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Synthesis and biological evaluation of gramicidin S dimers

Grotenbreg, Gijsbert M.; Witte, Martin D.; Hooft, Peter A.V. van; Spalburg, Emile; Reiß, Philipp; Noort, Daan; Neeling, Albert J. de; Koert, Ulrich; Marel, Gijsbert A. van der; Overkleeft, Herman S.

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Supporting Information for

Synthesis and biological evaluation of gramicidin S dimers

Gijsbert M. Grotenbreg, Martin D. Witte, Peter A. V. van Hooft, Emile Spalburg,
Philipp Reiß, Daan Noort, Albert J. de Neeling, Ulrich Koert, Gijsbert A. van der Marel,
Herman S. Overkleeft and Mark Overhand

Selected NMR spectra [‡]

(in CD₃OH, at 298 K, at 400 MHz)

Compound 13	¹ H	Page 2-5
Compound 13	TOCSY	Page 6,7
Compound 14	¹ H	Page 8-11
Compound 14	TOCSY	Page 12,13
Compound 17	¹ H	Page 14-17
Compound 18	¹ H	Page 18-21
Compound 21	¹ H	Page 22-25
Compound 22	¹ H	Page 26-29
Compound 23	¹ H	Page 30-33
Compound 23	TOCSY	Page 34-36

[‡] Variation in the experimental conditions, such as the solvent system or temperature, could not resolve the severe overlap of resonances in the ¹H NMR spectra due to the high degree of symmetry present in the gramicidin S analogues and the dimers thereof.

Current Data Parameters		gsl542003	
NAME			
EXPNO	1		
PROCNO	8		
F2 - Acquisition Parameters:			
Date_	20030405		
Time	18.03		
INSTRUM	avarage40		
PROBHD	5 mm BBI 1H/13		
PULPROG	zgpg30		
TD	1228		
SOLVENT	Me2D		
DS	64		
NS	0		
SWH	3720.238 Hz		
FIDRES	0.193480 Hz		
AQ	2.5842931 sec		
RG	161.3		
DW	134.400 usec		
DE	38.50 usec		
DI1	1.00000000 sec		
DI2	0.00002000 sec		
DI3	0.00000300 sec		
===== CHANNEL f1 =====			
NUC1	1H		
P1	7.30 usec		
P11	4.00 dB		
P19	52.29 dB		
SFO1	400.1319450 MHz		
F2 - Processing parameters			
SF	400.1300114 MHz		
SF1	37378		
WDW	GM		
SSB	0		
LB	-0.20 Hz		
GB	0.4		
PC	1.00		

mwe1101 (epje 1) 298 K

Current Data Parameters	gfs42003
NAME	
EXPNO	1
PROCNO	8
F2 - Acquisition Parameters	
Date_	20030405
Time	18.03
INSTRUM	BRUKER
PROBHD	5 mm BBI 1H/29
PULPROG	zgpg2
TD	18228
SOLVENT	MeOD
DS	0
NS	6
SWH	3720.238 Hz
FIDRES	0.193480 Hz
AQ	2.5842931 sec
RG	161.3
DW	134.400 usec
DE	38.750 usec
DI1	0.00000000 sec
DI2	0.00002000 sec
DI3	0.00000300 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 usec
P11	4.00 dB
P2	52.29 dB
PF01	400.1319405 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300114 MHz
WFO	GM
SSB	0
LB	-0.20 Hz
GB	0.4
PB	1.00

mwe1101 (epje 1) 298 K

```

Current Data Parameters
NAME          gljs04203
EXPNO         9
PROCNO        1
F2 - Acquisition Parameters
Date_         20030405
Time          18.03
INSTRUM       avance400
PROBHD        5 mm BBI 1H-BB
PULPROG       zgpg
TD            19228
SOLVENT       MeOD
NS            64
DS            0
SWH           3720.238 Hz
FIDRES        0.193480 Hz
AQ            2.5842931 sec
RG            161.3
DW            134.400 usec
DE            300.0 K
TE            8.50 usec
D1            1.00000000 sec
d12           0.00000000 sec
d13           0.00000300 sec

===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL9           52.29 dB
SFO1          400.119405 MHz

F2 - Processing parameters
SI            32768
SF            400.1300114 MHz
WDW           GM
SSB           0
LB            -0.20 Hz
GB            0.4
PC            1.00
  
