Supporting Information for *Organic Letters*

Palladium Catalyzed Regiocontrolled α -Arylation of Trimethylsilyl Enol Ethers with Aryl Halides

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General procedure for Pd-catalyzed arylation: To a mixture of the TMS enol ether (1 mmol), aryl halide (0.5 mmol), 2.5 mol% of Pd₂(dba)₃ (11.4 mg), and Bu₃SnF (309 mg, 1 mmol) under nitrogen was added a solution of ^tBu₃P (7.5 μ L) in benzene (2 mL) at room temperature. The resultant mixture was heated to reflux. After cooling to room temperature, the reaction mixture was diluted with ether (20 mL) (when tin residue precipitated, it was removed by decantation with ether), washed with 1N aqueous NaOH twice (5 mL each) followed by brine (5 mL x 2), dried (MgSO₄), and concentrated. The residue was purified by flash column chromatography on silica gel.

3a: ¹H NMR (CDCl₃) δ : 1.75-1.85 (m, 2H), 1.94-2.02 (m, 2H), 2.10-2.15 (m, 1H), 2.22-2.26 (m, 1H), 2.40-2.46 (m, 1H), 2.49-2.53 (m, 1H), 3.56 (dd, J = 5.5, 12.5 Hz, 1H), 3.78 (s, 3H), 6.87 (d, J = 8.5 Hz, 2H), 7.05 (d, J = 8.5 Hz, 2H). ¹³C NMR (CDCl₃) δ : 25.3, 27.8, 35.2, 42.1, 55.1, 56.5, 113.7, 129.3, 130.8, 158.3, 210.6.

3b: ¹H NMR (CDCl₃) δ : 1.76-1.86 (m, 2H), 1.95-2.05 (m, 2H), 2.09-2.14 (m, 1H), 2.21-2.27 (m, 1H), 2.40-2.46 (m, 1H), 2.49-2.53 (m, 1H), 2.93 (s, 6H), 3.53 (dd, J

= 5.5, 12 Hz, 1H), 6.72 (d, J = 8.5 Hz, 2H), 7.01 (d, J = 8.5 Hz, 2H). ^{13}C NMR (CDCl_3) δ : 25.3, 27.9, 35.1, 40.7, 42.1, 56.4, 112.7, 126.6, 129.0, 149.6, 211.2.

3c: ^1H NMR (CDCl_3) δ : 1.74-1.86 (m, 2H), 1.93-2.17 (m, 3H), 2.22-2.28 (m, 1H), 2.39-2.53 (m, 2H), 3.59 (dd, J = 5.2, 12 Hz, 1H), 7.13 (d, J = 7.2 Hz, 2H), 7.24 (t, J = 7.2 Hz, 1H), 7.32 (t, J = 7.2 Hz, 2H). ^{13}C NMR (CDCl_3) δ : 25.2, 27.7, 30.2, 35.0, 42.0, 57.2, 126.7, 128.2, 128.4, 138.6, 210.2.

3d: ^1H NMR (CDCl_3) δ : 1.78-1.89 (m, 2H), 1.96-2.07 (m, 2H), 2.19-2.24 (m, 1H), 2.29-2.33 (m, 1H), 2.47-2.58 (m, 2H), 3.75 (dd, J = 5.5, 12.5 Hz, 1H), 7.31 (d, J = 8.5 Hz, 2H), 8.18 (d, J = 8.5 Hz, 2H). ^{13}C NMR (CDCl_3) δ : 25.2, 27.6, 35.1, 42.1, 57.2, 123.4, 129.6, 146.3, 146.8, 208.7.

3e: ^1H NMR (CDCl_3) δ : 1.79-1.88 (m, 2H), 1.98-2.07 (m, 2H), 2.12-2.20 (m, 1H), 2.26-2.30 (m, 1H), 2.44-2.56 (m, 2H), 3.67 (dd, J = 5.5, 12.5 Hz, 1H), 3.90 (s, 3H), 7.21 (d, J = 8.5 Hz, 2H), 8.01 (d, J = 8.5 Hz, 2H). ^{13}C NMR (CDCl_3) δ : 25.3, 27.7, 35.0, 42.2, 52.0, 57.4, 128.6, 128.7, 129.6, 144.0, 166.9, 209.4.

