Supporting Information for Letter Entitled

“N-Heterocyclic Carbene Catalyzed Mukaiyama Aldol Reactions”

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General procedures:

All reactions were performed in oven-dried glassware under nitrogen with magnetic or mechanical stirring. All commercial reagents were used as received. Flash chromatography was performed using 230-400 mesh silica gel. HPLC analyses were performed on a 4.6 mm x 10 cm column with particle size of 2 micron; at wavelength 220 nm, at 25 °C. Mobile phases are A: water with 0.05% TFA, B: MeCN with 0.05% TFA. Gradient conditions are 90% A to 10% A in 15 min, hold 5 min, back to 90% A followed by a 3-min post run.

Procedure A: Aldol reactions between aldehydes and methyl trimethylsilyl dimethylketene acetal (2):

To aldehyde (3.0 mmol) in a dry flask under N₂ were added THF (anhydrous, 15 mL), methyl trimethylsilyl dimethylketene acetal (0.66 g, 3.60 mmol based on 95% purity) and

carbene **5** (5 mg, 0.014 mmol). The mixture was stirred at 23 °C for 3 h. HCl solution (1 N, 3 mL) was added and the solution was stirred at 23 °C for 1 h. Saturated NaHCO₃ aq solution (3 mL) and water (3 mL) were added. Dichloromethane (50 mL) was added and the aqueous layer was extracted with dichloromethane (50 mL). Organic layers were combined and solvents were removed under vacuum to give the crude residue, which was purified by silica gel flash chromatography (ethyl acetate/hexanes) to give pure product.

Compound **6a** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (5-35% EtOAc/hexanes) in 77% yield. ¹H NMR (CDCl₃, 400 MHz) δ 7.74-7.83 (m, 4H), 7.41-7.49 (m, 3H), 5.05 (d, *J* = 4.2 Hz, 1H), 3.72 (s, 3H), 3.28 (d, *J* = 4.2 Hz, 1H), 1.18 (s, 3H), 1.14 (s, 3H). ¹³C NMR (CDCl₃, 100 MHz) δ 178.3, 137.5, 133.0, 132.8, 128.1, 127.6, 127.3, 126.7, 126.1, 126.0, 125.7, 78.8, 52.2, 48.0, 23.2, 19.2.

Compound **6b** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (10-35% EtOAc/hexanes) in 76% yield. ¹H NMR (CDCl₃, 400 MHz) δ 7.29 (m, 5H), 4.89 (d, *J* = 4.2 Hz, 1H), 3.72 (s, 3H), 3.08 (d, *J* = 4.2 Hz, 1H), 1.14 (s, 3H), 1.11 (s, 3H). ¹³C NMR (CDCl₃, 100 MHz) δ 178.2, 139.9, 127.8, 127.7, 78.7, 52.1, 47.7, 23.0, 19.0.

Compound **6c** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (5-35% EtOAc/hexanes) in 83% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 8.15-8.17 (m, 1H), 7.79-7.87 (m, 2H), 7.67-7.69 (m, 1H), 7.44-7.52 (m, 3H), 5.94 (d, J = 3.9 Hz, 1H), 3.74 (s, 3H), 3.13 (d, J = 4.0 Hz, 1H), 1.25 (s, 3H), 1.08 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 178.5, 136.2, 133.5, 131.8, 128.9, 128.4, 126.1, 125.8, 125.3, 125.0, 123.7, 72.9, 52.2, 48.7, 23.9, 19.0.

Compound **6d** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (5-25% EtOAc/hexanes) in 83% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 7.18 (d, J = 8.1 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 4.86 (d, J = 4.2 Hz, 1H), 3.72 (s, 3H), 2.99 (d, J = 4.3 Hz, 1H), 2.34 (s, 3H), 1.14 (s, 3H), 1.10 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 178.2, 137.4, 137.0, 128.5, 127.5, 78.6, 52.1, 47.7, 23.1, 21.1, 19.0.

Compound **6e** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (10-40% EtOAc/hexanes) in 91% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 7.21 (d, J = 8.6 Hz, 2H), 6.85 (d, J = 8.6 Hz, 2H), 4.85 (d, J = 4.1 Hz, 1H), 3.80 (s, 3H), 3.72 (s, 3H), 3.03 (d, J = 4.1 Hz, 1H), 1.13 (s, 3H), 1.09 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 178.3, 159.1, 132.1, 128.7, 113.2, 78.3, 55.2, 52.1, 47.8, 23.0, 19.0.

