Supporting Information

A Facile Regiocontrol in the Palladium-Catalyzed Annulation of Fluorine-Containing Internal Alkynes with Variously Substituted 2-Iodoanilines: A New Regioselective Synthesis of 2- or 3-Fluoroalkylated Indole Derivatives

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Typical Procedure for the palladium-catalyzed annulation reaction in the presence of $\text{Pd(PPh}_3)_4$.

$\text{Pd(PPh}_3)_4$ (0.106 g, 0.097 mmol), Et_3N (0.068 mL, 0.488 mmol), the 2-iodoaniline (0.19 g, 0.976 mmol), the alkyne **1a** (0.1 g, 0.488 mmol), DMF (4.0 mL) were added to a flask equipped with a stirring bar. After being heated for 8 h at 80 °C, the mixture was quenched with aq. NaHCO_3 , and extracted with Et_2O three times. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated in *vacuo*. The residue was chromatographed on silica gel using hexane-benzene (1 : 1) to afford indoles **2a** and **3a** in 79% combined yield.

Typical Procedure for the palladium-catalyzed annulation reaction in the presence of $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3 + \text{P}(o\text{-Tol})_3$.

$\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ (0.05 g, 0.048 mmol) and $\text{P}(o\text{-Tol})_3$ (0.12g, 0.39 mmol) in DMF (4.0 mL) were stirred for 5 min. To this mixture were added 2-iodoaniline (0.19 g, 0.976 mmol), alkyne **1a** (0.1 g, 0.488 mmol) and Et_3N (0.068 mL, 0.488 mmol). After being heated for 8 h at 80 °C, the mixture was quenched with aq. NaHCO_3 , and extracted with Et_2O three times. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated in *vacuo*. The residue was purified by silica gel column chromatography hexane-benzene (1 : 1) to afford the indoles **2a** and **3a** in 85% combined yield.

Current Data Parameters
NAME chae-4-24
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030424
Time 20.37
INSTRUM DRX500
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860212 sec
RG 143.7
RG 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
P1 9.30 usec
SFO1 500.130885 MHz
NUC1 1H
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 500.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 25.00 cm
FLP 10.000 ppm
F1 5001.30 Hz
F2p -1.000 ppm
F2 -500.13 Hz
PPMCM 0.44000 ppm/cm
HZCM 220.05721 Hz/cm

2a

S2

Current Data Parameters
NAME chae-4-24
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090424
Time 20.34

INSTRUM DR6500

PROBHD 5 mm Multinu

PULPROG zgpg30

TD 65536

SOLVENT CCl3

NS 256

DS 2

SWH 39682.519 Hz

FIDRES 0.60507 Hz

AQ 0.8258036 sec

RG 8192

DW 12.600 usec

DE 7.50 usec

TE 300.0 K

d11 0.03000000 sec

d12 0.00002000 sec

PL13 18.00 dB

D1 0.50000000 sec

CPDPRG2 waltz16

PCPD2 100.00 usec

SFO2 500.132005 MHz

NUC2 ¹H

PL2 -6.00 dB

PL12 18.00 dB

P1 5.70 usec

SFO1 125.7736214 MHz

NUC1 ¹³C

PL1 -2.00 dB

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 25.00 cm

FLP 200.000 ppm

F1 25151.56 Hz

F2P -10.000 ppm

F2 -1257.58 Hz

PPMCM 8.40000 ppm/cm

HZCM 1055.36548 Hz/cm

ppm

131.17
128.69

77.28
77.03
76.78

2a

S3

Indole-3-Cl (minor)

3a

Current Data Parameters
 NAME chae-7.16-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030716
 Time 18.27
 INSTRUM drx500
 PROBHD 5 mm Multinuc1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 287.4
 DM 48.400 usec
 DE 6.00 usec
 TE 295.8 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCNMRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 -6.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 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
 CY 12.50 cm
 F1P 10.000 ppm
 F1 5001.30 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 275.07150 Hz/cm

S4

Indole-p-Cl (minor)

3a

Current Data Parameters
NAME chae-7-16-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030716
Time 18.36

INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 4597.6
DE 16.550 usec
TE 296.5 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.777942 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCH 10.50000 ppm/cm
HZCM 1320.45679 Hz/cm

S5

2b

Current Data Parameters
NAME chae-5-22
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090522
Time 18.11
INSTRUM DEX500
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.31564 Hz
AQ 1.5860212 sec
RG 322.5
DB 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
P1 9.30 usec
SFO1 500.130085 MHz
NUC1 1H
PUL -6.00 dB

F2 - Processing parameters
SI 16384
SF 500.130031 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CK 25.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
FREQN 0.46000 ppm/cm
HZCM 220.05721 Hz/cm

S6

Current Data Parameters
NAME chae-5-22
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20010522
Time 18.18
INSTRUM DEX500
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 39682.519 Hz
FIDRES 0.605507 Hz
AQ 0.825015 sec
RG 619.2
DE 12.500 usec
TE 300.0 K
D1 0.5000000 sec
D11 0.0300000 sec
D12 0.0600000 sec
D13 18.00 dB
CPDPRG2 waltz16
PCPD2 100.00 usec
SFO2 500.132005 MHz
NUC2 1H
PUL2 -6.00 dB
PL2 18.00 dB
PL 5.10 usec
SFO1 125.773214 MHz
NUC1 13C
PL1 -2.00 dB

F2 - Processing parameters
SI 32768
SF 125.7577958 MHz
WDW EX
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR Plot parameters
CX 25.00 cm
FLP 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PWCN 8.40000 ppm/cm
HZCN 1056.36548 Hz/cm

