Novel synthesis, reactivity and stereochemistry of substituted 3-trifluoromethyl and 3- perfluoroalkyl 3-phenoxy-prop-2-enal.

Salem El Kharrat, Laurent Philippe^{}, Hubert Blancou.*

Organisation Moléculaire Evolution et Matériaux Fluorés
Université Montpellier II Place E. Bataillon
34095 Montpellier cedex 05
France.

*Tel: (33) 467144678, Fax: (33) 467631046

E-mail: philippe.laurent@univ-montp2.fr

Supporting Information II: list of contents

S2-S46: Copy of ^1H , ^{13}C , Cosy ^1H - ^1H or ^{13}C - ^1H and ^{19}F NMR spectrum of compounds: **4, 5, 6, 7** and **8a-8b**.

F2 - Acquisition Parameters
Date_ 20060226
Time 18.40
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT C6D6
NS 16
DS 2
SWH 4844.961 Hz
FIDRES 0.147856 Hz
AQ 3.381677 sec
RG 327.161
DW 103.200 usec
DE 8.00 usec
TE 300.0 K
D1 1.00000000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 6.50 usec
PL1 -3.00 dB
SFO1 300.1322660 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S2

Current Data Parameters
 NAME FED27-2006
 EXNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060227
 Time 14.02
 INSTRUM spect
 PROBD 5 mm QNP
 PULPROG zgpg30
 TD 65536
 SOLVENT C6D6
 NS 1024
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.27478 Hz
 AQ 1.8219508 sec
 RG 2896.3
 DW 27.800 usec
 DE 8.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 d12 0.00020000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 6.70 usec
 PL1 -3.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 wait216
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 22.00 dB
 PL13 22.00 dB
 SFO2 300.1312005 MHz

F2 - Processing Parameters
 SI 32768
 SF 75.4676627 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

F2 - Acquisition Parameters
Date_ 20060226
Time 18.44
INSTRUM spect
PROBHD 5 mm QNP
PULPROG zgpg30
TD 131072
SOLVENT CDCl3
DS 16
SWH 25062.656 Hz
FIDRES 0.191213 Hz
AQ 2.6149364 sec
RG 128.000
DE 1.5000000
TE 300.0 K
D1 5.0000000 sec
===== CHANNEL f1 =====
NUC1 19F
P2 9.50 usec
PL1 -6.00 dB
SFO1 282.3761038 MHz
F2 - Processing parameters
SI 65536
SF 282.4043400 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

cis + 7

2409.25
2408.25
2232.53
2230.59
2225.18
2222.02
2218.63
2216.85
2210.83
2208.32
2198.54
2196.24
2190.98
2189.78
2187.68
2184.33
2182.37
2179.84
2178.65
2177.16
2175.38
2175.92
2170.59
2168.86
2163.64
2162.03
2157.44
2155.91
2153.40
2145.52
2144.20
2142.89
2139.18
2136.99
2134.34
2130.81
2129.51
2128.40
2127.35
2125.65
2120.92
2120.40
2120.46
2118.46
2117.35
2114.94
2112.34
2110.69
2109.63
2108.85
2101.49
2100.18
2098.08
2096.60
2094.26
2092.98
2091.85
2087.85
2083.54
2082.30
2075.20
2073.71
2063.63
2062.18

(4) CD₃CN

9.0 8.5 8.0 7.5 7.0 6.5 6.0 ppm

S9

Current Data Parameters
NAME Mar18-2006
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060318
Time 18.15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
F1 32768
SOLVENT CDCl₃
NS 16
DS 2
SWH 4844.961 Hz
FIDRES 0.147856 Hz
AQ 3.3817077 sec
RG 103.228
DE 103.228 usec
TE 300.0 K
D1 1.00000000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 6.50 usec
PL1 -3.00 dB
SFO1 300.1322660 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Current Data Parameters
 NAME: 4010-2003
 EXNO: 3
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20031118
 Time: 19.10
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/13
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CD3CN
 NS: 512
 DS: 4
 SWH: 17985.611 Hz
 FIDRES: 0.277459 Hz
 AQ: 1.871158 sec
 RG: 116384
 DW: 27.800 usec
 DE: 8.00 usec
 TE: 300.0 K
 NUC1: 13C
 P1: 6.70 usec
 PL1: 13.40 usec
 PL12: -3.00 dB
 SFO1: 75.4752953 MHz

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 6.70 usec
 PL1: 13.40 usec
 PL12: -3.00 dB
 SFO1: 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2: waltz16
 NUC2: 1H
 P2: 8.50 usec
 PL2: 19.00 usec
 PL12: 100.00 usec
 PL12: 0.00 dB
 PL12: 22.00 dB
 SFO2: 300.1312005 MHz

F2 - Processing Parameters
 SI: 32768
 SF: 75.4677490 MHz
 WDW: EM
 SSB: 0
 GB: 0
 PC: 1.40