3f: ^1H NMR (CDCl_3) δ : 1.76-1.87 (m, 2H), 1.98-2.08 (m, 2H), 2.11-2.06 (m, 1H), 2.24-2.28 (m, 1H), 2.41-2.48 (m, 1H), 2.50-2.55 (m, 1H), 3.59 (dd, J = 5.5, 12 Hz, 1H), 3.79 (s, 3H), 6.69 (d, J = 2 Hz, 1H), 6.73 (d, J = 8 Hz, 1H), 6.81 (dd, J = 2, 8 Hz, 1H), 7.25 (t, J = 8 Hz, 1H). ^{13}C NMR (CDCl_3) δ : 25.2, 27.7, 34.9, 42.1, 55.1, 57.3, 112.1, 114.4, 120.8, 129.3, 140.3, 159.5, 210.2.

3g: ^1H NMR (CDCl_3) δ : 1.73-1.84 (m, 2H), 1.98-2.05 (m, 2H), 2.13-2.21 (m, 2H), 2.44-2.53 (m, 2H), 3.75 (s, 3H), 3.93 (dd, J = 5.5, 12.5 Hz, 1H), 6.86 (d, J = 8 Hz, 1H), 6.94 (t, J = 8 Hz, 1H), 7.11 (d, J = 8 Hz, 1H), 7.23 (t, J = 8 Hz, 1H). ^{13}C NMR (CDCl_3) δ : 25.5, 27.4, 33.2, 42.1, 50.9, 55.3, 110.4, 120.4, 127.7, 127.8, 128.6, 156.8, 209.7.

3h: ^1H NMR (CDCl_3) δ : 1.73-1.88 (m, 2H), 1.98-2.08 (m, 2H), 2.14-2.27 (m, 2H), 2.19 (s, 3H), 2.43-2.57 (m, 2H), 3.57 (dd, J = 5.2, 12.8 Hz, 1H), 7.11-7.22 (m,

4H). ^{13}C NMR (CDCl_3) δ : 19.6, 25.8, 27.7, 34.1, 42.4, 53.7, 125.8, 126.7, 127.5, 130.1, 136.0, 137.3, 209.8.

3i: ^1H NMR (CDCl_3) δ : 1.75-1.89 (m, 2H), 2.01-2.12 (m, 2H), 2.15-2.18 (m, 1H), 2.33-2.38 (m, 1H), 2.50-2.53 (m, 2H), 4.28 (dd, $J = 5.5, 12.5$ Hz, 1H), 7.34 (d, $J = 8$ Hz, 1H), 7.39 (t, $J = 8$ Hz, 1H), 7.57 (t, $J = 8$ Hz, 1H), 7.95 (1H, d, $J = 8$ Hz). ^{13}C NMR (CDCl_3) δ : 25.2, 26.9, 33.4, 41.9, 53.2, 124.6, 127.5, 130.1, 133.0, 133.8, 149.0, 207.9.

5: ^1H NMR (CDCl_3) δ : 0.83 (d, $J = 6.5$ Hz, 3H), 1.54-1.62 (m, 1H), 1.76-1.88 (m, 1H), 1.99-2.14 (m, 3H), 2.39-2.46 (m, 1H), 2.50-2.53 (m, 1H), 3.15 (d, $J = 11.5$ Hz, 1H), 3.79 (s, 3H), 6.88 (d, $J = 8.5$ Hz, 2H), 6.99 (d, $J = 8.5$ Hz, 2H). ^{13}C NMR (CDCl_3) δ : 21.1, 25.8, 34.2, 40.6, 41.6, 55.0, 64.1, 113.5, 129.4, 130.0, 158.2, 210.2.