S7

sample

S8

Current Data Parameters
 NAME chae-7.5-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030705
 Time 18.30
 INSTRUM drx500
 PROBD 5 mm Multinuc1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 128
 DM 48.400 usec
 DE 6.00 usec
 TE 295.7 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 -6.00 dB
 SF01 500.1300885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300286 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 10.000 ppm
 F1 5001.30 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 275.07150 Hz/cm

3b

Current Data Parameters
NAME chae-7.5-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030705
Time 18.38
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30030.029 Hz
FIDRES 0.45622 Hz
AQ 1.0912244 sec
RG 3649.1
DM 16.550 usec
DE 6.00 usec
TE 296.4 K
D1 0.50000000 sec
d11 0.03000000 sec
MGREST 0.00000000 sec
MCIRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577960 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 DPM
F1 25151.56 Hz
F2P -10.000 DPM
F2 -1257.58 Hz
PRACH 10.50000 DPM/cm
HZCM 1320.45679 Hz/cm

S9

Current Data Parameters
NAME chae-5-28
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030528
Time 20.53
INSTRUM DRX500
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
FIDRES 0.115264 Hz
AQ 1.5860212 sec
RG 322.5
DE 48.400 usec
TE 300.0 K
D1 1.00000000 sec
P1 9.30 usec
SFO1 500.130885 MHz
NUC1 1H
P11 -6.00 dB

F2 - Processing parameters
SI 16384
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 25.00 cm
FLP 10.000 ppm
F1 5001.30 Hz
F2p -1.000 ppm
F2 -500.13 Hz
PPMCM 0.44000 ppm/cm
HZCM 220.05721 Hz/cm

S10

Current Data Parameters
NAME Chae-5-28
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050528
Time 21.00
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CMC13
NS 256
DS 2
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258035 sec
RG 9195.2
DW 12.600 usec
DE 7.50 usec
TE 300.2 K
d1 0.03000000 sec
d11 0.0002000 sec
d12 18.00 dB
d13 0.50000000 sec
D1 wait216
CDEPRG2
PCPD2 100.00 usec
SF02 500.132005 MHz
NUC2 1H
PI2 -6.00 dB
PI12 18.00 dB
P1 5.70 usec
SF01 125.7735214 MHz
NUC1 13C
PI1 -2.00 dB

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 25.00 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCK 8.40000 ppm/cm
HZCM 1055.36548 Hz/cm

S11

2c

sample

7.0000
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0.0400
0.0200
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Current Data Parameters
NAME Chae-7.3-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030703
Time 16.16

INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2

SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 406.4
DM 48.400 usec
DE 6.00 usec
TE 295.9 K

D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.130085 MHz

F2 - Processing parameters
SI 32768
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
CY 12.50 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCW 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S12

133	7.77
130	8.76
130	8.66
123	3.41
123	1.71
121	5.72
119	8.63
119	8.52
114	1.11
110	9.65
77	2.57
77	0.03
76	7.49

5.7 2.57

3c

Current Data Parameters
NAME C148-315-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040223
Time 21.05

INSTRUM drx500
PROBHD 5 mm Mu:innucl
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 256
DS 2

SWH 30030.025 Hz
FIDRES 0.458222 Hz
AQ 1.0912242 sec
RG 1145.4

DW 16.350 usec
DE 6.00 usec
TE 296.9 K
D1 0.50000000 sec
d11 0.03000000 sec
XDPREST 0.30000000 sec
MCNMR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
C13PRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577942 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.10

1D NMR plot parameters
CX 20.00 cm
CY 11.09 cm
Z1P 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCM 10.50000 ppm/cm
HZCM 1320.45675 Hz/cm

S13

Rxn318

Current Data Parameters
 NAME chae-R318
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters:
 Date_ 20040420
 Time 19.21
 INSTRUM dtx500
 PROBD 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 406.4
 DW 48.400 usec
 DE 6.00 usec
 TE 296.2 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWPRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL -6.00 dB
 SFO1 500.130885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300150 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S14

2d

Current Data Parameters
NAME chae-6-4
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030604
Time 20.19
INSTRUM DEXY00
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 39682.539 Hz
FIDRES 0.60507 Hz
AQ 0.325036 sec
RG 2048
DM 12.600 usec
DE 7.50 usec
TE 300.0 K
d11 0.0300000 sec
d12 0.0002000 sec
PUL3 18.00 dB
D1 0.5000000 sec
waitz16
CPOPRG2
PCPD2 100.00 usec
SFO2 500.132005 MHz
NUC2 1H
PUL2 -6.00 dB
PL12 18.00 dB
P1 5.70 usec
SFO1 125.773214 MHz
NUC1 13C
PL1 -2.00 dB

F2 - Processing parameters
SF 125.773214 MHz
WDW EN
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 25.00 cm
F1P 200.000 ppm
F1 23151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMXX 8.40000 ppm/cm
HZCM 1056.35348 Hz/cm

S15

sample

7.3553
7.3535
7.3516
7.3497
7.3478
7.3459
7.3440
7.3421
7.3402
7.3383
7.3364
7.3345
7.3326
7.3307
7.3288
7.3269
7.3250
7.3231

4.4475
4.4293
4.4150
4.4007

1.5060
1.4396
1.4253
1.4111

0.0000

3d

Current Data Parameters
NAME chae-R318-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040528
Time 19.51
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 724.1
DM 48.400 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.130085 MHz

F2 - Processing parameters
SI 32768
SF 500.1300147 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.69 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S16

13C 256
 114 256
 135 415
 135 245
 140 445
 129 415
 129 006
 128 950
 128 398
 123 791
 121 838
 120 108
 111 327
 77 254
 77 000
 76 746
 61 372
 14 256

