

Supplementary material

Diastereoselective Synthesis of (\pm) 1',4'-Dimethyluridine

Guillaume Sautrey, Damien Bourgeois,* Christian Périgaud

Institut des Biomolécules Max Mousseron (IBMM) UMR 5247 CNRS-UM 1-UM 2 Université Montpellier 2, CC
1705, Place Eugène Bataillon, 34095 Montpellier Cedex 5, France.

^1H and ^{13}C NMR Spectral Data

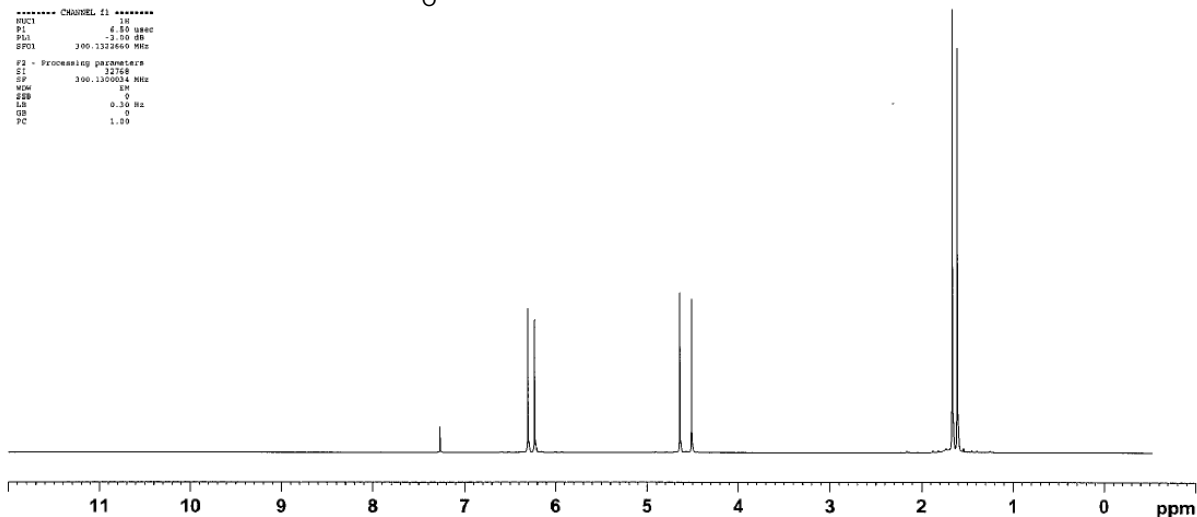
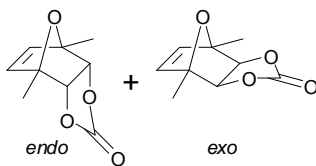
Compound 3 (endo/exo mixture)

```
Current Data Parameters
NAME 45-cp-0511009
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090513
Time 13:54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 2
DS 2
SWH 4844.963 Hz
FIDRES 0.147856 Hz
AQ 3.3817077 sec
RG 256
DR 102.200 usec
DE 8.00 usec
TE 300.0 K
D1 1.09600000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 4.00 usec
PL1 0.00 dB
PL3 300.1300014 MHz
PP1 0

F2 - Processing parameters
SI 32768
SF 300.1300014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



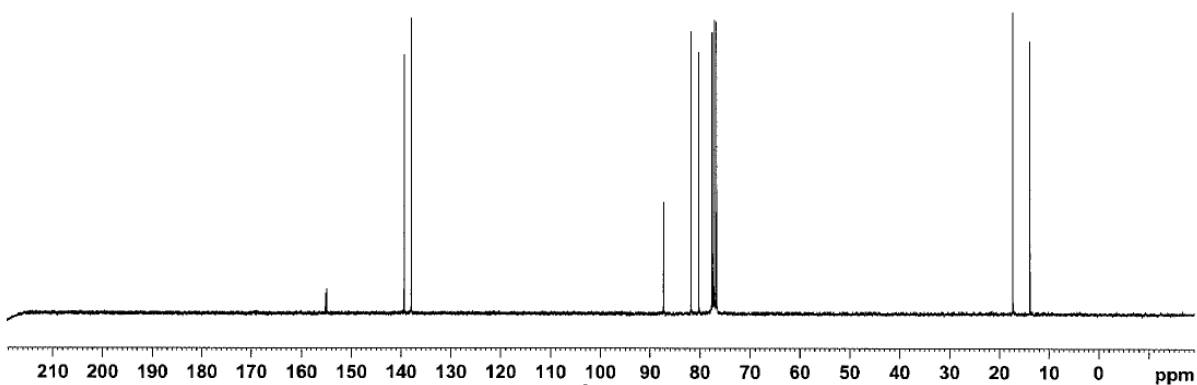
```
Current Data Parameters
NAME 45-cp-0511009
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090513
Time 13:52
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2
DS 2
SWH 12945.611 Hz
FIDRES 0.278419 Hz
AQ 1.8110004 sec
RG 256
DR 37.800 usec
DE 8.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.00000000 sec
d12 0.00000000 sec

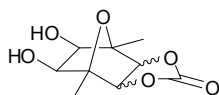
----- CHANNEL f1 -----
NUC1 13C
P1 4.00 usec
PL1 0.00 dB
PL3 75.477460 MHz
PP1 0

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 13C
P2 10.00 usec
PL2 0.00 dB
PL3 75.477460 MHz
PP2 0

F2 - Processing parameters
SI 32768
SF 75.477460 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```



