Supporting Information

Expanding Organoboron Chemistry. Epoxidation of Potassium Organotrifluoroborates

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General Methods and Materials. ^1H , ^{13}C and ^{19}F NMR spectra were measured on spectrometers at 500.13, 125.75 and 470.55 MHz, respectively. ^{11}B NMR spectra at 64.2 MHz were obtained on a spectrometer equipped with the appropriate decoupling accessories. The melting points were uncorrected. Standard flash chromatography procedures were followed using 32-63 μm silica gel. CI mass spectra were obtained at 70 eV with direct inlet injection. THF was distilled from sodium/benzophenone, and all water used was degassed with argon. The cross-coupling reactions were carried out under an argon atmosphere. Oxone, palladium catalysts, Cs_2CO_3 , and 4-bromobenzonitrile were commercially available. Dimethyldioxirane (solution in acetone) was prepared following established literature protocol.¹

Potassium 3-Phenylsulfonylpropyltrifluoroborate (1). To a solution of allyl phenyl sulfide (1 g, 6.6 mmol, 1 equiv) in CH_2Cl_2 (25 mL) was added a solution of $\text{HBBBr}_2\text{SMe}_2$ (1 M in CH_2Cl_2 , 13.3 mL, 13.3 mmol, 2 equiv). The resulting suspension was stirred at reflux for 24 h and then allowed to warm to rt. The mixture was cooled to 0 $^\circ\text{C}$ and water and ether were slowly added. The suspension was stirred for 30 min. The mixture was extracted with ether, and the combined organic extracts were dried over MgSO_4 and then filtered. After removal of the solvents the white solid was purified by crystallization in hexane/ether providing 1 g of the boronic acid (80% yield). ^1H NMR (CDCl_3) δ 7.32-7.23 (m, 4H), 7.11 (t, J = 1.2 Hz, 1H), 2.97-2.92 (m, 2H), 1.82-1.74 (m, 2H), 1.02-0.0 (m, 2H); ^{11}B NMR (CDCl_3) δ 33.5 (m). A part (770 mg, 3.9 mmol) of the resulting product was dissolved in ether (20 mL) and KHF_2 (915 mg, 11.7 mmol, 3 equiv) was added followed by the addition of water (1 mL) over 1 h. The mixture was extracted with acetone and the combined extracts were concentrated and then held under high vacuum for 30 min. The resulting white solid was purified by dissolution in hot acetone and precipitating with ether, providing **3b** as a flaky white solid (935 mg, 93% yield). mp 289 $^\circ\text{C}$; ^1H NMR ($\text{DMSO}-d_6$) δ 7.27-7.23 (m, 4H), 7.11 (t, J = 1.2 Hz, 1H), 2.83 (t, J = 7.8 Hz, 2H), 1.47-1.44 (m, 2H), 0.07-0.05 (m, 2H); ^{13}C NMR ($\text{DMSO}-d_6$) δ 137.7, 128.7 (2C), 127.2 (2C), 124.7, 35.4, 25.8; ^{19}F NMR ($\text{DMSO}-d_6$) δ -136.7; ^{11}B NMR ($\text{DMSO}-d_6$) δ 5.73 (m).

Preparation of Potassium 3-Phenylsulfonylpropyltrifluoroborate (2) To a CH_2Cl_2 solution (0.5 M) of 3-(phenylsulfonyl)propyltrifluoroborate **1** (114 mg, 0.44 mmol, 1 equiv) was added *m*-CPBA (153 mg, 0.88 mmol, 2 equiv) at rt. The resulting mixture was stirred for 1 h. A white solid appeared in the reaction mixture. Filtration of the solid and several washings with CH_2Cl_2 afforded the desired sulfone derivative as white solid (90 mg, 70% yield). mp 237 °C; ^1H NMR ($\text{DMSO}-d_6$) δ 7.84 (dd, $J = 8.1$ and 1.4 Hz, 2H), 7.72 (t, $J = 8.4$ Hz, 1H), 7.64 (t, $J = 8.1$ Hz, 2H), 3.10-3.06 (m, 2H), 1.41-1.34 (m, 2H), -0.02-(-0.07) (m, 2H); ^{13}C NMR ($\text{DMSO}-d_6$) δ 140.1, 134.2, 130.1 (2C), 128.4 (2C), 59.1, 19.9; ^{19}F NMR ($\text{DMSO}-d_6$) δ -137.6 (m); ^{11}B NMR ($\text{DMSO}-d_6$) δ 4.91.

Potassium *trans*-2-(Chloromethyl)-ethenyltrifluoroborate (3c). To a solution of *trans*-2-(chloromethyl)ethenylboronic acid (1.2 g, 9.9 mmol, 1 equiv) in MeOH (10 mL) was added KHF_2 (2.4 g, 30 mmol, 3 equiv) followed by the addition of water (1 mL) over 1 h. The reaction mixture was extracted with acetone and the combined organic extracts were concentrated and then held under high vacuum for 30 min. The resulting white solid was purified by dissolution in hot acetone and precipitating with ether, affording **3c** as a white solid (1.2 g, 68% yield). mp >280 °C; ^1H NMR (acetone- d_6) δ 5.78-5.71 (m, 2H), 4.01 (m, 2H); ^{13}C NMR (acetone- d_6) δ 142.8 (m), 131.4, 49.7; ^{19}F NMR (acetone- d_6) δ -142.8 (m); ^{11}B NMR (acetone- d_6) δ 4.6 (m).