3d

Current Data Parameters
 Name 1036-311-2
 ExpNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040308
 Time 20.45
 INSTRUM crysco
 PROBHD 5 mm Multinuc1
 PULPROG zgpg30
 TD 65536
 FIDRES 0.0013
 SOLVENT DMSO
 NS 256
 DS 2
 SWH 30030.329 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912244 sec
 R3 1623.5
 DM 16.590 usec
 DE 6.00 usec
 TE 295.4 K
 D1 0.50000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCNRC 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.70 usec
 PL1 -2.00 dB
 SFO1 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 -6.00 dB
 PL12 13.74 dB
 PL13 13.74 dB
 SFO2 500.132005 MHz

F2 - Processing Parameters
 SI 32768
 SF 125.7577960 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 0.10

1D NMR Plot Parameters
 CX 20.00 cm
 CY 10.91 cm
 F1P 200.000 ppm
 F1 25151.56 Hz
 F2P -10.000 ppm
 F2 -1257.58 Hz
 PPMCM 10.50000 ppm/cm
 HZCM 1320.45679 Hz/cm

S17

Current Data Parameters
NAME cha-5-2
EXNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030602
Time 11:59
INSTRUM DR2500
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SFO 10130.578 Hz
FIDRES 0.315664 Hz
AQ 1.5860212 sec
RG 645.1
BW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
P1 9.30 usec
SFO1 500.130085 MHz
NUC1 1H
P11 -6.00 dB

F2 - Processing parameters
SI 16364
SF 500.130080 MHz
RG 0
RM 0
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 25.80 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -500.13 Hz
F2 0.44000 ppm/cm
FPCW 220.05724 Hz/cm

S18

2e

Current Data Parameters
 NAME chae-6-2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030602
 Time 12.06
 INSTRUM DEX500
 PROBRD 5 mm Maltinu
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 2
 SM 39682.539 Hz
 FIDRES 0.60507 Hz
 AQ 0.8258036 sec
 RG 3251
 RW 12.600 usec
 DE 7.50 usec
 TE 300.0 K
 dt1 0.0300000 sec
 dt2 0.0002000 sec
 PC13 18.00 dB
 DI 0.5000000 sec
 CDEPRG2 waltz16
 POPP2 100.00 usec
 SFO2 500.1320005 MHz
 NUC2 1H
 PC2 -6.00 dB
 PC12 18.00 dB
 PL 5.70 usec
 SFO1 125.7736214 MHz
 NUC1 13C
 PC1 -2.00 dB

F2 - Processing parameters
 SI 37768
 SF 125.7577934 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 25.00 cm
 P1P 200.000 ppm
 F1 25351.56 Hz
 F2 10.000 ppm
 F2 1251.58 Hz
 PFRCK 8.46000 ppm/cm
 HZCM 1056.36348 Hz/cm

S19

Rxn317-2

Current Data Parameters
NAME chae-R317-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040417
Time 17.40
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 574.7
DM 48.400 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWIRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.1330885 MHz

F2 - Processing Parameters
SI 32768
SF 500.1300144 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 3.98 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCH 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S20

3e

Current Data Parameters
NAME chae-6-9
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030609
Time 11.08
INSTRUM DES500
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SFO/RENT CQC13
NS 256
DS 2
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.9258036 sec
RG 5792.6
DM 12.600 usec
DE 7.50 usec
TE 300.0 K
PC 0.0300000 sec
d11 0.0002000 sec
d12 18.00 dB
d13 0.5000000 sec
D1 CDEPRG2
WALTZ16
PCPD2 120.00 usec
SFO2 500.132003 MHz
NUC2 1H
P2 18.00 dB
F2 3.70 usec
SFO1 125.773214 MHz
NUC1 13C
P1 2.00 dB
F1 1.40

F2 - Processing parameters
SI 32768
SF 125.777956 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 25.00 cm
FIP 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCM 8.40000 ppm/cm
HZCM 1056.35546 Hz/cm

S21

sample

2f

2f

Current Data Parameters
NAME chae-6-11
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030611
Time 11.58
INSTRUM DRX500
PROBHD 5 mm Naltru
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 39682.539 Hz
FIDRES 0.605507 Hz
AQ 0.8258036 sec
RG 4096
DB 12.600 usec
DE 7.50 usec
TE 300.0 K
d11 0.03000000 sec
d12 0.00020000 sec
PC13 18.00 db
DI 0.50000000 sec
CPOPRG2 waltz16
PCPD2 100.00 usec
SFO2 500.132005 MHz
NUC2 1H
PC2 -6.00 db
PC12 18.00 db
PI 5.70 usec
SFO1 125.773614 MHz
NUC1 13C
PC1 -2.00 db

F2 - Processing parameters
SI 32768
SF 125.7577913 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CY 325.00 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1251.56 Hz
FREQ4 8.40000 ppm/cm
HZCM 1056.36546 Hz/cm

S23

sample

3f

7.3524
7.3491
7.3484
7.3511
7.3507
7.3479
7.3454
7.3456
7.3461
7.3443
7.3682
7.3656
7.3531
7.3506
7.3164
7.3143
7.2670
7.2392

2.3739

1.2567

0.0760
0.0001
0.0063

Current Data Parameters
NAME chae-R319-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040521
Time 16.35
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719823 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 296.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.1330985 MHz

F2 - Processing parameters
SI 32768
SF 500.1300238 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 5.39 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCW 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S24

