

Synthesis and glycosidase inhibition of *N*-substituted derivatives of 1,4-dideoxy-1,4-imino-D-mannitol (DIM)

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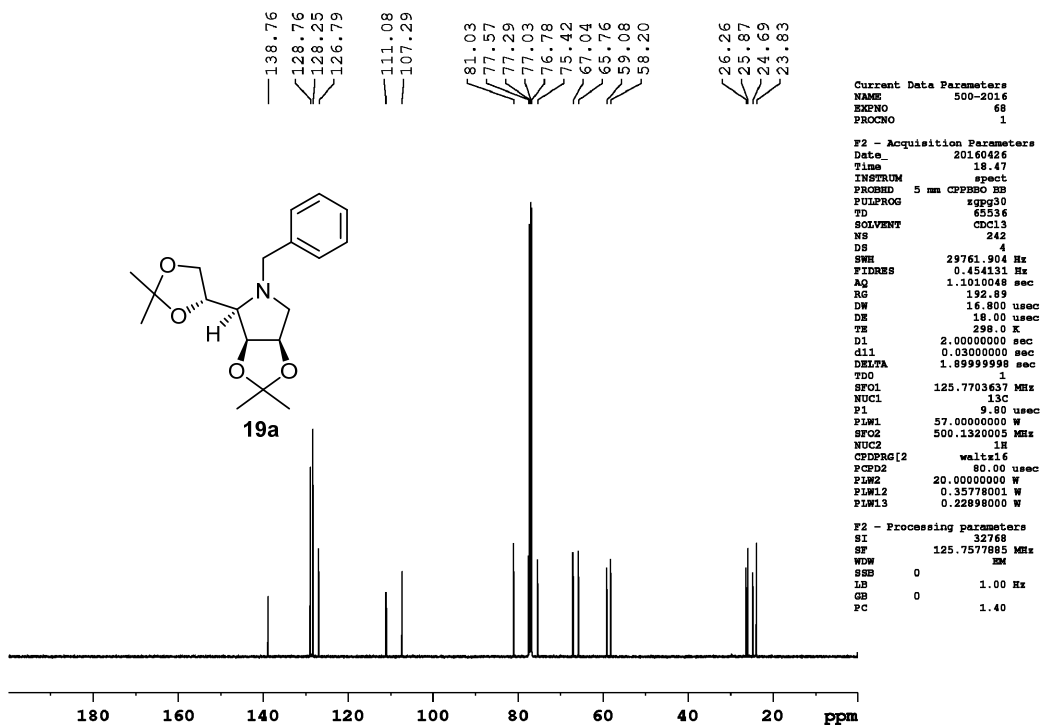
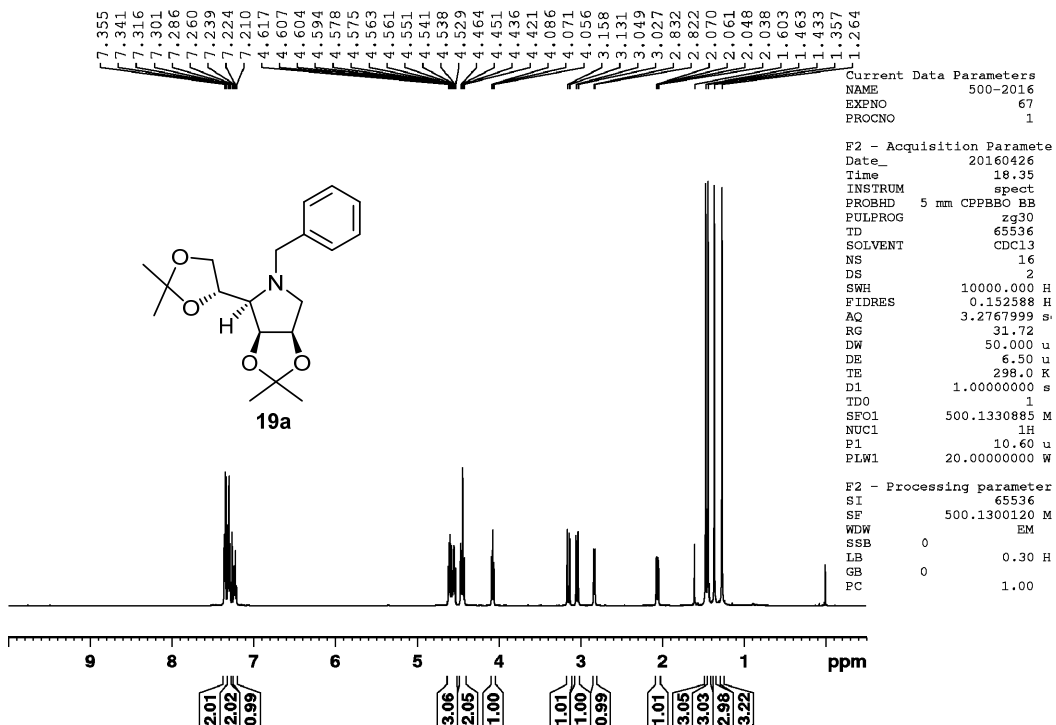
Supplementary Information

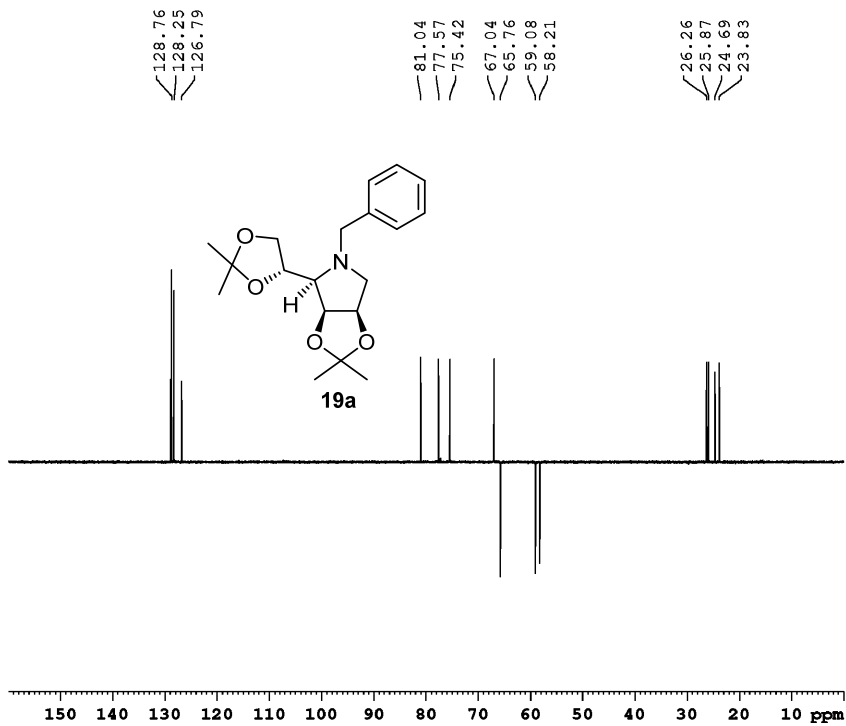
NMR spectra and Infrared spectra for
compound 18i, 19a-i, 20a-i, 26, 27g, 28a-g, 29a-h and 30

and

X-Ray Crystallographic Data for compound 11

Compound 19a:



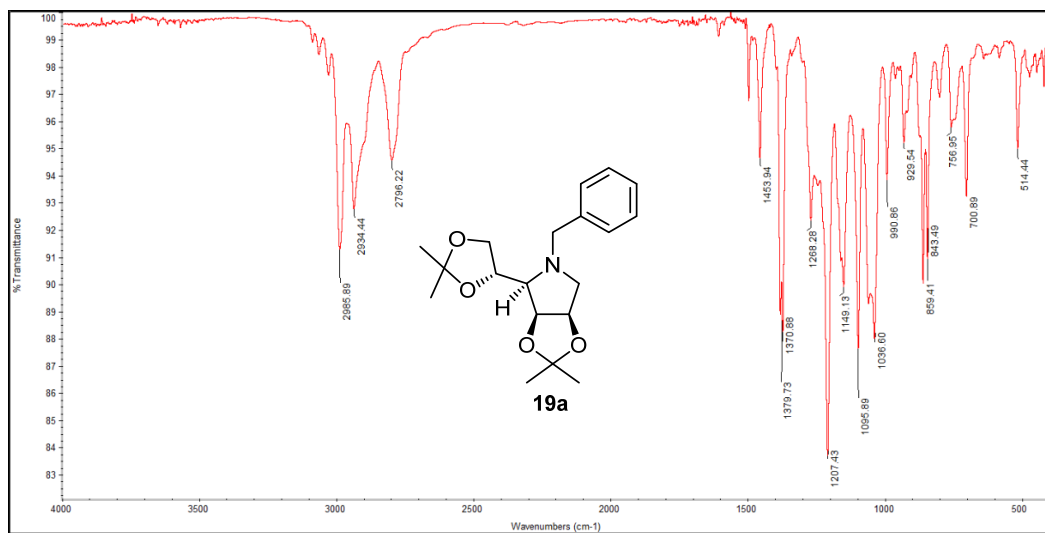


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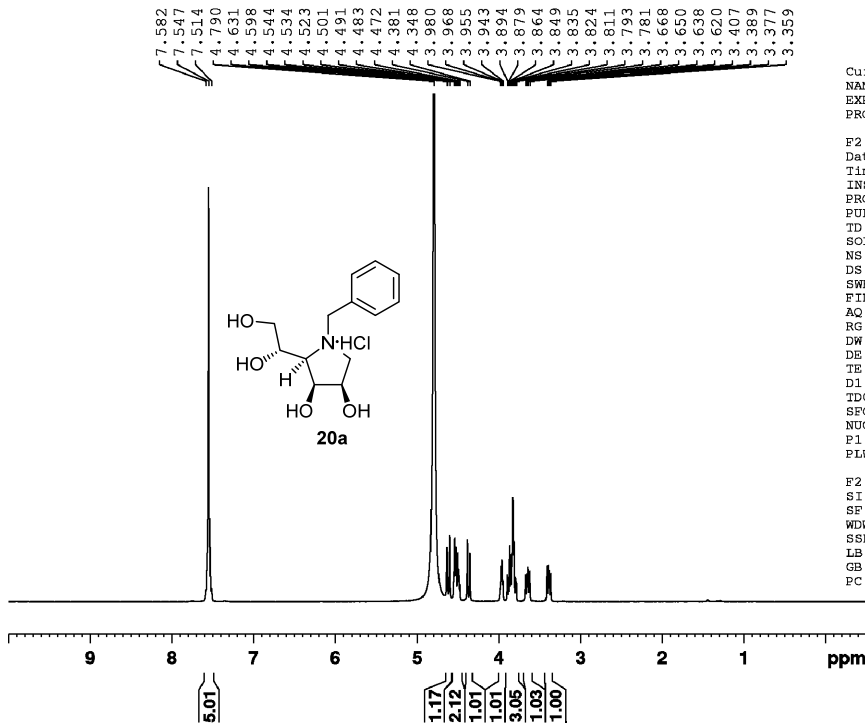
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EXPNO     69
PROCNO    1

F2 - Acquisition Parameters
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PULPROG   deptzg13b
TD         65536
SOLVENT   CDCl3
NS         66
DS         4
SWH        20161.291 Hz
FIDRES    0.307697 Hz
AQ         1.6282928 sec
RG         192.89
SQ         21.400 usec
DE         18.00 usec
TE         298.0 K
CQF2      145.000000
D1         2.0000000 sec
d2         0.00344828 sec
d12       0.0002000 sec
DELTA     0.0001248 sec
TD0       1
SFO1      125.7678486 MHz
NUC1       13C
P1         9.80 usec
P13       2000.00 usec
SFO0      0 W
FLM1      57.0000000 W
SFO5      500.1315995 MHz
SFOAL5    0.500
SFOFFAS   0 Hz
SWS       8.36410046 W
SFO2      500.1315995 MHz
NDCS      18
CQDPRG2   waltz16
P3         10.70 usec
P4         21.40 usec
PCPD2     80.00 usec
FLM3      20.0000000 W
FLM12     0.35778001 W

F2 - Processing parameters
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WDW        EM
SSB        0
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GB         0
PC         1.40
  
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Compound 20a:

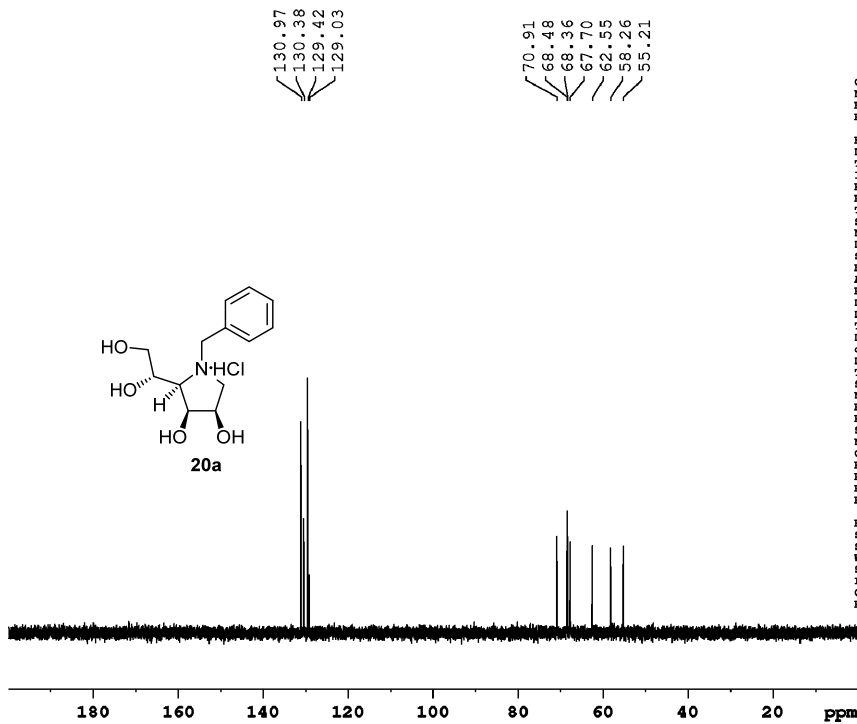


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Current Data Parameters
NAME      400-2016
EXPNO    138
PROCNO   1

F2 - Acquisition Parameters
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PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       32768
SOLVENT  D2O
NS       16
DS       0
SWH      8012.820 H
FIDRES   0.244532 H
AQ       2.0447233 s
RG       206.33
DW       62.400 u
DE       6.50 u
TE       299.7 K
D1       2.00000000 s
TDO      1
SFO1    400.2424716 M
NUC1     1H
P1       14.80 u
PLW1    12.00000000 W

F2 - Processing parameter
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WDW      EM
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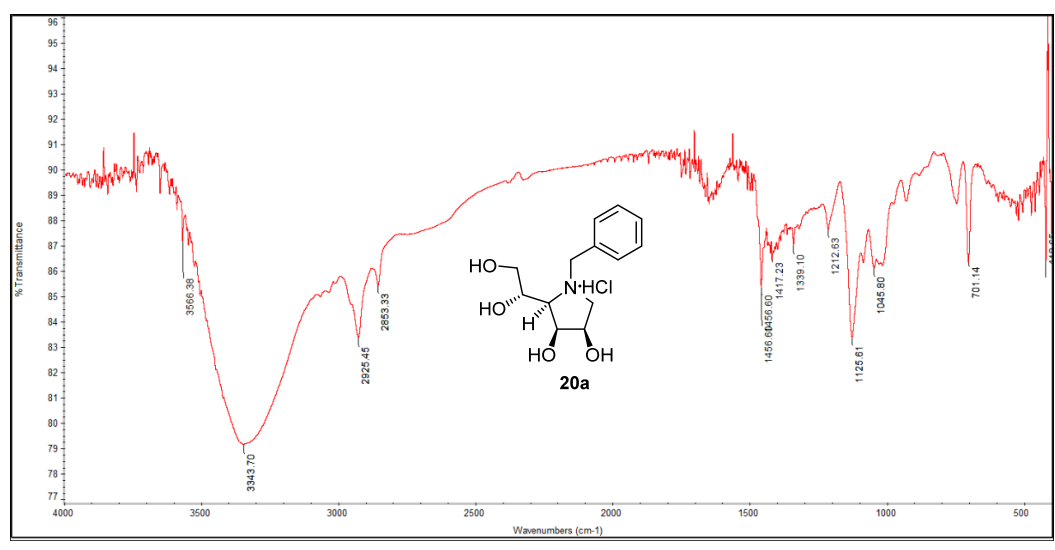
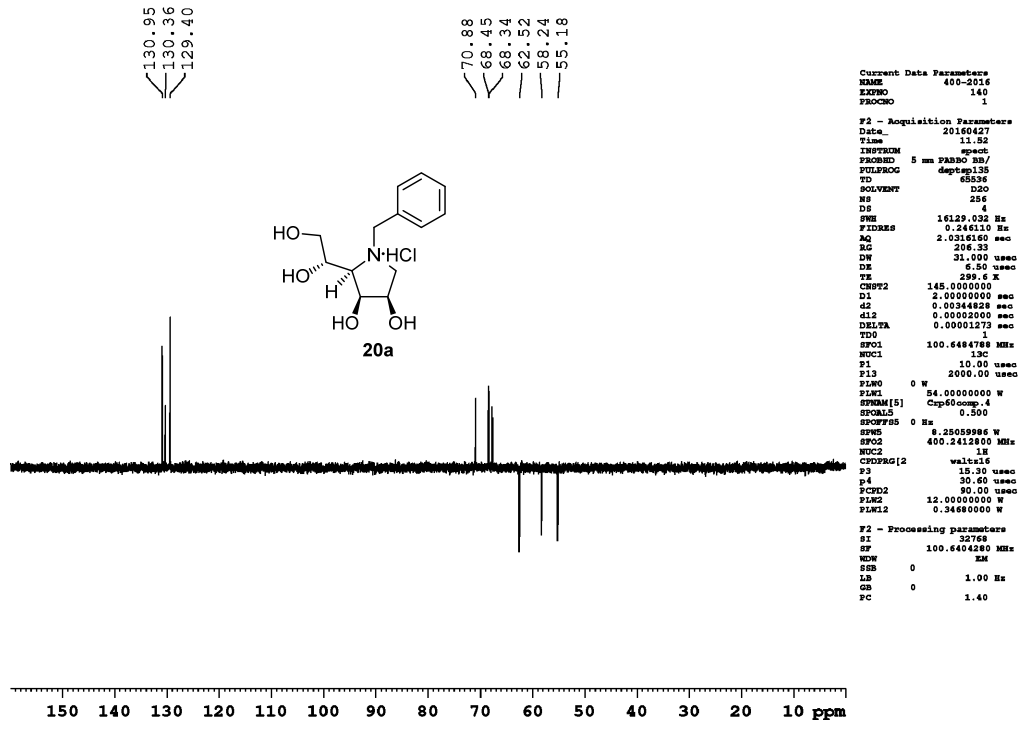


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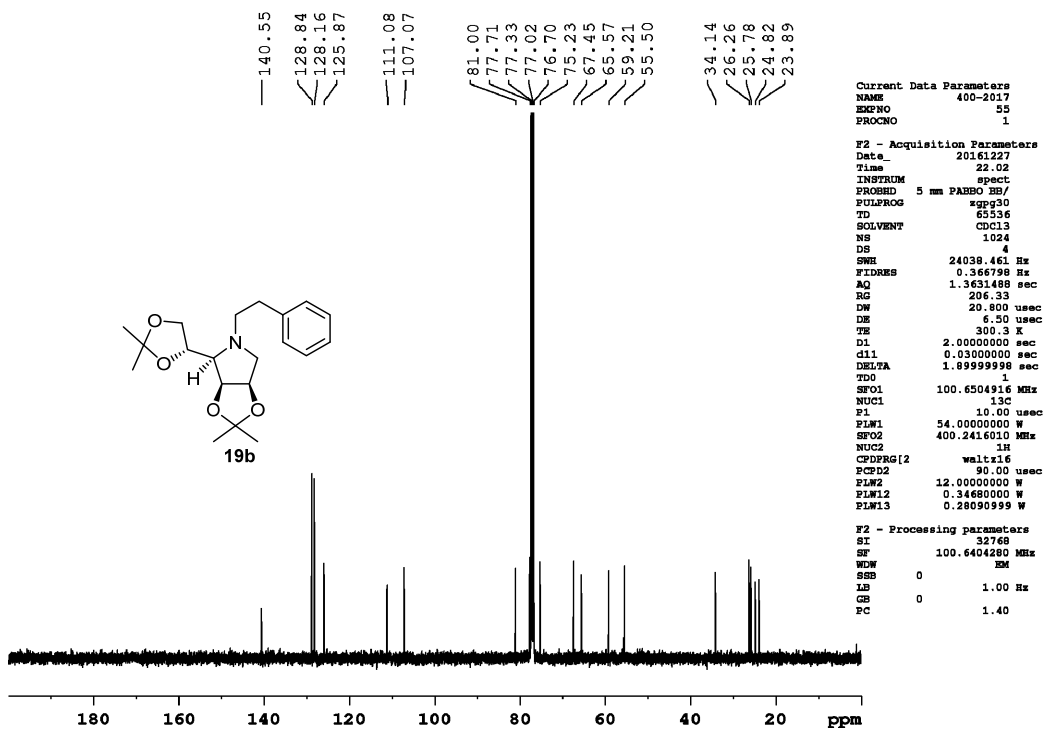
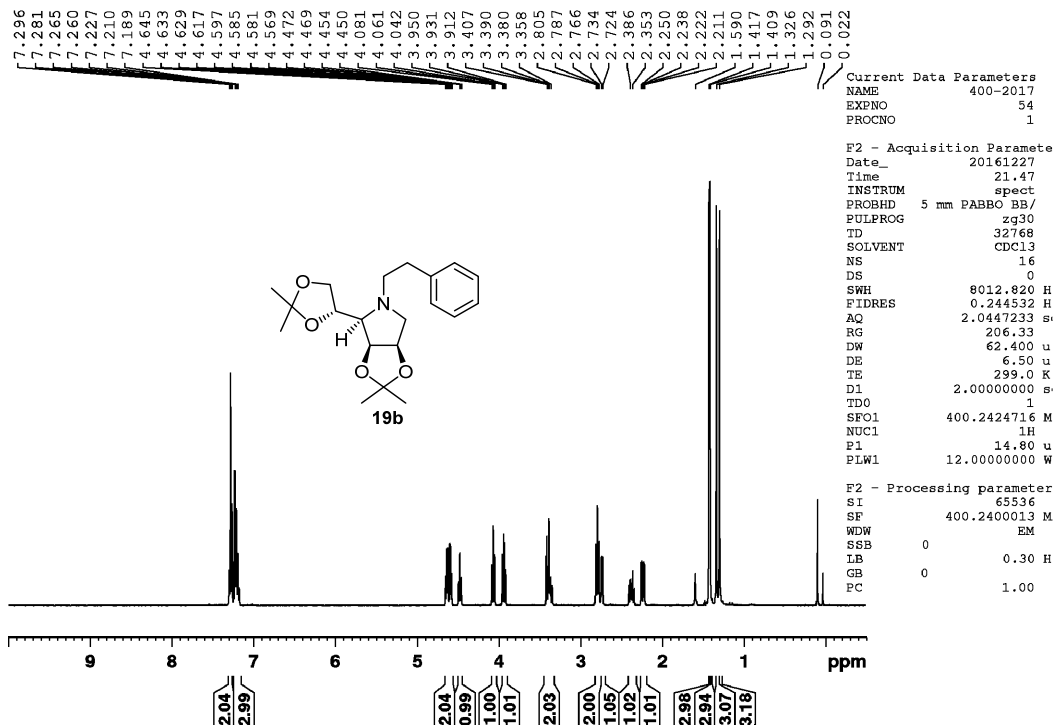
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EXPNO    139
PROCNO   1

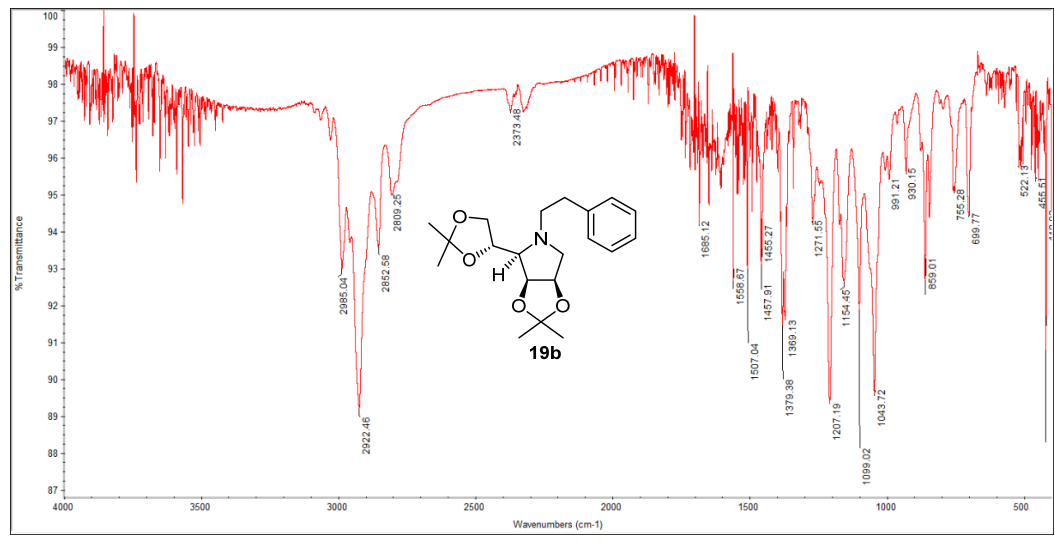
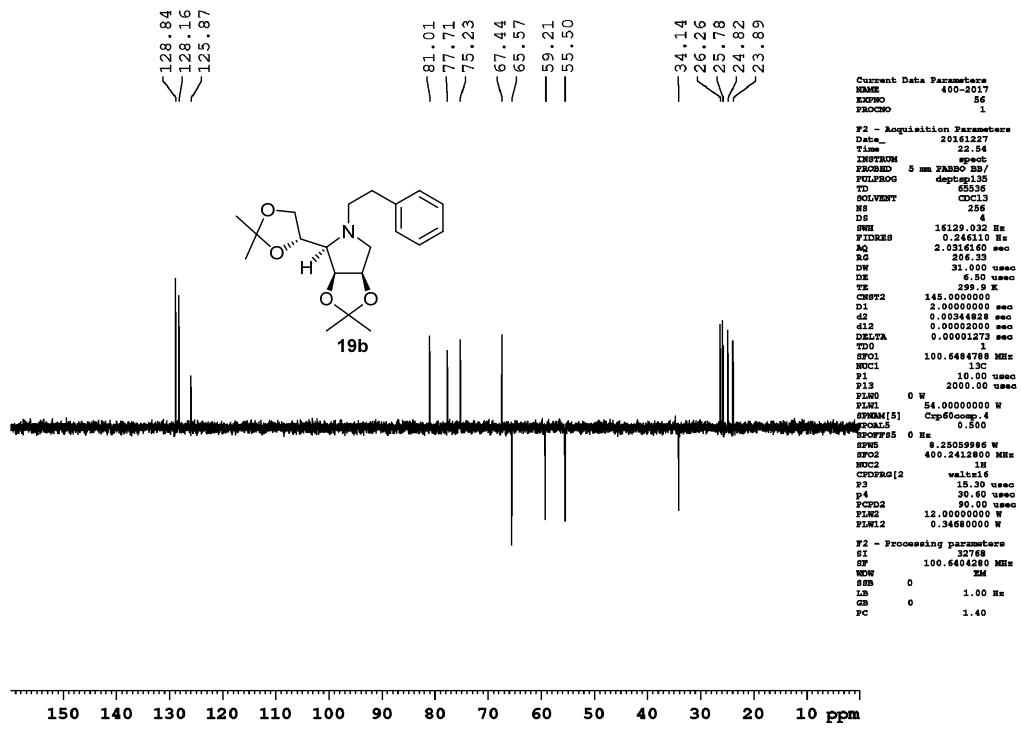
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INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  D2O
NS       1024
DS       4
SWH      24038.461 Hx
FIDRES   0.366798 Hx
AQ       1.3631488 sec
RG       206.33
DW       20.800 usec
DE       6.50 usec
TE       301.1 K
D1       2.00000000 sec
d11      0.03000000 sec
DELTA    1.89999998 sec
TDO      1
SFO1    100.6504916 MHz
NUC1     13C
P1       10.00 usec
PLW1    54.00000000 W
SFO2    400.2416010 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2   90.00 usec
PLW2    12.00000000 W
PLW12   0.34680000 W
PLW13   0.28090999 W

F2 - Processing parameters
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WDW      EM
SSB      0
LB       1.00 Hx
GB       0
PC       1.40
    
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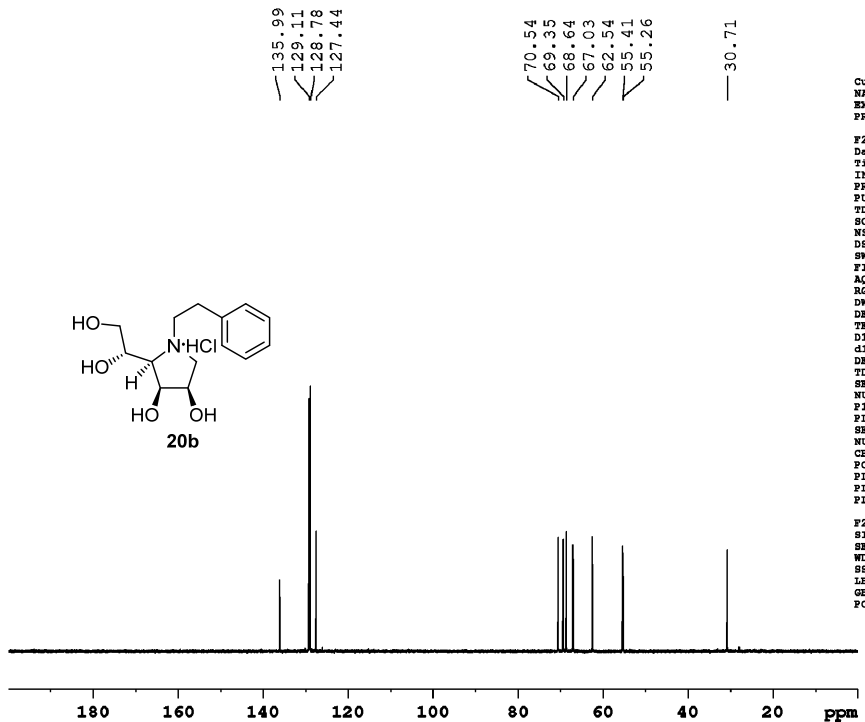
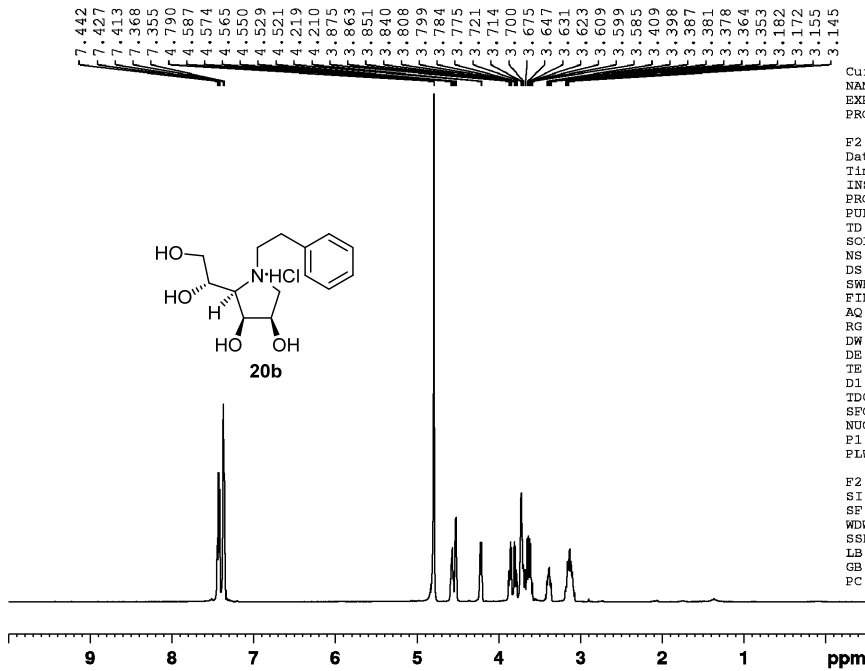


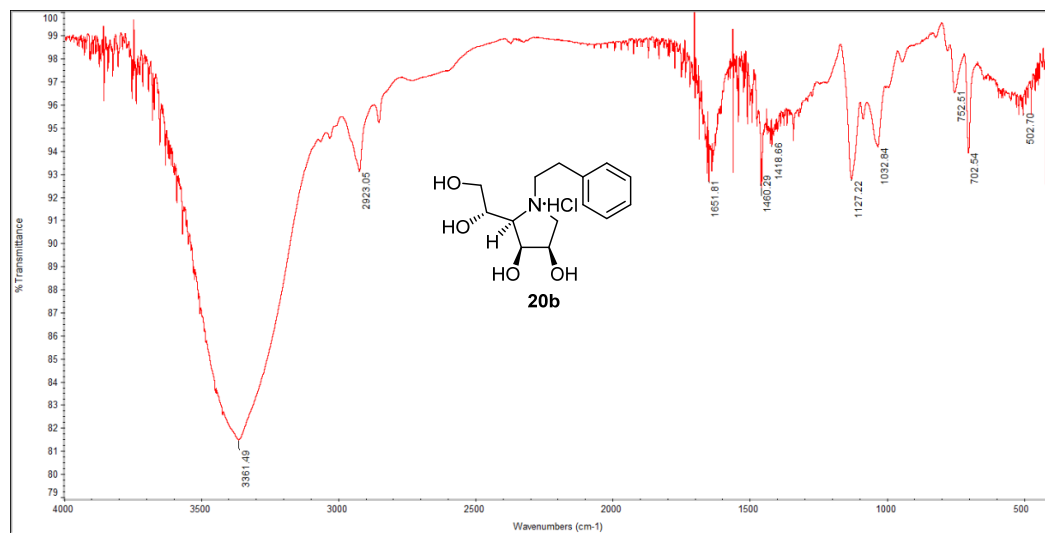
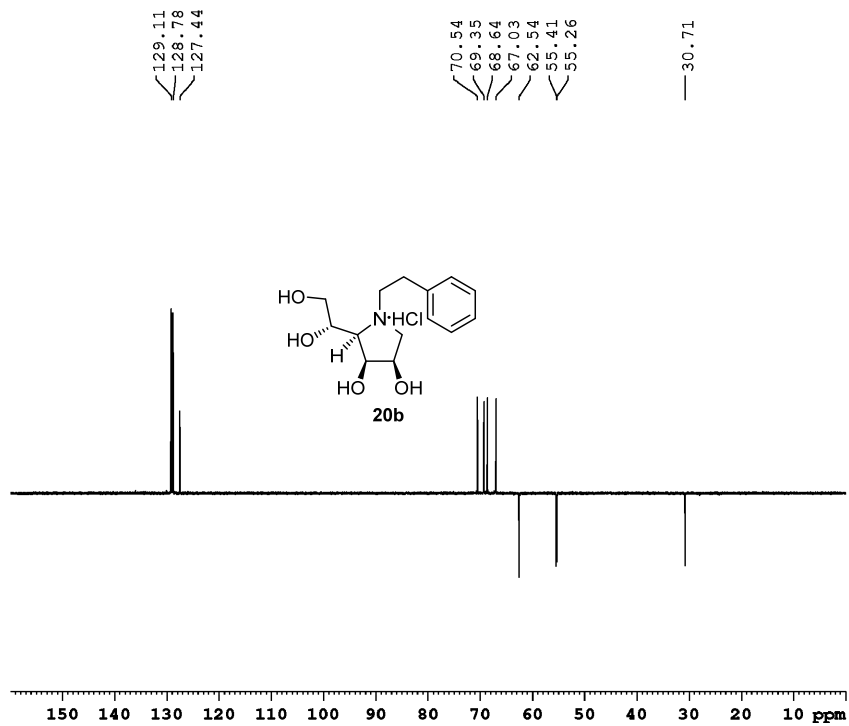
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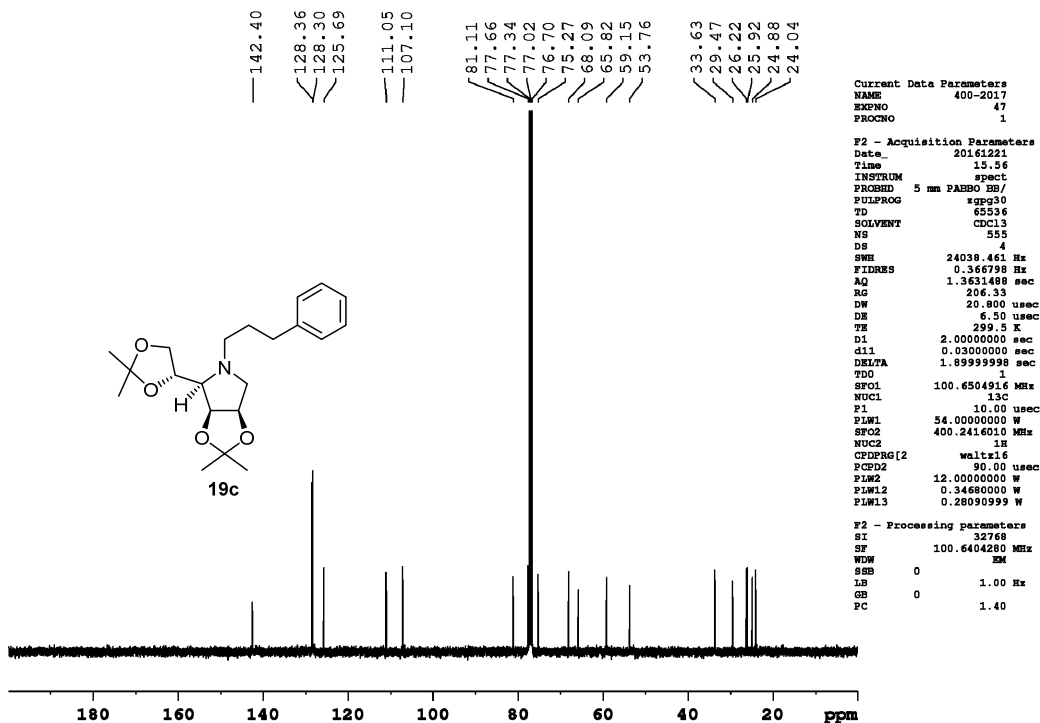
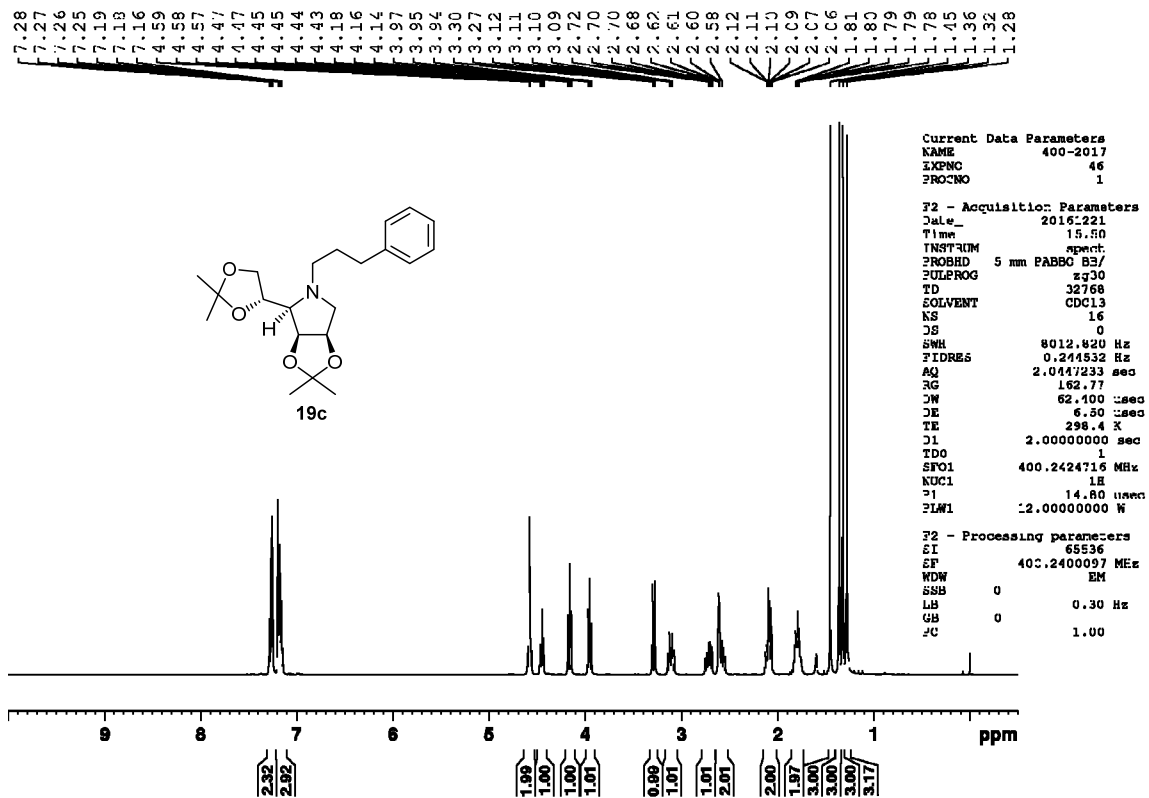


