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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; Overkleef, 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 CD<sub>3</sub>OH, at 298 K, at 400 MHz)

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

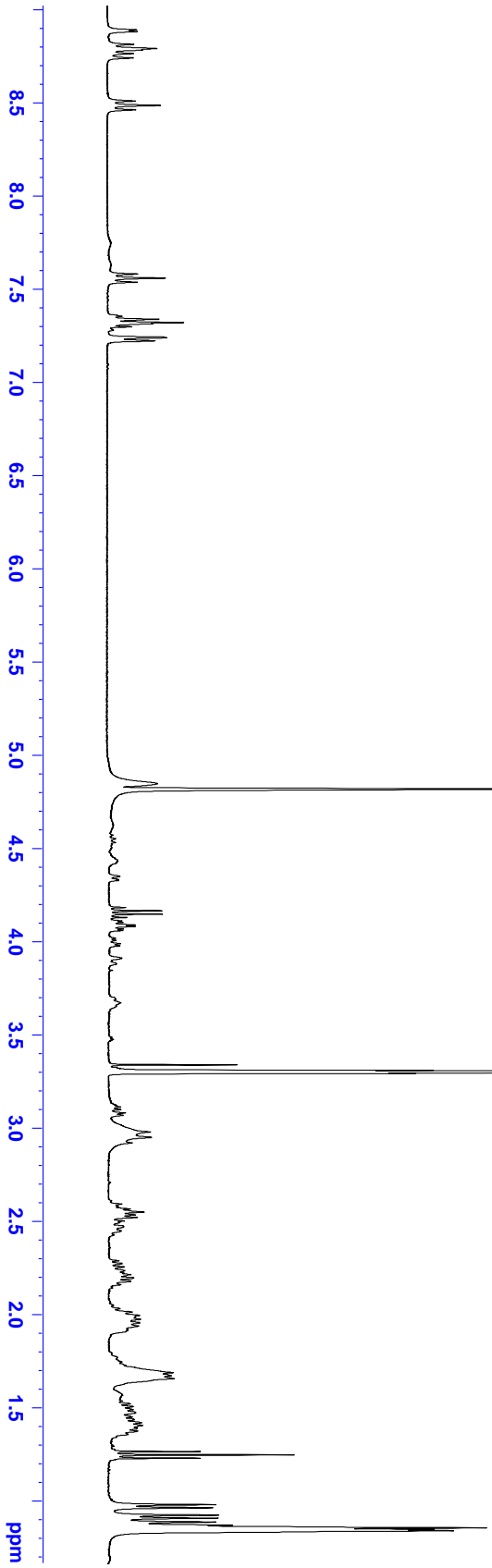
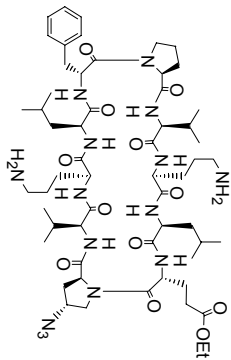
‡ Variation in the experimental conditions, such as the solvent system or temperature, could not resolve the severe overlap of resonances in the <sup>1</sup>H NMR spectra due to the high degree of symmetry present in the gramicidin S analogues and the dimers thereof.

mwe1101 (epje 1) 298 K

8.815  
8.792  
8.765  
8.742  
8.510  
8.487  
8.463

7.582  
7.560  
7.538  
7.356  
7.339  
7.321  
7.299  
7.240  
7.224

4.846  
4.819  
4.430  
4.349  
4.327  
4.183  
4.165  
4.147  
4.129  
4.110  
4.102  
4.089  
4.081  
4.067  
4.059  
3.988  
3.976  
3.911  
3.671  
3.338  
3.308  
3.304  
3.300  
3.296  
3.293  
3.112  
3.099  
3.080  
3.067  
3.067  
2.978  
2.949  
2.920  
2.591  
2.565  
2.548  
2.533  
2.519  
2.500  
2.470  
2.447  
2.287  
2.269  
2.254  
2.234  
2.212  
2.195  
2.175  
2.159  
2.030  
2.012  
1.994  
1.973  
1.953  
1.937



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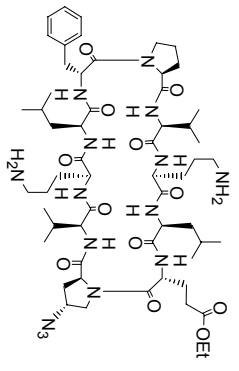
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PULPROG      zgpg
TD            19228
SOLVENT      MeOD
NS            64
DS            0
SWH           3720.238 Hz
FIDRES       0.193480 Hz
AQ           2.5842931 sec
RG           161.3
DW           134.400 usec
DE           8.50 usec
TE           300.0 K
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d13          0.00000300 sec

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PL1           4.00 dB
PL2           52.29 dB
SFO1          400.1319405 MHz

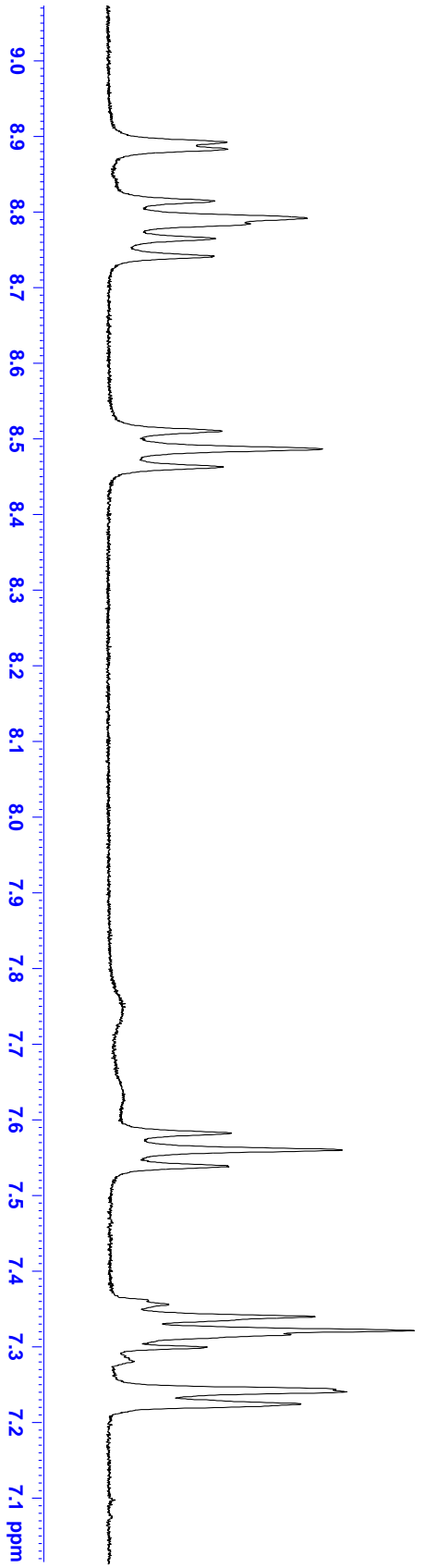
F2 - Processing parameters
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SF            400.1300114 MHz
WDW           GM
SSB           0
LB            -0.20 Hz
GB            0.4
PC            1.00
  
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mwe1101 (epje 1) 298 K

- 8.892
- 8.883
- 8.815
- 8.792
- 8.765
- 8.742
- 8.510
- 8.487
- 8.463
- 7.582
- 7.560
- 7.538
- 7.356
- 7.339
- 7.321
- 7.299
- 7.240
- 7.224