F2 - Acquisition Parameters
Date_ 20011112
Time 7.08
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT C6D6
NS 16
DS 484.961 Hz
SWH 0.147856 Hz
FIDRES 3.3817077 sec
AQ 512
RG 103.200 usec
DE 8.00 usec
TE 300.0 K
D1 1.0000000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 6.50 usec
PL1 -3.00 dB
SFO1 300.1322660 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EN
SSB 0
GB 0
PC 1.00

```

F2 - Acquisition Parameters
-----
Date_      Time_      20051110
Time_      18.09
INSTRUM    spect
PROBHD      5 mm QNP 1H/13
PULPROG     zgpg30
SOLVENT      DMSO-d6
NS           6526
DS           1024
SFS          4
===== CHANNEL f1 =====
NUC1         13C
P1           6.70 usec
PL1          -3.00 dB
SFO1         75.4752953 MHz
===== CHANNEL f2 =====
NUC2         1H
P2           100.00 usec
PL2          0.00 dB
SFO2         300.1324005 MHz
===== CHANNEL f3 =====
NUC3         1H
P3           100.00 usec
PL3          0.00 dB
SFO3         300.1324005 MHz
===== CHANNEL f4 =====
NUC4         1H
P4           100.00 usec
PL4          0.00 dB
SFO4         300.1324005 MHz
===== CHANNEL f5 =====
NUC5         1H
P5           100.00 usec
PL5          0.00 dB
SFO5         300.1324005 MHz
===== CHANNEL f6 =====
NUC6         1H
P6           100.00 usec
PL6          0.00 dB
SFO6         300.1324005 MHz
===== CHANNEL f7 =====
NUC7         1H
P7           100.00 usec
PL7          0.00 dB
SFO7         300.1324005 MHz
===== CHANNEL f8 =====
NUC8         1H
P8           100.00 usec
PL8          0.00 dB
SFO8         300.1324005 MHz
===== CHANNEL f9 =====
NUC9         1H
P9           100.00 usec
PL9          0.00 dB
SFO9         300.1324005 MHz
===== CHANNEL f10 =====
NUC10        1H
P10          100.00 usec
PL10         0.00 dB
SFO10        300.1324005 MHz
===== CHANNEL f11 =====
NUC11        1H
P11          100.00 usec
PL11         0.00 dB
SFO11        300.1324005 MHz
===== CHANNEL f12 =====
NUC12        1H
P12          100.00 usec
PL12         0.00 dB
SFO12        300.1324005 MHz
===== CHANNEL f13 =====
NUC13        1H
P13          100.00 usec
PL13         0.00 dB
SFO13        300.1324005 MHz
===== CHANNEL f14 =====
NUC14        1H
P14          100.00 usec
PL14         0.00 dB
SFO14        300.1324005 MHz
===== CHANNEL f15 =====
NUC15        1H
P15          100.00 usec
PL15         0.00 dB
SFO15        300.1324005 MHz
===== CHANNEL f16 =====
NUC16        1H
P16          100.00 usec
PL16         0.00 dB
SFO16        300.1324005 MHz
===== CHANNEL f17 =====
NUC17        1H
P17          100.00 usec
PL17         0.00 dB
SFO17        300.1324005 MHz
===== CHANNEL f18 =====
NUC18        1H
P18          100.00 usec
PL18         0.00 dB
SFO18        300.1324005 MHz
===== CHANNEL f19 =====
NUC19        1H
P19          100.00 usec
PL19         0.00 dB
SFO19        300.1324005 MHz
===== CHANNEL f20 =====
NUC20        1H
P20          100.00 usec
PL20         0.00 dB
SFO20        300.1324005 MHz
===== CHANNEL f21 =====
NUC21        1H
P21          100.00 usec
PL21         0.00 dB
SFO21        300.1324005 MHz
===== CHANNEL f22 =====
NUC22        1H
P22          100.00 usec
PL22         0.00 dB
SFO22        300.1324005 MHz
===== CHANNEL f23 =====
NUC23        1H
P23          100.00 usec
PL23         0.00 dB
SFO23        300.1324005 MHz
===== CHANNEL f24 =====
NUC24        1H
P24          100.00 usec
PL24         0.00 dB
SFO24        300.1324005 MHz
===== CHANNEL f25 =====
NUC25        1H
P25          100.00 usec
PL25         0.00 dB
SFO25        300.1324005 MHz
===== CHANNEL f26 =====
NUC26        1H
P26          100.00 usec
PL26         0.00 dB
SFO26        300.1324005 MHz
===== CHANNEL f27 =====
NUC27        1H
P27          100.00 usec
PL27         0.00 dB
SFO27        300.1324005 MHz
===== CHANNEL f28 =====
NUC28        1H
P28          100.00 usec
PL28         0.00 dB
SFO28        300.1324005 MHz
===== CHANNEL f29 =====
NUC29        1H
P29          100.00 usec
PL29         0.00 dB
SFO29        300.1324005 MHz
===== CHANNEL f30 =====
NUC30        1H
P30          100.00 usec
PL30         0.00 dB
SFO30        300.1324005 MHz
===== CHANNEL f31 =====
NUC31        1H
P31          100.00 usec
PL31         0.00 dB
SFO31        300.1324005 MHz
===== CHANNEL f32 =====
NUC32        1H
P32          100.00 usec
PL32         0.00 dB
SFO32        300.1324005 MHz
===== CHANNEL f33 =====
NUC33        1H
P33          100.00 usec
PL33         0.00 dB
SFO33        300.1324005 MHz
===== CHANNEL f34 =====
NUC34        1H
P34          100.00 usec
PL34         0.00 dB
SFO34        300.1324005 MHz
===== CHANNEL f35 =====
NUC35        1H
P35          100.00 usec
PL35         0.00 dB
SFO35        300.1324005 MHz
===== CHANNEL f36 =====
NUC36        1H
P36          100.00 usec
PL36         0.00 dB
SFO36        300.1324005 MHz
===== CHANNEL f37 =====
NUC37        1H
P37          100.00 usec
PL37         0.00 dB
SFO37        300.1324005 MHz
===== CHANNEL f38 =====
NUC38        1H
P38          100.00 usec
PL38         0.00 dB
SFO38        300.1324005 MHz
===== CHANNEL f39 =====
NUC39        1H
P39          100.00 usec
PL39         0.00 dB
SFO39        300.1324005 MHz
===== CHANNEL f40 =====
NUC40        1H
P40          100.00 usec
PL40         0.00 dB
SFO40        300.1324005 MHz
===== CHANNEL f41 =====
NUC41        1H
P41          100.00 usec
PL41         0.00 dB
SFO41        300.1324005 MHz
===== CHANNEL f42 =====
NUC42        1H
P42          100.00 usec
PL42         0.00 dB
SFO42        300.1324005 MHz
===== CHANNEL f43 =====
NUC43        1H
P43          100.00 usec
PL43         0.00 dB
SFO43        300.1324005 MHz
===== CHANNEL f44 =====
NUC44        1H
P44          100.00 usec
PL44         0.00 dB
SFO44        300.1324005 MHz
===== CHANNEL f45 =====
NUC45        1H
P45          100.00 usec
PL45         0.00 dB
SFO45        300.1324005 MHz
===== CHANNEL f46 =====
NUC46        1H
P46          100.00 usec
PL46         0.00 dB
SFO46        300.1324005 MHz
===== CHANNEL f47 =====
NUC47        1H
P47          100.00 usec
PL47         0.00 dB
SFO47        300.1324005 MHz
===== CHANNEL f48 =====
NUC48        1H
P48          100.00 usec
PL48         0.00 dB
SFO48        300.1324005 MHz
===== CHANNEL f49 =====
NUC49        1H
P49          100.00 usec
PL49         0.00 dB
SFO49        300.1324005 MHz
===== CHANNEL f50 =====
NUC50        1H
P50          100.00 usec
PL50         0.00 dB
SFO50        300.1324005 MHz
===== CHANNEL f51 =====
NUC51        1H
P51          100.00 usec
PL51         0.00 dB
SFO51        300.1324005 MHz
===== CHANNEL f52 =====
NUC52        1H
P52          100.00 usec
PL52         0.00 dB
SFO52        300.1324005 MHz
===== CHANNEL f53 =====
NUC53        1H
P53          100.00 usec
PL53         0.00 dB
SFO53        300.1324005 MHz
===== CHANNEL f54 =====
NUC54        1H
P54          100.00 usec
PL54         0.00 dB
SFO54        300.1324005 MHz
===== CHANNEL f55 =====
NUC55        1H
P55          100.00 usec
PL55         0.00 dB
SFO55        300.1324005 MHz
===== CHANNEL f56 =====
NUC56        1H
P56          100.00 usec
PL56         0.00 dB
SFO56        300.1324005 MHz
===== CHANNEL f57 =====
NUC57        1H
P57          100.00 usec
PL57         0.00 dB
SFO57        300.1324005 MHz
===== CHANNEL f58 =====
NUC58        1H
P58          100.00 usec
PL58         0.00 dB
SFO58        300.1324005 MHz
===== CHANNEL f59 =====
NUC59        1H
P59          100.00 usec
PL59         0.00 dB
SFO59        300.1324005 MHz
===== CHANNEL f60 =====
NUC60        1H
P60          100.00 usec
PL60         0.00 dB
SFO60        300.1324005 MHz
===== CHANNEL f61 =====
NUC61        1H
P61          100.00 usec
PL61         0.00 dB
SFO61        300.1324005 MHz
===== CHANNEL f62 =====
NUC62        1H
P62          100.00 usec
PL62         0.00 dB
SFO62        300.1324005 MHz
===== CHANNEL f63 =====
NUC63        1H
P63          100.00 usec
PL63         0.00 dB
SFO63        300.1324005 MHz
===== CHANNEL f64 =====
NUC64        1H
P64          100.00 usec
PL64         0.00 dB
SFO64        300.1324005 MHz
===== CHANNEL f65 =====
NUC65        1H
P65          100.00 usec
PL65         0.00 dB
SFO65        300.1324005 MHz
===== CHANNEL f66 =====
NUC66        1H
P66          100.00 usec
PL66         0.00 dB
SFO66        300.1324005 MHz
===== CHANNEL f67 =====
NUC67        1H
P67          100.00 usec
PL67         0.00 dB
SFO67        300.1324005 MHz
===== CHANNEL f68 =====
NUC68        1H
P68          1
```