```

mwel101 (epje 1) 298 K

Current Data Parameters
NAME g1js042003
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters:
Date_ 20030405
Time 18.03
INSTRUM avance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 13228
FIDRES 0.193480 Hz
RG 161.3
DW 134.400 us
TE 300.0 K
D1 1.00000000 sec
d12 0.00002000 sec
d13 0.00003000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 us
PL1 4.00 dB
PL2 52.29 dB
SFO1 400.1319405 MHz
F2 - Processing parameters
SI 32768
SF 400.1300114 MHz
WDW GM
SSB 0
LB -0.20 Hz
GB 0.4
PC 1.00

mwel101 (epje 1) 298 K, cleanTOCSY Tmix=70msec

Current Data Parameters	
NAME	gsjso42003
EXPNO	9
PROCNO	1
F2 - Acquisition Parameters	
Date_	20030405
Time	18.34
INSTRUM	5 mm
PROBHD	BB1-H-BB
PULPROG	zgpg30
TD	65536
NUC1	13C
NUC2	13C
DE	125
SWH	3720.238 Hz
FIDRES	1.816522 Hz
AQ	0.2753012 sec
RG	2048
DW	134.400 usec
DE	8.50 usec
TE	300.0 K
d0	0.0000030 sec
d1	1.00000000 sec
d11	0.03000000 sec
d12	0.00000000 sec
d13	0.00001400 sec
D20	0.0006500 sec
IN0	0.00026880 sec
I1	18
MOREST	0.00000000 sec
MCWK	0.00939939 sec
SFILT	256
===== CHANNEL f1 =====	
NUC1	1H
F1	6.10 usec
P1	15.00 usec
P2	25.00 usec
P3	50.00 usec
P7	2500.00 usec
P17	4.00 dB
P19	52.29 dB
P10	16.50 dB
SFO1	400.1319388 MHz
F1 - Acquisition Parameters	
NU0	1
TD	512
SFO1	400.1319388 MHz
PRF1	7.2.928 Hz
SW	9.298 ppm
PRMODE	States-TPPI
F2 - Processing Parameters	
SF	2048
SF	400.1300114 MHz
WDW	OSINE
SSB	2.3
LB	0.00 Hz
GB	0
PC	1.00
F1 - Processing Parameters	
SF	1024
MC2	States-TPPI
SF	400.1300064 MHz
WDW	OSINE
SSB	2.1
LB	0.00 Hz
GB	0

mwc1101 (epje 1) 298 K

Current Data Parameters	
NAME	gls042003
EXPNO	1
PROCNO	6
F2 - Acquisition Parameters	
Date_	20030905
Time	12.00
INSTRUM	avance400
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpg
TD	1928
SOLVENT	Medol
DS	0
NS	64
SWH	4807.692 Hz
FIDRES	0.250036 Hz
AQ	1.9997621 sec
RG	456.1
RG	10.0 use
DM	8.50 use
DE	300.0 K
TE	300.0 K
D1	1.00000000 sec
d12	0.00020000 sec
d13	0.00000300 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 use
P11	4.00 dB
P2	55.49 dB
SFO1	400.131939 MHz
F2 - Processing parameters	
SI	400.130015 MHz
SF	32768
WVM	GM
SSB	0
LB	-1.61 Hz
GB	0.4
PC	1.00

mwc1101 (epje 1) 298 K

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Current Data Parameters	
NAME	gfs042003
EXPNO	1
PROCNO	6
F2 - Acquisition Parameters	
Date_	20030405
Time	13.61
PROBHD	5 mm BBI 1H-2B
PULPROG	zgpg
TD	19228
SOLVENT	MeOD
DS	0
NS	4807.692 Hz
SWH	0.250065 Hz
FIDRES	1.9997621 sec
AQ	456.1
RG	104.000 usec
DM	30.70 usec
WE	0.0000000 sec
TE	1.00000000 sec
D1	0.00002000 sec
d12	0.00000300 sec
d13	
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 usec
PL1	4.00 dB
PR1	52.29 dB
SFO1	400.119379 MHz
F2 - Processing parameters	
SI	32768
SF	400.1190115 MHz
MW	GM
SSB	0
LB	-1.61 Hz
GB	0.4
PC	1.00

