Supporting Information

Laurendecumallenes A—B and Laurendecumenynes A—B, Halogenated Nonterpenoid C₁₅-acetogenins from the Marine Red Alga *Laurencia decumbens* (Rhodomelaceae)

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S7, HMBC spectrum of compound **1**;

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S14, ^1H NMR spectrum of compound **3**;

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Compound 1

¹H NMR

Current Data Parameters

NAME lpe-8
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061024
Time 15.05
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 161.3
DW 48.400 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 1H
P1 11.40 usec
PL1 -1.00 dB
SFO1 500.1330885 MHz

F2 - Processing parameters

SI 32768
SF 500.1300137 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 22.00 cm
CY 0.00 cm
F1P 7.500 ppm
F1 3750.98 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.34091 ppm/c
HZCM 170.49886 Hz/cm

¹³C NMR and DEPT

Current Data Parameters
NAME lpe-8
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061024
Time 15.16
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 518
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 302.7 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577877 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 210.000 ppm
F1 26409.13 Hz
F2P 5.000 ppm
F2 628.79 Hz
PPMCM 9.31818 ppm/c
HZCM 1171.83386 Hz/cm

COSY

Current Data Parameters
NAME lpe-8
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061024
Time 15.53
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG cosygpgqf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 6666.667 Hz
FIDRES 3.255208 Hz
AQ 0.1537250 sec
RG 228.1
OW 75.000 usec
OE 6.00 usec
TE 301.5 K
d0 0.00000300 sec
d1 1.48689198 sec
d13 0.00000400 sec
n16 0.00020000 sec
IN0 0.00015000 sec
MCREST 0.00000000 sec
MCNRC 1.48689198 sec

----- CHANNEL f1 -----
NUC1 1H
P0 11.40 usec
P1 11.40 usec
PL1 -1.00 dB
SF01 500.1330069 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 158
SF01 500.133 MHz
FIDRES 42.194092 Hz
SW 13.330 ppm
Fnm00E QF

F2 - Processing parameters
SI 1024
SF 500.1300137 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300137 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 8.000 ppm
F2LO 4001.04 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1PLO 8.000 ppm
F1LO 4001.04 Hz
F1PHI 0.000 ppm
F1HI 0.00 Hz
F2PPMCM 0.53333 ppm/cm
F2HZCM 266.73599 Hz/cm
F1PPMCM 0.53333 ppm/cm
F1HZCM 266.73599 Hz/cm

HSQC

Current Data Parameters
NAME lpe-8
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061024
Time 16.12
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG hsqcetgps12
TD 1024
SOLVENT CDCl3
NS 8
DS 16
SWH 6666.867 Hz
FIDRES 6.510417 Hz
AQ 0.0769250 sec
RG 16384
DN 75.000 usec
DE 6.00 usec
TE 300.5 K
ONST2 145.000000
d0 0.0000300 sec
d1 1.50000000 sec
d4 0.00172414 sec
d11 0.03000000 sec
d13 0.00000400 sec
d16 0.00020000 sec
d24 0.0006207 sec
DELTA 0.00127880 sec
DELTA1 0.00120800 sec
DELTA2 0.0006207 sec
DELTA3 0.00052414 sec
TNO 0.0001656 sec
MCREST 0.00000000 sec
MCWRK 0.25000051 sec
STICHT 128

***** CHANNEL f1 *****
NUC1 1H
P1 11.40 usec
p2 22.80 usec
P2B 1000.00 usec
PL1 0.00 dB
SF01 500.1330069 MHz

***** CHANNEL f2 *****
CPDPRG2 garp
NUC2 13C
P3 11.00 usec
p4 22.00 usec
PCPD2 70.00 usec
PL2 2.60 dB
PL12 18.90 dB
SF02 125.7716224 MHz

***** GRADIENT CHANNEL *****
GPMAN1 SINE 100
GPMAN2 SINE 100
GPMAN3 SINE 100
GPMAN4 SINE 100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P18 600.00 usec