Compound **6f** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (5-35% EtOAc/hexanes) in 81% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 7.29 (d, J = 8.4 Hz, 2H), 7.22 (d, J = 8.4 Hz, 2H), 4.85 (d, J = 3.5 Hz, 1H), 3.70 (s, 3H), 3.37 (d, J = 4.1 Hz, 1H), 1.11 (s, 3H), 1.08 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 178.1, 138.5, 133.5, 129.0, 127.9, 77.9, 52.2, 47.6, 22.8, 19.0.

Compound **6g** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (5-30% EtOAc/hexanes) in 68% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 7.62 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 8.2 Hz, 2H), 4.95 (d, J = 4.3 Hz, 1H), 3.73 (s, 3H), 3.38 (d, J = 4.3 Hz, 1H), 1.13 (s, 3H), 1.11 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 177.8, 145.3, 131.6, 128.5, 118.7, 111.6, 77.9, 52.4, 47.6, 22.8, 19.1.

Compound **6h** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (10-30% EtOAc/hexanes) in 75% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 8.19 (d, J = 8.8 Hz, 2H), 7.50 (d, J = 8.8 Hz, 2H), 5.00 (d, J = 4.3 Hz, 1H), 3.74 (s, 3H), 3.40 (d, J = 4.3 Hz, 1H), 1.15 (s, 3H), 1.13 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 177.8, 147.5, 147.2, 128.6, 123.0, 77.8, 52.4, 47.6, 22.8, 19.2.

Compound **6i** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (7-20% EtOAc/hexanes) in 74% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 7.27-7.42 (m, 5H), 6.66 (d, J = 15.9 Hz, 1H), 6.24 (dd, J = 7.1, 15.8 Hz, 1H), 4.38 (t, J = 5.9 Hz, 1H), 3.74 (s, 3H), 2.90 (d, J = 5.6 Hz, 1H), 1.27 (s, 3H), 1.26 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 177.9, 136.6, 132.9, 128.6, 127.8, 127.5, 126.6, 77.8, 52.1, 47.2, 22.8, 20.0.

Compound **6j** was prepared by using **Procedure A** and isolated by silica gel flash chromatography (5-15% EtOAc/hexanes) in 61% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 3.66 (s, 3H), 3.48 (d, J = 8.0 Hz, 1H), 2.48 (d, J = 8.0 Hz, 1H), 1.26 (s, 6H), 0.94 (s, 9H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 178.5, 83.2, 51.8, 47.0, 37.0, 27.7, 25.8, 22.7. HRMS calcd for $[\text{M}+\text{H}]^+$ $\text{C}_{10}\text{H}_{21}\text{O}_3$, m/z 189.1485, found: 189.1477. IR (cm^{-1}): 3118, 2938, 1700, 1473, 1238, 623.

Compound **6k** was prepared by using **Procedure A** and isolated without chromatography in 60% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 3.70 (s, 3H), 3.38 (s, 1H), 2.87 (brs, 1H), 1.85 (m, 1H), 1.28 (s, 3H), 1.19 (s, 3H), 0.97 (d, J = 6.9 Hz, 3H), 0.80 (d, J = 6.8 Hz, 3H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 178.6, 81.7, 51.9, 45.9, 29.9, 23.9, 22.4, 21.7, 16.1.

Procedure B: Aldol reaction between 2,2,2-trifluoroacetophenone (1m) and methyl trimethylsilyl dimethylketene acetal (2):

