Supporting Information for

Fluoride-assisted Regioselective Conversion of Functionalized Furans to α -Substituted γ -Hydroxybutenolides using Singlet Oxygen

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7.38
7.37
7.37
7.25
6.35
6.30
5.87
5.51
5.50
3.76
3.07
3.06
1.64

Current Data Parameters
NAME Copy of snp-d-86-a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060809
Time_ 19.37
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 2
DS 0
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 181
DW 83.400 use
DE 20.00 use
TE 295.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 use
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 65536
SF 399.9000145 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME Copy of snp-d-86-a
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060809
Time_ 19.52
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 237
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 10321.3
DW 19.900 usec
DE 20.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548909 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1.22
1.23
1.24
1.26
1.28
1.30
1.33
 3.12
4.19
4.21
4.22
4.24
5.50
5.84
5.85
5.85
5.85
6.29
6.29
6.35
6.35
6.35
6.35
6.35
6.35
6.36
6.36
7.25
7.37
7.37
7.37
7.37
7.37
7.38
7.38
7.38
7.38
7.39

Current Data Parameters
 NAME Copy of snp-d-86-b
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060809
 Time_ 18.07
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 CDC13
 NS 128
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.091480 Hz
 AQ 5.4657526 sec
 RG 181
 DW 83.400 usec
 DE 20.00 usec
 TE 296.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 0.00 dB
 SFO1 399.9023994 MHz

F2 - Processing parameters
 SI 65536
 SF 399.9000141 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

```

Current Data Parameters
NAME      Copy of snp-d-86-t
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20060809
Time_     18.27
INSTRUM   spect
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg
TD         66560
SOLVENT   CDCl3
NS         395
DS         2
SWH        25125.629 Hz
FIDRES     0.377488 Hz
AQ         1.3245940 sec
RG         3649.1
DW         19.900 use
DE         20.00 use
TE         296.2 K
D1         2.0000000 sec
d11        0.0300000 sec
MCREST    0.0000000 sec
MCWRK     0.0150000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         11.00 use
PL1        0.00 dB
SF01       100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      100.00 use
PL2        0.00 dB
PL12       20.70 dB
PL13       24.00 dB
SF02       399.9015996 MHz

F2 - Processing parameters
SI         32768
SF         100.5548892 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

7.39
7.38
7.38
7.26
7.26
6.36
6.36
6.36
6.30
5.86
5.85
5.52
5.50
4.19
4.17
4.15
3.10
3.10
3.09
3.09
1.67
1.66
1.66
1.64
1.62
1.60
1.41
1.40
1.38
1.36
1.34
0.95
0.93
0.91

Current Data Parameters
 NAME Copy of snp-d-86-e
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060809
 Time 18.39
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.091480 Hz
 AQ 5.4657526 sec
 RG 181
 DW 83.400 usec
 DE 20.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 0.00 dB
 SFO1 399.9023994 MHz

F2 - Processing parameters
 SI 65536
 SF 399.9000107 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME Copy of snp-d-86-e
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060809
 Time 19.34
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 66560
 SOLVENT CDCl3
 NS 986
 DS 2
 SWH 25125.629 Hz
 FIDRES 0.377488 Hz
 AQ 1.3245940 sec
 RG 3649.1
 DW 19.900 usec
 DE 20.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 100.5659560 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 20.70 dB
 PL13 24.00 dB
 SFO2 399.9015996 MHz

F2 - Processing parameters
 SI 32768
 SF 100.5548886 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

7.38
7.38
7.38
7.37
7.26
7.26
7.26
6.36
6.36
6.36
6.30
6.30
6.29
5.86
5.85
5.85
5.85
5.85
5.50
4.17
4.15
4.13
3.64
3.63
3.61
3.13
3.11
1.66
1.64
1.62
1.62
1.61
1.57
1.55
1.54
1.26
0.89
0.88
0.88
0.86

3d

Current Data Parameters
 NAME snp-d-86-fp
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061216
 Time 15.50
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 181
 DW 83.400 usec
 DE 20.00 usec
 TE 298.2 K
 D1 2.0000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 0.00 dB
 SFO1 399.9023994 MHz

F2 - Processing parameters
 SI 32768
 SF 399.9000111 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00


