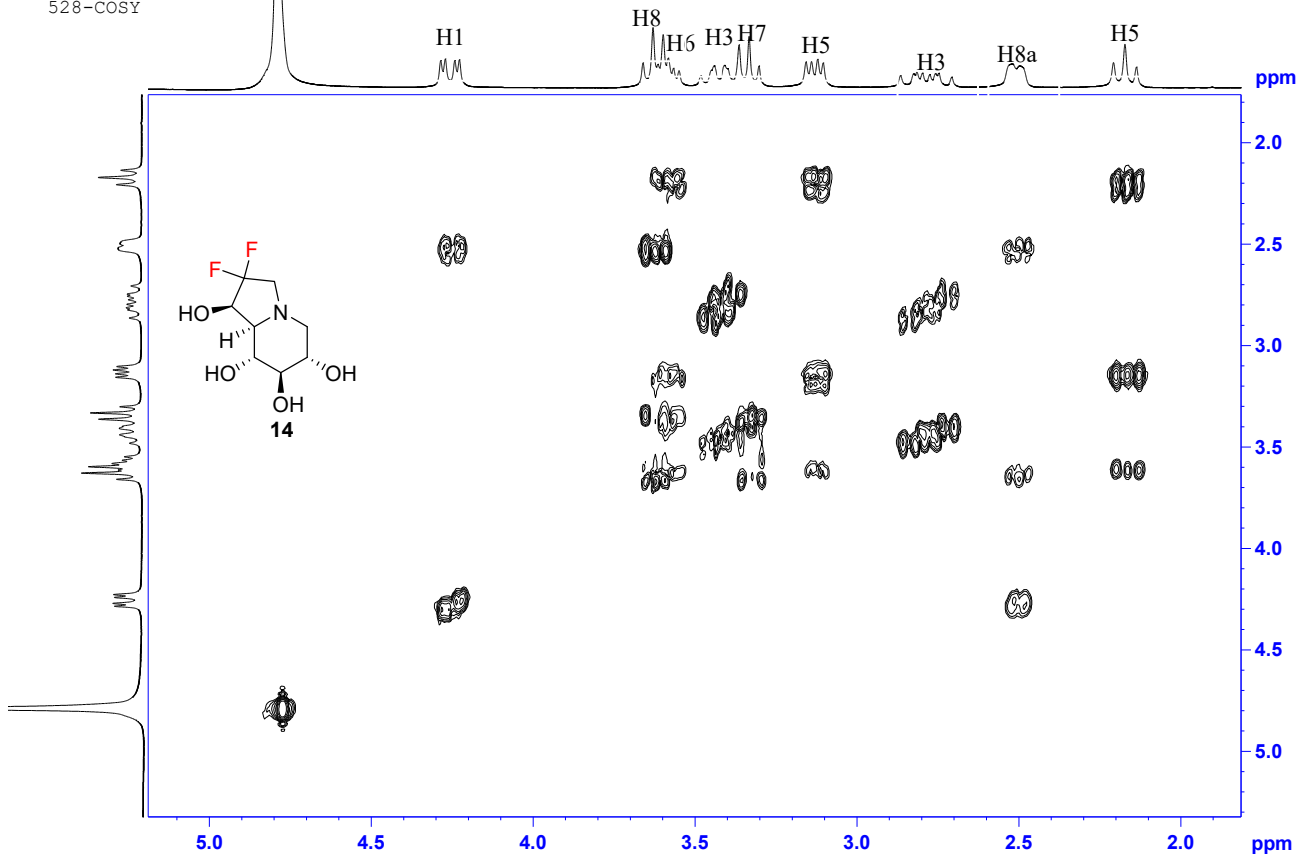
NAME 19F  
EXPNO 95  
PROCNO 1  
Date\_ 20151109  
Time 23.28  
INSTRUM spect  
PROBHD 5 mm PATBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT D2O  
NS 16  
DS 0  
SWH 56497.176 Hz  
FIDRES 0.862078 Hz  
AQ 0.5800524 sec  
RG 1024  
DW 8.850 usec  
DE 12.64 usec  
TE 298.6 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
D12 0.0000200 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 19F  
P1 23.50 usec  
PL1 0.00 dB  
PL1W 25.11886406 W  
SFO1 564.6299194 MHz

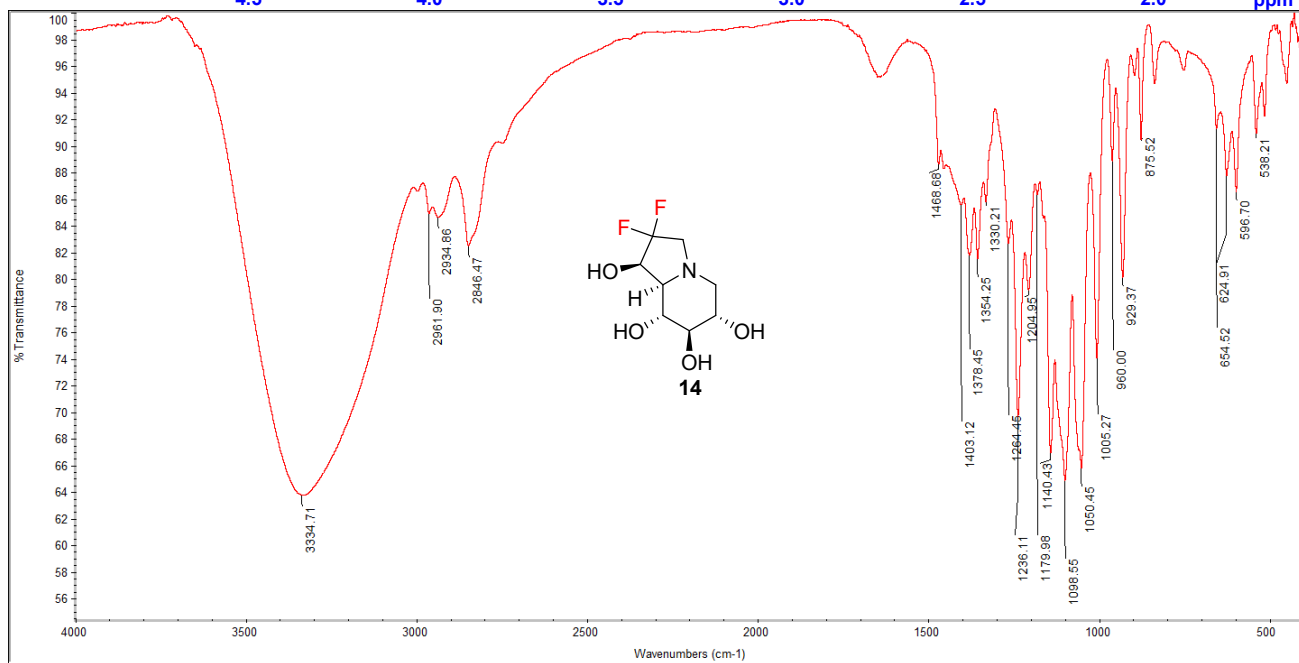
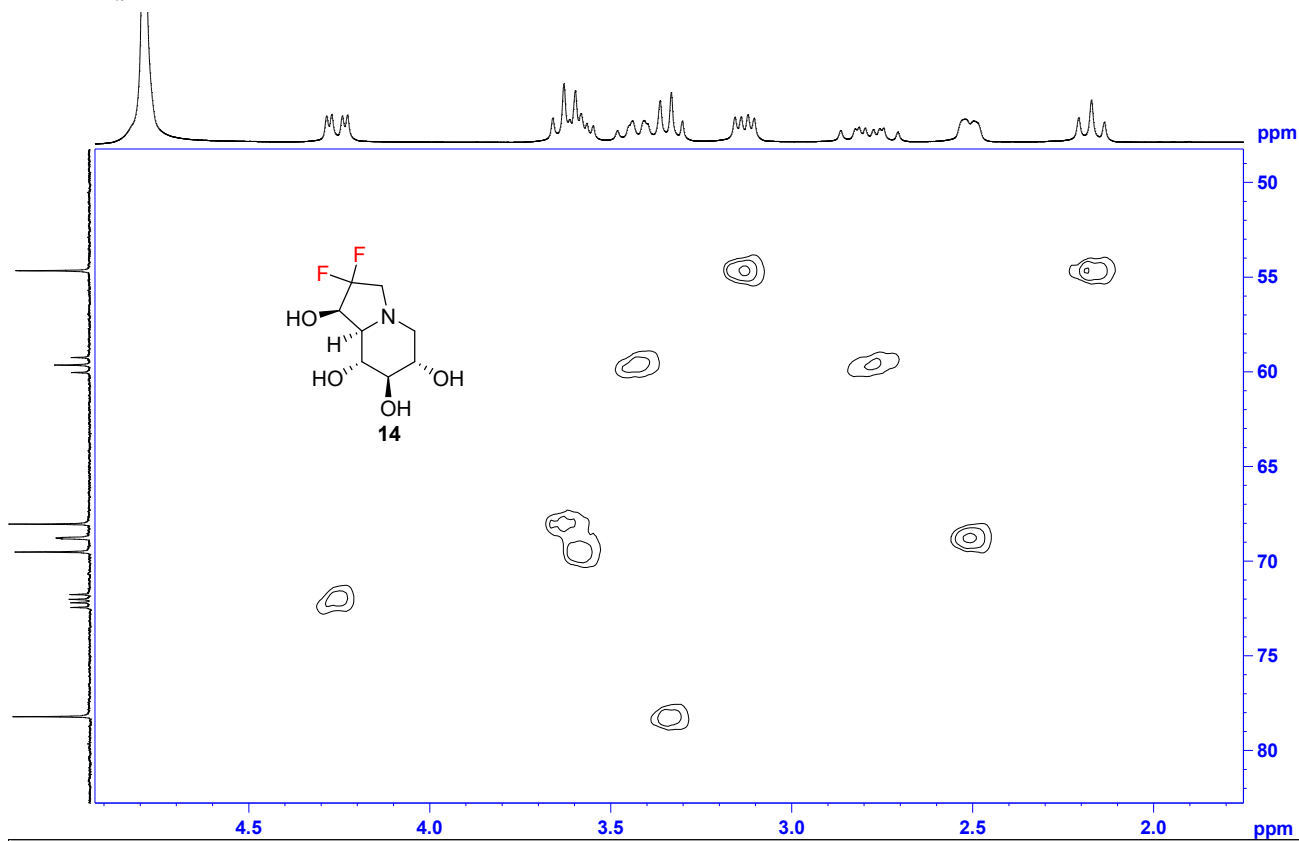
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 70.00 usec  
PL2 -0.60 dB  
PL12 14.72 dB  
SFO2 600.1324005 MHz  
SI 65536  
SF 564.6863880 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



528-COSY



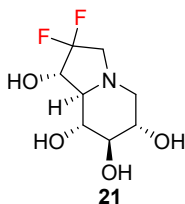
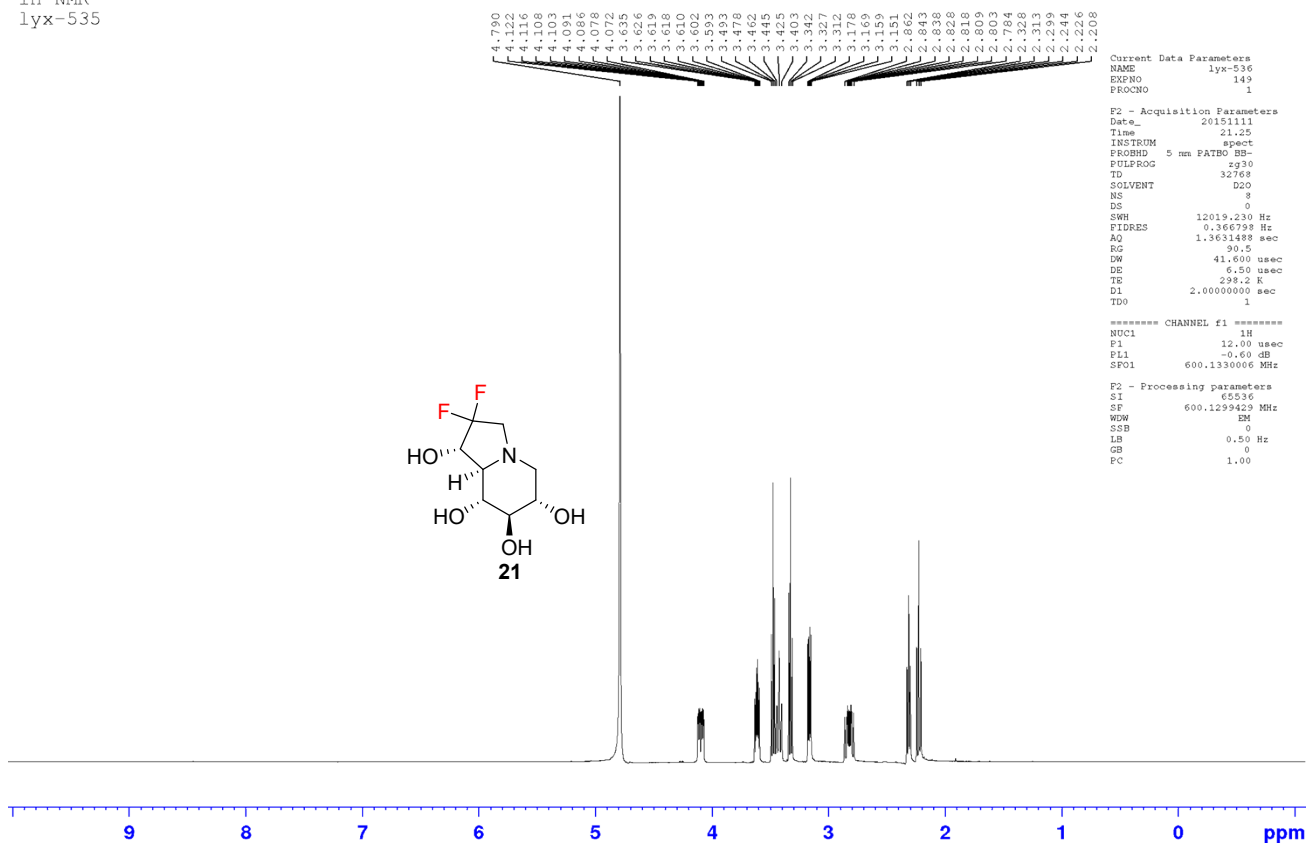
528-HSQCETGP



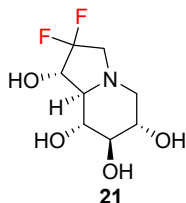
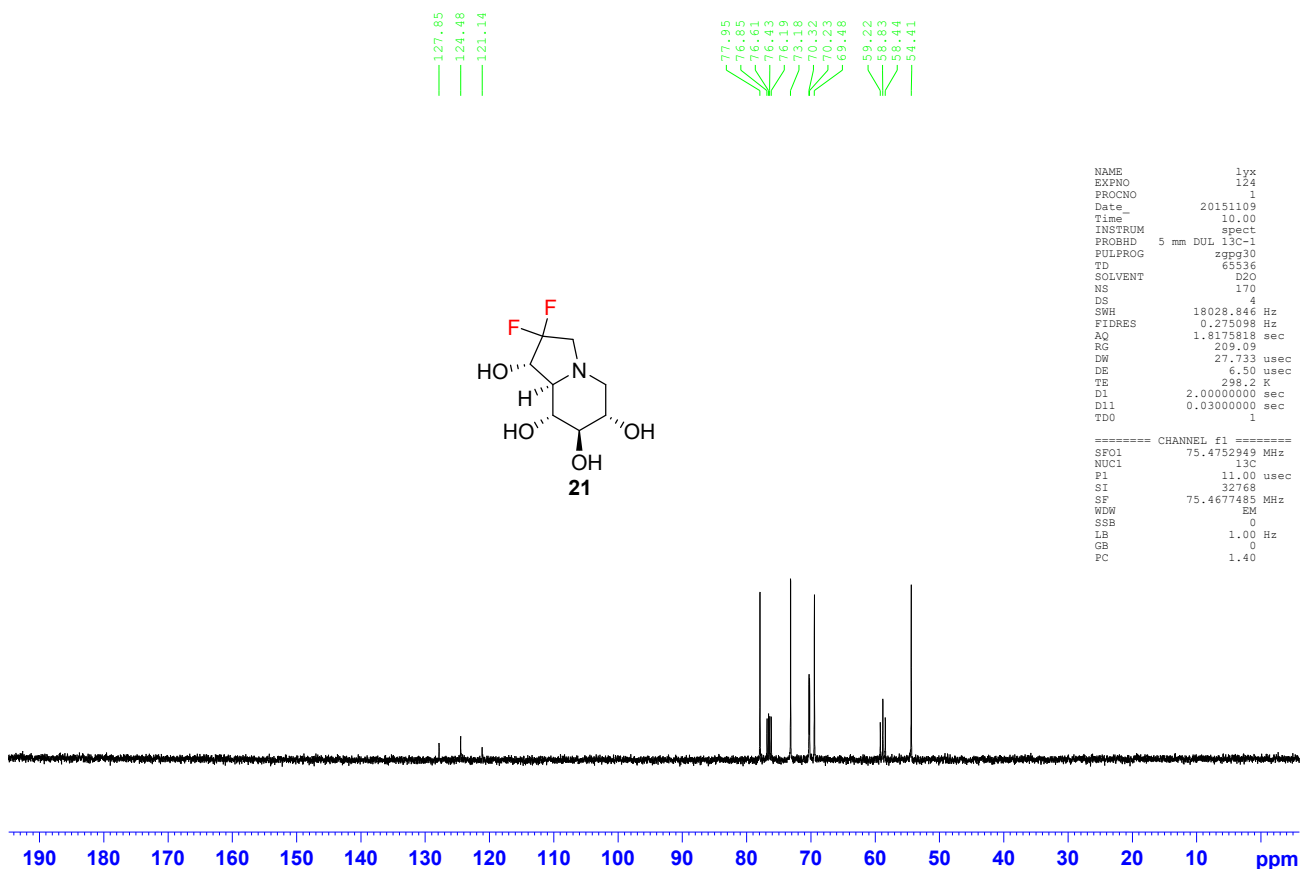


Compound 21:

<sup>1</sup>H NMR  
lyx-535

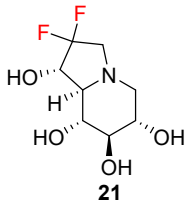


lyx-535-C13

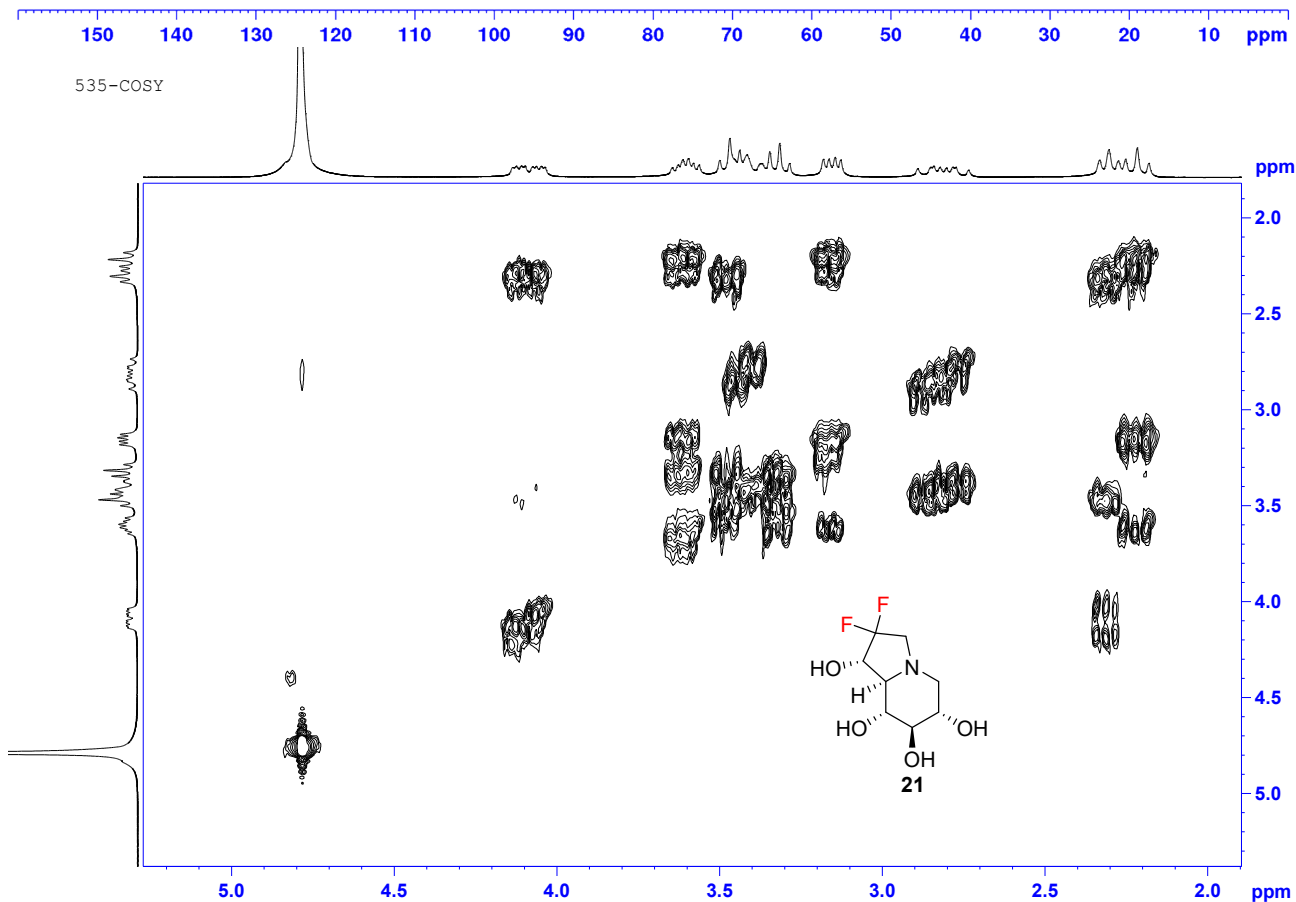
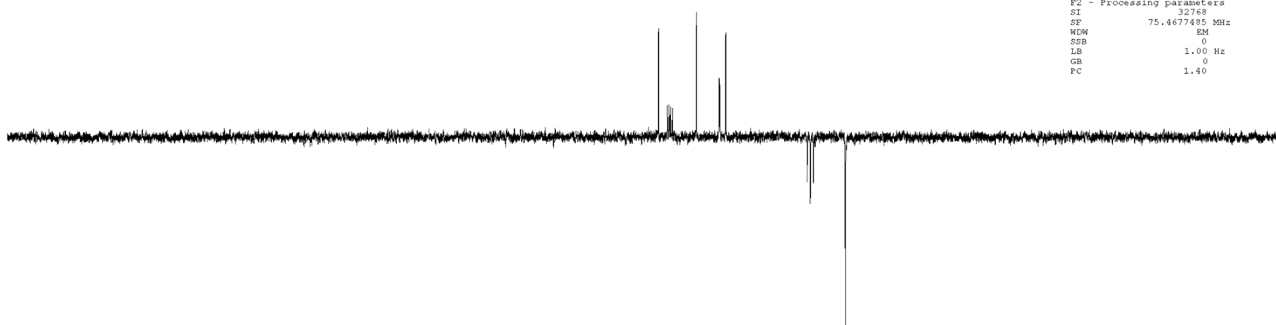


77.05  
76.05  
76.43  
76.19  
73.18  
70.32  
69.48  
59.22  
58.83  
58.44  
54.41

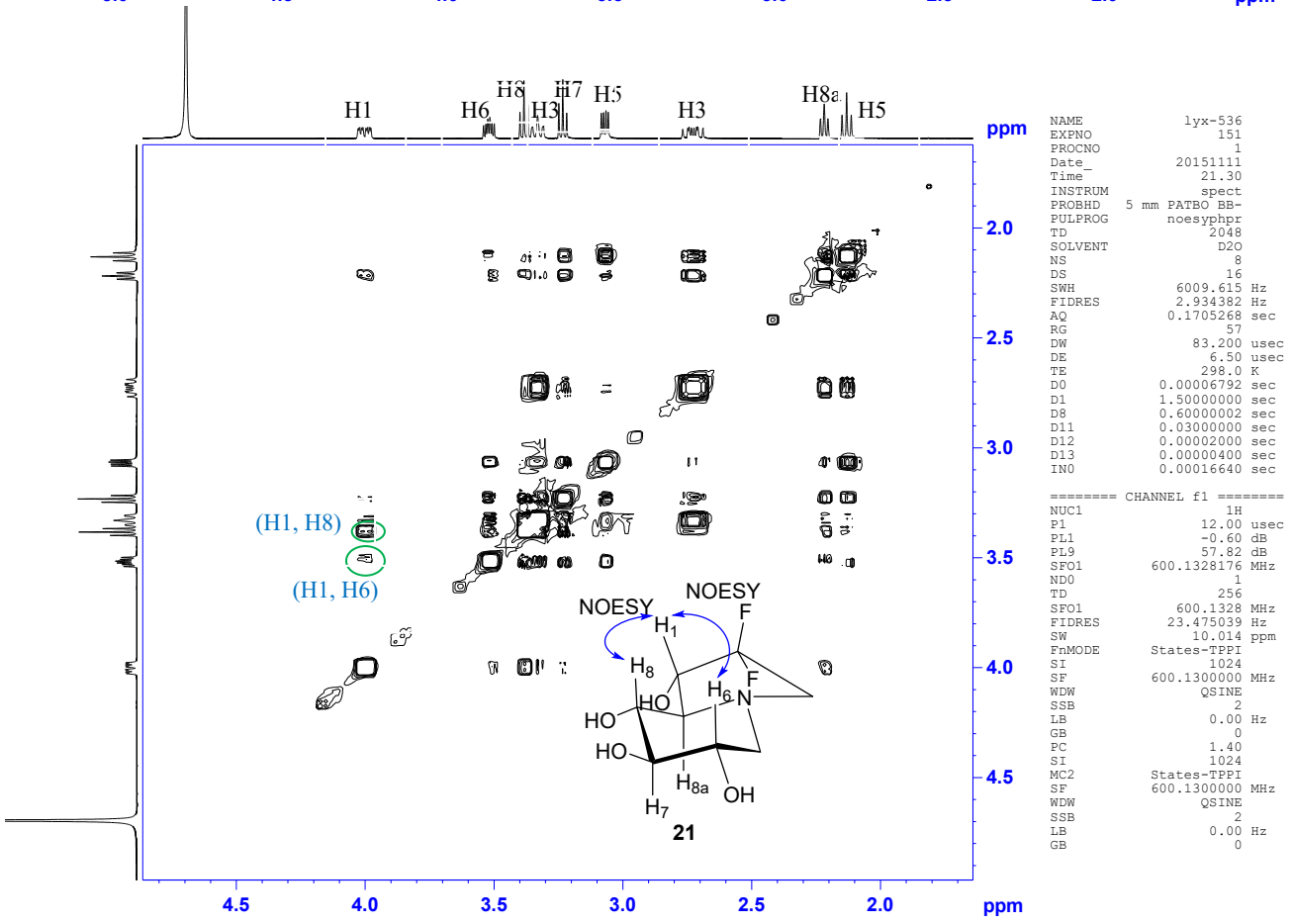
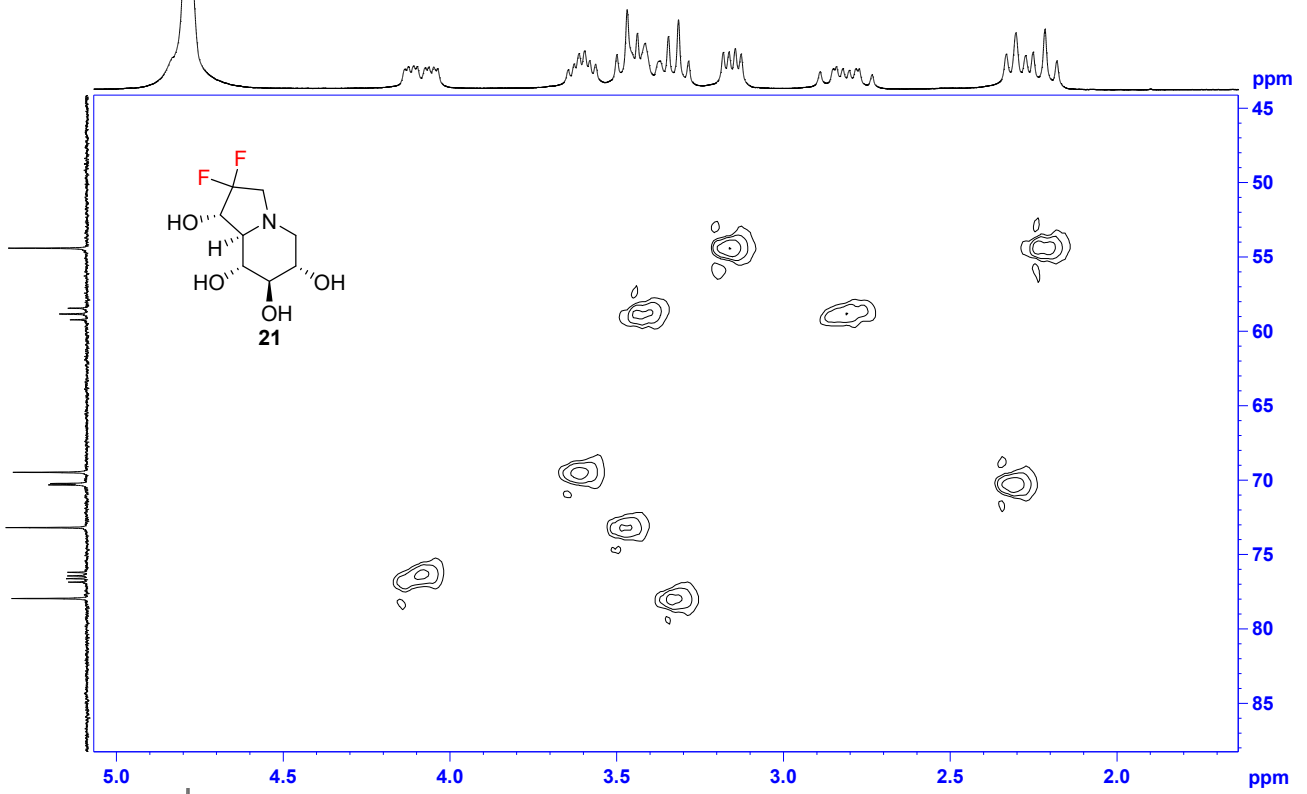
Current Data Parameters  
 NAME lyx  
 EXPNO 155  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20151209  
 Time 10.13  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG deptsp135  
 TD 65536  
 SOLVENT D2O  
 NS 101  
 DS 4  
 SWH 12077.295 Hz  
 FIDRES 0.184235 Hz  
 AQ 2.7131963 sec  
 RG 209.09  
 DW 81.400 usec  
 DE 6.50 usec  
 TE 298.2 K  
 CNST2 145.000000  
 D1 2.00000000 sec  
 D2 0.0034823 sec  
 D12 0.00002000 sec  
 TD0 1



----- CHANNEL f1 -----  
 SFO1 75.4737854 MHz  
 NUC1 13C  
 P1 11.00 usec  
 P13 2000.00 usec  
 PLW0 0 W  
 PLW1 195.00000000 W  
 SPNAM[5] Csp6comp.4  
 SFOAL5 0.500  
 SFOF25 0 Hz  
 SPW5 36.04999924 W  
 ----- CHANNEL f2 -----  
 SFO2 300.1309559 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 F3 19.00 usec  
 F4 20.00 usec  
 PCPD2 90.00 usec  
 PLW2 14.00000000 W  
 PLW12 0.17284000 W  
 F2 - Processing parameters  
 SI 32769  
 SF 75.4677854 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



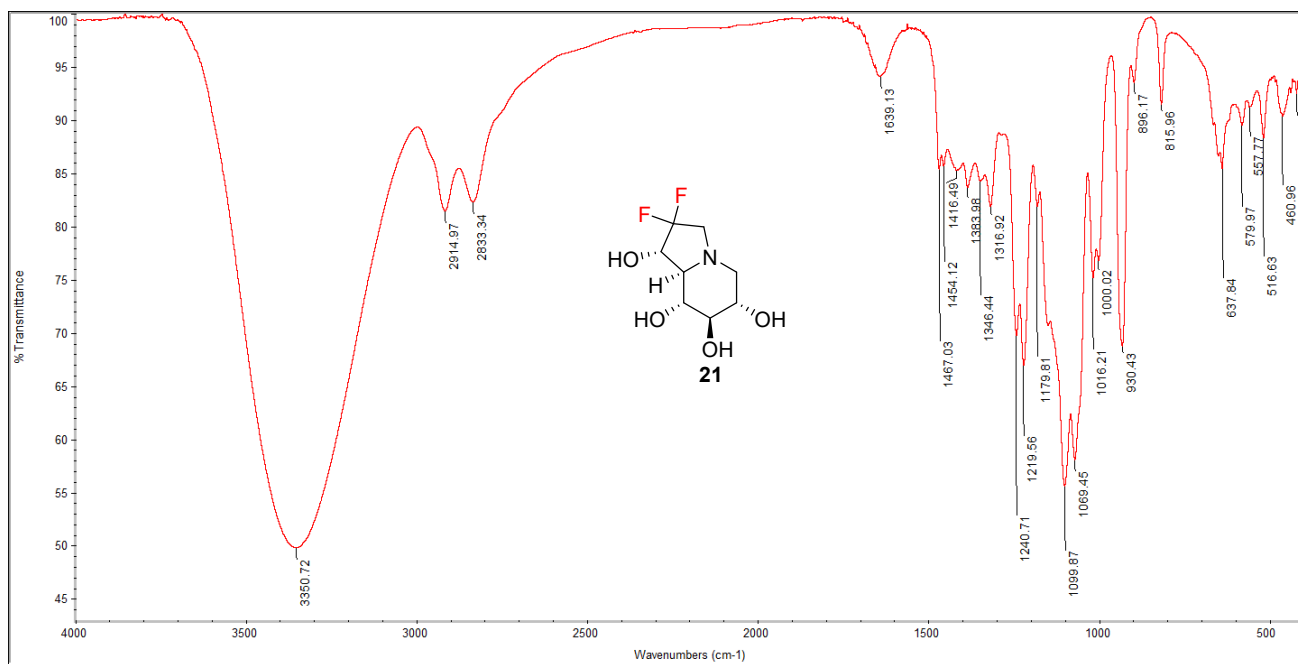
535-HSQCETGP



```

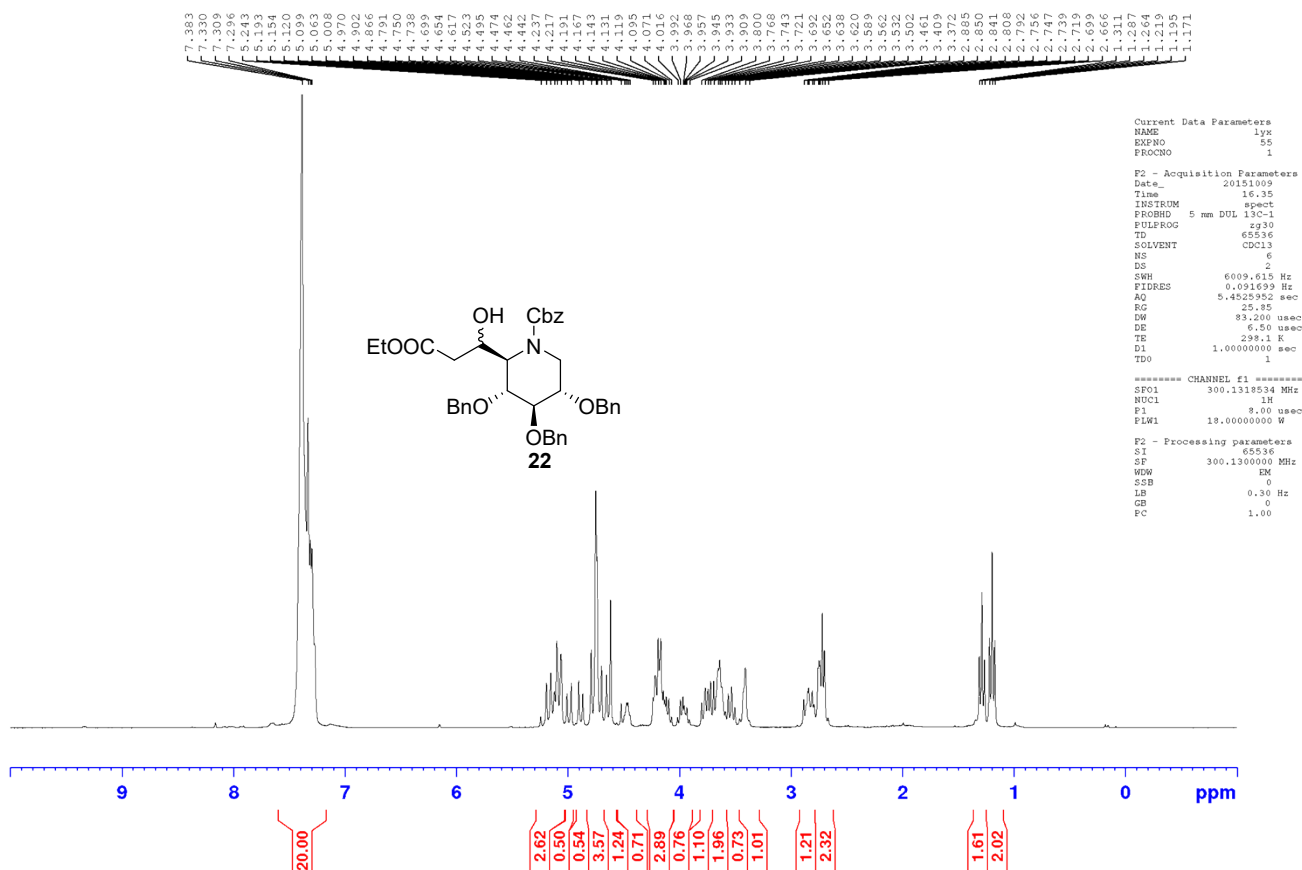
NAME          lyx-536
EXPNO         151
PROCNO        1
Date_         20151111
Time_         21.30
INSTRUM       spect
PROBHD        5 mm PATBO BB-
FULPROG       noesyphpr
TD            2048
SOLVENT       D2O
NS            8
DS            16
SWH           6009.615 Hz
FIDRES        2.934382 Hz
AQ            0.1705268 sec
RG            57
DW            83.200 usec
DE            6.50 usec
TE            298.0 K
D0            0.00006792 sec
D1            1.50000000 sec
D8            0.60000002 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
IN0           0.00016640 sec

===== CHANNEL f1 =====
NUC1          1H
P1            12.00 usec
PL1           -0.60 dB
PL9           57.82 dB
SF01         600.1328176 MHz
ND0           1
TD            256
SF01         600.1328 MHz
FIDRES        23.475039 Hz
SW            10.014 ppm
FnmODE        States-TFPI
SI            1024
SF           600.1300000 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           States-TFPI
SF           600.1300000 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
    
```

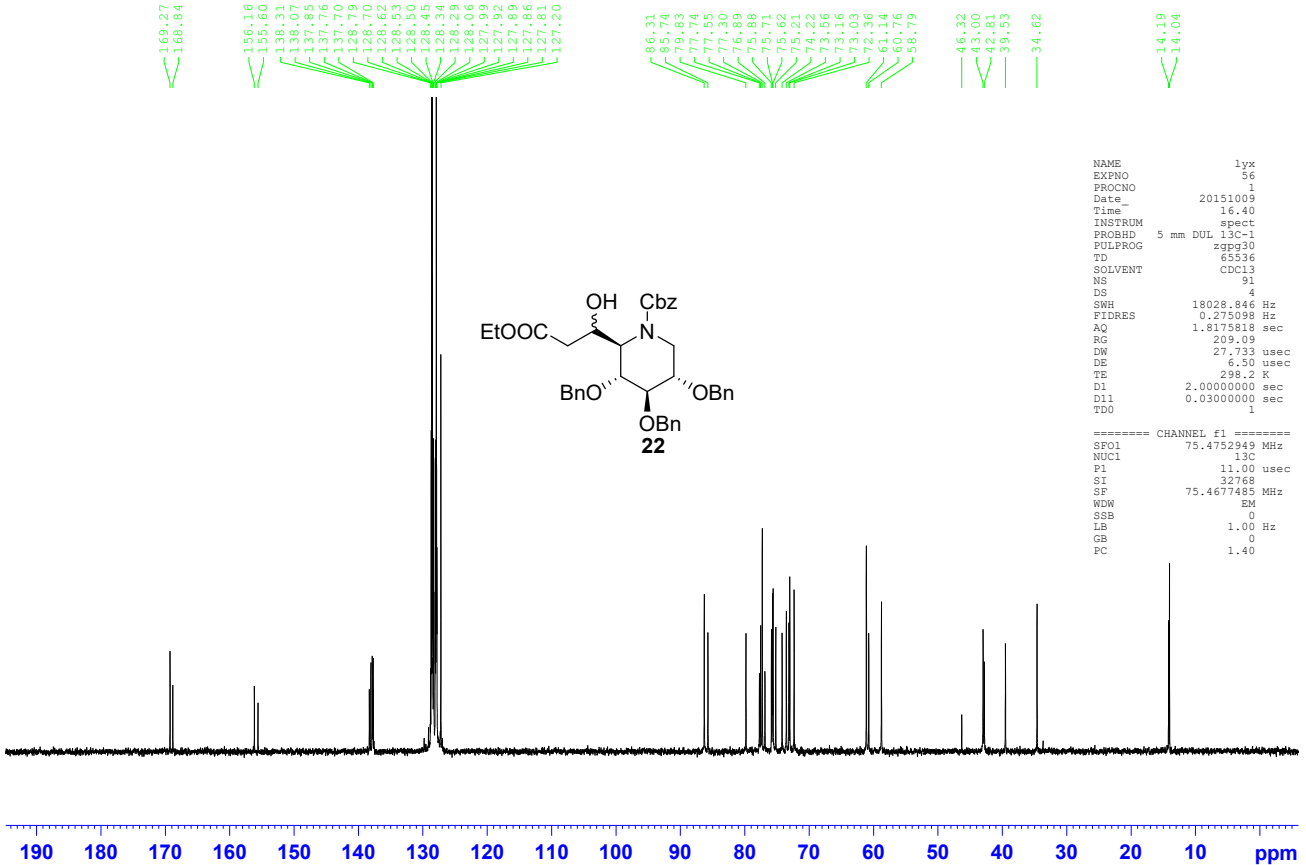


Compound 22:

lyx-512d-CH2



lyx-512d-C13

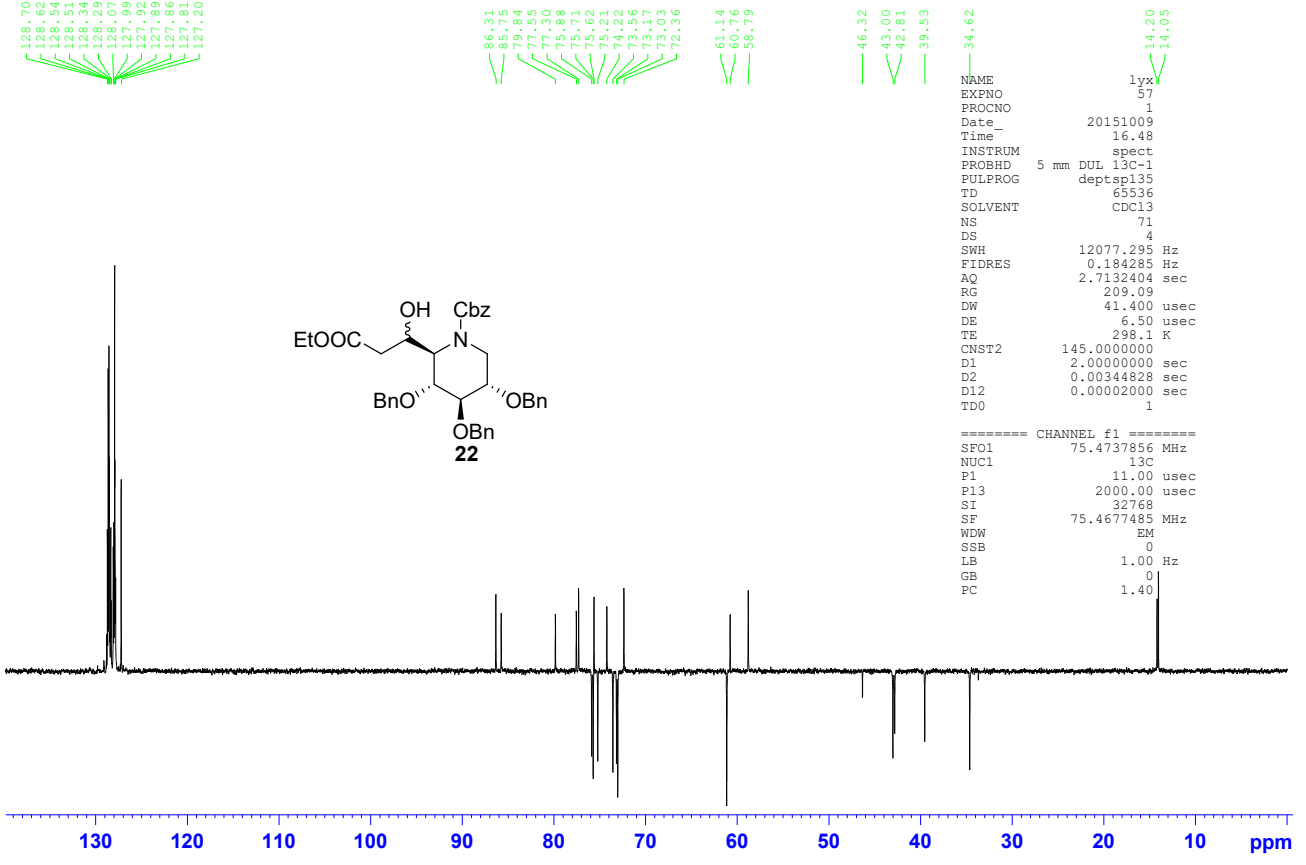


```

NAME lyx
EXPNO 56
PROCNO 1
Date_ 20151009
Time 16.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 91
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 209.09
DW 27.733 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 75.4752949 MHz
NUC1 13C
P1 11.00 usec
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

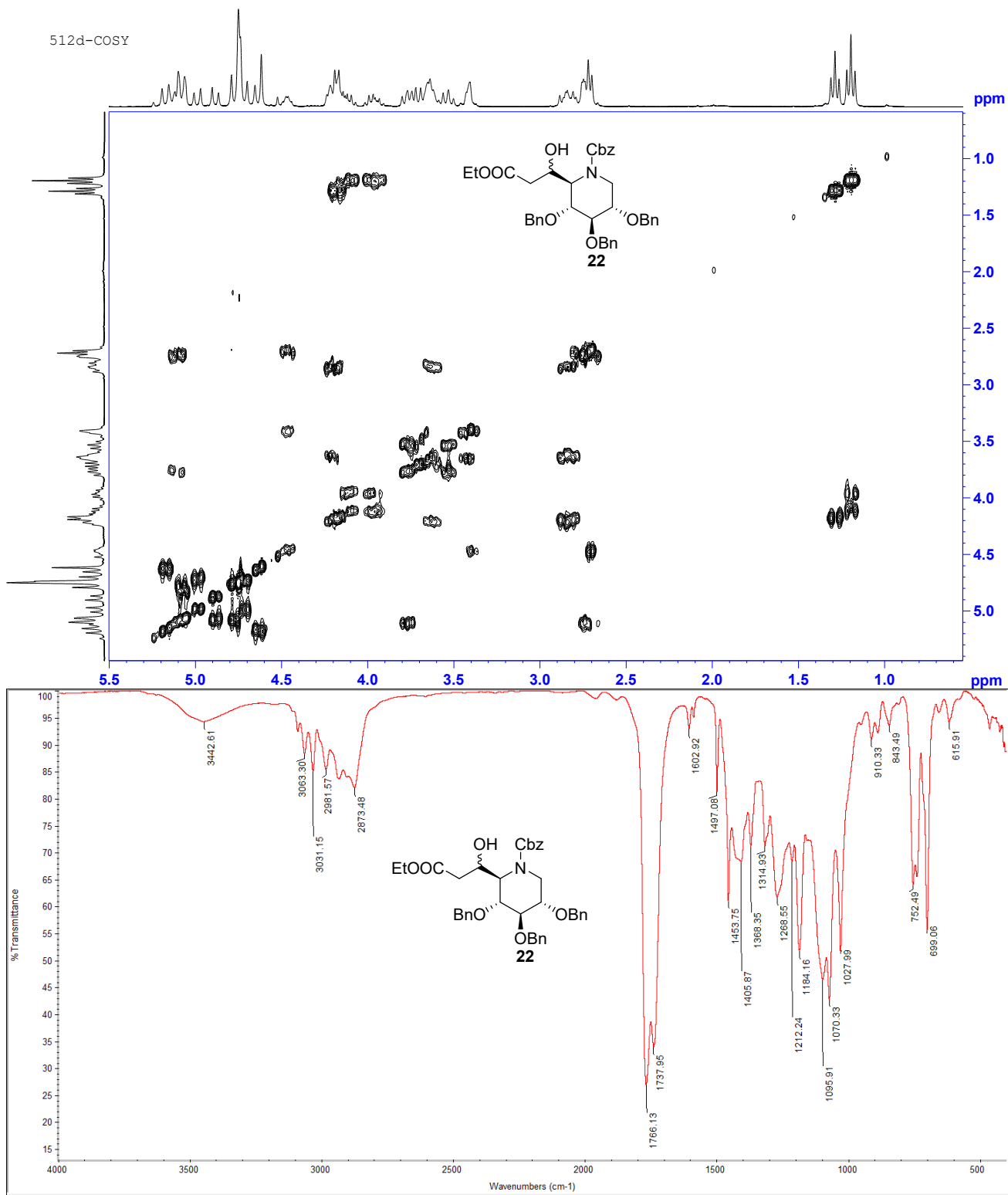
lyx-512d-dept135



```

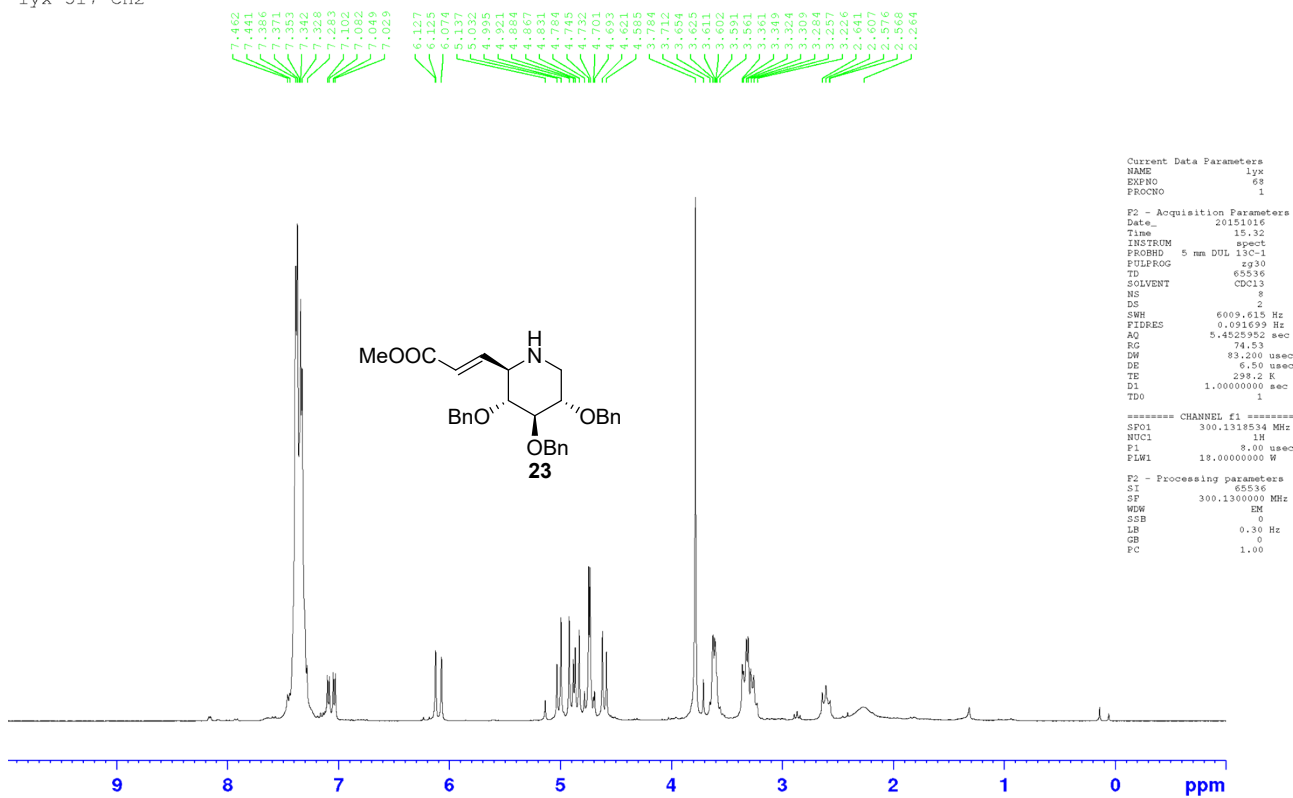
NAME lyx
EXPNO 57
PROCNO 1
Date_ 20151009
Time 16.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 71
DS 4
SWH 12077.295 Hz
FIDRES 0.184285 Hz
AQ 2.7132404 sec
RG 209.09
DW 41.400 usec
DE 6.50 usec
TE 298.1 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
SF01 75.4737856 MHz
NUC1 13C
P1 11.00 usec
P13 2000.00 usec
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

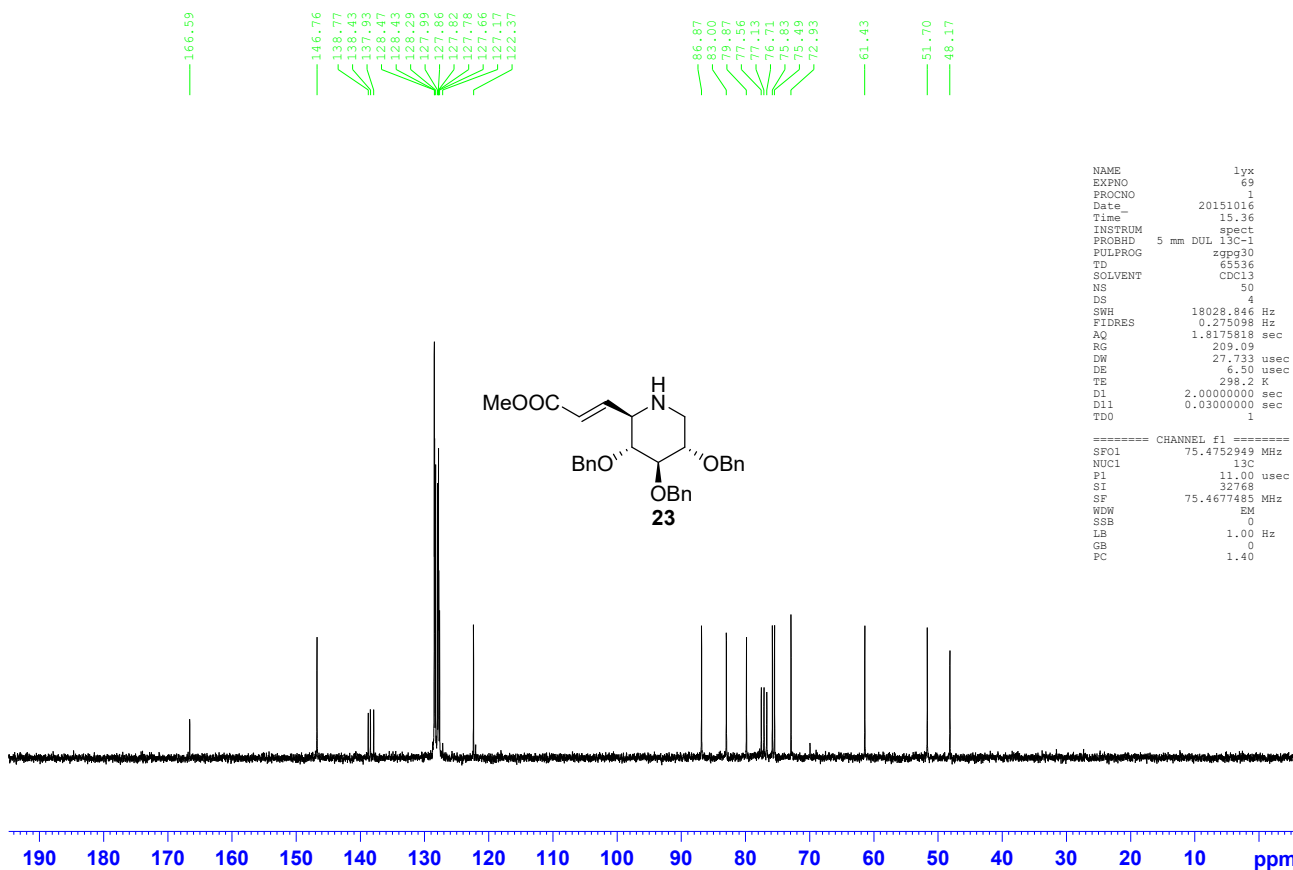


Compound **23**:

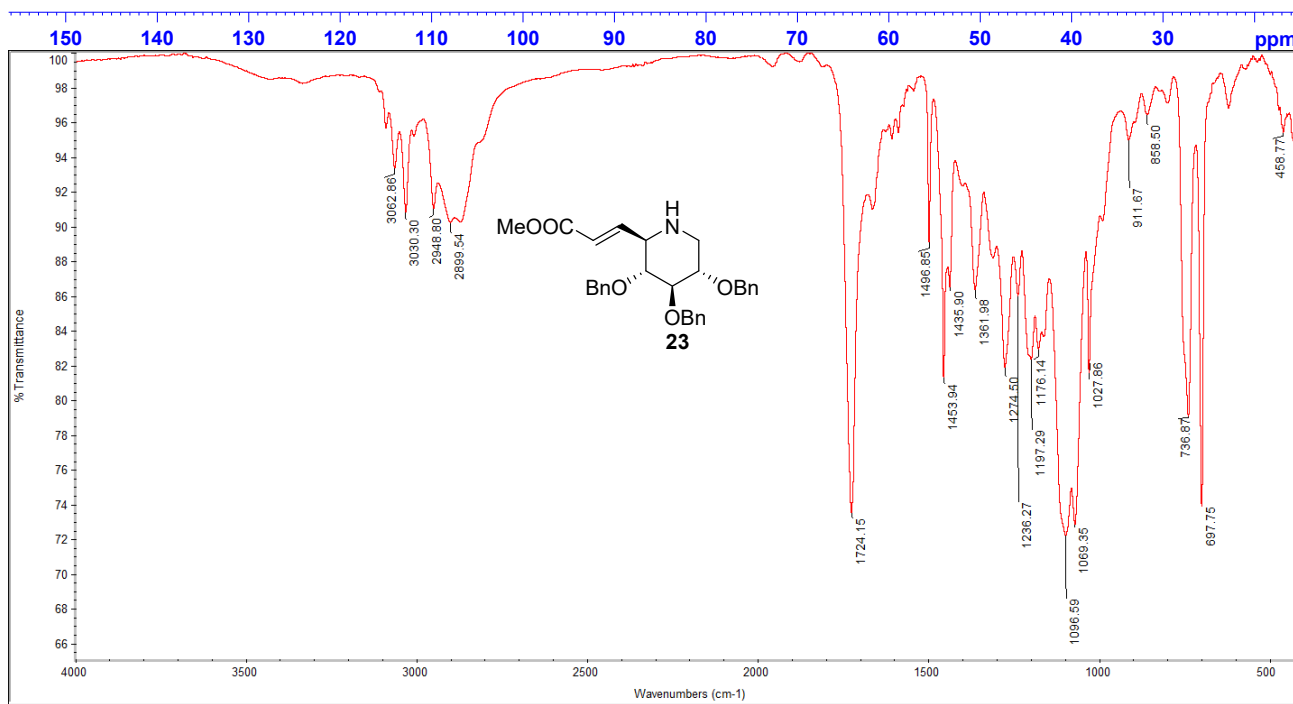
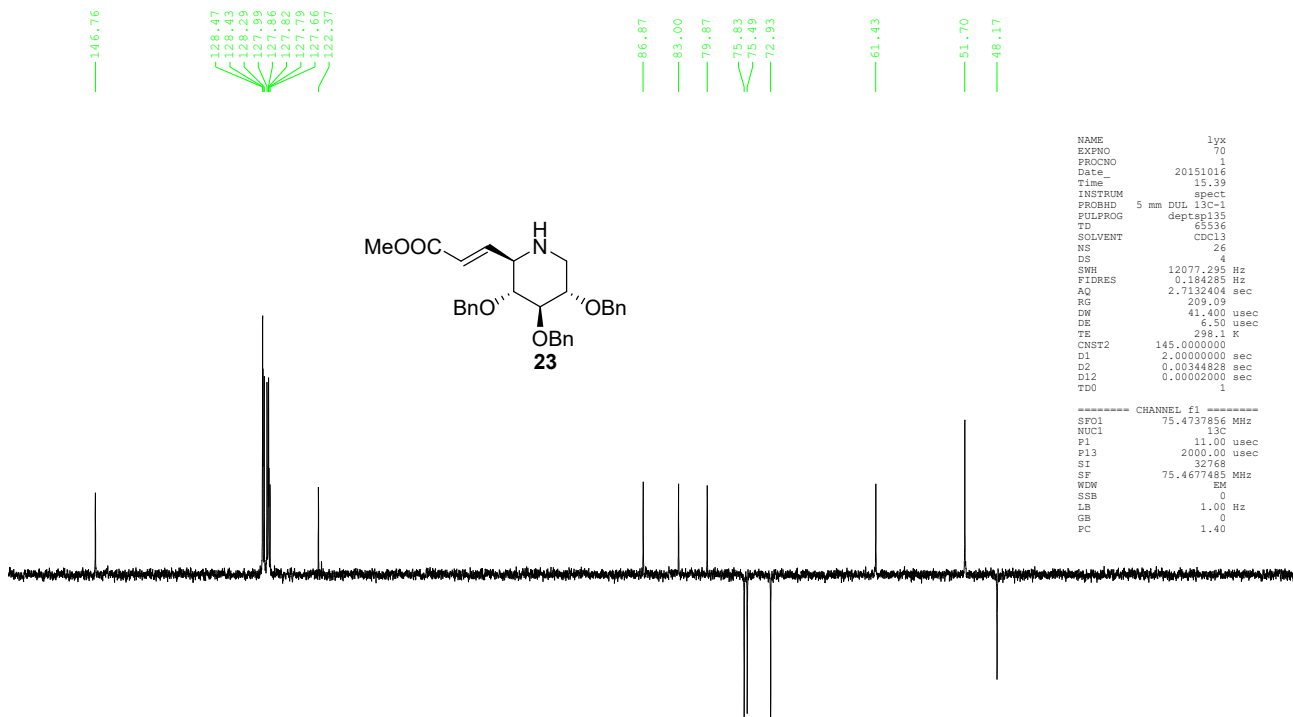
lyx-517-CH2



lyx-517-C13



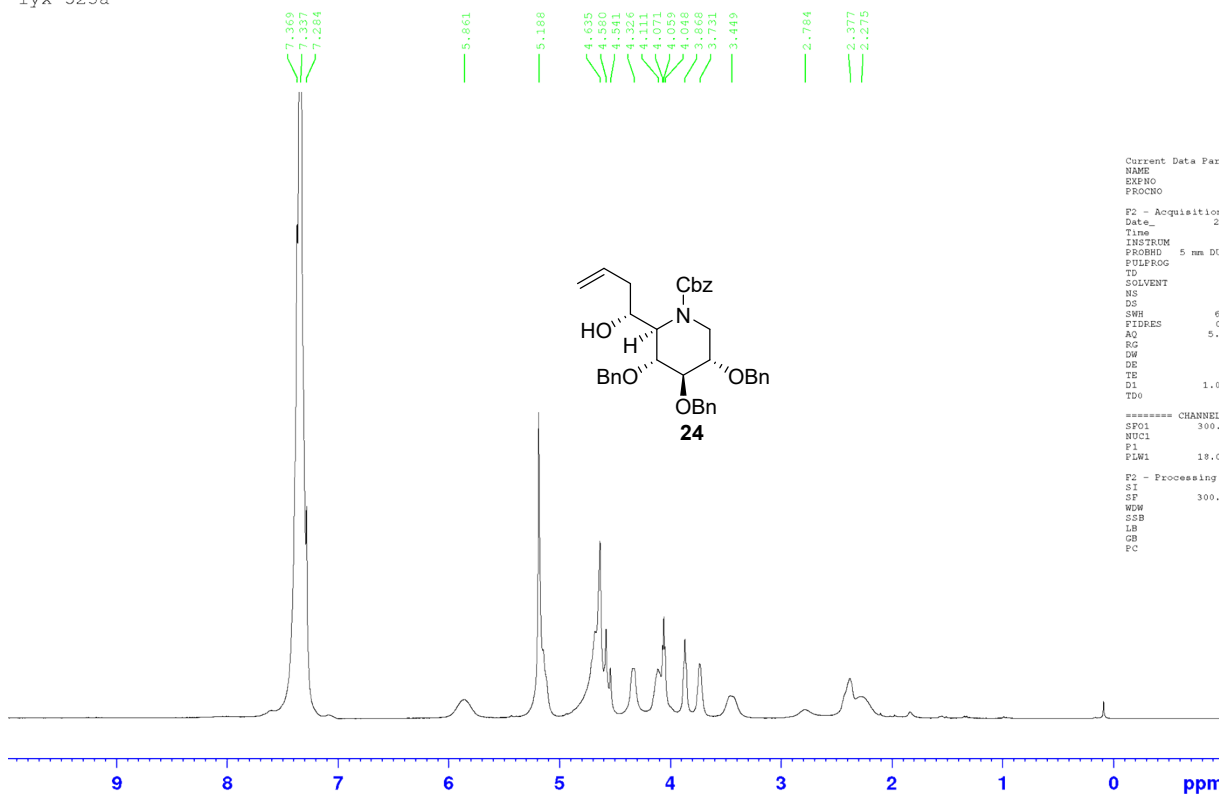
lyx-517-dept135





Compound 24:

lyx-523a



```

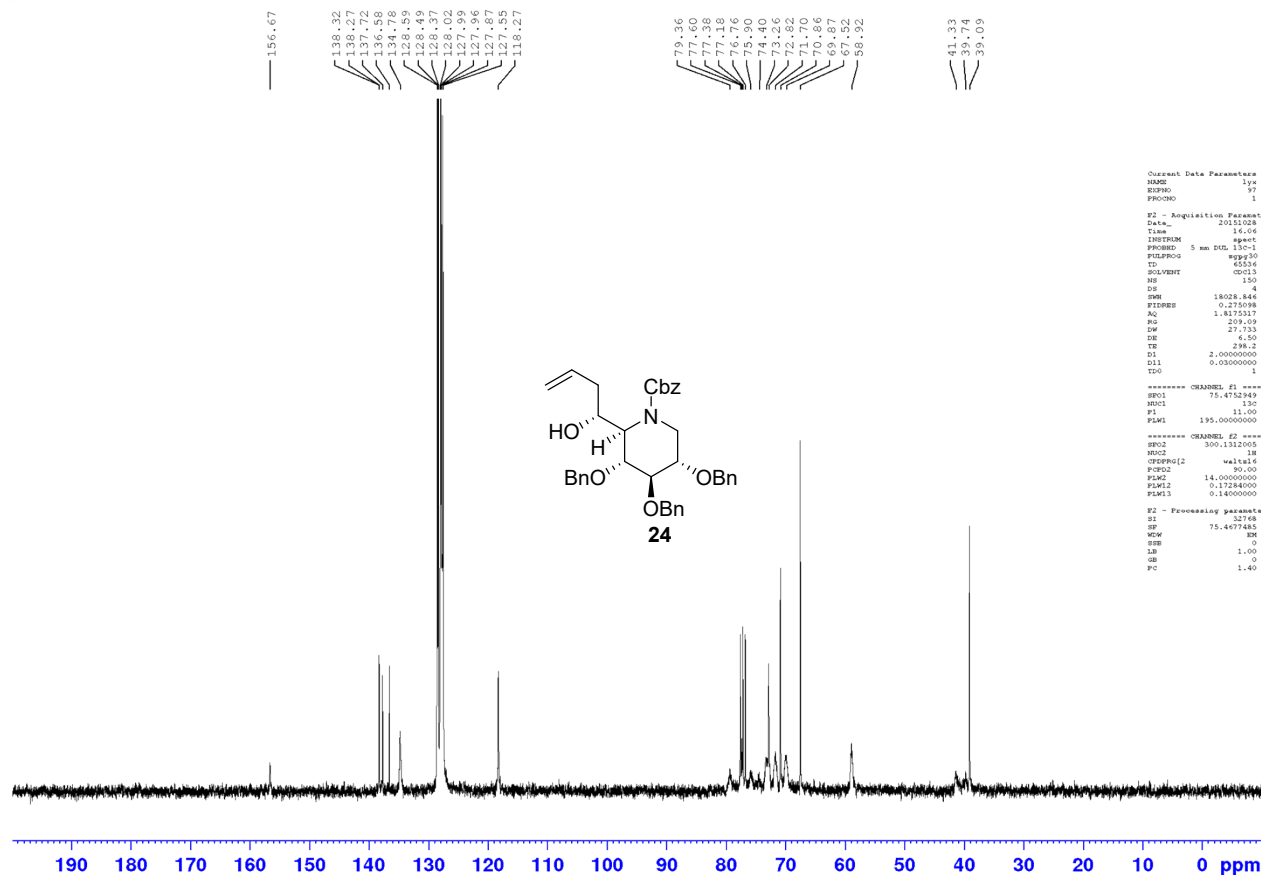
Current Data Parameters
NAME lyx
EXPNO 96
PROCNO 1

F2 - Acquisition Parameters
Date_ 20151028
Time 16.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4522952 sec
RG 56.57
DW 83.200 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 300.1318534 MHz
NUC1 1H
P1 8.00 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```

lyx-523a-C13