mwc1101 (epje 1) 298 K

Current Data Parameters		gsl542003	
NAME			
EXPNO	6		
PROCNO	1		
F2 - Acquisition Parameters:			
Date_	20030405		
Time	15.21		
INSTRUM	AVANCE400		
PROBHD	5 mm BBI		
PULPROG	zgpg30		
TD	19228		
SOLVENT	MeOD		
NS	64		
DS	0		
SWH	4807.692 Hz		
FIDRES	0.250036 Hz		
AQ	1.9997621 sec		
RG	456.1		
DW	104.000 usec		
DE	6.35 usec		
DI1	1.00000000 sec		
DI2	0.00002000 sec		
DI3	0.00000300 sec		
===== CHANNEL f1 =====			
NUC1	1H		
P1	7.30 usec		
P11	4.00 dB		
P19	52.25 dB		
SFO1	400.119379 MHz		
F2 - Processing parameters			
SF	400.119375 MHz		
SR	32766		
WWM	GM		
SSB	0		
LB	-1.61 GHz		
GB	0.4		
PC	1.00		

mwc1101 (epje 1) 298 K

Current Data Parameters	
NAME	gls042003
EXPNO	6
PROCNO	1
F2 - Acquisition Parameters:	
Date_	20030405
Time	13.21
INSTRUM	5 mm BBI XPPS
PULPROG	zgpg30
TD	13228
SOLVENT	MeOD
DS	64
NS	0
SWH	4807.692 Hz
FIDRES	0.250036 Hz
AQ	1.9997621 sec
RG	456.1
DW	104.000 usec
DE	36.35 usec
DI1	1.00000000 sec
DI2	0.00002000 sec
DI3	0.00000300 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 usec
P11	4.00 dB
SF1	55.2979 MHz
SFO1	400.115239 MHz
F2 - Processing parameters	
SI	32766
SR	400.110015 MHz
WDW	GM
SSB	0
LB	-1.61 Hz
GB	0.4
PB	1.00

mwcl101 (epje 1) 298 K, cleanTOCSY Tmix=70msec

Current Data Parameters	
NAME	g1jso42003
EXPO	7
PRONO	1
P2 - Acquisition Parameters	
Date_	20030405
Time	15.39
INSTRUM	avance400
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpg30
TD	404
SOLVENT	CDC13
DS	128
SWH	3720.28 Hz
FIDRES	1.816522 Hz
AQ	0.2753102 sec
RG	2048
DM	134.400 usec
DE	8.50 usec
TE	300.0 K
d0	0.00000300 sec
d1	1.00000000 sec
d11	0.03000000 sec
d12	0.00000400 sec
d13	0.00000400 sec
d20	0.00005000 sec
INO	0.00026880 sec
IN0	18
MCRSTRT	0.00000000 sec
MCRMRK	0.00999999 sec
STLCNT	256
===== CHANNEL f1 =====	
NUC1	1H
P1	8.10 usec
P5	16.67 usec
P6	5.00 usec
P7	5.00 usec
P17	2500.00 usec
PL1	4.00 dB
PL9	52.29 dB
PL10	16.50 dB
SFO1	400.119375 MHz
P1 - Acquisition Parameters	
ND0	1
TD	512
SFO1	400.1318 MHz
FIDRES	7.266099 Hz
PR	1.00000000 ppm
PHMOD	States-TF2
P2 - Processing Parameters	
SI	2048
SF	400.1100118 MHz
WDW	OSINE
SSB	2.3
LB	0.00 Hz
GB	0
PC	1.00
P1 - Processing Parameters	
SI	States-TF2
MC2	400.1100065 MHz
SF	400.1100065 MHz
WDW	OSINE
SSB	2.1
LB	0.00 Hz
GB	0

mwcl101 (epje 1) 298 K, cleanTOCSY Tmix=70msec

Current Data Parameters	
NAME	g1js042003
EXPNO	7
PROCNO	1

```
F2 - Acquisition Parameters
Date_      20030405
Time       15.39
```

INSTRUM	avance400
PROBHD	5 mm BBI 1H-BB
PULPROG	clmlevhpr
TD	2048
SOLVENT	CDCI3
NS	9