S15

```

F2 - Acquisition Parameters
Date_ 20051110
Time_ 14:12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DE 27.800 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 6.70 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677324 MHz
WDW EM
SSB 0
LB 1.0 Hz
GB 0
PC 1.40

```

SF 235.360
 SY 235.360
 O1 1926.311
 SI 65336
 TD 65336
 SH 71428.571
 HZ/PT 2.180
 PW 4.0
 RD 5.000
 AQ .459
 RG 8
 NS 64
 TE 297
 FW 89300
 O2 3711.228
 DP 21H P0
 LB .300
 GB 0.00
 CY 35.00
 CY 18.00
 F1 -70.000P
 F2 -129.997P
 HZ/CM 403.455
 PPM/CM 1.714
 SR 10136.04

415.28

1033.78
1031.82
1027.89
1024.47
966.99
963.94
960.82
897.78
846.09
802.48
802.40
818.29
763.37
794.07

1332.41
1328.46
1318.73

1510.76
1504.42
1506.81
1505.01
1503.54
1502.88
1501.76
1501.10
1500.39
1499.86
1499.17
1498.83
1498.28

HERTZ

JT0305.113
AU PROG:
X00.AU
DATE 3-7-2
TIME 14:00
SF 250.133
SY 250.0
O1 4318.857
S1 32788
T0 32788
SW 5000.000
HZ/P1 .305
PW 0.0
RD 0.0
AQ 3.277
RG 16
NS 64
TE 297
FW 6300
O2 2714.499
DP 63L P0
LB 0.300
GB 0.0
CX 35.00
F1 19.202P
F2 7.795P
HZ/CM 71.463
PPM/CM .286
SR 2854.01
D1 1.0000000
P0 1.60
RGA
RD 0.0
PW 0.0
DE 125.00
NS 64
DS 2

Current Data Parameters
NAME: Jul10
EXPNO: 73
PROCNO: 1

F2 - Acquisition Parameters
Date_: 500000
Time: 14.16
INSTRUM: spect
PROBHD: 5 mm Dual 13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 10293
DS: 2
SWH: 31847.133 Hz
FIDRES: 0.465949 Hz
AQ: 1.0289652 sec
RG: 64
DM: 15.700 usec
DE: 4.50 usec
TE: 300.0 K
D12: 0.0002000 sec
PL13: 20.00 dB
D1: 1.0000000 sec
CPDPRG2: waltz16
PCPD2: 100.00 usec
SF02: 400.1316005 MHz
NUC2: 1H
PL2: -6.00 dB
PL12: 17.00 dB
P1: 6.00 usec
DE: 4.50 usec
SF01: 100.6254358 MHz
NUC1: 13C
PL1: -6.00 dB
D11: 0.03000000 sec

F2 - Processing parameters
SI: 32768
SF: 100.6127290 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 30.00 cm
F1P: 215.000 ppm
F1: 21631.74 Hz
F2P: -5.000 ppm
F2: -503.06 Hz
PPM0M: 7.33333 ppm/cm
HZ0M: 737.82672 Hz/cm

Current Data Parameters
 NAME 548H3
 EXPNO 3
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20030425
 Time 14.29
 INSTRUM spect
 PULPROG zgpg30
 TD 131072
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 25062.656 Hz
 FIDRES 0.191213 Hz
 AQ 2.6149364 sec
 RG 724.1
 IN 1950 usec
 DE 8.00 usec
 TE 300.0 K
 D1 5.0000000 sec
 ===== CHANNEL f1 =====
 NUC1 19F
 P1 9.50 usec
 PL1 -6.00 dB
 SFO1 282.3761058 MHz
 F2 - Processing parameters
 SI 65536
 SF 282.403460 MHz
 WDW EM
 SS 0
 LB 0.30 Hz
 GB 0
 PC 1.00

F2 - Acquisition Parameters
 Date_ 20040629
 Time 17.40
 INSTRUM spect
 PROBD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 4844.961 Hz
 FIDRES 0.1775 Hz
 AQ 3.381707 sec
 RG 71.8
 DW 103.200 usec
 DE 8.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SFO1 300.1322660 MHz
 =====
 F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 DS 4
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ion Parameters
Date_ 20040629
Time 18.33
INSTRUM spect
PULPROG 5 mm QNP
TD 65536
SOLVENT DMSO
NS 1024
SF 17985.611 Hz
AQ 0.274439 sec
RG 1149.4
DW 27.800 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00020000 sec
NEL f1 =====
NEL f2 =====
===== CHANNEL f1 =====
NUC1 13C
P1 6.70 usec
PL1 -3.00 dB
SF01 75.4752953 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL3 22.00 dB
PL13 22.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SF 75.4677667 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