F1 - Acquisition parameters
NUC 13C
TD 113
SF01 125.7716 MHz
FIDRES 267.156464 Hz
SW 240.028 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.1300137 MHz
WDW GSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 125.7577877 MHz
WDW GSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 20.00 cm
CX1 15.00 cm
FAPLO 7.508 ppm
F2L0 3754.91 Hz
F2PHI -0.003 ppm
F2H1 -1.61 Hz
F1PL0 110.010 ppm
F1L0 13834.62 Hz
F1PHI -0.171 ppm
F1H1 -21.52 Hz
F2PPMCH 0.37550 ppm/c
F2HZCH 187.82552 Hz/c
F1PPMCH 7.34541 ppm/c
F1HZCH 923.74213 Hz/c

HMBC

Current Data Param
NAME lpe-8
EXPNO 7
PROCNO 1

F2 - Acquisition Param
Date_ 20061024
Time 16.37
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG hmcgplpndqf
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 6510.417 Hz
FIDRES 3.178914 Hz
AQ 0.1574132 sec
RG 16384
OW 76.800 usec
DE 6.00 usec
TE 300.5 K
CNS2 145.0000000
CNS13 7.0000000
d0 0.0000300 sec
d1 1.50000000 sec
d2 0.00344828 sec
d6 0.07142857 sec
D16 0.00020000 sec
IN0 0.00001856 sec
MCRES1 0.00000000 sec
MCWPK 1.50000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 11.40 usec
p2 22.80 usec
PL1 -1.00 dB
SF01 500.1331508 MHz

----- CHANNEL f2 -----
NUC2 13C
P3 11.00 usec
PL2 2.60 dB
SF02 125.7716224 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition param
N00 2
TD 188
SF01 125.7716 MHz
FIDRES 160.578079 Hz
SW 240.028 ppm
F0MODE OF

F2 - Processing param
SI 2048
SF 500.1300137 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing param
SI 1024
MC2 OF
SF 125.7577877 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot param:
CX2 20.00 cm
CX1 15.00 cm
F2PLO 6.500 ppm
F2LO 3250.84 Hz
F2PHI -0.001 ppm
F2HI -0.46 Hz
F1PLO 210.111 ppm
F1LO 26423.06 Hz
F1PHI -0.171 ppm
F1HI -21.52 Hz
F2PMCH 0.32605 ppm
F2HCH 162.56525 Hz/
F1PMCH 14.01879 ppm
F1HCH 1762.97180 Hz/

ppm 6 5 4 3 2 1

Compound 2

Current Data Parameters
NAME lpe-9
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061025
Time 18.30
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 287.4
DW 48.400 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCNPK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.40 usec
PL1 -1.00 dB
SF01 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300140 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 7.500 ppm
F1 3750.98 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.34091 ppm/c
HZCM 170.49886 Hz/cm

¹³C NMR and DEPT

Current Data Parameters
NAME lpe-9
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061025
Time 19.21
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG zgdc30
TD 65536
SOLVENT CDC13
NS 4096
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 16384
DW 16.650 usec
DE 6.00 usec
TE 304.3 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577859 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 210.000 ppm
F1 26409.13 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPHMC 9.54545 ppm/c
HZCM 1200.41516 Hz/cm

COSY

Current Data Parameters
NAME lpe-9
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061026
Time 1.54
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG cosygpgf
TD 2048
SOLVENT CDC13
NS 4
DS 8
SWH 6666.667 Hz
FIDRES 3.255208 Hz
AQ 0.1537250 sec
RG 228.1
DM 75.000 usec
DE 5.00 usec
TE 301.5 K
d0 0.00000300 sec
d1 1.48689198 sec
d13 0.00000400 sec
d16 0.00020000 sec
IN0 0.00015000 sec
MCREST 0.00000000 sec
MCWRK 1.48689198 sec