Compound 4



Major isomer

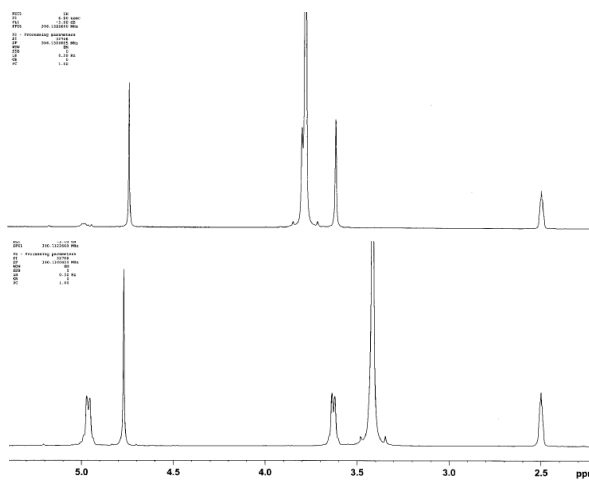
```

Current Data Parameters
NAME: 41-pp-05072009
EXPNO: 11
PROCNO: 1

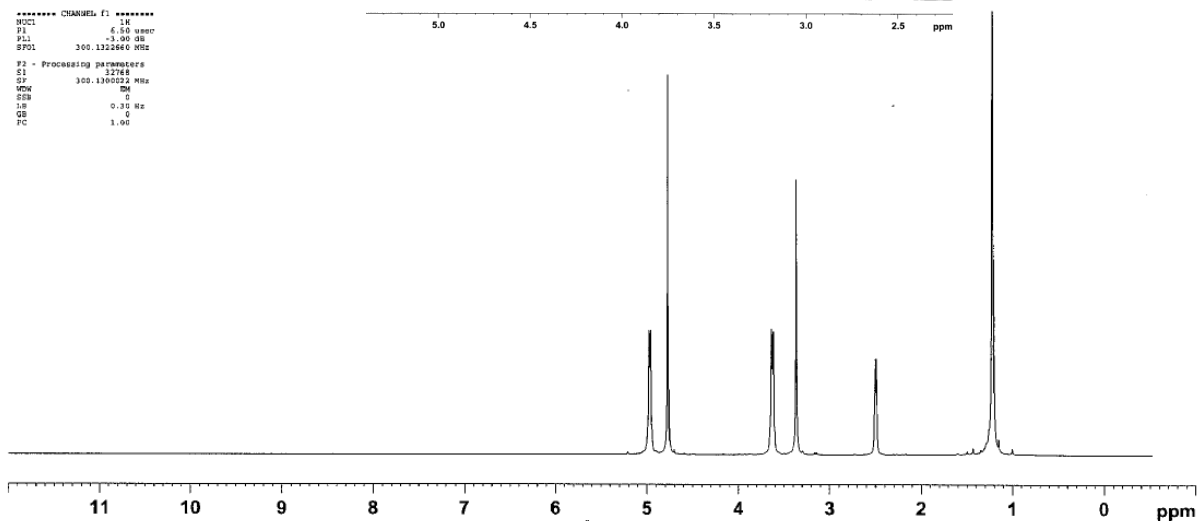
F1 - Acquisition Parameters
Date_ 20090907
Time: 22:49
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 16
DS: 2
SWH: 4844.561 Hz
FIDRES: 0.247856 Hz
AQ: 3.3817277 sec
RG: 256
DQ: 103.200 usec
DE: 8.90 usec
TE: 300.2 K
SI: 1.0000000 sec

***** CHANNEL f1 *****
NUC1: 13C
P1: 6.50 usec
PL1: -1.00 dB
SFO1: 300.1322660 MHz

F2 - Processing parameters
SI: 32768
SF: 300.1300222 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00
    
```



(with D₂O)



```

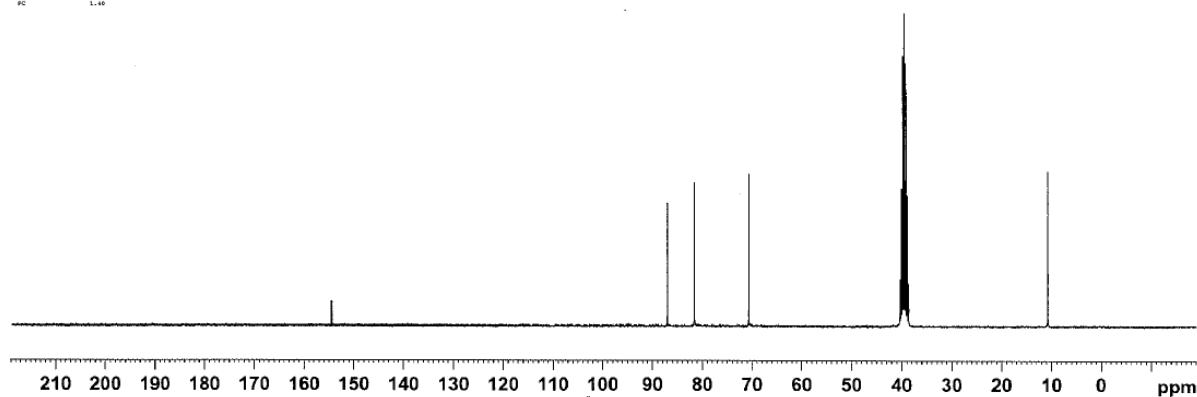
Current Data Parameters
NAME: 41-pp-05072009
EXPNO: 11
PROCNO: 1

F2 - Acquisition Parameters
Date_ 20090907
Time: 22:49
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 16
DS: 2
SWH: 12946.412 Hz
FIDRES: 0.277649 Hz
AQ: 1.1228194 sec
RG: 256
DQ: 103.200 usec
DE: 8.90 usec
TE: 300.2 K
SI: 1.0000000 sec
SFO1: 300.1300222 MHz
SFO2: 125.7611940 MHz

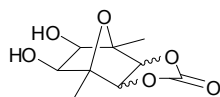
***** CHANNEL f1 *****
NUC1: 13C
P1: 6.50 usec
PL1: -1.00 dB
SFO1: 300.1322660 MHz

***** CHANNEL f2 *****
CPDPRG2: waltz16
NUC2: 13C
P2: 100.00 usec
PL2: 0.00 dB
PL12: 20.00 dB
PL13: 20.00 dB
SFO2: 125.7611940 MHz
SFO3: 300.1322660 MHz

F2 - Processing parameters
SI: 32768
SF: 300.1300222 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 1.00
    
```



Compound 4



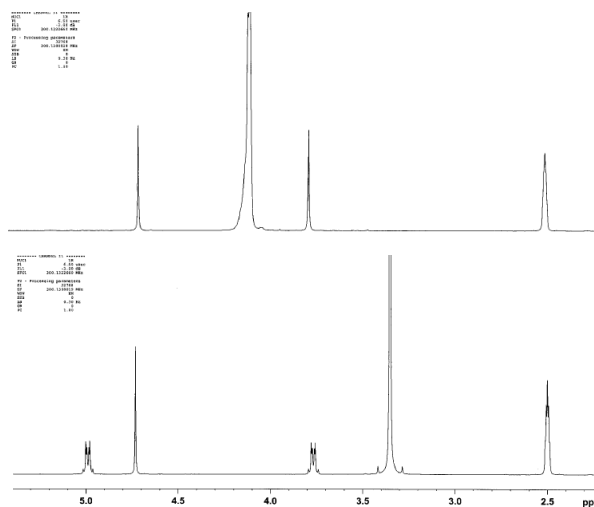
Minor isomer

```
Current Data Parameters
NAME 10-ep-0324209
EXPNO 11
PROCNO 1

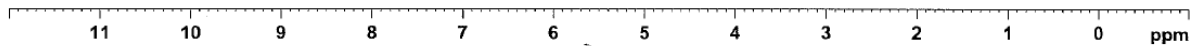
F2 - Acquisition Parameters
Date_ 20070315
Time 2.48
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT H2O
AQ 12.568
RG 320
SR 409.4
SWH 4844.961 Hz
FIDRES 0.147656 Hz
AQ 3.3817077 sec
RG 409.4
SW 103.200 usec
DE 8.00 usec
TE 300.2 K
DS 1.0000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 6.50 usec
PL1 -2.00 dB
SFO1 300.1322660 MHz

F2 - Processing parameters
SI 32768
SF 360.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



(with D₂O)



