Supporting Information

Highly Efficient Pd-Catalyzed Carbonylative Cross-Coupling Reactions Using Tetraorganoindates

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Experimental data for compounds **4 – 21** : S2 – S5

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Methyl 4-methylphenyl ketone (4) ^1H NMR (400 MHz, CDCl_3) δ 7.86 (d, $J = 8.11$ Hz, 2H), 7.26 (d, $J = 7.95$ Hz, 2H), 2.58 (s, 3H), 2.41 (s, 3H), ^{13}C NMR (400 MHz, CDCl_3) δ 198.3, 144.3, 135.1, 129.7, 128.9, 26.9, 22.0; IR (film) 1678, 1606 cm^{-1} ; HRMS (EI) for $\text{C}_9\text{H}_{10}\text{O}$ [M^+] calcd 134.0732, found 134.0729.

Isopropyl 4-methylphenyl ketone (5) ^1H NMR (400 MHz, CDCl_3) δ 7.86 (d, $J = 8.18$ Hz, 2H), 7.26 (d, $J = 8.17$ Hz, 2H), 3.50-3.57(m, 1H), 2.41 (s, 3H), 1.21 (d, $J = 6.74$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.6, 143.9, 134.1, 129.7, 128.9, 35.6, 22.0, 19.6; IR (film) 1715, 1682, 1609 cm^{-1} ; HRMS (EI) for $\text{C}_{11}\text{H}_{14}\text{O}$ calcd [M^+] 162.1045, found 162.1046.

Isobutyl 4-methylphenyl ketone (6) ^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, $J = 8.42$ Hz, 2H), 7.25 (d, $J = 8.10$ Hz, 2H), 2.80 (d, $J = 6.83$ Hz, 2H), 2.41 (s, 3H), 2.29 (m, 1H), 0.98 (d, $J = 6.60$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 200.0, 143.6, 135.0, 129.2, 128.3, 47.4, 25.3, 22.8, 21.6; IR (film) 1675, 1606 cm^{-1} ; HRMS (EI) for $\text{C}_{12}\text{H}_{16}\text{O}$ [M^+] calcd 176.1201, found 176.1210.

***sec*-Butyl 4-methylphenyl ketone (7)** ^1H NMR (400 MHz, CDCl_3) δ 7.86 (d, $J = 8.17$ Hz, 2H), 7.26 (d, $J = 8.04$ Hz, 2H), 3.35-3.40 (m, 1H), 2.41 (s, 3H), 1.79-1.86 (m, 1H), 1.44-1.52 (m, 1H), 1.18 (d, $J = 6.88$ Hz, 3H), 0.91 (t, $J = 7.44$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.2, 143.5, 134.3, 129.3, 128.4, 42.0, 21.6, 16.9, 11.8; IR (film) 1675, 1607 cm^{-1} ; HRMS (EI) for $\text{C}_{12}\text{H}_{16}\text{O}$ [M^+] calcd 176.1201, found 176.1208.

4-Methylphenyl phenylethynyl ketone (8) ^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, $J = 8.20$ Hz, 2H), 7.67-7.70 (m, 2H), 7.46-7.50(m, 1H), 7.40-7.44(m, 2H), 7.31 (d, $J = 8.05$ Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 177.8, 145.3, 134.6, 133.0, 130.7, 129.7, 129.4, 128.8, 120.3, 92.6, 87.0, 21.9; IR (film) 2200, 1633, 1604 cm^{-1} ; HRMS (EI) for $\text{C}_{16}\text{H}_{12}\text{O}$ [M^+] calcd 220.0888, found 220.0888.

4-Methylphenyl phenyl ketone (9) ^1H NMR (400 MHz, CDCl_3) δ 7.78 (d, $J = 7.09$ Hz, 2H), 7.72 (d, $J = 8.07$ Hz, 2H), 7.57 (t, $J = 6.87$ Hz, 1H), 7.47 (t, $J = 7.46$ Hz, 2H), 7.27 (d, $J = 7.87$ Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.9, 143.7, 138.4, 135.3, 132.6, 130.7, 130.4, 129.4, 128.6, 22.1; IR (film) 1654, 1605 cm^{-1} ; HRMS (EI) for $\text{C}_{14}\text{H}_{12}\text{O}$ [M^+] calcd 196.0888, found 196.0896.

Methyl 4-methoxyphenyl ketone (10) ^1H NMR (400 MHz, CDCl_3) δ 7.94 (d, $J = 8.91$ Hz, 2H), 6.93 (d, $J = 8.93$ Hz, 2H), 3.87 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.2, 163.9, 131.0, 130.7, 114.1, 55.9, 26.7; IR (film) 1672, 1600 cm^{-1} ; HRMS (EI) for $\text{C}_{16}\text{H}_{12}\text{O}$ [M^+] calcd 150.0681, found 150.0679.