NS	8
DS	128
SWH	3720.238 Hz
FIDRES	1.816522 Hz
AQ	0.2753012 sec
RG	2048

AN	2010
DW	134.400 use
DE	8.50 use
TE	300.0 K
d0	0.00000300 sec
D1	1.00000000 sec

d11	0.0300000	sec
d12	0.0000200	sec
d13	0.0000400	sec
D20	0.0000650	sec
INO	0.0002680	sec

```

===== CHANNEL f1 =====
L1      18
MCREST  0.0000000 sec
MCMRK   0.0099999 sec
STICNT  256

```

	CHROMIUM	1H
NUCl		
p1	6.10	use
p5	16.67	use
p6	25.00	use
p7	50.00	use

PL7	2500.00	use
PL1	4.00	dB
PL9	52.29	dB
PL10	16.50	dB
SFO1	400.1319375	MHz

```

F1 - Acquisition parameters
ND0      1
TD      512
SF01    400.1319 MHz
FIDRES  7.266090 Hz

```

F2 - Processing parameters	
SI	2048

SF	400.1300115	MHz
WDW	Q5INE	
SSB	2.3	
LB	0.00	Hz
GB	0	
PC	1.00	

PC	1.00
F1 - Processing parameters	
SI	1024
MC2	States-TPPI
SP	400.1300065 MHz

UNIT	QSSINE
MDW	2.1
SSB	0.00 Hz
LB	0
GB	

mwe0806 - dimer N3/Et turn 1H, bbi-av400

17

Current Data Parameters	
NAME	GJ5092004
EXNO	1
PRCNO	1
F2 - Acquisition Parameters	
Date-Time	20040915
INSTRUM	10.01
PROBHD	5 mm BI-IB-B
PULPRG	29PR
TD	12228
SOLVENT	H2O
NS	1024
SMH	4807.627 Hz
PIDFIRS	0.250036 Hz
AO	1.9997621 sec
RG	256
DW	104.000 usec
DE	8.50 usec
TE	298.0 K
D1	1.00000000 sec
g12	0.00002000 sec
MCSEST	0.00000000 sec
MCWRK	0.01500000 sec
===== CHANNEL f1 =====	
NUCL	1H
P1	7.30 usec
P1A	4.00 dB
P1B	5.00 dB
SFO1	400.1135975 MHz
F2 - Processing parameters	
SI	32768
WDW	400.1300435 MHz
SSB	EM
LB	0.00 Hz
GB	0
PC	1.00

mwe0806 - dimer N3/Et turn 1H, bbi-av400

17

Current Data Parameters
NAME G15092004
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time 10.01
INSTRUM avance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 19228
FIDRES 0.250036 Hz
AQ 1.9997621 sec
RG 256
DE 8.50 use
TE 298.0 K
D1 1.0000000 sec
d12 0.0000200 sec
MCPRST 0.00000000
MCRMK 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 use
PL1 4.00 dB
PL9 58.54 dB
SFO1 400.1319575 MHz
F2 - Processing parameters
SI 32768
SF 400.1300435 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

mwe0806 - dimer N3/Et turn 1H, bbi-av400

Current Data Parameters	
NAME	GJ5092004
EXNO	1
PROCN	1
F2 - Acquisition Parameters	
Date- Time	20040915 10.01
INSTRM	advance400
PROBHD	5 mm BBI I-H-BB
PULPRG	rspr
TD	19228
SOLVENT	H2O
NS	1024
NSM	4807.692 Hz
SMH	0.250036 Hz
FIDRES	1.9997621 sec
AO	256
RG	104.000 usec
DE	8.50 usec
TE	298.0 K
D1	1.00000000 sec
d12	0.00002000 sec
MCSEST	0.00000000 sec
MCWRK	0.01500000 sec
===== CHANNEL f1 =====	
NUC1	1H
F1	7.30 usec
PL1	4.00 dB
PD	5.00 dB
PTD	0.00 dB
SFO1	400.115975 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300435 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