7: ^1H NMR (CDCl_3) δ : 1.60-1.68 (m, 3H), 1.89-1.97 (m, 2H), 2.01-2.04 (m, 1H), 2.65 (br d, $J = 2.5$ Hz, 1H), 2.84 (br s, 1H), 3.06 (d, $J = 3.5$ Hz, 1H), 3.78 (s, 3H), 6.85 (d, $J = 9$ Hz, 2H), 7.19 (d, $J = 9$ Hz, 2H). ^{13}C NMR (CDCl_3) δ : 24.6, 27.9, 34.9, 41.6, 49.5, 55.2, 57.7, 113.9, 128.7, 129.3, 158.2, 217.6.

9: ^1H NMR (CDCl_3) δ : 0.96 (t, $J = 7$ Hz, 3H), 1.36 (d, $J = 7$ Hz, 3H), 2.31-2.43 (m, 2H), 3.71 (q, $J = 7$ Hz, 1H), 3.79 (s, 3H), 6.86 (d, $J = 8$ Hz, 2H), 7.13 (d, $J = 8$ Hz, 2H). ^{13}C NMR (CDCl_3) δ : 8.0, 17.6, 34.1, 51.8, 55.2, 114.2, 128.8, 133.0, 158.6, 211.9.

11: ^1H NMR (CDCl_3) δ : 1.43-1.47 (m, 1H), 1.53-1.63 (m, 1H), 1.97-2.14 (m, 4H), 2.76 (m, 1H), 3.19 (d, $J = 17.5$ Hz, 1H), 3.42-3.47 (m, 2H), 6.95-6.99 (m, 1H), 7.13-7.15 (m, 1H), 7.17-7.22 (m, 2H). ^{13}C NMR (CDCl_3) δ : 17.0, 37.3, 37.9, 38.1, 45.7, 52.2, 126.7, 126.7, 127.0, 128.2, 136.0, 138.4, 215.8.

13: ^1H NMR (CDCl_3) δ : 2.19 (dt, $J = 14, 3$ Hz, 1H), 2.25 (dt, $J = 14, 3$ Hz, 1H), 2.36 (dd, $J = 14, 5.6$ Hz, 1H), 2.43 (dd, $J = 14, 5$ Hz, 1H), 2.83 (m, 1H), 3.36-3.48 (m, 3H), 3.66-3.84 (m, 4H), 6.95-6.98 (m, 1H), 7.08-7.10 (m, 1H), 7.13-7.21 (m,

2H). ^{13}C NMR (CDCl_3) δ : 38.2, 43.1, 43.5, 44.2, 49.5, 63.3, 64.7, 106.3, 126.2, 126.8, 127.3, 127.9, 134.8, 138.8, 214.5.

15: ^1H NMR (CDCl_3) δ : 1.30 (t, J = 7 Hz, 3H), 2.15-2.20 (m, 1H), 2.23-2.26 (m, 2H), 2.30-2.33 (m, 1H), 2.42-2.49 (m, 2H), 3.15 (d, J = 18 Hz, 1H), 3.53 (d, J = 18 Hz, 1H), 3.65 (br s, 1H), 4.21 (q, J = 7 Hz, 2H), 7.12 (m, 2H), 7.19-7.27 (m, 2H). ^{13}C NMR (CDCl_3) δ : 14.1, 33.9, 36.0, 36.7, 40.6, 52.3, 61.0, 126.2, 127.6, 128.6, 129.2, 134.3, 135.6, 176.2, 209.9.

17: ^1H NMR (CDCl_3) δ : 1.38-1.48 (m, 1H), 1.69-1.93 (m, 3H), 2.20-2.28 (m, 1H), 2.35-2.41 (m, 1H), 2.70 (dd, J = 2.4, 15.6 Hz, 1H), 2.89-2.97 (m, 1H), 3.07 (dd, J = 6.8, 15.6 Hz, 1H), 3.85 (d, J = 7.2 Hz, 1H), 7.11-7.28 (m, 4H). ^{13}C NMR (CDCl_3) δ : 23.4, 27.8, 38.7, 39.4, 42.1, 58.5, 124.2, 125.3, 126.6, 127.3, 140.1, 142.8, 211.2.