Ethyl 3-acetylbenzoate (11) ^1H NMR (400 MHz, CDCl_3) δ 8.60 (s, 1H), 8.24(d, $J = 7.73$ Hz, 1H), 8.15(d, $J = 7.73$ Hz, 1H), 7.56(t, $J = 7.76$ Hz, 1H), 4.42(q, $J = 7.11$ Hz, 2H), 2.66 (s, 3H), 1.43(t, $J = 7.14$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.3, 165.8, 137.3, 133.9, 132.2, 131.1, 129.5, 128.8, 61.4, 26.8, 14.3; IR (film) 1714, 1688 cm^{-1} ; HRMS (EI) for $\text{C}_{11}\text{H}_{12}\text{O}_3$ [M^+] calcd 192.0786, found 192.0784.

4-Benzoyl phenol (12) ^1H NMR (400 MHz, CDCl_3) δ 7.75-7.80 (m, 4H), 7.56-7.59(m, 1H), 7.48 (t, $J = 7.57$ Hz, 2H), 6.92-7.26 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.7, 160.6, 138.1, 133.1, 132.2, 129.9, 129.7, 128.3, 115.4; IR (film) 3298, 1638, 1602 cm^{-1} ; HRMS (EI) for $\text{C}_{13}\text{H}_{10}\text{O}_2$ [M^+] calcd 198.0681, found 198.0683.

4-Chlorophenyl *n*-butyl ketone (13) ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 8.54$ Hz, 2H), 7.43 (d, $J = 8.55$ Hz, 2H), 2.94 (t, $J = 7.43$ Hz, 2H), 1.68-1.75 (m, 2H), 1.35-1.43 (m, 2H), 0.95 (t, $J = 7.33$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 199.3, 139.3, 135.4, 129.5, 128.9, 38.3, 26.4, 22.5, 13.9; IR (film) 1685 cm^{-1} ; HRMS (EI) for $\text{C}_{11}\text{H}_{13}\text{O}$ [M^+] calcd 196.0655, found 196.0654.

1,4-Diacetylbenzene (14) ^1H NMR (400 MHz, CDCl_3) δ 8.01 (s, 4H), 2.65 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.5, 140.2, 128.5, 26.4; IR (film) 1685 cm^{-1} ; HRMS (EI) for $\text{C}_{10}\text{H}_{10}\text{O}_2$ [M^+] calcd 162.0681, found 162.0687.

1,4-Diisobutrylbenzene (15) ^1H NMR (400 MHz, CDCl_3) δ 8.02 (s, 4H), 3.53-3.60 (m, 2H), 1.23 (d, $J = 6.91$ Hz, 12H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.3, 139.7, 128.9, 36.2, 19.4; IR (film) 2961, 1683 cm^{-1} ; HRMS (EI) for $\text{C}_{14}\text{H}_{18}\text{O}_2$ [M^+] 218.1307, found 218.1306.

Isopropyl 2-naphthyl ketone (16) ^1H NMR (400 MHz, CDCl_3) δ 8.48 (s, 1H), 8.03 (dd, $J = 1.72$, 1.64, 1H), 7.97 (d, $J = 7.94$ Hz, 1H), 7.87-7.92 (m, 2H), 7.53-7.62 (m, 2H), 3.70-3.77 (m, 1H), 1.28 (d, $J = 6.92$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.5, 135.5, 133.6, 132.6, 129.7, 129.5, 128.5, 128.3, 127.7, 126.7, 124.4, 35.4, 19.3; IR (film) 1677 cm^{-1} ; HRMS (EI) for $\text{C}_{14}\text{H}_{14}\text{O}$ [M^+] calcd 198.1045, found 198.1044.

3-Acetyl quinoline (17) ^1H NMR (400 MHz, CDCl_3) δ 9.44 (d, $J = 2.13$ Hz, 1H), 8.72 (d, $J = 2.05$ Hz, 1H), 8.17 (d, $J = 8.46$ Hz, 1H), 7.96 (d, $J = 8.12$ Hz, 1H), 7.83-7.87 (m, 1H), 7.64 (t, $J = 7.22$ Hz, 1H), 2.75 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 195.7, 148.8, 148.2, 136.4, 131.0, 128.5, 128.4, 128.3, 126.6, 125.8, 25.8; IR (film) 1711 cm^{-1} ; HRMS (EI) for $\text{C}_{11}\text{H}_9\text{ON}$ [M^+] calcd 171.0684, found 171.0683.

Isopropyl 2-thienyl ketone (18) ^1H NMR (400 MHz, CDCl_3) δ 7.72-7.73 (m, 1H), 7.62-7.64 (m, 1H), 7.13-7.41 (m, 1H), 3.36-3.41 (m, 1H), 1.25 (d, $J = 6.73$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.9, 144.1, 133.8, 131.9, 128.4, 37.6, 19.8; IR (film) 1659 cm^{-1} ; HRMS (EI) for $\text{C}_8\text{H}_{10}\text{OS}$ [M^+] calcd 154.0452, found 154.0453.