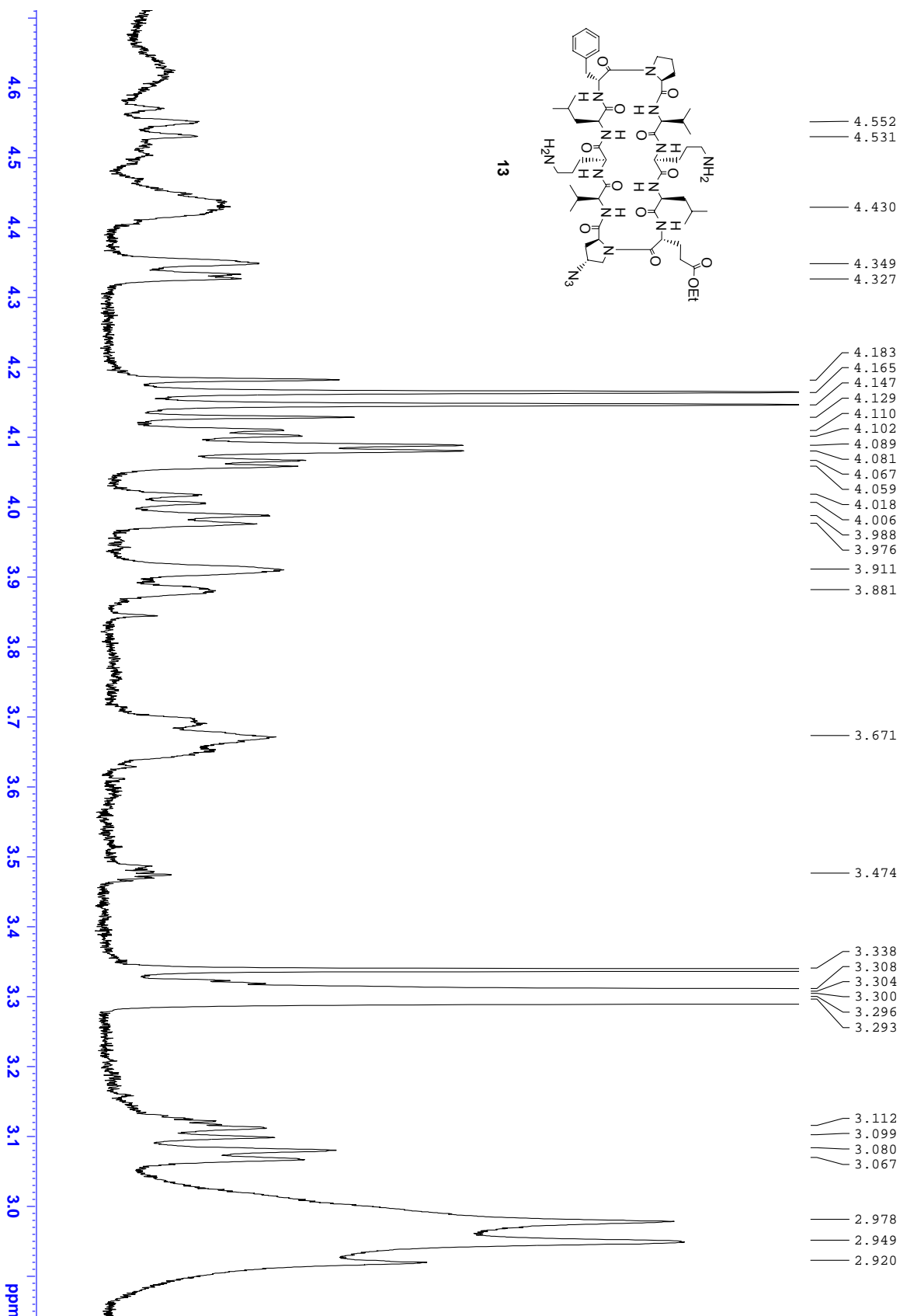


13



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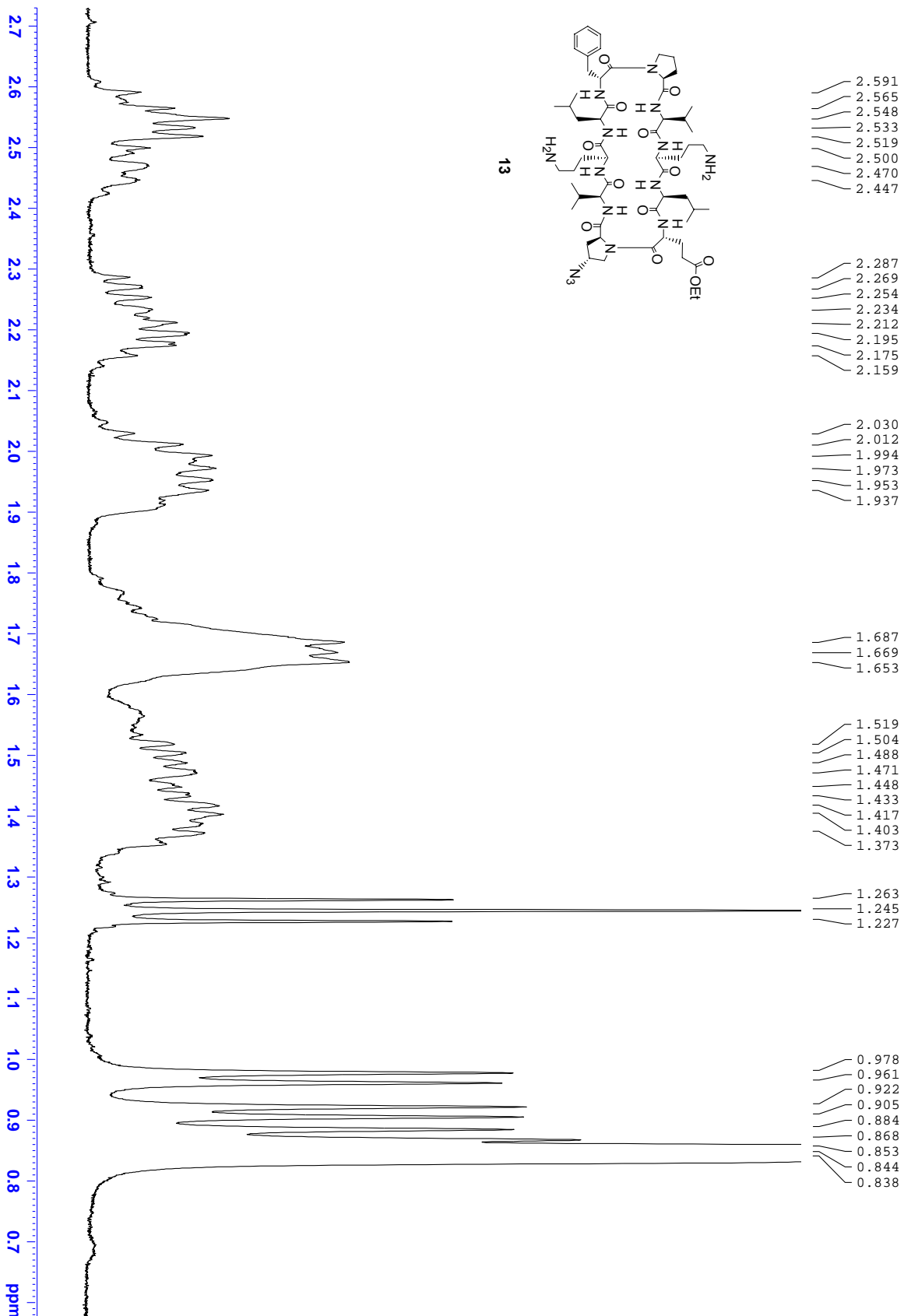
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EXPNO         8
PROCNO       1
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PULPROG      zgpg
TD            19228
SOLVENT      MeOD
NS            64
DS            0
SWH           3720.238 Hz
FIDRES       0.193480 Hz
AQ           2.5842931 sec
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
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
  
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Current Data Parameters
NAME          glj504203
EXPNO         9
PROCNO       1
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F2 - Acquisition Parameters
Date_         20030405
Time         18.03
INSTRUM      avance400
PROBHD       5 mm BBI 1H-5B
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           8.50 usec
TE           300.0 K
D1           1.00000000 sec
d12          0.00020000 sec
d13          0.00003000 sec
-----
CHANNEL f1
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL2           52.29 dB
SFO1         400.1319405 MHz
-----
F2 - Processing parameters
SI            32768
SP           400.1300114 MHz
WDW          GM
SSB          0
LB           -0.20 Hz
GB           0.4
PC           1.00
  
```

mwe1101 (epje 1) 298 K

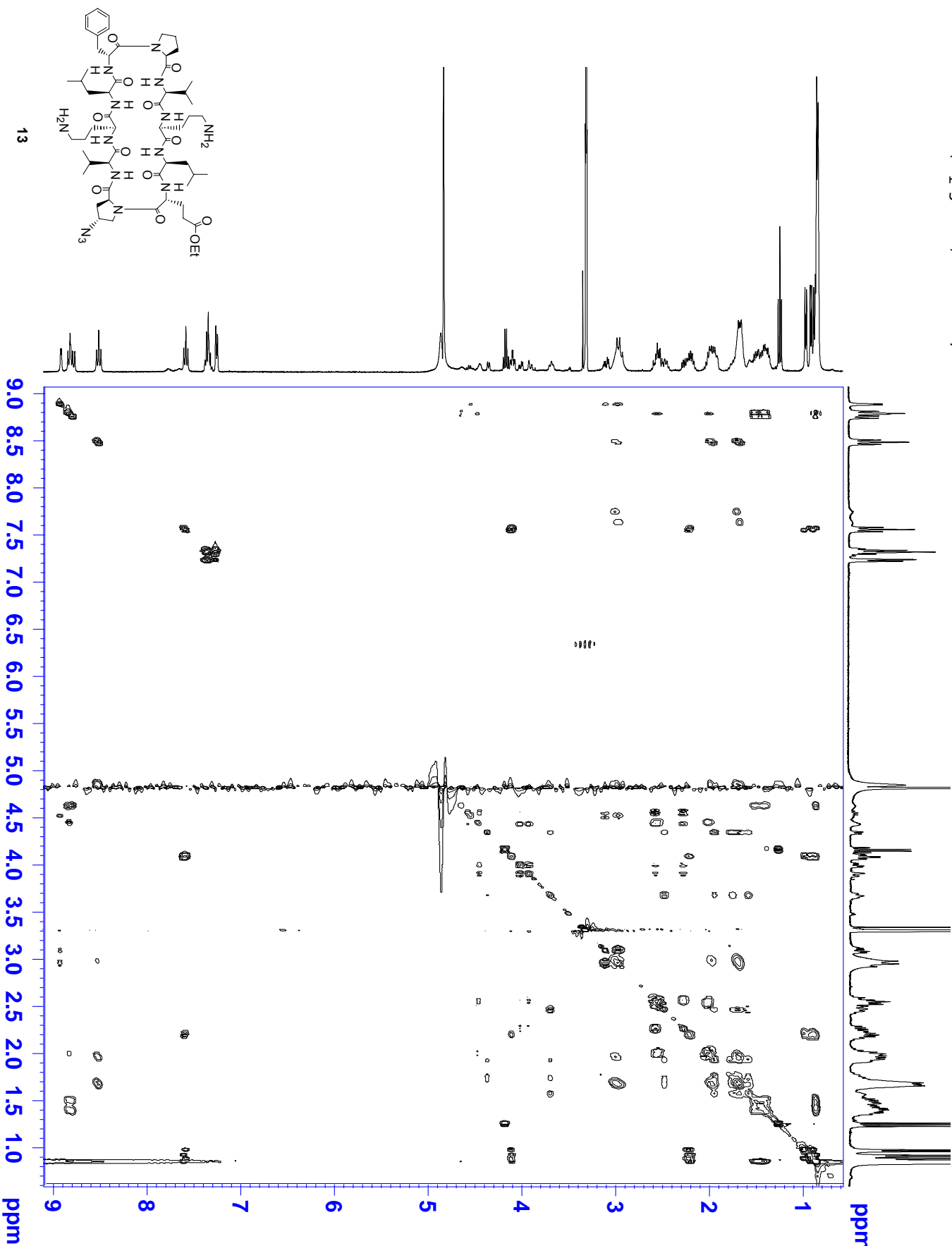


2.591	2.287	2.030	1.687	1.519	1.263	0.978
2.565	2.269	2.012	1.669	1.504	1.245	0.961
2.548	2.254	1.994	1.653	1.488	1.227	0.922
2.533	2.234	1.973		1.471		0.905
2.519	2.212	1.953		1.448		0.884
2.500	2.195	1.937		1.433		0.868
2.470	2.175			1.417		0.853
2.447	2.159			1.403		0.844
				1.373		0.838