```

Current Data Parameters
NAME      snp-d-86-fp
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20061216
Time_     16.39
INSTRUM   spect
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg
TD         66560
SOLVENT   CDCl3
NS         803
DS         2
SWH        25125.629 Hz
FIDRES     0.377488 Hz
AQ         1.3245940 sec
RG         3649.1
DW         19.900 usec
DE         20.00 usec
TE         298.2 K
D1         2.00000000 sec
d11        0.03000000 sec
MCREST    0.00000000 sec
MCWRK     0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         11.00 usec
PL1        0.00 dB
SFO1       100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      100.00 usec
PL2        0.00 dB
PL12       20.70 dB
PL13       24.00 dB
SFO2       399.9015996 MHz

F2 - Processing parameters
SI         32768
SF         100.5548879 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

```

7.41
7.41
7.41
7.41
7.41
7.41
7.41
7.39
7.39
7.39
7.39
7.26
6.40
6.39
6.38
6.37
6.37
6.37
6.37
6.37
6.37
5.95
5.95
5.95
5.95
5.95
5.55
4.44
4.42
4.42
4.42
4.41
3.72
3.71
3.70
3.69

3e

Current Data Parameters
NAME snp-d-55
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060530
Time 13.15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 256
DW 83.400 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 65536
SF 399.9000114 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME snp-d-55
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060530
Time_ 13.49
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 654
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 8192
DW 19.900 use
DE 20.00 use
TE 298.2 K
D1 2.0000000 sec
d11 0.0300000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 use
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 use
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548874 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Current Data Parameters	
NAME	snp-d-54b
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters	
Date_	20060602
Time_	10.53
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	5995.204 Hz
FIDRES	0.091480 Hz
AQ	5.4657526 sec
RG	812.7
DW	83.400 usec
DE	20.00 usec
TE	298.2 K
D1	2.0000000 sec
MCREST	0.0000000 sec
MCWRK	0.01500000 sec

```
===== CHANNEL f1 =====
NUC1      1H
P1        10.80 usec
PL1       0.00 dB
SF01      399.9023994 MHz
```

F2 - Processing parameters	
SI	6536
SE	399.900117 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

Current Data Parameters
NAME snp-d-54b
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060602
Time 11.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 365
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 13004
DW 19.900 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548873 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7.37
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.31
7.30
7.29
7.28
7.26
7.25
6.36
6.36
6.36
6.36
6.36
6.35
6.35
6.35
6.35
6.35
5.90
5.90
5.90
5.90
5.90
5.54
5.20
4.70

3g

S14

Current Data Parameters
NAME Copy (3) of snp-d-86-c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060810
Time_ 14.39
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 512
DW 83.400 usec
DE 20.00 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 10.80 usec
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters

SI 32768
SF 399.9000132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME Copy (3) of snp-d-86-c
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060810
Time_ 17.46
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 950
DS 4
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 18390.4
DW 19.900 usec
DE 20.00 usec
TE 296.2 K
D1 3.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters

SI 32768
SF 100.5548889 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

Current Data Parameters
NAME snp-d-63a-7
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060602
Time_ 15.44
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 181
DW 83.400 use
DE 20.00 use
TE 298.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 use
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 32768
SF 399.9000113 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME snp-d-54b
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060602
Time_ 11.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 365
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 13004
DW 19.900 use
DE 20.00 use
TE 298.2 K
D1 2.0000000 sec
d11 0.0300000 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 use
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 use
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548873 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7.26
7.12
7.12
7.12
7.12
6.45
6.45
6.42
6.13
6.08
6.04
5.36
5.32

H_{8b}5a

H_{8b}4a

3.79
3.77

Current Data Parameters
NAME snp-e-20-all
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070221
Time_ 14.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDC13
NS 50
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 20.2
DW 83.400 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters

SI 32768
SF 399.9000107 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

S18

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7.12

6.43

6.14
6.05

5.33

3.79

Current Data Parameters
NAME snp-e-20-Single isomer
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070224
Time 21.50
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 256
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 71.8
DW 83.400 usec
DE 20.00 usec
TE 296.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 10.80 usec
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters

SI 32768
SF 399.9000108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME snp-e-20-fp-single
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070228
 Time_ 19.35
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 66560
 SOLVENT CDCl3
 NS 4083
 DS 2
 SWH 25125.629 Hz
 FIDRES 0.377488 Hz
 AQ 1.3245940 sec
 RG 10321.3
 DW 19.900 usec
 DE 20.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.30 usec
 PL1 0.00 dB
 SFO1 100.5659560 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 20.70 dB
 PL13 24.00 dB
 SFO2 399.9015996 MHz

F2 - Processing parameters
 SI 32768
 SF 100.554883 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1.224
 1.229
 1.30
 1.30
 1.31
 1.32
 1.32
 2.07
 4.19
 4.21
 4.23
 4.25
 5.31
 6.03
 6.12
 6.42
 7.11
 7.26

Current Data Parameters
 NAME snp-e-25fp single
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070228
 Time 22.49
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 114
 DW 83.400 usec
 DE 20.00 usec
 TE 293.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 0.00 dB
 SFO1 399.9023994 MHz

F2 - Processing parameters
 SI 32768
 SF 399.9000112 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Current Data Parameters
NAME snp-e-25fp single
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070303
Time 0.11
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 5120
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 5792.6
DW 19.900 usec
DE 20.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.30 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170.74
166.45
146.62
138.60
138.14
137.94
128.77
128.51
97.80
77.82
77.50
77.18
66.51
66.38
61.96
14.52

6.45 6.40 ppm

Current Data Parameters
 NAME snp-d-133-p
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061104
 Time 11.56
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 128
 DS 2
 SWH 3881.988 Hz
 FIDRES 0.118469 Hz
 AQ 4.2205682 sec
 RG 80.6
 DW 128.800 usec
 DE 20.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 0.00 dB
 SFO1 399.9020183 MHz

F2 - Processing parameters
 SI 32768
 SF 399.9000121 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