```
Current Data Parameters
NAME 10-ep-0324209
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070315
Time 21.45
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT H2O
AQ 12.568
RG 320
SR 409.4
SWH 4844.961 Hz
FIDRES 0.147656 Hz
AQ 3.3817077 sec
RG 409.4
SW 103.200 usec
DE 8.00 usec
TE 300.2 K
DS 1.0000000 sec

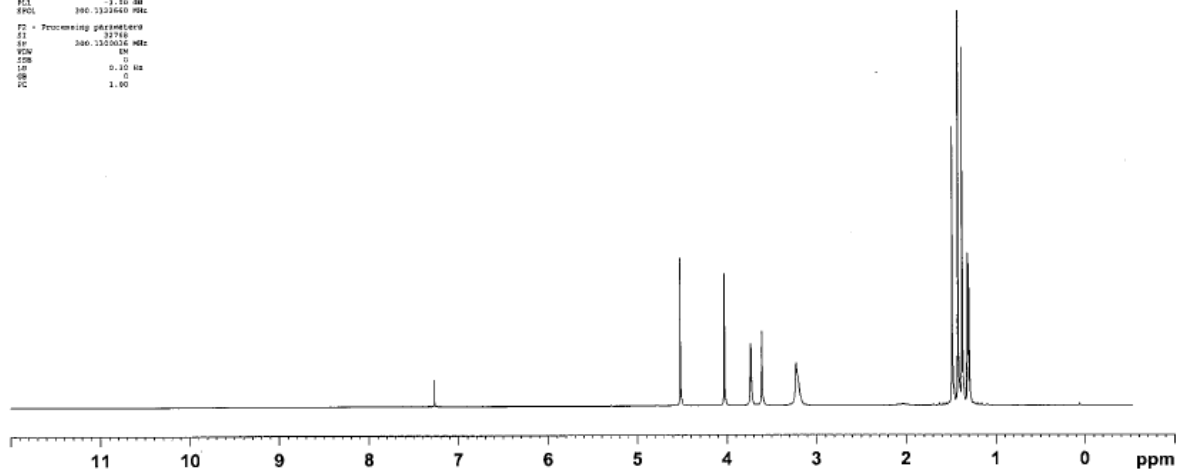
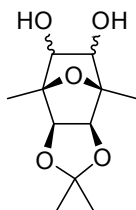
----- CHANNEL f1 -----
NUC1 13C
P1 6.50 usec
PL1 -2.00 dB
SFO1 300.1322660 MHz

----- CHANNEL f2 -----
NUC2 1H
P2 13.00 usec
PL2 0.00 dB
SFO2 500.1360540 MHz

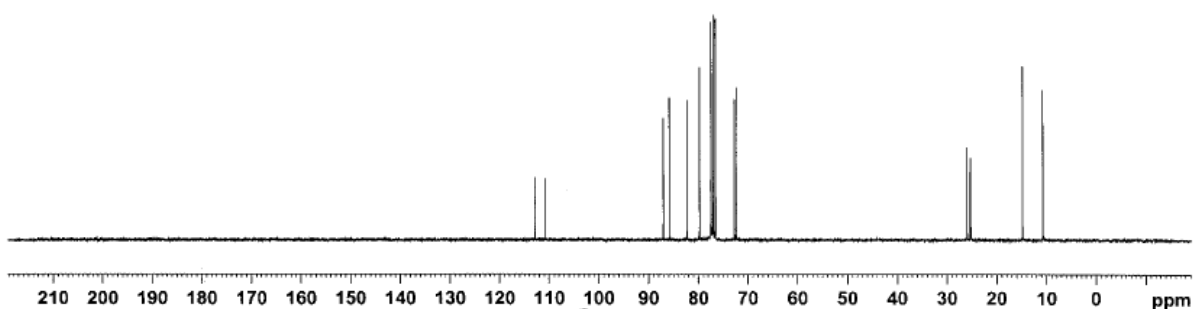
F2 - Processing parameters
SI 32768
SF 360.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40
```

Compound 5 (mixture of isomers)

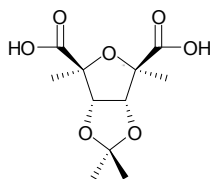
```
Current Data Parameters
NAME 49-09-03164009
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090217
Time 2:01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
RG 327.00
SOLVENT CDCl3
NS 2
DS 2
SWH 4844.801 Hz
FIDRES 0.147856 Hz
AQ 1.2817771 sec
RG 361.9
AQ 163.260 usec
SE 8.00 usec
TE 300.2 K
SI 1.0260700 sec
***** CHANNEL F1 *****
NUC1 13C
P1 4.70 usec
PL1 -2.50 dB
RFCL 100.625460 MHz
F2 - Processing parameters
SI 32768
SF 100.625016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



```
Current Data Parameters
NAME 49-09-03164009
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090217
Time 2:01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
RG 327.00
SOLVENT CDCl3
NS 2
DS 2
SWH 4844.801 Hz
FIDRES 0.147856 Hz
AQ 1.2817771 sec
RG 361.9
AQ 163.260 usec
SE 8.00 usec
TE 300.2 K
SI 1.0260700 sec
***** CHANNEL F1 *****
NUC1 13C
P1 4.70 usec
PL1 -2.50 dB
RFCL 100.625460 MHz
F2 - Processing parameters
SI 32768
SF 100.625016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```



Compound 6



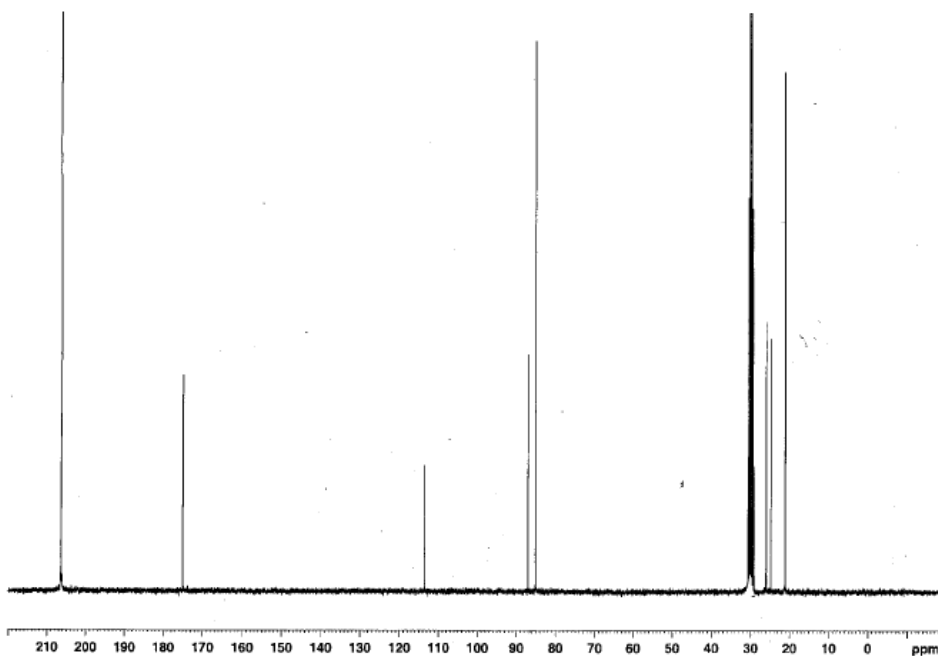
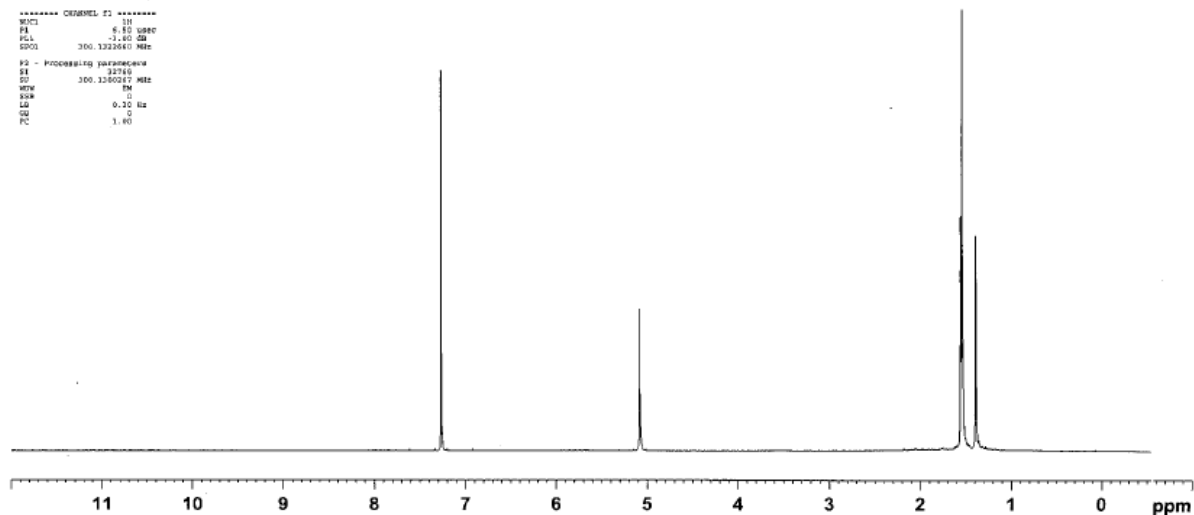
```