mwe0806 - dimer N3/Et turn 1H, bbi-av400

Current Data Parameters	
NAME	G15092004
EXNO	1
PROCN0	1
F2 - Acquisition Parameters	
Date_	20040915
Time	10:01
INSTRUM	avance400
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpg30
TD	19228
SOLVENT	H2O
NS	1024
DS	0
SWH	4807.692 Hz
F2H1	0.25003 Hz
F2H2	0.25003 Hz
F2H3	1.9997821 sec
RG	256
DM	104.000 usec
DE	8.50 usec
TE	298.0 K
D1	1.0000000 sec
d12	0.0002000 sec
MCESTRT	0.0000000 sec
MCWRK	0.0150000 sec
===== CHANNEL f1 =====	
NUC01	1H
P1	7.30 usec
PL1	4.00 dB
PL2	58.54 dB
SFO1	400.1319975 MHz
F2 - Processing parameters	
SF	400.1300435 MHz
WDW	32768
SSB	EM
LB	0
GB	0.00 Hz
PB	0
PC	1.00

mw0801 - dimer N3/Et sheet 1H, bbi-av400

18

Current Data Parameters
NAME G1j5092004
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time 13.00
INSTRUM advance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 19228
SOLVENT MeOD
NS 1024
DS 0
SWH 4807.692 Hz
FIDRES 0.250036 Hz
AQ 1.9997621 sec
RG 256
DW 104.000 usec
DE 8.50 usec
TE 283.0 K
D1 1.0000200 sec
d12 0.0000200 sec
MCOREST 0.0000000 sec
MCWRX 0.0150000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 usec
PL1 4.00 dB
PL9 60.89 dB
SF01 400.1319575 MHz
F2 - Processing parameters
SI 400.1300436 MHz
SF 32768
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

18

Current Data Parameters	
NAME	Gljs092004
EXPNO	4
PROCNO	1
F2 - Acquisition Parameters	
Date_	20040915
Time	13.00
INSTRUM	avance400
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpr
TD	19228
SOLVENT	MeOD
NS	1024
DS	0
SWH	4807.692 Hz
FIDRES	0.250036 Hz
AQ	1.9997621 sec
RG	256
DW	104.000 use
DE	8.50 use
TE	298.0 K
DE	1.0000000 sec
DE	0.0000000 sec
MCPRST	0.0000000 sec
MCRRK	0.0150000 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 use
PL1	4.00 dB
PL9	60.89 dB
SFO1	400.1319575 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300436 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

mwc0801 - dimer N3/Et sheet 1H, bbi-av400

Current Data Parameters
NAME G1j5032004
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time 13.00
INSTRUM avance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 19228
SOLVENT MeOD
NS 1024
DS 0
SWH 4807.692 Hz
FIDRES 0.250036 Hz
AQ 1.9997621 sec
RG 256
DW 104.000 usec
DE 8.50 usec
TE 300.2 K
D1 1.00002000 sec
d12 0.00002000 sec
MCOREST 0.00000000 sec
MCWRX 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 usec
PL1 4.00 dB
PL9 60.89 dB
SF01 400.1319575 MHz
F2 - Processing parameters
SI 400.1300436 MHz
SF 400.1300436 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

mwc0801 - dimer N3/Et sheet 1H, bbi-av400

Current Data Parameters	
NAME	GIJsg92004
EXNO	4
PROCN0	1
F2 - Acquisition Parameters	
Date_	20040915
Time	13.00
INSTRUM	avance400
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpgg
TD	19228
SOLVENT	MEOd
NS	1024
DS	0
SWH	4807.692 Hz
F2H1	0.250033 Hz
FINDRES	1.9997621 sec
RG	256
DM	104.000 usec
DE	8.50 usec
TE	298.0 K
D1	1.0000000 sec
d12	0.0000200 sec
MCESTRT	0.0000000 sec
MCWRK	0.01500000 sec
===== CHANNEL f1 =====	
NUC01	1H
P1	7.30 usec
PL1	4.00 dB
PL2	60.89 dB
SFO1	400.1319975 MHz
F2 - Processing parameters	
SI	32768
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PB	1.00

mwel501 - dimer NH2/COOH turn 1H, bbi-av400

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Current Data Parameters
NAME G1j502004
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time 11.43
INSTRUM avance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 19228
SOLVENT MeOD
NS 1024
DS 0
SWH 4807.692 Hz
FIDRES 0.250036 Hz
AQ 1.997621 sec
RG 256
DW 104.000 usec
DE 8.50 usec
TE 300.2 K
D1 1.0000200 sec
d12 0.0000200 sec
MCREST 0.0000000 sec
MCMRK 0.0150000 sec
==== CHANNEL f1 =====
NUC1 1H
P1 7.30 usec
PL1 4.00 dB
PL9 58.54 dB
SFO1 400.1319575 MHz
F2 - Processing parameters
SI 32768
SF 400.1300435 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