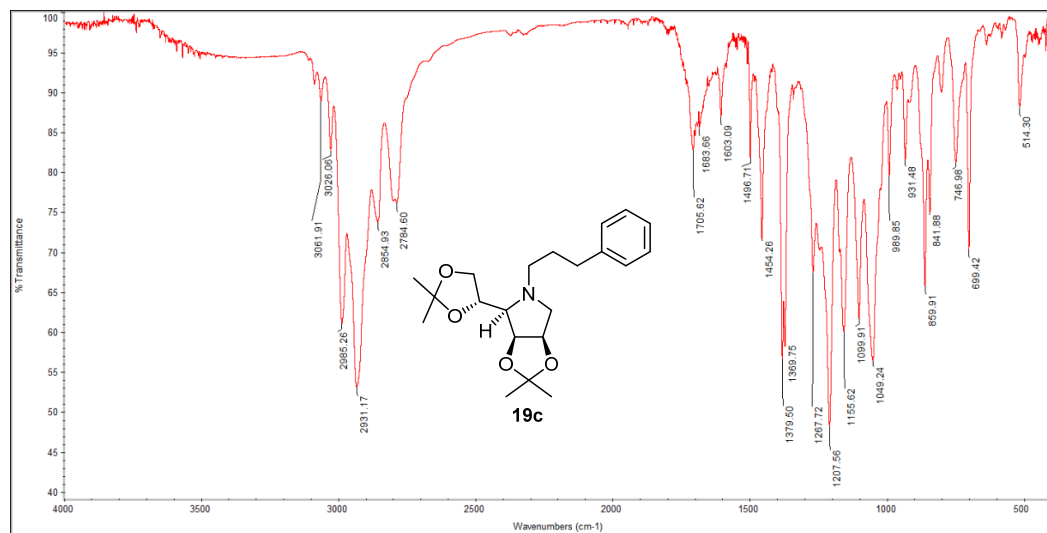
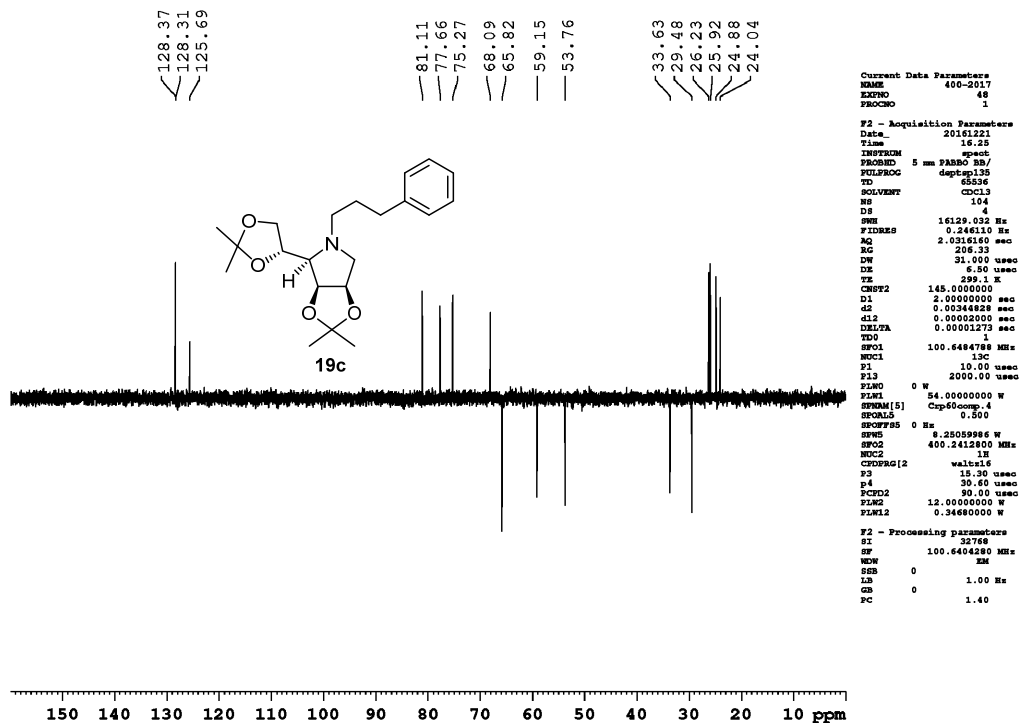
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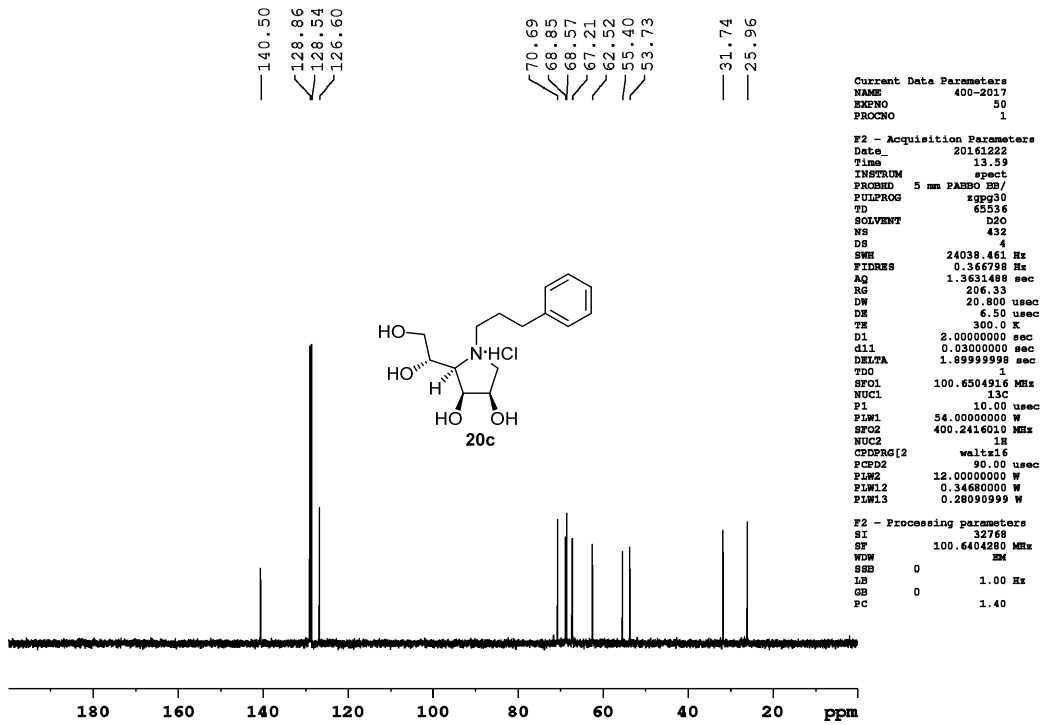
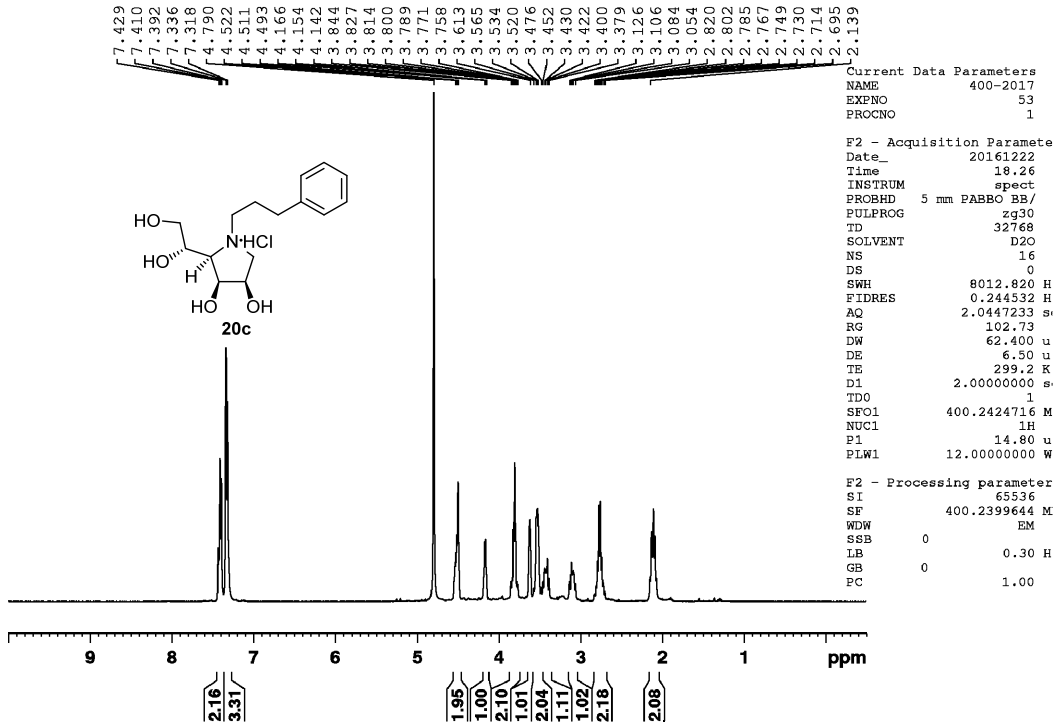


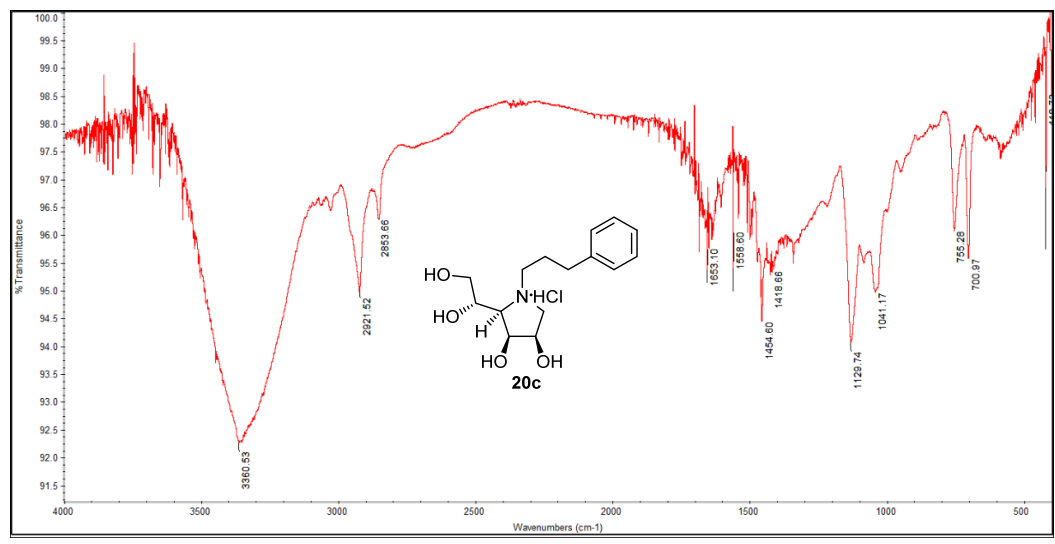
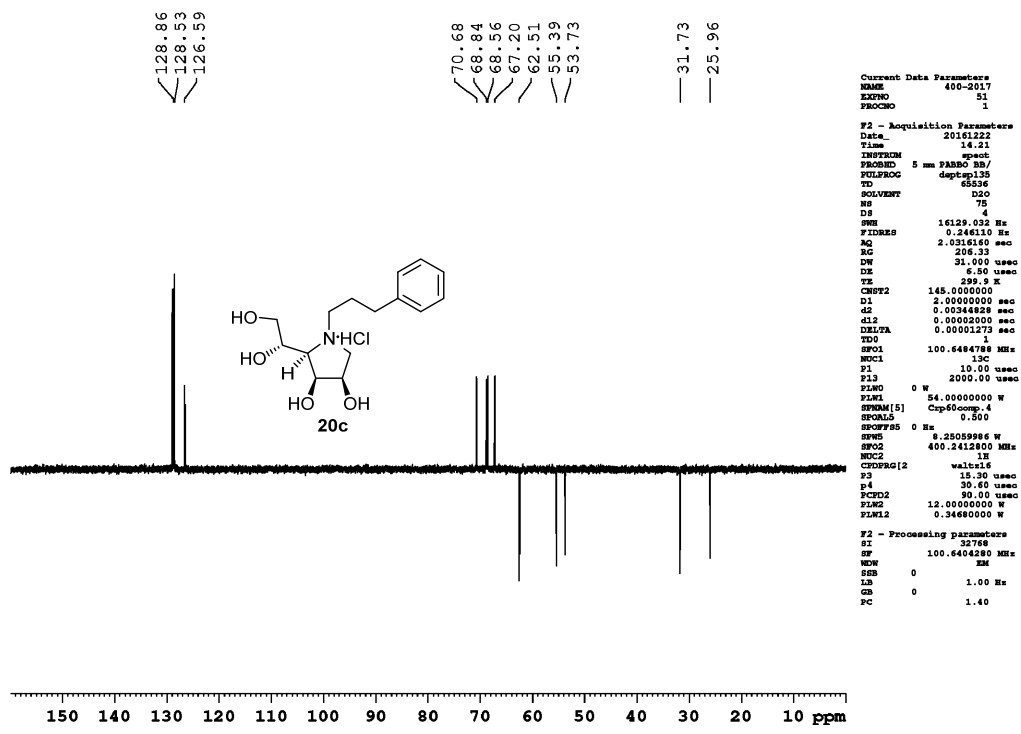
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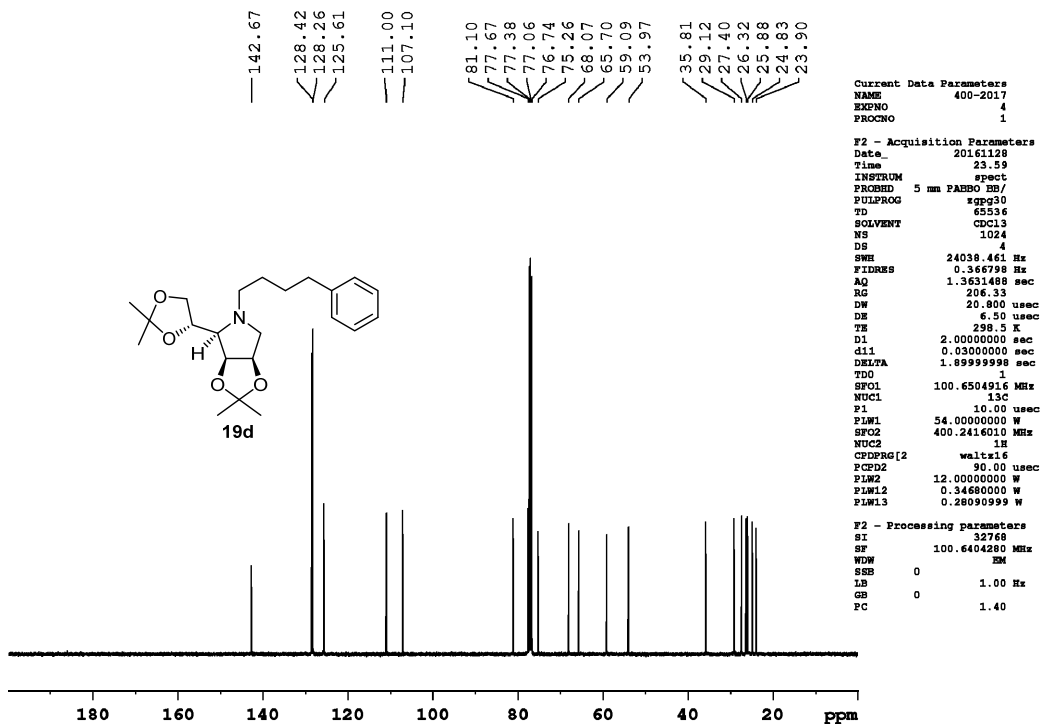
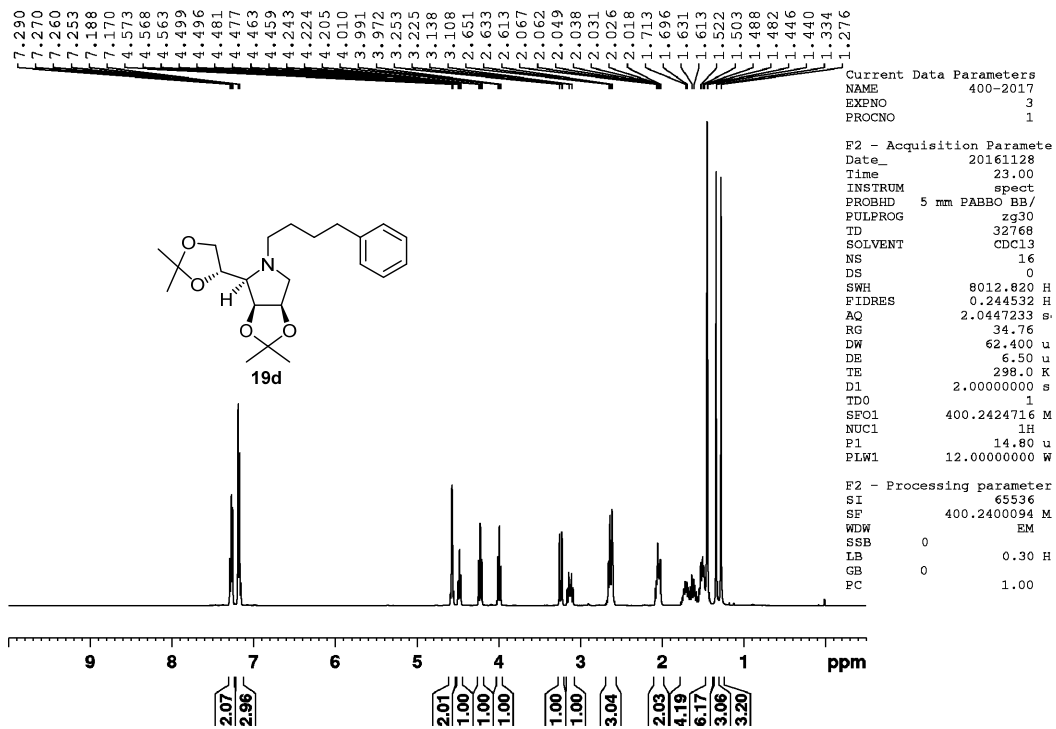


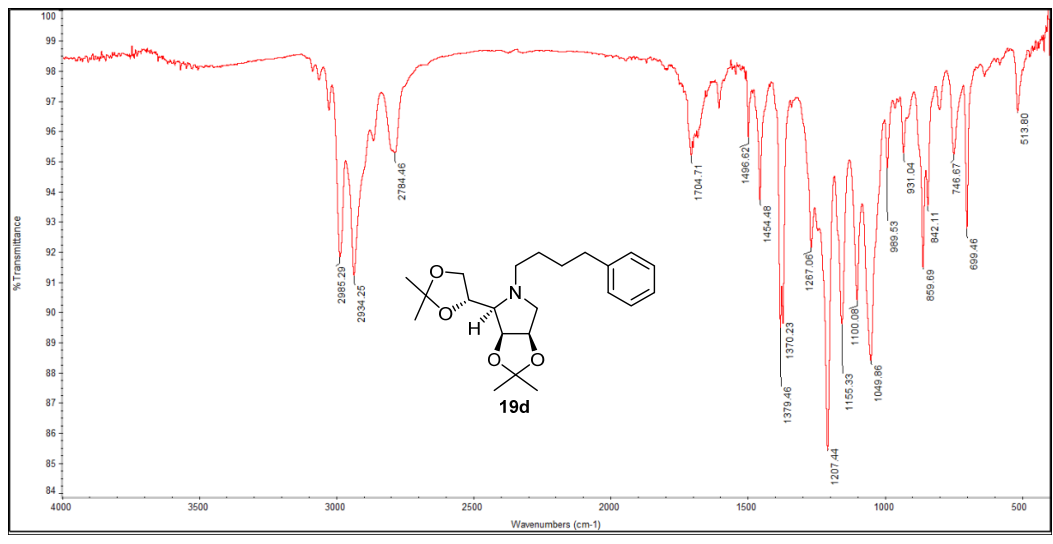
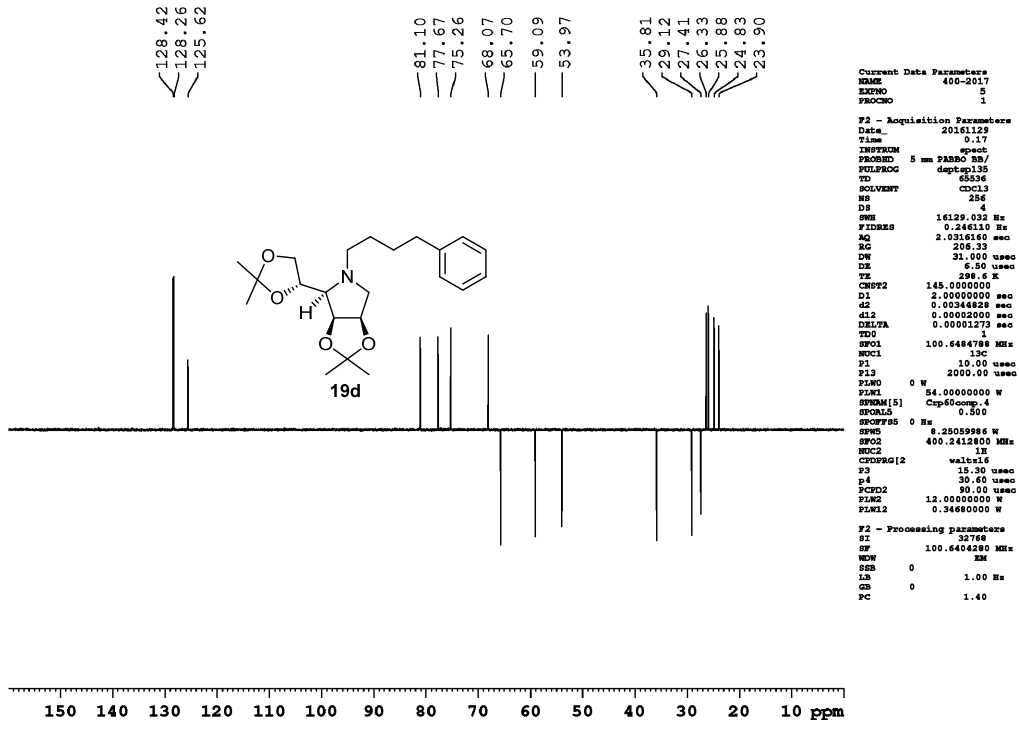
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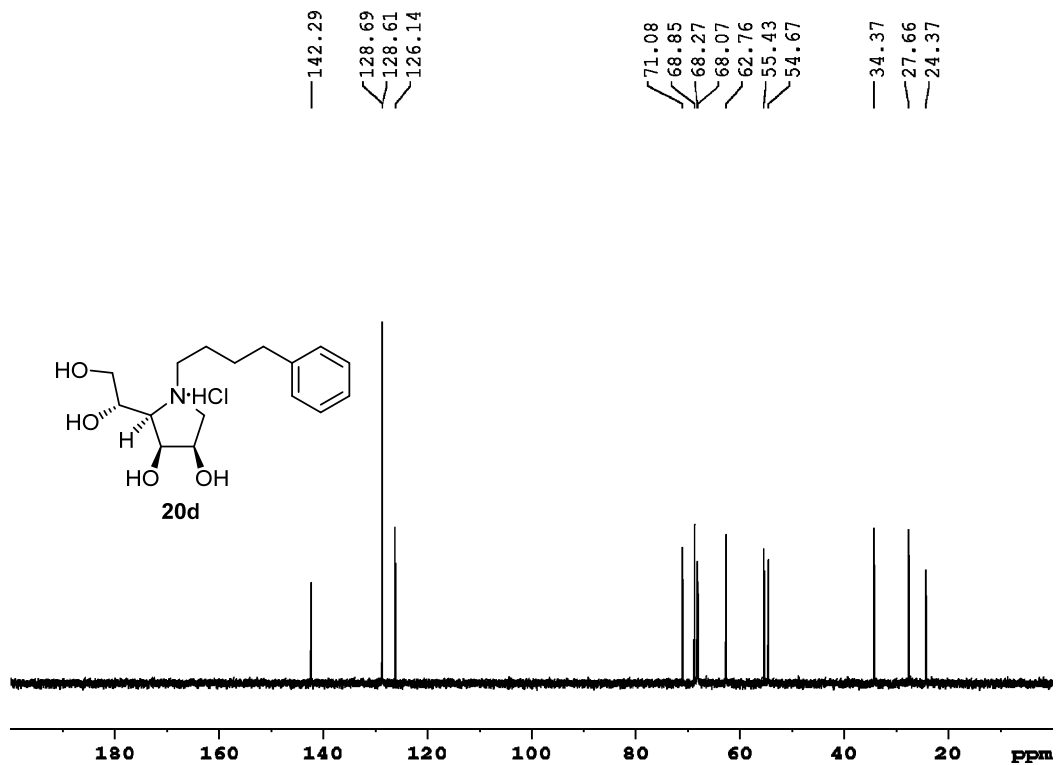
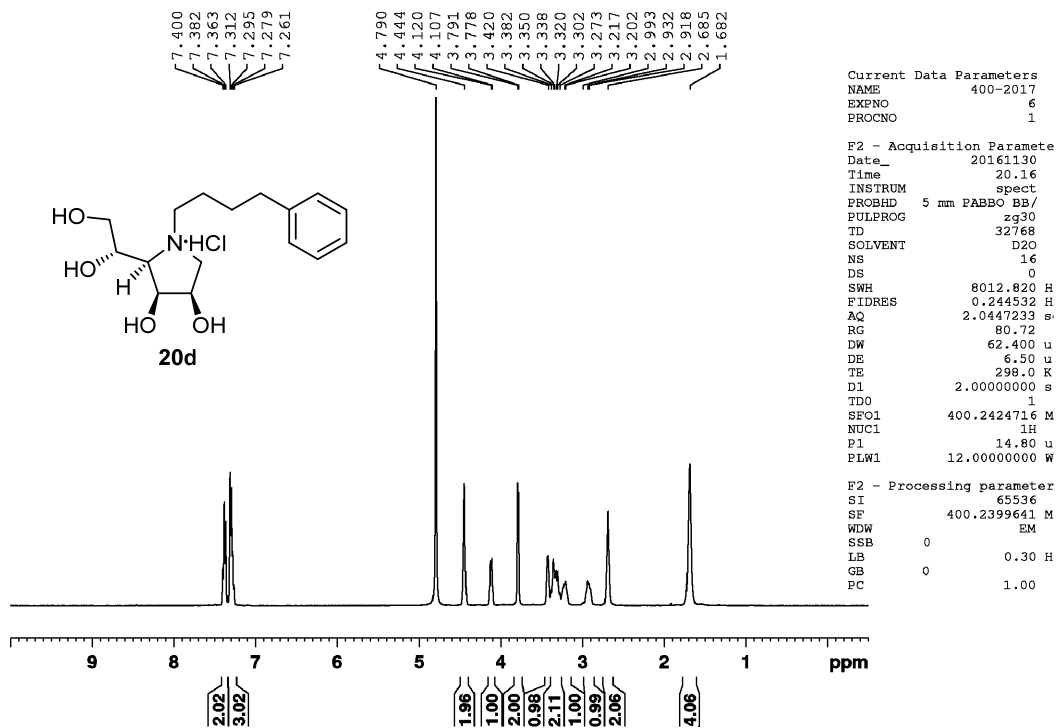


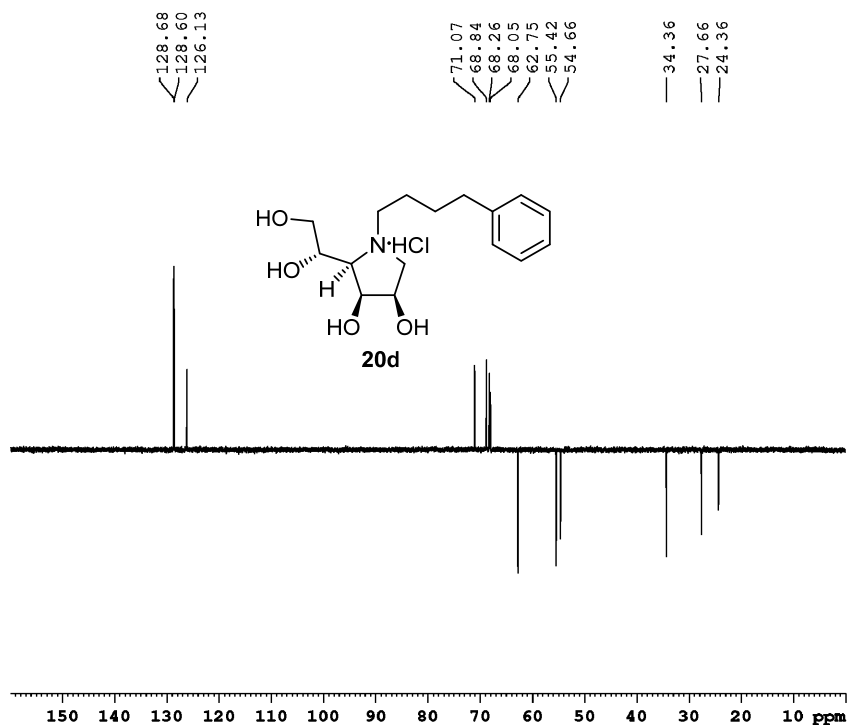
Compound 19d:





Compound **20d**:



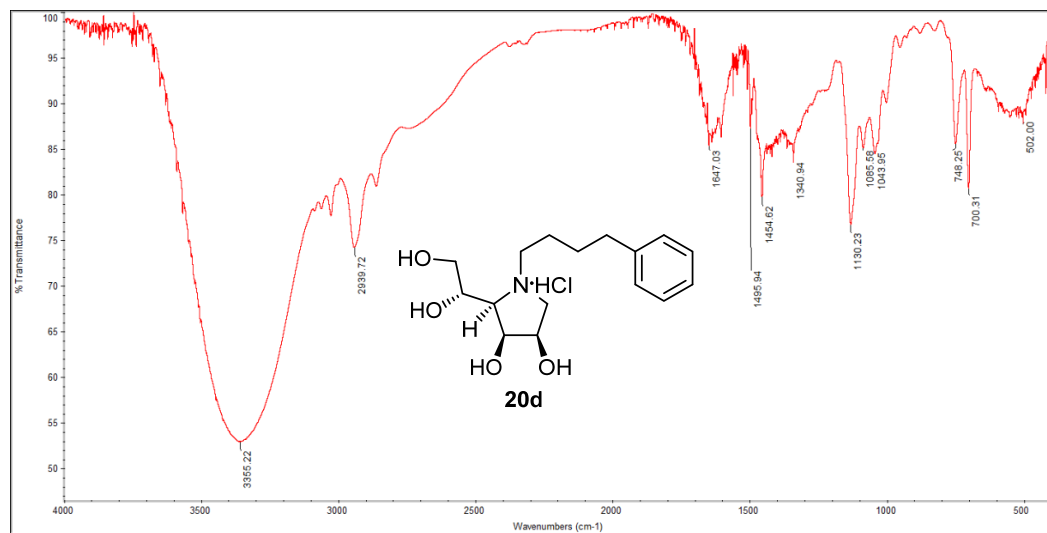


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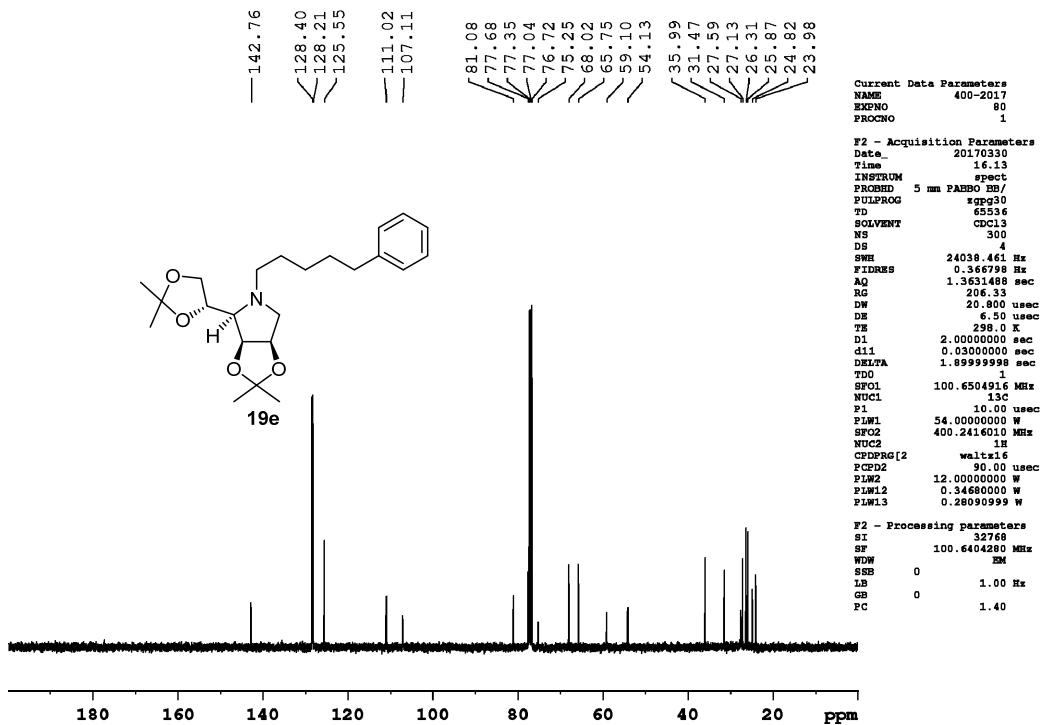
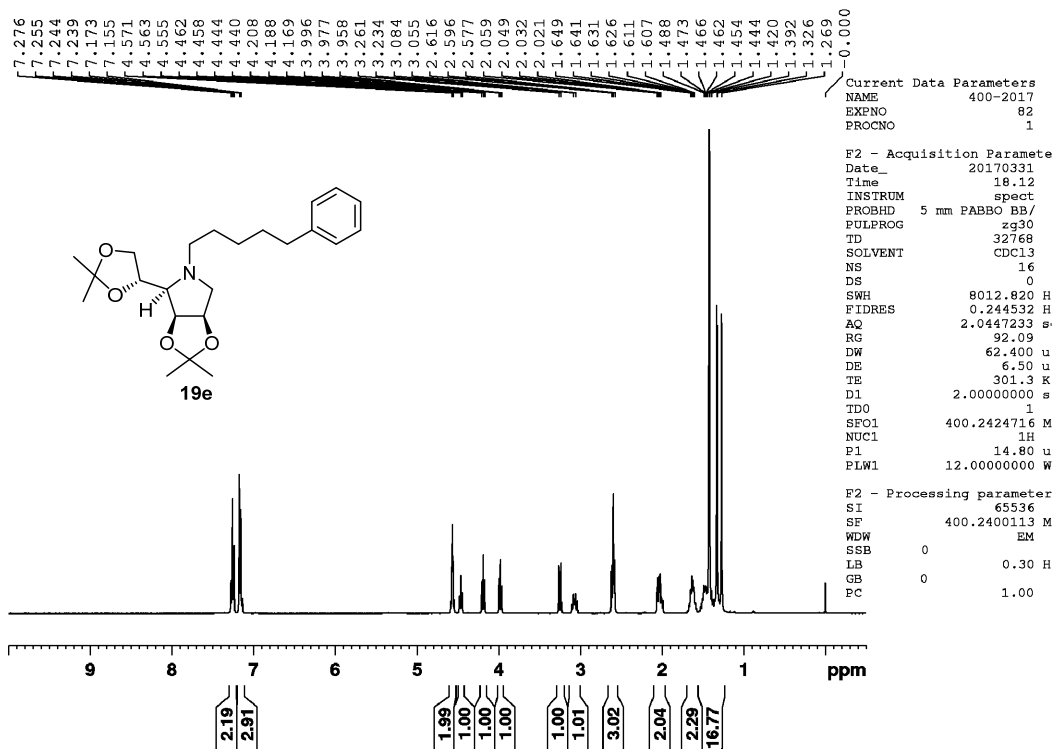
Current Data Parameters
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EXPNO    8
PROCNO    1

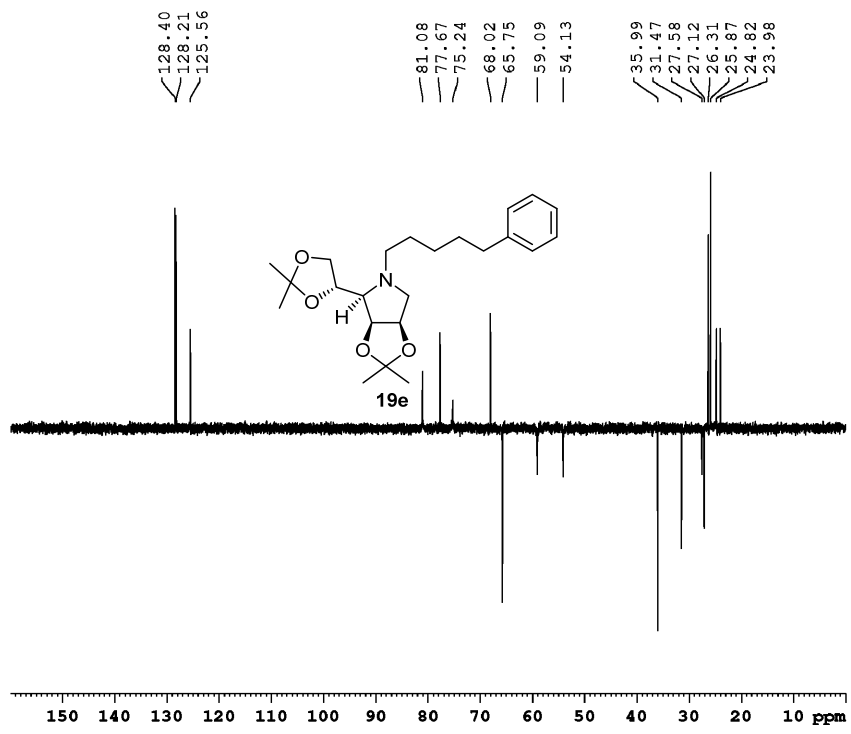
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Time     21.33
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  D2O
NS        256
DS        4
SWH       16129.032 Hz
FIDRES    0.244110 Hz
AQ        2.0316160 sec
RG         206.33
AQ        31.000 usec
DE         6.50 usec
TE        299.2 K
CHRT2     145.0000000
D1         2.000000000 sec
d2         0.0034828 sec
d12        0.00002000 sec
DELTA     0.00001270 sec
TD0        1
SFO1      100.6484788 MHz
NUC1       13C
P1         10.00 usec
PL1        2000.00 usec
PL2        0 W
PLM1       54.00000000 W
SFO2      8.25059986 W
SFO2       400.2412800 MHz
NUC2       1H
CPDPRG2   waltz16
P3         15.30 usec
P4         30.60 usec
PCD2       90.00 usec
PLM2       12.00000000 W
PLM2       0.34680000 W

F2 - Processing parameters
SI         32768
SF         100.6406280 MHz
WDW        RM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
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Compound 19e:



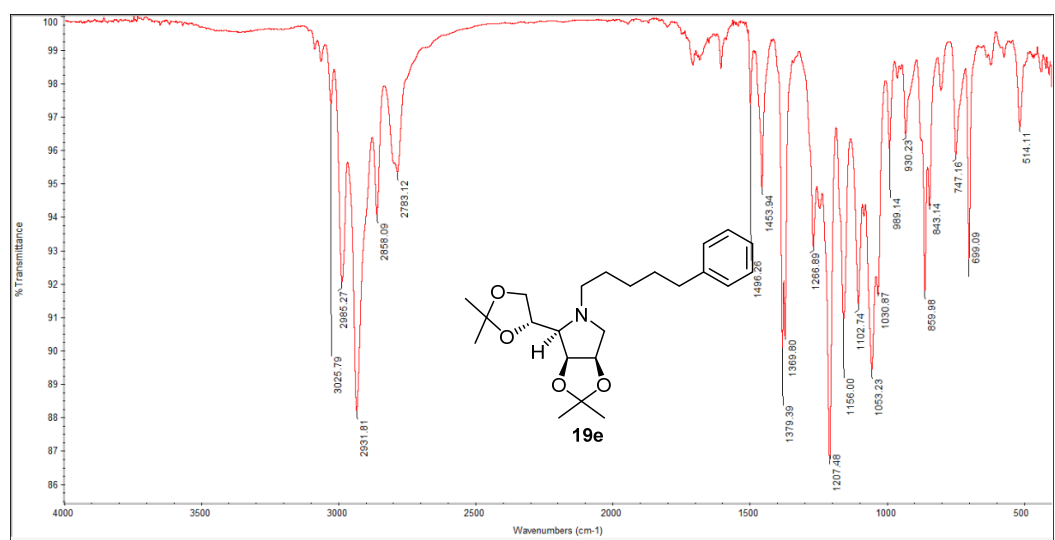


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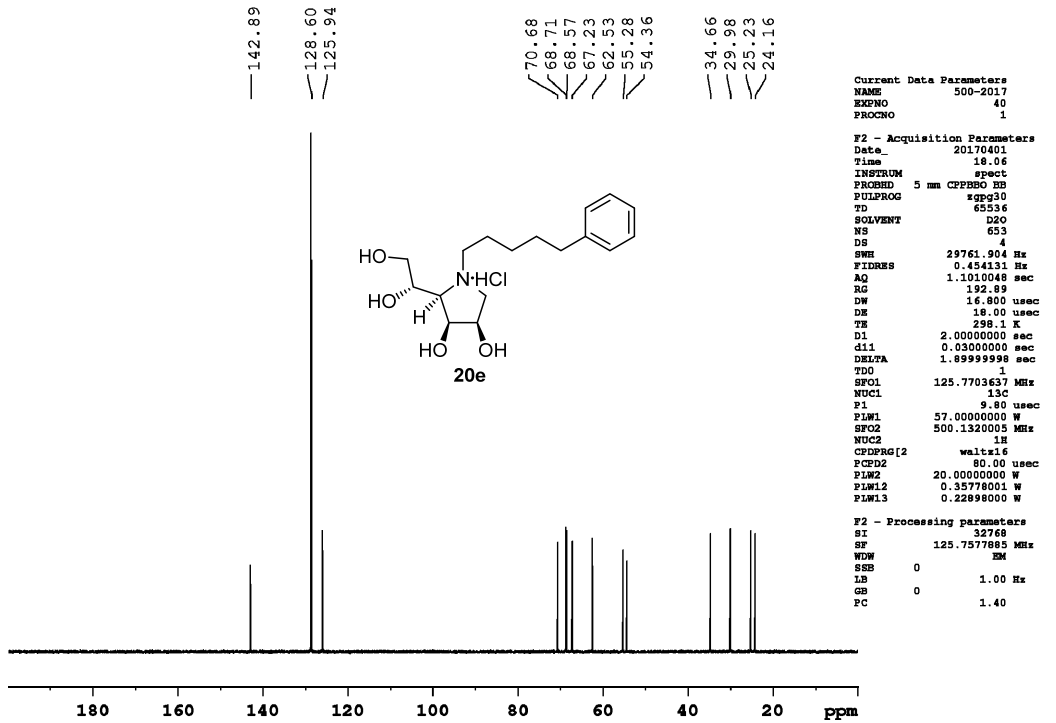
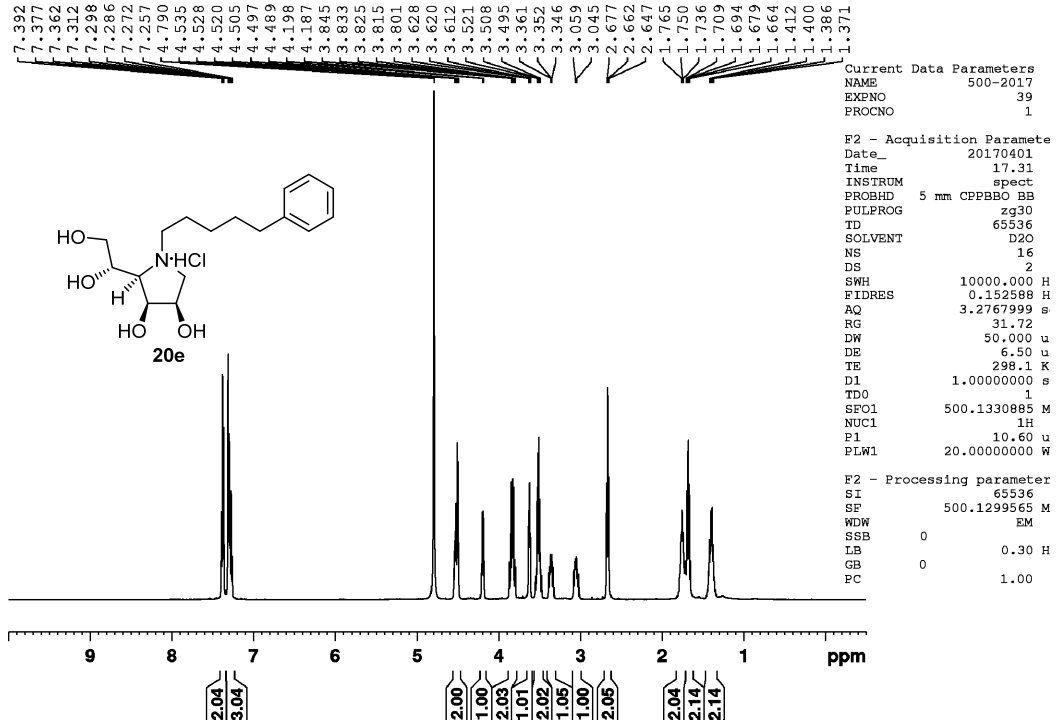
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NAME      400-2017
EXPNO     81
PROCNO    1

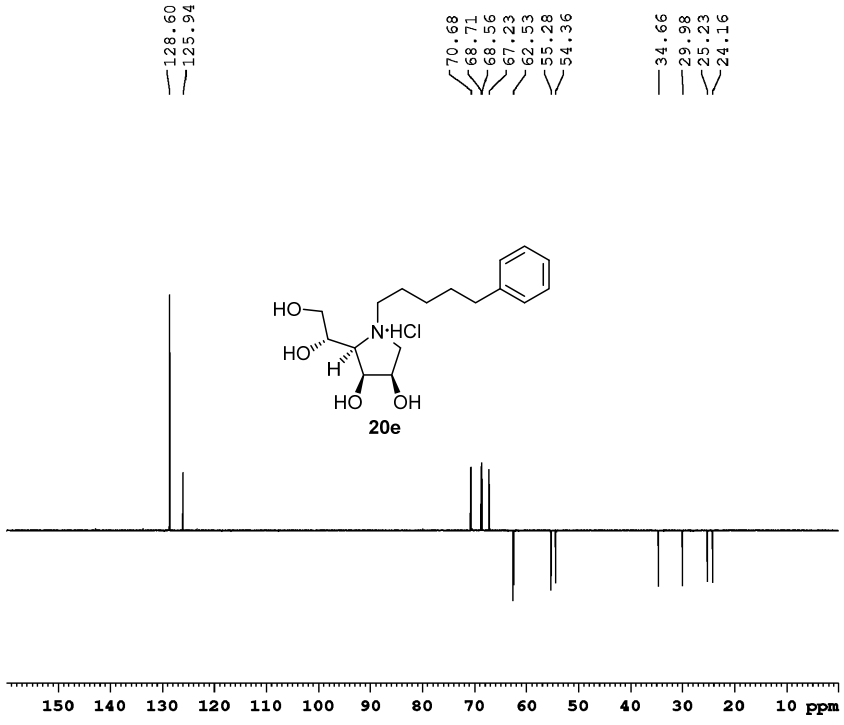
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PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         128
DS         4
SWH        16129.032 Hz
FIDRES     0.246115 Hz
AQ         2.0316160 sec
RG         206.33
SQ         31.300 usec
DE         6.80 usec
TE         299.0 K
CQF2       145.000000
D1         2.0000000 sec
d2         0.00344828 sec
d12        0.0002000 sec
DELTA     0.0001273 sec
TD0        1
SFO1       100.6484788 MHz
NUC1       13C
P1         10.00 usec
P12        2000.00 usec
PL1        0 W
PL12       0 W
PL121      54.0000000 W
SFO1M1[5] Csp50comp-4
SFOAL1     0.500
SFOFFAS    0 Hz
SWS        8.25059986 W
SFO2       400.2412800 MHz
NUC2       1H
CQFPR2[2] waltz16
P3         15.30 usec
P4         30.60 usec
PCPD2      90.00 usec
PLAS       12.0000000 W
PLM12      0.34680000 W

F2 - Processing parameters
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PC         1.40
  
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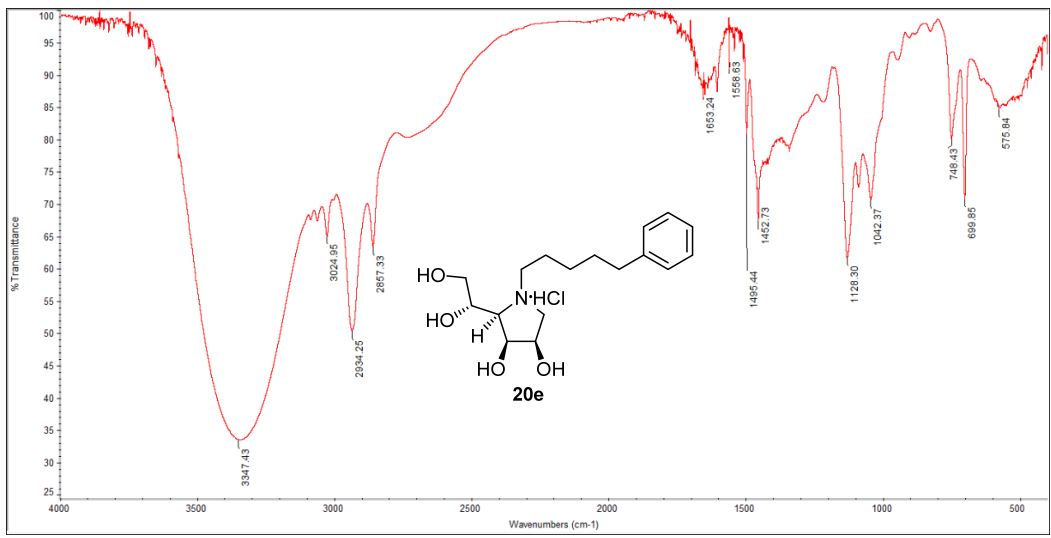