Potassium Isopropenyltrifluoroborate (3d)². To a solution of trimethylborate (6.2 g, 59 mmol, 3 equiv) in THF (25 mL) was added dropwise isopropenylmagnesium bromide (0.5 M THF solution, 40 mL, 20 mmol, 1 equiv) at rt. After stirring for 2 h, the mixture was cooled to 0 °C and an aqueous HCl solution (1 N, 50 mL) was added. The mixture was extracted with ether. The combined organic extracts were dried over MgSO_4 and filtered. After removal of the solvent the corresponding boronic acid was obtained as a white solid and used without further purification (1.5 g, 91% yield). A part (1.3 g, 14 mmol) of the resulting product was dissolved in ether (25 mL) and KHF_2 (4.1 g, 52 mmol, 3.5 equiv) was added followed by the addition of water (1.5 mL) over 1 h. The mixture was extracted with acetone and the combined organic extracts were concentrated and then held under high vacuum for 30 min. The resulting white solid was purified by dissolving in hot acetone and precipitating with ether, providing **3d** as a white solid (1.8 g, 90% yield).

Potassium 3-Butenyltrifluoroborate (5). To a solution of trimethylborate (7.7 g, 74 mmol, 3 equiv) in THF (100 mL) was added dropwise 3-butenylmagnesium bromide (0.5 M THF solution, 50 mL, 25 mmol, 1 equiv) at 0 °C. The mixture was allowed to warm to rt and stirred for 2 h, then cooled to 0 °C. An aqueous HCl solution (1 N, 100 mL) was added. The mixture was extracted with ether, and the combined organic extracts were dried over MgSO_4 and filtered. After removal of the solvent the corresponding boronic acid (2 g, 83% yield) was obtained as a white solid and used without further purification. The resulting product (2 g, 20 mmol, 1 equiv) was dissolved in ether (50 mL) and KHF_2 (4.6 g, 60 mmol, 3 equiv) was added followed by the addition of water (3 mL) over 1 h. The mixture was extracted with acetone and the combined organic extracts were concentrated and then held under high vacuum for 30 min. The resulting white solid was purified by dissolution in hot acetone and precipitating with ether, affording a white solid (2.3 g, 71% yield). mp 260 °C (decomp); ^1H NMR (acetone- d_6) δ 5.93-5.88 (m, 1H), 4.83 (dt, $J = 15.2$ and 1.5 Hz, 1H), 7.68 (dt, $J = 17.4$ and 1.4 Hz, 1H), 1.86-1.82 (m, 2H), 0.20 (m, 2H); ^{13}C NMR (acetone- d_6) δ 145.7, 110.6, 30.9; ^{19}F NMR ($\text{DMSO}-d_6$) δ -141.7 (m); ^{11}B NMR (acetone- d_6) δ 7.36 (m).

General Procedure for Epoxidation of Potassium Organotrifluoroborates with Dimethyldioxirane. **Potassium *trans*-2-Octyl-1-trifluoroboratooxirane (4a).** To a solution of potassium *trans*-1-dec-1-enyltrifluoroborate³ **3a** (806 mg, 3.2 mmol, 1 equiv) in acetone (1 M) was added dimethyldioxirane (88 mL, 0.05 M acetone solution, 1.2 equiv) at rt. After stirring for 30 min a white precipitate appeared. Acetone was partially removed under vacuum (approximately half of the volume), and ether was added to induce further precipitation. After filtration, the oxiranyltrifluoroborate **4a** was obtained as a white solid (730 mg, 85% yield). mp 195 °C; ^1H NMR ($\text{DMSO}-d_6$) δ 2.42-2.41 (m, 1H), 1.39-1.38 (m, 1H), 1.31-1.24 (m, 14H), 0.85 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR ($\text{DMSO}-d_6$) δ 54.1, 54.1 (m), 33.8, 31.2, 29.0, 28.9, 28.6, 26.2, 22.0, 13.8; ^{19}F NMR ($\text{DMSO}-d_6$) δ -143.8 (m); ^{11}B NMR ($\text{DMSO}-d_6$) δ 1.88 (m).

Potassium *trans*-2-Phenyl-1-trifluoroboratooxirane (4b). The reaction was carried out at -78 °C. Reaction time 10 min, yield 70%. mp 210 °C (decomp); ^1H NMR ($\text{DMSO}-d_6$) δ 7.26 (t, $J = 7.5$ Hz, 2H), 7.19-7.15 (m, 3H), 3.39 (m, 1H), 1.78-1.77 (m, 1H); ^{13}C NMR ($\text{DMSO}-d_6$) δ 142.0, 128.1 (2C), 126.6, 125.1 (2C), 61.7 (m), 54.5; ^{19}F NMR ($\text{DMSO}-d_6$) δ -144.3 (m); ^{11}B NMR ($\text{DMSO}-d_6$) δ 392 (m).