To 2, 2, 2-Trifluoroacetophenone (0.53 g, 3.0 mmol) in a dry flask under N₂ were added THF (anhydrous, 15 mL), methyl trimethylsilyl dimethylketene acetal (0.66 g, 3.60 mmol based on 95% purity) and carbene **5** (5 mg, 0.014 mmol). The mixture was stirred at 23 °C for 3 h. HCl aq solution (1 N, 3 mL) was added and most of the solvent was evaporated under vacuum. Methanol (15 mL) and HCl aq solution (1 N, 3 mL) was added and the solution was stirred at 23 °C for 10 days. Saturated NaHCO₃ solution (3 mL) and water (3 mL) were added and most of the solvent was evaporated under vacuum. Dichloromethane (50 mL) was added and the aqueous layer was extracted with dichloromethane (50 mL). Organic layers were combined and solvents were removed under vacuum to give the crude residue, which was purified by silica gel flash chromatography (10% ethyl acetate/hexanes) to give pure product **6m** as a colorless oil (0.71 g, 87% yield). ¹H NMR (CDCl₃, 400 MHz) δ 7.70 (m, 2H), 7.38 (m, 3H), 5.76 (s, 1H), 3.81 (s, 3H), 1.35 (s, 3H), 1.08 (s, 3H). ¹³C NMR (CDCl₃, 100 MHz) δ 178.2, 133.9, 128.7, 127.9, 127.7, 126.1 (q, *J*_{C-F} = 286 Hz), 80.5 (q, *J*_{C-F} = 26 Hz), 53.2, 46.8, 23.8, 20.5. HRMS: calcd for [M+H]⁺ C₁₃H₁₆F₃O₃, *m/z* 277.1046, found: *m/z* 277.1042. IR (cm⁻¹): 2958, 1699, 1474, 1451, 1437, 1287, 1267, 1195, 1150, 1069, 973, 937, 918, 763, 729, 705, 634, 540, 499.

Procedure C: Aldol reactions between aldehydes and 1-phenyl-1-(trimethylsilyloxy)ethylene (7):

To aldehyde (3.0 mmol) in a dry flask under N₂ were added THF (anhydrous, 15 mL) and 1-phenyl-1-(trimethylsilyloxy)ethylene (0.75 mL, 3.60 mmol based on 98% purity). The solution was cooled to -30 °C and carbene **5** (5 mg, 0.014 mmol) was added in one portion. The mixture was stirred at 0 °C for 65 h. HCl aq solution (1 N, 3 mL) was added and the solution was stirred at 23 °C for 1 h. Saturated NaHCO₃ aq solution (3 mL) and water (3 mL) were added. Dichloromethane (60 mL) was added and the aqueous layer was extracted with dichloromethane (30 mL). Organic layers were combined and solvents were removed under vacuum to give the crude residue, which was purified by silica gel flash chromatography (ethyl acetate/hexanes) to give product in yield indicated below.

Compound **8d** was prepared by using **Procedure C** and isolated by silica gel flash chromatography (10% EtOAc/hexanes) in 74% yield. ¹H NMR (CDCl₃, 400 MHz) δ 7.96-7.94 (m, 2H), 7.60-7.56 (m, 1H), 7.48-7.44 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 5.32-5.30 (m, 1H), 3.54-3.53 (m, 1H), 3.37 (d, *J* = 3.0 Hz, 1H), 3.35 (s, 1H), 2.35 (s, 3H). ¹³C NMR (CDCl₃, 100 MHz) δ 200.2, 140.0, 137.4, 136.6, 133.6, 129.2, 128.7, 128.2, 125.7, 69.9, 47.4, 21.1.

Compound **8e** was prepared by using **Procedure C** and isolated by silica gel flash chromatography (5-30% EtOAc/hexanes) in 10% yield. ¹H NMR (CDCl₃, 400 MHz) δ

7.97-7.95 (m, 2H), 7.59-7.57 (m, 1H), 7.49-7.45 (m, 2H), 7.38-7.36 (m, 2H), 6.93-6.90 (m, 2H), 5.28-5.32 (m, 1H), 3.82 (s, 3H), 3.53 (d, $J = 2.9$ Hz, 1H), 3.37 (d, $J = 3.2$ Hz, 1H), 3.36 (s, 1H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 200.3, 159.1, 136.6, 135.1, 133.6, 128.7, 128.2, 127.0, 113.9, 69.7, 55.3, 47.3.