```

Current Data Parameters
NAME          g1j5042003
EXPNO         8
PROCNO       1
F2 - Acquisition Parameters:
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Time_        18.03
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PROBHD       5 mm BBI 1H-RR
PULPROG      zgpg
TD            13228
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           0.00002000 sec
d13           0.00000300 sec
===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
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
  
```

mwe1101 (epje 1) 298 K, cleanTOCSY Tmix=70msec



Current Data Parameters  
 NAME g13s042003  
 EXPNO 9  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20030405  
 Time 18.34  
 INSTRUM advance400  
 PROBRD 5 mm BBI 1H-2B  
 PULPROG cmlleppr2  
 TD 65536  
 SOLVENT CDCl3  
 NS 32  
 DS 256  
 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 0.0000000 sec  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 d13 0.0000400 sec  
 D20 0.0006500 sec  
 INO 0.00026880 sec  
 I1 18  
 MCREST 0.0000000 sec  
 MCWRK 0.00999999 sec  
 STICNT 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 52.29 dB  
 PL10 16.50 dB  
 SFO1 400.1319388 MHz

F1 - Acquisition Parameters

NUC2 1H  
 SFO1 400.1319 MHz  
 FIDRES 7.266090 Hz  
 SW 9.298 ppm  
 FMODE States-TPPI

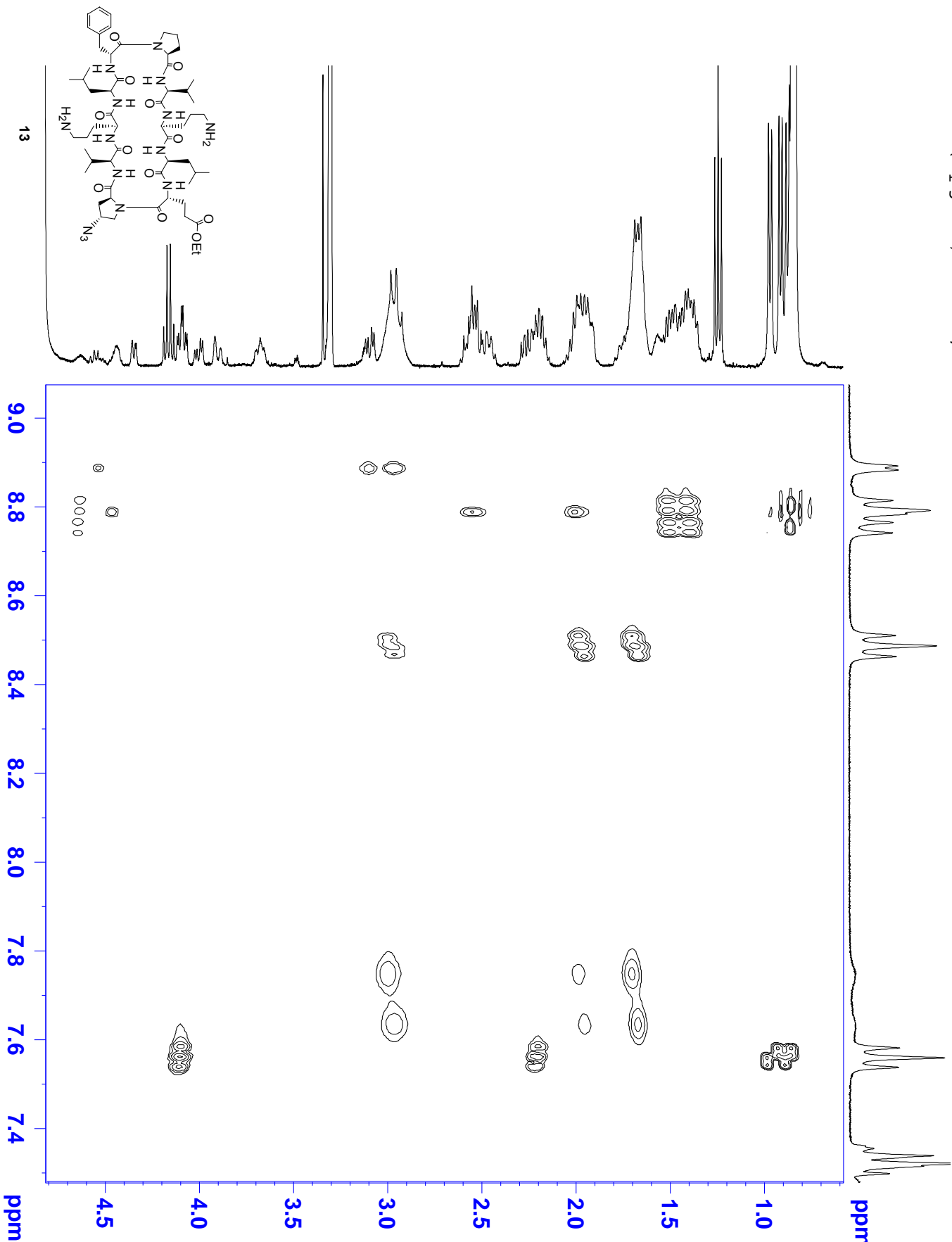
F2 - Processing Parameters

SI 2048  
 SF 400.1300114 MHz  
 WDW QSI  
 SSB 2.3 Hz  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

F1 - Processing Parameters

SI 1024  
 States-TPPI  
 MC2 400.1300064 MHz  
 SF 400.1300064 MHz  
 QSI  
 SSB 2.1 Hz  
 LB 0.00 Hz  
 GB 0

mwe1101 (epje 1) 298 K, cleanTOCSY Tmix=70msec



Current Data Parameters  
 NAME g1j3042003  
 EXPNO 9  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20030405  
 Time 18.34

INSTRUM advance400  
 PROBRD 5 mm BBI JH-285  
 PULPROG zgpg30

TD 65536  
 F2 298.15  
 SOLVENT CDCl3

NS 32  
 DS 256  
 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

TD 65536  
 D0 1.0000000 sec  
 D1 0.0300000 sec

d11 0.0000200 sec  
 d12 0.0000400 sec  
 d13 0.0000650 sec

D20 0.00026880 sec  
 IN0 0.00026880 sec  
 I1 18

MCREST 0.0000000 sec  
 MCMRK 0.00999999 sec  
 STICNT 256

===== CHANNEL f1 =====  
 NUC1 <sup>1</sup>H  
 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 52.29 dB

PL10 16.50 dB  
 SFO1 400.1319388 MHz

F1 - Acquisition Parameters  
 MD 512  
 SFO1 400.1319 MHz

FIDRES 7.266090 Hz  
 SW 9.298 ppm  
 FMODE States-TPPI

F2 - Processing parameters  
 SI 2048  
 SF 400.1300114 MHz

WDW QSI  
 SSB 2.3 Hz  
 GB 0.00 Hz

PC 1.00  
 F1 - Processing parameters  
 SI 1024

States-TPPI  
 MC2 400.1300064 MHz  
 SF QSI

WDW QSI  
 SSB 2.1 Hz  
 GB 0.00 Hz

PC 1.00

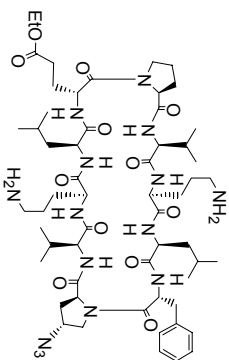
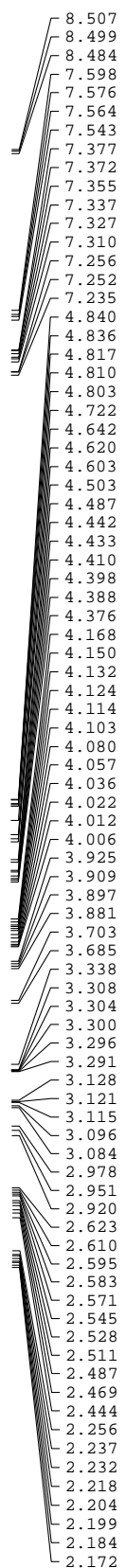
F1 - Processing parameters  