Current Data Parameters
NAME 32-cp-01201015
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080210
Time 12.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT ACETONE
NS 2
DS 2
SWH 4844.814 Hz
FIDRES 0.147050 Hz
AQ 0.0417070 sec
RG 1280.0
DM 103.090 usec
DE 6.80 usec
TE 300.2 K
DQ 1.0000000 sec

***** CHANNEL F1 *****
NUC1 13C
P1 6.80 usec
PL1 -1.80 dB
SFO1 100.1252660 MHz

F2 - Processing parameters
SI 32768
SF 100.1252660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.80
    
```



```

Current Data Parameters
NAME 32-cp-01201008
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080229
Time 4.22
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 4
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2896.0
DM 27.890 usec
DE 6.90 usec
TE 300.2 K
DQ 1.0000000 sec
SFO1 100.6261260 MHz
SFO2 75.4752853 MHz

***** CHANNEL F1 *****
NUC1 13C
P1 6.70 usec
PL1 -2.00 dB
SFO1 75.4752853 MHz

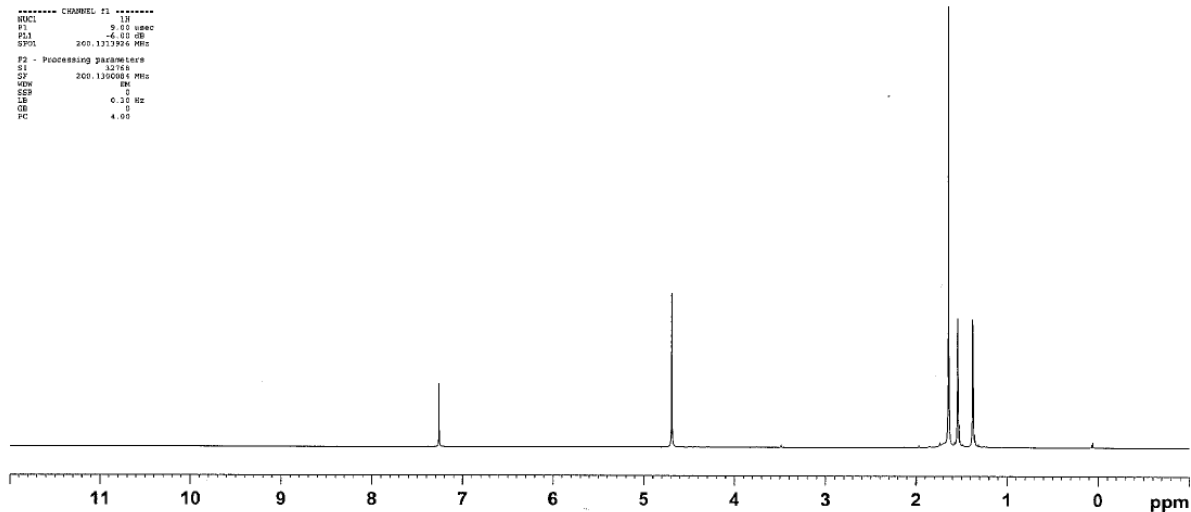
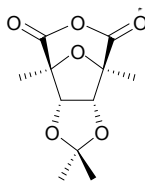
***** CHANNEL F2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL1 0.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 300.1311000 MHz

F2 - Processing parameters
SI 32768
SF 75.4676811 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