Potassium *trans*-2-(Chloromethyl)-1-trifluoroboratooxirane (4c). Reaction time 40 min, yield 71%. mp 123 °C; ¹H NMR (acetone-*d*₆) δ 3.80 (dd, *J* = 11.3 and 3.2 Hz, 1H), 3.30 (dd, *J* = 11.3 and 7.6 Hz, 1H), 2.96-2.93 (m, 1H), 1.83-1.81 (m, 1H); ¹³C NMR (acetone-*d*₆) δ 55.9, 50.0; ¹⁹F NMR (acetone-*d*₆) δ -148.5 (q, *J* = 47.7 Hz); ¹¹B NMR (acetone-*d*₆) δ 2.62 (q, *J* = 54.5 Hz).

Potassium 1-Methyl-1-trifluoroboratooxirane (4d). Reaction time 1 h, yield 80%. mp 130 °C; ¹H NMR (DMSO-*d*₆) δ 3.07-3.05 (m, 2H), 0.80 (s, 3H); ¹³C NMR (DMSO-*d*₆) δ 55.9, 50.0; ¹⁹F NMR (DMSO-*d*₆) δ -149.7 (m); ¹¹B NMR (DMSO-*d*₆) δ 3.58 (m).

Potassium 2-Oxiranylethyltrifluoroborate (6). Reaction time 1 h, yield 70%. mp 192 °C; ¹H NMR (DMSO-*d*₆) δ 2.79-2.74 (m, 1H), 2.55 (dd, *J* = 4.3 and 3.3 Hz, 1H), 2.27 (dd, *J* = 5.3 and 2.7 Hz, 1H), 1.44-1.39 (m, 1H), 1.16-1.11 (m, 1H), -0.002 (m, 2H); ¹³C NMR (DMSO-*d*₆) δ 54.4, 46.4, 28.8; ¹⁹F NMR (DMSO-*d*₆) δ -137.8 (m); ¹¹B NMR (DMSO-*d*₆) δ 5.88 (m).

Procedure for the Cross-Coupling of Potassium 2-Oxiranylethyltrifluoroborate. Preparation of 4-(4-Cyanophenyl)-1,2-butanediol (8). To a suspension of **6** (50 mg, 0.28 mmol), Cs₂CO₃ (275 mg, 0.84 mmol), PdCl₂(dppf)-CH₂Cl₂ (20 mg, 0.025 mmol), and 4-bromobenzonitrile (45 mg, 0.25 mmol) in THF (3 mL) was added water (0.3 mL) under an argon atmosphere. The reaction mixture was stirred at reflux temperature for 8 h, then cooled to rt, diluted with water (10 mL) and extracted with ether (15 mL x 3). The combined organic extracts were washed with brine (20 mL) and then dried over MgSO₄. The solvent was removed *in vacuo* and the crude product was purified by silica gel column chromatography (eluting with hexane/EtOAc = 3/1) to yield **8** (35 mg, 74%). *R*_f = 0.25 (EtOAc/hexane = 1/3); mp 59 °C; ¹H NMR (CDCl₃) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 3.72-3.68 (m, 1H), 2.68-3.65 (m, 1H), 3.48 (dd, *J* = 10.7 and 6.1 Hz, 1H), 2.91-2.86 (m, 1H), 2.79-2.73 (m, 1H), 1.80-1.72 (m, 2H); ¹³C NMR (CDCl₃) δ 147.5, 132.2 (2C), 129.2 (2C), 118.9, 109.9, 71.1, 66.7, 34.0, 31.9; HRMS (EI) calcd for C₁₁H₁₃NO₂ (M+H)⁺ 192.1024, found 192.1026.

Preparation of 4-(2-Oxiranylethyl)benzonitrile (9). Following the above procedure but using a ratio 40:1 of THF/H₂O as solvent. The crude product was purified by silica gel column chromatography (eluting with hexane/EtOAc = 8/1) to yield **9** (38 mg, 80%). *R*_f = 0.30 (hexane/EtOAc = 1/7); ¹H NMR (CDCl₃) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 2.95-2.93 (m, 1H), 2.90-2.78 (m, 2H), 3.74 (t, *J* = 4.6 Hz, 1H), 2.49 (dd, *J* = 4.8 and 2.6 Hz, 1H), 1.96-1.92 (m, 1H), 1.82-1.77 (m, 1H); ¹³C NMR (CDCl₃) δ 146.8, 132.3 (2C), 129.1 (2C), 118.9, 110.0, 51.3, 47.1, 33.7, 32.4; HRMS (EI) calcd for C₁₁H₁₃NO₂ (M+H)⁺ 174.0922, found 174.0918.

(1) Adam, W.; Chan, Y-Y.; Cremer, D.; Gauss, J. Scheutzw, D. Schindler, M. *J. Org. Chem.* **1987**, *52*, 2800-2803.

(2) For characterization of **3c**: Molander, G. A.; Rodriguez, M. *Org. Lett.* **2002**, *4*, 107-109.