Compound **8f** was prepared by using **Procedure C** and isolated by silica gel flash chromatography (10-30% EtOAc/hexanes) in 60% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 7.96-7.94 (m, 2H), 7.62-7.58 (m, 1H), 7.49-7.45 (m, 2H), 7.39-7.33 (m, 4H), 5.34-5.31 (m, 1H), 3.67 (d, $J = 3.0$ Hz, 1H), 3.35-3.29 (m, 2H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 200.0, 141.4, 136.4, 133.8, 133.3, 128.8, 128.7, 128.1, 127.2, 69.4, 47.2.

Compound **8h** was prepared by using **Procedure C** and isolated by silica gel flash chromatography (10% EtOAc/hexanes) in 84% yield. ^1H NMR (CDCl_3 , 400 MHz) δ 8.26-8.22 (m, 2H), 7.96-7.94 (m, 2H), 7.64-7.60 (m, 3H), 7.51-7.47 (m, 2H), 5.47-5.45 (m, 1H), 3.87 (d, $J = 2.9$ Hz, 1H), 3.45-3.31 (m, 2H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 199.5, 150.2, 147.4, 136.1, 134.1, 128.9, 128.2, 126.6, 123.8, 69.2, 47.0.

Compound **8n** was prepared by using **Procedure C** and isolated by silica gel flash chromatography (5-30% EtOAc/hexanes) in 25% yield. ^1H NMR (CDCl_3 , 400 MHz) δ

7.95-7.92 (m, 2H), 7.61-7.56 (m, 1H), 7.49-7.45 (m, 2H), 7.31-7.17 (m, 5H), 4.26-4.23 (m, 1H), 3.37 (brs, 1H), 3.17 (dd, $J = 17.7, 2.8$ Hz, 1H), 3.07 (dd, $J = 17.7, 8.9$ Hz, 1H), 2.93-2.86 (m, 1H), 2.80-2.72 (m, 1H), 1.98-1.91 (m, 1H), 1.85-1.80 (m, 1H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 200.9, 141.9, 136.7, 133.6, 128.7, 128.5, 128.4, 128.1, 125.9, 67.0, 45.0, 38.1, 31.9.

Procedure D: Aldol reaction between 2,2,2-trifluoroacetophenone (1m) and 1-phenyl-1-(trimethylsilyloxy)ethylene (7):

To 2, 2, 2-Trifluoroacetophenone (0.53 g, 3.0 mmol) in a dry flask under N_2 were added THF (anhydrous, 15 mL) and 1-phenyl-1-(trimethylsilyloxy)ethylene (0.75 mL, 3.60 mmol based on 98% purity). The solution was cooled to $-30\text{ }^\circ\text{C}$ and carbene **5** (5 mg, 0.014 mmol) was added in one portion. The mixture was stirred at $0\text{ }^\circ\text{C}$ for 65 h. HCl aq solution (1 N, 3 mL) was added and most of the solvent evaporated under vacuum. Methanol (15 mL) and HCl aq solution (1 N, 3 mL) was added and the solution was stirred at $23\text{ }^\circ\text{C}$ for 70 h. Saturated NaHCO_3 solution (3 mL) and water (3 mL) were added. Most of the solvents were evaporated under vacuum and dichloromethane (60 mL) was added and the aqueous layer was extracted with dichloromethane (30 mL). Organic layers were combined and solvents were removed under vacuum to give the crude residue, which was purified by silica gel flash chromatography (5% ethyl acetate/hexanes) to give pure product **8m** as a colorless oil (0.84 g, 95% yield). ^1H NMR (CDCl_3 , 400 MHz) δ 7.93-7.91 (m, 2H), 7.63-7.59 (m, 3H), 7.49-7.45 (m, 2H), 7.37-7.29 (m, 3H), 5.70 (s, 1 H), 4.04 (d, $J = 17.3$ Hz, 1H), 3.64 (d, $J = 17.4$ Hz, 1H). ^{13}C NMR (C_6D_6 , 100 MHz) δ

199.8, 138.4, 136.6, 134.1, 128.81, 128.78, 128.6, 128.4, 126.8, 125.5 (q, $J_{\text{C-F}} = 283 \text{ Hz}$),
76.9 (q, $J_{\text{C-F}} = 28 \text{ Hz}$), 40.2.