Compound 7

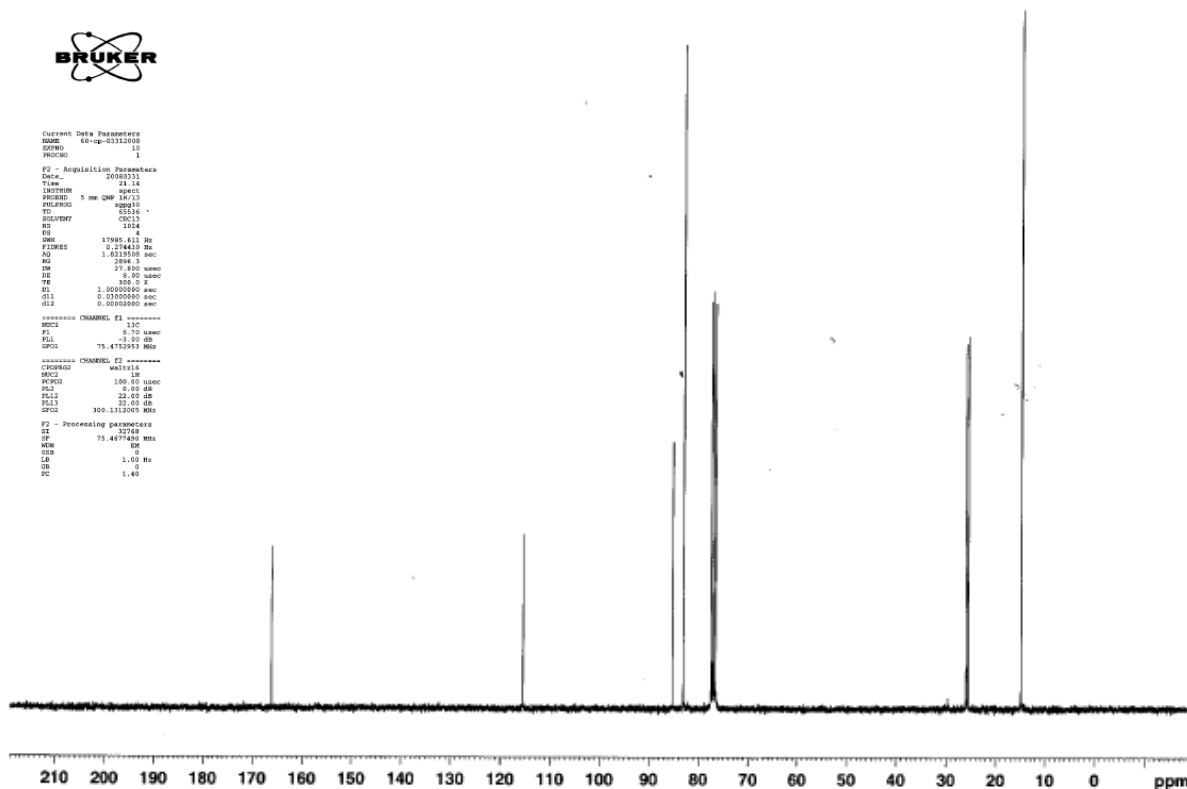
```

Current Data Parameters
NAME 11-cp-05042009
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090504
Time 17:55
INSTRUM spect
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2
DS 2
SWH 3221.649 Hz
FIDRES 0.000589 Hz
AQ 10.1712170 sec
RG 312.2
AQ 155.200 usec
DE 16.00 usec
TE 296.2 K
SI 1.0000000 sec
TEU 1
    
```



```

Current Data Parameters
NAME 08-cp-03112008
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080331
Time 21:14
INSTRUM spect
PROBHD 5 mm QNP 1H/29
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 17985.413 Hz
FIDRES 0.274430 Hz
AQ 1.6110100 sec
RG 2854.3
AQ 77.100 usec
DE 8.00 usec
TE 300.2 K
SI 1.0000000 sec
d11 0.0300000 sec
d12 0.0000000 sec
    
```



Compound 8

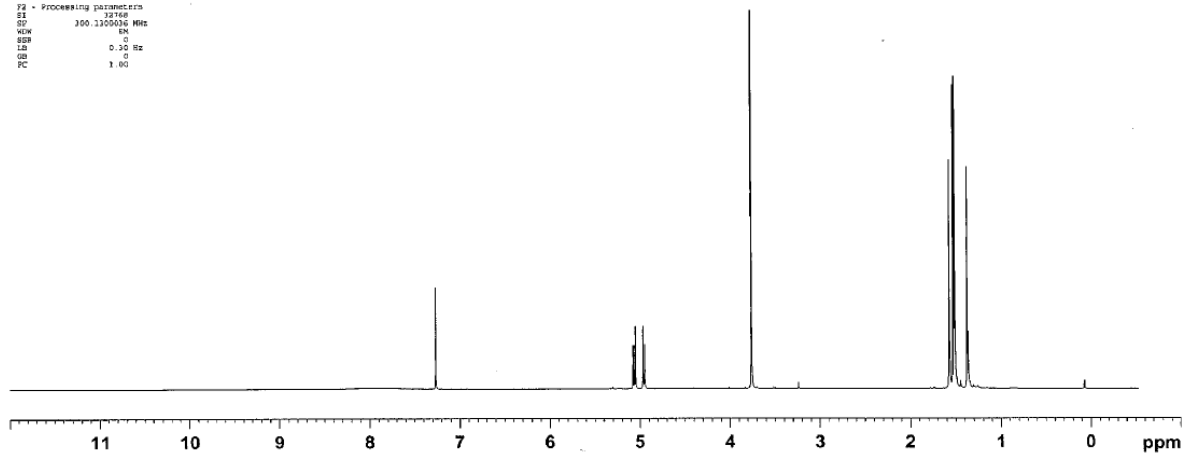
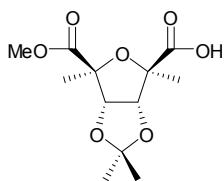
```

Current Data Parameters
NAME 42-cp-05102008
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080311
Time 8:42
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4944.961 Hz
FIDRES 0.149506 Hz
AQ 3.3817077 sec
RG 300
SQ 103.200 uS
RG 300
TE 300.2 K
SI 1.00000000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 6.70 uS
PL1 -3.90 dB
SFO1 300.322660 MHz

F2 - Processing parameters
SI 32768
SF 300.320016 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
    
```



```

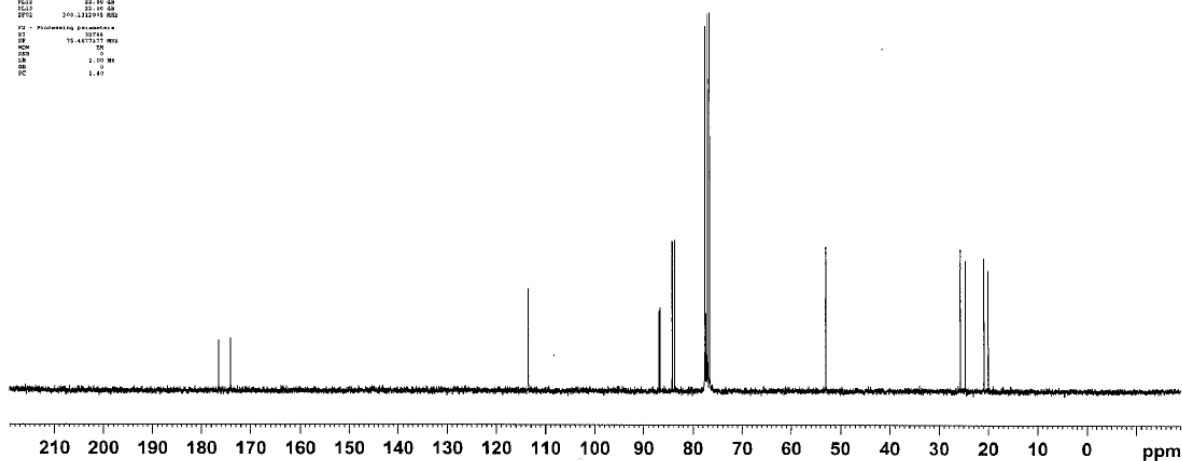
Current Data Parameters
NAME 42-cp-05102008
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080311
Time 8:42
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 12744.11 Hz
FIDRES 1.274519 Hz
AQ 3.3817077 sec
RG 300
SQ 27.440 uS
RG 300
TE 300.2 K
SI 1.00000000 sec
SFO1 127.485126 MHz

***** CHANNEL f1 *****
NUC1 13C
P1 6.70 uS
PL1 -3.90 dB
SFO1 127.485126 MHz

***** CHANNEL f2 *****
PULPROG waltz16
NUC2 13C
P2 10.00 uS
PL2 0.00 dB
SFO2 101.625126 MHz

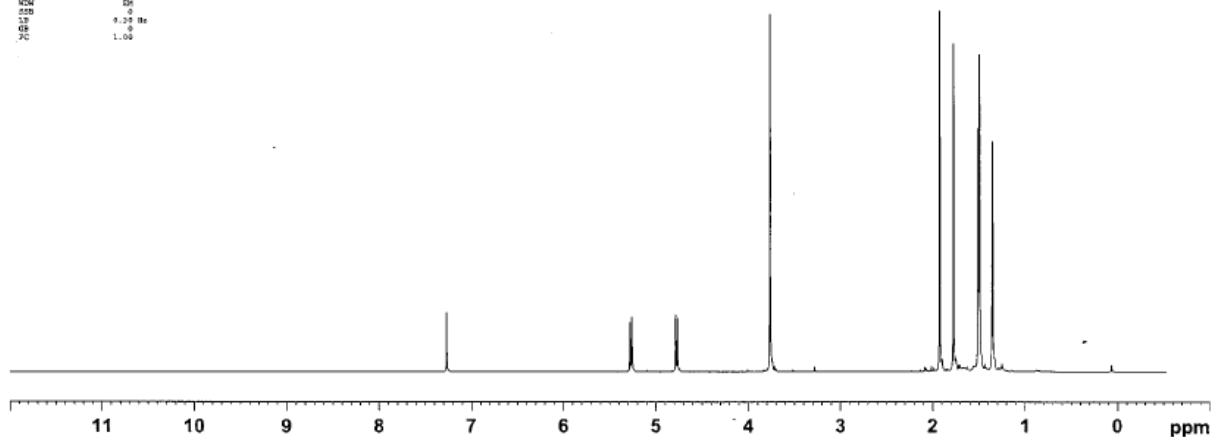
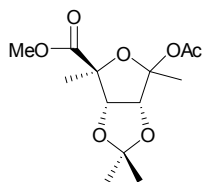
F2 - Processing parameters
SI 32768
SF 127.487317 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
    
```