```

Current Data Parameters
NAME lyx
EXPNO 97
PROCNO 1

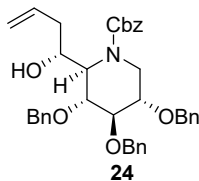
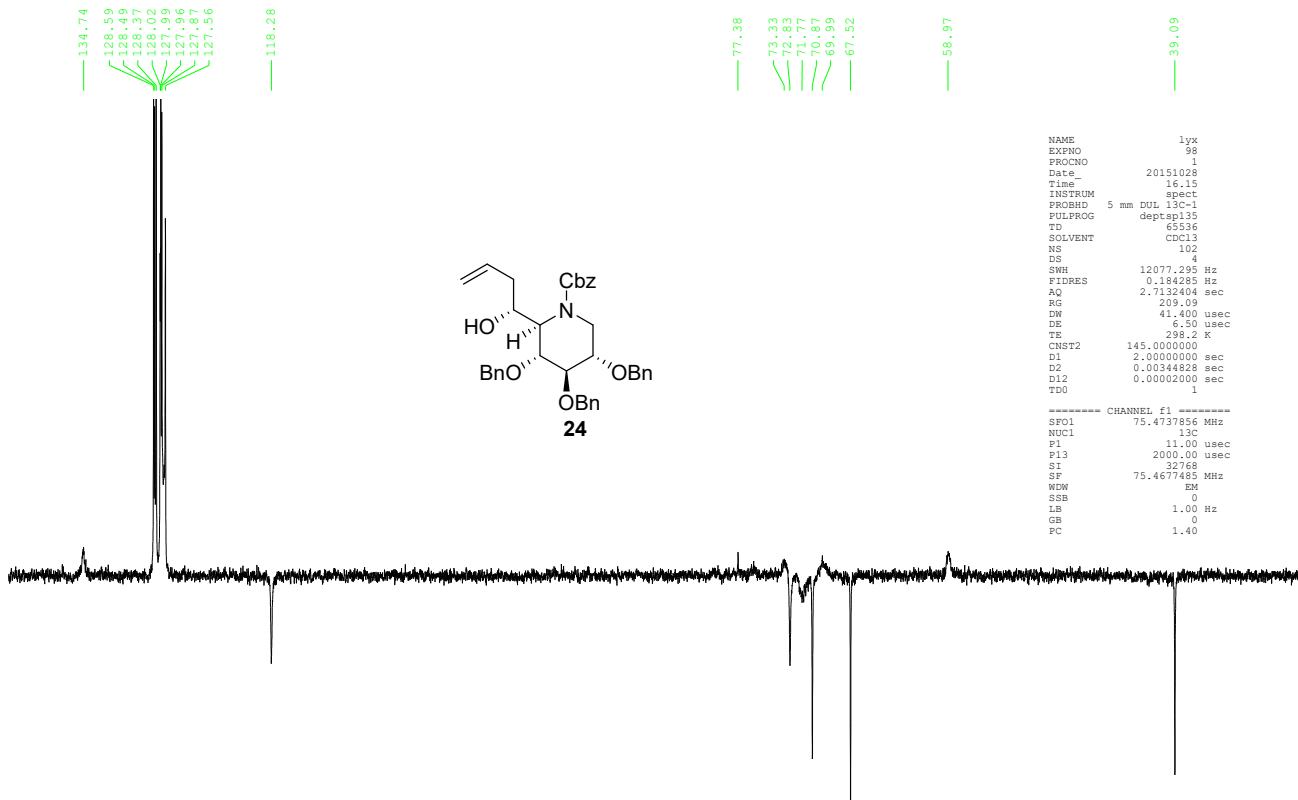
F2 - Acquisition Parameters
Date_ 20151028
Time 14.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG waltz16
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 18028.844 Hz
FIDRES 0.27509 Hz
AQ 1.8175517 sec
RG 239.09
DW 27.753 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 75.4752549 MHz
NUC1 13C
P1 11.00 usec
PLW1 195.00000000 W

===== CHANNEL f2 =====
SFO2 300.1312005 MHz
NUC2 1H
P2 8.00 usec
PLW2 14.00000000 W
===== CHANNEL f3 =====
SFO3 0.12284000 MHz
NUC3 13C
P3 0.14000000 W

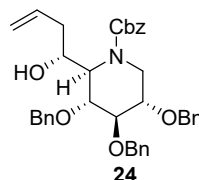
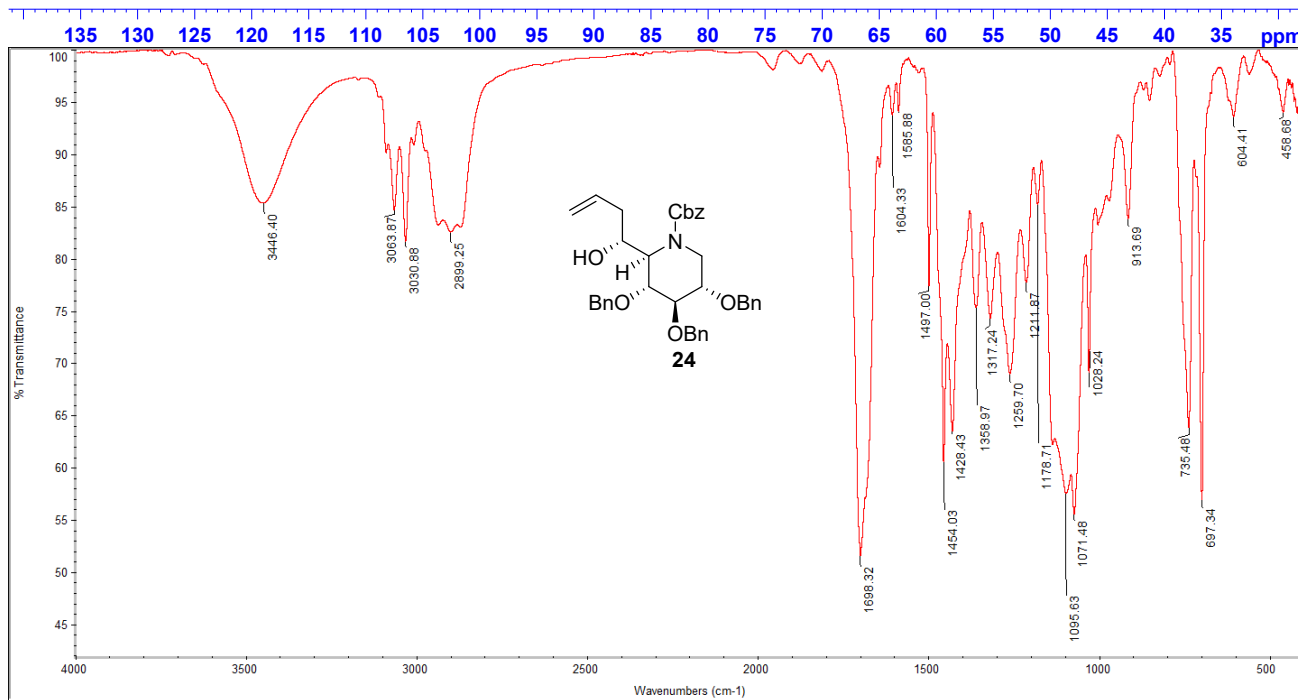
F2 - Processing parameters
SI 65536
SF 75.4674683 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

lyx-523a-dept135



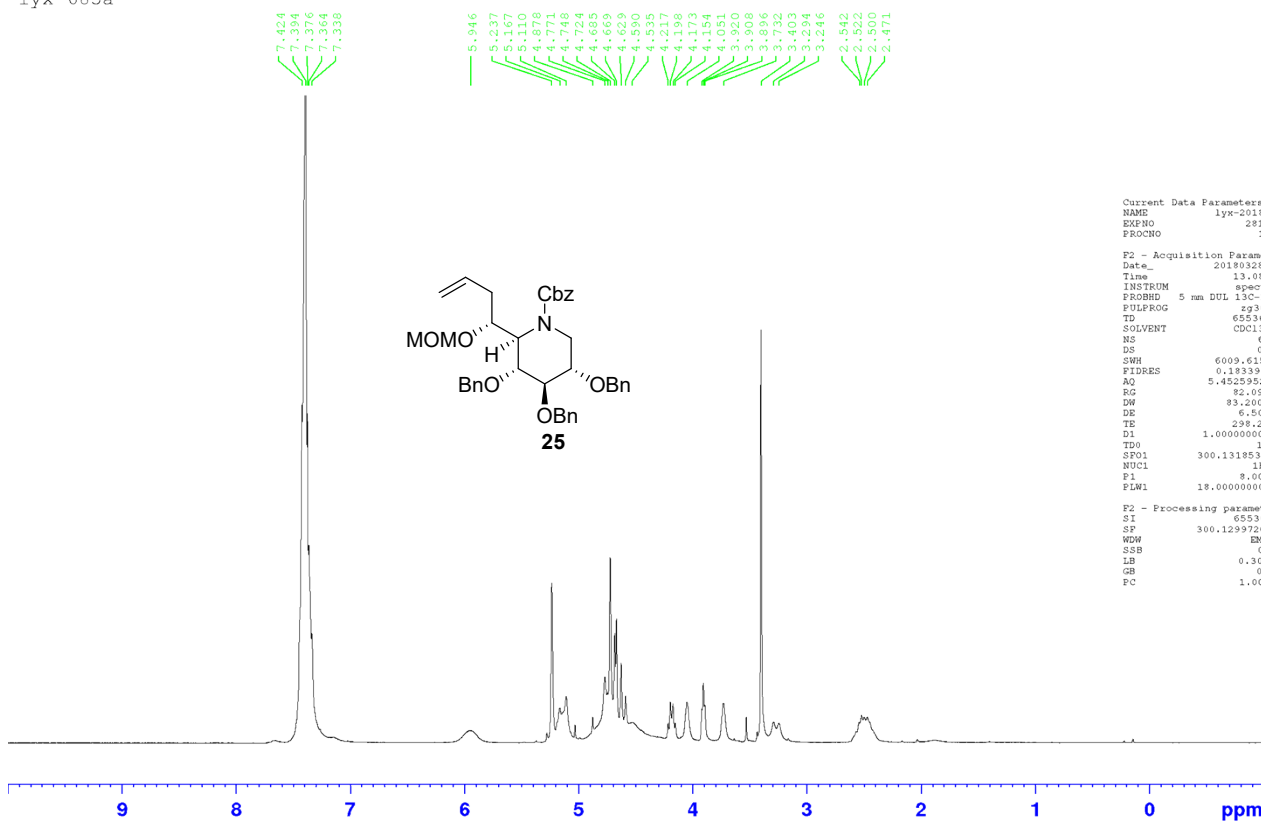
```

NAME          lyx
EXPNO         99
PROCNO        1
Date_         20151028
Time          16.15
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       deptsp135
TD            6536
SOLVENT       CDCl3
NS            102
DS            4
SWH           12077.295 Hz
FIDRES        0.184285 Hz
AQ            2.7132404 sec
RG            209.09
DW            41.400 usec
DE            6.50 usec
TE            298.2 K
CNST2         145.0000000
D1            2.0000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TDO           1
----- CHANNEL f1 -----
SFO1          75.4737856 MHz
NUC1          13C
P1            11.00 usec
PL1           2000.00 usec
SI            32768
SF            75.4677485 MHz
WWS          EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```



Compound 25:

lyx-685a

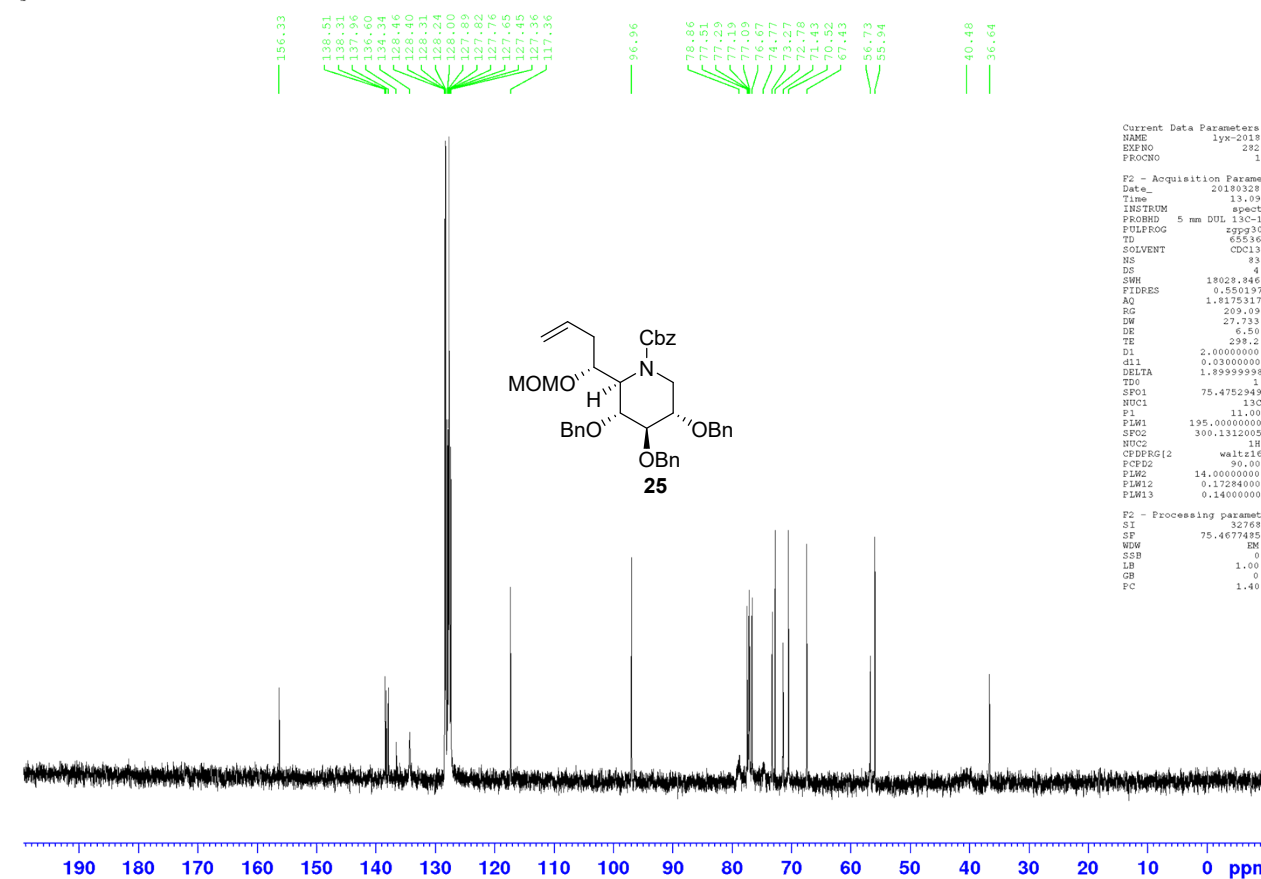


Current Data Parameters  
 NAME lyx-2018  
 EXPNO 281  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180328  
 Time 13.09 h  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 6  
 DS 0  
 SWH 6009.615 Hz  
 FIDRES 0.183399 Hz  
 AQ 5.4522952 sec  
 RG 82.09  
 DW 83.200 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TDO 0  
 SFO1 300.1318534 MHz  
 NUC1 13  
 P1 8.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1299736 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

lyx-685a



Current Data Parameters  
 NAME lyx-2018  
 EXPNO 282  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180328  
 Time 13.09 h  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 83  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.550197 Hz  
 AQ 1.8175317 sec  
 RG 209.09  
 DW 27.733 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.8989398 sec  
 TDO 1  
 SFO1 75.4752949 MHz  
 NUC1 13C  
 P1 11.00 usec  
 PLW1 195.00000000 W  
 SFO2 300.1312005 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 14.00000000 W  
 PLW12 0.1728400 W  
 PLW13 0.14000000 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4677485 MHz  
 WDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

lyx-685a

134.31  
128.46  
128.30  
128.33  
128.24  
128.00  
127.89  
127.82  
127.76  
127.64  
127.45  
127.36  
117.36

96.97

77.19  
73.27  
72.78  
71.43  
70.52  
67.43

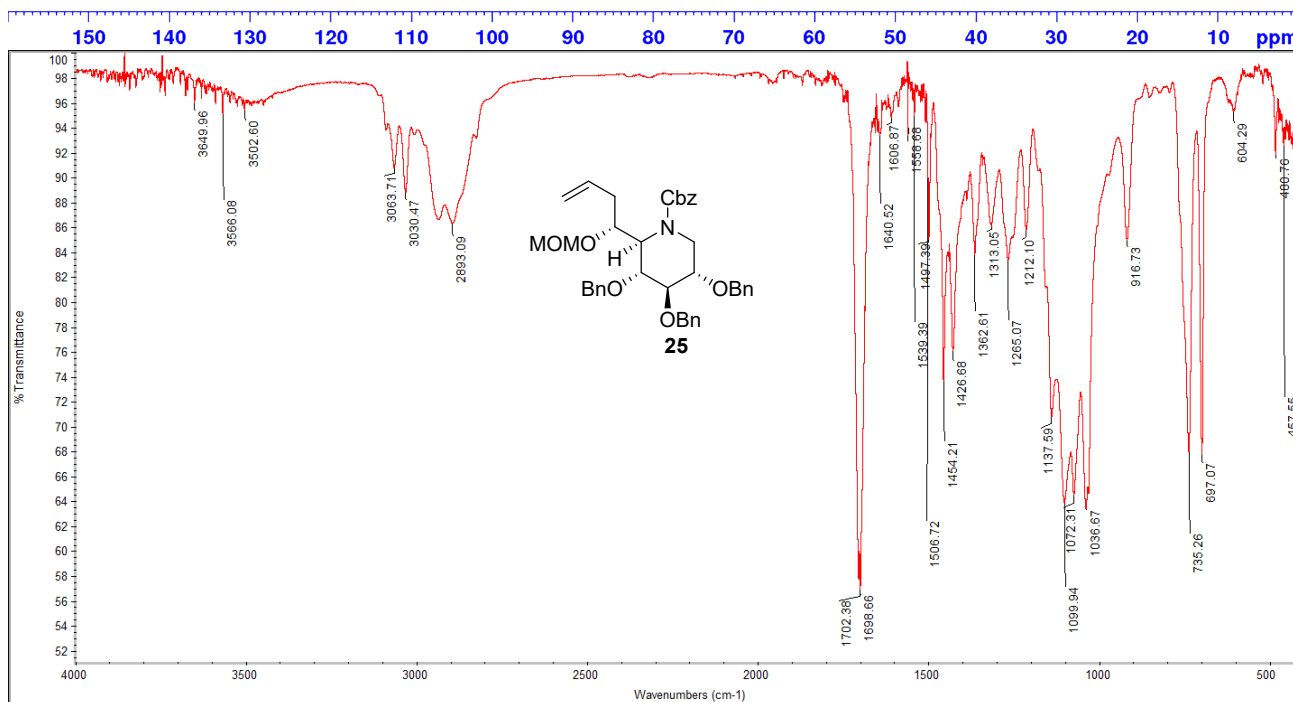
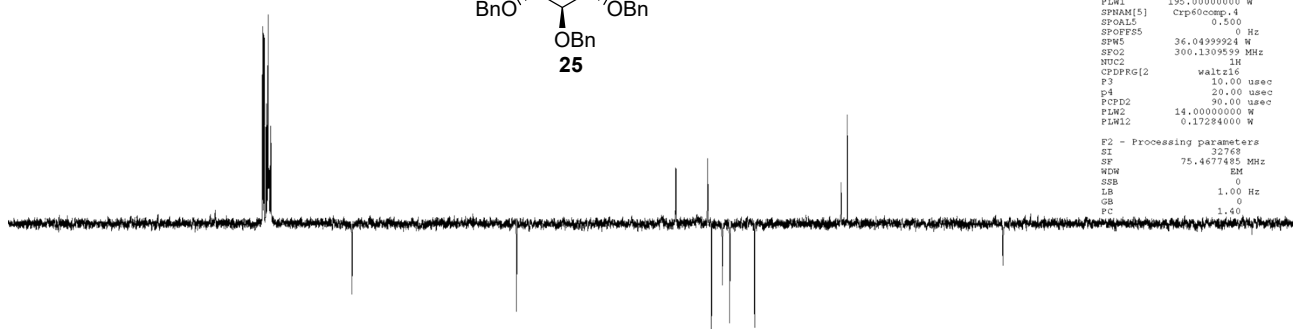
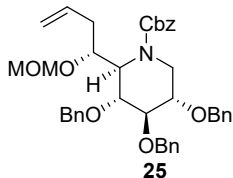
56.73  
55.94

36.64

Current Data Parameters  
NAME lyx-2018  
EXPNO 282  
PROCNO 1

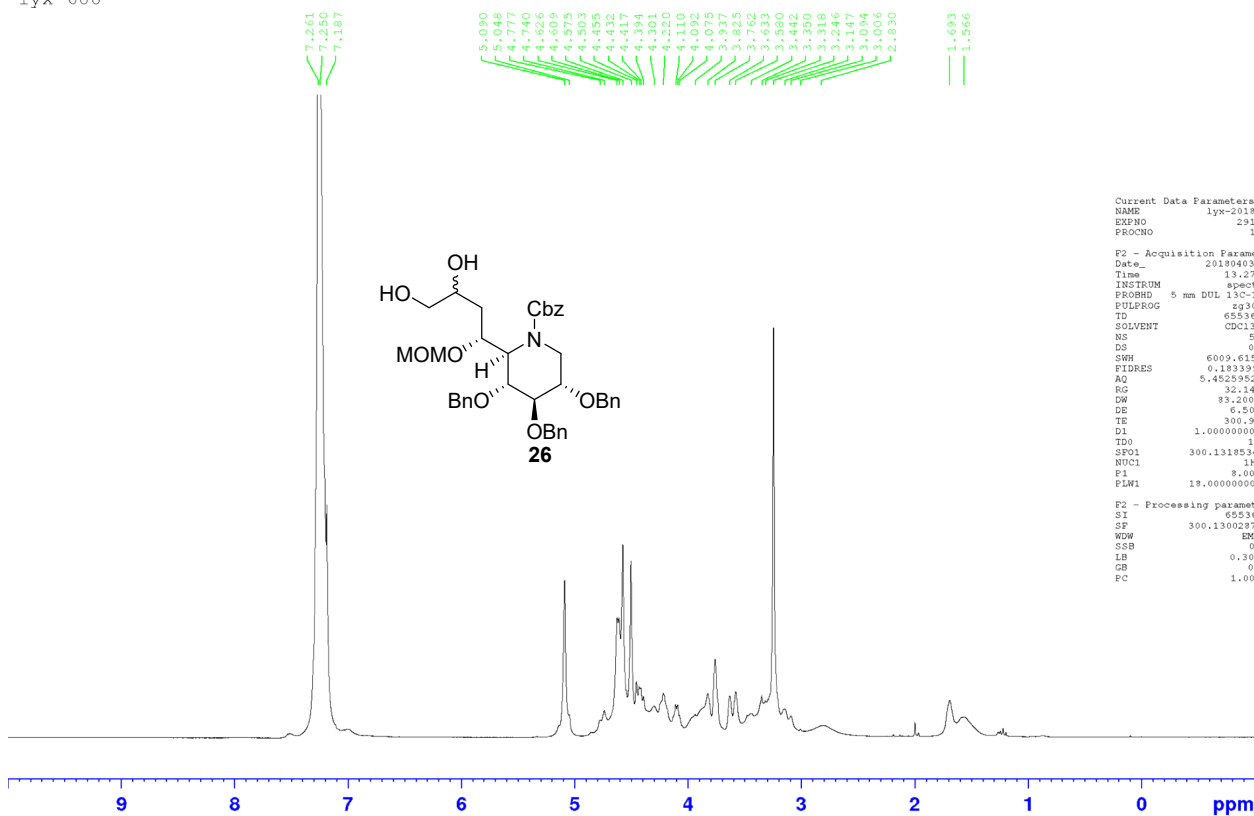
F2 - Acquisition Parameters  
Date\_ 20190328  
Time 13.15 h  
INSTRUM spect  
PROBHD 5 mm DDL 13c-1  
PULPROG zgpg30  
ID 65536  
SOLVENT cdcl3  
NS 51  
DS 4  
SWH 12077.285 Hz  
FIDRES 0.368570 Hz  
AQ 2.7131963 sec  
RG 299.08  
DM 41.400 usec  
DE 6.50 usec  
TE 298.2 K  
CNS2 145.0000000  
SI 2.000000000 sec  
d1 0.00344828 sec  
d12 0.00002000 sec  
DETA 0.00001801 sec  
TD 1  
SFO1 75.4737966 MHz  
NUC1 13c  
P1 11.00 usec  
P13 2000.00 usec  
PLA0 0 W  
PLM1 195.0000000 W  
SFOF5 SPMAM[5]  
SFOAL5 0.500  
SFOCF5 0 Hz  
SFM5 36.04999924 W  
SFO2 300.1309599 MHz  
NUC2 1H  
CPDPRG2 waltz16  
F3 10.00 usec  
P4 20.00 usec  
PCPD2 90.00 usec  
PLM2 14.00000000 W  
PLW12 0.17284000 W

F2 - Processing Parameters  
SI 32768  
SF 75.4677485 MHz  
WDW EM  
SSB 0  
B 1.00 Hz  
GB 0  
PC 1.40



Compound 26:

lyx-688



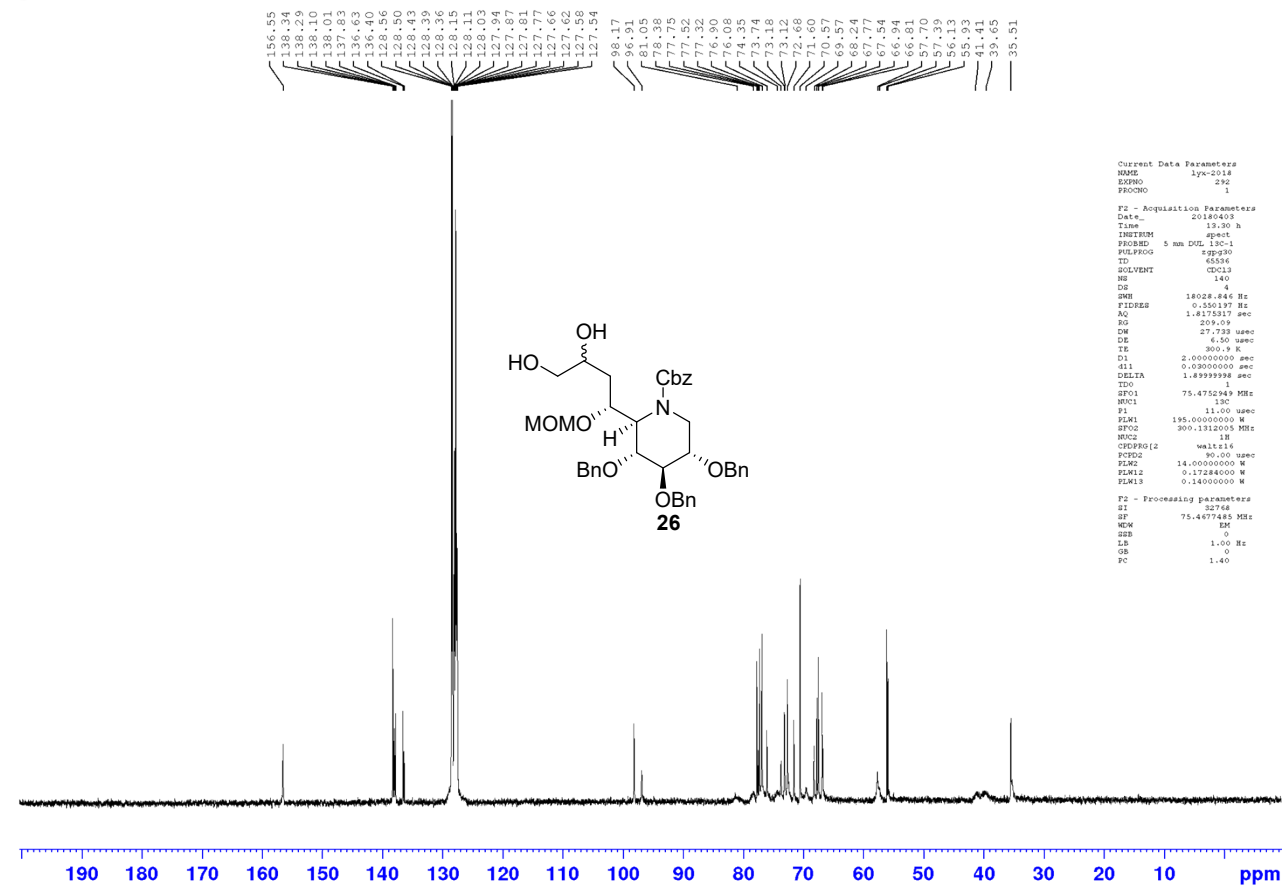
```

Current Data Parameters
NAME      lyx-2018
EXPNO    231
PROCNO   1

F2 - Acquisition Parameters
Date_    20180403
Time     13.27 h
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        5
DS        0
SWH       6009.615 Hz
FIDRES   0.133399 Hz
AQ        5.4525952 sec
RG        32.14
DW        93.200 usec
DE        6.50 usec
TE        300.2 K
D1        1.0000000 sec
TDO       1
SFO1     300.1318534 MHz
NUC1      1H
P1        8.00 usec
PLW1     19.0000000 W

F2 - Processing parameters
SI        65536
SF        300.1300287 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

lyx-688



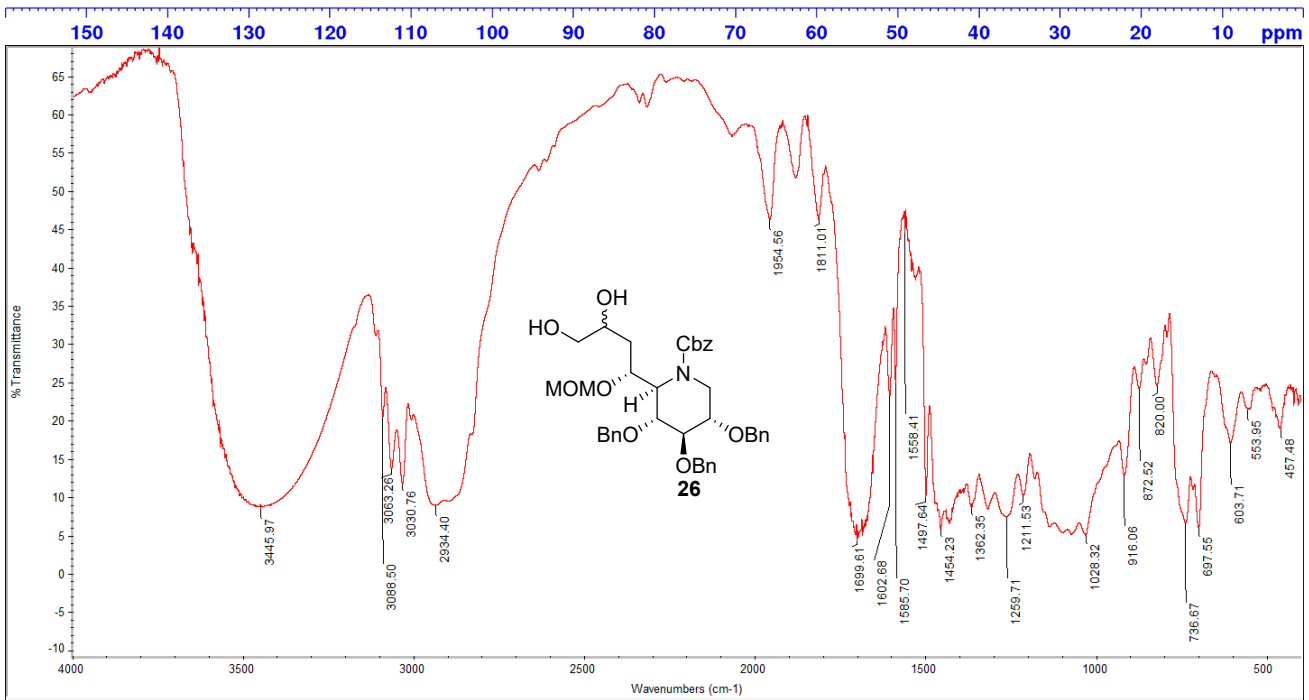
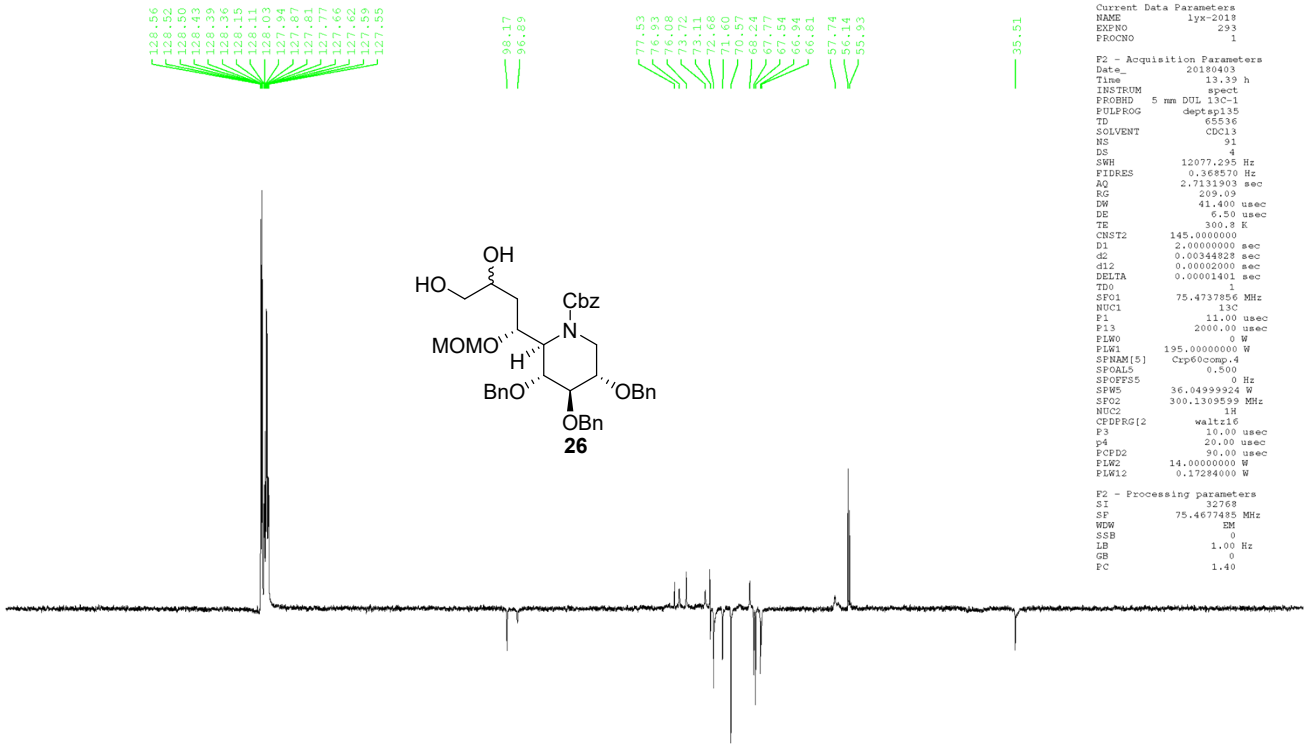
```

Current Data Parameters
NAME      lyx-2018
EXPNO    232
PROCNO   1

F2 - Acquisition Parameters
Date_    20180403
Time     13.30 h
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  zgpg30
TD        6554
SOLVENT  CDCl3
NS        4
DS        0
SWH       18028.846 Hz
FIDRES   0.550197 Hz
AQ        1.4375317 sec
RG        259.09
DW        27.728 usec
DE        6.50 usec
TE        300.2 K
D1        2.0000000 sec
d11       0.0300000 sec
DELTA    1.4999998 sec
TDO       1
SFO1     75.4752485 MHz
NUC1      13C
P1        11.00 usec
PLW1     195.0000000 W
SFO2     300.1318534 MHz
NUC2      1H
CHPROG2  waltz16
PCPD2    90.00 usec
PLM2    14.0000000 W
PLM12   0.1728000 W
PLM13   0.1400000 W

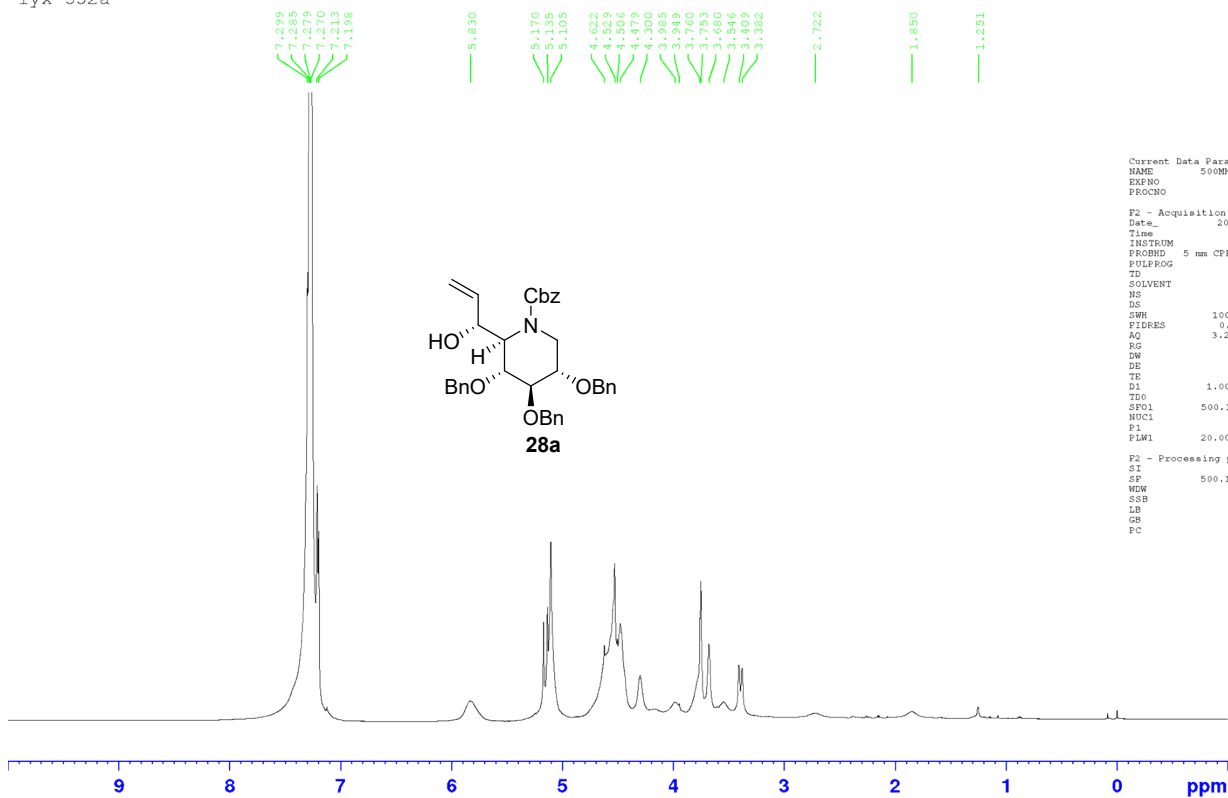
F2 - Processing parameters
SI        65536
SF        75.4677485 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```

lyx-688



Compound **28a**:

lyx-552a



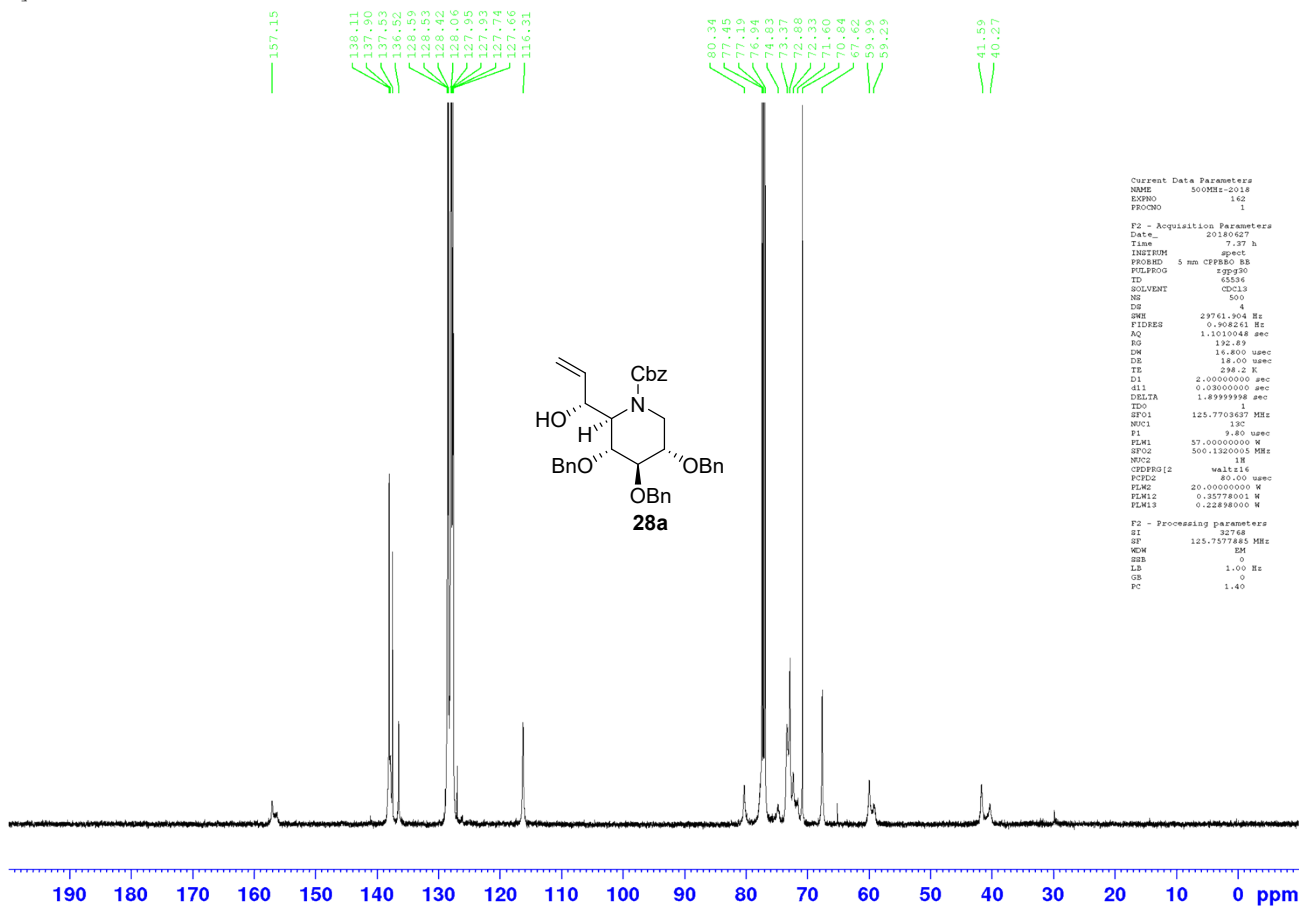
```

Current Data Parameters
NAME      500MHz-2018
EXPNO    161
PROCNO   1

F2 - Acquisition Parameters
Date_    20180627
Time     7.10 h
INSTRUM  spect
PROBHD   5 mm CPBPRB B3
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ        3.2769999 sec
RG         16.14
DW         50.000 usec
DE         6.50 usec
TE        298.2 K
D1        1.00000000 sec
TDO       1
SF01      500.1330885 MHz
NUC1      1H
P1        11.50 usec
PLW1      20.0000000 W

F2 - Processing parameters
SI        65536
SF        500.1330419 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
FC        1.00
    
```

lyx-552a

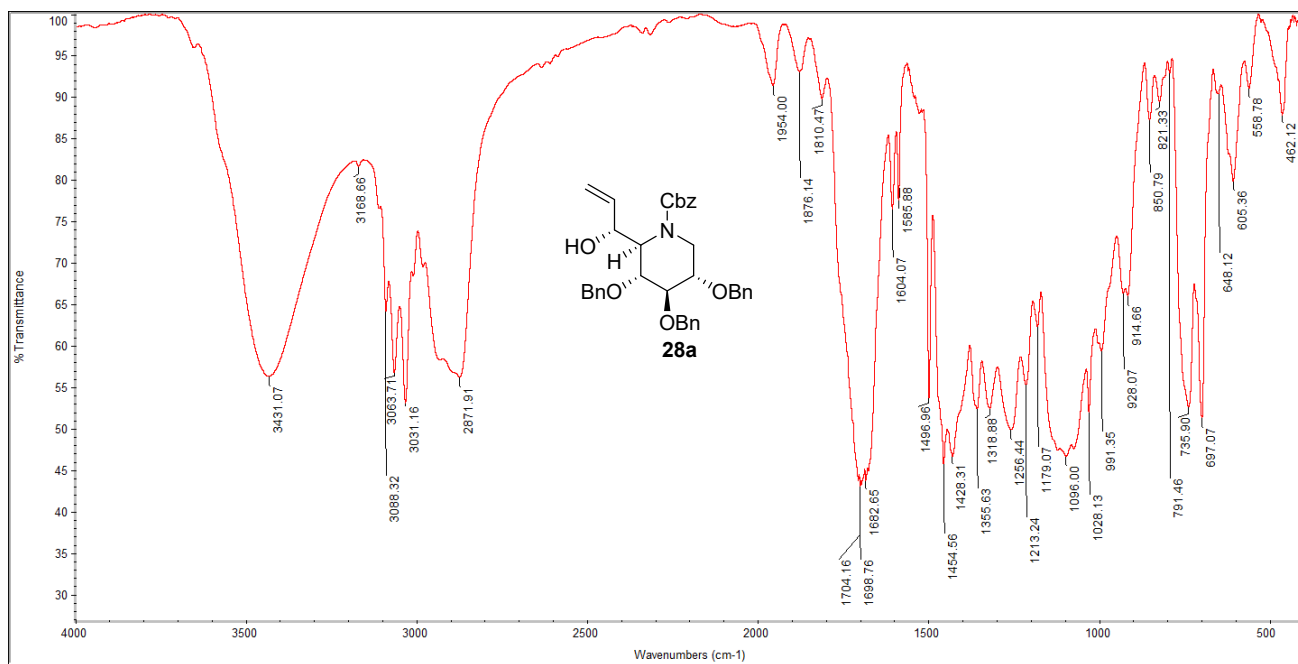


```

Current Data Parameters
NAME      500MHz-2018
EXPNO    162
PROCNO   1

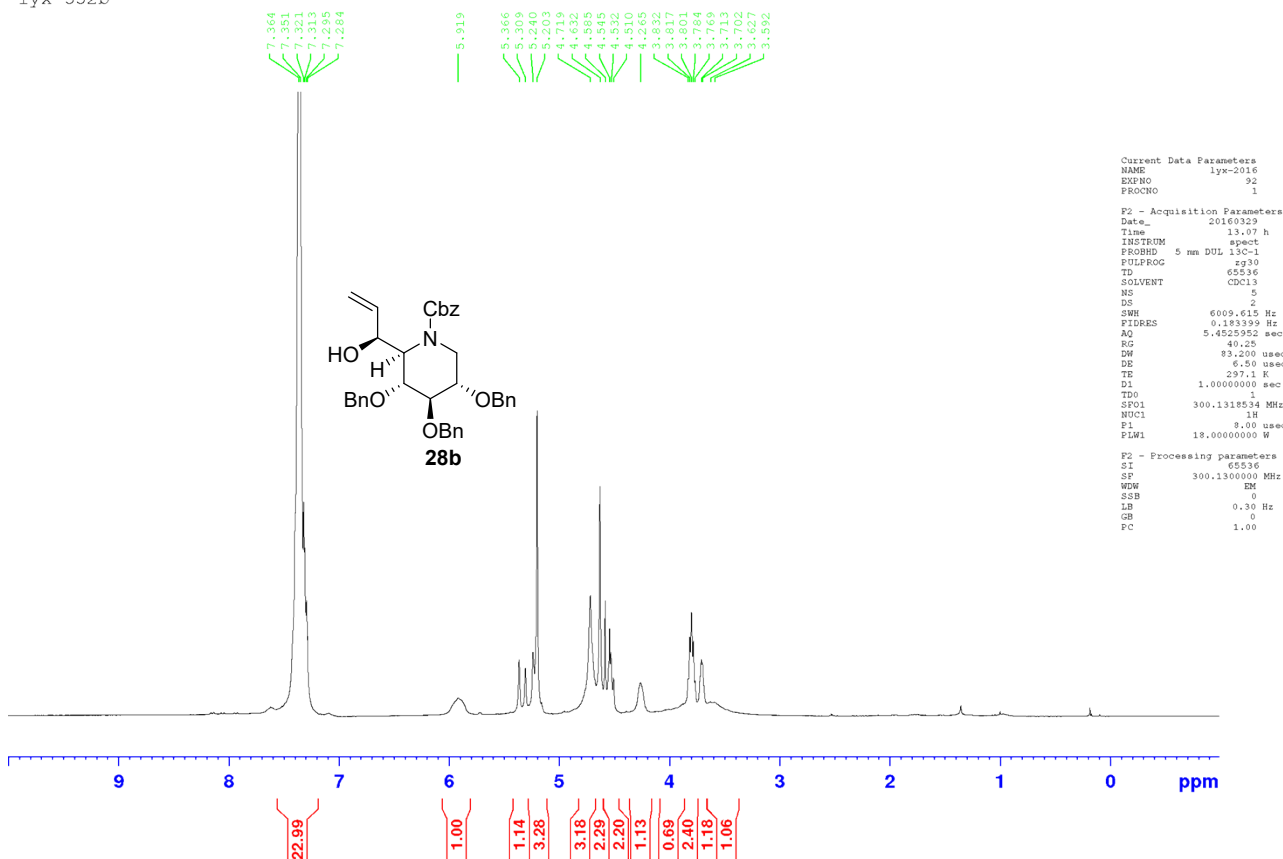
F2 - Acquisition Parameters
Date_    20180627
Time     7.37 h
INSTRUM  spect
PROBHD   5 mm CPBPRB B3
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        500
DS        4
SWH       23761.904 Hz
FIDRES    0.908241 Hz
AQ        1.1010048 sec
RG         192.89
DW         14.800 usec
DE         14.00 usec
TE        298.2 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA     1.48999998 sec
TDO       1
SF01      125.770467 MHz
NUC1      13C
P1        9.80 usec
PLW1      57.0000000 W
SF02      500.1320005 MHz
NUC2      1H
CPDPRG2  waltz16
FIDRES2   80.000 usec
FLM2     20.0000000 W
FLM12    0.2377800 W
FLM13    0.2288800 W

F2 - Processing parameters
SI        32768
SF        125.7577885 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```



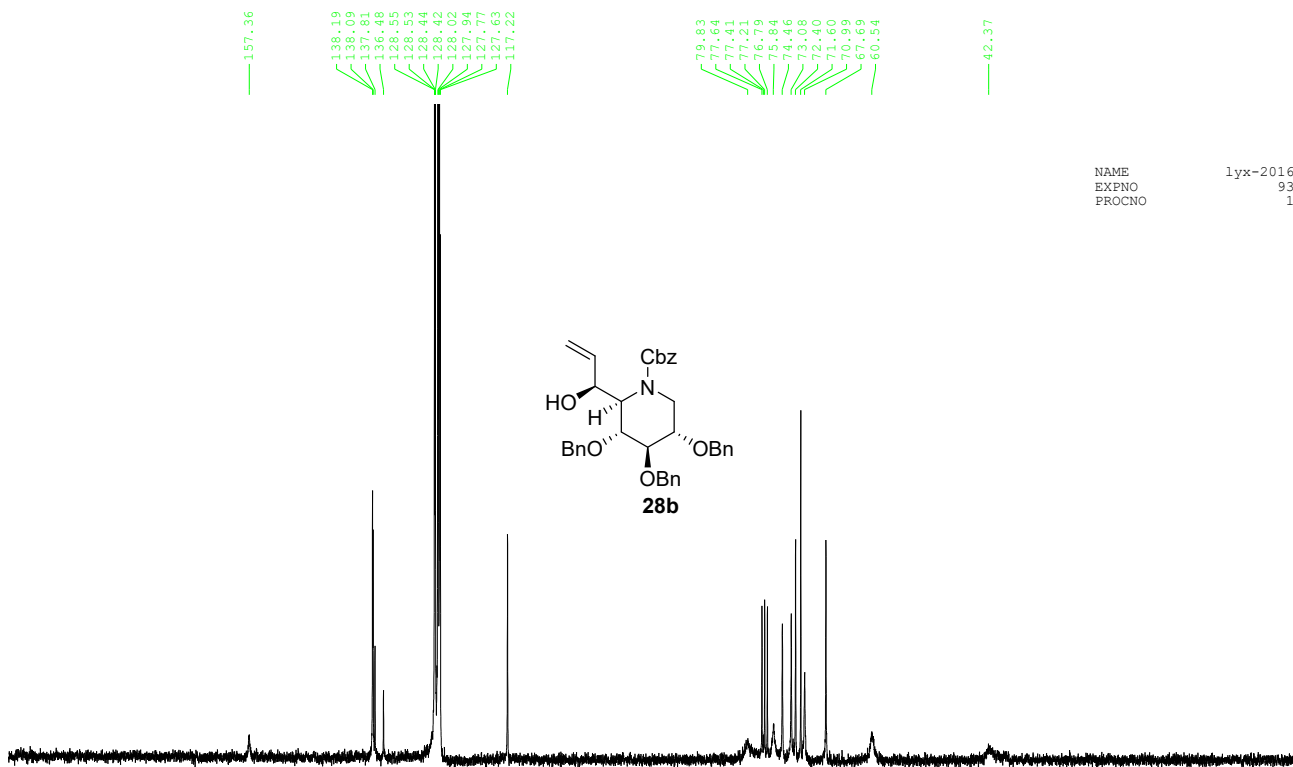
Compound 28b:

lyx-552b





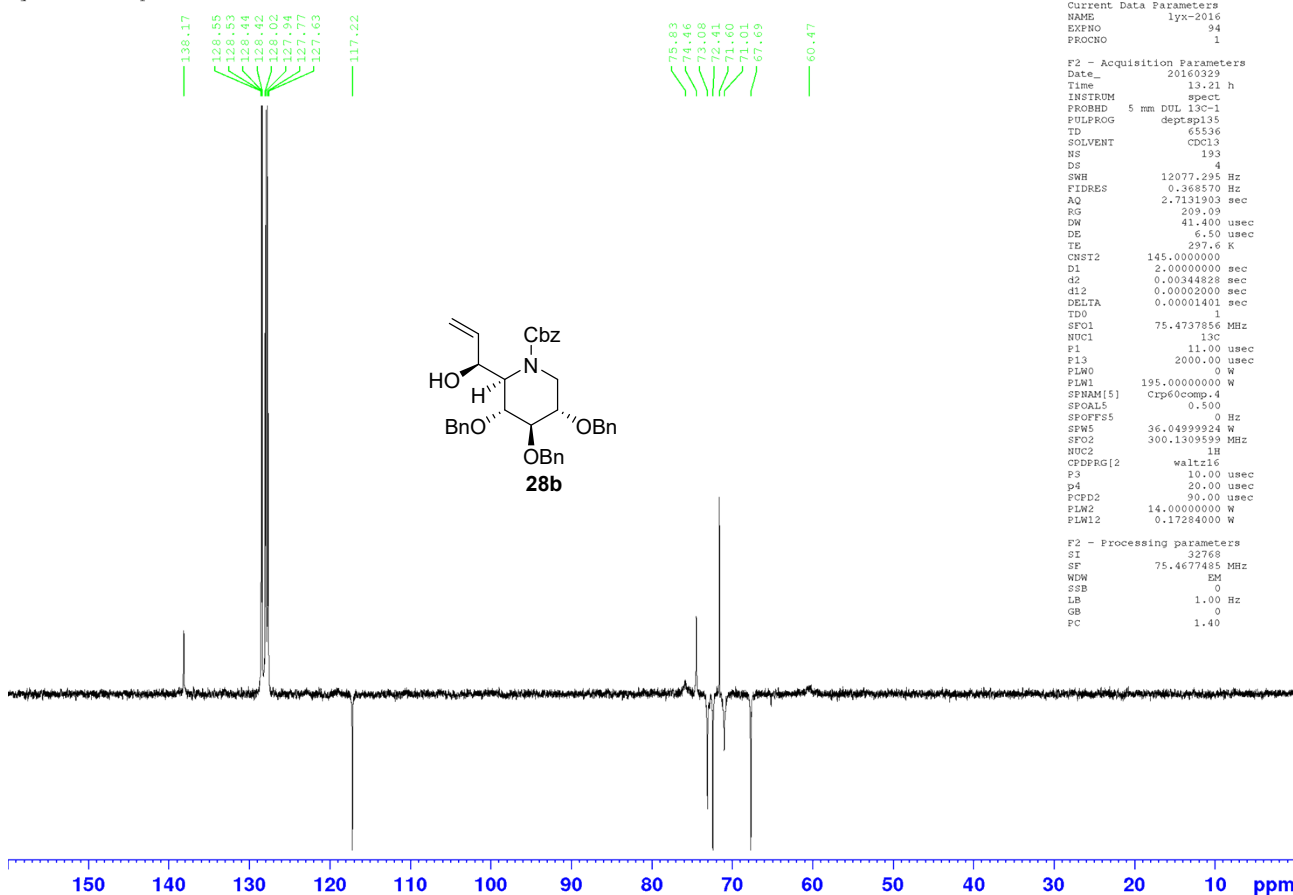
lyx-552b-C13



NAME lyx-2016  
EXPNO 93  
PROCNO 1

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

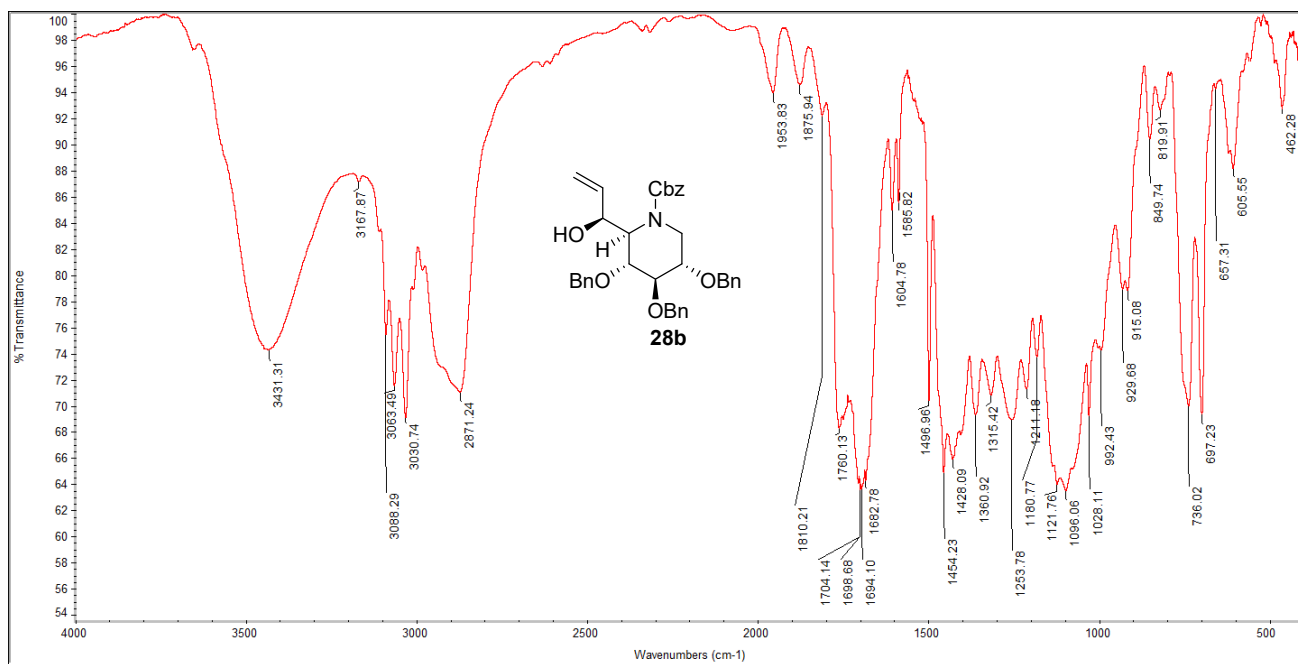
lyx-552b-dept135



Current Data Parameters  
NAME lyx-2016  
EXPNO 94  
PROCNO 1

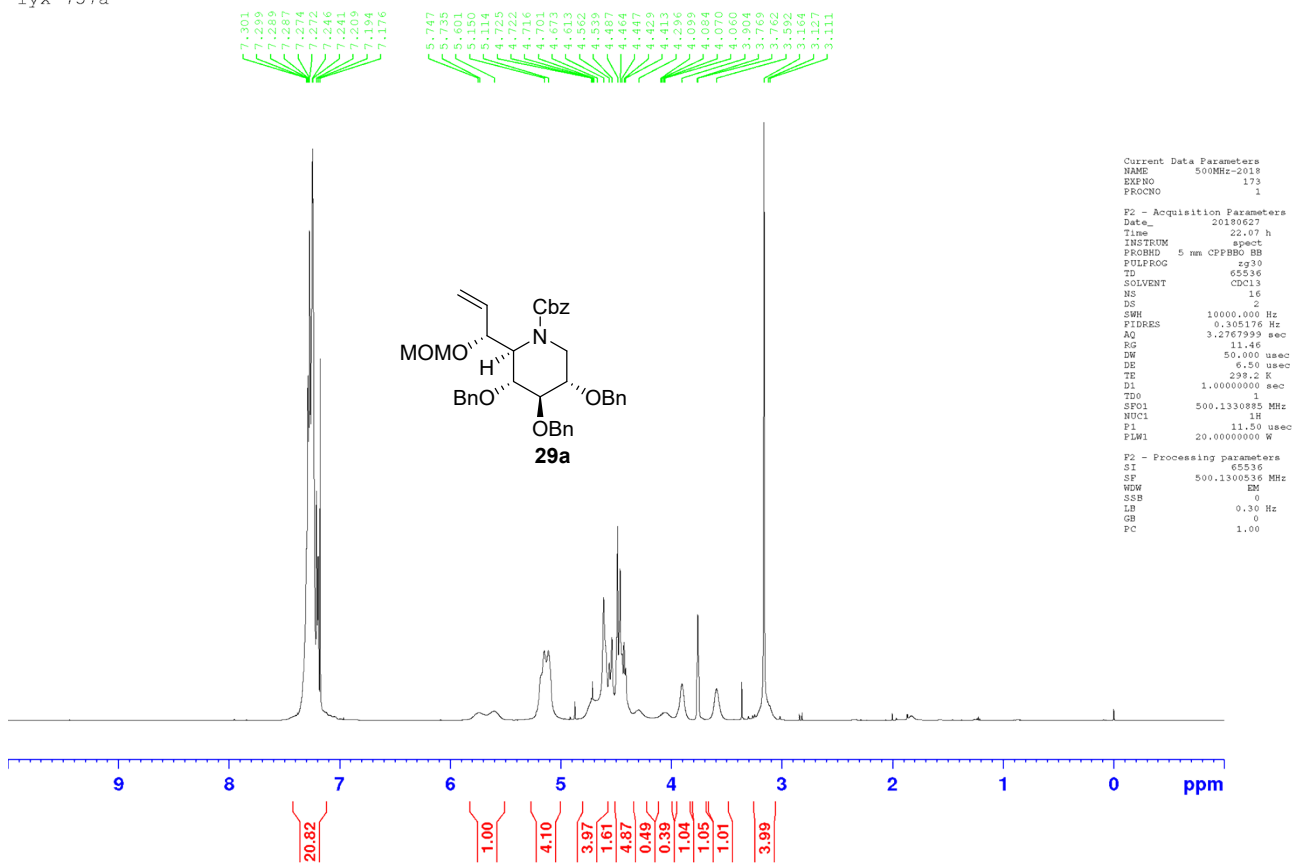
F2 - Acquisition Parameters  
Date\_ 20160329  
Time 13.21 h  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG deptsp135  
TD 65536  
SOLVENT cdcl3  
NS 193  
DS 4  
SWH 12077.295 Hz  
FIDRES 0.368570 Hz  
AQ 2.7131903 sec  
RG 209.09  
DM 41.400 usec  
DE 6.50 usec  
TE 297.6 K  
CHST2 145.000000 sec  
D1 2.00000000 sec  
d2 0.00344828 sec  
d12 0.00002000 sec  
DELTA 0.00001401 sec  
TDO 1  
SF01 75.4737856 MHz  
NUC1 13c  
P1 11.00 usec  
PL13 2000.00 usec  
PLM0 0 W  
PLM1 195.00000000 W  
SFNAM[5] Cxp60comp.4  
SF0AL5 0.500  
SFOFF55 0 Hz  
SF05 36.04999924 W  
SF02 300.13095939 MHz  
NUC2 1H  
CPDPRG2 waltz16  
P3 10.00 usec  
p4 20.00 usec  
PCPD2 90.00 usec  
PLM2 14.00000000 W  
PLW12 0.17284000 W