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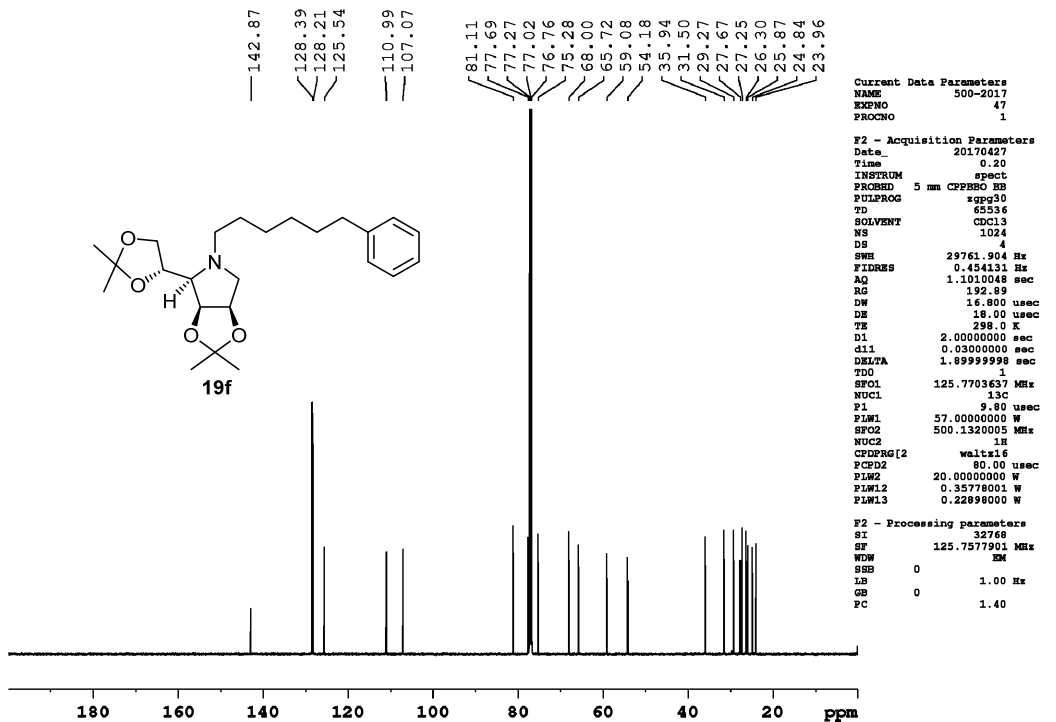
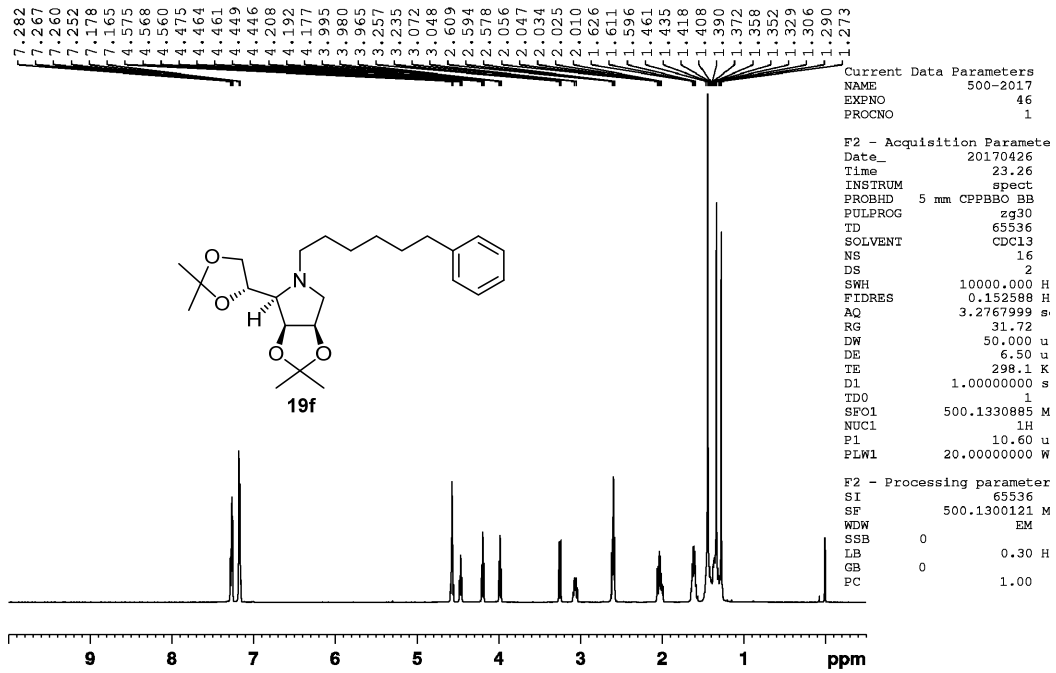


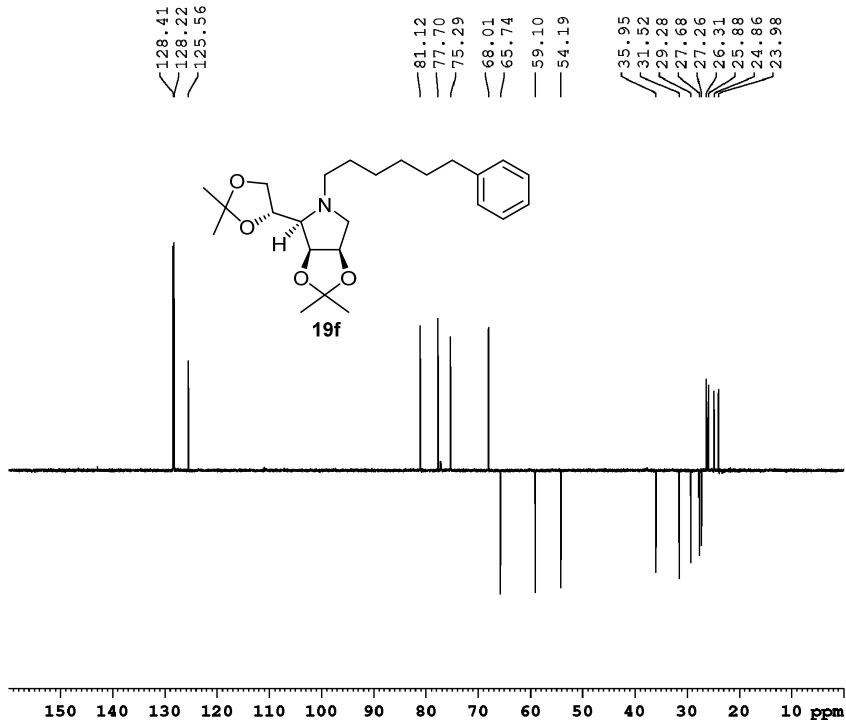


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 PROCNO 1
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 Time 18.17
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 PROCNO 5 nm CPFGPO 3B
 PULPROG deptap135
 ID 85536
 SOLVENT D₂O
 NS 170
 DS 4
 SWH 20161.291 Hz
 FIDRES 0.207637 Hz
 AQ 1.6232328 sec
 RG 192.89
 DW 24.800 usec
 DE 18.00 usec
 TE 300.2 K
 CHT2 145.0000000
 D1 2.0000000 sec
 d2 0.00344828 sec
 d12 0.0002000 sec
 DELTA 0.0001248 sec
 TD 1
 FPC1 125.7678486 MHz
 NUC1 13C
 P1 9.80 usec
 P13 2000.00 usec
 P180 0 W
 PL1 57.0000000 W
 PPM[5] Cap60comp-0
 PPOALS 0.500
 PPOFFS 0 Hz
 PPS 8.36410046 W
 PFC2 500.1315995 MHz
 NUC2 1H
 CDEPRG[2] waltz16
 P3 10.70 usec
 P4 21.40 usec
 PCD2 80.00 usec
 PARS 20.0000000 W
 PL12 0.35778001 W
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 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 GB 0 1.00 Hz
 PC 1.40



Compound 19f:



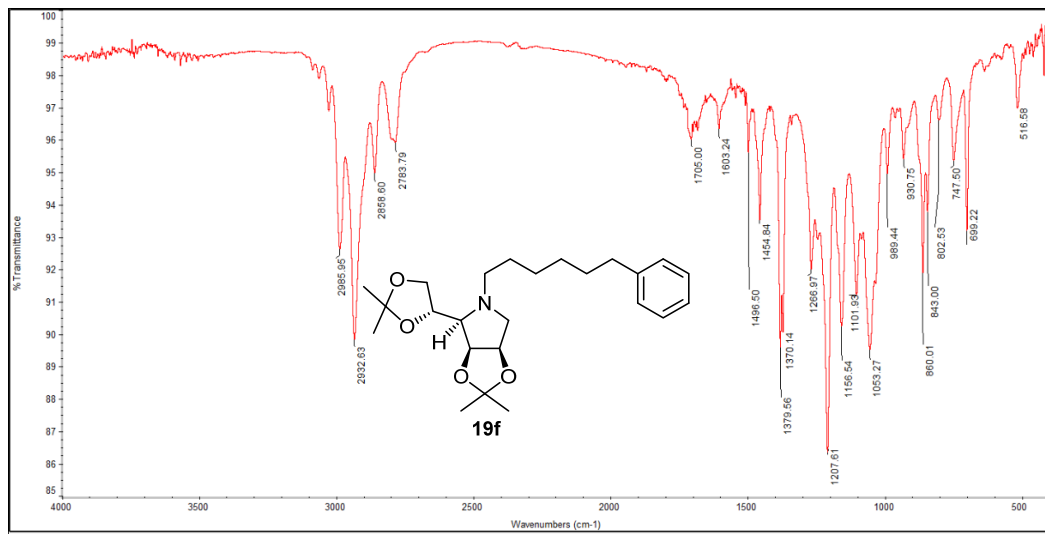


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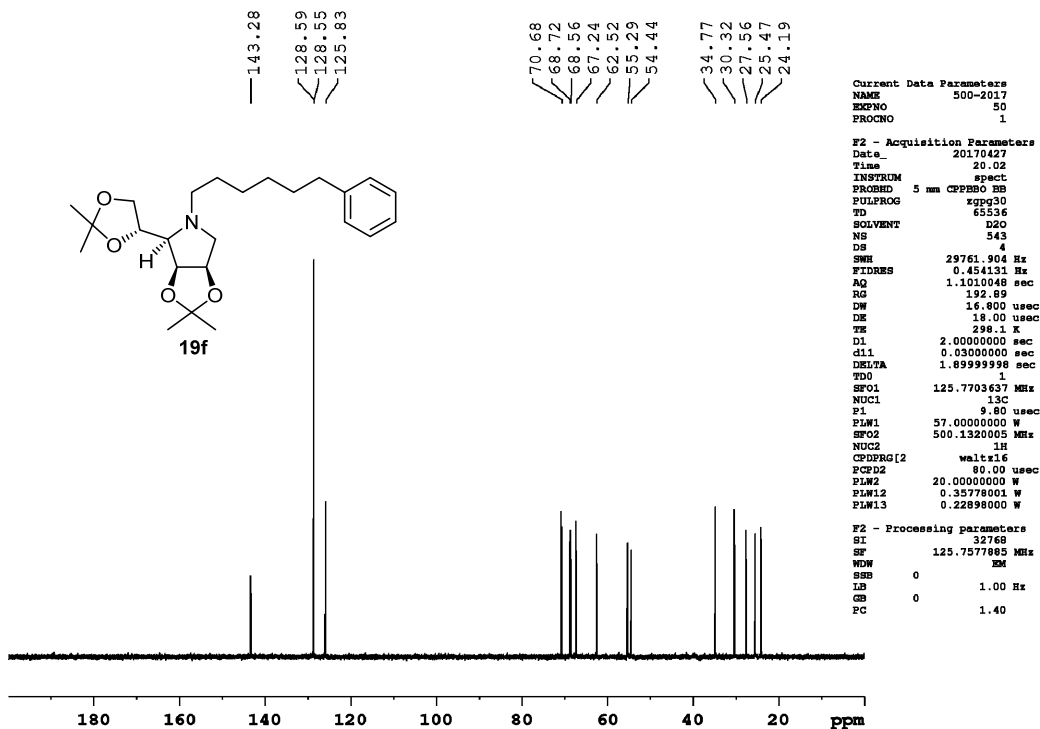
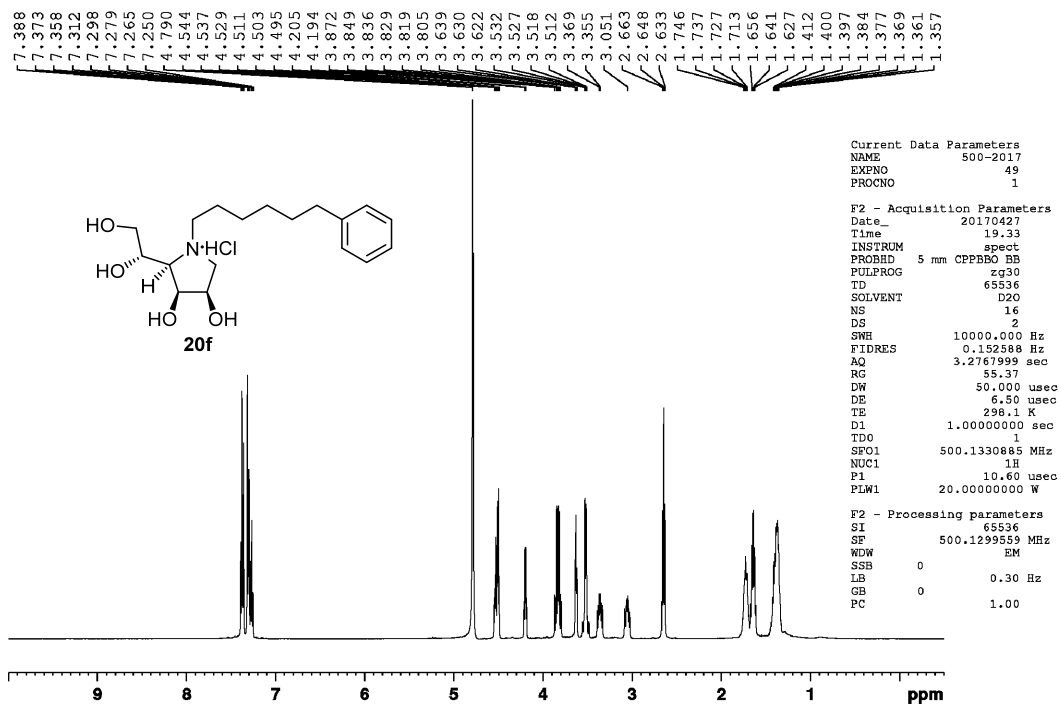
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EXPNO    48
PROCNO   1

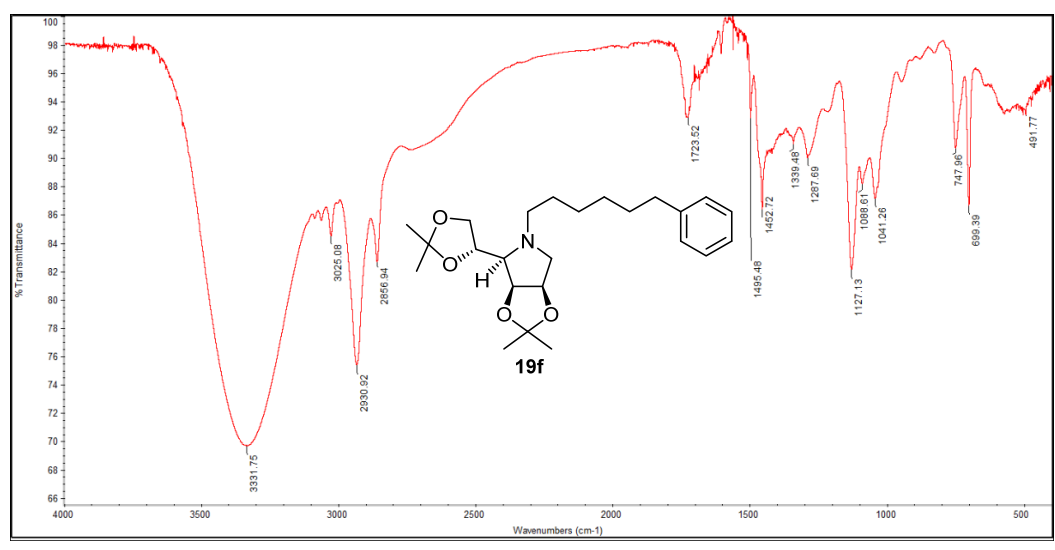
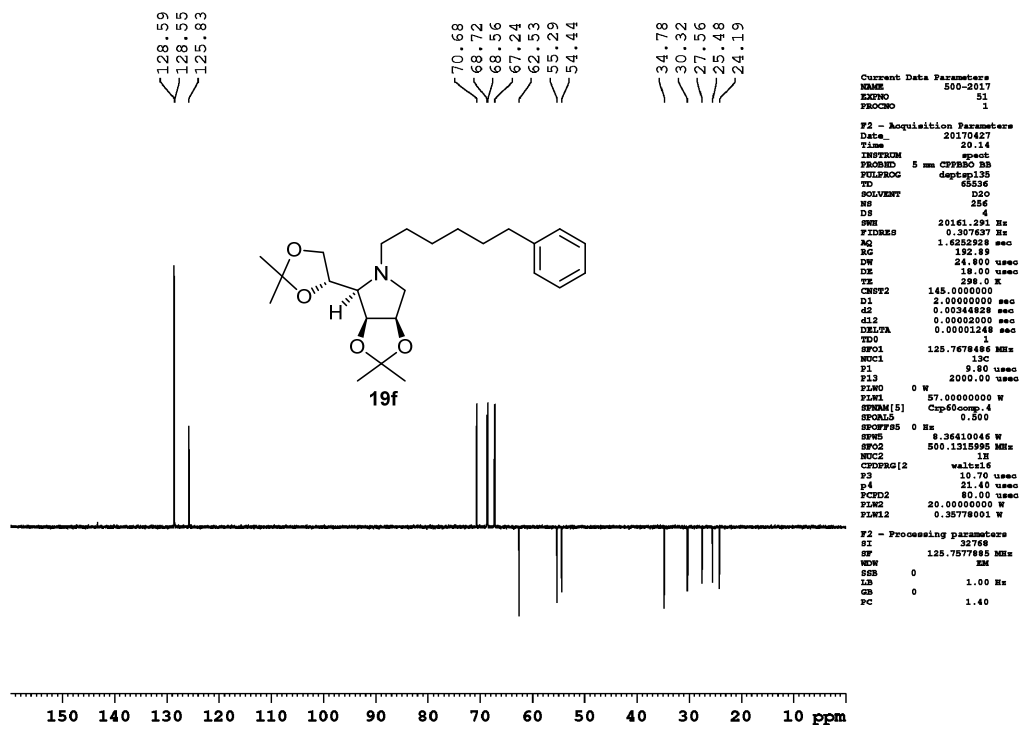
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PULPROG  zgpg30
ID       63536
SOLVENT  CDCl3
NS       256
DS       4
SWH      20161.291 Hz
FIDRES   0.307697 Hz
AQ       1.6282928 sec
RG       192.89
SQ       24.800 usec
DE       18.00 usec
TE       296.1 K
CQF2     145.0000000
D1       2.00000000 sec
d2       0.00344828 sec
d12      0.00052000 sec
DELTA    0.0001248 sec
TD       1
SFO1     125.7678486 MHz
NUC1     13C
P1       9.80 usec
PL1      0 W
SFO2     0 W
P2       2000.00 usec
PL2      0 W
SFO3     57.00000000 W
PL3      0 W
SFO4     57.00000000 W
PL4      0 W
SFO5     57.00000000 W
PL5      0 W
SFO6     57.00000000 W
PL6      0 W
SFO7     57.00000000 W
PL7      0 W
SFO8     57.00000000 W
PL8      0 W
SFO9     57.00000000 W
PL9      0 W
SFO10    57.00000000 W
PL10     0 W
SFO11    57.00000000 W
PL11     0 W
SFO12    57.00000000 W
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F2 - Processing parameters
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PC       1.40
  
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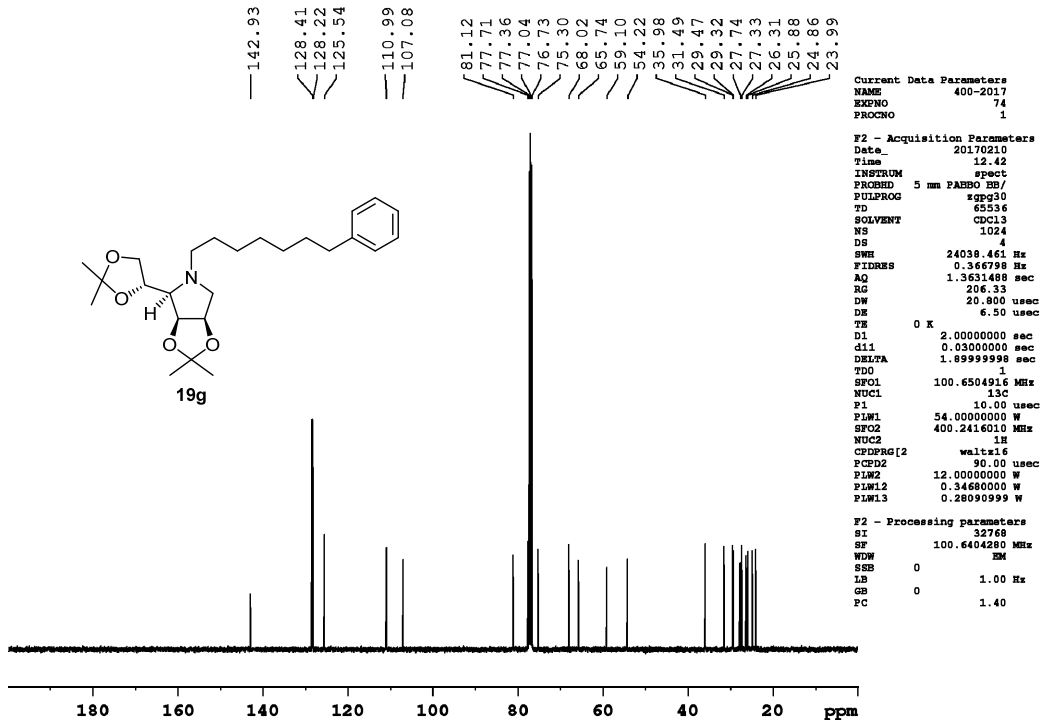
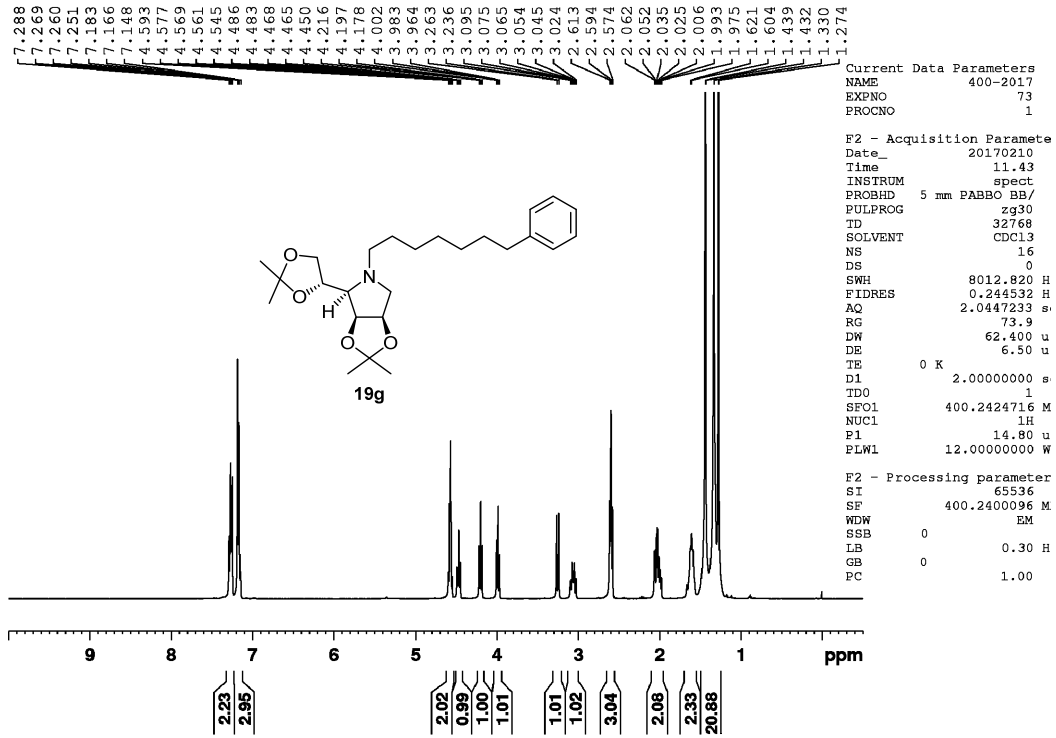


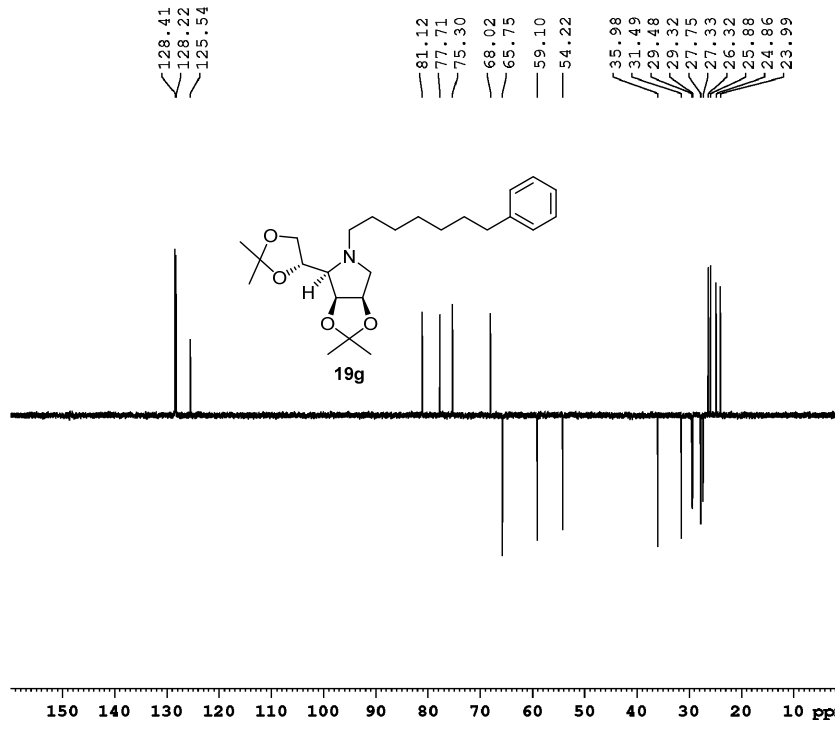
Compound 20f:





Compound 19g:

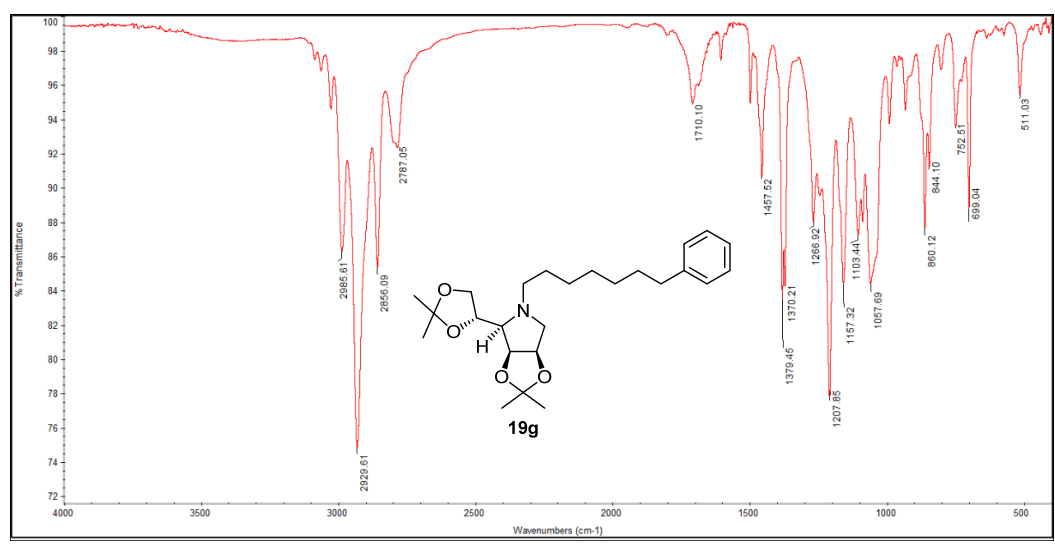




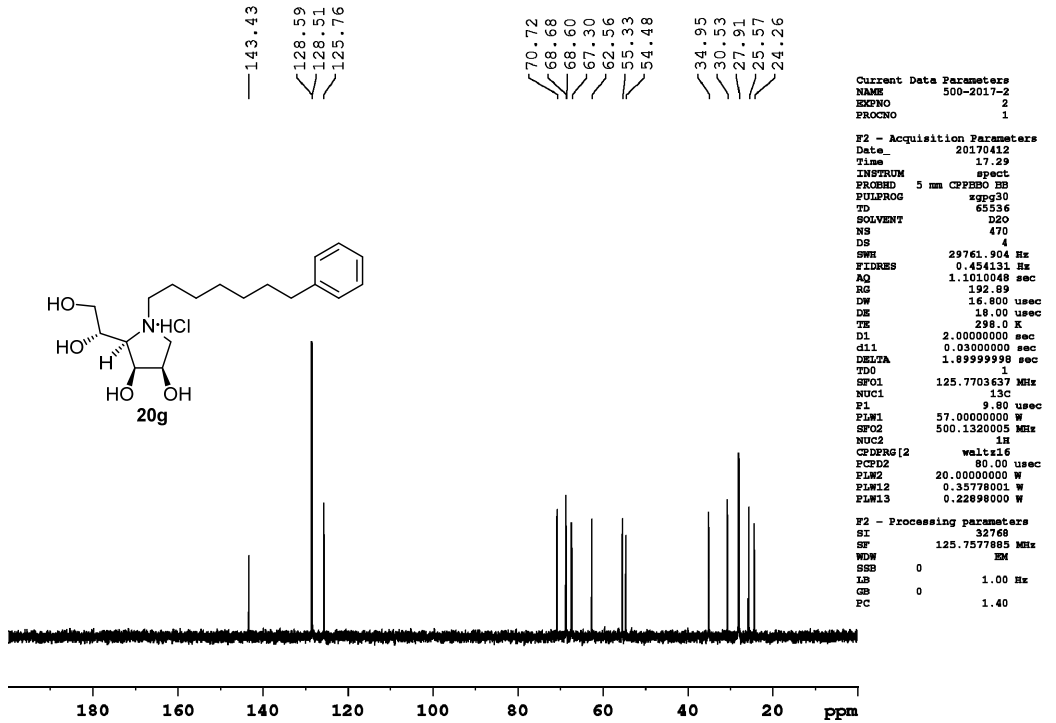
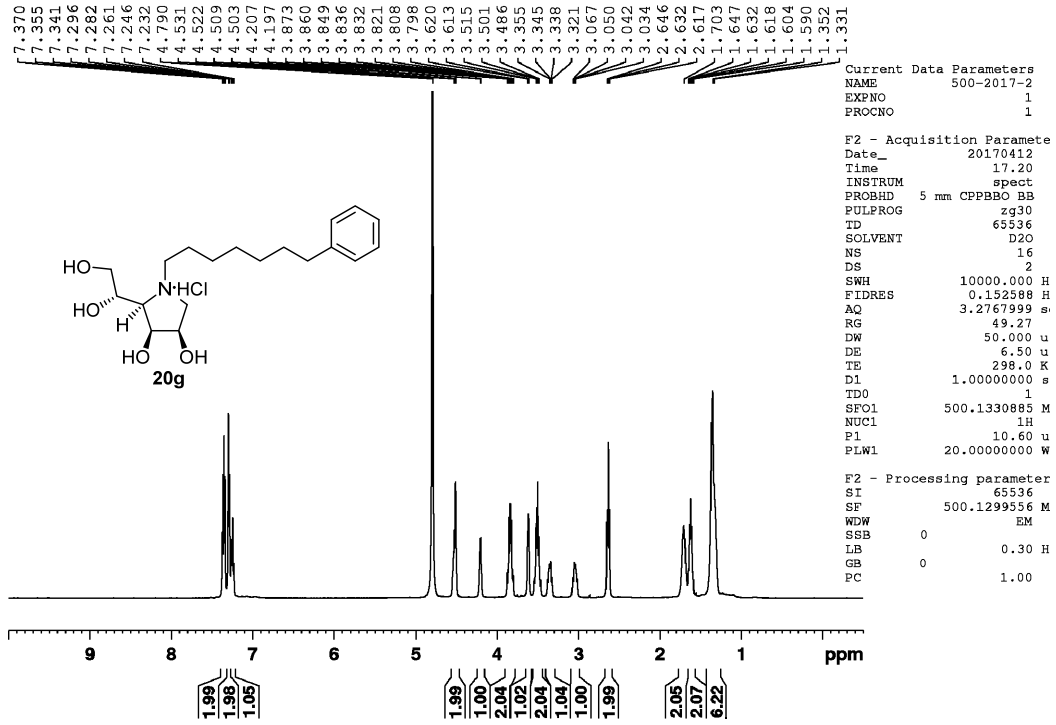
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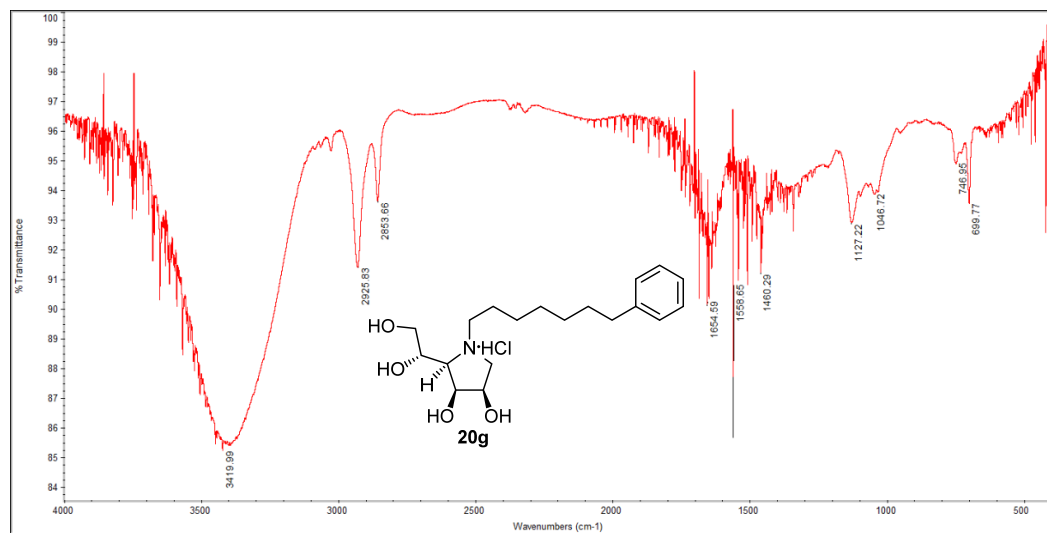
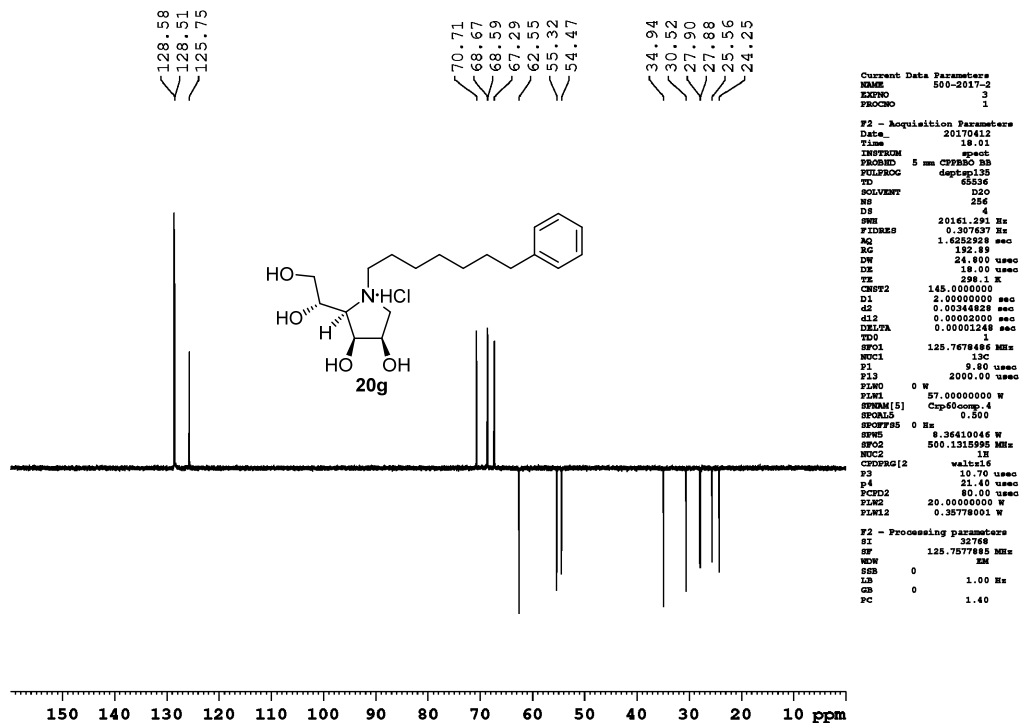
Current Data Parameters
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EXPNO        75
PROCNO       1

F2 - Acquisition Parameters
Date_         20170210
Time          13.00
INSTRUM      spect
PROBHD       5 mm PABBO BB7
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           286
DS           4
SWH          16129.032 Hz
FIDRES      0.246110 Hz
AQ          2.0316160 sec
RG           206.33
SQ          31.900 usec
DE           6.80 usec
TE           0 K
CMT2         145.000000
D1           2.0000000 sec
d2           0.00344828 sec
d12          0.0002000 sec
DELTA       0.0001273 sec
TD0          1
SFO1        100.6484788 MHz
NUC1         13C
P1           10.00 usec
P13          2000.00 usec
SFO         0 W
P14          15.30 usec
SFO         30.60 usec
PCPD2       90.00 usec
SFO         12.0000000 W
P15         0.34680000 W
F2 - Processing parameters
SI           32768
SF           100.6404280 MHz
WDW          EM
SSB          0
GB           1.00 Hz
PC           1.40
  
```

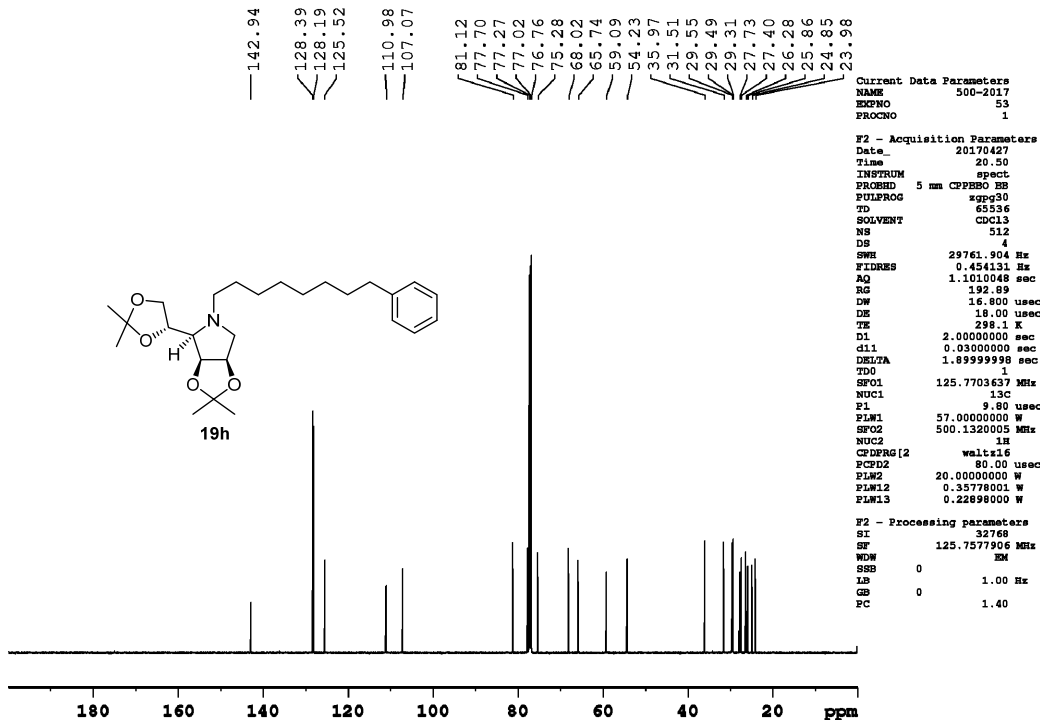
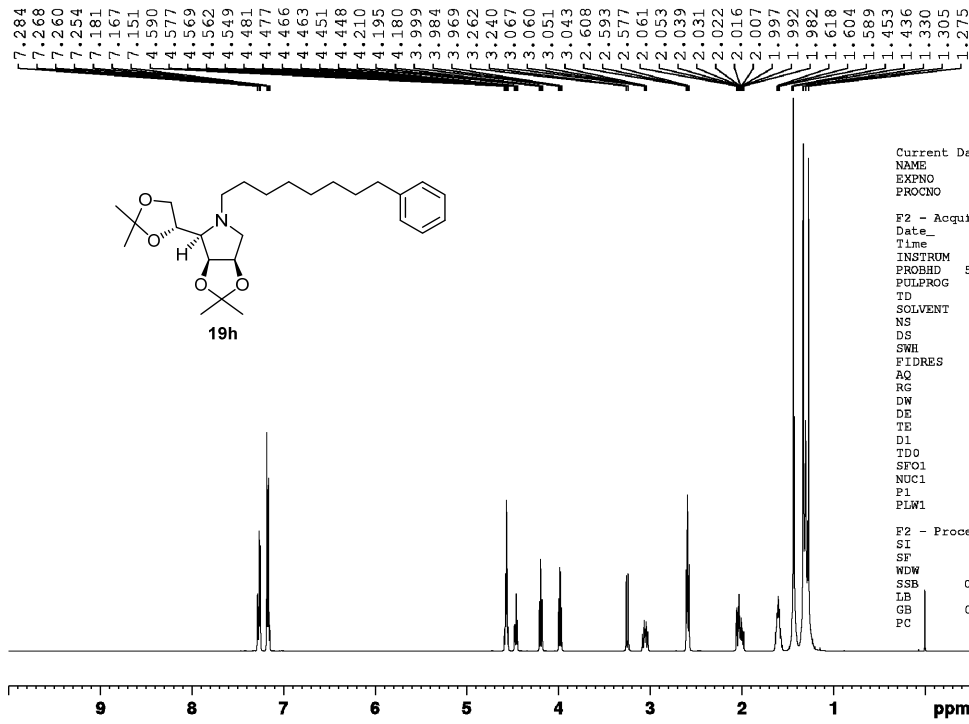


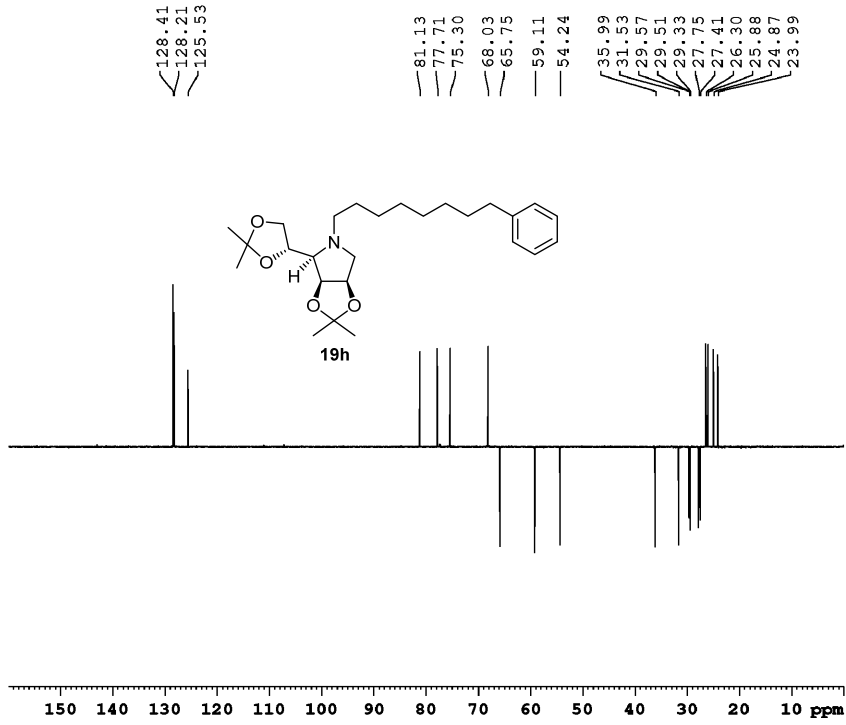
Compound 20g:





Compound 19h:



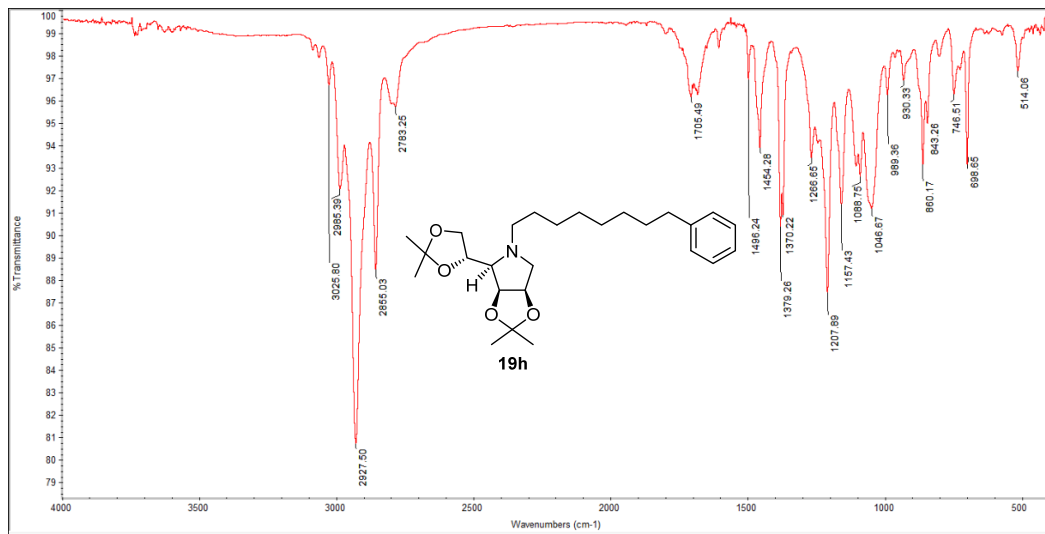