4-Methyl-1-phenylhex-1-en-3-one (19) ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, $J = 16.07$ Hz, 1H), 7.58-7.56 (m, 2H), 7.40-7.38 (m, 3H), 6.82 (d, $J = 16.02$ Hz, 1H), 2.76-2.81 (m, 1H), 1.74-1.82 (m, 1H), 1.44-1.52 (m, 1H), 1.16 (d, $J = 6.79$ Hz, 3H), 0.93 (t, $J = 7.47$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 204.2, 142.8, 135.1, 130.8, 129.3, 128.7, 125.4, 46.7, 26.7, 16.6, 12.2; IR (film) $1703, 1638\text{ cm}^{-1}$; HRMS (EI) for $\text{C}_{13}\text{H}_{16}\text{O}$ [M^+] calcd 188.1201, found 188.1203.

Benzyl isopropyl ketone (20) ^1H NMR (400 MHz, CDCl_3) δ 7.30-7.34 (m, 2H), 7.24-7.27 (m, 1H), 7.19-7.21 (m, 2H), 3.74 (s, 2H), 2.69-2.76 (m, 1H), 1.10 (d, $J = 6.95$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 212.0, 134.4, 129.5, 128.6, 126.9, 47.7, 40.1, 18.3; IR (film) 1712 cm^{-1} ; HRMS (EI) for $\text{C}_{11}\text{H}_{14}\text{O}$ [M^+] calcd 162.1045, found 162.1045.

Benzil (21) ^1H NMR (400 MHz, CDCl_3) δ 7.79-7.81 (m, 4H), 7.57-7.61 (m, 2H), 7.46-7.50 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 196.73, 137.55, 132.39, 130.02, 128.24; IR (film) 1658, 1599, 1279, 909 cm^{-1} ; HRMS (EI) calcd for $\text{C}_{14}\text{H}_{10}\text{O}_2$ M^+ 210.0681, found 210.0681.

SWL-001

2

Hz
3149.53
3141.42
2905.39
2897.60

1182.58
1175.17
1167.69
1032.65
975.77
963.53
700.03
692.72
685.17
677.67
670.06
635.67
573.87
566.34
558.80
551.40
387.22
379.88
372.54

28.44
0.00

Current Data Parameters
NAME mar-02
EXPNO 203
PROCNO 1

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TO 32768
SOLVENT CDCl3
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DS 0
SWH 8223.695 Hz
FIDRES 0.250957 Hz
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RG 362
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DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

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F2 - Processing parameters
SI 16384
SF 400.130097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
CX 30.00 cm
FJP 8.100 ppm
F1 3241.05 Hz
F2 -40.01 Hz
PPM0 0.27333 ppm/cm
HZCM 109.36888 Hz/cm

SML-001

Current Data Parameters

NAME	EXPNO	PROCNO
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F2 - Acquisition Parameters

Date_	Time
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PULPROG zgpg30

TD 65536

TO 0.0013

SOLVENT CDCl3

NS 2048

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FIDRES 0.465949 Hz

AQ 1.028962 sec

RG 1625.5

DM 15.700 usec

DE 6.00 usec

TE 300.0 K

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D11 0.0300000 sec

D12 0.0002000 sec

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

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

OPPRG2	WALTZ16	NUC2	PC2	PL2	PL3	SC2
waltz16		1H	105.00 usec	-2.00 dB	18.00 dB	400.1324708 MHz

F2 - Processing parameters

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

10 NMR P111 parameters

CX	F1P	F1	F2P	F2	PPMCM	HZCM
30.00 cm	220.000 ppm	22134.81 Hz	-5.000 ppm	-503.66 Hz	7.50000 ppm/	754.59510 Hz/c

SWL-057-P

Current Data Parameters
NAME Jun-02
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020604
Time 14.31

INSTRUM spect
PROBHD 5 mm DAI 13
PULPROG zgpg30
TO 65536
SOLVENT CDCl3
NS 789
DS 2
SWH 31947.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 1629.5
DM 15.700 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
D12 0.0002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.625356 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 105.00 usec
PL2 -2.00 dB
SFO2 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127250 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10 NMR plot parameters
CX 30.00 cm
FAP 220.000 ppm
F1 22134.80 Hz
FAP -5.000 ppm
F2 -503.05 Hz
PPMCM 7.5000 ppm/cm
HCHM 754.59546 Hz/cm

SML-260

Current Data Parameters
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 EXPNO 117
 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zgpg30
 TD 65536
 TO 65536
 SOLVENT CDCl3
 NS 1935
 DS 2
 SM 31847.133 Hz
 FIDRES 0.465348 Hz
 AQ 1.0296652 sec
 RG 1625.5
 DM 15.770 usec
 DE 6.00 usec
 TE 300.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 D12 0.0002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -2.00 dB
 SFO1 100.6254359 MHz

===== CHANNEL f2 =====
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 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 15.00 dB
 PL13 17.00 dB
 SFO2 400.1324709 MHz

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
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 F1P 220.000 ppm
 F1 22134.80 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCK 7.50000 ppm/cm
 HZCM 754.53546 Hz/cm