153.76
153.55
153.13
152.73

140.83
140.79
140.64

EEE

8a, DMSO D₆

C₃ EEE

C₁ EEE

F2 - Acquisition Parameters
Date_ 20040629
Time 18.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1149.4
DE 2776.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00000000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 6.70 usec
PL1 3.00 dB
SFO1 75.4752953 MHz
===== CHANNEL f2 =====
CFDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 22.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz
F2 - Processing Parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ion Parameters
20040629
17.40
spect
QNP 1H/13
32768
DMSO
16
2
4844.961 Hz
0.127656 Hz
3.58716 sec
71.8
103.200 usec
8.00 usec
300.0 K
300.0 K
1.00000000 sec
NEL f1 =====
1H
6.50 usec
-3.00 dB
00.1322860 MHz ==
ng parameters
32768
00.1300000 MHz z
EM
0.30 Hz
1.00 z

```

F2 - Acquisition Parameters
Date_      20000629
Time       17.41
Program    SDR
PROB       5 mm QNP 1H/13
PULPROG    zgpg30
TD          65536
SOLVENT     DMSO
NS          2
DS          4
SWH         25650.73 Hz
FIDRES      0.191233 Hz
SAMPLING    2.6151314 sec
RG          645.1
AQ          19.511 usec
RG2         38.00 usec
DE          0.0 K
TE          300.0 K
D1          5.0000000 sec
===== CHANNEL f1 =====
NUC1        13C
P1          19f
PL1         0.50 usec
PC1         0.00 dB
===== CHANNEL f2 =====
NUC2        1H
P2          19f
PL2         0.50 usec
PC2         0.00 dB
===== CHANNEL f3 =====
NUC3        13C
P3          19f
PL3         0.50 usec
PC3         0.00 dB
===== CHANNEL f4 =====
NUC4        13C
P4          19f
PL4         0.50 usec
PC4         0.00 dB
===== CHANNEL f5 =====
NUC5        13C
P5          19f
PL5         0.50 usec
PC5         0.00 dB
===== CHANNEL f6 =====
NUC6        13C
P6          19f
PL6         0.50 usec
PC6         0.00 dB
===== CHANNEL f7 =====
NUC7        13C
P7          19f
PL7         0.50 usec
PC7         0.00 dB
===== CHANNEL f8 =====
NUC8        13C
P8          19f
PL8         0.50 usec
PC8         0.00 dB
===== CHANNEL f9 =====
NUC9        13C
P9          19f
PL9         0.50 usec
PC9         0.00 dB
===== CHANNEL f10 =====
NUC10       13C
P10         19f
PL10        0.50 usec
PC10        0.00 dB
===== CHANNEL f11 =====
NUC11       13C
P11         19f
PL11        0.50 usec
PC11        0.00 dB
===== CHANNEL f12 =====
NUC12       13C
P12         19f
PL12        0.50 usec
PC12        0.00 dB
===== CHANNEL f13 =====
NUC13       13C
P13         19f
PL13        0.50 usec
PC13        0.00 dB
===== CHANNEL f14 =====
NUC14       13C
P14         19f
PL14        0.50 usec
PC14        0.00 dB
===== CHANNEL f15 =====
NUC15       13C
P15         19f
PL15        0.50 usec
PC15        0.00 dB
===== CHANNEL f16 =====
NUC16       13C
P16         19f
PL16        0.50 usec
PC16        0.00 dB
===== CHANNEL f17 =====
NUC17       13C
P17         19f
PL17        0.50 usec
PC17        0.00 dB
===== CHANNEL f18 =====
NUC18       13C
P18         19f
PL18        0.50 usec
PC18        0.00 dB
===== CHANNEL f19 =====
NUC19       13C
P19         19f
PL19        0.50 usec
PC19        0.00 dB
===== CHANNEL f20 =====
NUC20       13C
P20         19f
PL20        0.50 usec
PC20        0.00 dB
===== CHANNEL f21 =====
NUC21       13C
P21         19f
PL21        0.50 usec
PC21        0.00 dB
===== CHANNEL f22 =====
NUC22       13C
P22         19f
PL22        0.50 usec
PC22        0.00 dB
===== CHANNEL f23 =====
NUC23       13C
P23         19f
PL23        0.50 usec
PC23        0.00 dB
===== CHANNEL f24 =====
NUC24       13C
P24         19f
PL24        0.50 usec
PC24        0.00 dB
===== CHANNEL f25 =====
NUC25       13C
P25         19f
PL25        0.50 usec
PC25        0.00 dB
===== CHANNEL f26 =====
NUC26       13C
P26         19f
PL26        0.50 usec
PC26        0.00 dB
===== CHANNEL f27 =====
NUC27       13C
P27         19f
PL27        0.50 usec
PC27        0.00 dB
===== CHANNEL f28 =====
NUC28       13C
P28         19f
PL28        0.50 usec
PC28        0.00 dB
===== CHANNEL f29 =====
NUC29       13C
P29         19f
PL29        0.50 usec
PC29        0.00 dB
===== CHANNEL f30 =====
NUC30       13C
P30         19f
PL30        0.50 usec
PC30        0.00 dB
===== CHANNEL f31 =====
NUC31       13C
P31         19f
PL31        0.50 usec
PC31        0.00 dB
===== CHANNEL f32 =====
NUC32       13C
P32         19f
PL32        0.50 usec
PC32        0.00 dB
===== CHANNEL f33 =====
NUC33       13C
P33         19f
PL33        0.50 usec
PC33        0.00 dB
===== CHANNEL f34 =====
NUC34       13C
P34         19f
PL34        0.50 usec
PC34        0.00 dB
===== CHANNEL f35 =====
NUC35       13C
P35         19f
PL35        0.50 usec
PC35        0.00 dB
===== CHANNEL f36 =====
NUC36       13C
P36         19f
PL36        0.50 usec
PC36        0.00 dB
===== CHANNEL f37 =====
NUC37       13C
P37         19f
PL37        0.50 usec
PC37        0.00 dB
===== CHANNEL f38 =====
NUC38       13C
P38         19f
PL38        0.50 usec
PC38        0.00 dB
===== CHANNEL f39 =====
NUC39       13C
P39         19f
PL39        0.50 usec
PC39        0.00 dB
===== CHANNEL f40 =====
NUC40       13C
P40         19f
PL40        0.50 usec
PC40        0.00 dB
===== CHANNEL f41 =====
NUC41       13C
P41         19f
PL41        0.50 usec
PC41        0.00 dB
===== CHANNEL f42 =====
NUC42       13C
P42         19f
PL42        0.50 usec
PC42        0.00 dB
===== CHANNEL f43 =====
NUC43       13C
P43         19f
PL43        0.50 usec
PC43        0.00 dB
===== CHANNEL f44 =====
NUC44       13C
P44         19f
PL44        0.50 usec
PC44        0.00 dB
===== CHANNEL f45 =====
NUC45       13C
P45         19f
PL45        0.50 usec
PC45        0.00 dB
===== CHANNEL f46 =====
NUC46       13C
P46         19f
PL46        0.50 usec
PC46        0.00 dB
===== CHANNEL f47 =====
NUC47       13C
P47         19f
PL47        0.50 usec
PC47        0.00 dB
===== CHANNEL f48 =====
NUC48       13C
P48         19f
PL48        0.50 usec
PC48        0.00 dB
===== CHANNEL f49 =====
NUC49       13C
P49         19f
PL49        0.50 usec
PC49        0.00 dB
===== CHANNEL f50 =====
NUC50       13C
P50         19f
PL50        0.50 usec
PC50        0.00 dB
===== CHANNEL f51 =====
NUC51       13C
P51         19f
PL51        0.50 usec
PC51        0.00 dB
===== CHANNEL f52 =====
NUC52       13C
P52         19f
PL52        0.50 usec
PC52        0.00 dB
===== CHANNEL f53 =====
NUC53       13C
P53         19f
PL53        0.50 usec
PC53        0.00 dB
===== CHANNEL f54 =====
NUC54       13C
P54         19f
PL54        0.50 usec
PC54        0.00 dB
===== CHANNEL f55 =====
NUC55       13C
P55         19f
PL55        0.50 usec
PC55        0.00 dB
===== CHANNEL f56 =====
NUC56       13C
P56         19f
PL56        0.50 usec
PC56        0.00 dB
===== CHANNEL f57 =====
NUC57       13C
P57         19f
PL57        0.50 usec
PC57        0.00 dB
===== CHANNEL f58 =====
NUC58       13C
P58         19f
PL58        0.50 usec
PC58        0.00 dB
===== CHANNEL f59 =====
NUC59       13C
P59         19f
PL59        0.50 usec
PC59        0.00 dB
===== CHANNEL f60 =====
NUC60       13C
P60         19f
PL60        0.50 usec
PC60        0.00 dB
===== CHANNEL f61 =====
NUC61       13C
P61         19f
PL61        0.50 usec
PC61        0.00 dB
===== CHANNEL f62 =====
NUC62       13C
P62         19f
PL62        0.50 usec
PC62        0.00 dB
===== CHANNEL f63 =====
NUC63       13C
P63         19f
PL63        0.50 usec
PC63        0.00 dB
===== CHANNEL f64 =====
NUC64       13C
P64         19f
PL64        0.50 usec
PC64        0.00 dB
===== CHANNEL f65 =====
NUC65       13C
P65         19f
PL65        0.50 usec
PC65        0.00 dB
===== CHANNEL f66 =====
NUC66       13C
P66         19f
PL66        0.50 usec
PC66        0.00 dB
===== CHANNEL f67 =====
NUC67       13C
P67         19f
PL67        0.50 usec
PC67        0.00 dB
===== CHANNEL f68 =====
NUC68       13C
P68         19f
PL68        0.50 usec
PC68        0.00 dB
===== CHANNEL f69 =====
NUC69       13C
P69         19f
PL69        0.50 usec
PC69        0.00 dB
===== CHANNEL f70 =====
NUC70       13C
P70         19f
PL70        0.50 usec
PC70        0.00 dB
===== CHANNEL f71 =====
NUC71       13C
P71         19f
PL71        0.50 usec
PC71        0.00 dB
===== CHANNEL f72 =====
NUC72       13C
P72         19f
PL72        0.50 usec
PC72        0.00 dB
===== CHANNEL f73 =====
NUC73       13C
P73         19f
PL73        0.50 usec
PC73        0.00 dB
===== CHANNEL f74 =====
NUC74       13C
P74         19f
PL74        0.50 usec
PC74        0.00 dB
===== CHANNEL f75 =====
NUC75       13C
P75         19f
PL75        0.50 usec
PC75        0.00 dB
===== CHANNEL f76 =====
NUC76       13C
P76         19f
PL76        0.50 usec
PC76        0.00 dB
===== CHANNEL f77 =====
NUC77       13C
P77         19f
PL77        0.50 usec
PC77        0.00 dB
===== CHANNEL f78 =====
NUC78       13C
P78         19f
PL78        0.50 usec
PC78        0.00 dB
===== CHANNEL f79 =====
NUC79       13C
P79         19f
PL79        0.50 usec
PC79        0.00 dB
===== CHANNEL f80 =====
NUC80       13C
P80         19f
PL80        0.50 usec
PC80        0.00 dB
===== CHANNEL f81 =====
NUC81       13C
P81         1
```