----- CHANNEL f1 -----
NUC1 1H
P0 11.40 usec
P1 11.40 usec
PL1 -1.00 dB
SFO1 500.1330069 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
N00 1
TD 256
SFO1 500.133 MHz
FIDRES 26.041666 Hz
SW 13.330 ppm
FnmODE QF

F2 - Processing parameters
SI 1024
SF 500.1300140 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300140 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

20 NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 7.500 ppm
F2LO 3750.98 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1PLO 7.500 ppm
F1LO 3750.98 Hz
F1PHI 0.000 ppm
F1HI 0.00 Hz
F2PPMCM 0.50000 ppm/cm
F2HZCM 250.06500 Hz/cm
F1PPMCM 0.50000 ppm/cm
F1HZCM 250.06500 Hz/cm

HSQC

Current Data Parameters
NAME lpe-8
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061026
Time 2.23
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG hsqcetgps12
TD 1024
SOLVENT CDCl3
NS 8
DS 16
SMH 6666.667 Hz
FIDRES 6.510417 Hz
AQ 0.0769250 sec
RG 16384
DM 75.000 usec
DE 6.00 usec
TE 300.4 K
CHST2 145.0000000
d0 0.0000000 sec
d1 1.5000000 sec
d4 0.00172414 sec
d11 0.03000000 sec
d13 0.00000460 sec
d16 0.00000000 sec
d24 0.0006207 sec
DELTA 0.00127880 sec
DELTA1 0.00120800 sec
DELTA2 0.0006207 sec
DELTA3 0.00056414 sec
TMO 0.0001655 sec
MORST 0.00000000 sec
MORWK 0.25000051 sec
STCNT 128

***** CHANNEL f1 *****
NUC1 1H
P1 11.40 usec
P2 22.80 usec
P2B 1000.00 usec
PL1 -1.00 dB
SF01 500.130069 MHz

***** CHANNEL f2 *****
CPOPRG2 gcpd
NUC2 13C
P3 11.00 usec
P4 22.00 usec
PCPD2 70.00 usec
PL2 2.60 dB
PL12 16.90 dB
SF02 125.7716224 MHz

***** GRADIENT CHANNEL *****
GPRAM1 SINE.100
GPRAM2 SINE.100
GPRAM3 SINE.100
GPRAM4 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
NUC 13C
TD 256
SF01 125.7716 MHz
FIDRES 117.924530 Hz
SM 240.028 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.1300140 MHz
WDW OSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 125.7577859 MHz
WDW OSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 20.00 cm
CX1 15.00 cm
F2PLO 7.500 ppm
F2LO 3750.98 Hz
F2PHI 0.000 ppm
F2H1 0.00 Hz
F1PLO 110.000 ppm
F1LO 13633.36 Hz
F1PHI 0.000 ppm
F1H1 0.00 Hz
F2PNUC 0.37500 ppm/c
F2H2CN 187.54875 Hz/c
F1PNUC 7.33333 ppm/c
F1H2CN 922.22375 Hz/c

HMBC

Current Data Param
NAME lpe-9
EXPNO 7
PROCNO 1

F2 - Acquisition Param
Date_ 20061026
Time 3.19
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG hmcgplndqf
TD 2048
SOLVENT COC13
NS 8
DS 16
SWH 6510.417 Hz
FIDRES 3.178914 Hz
AQ 0.1574132 sec
RG 16384
DW 76.800 usec
DE 6.00 usec
TE 300.6 K
CNS2 145.000000
CNS13 7.000000
d0 0.00000300 sec
d1 1.50000000 sec
d2 0.00344828 sec
d6 0.07142857 sec
d16 0.00020000 sec
IN0 0.0001656 sec
MCHES1 0.00000000 sec
MCHWK -1.50000000 sec

----- CHANNEL f1 ----
NUC1 1H
P1 11.40 usec
p2 22.80 usec
PL1 -1.00 dB
SF01 500.1331508 MHz