```

Current Data Parameters
NAME      snp-d-133-p
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20061104
Time_     14.30
INSTRUM   spect
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg
TD         66560
SOLVENT   CDCl3
NS         2779
DS         2
SWH        25125.629 Hz
FIDRES     0.377488 Hz
AQ         1.3245940 sec
RG          3649.1
DW          19.900 use
DE          20.00 use
TE         298.2 K
D1          2.0000000 sec
d11         0.0300000 sec
MCREST     0.0000000 sec
MCWRK      0.0150000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         11.00 use
PL1        0.00 dB
SFO1       100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      100.00 use
PL2         0.00 dB
PL12       20.70 dB
PL13       24.00 dB
SFO2       399.9015996 MHz

F2 - Processing parameters
SI          32768
SF         100.5548878 MHz
WDW         no
SSB         0
LB          0.00 Hz
GB          0
PC          1.40

```

H_{8b}5d **H_{8b}4d**

Current Data Parameters
NAME snp-d-165-l-2c-4
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061218
Time 21.26
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 128
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 181
DW 83.400 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 32768
SF 399.9000110 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME snp-d-165-L-2c-4
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061219
Time_ 6.02
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 9216
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 9195.2
DW 19.900 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548863 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

7.12
7.12
7.11
6.51
6.16
6.10
6.10
6.10
5.36
4.46
4.45
4.44
4.44
4.43
4.42
3.75
3.73
3.72

Current Data Parameters
NAME snp-d-138-p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061110
Time_ 19.31
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 512
DW 83.400 use
DE 20.00 use
TE 298.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 use
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 65536
SF 399.9000117 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

7.12
 7.12
 7.12
 6.51
 6.16
 6.10
 5.36
 4.46
 4.45
 4.45
 4.44
 4.43
 4.43
 3.75
 3.73
 3.72

Current Data Parameters
 NAME snp-d-138-pp
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061110
 Time 19.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 CDC13
 NS 16
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.091480 Hz
 AQ 5.4657526 sec
 RG 512
 DW 83.400 usec
 DE 20.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 0.00 dB
 SFO1 399.9023994 MHz

F2 - Processing parameters
 SI 65536
 SF 399.9000117 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

Current Data Parameters

NAME snp-d-138-pp
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061111
Time_ 6.35
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 10240
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 6502
DW 19.900 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====

NUC1 13C
P1 11.00 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters

SI 32768
SF 100.5548868 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

H_{8a},4f

Current Data Parameters
NAME snp-d-137-nmr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061109
Time_ 18.09
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 2
DS 0
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 181
DW 83.400 use
DE 20.00 use
TE 298.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 use
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 65536
SF 399.9000112 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME snp-e-31-p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters	
Date_	20070311
Time	19.30
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	0
SWH	5995.204 Hz
FIDRES	0.091480 Hz
AQ	5.4657526 sec
RG	406.4
DW	83.400 use
DE	20.00 use
TE	298.2 K
D1	2.0000000 sec
MCREST	0.0000000 sec
MCWRK	0.0150000 sec

7.36
7.35
7.34
7.26
7.25
7.02
6.46
6.05
6.03
5.33
5.20
5.19
5.18

6.6 6.5 6.4 ppm

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

5.94
1.00
1.08
2.16
1.04
2.12

Current Data Parameters
NAME snp-e-19 -all-2d
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070228