Compound 9

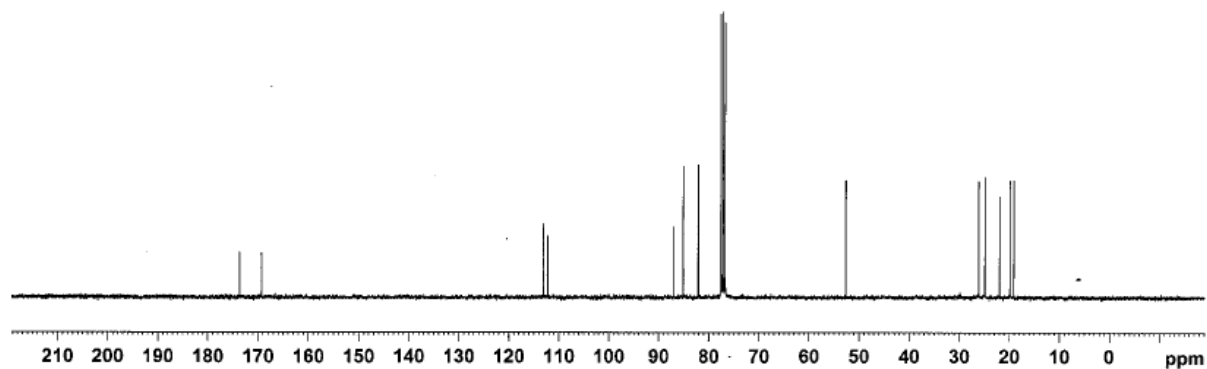
```

Current Data Parameters
NAME: 14-cp-12012806
EXPNO: 1
PROCNO: 1
PROCPS: 1
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
AQ: 0.147856 sec
RG: 326
SI: 103.200 MHz
SF: 500.136 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00
===== CHANNEL f1 =====
NUC1: 13C
P1: 6.00 usec
PL1: -2.00 dB
SFO1: 100.628360 MHz
F2 - Processing parameters
SI: 32768
SF: 100.628360 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00
    
```



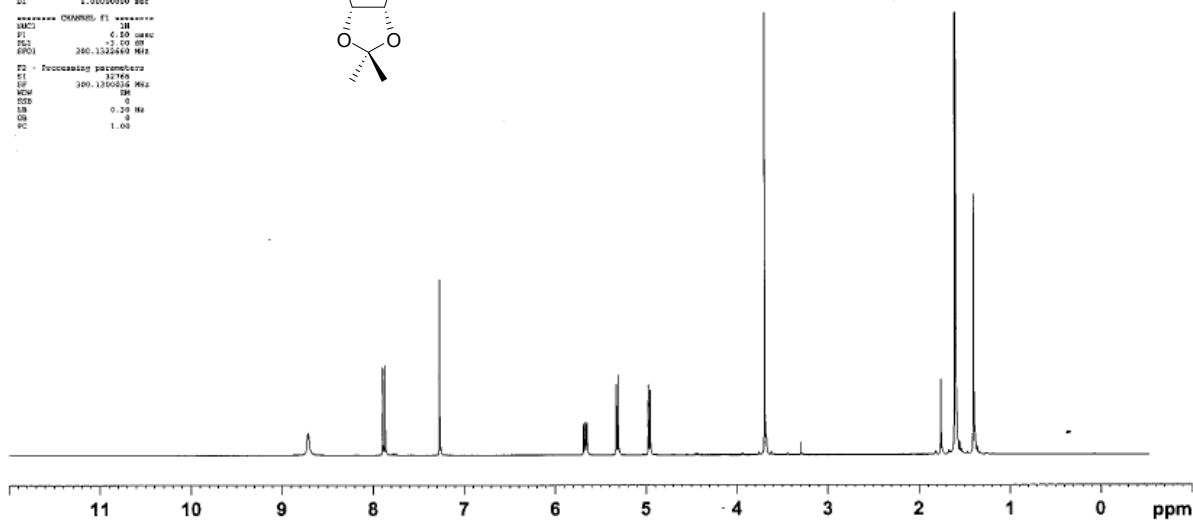
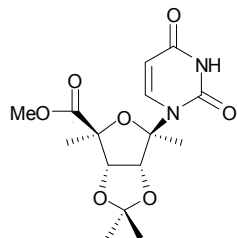
```

Current Data Parameters
NAME: 14-cp-12012810
EXPNO: 1
PROCNO: 1
PROCPS: 1
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
AQ: 0.147856 sec
RG: 326
SI: 103.200 MHz
SF: 500.136 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00
===== CHANNEL f1 =====
NUC1: 13C
P1: 6.00 usec
PL1: -2.00 dB
SFO1: 100.628360 MHz
F2 - Processing parameters
SI: 32768
SF: 100.628360 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.00
    
```