----- CHANNEL f2 ----
NUC2 13C
P3 11.00 usec
PL2 2.60 dB
SF02 125.7716224 MHz

----- GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 50.00 %
GPZ1 30.00 %
GPZ2 40.10 %
P16 1000.00 usec

F1 - Acquisition param
N00 2
TD 256
SF01 125.7716 MHz
FIDRES 117.924530 Hz
SW 240.028 ppm
F0MODE OF

F2 - Processing param
SI 2048
SF 500.1300140 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing param
SI 1024
NC2 OF
SF 125.7577859 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot paramet
CX2 20.00 cm
CX1 15.00 cm
F2P0 7.500 ppm
F2L0 3750.98 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1P0 210.000 ppm
F1L0 26409.13 Hz
F1PHI -0.000 ppm
F1HI -0.00 Hz
F2P0MCH 0.37500 ppm
F2H0MCH 187.54875 Hz/
F1P0MCH 14.00000 ppm
F1H0MCH 1760.60901 Hz/

GOESY

^1H NMR ns = 64

goesy Tm = 2s o1p= 5.48 ns =1024

goesy Tm = 1.3s o1p= 4.80 ns = 1024

goesy Tm = 0.8s o1p= 4.35 ns = 1024

goesy Tm = 0.8s o1p= 4.13 ns = 1024

goesy Tm = 0.65s o1p=3.91 ns =1024

goesy Tm = 0.65s o1p=3.84 ns = 1024

goesy Tm = 0.60s o1p=2.45 ns =4096

goesy Tm = 0.60s o1p=2.22 ns =1024

¹H NMR

Current Data Parameters
 NAME lpe-6
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20061014
 Time 14.08
 INSTRUM av500
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 16
 DS c
 SWH 10330.578 Hz
 FIDRES 0.315264 Hz
 AQ 1.5860696 sec
 RG 161.3
 DW 48.400 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.40 usec
 PL1 -1.00 dB
 SF01 500.1330885 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300140 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 0.00 cm
 F1P 7.500 ppm
 F1 3750.98 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPMCM 0.34091 ppm/c
 HZCM 170.49886 Hz/cm

¹³C NMR and DEPT

Current Data Parameters

NAME lpe-6
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20061014
Time 14.48
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG zgdc30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 16384
CH 10.0000000
DE 6.00 usec
TE 304.7 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 ¹³C
P1 11.00 usec
PL1 2.20 dB
SF01 125.7703643 MHz

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

CPDPRG2 waltz16
NUC2 ¹H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters

SI 32768
SF 125.7577859 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 22.00 cm
CY 0.00 cm
F1P 145.000 ppm
F1 18234.88 Hz
F2P 8.000 ppm
F2 1006.06 Hz
PPMCM 6.22727 ppm/c
HZCM 783.12805 Hz/cm

COSY

Current Data Parameters
NAME lpe-6
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061014
Time 15.04
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG cosygpgqf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 6666.667 Hz
FIDRES 3.255208 Hz
AQ 0.1537250 sec
RG 228.1
DM 75.000 usec
DE 6.00 usec
TE 302.5 K
d0 0.00000300 sec
D1 1.48689198 sec
d13 0.0000400 sec
D16 0.00020000 sec
IN0 0.00015000 sec
MCREST 0.00000000 sec
MCWPR 1.48689198 sec

***** CHANNEL f1 *****
NUC1 1H
P0 11.40 usec
P1 11.40 usec
PL1 -1.00 dB
SF01 500.1330069 MHz

***** GRADIENT CHANNEL *****
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 125
SF01 500.133 MHz
FIDRES 53.333332 Hz
SW 13.330 ppm
FnmODE QF

F2 - Processing parameters
SI 1024
SF 500.1300140 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 500.1300140 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 8.000 ppm
F2LO 4001.04 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1PLO 8.000 ppm
F1LO 4001.04 Hz
F1PHI 0.000 ppm
F1HI 0.00 Hz
F2PPMCM 0.53333 ppm/cm
F2HZCM 266.73599 Hz/cm
F1PPMCM 0.53333 ppm/cm
F1HZCM 266.73599 Hz/cm