(3) Molander, G. A.; Bernardi, C. R. *J. Org. Chem.* **2002**, *67*, 8424-8429.

ppm
S4

7.27537
7.27164
7.26946
7.26326
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7.25482
7.25070
7.24590
7.24157
7.23775
7.23572
7.23406
7.11385
7.11144

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2.83384
2.81847
2.50754
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2.49826
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Current Data Parameters
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EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20021001
Time: 18.22
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl₃
NS: 47
DS: 2
SWH: 6009.615 Hz
FIDRES: 0.181399 Hz
AQ: 2.7363477 sec
RG: 812.7
DM: 83.200 usec
DE: 5.00 usec
TE: 300.0 K
D1: 1.00000000 sec
***** CHANNEL f1 *****
NUC1: 1H
P1: 7.50 usec
PL1: 0.00 dB
SFO1: 500.13625019 MHz
F2 - Processing parameters
SI: 32768
SF: 500.1360084 MHz
WDW: EM
SSB: 0
LB: -0.50 Hz
GB: 0.7
PC: 1.00
1D NMR plot parameters
CX: 22.00 cm
F1P: 10.000 ppm
F1: 500.1360084 MHz
F2P: -0.500 ppm
F2: -250.119 Hz
PPMCH: 0.47727 ppm/cm
HZCN: 238.82248 Hz/cm

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39.508
39.342
39.175
39.009
35.415
25.812

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127.255
124.704

Current Data Parameters
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EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20021004
Time 10.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 206
DS 4
SWH 31416.54 Hz
FIDRES 0.419916 Hz
AQ 1.040724 sec
RG 4096
DM 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0100000 sec
D12 0.0002000 sec

===== CHANNEL f1 =====
NUC1 13C
PC 10 usec
PA 1.00 dB
PL1 2.00 dB
SFO1 125.8169556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL3 26.00 dB
PL13 26.00 dB
SFO2 500.1320016 MHz

F2 - Processing parameters
SI 32768
SF 125.8232140 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
F1P 225.000 ppm
F1 28310.23 Hz
F2P -5.500 ppm
F2 -52.81 Hz
FREQH 30.25600 ppm/cm
FREQV 1289.66823 Hz/cm

ppm

137.15

Current Data Parameters
NAME mr01291
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030129
Time 10.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgfhgdn
TD 131072
SOLVENT DMSO
NS 245
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 1024
DW 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 19F
P1 10.60 usec
PL1 -3.00 dB
SFO1 470.7901483 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters
SI 65536
SF 470.8373320 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ID NMR plot parameters
CX 20.00 cm
FLP -104.548 ppm
F1 -49225.13 Hz
F2P -150.759 ppm
F2 -70983.11 Hz
PPMCH 2.31056 ppm/cm
HZCM 1087.89905 Hz/cm

ppm

PPM

Current Data Parameters
 NAME me2011
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030201
 Time 15.04
 INSTRUM spect
 PROBMOD 5 mm QNP 1H/1
 PULPROG zg30
 TD 32768
 SFO1 500.1360000 MHz
 SOLVENT CDCl3
 NS 45
 DS 2
 SWH 609.615 Hz
 FIDRES 0.161339 Hz
 AQ 2.7261477 sec
 RG 574.7
 DW 83.200 usec
 DB 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
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 SFO1 500.1360000 MHz

F2 - Processing parameters
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 SF 500.1360000 MHz
 WDW EM
 SSB 0
 LB -0.50 Hz
 GB 0.3
 PC 1.00

1D NMR plot parameters
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 F2 546.81 Hz
 F3 -1.055 ppm
 F4 -527.81 Hz
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 HZCH 273.10634 Hz/cm

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130.177
128.465

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40.372
40.205
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19.945

ppm

Current Data Parameters
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EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030222
Time 12.01
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PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 464
DS 4
SWH 31446.541 Hz
FIDRES 0.4778936 Hz
AQ 1.04220000 sec
RG 4096
DM 15.900 umsec
DE 6.00 umsec
TE 300.0 K
D1 1.00000000 sec
D11 0.01000000 sec
D12 0.00020000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 umsec
PL1 3.00 dB
SFO1 125.835556 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 umsec
PL2 0.00 dB
PL12 26.00 dB
PL13 26.00 dB
SFO2 500.1320016 MHz

F2 - Processing parameters
SI 32768
SF 125.8231160 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
F1P 234.956 ppm
F1 29562.86 Hz
F2P -14.971 ppm
F2 -1803.68 Hz
FREQ 111.6050000 MHz/cm
HZCM 1423.00010 Hz/cm

-137.64

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Current Data Parameters
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EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
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PULPROG   zgfhggn
TD         131072
SOLVENT   DMSO
NS         153
DS         4
SWH        100000.000 Hz
FIDRES     0.762919 Hz
AQ          0.6554100 sec
RG          1024
DM          5.000 usec
DE          6.000 usec
TE         300.0 K
D1          1.00000000 sec
D11         0.03000000 sec
D12         0.00002000 sec

===== CHANNEL f1 =====
NUC1       19F
P1          10.60 usec
PL1         -3.00 dB
SF01       470.7901483 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       100.00 usec
PL2          0.00 dB
PL12        26.00 dB
SF02        500.3920016 MHz

F2 - Processing parameters
SI          65536
SF          470.837320 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

1D NMR plot parameters
CX          20.00 cm
F1P         6.194 ppm
F1          2916.28 Hz
F2P        -206.194 ppm
F2         -97083.72 Hz
PPMCM       10.61938 ppm/cm
HZCM        4999.99951 Hz/cm

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2.04948
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4.02250
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ppm