S25

Current Data Parameters

NAME	chae-7.14-1
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20030714
Time	17.16
INSTRUM	dfx500
PROBHD	5 mm WJ11nuc1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	30030.029 Hz
FIDRES	0.456222 Hz
AQ	1.0912244 sec
RG	10321.3
DW	16.650 usec
DE	6.00 usec
TE	296.5 K
D1	0.50000000 sec
d11	0.03000000 sec
WCREST	0.00000000 sec
MCWRR	0.01500000 sec

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

NUC1	¹³ C
P1	5.70 usec
PL1	-2.00 dB
SFO1	125.7703643 MHz

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

CPDPRG2	waltz16
NUC2	¹ H
PCPD2	100.00 usec
PL2	-6.00 dB
PL12	13.74 dB
PL13	13.74 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577942 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
CY	12.50 cm
F1P	200.000 ppm
F1	25151.56 Hz
F2P	-10.000 ppm
F2	-1257.58 Hz
ppmCM	10.50000 ppm/cm
HZCM	1320.45679 Hz/cm

sample

8.4820
8.6215
7.6350
7.5162
7.4451
7.4284
7.3377
7.3358
7.3898
7.3848
7.3931
7.3806
7.3757
7.3725
7.3677
7.2136
7.2119

28

0.0857
-0.0000

Current Data Parameters
NAME chae-R320
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040525
Time 16.23
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DM 48.400 usec
DE 6.00 usec
TE 296.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCNMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1300885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300339 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.58 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S26

28

Current Data Parameters
NAME chae-7.4-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030704
Time 16.42

INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 1290.2
DM 16.650 usec
DE 6.00 usec
TE 296.6 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577951 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPNCH 10.50000 ppm/cm
HZCH 1320.45679 Hz/cm

S27

sample

3g

Current Data Parameters
NAME chae-R320-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040521
Time 21.10
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 228.1
DM 48.400 usec
DE 6.00 usec
TE 296.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCNRMK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300241 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 5.58 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S28

3g

Current Data Parameters

NAME chae-7.17-1

EXPNO 2

PROCNO 1

F2 - Acquisition Parameters

Date_ 20030717

Time 16.47

INSTRUM drx500

PROBHD 5 mm Multinucl

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 256

DS 2

SWH 30030.029 Hz

FIDRES 0.458222 Hz

AQ 1.0912244 sec

R6 3649.1

RG 16.650 usec

DE 6.00 usec

TE 296.7 K

D1 0.50000000 sec

d11 0.03000000 sec

MCREST 0.00000000 sec

MCIRK 0.01500000 sec

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

NUC1 13C

P1 5.70 usec

PL1 -2.00 dB

SFO1 125.7703643 MHz

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

CPROPG2 waltz16

NUC2 1H

PCPD2 100.00 usec

PL2 -6.00 dB

PL12 13.74 dB

PL13 13.74 dB

SFO2 500.1320005 MHz

F2 - Processing parameters

SF 32768

SF 125.7577942 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

10 NMR plot parameters

CX 20.00 cm

CY 12.50 cm

FAP 200.000 ppm

F1 25151.56 Hz

F2 -10.000 ppm

F2 -1257.58 Hz

PPMCM 10.50000 ppm/cm

HZCM 1320.45679 Hz/cm

S29

sample

2h

S30

Current Data Parameters
NAME Chae-R351
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030927
Time 15.11
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DW 48.400 usec
DE 6.00 usec
TE 295.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWAK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1300885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300295 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 11.57 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

ppm

2h

Current Data Parameters
NAME Chae-R351
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030927
Time 15.21

INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2

SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 3649.1
DM 16.650 usec
DE 5.00 usec
TE 296.5 K
D1 0.50000000 sec
d11 0.03000000 sec
MCRES1 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577951 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.10

1D NMR Plot Parameters
CX 20.00 cm
CY 11.34 cm
FAP 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCM 10.50000 ppm/cm
HZCM 1320.45679 Hz/cm

S31

sample

7.5411
7.5362
7.5257
7.5201
7.5074
7.5043
7.4956
7.4946
7.4909
7.4805
7.4713
7.4605
7.4572
7.4436
7.4343

2.95281
2.93731
2.92230
2.72757
2.71242
2.69712
2.68741
2.67162
2.65662
2.64099
2.62594
1.55292
1.25509
0.07026
0.00633
0.00017

3h

Current Data Parameters
NAME chae-R351-2
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040618
Time 16.43

INSTRUM dpx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2

SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 724.1

DW 48.400 usec
DE 6.00 usec
TE 297.2 K

D1 1.00000000 sec
MCREST 0.00000000 sec
MCNMR 0.01500000 sec

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

NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.1300885 MHz

F2 - Processing parameters

SF 500.1300140 MHz
WDW EM
SSB 0

LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
CY 3.50 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S32

141 200
 134 342
 128 348
 128 348
 126 348
 122 348
 121 348
 119 348
 110 348

77 255
 77 001
 76 747

35 342
 31 150
 26 465

3h

Current Data Parameters
 NAME: 07ae-f351-2
 EXPNO: 3
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20040218
 Time: 19.11
 INSTRUM: drx500
 PROBRD: 5 mm KUL1nuc
 PULPROG: zgpg30
 TD: 35536
 SOLVENT: CDCl3
 NS: 256
 DS: 2
 SMH: 30030.029 Hz
 FIDRES: 0.458222 Hz
 AQ: 1.091224 sec
 RG: 3649.1
 DW: 16.650 usec
 DE: 6.00 usec
 TE: 296.8 K
 D1: 0.50000000 sec
 D11: 0.03000000 sec
 MCREST: 0.00000000 sec
 MCWRR: 0.01500000 sec