SML-102

Current Data Parameters
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 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20020907
 Time 11.47
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 PULPROG zgpg30
 TO 2030
 10 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SMH 823.655 Hz
 FIDRES 0.250587 Hz
 AQ 1.5923444 sec
 RG 63
 DW 60.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 10.80 usec
 PL1 -2.00 dB
 SFO1 400.1324710 MHz
 F2 - Processing parameters
 SI 16384
 SF 400.130085 MHz
 MCW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 30.00 cm
 F1P 8.100 ppm
 F1 3241.05 Hz
 F2P -0.100 ppm
 F2 -40.01 Hz
 PPMCK 0.27333 ppm/cm
 HZCK 109.36888 Hz/cm

SML-102

Current Data Parameters

NAME	EXPNO	PROCNO
SML-102	218	1

F2 - Acquisition Parameters

Date_	Time
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PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 1141
DS 2
SWH 31847.133 Hz
FIDRES 0.485349 Hz
AQ 1.0289552 sec
RG 2048
RW 19.700 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

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

NUC1	13C
P1	10.50 usec
PL1	-1.00 dB
SFO1	100.625458 MHz

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

NUC2	1H
PCPD02	100.00 usec
PL2	-2.00 dB
PL12	18.00 dB
PL13	20.00 dB
SFO2	400.1324706 MHz

F2 - Processing parameters

SF	32768
SI	100.6127671 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

¹H NMR plot parameters

FX	30.00 cm
F1P	220.000 ppm
F1	22134.81 Hz
F2P	-50.000 ppm
F2	-503.06 Hz
PRICK	7.50000 ppm/cm
HZCM	754.59570 Hz/cm

SML-101

Hz
3150.12
3141.95
2909.23
2906.20
2901.19

1362.33
1355.61
1348.83
1342.11

964.43
743.98
737.08
730.14
723.03
716.20
662.80
607.83
600.65
593.76
586.82
579.81
533.47
527.17
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386.92
371.48
364.04
355.50

0.00

Current Data Parameters
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EXPNO: 30
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20020905
Time: 11.12
INSTRUM: spect
PROBHD: 5 mm Dui1 13
PULPROG: zg30
TD: 32768
SOLVENT: CDCl3
NS: 16
DS: 0
SWH: 8223.665 Hz
FIDRES: 0.250967 Hz
AQ: 1.9923444 sec
RG: 181
DM: 60.800 usec
DE: 5.00 usec
TE: 300.0 K
D1: 1.00000000 sec
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NUC1: 1H
P1: 10.80 usec
PL1: -2.00 dB
SFO1: 400.1324710 MHz
F2 - Processing parameters
SI: 16384
SF: 400.130084 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
10 NMR plot parameters
CX: 30.00 cm
CJ: 8.100 ppm
F1: 3241.05 Hz
F2: -40.01 Hz
PPMCM: 0.27333 ppm/cm
HZCM: 109.36888 Hz/cm

SWL-101

Current Data Parameters
 NAME sep-02
 EXPNO 217
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020923
 Time 14:57
 INSTRUM spect
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 PULPROG zgpg30
 TD 299930
 SOLVENT CDCl3
 NS 624
 DS 2
 SWH 31847.133 Hz
 FIDRES 0.485949 Hz
 AQ 1.028952 sec
 RG 3649.1
 DW 15.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 -1.00 dB
 SFO1 100.525459 MHz

===== CHANNEL f2 =====
 CDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SFO2 400.1324708 MHz

F2 - Processing Parameters
 SI 32768
 SF 160.5127671 MHz
 MW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
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 F1 2213.61 Hz
 F2P -5.000 GHz
 F2 -503.06 Hz
 PRICK 7.50000 GHz/cm
 HZCM 754.59570 Hz/cm

SMU 316-2

Current Data Parameters
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EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.5923444 sec
RG 161.3
DM 60.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
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PL1 -2.00 dB
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F2 - Processing parameters
SI 16384
SF 400.130090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10 NMR plot parameters
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F2 -40.01 Hz
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HZCM 114.70364 Hz/cm

SWL 316-2

Current Data Parameters

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PROCNO	1

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RG	1625.5
DM	15.700 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
D12	0.0002000 sec

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

NUC1	13C
P1	9.50 usec
PL1	-2.00 dB
SFO1	100.6254598 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-2.00 dB
PL12	15.00 dB
PL13	17.00 dB
SFO2	400.1324709 MHz

F2 - Processing parameters

SI	32768
SF	100.612779 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	30.00 cm
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F2P	20625.62 Hz
F2	-5.000 ppm
F2P	-503.05 Hz
PPMCM	7.00000 ppm/cm
HZCM	704.28937 Hz/cm

Current Data Parameters
NAME: oct-02
EXPNO: 298
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20021028
Time: 13.18
INSTRUM: spect
PROBHD: 5 mm Dual 13
PULPROG: zg30
TO: 32768
SOLVENT: CDCl3
NS: 20
DS: 0
SWH: 8223.686 Hz
FIDRES: 0.250987 Hz
AQ: 1.992444 sec
RG: 128
DM: 60.800 usec
DE: 6.00 usec
TE: 300.0 K
D1: 1.00000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 9.50 usec
PL1: -2.00 dB
SFO1: 400.1324710 MHz