Current Data Parameters
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EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 46
DS 2
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FIDRES 0.18139 Hz
AQ 2.723847 sec
RG 327.4
SFO 500.136099 MHz
DQ 83.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 0.00 dB
SFO1 500.136099 MHz

F2 - Processing parameters
SI 32768
SF 500.136099 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.3
PC 1.00

1D NMR Plot Parameters
CX 22.00 cm
P1P 10.000 ppm
F1 500.1360 Hz
F2P 250.1360 ppm
F3 250.1360 ppm
F4 0.47227 ppm/cm
FREQN 210.82248 Hz/cm

Current Data Parameters
 NAME m02241
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030225
 Time 12.42

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 PULPROG zgfhgqn
 TD 131072
 SOLVENT C6D6
 NS 29
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6554100 sec
 RG 1024
 DW 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 19F
 P1 10.60 usec
 PL1 -3.00 dB
 SFO1 470.7901483 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SFO2 500.3920016 MHz

F2 - Processing parameters
 SI 65536
 SF 470.8372320 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
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 F1 2916.28 Hz
 F2P -206.194 ppm
 F2 -97083.72 Hz
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 HZCM 4999.99951 Hz/cm

142.73
 142.86

ppm

Current Data Parameters
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PROCNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030225
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INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 481
DS: 4
SWH: 31445.541 Hz
FIDRES: 0.449816 Hz
AQ: 1.042072 sec
RG: 4096
BW: 15.500 usec
DE: 6.00 usec
TE: 300.0 K
D1: 3.0000000 sec
D11: 0.0100000 sec
D12: 0.0002000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 7.50 usec
PL1: 0.00 dB
SFO1: 125.819950 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 usec
PL2: 0.00 dB
PL12: 26.00 dB
PL13: 26.00 dB
SFO2: 500.132001 MHz

F2 - Processing parameters
SI: 32768
SF: 125.819950 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 22.00 cm
P1P: 225.000 ppm
F1: 28310.19 Hz
F2P: -0.500 ppm
F2: -0.279 Hz
PRCH: 10.25000 MHz/cm
HZCN: 1289.68628 Hz/cm

4 88752
4 15771

ppm

S15

2.50356
 2.49986
 2.49614
 2.42502
 2.41848
 1.39417
 1.38778
 1.38145
 1.31947
 1.29272
 1.27896
 1.24764
 0.87228
 0.85862
 0.84452

Current Data Parameters
 NAME: m01101
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20010130
 Time: 12.54
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/1
 PULPROG: zg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 10
 DS: 2
 SWH: 6009.615 Hz
 FIDRES: 0.183399 Hz
 AQ: 2.7163477 sec
 RG: 362
 DM: 83.200 usec
 DE: 6.00 usec
 TE: 100.0 K
 D1: 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 1.50 usec
 PL1: 0.00 dB
 SFO1: 500.1325019 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 500.1300081 MHz
 WDW: EM
 SSB: 0
 LB: -0.50 Hz
 GB: 0.3
 PC: 1.00
 ID: NMR plot parameters
 CZ: 22.00 cm
 F1P: 10.000 ppm
 F1: 5003.90 Hz
 F2P: -0.500 ppm
 F2: -250.19 Hz
 PPMCH: 0.47727 ppm/cm
 HZCM: 238.82248 Hz/cm

4a

-143.87

Current Data Parameters
 NAME mr01301
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20030130
 Time 12:57
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgfhgqn
 TD 131072
 SOLVENT C6D6
 NS 140
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6554100 sec
 RG 1024
 DW 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

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

NUC1 ¹⁹F
 P1 10.60 usec
 PL1 -3.00 dB
 SFO1 470.7901483 MHz

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

CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SFO2 500.3920016 MHz

F2 - Processing parameters

SI 65536
 SF 470.8372320 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 FIP -92.202 ppm
 FI -43412.32 Hz
 F2P -180.458 ppm
 F2 -84966.13 Hz
 PPMCM 4.41276 ppm/cm
 HZCM 2077.69092 Hz/cm

1.88365

ppm

4a

7.26486
7.24992
7.18266
7.17578
7.15962

3.39608
3.39003
2.50018
2.08480
1.78325

ppm

Current Data Parameters
NAME millil
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20011114
Time 15:48
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 17
DS 2
SWH 6009.615 Hz
FIDRES 0.181399 Hz
AQ 2.726177 sec
RG 362
DW 83.200 usec
DE 1.700 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 0.00 dB
SFO1 500.1365013 MHz

F2 - Processing parameters
SI 32768
SF 500.1365013 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.3
PC 1.00

1D NMR plot parameters
CX 22.00 cm
F1P 10.000 ppm
F1 500.90 Hz
F2P -0.500 ppm
F2 -250.19 Hz
PPOCK 0.47727 ppm/cm
RGCK 238.32240 Hz/cm

Integral

Current Data Parameters
NAME: m01102
EXPNO: 5
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030130
Time: 21.30
INSTRUM: spect
PROBHD: 5 mm QNP 1H/1
PULPROG: zgpg
TD: 65536
SOLVENT: CDCl3
NS: 1490
DS: 4
SWH: 31446.644 Hz
FIDRES: 0.078916 Hz
AQ: 1.0420724 sec
RG: 7298.2
RW: 15.900 usec
DE: 6.00 usec
TE: 300.0 K
D1: 4.00000000 sec
D11: 0.03000000 sec
D12: 0.00002000 sec