===== CHANNEL f1 =====
 NUC1: 13C
 P1: 5.70 usec
 PL1: -2.00 dB
 SF01: 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2: waltz16
 NUC2: 1H
 PCPD2: 100.00 usec
 PL2: -6.00 dB
 PL12: 13.74 dB
 PL13: 13.74 dB
 SF02: 500.1320005 MHz

F2 - Processing Parameters
 SI: 32768
 SF: 125.7577942 MHz
 WDW: EM
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.40

1D NMR plot parameters
 CX: 20.00 cm
 CY: 10.98 cm
 F1P: 200.000 ppm
 F1: 25151.56 Hz
 F2P: -10.000 ppm
 F2: -1257.58 Hz
 PPMCM: 10.50000 ppm/cm
 HZCM: 1320.45679 Hz/cm

[illegible]

21

Current Data Parameters	
NAME	Value
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Date_	20040211
Time	18.48
INSTRUM	dfx500
PROBHD	5 mm Multinuc1
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	256
DM	48.400 usec
DE	5.00 usec
TE	295.4 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCPRK	0.01500000 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	10.30 usec
PL1	-6.00 dB
SFO1	500.1330885 MHz
F2 - Processing parameters	
SI	32768
SF	500.1300222 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00
1D NMR plot parameters	
CX	20.00 cm
CY	9.97 cm
F1P	10.000 ppm
F1	5001.30 Hz
F2P	-1.000 ppm
F2	-500.13 Hz
PPMQM	0.55000 ppm/cm
HZCM	275.07150 Hz/cm

S34

2i

Current Data Parameters
 NAME Case-3403
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040211
 Time 18.56
 INSTRUM grx500
 PQA040 5 mm Multinuc1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 2
 SWH 30030.029 Hz
 FIDRES 0.459222 Hz
 AQ 1.0912244 sec
 RG 5792.6
 DW 16.650 usec
 DE 6.00 usec
 TE 296.5 K
 D1 0.50000000 sec
 d11 0.03000000 sec
 MCOREST 0.00000000 sec
 KCMRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.70 usec
 PL1 -2.00 dB
 SF01 125.7703643 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD02 100.00 usec
 PL2 -5.00 dB
 PL12 13.74 dB
 PL13 13.74 dB
 SF02 500.1320005 MHz

F2 - Processing Parameters
 SI 32768
 SF 125.7577932 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 0.05

1D NMR Plot Parameters
 CX 20.00 cm
 CY 21.35 cm
 FJP 200.000 ppm
 F1 25151.56 Hz
 F2 -10.000 ppm
 F2 -1257.58 Hz
 PPMCM 10.50000 ppm/cm
 HZCM 1320.45679 Hz/cm

S35

sample

Current Data Parameters
 NAME chae-R400-2
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040622
 Time 17.53
 INSTRUM drx500
 PROBD 5 mm Multinuc1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 406.4
 DM 48.400 usec
 DE 6.00 usec
 TE 297.8 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWPK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 -6.00 dB
 SFO1 500.130085 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300185 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 3.99 cm
 F1P 10.000 ppm
 F1 5001.30 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 275.07150 Hz/cm

S36

3i

Current Data Parameters

NAME	CH3-R400-2
EXPNO	2
F2PROCNO	1

F2 - Acquisition Parameters

Date_	20040217
Time	18.24
INSTRUM	CPX500
PROBHD	5 mm Multinuc1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	256
DS	2
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912244 sec
RG	3649.1
DE	16.650 usec
TE	296.5 K
D1	0.50000000 sec
d11	0.03000000 sec
MGEST	0.00000000 sec
MGMRK	0.01500000 sec

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

NUC1	13C
P1	5.70 usec
PL1	-2.00 dB
SFO1	125.7703643 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	-6.00 dB
PL12	13.74 dB
PL13	13.74 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577932 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	0.10

1D NMR plot parameters

CX	20.00 cm
CY	22.28 cm
F1P	200.000 ppm
F1	25151.56 Hz
F2P	-10.000 ppm
F2	-1257.58 Hz
PRMCM	10.50000 PPM/cm
HZCM	1320.45679 Hz/cm

S37

2j

130 106
133 125
140 796
129 106
126 201
129 844
121 111
120 285
111 825
109 830

77 252
76 998
76 744

Current Data Parameters
NAME Chae-7.1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030701
Time 15.23

INSTRUM dtx500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT DMS
NS 256
DS 2

SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 1824.6
DM 16.650 usec
DE 6.00 usec
TE 296.5 K

D1 0.50000000 sec
d11 0.03000000 sec
MCHEST 0.00000000 sec
MCPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577951 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 23151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCK 10.50000 ppm/cm
HZCK 1320.45679 Hz/cm

S39

sample

1.0000
1.9923
2.0194
1.1434
0.9927

1.7391
0.0818
0.0000

2k

Current Data Parameters
NAME chae-R345
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030823
Time 14.47
INSTRUM grx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DM 48.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.130885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300219 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S40

2k

Current Data Parameters
NAME: 346-R345
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20030823
Time: 14.55
INSTRUM: drx500
PROBHD: 5 mm Multinuc1
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 256
DS: 2
SWH: 30030.029 Hz
FIDRES: 0.458222 Hz
AQ: 1.0912244 sec
RG: 3649.1
DM: 16.650 usec
DE: 6.00 usec
TE: 296.9 K
D1: 0.50000000 sec
d11: 0.03000000 sec
MCHEST: 0.00000000 sec
MCMRK: 0.01500000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 5.70 usec
PL1: -2.00 dB
SFO1: 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2: waltz16
NUC2: 1H
PCPD2: 100.00 usec
PL2: -6.00 dB
PL12: 13.74 dB
PL13: 13.74 dB
SFO2: 500.1320005 MHz