2

4

6

ppm

HSQC

Current Data Parameters
NAME 1de-6
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20061014
Time 15:18
INSTRUM v5500
PROBHD 5 mm BBO BB-1H
PULPROG hsqcetgps12
TD 1024
SOLVENT CDCl3
NS 8
DS 16
SWH 6666.667 Hz
FIDRES 6.510417 Hz
AQ 0.0769250 sec
RG 16384
DM 75.000 usec
DE 6.00 usec
TE 301.4 K
CHS12 145.000000
d0 0.00000300 sec
d1 1.50000000 sec
d4 0.00172414 sec
d11 0.03000000 sec
d13 0.00000400 sec
d16 0.00020000 sec
d24 0.00006207 sec
DELTA 0.00127880 sec
DELTA1 0.00120800 sec
DELTA2 0.00006207 sec
DELTA3 0.00052414 sec
RG 0.00001856 sec
NCREST 0.00000000 sec
NCRMK 0.25000051 sec
STICHT 128

***** CHANNEL f1 *****
NUC1 1H
P1 11.40 usec
P2 22.80 usec
P2B 1000.00 usec
PL1 -1.00 dB
SFO1 500.133069 MHz

***** CHANNEL f2 *****
CPDPRG2 gpr2
NUC2 13C
P3 11.00 usec
P4 22.00 usec
PCPD2 70.00 usec
PL2 2.60 dB
PL12 18.90 dB
SFO2 125.7716224 MHz

***** GRADIENT CHANNEL *****
GPMAN1 SINE:100
GPMAN2 SINE:100
GPMAN3 SINE:100
GPMAN4 SINE:100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 800.00 usec

F1 - Acquisition parameters
NUC 13C
TD 90
SFO1 125.7716 MHz
FIDRES 335.420719 Hz
SW 240.028 ppm
FwMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.1300140 MHz
WDW DSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 125.7571955 MHz
WDW DSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 20.00 cm
CX1 15.00 cm
F2P0 6.500 ppm
F2L0 3250.84 Hz
F2H1 0.000 ppm
F2H0 0.00 Hz
F1L0 150.000 ppm
F1L1 18863.67 Hz
F1H1 0.000 ppm
F1H0 0.00 Hz
F2PWH 0.32500 ppm/c
F2XZH 162.54225 Hz/cm
F1PWH 10.00000 ppm/c
F1XZH 1257.57788 Hz/cm

HMBC

Current Data Param
NAME lpe-6
EXPNO 7
PROCNO 1

F2 - Acquisition Param
Date_ 20061103
Time 10.11
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG hmcgplndqf
TD 2048
SOLVENT CDCl3
NS 16
DS 16
SWH 6510.417 Hz
FIDRES 3.178914 Hz
AQ 0.1574132 sec
RG 16384
DM 76.800 usec
DE 6.00 usec
TE 300.4 K
CNS12 145.0000000
CNS13 8.0000000
d0 0.00000300 sec
d1 1.50000000 sec
d2 0.00344020 sec
d6 0.06250000 sec
D16 0.00020000 sec
TD0 0.0001656 sec
MCREST 0.0000000 sec
MCNMR 1.5000000 sec

----- CHANNEL f1 ----
NUC1 1H
P1 11.40 usec
p2 22.80 usec
PL1 -1.00 dB
SF01 500.1331508 MHz

----- CHANNEL f2 ----
NUC2 13C
P3 11.00 usec
PL2 2.00 dB
SF02 125.7716224 MHz

----- GRADIENT CHANNEL
GPMAN1 SINE 100
GPMAN2 SINE 100
GPMAN3 SINE 100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition param
ND0 2
TD 93
SF01 125.7716 MHz
FIDRES 324.609467 Hz
SW 240.028 ppm
FhMODE OF