***** CHANNEL f1 *****
NUC1: 13C
P1: 7.50 usec
PL1: 0.00 dB
SFO1: 125.8169556 MHz

***** CHANNEL f2 *****
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 usec
PL2: 0.00 dB
PL12: 26.00 dB
PL13: 26.00 dB
SFO2: 500.3620016 MHz

F2 - Processing parameters
SI: 32768
SF: 125.8169556 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40

1D NMR plot parameters
CX: 22.00 cm
F1P: 234.956 ppm
F1: 2354.97 Hz
F2P: 144.350 ppm
F2: -1483.44 Hz
FREQ: 111.36030 ppm/cm
HZCM: 1423.38953 Hz/cm

144.30

Current Data Parameters
NAME mr01302
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030130
Time 15.33
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgfhgqn
TD 131072
SOLVENT C6D6
NS 182
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 1024
DW 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

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

NUC1 19F
P1 10.60 usec
PL1 -3.00 dB
SFO1 470.7901483 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SFO2 500.3920016 MHz

F2 - Processing parameters

SI 65536
SF 470.837320 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 6.194 ppm
F1 2916.28 Hz
F2P -206.194 ppm
F2 -97083.72 Hz
PPMCM 10.61938 ppm/cm
HZCM 4999.99951 Hz/cm

3.92055

ppm

S23

4c

Current Data Parameters
 NAME: m2011
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20030201
 Time: 14.48
 INSTRUM: spect
 PULPROG: 5 mm QNP 1H/1
 zg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 20
 DS: 4
 SWH: 6009.615 Hz
 FIDRES: 0.181359 Hz
 AQ: 2.726197 sec
 RG: 456.1
 DW: 83.200 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.0000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.1325015 MHz

F2 - Processing parameters
 SI: 32768
 SF: 500.1300124 MHz
 WDW: EM
 SSF: 0
 LB: -0.50 Hz
 GB: 0.3
 PC: 1.00

1D NMR plot parameters
 CA: 2.00 cm
 FID: 10.900 cm
 FI: 5194.32 Hz
 F2: -1.030 ppm
 F3: -515.10 Hz
 PPMCK: 0.54590 ppm/cm
 HZCM: 273.16434 Hz/cm

4c

Current Data Parameters
NAME m02061
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030212
Time 12.16
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT AcetD
NS 710
DS 4
SWH 31446.541 Hz
FIDRES 0.479816 Hz
AQ 1.0420724 sec
RG 5792.6
DM 15.900 usec
DE 6.00 usec
TE 300.2 K
D1 4.0000000 sec
D11 0.0200000 sec
D12 0.0002000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 7.50 usec
PL1 3.00 dB
SFO1 125.8169556 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 500.1320016 MHz

F2 - Processing parameters
SI 32768
SF 125.820386 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
P1P 225.000 ppm
F1 28310.19 Hz
F2P -0.500 ppm
F2 -62.91 Hz
PPMCK 10.25000 ppm/cm
HZCN 1285.68616 Hz/cm

ppm
206.344
206.267

ppm

200

150

100

50

4c

Current Data Parameters
NAME mr2011
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030201
Time 14.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgfhgqn
TD 131072
SOLVENT C6D6
NS 88
DS 4
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6554100 sec
RG 1024
LW 5.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 19F
P1 10.60 usec
PL1 -3.00 dB
SF01 470.7901483 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
SF02 500.3920016 MHz

F2 - Processing parameters
SI 65536
SF 470.8372320 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 6.194 ppm
F1 2916.28 Hz
F2P -206.194 ppm
F2 -97083.72 Hz
PPMCH 10.61938 ppm/cm
HZCM 4999.99951 Hz/cm

3.04849
2 1.9832

ppm

Current Data Parameters
 NAME M11062
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20021106
 Time 11.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 32768
 SFO 500.136079 MHz
 CQ 13
 NS 16
 DS 2
 SWH 6009.615 Hz
 FIDRES 0.181199 Hz
 AQ 2.7163477 sec
 RG 322.5
 DM 83.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

***** CHANNEL f1 *****
 NUCL 13C
 P1 1.50 usec
 PL1 0.00 dB
 SFO1 500.136079 MHz

F2 - Processing parameters
 SI 32768
 SF 500.136079 MHz
 WDW EM
 SSB 0
 GB 0.50 Hz
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 P1P 10.000 ppm
 P1 5003.90 Hz
 P2P -0.500 ppm
 P2 -250.19 Hz
 PPMCH 0.47727 ppm/cm
 HZCH 228.82248 Hz/cm

ppm

Integral

ppm

4d

Current Data Parameters
 NAME m02241
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20010225
 Time 14.16
 INSTRUM spect
 PROBRW 5 mm QNP
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 700
 DS 4
 SWH 31446.541 Hz
 FIDRES 0.479816 Hz
 AQ 1.6120724 sec
 RG 4096
 DW 15.900 usec
 DE 6.00 usec
 TE 300.0 K
 D1 3.0000000 sec
 D11 0.0300000 sec
 D12 0.0002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.50 usec
 PL1 3.00 dB
 SFO1 125.8199556 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 25.00 dB
 PL3 25.00 dB
 SFO2 500.1370016 MHz