3a

Current Data Parameters
NAME C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000725
Time 10.02
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 92
DS 0
SWH 39682.539 Hz
FIDRES 0.505507 Hz
AQ 0.8258036 sec
RG 1024
DW 12.600 usec
DE 7.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SFO1 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7578055 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27666.71 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCH 11.25000 ppm/cm
HZCM 1414.77527 Hz/cm

3a

Current Data Parameters
NAME H-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000725
Time 9.56
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 32
DW 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SFO1 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300207 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 4001.04 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCH 0.41000 ppm/cm
HZCM 205.05331 Hz/cm

3b

Current Data Parameters
NAME proton
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000902
Time 18.50
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DSH 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 256
DM 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SF01 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 4001.04 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 205.05330 Hz/cm

3b

Current Data Parameters
NAME 13C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000902
Time 18.52
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 13591
DSH 0
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 2048
DM 12.600 usec
DE 7.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SF01 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577922 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27656.71 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCM 11.36000 ppm/cm

3c

Current Data Parameters
NAME dE1AULC
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000726
Time 8.12
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgdc
TD 65536
SOLVENT CDC13
NS 146
DS
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 9195.2
DM 12.600 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
PL1 -3.00 dB
SF01 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 28.00 dB
SF02 500.1317628 MHz

F2 - Processing parameters
SI 32768
SF 125.7578152 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 238.554 ppm
F1 30000.01 Hz
F2P -7.952 ppm
F2 -1000.00 Hz
PPMCM 12.32526 ppm/cm
HZCM 1550.00049 Hz/cm

3c

Current Data Parameters
NAME H-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000726
Time 15.44
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDC13
NS 4
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 15
DM 83.200 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 8.50 usec
PL1 0.00 dB
SF01 400.1328009 MHz

F2 - Processing parameters
SI 16384
SF 400.1300261 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.200 ppm
F2 -80.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 164.05331 Hz/cm

3d

Current Data Parameters
NAME default
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000728
Time 14.39
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 144
DS 1
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 9195.2
DM 12.600 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
PL1 -3.00 dB
SF01 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 26.00 dB
SF02 500.1317628 MHz

F2 - Processing parameters
SI 32768
SF 125.7578031 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 238.554 ppm
F1 30000.00 Hz
F2P -7.952 ppm
F2 -1000.00 Hz
PPMCM 12.32528 ppm/cm
HZCM 1550.00037 Hz/cm

3d

Current Data Parameters
NAME test
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20011226
Time 11.54
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 128
DM 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SF01 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 9.000 ppm
F1 4501.17 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.46000 ppm/cm
HZCM 230.05980 Hz/cm

3e

Current Data Parameters
NAME C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000721
Time 17.19
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 268
DS 0
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 1024
DW 12.600 usec
DE 7.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SFO1 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577970 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27666.71 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCM 11.25000 ppm/cm
HZCM 1414.77527 Hz/cm

3e

Current Data Parameters
NAME H-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000721
Time 17.04
INSTRUM spect
PROBHD 5 mm GNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 64
DW 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SFO1 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 4251.10 Hz
F1 8.500 ppm
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.43500 ppm/cm
HZCM 217.55655 Hz/cm

3f

Current Data Parameters
NAME proton
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20000902
Time 7.18
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 64
DM 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SF01 500.135009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300149 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 4001.04 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 205.05330 Hz/cm

3f

Current Data Parameters
NAME 13C-NMR
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20000902
Time 7.24
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 160
DS 0
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 2048
DM 12.600 usec
DE 7.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SF01 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577970 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27666.71 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCM 11.25000 ppm/cm