F2 - Processing param
SI 2048
SF 500.1300140 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing param
SI 1024
MC2 OF
SF 125.757859 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot param:
CX2 20.00 cm
CX1 15.00 cm
F2PL0 7.505 ppm
F2L0 3753.52 Hz
F2PHI -0.002 ppm
F2HI -0.78 Hz
F1PL0 150.112 ppm
F1L0 18877.73 Hz
F1PHI -0.156 ppm
F1HI -19.68 Hz
F2PHICH 0.37633 ppm
F2LCH 187.71490 Hz/
F1PHICH -10.01789 ppm
F1LCH 1259.82703 Hz/

ppm 7 6 5 4 3 2 1

¹H NMR

Current Data Parameters

NAME 1pb1-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060907
Time 15.11
INSTRUM av500
PROBHD 5 mm BB0 BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.315264 Hz
AQ 1.5860696 sec
RG 80.6
DW 48.400 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 1H
P1 11.40 usec
PL1 -1.00 dB
SF01 500.1330885 MHz

F2 - Processing parameters

SI 32768
SF 500.1300137 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 22.00 cm
CY 0.00 cm
F1P 7.500 ppm
F1 3750.98 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.34091 ppm/c
HZCM 170.49884 Hz/cm

¹³C NMR and DEPT

Current Data Parameters
NAME lpb1-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060907
Time 15.24
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG zgdc30
TD 65536
SOLVENT CDC13
NS 288
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 16384
DW 16.650 usec
DE 0.00 usec
TE 303.8 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577887 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 0.00 cm
F1P 145.000 ppm
F1 18234.88 Hz
F2P 5.000 ppm
F2 628.79 Hz
PPMCM 6.36364 ppm/cm
HZCM 800.27679 Hz/cm

COSY

Current Data Parameters

NAME ipbl-1
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060907
Time 16.00
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG cosygpgf
TD 2048
SOLVENT CDCl3
NS 4
DS 8
SWH 6666.667 Hz
FIDRES 3.255208 Hz
AQ 0.1537250 sec
RG 228.1
DN 75.000 usec
DE 6.00 usec
TE 302.4 K
d0 0.0000300 sec
D1 1.48689198 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00015000 sec
MCREST 0.00000000 sec
MCMRK 1.48689198 sec

----- CHANNEL f1 -----
NUC1 1H
P0 11.40 usec
P1 11.40 usec
PL1 -1.00 dB
SF01 500.1330069 MHz

----- GRADIENT CHANNEL -----
GPNAM1 SINE 100
GPNAM2 SINE 100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters

ND0 1
TD 161
SF01 500.133 MHz
FIDRES 41.407867 Hz
SW 13.330 ppm
FnMODE QF

F2 - Processing parameters

SI 1024
SF 500.1300137 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters

SI 1024
MC2 QF
SF 500.1300137 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters

CX2 15.00 cm
CX1 15.00 cm
F2PLO 7.440 ppm
F2LO 3720.97 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1PLO 7.440 ppm
F1LO 3720.97 Hz
F1PHI 0.000 ppm
F1HI 0.00 Hz
F2PPMCM 0.49600 ppm/cm
F2HZCM 248.06448 Hz/cm
F1PPMCM 0.49600 ppm/cm
F1HZCM 248.06448 Hz/cm

HSQC

Current Data Parameters
NAME 1p01-1
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060907
Time 16.19
INSTRUM av500
PROBHD 5 mm BBO 80-1H
PULPROG hsqcattg12
TD 1024
SOLVENT CDCl3
NS 8
DS 16
SWH 6586.687 Hz
FIDRES 6.510417 Hz
AQ 0.0768250 sec
RG 16384
DN 75.000 usec
DE 6.00 usec
TE 301.4 K
CH22 145.000000
d0 0.0000300 sec
d1 1.5000000 sec
d4 0.00172414 sec
d11 0.0300000 sec
d13 0.0000000 sec
d16 0.0002000 sec
d24 0.0006207 sec
DELTA 0.00127880 sec
DELTA1 0.00120800 sec
DELTA2 0.0006207 sec
DELTA3 0.00052414 sec
IN0 0.00001856 sec
MORSE1 0.0000000 sec
MORSE2 0.2500001 sec
ST12H 128