F2 - Processing parameters
 SI 32768
 SF 125.822244 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 SI 32768
 SF 125.822244 MHz
 F1 234.605 ppm
 F2 29518.80 Hz
 F3 -15.451 ppm
 F4 -1944.10 Hz
 PPMCH 11.36620 ppm/cm
 HZCH 1430.13184 Hz/cm

4d

-149.60

Current Data Parameters
 NAME m02241
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030225
 Time 13.28
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgfhqgn
 TD 131072
 SOLVENT C6D6
 NS 60
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6554100 sec
 RG 1625.5
 DW 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 19F
 P1 10.60 usec
 PL1 -3.00 dB
 SFO1 470.7901483 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SFO2 500.3920016 MHz

F2 - Processing parameters
 SI 65536
 SF 470.8372320 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 6.194 ppm
 F1 2916.28 Hz
 F2P -206.194 ppm
 F2 -97083.72 Hz
 PPMCM 10.61938 ppm/cm
 HZCM 4999.99951 Hz/cm

3.58419

ppm

4d

5

ppm

Current Data Parameters
 NAME: m11264
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20021126
 Time: 20:29
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/13
 PULPROG: zgpg30
 TO: 32768
 SOLVENT: CDCl3
 NS: 41
 DS: 1
 SWH: 8064.516 Hz
 FIDRES: 0.246110 Hz
 AQ: 2.0316660 sec
 RG: 256
 DW: 62.000 usec
 DE: 66.37 usec
 TE: 300.2 K
 NUC1: 13C
 P1: 1.0000000 sec
 PL1: 12.00 usec
 SF01: 500.3822518 MHz
 NUCLEUS: 13C
 F2 - Processing parameters
 SI: 32768
 SF: 500.3800126 MHz
 WDW: EM
 SSB: 0
 LB: -0.50 Hz
 GB: 0.3
 PC: 1.40
 1D NMR plot parameters
 CX: 22.00 cm
 FIP: 10.000 ppm
 FI: 5003.90 Hz
 F2P: -0.500 ppm
 F2: -250.19 Hz
 PPH0H: 0.47727 ppm/
 HZCM: 230.82248 Hz/c

S32

Current Data Parameters
NAME ml1264
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20021126
Time 20.32
INSTRUM amx500
PROBHD 5 mm Dual 13
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 55
DS 2
SWH 33333.332
FIDRES 0.508626
AQ 0.9830900
RG 16384
DW 15.000
DE 18.75
TE 300.0
HL1 40
D1 5.0000000
CPOPRG waltz16
P31 107.00
S4 24
D11 0.0300000
S2 18
P1 5.00
SF01 125.8382148
NUCLEUS 13C

F2 - Processing parameters
S1 32768
SF 125.8230578
WDW EM
SSB 0
LB 1.50
GB 0
PC 1.40

1D NMR plot parameters
CX 21.00
FIP 225.000
F1 28310.19
F2P -0.500
F2 -62.91
PPMCM 10.73810
HZCM 1351.09998

Current Data Parameters
 NAME ml1271
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20021127
 Time 12.20
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgfhgqn
 TD 131072
 SOLVENT C6D6
 NS 78
 DS 4
 SWH 100000.000 Hz
 FIDRES 0.762939 Hz
 AQ 0.6554100 sec
 RG 1024
 DW 5.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 19F
 P1 10.60 usec
 PL1 -3.00 dB
 SFO1 470.790483 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 0.00 dB
 PL12 26.00 dB
 SFO2 500.3920016 MHz

F2 - Processing parameters
 SI 65536
 SF 470.8172320 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 6.194 ppm
 F1 2916.28 Hz
 F2P -206.194 ppm
 F2 -97083.72 Hz
 PPMCM 10.61938 ppm/cm
 HZCM 4999.99951 Hz/cm

141.72
 141.86

7.80748
6.92486

PPM

6

6

Current Data Parameters
 NAME: 1001151
 EXPNO: 7
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20030215
 Time: 13.24
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/1
 PULPROG: zgpg
 TD: 65536
 SFO: 500.132016 MHz
 SOLVENT: DMSO
 NS: 178
 DS: 4
 SWH: 31446.541 Hz
 FIDRES: 0.479816 Hz
 AQ: 1.0420724 sec
 RG: 14596.5
 DW: 15.900 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 3.00000000 sec
 D11: 0.01000000 sec
 D12: 0.00020000 sec

***** CHANNEL f1 *****
 NUC1: 13C
 P1: 7.50 usec
 PL1: 3.00 dB
 SFO1: 125.8169556 MHz

***** CHANNEL f2 *****
 CPOPRG2: waltz16
 NUC2: 1H
 P2: 100.00 usec
 PL2: 0.00 dB
 PL12: 26.00 dB
 PL13: 26.00 dB
 SFO2: 500.132016 MHz

F2 - Processing parameters
 SI: 32768
 SF: 125.822331 MHz
 WDW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CX: 21.00 cm
 F1: 271.450 ppm
 F2: 29518.450 ppm
 F3: 215.450 ppm
 F4: -1544.10 Hz
 FPMCH: 11.16620 ppm/cm
 HZCN: 1430.13196 Hz/cm