 SI 1024  
 States-TPPI

MC2 400.1300064 MHz  
 SF QSI  
 WDW QSI

SSB 2.1 Hz  
 GB 0.00 Hz

PC 1.00



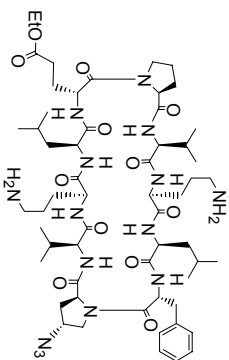


Current Data Parameters  
 NAME g1j504203  
 EXPRNO 6  
 PROCNO 1  
 P2 - Acquisition Parameters  
 Date\_ 20030405  
 Time 15 21  
 INSTRUM avance400  
 PROBRD 5 mm BBI 1H-BB  
 PULPROG zgpr  
 TD 19228  
 SOLVENT MeOD  
 NS 64  
 DS 0  
 SMH 4807.692 Hz  
 FIDRES 0.250036 Hz  
 AQ 1.9997621 sec  
 RG 456.1  
 DW 104.000 usec  
 DE 8.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 D12 0.0000000 sec  
 D13 0.0000000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.30 usec  
 PL1 4.00 dB  
 PL9 52.29 dB  
 SFO1 400.1319379 MHz  
 P2 - Processing parameters  
 SI 32768  
 SF 400.1300115 MHz  
 WDW GM  
 SSB 0  
 LB -1.61 Hz  
 GB 0.4  
 PC 1.00

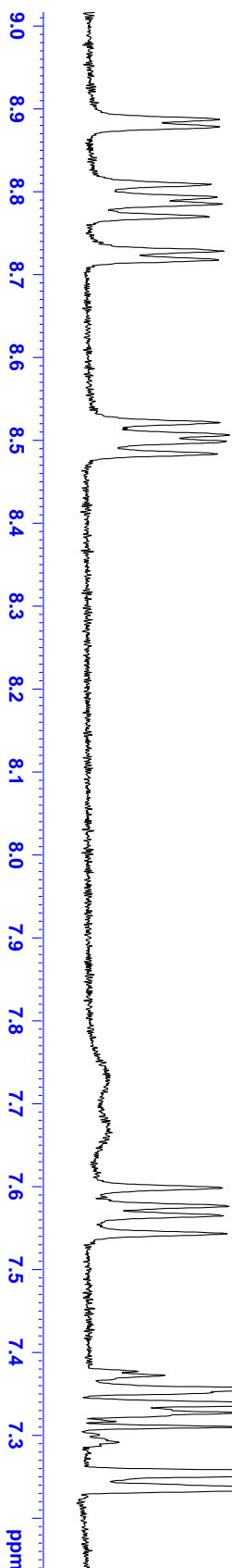
8.887  
8.879  
8.809  
8.793  
8.785  
8.770  
8.728  
8.718  
8.522  
8.507  
8.499  
8.484

7.598  
7.576  
7.564  
7.543

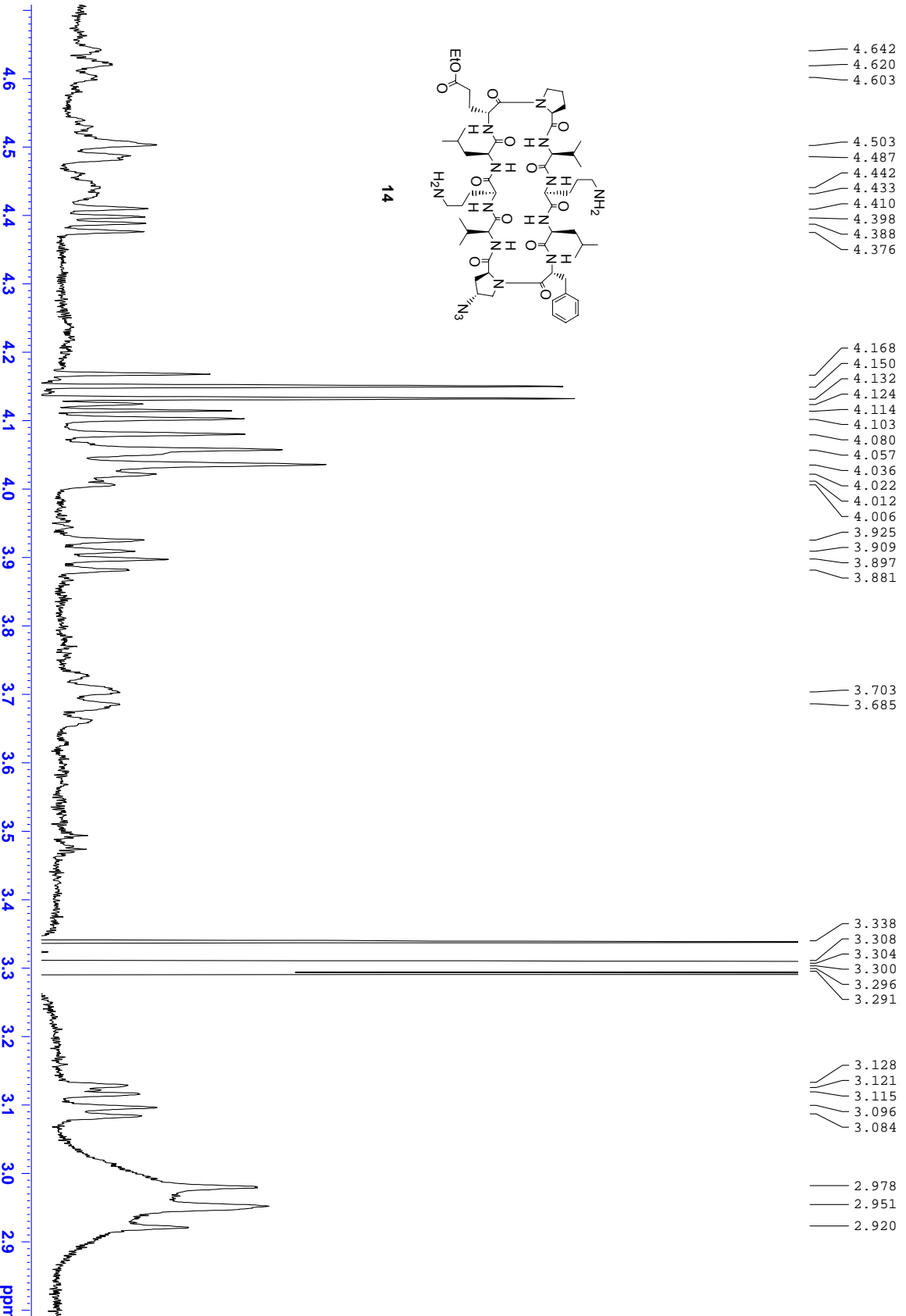
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7.355  
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7.327  
7.310  
7.256  
7.252  
7.235



14

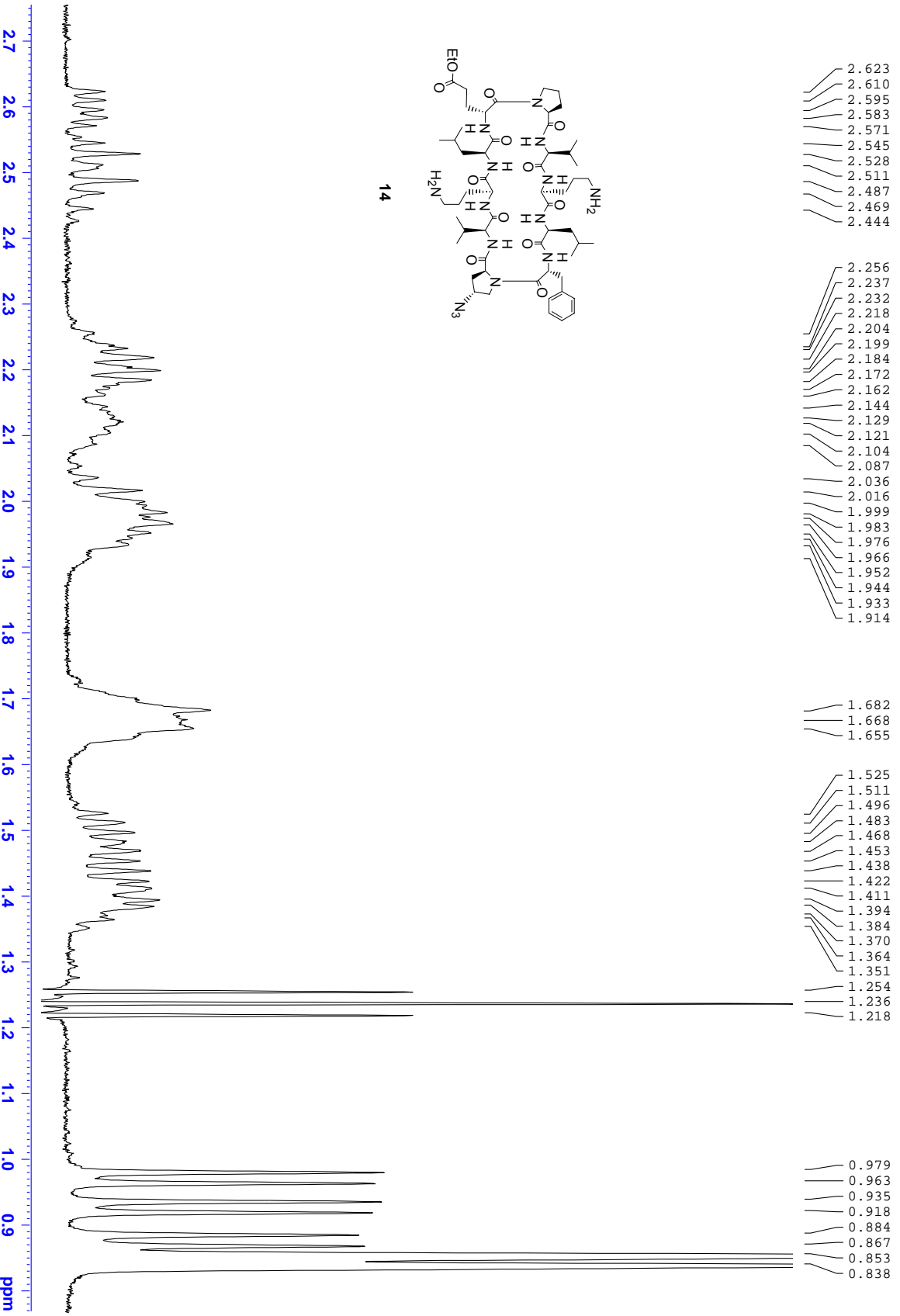


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PROCNO 1  
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PROBHD 5 mm BBI 1H-BB  
PULPROG zgpg  
TD 19228  
SOLVENT MeOD  
NS 64  
DS 0  
SWH 4807.692 Hz  
FIDRES 0.250036 Hz  
AQ 1.9997621 sec  
RG 456.1  
DM 104.000 use  
DE 8.50 use  
TE 300.0 K  
D1 1.0000000 sec  
D12 0.000200 sec  
D13 0.0000300 sec  
===== CHANNEL f1 =====  
NUC1 1H  
P1 7.30 use  
PL1 4.00 dB  
PL2 52.29 dB  
SFO1 400.1319379 MHz  
F2 - Processing parameters  
SI 32768  
SF 400.1300115 MHz  
WDW GM  
SSB 0  
LB -1.61 Hz  
GB 0.4  
PC 1.00



Current Data Parameters  
 NAME g1j5042003  
 EXPNO 6  
 PROCNO 1  
 F2 - Acquisition Parameters:  
 Date\_ 20030405  
 Time 15:21  
 INSTRUM avance400  
 PROBRD 5 mm BBI 1H-RR  
 PULPROG zgpg  
 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 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 52.29 dB  
 SFO1 400.131979 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 400.1300115 MHz  
 WDW GM  
 SSB 0  
 LB -1.61 Hz  
 GB 0.4  
 PC 1.00

14

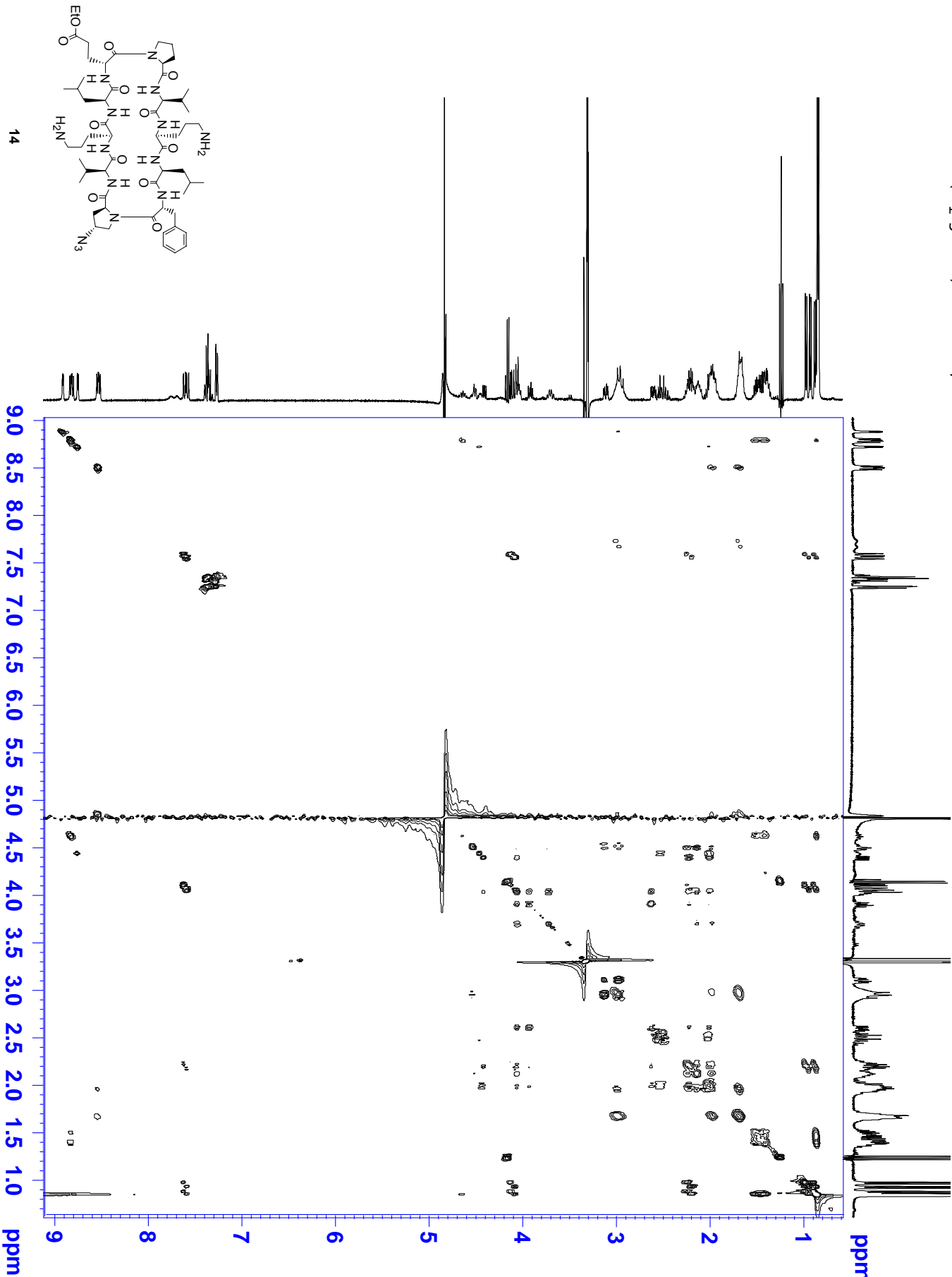


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2.610	2.237	1.668	1.511	0.963
2.595	2.232	1.655	1.496	0.935
2.583	2.218		1.483	0.918
2.571	2.204		1.468	0.884
2.545	2.199		1.453	0.867
2.528	2.184		1.438	0.853
2.511	2.172		1.422	0.838
2.487	2.162		1.411	
2.469	2.144		1.394	
2.444	2.129		1.384	
	2.121		1.370	
	2.104		1.364	
	2.087		1.351	
	2.036		1.254	
	2.016		1.236	
	1.999		1.218	
	1.983			
	1.976			
	1.966			
	1.952			
	1.944			
	1.933			
	1.914			

Current Data Parameters  
 NAME g1j5042003  
 EXPNO 6  
 PROCNO 1  