mwel501 - dimer NH2/COOH turn 1H, bbi-av400

21

~~7.665~~
~~7.642~~
~~7.621~~
~~7.599~~

7.247
7.242
7.226
7.208
7.187
7.164
7.160
7.144

Current Data Parameters	
NAME	G3092004
EXPNO	3
PROCNO	1
F2 - Acquisition Parameters	
Date_	20040915
Time	11.43
INSTRUM	avance400
PROBHD	5 mm BBI 1H-4B0
PULPROG	zgpg
TD	19228
SOLVENT	MeOD
NS	1024
DS	0
SWH	4897.680 Hz
F2	0.950023 Hz
AQ	1.9997621 sec
RG	325
DE	104.000 usec
DD	8.50 usec
TE	298.0 K
D1	1.00000000 sec
d12	0.00020000 sec
MC2	0.00000000 sec
MEMRK	0.01500000 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 usec
PL1	4.00 dB
P2	58.54 dB
SFO1	400.131975 MHz
F2 - Processing parameters	
SF2	400.130045 MHz
WOW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

mwel501 - dimer NH2/COOH turn 1H, bbi-av400

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Current Data Parameters
NAME G1j5092004
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time 11.43
INSTRUM avance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 19228
SOLVENT MeOD
NS 1024
DS 0
SWH 4807.692 Hz
FIDRES 0.25036 Hz
AQ 1.9997621 sec
RG 256
DW 104.000 usec
DE 8.50 usec
TE 300.2 K
D1 1.00002000 sec
d12 0.00002000 sec
MCOREST 0.00000000 sec
MCWRX 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 usec
PL1 4.00 dB
PL9 58.54 dB
SF01 400.1319575 MHz
F2 - Processing parameters
SI 32768
SF 400.1300435 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

mwel501 - dimer NH2/COOH turn 1H, bbi-av400

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Current Data Parameters
NAME GJ5092004
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time_ 11.43
INSTRUM avance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpr
TD 19228
SOLVENT MeOD
NS 1024
DS 0
SWH 4807.692 Hz
FIDRES 0.250036 Hz
AQ 1.9997621 sec
RG 286
DW 104.000 usec
DE 8.50 usec
TE 298.0 K
D1 1.0000000 sec
d12 0.0000200 sec
MCOREST 0.0000000 sec
MCORRK 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 usec
PL1 4.00 dB
PL9 58.54 dB
SFO1 400.1319575 MHz
F2 - Processing parameters
SI 32768
SF 400.1300435 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

mwcl501 - dimer NH₂/COOH sheet 1H, bbi-av400

Current Data Parameters	
NAME	GJ5092004
EXNO	1
PROCN	5
P2 - Acquisition Parameters	
Date_	20040915
Time	14.09
INSTRUM	advance03
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpr
TD	19228
SOLVENT	MeOD
NS	1024
DS	
SS	4807.632 Hz
F1	0.250036 Hz
F2	
FIDRES	1.99976721 sec
AQ	256
RG	
DE	104.000 usec
DM	8.50 usec
TE	298.0 K
D1	1.00000000 sec
d12	0.00002000 sec
MCESTR	0.00000000 sec
MCWRK	0.01500000 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 usec
PL1	4.00 dB
PL2	60.08 dB
SFO1	400.119379 MHz
P2 - Processing parameters	
SF	400.130043 MHz
WDW	32768
SSB	EM
LB	0.00 Hz
GB	0
PC	1.00

mmw1501 - dimer NH₂/COOH sheet 1H, bbi-av400

Current Data Parameters	
NAME	G15092004
EXNO	5
PROCN0	1
F2 - Acquisition Parameters	
Date_	20040915
Time	14.09
INSTRUM	avanc4e00
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpgzr
TD	19228
SOLVENT	MeOD
NS	1024
DS	0
SWH	4807.692 Hz
FIDRES	0.050033 Hz
AQ	1.9937623 sec
RG	256
DM	104.000 usec
DE	8.50 usec
TE	298.0 K
D1	1.00000000 sec
d12	0.00002000 sec
MCESTRT	0.00000000 sec
MCWRK	0.01500000 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 usec
PL1	4.00 dB
PL2	60.89 dB
SFO1	400.1319579 MHz
F2 - Processing parameters	
SF	400.1300433 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