3g

Current Data Parameters
NAME C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000725
Time 20.19
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 67
DS 0
SWH 39682.538 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 1024
DM 12.500 usec
DE 7.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SF01 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7578128 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27666.72 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCM 11.25000 ppm/cm
HZCM 1414.77539 Hz/cm

3g

Current Data Parameters
NAME H-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000725
Time 20.14
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 16
DM 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SF01 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300305 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 4001.04 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 205.05331 Hz/cm

Current Data Parameters
NAME dEfaULc
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000729
Time 17.14
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 108
DS 0
SWH 30211.480 Hz
FIDRES 0.921981 Hz
AQ 0.5423604 sec
RG 9195.2
OW 16.550 usec
DE 23.64 usec
TE 300.0 K
d11 0.03000000 sec
PL12 20.00 dB
CPDPRG2 waltz16
PCPD2 105.00 usec
SF02 400.1329209 MHz
NUC2 1H
PL2 120.00 dB
D1 1.50000000 sec
P1 6.80 usec
SF01 100.6223610 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 100.6127846 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.25000 ppm/cm
HZCM 1131.89380 Hz/cm

Current Data Parameters
NAME H-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000729
Time 17.10
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 20.2
OW 83.200 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 8.50 usec
PL1 0.00 dB
SF01 400.1328009 MHz

F2 - Processing parameters
SI 16384
SF 400.1300272 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.200 ppm
F2 -80.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 164.05331 Hz/cm

3i

Current Data Parameters
NAME default
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 990608
Time 16.52
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 300
DS 0
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 1024
DM 12.600 usec
DE 7.50 usec
TE 300.0 K
D11 0.03000000 sec
PL12 20.00 dB
CPOPRG2 waltz16
PCPD2 100.00 usec
SF02 500.1320005 MHz
NUC2 1H
PL2 120.00 dB
D1 2.00000000 sec
P1 5.00 usec
SF01 125.7736214 MHz
NUC1 13C
PL1 0.00 dB

F2 - Processing parameters
SI 32768
SF 125.7578237 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27656.72 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCM 11.25000 ppm/cm
HZCM 1414.77551 Hz/cm

3i

Current Data Parameters
NAME default
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 990608
Time 16.32
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 5208.333 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 16
DM 96.000 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 5.00 usec
SF01 500.1320118 MHz
NUC1 1H
PL1 0.00 dB

F2 - Processing parameters
SI 16384
SF 500.1299992 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 9.000 ppm
F1 4501.17 Hz
F2P -100.03 Hz
F2 -100.03 Hz
PPMCM 0.46000 ppm/cm
HZCM 230.05980 Hz/cm

5

Current Data Parameters
NAME C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000725
Time 20.28
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 93
DS 0
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 1024
DM 12.600 usec
DE 7.50 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SF01 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7578164 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27666.72 Hz
F2P -5.000 ppm
F2 -528.79 Hz
PPMCH 11.25000 ppm/cm
HZCM 1414.77551 Hz/cm

5

Current Data Parameters
NAME H-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000725
Time 20.23
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 16
DM 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.0000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SF01 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 4001.04 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCH 0.41000 ppm/cm
HZCM 205.05330 Hz/cm

Current Data Parameters
NAME default
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000729
Time 20.52
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgdc
TO 65536
SOLVENT CDC13
NS 4326
DS 1
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 9195.2
DW 12.600 usec
DE 4.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 8.00 usec
PL1 -3.00 dB
SF01 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 28.00 dB
SF02 500.1317628 MHz

F2 - Processing parameters
SI 32768
SF 125.7577934 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 238.554 ppm
F1 30000.00 Hz
F2P -7.952 ppm
F2 -1000.00 Hz
PPMCM 12.32826 ppm/cm
HZCM 1550.00012 Hz/cm

Current Data Parameters
NAME default
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000729
Time 20.11
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg
TO 32768
SOLVENT CDC13
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 228.1
DW 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SF01 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 7.998 ppm
F1 4000.00 Hz
F2P -0.200 ppm
F2 -100.00 Hz
PPMCM 0.49989 ppm/cm
HZCM 205.00002 Hz/cm