F2 - Processing parameters  
SI 32768  
SF 75.4677485 MHz  
WCM EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



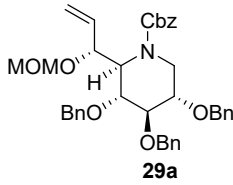
Compound **29a**:

lyx-757a



lyx-757a

156.37  
 138.52  
 138.33  
 138.07  
 136.85  
 135.52  
 128.49  
 128.45  
 128.38  
 128.31  
 127.80  
 127.74  
 127.54  
 127.50  
 119.41  
 94.34  
 78.60  
 78.08  
 77.50  
 77.45  
 76.26  
 76.25  
 74.53  
 73.93  
 73.11  
 72.66  
 71.25  
 70.64  
 67.32  
 57.47  
 57.01  
 55.81  
 55.66  
 40.75  
 39.66

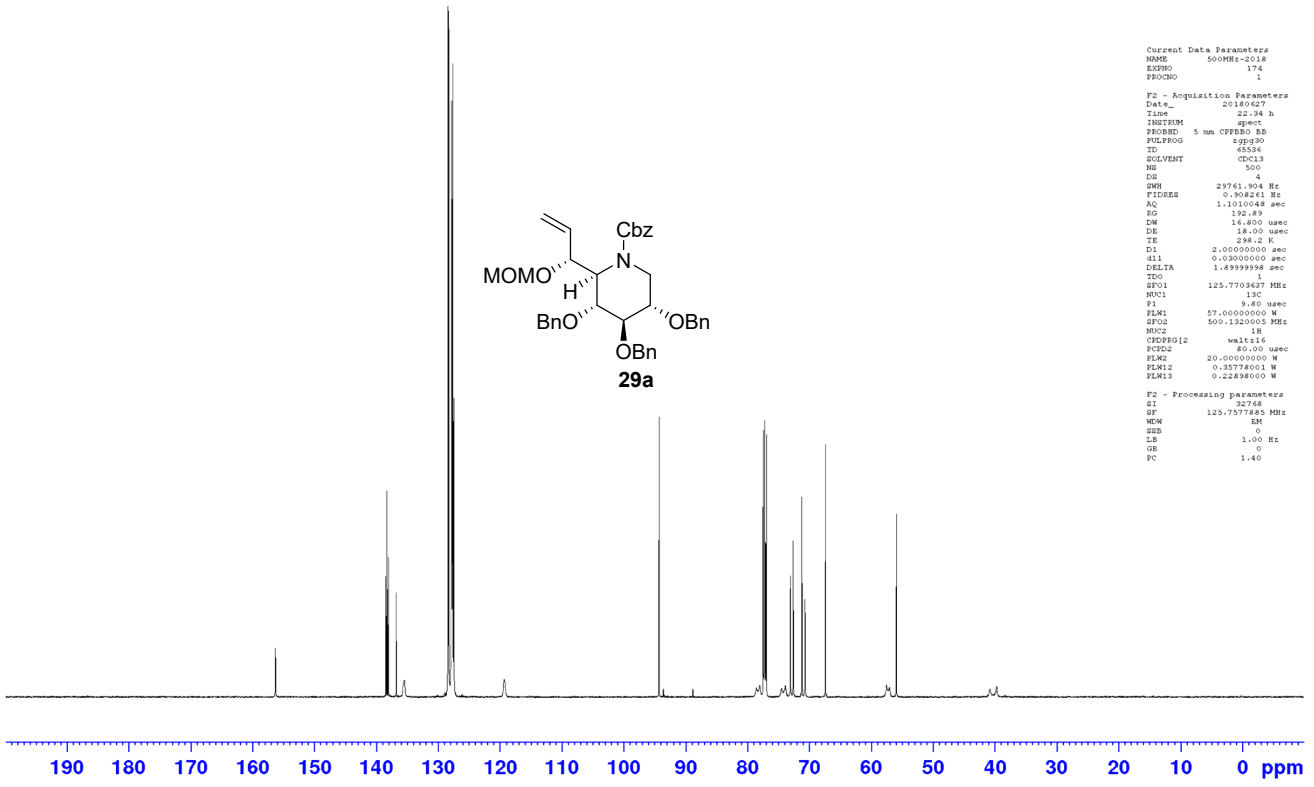


```

Current Data Parameters
NAME      500MHz-2018
EXPNO     1
PROCNO    1

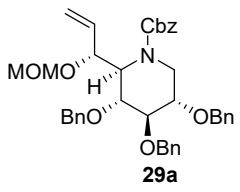
F2 - Acquisition Parameters
Date_     20180427
Time      22:34 h
INSTRUM   spect
PROBHD    5 mm CPBPR0 BB
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         500
DS         4
SWH        29741.004 Hz
FIDRES     0.908261 Hz
AQ         1.1010048 sec
RG         192.89
DM         14.800 usec
DE         18.00 usec
TE         298.2 K
d11        2.00000000 sec
d12        0.03000000 sec
DELTA      1.49999998 sec
TEO        1
SF01       125.7703627 MHz
NUC1       13C
P1         9.80 usec
PL1        57.00000000 W
SF02       500.1320005 MHz
NUC2       1H
PCPGP2     wait16
PCPD2      80.00 usec
PLM2       20.00000000 W
PLM12      0.35778001 W
PLM13      0.22898000 W

F2 - Processing Parameters
SI         2768
SF         125.7577885 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
  
```



lyx-757a

135.49  
 128.49  
 128.36  
 128.31  
 127.90  
 127.85  
 127.74  
 127.54  
 127.50  
 119.44  
 94.34  
 78.64  
 78.47  
 78.03  
 77.45  
 77.16  
 74.58  
 73.88  
 72.66  
 72.65  
 71.25  
 70.64  
 67.32  
 57.49  
 56.97  
 55.82  
 55.71  
 40.78  
 39.64  
 38.23

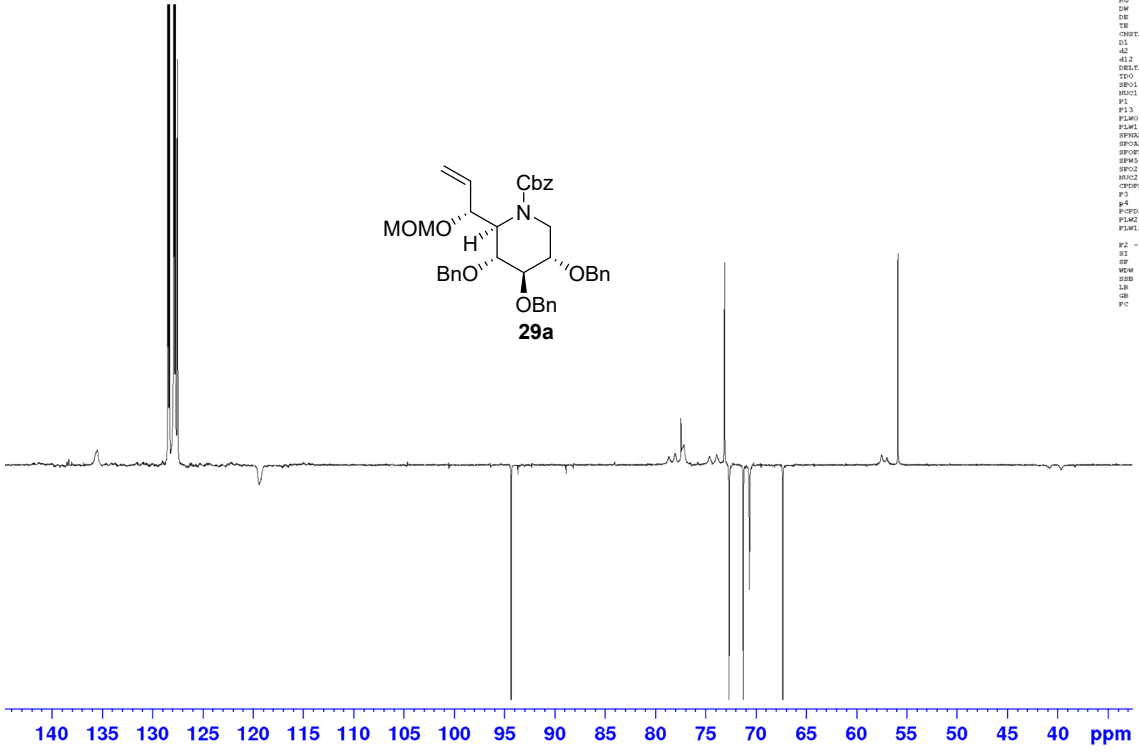


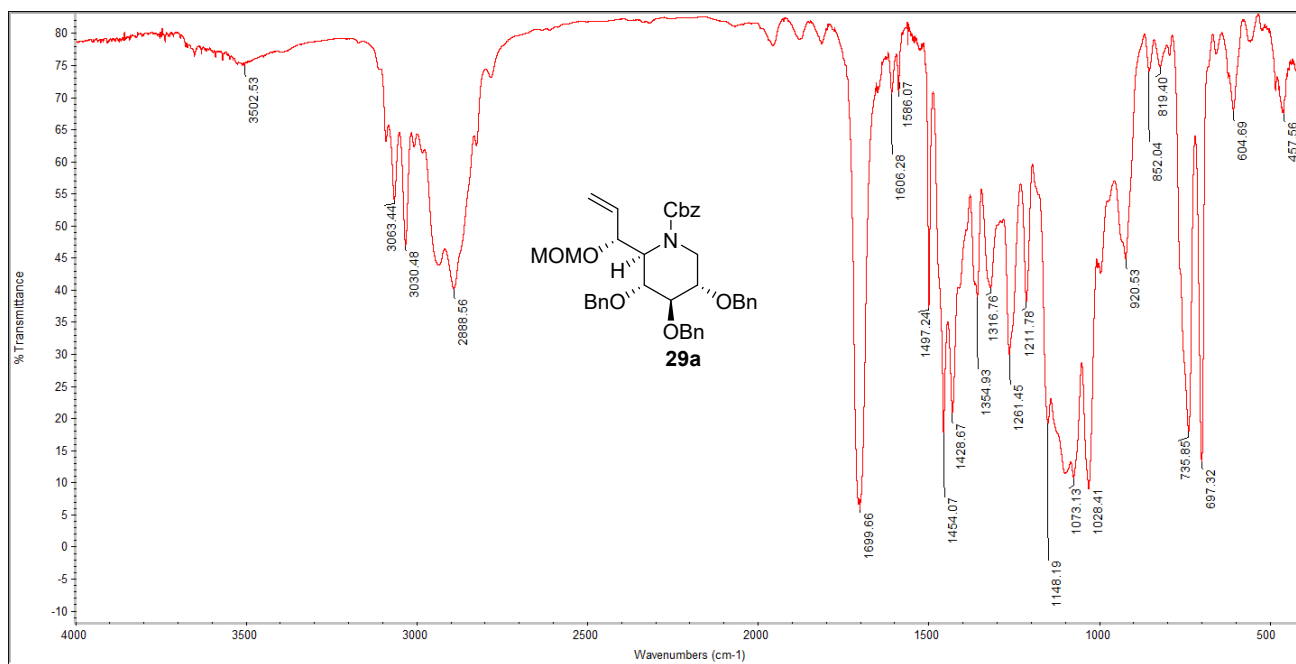
```

Current Data Parameters
NAME      500MHz-2018
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20180427
Time      22:51 h
INSTRUM   spect
PROBHD    5 mm CPBPR0 BB
PULPROG   zgpg135
TD         65536
SOLVENT   CDCl3
NS         500
DS         4
SWH        20141.291 Hz
FIDRES     0.415274 Hz
AQ         1.4252928 sec
RG         192.89
DM         24.800 usec
DE         18.00 usec
TE         298.2 K
d11        2.00000000 sec
d12        0.00348828 sec
d13        0.00001000 sec
DELTA      0.00001248 sec
TEO        1
SF01       125.7678484 MHz
NUC1       13C
P1         9.80 usec
PL1        57.00000000 W
PLM0       0 W
PLM1       2000.00 usec
SF02       500.1315995 MHz
NUC2       1H
PCPGP2     wait16
P3         10.70 usec
P4         21.40 usec
PCPD2      80.00 usec
PLM2       20.00000000 W
PLM12      0.35778001 W

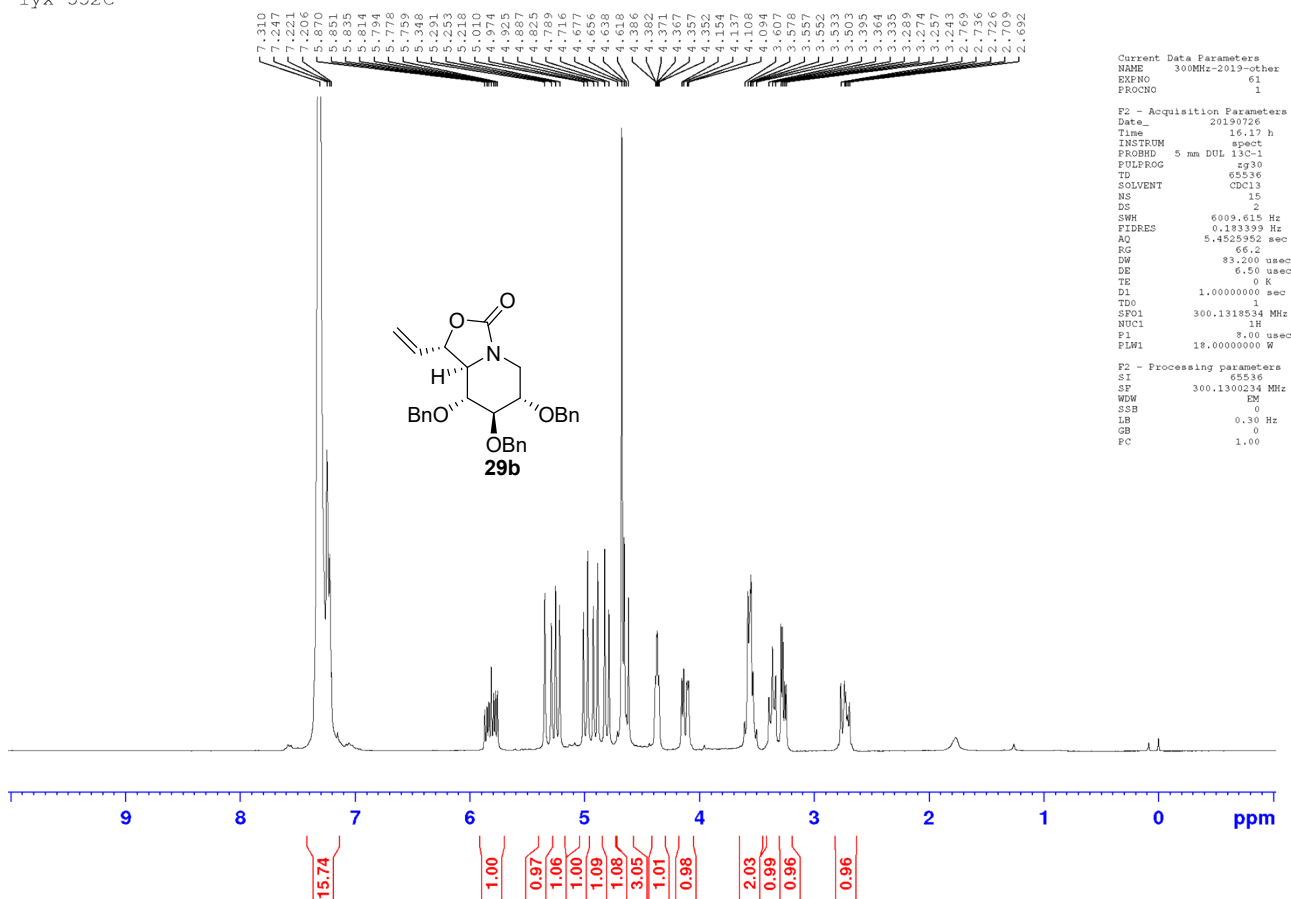
F2 - Processing Parameters
SI         2768
SF         125.7577885 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
  
```



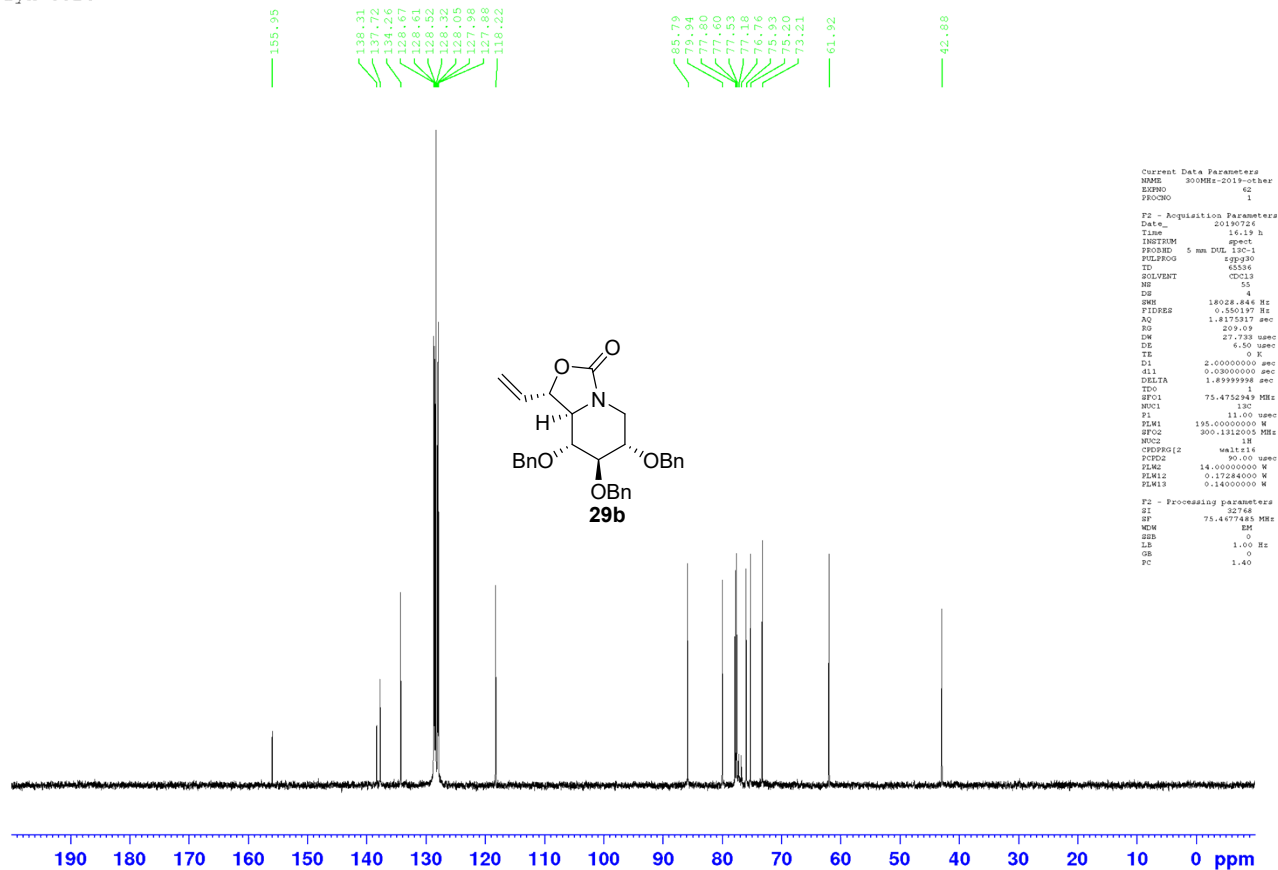


Compound **29b**:

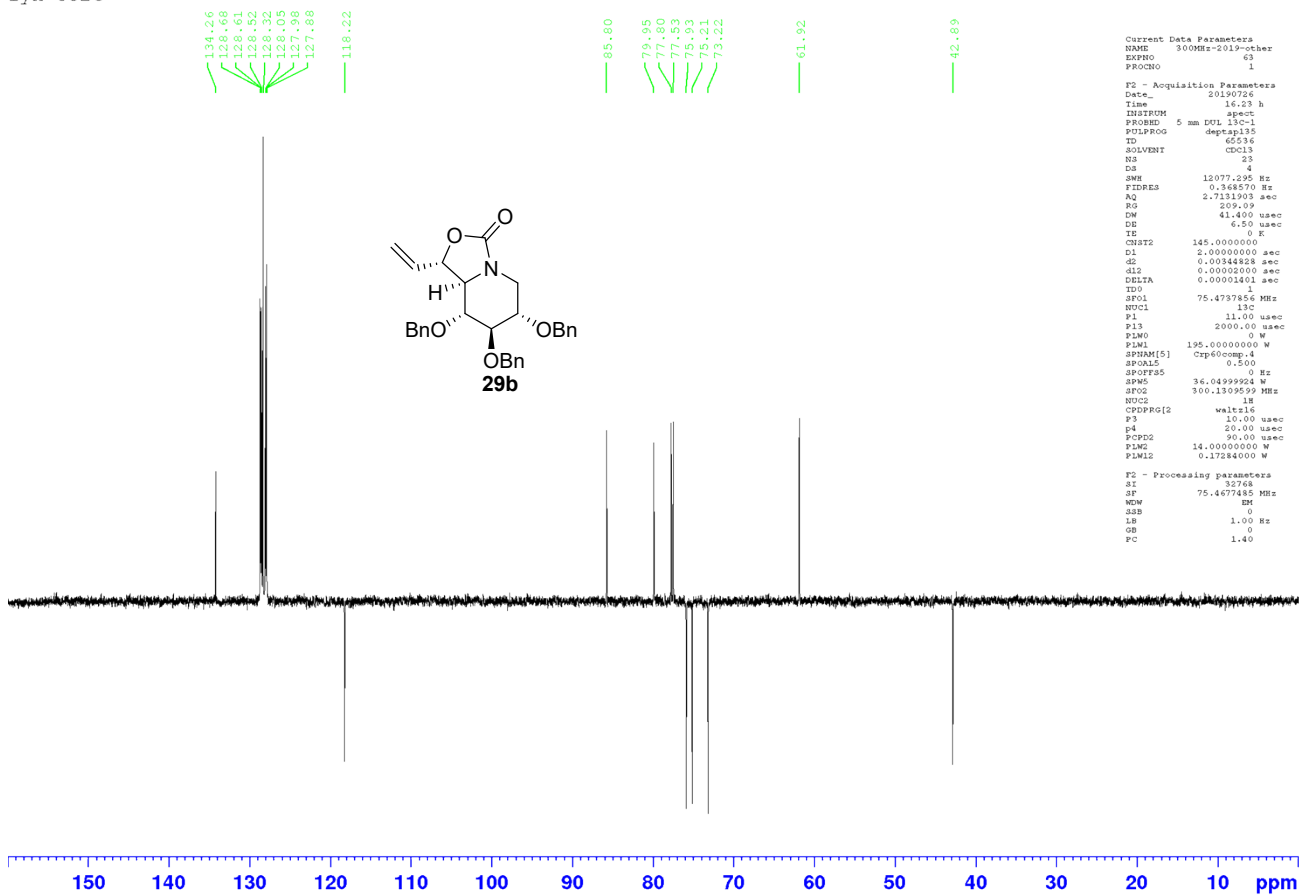
lyx-552c

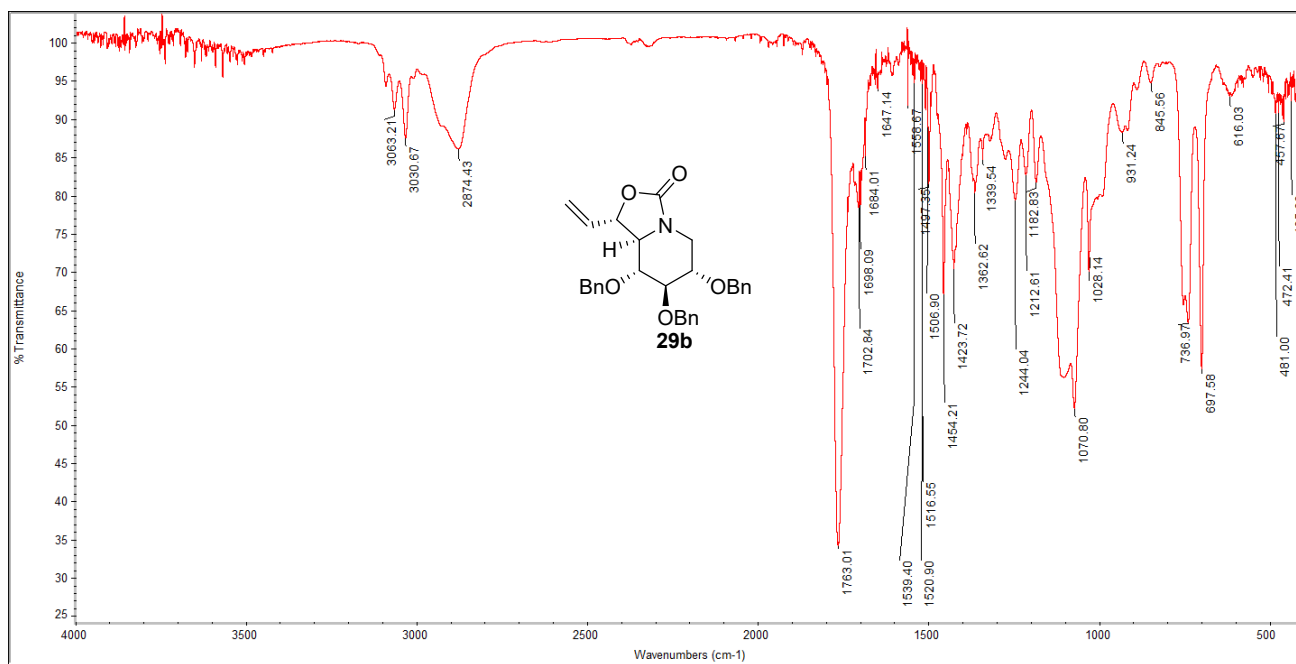


lyx-552c



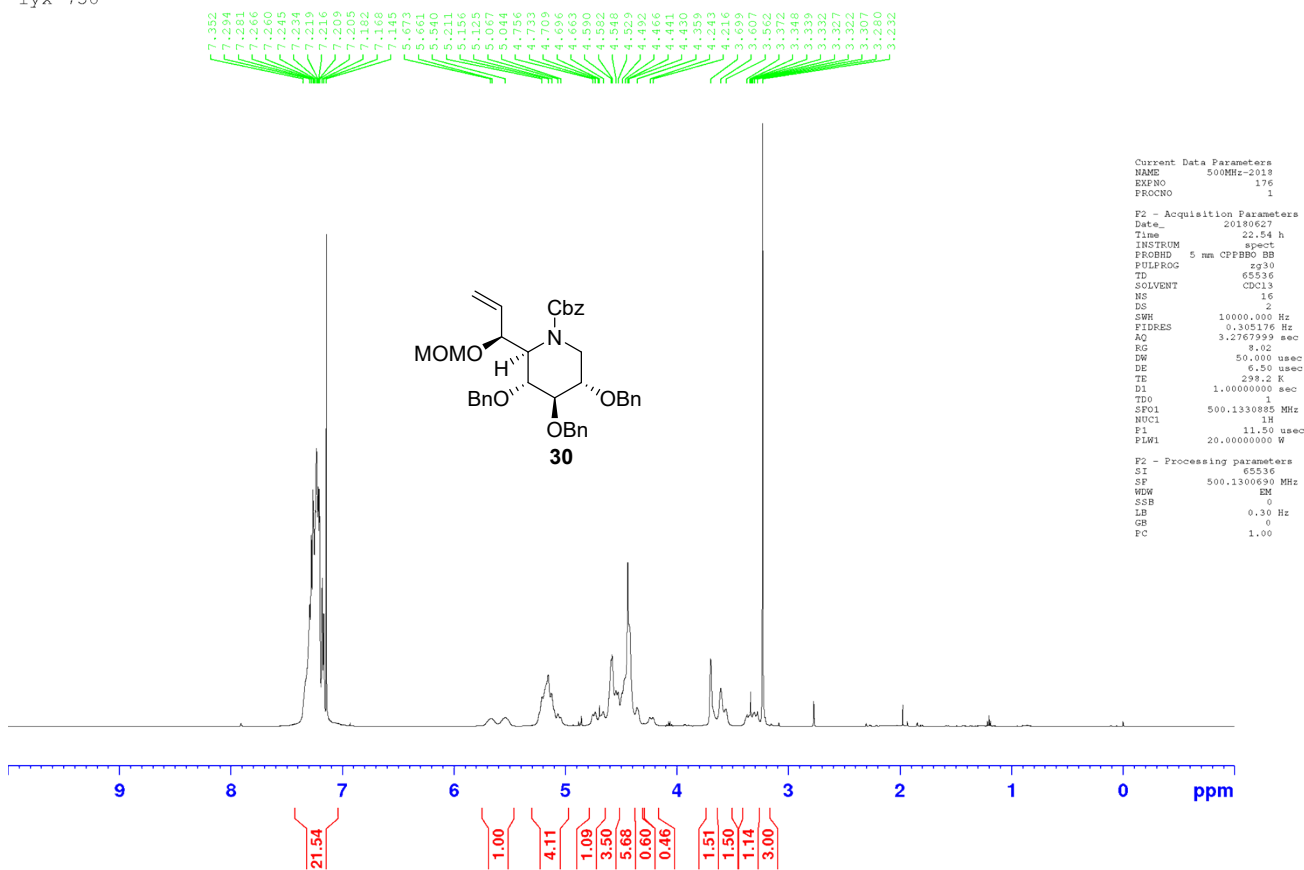
lyx-552c





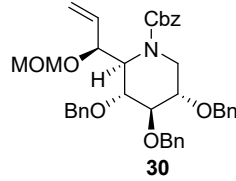
Compound 30:

lyx-758



lyx-758

156.96  
156.79  
138.43  
138.35  
138.02  
137.34  
137.04  
135.75  
128.56  
128.40  
127.98  
127.71  
127.68  
127.54  
120.27  
120.14  
93.59  
77.77  
77.65  
77.60  
77.14  
76.92  
75.16  
74.51  
74.19  
73.16  
72.72  
72.72  
71.86  
71.86  
70.51  
67.29  
67.10  
58.26  
57.57  
55.91  
55.63  
55.63  
40.04  
38.91



```

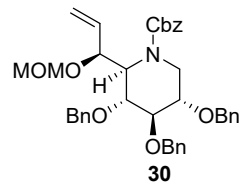
Current Data Parameters
NAME      500MHz-2018
EXPNO     177
PROCNO    1

F2 - Acquisition Parameters
Date_     20180627
Time      23:21 h
INSTRUM   spect
PROBHD    5 mm CPBPR0 BB
PULPROG   zgpg30
ID         65336
SOLVENT   CDCl3
NS         500
DS         4
SWH        29761.904 Hz
FIDRES     0.904261 Hz
AQ         1.1010048 sec
RG         192.89
DM         16.800 usec
DE         18.00 usec
TE         298.1 K
D1         2.00000000 sec
d11        0.00000000 sec
DELTA     1.89999998 sec
TD0        1
SFO1       125.770437 MHz
NUC1       13C
P1         9.80 usec
P1M1       57.00000000 M
SFO2       500.1313995 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
P2        20.00000000 M
P2M2       0.25778001 M
P2M3       0.25778001 M

F2 - Processing parameters
SI         32768
SF         125.7577885 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

lyx-758

135.75  
128.56  
128.40  
127.98  
127.91  
127.71  
127.68  
127.54  
120.27  
120.14  
93.59  
77.78  
77.78  
77.59  
76.92  
75.17  
74.51  
74.19  
73.16  
72.73  
72.60  
72.60  
71.81  
71.81  
67.30  
67.10  
58.27  
57.56  
55.81  
55.63  
40.04  
38.91

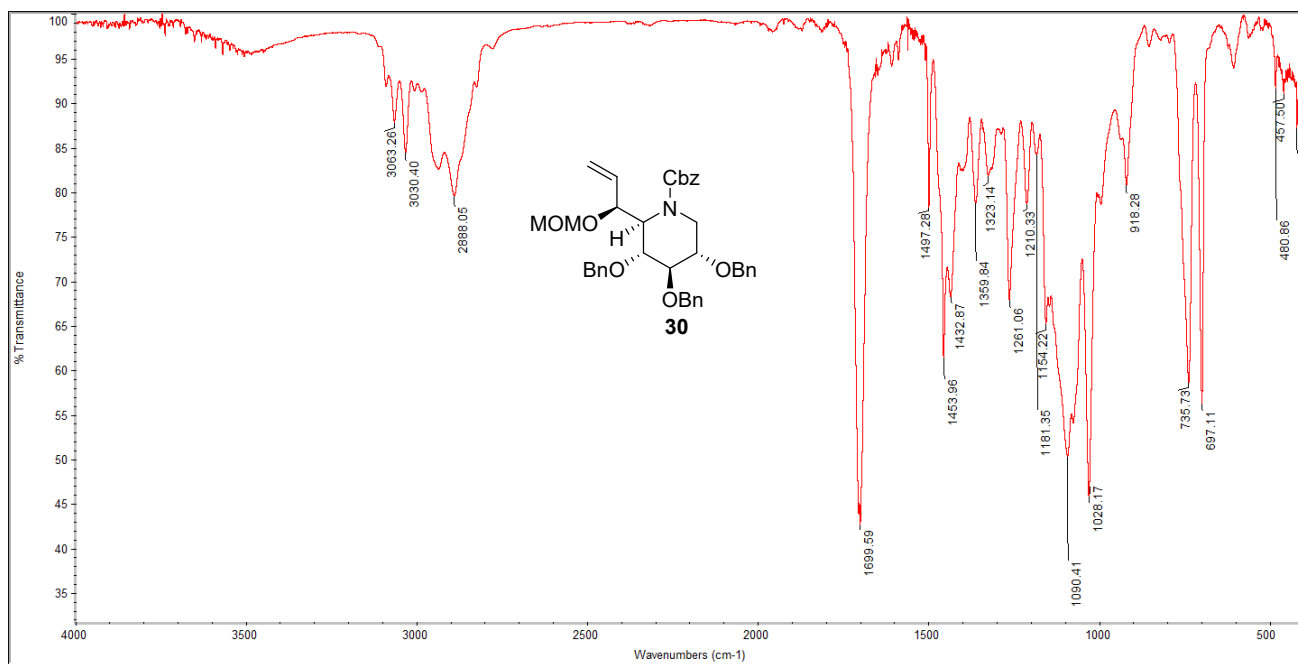


```

Current Data Parameters
NAME      500MHz-2018
EXPNO     178
PROCNO    1

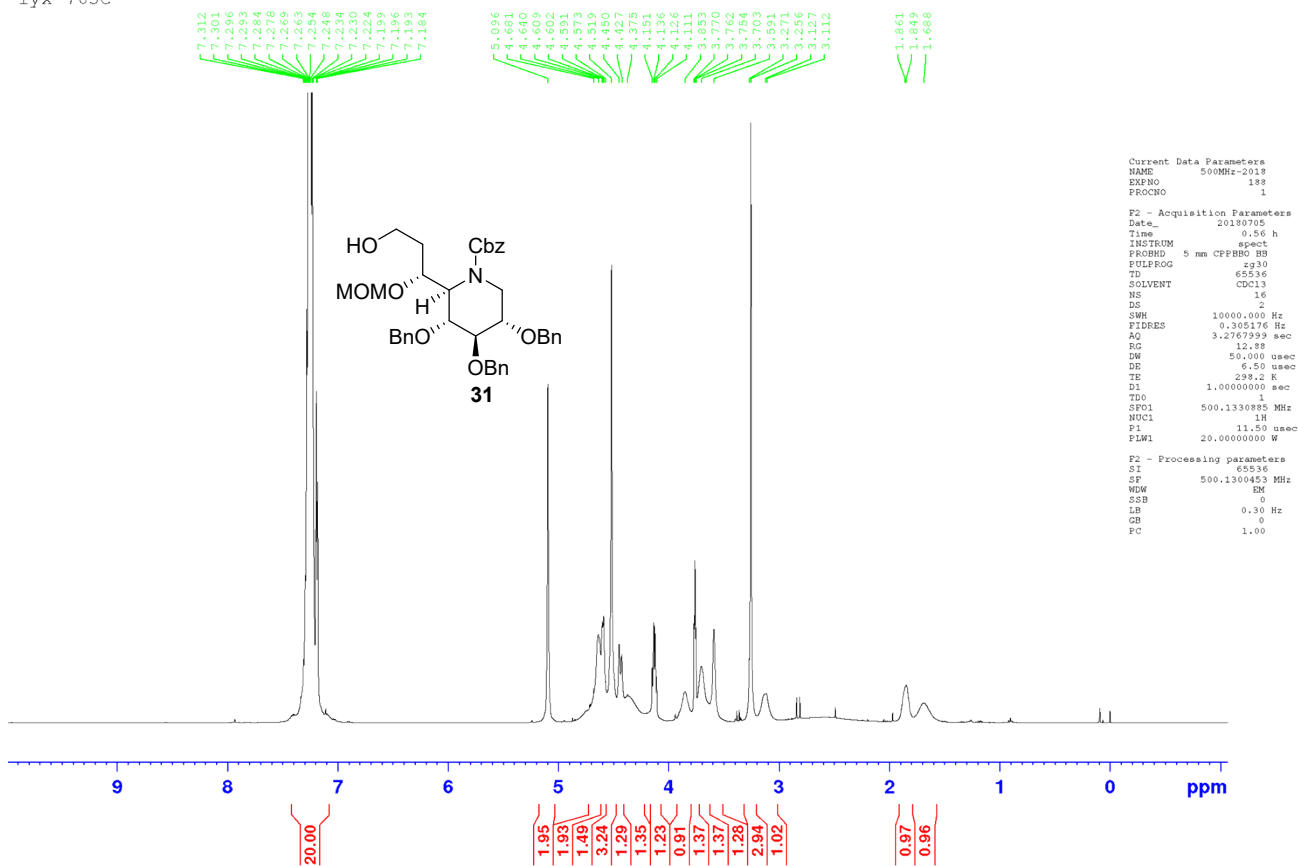
F2 - Acquisition Parameters
Date_     20180627
Time      23:27 h
INSTRUM   spect
PROBHD    5 mm CPBPR0 BB
PULPROG   deptap155
ID         65336
SOLVENT   CDCl3
NS         256
DS         4
SWH        29761.904 Hz
FIDRES     0.415274 Hz
AQ         1.4232928 sec
RG         192.89
DM         16.800 usec
DE         18.00 usec
TE         298.1 K
D1         2.00000000 sec
d11        0.00000000 sec
DELTA     0.00000000 sec
TD0        1
SFO1       125.7478446 MHz
NUC1       13C
P1         9.80 usec
P1M1       57.00000000 M
SFO2       500.1313995 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
P2        20.00000000 M
P2M2       0.25778001 M
P2M3       0.25778001 M

F2 - Processing parameters
SI         32768
SF         125.7577885 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



Compound 31:

lyx-763c



```

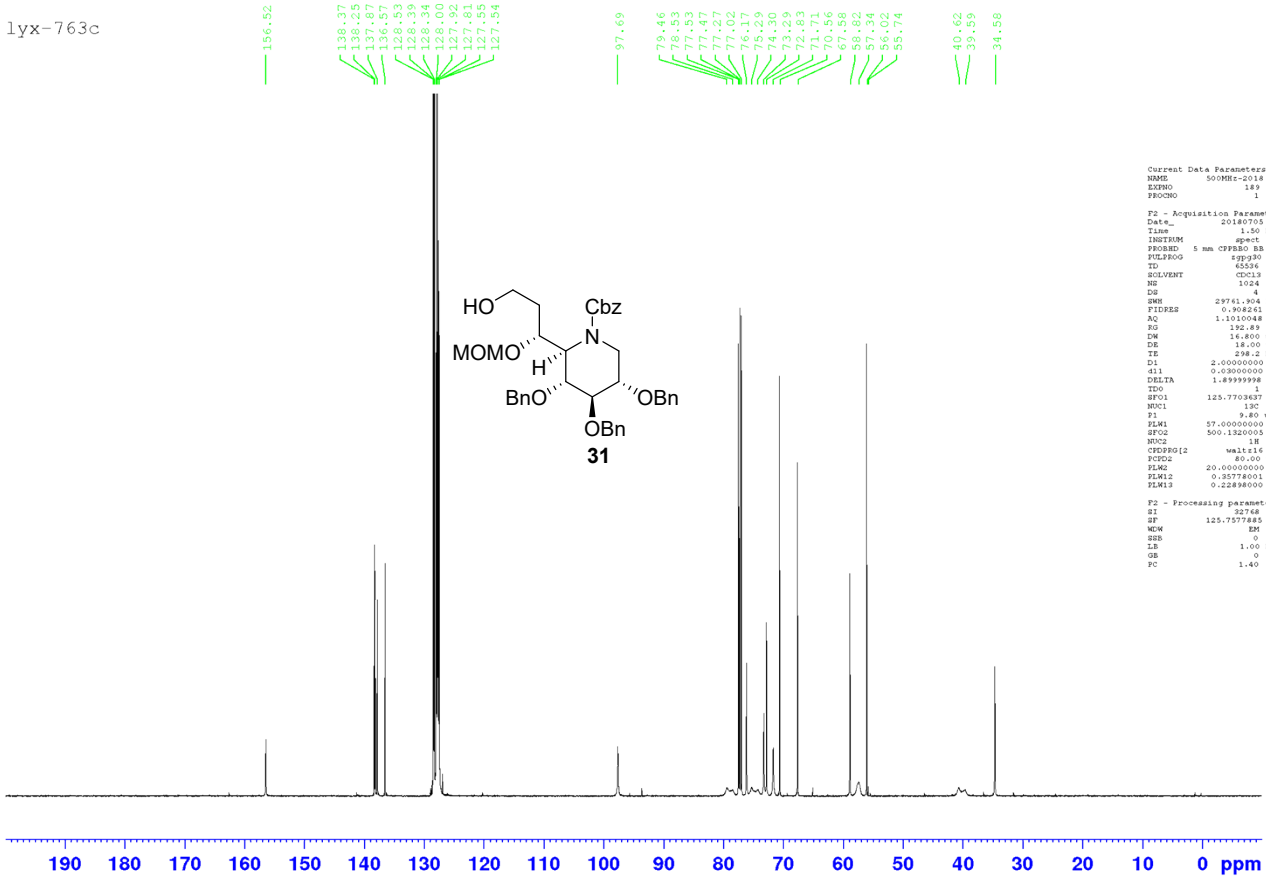
Current Data Parameters
NAME      500MHz-2018
EXPNO    198
PROCNO   1

F2 - Acquisition Parameters
Date_    20180705
Time     0.56 h
INSTRUM  spect
PROBHD   5 mm CPFBH1-EB
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ        3.2767399 sec
RG         12.88
DM         50.000 usec
DE         6.50 usec
TE        298.2 K
D1         1.00000000 sec
D11        1
SFO1      500.1330885 MHz
NUC1       1H
P1         11.50 usec
PL1        20.00000000 W

F2 - Processing parameters
SI         65536
SF         500.1300453 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



lyx-763c



```

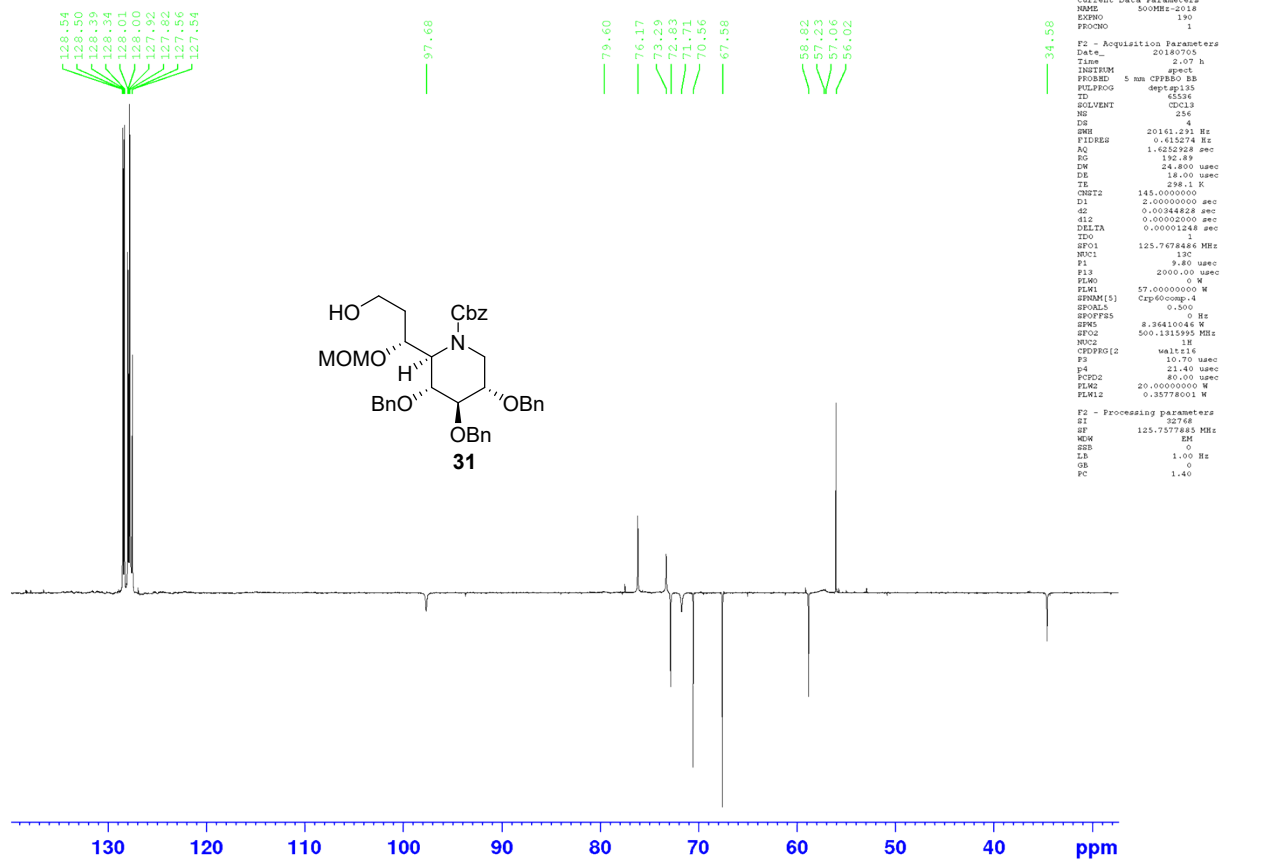
Current Data Parameters
NAME 20180705
EXPNO 189
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180705
Time 1.50 h
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.804 Hz
FIDRES 0.302261 Hz
AQ 1.1010048 sec
RG 192.89
DM 14.800 usec
DE 18.00 usec
TE 298.2 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999999 sec
TD0 1
SFO1 125.770367 MHz
NUC1 13C
P1 9.80 usec
PLM1 57.0000000 MHz
SFO2 500.1320000 MHz
NUC2 1H
CPCPRG2 waltz16
PCPD2 80.00 usec
PLM2 20.0000000 MHz
PLM12 0.35778001 M
PLM13 0.22880000 M

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```

lyx-763c



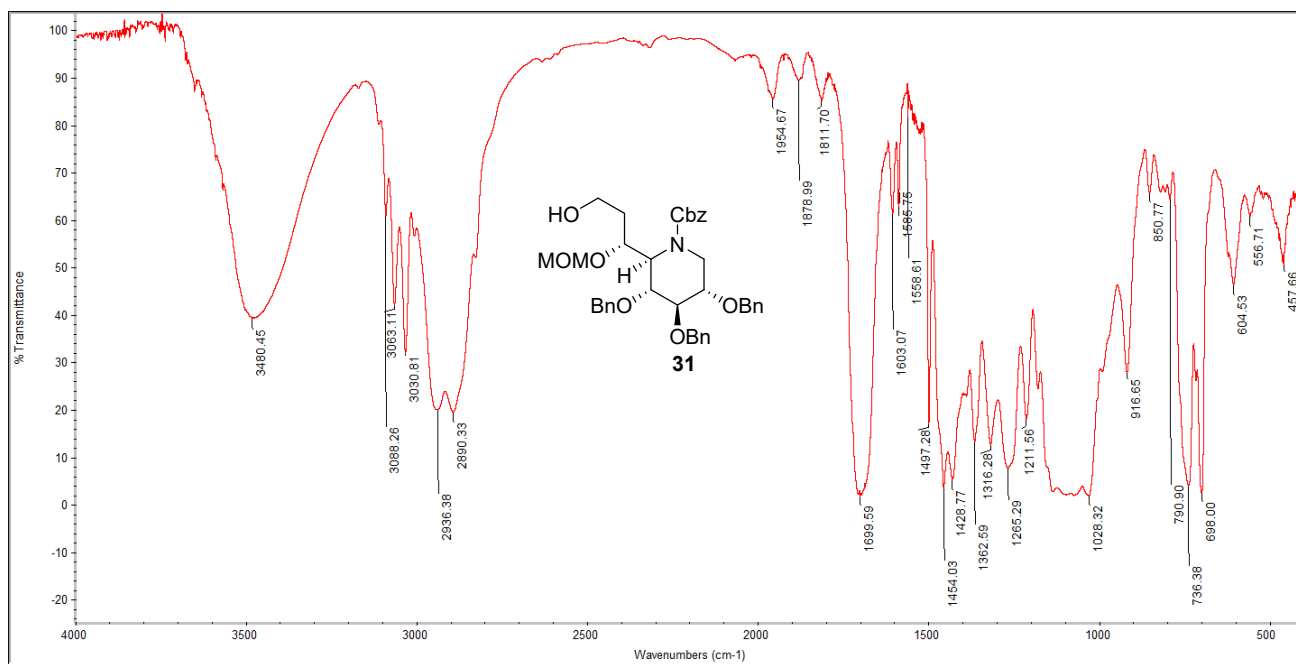
```

Current Data Parameters
NAME 20180705
EXPNO 189
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180705
Time 2.07 h
INSTRUM spect
PROBHD 5 mm CPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 20161.291 Hz
FIDRES 0.415274 Hz
AQ 1.4232728 sec
RG 192.89
DM 14.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.0000000 sec
d11 0.03000000 sec
d12 0.00020000 sec
DELTA 0.0001248 sec
TD0 1
SFO1 125.7478484 MHz
NUC1 13C
P1 9.80 usec
PLM1 57.0000000 MHz
SFO2 500.1315995 MHz
NUC2 1H
CPCPRG2 waltz16
PCPD2 80.00 usec
PLM2 20.0000000 MHz
PLM12 0.35778001 M

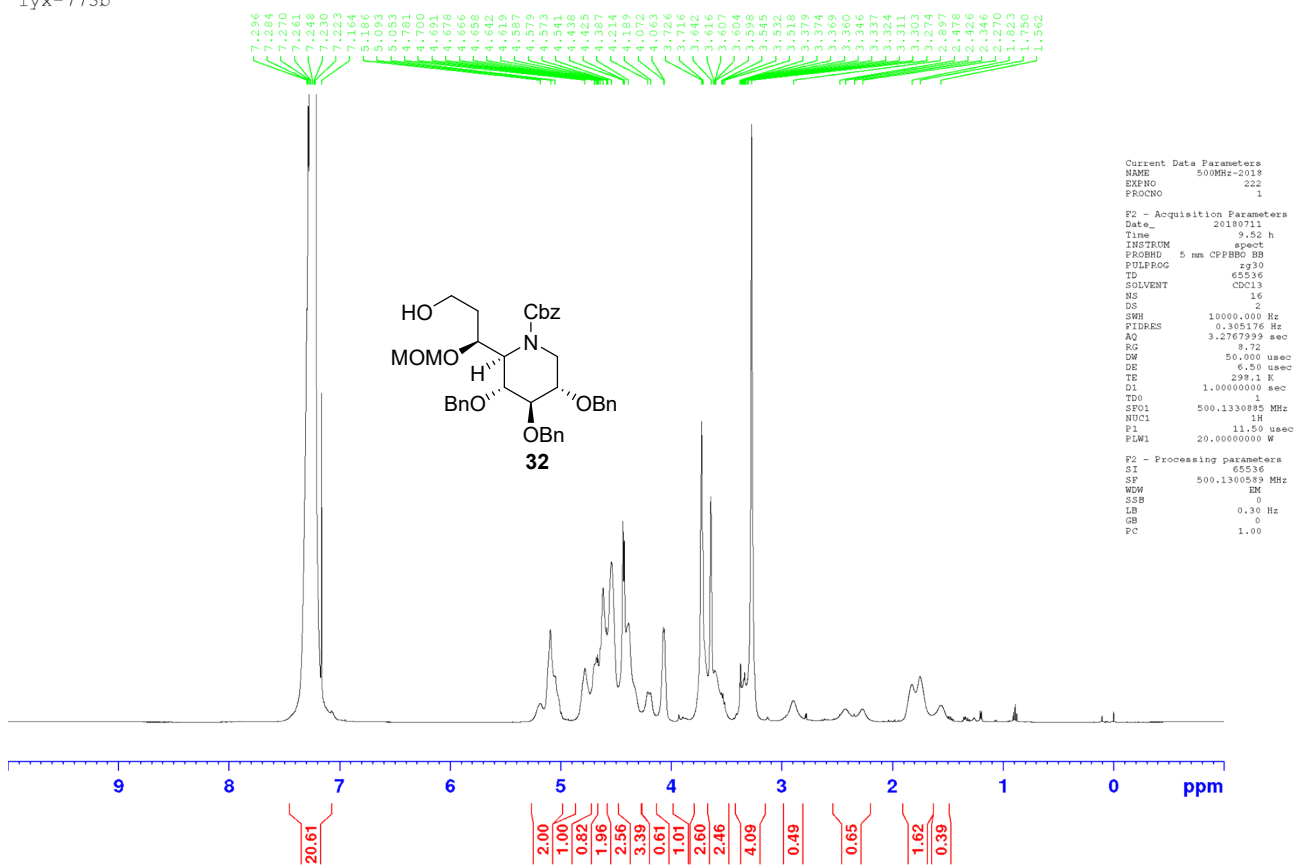
F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```



Compound 32:

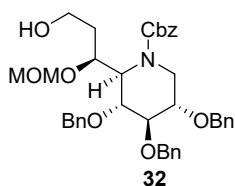
lyx-773b



Current Data Parameters  
 NAME 500MHz-2018  
 EXNO 222  
 F2NAME  
 F2 - Acquisition Parameters  
 Date\_ 20180711  
 Time 9.52 h  
 INSTRUM spect  
 PROBHD 5 mm CFPBBO BB  
 PULPROG zg30  
 TD 65536  
 TE 300.2 K  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 10060.000 Hz  
 FIDRES 0.240176 Hz  
 AQ 3.276739 sec  
 RG 8.72  
 SW 50.000 usec  
 DE 6.50 usec  
 TE 299.1 K  
 D1 1.00000000 sec  
 TDO 1  
 SPOL 500.1330889 MHz  
 NUCL 1H  
 P1 11.50 usec  
 PLWL 20.00000000 W  
 F2 - Processing parameters  
 SI 65536  
 SF 500.1330889 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

lyx-773b

137.18  
136.92  
138.44  
138.25  
137.91  
136.67  
128.54  
128.48  
128.43  
128.07  
127.86  
127.78  
127.62  
97.06  
81.47  
78.35  
77.63  
77.57  
77.37  
77.17  
76.10  
75.50  
74.93  
74.22  
73.61  
73.39  
73.10  
72.36  
70.56  
69.09  
58.89  
56.10  
42.04  
40.02  
34.55



```

Current Data Parameters
NAME      500MHz-2018
EXPNO     223
PROCNO    1

F2 - Acquisition Parameters
Date_     20180711
Time      10:47 h
INSTRUM   spect
PROBHD    5 mm CPBBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SMB       29761.904 Hz
FIDRES    0.368241 Hz
AQ         1.1010048 sec
RG         192.89
DM         14.800 usec
DE         18.00 usec
TE         298.2 K
D1         2.00000000 sec
d11        0.00000000 sec
DELTA     1.49999998 sec
TD0        1
SFO1      125.7703637 MHz
NUC1       13C
P1         9.80 usec
PLM1       57.00000000 W
SFO2      500.1320000 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PLM2      20.00000000 W
PLM12     0.35778001 W
PLM13     0.22898000 W

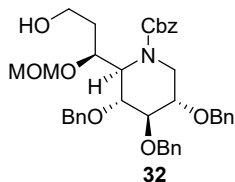
F2 - Processing parameters
SI         32768
SF         125.7577885 MHz
WDW        RM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

lyx-773b

128.54  
128.48  
128.43  
128.07  
127.88  
127.74  
127.62  
97.06  
81.51  
78.34  
77.57  
76.08  
74.93  
74.25  
73.61  
73.10  
70.56  
67.60  
59.10  
58.89  
56.10  
42.01  
34.54



```

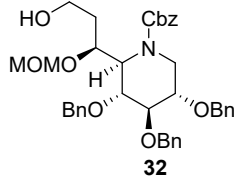
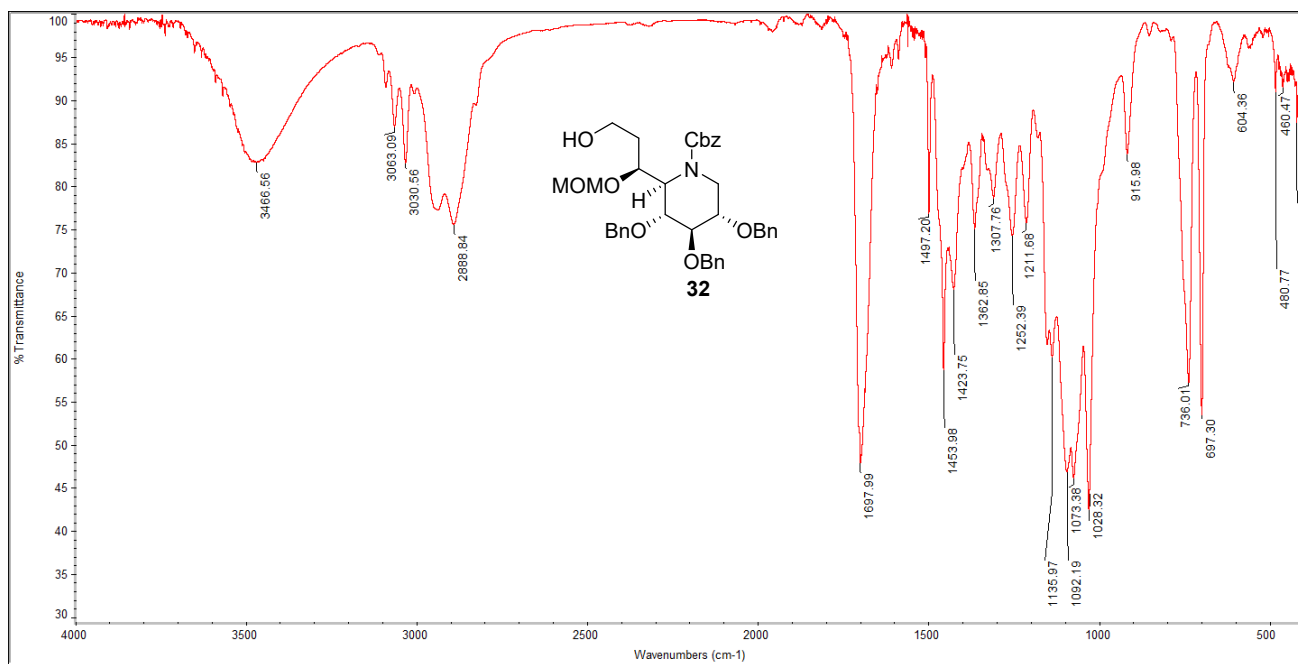
Current Data Parameters
NAME      500MHz-2018
EXPNO     224
PROCNO    1

F2 - Acquisition Parameters
Date_     20180711
Time      11:03 h
INSTRUM   spect
PROBHD    5 mm CPBBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         4
SMB       20161.291 Hz
FIDRES    0.415274 Hz
AQ         1.6252028 sec
RG         192.89
DM         14.800 usec
DE         18.00 usec
TE         298.1 K
D1         2.00000000 sec
d12        0.00000000 sec
DELTA     0.00001248 sec
TD0        1
SFO1      125.7678486 MHz
NUC1       13C
P1         9.80 usec
PLM1       57.00000000 W
SFO2      500.1315950 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     80.00 usec
PLM2      20.00000000 W
PLM12     0.35778001 W

F2 - Processing parameters
SI         32768
SF         125.7577885 MHz
WDW        RM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

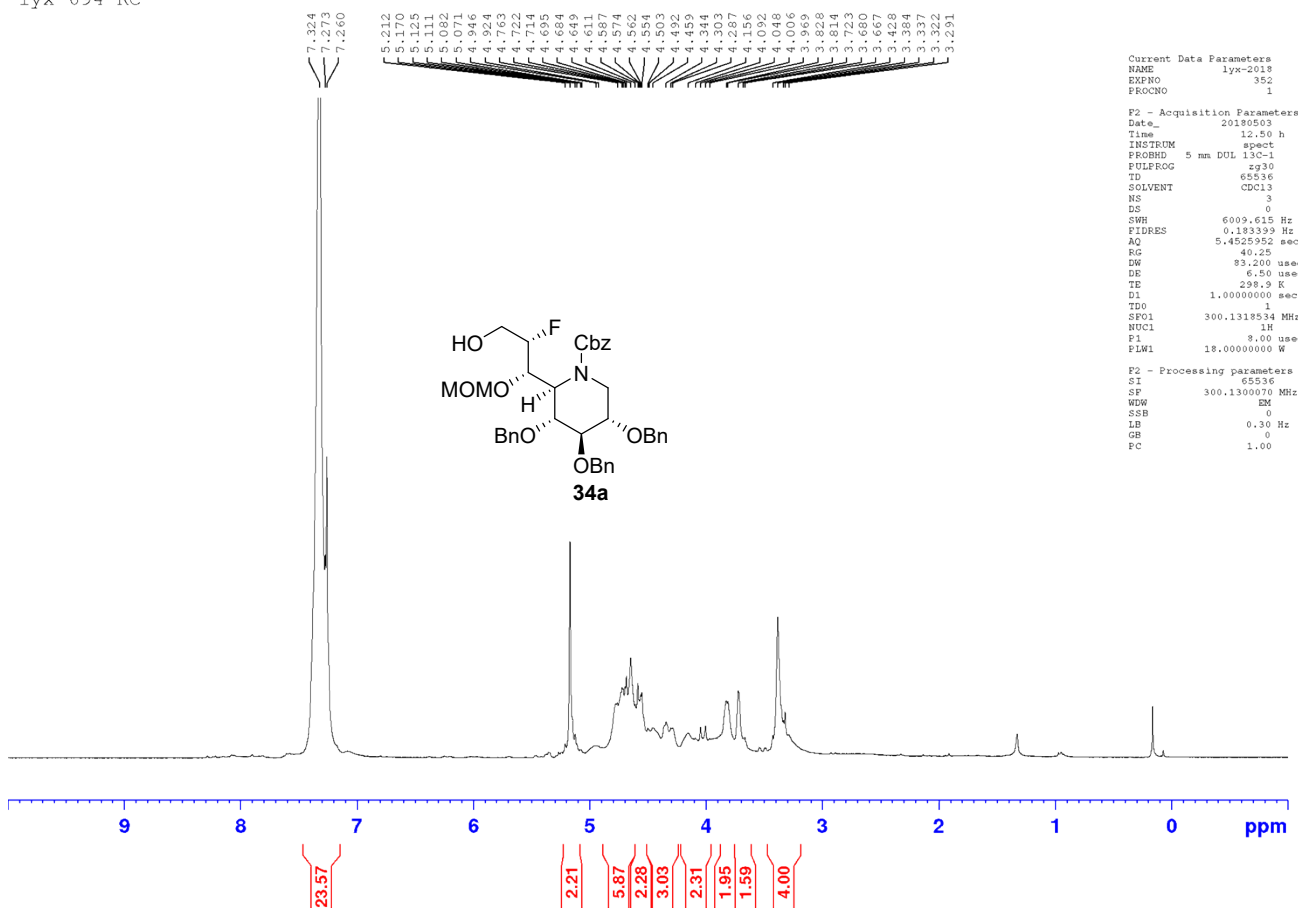
```