F2 - Processing Parameters
SI: 32768
SF: 125.7577951 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 0.10

10 NMR plot parameters
CY: 20.00 cm
CX: 12.50 cm
F1P: 200.000 ppm
F1: 25151.56 Hz
F2P: -10.000 ppm
F2: -1257.58 Hz
PPMCM: 10.50000 ppm/cm
HZCM: 1320.45679 Hz/cm

S41

Rxn345-2

3k

Current Data Parameters
NAME chae-R345-2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters:
Date_ 20040420
Time 19.14

INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 812.7
DW 48.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

S42

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

NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

140.135
129.604
121.075
112.240
77.261
77.003
76.750

3k

Current Data Parameters
NAME chae-345-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030908
Time 11.14

INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30030.029 HZ
FIDRES 0.458222 HZ
AQ 1.0912244 sec
RG 812.7
DM 16.650 usec
DE 6.00 usec
TE 297.0 K
D1 0.50000000 sec
d11 0.03000000 sec
ICREST 0.00000000 sec
WCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577987 MHz
WDW EM
SSB 0
LB 1.00 HZ
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 DPM
F1 25151.56 HZ
F2P -10.000 DPM
F2 -1257.58 HZ
PRPCH 10.50000 DPM/cm
HZCM 1320.45579 HZ/cm

S43

sample

21

Current Data Parameters
NAME chae-R340
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030728
Time 18.47
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DM 48,400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.1330885 MHz

F2 - Processing Parameters
SI 32768
SF 500.1300286 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 11.61 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S44

133.484	77.256
133.201	77.002
131.172	76.748
131.068	
130.761	
128.638	
128.334	
127.295	
127.102	
127.626	
121.484	
121.191	
120.485	
120.026	
117.999	
117.978	
111.418

21

Current Data Parameters
NAME Chae-R340
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030728

Time 18.56
INSTRUM drx500
PROBHD 5 mm WJ11nuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2

SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 3649.1
DM 16.650 usec
DE 6.00 usec
TE 296.9 K
D1 0.50000000 sec
d11 0.03000000 sec
MOOREST 0.00000000 sec
MCWAK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577951 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.96 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCM 10.50000 ppm/cm
HZCM 1320.45679 Hz/cm

S45

sample

31

Current Data Parameters
NAME chae-R340
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030731
Time 17.20
INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 287.4
DM 48.400 usec
DE 6.00 usec
TE 296.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.1330885 MHz

F2 - Processing Parameters
SI 32768
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
CY 11.07 cm
F1P 10.000 DPM
F1 5001.30 Hz
F2P -1.000 DPM
F2 -500.13 Hz
PPMCM 0.55000 DPM/cm
HZCM 275.07150 Hz/cm

S46

2m

Current Data Parameters
NAME chae-7.24-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030724
Time 19.40
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SM 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 9195.2
DM 16.650 usec
DE 6.00 usec
TE 296.7 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCMBK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577932 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10 NMR plot parameters
CX 20.00 cm
CY 11.24 cm
F1p 200.000 ppm
F1 25151.56 Hz
F2p -10.000 ppm
F2 -1257.58 Hz
PPMCM 10.50000 ppm/cm
HZCM 1320.45679 Hz/cm

S49

RX-333-2

Current Data Parameters
NAME: RX-333-2
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20060629
Time: 17.24
INSTRUM: spect
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 2
DS: 2
SWH: 10150.578 Hz
FIDRES: 0.167632 Hz
AQ: 3.1719923 sec
RG: 912.3
CW: 48.400 usec
TE: 296.2 K
DE: 6.00 usec
TE: 296.2 K
D1: 1.00000000 sec
dCREST: 0.00000000 sec
dCMR: 0.01500000 sec
===== CHANNEL f1 =====
NUC1: 1H
P1: 10.30 usec
PL1: -6.00 dB
SF01: 500.1300935 MHz
F2 - Processing parameters
SI: 32768
SF: 500.1300125 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
2D NMR plot parameters
CX: 20.00 cm
CY: 4.72 cm
F1: 12.000 ppm
F2: 5001.56 Hz
F2P: -1.000 ppm
F2: -500.13 Hz
PPMCH: 0.65000 ppm/cm
HZCM: 325.08450 Hz/cm

S50

77 253
 76 999
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3m

Current Date: 06/06/2015
NAME: J. G. G. G. G.
EXPENSE: 2
FIDUCY: 1

F2 - Acquisition Performance

Time	19	23
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55:33 ID

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30330. 123

1.09:2.44

12. 0

293.6

01	0.30000100
01	0.03000100

MCHES1	0.60000E+00
MCMBK	0.01500E+00

CHANNEL 11

	NUC1	P1
30	5	70

9.1	-2 00
9.01	4 25 770 36 44

----- CHAINE £3

```
CFDPAGE2      wallt::1:
MIG3
```

FCPD2	100 00
100 00	100 00

PL12 13 7.