F2 - Processing parameters
SI: 16384
SF: 400.1300115 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 30.00 cm
F1P: 8.100 ppm
F1: 3241.05 Hz
F2P: -0.100 ppm
F2: -40.01 Hz
PPHQM: 0.27353 ppm/cm
HZCM: 109.38889 Hz/cm

SWL-125-P

Current Data Parameters
NAME oct-02
EXPNO 418
PROCNO 1
F2 - Acquisition Parameters
Date_ 20021031
Time 15:52
INSTRUM spect
PROBHD 5 mm QNP 13
PULPROG zgpg30
TO 29930
TD 65536
SOLVENT CDCl3
NS 515
DS 2
SWH 31647.133 Hz
FIDRES 0.485949 Hz
AQ 1.0285632 sec
RG 1525.5
DM 15.700 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.625359 MHz
===== CHANNEL f2 =====
CDEPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
10 NMR plot parameters
CX 30.00 cm
FLP 220.000 MHz
F1 22134.80 Hz
F2P 503.000 MHz
F2 -503.06 Hz
FREQM 750.000 MHz/cm
H2CM 754.35946 Hz/cm

SWL-269

Current Data Parameters
 NAME Jun-03
 EXPNO 45
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030619
 Time 13.36
 INSTRUM spect
 PRCBH0 5 mm Dual 13
 PULPROG zg30
 TD 32768
 FIDRES 0.250567 Hz
 AQ 1.9923444 sec
 RG 181
 DW 60.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 11.50 usec
 PL1 -2.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 16394
 SF 400.130000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 30.00 cm
 F1P 8.100 ppm
 F1 3241.05 Hz
 F2P -0.100 ppm
 F2 -40.01 Hz
 PPMCH 0.2733 ppm/cm
 HZCM 109.36888 Hz/cm

SML-269

Current Data Parameters

NAME	VALUE
EXPNO	100-03
PROCNO	48
PROCNO	1

F2 - Acquisition Parameters

Date_	Time
20030619	16.01

INSTRUM spect

PROBHD 5 mm Dual 13

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 301

DS 2

SWH 31847.133 Hz

FIDRES 0.465949 Hz

AQ 1.0289692 sec

RG 3649.1

OW 15.700 Lsec

DE 6.00 Lsec

TE 300.0 K

D1 2.00000000 sec

D11 0.03000000 sec

D12 0.00002000 sec

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

NUC1	13C
P1	9.50 Lsec
PL1	-2.00 dB
SFO1	100.6254358 MHz

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

OPPRG2	wa1z16
MIC2	1H
PCPD2	100.00 Lsec
PL2	-2.00 dB
PL12	15.00 dB
PL13	17.00 dB
SFO2	400.1324706 MHz

F2 - Processing parameters

SI	32768
SF	100.6127790 MHz
NDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

10 NMR plot parameters

FX	30.00 cm
F1P	220.000 ppm
F1	22134.80 Hz
F2P	-5.000 ppm
F2	-503.06 Hz
PRICK	7.50000 ppm/cm
HZCM	754.53546 Hz/cm

SNL-071

Current Data Parameters
NAME Jun-02
EXPNO 162
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020828
Time 5.15
INSTRUM spect
PROBHD 5 mm DUA1 13
PULPROG zgpg30
TO 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0285652 sec
RG 1149.4
OW 15.700 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00020000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.625359 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6127664 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
FLP 230.000 ppm
F1 23140.94 Hz
FAP 5.000 ppm
F2 -503.06 Hz
FREQM 7.69333 MHz/cm
WICH 766.13366 Hz/cm

SML-315

12

Current Data Parameters
NAME sep-03
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030919
Time 13.28
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9823444 sec
RG 362
DM 60.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 11.50 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.130088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1p 8.100 ppm
F1 3241.05 Hz
F2p -0.100 ppm
F2 -40.01 Hz
PPCKM 0.27333 ppm/cf
HZCM 109.36888 Hz/cm

SWL-315

SM-317-1

Hz
3164.66
3162.79
3158.03
3156.12
3153.76

2977.11
2975.33
2970.40
2960.56
2906.66

1181.88
1174.50
1167.02

700.22
692.80
690.84
685.29
677.81
670.21
640.87
573.79
566.27
558.69
551.32
490.77
483.76
476.75
392.51
388.59
385.21
381.33
373.94

0.00

13

Current Data Parameters
NAME OCT-03
EXPNO 73
PROCNO 1

F2 - Acquisition Parameters
Date_ 20031027
Time 14.28
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 40
DS 0
SWH 8223.685 Hz
FIDRES 0.250957 Hz
AQ 1.9923444 sec
RG 1181
DM 60.800 us/c
DE 6.00 us/c
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 us/c
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 16384
SF 400.1300770 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1 8.200 ppm
F2 3281.07 Hz
F3 -0.100 ppm
F4 -40.01 Hz
F5 0.27057 ppm/cm
F6 110.70254 Hz/cm