9

Current Data Parameters
NAME 13C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000909
Time 17.58
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg
TO 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 39682.539 Hz
FIDRES 0.505507 Hz
AQ 0.8298036 sec
RG 2048
OW 12.600 usec
DE 7.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SFO1 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577922 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27666.71 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCM 11.25000 ppm/cm
HZCM 1414.77515 Hz/cm

9

Current Data Parameters
NAME proton
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000909
Time 17.52
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TO 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 256
OW 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SFO1 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 4001.04 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 205.05330 Hz/cm

11

Current Data Parameters
NAME 13C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000911
Time 9.28
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 131
DS 0
SWH 39682.539 Hz
FIDRES 0.505507 Hz
AQ 0.8259036 sec
RG 8192
DM 12.600 usec
DE 7.50 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.03000000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SF01 125.7736214 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577982 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27566.71 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCM 11.25000 ppm/cm
HZCM 1414.77527 Hz/cm

11

Current Data Parameters
NAME proton
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000911
Time 9.21
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 64
DM 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SF01 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 4001.04 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 205.05330 Hz/cm

Current Data Parameters
NAME 13C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000920
Time 17.10
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 43
DS 0
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 2048
DM 12.500 usec
DE 7.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

***** CHANNEL f1 *****
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SF01 125.7736214 MHz

***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7578043 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27668.71 Hz
F2P -5.000 ppm
F2 -628.79 Hz
PPMCM 11.25000 ppm/cm
HZCM 1414.77527 Hz/cm

Current Data Parameters
NAME dEFAulh
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000920
Time 18.14
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 90.5
DM 62.400 usec
DE 7.00 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
SF01 400.1328009 MHz
NUC1 1H
PL1 -5.00 dB

F2 - Processing parameters
SI 32768
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.200 ppm
F2 -80.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 164.05330 Hz/cm

15

Current Data Parameters
NAME 13C-NMR
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000909
Time 9.00
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 153
DS 0
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 2048
DW 12.600 usec
DE 7.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.00 usec
PL1 0.00 dB
SFO1 125.7736214 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 20.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577994 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 27666.71 Hz
F2P -5.000 ppm
F2 -629.79 Hz
PPMCM 11.25000 ppm/cm
HZCM 1414.77527 Hz/cm

15

Current Data Parameters
NAME proton
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000909
Time 8.53
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 64
DW 62.400 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 5.00 usec
PL1 0.00 dB
SFO1 500.1335009 MHz

F2 - Processing parameters
SI 16384
SF 500.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 4001.04 Hz
F2P -0.200 ppm
F2 -100.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 205.05330 Hz/cm

Current Data Parameters
NAME dEfaulc
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000921
Time 13.29
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT C6D6
NS 256
DS 0
SWH 30211.480 Hz
FIDRES 0.921981 Hz
AQ 0.5423604 sec
RG 9195.2
DW 16.550 usec
DE 23.64 usec
TE 300.0 K
d11 0.03000000 sec
PL12 20.00 dB
CPDPRG2 waltz16
PCPD2 105.00 usec
SFO2 400.1329209 MHz
NUC2 1H
PL2 120.00 dB
D1 1.50000000 sec
P1 6.80 usec
SFO1 100.6223610 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 100.6127772 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 22134.81 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.25000 ppm/cm
HZCM 1131.89380 Hz/cm

17

Current Data Parameters
NAME dEfaulh
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20000921
Time 13.21
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 40.3
DW 62.400 usec
DE 7.00 usec
TE 300.0 K
D1 1.00000000 sec
P1 7.70 usec
SFO1 400.1326009 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters
SI 32768
SF 400.1300110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 8.000 ppm
F1 3201.04 Hz
F2P -0.200 ppm
F2 -80.03 Hz
PPMCM 0.41000 ppm/cm
HZCM 164.05330 Hz/cm