***** CHANNEL f1 *****
NUC1 13C
P1 11.40 usec
p2 22.80 usec
P28 1000.00 dB
PL1 1.00 dB
SF01 500.130069 MHz

***** CHANNEL f2 *****
CPDPRG2 gpr0
NUC2 13C
P3 11.00 usec
p4 22.00 usec
PCPD2 70.00 usec
PL2 2.00 dB
PL12 18.90 dB
SF02 125.7716224 MHz

***** GRADIENT CHANNEL *****
GRANA1 SINE.100
GRANA2 SINE.100
GRANA3 SINE.100
GRANA4 SINE.100
GP11 0.00 %
GP12 0.00 %
GP13 0.00 %
GP14 0.00 %
GP11 0.00 %
GP12 0.00 %
GP13 0.00 %
GP14 0.00 %
GP21 80.00 %
GP22 20.10 %
GP23 11.00 %
GP24 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
ND0 2
TD 91
SF01 125.7716 MHz
FIDRES 331.743713 Hz
SM 240.028 ppm
FWDODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 500.1300137 MHz
WDW OSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
WDW echo-antiecho
SF 125.7577887 MHz
WDW OSINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 20.00 cm
CX1 15.00 cm
F2PLO 6.714 ppm
F2LO 3357.77 Hz
F2PHI -0.042 ppm
F2H1 -21.14 Hz
F2PLO 150.559 ppm
F1LO 18933.84 Hz
F1PHI 2.166 ppm
F1H1 272.38 Hz
F2PWH 0.33780 ppm/c
F2H2H 180.94531 Hz/c
F1PWH 9.85286 ppm/c
F1H2H 1244.10376 Hz/c

Current Data Parameters
NAME lpb1-1
EXPNO 7
PROCNO 1

HMBC

F2 - Acquisition Parameters
Date_ 20060907
Time 16.39
INSTRUM av500
PROBHD 5 mm BBO BB-1H
PULPROG hmcgplndqf
TD 2048
SOLVENT CDCl3
NS 8
DS 16
SWH 6510.417 Hz
AQ 0.1574132 sec
FIDRES 3.178914 Hz
RG 16384
DM 76.800 usec
DE 6.00 usec
TE 301.5 K
CHST2 145.000000
CHST13 7.000000
d0 0.0000300 sec
d1 1.5000000 sec
d2 0.00344628 sec
d5 0.07142857 sec
d16 0.00020000 sec
INQ 0.0001656 sec
MCREST 0.0000000 sec
MCNPK 1.5000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 11.40 usec
p2 22.80 usec
PL1 -1.00 dB
SF01 500.1331508 MHz

----- CHANNEL f2 -----
NUC2 13C
P3 11.00 usec
PL2 2.50 dB
SF02 125.7716224 MHz

----- GRADIENT CHANNEL -----
GPMAN1 SINE 100
GPMAN2 SINE 100
GPMAN3 SINE 100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 2
TD 115
SF01 125.7716 MHz
FIDRES 262.510254 Hz
SW 240.028 ppm
FHM00 OF

F2 - Processing parameters
SI 2048
SF 500.1300137 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 OF
SF 125.7577887 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CK2 20.00 cm
CK1 15.00 cm
F2PL0 6.500 ppm
F2L0 3250.84 Hz
F2PHI 0.000 ppm
F2HI 0.00 Hz
F1PL0 150.090 ppm
F1L0 18874.97 Hz
F1PHI -0.000 ppm
F1HI -0.00 Hz
F2PMCH 0.32500 ppm/cm
F2HZCH 162.54225 Hz/cm
F1PMCH 10.00599 ppm/cm
F1HZCH 1258.33154 Hz/cm