SMIL-317-1

Current Data Parameters

NAME	021-03
EXPNO	74
PROCNO	1

F2 - Acquisition Parameters

Date_	20031027
Time	15.00
INSTRUM	spect
PROBHD	5 mm Dual 13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1310
DS	2
SWH	31847.133 Hz
FIDRES	0.485949 Hz
AQ	1.028952 sec
RG	3649.1
DW	15.700 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
D12	0.00020000 sec

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

NUC1	13C
P1	9.50 usec
PL1	-2.00 dB
SFO1	100.6254258 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-2.00 dB
PL12	15.00 dB
PL13	17.00 dB
SFO2	400.1324708 MHz

F2 - Processing parameters

SI	32768
SF	100.6127570 MHz
MDW	FM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	30.00 cm
F1P	220.000 GHz
F2P	22134.61 Hz
F2	-5.000 GHz
PPMCM	7.50000 ppm/cm
HZCM	754.59570 Hz/cm

SML-124-2

14

Current Data Parameters

NAME	oct-02
EXPNO	310
PROCNO	1

F2 - Acquisition Parameters

Date_	20021028
Time	17.56
INSTRUM	spect
PROBHD	5 mm Dual 13
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	20
DS	0
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	362
DM	60.800 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec

***** CHANNEL f1 *****

NUC1

P1	9.50 usec
PL1	-2.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	16384
SF	400.1300069 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

10 NMR plot parameters

CX	30.00 cm
F1P	8.500 ppm
F1	3401.10 Hz
F2P	-0.100 ppm
F2	-40.01 Hz
PPMCM	0.28657 ppm/cm
HZCM	114.70384 Hz/cm

SWL-124-2

Current Data Parameters

NAME	Oct-02
EXPNO	311
PROCNO	1

F2 - Acquisition Parameters

Date_	20021028
Time	18.05
INSTRUM	spect
PROBHD	5 mm QNP1 13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	2
SWH	31947.133 Hz
FIDRES	0.485949 Hz
AQ	1.028662 sec
RG	3649.1
DM	15.700 USEC
DE	6.00 USEC
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec

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

NUC1	13C
P1	10.50 USEC
PL1	-1.00 dB
SFO1	100.6254358 MHz

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

CPDPRG2	WALTZ16
NUC2	1H
PCPD2	100.00 USEC
PL2	-2.00 dB
PL12	18.00 dB
PL13	20.00 dB
SFO2	400.1324708 MHz

F2 - Processing parameters

SI	32768
SF	100.6127672 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR Plot Parameters

CX	30.00 cm
F1P	220.000 ppm
F2P	22134.81 Hz
F2	-5.000 ppm
F2	-503.05 Hz
PPMCM	7.50000 ppm/cm
HZCM	754.53570 Hz/cm

SML-131-P

15

Current Data Parameters
 NAME: SML-131-P
 EXPNO: 411
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20021031
 Time: 12.39
 INSTRUM: spect
 PULPROG: zgpg30
 PULPROG: zgpg30
 SOLVENT: CDCl3
 NS: 20
 DS: 0
 SWH: 8223.565 Hz
 FIDRES: 0.250567 Hz
 AQ: 1.9923444 sec
 RG: 181
 CW: 60.000 usec
 DE: 300.0 K
 TE: 300.0 K
 D1: 1.00000000 sec
 ***** CHANNEL f1 *****
 NUC1: 13C
 P1: 9.50 usec
 PL1: -2.00 dB
 SFO1: 400.1324710 MHz
 F2 - Processing parameters
 SI: 16384
 SF: 400.130054 MHz
 KW: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00
 1D NMR plot parameters
 CX: 30.00 cm
 F1P: 8.500 ppm
 F1: 3401.10 Hz
 F2P: -40.01 Hz
 F2: 0.28657 ppm/cm
 PRGM: hzgcm
 HZCM: 114.70394 Hz/cm

SWH-131-P

Current Data Parameters
 NAME oct-02
 EXPNO 412
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20021031
 Time 13.07
 INSTRUM spect
 PROBHD 5 mm Dual 13
 PULPROG zgpg30
 TO 65536
 SOLVENT CDCl3
 NS 624
 DS 2
 SWH 31847.133 Hz
 FIDRES 0.485949 Hz
 AQ 1.0289652 sec
 RG 1625.5
 DM 15.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 -1.00 dB
 SFO1 100.625458 MHz
 ===== CHANNEL f2 =====
 C13PRG2 waltz16
 NUC2 1H
 P1 100.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SFO2 400.132408 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.617290 MHz
 MW CW
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40
 10 NMR plot parameters
 CY 30.00 ct
 F1P 230.000 ppm
 F1 2213.80 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMCK 7.50000 ppm/cm
 HZCK 754.59546 Hz/cm

SWL-333-2

Current Data Parameters
 NAME: 20031031
 EXPNO: 113
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20031031
 Time: 16.54
 INSTRUM: spect
 PROBHD: 5 mm Dual 13
 PULPROG: zg30
 TD: 32768
 SOLVENT: CDCl3
 NS: 20
 DS: 0
 SWH: 8223.685 Hz
 FIDRES: 0.280967 Hz
 AQ: 1.9923444 sec
 RG: 406.4
 DW: 60.800 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 11.50 usec
 PL1: -2.00 dB
 SFO1: 400.1324710 MHz