SFC2 500.132000

F2 - Processing parameter

SF 125.757793

555

68

10

- D WEN PLOT DIFFERENCE
CX 20.0

C1	10.3
F1P	200.00

F1	23151.3
=2P	-10.00

F2	-1257.5
PPHCM	10.5000

727M : 320.456/

S51

Indole-methoxyaniline

```
Current Data Parameters
NAME          chae-7.15-1
EXPNO         1
PROCNO        1
```

```
F2 - Acquisition Parameters
Date_ 20030715
```

```
INSTRUM      drx500
PROBHD      5 mm Multinuc1
PULPROG      zg30
```

SOLVENT	CDC13
NS	16

SW1	10350.578 HZ
FIDRES	0.157632 HZ
AD	3.4740000

DW	48.400 usec
DE	6.00 usec

U1	1.00000000 sec
MCREST	0.00000000 sec

```
===== CHANNEL f1 =====
NIG1 1H
```

PL1	-6.00 dB
SFO1	500.1330885 MHz

Processing parameters	
SI	32768
CF	500, 400, 400, 400

SSB	0
LB	0.30 Hz

1.00

10.000 mm	10.000 mm
12.50 cm	12.50 cm
10.000 mm	10.000 mm

F2P	-1.000 ppm
F2	-500.13 Hz

273.0/130 H2/C

S52

Indole-methoxylaniline

2n

Current Data Parameters
NAME chae-7.15-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030715
Time 18.05
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 4096
DM 16.650 usec
DE 6.00 usec
TE 298.5 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCIRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SF02 500.1320005 MHz

F2 - Processing Parameters
SI 32768
SF 125.7577932 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCM 10.50000 ppm/cm
HZCM 1320.45691 Hz/cm

S53

sample

1.0000
1.1085
2.2848
2.1988
1.0889
1.0910

3.84839

1.60709

0.07448

0.00022

Integral

1.0000

1.1085

2.2848

2.1988

1.0889

1.0910

3.2379

ppm

6

6

4

2

0

Current Data Parameters
NAME chae-7,22-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030722
Time 19.20

INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2

SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 322.5
DW 48.400 usec
DE 6.00 usec
TE 296.0 K

D1 1.000000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300178 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 11.22 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

3n

S54

S55

Current Data Parameters

NAME chae-7-22-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030722
Time 19.28
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 3649.1
DM 16.650 usec
DE 6.00 usec
TE 296.7 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNMR 0.01500000 sec

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

NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SF01 125.7703643 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SF02 500.1320005 MHz

F2 - Processing parameters

SI 32768
SF 125.7577942 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 12.50 cm
FIP 200.000 ppm
F1 25151.56 Hz
F2 -1257.58 Hz
PPMCM 10.50000 ppm/cm
HZCM 1320.45679 Hz/cm

sample

7.3621
7.3464
7.3042
7.2977
7.2833
7.2773
7.2613
7.2410
7.2270
7.2170
7.2042

1.6717
1.2543
0.0062
0.0061

20

Current Date Parameters
NAME 10a-F14J
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20030825
Time 18.45

INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMS-D6
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 406.4
DM 48.400 usec
DE 6.00 usec
TE 296.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SFO1 500.1300885 MHz

F2 - Processing Parameters
SI 32768
SF 500.1300153 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR Plot Parameters
CX 20.00 cm
CY 10.58 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCH 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

S56

S57

```

===== CHANNEL f1 =====
NUC1      13C
P1         5.70 usec
PL1        -2.00 dB
SF01      125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2        -6.00 dB
PL12       13.74 dB
PL13       13.74 dB
SF02       500.1320005 MHz

F2 - Processing parameters
SI         32768
SF         125.7577932 MHz
WDW         EM
SSB         0
LB         1.00 Hz
GB          0
PC          0.10

F1 - Acquisition Parameters
Date_      20030826
Time       18.53
INSTRUM    drx500
PROBHD     5 mm Multinuc1
PULPROG    zgpg30
TD          65536
SOLVENT    CDCl3
NS          256
DS          2
SWH         30030.029 Hz
FIDRES     0.458222 Hz
AQ          1.0912244 sec
RG          3649.1
DM          16.650 usec
DE          6.00 usec
TE          297.4 K
D1          0.50000000 sec
d11         0.03000000 sec
WDETEST    0.00000000 sec
MCMARK     0.01500000 sec

F2 - Acquisition Parameters
Date_      20030826
Time       18.53
INSTRUM    drx500
PROBHD     5 mm Multinuc1
PULPROG    zgpg30
TD          65536
SOLVENT    CDCl3
NS          256
DS          2
SWH         30030.029 Hz
FIDRES     0.458222 Hz
AQ          1.0912244 sec
RG          3649.1
DM          16.650 usec
DE          6.00 usec
TE          297.4 K
D1          0.50000000 sec
d11         0.03000000 sec
WDETEST    0.00000000 sec
MCMARK     0.01500000 sec

10 NMR plot parameters
CX         20.00 cm
CY         12.50 cm
F1P        200.000 DPM
F1         25151.56 Hz
F2P        -10.000 DPM
F2         -1257.58 Hz
PPMCM      10.50000 DPM/cm
HZCM       1330.45679 Hz/cm

```

sample

30

```

Current Data Parameters
NAME      03se-R344-2-2
EXPNO     1
PROCNO    1
PROCNAME  1

F2 - Acquisition Parameters
Date_     20030426
Time      19.45
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157532 Hz
AQ          3.1719923 sec
RG          405.4
CW          48.400 usec
DE          6.00 usec
TE          296.5 K
D1          1.00000000 sec
dCREST     0.00000000 sec
MCWK       0.01500000 sec

===== CHANNEL f1 =====
NUC1       1H
P1          10.30 usec
PL1         -6.00 dB
SF01       500.1330885 MHz

F2 - Processing parameters
SI          32768
SF          500.1300156 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

1D NMR plot parameters
CX          20.00 cm
CY          10.96 cm
F1P         10.000 ppm
F1          500.130 Hz
F2P         -1.000 ppm
F2          -500.13 Hz
PPMCK       0.55000 ppm/cm
HZCM        275.07150 Hz/cm
  
```

S58

sample

1.0000
5.2014
0.7942
3.1366
2.2242
6.5287
1.4507
5.3122
0.8654
5.3201
7.8459
3.5375
2.3369