Current Data Parameters
NAME Feb26-2006
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060226
Time 15.56
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT C6D6
NS 16
DS 2
SWH 4844.961 Hz
FIDRES 0.147856 Hz
AQ 3.387777 sec
RG 143.7
DW 103.200 usec
DE 8.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.50 usec
PL1 -3.00 dB
SFO1 300.1322660 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

2274.25
 2260.26
 2194.64
 2186.52
 2182.03
 2176.42
 2168.82
 2149.87
 2144.75
 2124.70
 2117.14
 2110.23
 2103.33
 2089.76
 2085.97
 2081.86
 2078.34
 2070.60
 2063.67
 2056.58
 2049.22
 1978.02
 1970.21
 1942.95
 1935.05
 1623.84
 1615.83
 1580.10
 1566.16

Current Data Parameters
 NAME Feb26-2006
 EXPNO 13
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060226
 Time 18:55
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 FULPROG zgpg30
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4844.961 Hz
 FIDRES 0.147856 Hz
 AQ 3.3817077 sec
 RG 143.7
 DR 103.250 usec
 DE 8.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 6.00 usec
 PL1 -3.00 dB
 SFO1 300.1322660 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 WDM 1.000000
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters	
NAME	Feb26-2006
EXPO	15
PROCNO	1
F2 - Acquisition parameters	
Date_	200606226
Time_	19:00
INSTRUM	PROBHD
PROBHD	5 mm QNP 1H/13
FULPROG	cosygpzg30
SOLVENT	CDCl3
NS	1
DS	2
SWH	2934.270 Hz
FIDRES	1.432750 sec
AQ	0.3450292 sec
RG	170.408 usec
DE	8.00 usec
TE	300.0 K
DT	0.3242802 sec
DI	1.3342800 sec
h1	0.00000400 sec
h13	0.00000400 sec
h16	0.00000400 sec
h17	0.00000400 sec
MKRGST	0.00000000 sec
MONPRG	1.33428002 sec
===== CHANNEL f1 =====	
NUC1	1H
P0	6.50 usec
P1	5.00 usec
PL1	0.00 dB
SP01	300.1311793 MHz
===== GRADIENT CHANNEL =====	
GVNM1	SINE.100
GVNM2	SINE.100
GVX1	0.00 dB
GVY1	0.00 dB
GVZ1	0.00 dB
GVX2	10.00 dB
GVY2	10.00 dB
GVZ2	10.00 dB
PL16	1000.00 usec
F2 - Acquisition parameters	
NUC0	128
SP01	300.13112 MHz
SP02	22.93777000 MHz
SW	8.777 ppm
FMODE	QF
F2 - Processing parameters	
SI	1024
SF	300.1300000 MHz
SSB	SING
GB	0.00 Hz
PC	1.40
FC	0
F1 - Processing parameters	
SI	1024
SW	8.777 ppm
SF	300.1300000 MHz
SSB	SING
GB	0.00 Hz
PC	0

Current Data Parameters		P2 - Acquisition Parameters		P2 - Processing Parameters	
NAME	Feb56-2006	Date	2.06020226	SI	32768
EXPNO	3	Time	16.48	SF	75.4677324 MHz
PRONO	1	INSTRUM	spect	EM	
		PROBHD	5 mm QNP 1H/13	WDW	1.00 Hz
		PULPROG	zgpg30	GB	0
		TD	65536	PC	1.40
		SOLVENT	CDCl ₃		
		NS	1024		
		DS	17985.61 Hz		
		F2 - F1	0.2743439 Hz		
		AQ	1.8219508 sec		
		RG	7592.6		
		DM	27.400 usec		
		DE	300.0 Hz		
		TE	0.03000000 sec		
		d1	0.03000000 sec		
		d11	0.00002000 sec		
		d12	0.00002000 sec		
		===== CHANNEL f1 =====			
		NUC1	13C		
		P1	6.70 usec		
		PL1	-3.00 dB		
		SFO1	75.4732953 MHz		
		===== CHANNEL f2 =====			
		CPDPRG2	waltz16		
		NUC2	1H		
		P2	100.00 usec		
		PL2	0.00 dB		
		PL12	22.00 dB		
		PL13	22.00 dB		
		SFO2	300.1312005 MHz		
		===== CHANNEL f3 =====			
		SI	32768		
		SF	75.4677324 MHz		
		WDW	EM		
		GB	1.00 Hz		
		PC	1.40