F2 - Processing Parameters
 SI: 16384
 SF: 400.130069 MHz
 WDM: EN
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 30.00 cm
 F1P: 10.500 ppm
 F1: 4201.37 Hz
 F2P: -0.500 ppm
 F2: -200.07 Hz
 PPM/CM: 0.36667 ppm/cm
 HZ/CM: 146.71434 Hz/cm

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Current Data Parameters
NAME          oct-03
EXPNO         119
PROCNO        1

F2 - Acquisition Parameters
Date_         20031111
Time          4.08
INSTRUM       spect
PROBHD        5 mm Dui1 13
PULPROG       zgpg30
TD            2090320
SFO           200.130
NUC1           13C
NUC2           13C
DE            1.4243
RG            3.2
SM            3184.7 13 Hz
FIDRES        0.468446 Hz
AQ            1.0398952 sec
RG2           1635.5
DE2           15.70 uSFC
PC            6.00 uSFC
T2            300.0 Hz
D1            2.0000000 sec
D11           0.0300000 sec
D12           0.0000000 sec

***** CHANNEL f1 *****
NUC1          13C
PC1           9.50 uSFC
P1            -2.00 dB
P1.1          100.6254268 MHz

***** CHANNEL f2 *****
CPROG2        waltz16
NUC2          1H
PC2           100.00 uSFC
P2            -2.00 dB
P2.1          15.00 dB
P1.12         17.00 dB
P1.13         17.00 dB
SFO2          400.1324708 MHz

F2 - Processing Parameters
SI            32768
SF            100.6121677 MHz
AQ            EM
NUC1          13C
NUC2          1H
SFO1          200.130 MHz
PC            1.40

10 NMR plot parameters
CX            30.00 cm
F1P           210.000 MHz
F1            212.28 68 Hz
F2P           -5.000 GHz
F2            -5.053 06 GHz
PCMD          F2:16567 spw/cm
WDW           HANN
GB            721.05811 Hz/cm

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SWL-329

Current Data Parameters
NAME: SWL-329
EXPNO: 75
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20031027
Time: 17.40
INSTRUM: spect
PROBHD: 5 mm QNP1 13
PULPROG: zgpg30
TD: 32768
SOLVENT: CDCl3
NS: 20
DS: 0
SWH: 8223.695 Hz
FIDRES: 0.250957 Hz
AQ: 1.992344 sec
RG: 181
DE: 60.800 usec
TE: 300.0 K
D1: 1.0000000 sec

===== CHANNEL f1 =====
NUC1: 1H
P1: 11.50 usec
PL1: -2.00 dB
SFO1: 400.1324710 MHz

F2 - Processing parameters
SI: 46384
SF: 400.130029 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

10 NMR plot parameters
CX: 30.00 cm
F1P: 10.000 ppm
F1: 400.130 Hz
F2P: -0.100 ppm
F2: -40.01 Hz
PPODM: 0.33667 ppm/cm
HZCM: 134.71043 Hz/cm

SML-329

Current Data Parameters
NAME oct-03
EXPNO 76
PROCNO 1
Date_ 20031027
Time 17:35
INSTRUM spect
PROBHD 5 mm Dui 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1857
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0286632 sec
RG 1290.2
DM 15.700 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.0002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SF01 100.6254358 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 17.00 dB
SF02 400.1324708 MHz

F2 - Processing parameters
SI 32768
SF 100.6128704 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 30.00 cm
F1P 205.000 ppm
F1 20625.64 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCH 704.29004 Hz/cm
HZCH

SML-330-3P

Current Data Parameters
NAME oct-03
EXPNO 111
PROCNO 1

F2 - Acquisition Parameters
Date_ 20031031
Time 16.44
INSTRUM spect
PROBHD 5 mm QNP 13
PULPROG zg30
TO 32768
SOLVENT DMS
NS 20
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 287.4
WE 50.800 usec
DE 5.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 -2.00 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

1D NMR plot parameters
CX 30.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -40.01 Hz
F2 0.27333 ppm/Ca
PPMCM 109.36888 Hz/cm
HZCM

SWL 330-3P

Current Data Parameters
 NAME oct-03
 EXPNO 118
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20031110
 Time 14.38
 INSTRUM spect
 PROBR0 5 mm Duj 13
 PULPROG zgpg30
 TD 65536
 ID 00536
 SOLVENT CDCl3
 NS 2048
 DS 2
 SWH 31847.133 Hz
 FIDRES 0.485949 Hz
 AQ 1.028952 sec
 RG 812.7
 DW 15.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.0002000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -2.00 dB
 SFO1 100.625458 MHz

===== CHANNEL f2 =====
 CPOPRG2 waltz16
 NUC2 1H
 P2 100.00 usec
 PL2 -2.00 dB
 PL12 15.00 dB
 PL13 17.00 dB
 SFO2 400.1324709 MHz

F2 - Processing Parameters
 SI 32768
 SF 100.6127290 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