130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 ppm

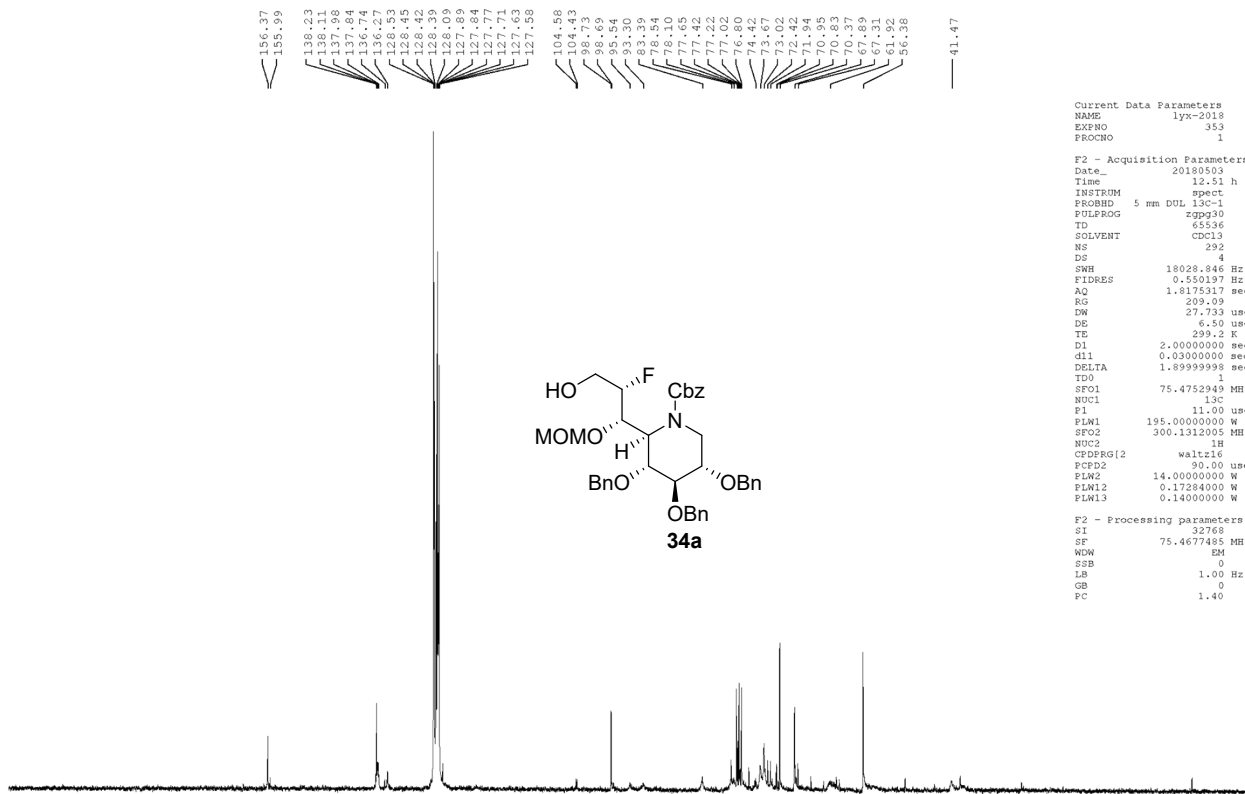


Compound 34a:

lyx-694-Rc



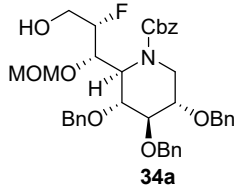
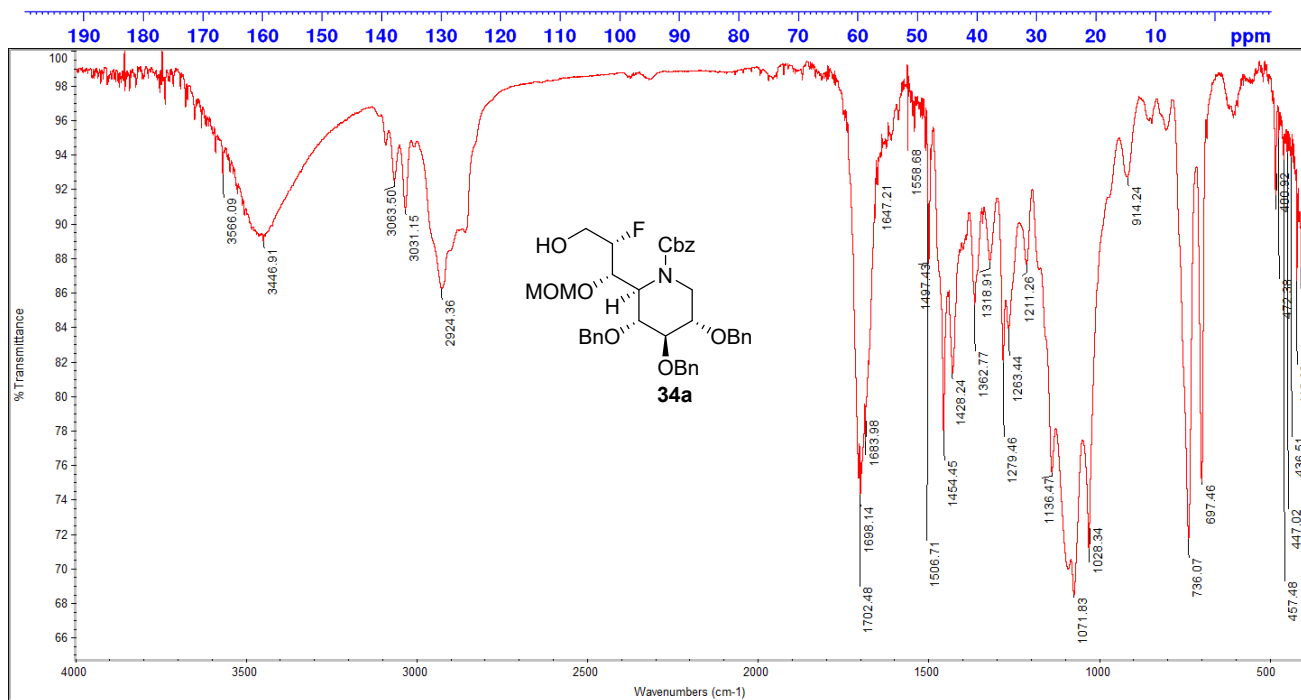
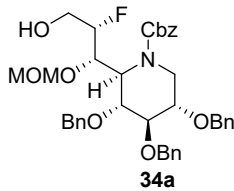
Current Data Parameters  
 NAME lyx-2018  
 EXPNO 352  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20180503  
 Time 12.50 h  
 INSTRUM spect  
 PROBHD 5 mm DDL 13C-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 3  
 DS 0  
 SWH 6009.615 Hz  
 FIDRES 0.183399 Hz  
 AQ 5.4525952 sec  
 RG 40.25  
 DW 83.200 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 1.00000000 sec  
 TEO 1  
 SFO1 300.1318534 MHz  
 NUC1 1H  
 F1 8.00 usec  
 PLW1 18.00000000 W  
 F2 - Processing parameters  
 SI 65536  
 SP 300.1300070 MHz  
 WW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME lyx-2018  
 EXPNO 353  
 PROCNO 1

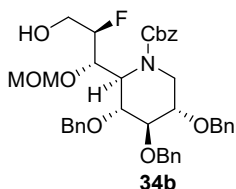
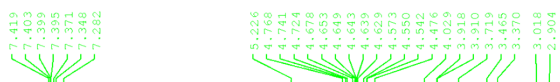
F2 - Acquisition Parameters  
 Date\_ 20180503  
 Time 12:51 h  
 INSTRUM spect  
 PROBHD 5 mm DUL 13C-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 292  
 DS 4  
 SWH 18028.846 Hz  
 FIDRES 0.550197 Hz  
 AQ 1.8175317 sec  
 RG 209.09  
 DW 27.733 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 DELTA 1.8999999 sec  
 ID0 1  
 SFO1 75.4752949 MHz  
 NUC1 13C  
 F1 11.90 usec  
 ELM1 195.0000000 W  
 SFO2 300.1312005 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 14.0000000 W  
 ELM2 0.1728400 W  
 ELM3 0.1400000 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4677485 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



# Compound 34b:

lyx-694-Sc

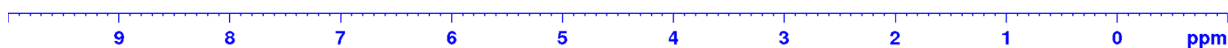


```

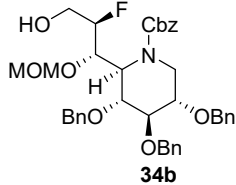
Current Data Parameters
NAME      500MHz-2018
EXPNO    27
PROCNO   1

F2 - Acquisition Parameters
Date_    20180423
Time     21.41 h
INSTRUM  spect
PROBHD   5 mm CPFBBO B3
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ         3.2767999 sec
RG         11.46
DW         50.000 usec
DE         6.50 usec
TE         298.1 K
D1         1.00000000 sec
TDO        1
SF01      500.1330885 MHz
NUC1      1H
P1         11.50 usec
PLW1      20.0000000 W

F2 - Processing parameters
SI         65536
SF         500.1330000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
FC         1.00
    
```



lyx-694-Sc



```

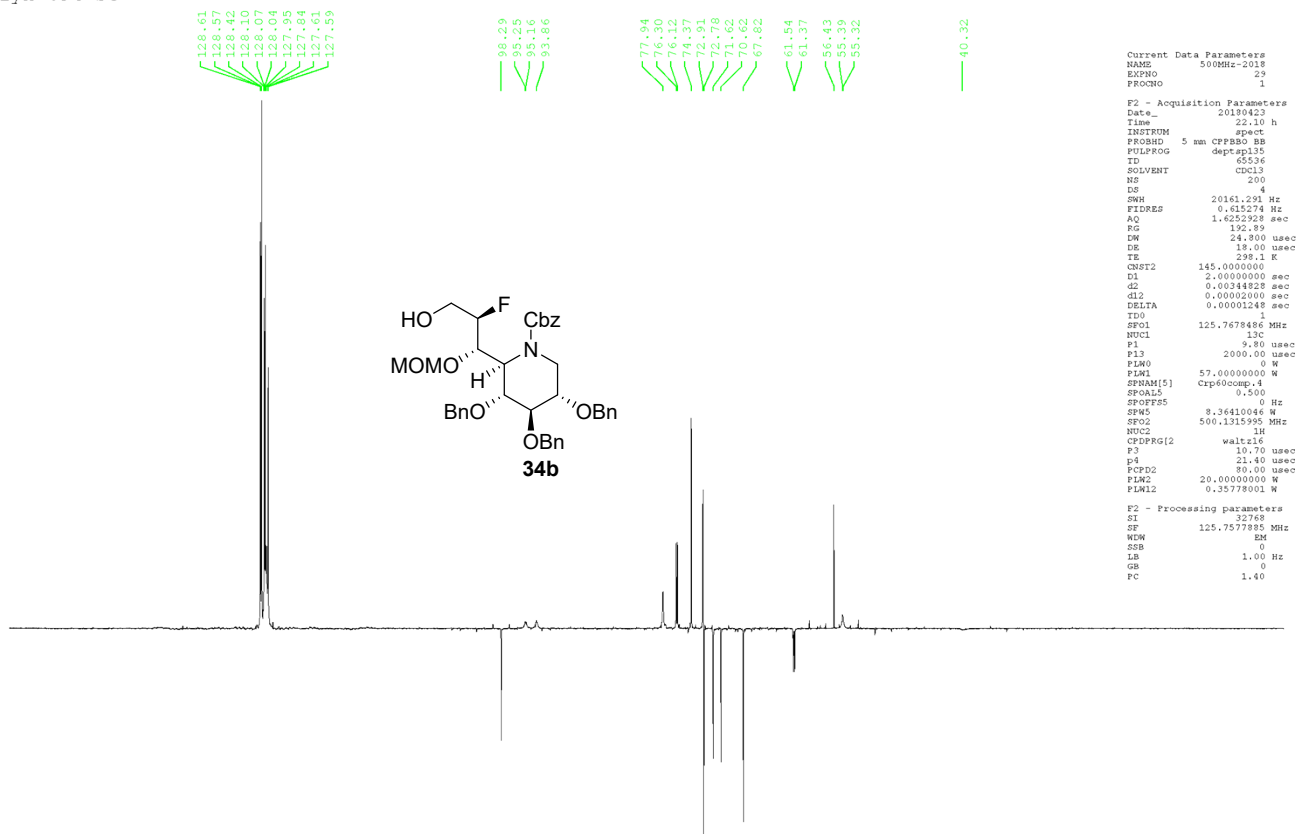
Current Data Parameters
NAME      500MHz-2018
EXPNO    28
PROCNO   1

F2 - Acquisition Parameters
Date_    20180423
Time     21.57 h
INSTRUM  spect
PROBHD   5 mm CPFBBO B3
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        4
SWH       29741.904 Hz
FIDRES    0.308241 Hz
AQ         1.1070048 sec
RG         192.89
DW         16.400 usec
DE         18.00 usec
TE         298.1 K
D1         2.00000000 sec
d11       0.03000000 sec
DELTA     1.49999998 sec
TDO        1
SF01      125.7703437 MHz
NUC1      13C
P1         9.80 usec
PLM1      57.0000000 W
SF02      500.1320005 MHz
NUC2      1H
CPDPRG2   waltz16
F0202     80.00 usec
PLM2      20.0000000 W
PLM12     0.35778001 W
PLM13     0.22878000 W

F2 - Processing parameters
SI         32768
SF         125.7577480 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
FC         1.40
    
```



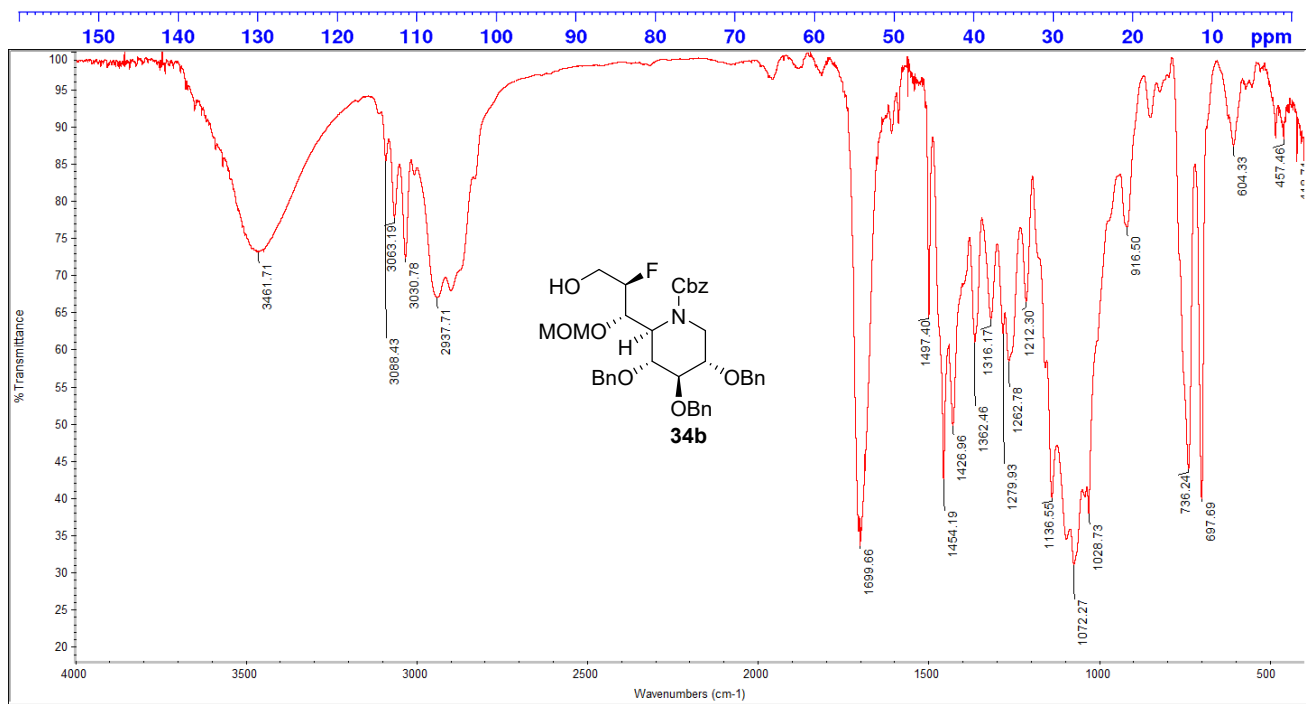
lyx-694-Sc



Current Data Parameters  
 NAME 500MHz-2018  
 EXPNO 29  
 PROCNO 1

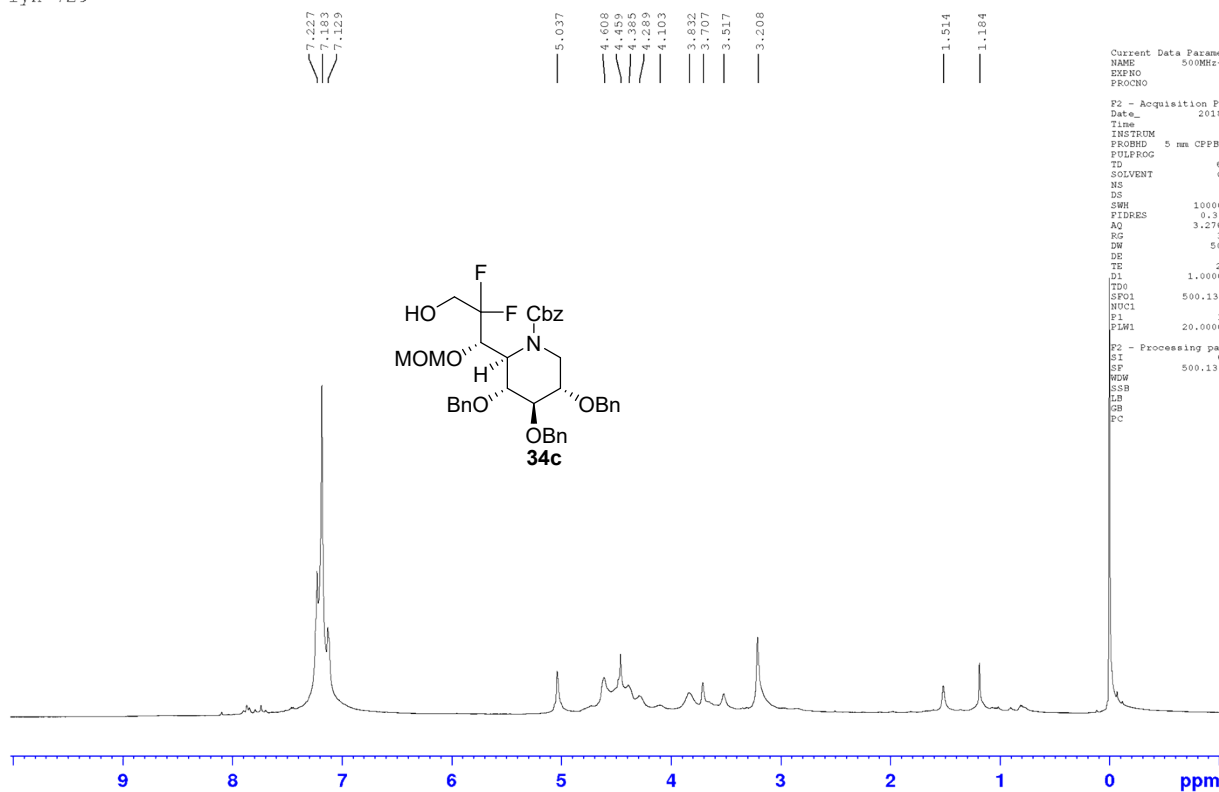
F2 - Acquisition Parameters  
 Date\_ 20180423  
 Time 22.10 h  
 INSTRUM spect  
 PULPROG 5 mm CFPBBO BB  
 DEPTPRG deptpr135  
 TD 65536  
 SOLVENT CDCl3  
 NS 200  
 DS 4  
 SWH 20161.291 Hz  
 FIDRES 0.615274 Hz  
 AQ 1.6252528 sec  
 RG 192.89  
 SQ 24.500 usec  
 DE 18.00 usec  
 TE 299.1 K  
 CNST2 145.0000000  
 D1 2.00000000 sec  
 d2 0.0014828 sec  
 d12 0.0002000 sec  
 DELTA 0.0001248 sec  
 ID0 1  
 SF01 125.7678486 MHz  
 NU1 13C  
 P1 9.80 usec  
 PL1 2000.0 usec  
 PLN0 0 W  
 PLN1 57.00000000 W  
 SFOA5[5] cps60000.4  
 SFOA5 0.500  
 SFOA5 0 Hz  
 SFO5 3.36410046 W  
 SFO2 500.1315995 MHz  
 NU2 1H  
 CPDPRG2 waltz16  
 P3 10.70 usec  
 p4 21.40 usec  
 PCPD2 80.00 usec  
 PLN2 20.00000000 W  
 PLN12 0.35778001 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7577885 MHz  
 MDN EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



Compound **34c**:

lyx-729



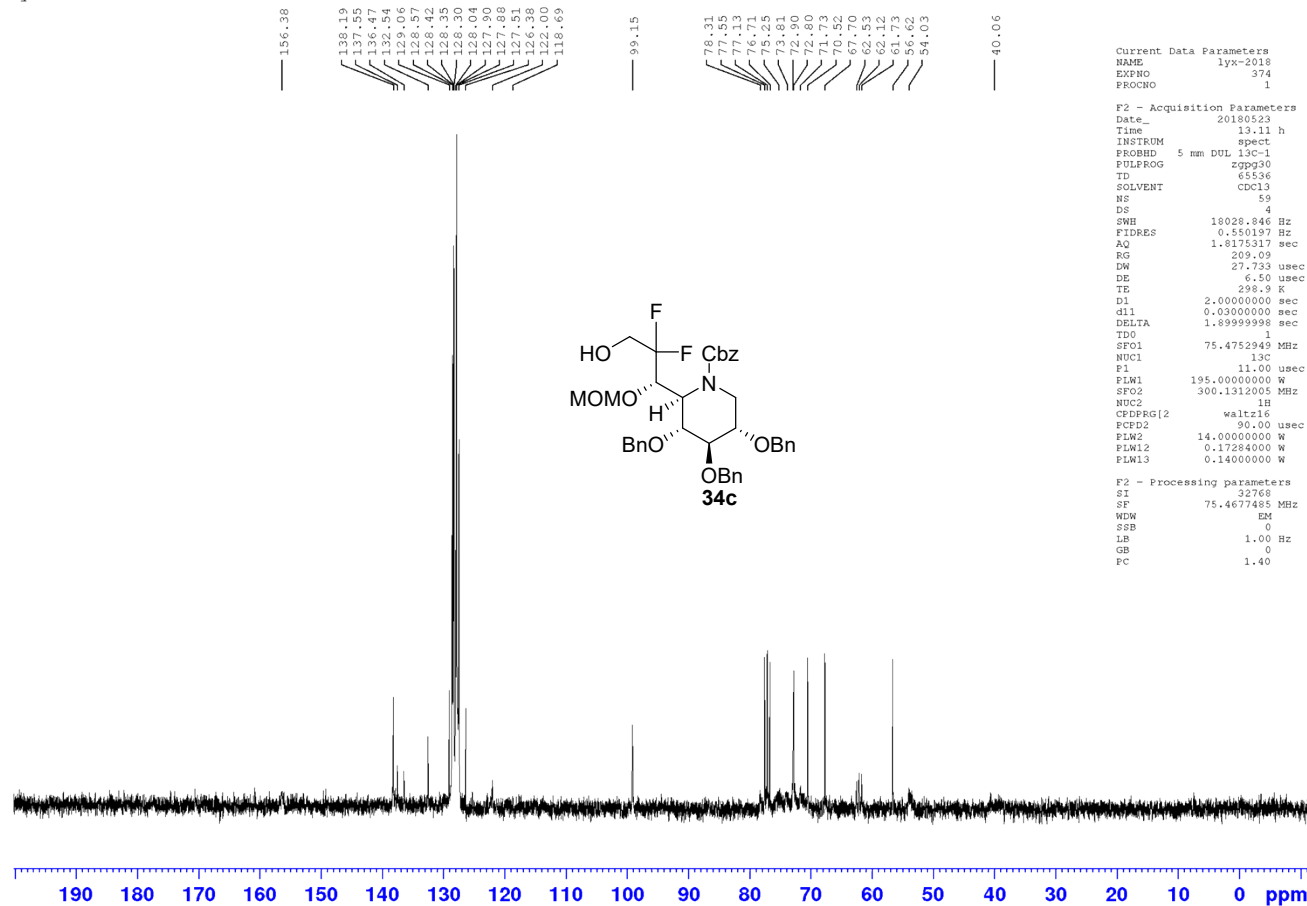
```

Current Data Parameters
NAME      500MHz-2018
EXPNO    123
PROCNO   1

F2 - Acquisition Parameters
Date_    20180531
Time     0.54 h
INSTRUM  spect
PROBHD   5 mm CFPBBO BB
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       10000.000 Hz
FIDRES    0.305176 Hz
AQ         3.2767999 sec
RG         31.72
DN         50.000 usec
DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec
D11        1
TD0        1
SFO1       500.1330885 MHz
NUC1       1H
P1         11.50 usec
PL1        20.00000000 W

F2 - Processing parameters
SI         65536
SF         500.1300494 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

lyx-729b



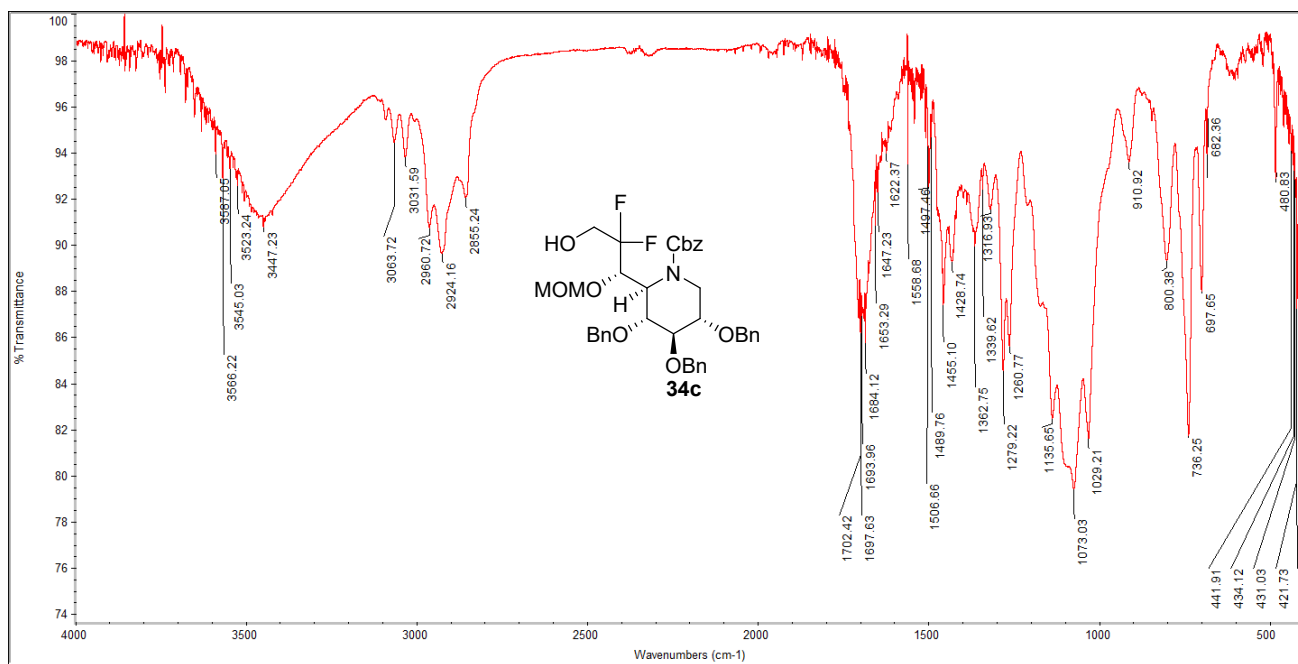
```

Current Data Parameters
NAME      lyx-2018
EXPNO    374
PROCNO   1

F2 - Acquisition Parameters
Date_    20180523
Time     13.11 h
INSTRUM  spect
PROBHD   5 mm DUL 13C-1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        59
DS        4
SWH       18028.846 Hz
FIDRES    0.550197 Hz
AQ         1.8175317 sec
RG         209.09
DN         27.733 usec
DE         6.50 usec
TE         298.9 K
D1         2.00000000 sec
d11        0.030000000 sec
DELTA     1.89999998 sec
TD0        1
SFO1       75.4752949 MHz
NUC1       13C
P1         11.00 usec
PL1        195.00000000 W
SFO2       300.1312005 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2     90.00 usec
PLM2      14.00000000 W
PLW12     0.17284000 W
PLW13     0.14000000 W

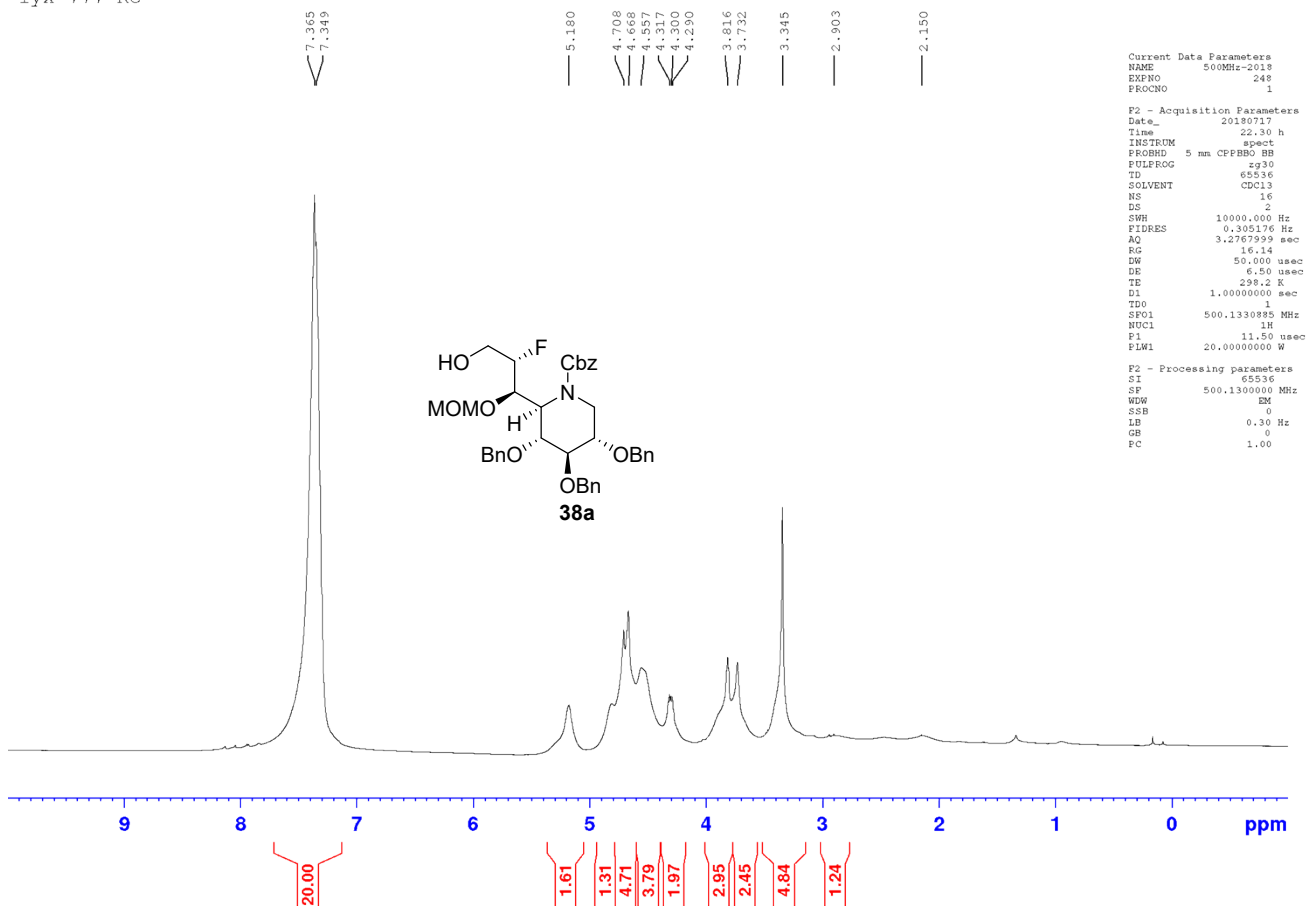
F2 - Processing parameters
SI         32768
SF         75.4677485 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```





Compound **38a**:

lyx-777-Rc

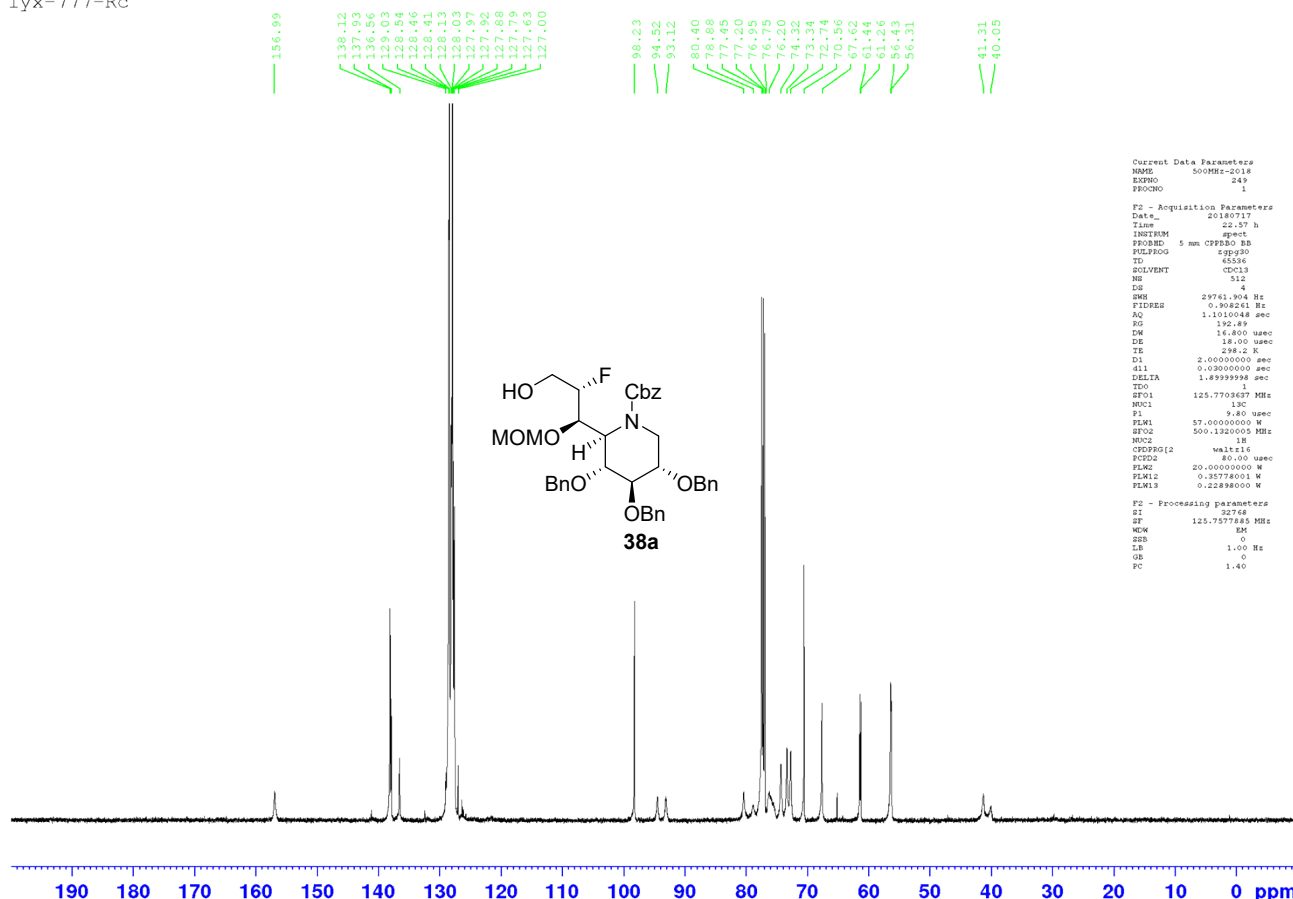


Current Data Parameters  
 NAME 500MHz-2018  
 EXPNO 248  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180717  
 Time 22.30 h  
 INSTRUM spect  
 PROBHD 5 mm CFPBBO BB  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 10000.000 Hz  
 FIDRES 0.305176 Hz  
 AQ 3.2767939 sec  
 RG 16.14  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TEO 1  
 SFO1 500.1330885 MHz  
 NUCL1 1H  
 P1 11.50 usec  
 PLW1 20.00000000 W

F2 - Processing parameters  
 SI 55536  
 SP 500.1300000 MHz  
 WW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

lyx-777-Rc

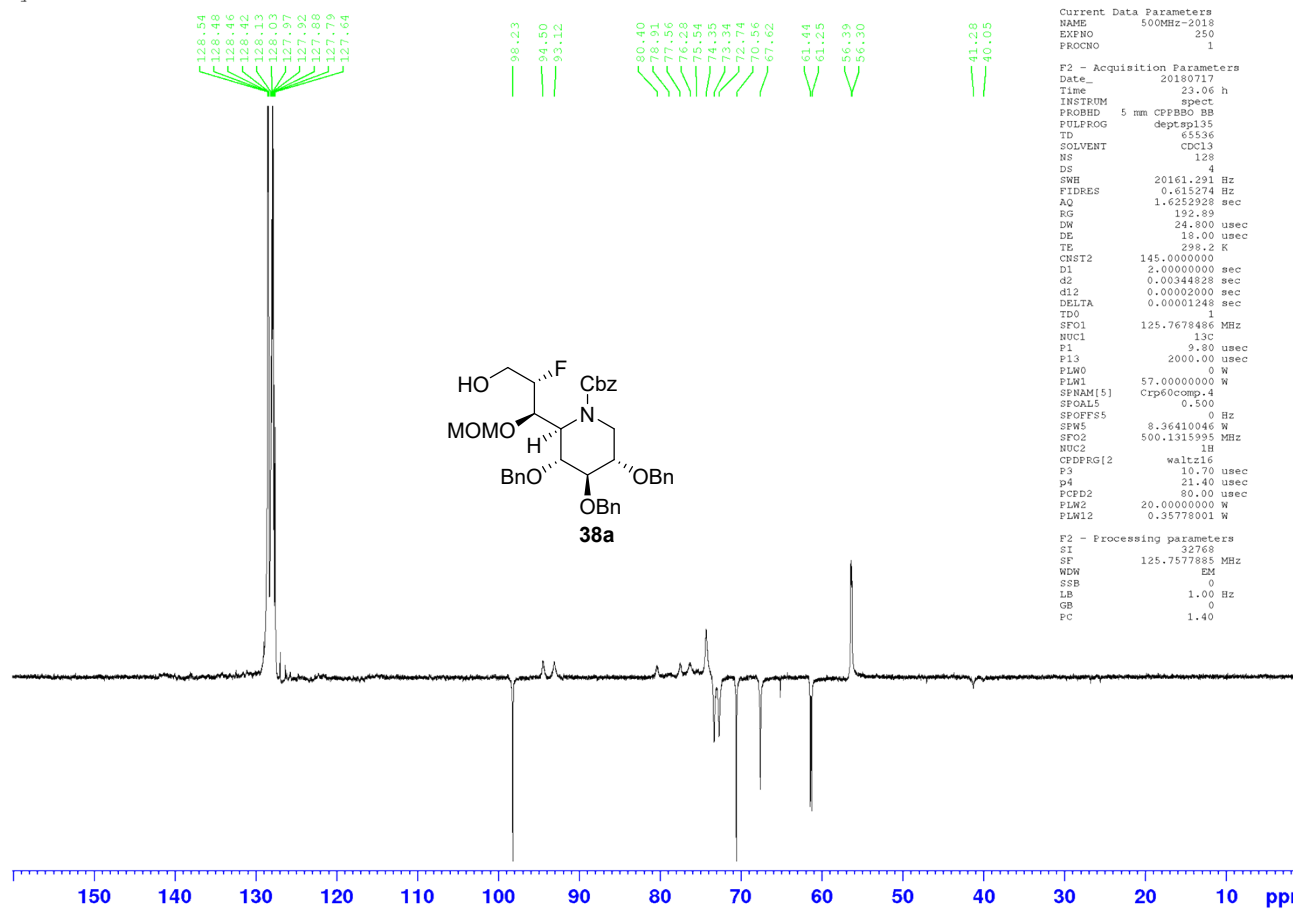


Current Data Parameters  
 NAME 500MHz-2018  
 EXPNO 249  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180717  
 Time 22:57 h  
 INSTRUM spect  
 FREQHED 5 mm CPBBO BB  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 12  
 DS 4  
 SWH 29741.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 1.1010048 sec  
 RG 192.89  
 DW 24.800 usec  
 DE 18.00 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 d11 0.00000000 sec  
 DELTA 1.89999994 sec  
 TDO 1  
 SFO1 125.770367 MHz  
 NUC1 13C  
 P1 9.80 usec  
 PL1 0.00000000 W  
 SFO2 500.1320005 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 P3 10.70 usec  
 PLM2 20.00000000 W  
 PLM12 0.35778001 W  
 PLM13 0.22888000 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7577885 MHz  
 EM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

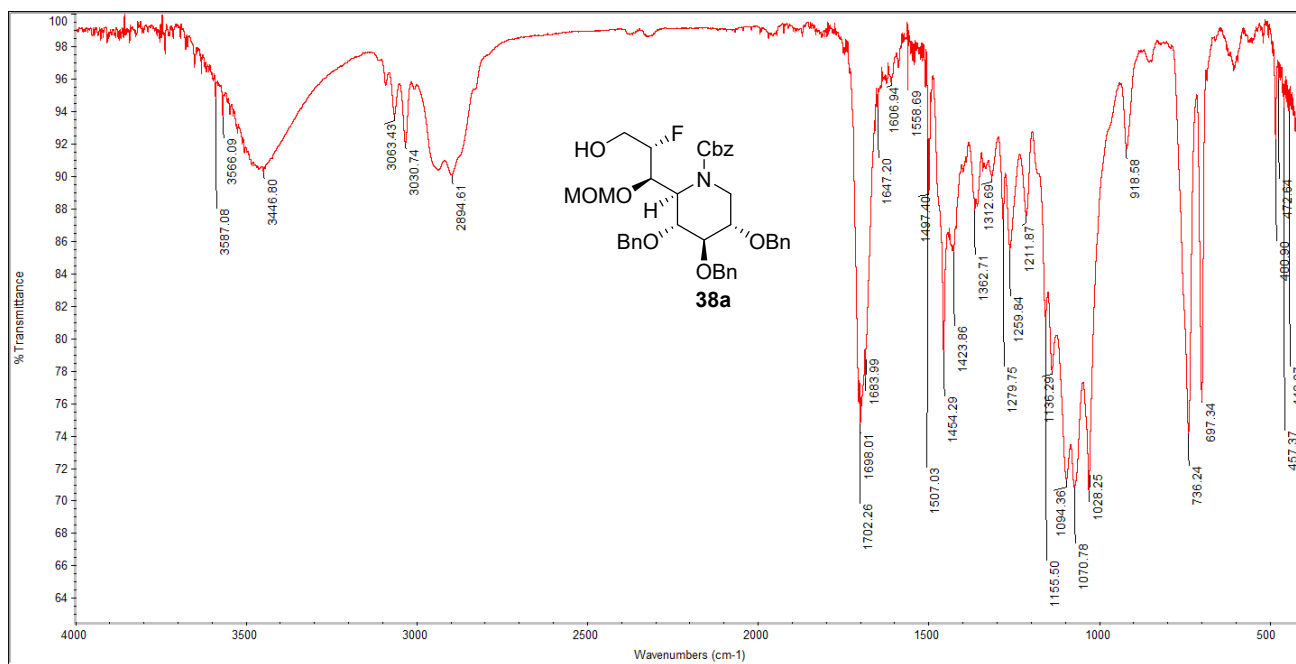
lyx-777-Rc



Current Data Parameters  
 NAME 500MHz-2018  
 EXPNO 250  
 PROCNO 1

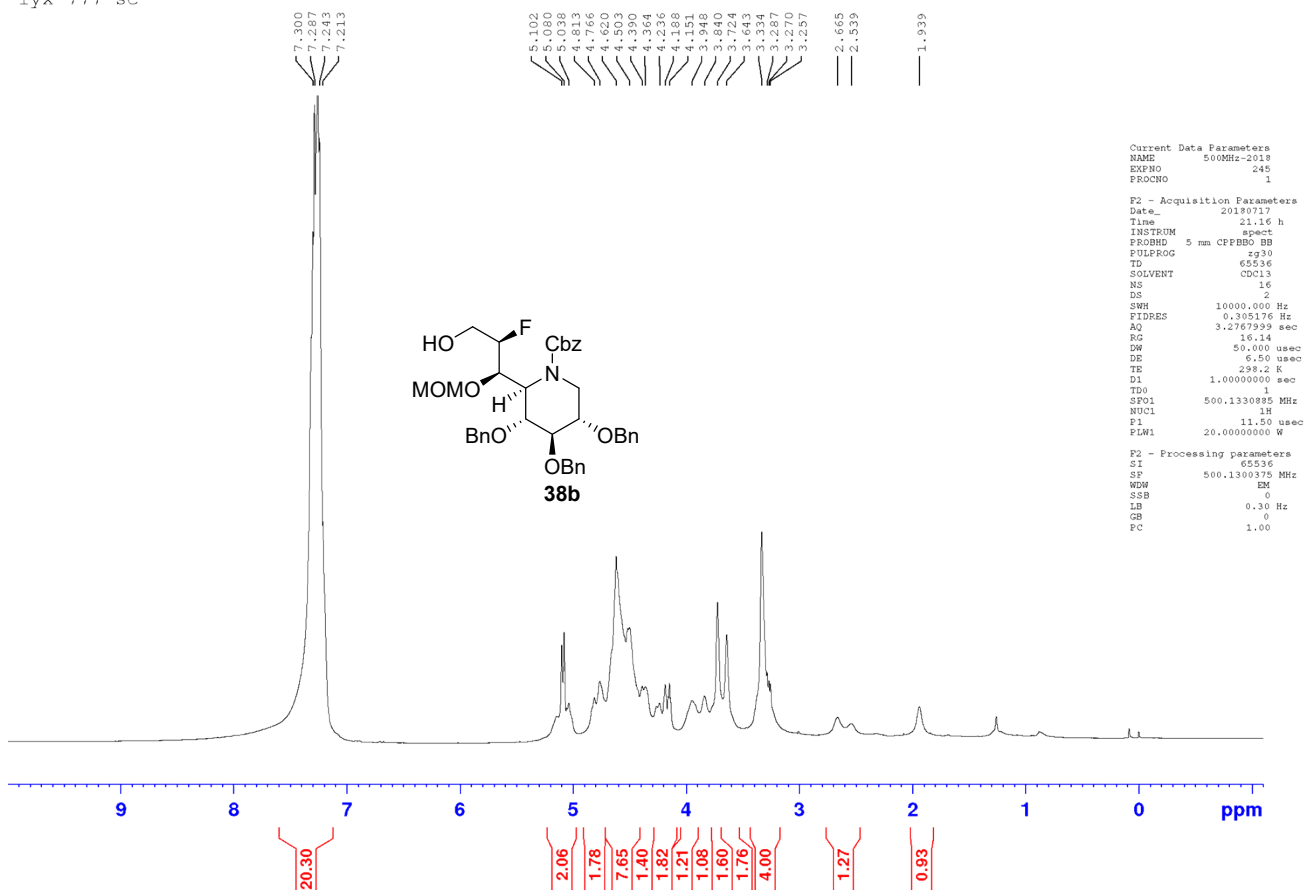
F2 - Acquisition Parameters  
 Date\_ 20180717  
 Time 23:06 h  
 INSTRUM spect  
 FREQHED 5 mm CPBBO BB  
 PULPROG deptspl35  
 TD 65536  
 SOLVENT CDCl3  
 NS 128  
 DS 4  
 SWH 20161.291 Hz  
 FIDRES 0.615274 Hz  
 AQ 1.6252928 sec  
 RG 192.89  
 DW 24.800 usec  
 DE 18.00 usec  
 TE 298.2 K  
 CNST2 145.00000000 sec  
 d1 0.00344828 sec  
 d2 0.00002000 sec  
 d12 0.00002000 sec  
 DELTA 0.00001248 sec  
 TDO 1  
 SFO1 125.7678486 MHz  
 NUC1 13C  
 P1 9.80 usec  
 PL1 0.00000000 W  
 SFO2 500.1315995 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 P3 10.70 usec  
 PLM2 20.00000000 W  
 PLM12 0.35778001 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7577885 MHz  
 EM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

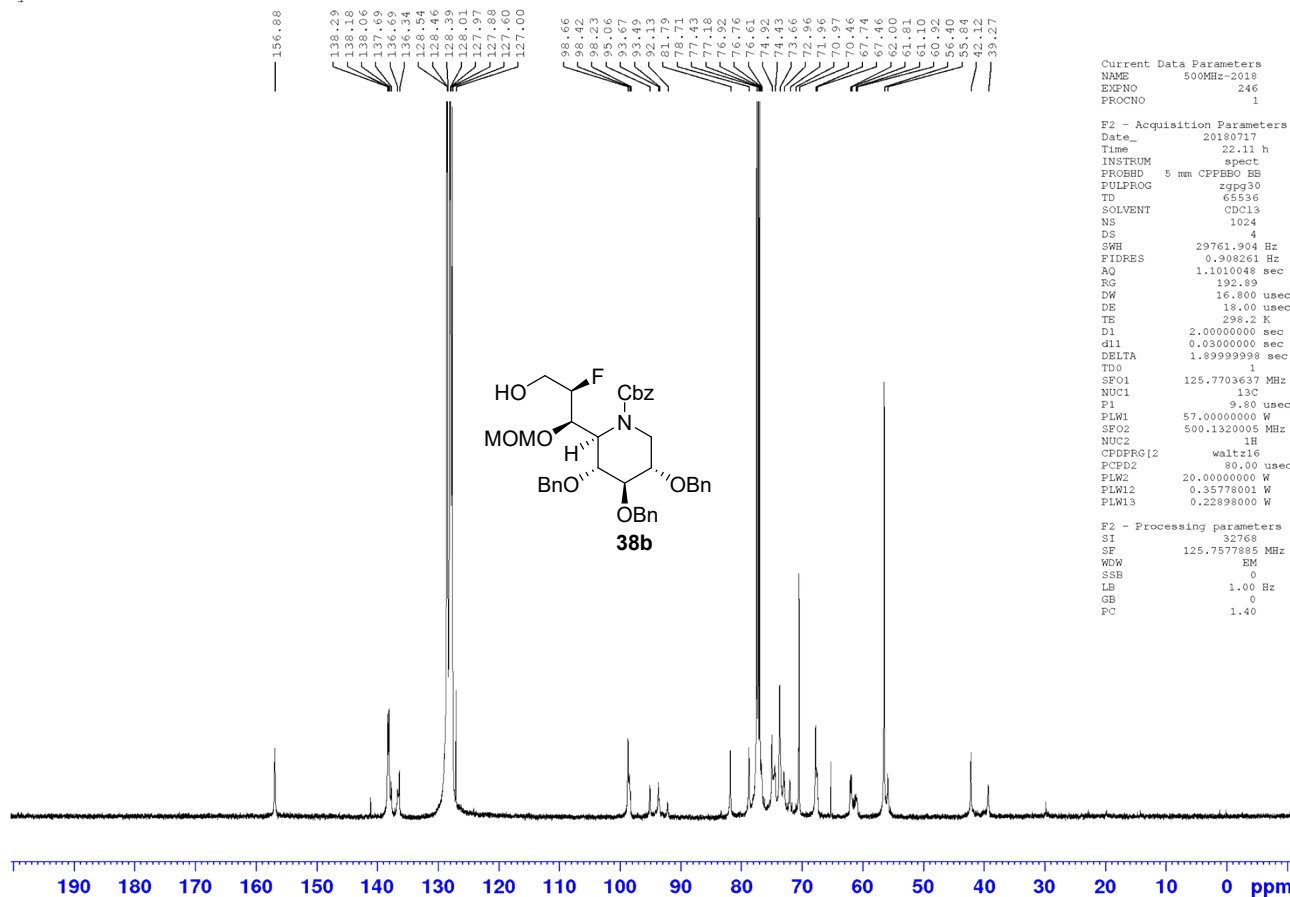


**Compound 38b:**

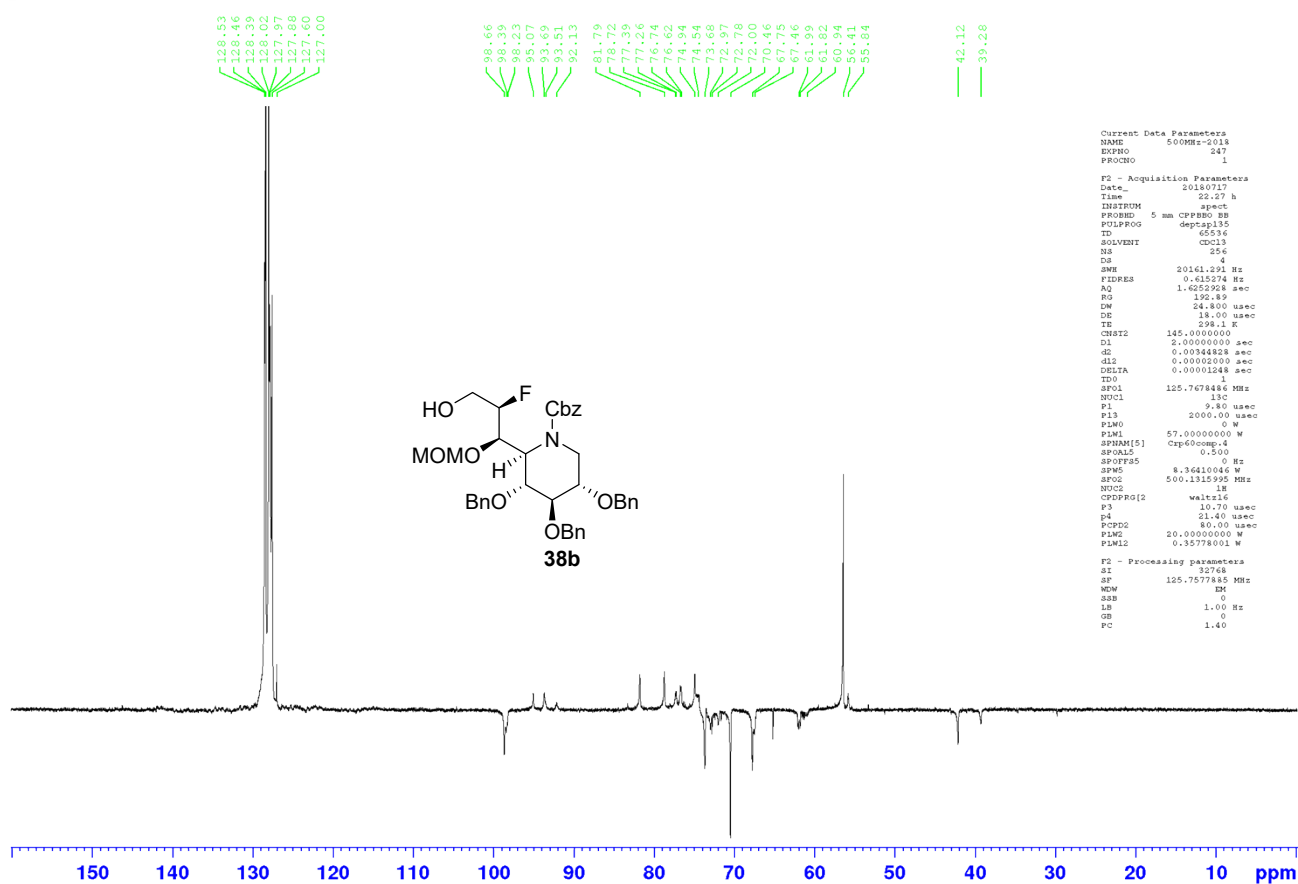
lyx-777-sc

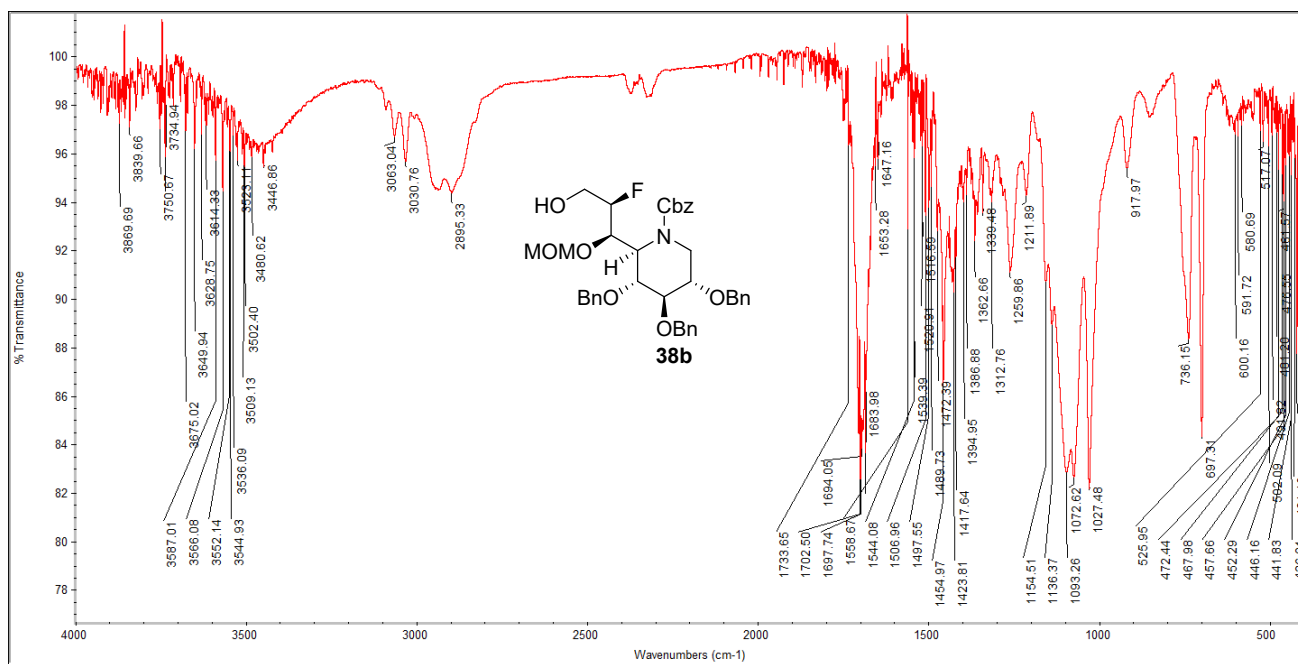


lyx-777-sc



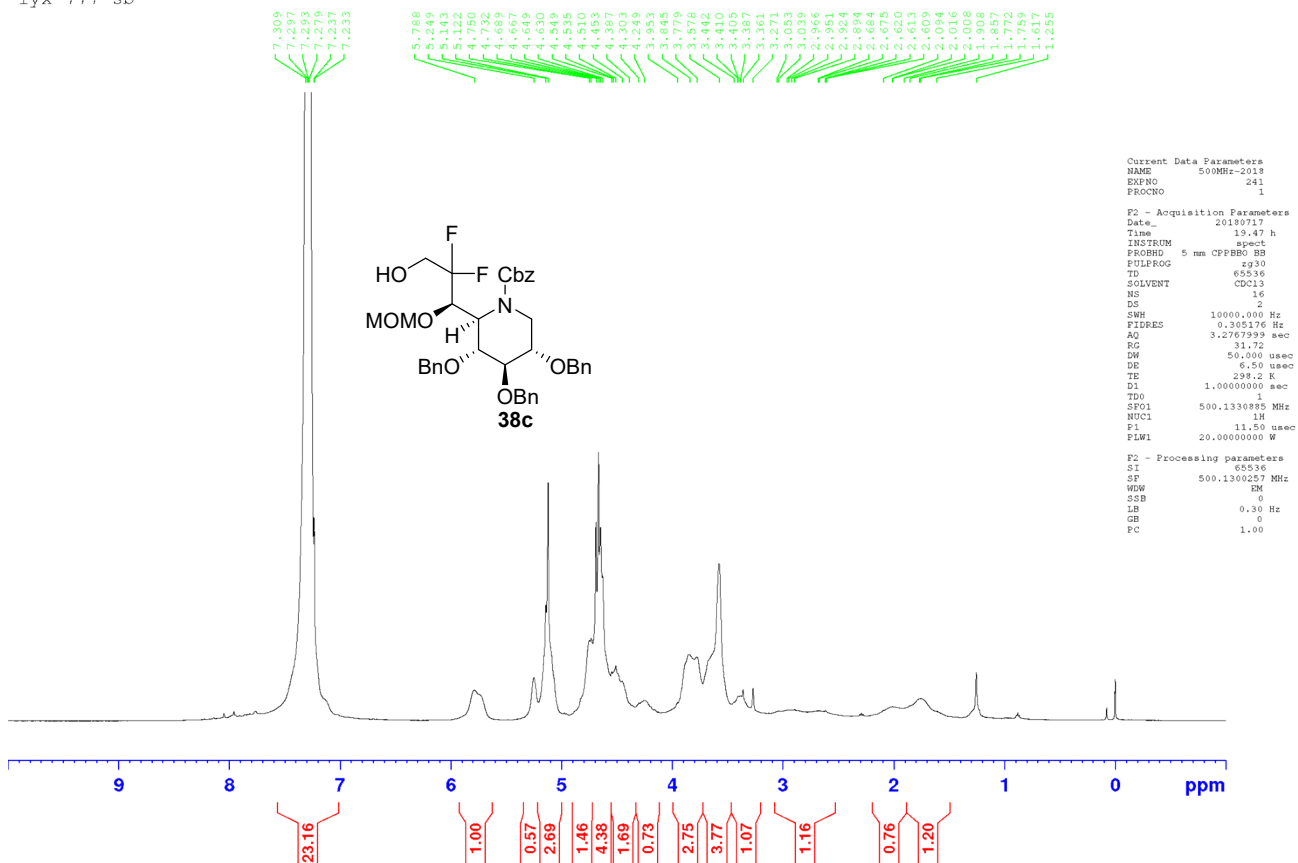
lyx-777-sc



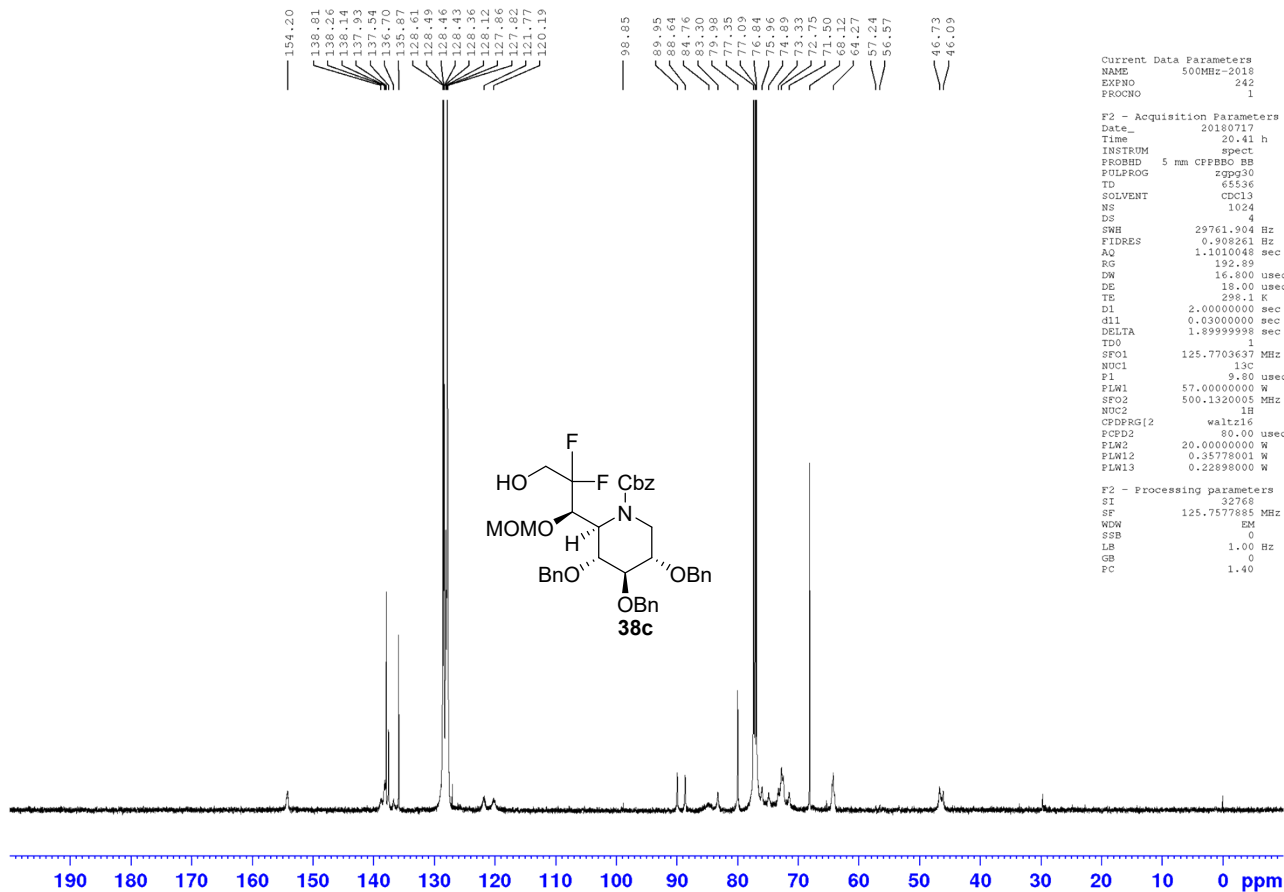


Compound 38c:

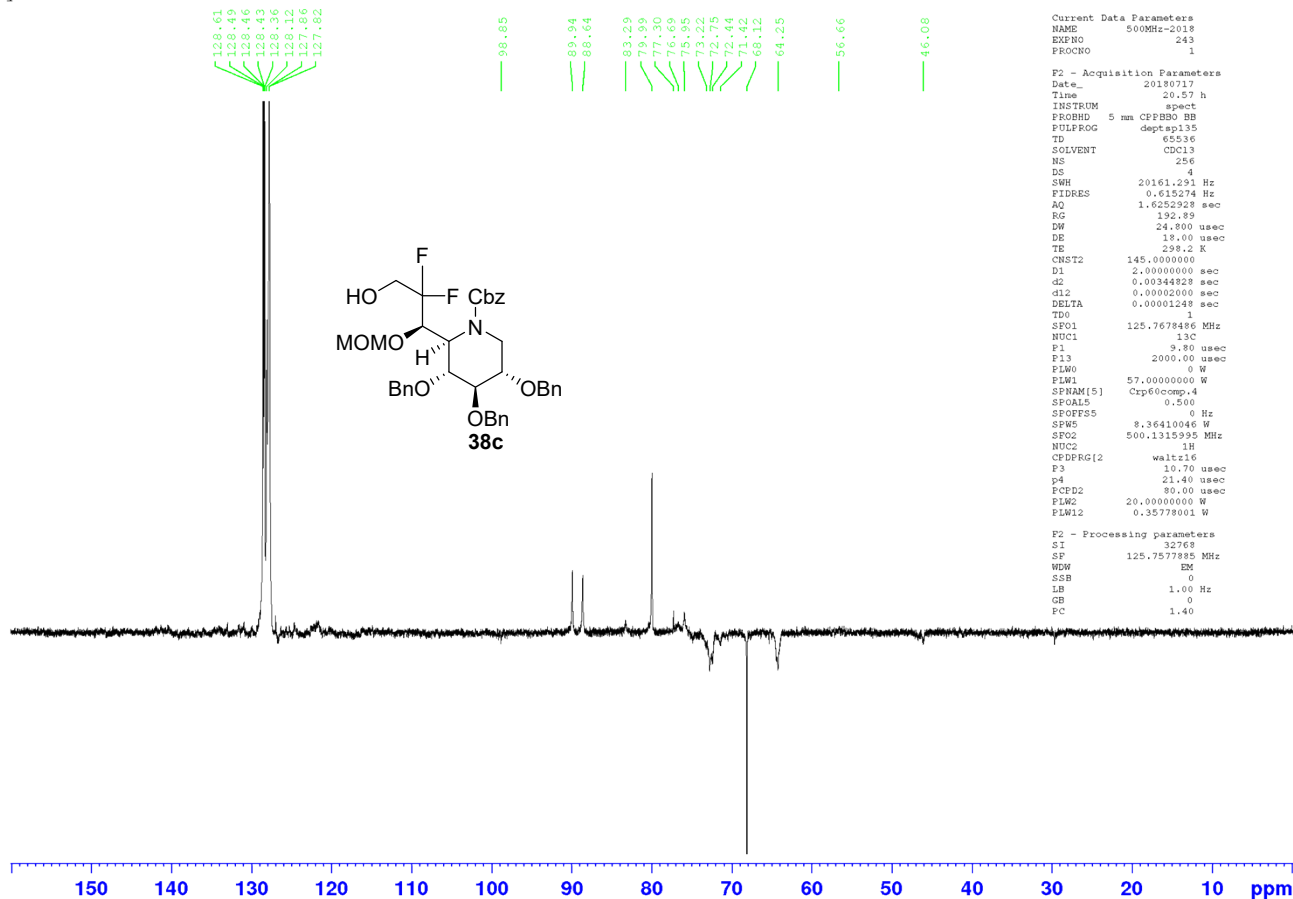
lyx-777-sb

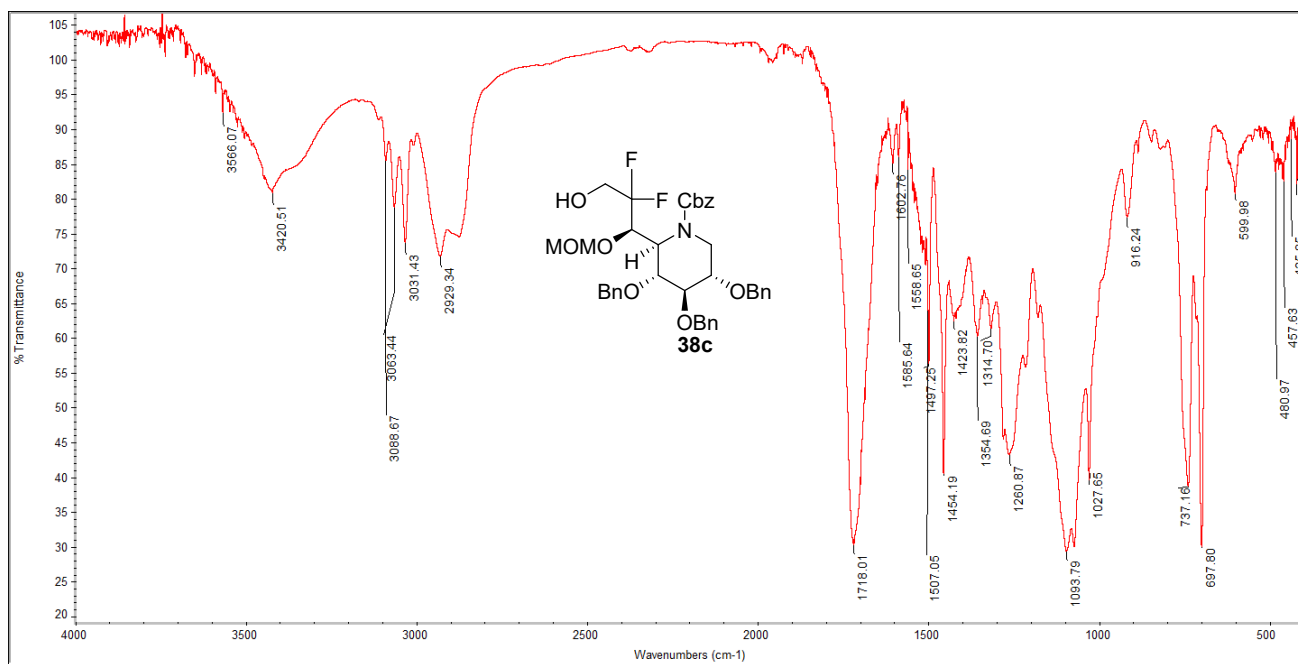


lyx-777-sb



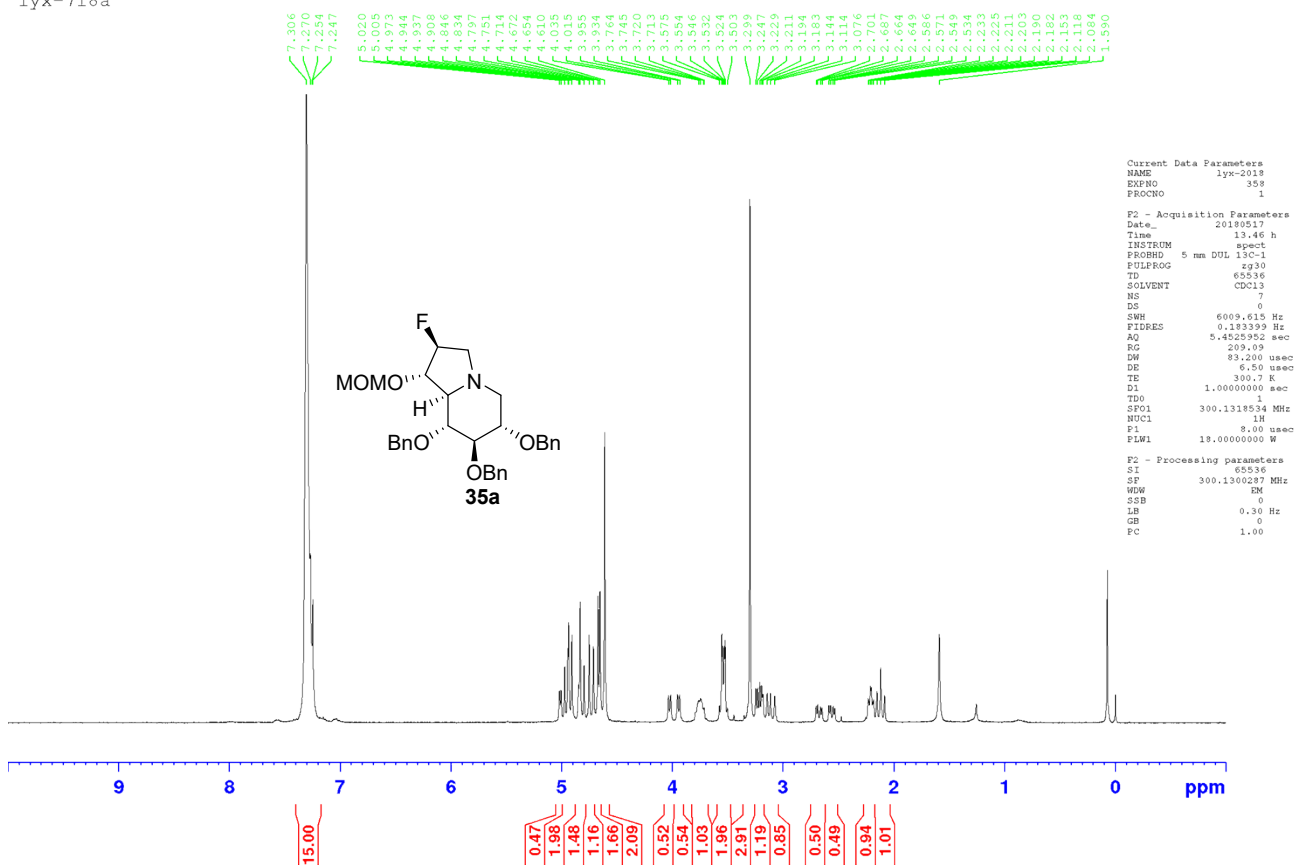
lyx-777-sb





Compound 35a:

lyx-718a



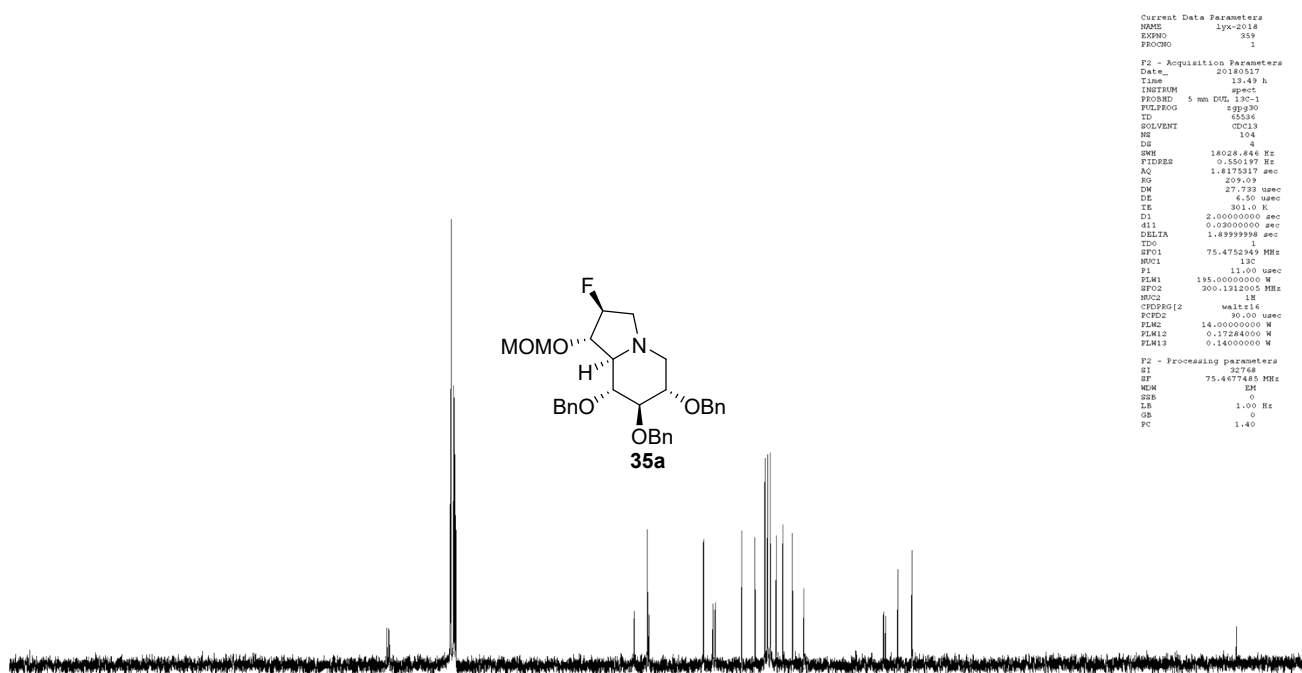
Current Data Parameters  
 NAME lyx-2018  
 EXPNO 359  
 FREQNO 1

F2 - Acquisition Parameters  
 Date\_ 20180917  
 Time 13.46 h  
 INSTRUM spect  
 PROBHD 5 mm DUL 150-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 7  
 DS 0  
 SWH 6009.618 Hz  
 FIDRES 0.183399 Hz  
 AQ 5.4522852 sec  
 RG 209.09  
 DM 83.200 usec  
 DE 6.50 usec  
 TE 300.7 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 300.1318534 MHz  
 NUC1 1H  
 P1 8.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1300287 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

lyx-718a

- 138.77
- 138.48
- 138.37
- 128.45
- 128.35
- 127.95
- 127.82
- 127.72
- 127.65
- 127.54
- 98.69
- 96.53
- 96.26
- 87.43
- 85.90
- 85.53
- 81.23
- 77.46
- 77.04
- 76.61
- 75.66
- 74.58
- 73.01
- 71.14
- 58.24
- 57.93
- 55.93
- 53.63

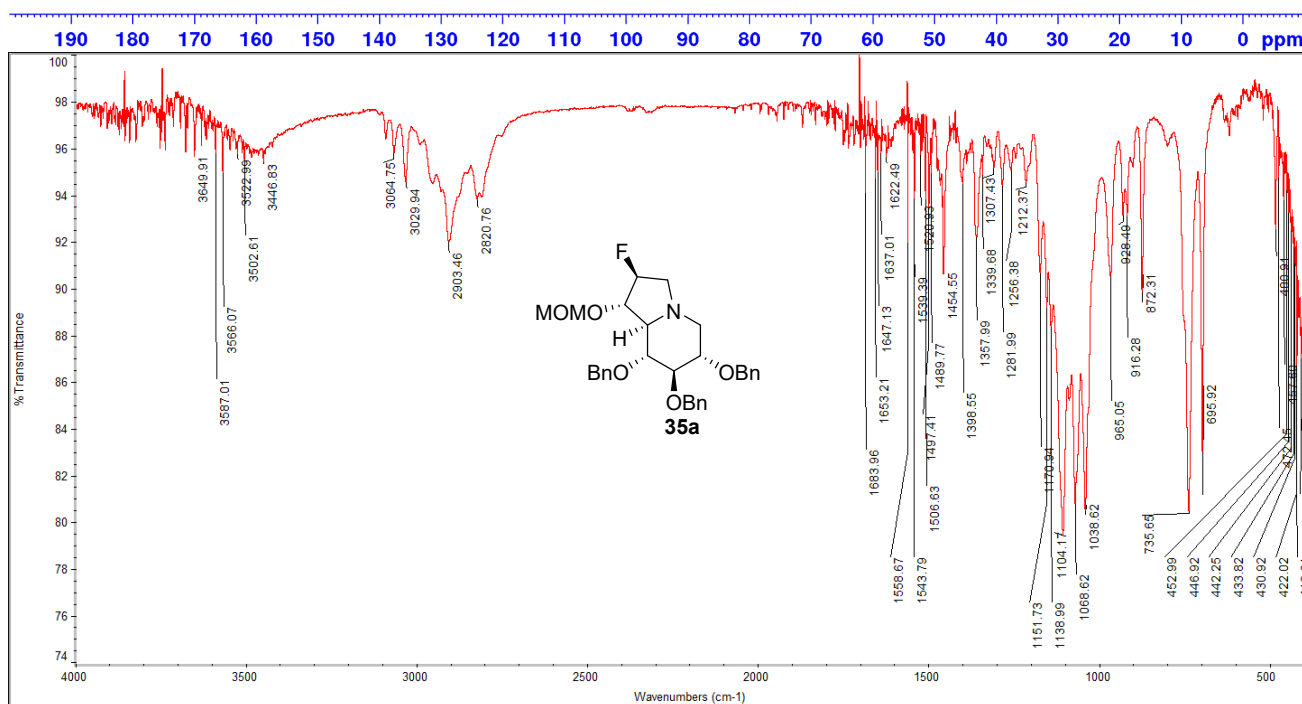


```

Current Data Parameters
NAME      lyx-0218
EXPNO    359
PROCNO   1

F2 - Acquisition Parameters
Date_    20180517
Time     13:49 h
INSTRUM  spect
PROBHD   5 mm DML 13C-1
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        104
DE        1.010 Hz
FIDRES   18028.446 Hz
AQ        0.550197 sec
RG        1.4175317 sec
RG        209.09
DM        27.733 usec
DE        6.50 usec
TE        301.0 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA     1.87999998 sec
TD0        1
SFO1      75.4752449 MHz
NUC1       13C
F1         11.50 usec
PLM1      195.0000000 W
SFO2      300.1312005 MHz
NUC2       1H
CFDP2G2  wait116
PCPD      30.00 usec
PLM2      14.0000000 W
PLM12     0.1728400 W
PLM13     0.1400000 W

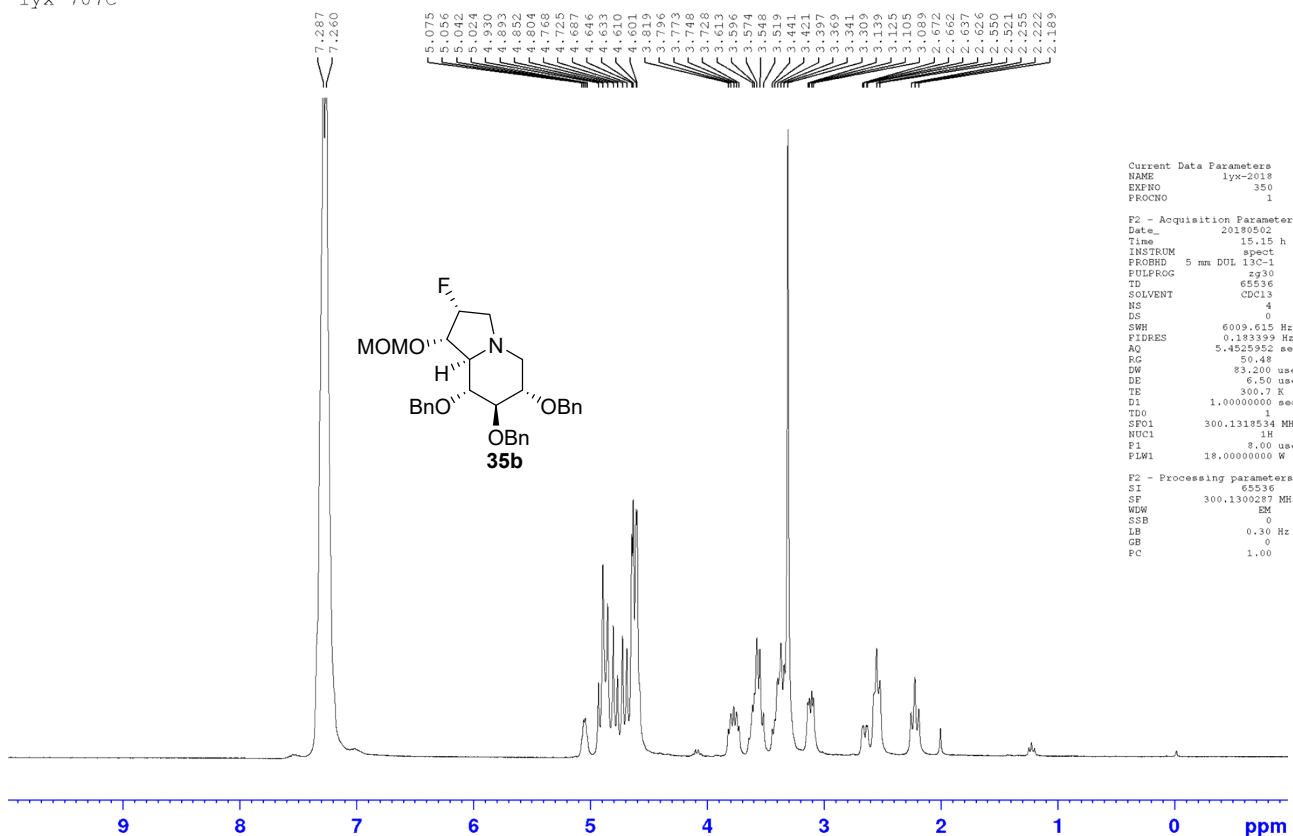
F2 - Processing parameters
SI         32768
SF         75.4677445 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```



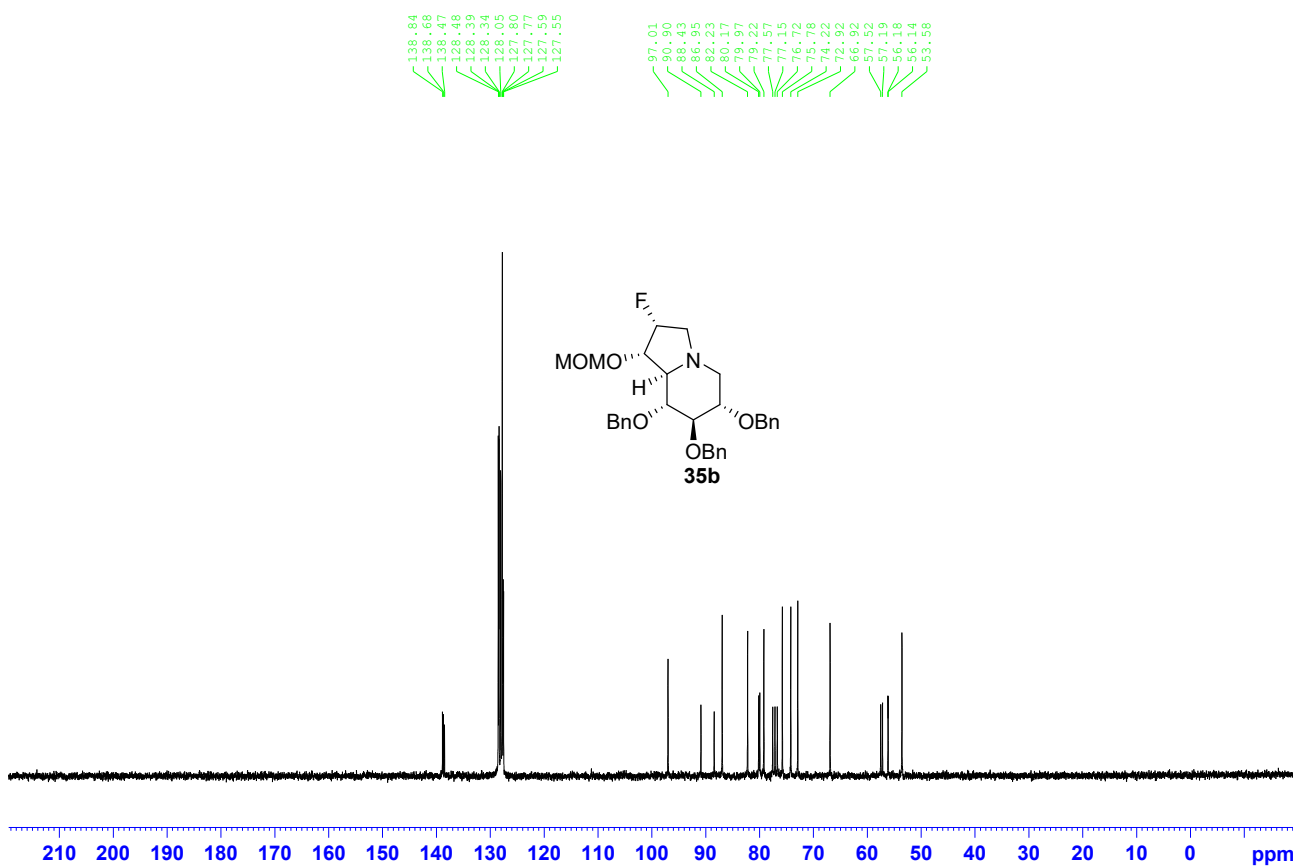


Compound **35b**:

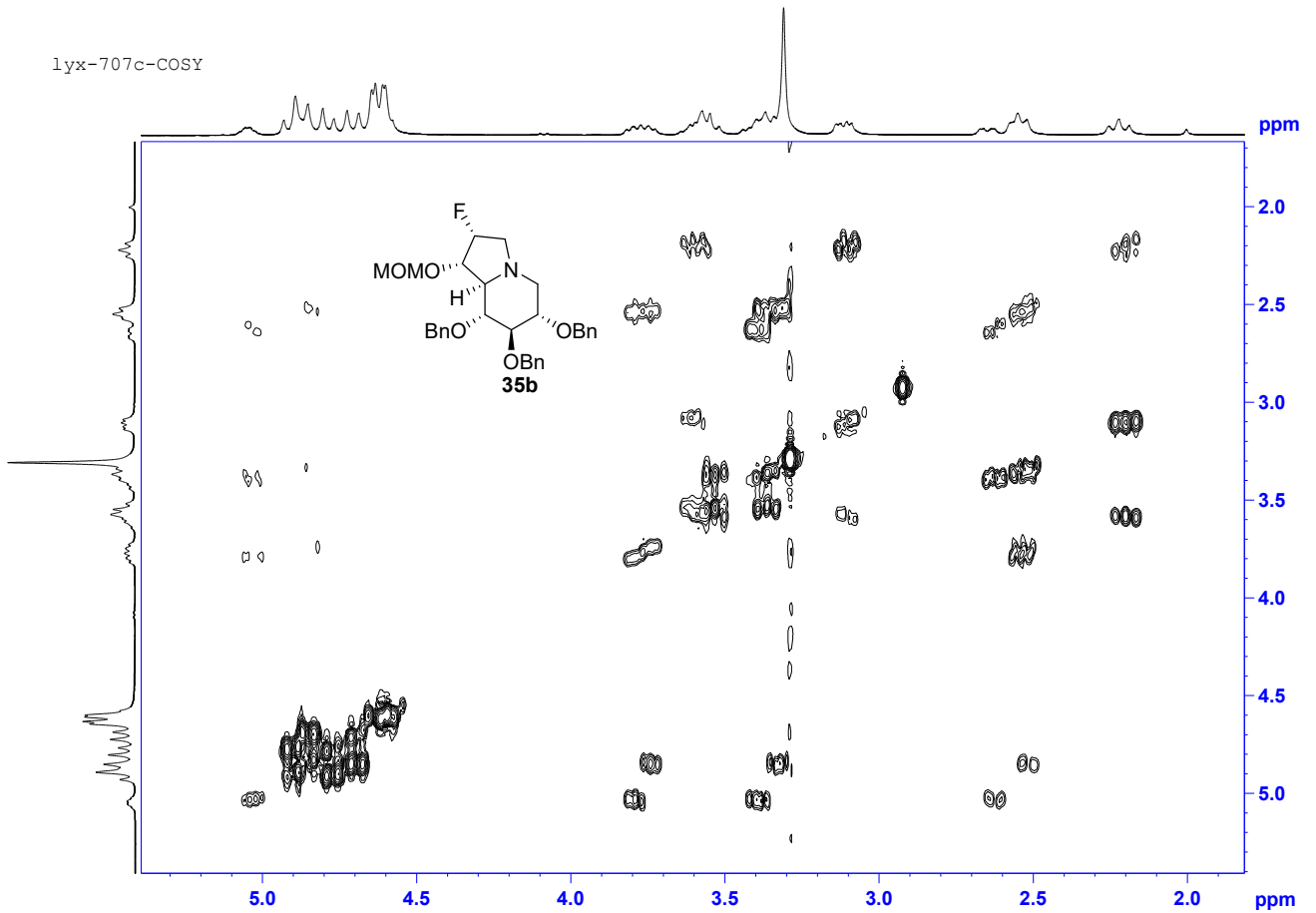
lyx-707c



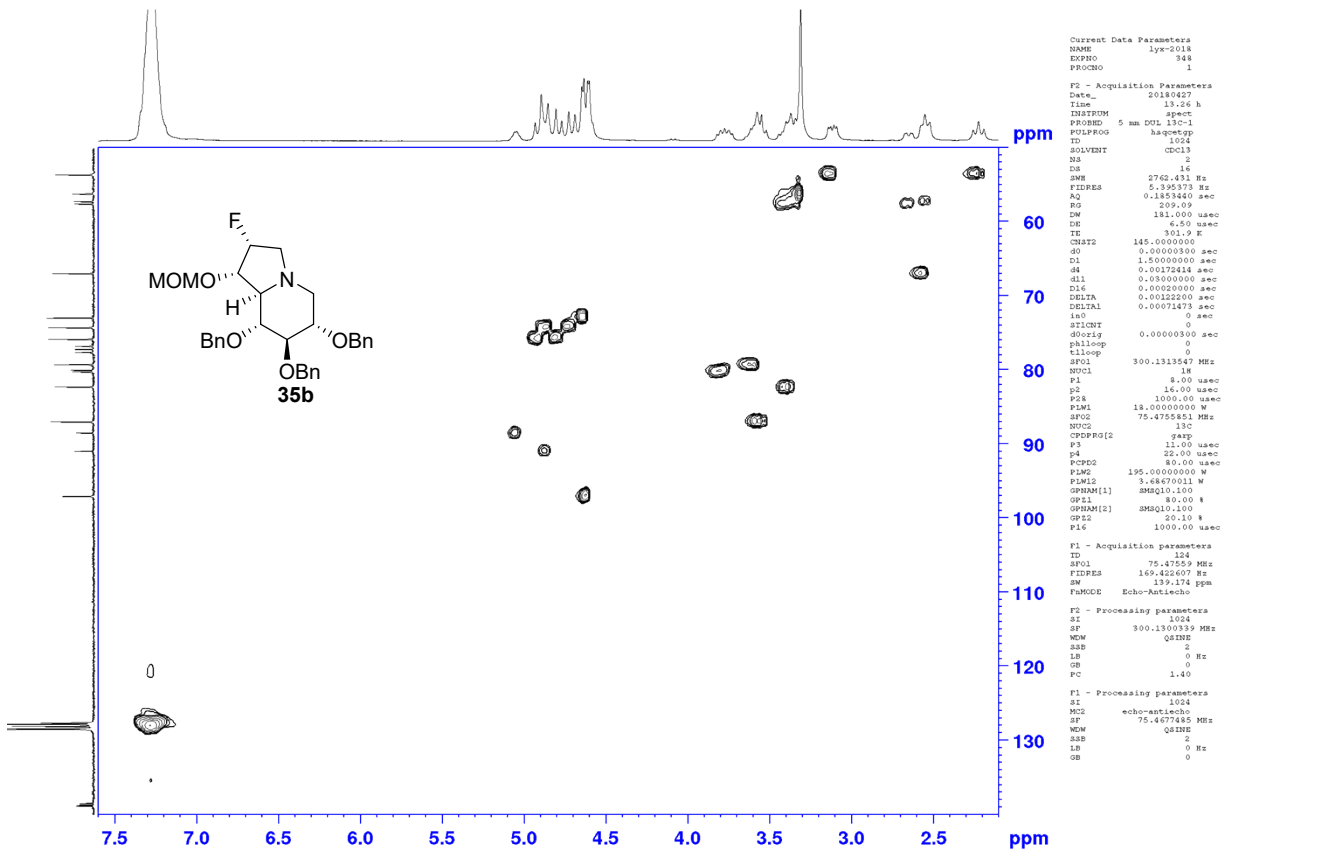
lyx-707c



lyx-707c-COSY



707c-HSQCETGP



```

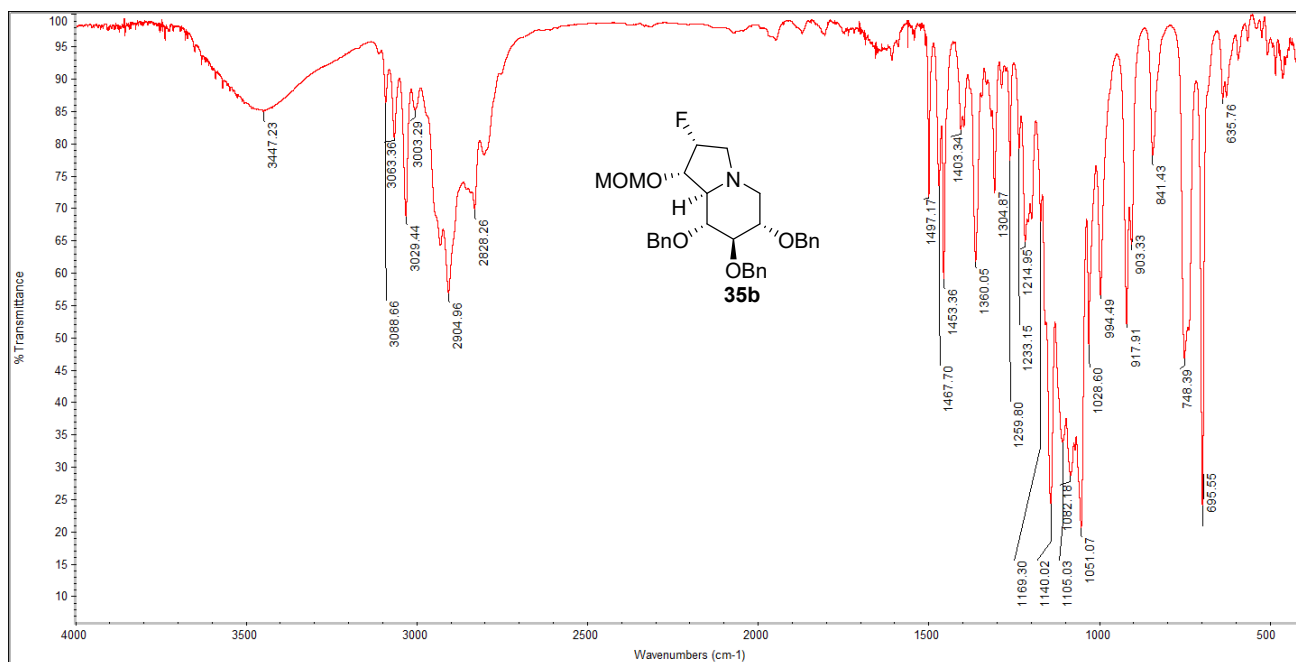
Current Data Parameters
NAME lyx-2018
EXPNO 344
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180427
Time 13:16 h
INSTRUM spect
PROBHD 5 mm DOL 13C-1
PULPROG zgpg30
TD 1024
SOLVENT h2o
NS 2
DS 4
SWH 2762.431 Hz
FIDRES 0.0000330 sec
AQ 0.1833400 sec
RG 209.09
CW 181.000 usec
DE 6.50 usec
TE 301.2 K
CNS12 145.0000000
D0 0.0000330 sec
D1 1.0000000 usec
d4 0.00172414 usec
d11 0.000000000 usec
D16 0.000200000 usec
DELTA 0.00222000 usec
DELTA1 0.00071473 usec
lno 0 usec
SFO1 300.1330597 MHz
SFO2 75.47559 MHz
P1 8.00 usec
P2 16.00 usec
P3 11.00 usec
P4 52.00 usec
PCPD2 195.0000000 W
PLM12 3.68670011 W
SFO1M1 300.1330597 MHz
SFO1M2 75.47559 MHz
SFO2M1 150.2661194 MHz
SFO2M2 75.47559 MHz
P16 1000.00 usec

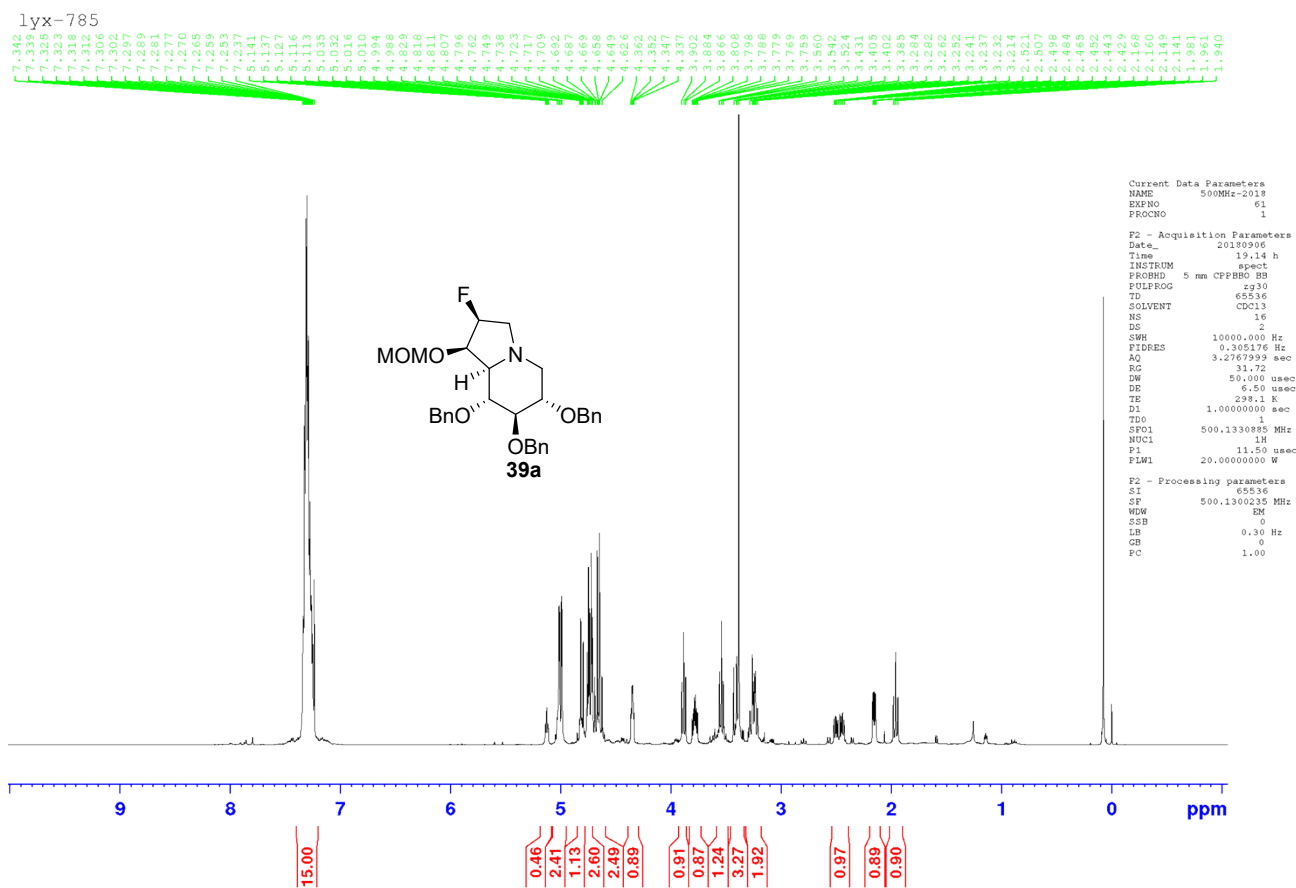
F1 - Acquisition parameters
ID 1024
SFO1 75.47559 MHz
FIDRES 169.422607 Hz
SW 139.174 ppm
PaMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 300.1300339 MHz
WDW QSHINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
WDW echo-antlecho
SF 75.4677485 MHz
WDW QSHINE
SSB 2
LB 0 Hz
GB 0
PC 1.40
    
```



Compound 39a:



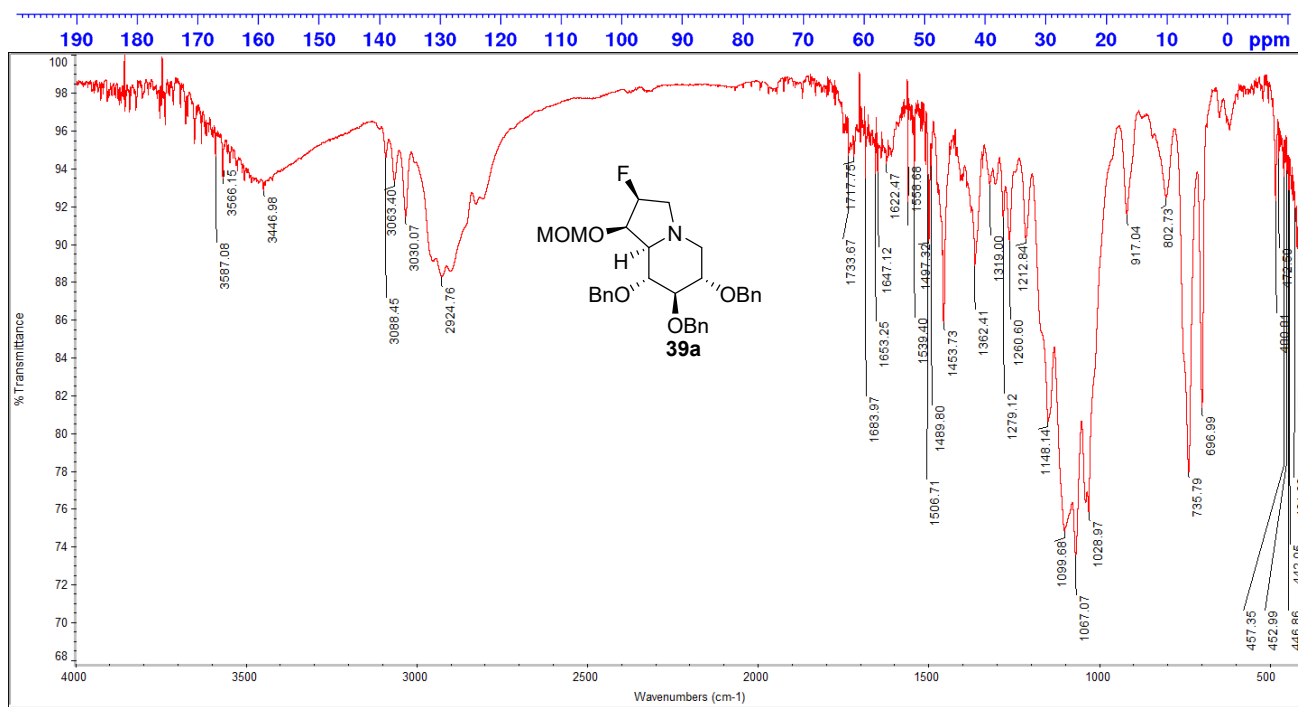
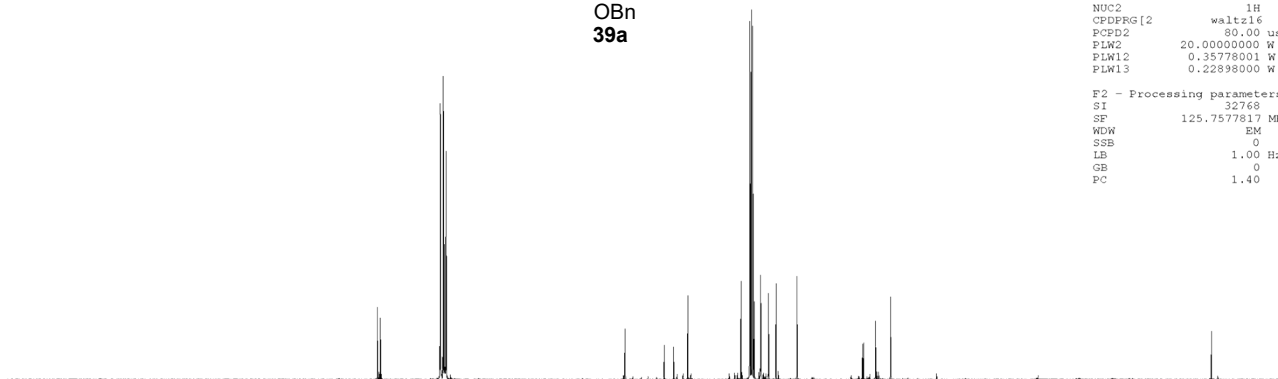
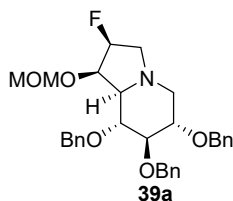
138.92  
138.91  
138.38  
128.60  
128.47  
128.47  
128.44  
128.03  
127.98  
127.97  
127.86  
127.83  
127.61  
127.50

97.99  
97.95  
91.49  
89.96  
87.61  
78.83  
77.40  
77.39  
76.89  
76.61  
75.61  
75.57  
75.50  
74.30  
73.03  
69.59  
58.56  
56.62  
56.60  
54.13

Current Data Parameters  
NAME 500MHz-2018  
EXPNO 62  
PROCNO 1

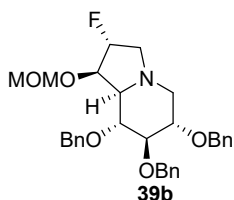
F2 - Acquisition Parameters  
Date\_ 20180906  
Time 19.41 h  
INSTRUM spect  
PROBHD 5 mm CFPBBO BB  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 512  
DS 4  
SWH 29761.904 Hz  
FIDRES 0.908261 Hz  
AQ 1.1010048 sec  
RG 192.89  
DW 16.800 usec  
DE 18.00 usec  
TE 298.1 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.89999998 sec  
TD0 1  
SF01 125.7703637 MHz  
NUC1 13C  
P1 9.80 usec  
PLW1 57.0000000 W  
SF02 500.1320005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 80.00 usec  
PLW2 20.0000000 W  
PLW12 0.35778001 W  
PLW13 0.22898000 W

F2 - Processing parameters  
SI 32768  
SF 125.7577817 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Compound **39b**:

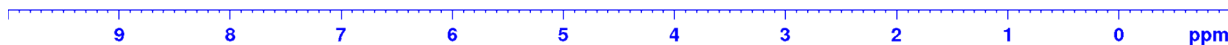
lyx-784



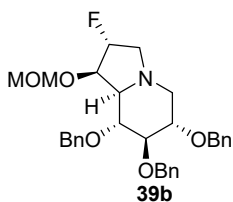
Current Data Parameters  
 NAME 400MHz-2019  
 EXPNO 22  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20191024  
 Time 8.36 h  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.489064 Hz  
 AQ 2.044723 sec  
 RG 39.92  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 TD 1  
 SFO1 400.2424716 MHz  
 NUC1 1H  
 P1 14.30 usec  
 PLW1 12.0000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2400000 MHz  
 WDW EM  
 SSB 0  
 LB 0.38 Hz  
 GB 0  
 PC 1.00



lyx-784



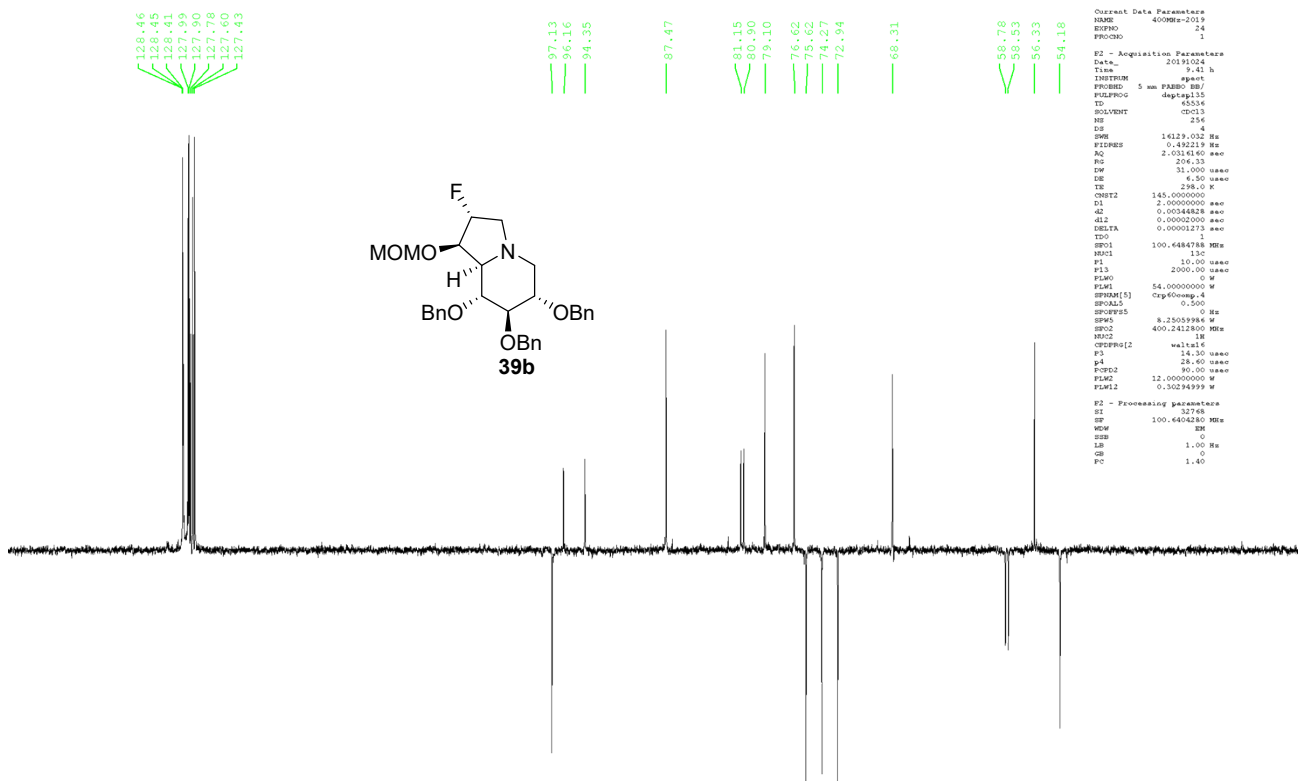
Current Data Parameters  
 NAME 400MHz-2019  
 EXPNO 22  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20191024  
 Time 8.36 h  
 INSTRUM spect  
 PROBRD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.753596 Hz  
 AQ 1.3631488 sec  
 RG 250.00  
 DW 20.800 usec  
 DE 4.50 usec  
 TE 298.0 K  
 D1 2.00000000 sec  
 d11 10.00 usec  
 DELTA 1.89999998 sec  
 TD 1  
 SFO1 100.6504916 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 54.0000000 W  
 SFO2 400.2416010 MHz  
 NUC2 1H  
 DELTAP2 10.00 usec  
 PLW2 12.0000000 W  
 PLW3 0.20294999 W  
 PLW4 0.24539000 W

F2 - Processing parameters  
 SI 26768  
 SF 100.6404280 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

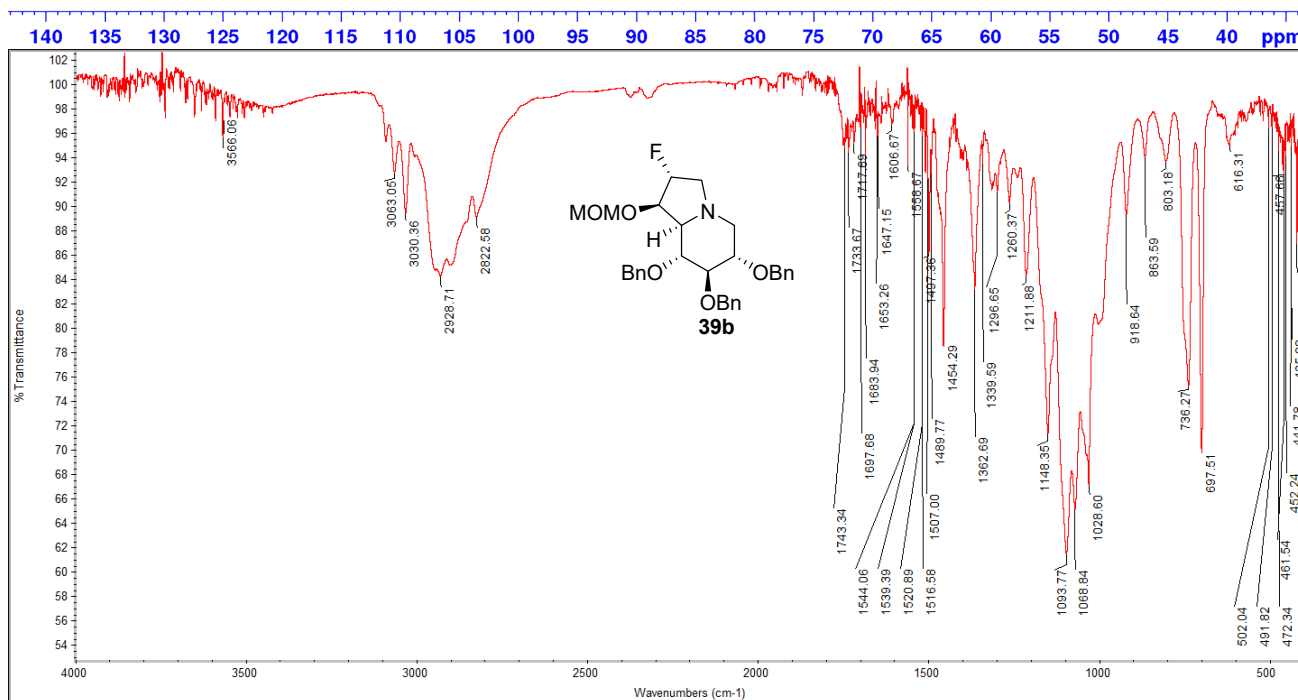


lyx-784



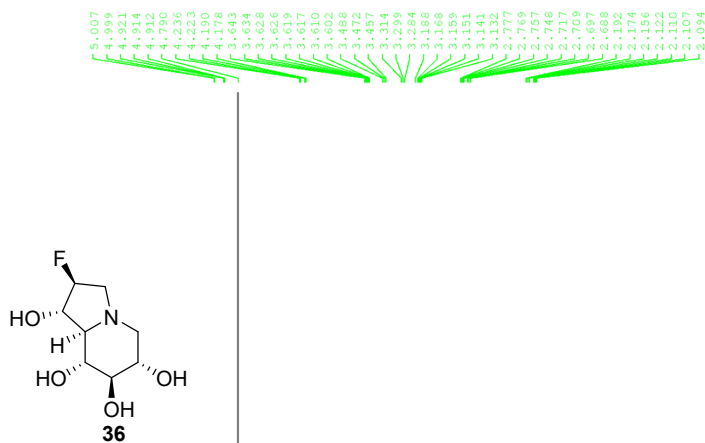
```

Current Data Parameters
NAME      400MHz-1019
EXPNO    1
PROCNO    1
Date_     20151024
Time      9:41
INSTRUM   spect
PROBHD    5 mm F4BBO BB7
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         4
SWH        16122.032 Hz
FIDRES     0.4822338 Hz
AQ         2.0314140 sec
RG         254.33
DW         31.05000000 sec
DE         4.50000000 sec
TE         298.0 K
CQ1P2     145.00000000
D1         2.0000000000 sec
d2         0.003484828 sec
d12        0.0000200000 sec
DELTA     0.000012133 sec
TDO        1
SFO1       100.6484748 MHz
HFO1       13C
F13        101.00000000 sec
P13        2000.00000000 sec
PL13       0
PL14       0
PL15       0
PL16       0
PL17       0
PL18       0
PL19       0
PL20       0
PL21       0
PL22       0
PL23       0
PL24       0
PL25       0
PL26       0
PL27       0
PL28       0
PL29       0
PL30       0
PL31       0
PL32       0
PL33       0
PL34       0
PL35       0
PL36       0
PL37       0
PL38       0
PL39       0
PL40       0
PL41       0
PL42       0
PL43       0
PL44       0
PL45       0
PL46       0
PL47       0
PL48       0
PL49       0
PL50       0
PL51       0
PL52       0
PL53       0
PL54       0
PL55       0
PL56       0
PL57       0
PL58       0
PL59       0
PL60       0
PL61       0
PL62       0
PL63       0
PL64       0
PL65       0
PL66       0
PL67       0
PL68       0
PL69       0
PL70       0
PL71       0
PL72       0
PL73       0
PL74       0
PL75       0
PL76       0
PL77       0
PL78       0
PL79       0
PL80       0
PL81       0
PL82       0
PL83       0
PL84       0
PL85       0
PL86       0
PL87       0
PL88       0
PL89       0
PL90       0
PL91       0
PL92       0
PL93       0
PL94       0
PL95       0
PL96       0
PL97       0
PL98       0
PL99       0
PL100      0
P2 - Processing parameters
SI         32768
SF         100.6484748 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



Compound 36:

<sup>1</sup>H NMR  
lyx-733



```

Current Data Parameters
NAME NOE-2018
EXPNO 29
PROCNO 1

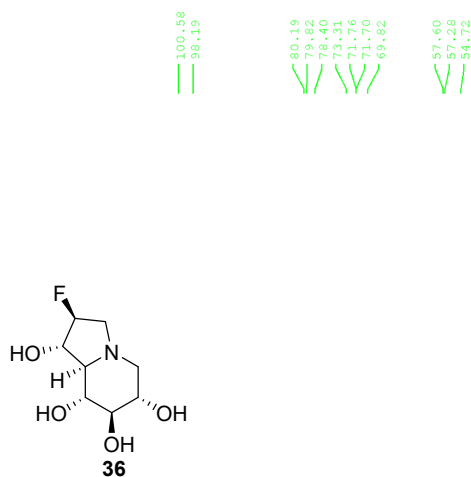
F2 - Acquisition Parameters
Date_ 20180525
Time 23.15
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg30
TD 65536
SOLVENT D2O
NS 1
DS 0
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262974 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 297.1 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.70 usec
PL1 0.50 dB
SFO1 600.1330123 MHz

F2 - Processing parameters
SI 32768
SF 600.1299429 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```



lyx-733



```

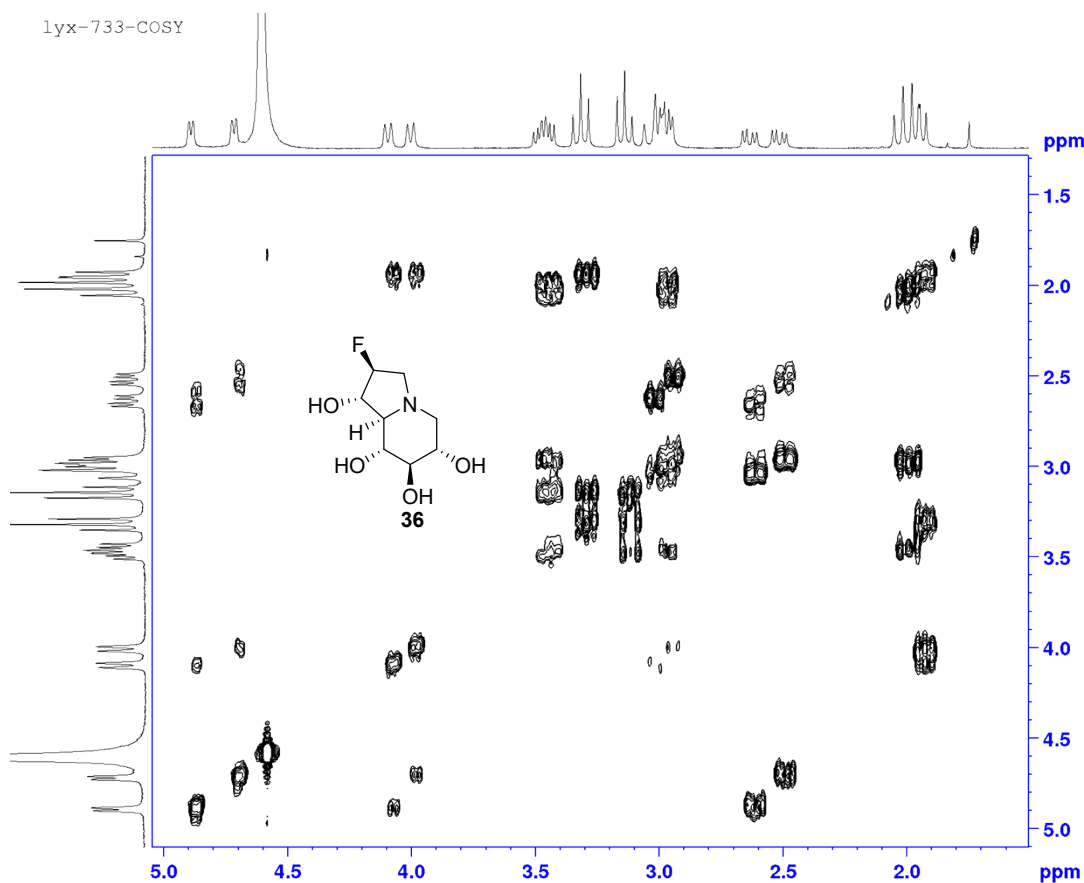
Current Data Parameters
NAME lyx-2018
EXPNO 385
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180525
Time 10.58 h
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 162
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 1.8175317 sec
RG 209.09
DW 27.733 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1
SFO1 75.4752949 MHz
NUC1 13C
P1 11.00 usec
PLW1 195.0000000 W
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 14.0000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```



lyx-733-COSY



```

Current Data Parameters
NAME      lyx-2018
EXPNO    387
PROCNO   1

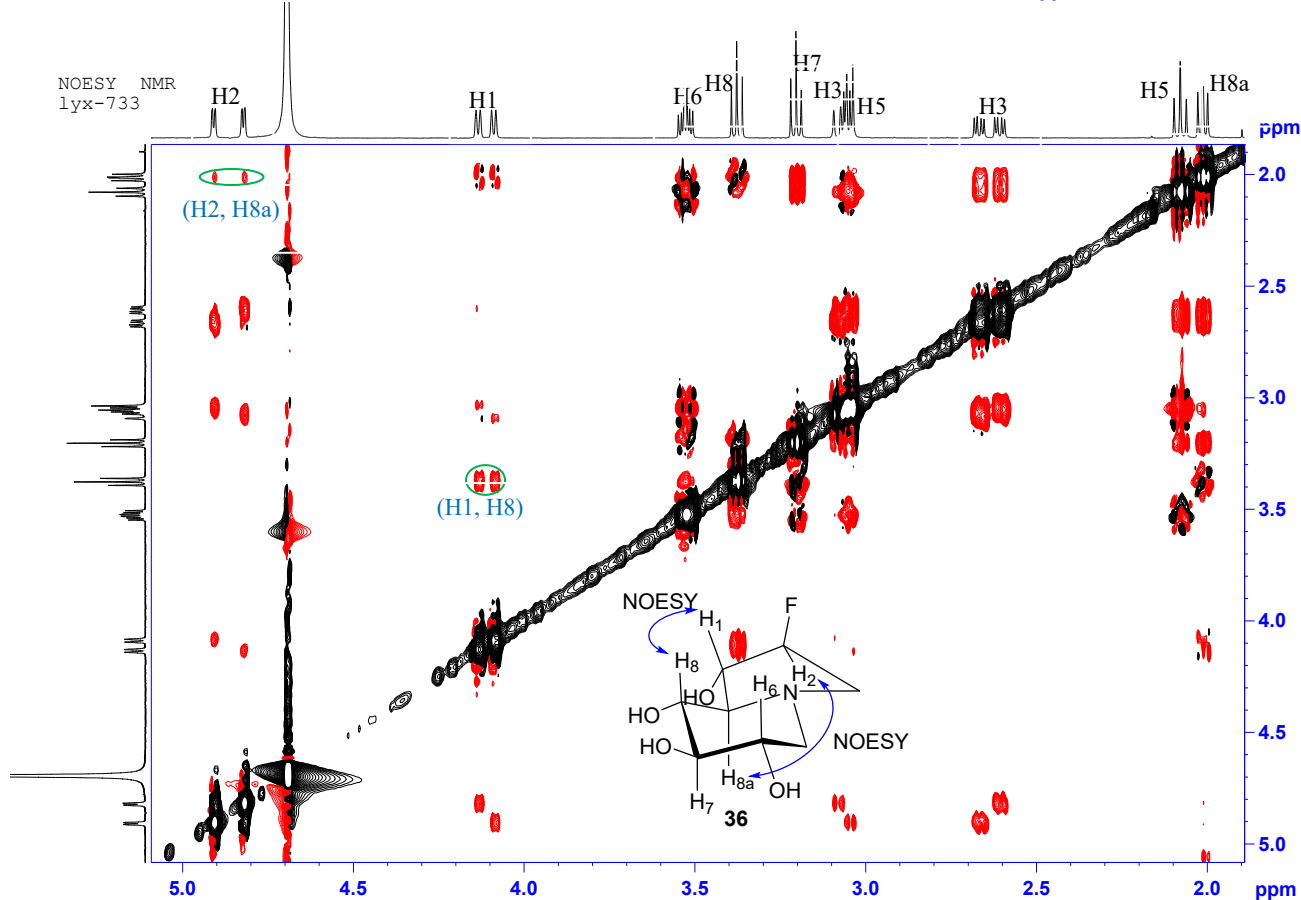
F2 - Acquisition Parameters
Date_    20180525
Time     11.08 h
INSTRUM  spect
PROBHD   5 mm DOL 13C-1
PULPROG  cosypppgf
TD        65536
SOLVENT  D2O
NS        1
DS        8
SMH       2304.147 Hz
FIDRES    2.250144 Hz
AQ         0.4444160 sec
RG         209.09
DN         217.000 usec
DE         8.50 usec
TE         300.2 K
d0         0.00000000 sec
d1         1.9117494 sec
d11        0.03000000 sec
d12        0.00002000 sec
d13        0.00002000 sec
d16        0.00020000 sec
in0        0 sec
STICHT    0
d0orip    0.00000000 sec
tiltop    0
SFO1      300.1312924 MHz
NUC1       13
P0         8.00 usec
P1         8.00 usec
P17        2590.00 usec
PLM1       18.00000000 W
PULSE1    1.79410001 W
GPNAM[1]  SMSQ10.100 W
CP1        10.00 %
P16        1000.00 usec

F1 - Acquisition parameters
TD         65536
SFO1      300.1313 MHz
FIDRES     48.503269 Hz
SN         7.677 ppm
FNUC1      13

F2 - Processing parameters
SI         1024
SF         300.1300360 MHz
WDW        QSI
SSB        0
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         300.1300355 MHz
WDW        QSI
SSB        0
LB         0 Hz
GB         0
    
```