Time_ 22.52
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDC13
NS 2
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 114
DW 83.400 use
DE 20.00 use
TE 293.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.80 use
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 32768
SF 399.9000132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME snp-e-19all
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070301
Time_ 8.23
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 3072
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 7298.2
DW 19.900 usec
DE 20.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 12.30 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548950 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Ratio: 25 : 1

Current Data Parameters
NAME snp-e-29-mixHRMS
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070306
Time 21.09
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.091480 Hz
AQ 5.4657526 sec
RG 724.1
DW 83.400 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 65536
SF 399.9000132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME snp-d-77-5
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060718
 Time 14.25
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 66560
 SOLVENT CDCl3
 NS 326
 DS 2
 SWH 25125.629 Hz
 FIDRES 0.377488 Hz
 AQ 1.3245940 sec
 RG 4096
 DW 19.900 usec
 DE 20.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 100.5659560 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 20.70 dB
 PL13 24.00 dB
 SFO2 399.9015996 MHz

F2 - Processing parameters
 SI 32768
 SF 100.5548923 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

7.42
7.41
7.41
7.41
7.41
7.41
7.37
7.37
7.37
7.36
7.26
6.66
6.38
6.38
6.37
6.37
6.36
5.93
5.93
5.93
5.92

3.75
2.10

7

Current Data Parameters
NAME snp-d-144-6
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061201
Time_ 10.02
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 90.5
DW 83.400 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 10.80 usec
PL1 0.00 dB
SFO1 399.9023994 MHz

F2 - Processing parameters
SI 32768
SF 399.9000114 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME snp-d-144-6
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061201
Time 11.00
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 1024
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 8192
DW 19.900 usec
DE 20.00 usec
TE 298.2 K
D1 2.0000000 sec
d11 0.0300000 sec
MCREST 0.0000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548872 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7

6.51
6.30
6.14
6.09
6.03

3.76
2.11

Current Data Parameters
NAME snp-d-153-3-
EXPNO
PROCNO

F2 - Acquisition Parameters
Date_ 200611
Time_ 16

INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1

DS 4
SWH 5995.173
FIDRES 0.091300
AQ 5.465700
RG 327.680
DE 20.000
TE 298.15

D1 2.000000
MCREST 0.000000
MCWRK 0.015000

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00
PL1 0.00
SFO1 399.902300

F2 - Processing parameters
SI 65536
SF 399.900000
WDW EM
SSB 0
LB 0.30
GB 0.00
PC 1

Current Data Parameters
NAME snp-d-153-3
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061202
Time_ 3.43
INSTRUM spect
PROBHD 5 mm TXI 1H/2H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 128
DS 0
SWH 8992.806 Hz
FIDRES 0.274439 Hz
AQ 1.8220063 sec
RG 181
DW 55.600 usec
DE 6.00 usec
TE 302.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SFO1 600.1821059 MHz

F2 - Processing parameters
SI 32768
SF 600.1800144 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

Current Data Parameters
NAME snp-d-153-3-FP
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061203
Time_ 12.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 66560
SOLVENT CDCl3
NS 3892
DS 2
SWH 25125.629 Hz
FIDRES 0.377488 Hz
AQ 1.3245940 sec
RG 14596.5
DW 19.900 usec
DE 20.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 0.00 dB
SFO1 100.5659560 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.70 dB
PL13 24.00 dB
SFO2 399.9015996 MHz

F2 - Processing parameters
SI 32768
SF 100.5548864 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

21.24

53.18

66.40

68.19

77.19

77.50

77.82

98.76

120.55

121.73

128.75

130.26

169.84