10 NMR plot parameters
 CX 30.00 cm
 FIP 220.000 DPM
 F1 22134.80 Hz
 F2P -5.000 DPM
 F2 -503.06 Hz
 PPMCM 7.50000 DPM/cm
 HZCM 754.55546 Hz/cm

SWL-136-P

19

Current Data Parameters
NAME nov-02
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 2002101
Time 20.05
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 32768
SOLVENT DMS
NS 40
DS 0
SWH 8223.665 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 181
DM 60.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing Parameters
SI 16384
SF 400.130061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -40.01 Hz
F2 0.2733 ppm/cm
P1MCM 109.36888 Hz/cm
HZCM

SW-136-P

Current Data Parameters
 NAME nov-02
 EXPNO 23
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20021101
 Time 20.21
 INSTRUM spect
 PROBRD 5 mm Dual 13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 416
 DS 2
 SFO1 31847.133 Hz
 FIDRES 0.485949 Hz
 AQ 1.0289652 sec
 RG 5160.6
 DW 15.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00020000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 -1.00 dB
 SFO1 100.6264558 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -2.00 dB
 PL12 18.00 dB
 PL13 20.00 dB
 SFO2 400.1364708 MHz

F2 - Processing Parameters
 SI 32768
 SF 100.612750 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 30.00 cm
 F1P 220.000 ppm
 F1 22134.80 Hz
 F2P -5.000 ppm
 F2 -503.06 Hz
 PPMKHZ 7.50000 ppm/cm
 HZCM 754.59546 Hz/cm

SM-305

Current Data Parameters
 NAME sep-03
 EXPNO 25
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030916
 Time 18.20
 INSTRUM spect
 PROBHD 5 mm QNP 13
 PULPROG zgpg30
 TO 32768
 SOLVENT CDCl3
 NS 20
 DS 0
 SWH 8231.685 Hz
 FIDRES 0.240867 Hz
 AQ 1.9923444 sec
 RG 181
 DM 60.800 ussec
 DE 5.00 ussec
 TE 300.0 K
 01 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 11.50 ussec
 PL1 -2.00 dB
 SF01 400.1324710 MHz

F2 - Processing parameters
 SI 16394
 SF 400.1300100 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 30.00 cm
 F1P 8.100 ppm
 F1 3241.05 Hz
 F2P -0.100 ppm
 F2 -40.01 Hz
 PPMCK 0.27333 ppm/cm
 HZCM 109.36689 Hz/cm

SML-305

Current Data Parameters

NAME	EXPNO	PROCNO
NAME	sep-03	36
EXPNO	1	1
PROCNO	1	1

F2 - Acquisition Parameters

Date_	Time
20030919	14.23

INSTRUM spect

PROBHD 5 mm Dual 13

PULPROG zgpg30

TO 65536

SOLVENT CDCl3

NS 1276

DS 2

SWH 31847.133 Hz

FIDRES 0.485949 Hz

AQ 1.028662 sec

RG 2560.3

DM 15.700 usec

DE 6.00 usec

TE 300.0 K

D1 2.00000000 sec

D11 0.03000000 sec

D12 0.00020000 sec

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

NUC1	P1	SFO1
¹³ C	9.50 usec	100.6234358 MHz
¹ H	-2.00 usec	

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

CPDPRG2	WALTZ16	NUC2	P2	SFO2
WALTZ16	1H			
PCPD2	100.00 usec			
PL2	-2.00 usec			
PL12	15.00 usec			
PL13	17.00 usec			
SFO2	400.1324709 MHz			

F2 - Processing parameters

SI	SF	WDW	SSB	LB	GB	PC
32768	100.6127677 MHz	EM	0	1.00 Hz	0	1.40

1D NMR plot parameters

EX	F1P	F2P	PPMCM	HZCM
30.00 cm	240.000 ppm	24147.06 Hz	-5.000 ppm	8.16667 ppm/cm
				821.6706 Hz/cm

SMU-332-1

21

Current Data Parameters
NAME oct-03
EXPNO 103
PROCNO 1

F2 - Acquisition Parameters
Date_ 20031031
Time 14.43
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.665 Hz
FIDRES 0.25967 Hz
AQ 1.992444 sec
RG 181
DW 60.800 usec
DE 5.00 usec
TE 300.0 K
D1 1.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 11.50 usec
PL1 -2.00 dB
SF01 400.1326710 MHz

F2 - Processing parameters
SI 16384
SF 400.130179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 8.100 ppm
F1 3241.05 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCH 0.2733 ppm/cm
HZCM 109.36888 Hz/cm

SWL-332-1

21

Current Data Parameters
NAME oct-03
EXPNO 104
PROCNO 1
F2 - Acquisition Parameters
Date_ 20031031
Time 14.56
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 231
DS 2
SWH 31847.133 Hz
FIDRES 0.465949 Hz
AQ 1.026562 sec
RG 3649.1
DE 15.700 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.0002000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
SFO1 100.6254358 MHz
===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -2.00 dB
PL12 15.00 dB
PL13 17.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
F1P 205.000 ppm
F1 20525.62 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCH 7.00000 ppm/cm
HZCH 704.28937 Hz/cm