```

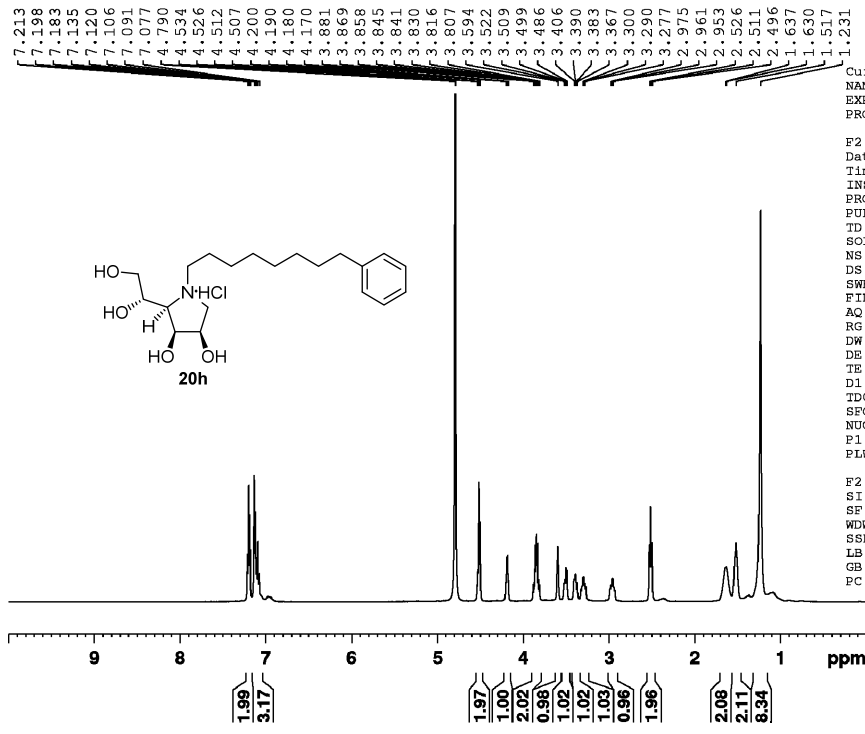
Current Data Parameters
NAME      500-2017
EXPNO     54
PROCNO    1

F2 - Acquisition Parameters
Date_     20170427
Time      21.06
INSTRUM   spect
PROBHD    5 mm CP2HBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         4
SWH        20161.291 Hz
FIDRES     0.207637 Hz
AQ         1.6252928 sec
RG         392.89
DW         24.800 usec
DE         18.00 usec
TE         298.1 K
CPDPR2    145.0000000
D1         2.0000000 sec
d12        0.00344428 sec
d13        0.00002000 sec
DELTA     0.00001248 sec
YD0        1
SFO1      125.7678486 MHz
NUC1       13C
P1         9.80 usec
P13        2000.00 usec
PL10       0 W
PL11       57.0000000 W
SFO1M15    Exp50comp-4
SFOALS     0.500
SFOFFAS    0 Hz
SWS        8.36410046 W
SFO2       500.1315995 MHz
NUC2       1H
CPDPRG2    waltz16
P3         10.70 usec
P4         21.40 usec
PCPD2     80.00 usec
PL12       20.0000000 W
PL13       0.3577800 W

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



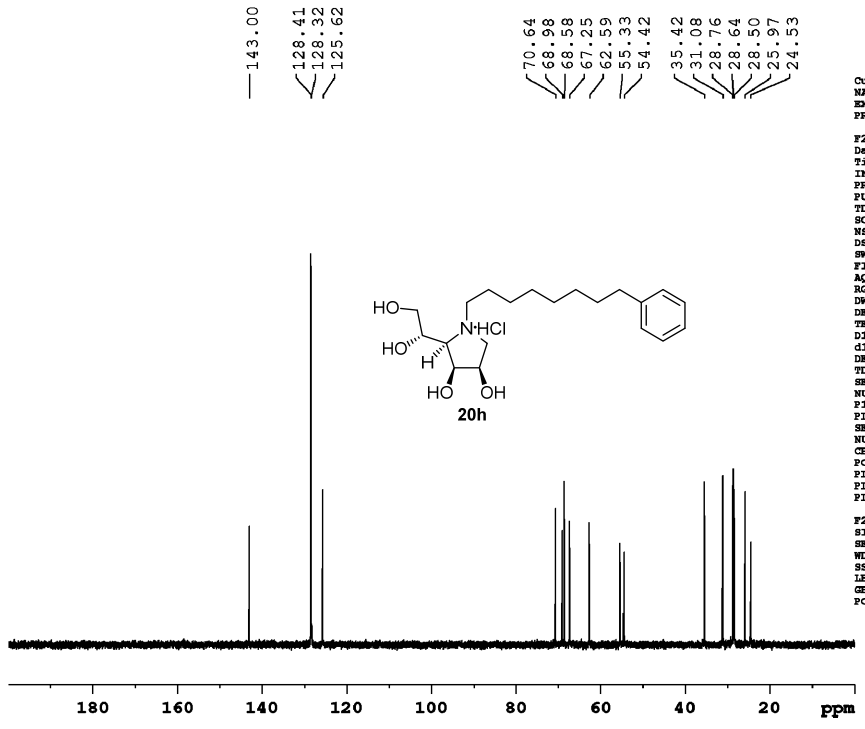
Compound 20h:



Current Data Parameters
 NAME 500-2017
 EXPNO 58
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170428
 Time 19.08
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zg30
 TD 65536
 SOLVENT D2O
 NS 16
 DS 2
 SWH 10000.000 H
 FIDRES 0.152588 H
 AQ 3.2767999 s
 RG 31.72
 DW 50.000 u
 DE 6.50 u
 TE 298.1 K
 DL 1.00000000 s
 TDO 1
 SFO1 500.1330885 M
 NUC1 1H
 P1 10.60 u
 PLW1 20.00000000 W

F2 - Processing parameter
 SI 65536
 SF 500.1299554 M
 WDW EM
 SSB 0
 LB 0.30 H
 GB 0
 PC 1.00



Current Data Parameters
 NAME 500-2017
 EXPNO 59
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170428
 Time 19.14
 INSTRUM spect
 PROBHD 5 mm CPPBBO BB
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 285
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 192.89
 DW 16.800 usec
 DE 18.00 usec
 TE 298.1 K
 DL 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1
 SFO1 125.7703637 MHz
 NUC1 13C
 P1 9.80 usec
 PLW1 57.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG2 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

128.41
128.32
125.62

70.64
68.08
68.08
67.23
62.59
55.33
54.42

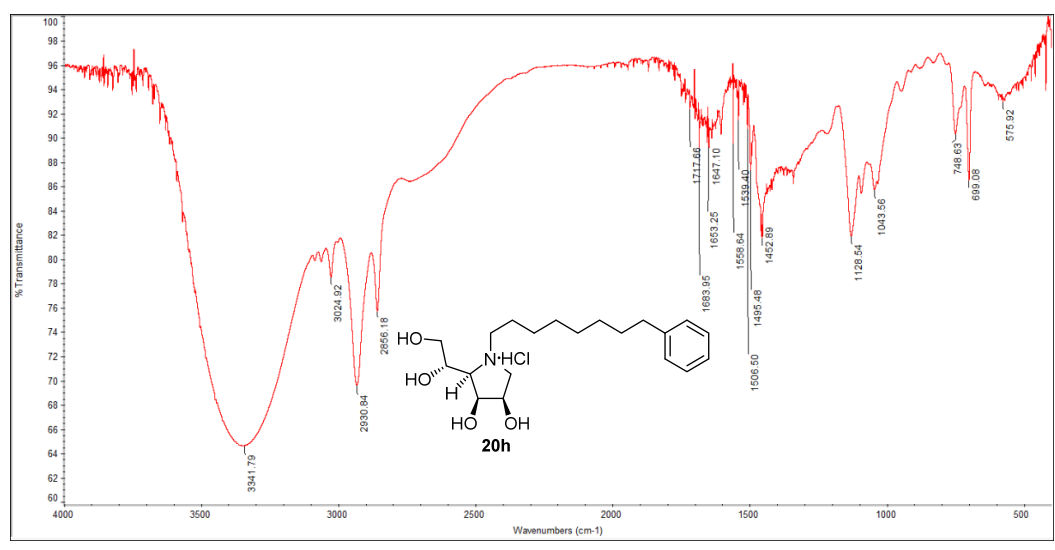
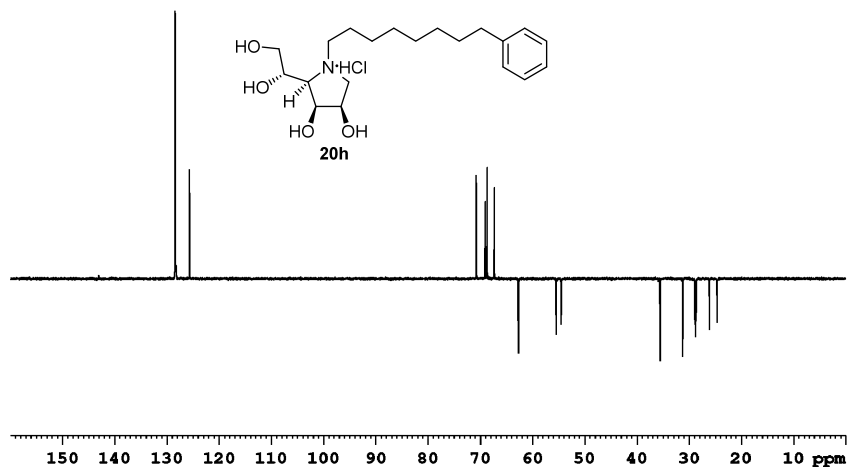
55.42
31.08
28.76
28.64
26.50
25.77
24.53

```

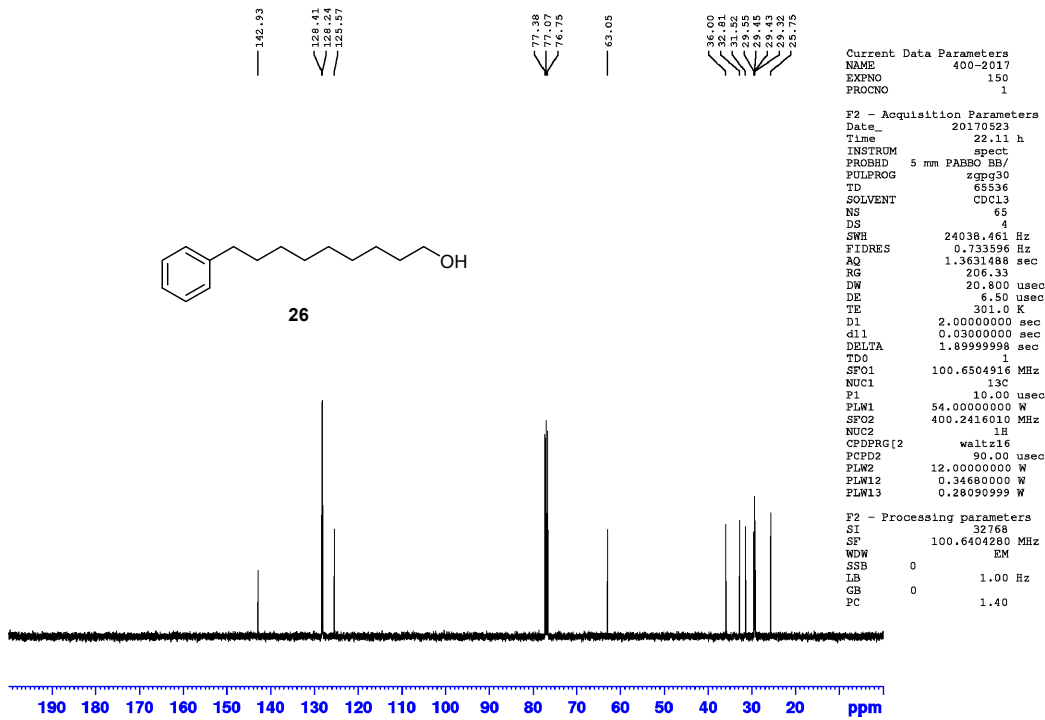
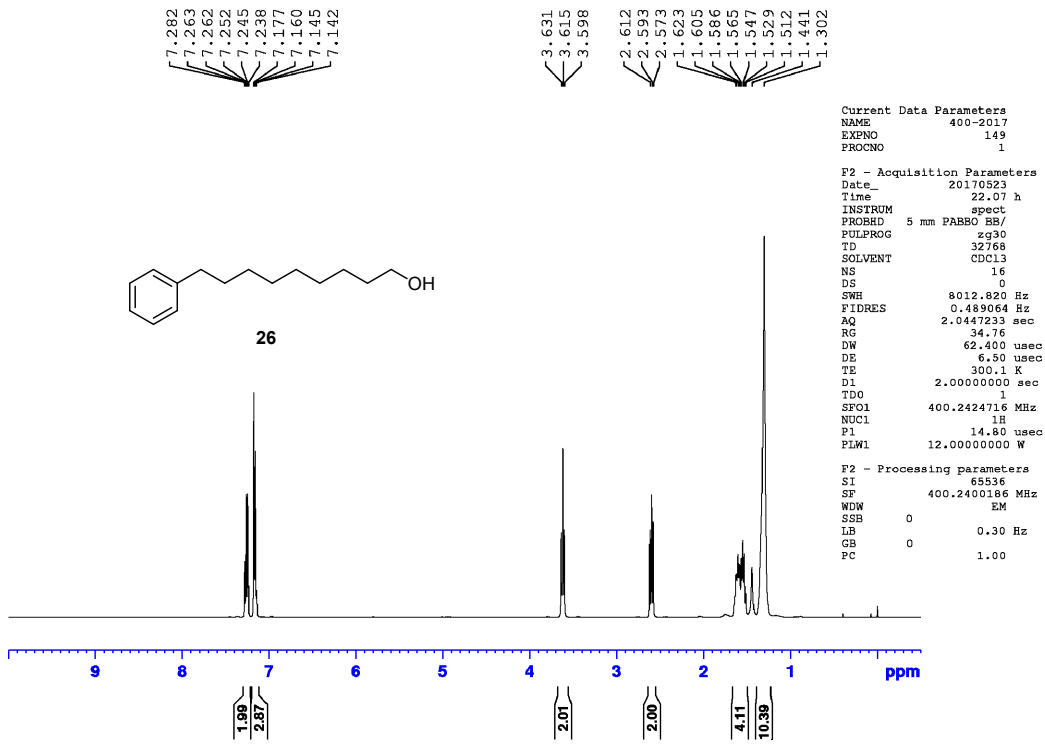
Current Data Parameters
NAME      500-2017
EXPNO    60
PROCNO   1

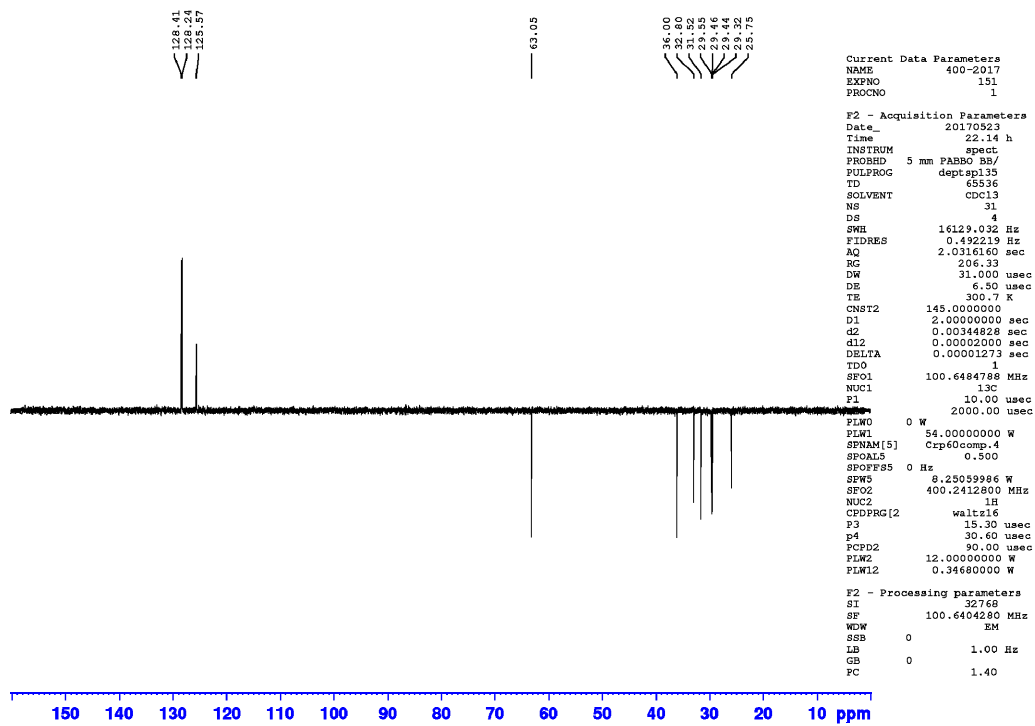
F2 - Acquisition Parameters
Date_    20170428
Time     19.25
INSTRUM  spect
PROBHD   5 mm CPBPRG3 BB
PULPROG  zgpg30
TD        65536
SOLVENT  D2O
DS        4
FWS      20161.291 Hz
AQ        0.307657 Hz
RG        1.6252528 sec
RG        192.89
DW        24.400 usec
DE        18.00 usec
TE        298.0 K
CHFT2    145.000000
D1        2.0000000 sec
d2        0.0034428 sec
d12       0.0002200 sec
DELTA    0.00001249 sec
TDO       1
SFO1     125.7678486 MHz
NUC1      13C
P1        9.80 usec
P12       2000.00 usec
PL10     0 W
PL12     57.0000000 W
SFO1(5)  Cp40comp 4
SFOAL5   0.200
SFOFF5   0 Hz
SWS      8.36410046 W
SFO2     500.1315995 MHz
NUC2      1H
CPDPRG2  waltz16
P3        10.70 usec
P4        21.40 usec
PCPD2    80.00 usec
PL10     20.0000000 W
PL12     0.35778001 W

F2 - Processing parameters
SI        32768
SF        125.7577865 MHz
WDW       EM
SSB       0
GB        0
PC        1.40
  
```

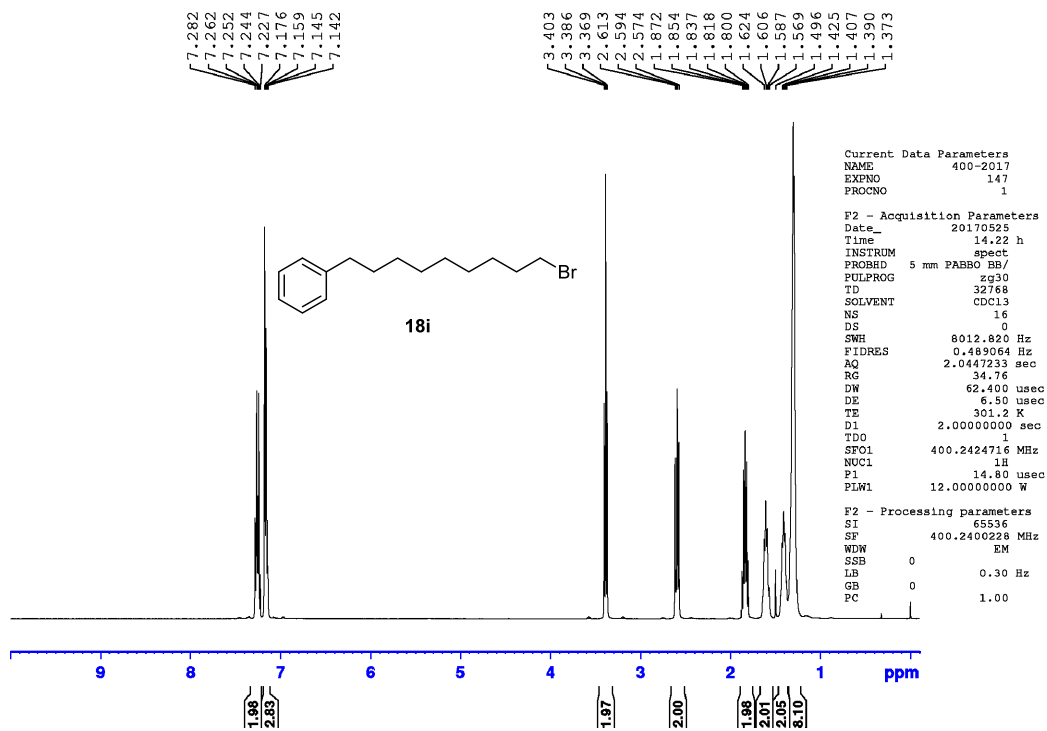


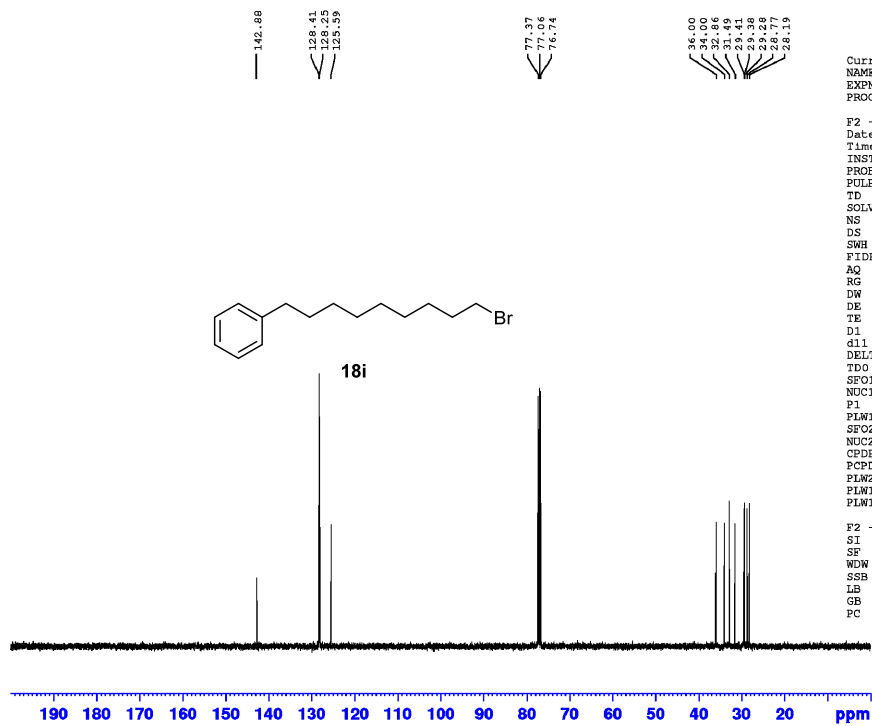
Compound 26:





Compound 18i:



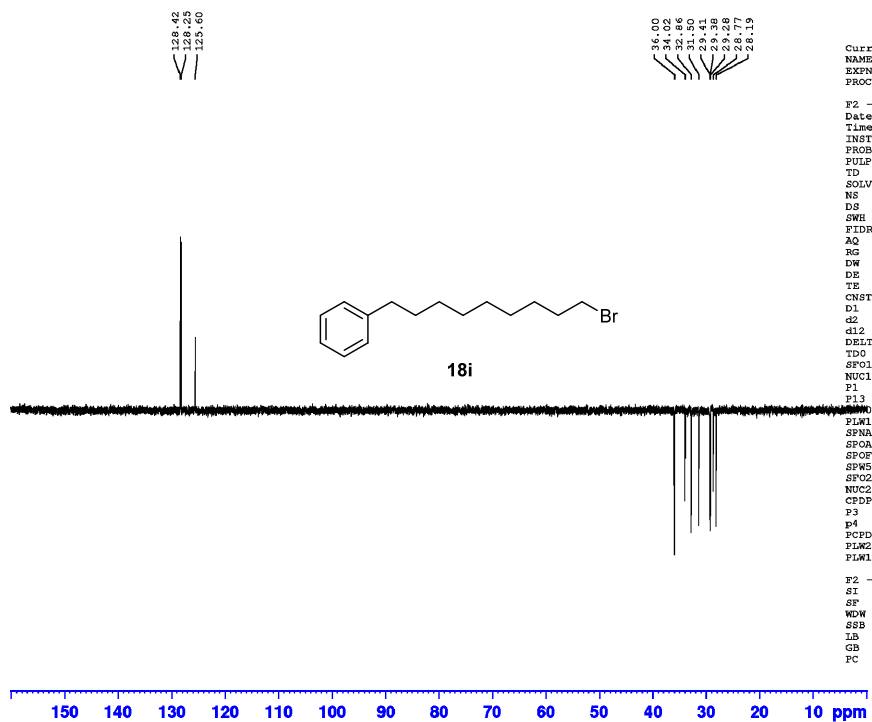


```

Current Data Parameters
NAME          400-2017
EXPNO        148
PROCNO       1

F2 - Acquisition Parameters
Date_        20170525
Time         14.29 h
INSTRUM      spect
PROBHD       5 mm PABBO BB/
PULPROG      zgpg30
TD           65536
SOLVENT      CDC13
NS           121
DS           4
SWH          24038.461 Hz
FIDRES       0.733596 Hz
AQ           1.3631488 sec
RG           206.33
DW           20.800 usec
DE           6.50 usec
TE           302.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TDO          1
SFO1         100.6504916 MHz
NUC1         13C
P1           10.00 usec
PLW1         54.00000000 W
SFO2         400.2416010 MHz
NUC2         1H
CPDPRG[2]   waltz16
PCPD2        90.00 usec
PLW2         12.00000000 W
PLW12        0.34680000 W
PLW13        0.28090999 W

F2 - Processing parameters
SI           32768
SF           100.6404280 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```



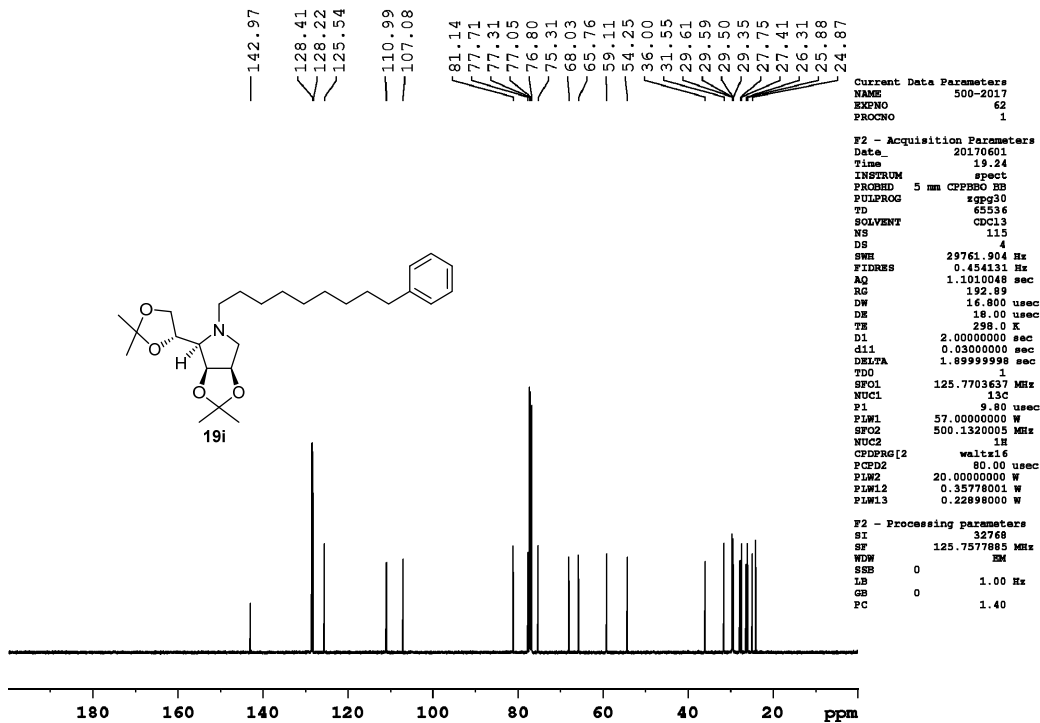
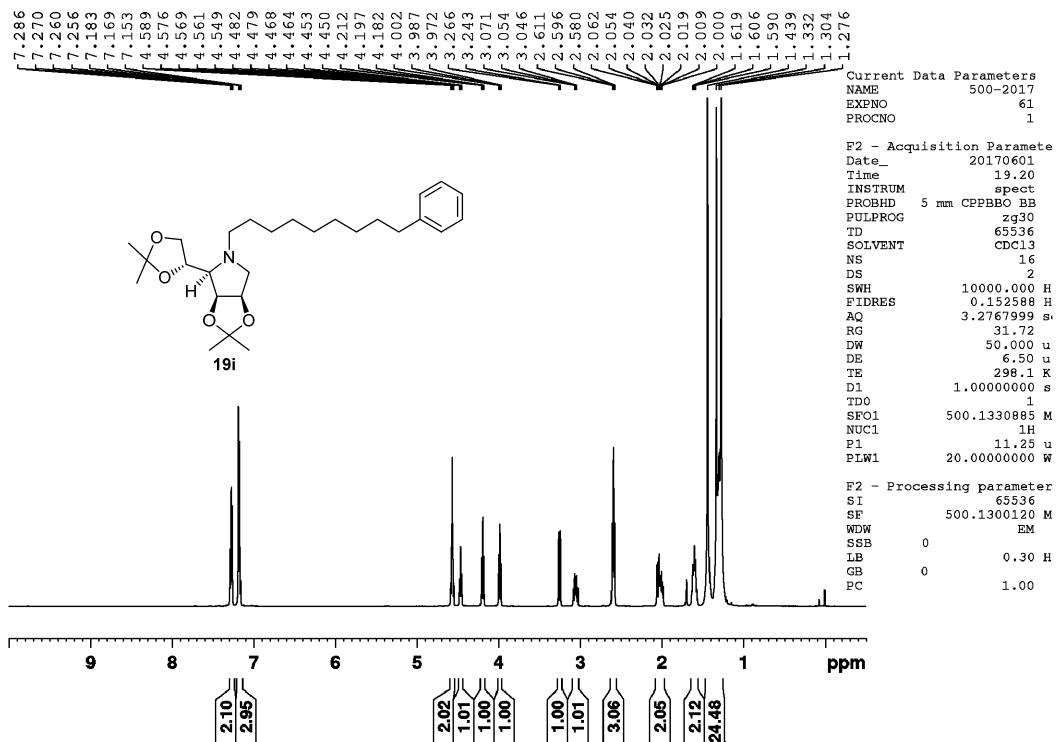
```

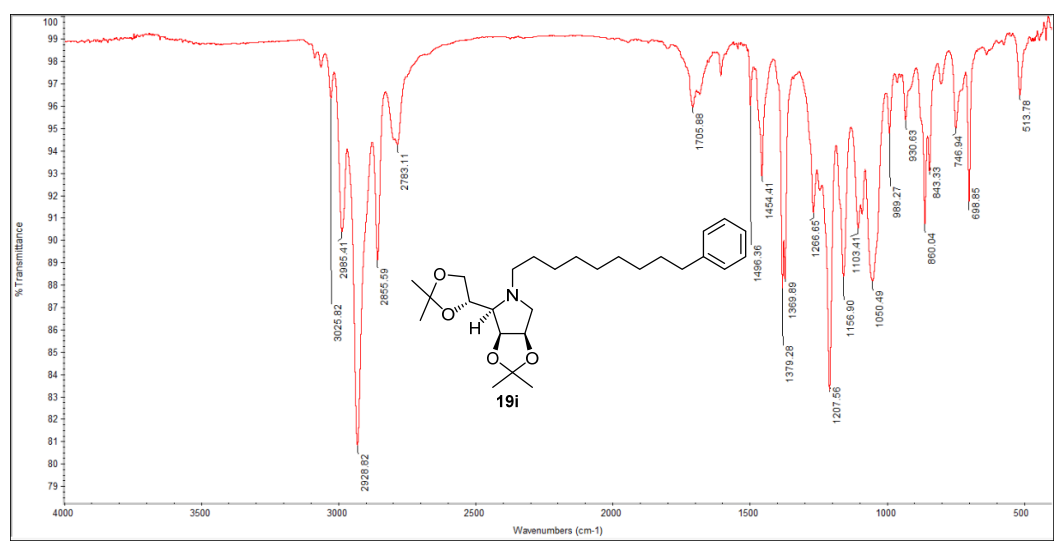
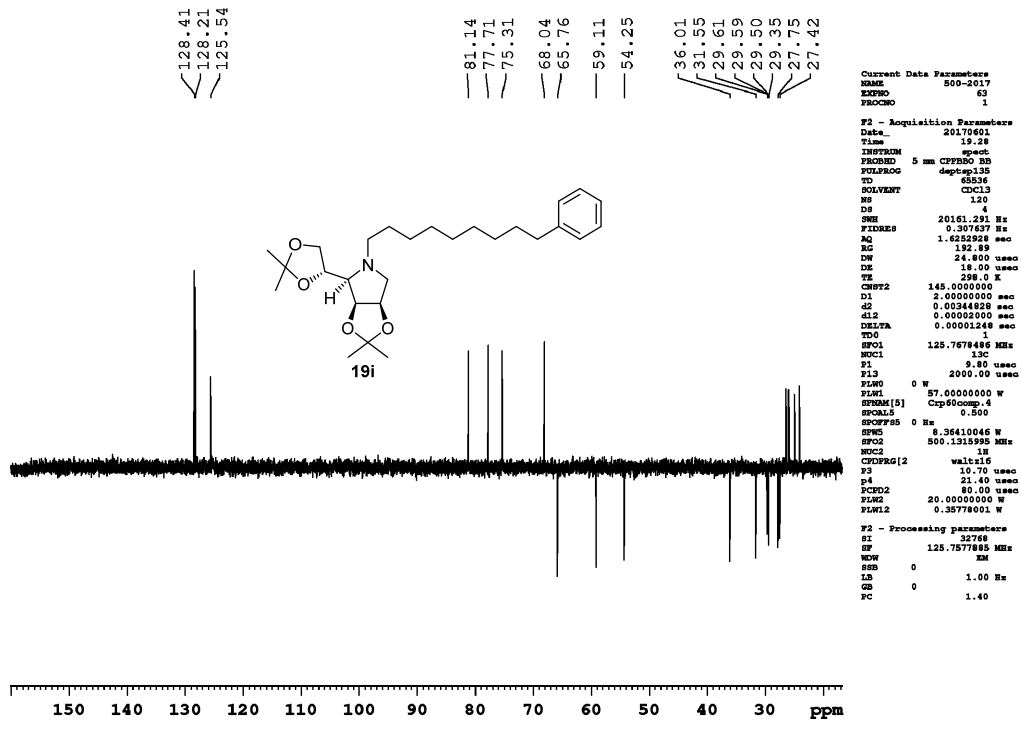
Current Data Parameters
NAME          400-2017
EXPNO        155
PROCNO       1

F2 - Acquisition Parameters
Date_        20170525
Time         14.33 h
INSTRUM      spect
PROBHD       5 mm PABBO BB/
PULPROG      deptsp135
TD           65536
SOLVENT      CDC13
NS           21
DS           4
SWH          16123.032 Hz
FIDRES       0.432219 Hz
AQ           2.0316160 sec
RG           206.33
DW           31.000 usec
DE           6.50 usec
TE           301.2 K
CNST2       145.0000000 sec
D1           2.00000000 sec
d2           0.00344828 sec
d12          0.00002000 sec
DELTA        0.00001273 sec
TDO          1
SFO1         100.6484788 MHz
NUC1         13C
P1           10.00 usec
P13          2000.00 usec
SFO5         0 W
PLW1         54.00000000 W
SPNAM[5]    Crp60comp.4
SFOAL5       0.500
SFOFFS5     0 Hz
SEW5         8.25059986 W
SFO2         400.2412800 MHz
NUC2         1H
CPDPRG[2]   waltz16
P3           15.30 usec
p4           30.60 usec
PCPD2        90.00 usec
PLW2         12.00000000 W
PLW12        0.34680000 W

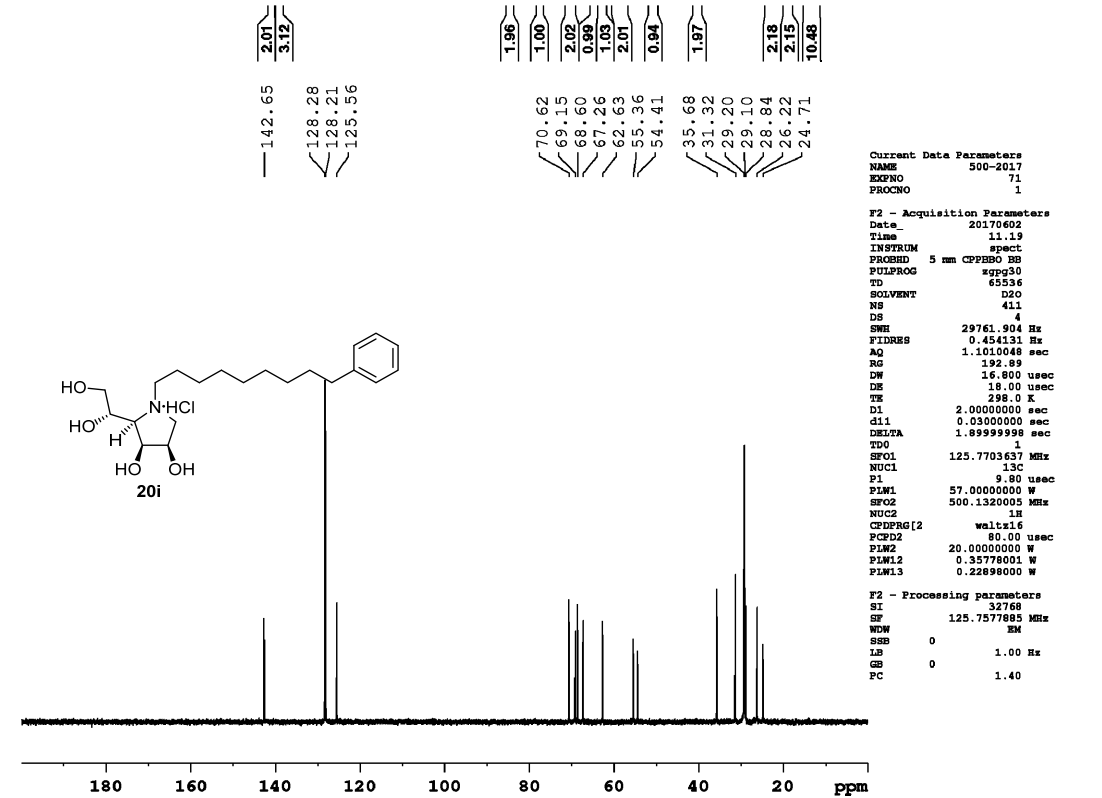
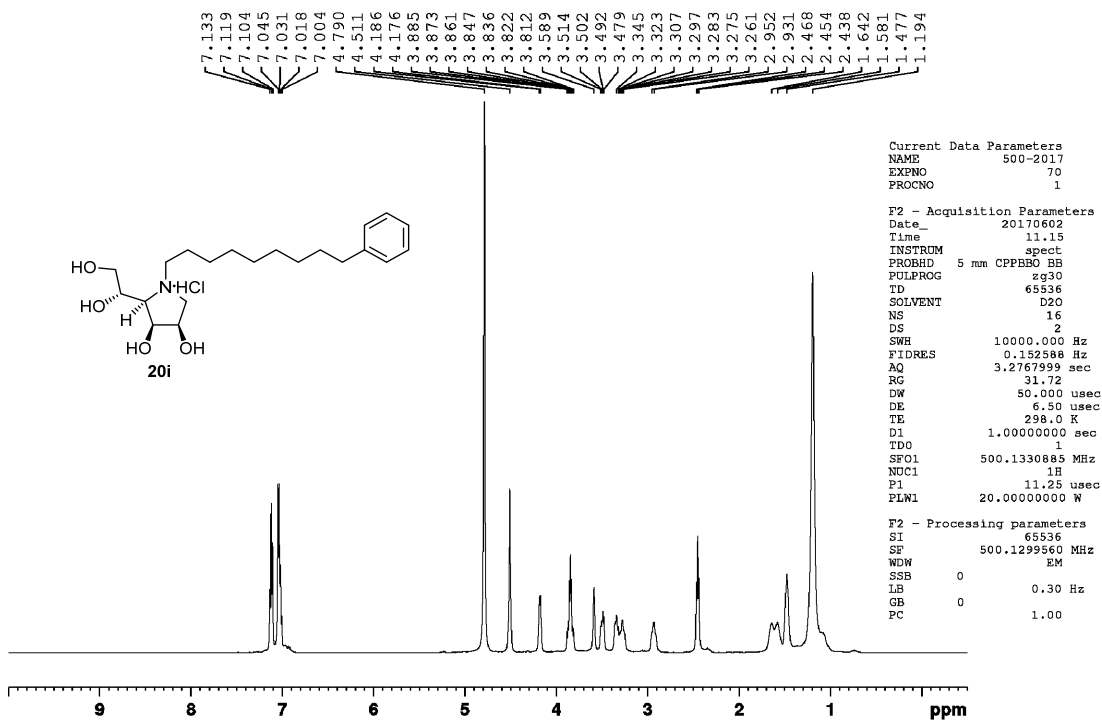
F2 - Processing parameters
SI           32768
SF           100.6404280 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

Compound 19i:





Compound 20i:



< 128.28
 < 128.21
 < 125.56

< 70.62
 < 69.15
 < 68.60
 < 67.26
 < 62.62
 < 55.36
 < 54.41

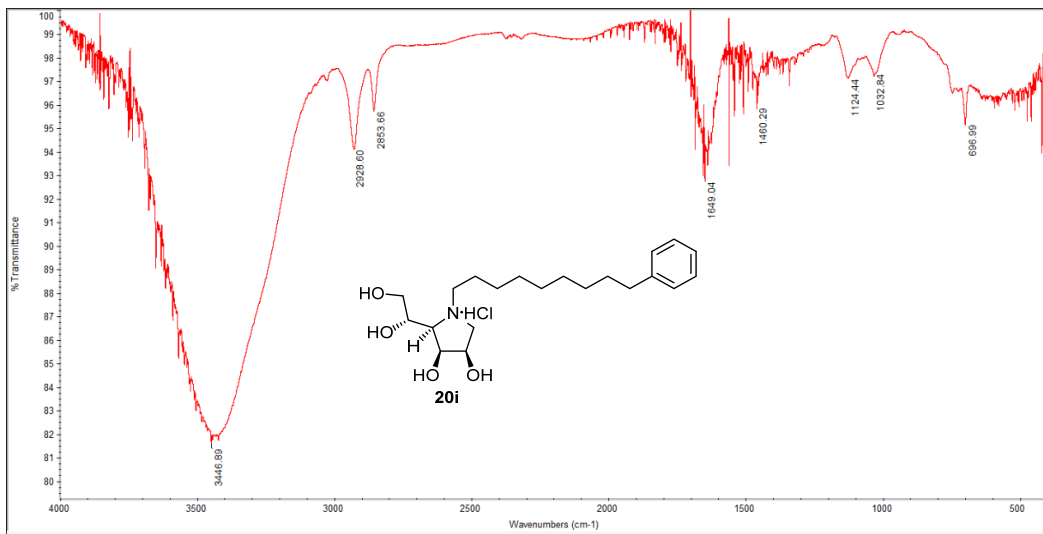
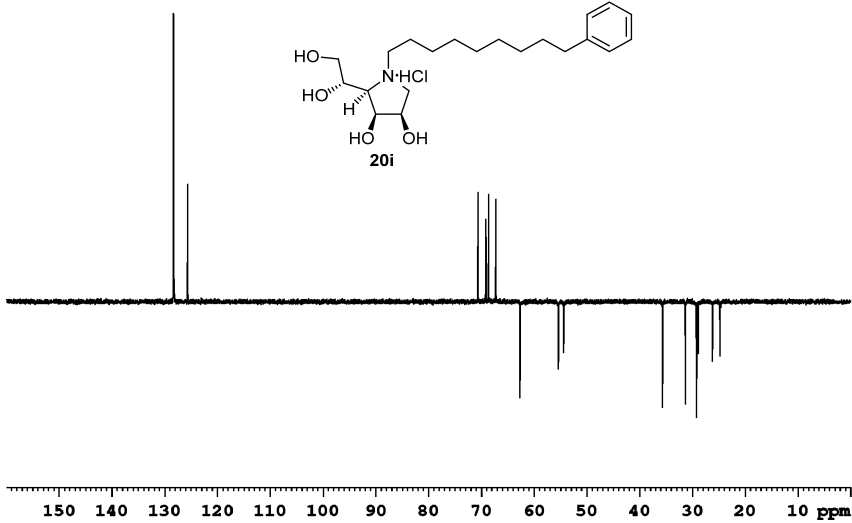
< 35.68
 < 31.32
 < 29.20
 < 29.10
 < 28.84
 < 26.21
 < 24.71

```

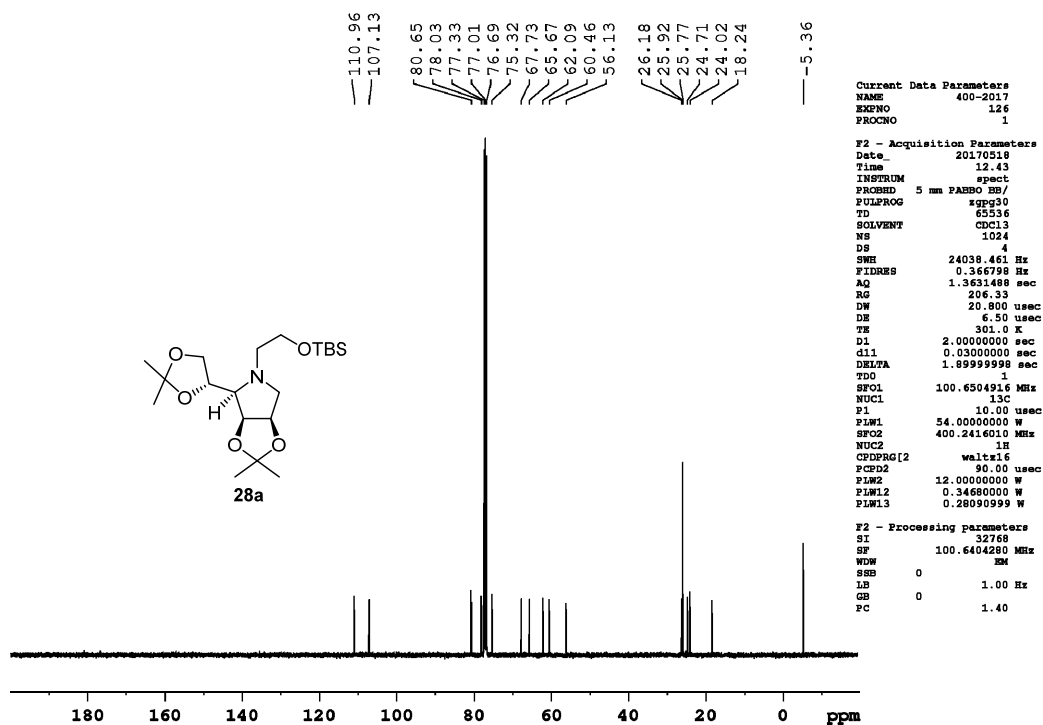
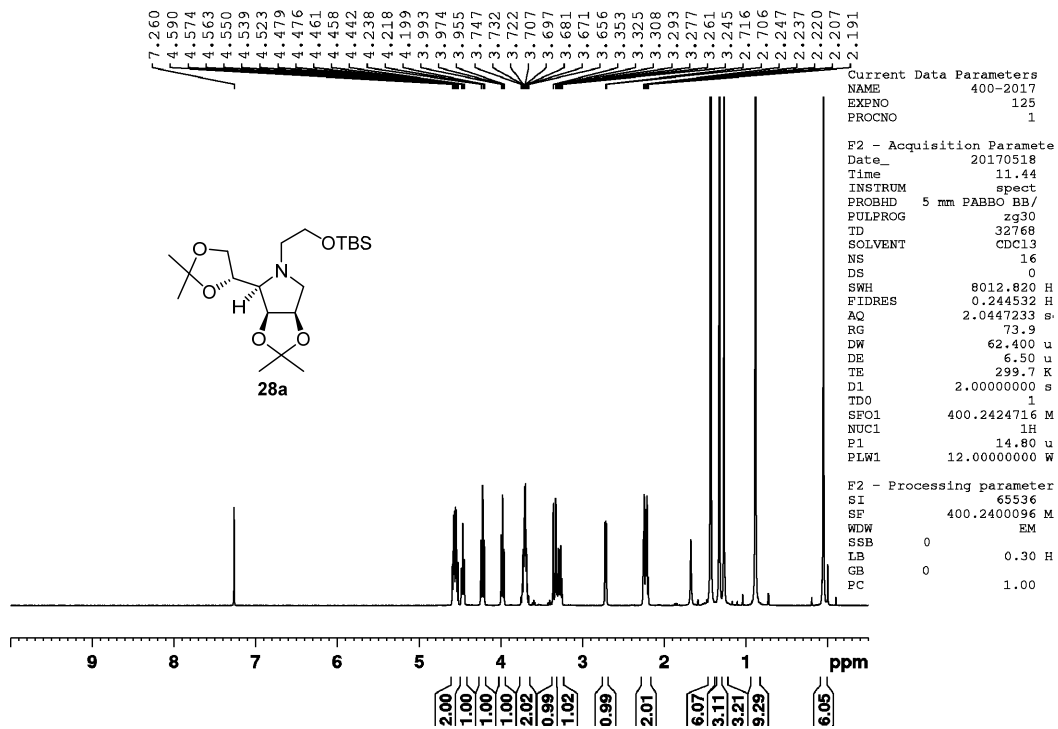
Current Data Parameters
NAME      500-2017
EXPNO    72
PROCNO   1

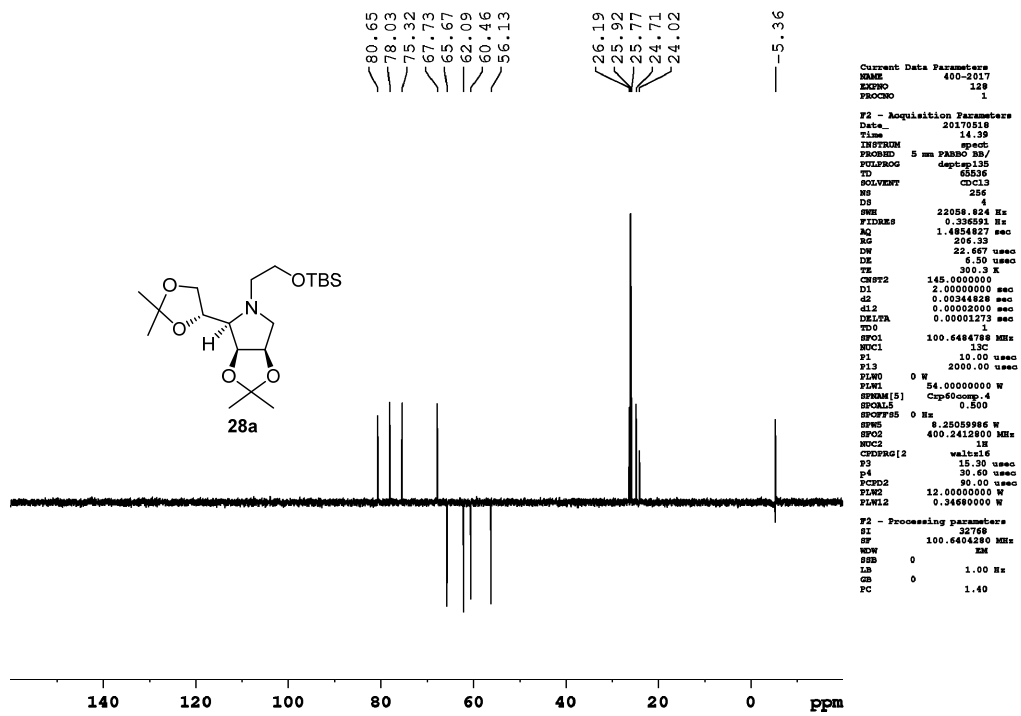
F2 - Acquisition Parameters
Data_    20170502
Time     11.41
INSTRUM  spect
PROBHD   5 mm CPMAS BB
PULPROG  zgpg30
TD       65536
SOLVENT  D2O
NS       64
DS       4
SWH      20161.291 Hz
FIDRES   0.307657 Hz
AQ       1.6252928 sec
RG       192.89
DW       24.800 usec
DE       18.00 usec
TE       298.0 K
CST2     145.0000000
D1       2.000000000 sec
d2       0.00344828 sec
d12      0.00002000 sec
DELTA    0.00001248 sec
TD0      1
SFO1     125.7678485 MHz
NUC1     13C
P1       9.80 usec
P13      2000.00 usec
PRG      0 W
PLW1     57.00000000 W
SFO1(S)  Csp400mgp-4
SFOAL5   0.500
SFOFF5   0 Hz
SWS      8.35410046 W
SFO2     500.1315995 MHz
MOC2     18
CROSSPRG[2] waltz16
P3       10.70 usec
P4       21.40 usec
PCPD2    80.00 usec
PLW2     20.00000000 W
PLW12    0.35776901 W

F2 - Processing parameters
SI       32768
SF       125.7678485 MHz
NUC      13C
SFB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```



Compound 28a:





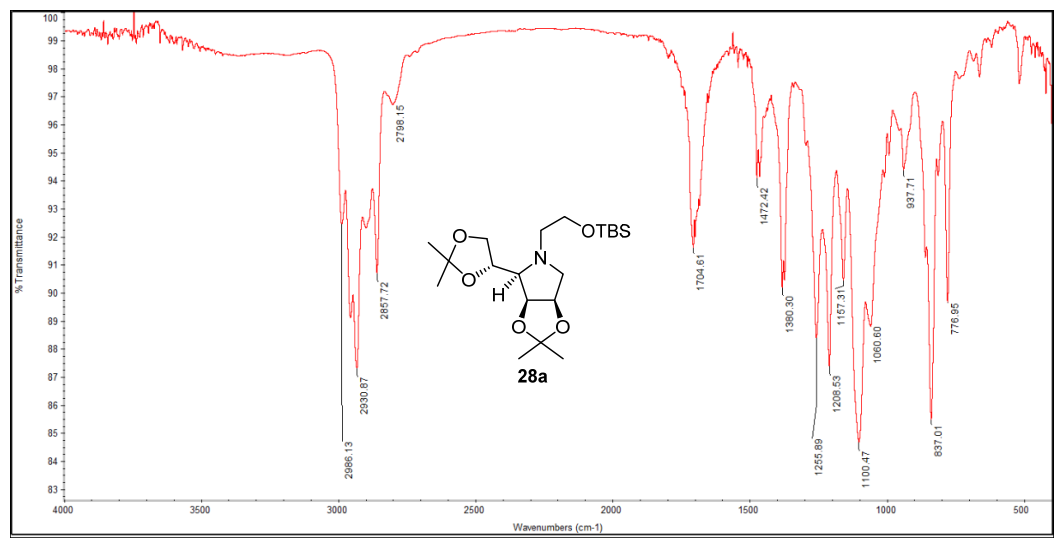
```

Current Data Parameters
NAME      400-2017
XDRNO    128
PROCNO    1

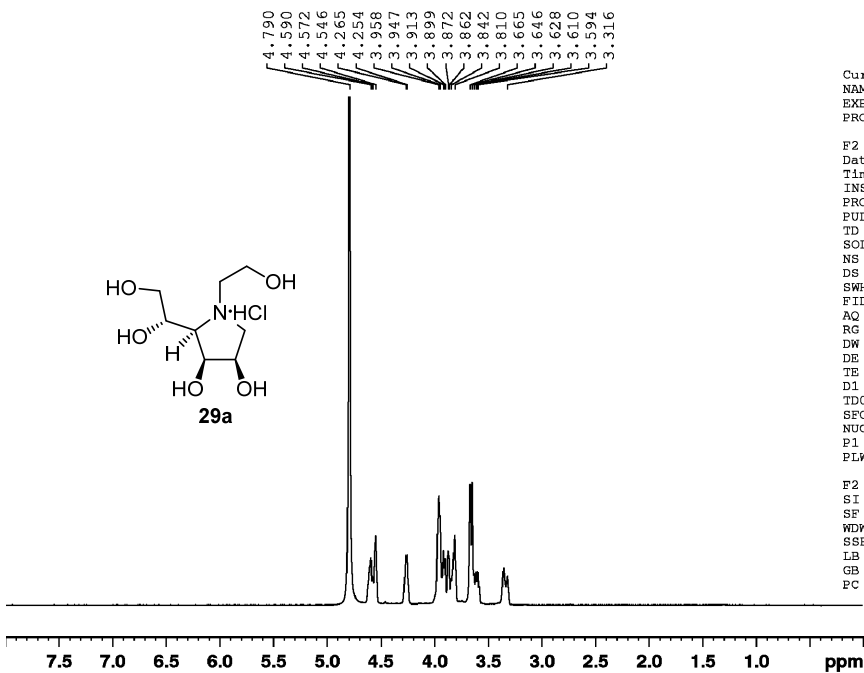
F2 - Acquisition Parameters
Data_     20170518
File      14_38
INSTRUM   spect
PROBHD    5 mm PABBO BBI/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         4
SHE        22058.824 Hz
FIDRES    0.336591 Hz
AQ         1.4854827 sec
RG         206.33
DN         22.867 usec
DE         6.50 usec
TE         300.3 K
CHFT2     145.000000
D1         2.0000000 sec
d2         0.00344828 sec
dL2        0.00000000 sec
DELTA     0.0001273 sec
SD0        1
SFO1      100.648478 MHz
NUC1       13C
P1         10.00 usec
P13        2000.00 usec
PLM0       0 W
PLM1       54.0000000 W
SFOAL5    Csp60comp.4
SFOAL5    0.800
SFOAL5    0 Hz
SFO5      8.25059986 W
SFO5      400.2412800 MHz
NUC2       1H
CHOPRG[2] waltz16
P2         15.30 usec
P4         30.60 usec
NCHD2     80.00 usec
PLM2      12.0000000 W
PLM12     0.34680000 W

F2 - Processing parameters
SI         32768
SF         100.6404280 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



Compound 29a:

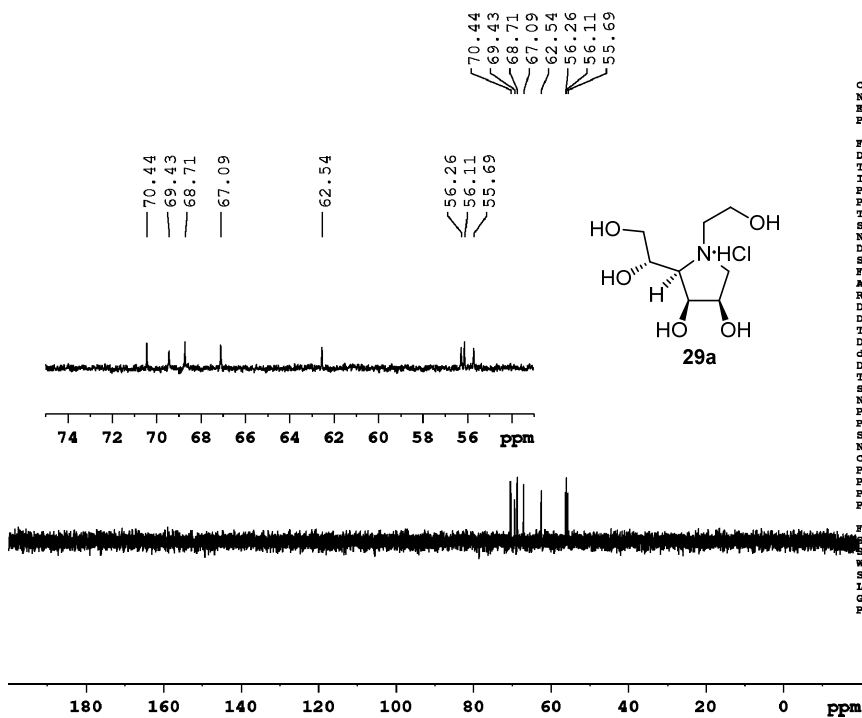


```

Current Data Parameters
NAME 400-2017
EXPNO 129
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170519
Time 11.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT D2O
NS 16
DS 0
SWH 8012.820 H
FIDRES 0.244532 H
AQ 2.0447233 s
RG 206.33
DW 62.400 u
DE 6.50 u
TE 298.4 K
D1 2.0000000 s
TDO 1
SFO1 400.2424716 M
NUC1 1H
F1 14.80 u
FLW1 12.0000000 W

F2 - Processing parameter
SI 65536
SF 400.2399647 M
WDW EM
SSB 0
LB 0.30 H
GB 0
FC 1.00
    
```

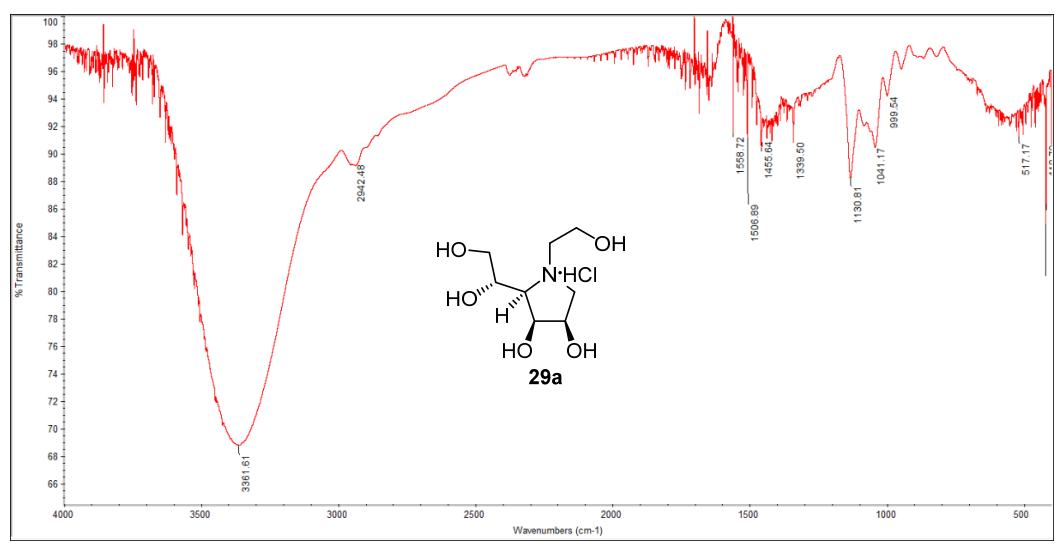
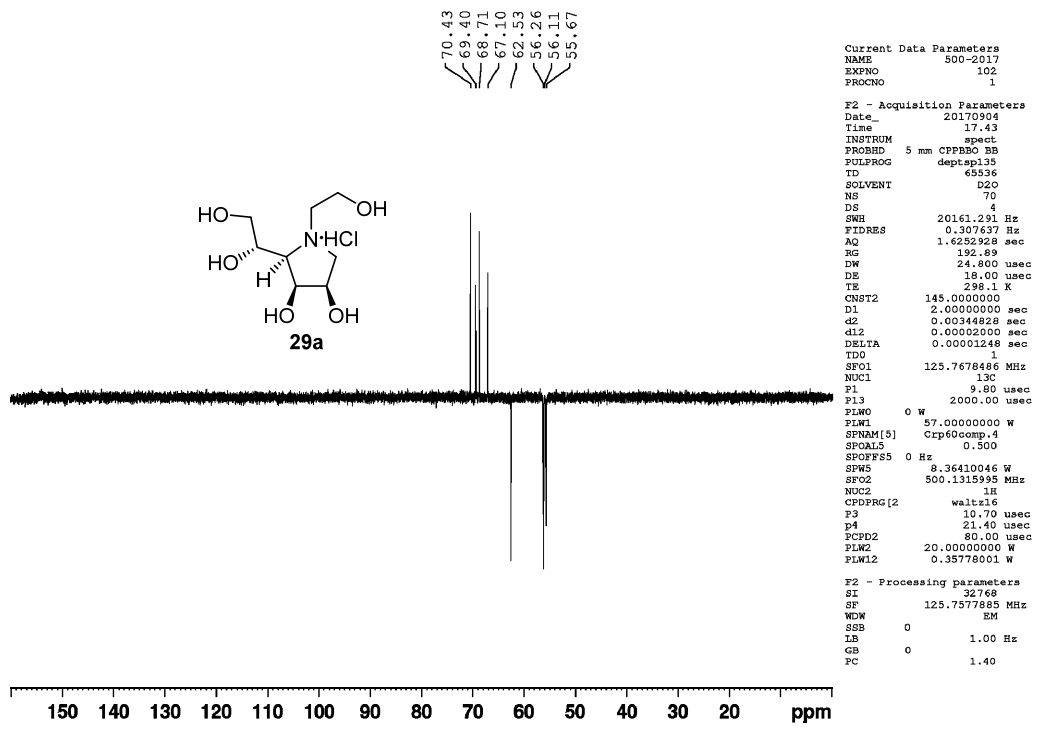


```

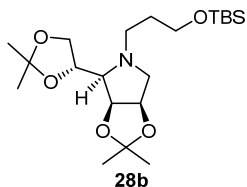
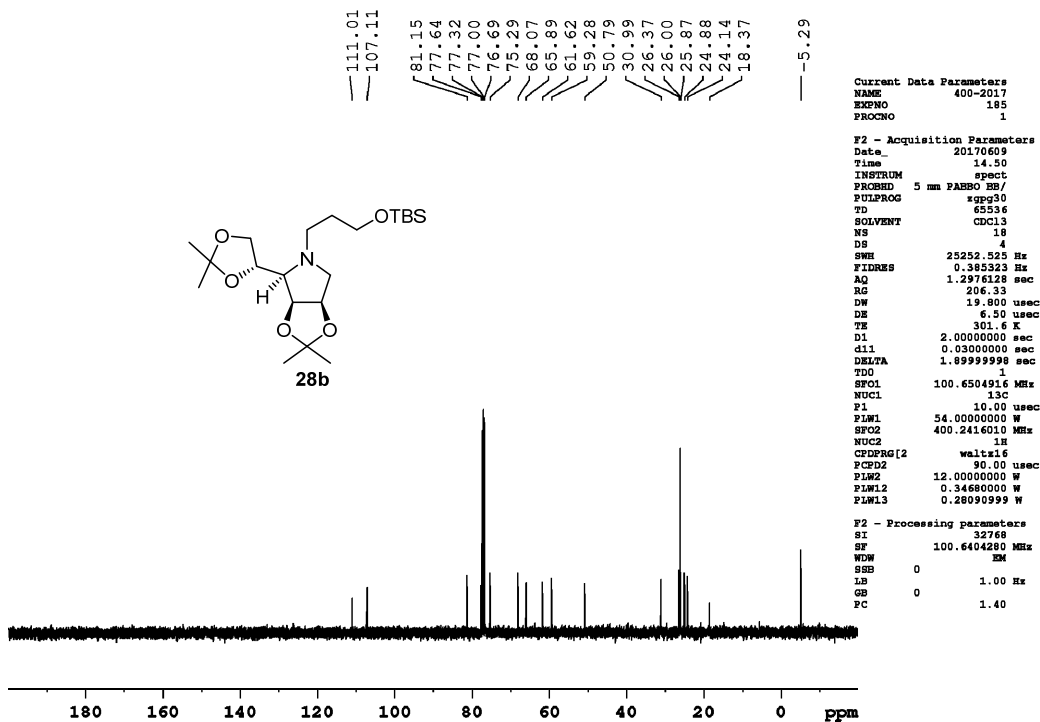
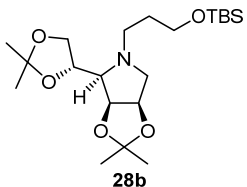
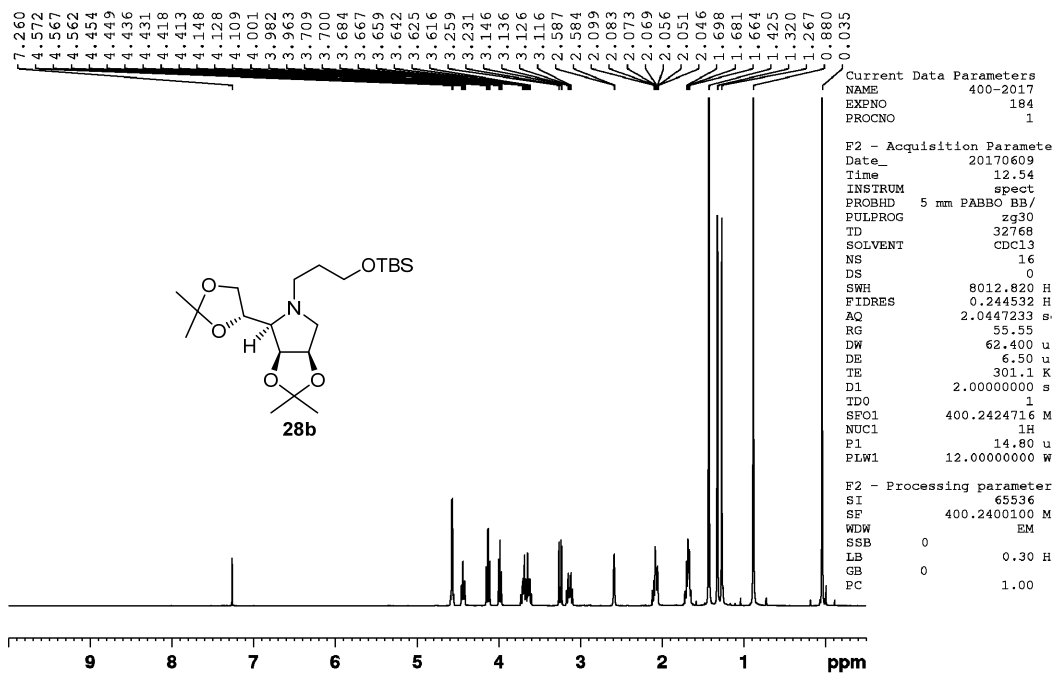
Current Data Parameters
NAME 400-2017
EXPNO 130
PROCNO 1

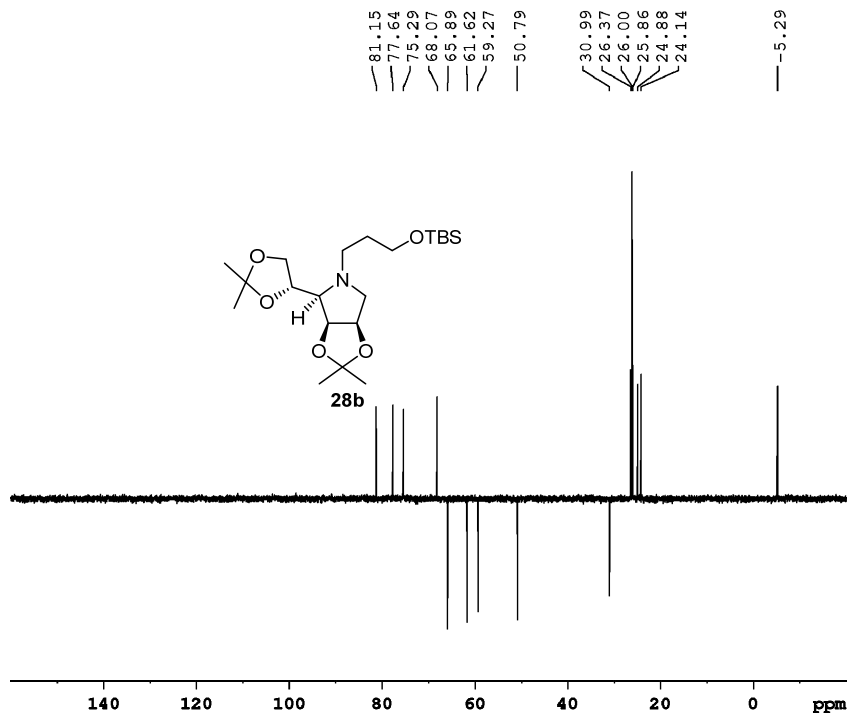
F2 - Acquisition Parameters
Date_ 20170519
Time 11.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT D2O
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 206.33
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TDO 1
SFO1 100.6504916 MHz
NUC1 13C
F1 10.00 usec
FLW1 54.0000000 W
SFO2 400.2416010 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 12.0000000 W
PLW12 0.3468000 W
PLW13 0.28690999 W

F2 - Processing parameters
SI 32768
SF 100.6404280 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40
    
```



Compound 28b:



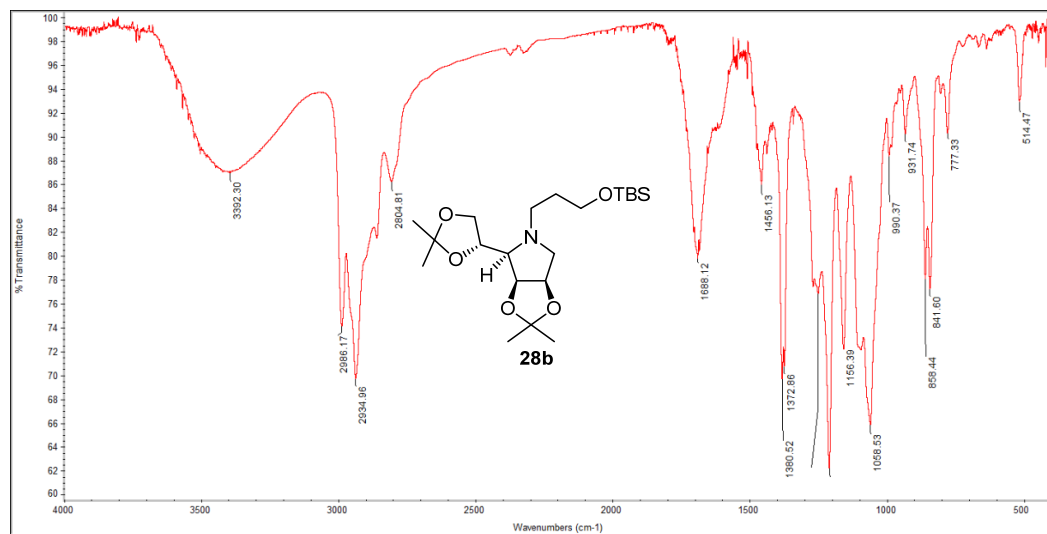


```

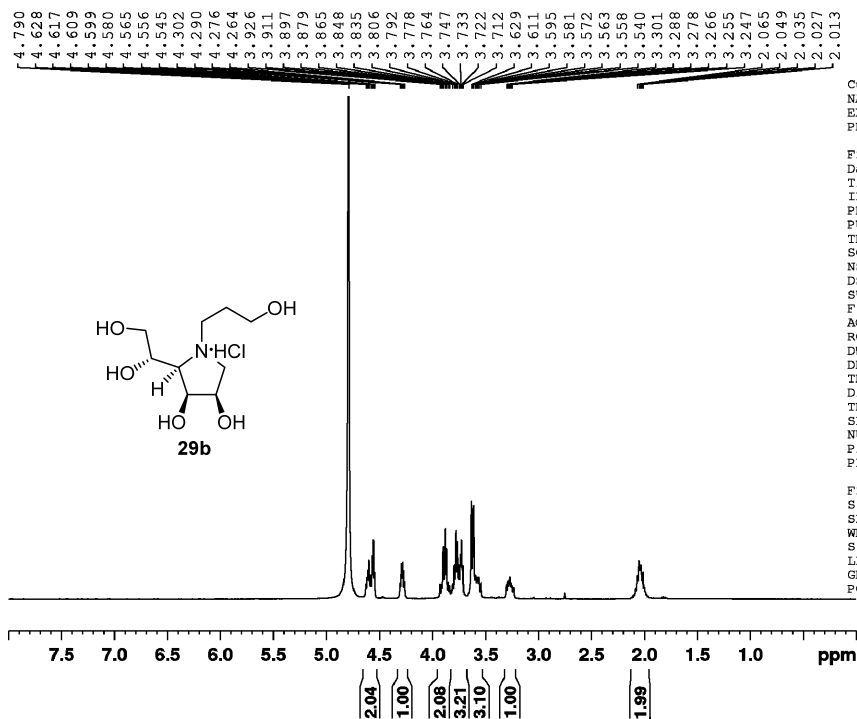
Current Data Parameters
NAME      400-2017
EXPNO    188
PROCNO   1

F2 - Acquisition Parameters
Date_    20170609
Time     14.36
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        76
DS        4
SWH       22058.824 Hz
FIDRES   0.336591 Hz
AQ        1.4854827 sec
RG        206.32
DW        22.487 usec
DE        6.50 usec
TE        301.5 K
CQF2     145.000000
D1        2.0000000 sec
d2        0.00344828 sec
d12       0.00002000 sec
DELTA    0.00001273 sec
WDS       1
SFO1     100.6484788 MHz
NUC1      13C
P1        13.00 usec
E13       2000.00 usec
PLMO      0 W
PLM1     54.0000000 W
SFRM[15]  Csp60comp.4
SFOALS    0.500
SFOFFAS  0 Hz
SFRS     8.25059986 W
SFO2     400.2412800 MHz
NUC2      1H
CQFPG[2]  waltz16
P2        15.30 usec
p4        30.60 usec
SFO2     90.00 usec
PLM2     12.0000000 W
PLM12    0.34680000 W

F2 - Processing parameters
SI        32768
SF        100.6404280 MHz
WDW       EM
SS        0
LB        1.00 Hz
GB        0
PC        1.40
  
```



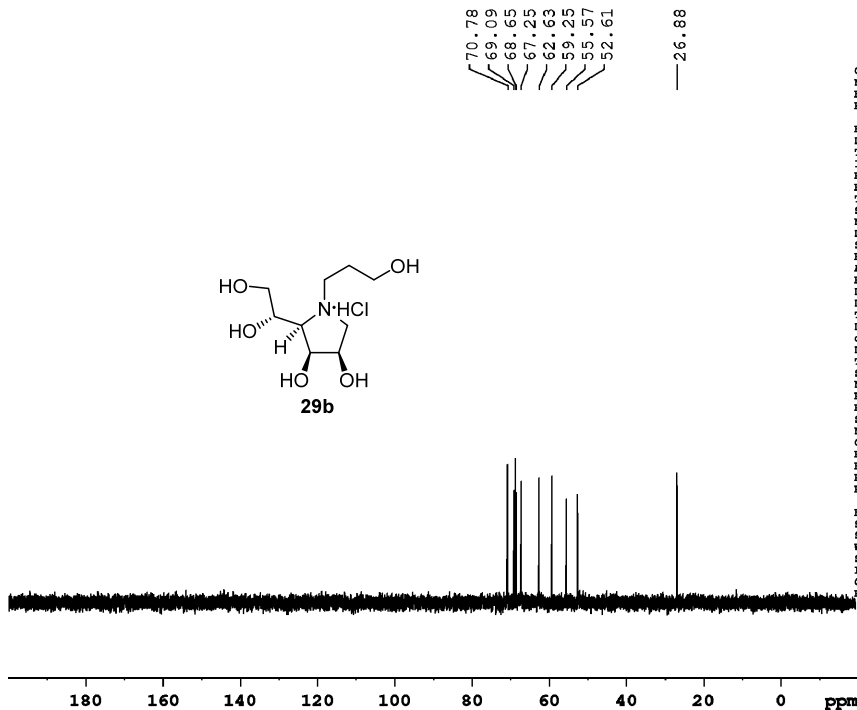
Compound 29b:



Current Data Parameters
 NAME 400-2017
 EXPNO 190
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170610
 Time 12.48
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT D2O
 NS 16
 DS 0
 SWH 8012.820 H
 FIDRES 0.244532 H
 AQ 2.0447233 s
 RG 116.67
 DW 62.400 u
 DE 6.50 u
 TE 301.8 K
 D1 2.0000000 s
 TD0 1
 SFO1 400.2424716 M
 NUC1 1H
 P1 14.80 u
 PLW1 12.0000000 W

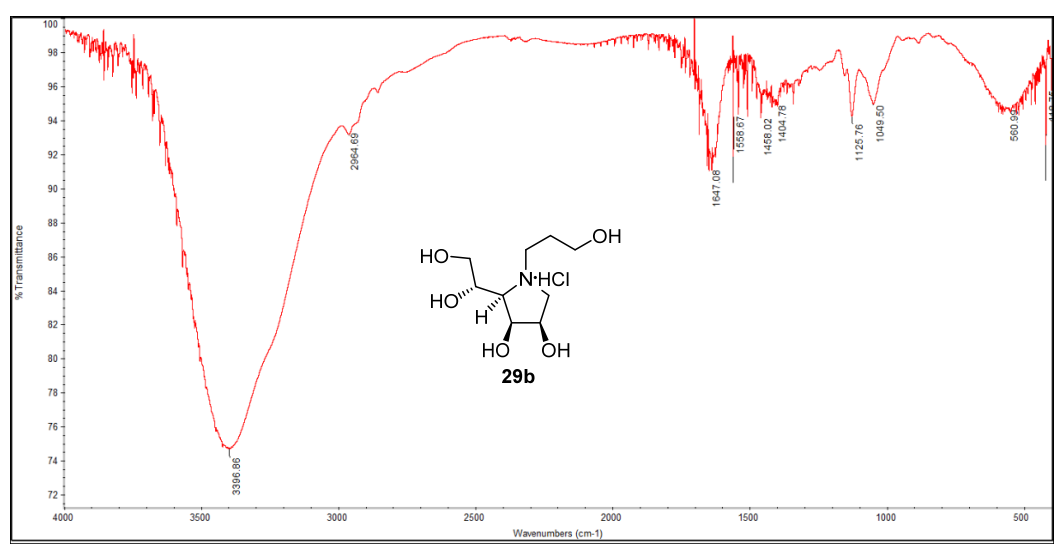
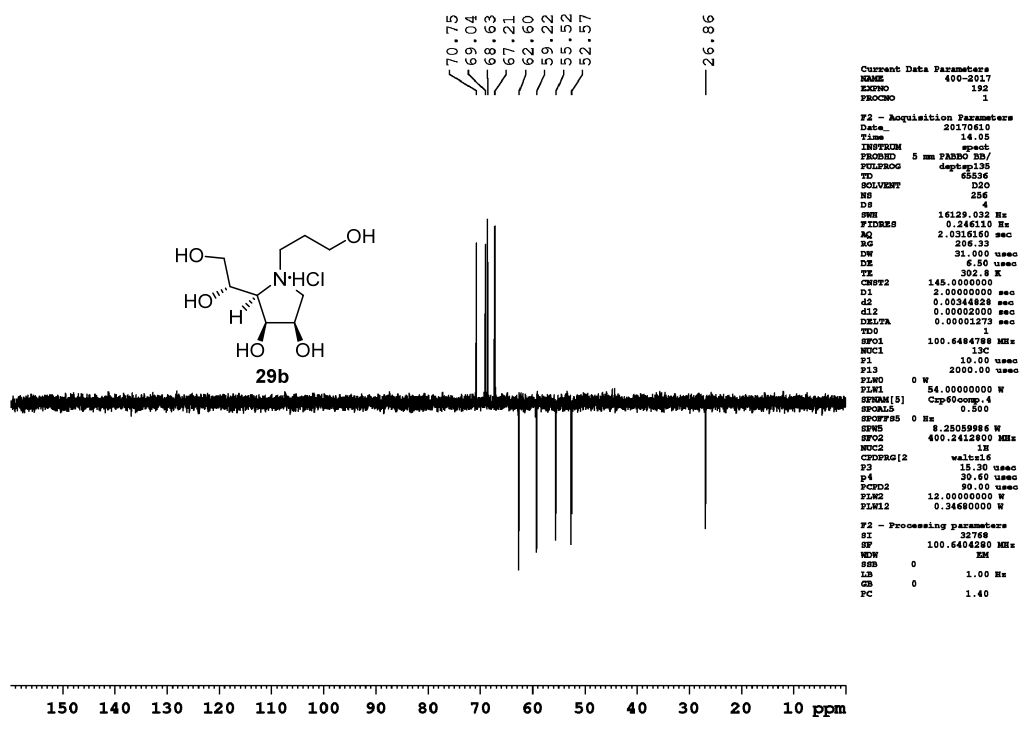
F2 - Processing parameter
 SI 65536
 SF 400.2399665 M
 WDW EM
 SSB 0
 LB 0.30 H
 GB 0
 PC 1.00



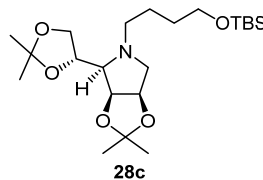
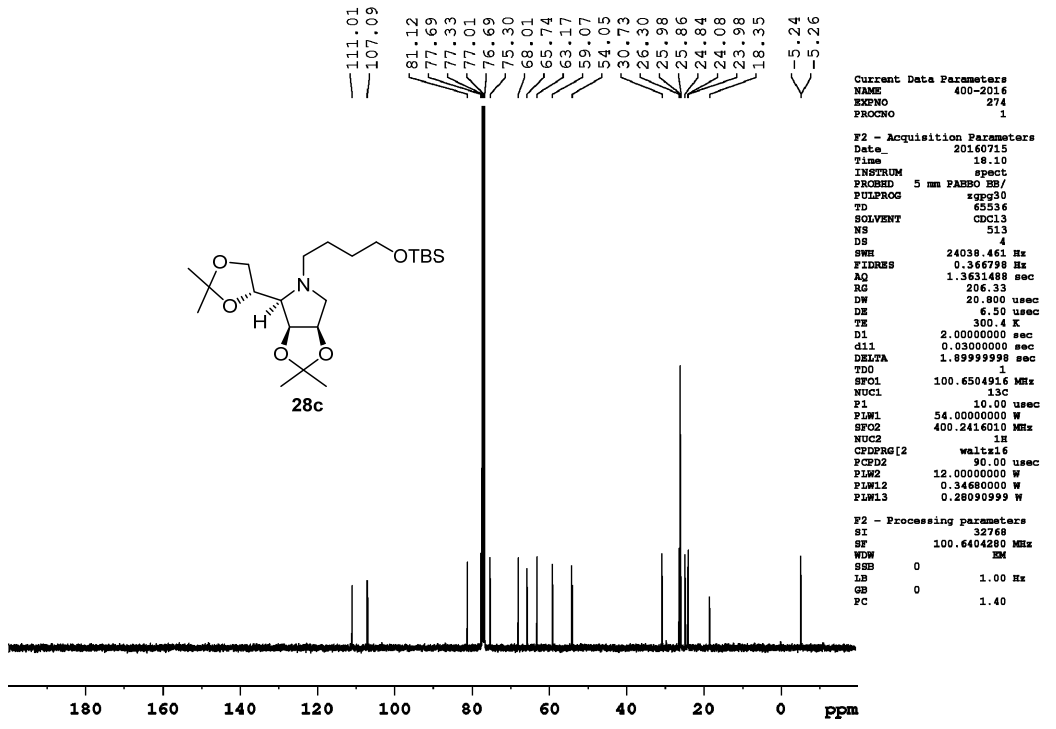
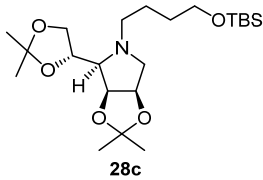
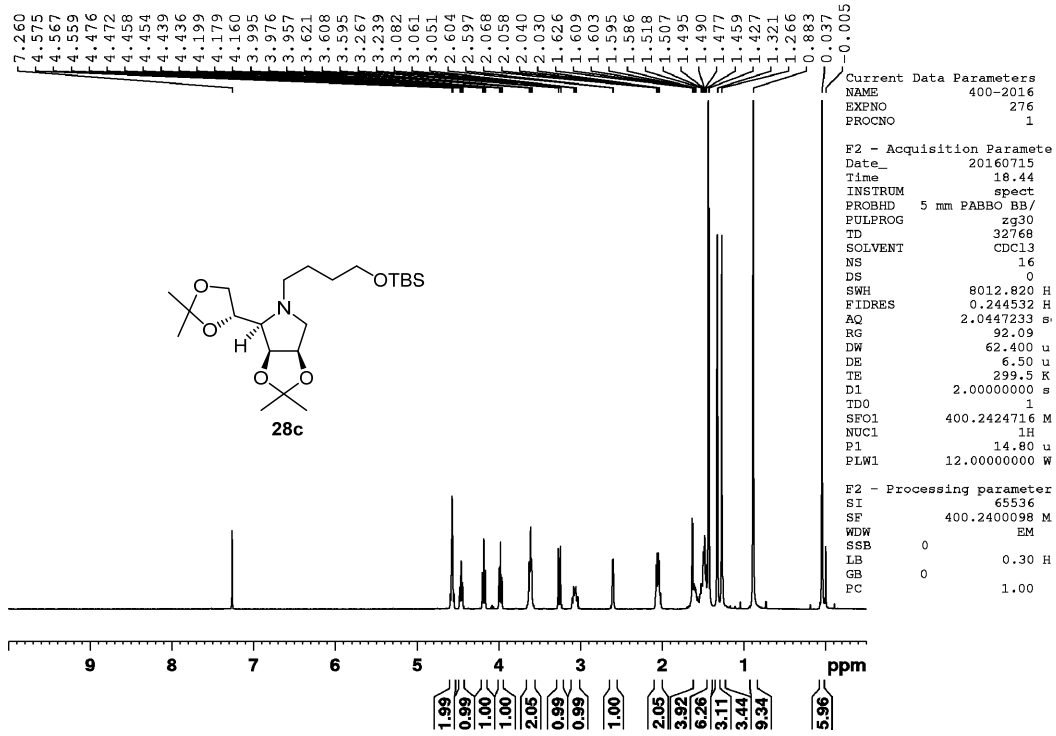
Current Data Parameters
 NAME 400-2017
 EXPNO 191
 PROCNO 1