mwcl501 - dimer NH2/COOH sheet 1H, bbi-av400

Current Data Parameters
NAME G1j502004
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time 14.09
INSTRUM advance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 19228
SOLVENT MeOD
NS 1024
DS 0
SWH 4807.692 Hz
FIDRES 0.25036 Hz
AQ 1.9997621 sec
RG 256
DW 104.000 usec
DE 8.50 usec
TE 283.0 K
D1 1.00000000 sec
d12 0.00002000 sec
MCREST 0.00000000 sec
MCWRX 0.01500000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 usec
PL1 4.00 dB
PL9 60.89 dB
SF01 400.1319579 MHz
F2 - Processing parameters
SI 400.1300433 MHz
SF 400.1300433 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

mwcl501 - dimer NH2/COOH sheet 1H, bbi-av400

Current Data Parameters
NAME G:\j5092004
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time_ 14.09
INSTRUM avance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 19228
SOLVENT MeOD
NS 1024
DS 0
SWH 4807.692 Hz
FIDRES 0.250036 Hz
AQ 1.9997621 sec
RG 286
DW 104.000 use
DE 8.50 use
TE 298.0 K
D1 1.0000000 sec
d12 0.0000200 sec
MCREST 0.0000000 sec
MCWRK 0.0150000 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 use
PL1 4.00 dB
PL9 60.89 dB
SFO1 400.1319579 MHz
F2 - Processing parameters
SI 32768
SF 400.1300433 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

dimer over turn 1h nmr av-400 ATM-bbigs probe

Current Data Parameters	
NAME	GJ5072003
EXPNO	2
PROCNO	1
F2 - Acquisition Parameters	
Date_	20030723
Time	10.20
INSTRUM	avance400
PROBHD	5 mm BBI-1H-5B
PULPROG	zgpg
TD	1928
SOLVENT	MeD
NS	128
DS	0
SWH	4807.652 Hz
FIDRES	0.250036 Hz
AQ	1.997621 sec
RG	228.1
DW	104.000 usec
DE	8.50 usec
TE	300.0 K
D1	1.00000000 sec
d12	0.00002000 sec
d13	0.00000300 sec
===== CHANNEL f1 =====	
NUC1	1H
PU	7.30 usec
P11	4.00 dB
P19	58.19 dB
SFO1	400.131863 MHz
F2 - Processing Parameters	
SI	131072
SF	400.1300369 MHz
MW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

dimer over turn 1h nmr av-400 ATM-bbigs probe

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Current Data Parameters
NAME G1j5072003
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030723
Time 10.20
INSTRUM advance400
PROBHD 5 mm BBI 1h-BB
PULPROG zgpg
TD 13228
SOLVENT MeOD
NS 128
DS 4
SWH 4807.692 Hz
FIDRES 0.250036 Hz
AQ 1.9997621 sec
RG 228.1
RW 104.000 usec
DE 8.50 usec
TE 300.0 K
D1 1.00000000 sec
d12 0.00002000 sec
d13 0.00000300 sec
===== CHANNEL f1 =====
NUC1 1H
P1 7.30 usec
PL1 4.00 dB
PL9 58.19 dB
SFO1 400.131863 MHz
F2 - Processing Parameters
SI 131072
SF 400.1300389 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

dimer over turn 1h nmr av-400 ATM-bbigs probe

Current Data Parameters	
NAME	GJ9072003
EXNO	1
PRCNO	2
F2 - Acquisition Parameters	
Date--	20030723
Time--	10.20
INTERUM	avance400
PROBHD	5 mm BBI 1H-BB
PULPROG	zgpr
TD	19228
SOLVENT	MeOD
NS	128
DS	0
SWH	4807.692 Hz
FIDRES	0.250036 Hz
AQ	1.9997621 sec
RG	228.1
DW	104.000 usec
DE	8.50 usec
TE	300.0 K
D1	1.00000000 sec
d12	0.00002000 sec
d13	0.00000300 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 usec
PL1	4.00 dB
PT1	58.10 dB
SFO1	400.1318863 MHz
F2 - Processing Parameters	
SI	131072
WDW	400.1300389 MHz
SSB	EM
LB	0
GB	0.50 Hz
PC	0
	1.00