NOESY NMR  
lyx-733

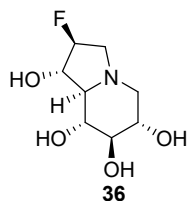




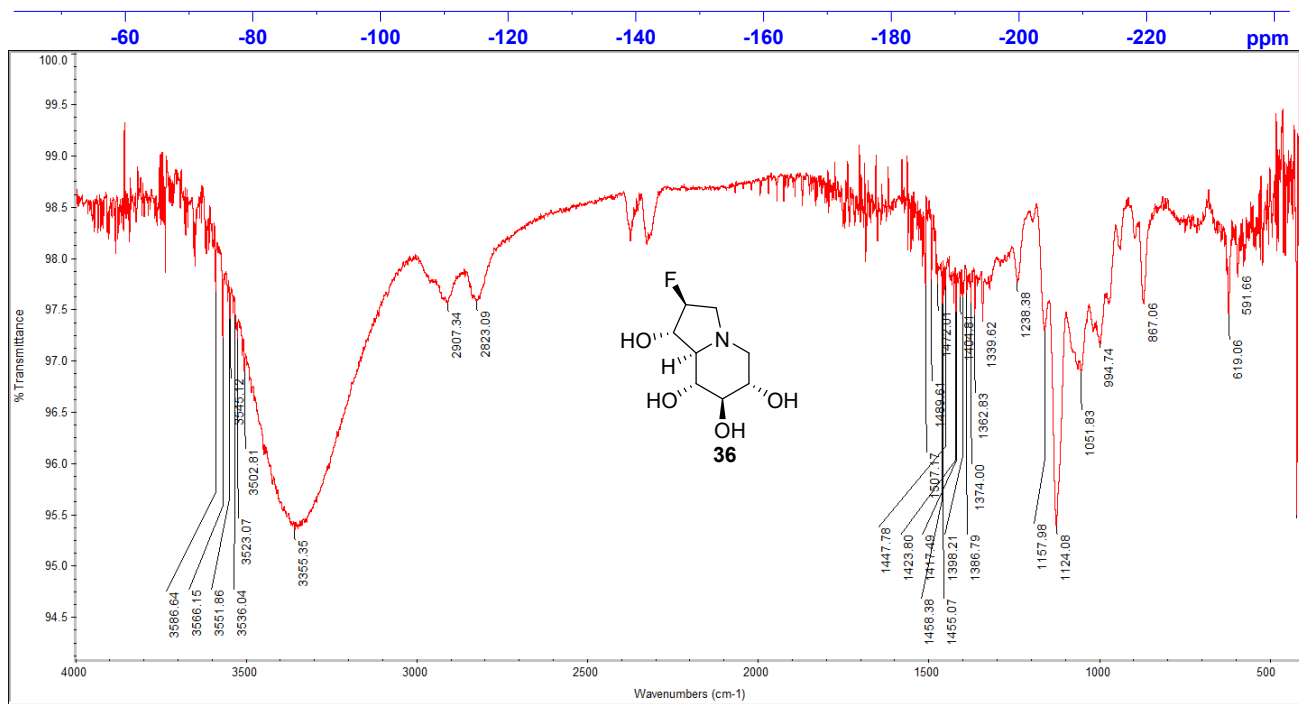
19F NMR  
733

-174.57

```
NAME          19F-2018
EXPNO         3
PROCNO        1
Date_         20180530
Time          9.48
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgfglqgn.2
TD            32768
SOLVENT       D2O
NS            16
DS            0
SWH           89285.711 Hz
FIDRES        2.724784 Hz
AQ            0.1835508 sec
RG            206.33
DW            5.600 usec
DE            6.50 usec
TE            301.9 K
D1            1.0000000 sec
D11           0.0300000 sec
D12           0.0000200 sec
TDO           1
```

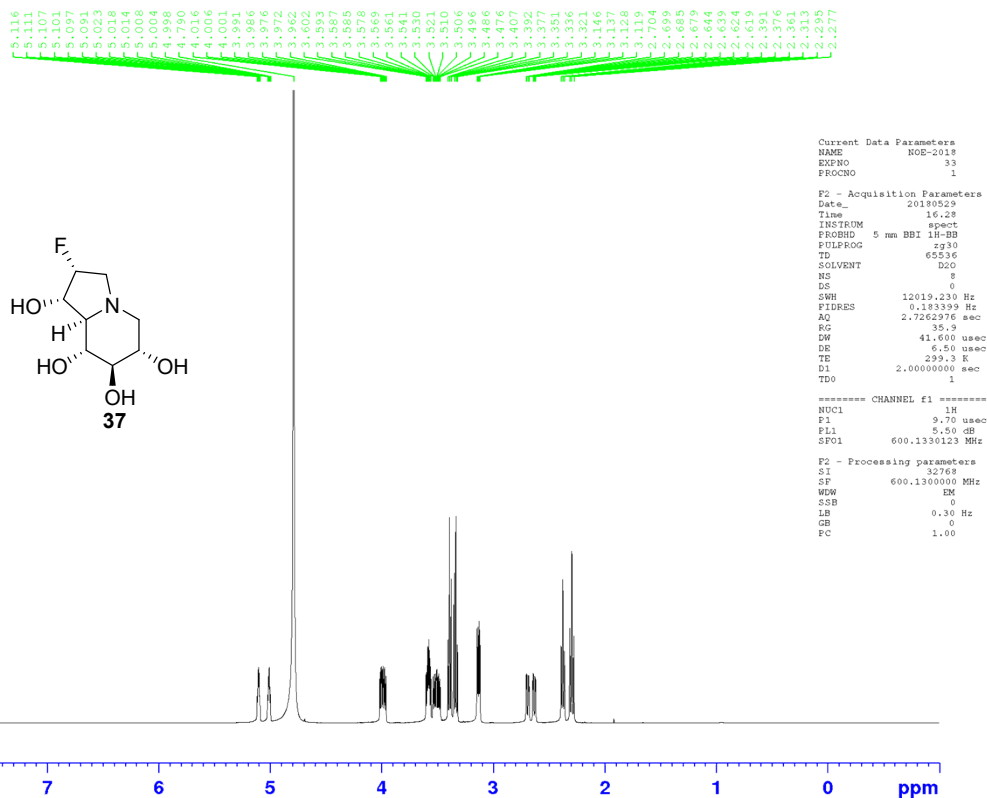


```
===== CHANNEL f1 =====
SFO1         376.5416137 MHz
NUC1         19F
P1           14.50 usec
SI           65536
SF           376.6018700 MHz
WDM          0
SSB          0
LB           3.00 Hz
GB           0
PC           1.00
```

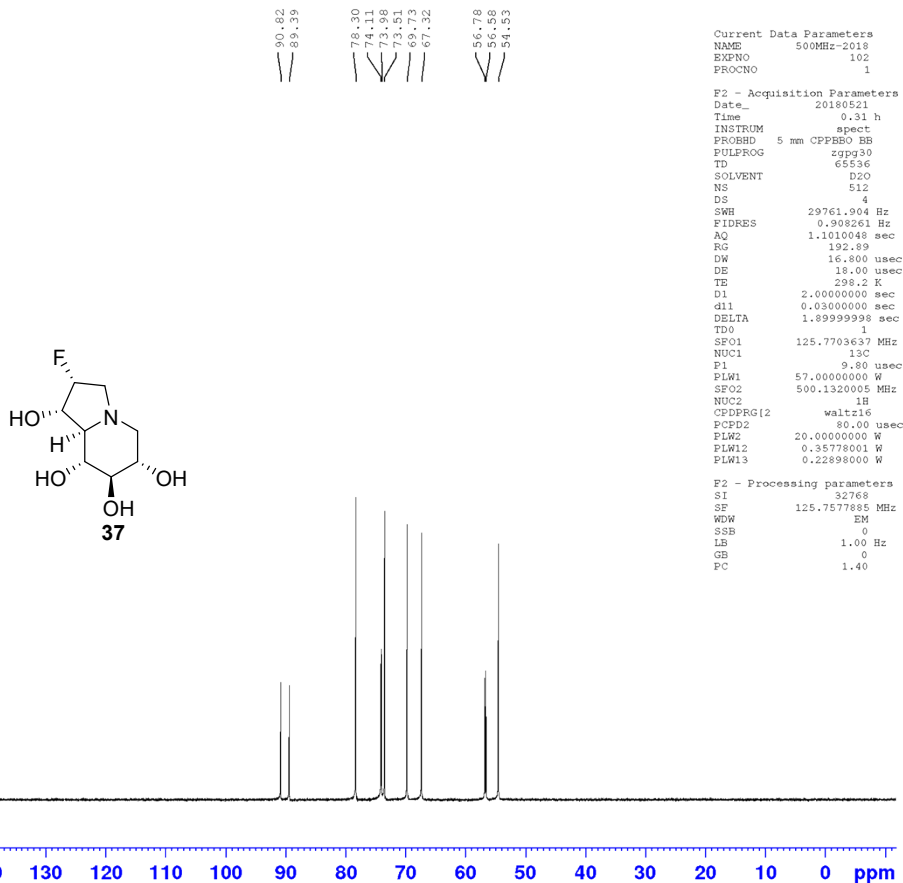


# Compound 37:

<sup>1</sup>H NMR  
lyx-714



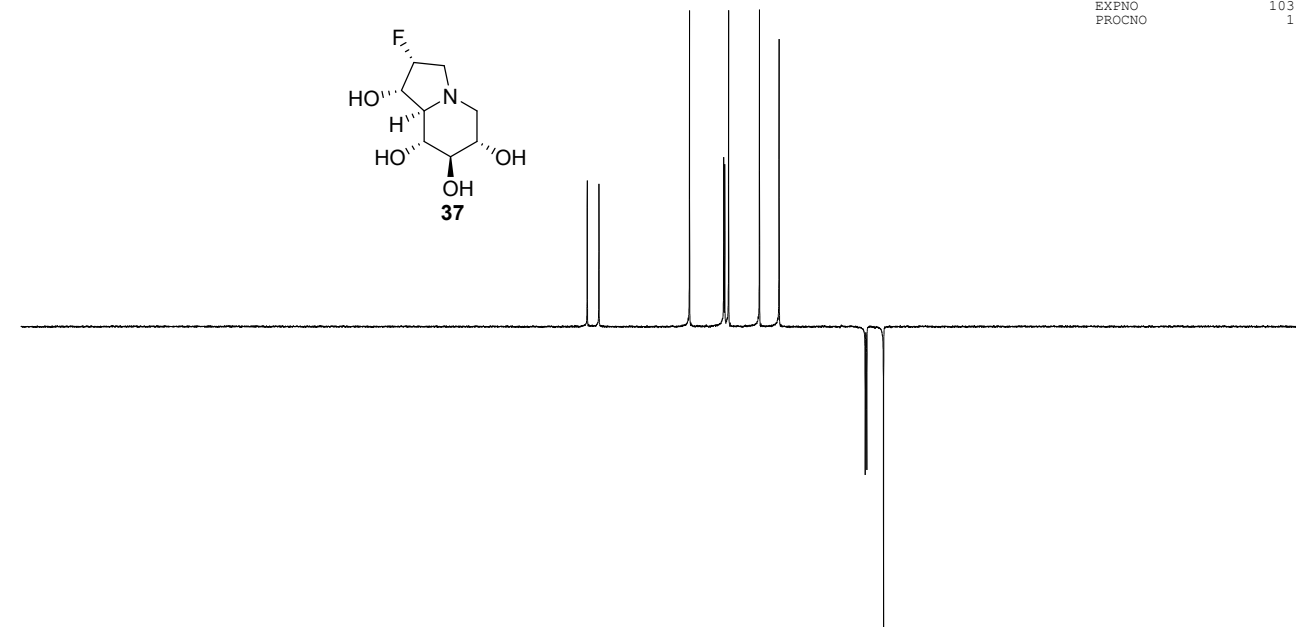
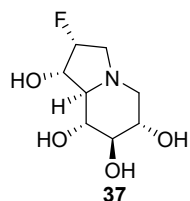
lyx-714



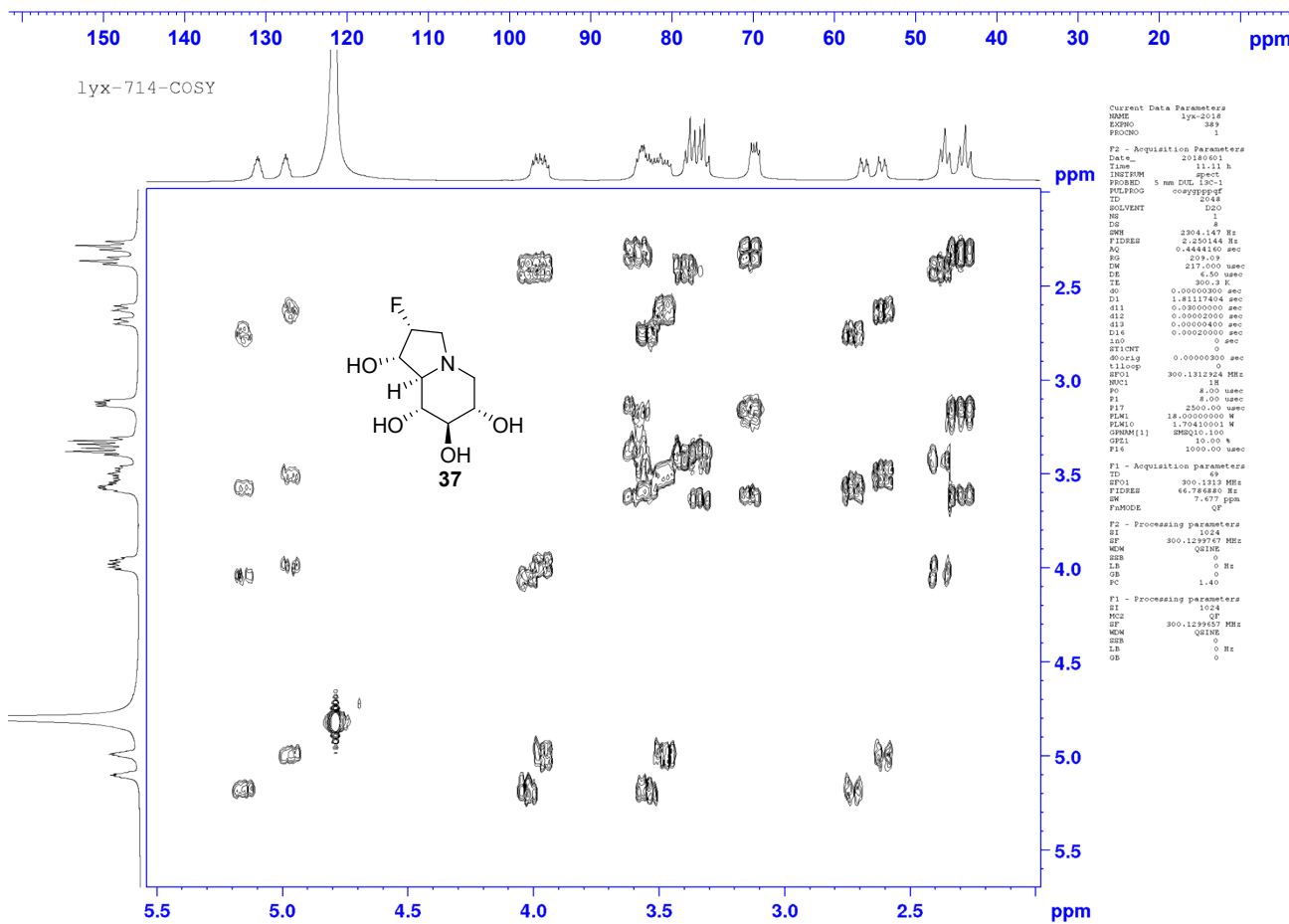
lyx-714

90.82  
89.39  
78.30  
74.11  
73.98  
73.51  
69.73  
67.32  
56.78  
56.58  
54.53

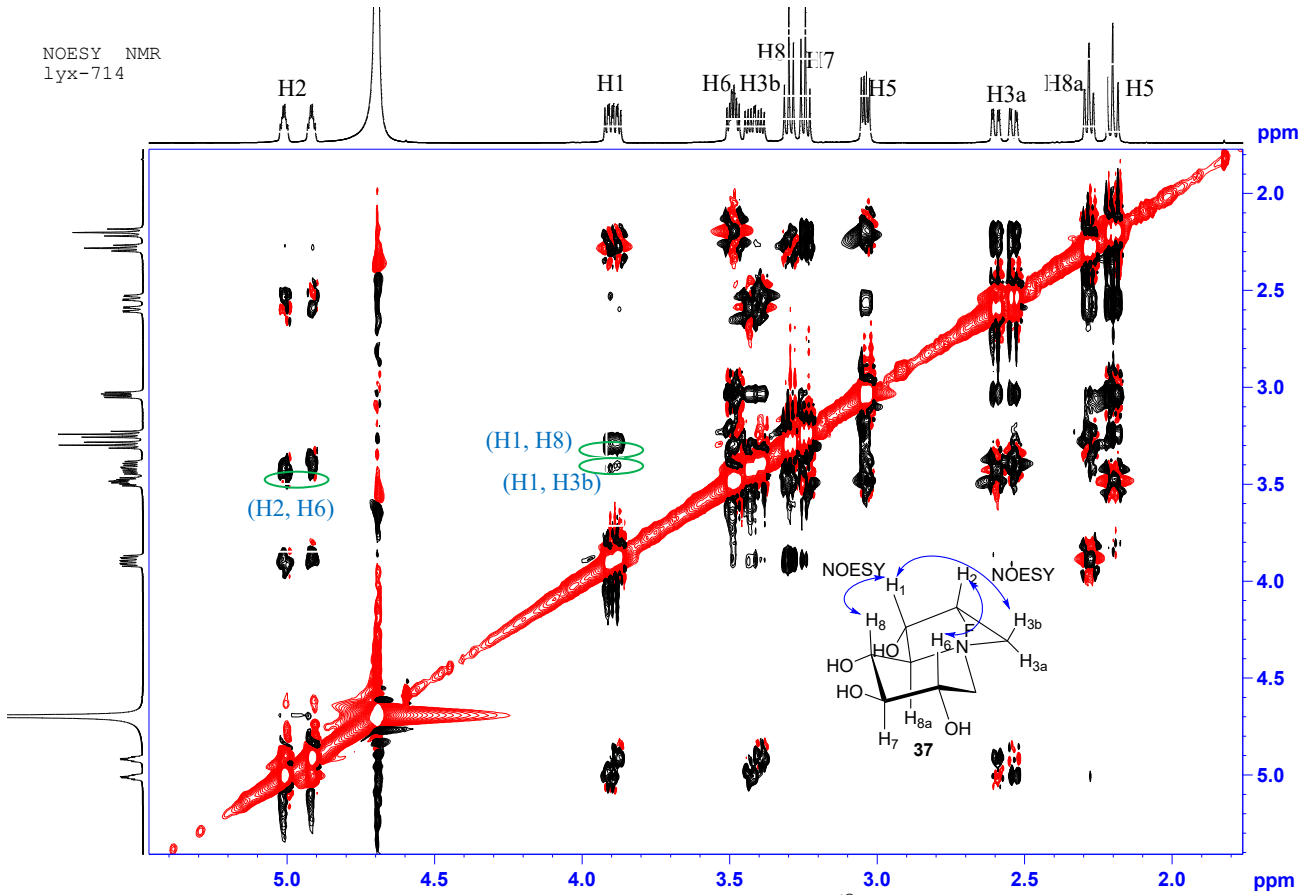
NAME 500MHz-2018  
EXPNO 103  
PROCNO 1



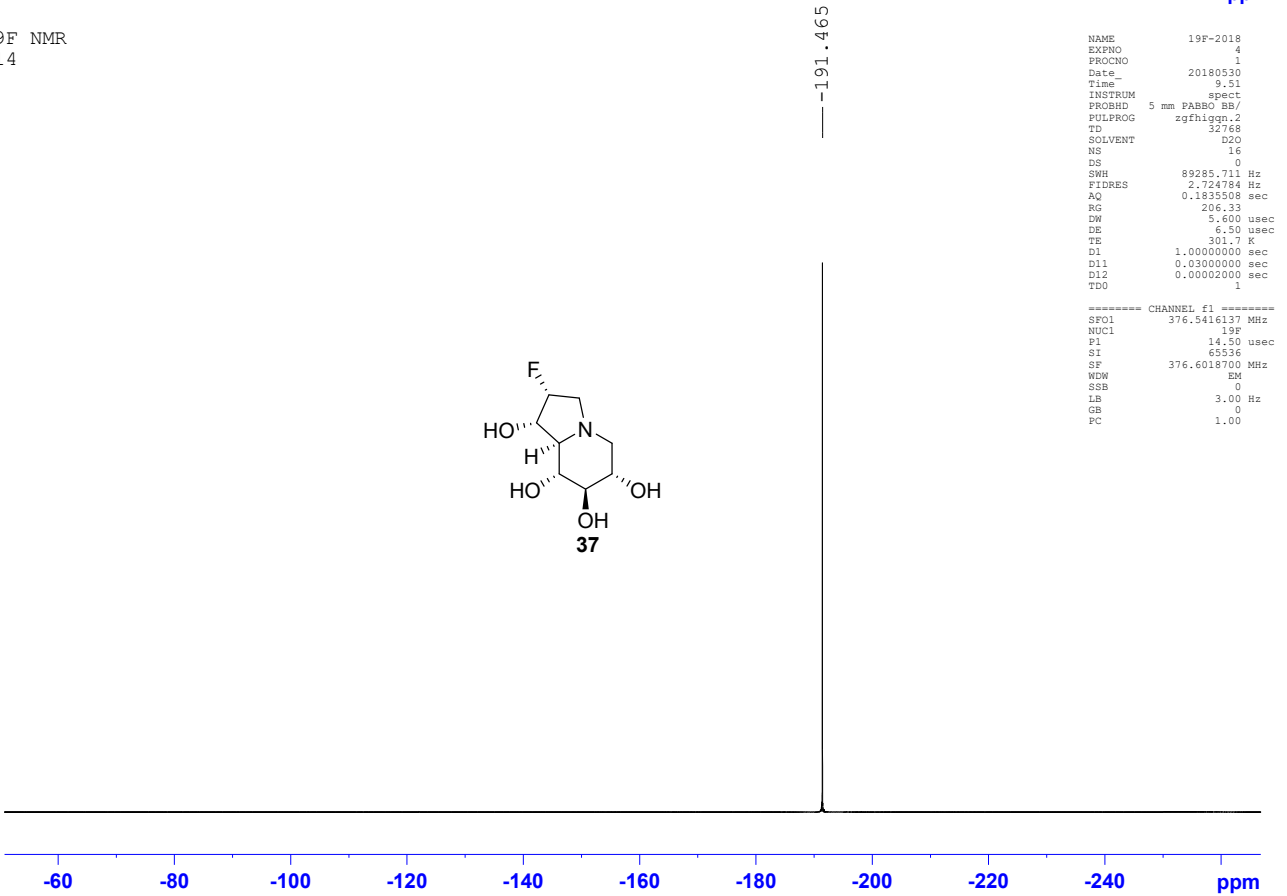
lyx-714-COSY



NOESY NMR  
lyx-714

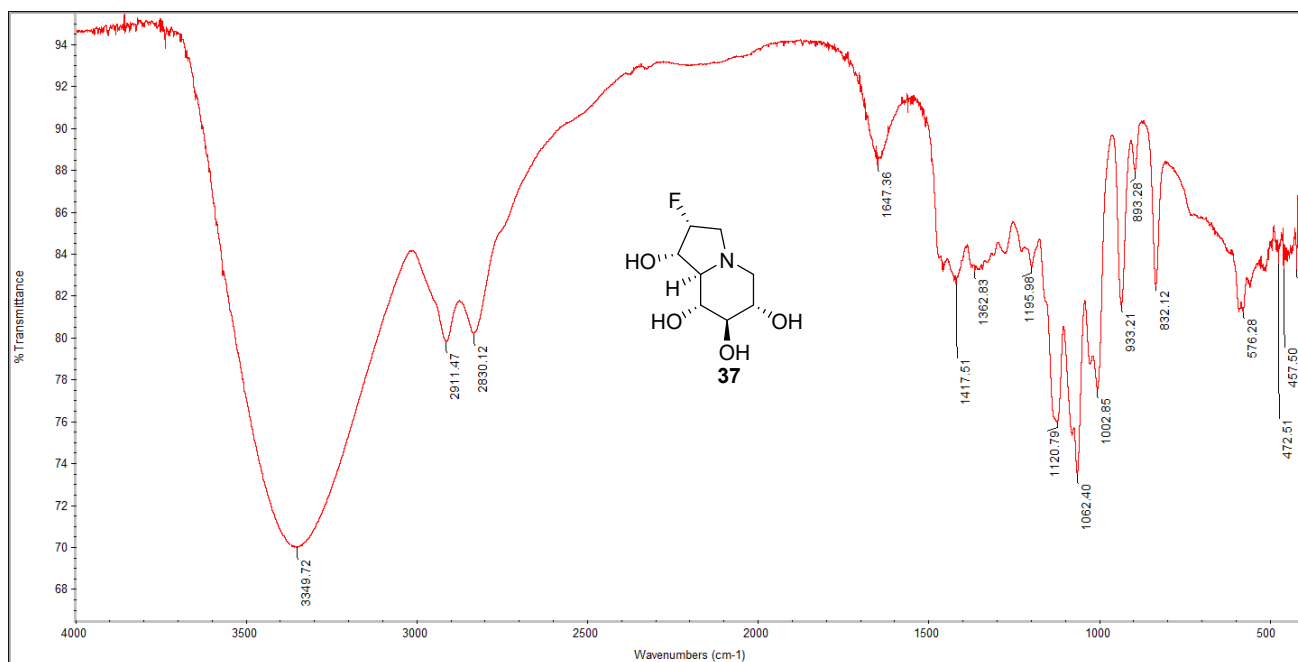


19F NMR  
714



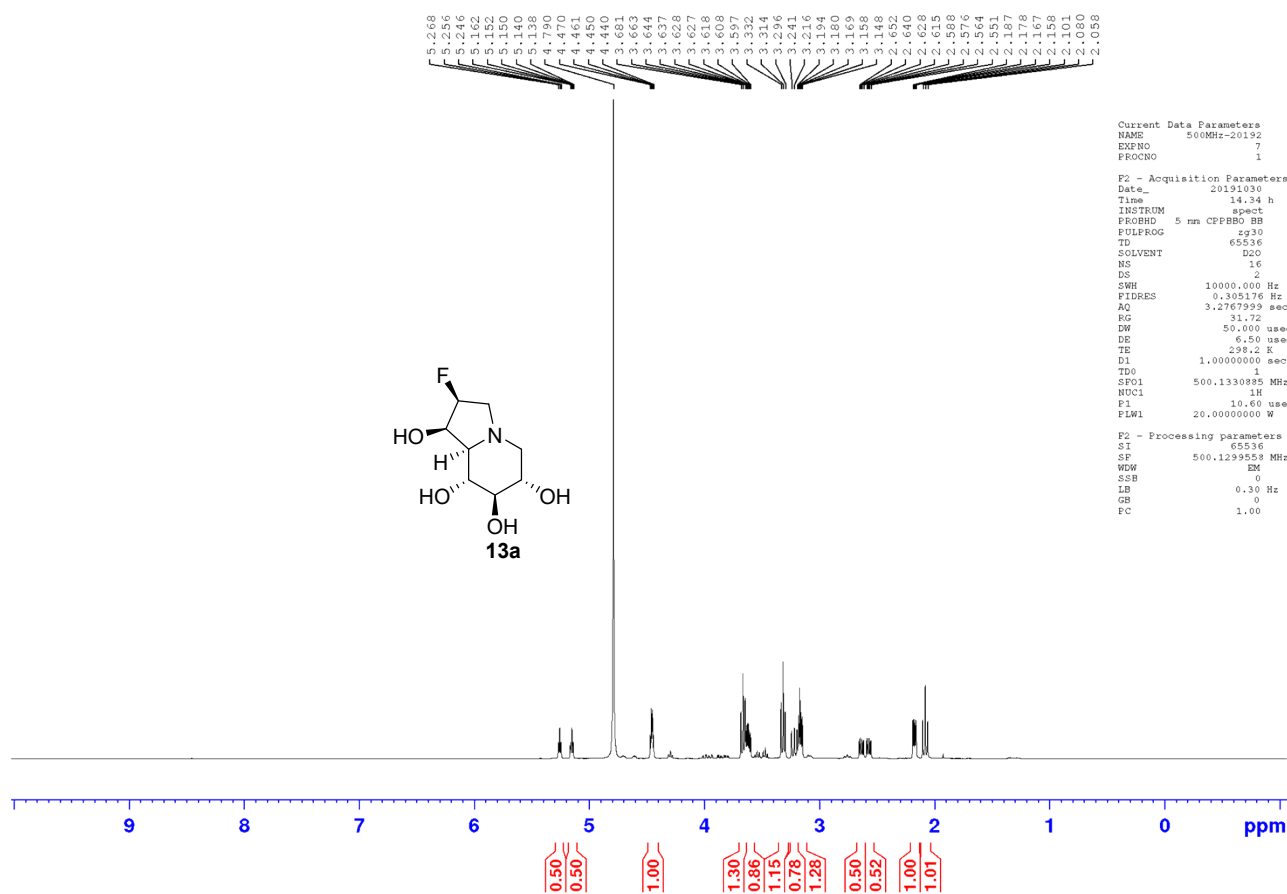
```

NAME          19F-2018
EXNO          4
PROCNO        1
Date          20180530
Time          9.51
INSTRUM       spect
PROBHD        5 mm PABBO BB/
PULPROG       zgfhlgpn.2
TD            32768
SOLVENT       D2O
NS            16
DS            0
SWH           89285.711 Hz
FIDRES        2.724784 Hz
AQ            0.1835508 sec
RG            206.33
DW            5.600 usec
DE            6.50 usec
TE            301.7 K
D1            1.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
TD0           1
----- CHANNEL f1 -----
SF01          376.5416137 MHz
NUC1          19F
P1            14.50 usec
SI            65536
SF            376.6018700 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.00
  
```



Compound 13a:

lyx-792



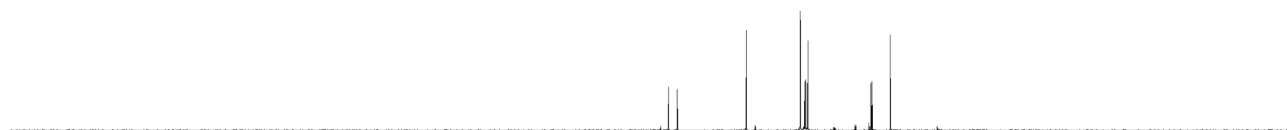
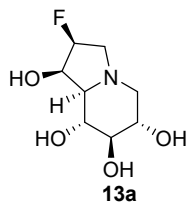
lyx-792

91.85  
90.07  
78.62  
69.72  
69.64  
68.96  
68.83  
68.44  
59.01  
57.91  
54.78

Current Data Parameters  
 NAME 500MHz-20192  
 EXPNO 8  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20191030  
 Time 15.29 h  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT D2O  
 NS 1024  
 DS 4  
 SWH 29761.904 Hz  
 FIDRES 0.908261 Hz  
 AQ 1.1010048 sec  
 RG 192.89  
 DW 16.800 usec  
 DE 18.00 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 1  
 SFO1 125.7703637 MHz  
 NUC1 13C  
 P1 9.80 usec  
 PLW1 57.0000000 W  
 SFO2 500.1320005 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 80.00 usec  
 PLW2 20.0000000 W  
 PLW12 0.35778001 W  
 PLW13 0.22898000 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7577885 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

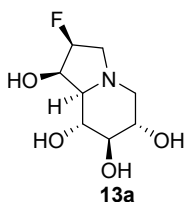
lyx-792

91.85  
90.07  
78.62  
69.72  
69.64  
68.96  
68.83  
68.44  
59.01  
57.91  
54.78

Current Data Parameters  
 NAME 500MHz-20192  
 EXPNO 9  
 PROCNO 1

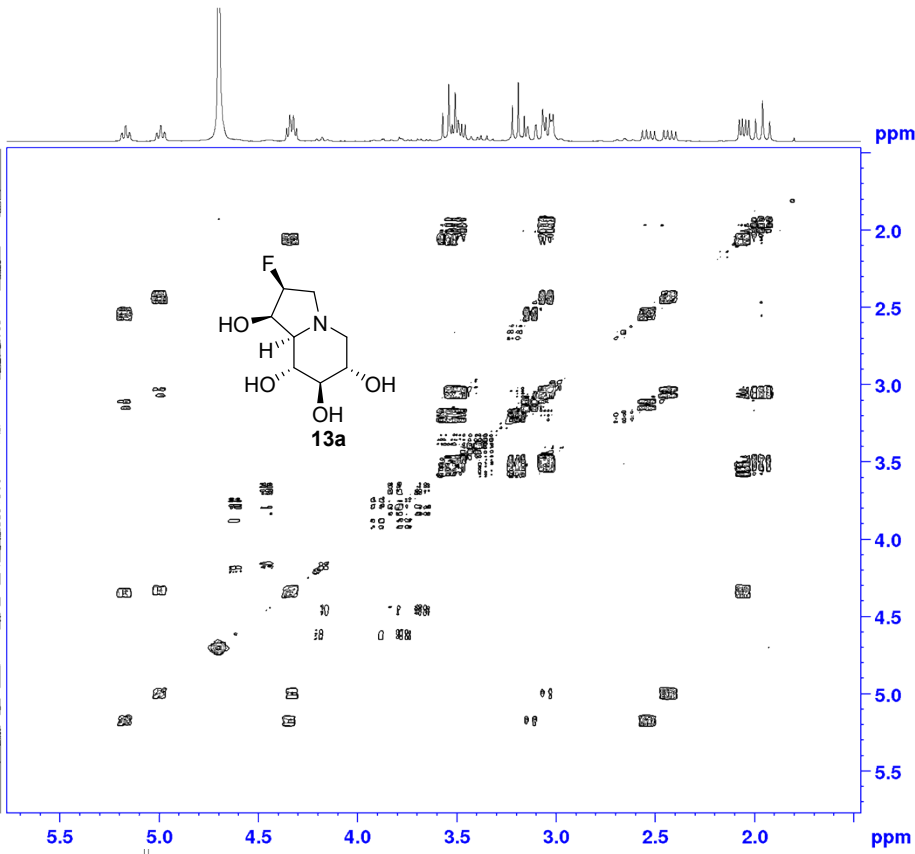
F2 - Acquisition Parameters  
 Date\_ 20191030  
 Time 15.45 h  
 INSTRUM spect  
 PROBHD 5 mm CPPBBO BB  
 PULPROG deptg135  
 TD 65536  
 SOLVENT D2O  
 NS 256  
 DS 4  
 SWH 20161.295 Hz  
 FIDRES 0.615274 Hz  
 AQ 1.6252929 sec  
 RG 192.89  
 DW 24.800 usec  
 DE 18.00 usec  
 TE 298.2 K  
 CNST2 145.0000000 sec  
 D1 2.00000000 sec  
 d2 0.00344829 sec  
 d12 0.00002000 sec  
 DELTA 0.0000248 sec  
 TD0 1  
 SFO1 125.7678488 MHz  
 NUC1 13C  
 P1 9.80 usec  
 PL1 2000.00 usec  
 PLW0 0 W  
 PLW1 57.0000000 W  
 SFO2 500.1315995 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 P3 10.70 usec  
 P4 21.40 usec  
 PCPD2 80.00 usec  
 PLW2 20.0000000 W  
 PLW12 0.35778001 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7577885 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

lyx-792



```

Current Data Parameters
NAME      lyx-2019
EXPNO    102
PROCNO   1

F2 - Acquisition Parameters
Date_    20191122
Time     13.15 h
INSTRUM  spect
PROBHD   5 mm CUL 1H-1
PULPROG  ooeypppprf
TD        2248
SOLVENT  D2O
NS        1
DS        8
SHE       1291.990 Hz
FIDRES   1.241709 Hz
AQ        0.725750 sec
RG        117.72
DM        387.000 usec
DE        6.50 usec
TE        311.4 K
DQ        0.00000000 sec
D1        1.46301401 sec
d11       0.00000000 sec
d12       0.00000000 sec
d13       0.00000000 sec
d14       0.00020000 sec
AQ        0 sec
STOCHT   0
SFO1     0.00000000 sec
tiltpp   0
NUC1     300.131054 MHz
PC        18
PC2       8.00 usec
P1        8.00 usec
P12       2500.00 usec
P2        18.00000000 sec
P2M1     1.70410001 W
GPM1(1)  SMSG10.100
P14      1000.00 usec

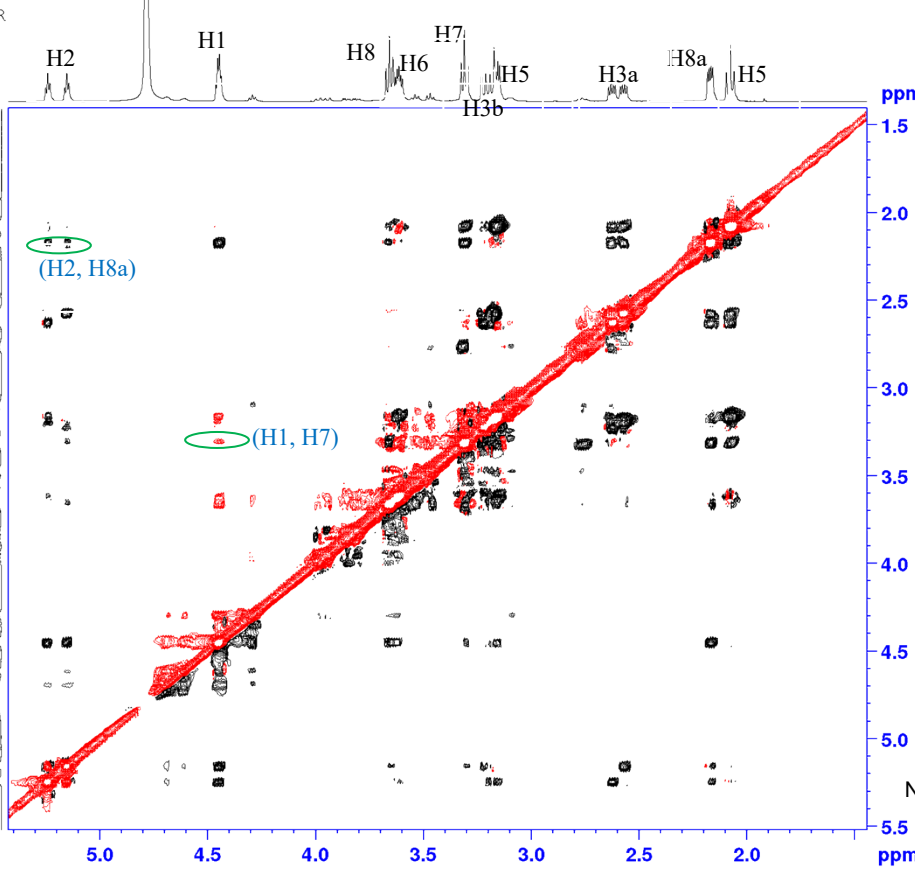
F1 - Acquisition parameters
TD        128
SFO1     300.1311 MHz
FIDRES   20.147338 Hz
SW        4.303 ppm
FMODE    QF

F2 - Processing parameters
SI        1024
SF        300.1300000 MHz
WDW       QFTT
SSB       0
LB        0 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
SF        300.1300000 MHz
WDW       QFTT
SSB       0
LB        0 Hz
GB        0

```

NOESY NMR  
lyx-792



```

Current Data Parameters
NAME      NOE-2019
EXPNO    9
PROCNO   1

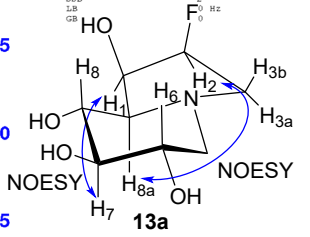
F2 - Acquisition Parameters
Date_    20191126
Time     16.10 h
INSTRUM  Avance
PROBHD   1124704_01003 (
PULPROG  noesypppprf
TD        2048
SOLVENT  H2O+d2o
NS        16
DS        16
SHE       7142.857 Hz
FIDRES   6.973446 Hz
AQ        0.1432600 sec
RG        57
DM        70.000 usec
DE        7.95 usec
TE        0.00000000 sec
DQ        1.50000000 sec
D1        0.13000001 sec
D11       0.03600000 sec
D12       0.00000000 sec
D13       0.00000000 sec
D14       0.00014000 sec
TDav     1
SFO1     600.1328206 MHz
NUC1     1
PC        15.00 usec
P1        30.60499954 W
P1M1     0.00027544 W
GPM1(1)  SMSG10.100
P14      1000.00 usec

F1 - Acquisition parameters
TD        256
SFO1     600.1328 MHz
FIDRES   55.813570 Hz
SW        11.902 ppm
FMODE    States-TPPI

F2 - Processing parameters
SI        2048
SF        600.1299487 MHz
WDW       QFTT
SSB       2
LB        0 Hz
GB        0
PC        1.00

F1 - Processing parameters
SI        1024
SF        600.1299470 MHz
WDW       QFTT
SSB       2
LB        0 Hz
GB        0

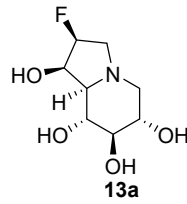
```



19F (1H decoupled) NMR  
792

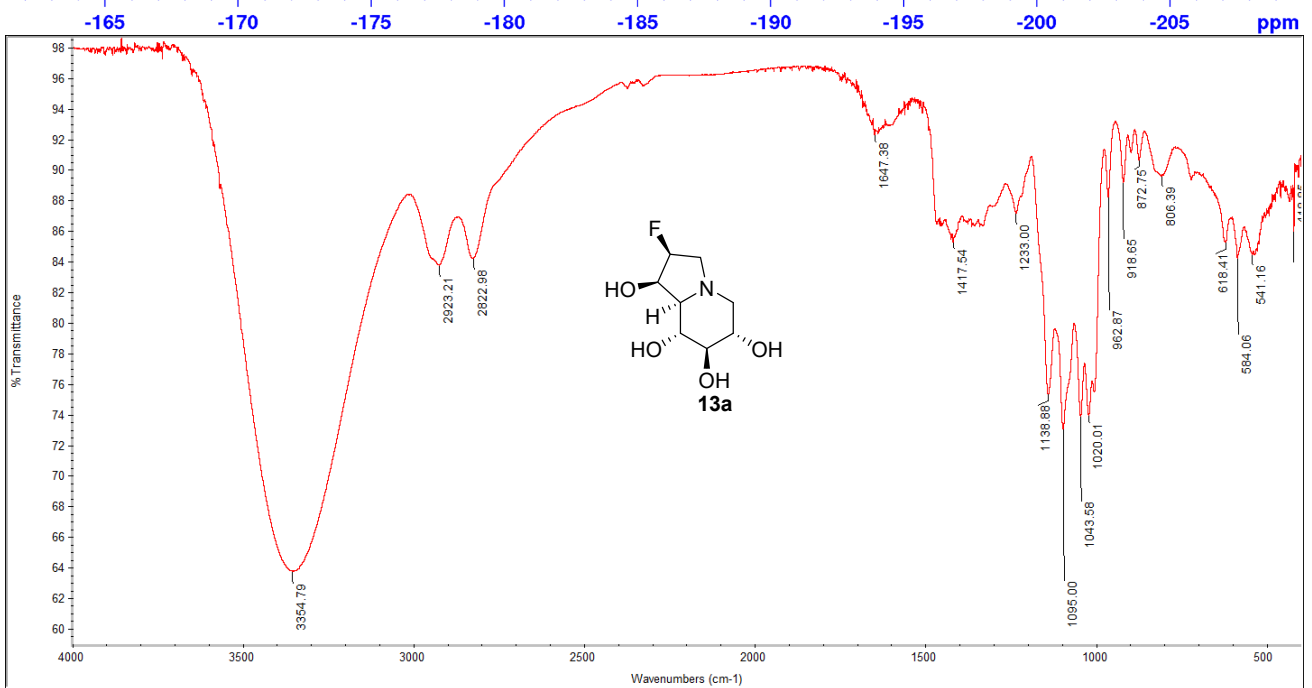
Current Data Parameters  
NAME NOE-2019  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20191106  
Time 13.54 h  
INSTRUM Avance  
PROBHD Z124704.0003 ( )  
PULPROG zgfhlgqn.2  
TD 65536  
SOLVENT H2O+D2O  
NS 32  
DS 0  
SWH 68493.148 Hz  
FIDRES 2.090245 Hz  
AQ 0.4784128 sec  
RG 29.2969  
DW 7.300 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
D12 0.00002000 sec  
TD0 1  
SFO1 564.5790976 MHz  
NUC1 19F  
P1 25.00 usec  
PLW1 45.41600037 W  
SFO2 600.1324005 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 30.60499954 W  
PLW12 1.40530002 W



-195.72

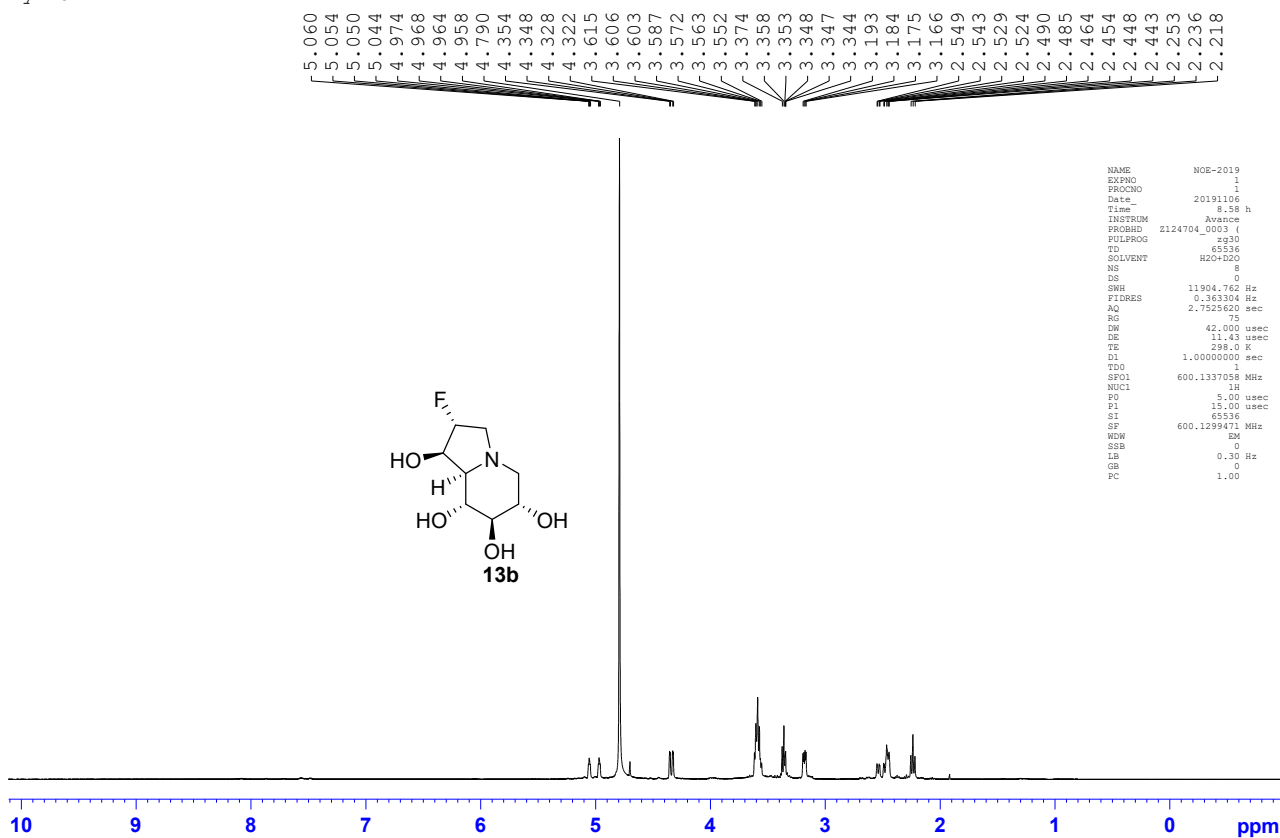
F2 - Processing parameters  
SI 65536  
SF 564.6863882 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00





Compound **13b**:

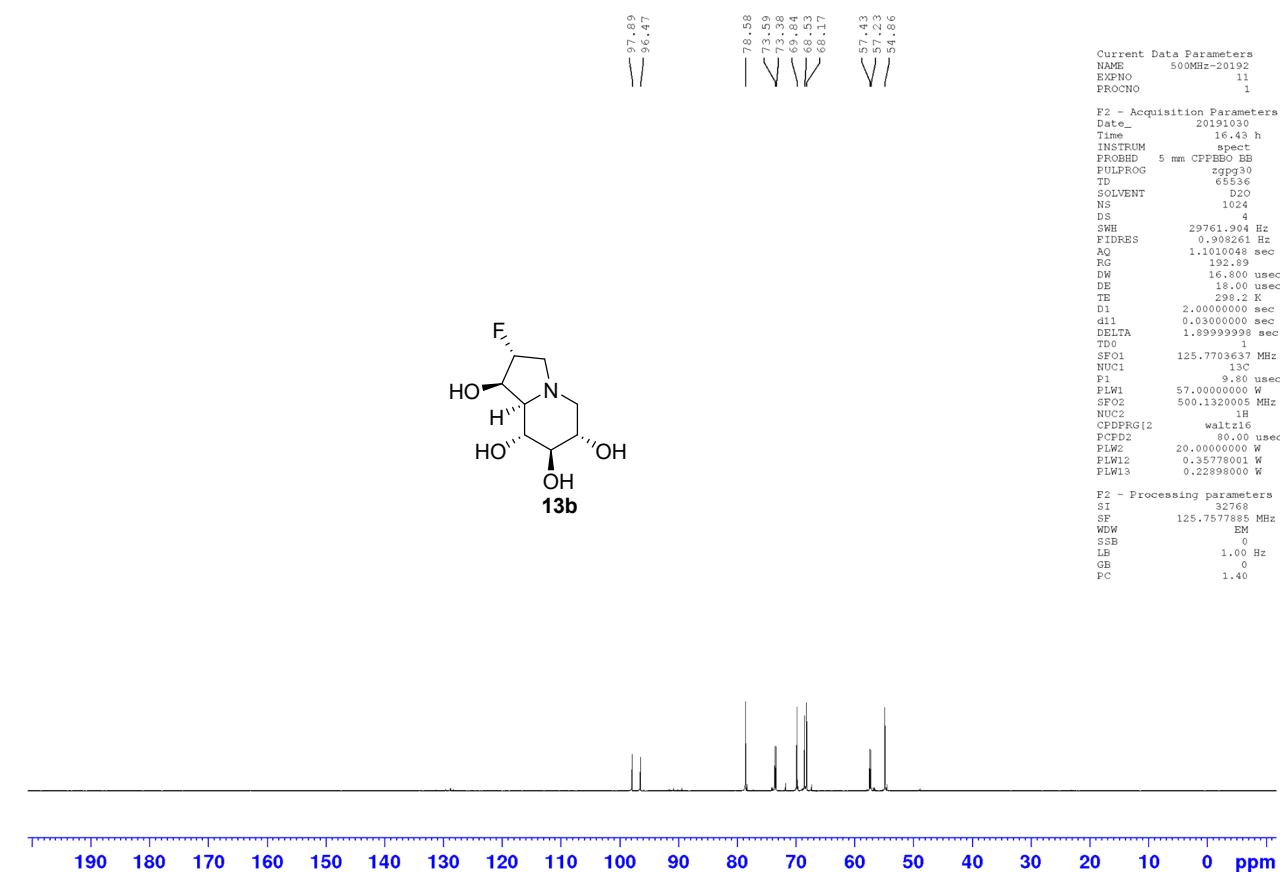
lyx-817



```

NAME      NOE-2019
EXPNO     1
PROCNO    1
Date_     20191106
Time      8.58 h
INSTRUM   Avance
PROBHD    2124704_0003 (
PULPROG   zg30
TD         65536
SOLVENT   H2O-D2O
NS         8
DS         0
SWH        11904.762 Hz
FIDRES     0.363304 Hz
AQ         2.7525620 sec
RG         75
RW         42.000 usec
DE         11.43 usec
TE         298.2 K
D1         1.00000000 sec
TDO        0
SFO1       600.1337058 MHz
NUC1       1H
PQ         5.00 usec
PL         15.00 usec
SI         65536
SF         600.1299471 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

lyx-817



```

Current Data Parameters
NAME      500MHz-20192
EXPNO     11
PROCNO    1

F2 - Acquisition Parameters
Date_     20191130
Time      16.43 h
INSTRUM   spect
PROBHD    5 mm CFPBBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   D2O
NS         1024
DS         4
SWH        29761.904 Hz
FIDRES     0.308261 Hz
AQ         1.1010048 sec
RG         192.89
RW         16.800 usec
DE         18.00 usec
TE         298.2 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA      1.899999998 sec
TDO        1
SFO1       125.7703637 MHz
NUC1       13C
PQ         9.80 usec
PLW1       57.00000000 W
SFO2       500.1320005 MHz
NUC2       1H
CFDPFG2    waltz16
PCPD2      80.00 usec
PLW2       20.00000000 W
PLW12      0.35778001 W
PLW13      0.22898000 W

F2 - Processing parameters
SI         32768
SF         125.7577885 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

lyx-817

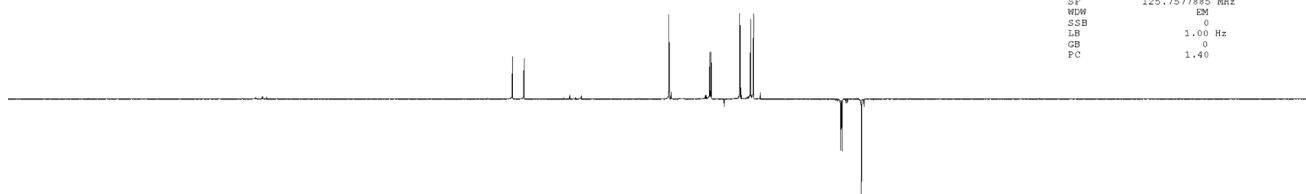
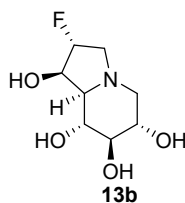
97.89  
96.47  
78.58  
73.59  
73.38  
69.84  
68.53  
68.17  
57.43  
57.23  
54.86

```

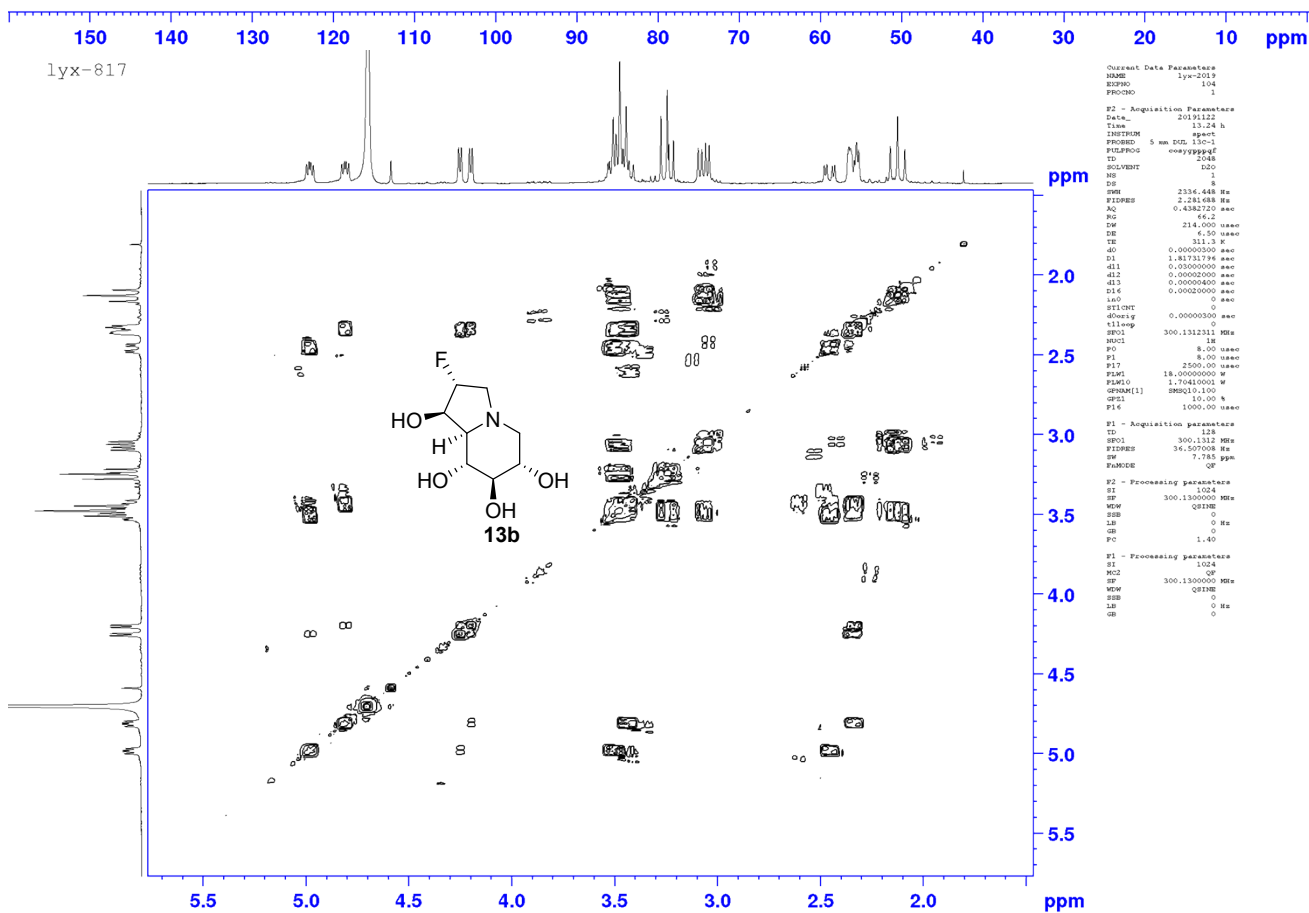
Current Data Parameters
NAME      500MHz-20192
EXPNO    12
PROCNO   1

F2 - Acquisition Parameters
Date_    20191030
Time     17.00 h
INSTRUM  spect
PROBHD   5 mm CFPBBO BB
PULPROG  zgpg30
TD        65536
SOLVENT  D2O
NS        256
DS        4
SWH       20161.291 Hz
FIDRES    0.615274 Hz
AQ         1.6252928 sec
RG         192.89
DW         24.800 usec
DE         18.00 usec
TE         298.2 K
CNS2      145.0000000
D1         2.000000000 sec
d2         0.00344828 sec
d12        0.00002000 sec
DELTA     0.00001248 sec
TD0        1
SF01      125.7678486 MHz
NUC1       13C
P1         9.80 usec
P13        2000.00 usec
PLM0       0 W
PLM1       57.00000000 W
SFOFF5     0 Hz
SFOFF5     0 Hz
SFOFF5     500.1315935 MHz
NUC2       1H
CEPPROG2  waltz16
P3         19.70 usec
p4         21.40 usec
PCPD2     30.00 usec
PLM2      20.00000000 W
PLM12     0.35778001 W

F2 - Processing parameters
SI         32768
SF         125.7577885 MHz
MSB        0
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```



lyx-817



```

Current Data Parameters
NAME      lyx-817
EXPNO    104
PROCNO   1

F2 - Acquisition Parameters
Date_    20191122
Time     13.24 h
INSTRUM  spect
PROBHD   5 mm BBO 150-3
PULPROG  zgpg30
TD        65536
SOLVENT  D2O
NS        256
DS        4
SWH       2334.248 Hz
FIDRES    2.281488 Hz
AQ         0.4382720 sec
RG         66.2
DW         24.000 usec
DE         15.50 usec
TE         311.3 K
d0         0.000000000 sec
d1         1.81731794 sec
d11        0.000000000 sec
d12        0.000020000 sec
d13        0.000000000 sec
d16        0.000020000 sec
IAC0       0 usec
STLCNT     0.000000000 sec
d0freq     300.1312311 MHz
NUC1       13C
P1         8.00 usec
P13        2500.00 usec
PLM1       18.00000000 W
PLM0       17.04100001 W
SFOFF1     88201.100
SFOFF1     1000.00 usec

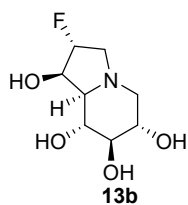
F2 - Acquisition parameters
TD         128
SF         300.13112 MHz
FIDRES     36.507008 Hz
SR         7.787 ppm
PULPROG    zgpg30

F2 - Processing parameters
SI         300.1300000 MHz
MSB        0
SSB        0 Hz
LB         0
GB         0
PC         1.40

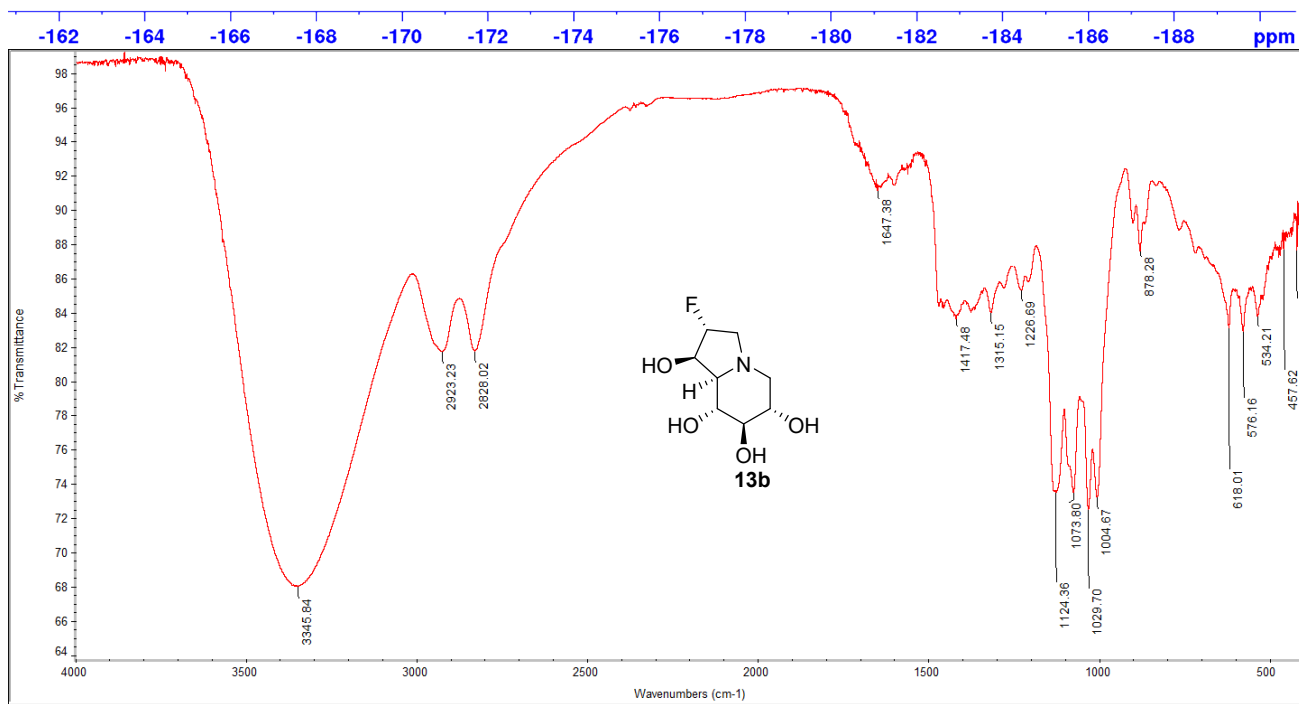
F1 - Processing parameters
SI         1024
NUC1       13C
SF         300.1300000 MHz
MSB        0
SSB        0 Hz
LB         0
GB         0
    