 F2 - Acquisition Parameters:  
 Date\_ 20030405  
 Time 15:421  
 INSTRUM avance400  
 PROBRD 5 mm BBI 1H-4B  
 PULPROG zgpg  
 TD 13228  
 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 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 52.29 dB  
 SFO1 400.131979 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 400.1300115 MHz  
 WDW GM  
 SSB 0  
 LB -1.61 Hz  
 GB 0.4  
 PC 1.00

14

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



Current Data Parameters  
 NAME g13s042003  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20030405  
 Time 15.39  
 INSTRUM advance400  
 PROBRD 5 mm BBI JH-25  
 PULPROG cmllepr2  
 TD 65536  
 SOLVENT CDCl3  
 NS 8  
 DS 128  
 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  
 TD 0.0000300 sec  
 D0 1.00000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec  
 d13 0.00004000 sec  
 D20 0.00065000 sec  
 INO 0.00026880 sec  
 IL 18  
 MCREST 0.00000000 sec  
 WCRK 0.00999999 sec  
 SFCNT 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 52.29 dB  
 PL10 16.50 dB  
 SFO1 400.131975 MHz

F1 - Acquisition Parameters

NUC0 512  
 SFO1 400.1319 MHz  
 FIDRES 7.266090 Hz  
 SW 9.298 ppm  
 FMODE States-TPPI

F2 - Processing parameters

SI 2048  
 SF 400.1300115 MHz  
 MDW QSIINE  
 SSB 2.3 Hz  
 LB 0.00 Hz  
 GB 1.00

F1 - Processing parameters

SI 1024  
 States-TPPI  
 MC2 400.1300065 MHz  
 SF QSIINE  
 MDW 2.1 Hz  
 SSB 0.00 Hz  
 LB 0  
 GB

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

Current Data Parameters  
 NAME g1j3042003  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20030405  
 Time 15.39

INSTRUM advance400  
 PROBRD 5 mm BBI JH-285  
 PULPROG ctmlepr2  
 TD 268432  
 SOLVENT CDCl3

DS 128  
 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

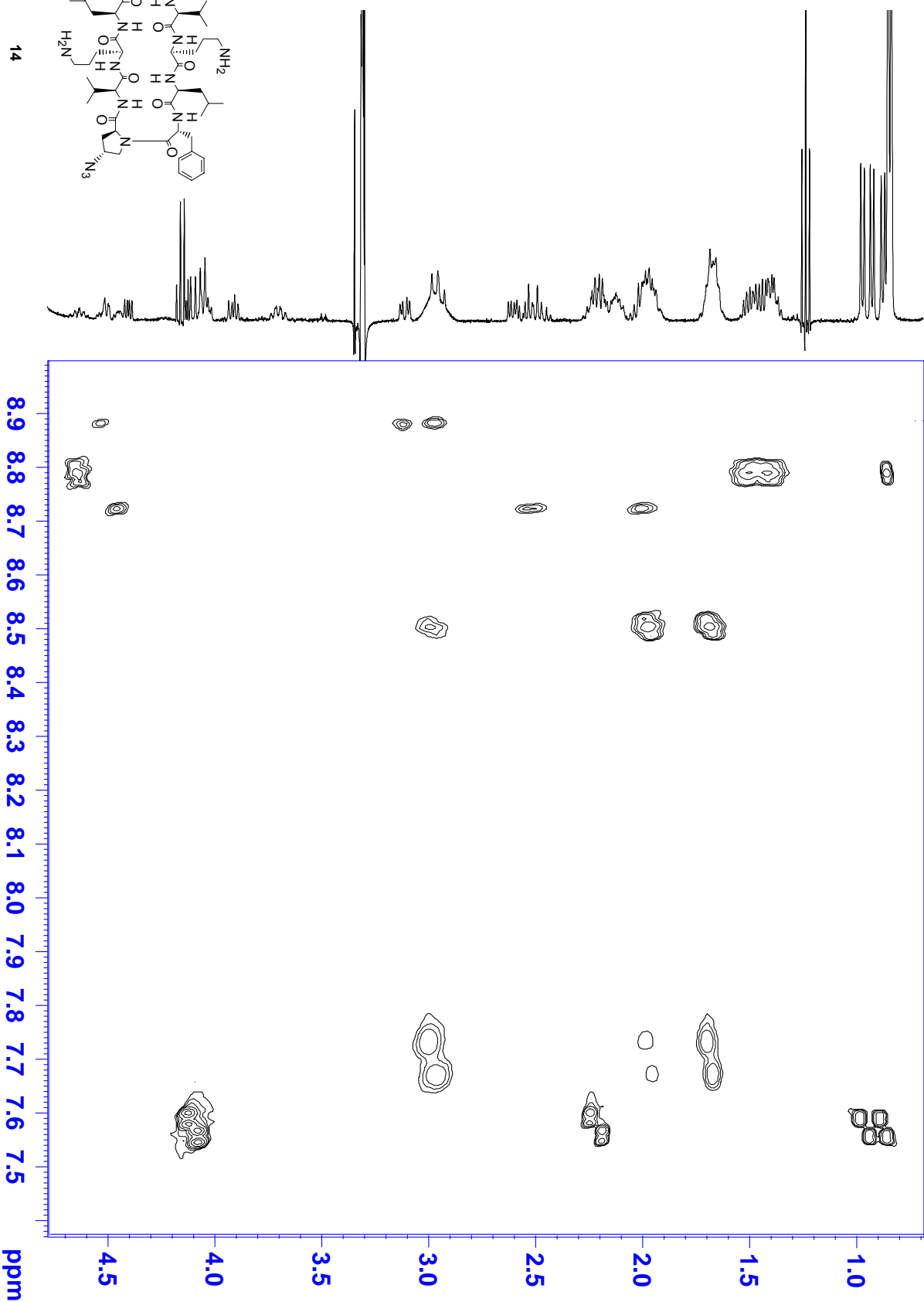
TD 1.0000000 sec  
 D1 0.0000000 sec  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 d13 0.00000400 sec  
 D20 0.00006500 sec  
 INO 0.00026880 sec  
 I1 18  
 MCREST 0.0000000 sec  
 MCWRK 0.00999999 sec  
 STCNT 256

===== CHANNEL f1 =====  
 NUC1 <sup>1</sup>H  
 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 52.29 dB  
 PL10 16.50 dB  
 SFO1 400.1319775 MHz

F1 - Acquisition Parameters  
 MD 512  
 SFO1 400.1319 MHz  
 FIDRES 7.266090 Hz  
 SW 9.298 ppm  
 FMODE States-TFPI

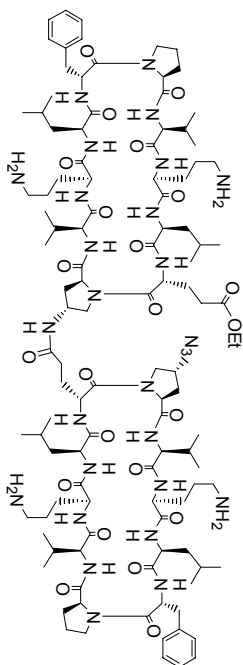
F2 - Processing parameters  
 SI 2048  
 SF 400.1300115 MHz  
 WDW QSI  
 SSB 2.3 Hz  
 LB 0.00 Hz  
 GB 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 States-TFPI  
 SF 400.1300065 MHz  
 QSI  
 SSB 2.1 Hz  
 LB 0.00 Hz  
 GB 0

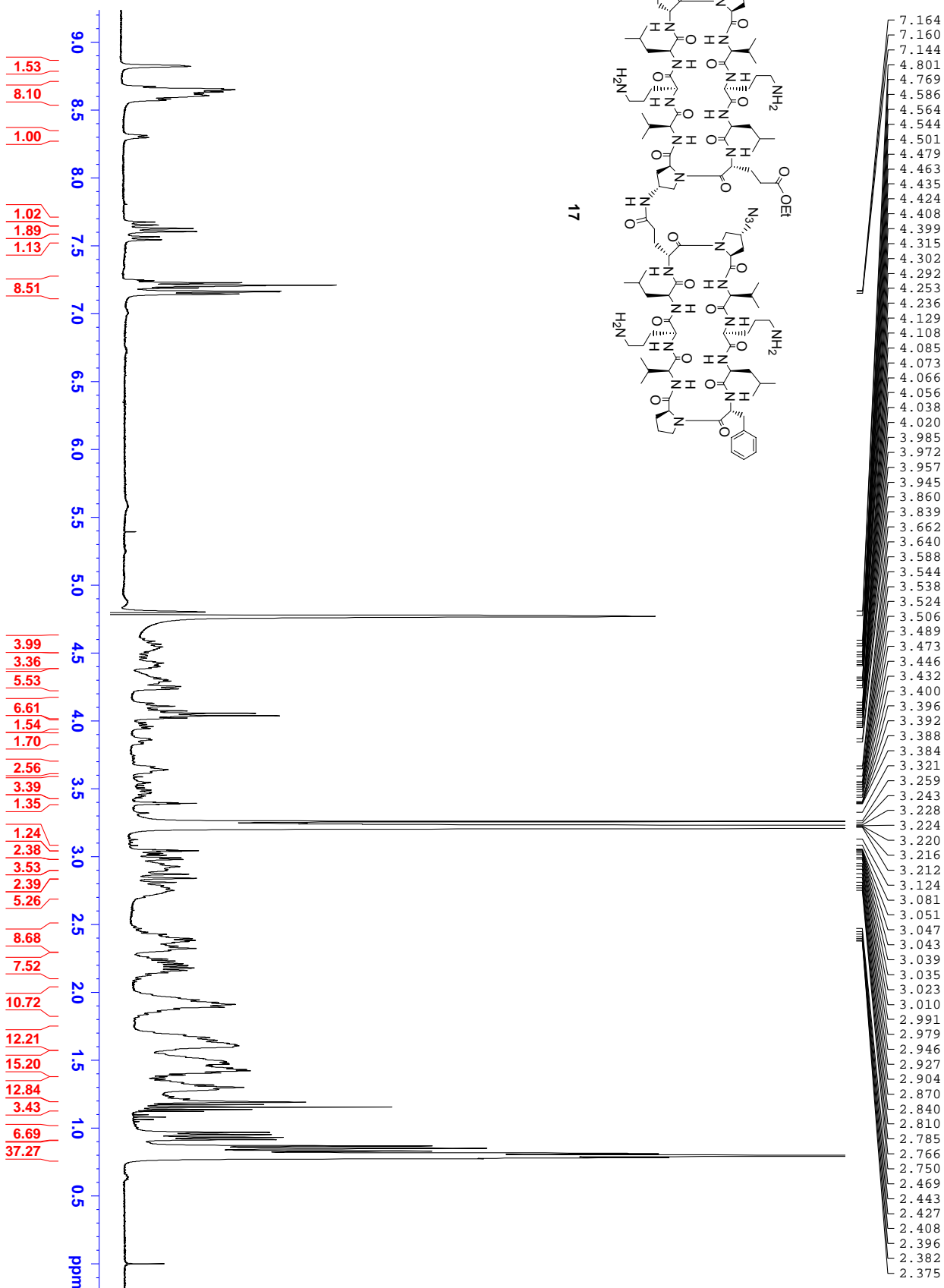


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mwe0806 - dimer N3/Et turn 1H, bbi-av400



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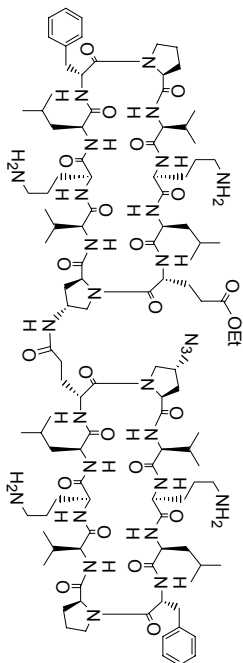
```