6

Current Data Parameters	
NAME	mr01311
EXPNO	4
PROCNO	1

[illegible]

```
===== CHANNEL f1 =====
===== 19F =====
NUC1
P1      10.60 usec
PL1     -3.00 dB
SF01    470.7901483 MHz
```

```
===== CHANNEL f2 =====
CPDRG2      waltz16
NUC2        1H
PCPD2       100.00 usec
PL2         0.00 dB
PLI2        26.00 dB
SF02        500.3920016 MHz
```

F2 - Processing parameters	
SI	65536
SF	470.8372320 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters	
CX	20.00 cm
F1P	6.194 ppm
F1	2916.28 Hz
F2P	-206.194 ppm
F2	-97083.72 Hz
PGMCM	10.61938 ppm/cm
H2CM	4999.99951 Hz/cm

6

6.35157
5.41907

```

Current Data Parameters
NAME      1
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20021205
Time      16.50
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         512
DS         4
SWH        6009.415 Hz
FIDRES     0.183399 Hz
AQ         2.7263477 sec
RG         203.2
DM         83.200 usec
DE         6.00 usec
TE         300.0 K
D1         1.0000000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
PL         0.00 dB
PC         0.00 dB
SFO1       500.1362919 MHz

F2 - Processing parameters
SI         32768
SF         500.1360157 MHz
WDW        EM
SSB        0
LB         0.3
GB         0.3
PC         1.00

1D NMR plot parameters
CQ         22.00 cm
P1P        10.000 ppm
F1         500.90 Hz
F2P        -0.500 ppm
F2         -250.19 Hz
PPMCH      0.47727 ppm/cm
HZCM       238.42248 Hz/cm

```

7.60438
7.58803
7.33364
7.31735
7.26964

2.95282
2.94729
2.93928
2.93364
2.89492
2.88323
2.87680
2.86312
2.84702
2.82968
2.78323
2.77400
2.76557
2.76577
2.49905
2.49370
2.48932
2.48403
1.96252
1.94850
1.82174
1.80462

ppm

Current Data Parameters
Date_ 20021212
Time 18.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
DS 3
SWH 600.615 Hz
FIDRES 0.18339 Hz
AQ 2.7263477 sec
RG 645.1
DM 83.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.50 usec
PL1 0.00 dB
SFO1 500.3925019 MHz

F2 - Processing parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F3 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F4 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F5 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F6 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F7 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F8 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F9 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F10 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F11 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F12 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F13 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F14 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F15 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F16 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F17 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F18 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F19 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F20 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F21 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F22 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F23 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F24 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F25 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F26 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F27 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F28 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F29 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F30 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F31 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F32 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F33 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F34 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F35 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F36 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F37 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F38 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F39 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F40 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F41 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F42 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F43 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F44 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F45 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F46 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F47 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F48 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F49 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

F50 - NMR plot parameters
SI 32768
SF 500.3900115 MHz
WDW EM
SSB 0
LB -0.50 Hz
GB 0.1
PC 1.00

31.939
34.073

66.703
71.113
76.748
77.002
77.256

109.905

118.966

129.242
132.259

147.522

ppm

```

Current Data Parameters
NAME      M12051
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20021205
Time      16.58
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg
TD         65536
SOLVENT   CDCl3
NS         146
DS         4
SWH        31446.541 Hz
FIDRES     0.479816 Hz
AQ         1.0420724 sec
RG         6096
DM         15.900 usec
DE         6.00 usec
TE         300.0 K
D1         3.00000000 sec
D11        0.01000000 sec
D12        0.00020000 sec

***** CHANNEL f1 *****
NUC1       13C
P1         7.50 usec
PL1        3.00 dB
SFO1       125.8169556 MHz

***** CHANNEL f2 *****
CPDPRG2    waltz16
NUC2       1H
P2         100.00 usec
PL2        0.00 dB
PUL2       28.00 dB
PL12       28.00 dB
SFO2       500.1320016 MHz

F2 - Processing parameters
SI         32768
SF         125.8231675 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

1D NMR plot parameters
CX         22.00 cm
P1P        25500 ppm
F1P        11.11111111 MHz
P2P        -0.500 ppm
F2P        -62.91 Hz
PPMCM      10.25000 ppm/cm
HZCM       1289.68750 Hz/cm

```

146.872
132.311
129.193
118.964
110.047
77.793
77.250
76.996
76.742
51.388
47.155
33.713
32.452

ppm

Current Data Parameters
NAME: m02222
EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
Date_ 20010222
Time 16.37
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 1919
DS 4
SWH 31446.541 Hz
FIDRES 0.479318 Hz
AQ 1.044578 sec
RG 327.064
RW 15.900 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
D11 0.0300000 sec
D12 0.0002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.50 usec
PL1 3.00 dB
SFO1 125.819558 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 26.00 dB
PL13 26.00 dB
SFO2 500.1320016 MHz

F2 - Processing parameters
SI 32768
SF 500.1320016 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
F1P 234.605 ppm
F1 29518.79 Hz
F2P -15.451 ppm
F2 -194.130 Hz
PPMCH 11.3850 ppm/cm
NUC1 13C