Current Data Parameters
Date Feb26-2005
Time 16:48
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060226
Time_ 16:48
INSTRUM 5 mm QNP 1H/13
PROBHD zgpg30
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 327.680
DE 27.800 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 6.70 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
===== CHANNEL f2 =====
CDPRG2 waltz16
NUC2 1H
PCPDZ 100.00 usec
PL2 0.00 dB
PL12 22.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677324 MHz
WDW EM
SSB 0
GB 1.00 Hz
PC 1.40

13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 ppm

155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 ppm

1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5 -3.0 -3.5 -4.0 -4.5 -5.0 -5.5 -6.0 -6.5 -7.0 -7.5 -8.0 -8.5 -9.0 -9.5 -10.0 -10.5 -11.0 -11.5 -12.0 -12.5 -13.0 -13.5 -14.0 -14.5 -15.0 -15.5 -16.0 -16.5 -17.0 -17.5 -18.0 -18.5 -19.0 -19.5 -20.0 -20.5 -21.0 -21.5 -22.0 -22.5 -23.0 -23.5 -24.0 -24.5 -25.0 -25.5 -26.0 -26.5 -27.0 -27.5 -28.0 -28.5 -29.0 -29.5 -30.0 -30.5 -31.0 -31.5 -32.0 -32.5 -33.0 -33.5 -34.0 -34.5 -35.0 -35.5 -36.0 -36.5 -37.0 -37.5 -38.0 -38.5 -39.0 -39.5 -40.0 -40.5 -41.0 -41.5 -42.0 -42.5 -43.0 -43.5 -44.0 -44.5 -45.0 -45.5 -46.0 -46.5 -47.0 -47.5 -48.0 -48.5 -49.0 -49.5 -50.0 -50.5 -51.0 -51.5 -52.0 -52.5 -53.0 -53.5 -54.0 -54.5 -55.0 -55.5 -56.0 -56.5 -57.0 -57.5 -58.0 -58.5 -59.0 -59.5 -60.0 -60.5 -61.0 -61.5 -62.0 -62.5 -63.0 -63.5 -64.0 -64.5 -65.0 -65.5 -66.0 -66.5 -67.0 -67.5 -68.0 -68.5 -69.0 -69.5 -70.0 -70.5 -71.0 -71.5 -72.0 -72.5 -73.0 -73.5 -74.0 -74.5 -75.0 -75.5 -76.0 -76.5 -77.0 -77.5 -78.0 -78.5 -79.0 -79.5 -80.0 -80.5 -81.0 -81.5 -82.0 -82.5 -83.0 -83.5 -84.0 -84.5 -85.0 -85.5 -86.0 -86.5 -87.0 -87.5 -88.0 -88.5 -89.0 -89.5 -90.0 -90.5 -91.0 -91.5 -92.0 -92.5 -93.0 -93.5 -94.0 -94.5 -95.0 -95.5 -96.0 -96.5 -97.0 -97.5 -98.0 -98.5 -99.0 -99.5 -100.0 -100.5 -101.0 -101.5 -102.0 -102.5 -103.0 -103.5 -104.0 -104.5 -105.0 -105.5 -106.0 -106.5 -107.0 -107.5 -108.0 -108.5 -109.0 -109.5 -110.0 -110.5 -111.0 -111.5 -112.0 -112.5 -113.0 -113.5 -114.0 -114.5 -115.0 -115.5 -116.0 -116.5 -117.0 -117.5 -118.0 -118.5 -119.0 -119.5 -120.0 -120.5 -121.0 -121.5 -122.0 -122.5 -123.0 -123.5 -124.0 -124.5 -125.0 -125.5 -126.0 -126.5 -127.0 -127.5 -128.0 -128.5 -129.0 -129.5 -130.0 -130.5 -131.0 -131.5 -132.0 -132.5 -133.0 -133.5 -134.0 -134.5 -135.0 -135.5 -136.0 -136.5 -137.0 -137.5 -138.0 -138.5 -139.0 -139.5 -140.0 -140.5 -141.0 -141.5 -142.0 -142.5 -143.0 -143.5 -144.0 -144.5 -145.0 -145.5 -146.0 -146.5 -147.0 -147.5 -148.0 -148.5 -149.0 -149.5 -150.0 -150.5 -151.0 -151.5 -152.0 -152.5 -153.0 -153.5 -154.0 -154.5 -155.0 -155.5 -156.0 -156.5 -157.0 -157.5 -158.0 -158.5 -159.0 -159.5 -160.0 -160.5 -161.0 -161.5 -162.0 -162.5 -163.0 -163.5 -164.0 -164.5 -165.0 -165.5 -166.0 -166.5 -167.0 -167.5 -168.0 -168.5 -169.0 -169.5 -170.0 -170.5 -171.0 -171.5 -172.0 -172.5 -173.0 -173.5 -174.0 -174.5 -175.0 -175.5 -176.0 -176.5 -177.0 -177.5 -178.0 -178.5 -179.0 -179.5 -180.0 -180.5 -181.0 -181.5 -182.0 -182.5 -183.0 -183.5 -184.0 -184.5 -185.0 -185.5 -186.0 -186.5 -187.0 -187.5 -188.0 -188.5 -189.0 -189.5 -190.0 -190.5 -191.0 -191.5 -192.0 -192.5 -193.0 -193.5 -194.0 -194.5 -195.0 -195.5 -196.0 -196.5 -197.0 -197.5 -198.0 -198.5 -199.0 -199.5 -200.0 -200.5 -201.0 -201.5 -202.0 -202.5 -203.0 -203.5 -204.0 -204.5 -205.0 -205.5 -206.0 -206.5 -207.0 -207.5 -208.0 -208.5 -209.0 -209.5 -210.0 -210.5 -211.0 -211.5 -212.0 -212.5 -213.0 -213.5 -214.0 -214.5 -215.0 -215.5 -216.0 -216.5 -217.0 -217.5 -218.0 -218.5 -219.0 -219.5 -220.0 -220.5 -221.0 -221.5 -222.0 -222.5 -223.0 -223.5 -224.0 -224.5 -225.0 -225.5 -226.0 -226.5 -227.0 -227.5 -228.0 -228.5 -229.0 -229.5 -230.0 -230.5 -231.0 -231.5 -232.0 -232.5 -233.0 -233.5 -234.0 -234.5 -235.0 -235.5 -236.0 -236.5 -237.0 -237.5 -238.0 -238.5 -239.0 -239.5 -240.0 -240.5 -241.0 -241.5 -242.0 -242.5 -243.0 -243.5 -244.0 -244.5 -245.0 -245.5 -246.0 -246.5 -247.0 -247.5 -248.0 -248.5 -249.0 -249.5 -250.0 -250.5 -251.0 -251.5 -252.0 -252.5 -253.0 -253.5 -254.0 -254.5 -255.0 -255.5 -256.0 -256.5 -257.0 -257.5 -258.0 -258.5 -259.0 -259.5 -260.0 -260.5 -261.0 -261.5 -262.0 -262.5 -263.0 -263.5 -264.0 -264.5 -265.0 -265.5 -266.0 -266.5 -267.0 -267.5 -268.0 -268.5 -269.0 -269.5 -270.0 -270.5 -271.0 -271.5 -272.0 -272.5 -273.0 -273.5 -274.0 -274.5 -275.0 -275.5 -276.0 -276.5 -277.0 -277.5 -278.0 -278.5 -279.0 -279.5 -280.0 -280.5 -281.0 -281.5 -282.0 -282.5 -283.0 -283.5 -284.0 -284.5 -285.0 -285.5 -286.0 -286.5 -287.0 -287.5 -288.0 -288.5 -289.0 -289.5 -290.0 -290.5 -291.0 -291.5 -292.0 -292.5 -293.0 -293.5 -294.0 -294.5 -295.0 -295.5 -296.0 -296.5 -297.0 -297.5 -298.0 -298.5 -299.0 -299.5 -300.0 -300.5 -301.0 -301.5 -302.0 -302.5 -303.0 -303.5 -304.0 -304.5 -305.0 -305.5 -306.0 -306.5 -307.0 -307.5 -308.0 -308.5 -309.0 -309.5 -310.0 -310.5 -311.0 -311.5 -312.0 -312.5 -313.0 -313.5 -314.0 -314.5 -315.0 -315.5 -316.0 -316.5 -317.0 -317.5 -318.0 -318.5 -319.0 -319.5 -320.0 -320.5 -321.0 -321.5 -322.0 -322.5 -323.0 -323.5 -324.0 -324.5 -325.0 -325.5 -326.0 -326.5 -327.0 -327.5 -328.0 -328.5 -329.0 -329.5 -330.0 -330.5 -331.0 -331.5 -332.0 -332.5 -333.0 -333.5 -334.0 -334.5 -335.0 -335.5 -336.0 -336.5 -337.0 -337.5 -338.0 -338.5 -339.0 -339.5 -340.0 -340.5 -341.0 -341.5 -342.0 -342.5 -343.0 -343.5 -344.0 -344.5 -345.0