S11

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 LB 0.30 Hz
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NAME
PROCNO 1

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S13

Current Data Parameters
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PROCNO 1

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FIDRES 0.252629 Hz
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514

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F2 - Processing parameters
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S15

Current Data Parameters
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 FIDRES 0.252629 Hz
 AQ 1.9792372 sec
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RG            8192
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LIS

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NAME	Oct11-2006
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RG	8192
DW	20.850 usec
DE	6.00 usec
TE	295.2 K
DL	0.50000000 sec
d11	0.03000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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NUC2	¹ H
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519

Current Data Parameters
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 PROCNO 1

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 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.252629 Hz
 AQ 1.9792372 sec
 RG 57
 DW 60.400 usec
 DE 6.00 usec
 TE 295.2 K
 DL 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.06 usec
 PL1 -2.00 dB
 SFO1 400.3332026 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.3300051 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

EXPNO 201
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061013
Time 3.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 13004
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
DI 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters
SI 32768
SF 100.6630590 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S21

Current Data Parameters
 NAME Oct12-2006
 EXPNO 210
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061012
 Time 16.24
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.252629 Hz
 AQ 1.9792372 sec
 RG 40.3
 DW 60.400 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 9.06 usec
 PL1 -2.00 dB
 SFO1 400.3332026 MHz

F2 - Processing parameters
 SI 32768
 SF 400.3300008 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

EXPNO 211
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061013
Time 5.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 9195.2
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNMR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters
SI 32768
SF 100.6630590 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Current Data Parameters
 NAME Oct11-2006
 EXPNO 270
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061011
 Time 15.38
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 322.5
 DW 60.400 usec
 DE 6.00 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130058 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

524

EXPNO 320
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061012
Time 3.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8196
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 9195.2
DM 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters
SI 32768
SF 100.6630592 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S25

Current Data Parameters
 NAME Oct11-2006
 EXPNO 310
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20061011
 Time 16.20
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 456.1
 DW 60.400 usec
 DE 6.00 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NAME Oct11-2006
EXPNO 341
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061012
Time 7.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6493
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters
SI 32768
SF 100.6630590 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

527

Current Data Parameters
 NAME Oct11-2006
 EXPNO 220
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061011
 Time 14.13
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 90.5
 DW 60.400 usec
 DE 6.00 usec
 TE 297.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

85

EXPNO 221
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061011
Time 21.04
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 143.7
DM 20.850 usec
DE 6.00 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 9.50 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 0.00 dB
PL12 17.00 dB
PL13 10.79 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S29

Current Data Parameters
NAME Oct13-2006
EXPNO 130
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061013
Time_ 15.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 50.8
DE 60.400 usec
TE 295.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.06 usec
PL1 -2.00 dB
SFO1 400.3332026 MHz

F2 - Processing parameters
SI 32768
SF 400.3300072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

===== CHANNEL f1 =====
 NAME Oct13-2006
 EXPNO 131
 PROCNO 1

===== CHANNEL f2 =====
 NAME Oct13-2006
 EXPNO 131
 PROCNO 1

===== Acquisition Parameters =====
 Date_ 20061014
 Time 4.24
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8192
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 16384
 DW 20.850 usec
 DE 6.00 usec
 TE 295.2 K
 D1 0.50000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.10 usec
 PL1 -3.00 dB
 SFO1 100.6731249 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 18.86 dB
 PL13 18.86 dB
 SFO2 400.3316013 MHz

===== Processing Parameters =====
 SI 32768
 SF 100.6630590 MHz
 MDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

133

Current Data Parameters
 NAME Nov15-2006
 EXPNO 80
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061115
 Time 10.24
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.252629 Hz
 AQ 1.9792372 sec
 RG 143.7
 DW 60.400 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.06 usec
 PL1 -2.00 dB
 SFO1 400.3332026 MHz

F2 - Processing parameters
 SI 32768
 SF 400.3300034 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NAME: NOV10-2000
EXPNO: 311
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20061116
Time: 21.19

INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
DS: 4096
SWH: 23980.814 Hz
FIDRES: 0.365918 Hz
AQ: 1.3664756 sec
RG: 8192
DW: 20.850 usec
DE: 6.00 usec
TE: 297.2 K
D1: 0.50000000 sec
d11: 0.03000000 sec
MCREST: 0.00000000 sec
MCWRK: 0.01500000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 8.10 usec
PL1: -3.00 dB
SFO1: 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 usec
PL2: -2.00 dB
PL12: 18.86 dB
PL13: 18.86 dB
SFO2: 400.3316013 MHz