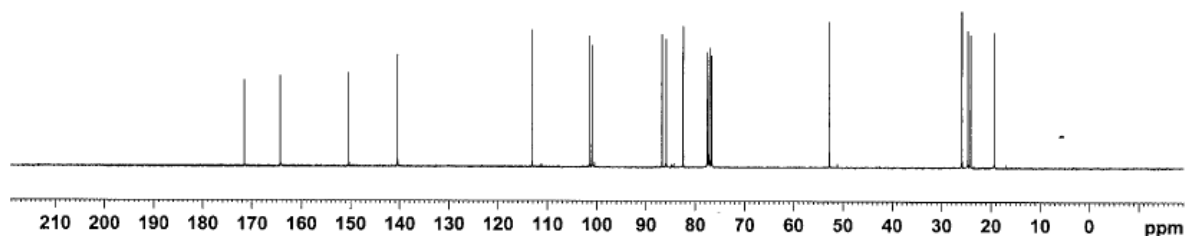


Compound 10

```
===== CHANNEL F1 =====  
NAME 45-01010101  
PROCNO 1  
F2 - Acquisition Parameters  
DATE_ 20090218  
TIME 11.18  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 4044.861 Hz  
FIDRES 0.147656 Hz  
AQ 1.1817077 sec  
RG 456.1  
CFW 100.2500 MHz  
CQ 8.50 MHz  
TE 300.0 K  
D1 1.01000000 sec  
===== CHANNEL F2 =====  
NAME 13  
P1 0.50 MHz  
P2 1.00 MHz  
SFO1 360.1325460 MHz  
F2 - Processing parameters  
SI 32768  
SF 360.1325460 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 1.00
```



```
===== CHANNEL F1 =====  
NAME 45-01010101  
PROCNO 1  
F2 - Acquisition Parameters  
DATE_ 20090218  
TIME 11.18  
INSTRUM spect  
PROBHD 5 mm QNP 1H/13  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 4  
SWH 4044.861 Hz  
FIDRES 0.147656 Hz  
AQ 1.1817077 sec  
RG 456.1  
CFW 100.2500 MHz  
CQ 8.50 MHz  
TE 300.0 K  
D1 1.01000000 sec  
===== CHANNEL F2 =====  
NAME 13  
P1 0.50 MHz  
P2 1.00 MHz  
SFO1 360.1325460 MHz  
F2 - Processing parameters  
SI 32768  
SF 360.1325460 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 1.00
```



Compound 11

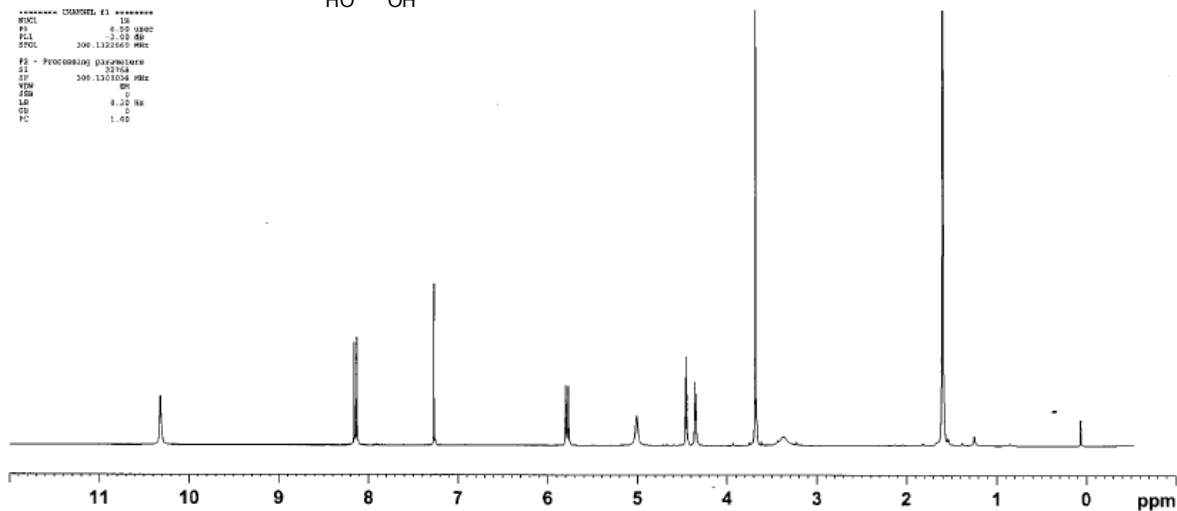
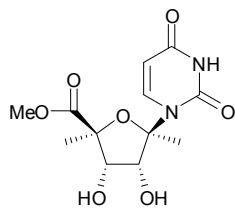
```

Current Data Parameters
NAME  11-11-111111
EXPNO  1
PROCNO  1

F2 - Acquisition Parameters
Date_  20090311
Time  13.25
INSTRUM  spect
PROBHD  5 mm QNP 1H/13
PULPROG  zgpg30
TD  65536
SOLVENT  CDCl3
NS  16
DS  2
SWH  4004.965 Hz
FIDRES  0.147866 Hz
AQ  3.2817077 sec
RG  256
DE  103.208 (kHz)
TE  300.2 K
PC  350.0 K
SI  1.5000000 sec

===== CHANNEL f1 =====
NUC1  13
P1  4.100 usec
PL1  -2.00 dB
SFO1  100.628360 MHz

F2 - Processing parameters
SI  65536
SF  100.628360 MHz
WDW  EM
SSB  0
LB  8.00 Hz
GB  0
PC  1.00
    
```



```

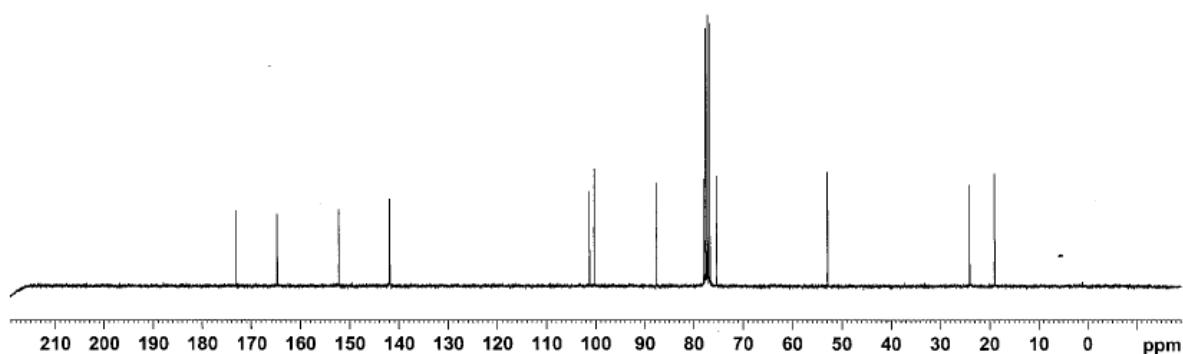
Current Data Parameters
NAME  11-11-111111
EXPNO  1
PROCNO  1

F1 - Acquisition Parameters
Date_  20090311
Time  4.45
INSTRUM  spect
PROBHD  5 mm QNP 1H/13
PULPROG  zgpg30
TD  65536
SOLVENT  CDCl3
NS  16
DS  2
SWH  17981.111 Hz
FIDRES  0.274411 Hz
AQ  3.2817077 sec
RG  256
DE  103.208 (kHz)
TE  300.2 K
PC  350.0 K
SI  1.5000000 sec

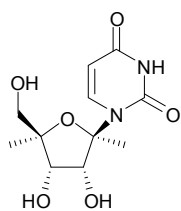
===== CHANNEL f1 =====
NUC1  13
P1  4.100 usec
PL1  -2.00 dB
SFO1  100.628360 MHz

===== CHANNEL f2 =====
NAME  13
EXPNO  1
PROCNO  1
PULPROG  zgpg30
TD  65536
SOLVENT  CDCl3
NS  16
DS  2
SWH  17981.111 Hz
FIDRES  0.274411 Hz
AQ  3.2817077 sec
RG  256
DE  103.208 (kHz)
TE  300.2 K
PC  350.0 K
SI  1.5000000 sec

===== CHANNEL f3 =====
NAME  13
EXPNO  1
PROCNO  1
PULPROG  zgpg30
TD  65536
SOLVENT  CDCl3
NS  16
DS  2
SWH  17981.111 Hz
FIDRES  0.274411 Hz
AQ  3.2817077 sec
RG  256
DE  103.208 (kHz)
TE  300.2 K
PC  350.0 K
SI  1.5000000 sec
    
```