```

<sup>19</sup>F (1H decoupled) NMR  
lyx-817

Current Data Parameters  
NAME NoE-2019  
EXPNO 3  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20191106  
Time 9.11 h  
INSTRUM Avance  
PROBHD Z124704\_0003 ( zfhigpn.2  
PULPROG zgfhigpn.2  
TD 65536  
SOLVENT H2O-D2O  
NS 16  
DS 0  
SWH 68493.148 Hz  
FIDRES 2.090245 Hz  
AQ 0.4784128 sec  
RG 29.2969  
DW 7.300 usec  
DE 6.50 usec  
TE 298.3 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
D12 0.00020000 sec  
TDO 1  
SFO1 564.5790976 MHz  
NUC1 19F  
F1 25.00 usec  
PLW1 45.41600037 W  
SFO2 600.1324005 MHz  
NUC2 1H  
CFPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 30.60499954 W  
PLW12 1.40530002 W  
F2 - Processing parameters  
SI 65536  
SF 564.6863882 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

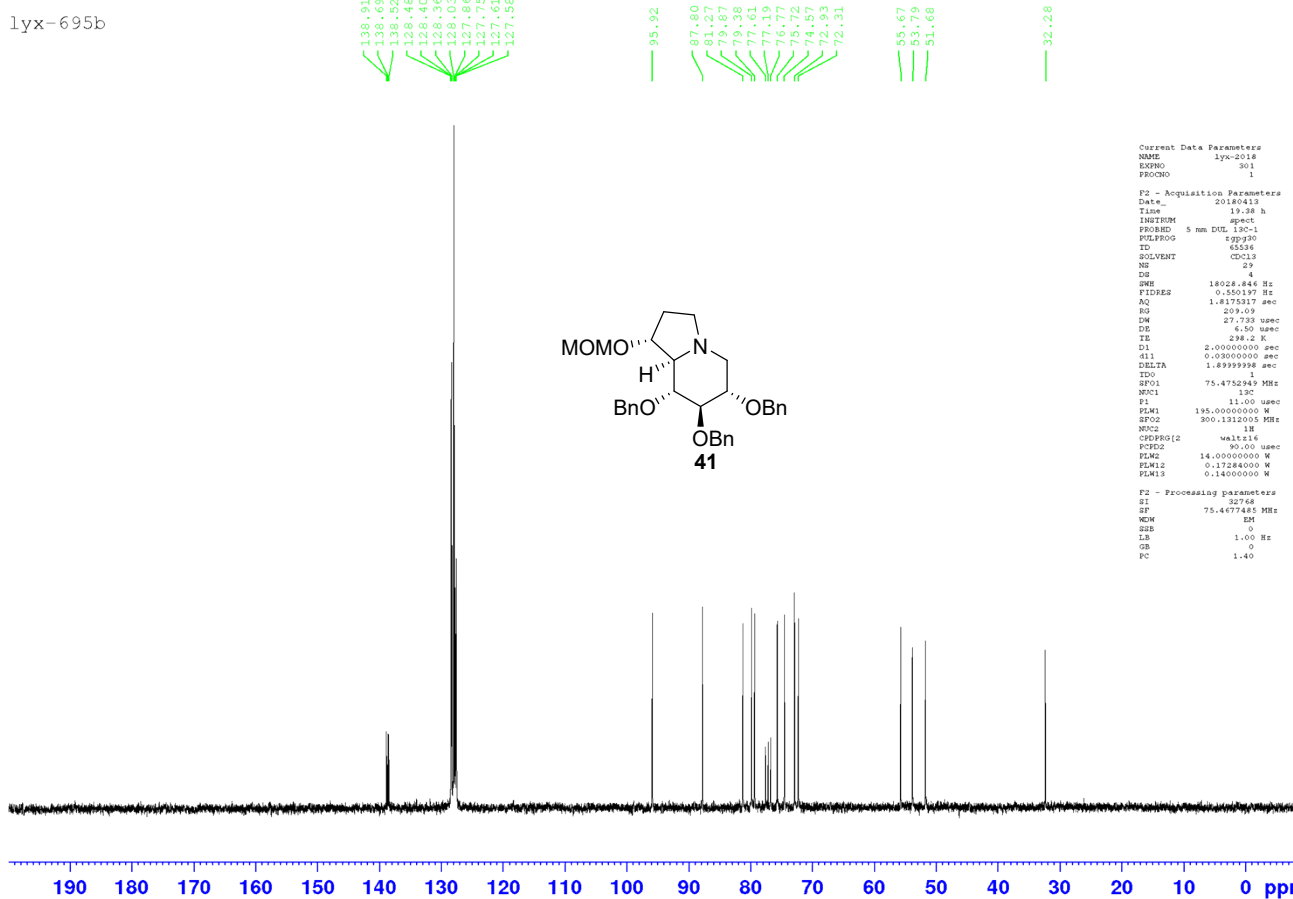
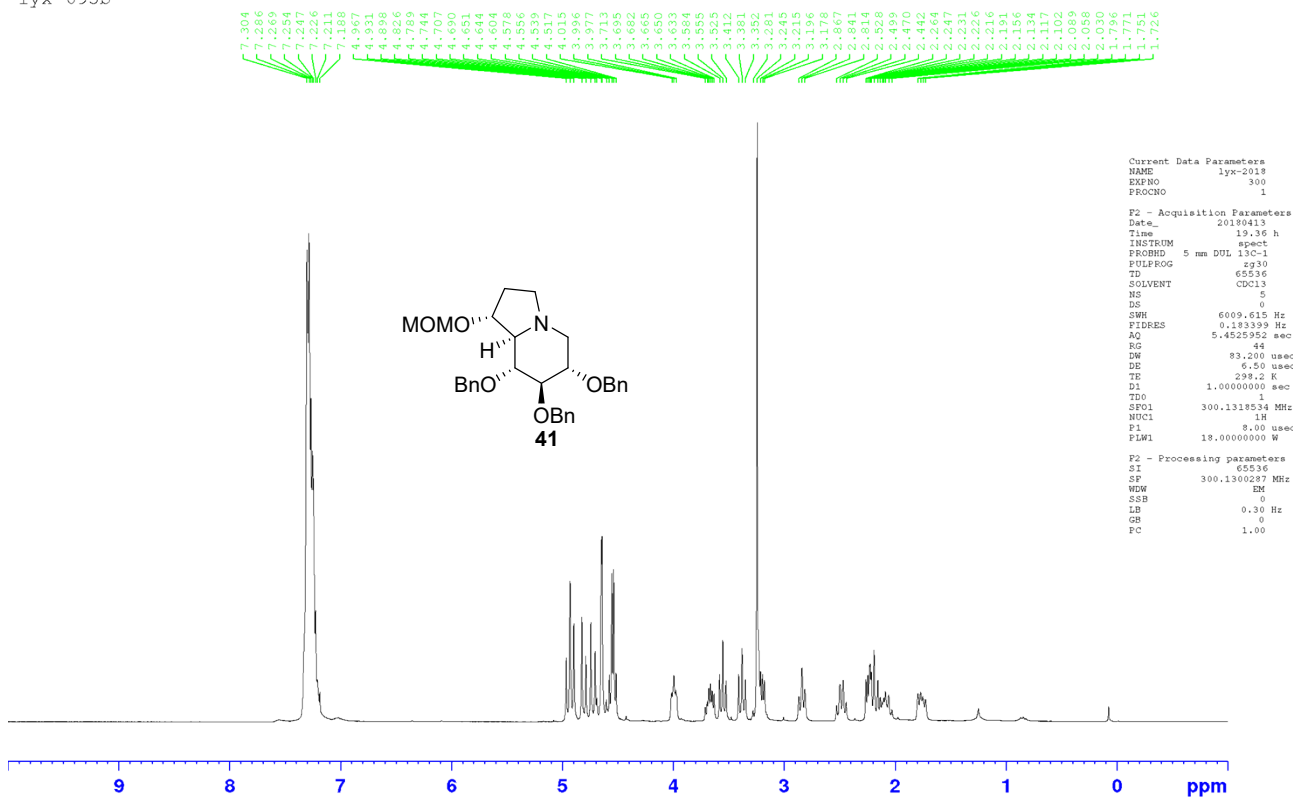


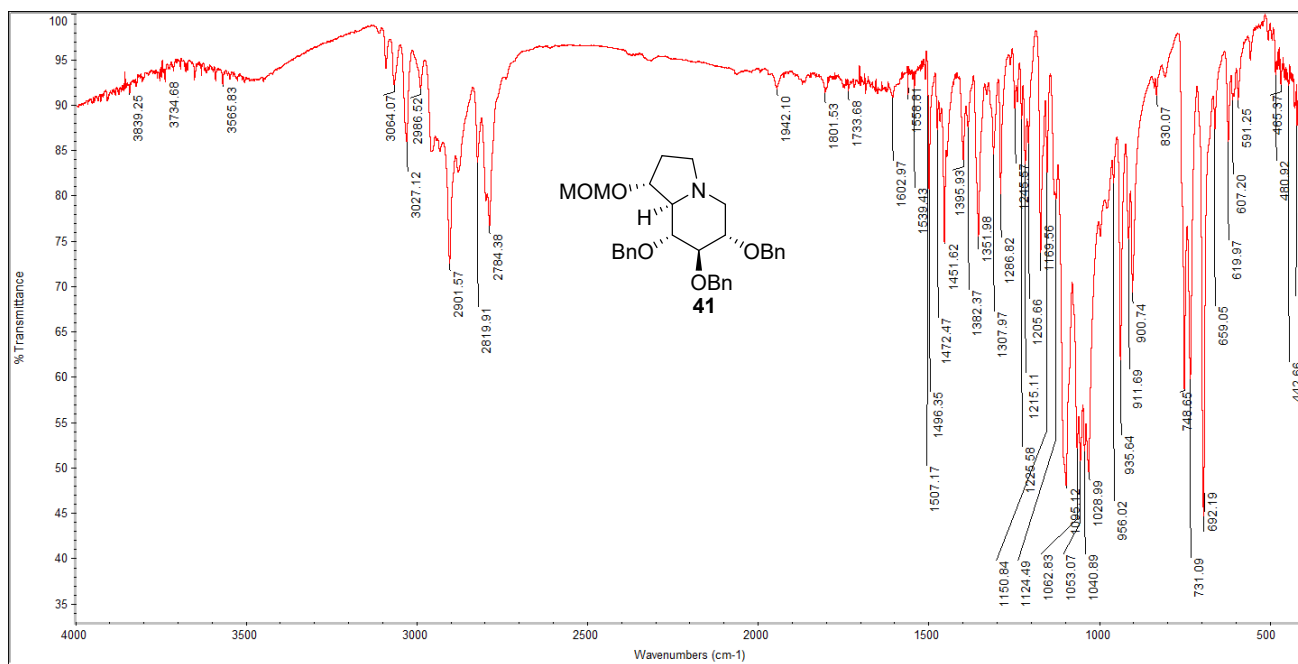
-176.81



Compound 41:

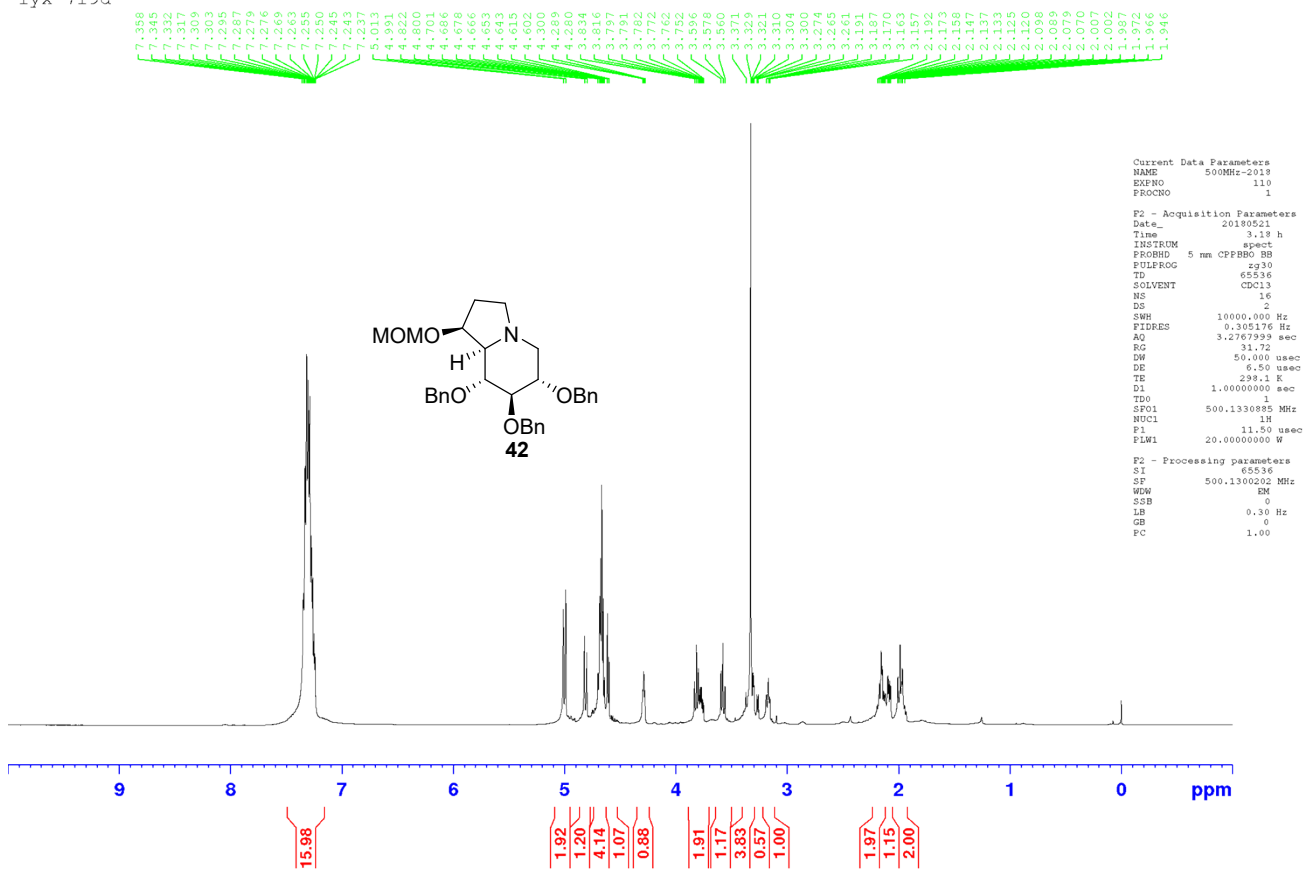
lyx-695b





Compound 42:

lyx-719d



lyx-719d

139.03  
138.94  
138.46  
128.42  
128.37  
127.97  
127.90  
127.70  
127.82  
127.70  
127.52  
127.47  
127.37

96.24

87.77  
79.28  
77.33  
77.12  
77.08  
76.82  
76.55  
75.50  
74.83  
74.68  
71.29

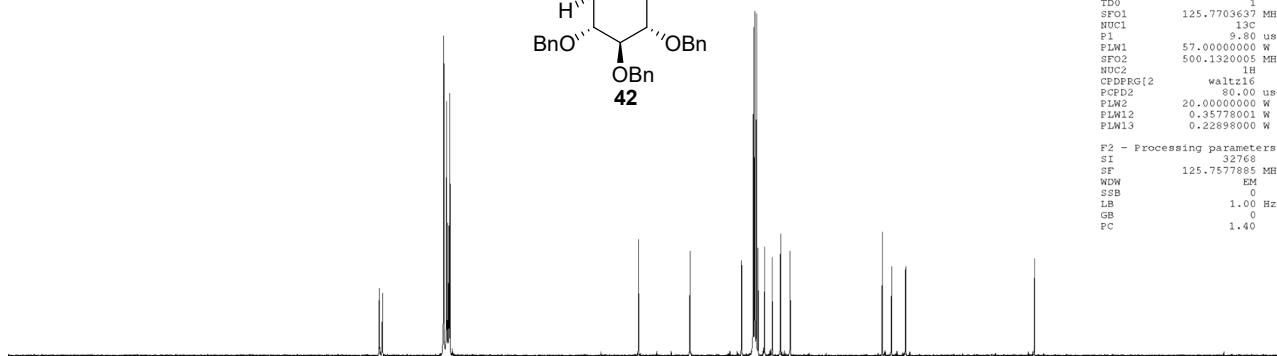
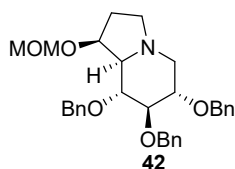
56.12  
54.61  
52.29

31.18

```
Current Data Parameters
NAME 500MHz-2018
EXPNO 111
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180521
Time 3.46 h
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 192.89
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1
SF01 125.7703637 MHz
NUC1 13C
P1 9.80 usec
PLW1 57.00000000 W
SF02 500.1320005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLM2 20.00000000 W
PLW2 0.35778001 W
FLM13 0.22898000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40
```



lyx-719d

128.42  
128.39  
128.37  
127.97  
127.90  
127.70  
127.82  
127.52  
127.37

96.24

87.77

79.28  
77.12  
76.55  
75.50  
74.23  
72.88  
71.29

56.12

54.61

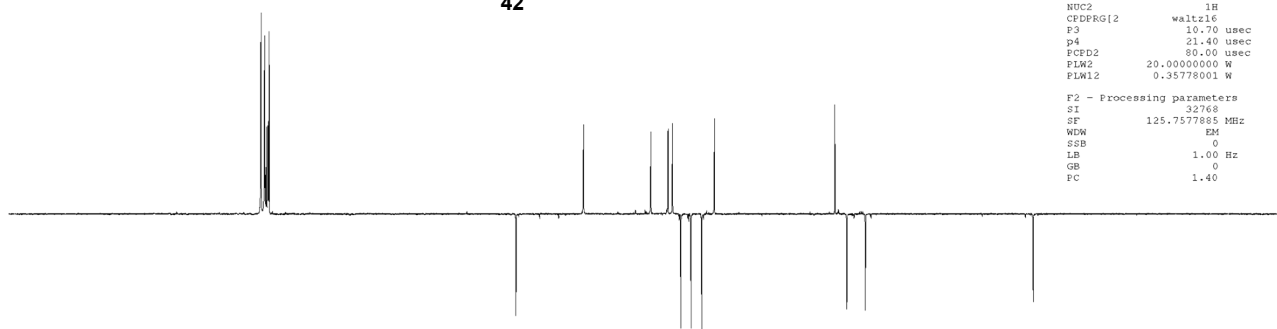
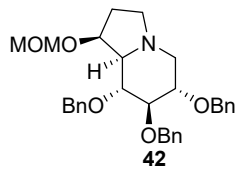
52.29

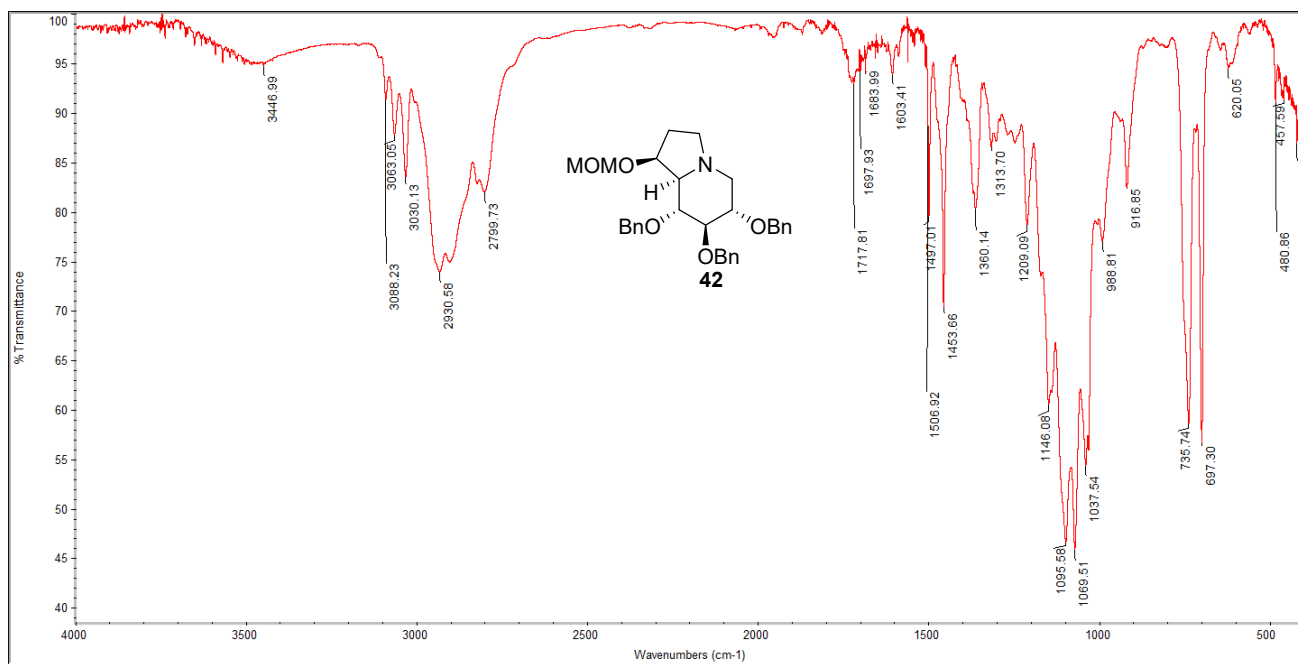
31.18

```
Current Data Parameters
NAME 500MHz-2018
EXPNO 112
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180521
Time 4.02 h
INSTRUM spect
PROBHD 5 mm CFPBBO BB
PULPROG deptcp135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 20161.291 Hz
FIDRES 0.615274 Hz
AQ 1.6252928 sec
RG 192.89
DW 24.800 usec
DE 18.00 usec
TE 298.2 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344928 sec
d12 0.00002000 sec
DELTA 0.00001248 sec
TDO 1
SF01 125.7678486 MHz
NUC1 13C
P1 9.80 usec
PL1 2000.00 usec
FLW0 0 W
FLW1 57.00000000 W
SFRAM(5) crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SFW5 8.36410046 W
SF02 500.1315985 MHz
NUC2 1H
CPDPRG2 waltz16
P3 10.70 usec
P4 21.40 usec
PCPD2 80.00 usec
PLM2 20.00000000 W
FLW2 0.35778001 W

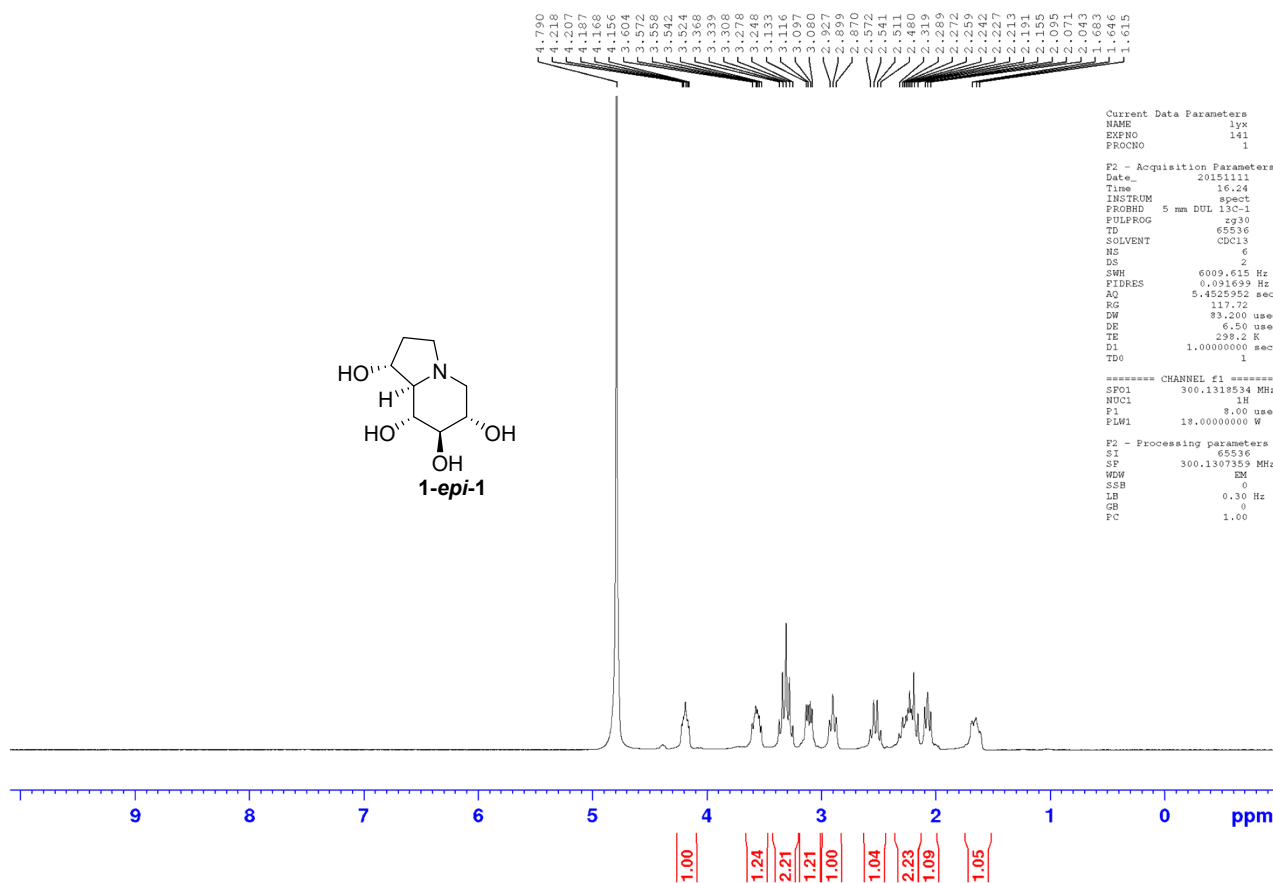
F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40
```





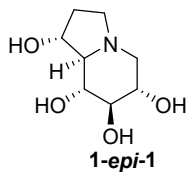
Compound **1-epi-1**:

lyx-538



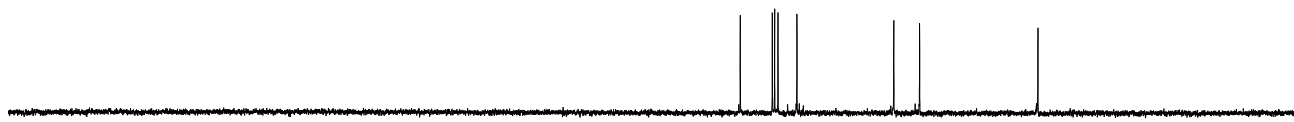
lyx-538-C13

81.19  
76.21  
75.85  
75.32  
72.38  
57.34  
53.33  
34.94



```
NAME lyx
EXPNO 142
PROCNO 1
Date_ 20151111
Time 16.26
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 58
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 209.09
DW 27.733 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
```

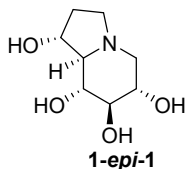
```
===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 11.00 usec
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

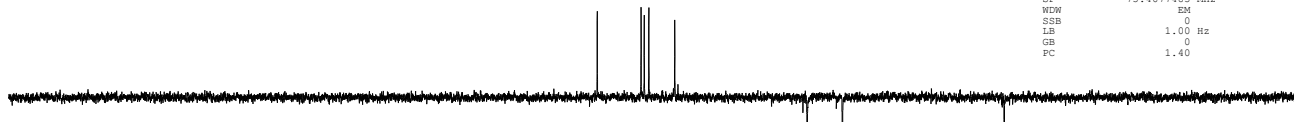
lyx-538-dept135

81.19  
76.21  
75.85  
72.39  
57.34  
53.33  
34.95



```
NAME lyx
EXPNO 143
PROCNO 1
Date_ 20151111
Time 16.21
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG deptg135
TD 65536
SOLVENT CDCl3
NS 33
DS 4
SWH 12077.295 Hz
FIDRES 0.184285 Hz
AQ 2.7132404 sec
RG 209.09
TW 41.400 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.00000000 sec
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TDO 1
```

```
===== CHANNEL f1 =====
SFO1 75.4737856 MHz
NUC1 13C
P1 11.00 usec
P13 2000.00 usec
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

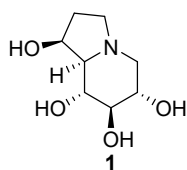
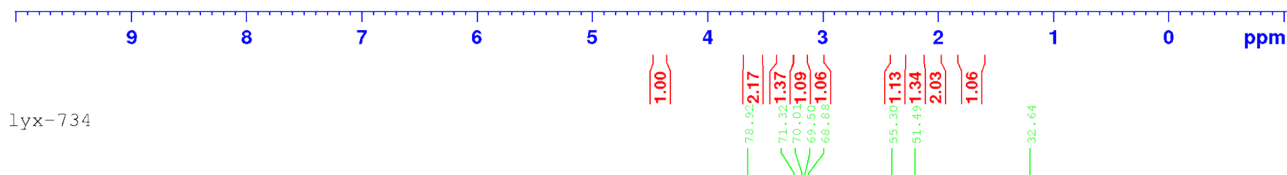
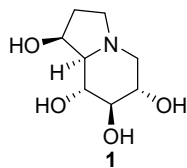
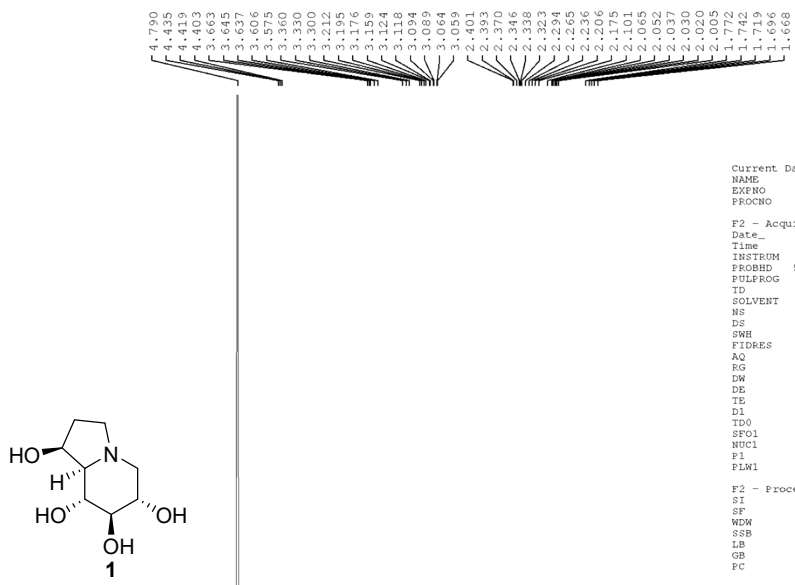


140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



Compound 1:

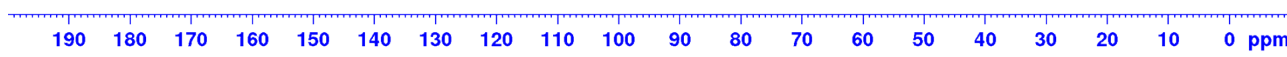
lyx-734



Current Data Parameters  
 NAME lyx-2018  
 EXPNO 384  
 PROCNO 1

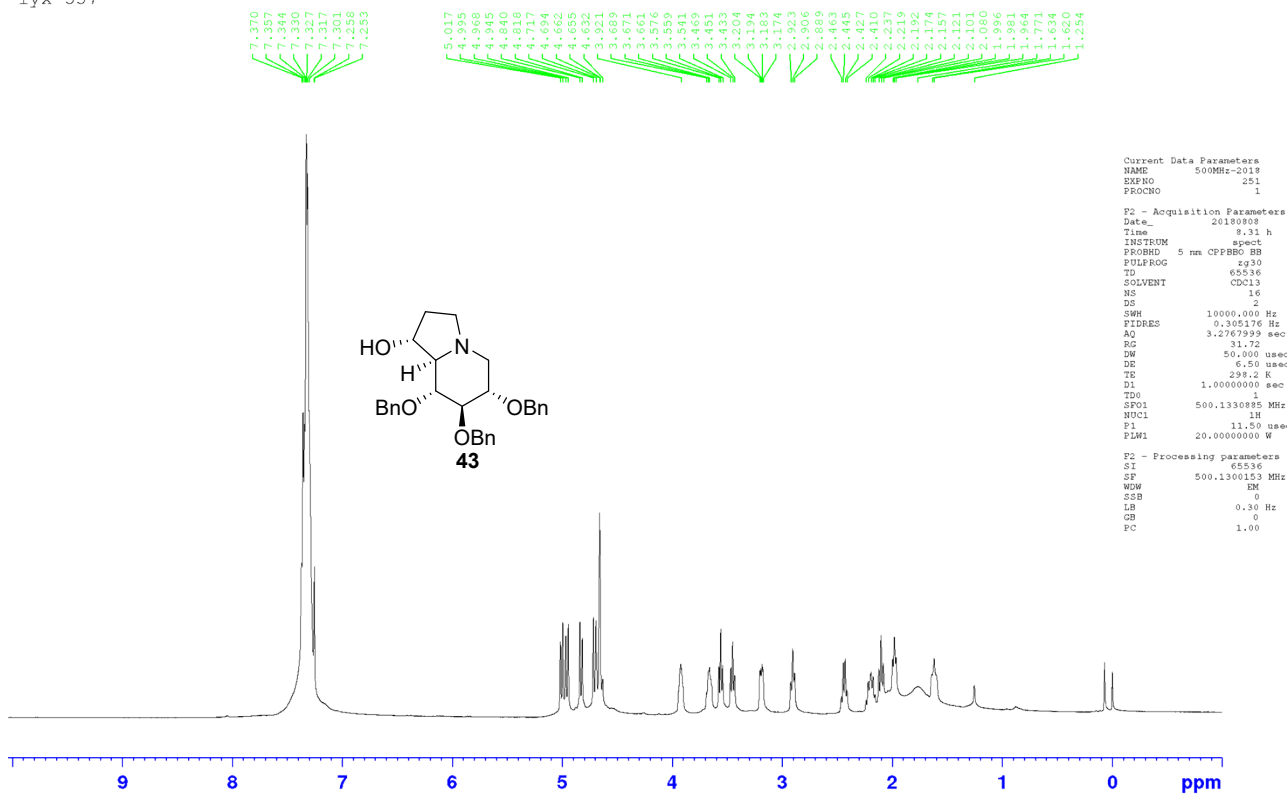
F2 - Acquisition Parameters  
 Date\_ 20180528  
 Time 14:10 h  
 INSTRUM spect  
 PROBHD 5 mm DUL 13c-1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT D2O  
 NS 121  
 DS 4  
 SWH 18028.844 Hz  
 FIDRES 0.550197 Hz  
 AQ 1.8175317 sec  
 RG 209.09  
 DM 27.733 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.0000000 sec  
 d11 0.03000000 sec  
 DELTA 1.8999999 sec  
 TD0 1  
 SFO1 75.4752949 MHz  
 NUC1 13C  
 P1 11.00 usec  
 PLW1 135.0000000 W  
 SFO2 300.1312063 MHz  
 NUC2 1H  
 CDEPRG12 waltz16  
 PDE2 30.00 usec  
 PFM2 14.00000000 W  
 PFM12 0.17284000 W  
 PFM13 0.14000000 W

F2 - Processing parameters  
 SI 32768  
 SF 75.4677423 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

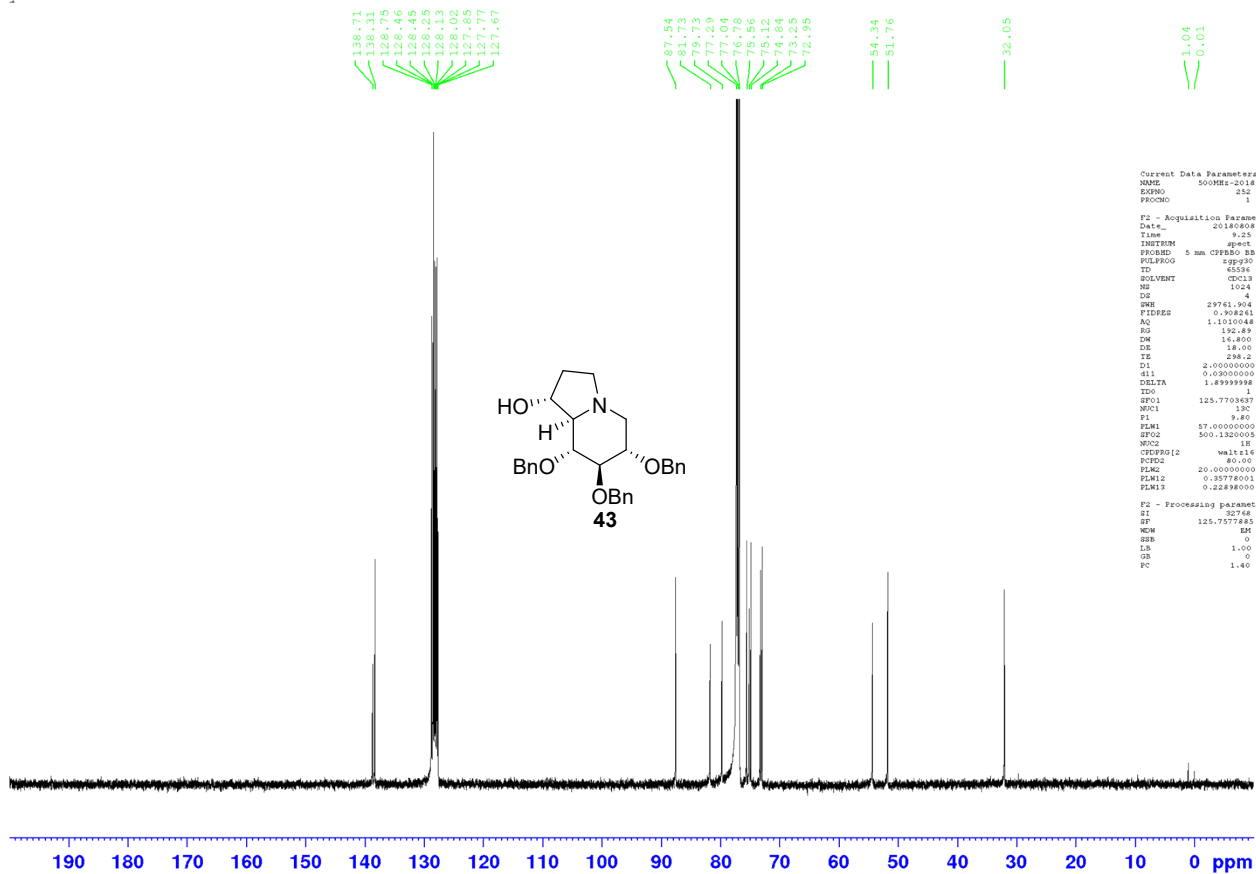


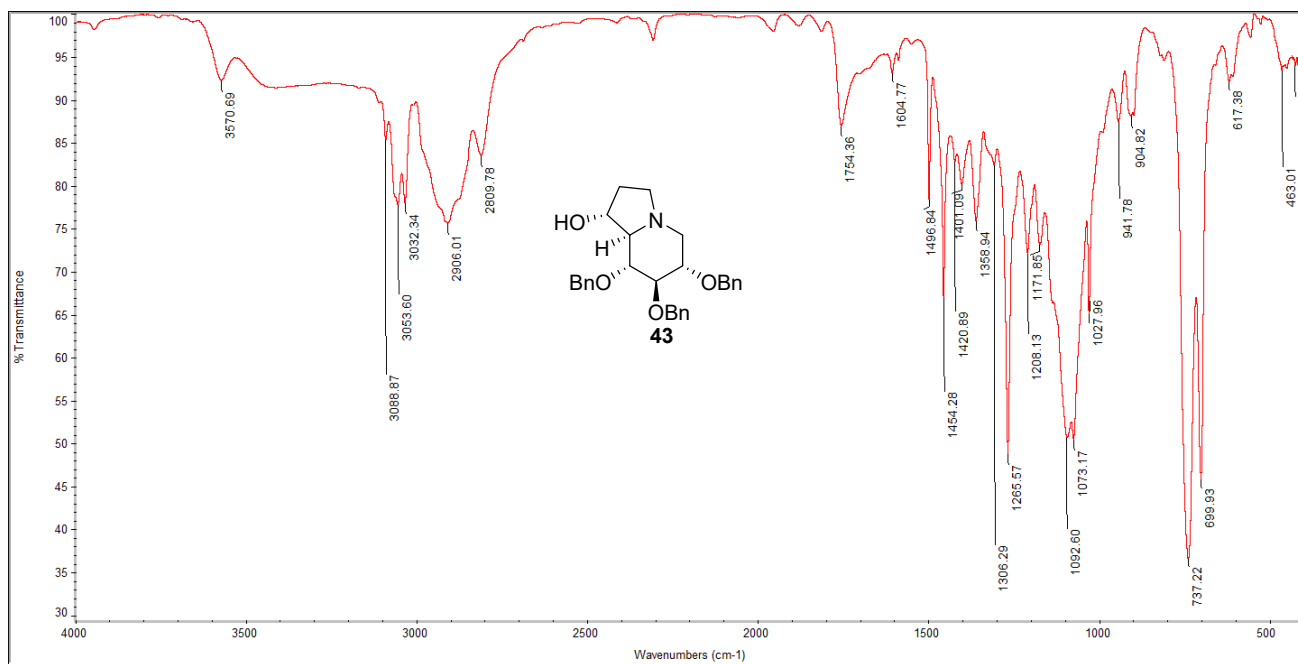
Compound 43:

lyx-537



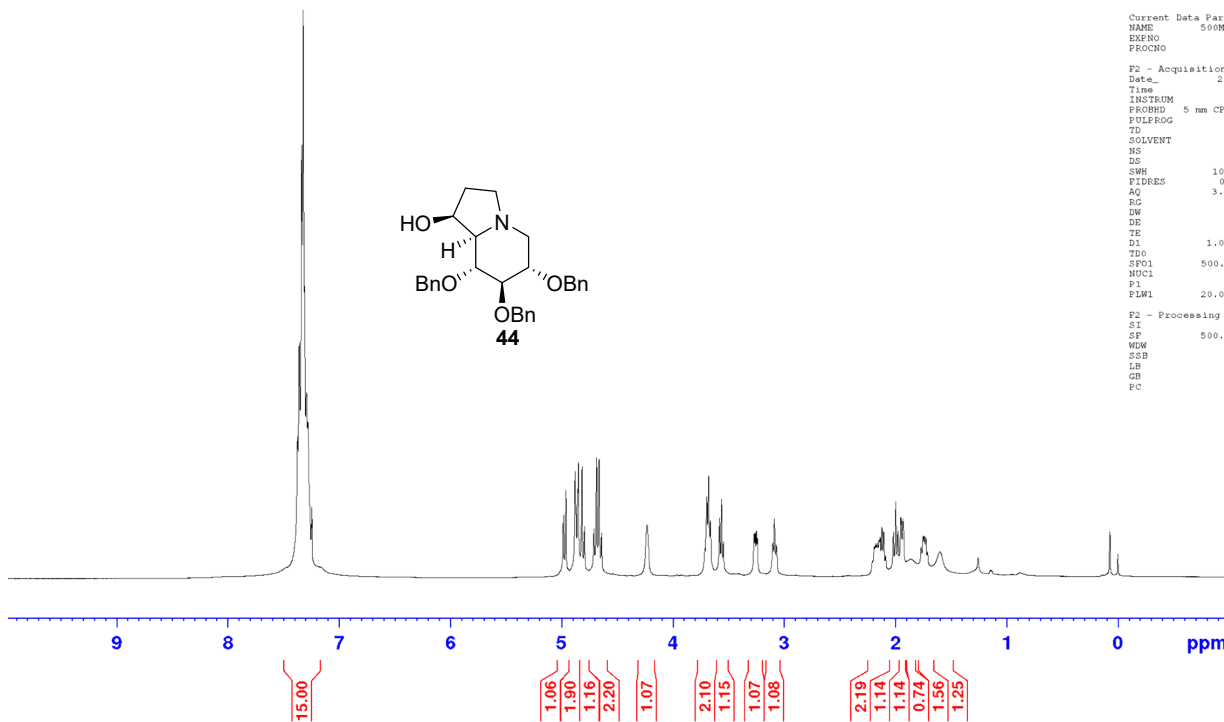
lyx-537





Compound 44:

lyx-542



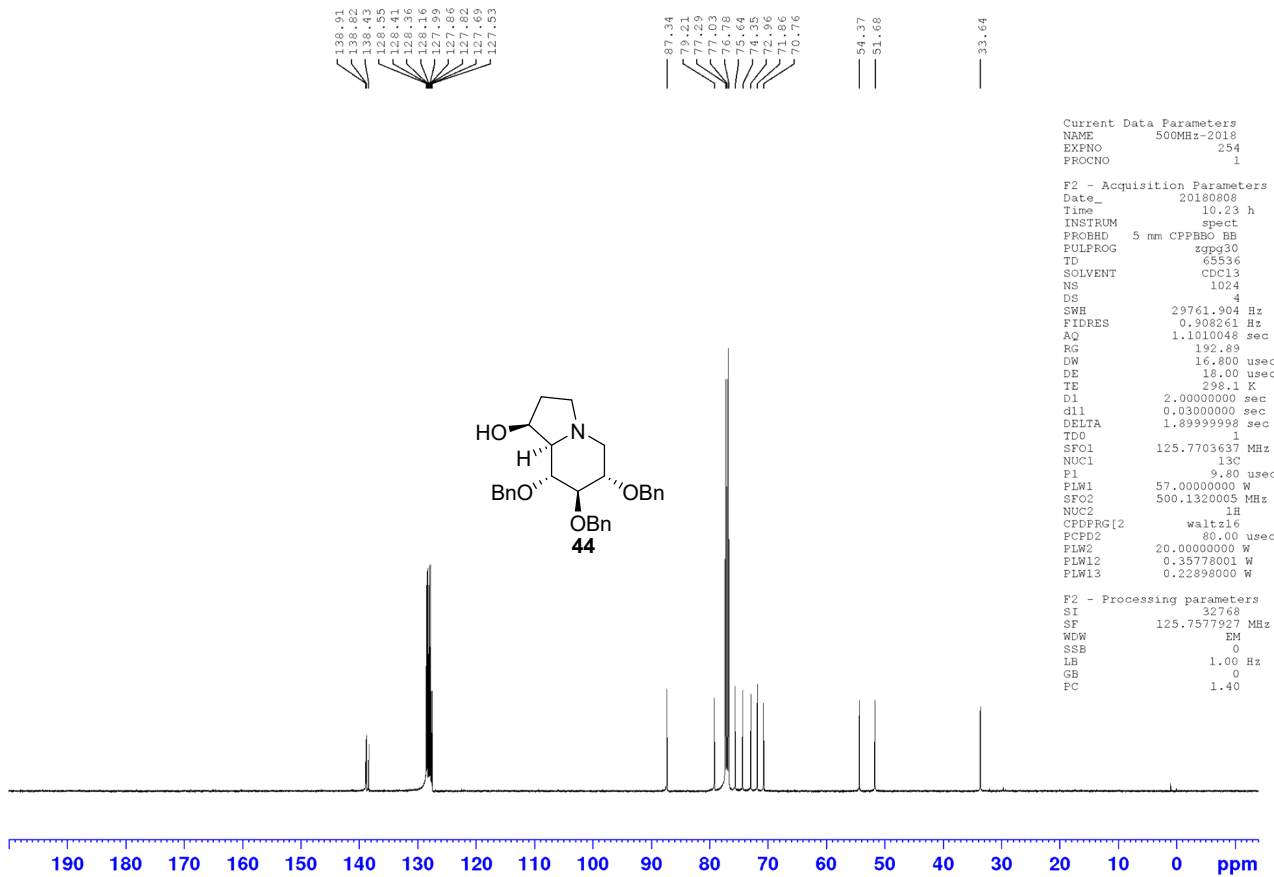
```

Current Data Parameters
NAME      500MHz-2018
EXPNO    253
PROCNO   1

F2 - Acquisition Parameters
Date_    20180809
Time     9.28 h
INSTRUM  spect
PROBHD   5 mm CPBPRB B3
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       16
DS       2
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       3.276739 sec
RG       31.72
DM       50.000 usec
DE       6.50 usec
TE       298.2 K
D1       1.00000000 sec
TDO      1
SFO1     500.1330885 MHz
NUC1     1H
P1       11.50 usec
PL1      20.00000000 W

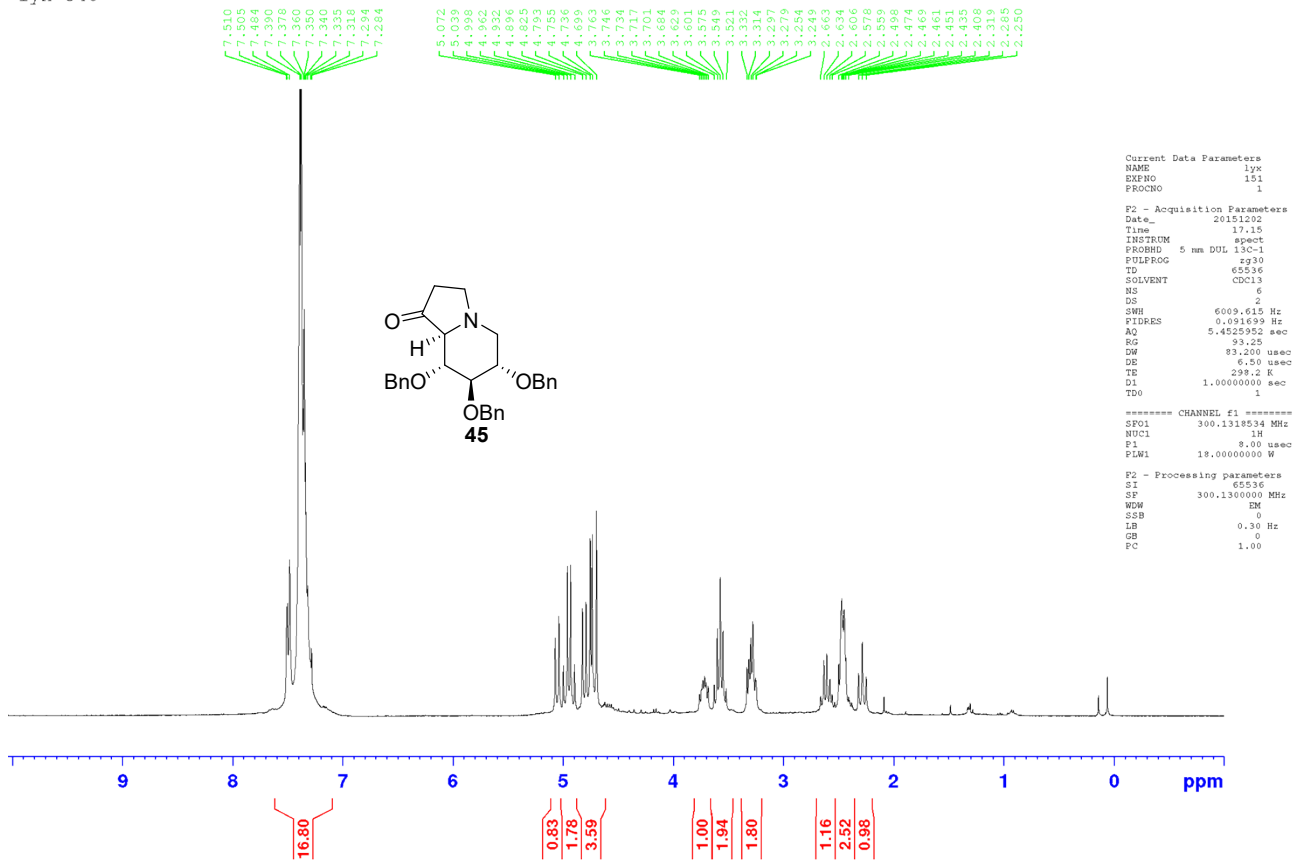
F2 - Processing parameters
SI       65536
SF       500.1330883 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

lyx-542

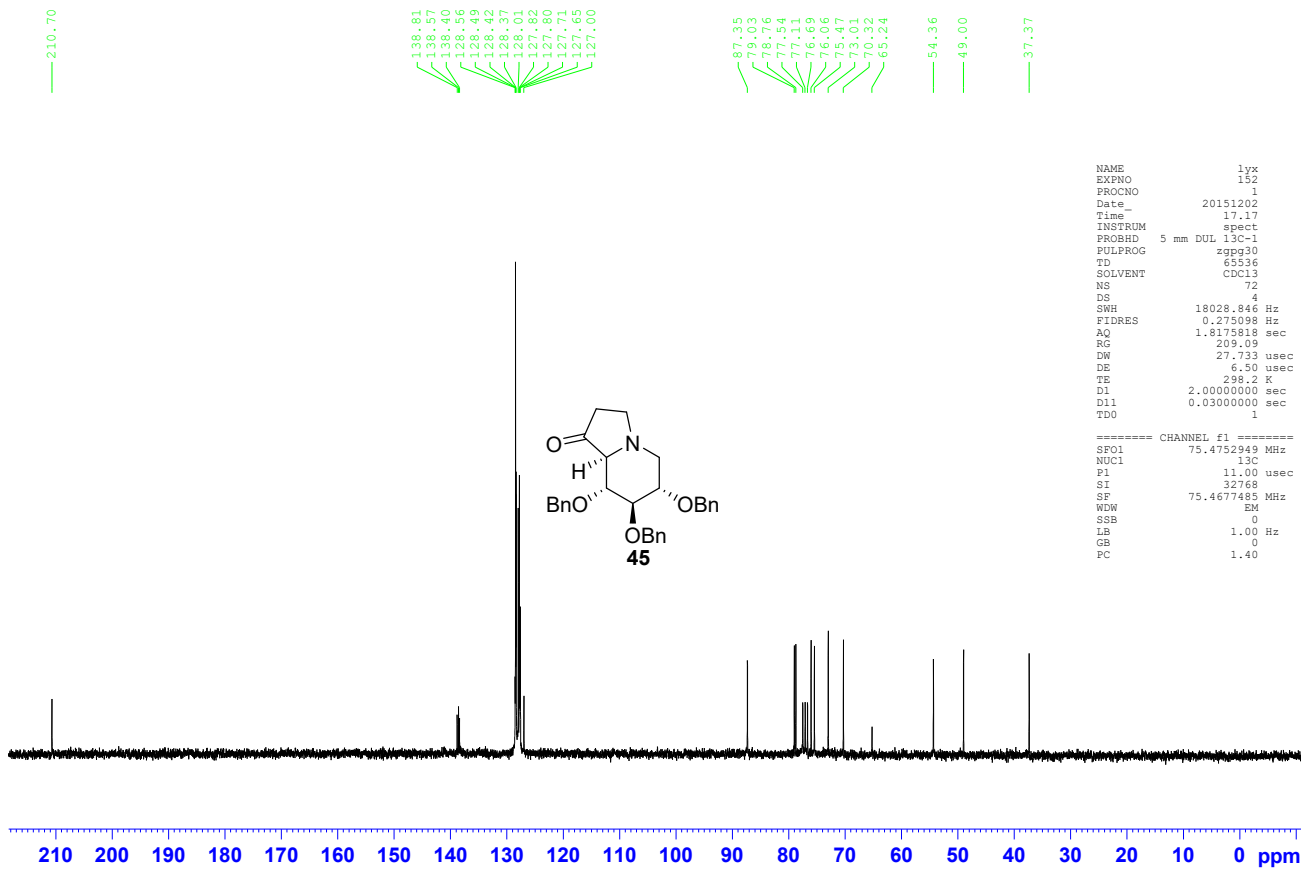


Compound 45:

lyx-540



lyx-540-C13



```

NAME lyx
EXPNO 152
PROCNO 1
Date_ 20151202
Time 17.17
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 72
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 209.09
DW 27.733 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

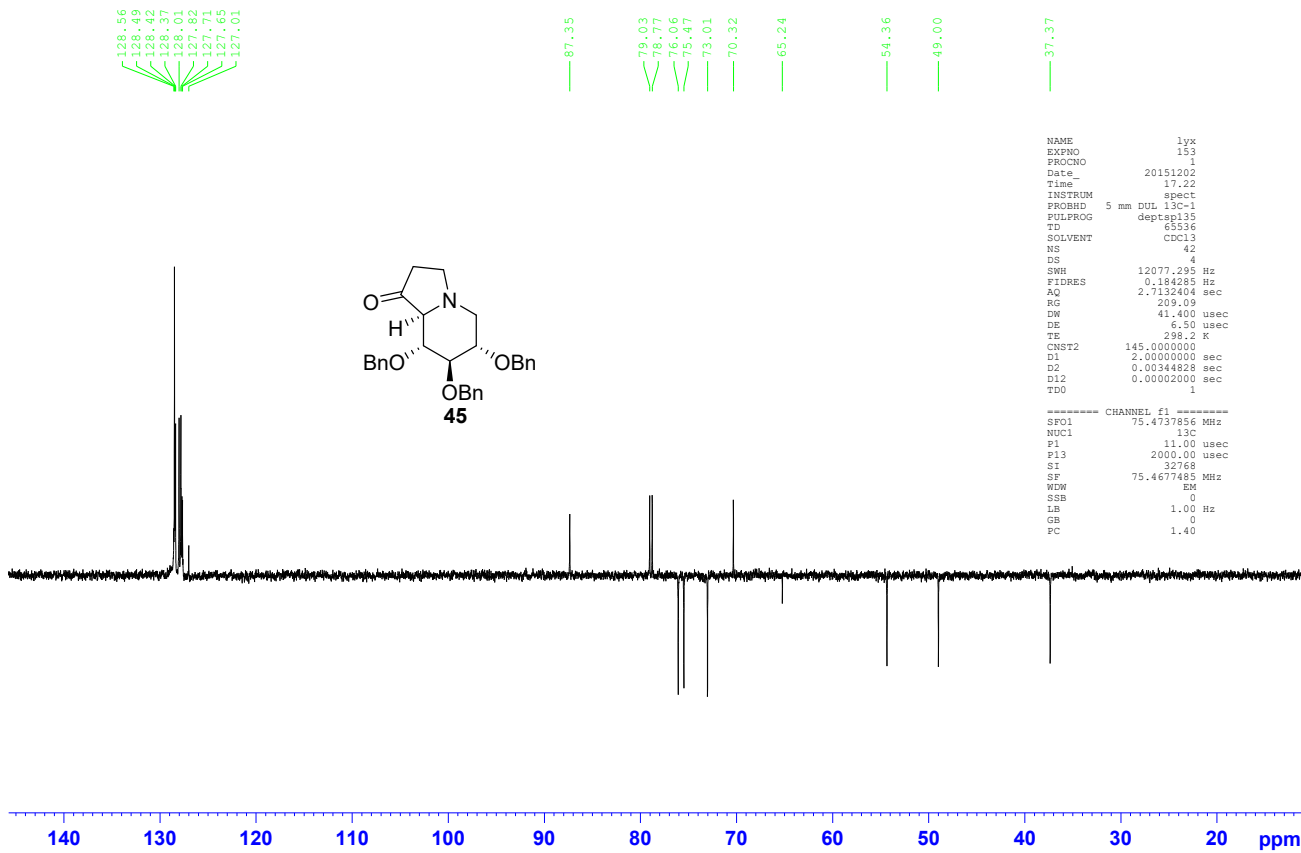
```

```

===== CHANNEL f1 =====
SFO1 75.4752949 MHz
NUC1 13C
P1 11.00 usec
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```

lyx-540-dept135



```

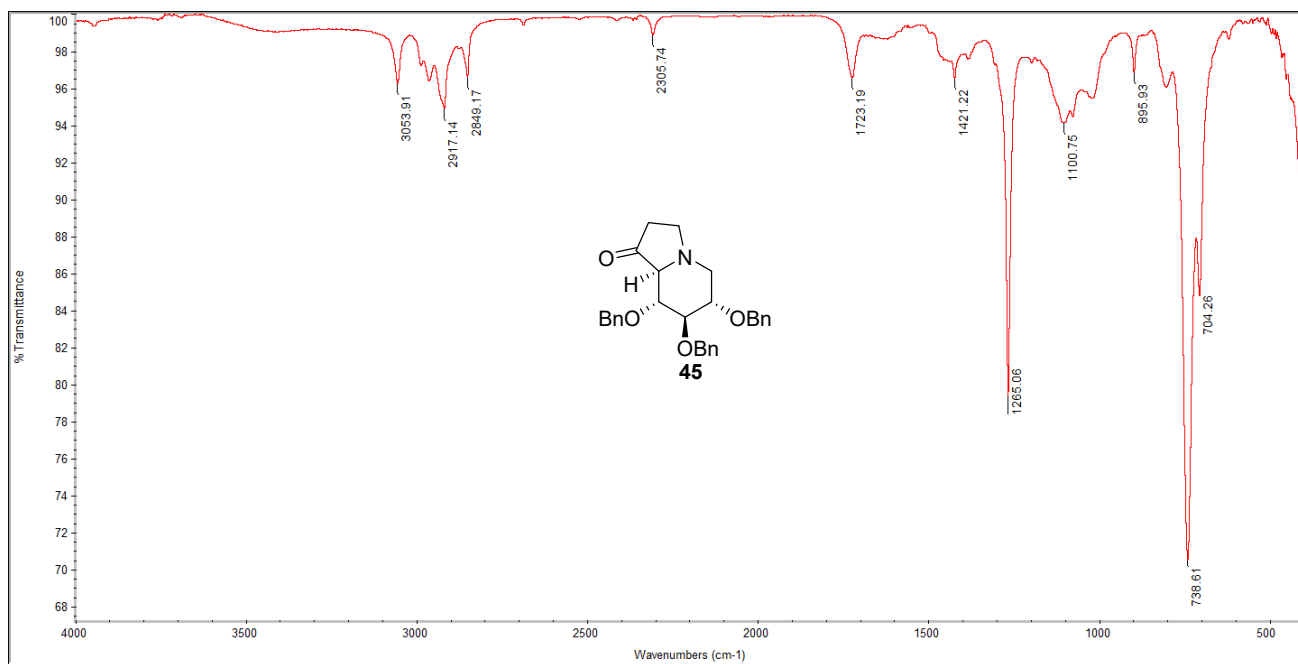
NAME lyx
EXPNO 153
PROCNO 1
Date_ 20151202
Time 17.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 42
DS 4
SWH 12077.295 Hz
FIDRES 0.184285 Hz
AQ 2.7132404 sec
RG 209.09
DW 41.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.0000200 sec
TDO 1

```

```

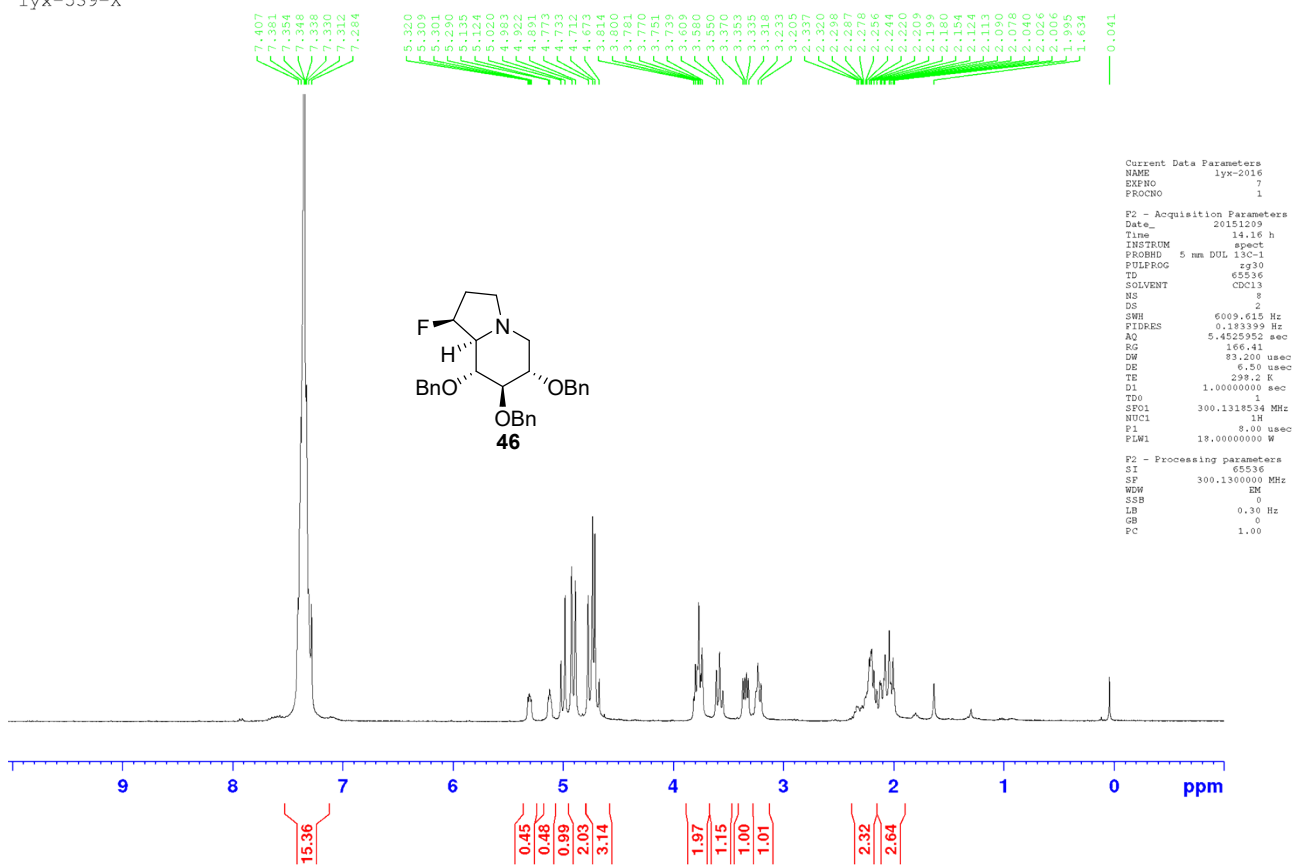
===== CHANNEL f1 =====
SFO1 75.4737856 MHz
NUC1 13C
P13 2000.00 usec
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```