Current Data Parameters
NAME          G13052004
EXPNO        1
PROCNO       1
F2 - Acquisition Parameters
Date_        20040915
Time         10.01
INSTRUM     avance400
PROBHD      5 mm BBI 1H-BB
PULPROG     zgpg
TD           19228
SOLVENT     H2O
NS           1024
DS           0
SWH          4807.692 Hz
FIDRES       0.250036 Hz
AQ           1.9997621 sec
RG           256
DW           104.000 usec
DE           236.0
TE           298.0 K
D1           1.00002000 sec
d12          0.00000000 sec
MCOREST     0.00000000 sec
MCMARK      0.01500000 sec

===== CHANNEL f1 =====
NUC1         1H
P1           7.30 usec
PL1          4.00 dB
PL19         58.54 dB
SFO1         400.1319575 MHz

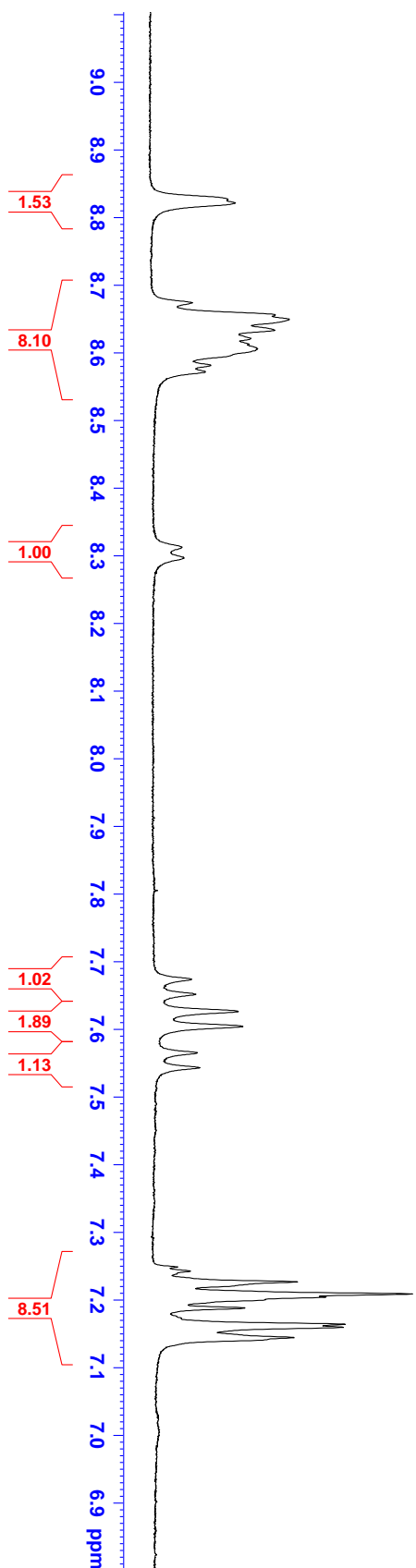
F2 - Processing parameters
SI           32768
SF           400.1300435 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
```

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



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8.821	8.673	8.312	7.674	7.249
8.649	8.633	8.296	7.652	7.242
8.620	8.606		7.627	7.227
8.581	8.571		7.604	7.209
			7.566	7.204
			7.543	7.188
				7.164
				7.160
				7.144



```

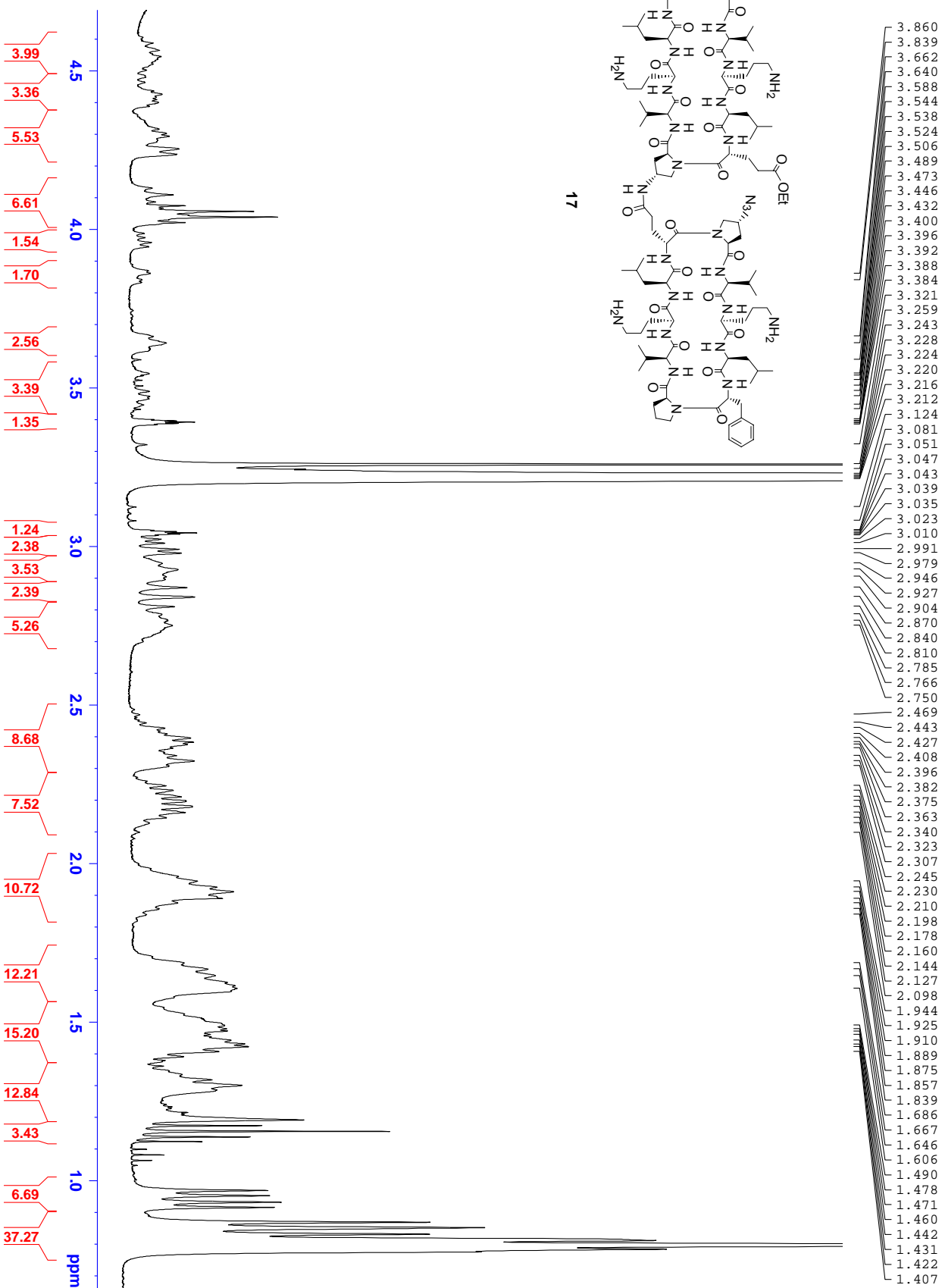
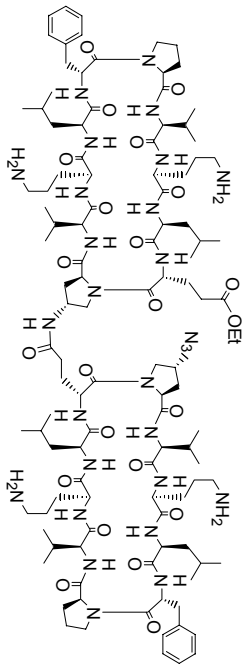
Current Data Parameters
NAME          G1J5092004
EXPNO         1
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time          10.01
INSTRUM      avance400
PROBHD       5 mm BBI 1H-BB
PULPROG      zgpr
TD            19228
H2O           H2O
SOLVENT      1024
NS            0
DS            0
SWH           4807.692 Hz
FIDRES        0.250036 Hz
AQ            1.9997621 sec
RG            256
DE            104.000 use
DM            8.50 use
PE            28.00 K
D1            1.0000200 sec
d12           0.0000200 sec
MCPRST       0.00000000
MCMRCK       0.01500000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            7.30 use
PL1           4.00 dB
PL2           58.54 dB
PL9
SF01          400.1319575 MHz

F2 - Processing parameters
SI            32768
SF            400.1300435 MHz
WDW           EM
SSB           0
LB            0
GB            0
PC            1.00
  
```



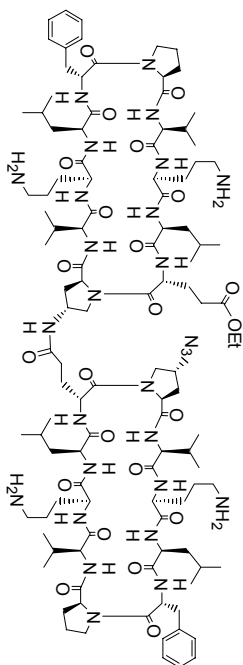
mwe0806 - dimer N3/Et turn 1H, bbi-av400



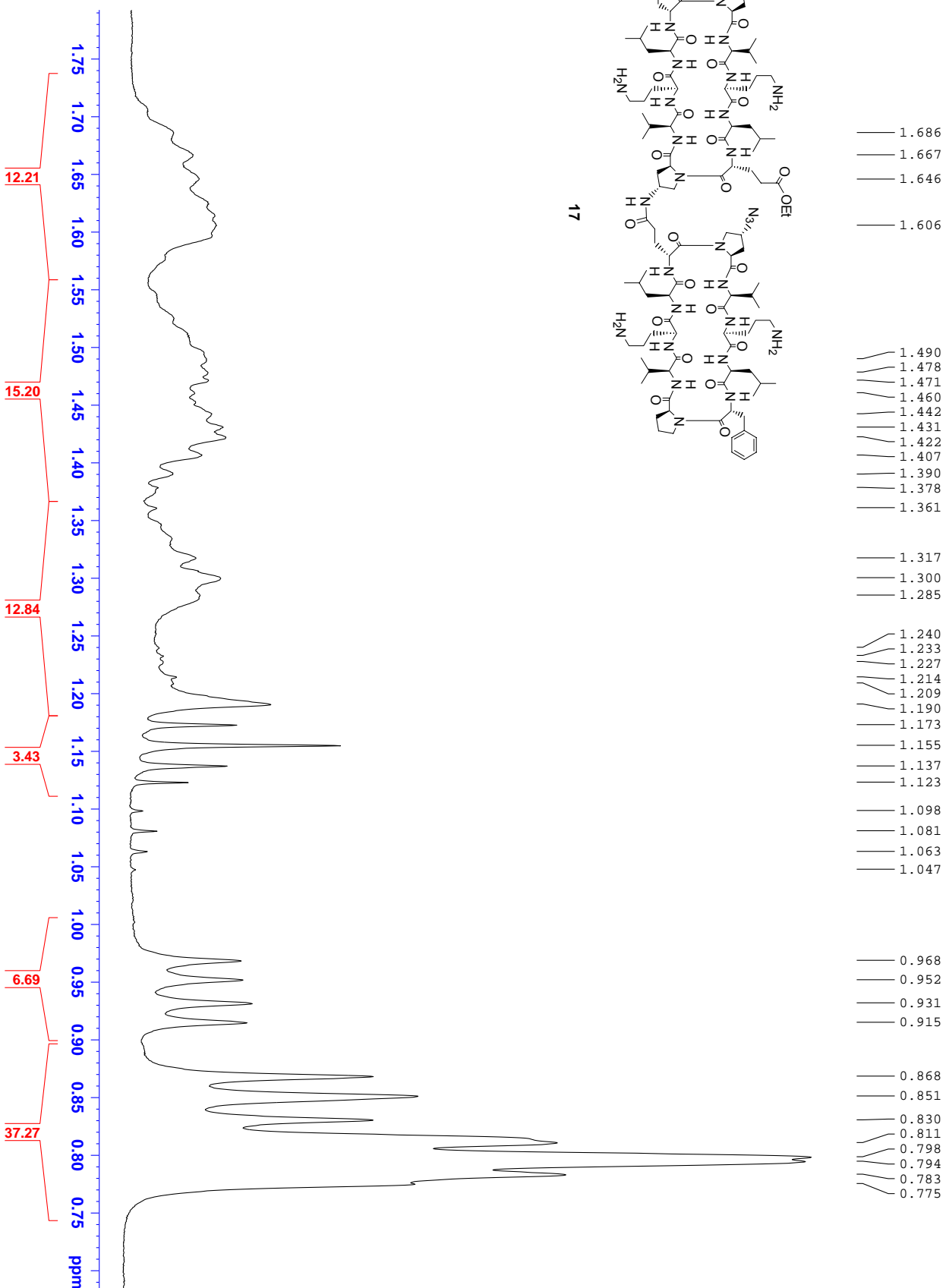
```