4b

Current Data Parameters
NAME Chae-326-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040311
Time 15:52
INSTRUM spect
PROBHD 5 mm WALTZ-16
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 362
DK 48.400 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
WREST 0.00000000 sec
MDWFK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -5.00 dB
SFO1 500.1330885 MHz

F2 - Processing Parameters

SI 32768
SF 500.1300175 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 8.39 cm
FAP 13.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
SFOCM 3.55000 ppm/cm
HZCM 275.37150 Hz/cm

S60

sample

Current Data Parameters
 NAME chae-7-4-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20030704
 Time 16.47
 INSTRUM drx500
 PROBHD 5 mm Multinuc1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.171923 sec
 RG 203.2
 DW 48.400 usec
 DE 6.00 usec
 TE 296.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCNMR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.30 usec
 PL1 -6.00 dB
 SFO1 500.1300885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300235 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 10.000 ppm
 F1 5001.30 Hz
 F2P -1.000 ppm
 F2 -500.13 Hz
 PPMCM 0.55000 ppm/cm
 HZCM 275.07150 Hz/cm

S61

5b

```

Current Data Parameters
NAME      cnae-7.4-2
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20030704
Time      16.55
INSTRUM   drx500
PROBHD    5 mm Multinuc1
PULPROG   zgpg30
TO        299930
TD         65536
SOLVENT   CDCl3
NS         256
DS         2
SWH        30030.029 HZ
FIDRES     0.458222 HZ
AQ         1.0912244 sec
RG         3251
DW         16.550 usec
DE         6.00 usec
TE         296.6 K
D1         0.50000000 sec
d11        0.03000000 sec
MCOREST    0.00000000 sec
MCKMR      0.01500000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         5.70 usec
PL1        -2.00 dB
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPOPRG2    waltz16
NUC2       1H
PCPD2      100.00 usec
PL2        -6.00 dB
PL12       13.74 dB
PL13       13.74 dB
SFO2       500.1320005 MHz

F2 - Processing parameters
SI         32768
SF         125.7577951 MHz
WDW        EM
SSB        0
LB         1.00 HZ
GB         0
PC         1.40

1D NMR plot parameters
CX         20.00 cm
CY         12.50 cm
F1P        200.000 ppm
F1         25151.56 Hz
F2P        -10.000 ppm
F2         -1257.58 Hz
PPMCM      10.50000 ppm/cm
HZCM       1320.45679 Hz/cm
  
```

S62

sample

4c

Current Data Parameters
NAME C93-R07-2
EXPNO 1
PROCNO 1
PROCPS 1
F2 - Acquisition Parameters
Date_ 20040215
Time 20.19
INSTRUM GPC500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
FIDRES 0.157622 Hz
AQ 3.1719823 sec
RG 327.4
DM 49.400 usec
DE 5.00 usec
TE 295.7 K
D1 1.0000000 sec
MCOREST 0.0000000 sec
MCNMRK 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -6.00 dB
SFO1 500.130085 MHz
F2 - Processing parameters
SI 32768
SF 500.1300210 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.46 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
ZPMQCM 0.35000 sec/27
HZCM 275.07150 Hz/cm

S63

0.00

145.759
132.860
130.966
131.010
129.006
128.325
127.928
123.419
123.087
123.964
126.621
119.492
118.041
110.944

77.252
76.998
76.744

31.841
31.594

4c

Current Data Parameters
NAME chae-R407-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040215
Time 20.28

INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912244 sec
RG 3649.1
WM 16.650 usec
DE 6.00 usec
TE 296.7 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577942 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.10

1D NMR plot parameters
CX 20.00 cm
CY 11.21 cm
F1P 200.000 DPM
F1 25151.56 Hz
F2P -10.000 DPM
F2 -1257.58 Hz
PPMCM 10.50000 DPM/cm
HZCM 1320.45679 Hz/cm

S64

sample

S65

Current Data Parameters
NAME chae-R407
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040218
Time 15.20
INSTRUM drx500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 128
DM 48.400 usec
DE 5.00 usec
TE 295.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 10.30 usec
PL1 -6.00 dB
SF01 500.130085 MHz

F2 - Processing parameters
SI 32768
SF 500.1300311 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 11.12 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -1.000 ppm
F2 -500.13 Hz
PPMCM 0.55000 ppm/cm
HZCM 275.07150 Hz/cm

133	553
131	600
130	492
129	294
129	286
129	607
128	725
127	610
125	402
123	058
120	607
119	528
119	517
110	936
102	265
102	238
77	256
77	002
76	748
30	529
30	281
30	032
29	784

5c

Current Data Parameters
NAME 1065-B407
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040218
Time 15:28

INSTRUM drx500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TO 65536
SOLVENT CDCl3
NS 256
DS 2
SMH 30030.029 HZ
FIDRES 0.458222 HZ
AQ 1.0912244 sec
RG 3649.1
DM 16.650 usec
DE 6.00 usec
TE 296.5 K
D1 0.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCNKR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 5.70 usec
PL1 -2.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 13.74 dB
PL13 13.74 dB
SFO2 500.1320005 MHz

F2 - Processing Parameters
SI 32768
SF 125.7577960 MHz
WDW EM
SSB 0
LB 1.00 HZ
GB 0
PC 0.10

1D NMR plot parameters
CX 20.00 cm
CY 11.16 cm
F1P 200.000 ppm
F1 25151.56 Hz
F2P -10.000 ppm
F2 -1257.58 Hz
PPMCH 10.50000 ppm/cm
HZCM 1320.45579 Hz/cm

S66

Stereochemical Assignment of 2h