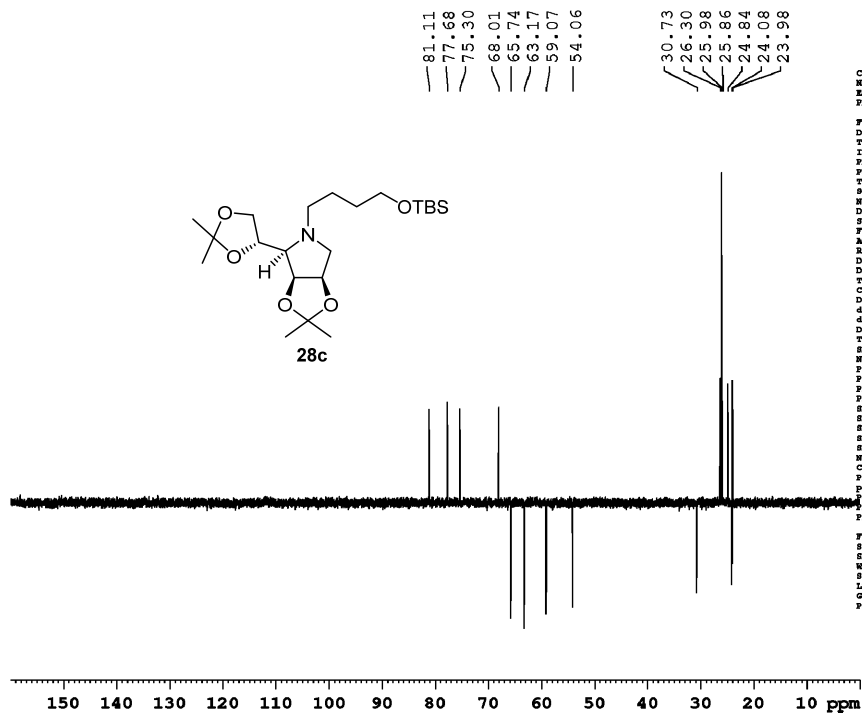
F2 - Acquisition Parameters
 Date_ 20170610
 Time 13.47
 INSTRUM spect
 PROBHD 5 mm FAPBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT D2O
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 206.33
 DW 20.800 usec
 DE 6.50 usec
 TE 303.3 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TD0 1
 SFO1 100.6504916 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 54.0000000 W
 SFO2 400.2416010 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.0000000 W
 PLW12 0.3468000 W
 PLW13 0.2809099 W

F2 - Processing parameters
 SI 32768
 SF 100.6404280 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Compound 28c:



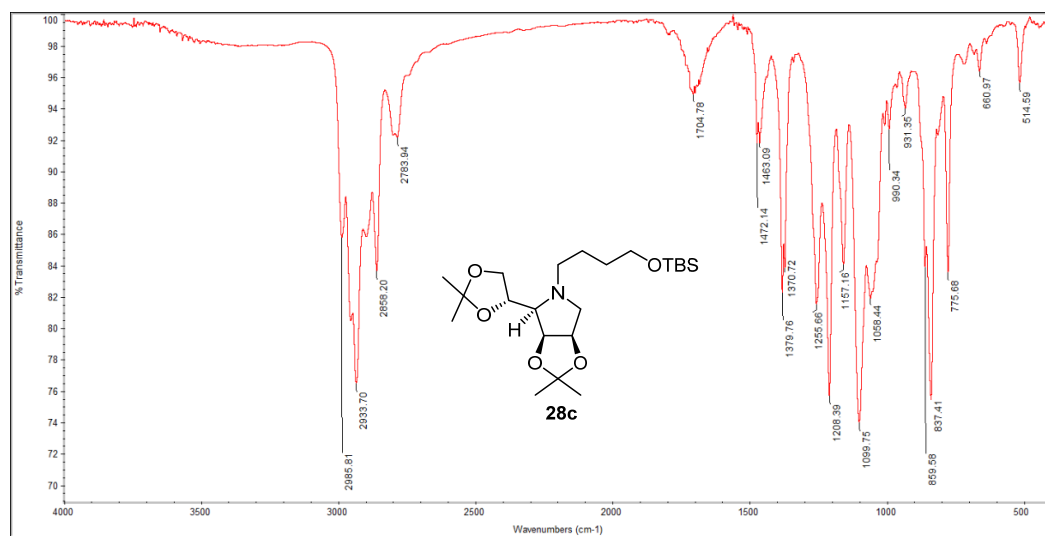


```

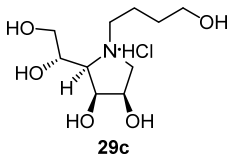
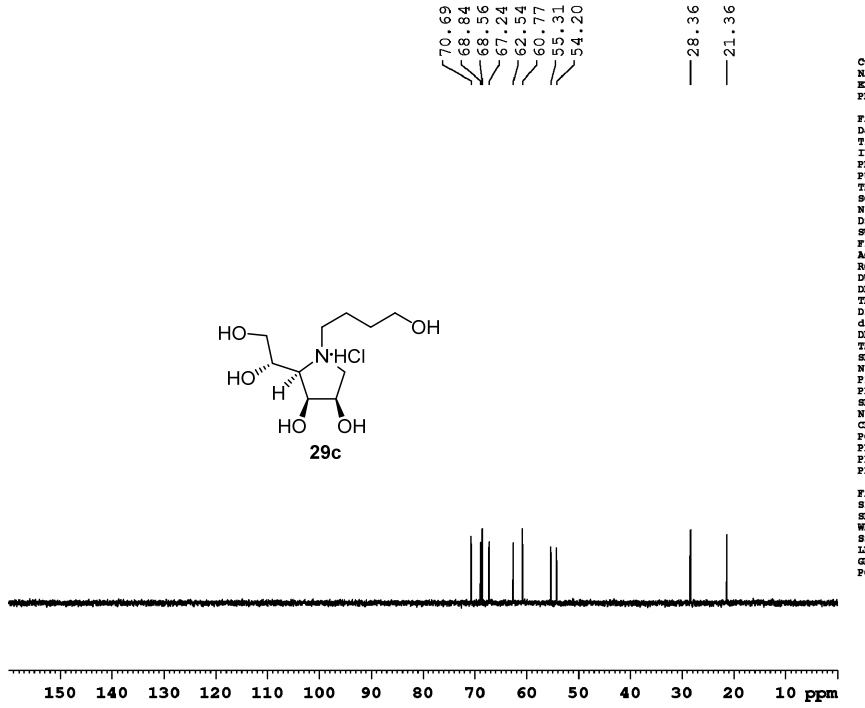
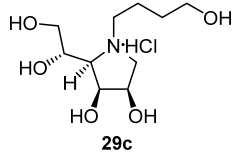
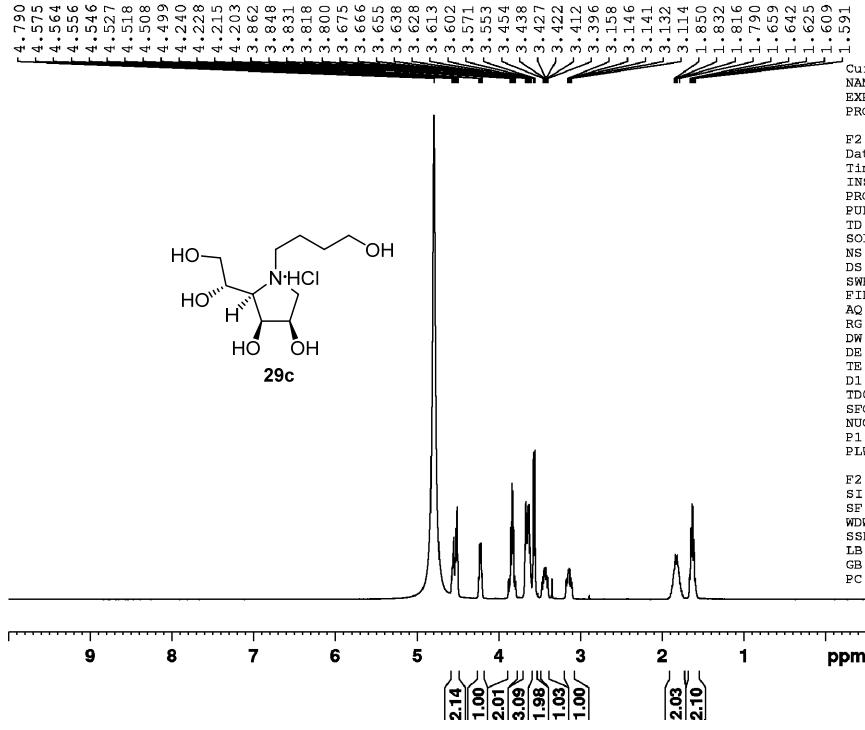
Current Data Parameters
NAME      400-2016
EXPNO    275
PROCNO    1

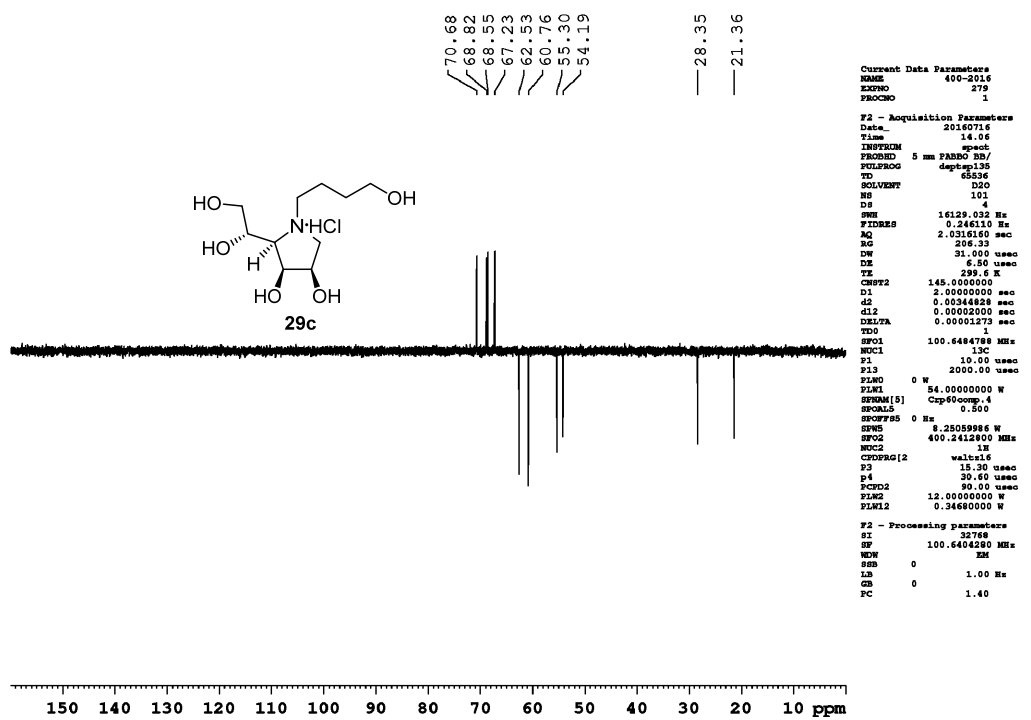
F2 - Acquisition Parameters
Date_     20160715
Time      18.36
INSTRUM   spect
PROBHD    5 mm PABBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         119
DS         4
SWH        16129.032 Hz
FIDRES     0.246110 Hz
AQ         2.0316160 sec
RG         206.33
DN         31.000 usec
DE         6.50 usec
TE         300.1 K
CNP2      145.0000000
D1         2.0000000 sec
ds         0.0004428 sec
d12        0.0002000 sec
DELTA     0.0001273 sec
TDC        1
SF01       100.6484788 MHz
NUC1       13C
P1         10.00 usec
PL13       2000.00 usec
PL12       0 W
PL14       54.0000000 W
SFOFF(5)  Csp60comp,4
SFOFF5     0.500
SFOFF5     0 Hz
SFOFF5     8.2555986 Hz
SFOFF5     400.2412800 MHz
MOC2       1H
CPCPRG2    waltz16
P3         15.30 usec
P4         30.60 usec
PCPD2      90.00 usec
PLW2       12.0000000 W
PLWL2      0.34680000 W

F2 - Processing parameters
SI         32768
SF         100.6404280 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC         1.40
  
```



Compound 29c:



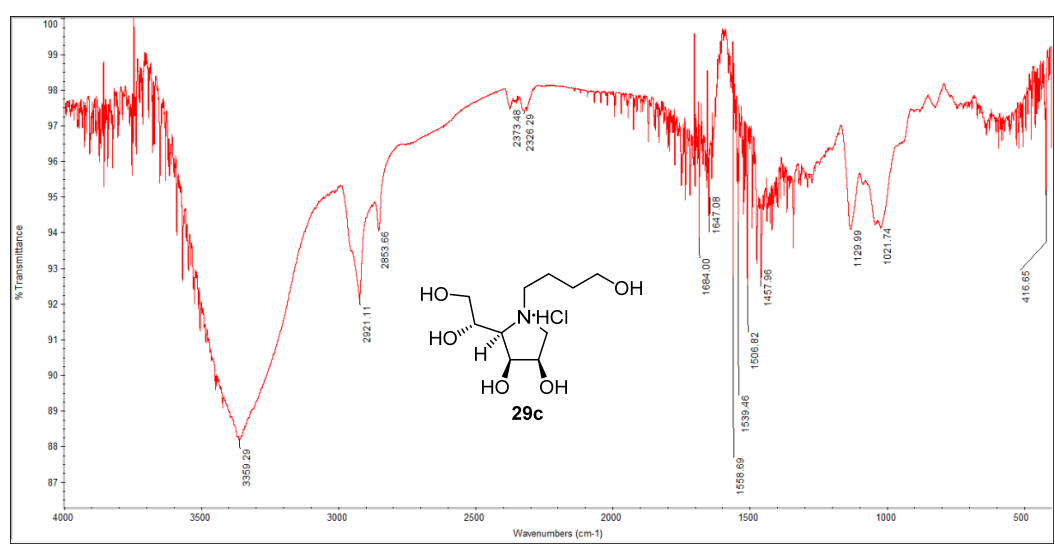


```

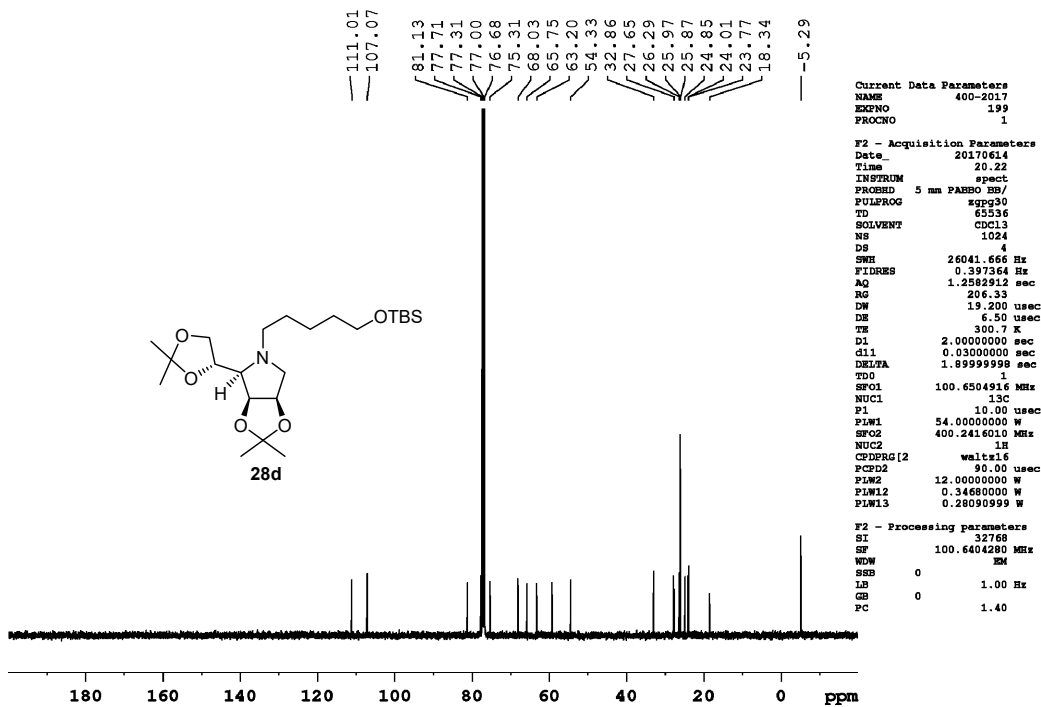
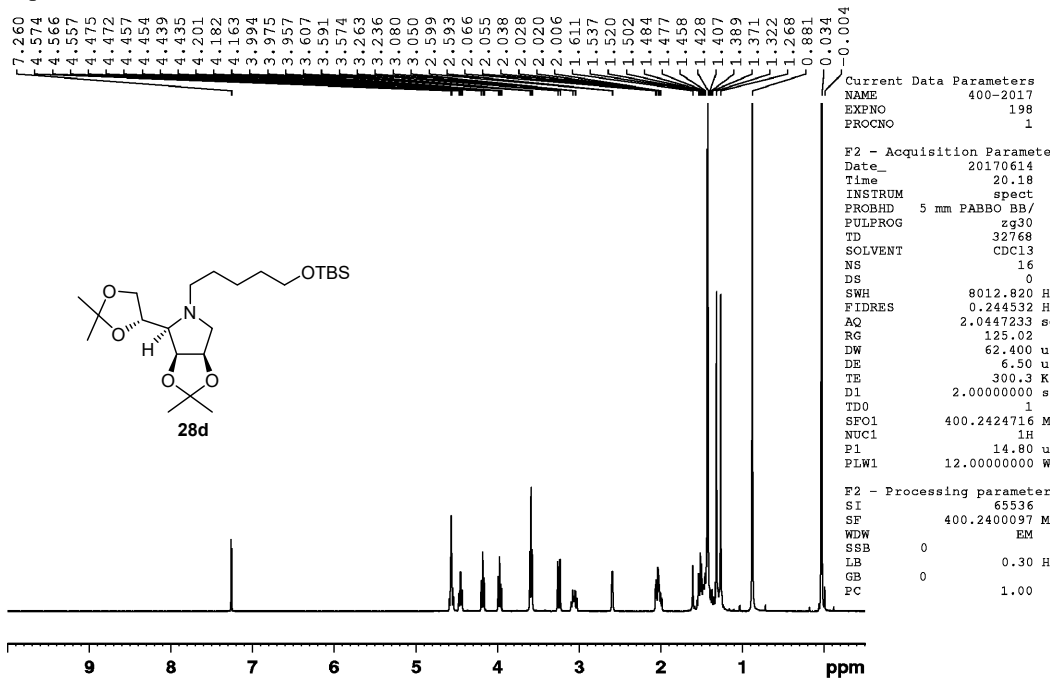
Current Data Parameters
NAME      400-2014
EXPNO    279
PROCNO   1

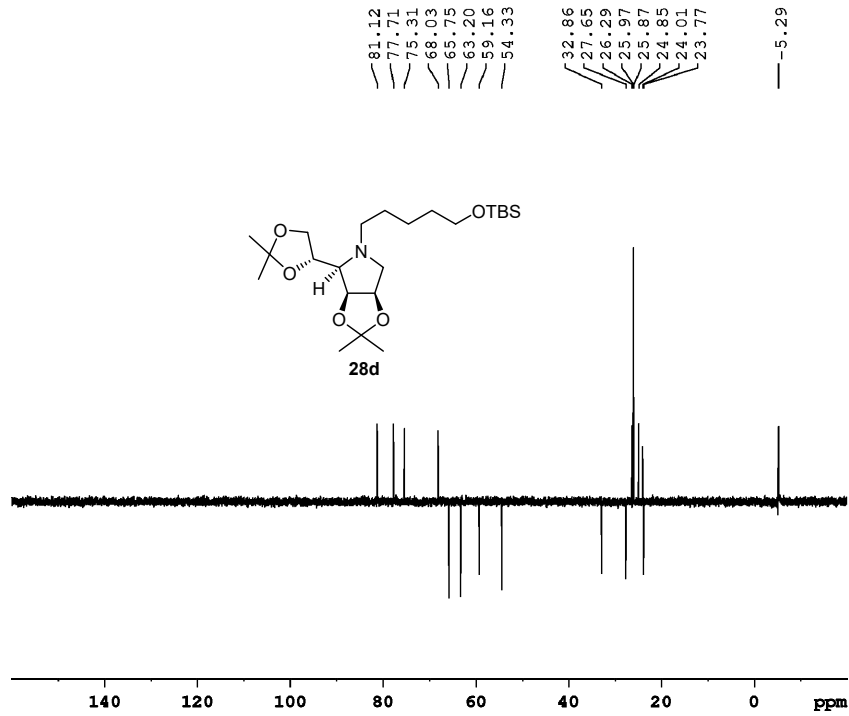
F2 - Acquisition Parameters
Date_    20160716
Time     14.06
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        101
DS        4
SWH       16129.932 Hz
FIDRES   0.246110 Hz
AQ        2.0216180 sec
RG         206.39
DW         31.000 usec
DE         6.50 usec
TE        299.6 K
CQF2      145.0000000
D1         2.0000000 sec
d2         0.00344628 sec
d12        0.00000000 sec
DELTA     0.00001273 sec
WFO       1
SFO1      100.6464780 MHz
NUC1       13C
P1         10.00 usec
E13        0 W
P13        2000.00 usec
PLMG       0 W
PLM1      54.0000000 W
SFOFMS[5] Csp60comp.4
SFOFMS    0.500
SFOFMS    0 Hz
SFOFMS    8.25059986 W
SFOFMS    400.2412800 MHz
NUC2       1H
CQF2G[2]  waltz16
P2         15.30 usec
P4         30.60 usec
PCPD2     90.00 usec
PLM2      12.0000000 W
PLM12     0.34680000 W

F2 - Processing parameters
SI         32768
SF         100.6404280 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         1.40
  
```



Compound 28d:





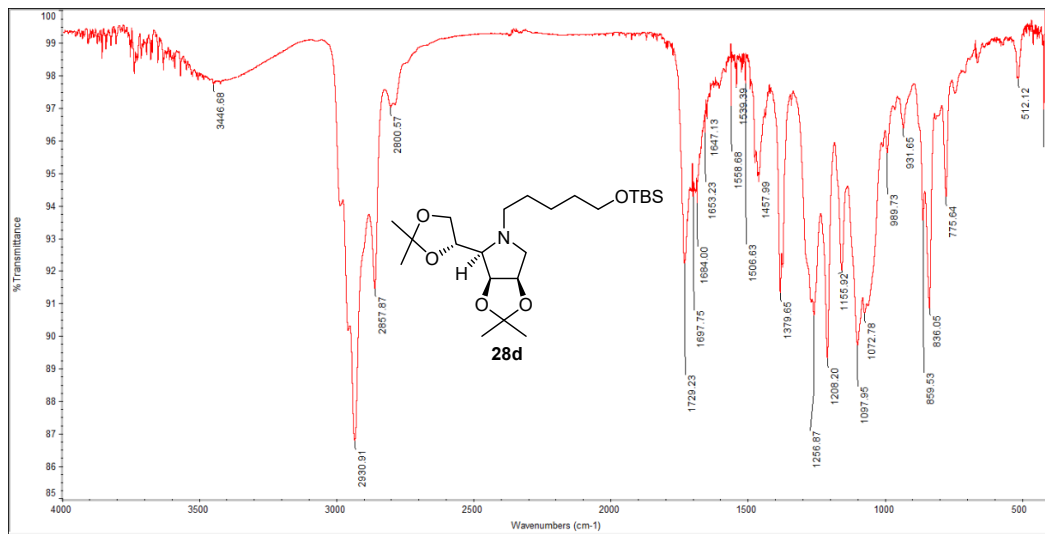
```

Current Data Parameters
NAME      400-2017
EXPNO    200
PROCNO   1

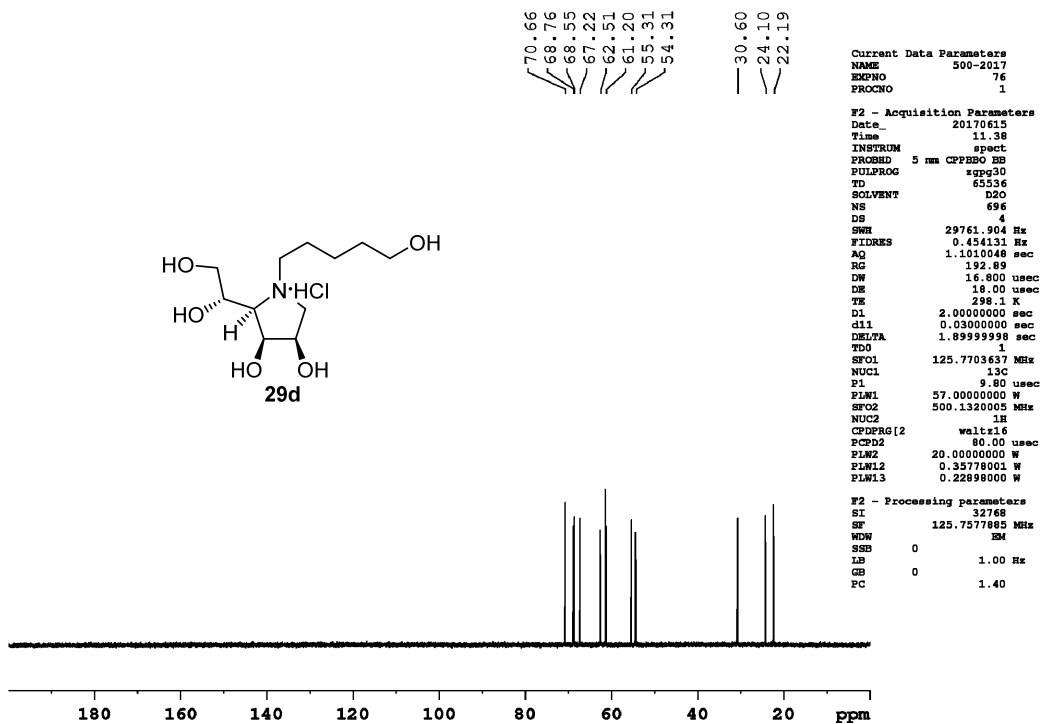
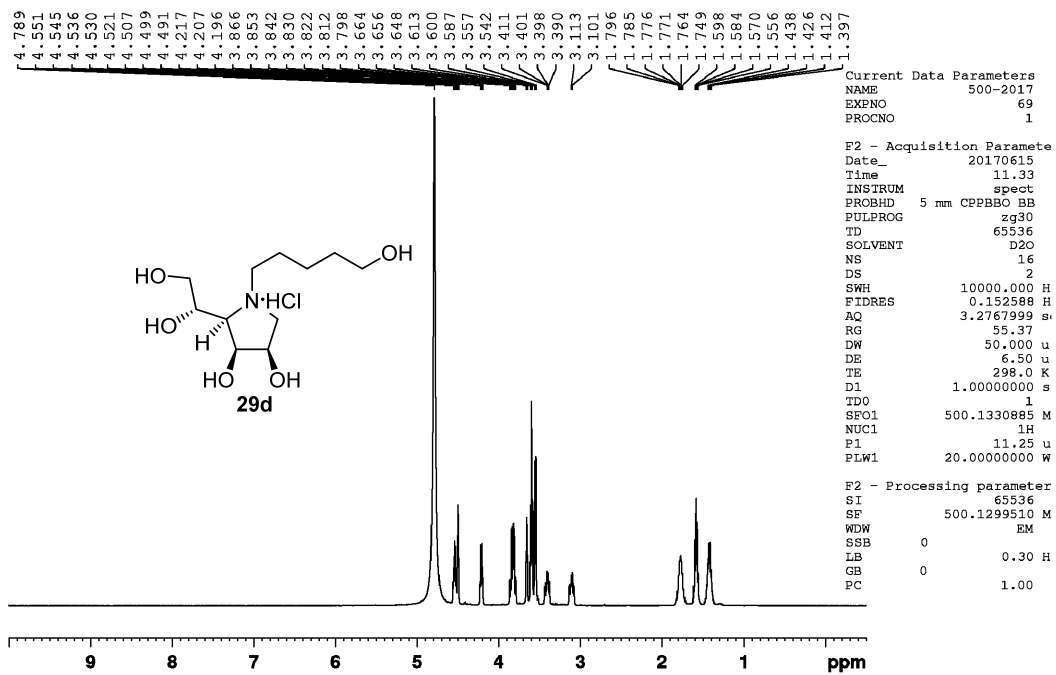
F2 - Acquisition Parameters
Date_    20170614
Time     21.34
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
TD        65536
SOLVENT  CDCl3
NS        256
DS        4
SWH       22058.824 Hz
FIDRES   0.336591 Hz
AQ        1.4824627 sec
RG        306.39
DW        22.687 usec
DE        6.50 usec
TE        301.3 K
CQF2     145.000000
SI        2.0000000 sec
d2       0.00344628 sec
d12      0.00000000 sec
DELTA    0.00001273 sec
YD0       100.646478 MHz
NUC1      13C
SI        10.00 usec
F13       2000.00 usec
PLMO      0 W
PLM1     54.0000000 W
SFOFF(5) Csp60comp.4
SFOFF5   0 Hz
SFOFF6   8.25059986 W
SFOFF7   400.2412800 MHz
NUC2      1H
CHOPRO2  waltz16
F3        15.30 usec
p4        30.60 usec
PCPD2     90.00 usec
PLM2     12.0000000 W
PLM12    0.34680000 W

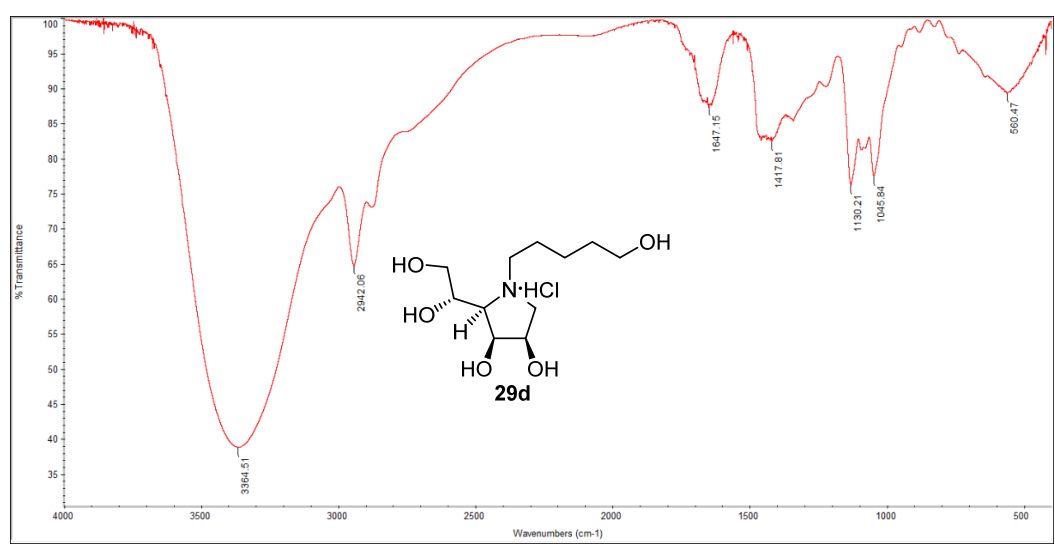
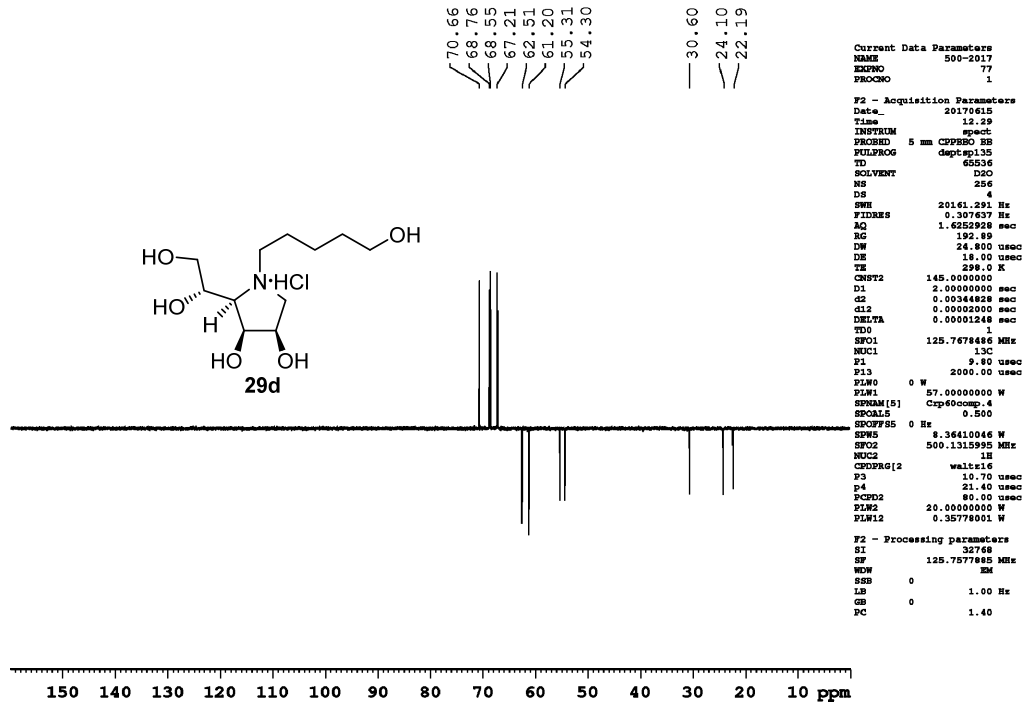
F2 - Processing parameters
SI        32768
SF        100.6404280 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

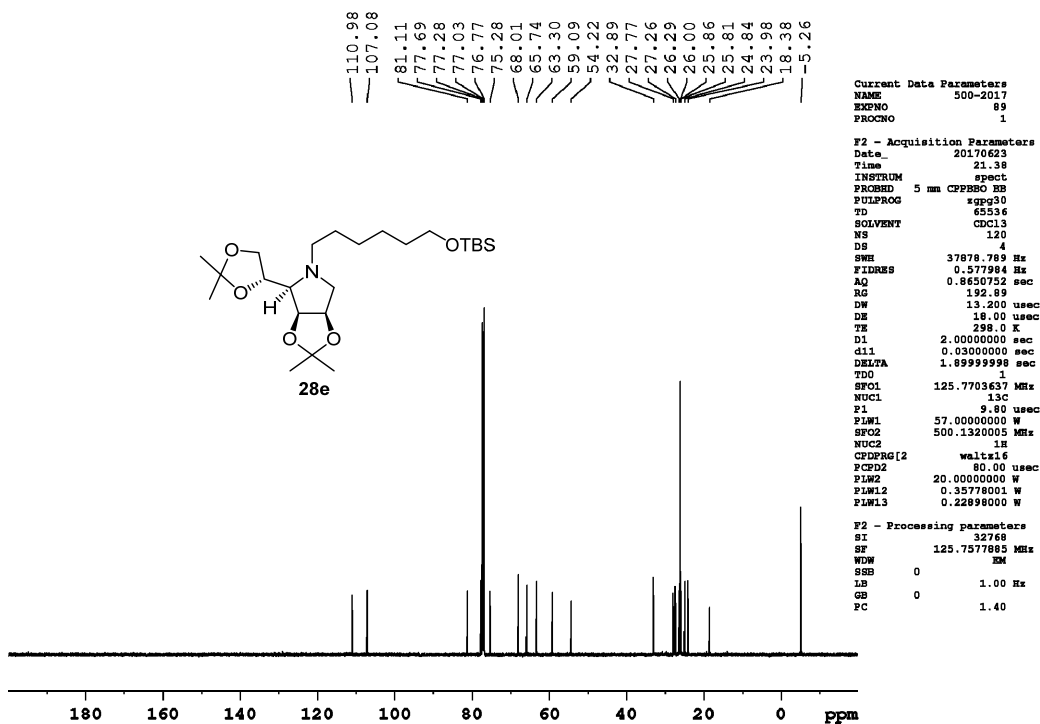
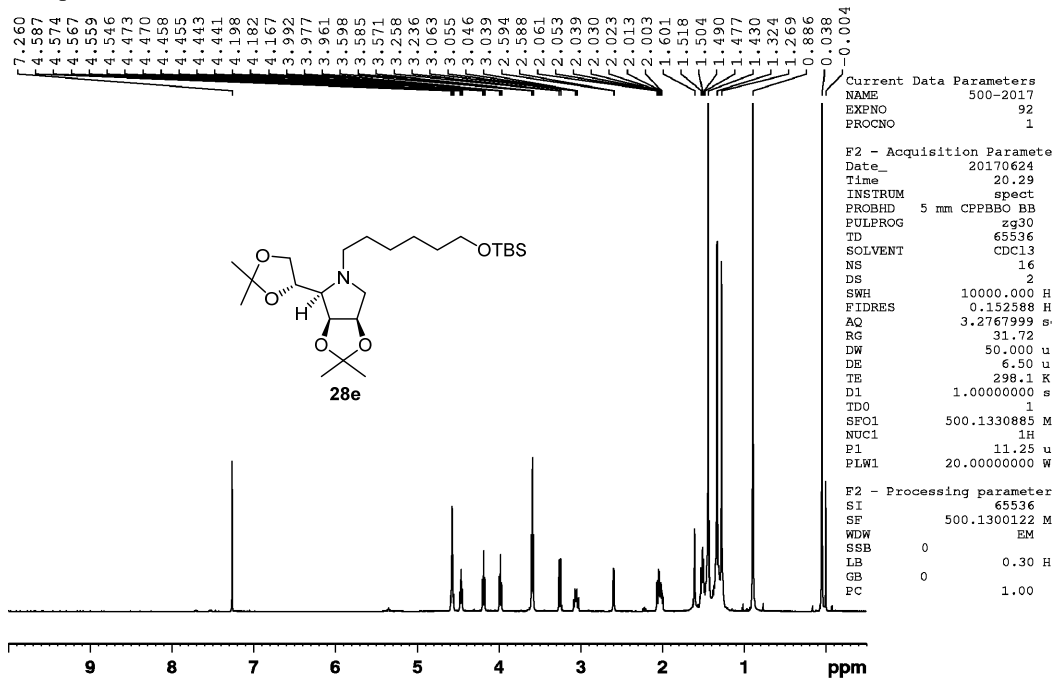


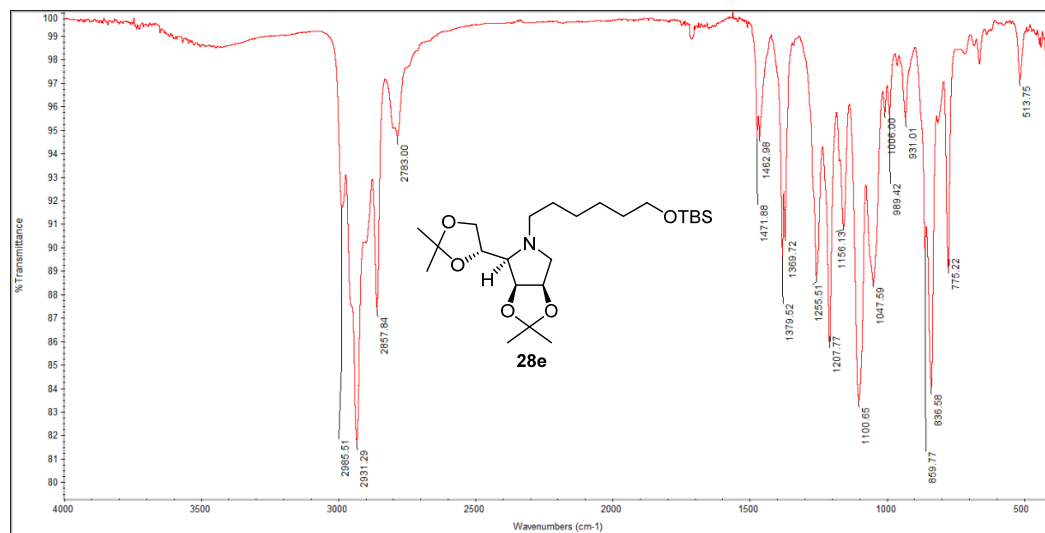
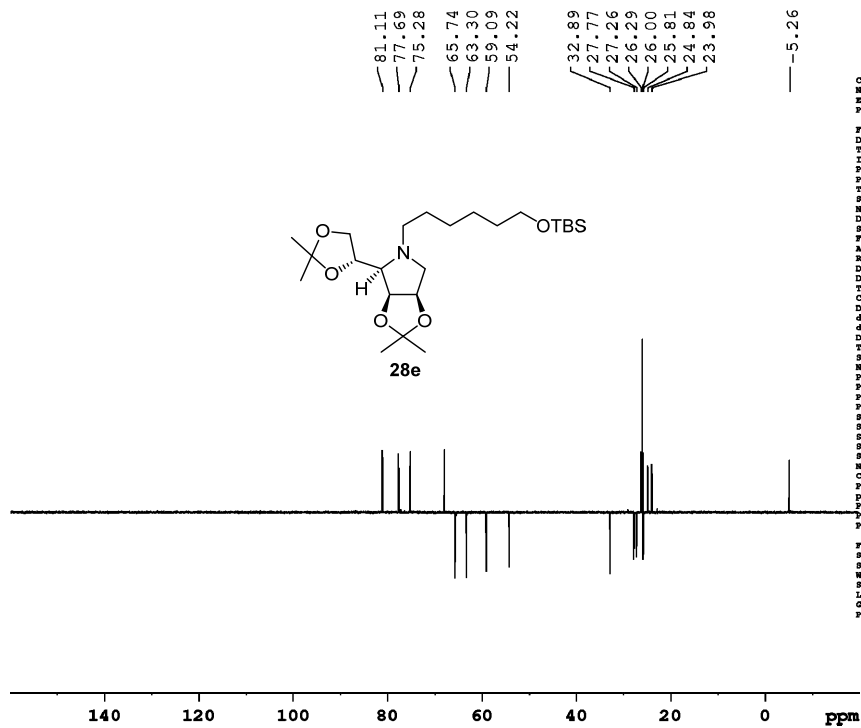
Compound 29d:



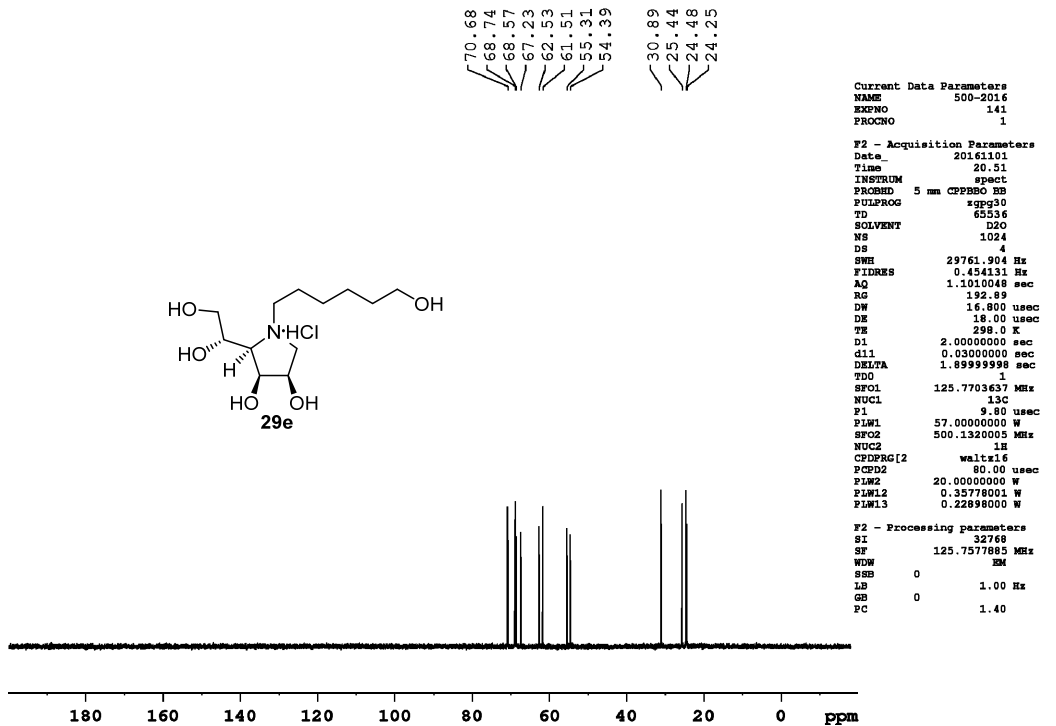
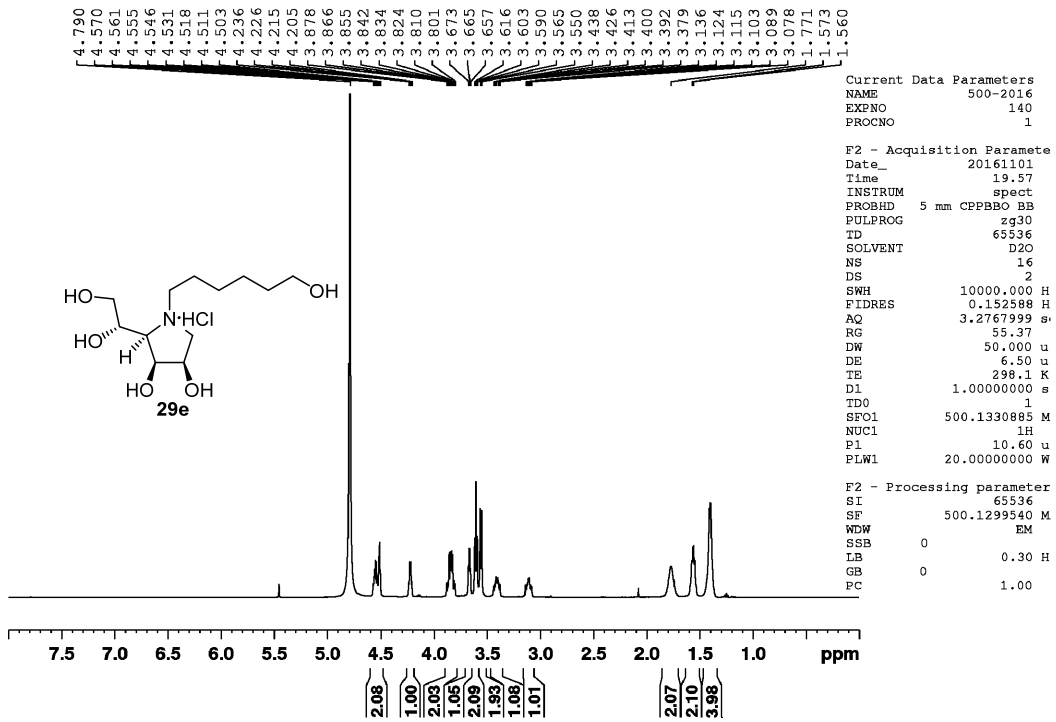


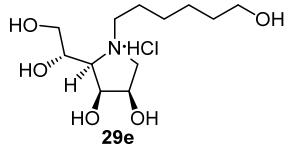
Compound 28e:





Compound 29e:





70.68
68.74
68.57
67.23
62.53
61.51
55.31
54.39

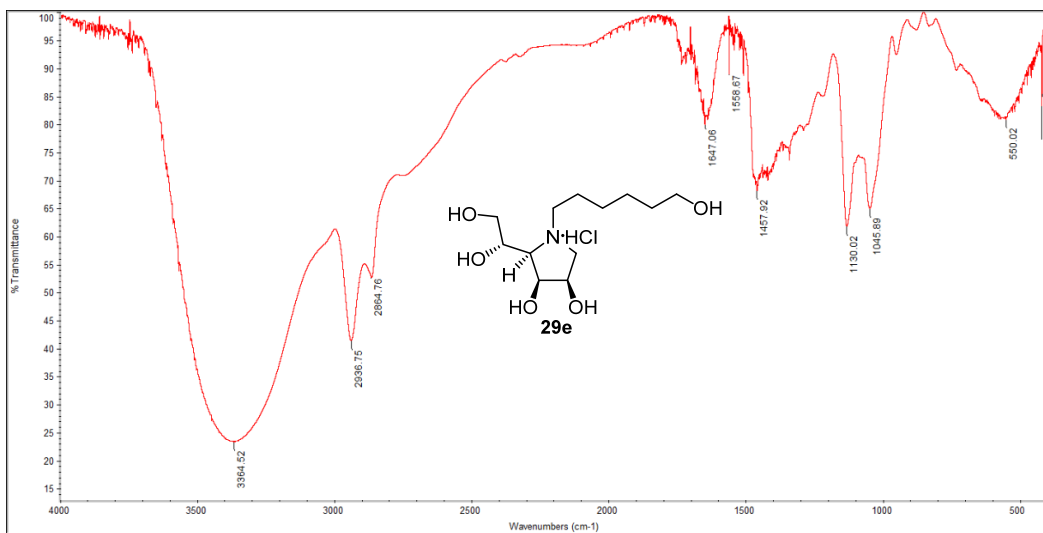
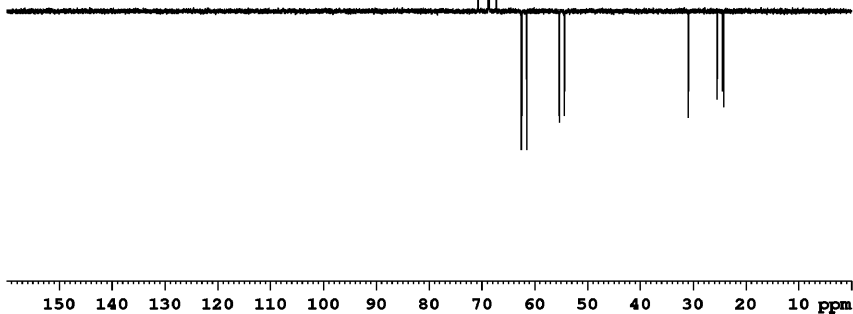
30.89
25.44
24.48
24.25