Current Data Parameters
NAME          G1J5092004
EXPNO         1
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time          10.01
INSTRUM       advanced400
PROBHD        5 mm BBI 1H-BB
PULPROG       zgpr
TD            19228
SOLVENT       H2O
NS            1024
DS            0
SWH           4807.692 Hz
AQ            0.250036 Hz
RG            1.9997621 sec
DE           256
DM           104.000 usec
DI           38.90
DE           28.00 K
D1           1.00000000 sec
d12          0.00000000 sec
MCOREST      0.00000000 sec
MCMRFX       0.01500000 sec
===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1          4.00 dB
PL2          58.54 dB
SF01         400.1319575 MHz
F2 - Processing parameters
SI           32768
SF           400.1300435 MHz
WDW          EM
SSB          0
GB           0
CB           0.00 Hz
DB           0
PC           1.00
  
```

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



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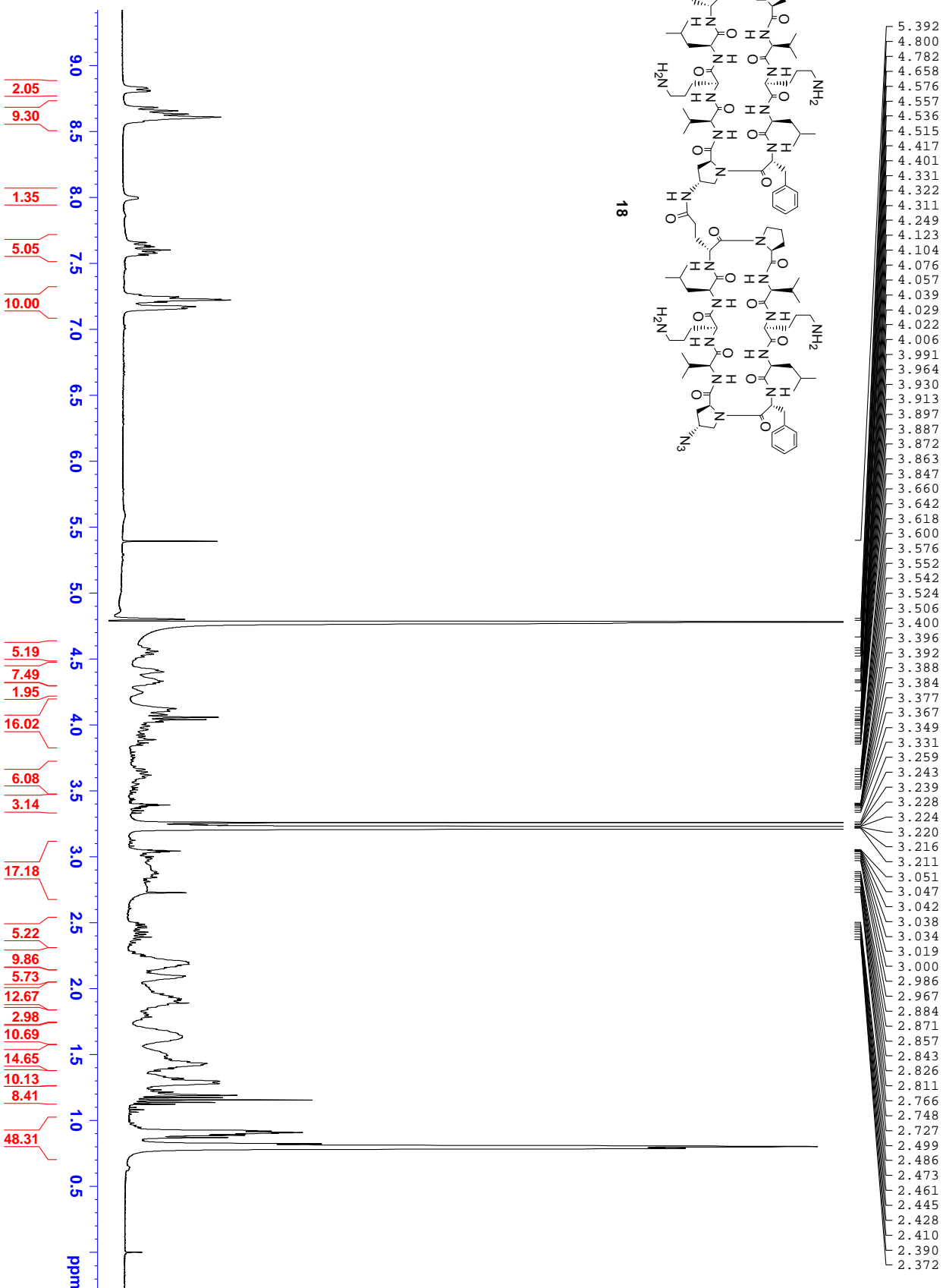
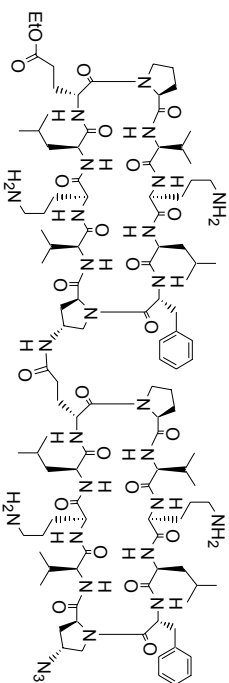
1.686	
1.667	
1.646	
1.606	
1.490	
1.478	
1.471	
1.460	
1.442	
1.431	
1.422	
1.407	
1.390	
1.378	
1.361	
1.317	
1.300	
1.285	
1.240	
1.233	
1.227	
1.214	
1.209	
1.190	
1.173	
1.155	
1.137	
1.123	
1.098	
1.081	
1.063	
1.047	
0.968	
0.952	
0.931	
0.915	
0.868	
0.851	
0.830	
0.811	
0.798	
0.794	
0.783	
0.775	

```

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   zgpr
TD         19228
SOLVENT    H2O
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         298.0 K
D1         1.00000000 sec
d12        0.00000000 sec
MCOREST    0.00000000 sec
MCWRK      0.01500000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         7.30 usec
PL1        4.00 dB
PL2
PL9        58.54 dB
SFO1       400.1319575 MHz

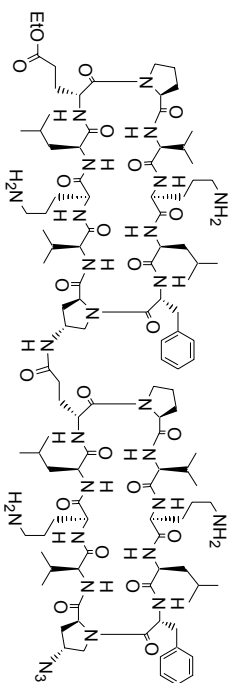
F2 - Processing parameters
SI         32768
SF         400.1300435 MHz
WDW        EM
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```



```

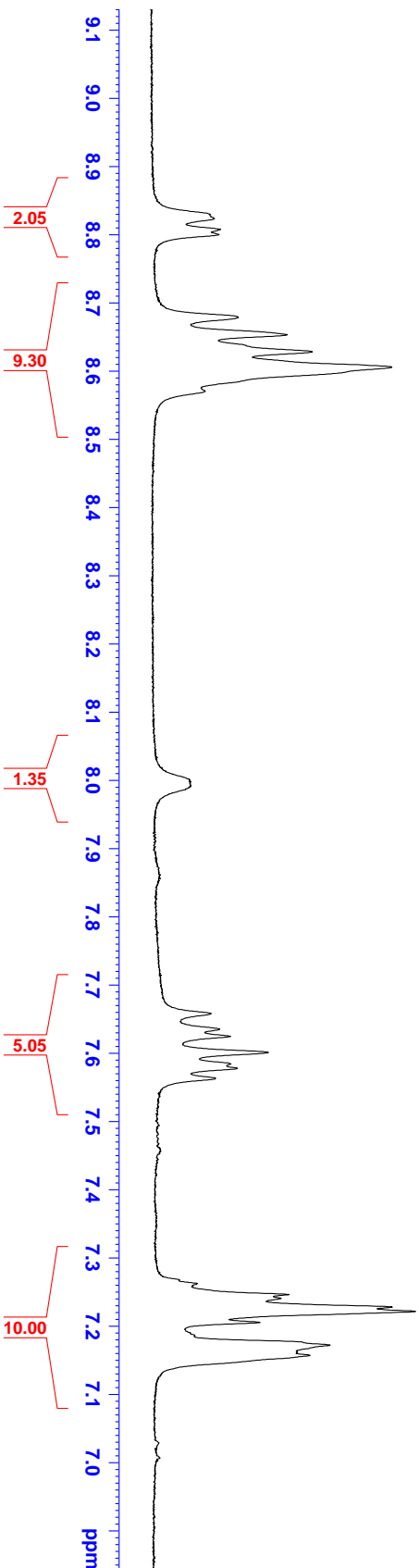
Current Data Parameters
NAME          G1J5092004
EXPNO        4
PROCNO       1
F2 - Acquisition Parameters
Date_        20040915
Time         13.00
INSTRUM      advanced400
PROBHD       5 mm BBI 1H-BB
PULPROG      zgpg
TD            19228
SOLVENT      MeOD
NS            1024
DS            0
SWH           4807.692 Hz
FIDRES        0.250036 Hz
AQ            1.9997621 sec
RG            256
DE            104.000 usec
TE            28.50
DE            28.50
D1            1.0000200 sec
d12           0.0000200 sec
MORREST      0.00000000 sec
MCWRRX       0.01500000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL2           60.89 dB
PL9           400.1319575 MHz
SF01          400.1300436 MHz
F2 - Processing parameters
SI            32768
SF            400.1300436 MHz
WDW           EM
SSB           0
GB            0
CB            0.00 Hz
DB            0
PC            1.00
    
```



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8.823	8.807	8.800
8.678	8.653	8.628
8.605	8.570	
7.992		
7.658	7.635	7.624
7.601	7.584	7.577
7.563		
7.262	7.246	7.240
7.227	7.221	7.205
7.171	7.157	