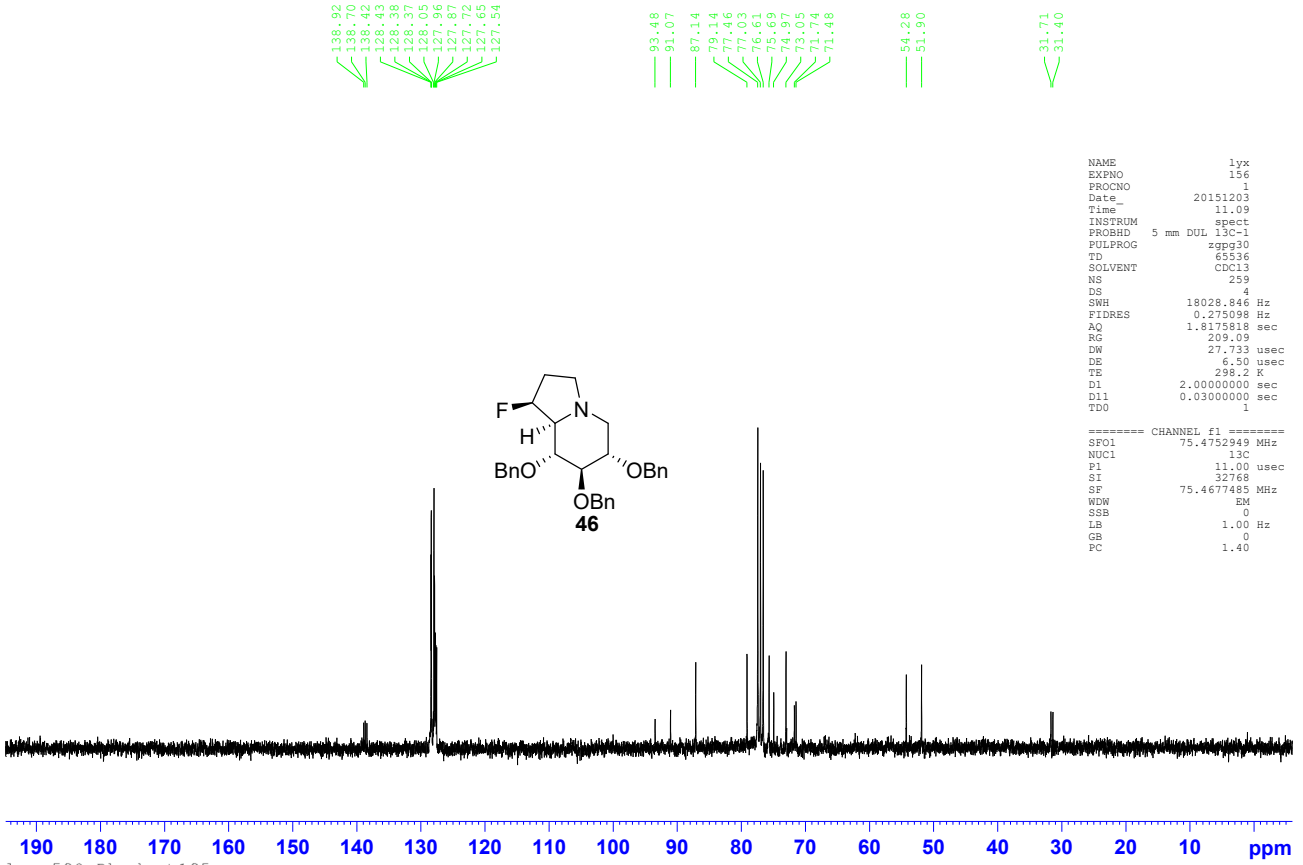


Compound 46:

lyx-539-X



lyx-539-Db-C13

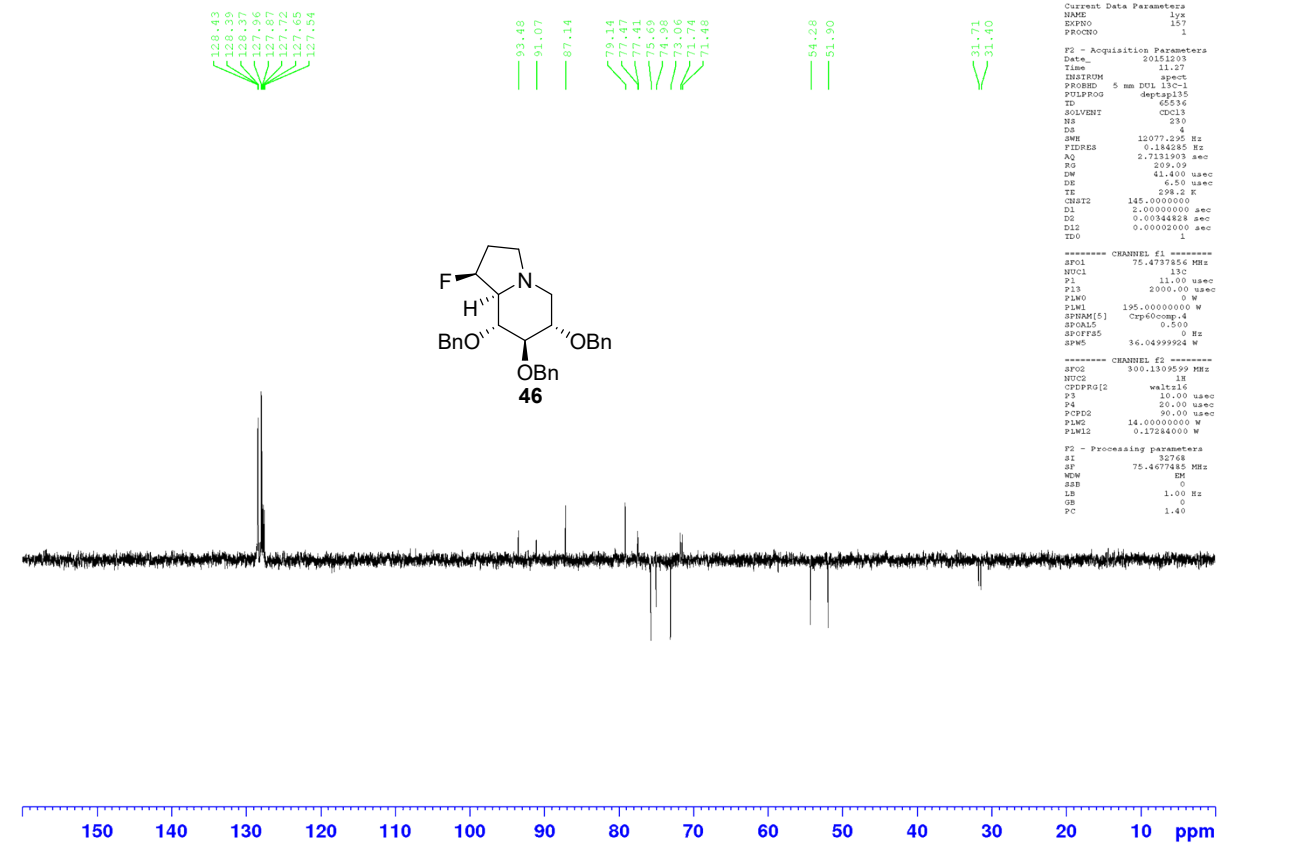


```

NAME          lyx
EXPNO         156
PROCNO        1
Date_         20151203
Time          11.09
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            259
DS            4
SWH           18028.846 Hz
FIDRES        0.275098 Hz
AQ            1.8175818 sec
RG            209.09
DW            27.733 usec
DE            6.50 usec
TE            298.2 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

===== CHANNEL f1 =====
SF01          75.4752949 MHz
NUC1          13C
P1            11.00 usec
SI            32768
SF            75.4677485 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

lyx-539-Db-dept135



```

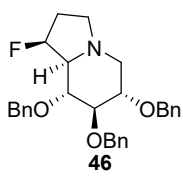
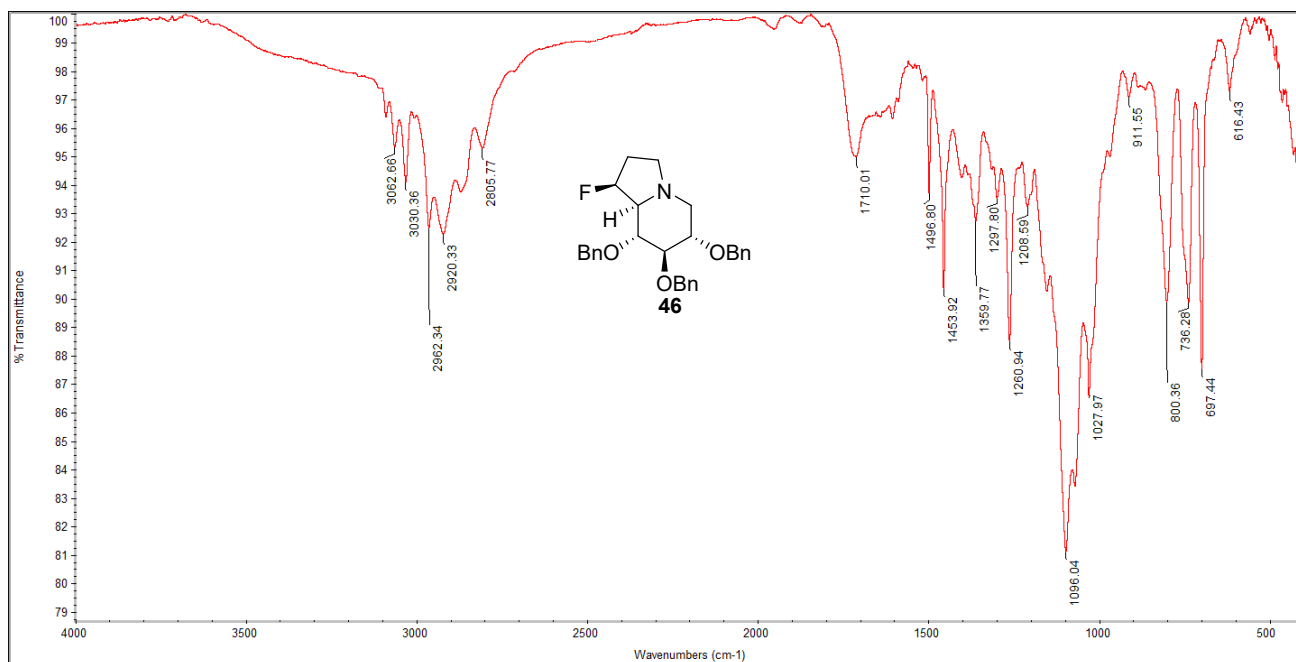
Current Data Parameters
NAME          lyx
EXPNO         157
PROCNO        1

F2 - Acquisition Parameters
Date_         20151203
Time          11.27
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       dept135
TD            65536
SOLVENT       CDCl3
NS            250
DS            4
SWH           12077.296 Hz
FIDRES        0.184285 Hz
AQ            2.123393 sec
RG            209.09
DW            41.400 usec
DE            6.50 usec
TE            298.2 K
CHX2          145.0000000 sec
D1            2.0000000 sec
DE            0.0084888 sec
D12           0.0000200 sec
TD0           1

===== CHANNEL f1 =====
SF01          75.4737856 MHz
NUC1          13C
P1            11.00 usec
P13           2000.00 usec
PLM0          0 W
PLM1          195.00000000 W
SPCAL5        0.500
SFOFF15       0 Hz
SPW5          36.04999924 W

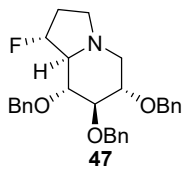
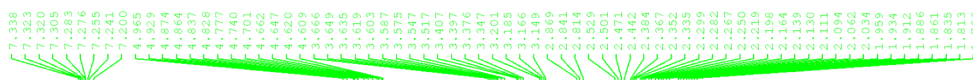
===== CHANNEL f2 =====
SF02          300.1309599 MHz
NUC2          135
CPDPRG2       waltz16
P3            10.00 usec
P4            20.00 usec
PCPD2        90.00 usec
PLM2          14.00000000 W
PLW2          0.17244000 W

F2 - Processing parameters
SI            32768
SF            75.4677485 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```



Compound 47:

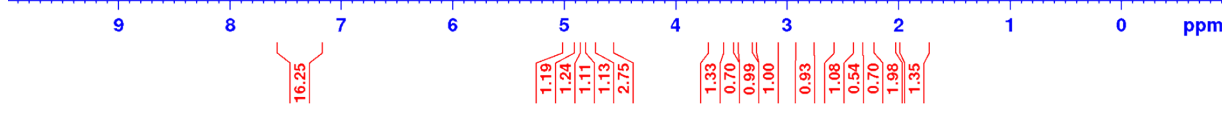
lyx-781



Current Data Parameters  
 NAME lyx-2018  
 EXNO 439  
 PROCNO 1

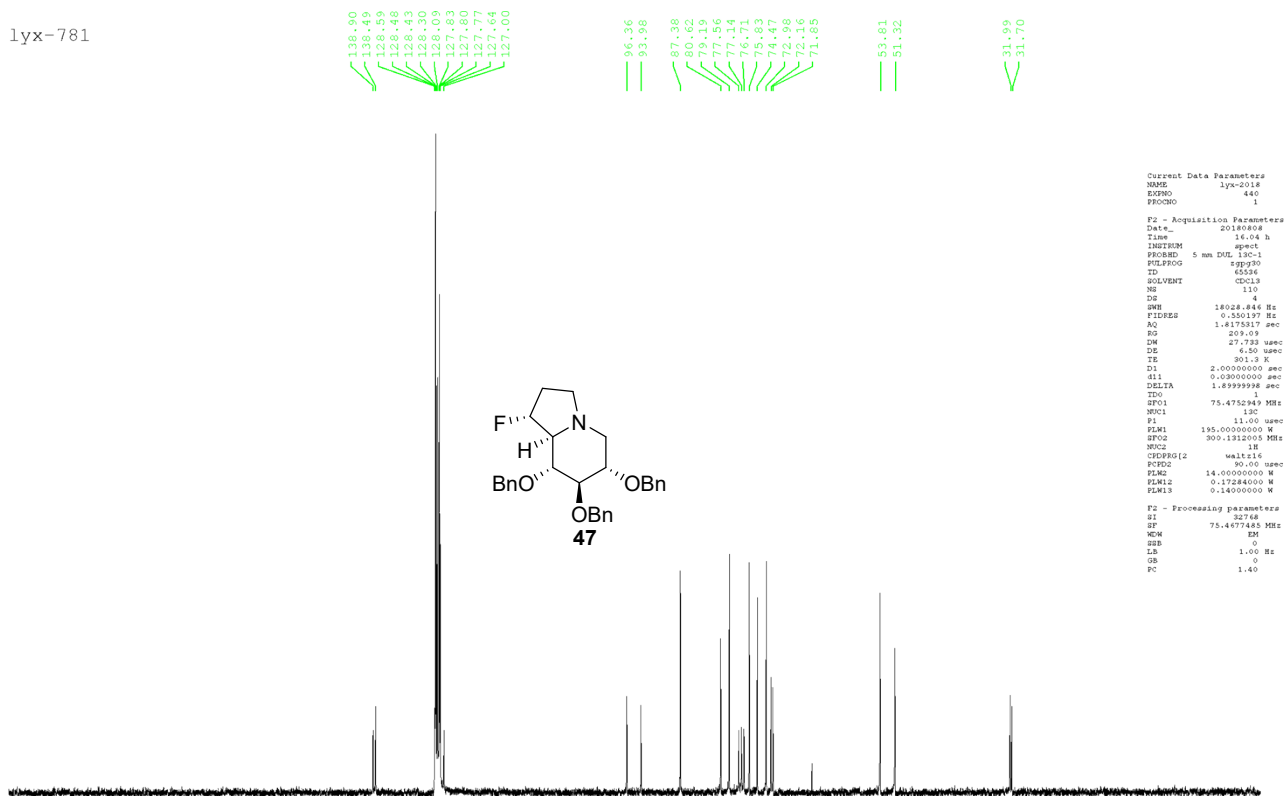
F2 - Acquisition Parameters  
 Date: 20180908  
 Time: 16.02 h  
 INSTRUM spect  
 PROBHD 5 mm DUL 15c-1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6009.615 Hz  
 FIDRES 0.188399 Hz  
 AQ 5.4525952 sec  
 RG 82.09  
 SW 83.400 usec  
 DE 6.50 usec  
 TE 301.1 K  
 D1 1.00000000 sec  
 TDO 1  
 SPOL 300.1318534 MHz  
 NUCL 1H  
 P1 8.00 usec  
 PLWL 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 300.1300251 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

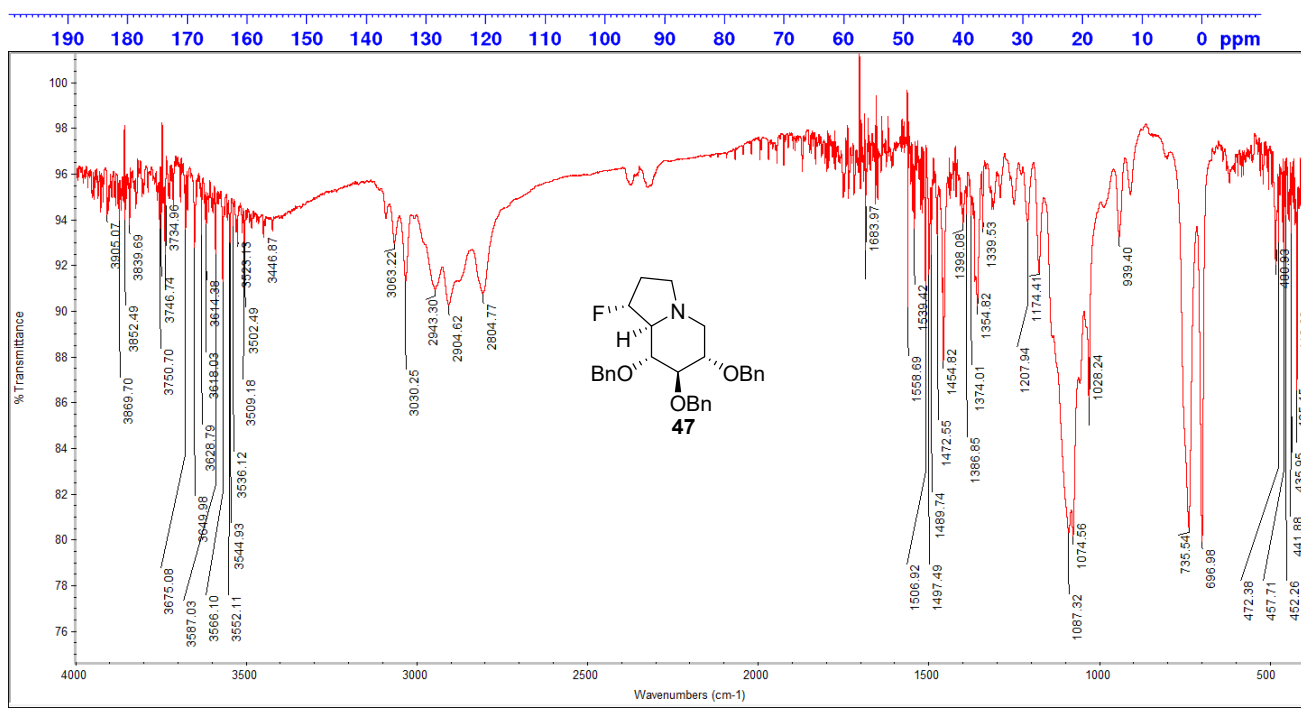




lyx-781

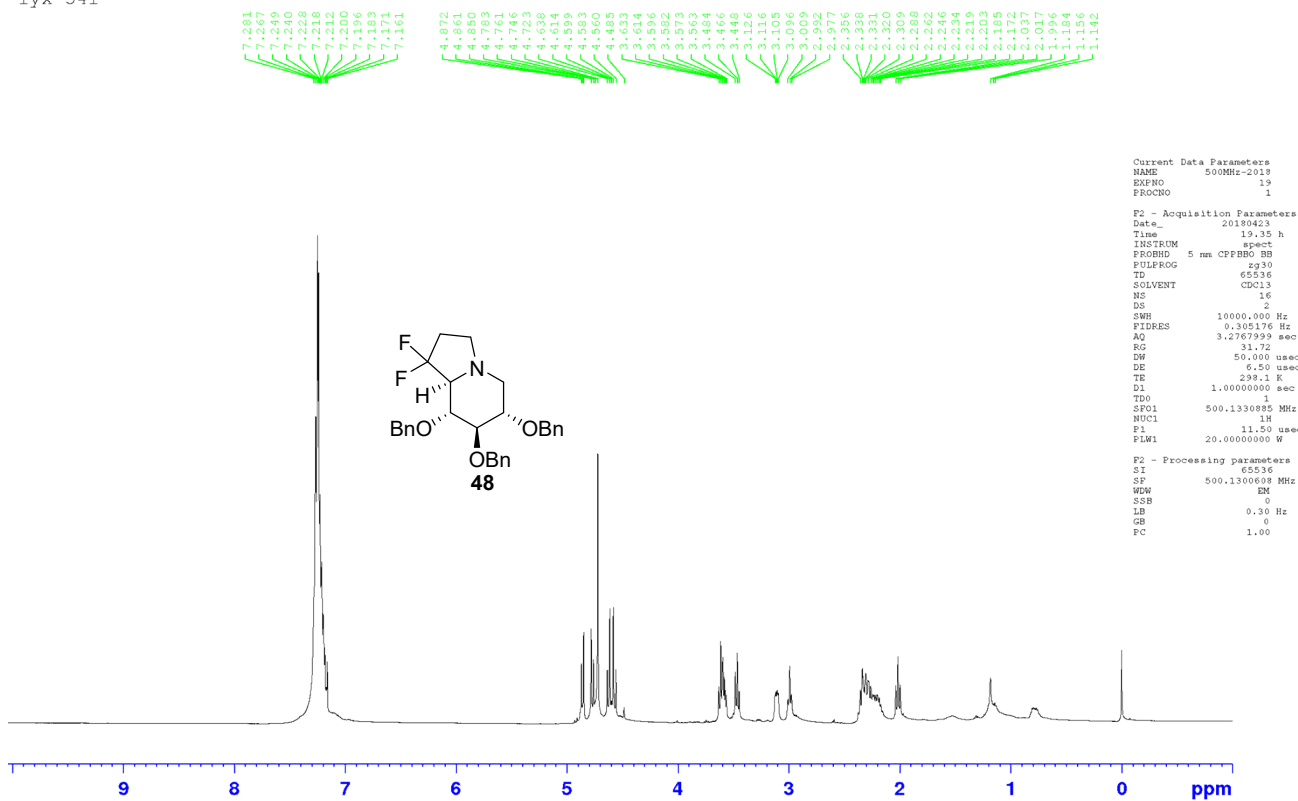


Current Data Parameters  
 NAME: lyx-2018  
 EXPNO: 480  
 SFOCNO: 1  
 F2 - Acquisition Parameters  
 Date\_: 20180808  
 Time: 14.04 h  
 INSTRUM: spect  
 PROBD: 5 mm DOL 13C-1  
 PULPROG: zgpg30  
 ID: 65336  
 SOLVENT: CDCl3  
 NS: 110  
 DS: 4  
 SWH: 18028.844 Hz  
 FIDRES: 0.350197 Hz  
 AQ: 1.8175317 sec  
 RG: 309.50  
 DM: 27.732 usec  
 DE: 8.50 usec  
 TE: 301.2 K  
 D1: 2.0000000 sec  
 d11: 0.0300000 sec  
 DELTA: 1.8999998 sec  
 ZD0:  
 SFO1: 75.4752949 MHz  
 NUC1: 13C  
 P1: 11.00 usec  
 PL1: 195.0000000 M  
 SFO2: 300.1312005 MHz  
 NUC2: 1H  
 P2: 14.0000000 usec  
 PL2: 0.0000000 M  
 PLM12: 0.17284000 M  
 PLM13: 0.14000000 M  
 F2 - Processing parameters  
 SI: 32768  
 SF: 75.4677485 MHz  
 MEW: EM  
 HSB: 1.00 Hz  
 LB: 0  
 GB: 1.40

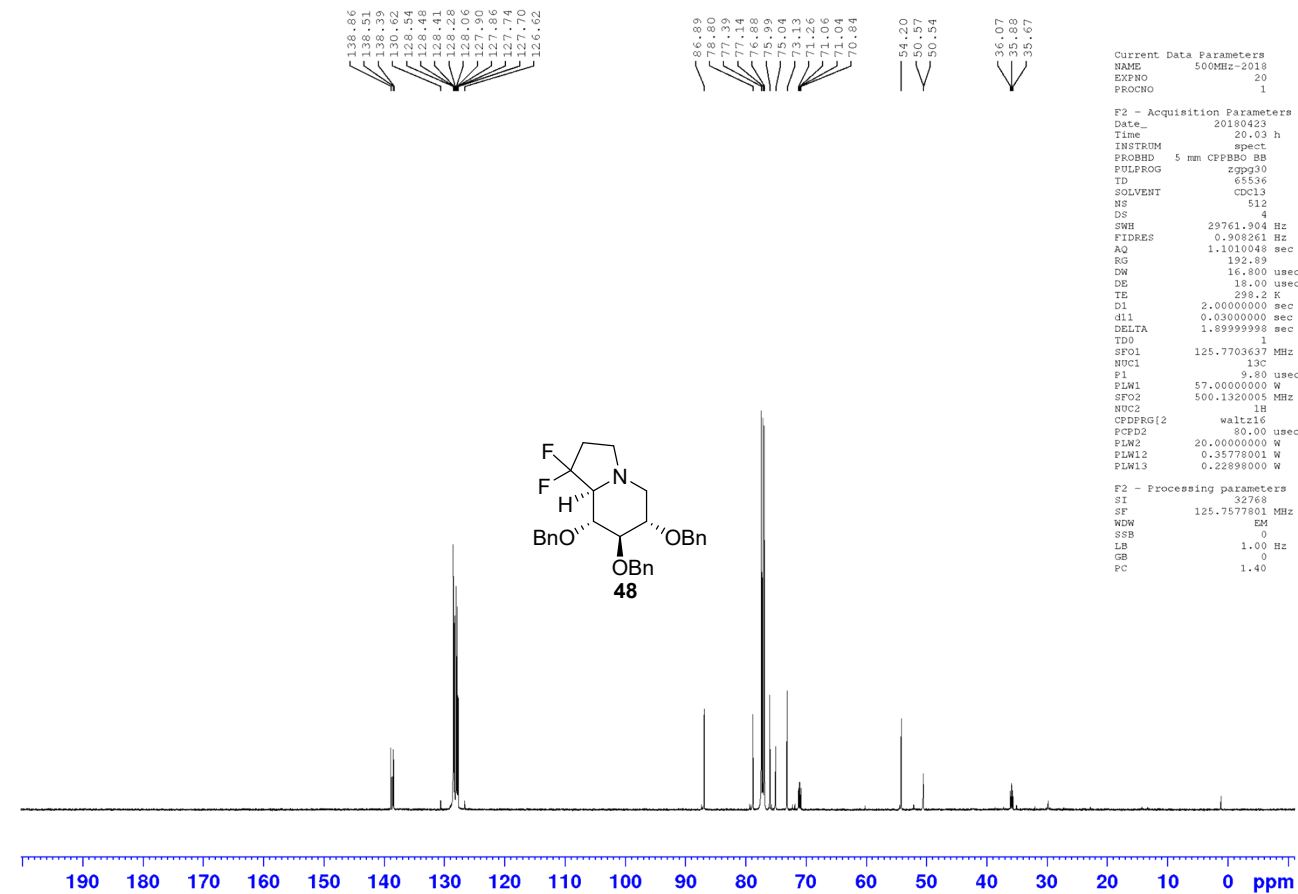


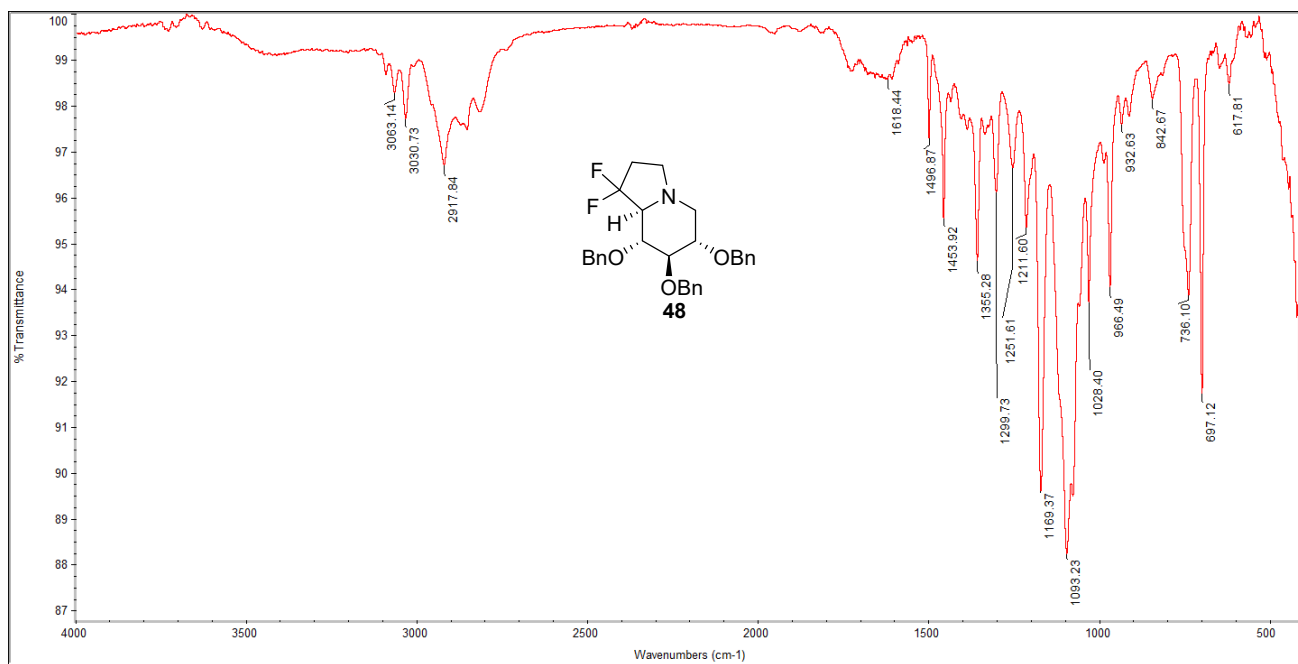
Compound 48:

lyx-541



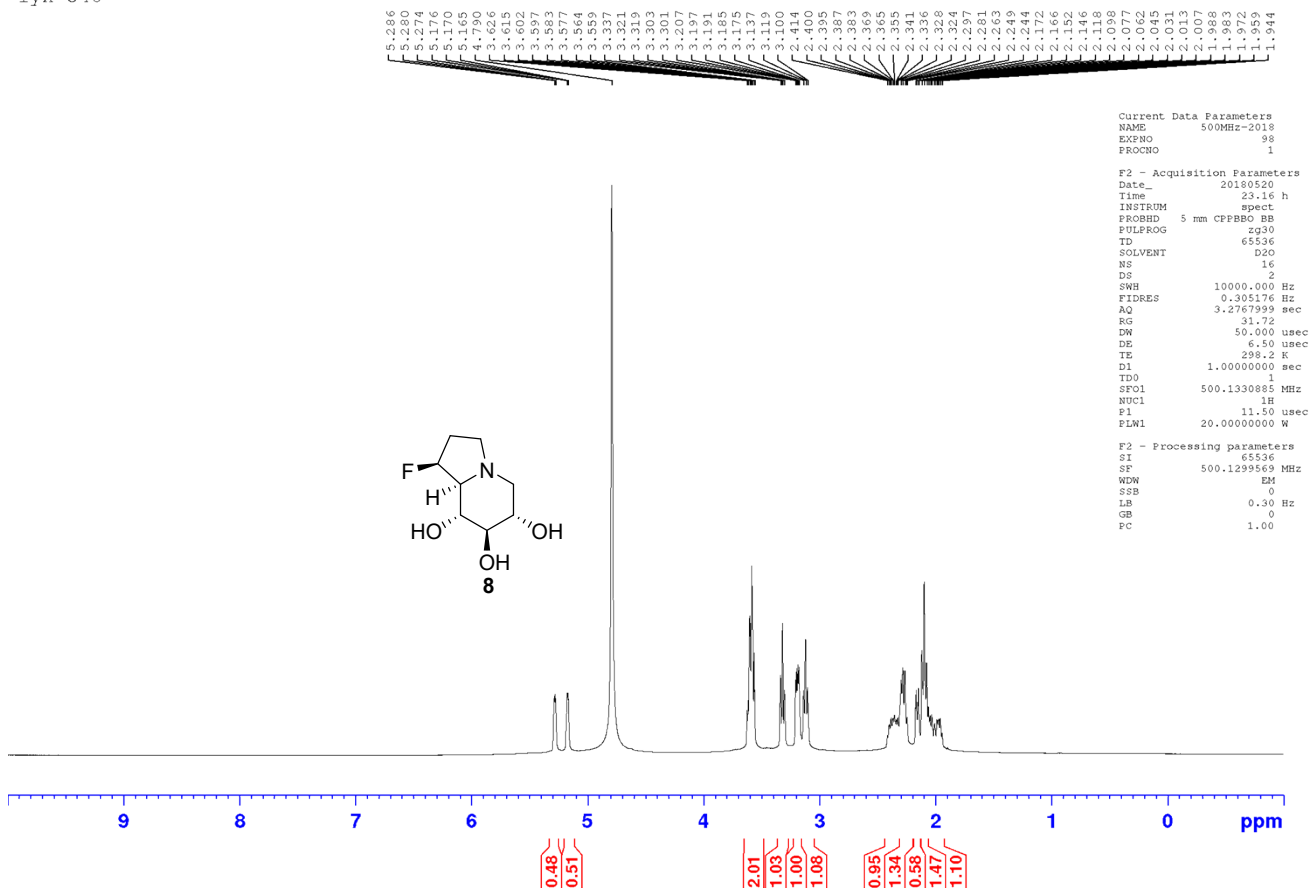
lyx-541



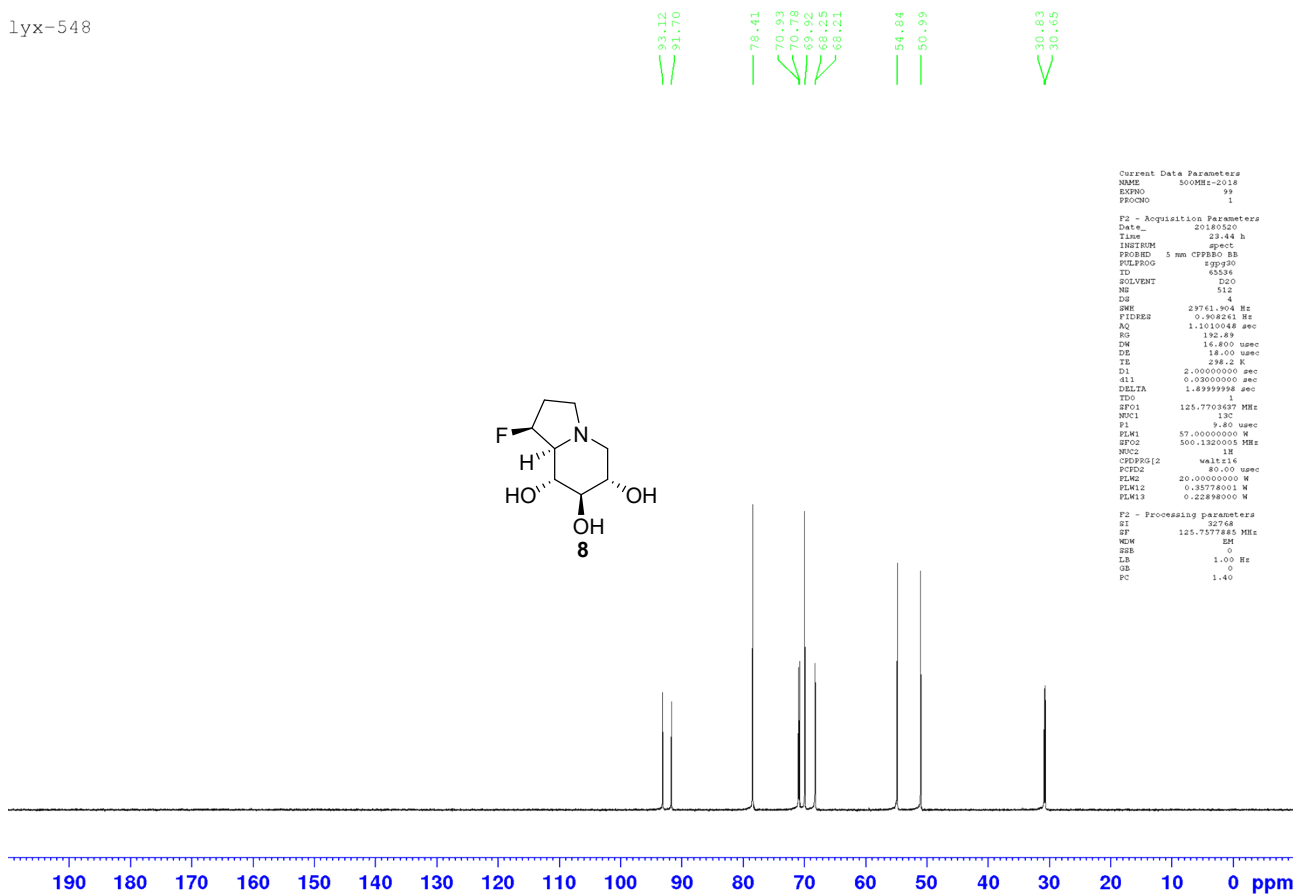


Compound 8:

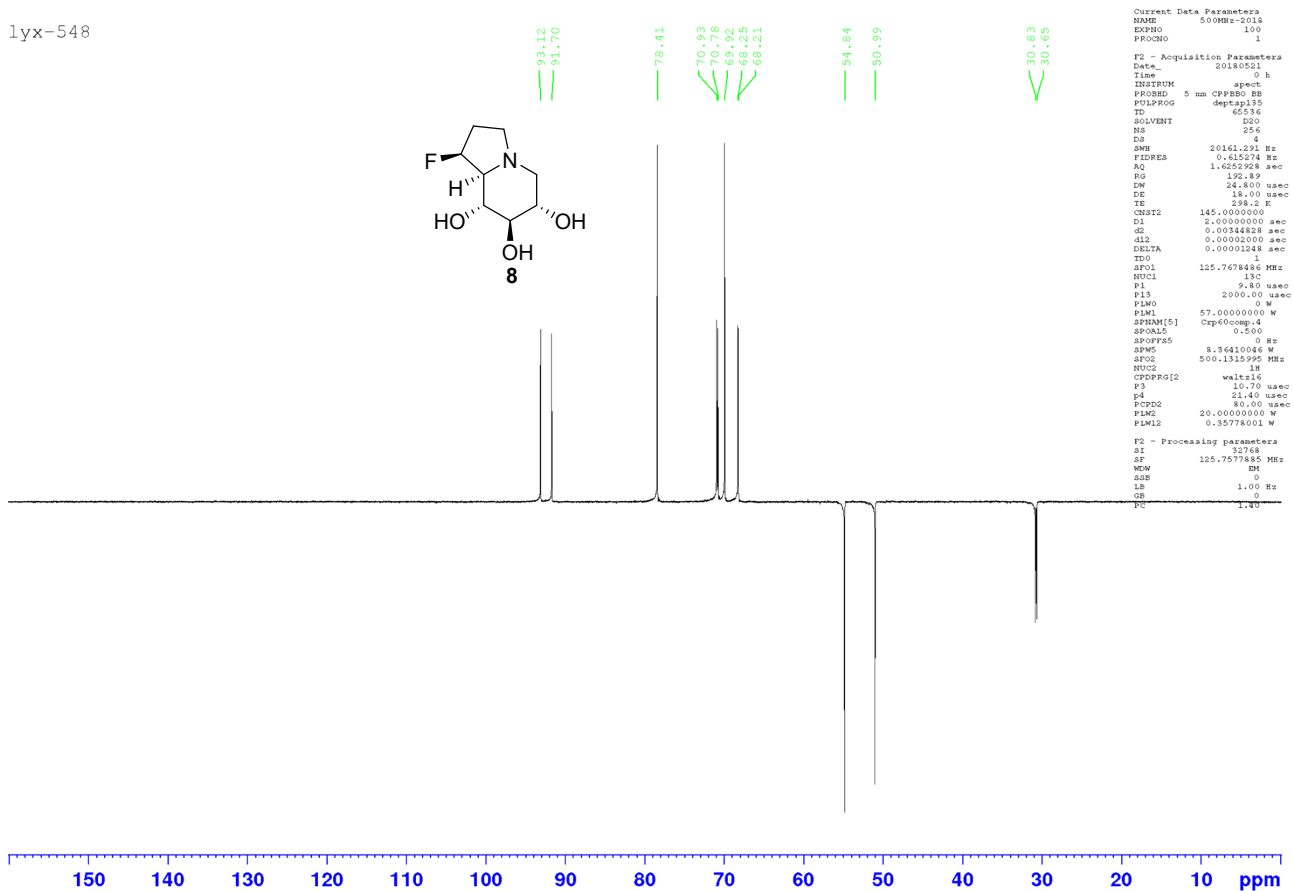
lyx-548



lyx-548



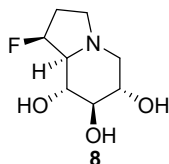
lyx-548



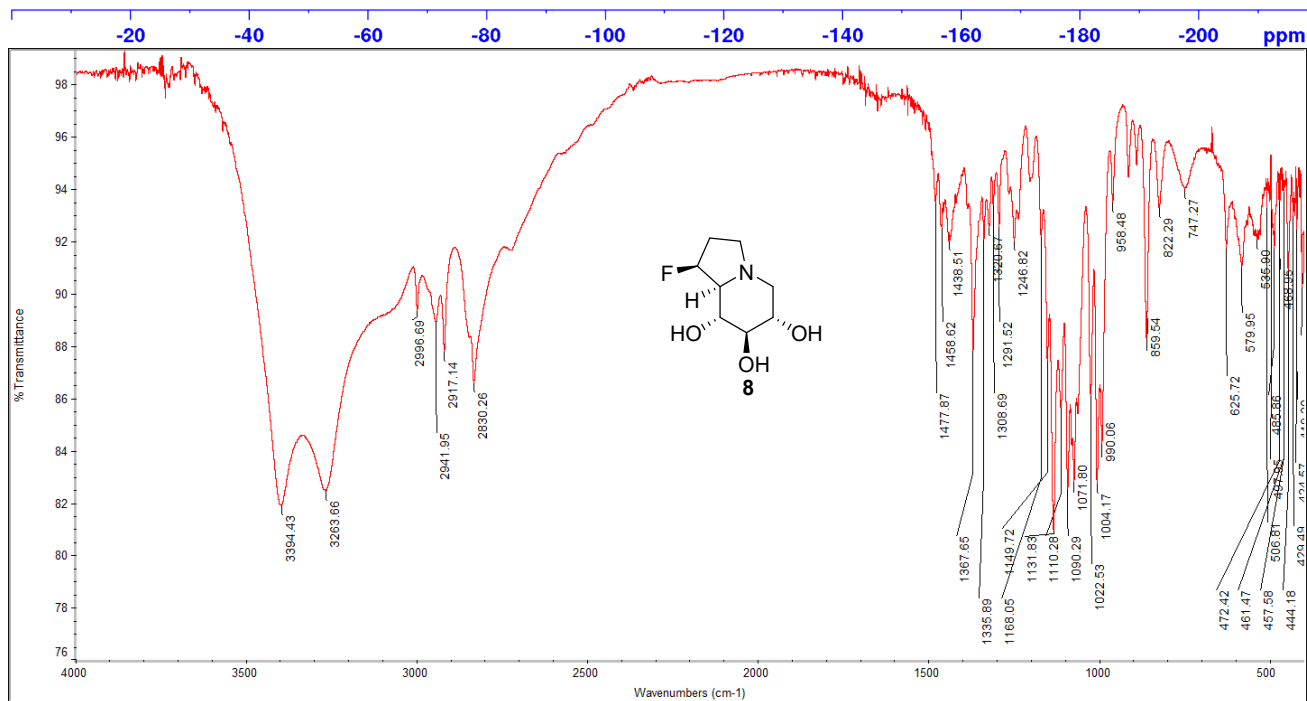
Current Data Parameters  
 NAME 19F-2021  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211103  
 Time 11.38 h  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgfhggn.2  
 TD 131072  
 SOLVENT CDC13  
 NS 16  
 DS 0  
 SWH 89285.711 Hz  
 FIDRES 1.362392 Hz  
 AQ 0.7340032 sec  
 RG 206.33  
 DW 5.600 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 TDO  
 rde1 0.0000650 sec  
 SFO1 376.5642094 MHz  
 NUC1 19F  
 P1 14.50 usec  
 PLW1 17.98900032 W  
 SFO2 400.2416010 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.30294999 W

F2 - Processing parameters  
 SI 6536  
 SF 376.6018696 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

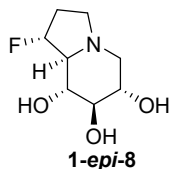
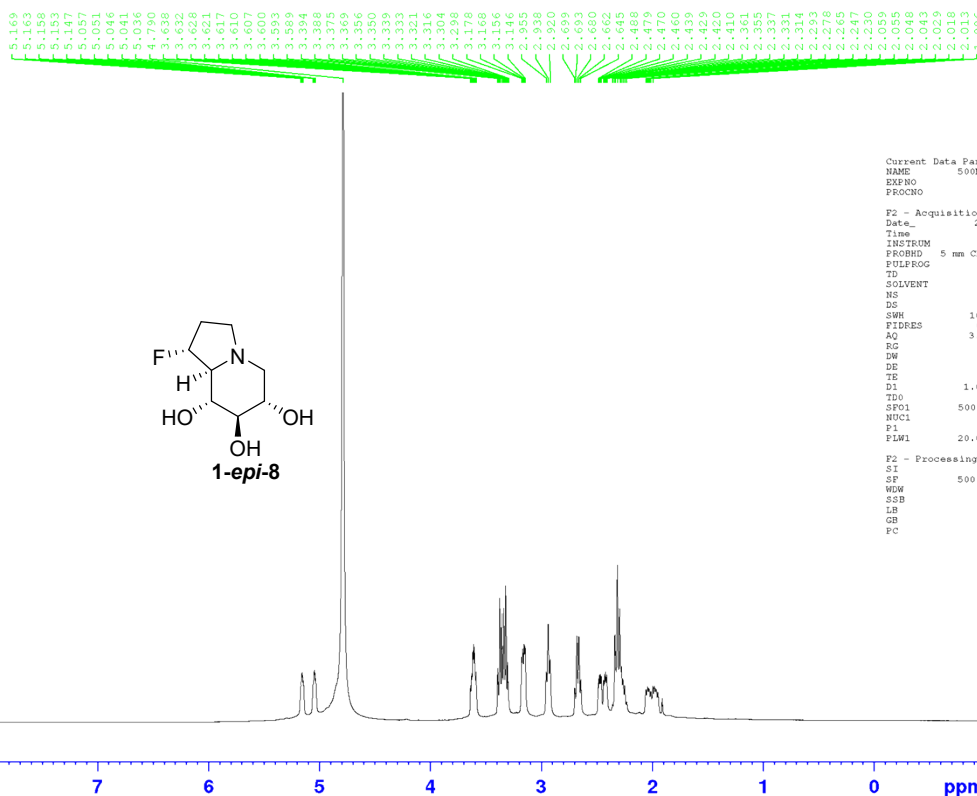


-163.73

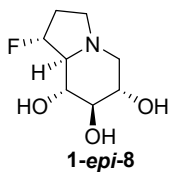
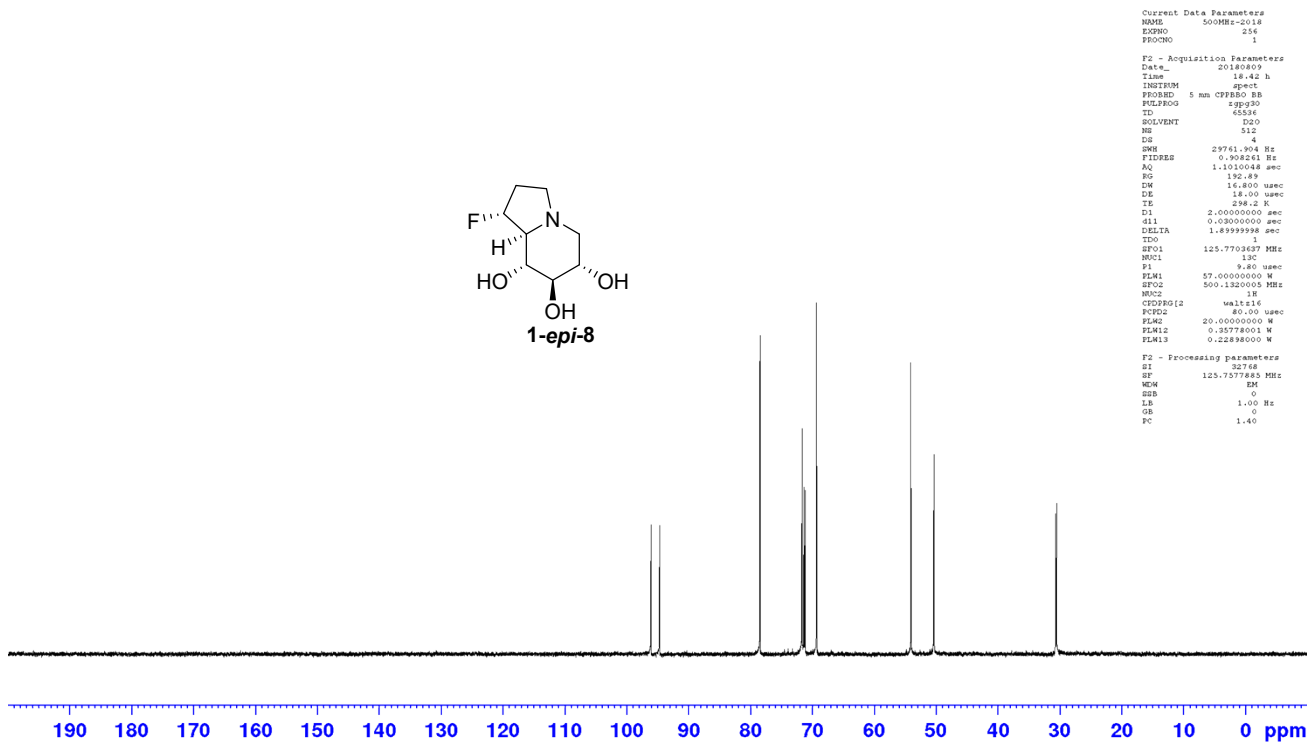


Compound **1-*epi*-8**:

lyx-786



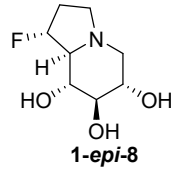
lyx-786



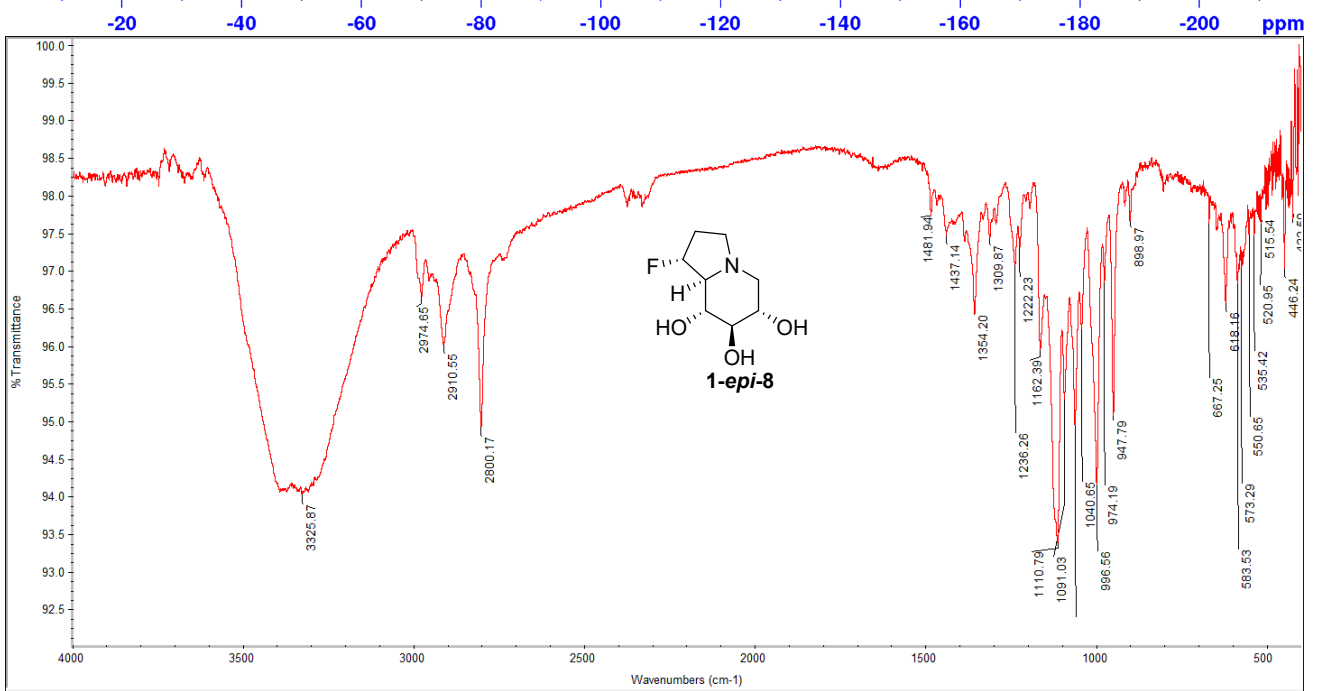
Current Data Parameters  
 NAME 19f-2021  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211103  
 Time 11.36 h  
 INSTRUM spect  
 PROBHD 5 mm F400 BB/  
 PULPROG zgpg30  
 TD 131072  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 89285.711 Hz  
 FIDRES 1.362392 Hz  
 AQ 0.7340032 sec  
 RG 206.33  
 DW 5.600 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 TDO 1  
 rdel1 0.00000650 sec  
 SFO1 376.5642094 MHz  
 NUC1 19F  
 P1 14.50 usec  
 PLW1 17.98900032 W  
 SFO2 400.2416010 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.30294399 W

F2 - Processing parameters  
 SI 65536  
 SF 376.6018696 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB  
 PC 1.00

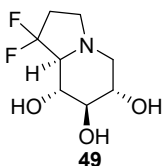
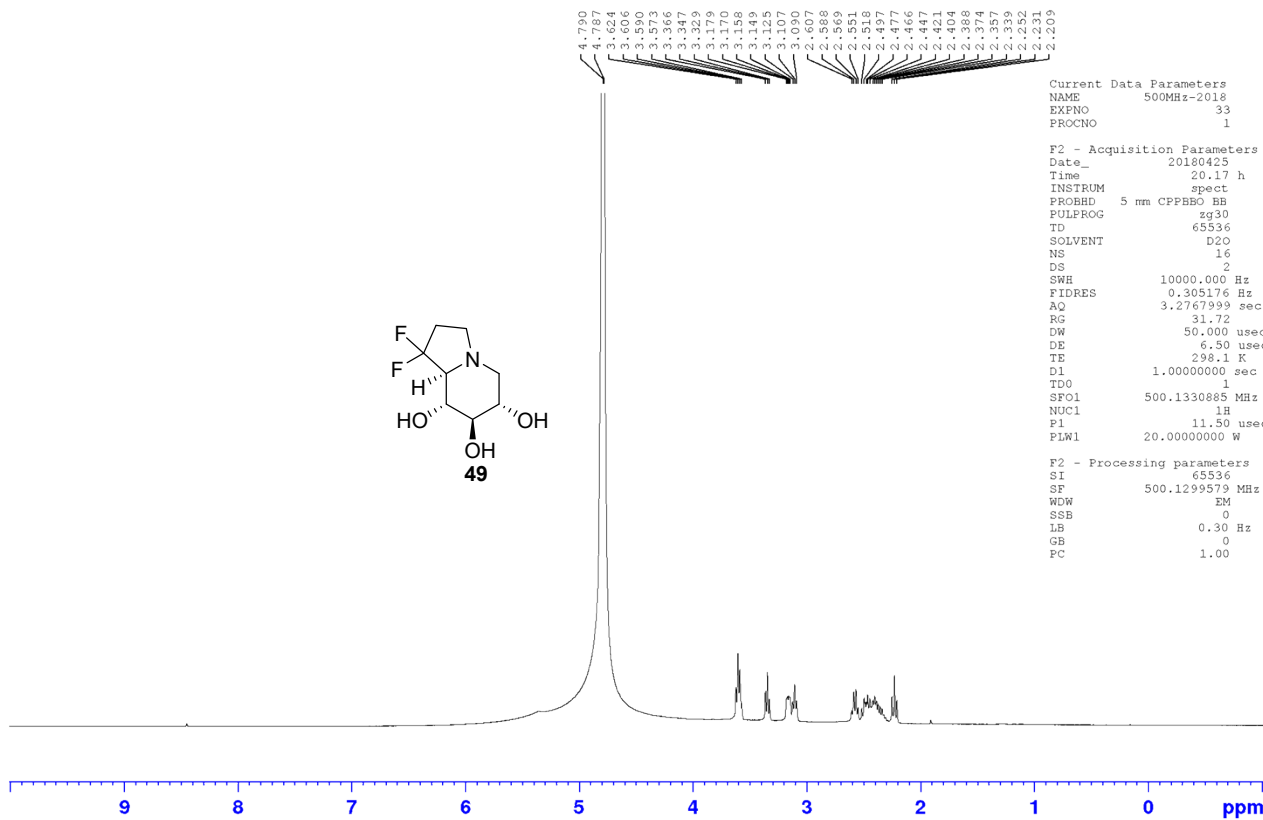


-173.75

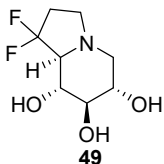
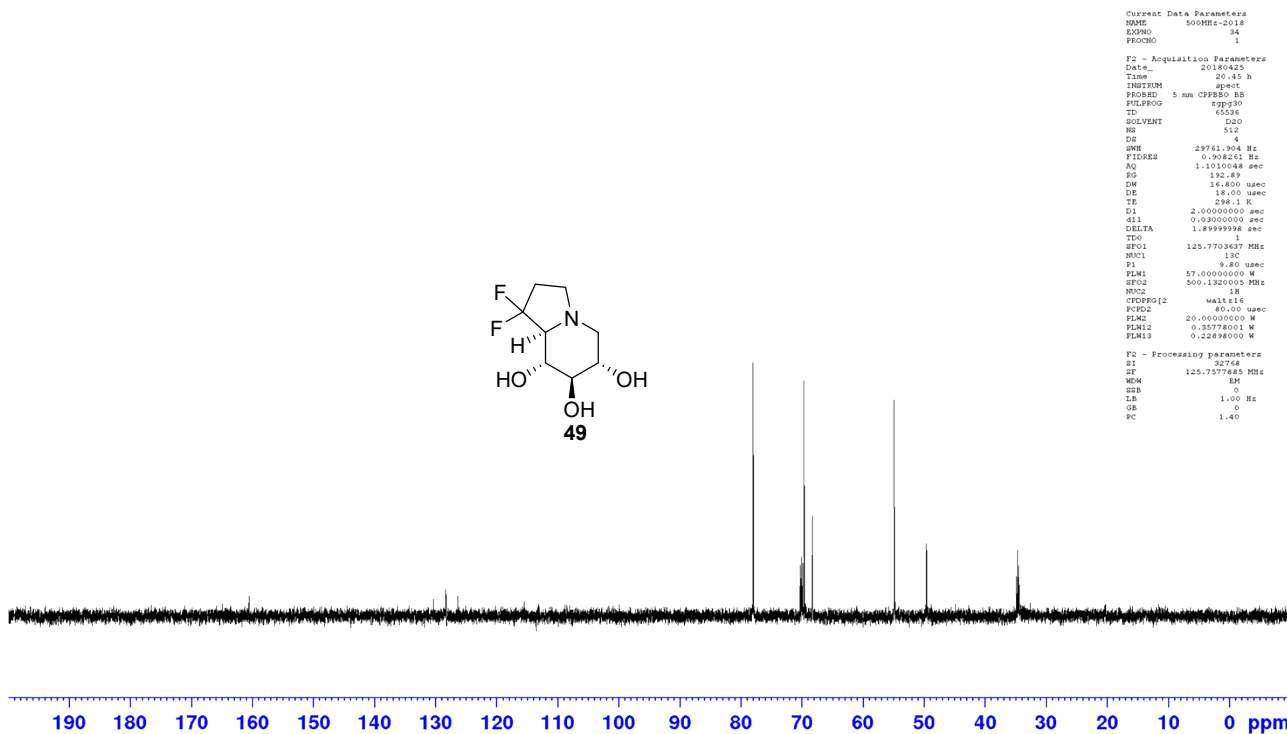


Compound 49:

lyx-549

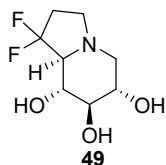


lyx-549





lyx-549



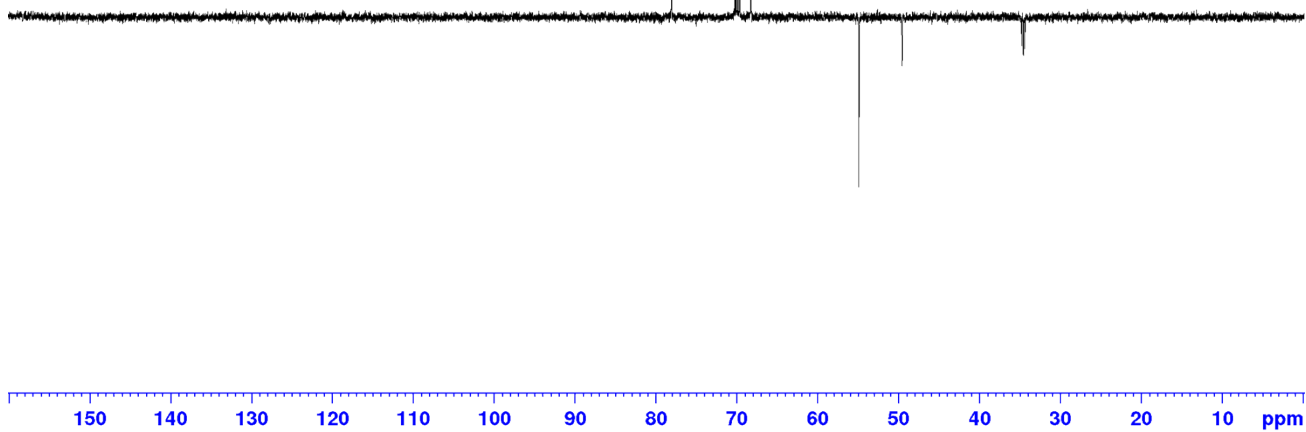
78.02  
70.21  
70.02  
70.00  
69.80  
69.56  
68.22  
68.19  
54.85  
49.51  
34.78  
34.38  
34.39

```

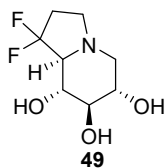
Current Data Parameters
NAME      300MHz-2018
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20180201
Time     21:01:16
INSTRUM  spect
PROBHD   5 mm QNP1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        256
DS        4
SWH       20141.232 Hz
FIDRES    0.412476 Hz
AQ         1.6232028 sec
RG         312.89
DM         24.800 usec
DE         18.00 usec
TE         298.2 K
D1         1.00000000 sec
d11        0.00000000 sec
d12        0.00044228 sec
d2         0.00020000 sec
DELTA     0.0001248 sec
TD0       1
SFO1     125.767844 MHz
NUC1      13C
P1         9.80 usec
PL1        0.00 usec
PL12       2000.00 usec
SFO2     57.0000000 MHz
SFO21     cryoProbe 4
SFO211    0.500
SFO212    0
SFO213    4.36410046 W
SFO214    500.1312993 MHz
NUC2      1H
SFO2      400.1464010 MHz
SFO21     1H
CPDPRG2   waltz16
P3         19.70 usec
P4         19.70 usec
PFD0      80.00 usec
PLW1      20.00000000 W
PLW2      0.33778001 W

F2 - Processing parameters
SI         32768
SF         125.767844 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



549



-95.72  
-96.33  
-101.99  
-102.60

```

Current Data Parameters
NAME      19F-2021
EXPNO    5
PROCNO   1

F2 - Acquisition Parameters
Date_    20211103
Time     11:41:16
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        131072
SOLVENT  CDCl3
NS        56
DS        0
SWH       89285.711 Hz
FIDRES    1.362392 Hz
AQ         0.7340032 sec
RG         206.33
DM         5.600 usec
DE         6.50 usec
TE         297.9 K
D1         1.00000000 sec
d11        0.03000000 sec
d12        0.00020000 sec
TD0       1
SFO1     376.5642094 MHz
NUC1      19F
P1         14.50 usec
PLW1      17.98900032 W
SFO2     400.2416010 MHz
NUC2      1H
CPDPRG2   waltz16
P3         30.00 usec
P4         12.00000000 W
PLW2      0.30294999 W

F2 - Processing parameters
SI         65536
SF         376.6018696 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