```

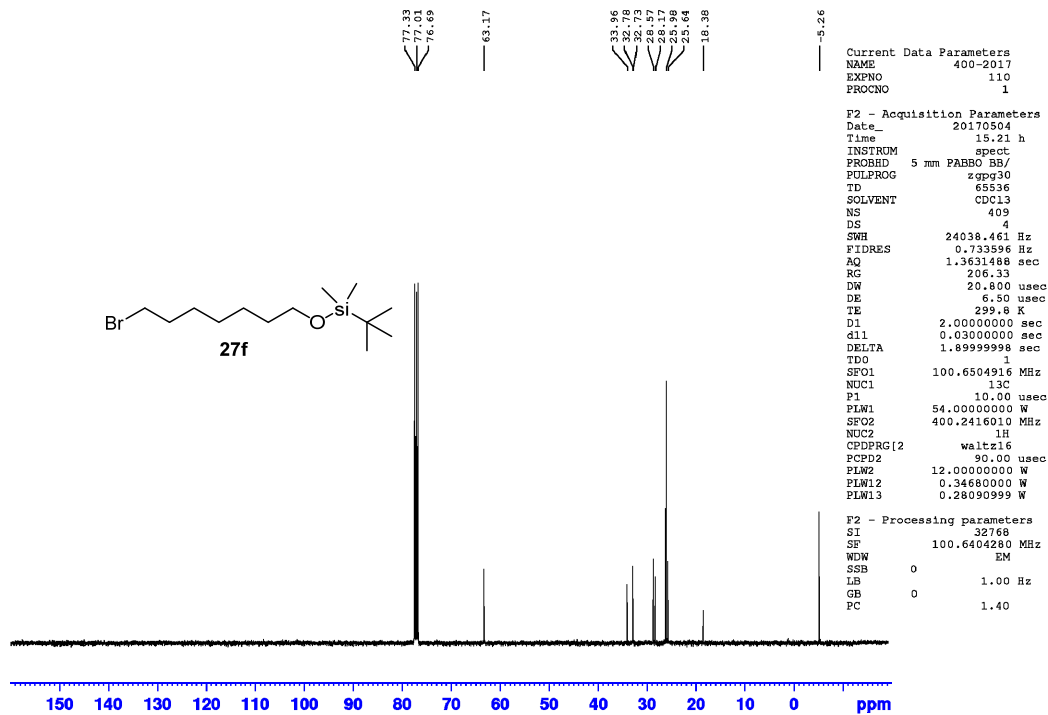
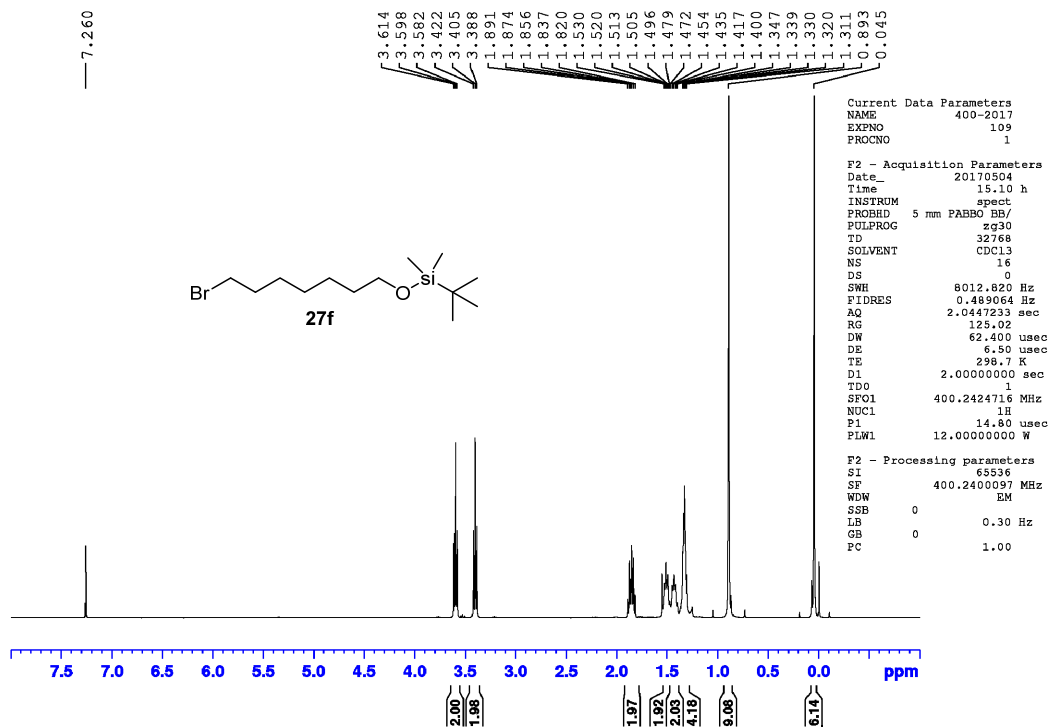
Current Data Parameters
NAME      500-2014
EXPNO     142
PROCNO    1

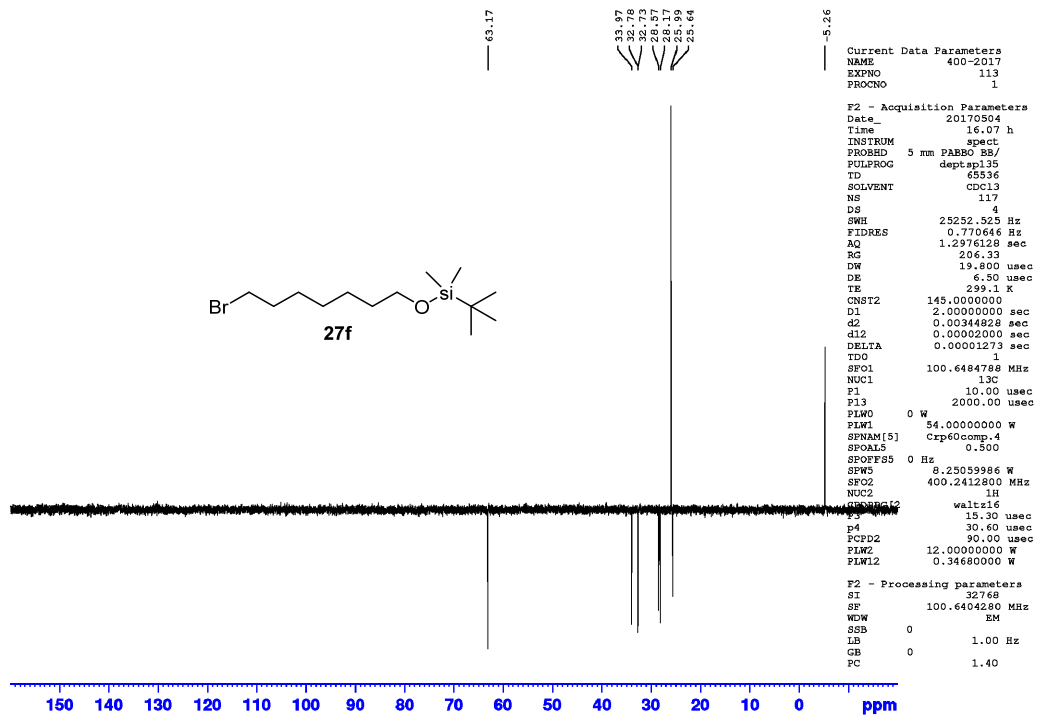
F2 - Acquisition Parameters
Date_     20161101
Time      21.07
INSTRUM   spect
PROBHD    5 mm CPYBBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   D2O
NS         256
DS         4
SHE       20161.391 Hz
FIDRES    0.307637 Hz
AQ         1.6282828 sec
RG         392.89
DW         24.800 usec
DE         18.00 usec
TE         298.0 K
CHFT2     145.0000000
D1         2.0000000 sec
d2         0.00344628 sec
d12        0.00000000 sec
DELTA     0.00001248 sec
FID        1
FPC1       125.7678484 MHz
NUC1       13C
P1         9.80 usec
P13        2000.00 usec
PLM0       0 W
PLM1       57.00000000 W
SFOCAL[S]  Csp60comp.4
SFOCAL5    0.500
SFOCAL5    0 Hz
SFO5       8.36410046 W
SFO3       500.1315995 MHz
NUC2       1H
CHOPRO[2] waltz16
p3         10.70 usec
p4         21.40 usec
PCPD2     80.00 usec
PLM2       20.00000000 W
PLM12     0.35778001 W

F2 - Processing parameters
SI         32768
SF         125.7577888 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

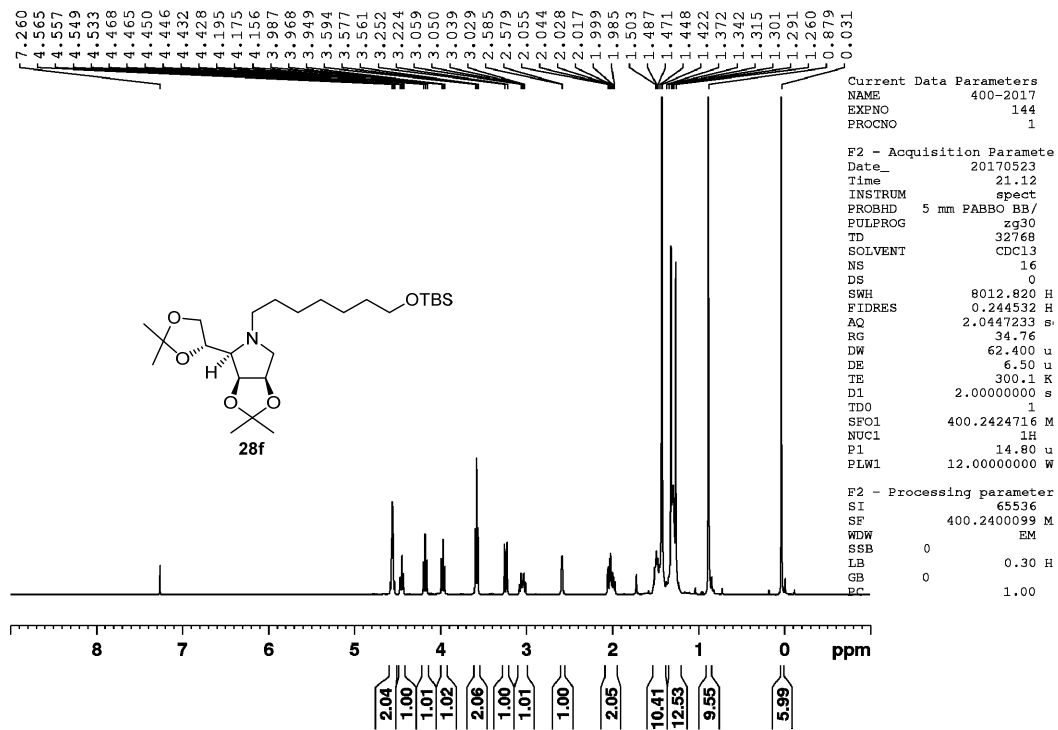


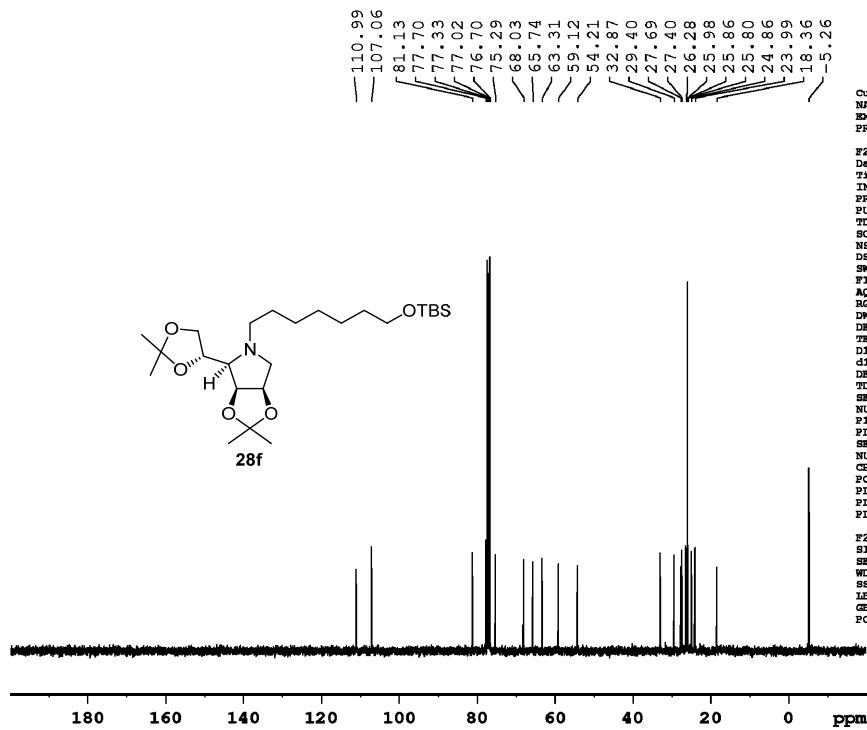
Compound 27f:





Compound 28f:



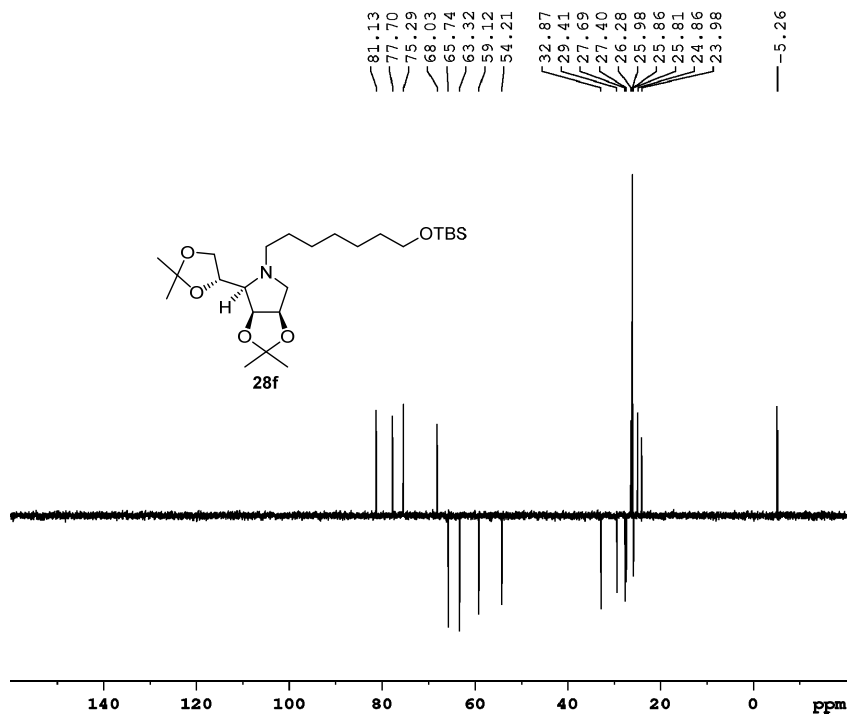


```

Current Data Parameters
NAME      400-2017
EXPNO    145
PROCNO   1

F2 - Acquisition Parameters
Data_    20170523
Time     21.21
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        218
DS        4
SWH       26041.666 Hz
FIDRES   0.397364 Hz
AQ        1.2582912 sec
RG        206.33
DW        19.200 usec
DE        6.50 usec
TE        300.2 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA    1.89999998 sec
TDO       1
SFO1     100.6504916 MHz
NUC1      13C
P1        10.00 usec
PLW1     54.00000000 W
SFO2     400.2416010 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2    90.00 usec
PLW2     12.00000000 W
PLW12    0.34680000 W
PLW13    0.28090999 W

F2 - Processing parameters
SI        32768
SF        100.6404280 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

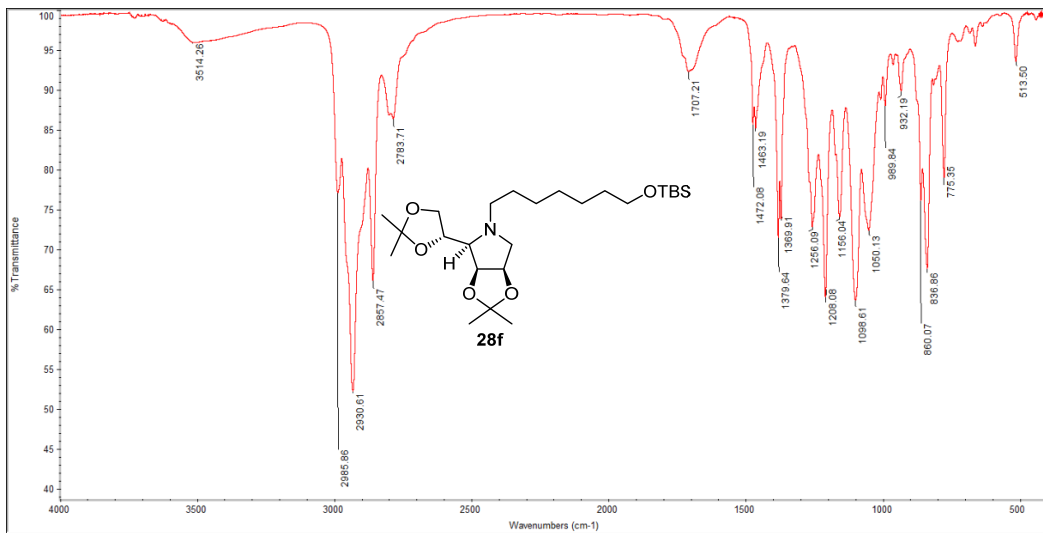


```

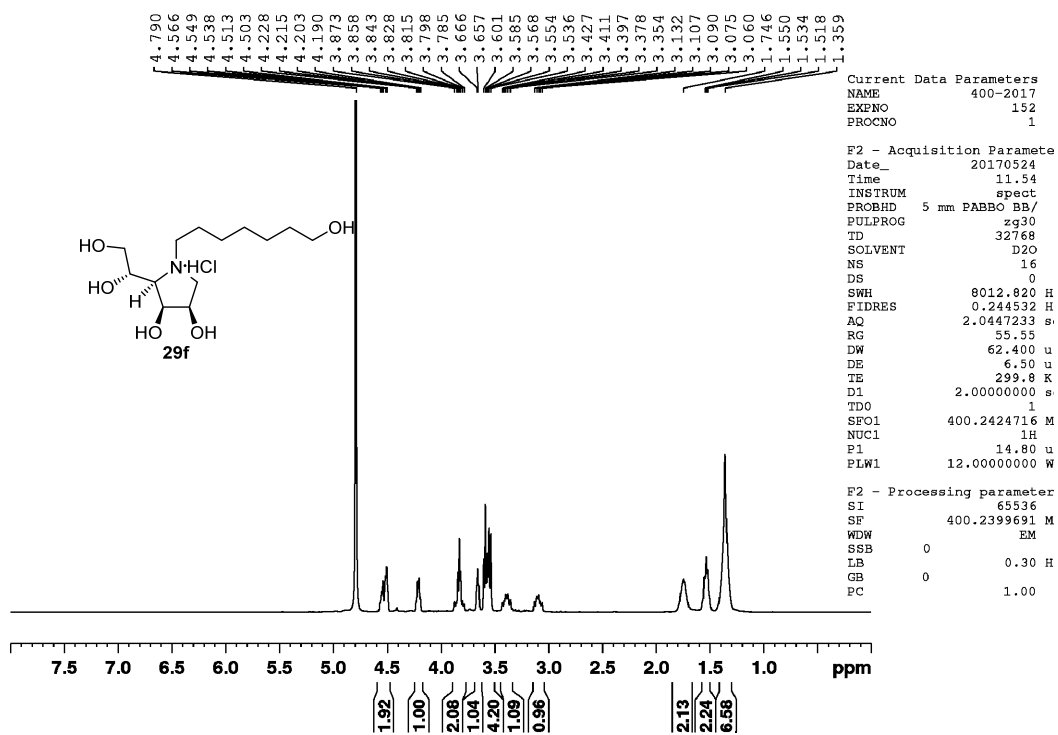
Current Data Parameters
NAME      400-2017
EXPNO    146
PROCNO   1

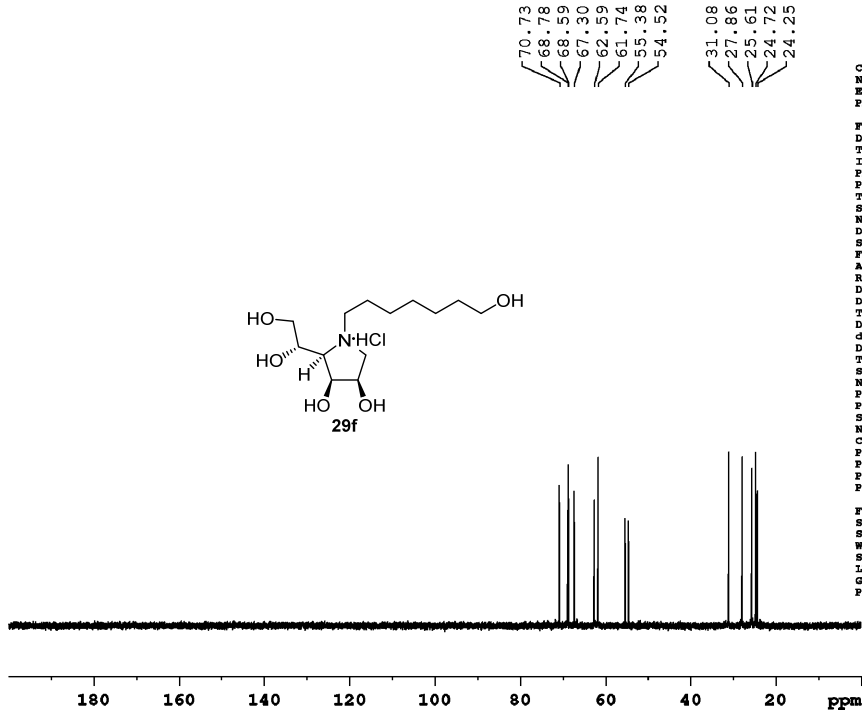
F2 - Acquisition Parameters
Data_    20170523
Time     21.29
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg130
VD        65536
SOLVENT  CDCl3
NS        64
DS        4
SWH       22058.824 Hz
FIDRES   0.336591 Hz
AQ        1.4854827 sec
RG        206.33
DW        22.687 usec
DE        6.50 usec
TE        300.4 K
CPDPRG2  waltz16
D1        2.00000000 sec
d2        0.00344828 sec
d12       0.00000000 sec
DELTA    0.00001273 sec
TDO       1
SFO1     100.6484788 MHz
NUC1      13C
P1        10.00 usec
P13       2000.00 usec
PLW0      0 W
PLW1     54.00000000 W
SFO1M[5] Crp60comp_4
SFO1M5   0.500
SFOFF5   0 Hz
SFO5     8.25039984 W
SFO6     400.2416010 MHz
MDC2     1H
CPDPRG2  waltz16
P4        15.30 usec
PCPD2    90.00 usec
PLW2     12.00000000 W
PLW12    0.34680000 W

F2 - Processing parameters
SI        32768
SF        100.6404280 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```



Compound 29f:



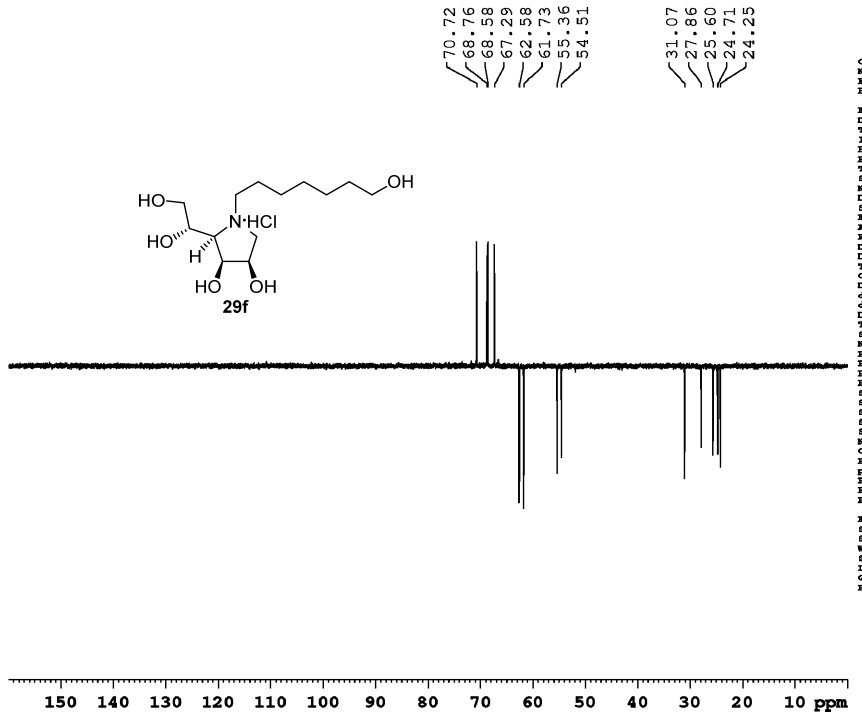


```

Current Data Parameters
NAME      400-2017
EXPNO    153
PROCNO   1

F2 - Acquisition Parameters
Date_    20170524
Time     12.24
INSTRUM  spect
PROBHD   5 mm F4BBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  D2O
NS        512
DS        4
SWH       24038.461 Hz
FIDRES   0.386798 Hz
AQ        1.3831488 sec
RG        206.33
DW        20.800 usec
DE        6.50 usec
TE        300.2 K
D1        2.0000000 sec
d11       0.0300000 sec
DELTA    1.8999999 sec
TDO       1
SFO1     100.6504916 MHz
NUC1      13C
P1        10.00 usec
ELW1     54.0000000 W
SFO2     400.2416010 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2    90.00 usec
ELW2     12.0000000 W
ELW12    0.3468000 W
ELW13    0.2809099 W

F2 - Processing parameters
SI        32768
SF        100.6404280 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

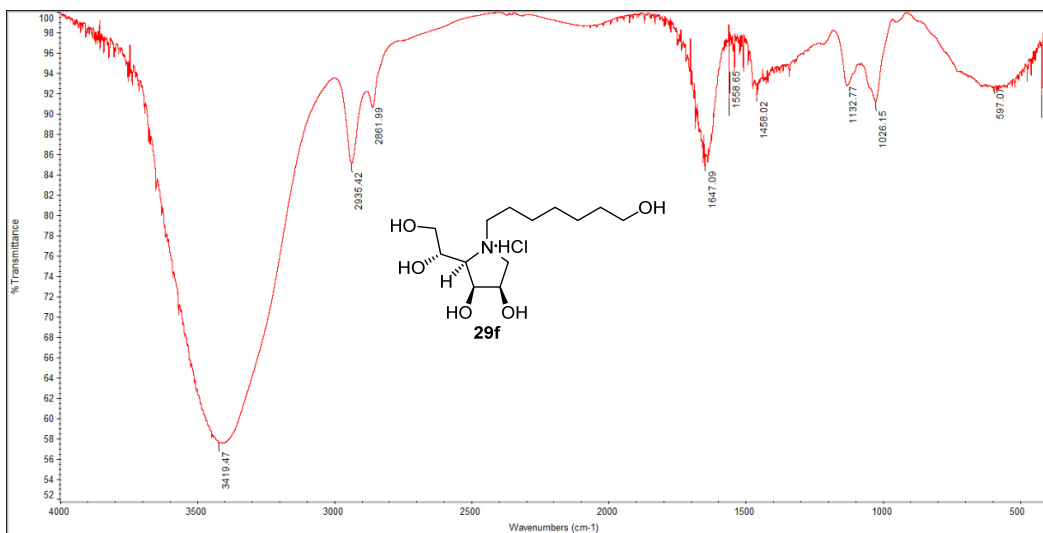


```

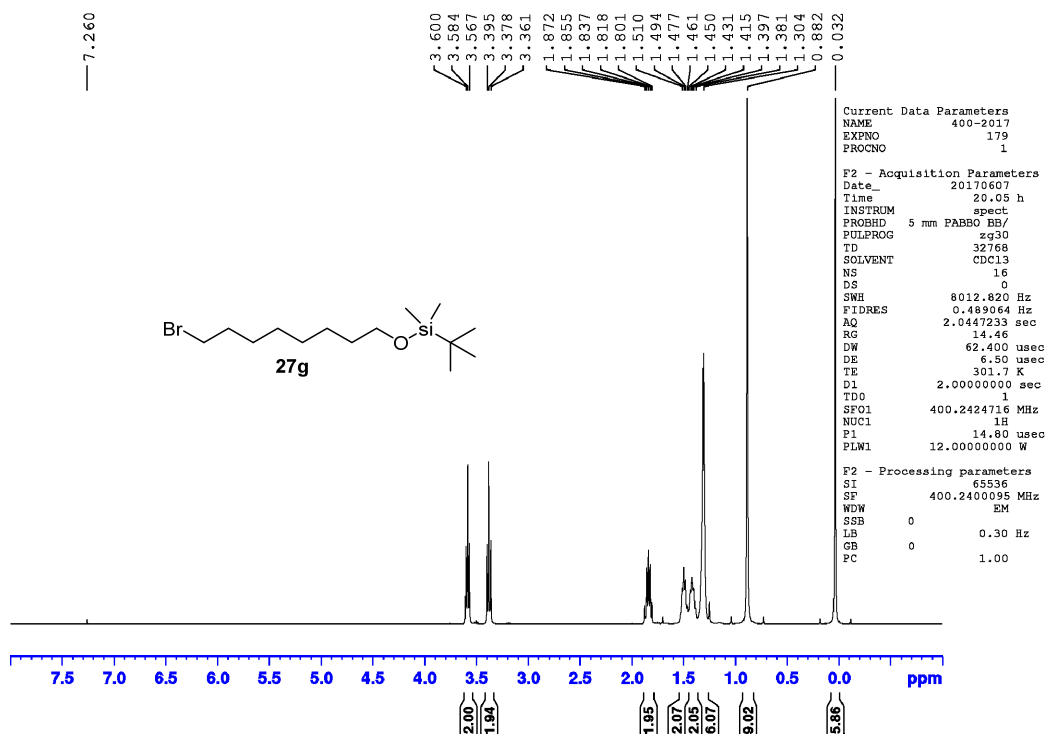
Current Data Parameters
NAME      400-2017
EXPNO    154
PROCNO   1

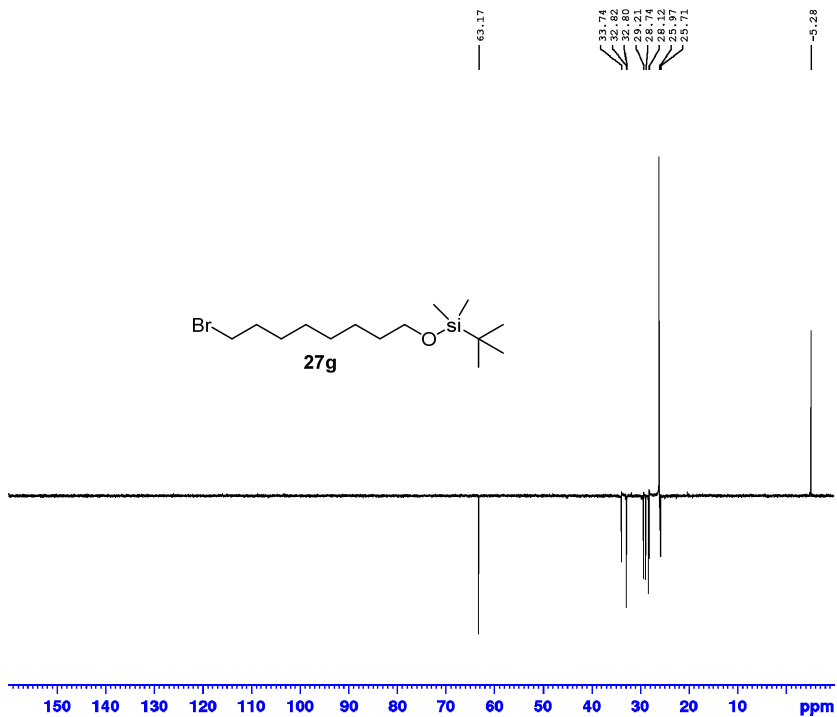
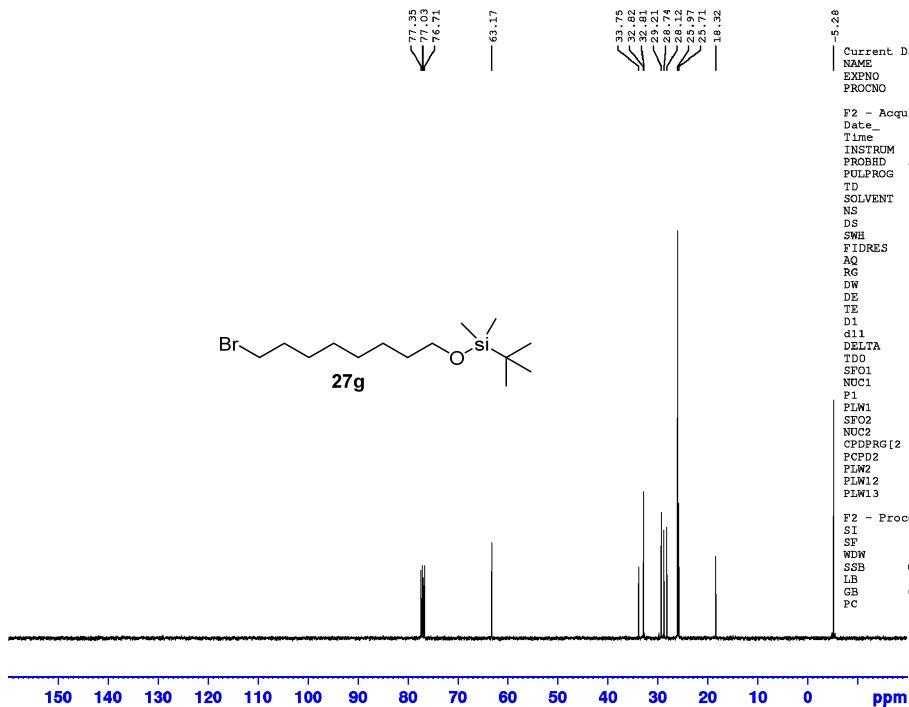
F2 - Acquisition Parameters
Date_    20170524
Time     12.33
INSTRUM  spect
PROBHD   5 mm F4BBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  D2O
NS        512
DS        4
SWH       16119.032 Hz
FIDRES   0.246110 Hz
AQ        2.0316180 sec
RG        206.33
DW        31.000 usec
DE        6.50 usec
TE        300.2 K
CPDPRG2  145.0000000
D1        2.0000000 sec
d2        0.00344828 sec
d12       0.0000200 sec
DELTA    0.0001272 sec
TDO       1
SFO1     100.6404788 MHz
NUC1      13C
P1        10.00 usec
ELW1     54.0000000 W
SFO2     400.2412800 MHz
NUC2      1H
CPDPRG2  waltz16
PCPD2    90.00 usec
ELW2     12.0000000 W
ELW12    0.3468000 W

F2 - Processing parameters
SI        32768
SF        100.6404280 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

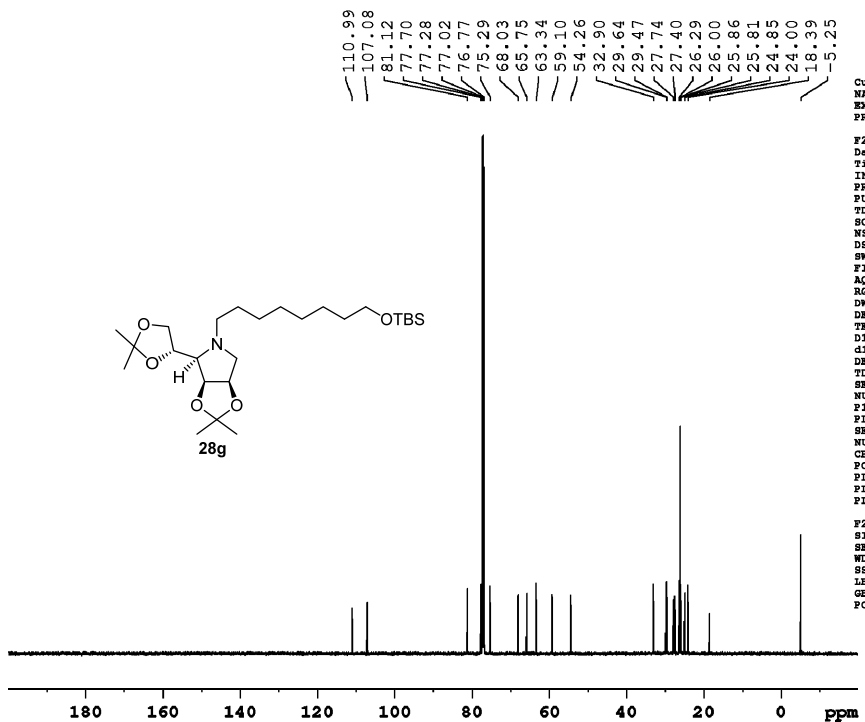
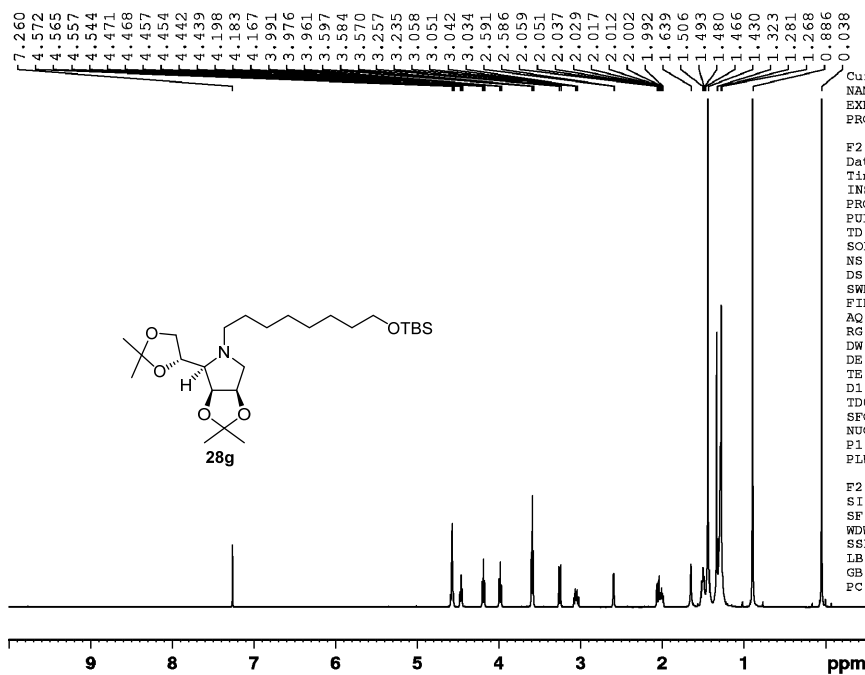


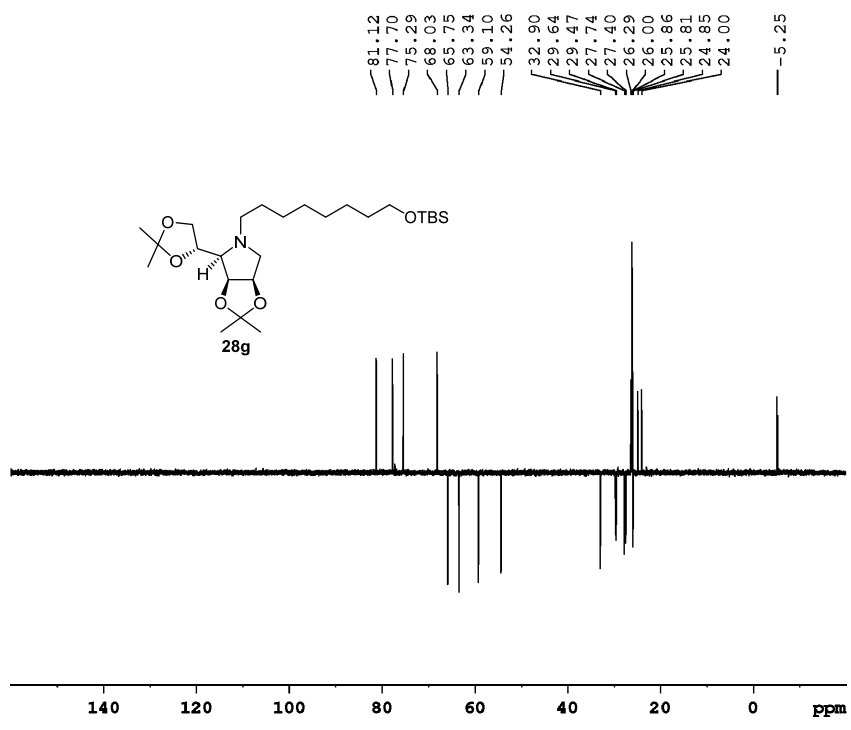
Compound 27g:





Compound 28g:



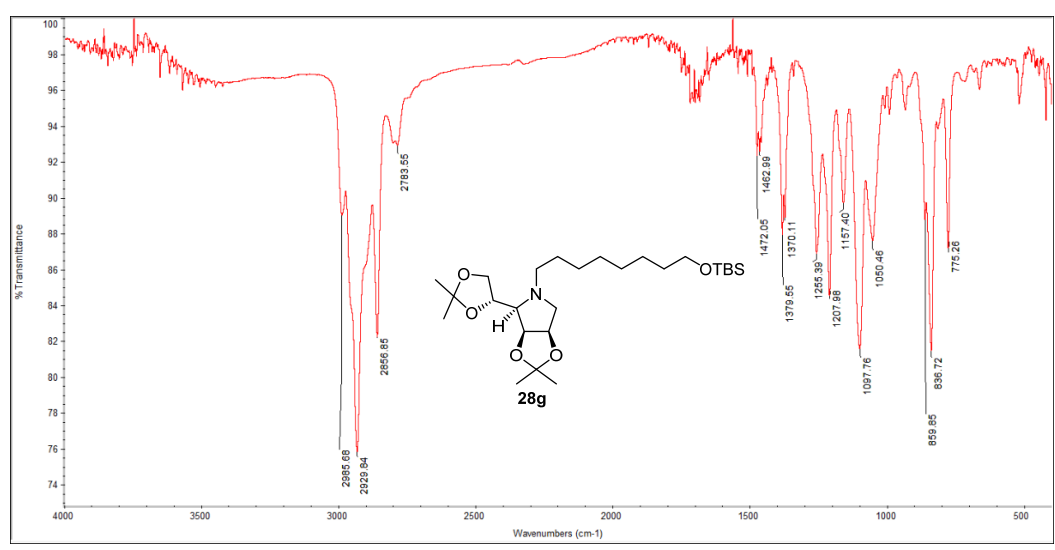


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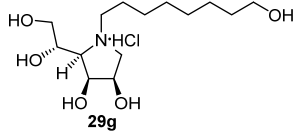
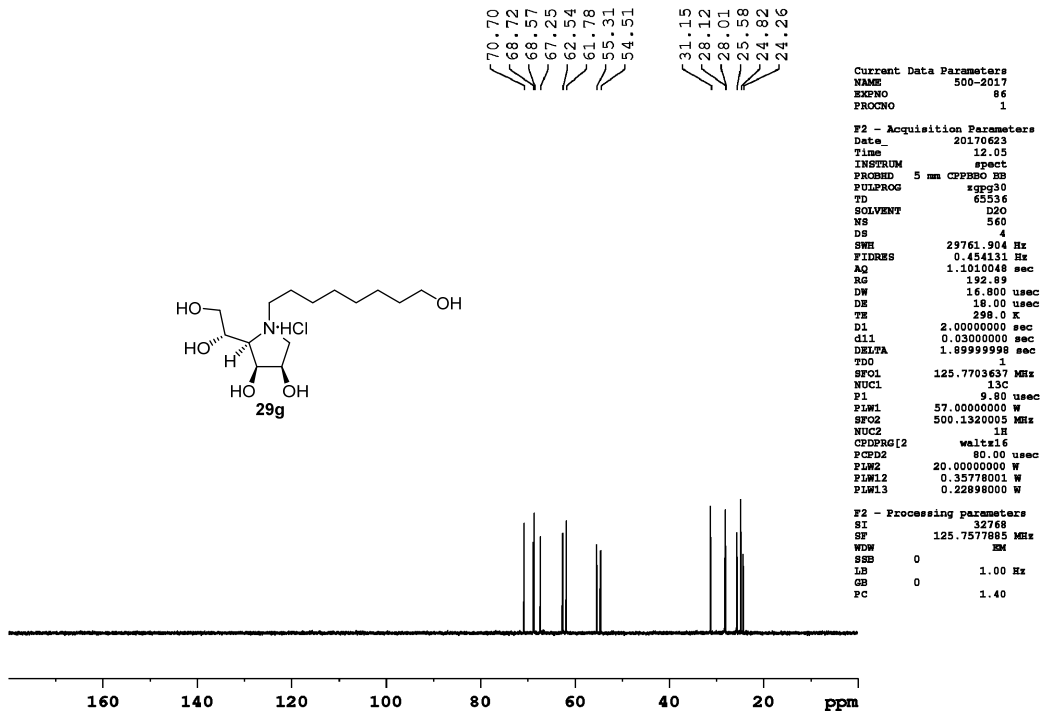
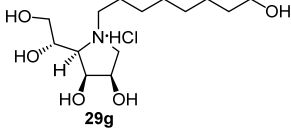
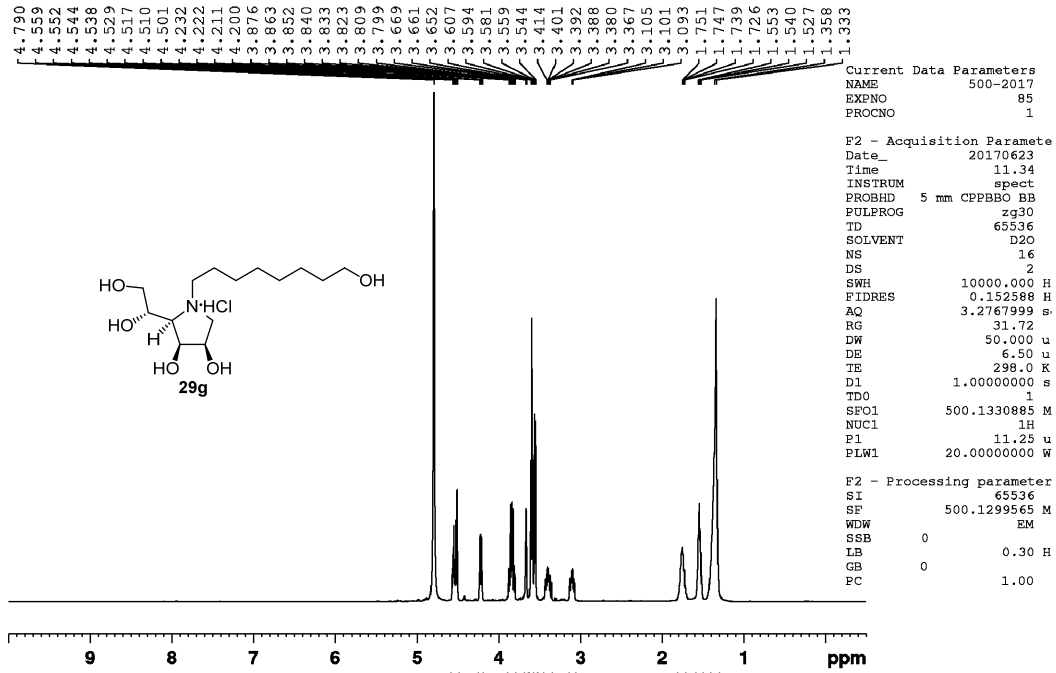
Current Data Parameters
NAME      500-2017
EXPNO     80
PROCNO    1

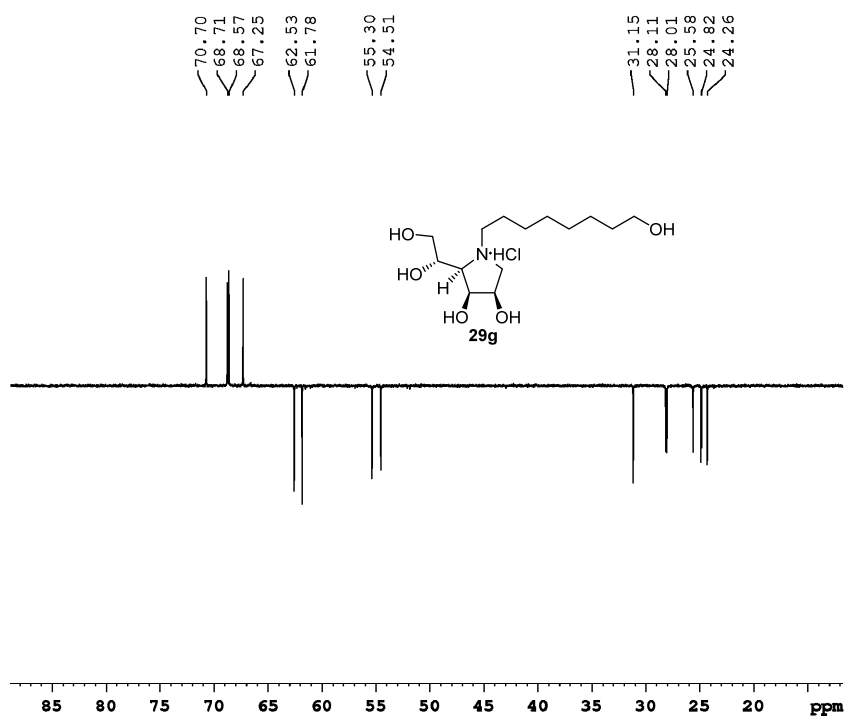
F2 - Acquisition Parameters
Date_     20170622
Time      12.36
INSTRUM   spect
PROBHD    5 mm CPYPRBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         52
DS         4
SWH        25252.525 Hz
FIDRES    0.385323 Hz
AQ         1.2976128 sec
RG         322.89
DW         19.800 usec
DE         18.00 usec
TE         298.1 K
CQPT2     145.000000
D1         2.0000000 sec
d2         0.00344828 sec
dL2        0.0000000 sec
DELTA     0.00001248 sec
TDO        1
SFO1      125.7678486 MHz
NUC1       13C
P1         9.80 usec
P13        2000.00 usec
PLP0       0 W
PLM1      57.0000000 W
SFO2       500.1315990 MHz
NUC2       1H
CQCPG2[2] waltz16
P2         10.70 usec
P4         21.40 usec
PCPD2     80.00 usec
PLM2      20.0000000 W
PLM12     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
  
```



Compound 29g:



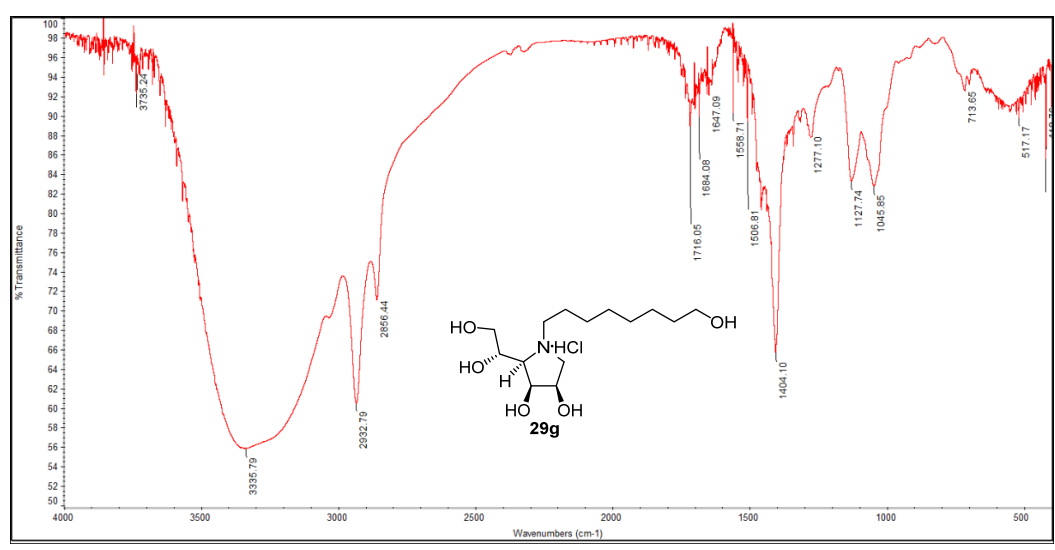


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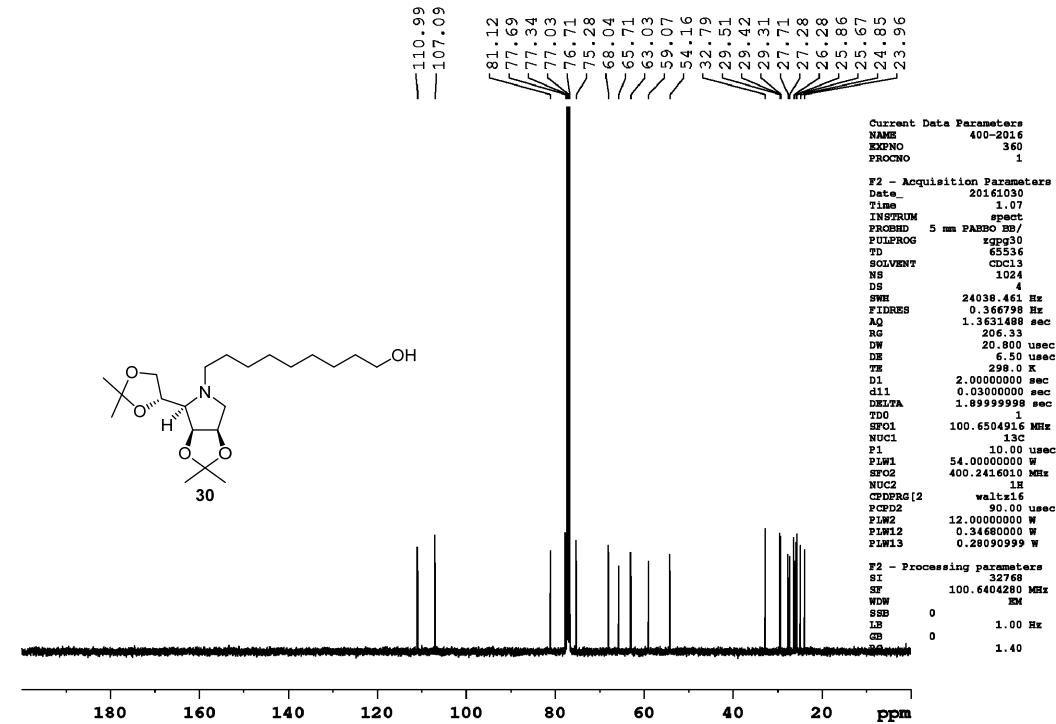
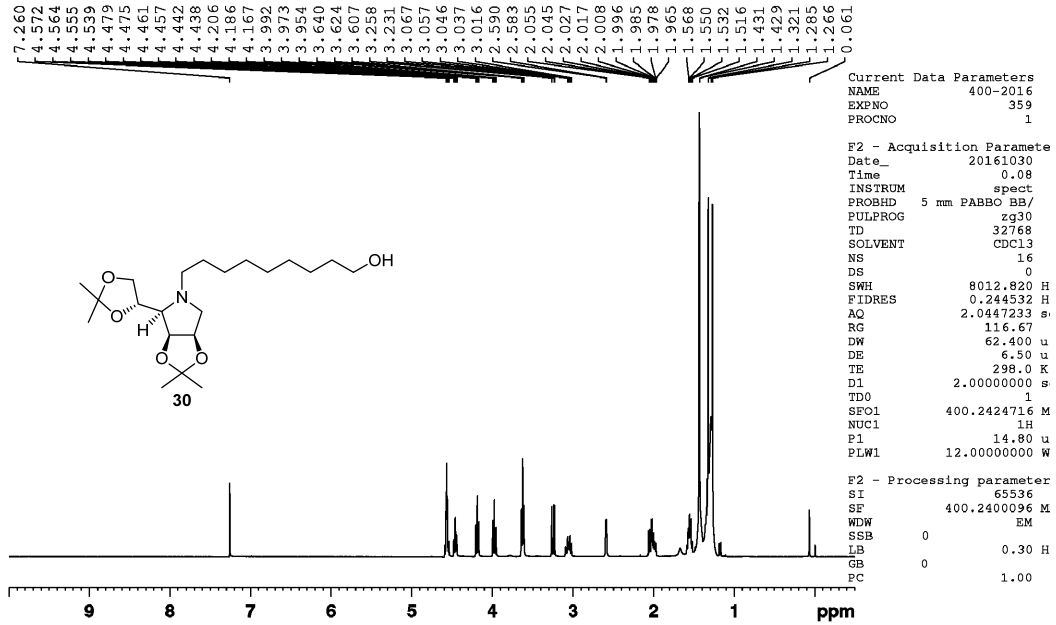
Current Data Parameters
NAME      500-2017
EXPNO     87
PROCNO    1

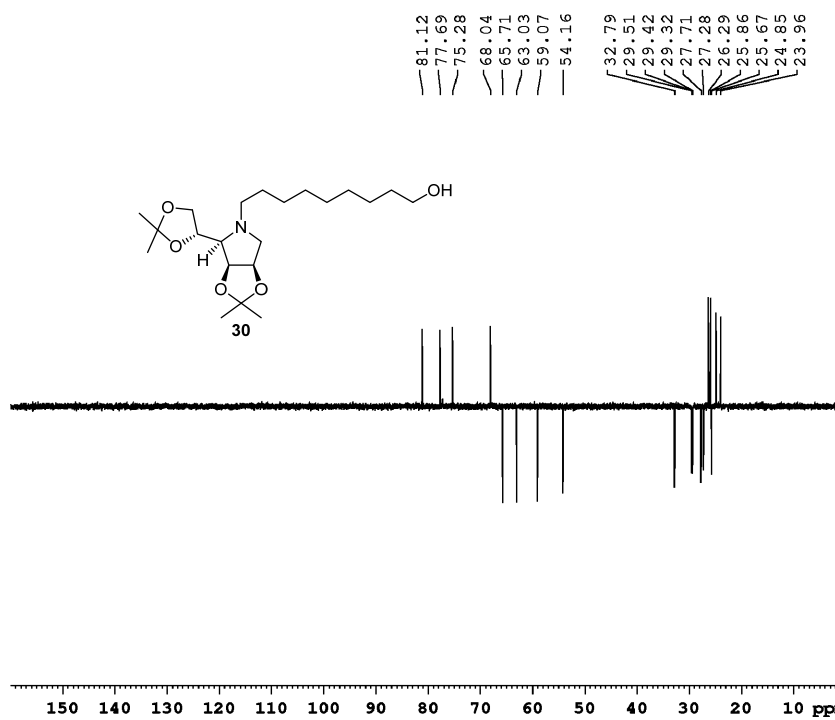
F2 - Acquisition Parameters
Date_     20170623
Time      12.15
INSTRUM   spect
PROBHD    5 mm CPYBBO BB
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         160
DS         4
SWH        20161.291 Hz
FIDRES    0.307637 Hz
AQ         1.6252928 sec
RG         192.89
DW         24.800 usec
DE         18.00 usec
TE         298.1 K
CQF2      148.0000000
D1         2.0000000 sec
d2         0.00344828 sec
d12        0.00000000 sec
DELTA     0.00001248 sec
SFO1      125.7678486 MHz
NUC1       13C
P1         9.80 usec
F13        2000.00 usec
PLWD      0 W
PLW1      57.00000000 W
SFO5M[5]  Csp60comp_4
SFOALS    0.850
SFOFF5    0 Hz
SWS       8.36410046 W
SFO2      500.1315985 MHz
NUC2       1H
CHRG2[2]  waltz16
P3         10.70 usec
P4         21.40 usec
SFO2      80.00 usec
PLW2      20.00000000 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
  
```



Compound 30:



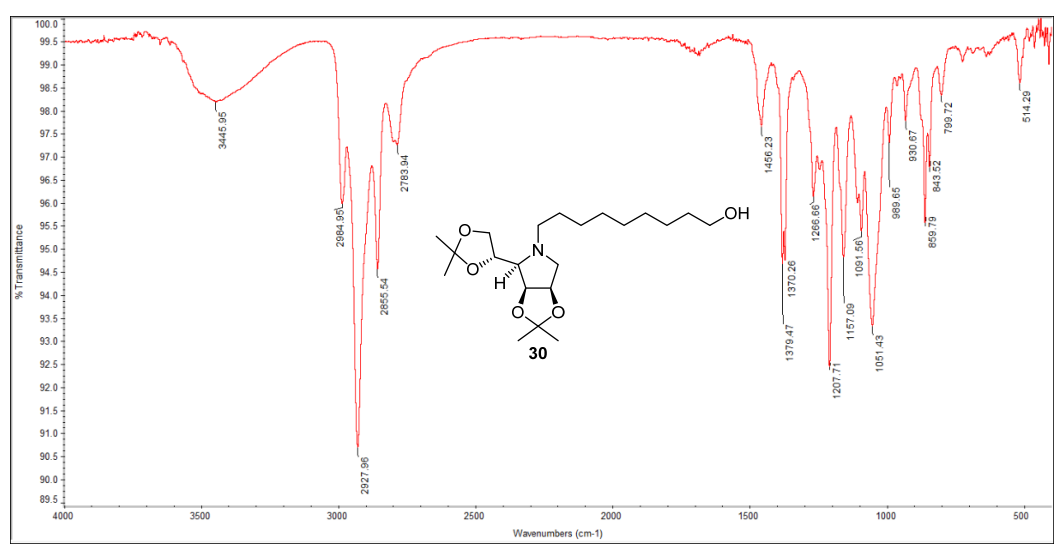


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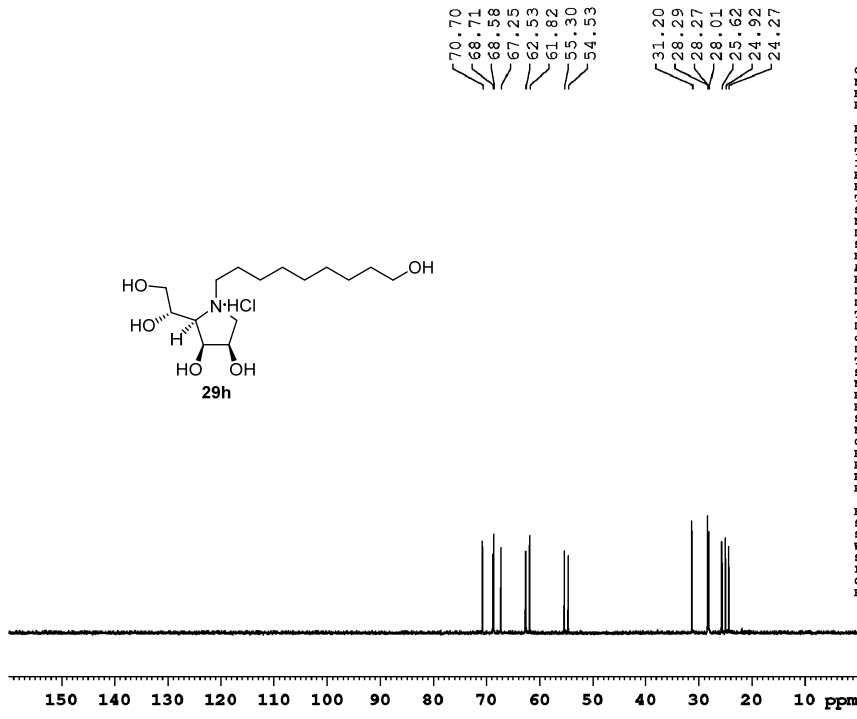
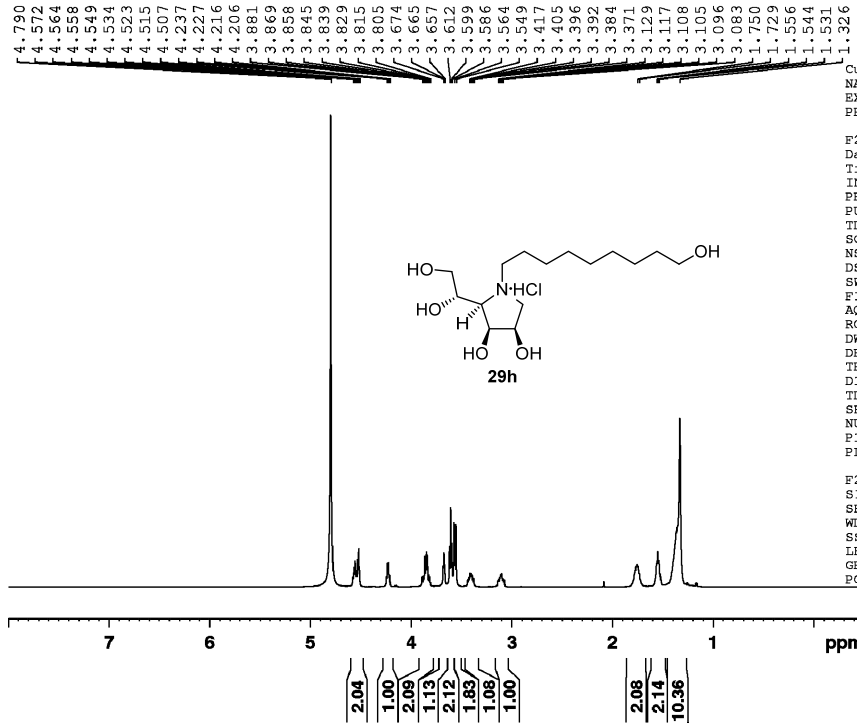
Current Data Parameters
NAME      400-2016
EXPNO    1
PROCNO   1

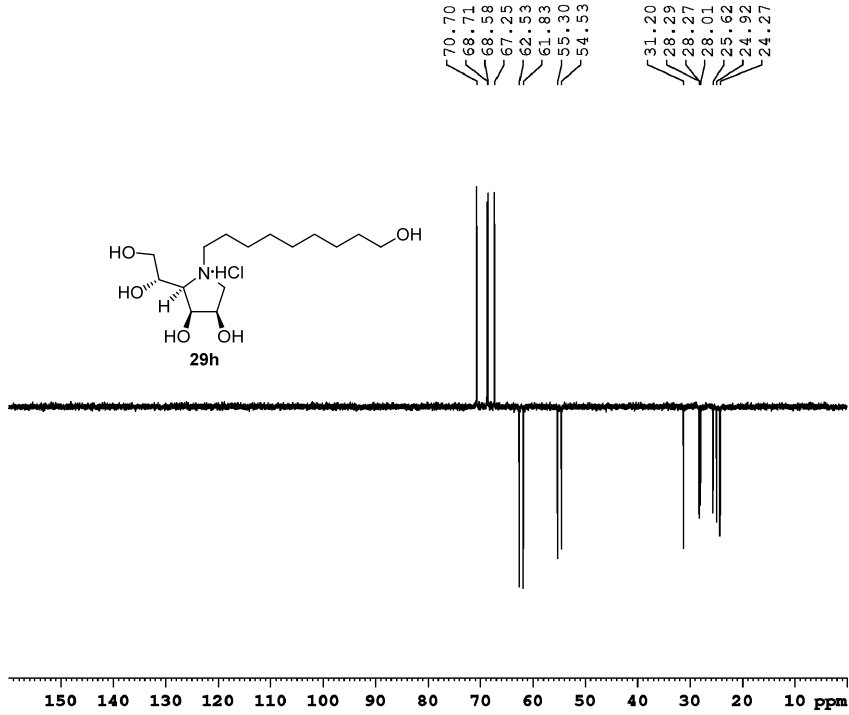
F2 - Acquisition Parameters
Date_    20161030
Time     1.26
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        256
DS        4
SWH       16129.932 Hz
FIDRES   0.246110 Hz
AQ        2.0216180 sec
RG         206.39
DW         31.000 usec
DE         6.50 usec
TE         298.0 K
CQF2      145.000000
SI         2.0000000 sec
d2         0.00344628 sec
d12        0.00002000 sec
DELTA     0.0001273 sec
WDW        2
SSB1      100.6464788 MHz
NUC1       13C
SI         10.00 usec
E13        0 W
2000.00 usec
FLM0
FLM1      54.0000000 W
SFRM[5]   Csp60comp.4
SFOALS    0.500
SFOFFS    0 Hz
SWS       8.25059986 W
SFC       400.2412800 MHz
NUC2       1H
CQCPG[2]  waltz16
SI         15.30 usec
p4         30.60 usec
SFO2      50.00 usec
FLM2      12.0000000 W
FLML2     0.34680000 W

F2 - Processing parameters
SI         32768
SF         100.6404280 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```



Compound 29h:



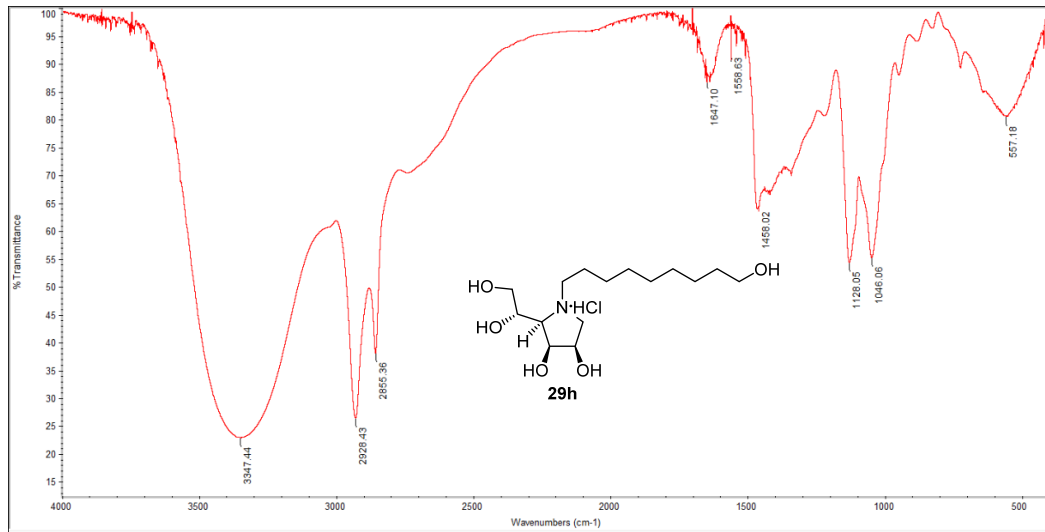


```

Current Data Parameters
NAME      500-2016
EXPNO     133
PROCNO    1

F2 - Acquisition Parameters
Date_     20161101
Time      2.46
INSTRUM   spect
PROBHD    5 mm CPYPRB0 B5
PULPROG   zgpg30
TD         65536
SOLVENT   D2O
NS         256
DS         4
SWH        20161.291 Hz
FIDRES    0.307637 Hz
AQ         1.6252926 sec
RG         192.89
DW         24.800 usec
DE         18.00 usec
TE         298.1 K
CHFT2     145.0000000
SI         2.0000000 sec
AQ2        0.00344828 sec
AQ2        0.00000000 sec
DELTA      0.00001249 sec
TDO        1
SFO1       125.7678484 MHz
NUC1        13C
P1          9.80 usec
P13        2000.00 usec
PLM0        0 W
PLM1       57.00000000 W
SFO2        500.1315995 MHz
NUC2        1H
PCYPRG2    waltz16
P3         10.70 usec
P4         21.40 usec
PCYPRG2    80.00 usec
PLM2       20.00000000 W
PLM12      0.35778001 W

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



3. X - Ray Crystallographic Data for compound 11

Structure deposited at the Cambridge Crystallographic Data Centre (CCDC 1908913)

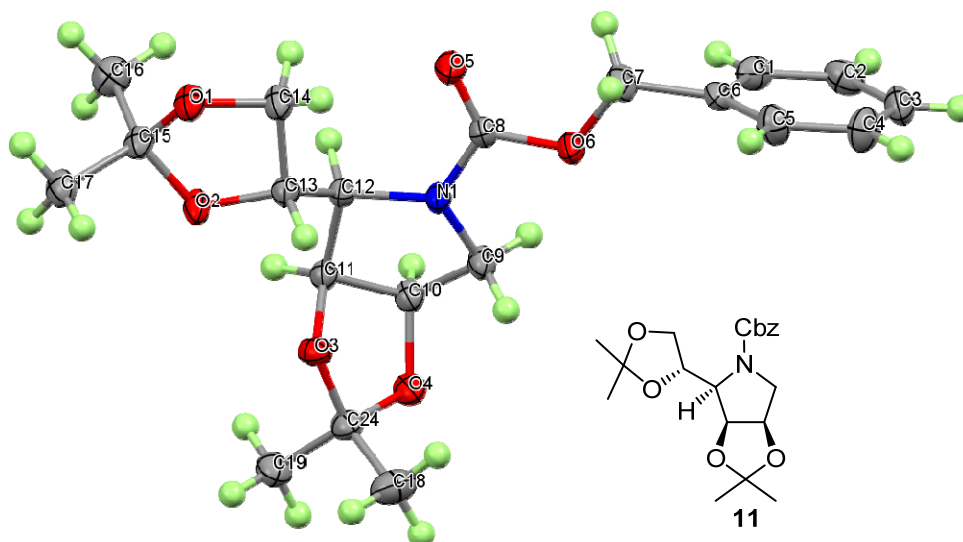


Fig1. X-Ray ellipsoid plots of **11**

Table 1. Crystal data and structure refinement for **11**.

Identification code	sa4466	
Empirical formula	C ₂₀ H ₂₇ N O ₆	
Formula weight	377.42	
Temperature	173.1500 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 11.118(2) Å	α = 90°.
	b = 7.8299(16) Å	β = 111.37(3)°.
	c = 11.760(2) Å	γ = 90°.
Volume	953.4(4) Å ³	
Z	2	
Density (calculated)	1.315 Mg/m ³	
Absorption coefficient	0.097 mm ⁻¹	
F(000)	404	
Crystal size	0.433 x 0.369 x 0.161 mm ³	
Theta range for data collection	2.159 to 27.468°.	
Index ranges	-14 ≤ h ≤ 14, -10 ≤ k ≤ 10, -15 ≤ l ≤ 15	
Reflections collected	10648	
Independent reflections	4309 [R(int) = 0.0237]	

Completeness to $\theta = 26.000^\circ$	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8871
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4309 / 1 / 248
Goodness-of-fit on F^2	1.074
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0318$, $wR_2 = 0.0758$
R indices (all data)	$R_1 = 0.0323$, $wR_2 = 0.0763$
Absolute structure parameter	0.4(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.162 and -0.144 $e.\text{\AA}^{-3}$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **11**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
O1	4999(1)	1330(2)	-3087(1)	27(1)
O2	5585(1)	4107(2)	-3098(1)	28(1)
O3	7732(1)	6416(2)	-1677(1)	25(1)
O4	8173(1)	8691(2)	-361(1)	28(1)
O5	6027(1)	2375(2)	614(1)	38(1)
O6	7604(1)	3710(2)	2157(1)	27(1)
N1	6978(1)	4793(2)	272(1)	21(1)
C1	7786(2)	3915(3)	4846(2)	30(1)
C2	8404(2)	4209(3)	6090(2)	32(1)
C3	9521(2)	3309(3)	6740(2)	33(1)
C4	10010(2)	2138(3)	6142(2)	36(1)
C5	9384(2)	1852(3)	4902(2)	32(1)
C6	8268(2)	2732(2)	4248(2)	25(1)
C7	7529(2)	2291(3)	2931(2)	35(1)
C8	6797(2)	3533(2)	976(2)	24(1)
C9	7685(2)	6353(2)	804(2)	25(1)
C10	7173(2)	7704(2)	-203(2)	22(1)
C11	6606(2)	6668(2)	-1376(1)	20(1)
C12	6142(2)	4977(2)	-1031(1)	19(1)
C13	6214(2)	3509(2)	-1867(1)	21(1)
C14	5458(2)	1875(2)	-1840(2)	27(1)
C15	4678(2)	2842(2)	-3801(2)	23(1)
C16	3318(2)	3445(3)	-4002(2)	33(1)
C17	4883(2)	2520(3)	-4983(2)	29(1)
C18	9908(2)	7410(3)	-857(2)	40(1)
C19	8166(2)	9193(3)	-2376(2)	34(1)
C24	8500(2)	7931(2)	-1332(2)	25(1)

Table 3. Bond lengths [Å] and angles [°] for **11**.

O1-C14	1.432(2)
O1-C15	1.420(2)
O2-C13	1.437(2)
O2-C15	1.440(2)
O3-C11	1.433(2)
O3-C24	1.431(2)
O4-C10	1.421(2)
O4-C24	1.447(2)
O5-C8	1.213(2)
O6-C7	1.458(2)
O6-C8	1.359(2)
N1-C8	1.350(2)
N1-C9	1.463(2)
N1-C12	1.481(2)
C1-H1	0.9300
C1-C2	1.390(3)
C1-C6	1.384(3)
C2-H2	0.9300
C2-C3	1.389(3)
C3-H3	0.9300
C3-C4	1.381(3)
C4-H4	0.9300
C4-C5	1.387(3)
C5-H5	0.9300
C5-C6	1.381(3)
C6-C7	1.505(3)
C7-H7A	0.9700
C7-H7B	0.9700
C9-H9A	0.9700
C9-H9B	0.9700
C9-C10	1.534(2)
C10-H10	0.9800
C10-C11	1.525(2)
C11-H11	0.9800
C11-C12	1.529(2)
C12-H12	0.9800

C12-C13	1.533(2)
C13-H13	0.9800
C13-C14	1.537(2)
C14-H14A	0.9700
C14-H14B	0.9700
C15-C16	1.518(3)
C15-C17	1.509(3)
C16-H16A	0.9600
C16-H16B	0.9600
C16-H16C	0.9600
C17-H17A	0.9600
C17-H17B	0.9600
C17-H17C	0.9600
C18-H18A	0.9600
C18-H18B	0.9600
C18-H18C	0.9600
C18-C24	1.515(3)
C19-H19A	0.9600
C19-H19B	0.9600
C19-H19C	0.9600
C19-C24	1.513(3)
C15-O1-C14	106.05(13)
C13-O2-C15	109.67(13)
C24-O3-C11	107.48(13)
C10-O4-C24	108.23(13)
C8-O6-C7	113.22(14)
C8-N1-C9	121.66(14)
C8-N1-C12	121.86(14)
C9-N1-C12	113.45(13)
C2-C1-H1	119.6
C6-C1-H1	119.6
C6-C1-C2	120.75(17)
C1-C2-H2	120.2
C3-C2-C1	119.64(18)
C3-C2-H2	120.2
C2-C3-H3	120.1
C4-C3-C2	119.73(18)

C4-C3-H3	120.1
C3-C4-H4	119.9
C3-C4-C5	120.13(18)
C5-C4-H4	119.9
C4-C5-H5	119.7
C6-C5-C4	120.68(19)
C6-C5-H5	119.7
C1-C6-C7	120.64(17)
C5-C6-C1	119.06(17)
C5-C6-C7	120.08(19)
O6-C7-C6	109.51(15)
O6-C7-H7A	109.8
O6-C7-H7B	109.8
C6-C7-H7A	109.8
C6-C7-H7B	109.8
H7A-C7-H7B	108.2
O5-C8-O6	123.63(16)
O5-C8-N1	125.14(16)
N1-C8-O6	111.23(15)
N1-C9-H9A	110.8
N1-C9-H9B	110.8
N1-C9-C10	104.77(13)
H9A-C9-H9B	108.9
C10-C9-H9A	110.8
C10-C9-H9B	110.8
O4-C10-C9	112.80(14)
O4-C10-H10	111.5
O4-C10-C11	104.84(14)
C9-C10-H10	111.5
C11-C10-C9	104.26(14)
C11-C10-H10	111.5
O3-C11-C10	100.75(13)
O3-C11-H11	112.6
O3-C11-C12	110.87(14)
C10-C11-H11	112.6
C10-C11-C12	106.76(13)
C12-C11-H11	112.6
N1-C12-C11	102.33(13)

N1-C12-H12	108.8
N1-C12-C13	115.51(14)
C11-C12-H12	108.8
C11-C12-C13	112.19(13)
C13-C12-H12	108.8
O2-C13-C12	106.34(14)
O2-C13-H13	110.1
O2-C13-C14	102.88(13)
C12-C13-H13	110.1
C12-C13-C14	117.00(14)
C14-C13-H13	110.1
O1-C14-C13	102.72(14)
O1-C14-H14A	111.2
O1-C14-H14B	111.2
C13-C14-H14A	111.2
C13-C14-H14B	111.2
H14A-C14-H14B	109.1
O1-C15-O2	105.13(13)
O1-C15-C16	111.90(16)
O1-C15-C17	108.41(15)
O2-C15-C16	108.93(15)
O2-C15-C17	109.55(15)
C17-C15-C16	112.64(16)
C15-C16-H16A	109.5
C15-C16-H16B	109.5
C15-C16-H16C	109.5
H16A-C16-H16B	109.5
H16A-C16-H16C	109.5
H16B-C16-H16C	109.5
C15-C17-H17A	109.5
C15-C17-H17B	109.5
C15-C17-H17C	109.5
H17A-C17-H17B	109.5
H17A-C17-H17C	109.5
H17B-C17-H17C	109.5
H18A-C18-H18B	109.5
H18A-C18-H18C	109.5
H18B-C18-H18C	109.5

C24-C18-H18A	109.5
C24-C18-H18B	109.5
C24-C18-H18C	109.5
H19A-C19-H19B	109.5
H19A-C19-H19C	109.5
H19B-C19-H19C	109.5
C24-C19-H19A	109.5
C24-C19-H19B	109.5
C24-C19-H19C	109.5
O3-C24-O4	105.63(13)
O3-C24-C18	108.09(16)
O3-C24-C19	111.55(15)
O4-C24-C18	110.04(16)
O4-C24-C19	108.33(16)
C19-C24-C18	112.96(17)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O1	35(1)	18(1)	23(1)	-2(1)	6(1)	-4(1)
O2	39(1)	23(1)	16(1)	-1(1)	3(1)	-11(1)
O3	28(1)	23(1)	28(1)	-6(1)	14(1)	-7(1)
O4	36(1)	24(1)	26(1)	-6(1)	12(1)	-11(1)
O5	42(1)	43(1)	22(1)	4(1)	4(1)	-22(1)
O6	31(1)	29(1)	17(1)	4(1)	3(1)	-8(1)
N1	24(1)	21(1)	15(1)	1(1)	3(1)	-3(1)
C1	25(1)	27(1)	35(1)	8(1)	9(1)	4(1)
C2	40(1)	29(1)	36(1)	-1(1)	22(1)	2(1)
C3	42(1)	34(1)	20(1)	2(1)	8(1)	-4(1)
C4	32(1)	39(1)	29(1)	4(1)	1(1)	9(1)
C5	34(1)	35(1)	27(1)	-1(1)	12(1)	7(1)
C6	26(1)	27(1)	20(1)	6(1)	7(1)	-5(1)
C7	45(1)	33(1)	22(1)	9(1)	4(1)	-11(1)
C8	24(1)	28(1)	17(1)	2(1)	6(1)	-4(1)
C9	30(1)	23(1)	18(1)	-2(1)	6(1)	-4(1)
C10	27(1)	19(1)	21(1)	-1(1)	9(1)	-2(1)
C11	21(1)	21(1)	17(1)	1(1)	5(1)	0(1)
C12	18(1)	21(1)	16(1)	1(1)	4(1)	-1(1)
C13	23(1)	21(1)	18(1)	0(1)	5(1)	-1(1)
C14	35(1)	21(1)	21(1)	0(1)	6(1)	-4(1)
C15	28(1)	17(1)	21(1)	-4(1)	5(1)	-4(1)
C16	33(1)	29(1)	36(1)	-3(1)	11(1)	3(1)
C17	36(1)	26(1)	23(1)	-6(1)	9(1)	-4(1)
C18	28(1)	38(1)	54(1)	1(1)	13(1)	-4(1)
C19	42(1)	32(1)	30(1)	2(1)	13(1)	-9(1)
C24	28(1)	23(1)	26(1)	-3(1)	10(1)	-6(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **11**.

	x	y	z	U(eq)
H1	7041	4521	4412	35
H2	8072	5003	6486	39
H3	9938	3495	7573	39
H4	10761	1540	6573	43
H5	9717	1060	4506	38
H7A	7891	1272	2712	42
H7B	6634	2063	2812	42
H9A	8607	6190	1023	30
H9B	7519	6686	1527	30
H10	6518	8430	-71	27
H11	5920	7280	-2016	24
H12	5245	5109	-1091	23
H13	7118	3229	-1719	26
H14A	6015	1021	-1306	32
H14B	4746	2115	-1572	32
H16A	2705	2638	-4508	50
H16B	3175	4540	-4396	50
H16C	3214	3539	-3229	50
H17A	5743	2100	-4808	43
H17B	4767	3567	-5435	43
H17C	4270	1689	-5456	43
H18A	10057	6573	-223	60
H18B	10439	8393	-535	60
H18C	10121	6932	-1512	60
H19A	8386	8715	-3027	52
H19B	8644	10230	-2097	52
H19C	7258	9436	-2667	52

Table 6. Torsion angles [°] for **11**.

O2-C13-C14-O1	27.32(17)
O3-C11-C12-N1	83.10(15)
O3-C11-C12-C13	-41.31(17)
O4-C10-C11-O3	32.53(16)
O4-C10-C11-C12	148.37(13)
N1-C9-C10-O4	-134.39(14)
N1-C9-C10-C11	-21.22(18)
N1-C12-C13-O2	-166.98(13)
N1-C12-C13-C14	78.81(19)
C1-C2-C3-C4	0.3(3)
C1-C6-C7-O6	72.6(2)
C2-C1-C6-C5	-0.6(3)
C2-C1-C6-C7	173.98(18)
C2-C3-C4-C5	-0.5(3)
C3-C4-C5-C6	0.1(3)
C4-C5-C6-C1	0.4(3)
C4-C5-C6-C7	-174.19(19)
C5-C6-C7-O6	-112.9(2)
C6-C1-C2-C3	0.3(3)
C7-O6-C8-O5	4.8(3)
C7-O6-C8-N1	-174.53(17)
C8-O6-C7-C6	-170.12(16)
C8-N1-C9-C10	-155.20(16)
C8-N1-C12-C11	173.14(15)
C8-N1-C12-C13	-64.7(2)
C9-N1-C8-O5	165.00(19)
C9-N1-C8-O6	-15.7(2)
C9-N1-C12-C11	12.56(18)
C9-N1-C12-C13	134.74(16)
C9-C10-C11-O3	-86.22(15)
C9-C10-C11-C12	29.62(17)
C10-O4-C24-O3	-3.93(18)
C10-O4-C24-C18	-120.36(16)
C10-O4-C24-C19	115.70(16)
C10-C11-C12-N1	-25.76(16)
C10-C11-C12-C13	-150.18(14)

C11-O3-C24-O4	26.04(17)
C11-O3-C24-C18	143.80(16)
C11-O3-C24-C19	-91.44(17)
C11-C12-C13-O2	-50.22(17)
C11-C12-C13-C14	-164.44(14)
C12-N1-C8-O5	6.0(3)
C12-N1-C8-O6	-174.66(14)
C12-N1-C9-C10	5.43(19)
C12-C13-C14-O1	143.45(15)
C13-O2-C15-O1	-14.42(18)
C13-O2-C15-C16	105.66(17)
C13-O2-C15-C17	-130.72(16)
C14-O1-C15-O2	32.84(18)
C14-O1-C15-C16	-85.25(17)
C14-O1-C15-C17	149.92(15)
C15-O1-C14-C13	-37.33(18)
C15-O2-C13-C12	-131.62(15)
C15-O2-C13-C14	-8.09(18)
C24-O3-C11-C10	-35.77(16)
C24-O3-C11-C12	-148.51(14)
C24-O4-C10-C9	94.92(16)
C24-O4-C10-C11	-17.90(18)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **11** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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