F2 - Processing parameters
SI: 32768
SF: 100.6630578 MHz
WDW: EM
SSB: 0
LB: 3.00 Hz
GB: 0
PC: 1.40

S33

Current Data Parameters
NAME Nov13-2006
EXPNO 250
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061113
Time 15.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.06 usec
PL1 -2.00 dB
SFO1 400.3332026 MHz

F2 - Processing parameters
SI 32768
SF 400.3300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

534

NAME Nov29-2006
EXPNO 290
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061129
Time 23.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 18390.4
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters

SI 32768
SF 100.6630590 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S35

Current Data Parameters
NAME Nov10-2006
EXPNO 170
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061110
Time_ 10.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 161.3
DE 60.400 usec
TE 296.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 9.06 usec
PL1 -2.00 dB
SFO1 400.3332026 MHz

F2 - Processing parameters
SI 32768
SF 400.3300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NAME NOV13-ZUUB
EXPNO 181
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061113
Time 21.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters

SI 32768
SF 100.6630614 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S37

Current Data Parameters
NAME Nov14-2006
EXPNO 150
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061114
Time 13.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8278.146 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.06 usec
PL1 -2.00 dB
SFO1 400.3332026 MHz

F2 - Processing parameters
SI 32768
SF 400.330075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

EXPNO 151
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061114
Time_ 21.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 18390.4
DW 20.850 usec
DE 6.00 usec
TE 295.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters

SI 32768
SF 100.6630600 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S39

Current Data Parameters
 NAME Nov20-2006
 EXPNO 70
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061120
 Time_ 10.18
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.252629 Hz
 AQ 1.9792372 sec
 RG 203.2
 DW 60.400 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.5000000 sec
 MCREST 0.0000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.06 usec
 PL1 -2.00 dB
 SFO1 400.3332026 MHz

F2 - Processing parameters
 SI 32768
 SF 400.3300074 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NAME Nov09-2006
EXPNO 291
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061109
Time_ 23.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters

SI 32768
SF 100.6630602 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

54

Current Data Parameters
 NAME Dec01-2006
 EXPNO 150
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061201
 Time 11.11
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.252629 Hz
 AQ 1.9792372 sec
 RG 203.2
 DW 60.400 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUCL1 1H
 P1 9.06 usec
 PL1 -2.00 dB
 SFO1 400.3332026 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.3300055 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NOV07-4006
EXPNO 281
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061109
Time 21.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DM 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing Parameters
SI 32768
SF 100.6630598 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S43

Current Data Parameters
 NAME Nov15-2006
 EXPNO 70
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061115
 Time_ 10.15
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.252629 Hz
 AQ 1.9792372 sec
 RG 181
 DW 60.400 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.06 usec
 PL1 -2.00 dB
 SFO1 400.3332026 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.3300088 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

544

NAME Nov16-2006
EXPNO 331
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061117
Time_ 1.58

INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 4

SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 14596.5
DM 20.850 usec
DE 6.00 usec
TE 296.2 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 100.6731249 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.86 dB
PL13 18.86 dB
SFO2 400.3316013 MHz

F2 - Processing parameters
SI 32768
SF 100.6630590 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

545

Current Data Parameters
 NAME Dec01-2006
 EXPNO 160
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061201
 Time_ 11.20
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 8278.146 Hz
 FIDRES 0.252629 Hz
 AQ 1.9792372 sec
 RG 50.8
 DW 60.400 usec
 DE 6.00 usec
 TE 295.2 K
 D1 1.50000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.06 usec
 PL1 -2.00 dB
 SFO1 400.3332026 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.3300188 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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Current Data Parameters
 NAME Nov30-2006
 EXPNO 140
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061130
 Time 23.28
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT C6D6
 NS 8192
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 8192
 DW 20.850 usec
 DE 6.00 usec
 TE 296.2 K
 D1 0.50000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 8.10 usec
 PL1 -3.00 dB
 SFO1 100.6731249 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 18.86 dB
 PL13 18.86 dB
 SFO2 400.3316013 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6630369 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40