§ 33

65.99

62.25

EEE

ZZE

36%

11%

Current Data Parameters
NAME: 2009226
EXPNO: 2
PROCNO: 1
F2 - Acquisition Parameters
File: 2009226
Date_ 2009226
Time: 14.13
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: C6D6
NS: 16
DS: 4
SWH: 25062.656 Hz
FIDRES: 0.181 Hz
AQ: 2.614364 sec
RG: 1824.6
DW: 19.950 usec
DE: 3.000 usec
TE: 300.0 K
D1: 5.00000000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 12.00 usec
PL1: -6.00 dB
SFO1: 282.3761058 MHz
F2 - Processing parameters
SI: 65536
SF: 282.4043460 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

Current Data Parameters
 NAME: 06115-206
 EXPNO: 2
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20060613
 Time: 14.16
 Time2: 14.16
 PULPROG: 5 mm QNP 1H/13
 PROBHD: 5 mm QNP 1H/13
 PULPROG: zg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 4844.94 Hz
 FWHM: 0.147866 Hz
 AQ: 3.3817077 sec
 RG: 256
 DW: 103.200 usec
 DE: 8.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

===== CHANNEL F1 =====
 NUC1: 1H
 PL1: 6.50 usec
 PL1: -3.00 dB
 SFO1: 300.1325660 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1300000 MHz
 MDW: EM
 SSB: 0
 LB: 0
 GB: 0
 PC: 1.00

Current Data Parameters
 NAME Junit3-2006
 EXPNO 6
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060611
 Time 14:21
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG cosygpcdf
 TD 2048
 SOLVENT C6D6
 NS 8
 DS 8
 SMH 3787.879 Hz
 FIDRES 1.849550 Hz
 AQ 0.2703860 sec
 RG 327.500
 DW 132.000 usec
 DE 8.00 usec
 TE 300.0 K
 d0 0.0000300 sec
 d1 1.4021042 sec
 d12 0.0000000 sec
 d13 0.0000000 sec
 d16 0.00010000 sec
 INO 0.00026400 sec
 MCREST 0.00000000 sec
 MCWRR 1.4021042 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P0 6.50 usec
 PL1 6.50 usec
 PL2 -3.00 dB
 SF01 300.1318426 MHz
 ===== GRADIENT CHANNEL =====
 GPMAM1 SINE.100
 GPMAM2 SINE.100
 GPX1 0.00
 GPC1 0.00
 GPV1 0.00
 GPV2 0.00
 GPZ1 10.00
 GPZ2 10.00
 F16 1000.00 usec
 F1 - Acquisition parameters
 ND0 1
 TD 128
 SF01 300.1318 MHz
 FIDRES 231.52624 Hz
 SFO1 12.000000 Ppm
 FPMODE QF
 F2 - Processing parameters
 SI 1024
 SF 300.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 300.1300000 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

2184.85
 2170.90
 2110.44
 2102.11
 2093.24
 2085.88
 2047.27
 2040.72
 2033.59
 2022.66
 2010.06
 2009.23
 2001.73
 1994.80
 1987.83
 1980.46
 1973.27
 1899.51
 1891.60
 1849.21
 1841.36
 1543.95
 1535.79
 1515.35
 1501.41

Current Data Parameters
 NAME JUN14-2006
 EXPNO 5
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060614
 Time 11:11:11
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl₃
 NS 16
 DS 4
 SWH 4844.961 Hz
 FIDRES 0.147856 Hz
 AQ 3.3817077 sec
 RG 1024
 DW 103.200 usec
 DE 19.00 usec
 TE 300.2 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 0.00 dB
 SFO1 300.1322660 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300715 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

C6H / C6D6
A3 C6D6 jpb

Current Data Parameters
NAME Jun14-2006
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060614
Time 12:52
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG cosygdaf
TD 65536
SOLVENT CDCl3
NS 8
DS 1
SWH 3019.324 Hz
FIDRES 0.3391988 Hz
AQ 0.3391988 sec
RG 574.7
DM 165.600 usec
DE 38.00 usec
TE 300.2 K
D0 0.00000300 sec
D1 1.33451998 sec
d13 0.00000400 sec
L16 0.00000000 sec
L20 0.00031320 sec
MCREST 0.00000000 sec
MCRK 1.33451998 sec

===== CHANNEL f1 =====
NUC1 1H
P0 6.50 usec
PL 6.50 usec
PL1 3.00 dB
SFO1 300.1314473 MHz

===== GRADIENT CHANNEL =====
GPM1 SINE 100
GPM2 SINE 100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GZ1 10.00 %
GZ2 10.00 %
P16 1000.00 usec

F1 - Acquisition Parameters
ND0 128
TD 128
SFO1 300.1314 MHz
FIDRES 23.588467 Hz
SFO2 100.626119 MHz
PQ 0.00
PR 0.00
PC 1.40

F2 - Processing parameters
SI 32768
SF 300.1300724 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
SF 300.1300724 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