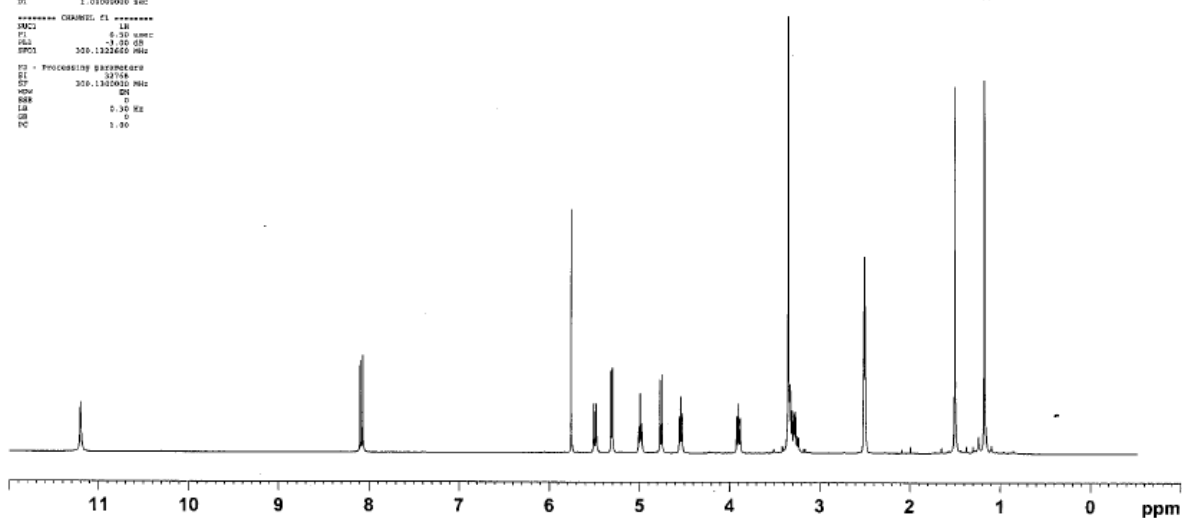
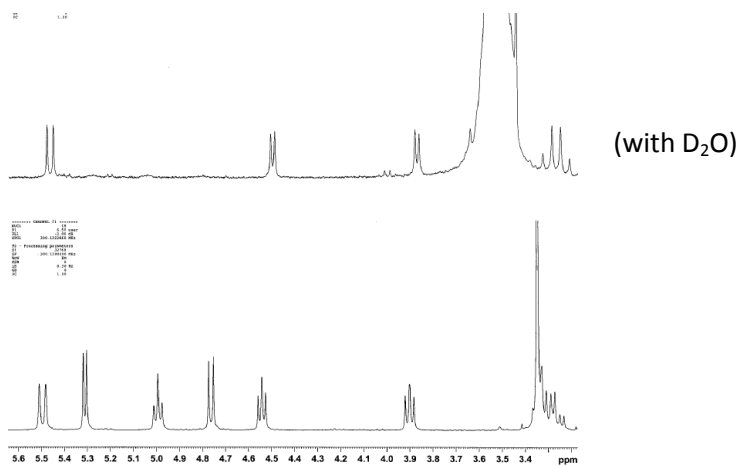


Compound 12



```

===== Data Parameters =====
NAME: 12-12-12-12-12-12
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20090110
Time : 14.32
INSTRUM : spect
PROBHD : 5 mm QNP 1H/13
PULPROG : zgpg30
TD : 32768
SOLVENT : DMSO
DS : 4
AQ : 0.88486570
FIDRES : 0.147864 Hz
AQ : 2.3217074 sec
RG : 406.4
WDW : EM
SSB : 0
LB : 100.000000
GB : 0
PC : 1.01000000 sec
===== CHANNEL f1 =====
NUC1 : 13
P1 : 0.30 sec
PL1 : -1.00 dB
SFO1 : 300.1320000 MHz
F2 - Processing parameters
SI : 32768
SF : 300.1320000 MHz
WDW : EM
SSB : 0
LB : 0.30 Hz
GB : 0
PC : 1.00
    
```



```

===== Data Parameters =====
NAME: 12-12-12-12-12-12
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ : 20090110
Time : 14.32
INSTRUM : spect
PROBHD : 5 mm QNP 1H/13
PULPROG : zgpg30
TD : 32768
SOLVENT : DMSO
DS : 4
AQ : 0.88486570
FIDRES : 0.147864 Hz
AQ : 2.3217074 sec
RG : 406.4
WDW : EM
SSB : 0
LB : 100.000000
GB : 0
PC : 1.01000000 sec
===== CHANNEL f1 =====
NUC1 : 13
P1 : 0.30 sec
PL1 : -1.00 dB
SFO1 : 300.1320000 MHz
F2 - Processing parameters
SI : 32768
SF : 300.1320000 MHz
WDW : EM
SSB : 0
LB : 0.30 Hz
GB : 0
PC : 1.00
    
```