dimer over turn 1h nmr av-400 ATM-bbigs probe

Current Data Parameters	
NAME	GJ5072003
EXNO	1
PROCN0	2
F2 - Acquisition Parameters	
Date--	20030723
Time--	10.20
INSTRUM	advance400
PROBHD	5 mm BBI II-HB
PULPROG	zgpr
TD	19228
SOLVENT	MeOD
NS	128
DS	0
SWH	4807.692 Hz
FIDRES	0.250036 Hz
AQ	1.9997621 sec
RG	228.1
DW	104.000 usec
DE	8.50 usec
TE	300.0 K
D1	1.00000000 sec
d12	0.00020000 sec
d13	0.00000300 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	7.30 usec
P11	4.00 dB
P19	58.19 dB
SFO1	400.1318863 MHz
F2 - Processing parameters	
SI	131072
SW	400.1300389 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

dimer over turn 1h nmr av-400 ATM-bbigs probe, cleanTOCSY Tmix=70msec

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Current Data Parameters
NAME G13s072003
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030723
Time 10.54
INSTRUM advance400
PROBHD 5 mm BBI 1H-2B
PULPROG clemeypr2
TD 65536
SOLVENT CDCl₃
NS 8
DS 256
SWH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2130420 sec
RG 2580.3
DW 104.000 usec
DE 8.50 usec
TE 300.0 K
D0 0.0000000 sec
D1 1.0000000 sec
d11 0.0300000 sec
d12 0.0000200 sec
d13 0.00000400 sec
D20 0.0006500 sec
IN0 0.00020800 sec
I1 0.00000000 sec
MCREST 0.0099999 sec
MCWRK 0.0099999 sec
STCNT 256
===== CHANNEL f1 =====
NUC1 1H
P1 6.10 usec
P5 16.67 usec
P6 25.00 usec
P7 50.00 usec
P17 2500.00 usec
PL1 4.00 dB
PL9 58.51 dB
PL10 16.50 dB
SFO1 400.1318941 MHz
F1 - Acquisition Parameters
NUC2 1H
SFO2 400.1318 MHz
FIDRES 9.390024 Hz
SW 12.015 ppm
FMODE States-TPPI
F2 - Processing parameters
SI 2048
SF 400.1300389 MHz
WDW QSI
SSB 2.3
LB 0.00 Hz
GB 1.40
PC 1.40
F1 - Processing parameters
SI 1024
SF 400.1300389 MHz
WDW QSI
SSB 2.1
LB 0.00 Hz
GB 0

dimer over turn 1h nmr av-400 ATM-bbigs probe, cleanTOCSY Tmix=70msec

dimer over turn 1h nmr av-400 ATM-bbigs probe, cleanTOCSY Tmix=70msec

Current Data Parameters
NAME G1js072003
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20030723
Time 10.54
INSTRUM avance400
PROBHD 5 mm BBI 1H-2B
PULPROG clemvprg2
TD 2448
SOLVENT CDCl3
NS 8
DS 256
SWH 4807.692 Hz
FIDRES 2.347506 Hz
AQ 0.2130420 sec
RG 2580.3
DW 104.000 usec
DE 300.0 K
TE 300.0 K
D1 0.0000000 sec
d11 0.0300000 sec
d12 0.0000200 sec
d13 0.0000400 sec
D20 0.0006500 sec
INO 0.0002080 sec
I1 18
MCREST 0.0000000 sec
MCWRK 0.0099999 sec
STLCNT 256

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

NUC1 1H
P1 6.10 usec
P5 16.67 usec
P6 25.00 usec
P7 50.00 usec
P17 2500.00 usec
PL1 4.00 dB
PL9 58.51 dB
PL10 16.50 dB
SFO1 400.1318841 MHz

F1 - Acquisition Parameters

NUC2 513
SFO2 400.1319 MHz
FIDRES 9.390024 Hz
SW 12.015 ppm
FMODE States-TPI1

F2 - Processing parameters

SI 2048
SF 400.1300389 MHz
WDW QSI
SSB 2.3 Hz
LB 0.00 Hz
GB 1.40

F1 - Processing parameters

SI 1024
States-TPI1
SF 400.1300389 MHz
WDW QSI
SSB 2.1 Hz
LB 0.00 Hz
GB 0