Current Data Parameters		F2 - Acquisition Parameters		F2 - Processing parameters	
NAME	Jun13-2006	Time	20060613	SI	32768
EXPNO	3	INSTRUM	spect	CFPACGE	wait1s
PROCNO	1	5	15	NIC2	1H
		TD	5 mm QNP 1H/13	CHANCEL F2 =====	
		PULPROG	zgpg30	PL1	6.70 usec
		TD0	65336	PL2	-3.00 dB
		TD1	14806 usec	PL3	75.475295 MHz
		TD2	2.800 usec	PL4	100.00 usec
		TD3	8.00 usec	PL5	0.00 dB
		TD4	300.0 K	PL6	22.00 dB
		TD5	1.00000000 sec	PL7	27.00 dB
		TD6	0.03000000 sec	PL8	44.00 dB
		TD7	0.00020000 sec	PL9	300.132003 MHz
		TD8	0.00020000 sec	SF02	300.132003 MHz
		===== CHANNEL f1 =====			
		NUC1	13C		
		PL1	6.70 usec		
		PL2	-3.00 dB		
		SF01	75.475295 MHz		
		===== CHANNEL f2 =====			
		NUC2	1H		
		PL1	100.00 usec		
		PL2	0.00 dB		
		PL3	22.00 dB		
		PL4	27.00 dB		
		PL5	44.00 dB		
		PL6	300.132003 MHz		
		===== CHANNEL f3 =====			
		SI	32768		
		CFPACGE	wait1s		
		NIC2	1H		
		PL1	100.00 usec		
		PL2	0.00 dB		
		PL3	22.00 dB		
		PL4	27.00 dB		
		PL5	44.00 dB		
		PL6	300.132003 MHz		
		===== CHANNEL f4 =====			
		SI	32768		
		CFPACGE	wait1s		
		NIC2	1H		
		PL1	100.00 usec		
		PL2	0.00 dB		
		PL3	22.00 dB		
		PL4	27.00 dB		
		PL5	44.00 dB		
		PL6	300.132003 MHz		
		===== CHANNEL f5 =====			
		SI	32768		
		CFPACGE	wait1s		
		NIC2	1H		
		PL1	100.00 usec		
		PL2	0.00 dB		
		PL3	22.00 dB		
		PL4	27.00 dB		
		PL5	44.00 dB		
		PL6	300.132003 MHz		
		===== CHANNEL f6 =====			
		SI	32768		
		CFPACGE	wait1s		
		NIC2	1H		
		PL1	100.00 usec		
		PL2	0.00 dB		
		PL3	22.00 dB		
		PL4	27.00 dB		
		PL5	44.00 dB		
		PL6	300.132003 MHz		
		===== CHANNEL f7 =====			
		SI	32768		
		CFPACGE	wait1s		
		NIC2	1H		
		PL1	100.00 usec		
		PL2	0.00 dB		
		PL3	22.00 dB		
		PL4	27.00 dB		
		PL5	44.00 dB		
		PL6	300.132003 MHz		
		===== CHANNEL f8 =====			
		SI	32768		
		CFPACGE	wait1s		
		NIC2	1H		
		PL1	100.00 usec		
		PL2	0.00 dB		

```

Current Data Parameters
NAME      JUN13-2005
EXPNO     1
PROCNO    1

P2 - Acquisition Parameters
Date_     20060613
Time      14.14
INSTRUM   spect
PROBHD    5 mm QNP
PULPROG   zgpg30
TD         131072
SOLVENT   CDCl3
NS         16
DS         4
SWH        25062.656 Hz
FIDRES     0.191213 Hz
AQ         2.618564 sec
RG         64
DM         19.950 usec
DE         8.00 usec
TE         300.0 K
D1         5.0000000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         19.0 usec
PL1        -6.00 dB
SFO1       282.1761058 MHz

P2 - Processing parameters
SI         65536
WDW        EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

```

Current Data Parameters
 NAME Jun14-2006
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060914
 Time 17.15
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 4844.961 Hz
 FIDRES 0.147856 Hz
 AQ 3.3817077 sec
 RG 256
 DE 103.200 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 13
 PL1 6.50 usec
 PL1 -3.00 dB
 SFO1 300.1322660 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300000 MHz
 EQ 0
 MCW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

A3 DMSO jpb

Current Data Parameters
 NAME Jun14-2006
 EXNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060614
 Time 18.05
 INSTRUM spect
 PROBHID 5 mm QNP 1H/13
 PULPROG cosygpcd
 FIDRES 0.165
 SOLVENT DMSO
 NS 1
 DS 8
 SWH 3188.775 Hz
 FIDRES 0.165 Hz
 AQ 0.321764 sec
 RG 0.321764 sec
 DW 156.800 usec
 DE 8.00 usec
 TE 300.2 K
 D1 0.00000000 sec
 d13 1.35090399 sec
 d16 0.00000000 sec
 INU 0.00010000 sec
 INUS 0.00010000 sec
 MCWST 1.35090399 sec
 MCWR 1.35090399 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.50 usec
 PL1 -3.00 dB
 SF01 300.1316066 MHz

===== GRADIENT CHANNEL =====
 GPM1 0.00 %
 GPM2 0.00 %
 GPX1 0.00 %
 GPV1 0.00 %
 GPZ1 0.00 %
 GPZ2 10.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 NS 128
 TD 128
 SF01 300.1316 MHz
 FIDRES 24.912308 Hz
 SW 10.625 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 300.1300000 MHz
 WDW SINE
 SSF 0.00 Hz
 LB 0
 GB 1.40
 PC

F1 - Processing parameters
 SI 1024
 SF 300.1300000 MHz
 WDW SINE
 SSF 0.00 Hz
 LB 0
 GB 1.40

Current Data Parameters
NAME Jun14-2006
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060614
Time 18.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 4844.561 Hz
FIDRES 0.141000 Hz
AQ 3.3817077 sec
RG 256
DM 102.200 usec
DE 8.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.50 usec
PL1 0.00 dB
SFO1 300.1322660 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

EEE
8b
DMSO D₆/D₂O

Current Data Parameters
NAME Jun14-2006
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060614
Time 18.05
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.22453 Hz
AQ 1.821508 sec
RG 1024
DW 27.800 usec
DE 8.00 usec
TE 300.0 K
D1 1.0000000 sec
d11 0.0000000 sec
d12 0.0000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 6.70 usec
PL1 -3.00 dB
SFO1 75.475293 MHz

===== CHANNEL f2 =====
C13PROG2 waltz16
NUC2 1H
P2 100.00 usec
PL2 0.00 dB
PL3 0.00 dB
PL13 22.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.65

Current Data Parameters
 NAME Jun14-2006
 PROCNO 1
 P2 - Acquisition Parameters
 Date_ 20060614
 Time 10:13
 INSTRUM spect
 PROBD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 131072
 SOLVENT DMSO
 NS 16
 DS 4
 SWH 25062.656 Hz
 FIDRES 0.191213 Hz
 AQ 2.6149364 sec
 RG 327.500
 FM 19.990 usec
 DE 8.00 usec
 TE 300.0 K
 D1 5.0000000 sec
 ===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 9.50 usec
 PL1 0.00 dB
 SF01 282.3761058 MHz
 P2 - Processing parameters
 SI 32768
 SF 282.4034460 MHz
 EQ 1
 MDW EM
 SSB 0
 GB 0
 PC 1.00