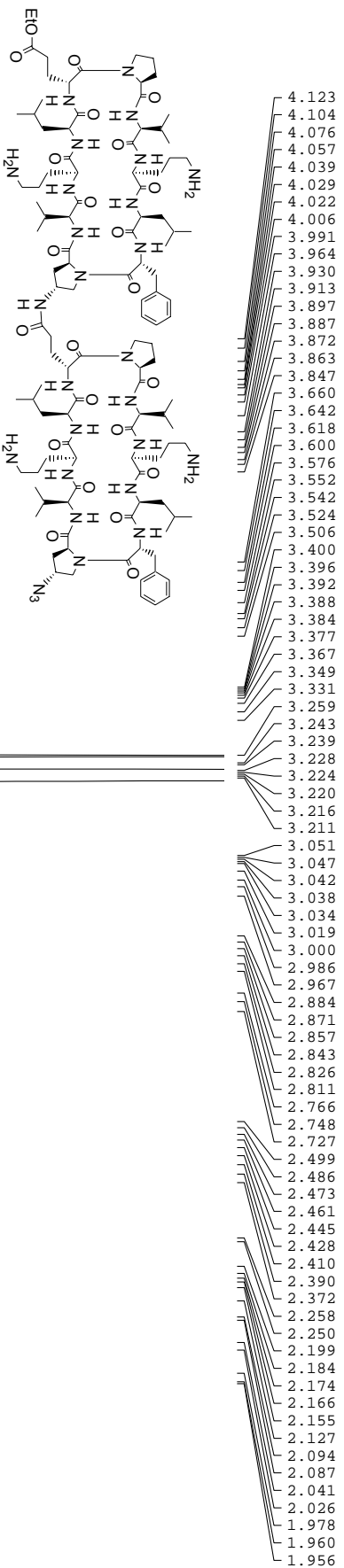
```

Current Data Parameters
NAME          G1J5092004
EXPNO         4
PROCNO       1
F2 - Acquisition Parameters
Date_        20040915
Time         13.00
INSTRUM     avance400
PROBHD      5 mm BBI 1H-BB
PULPROG     zgpr
TD          19228
MEOB       MeOD
SOLVENT     1024
NS          1024
DS          0
SWH         4807.692 Hz
AQ          0.250036 Hz
RG          1.9997621 sec
DE         286
DM         104.000 usec
DE         8.50 usec
TE         298.0 K
D1         1.00000000 sec
d12        0.00000000 sec
MCREPST    0.00000000
MCMRFX     0.01500000 sec

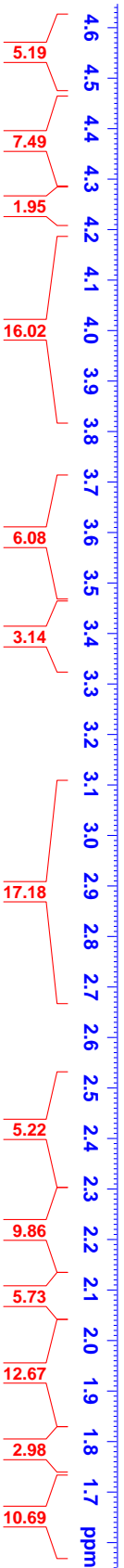
===== CHANNEL f1 =====
NUC1        1H
P1          7.30 usec
PL1         4.00 dB
PL2         60.89 dB
PL3         60.89 dB
SFO1        400.1319575 MHz

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



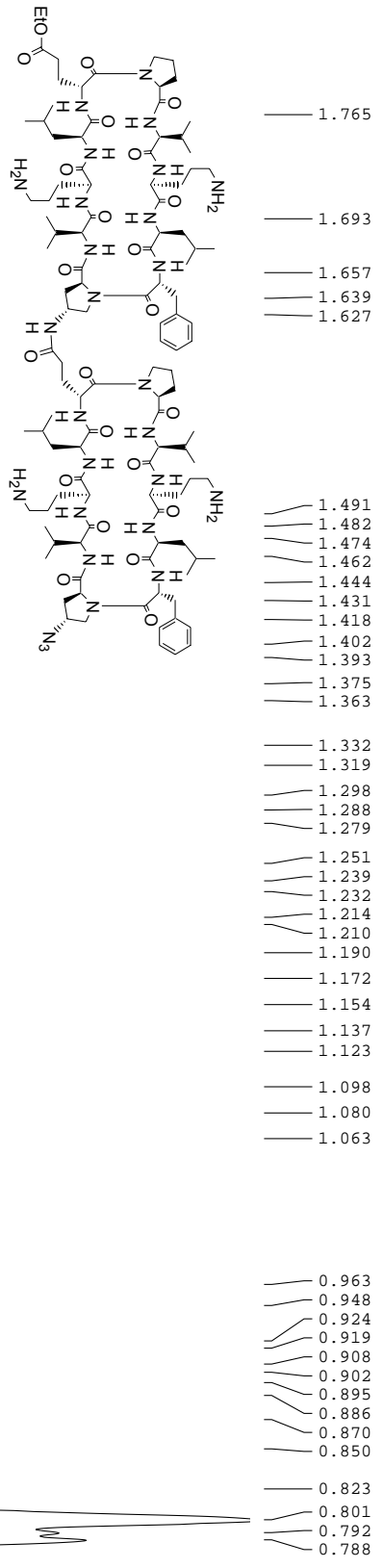
18



```

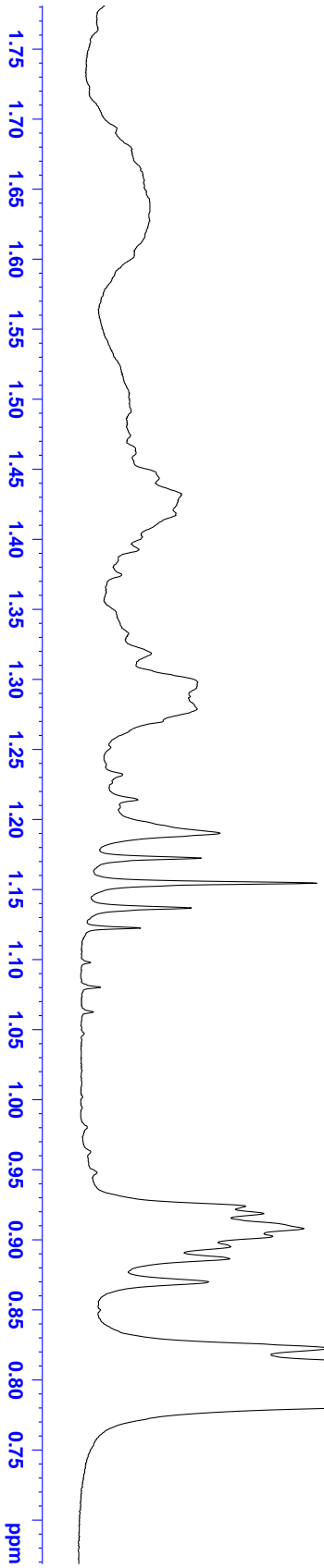
Current Data Parameters
NAME          G1J5052004
EXPNO         4
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time          13.00
INSTRUM       advanced400
PROBHD        5 mm BBI 1H-BB
PULPROG       zgpr
TD            19228
SOLVENT       MeOD
NS            1024
DS            0
SWH           4807.692 Hz
AQ            0.250036 Hz
RG            256
DE            104.000 usec
TE            28.90 K
D1            1.00002000 sec
d12           0.00002000 sec
MCWRRX       0.01500000 sec
===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL2           60.89 dB
SF01         400.1319575 MHz
F2 - Processing parameters
SI           32768
SF           400.1300436 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
```

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



1.765	1.491	1.332	1.098	0.963
1.693	1.482	1.319	1.080	0.948
1.657	1.474	1.298	1.000	0.924
1.639	1.462	1.288	0.919	0.908
1.627	1.444	1.279	0.902	0.895
	1.431	1.251	0.886	0.870
	1.418	1.239	0.850	0.823
	1.402	1.232	0.801	0.792
	1.393	1.214	0.788	
	1.375	1.210		
	1.363	1.190		
		1.172		
		1.154		
		1.137		
		1.123		
		1.098		
		1.080		
		1.063		
		0.963		
		0.948		
		0.924		
		0.919		
		0.908		
		0.902		
		0.895		
		0.886		
		0.870		
		0.850		
		0.823		
		0.801		
		0.792		
		0.788		

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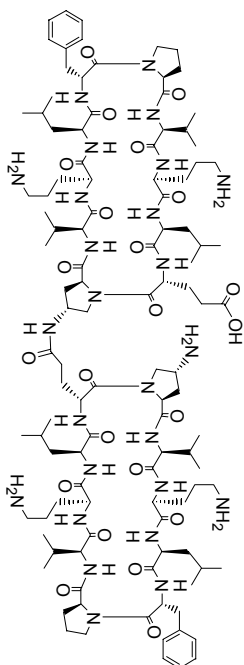
```

Current Data Parameters
NAME          G158092004
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            298.0 K
D1            1.0000200 sec
d12           0.0000000 sec
MCOREST      0.0000000 sec
MCWRK        0.01500000 sec

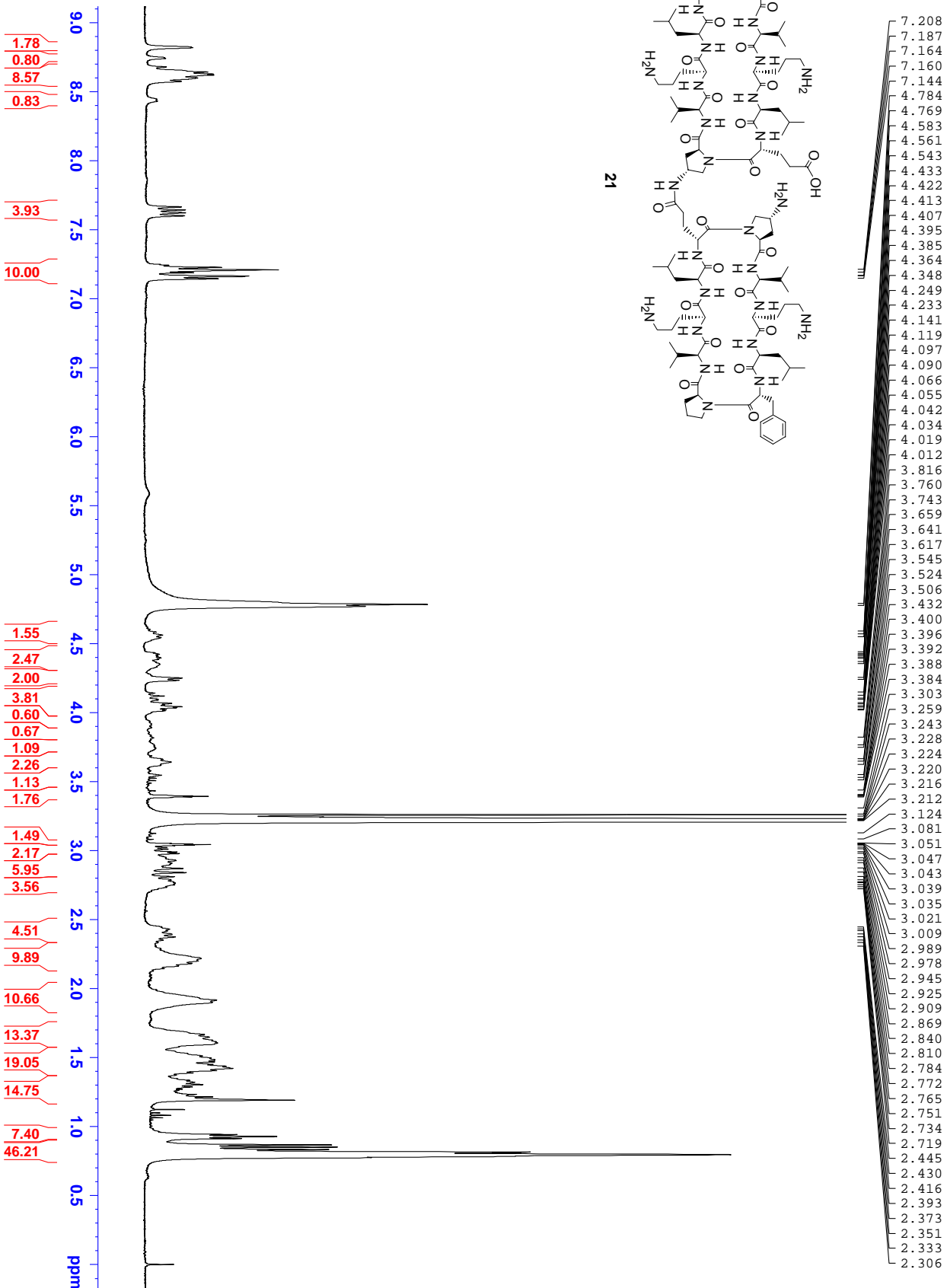
===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL9           60.89 dB
SFO1         400.1319575 MHz

F2 - Processing parameters
SI            32768
SF            400.1300436 MHz
WDW           EM
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
    
```

mwe1501 - dimer NH2/COOH turn 1H, bbi-av400

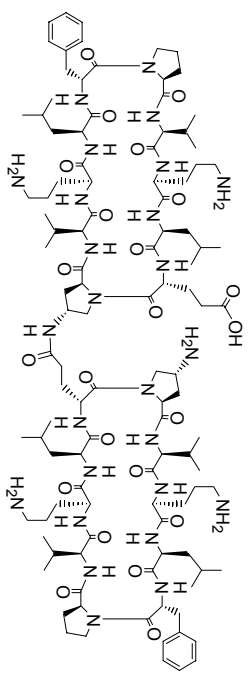


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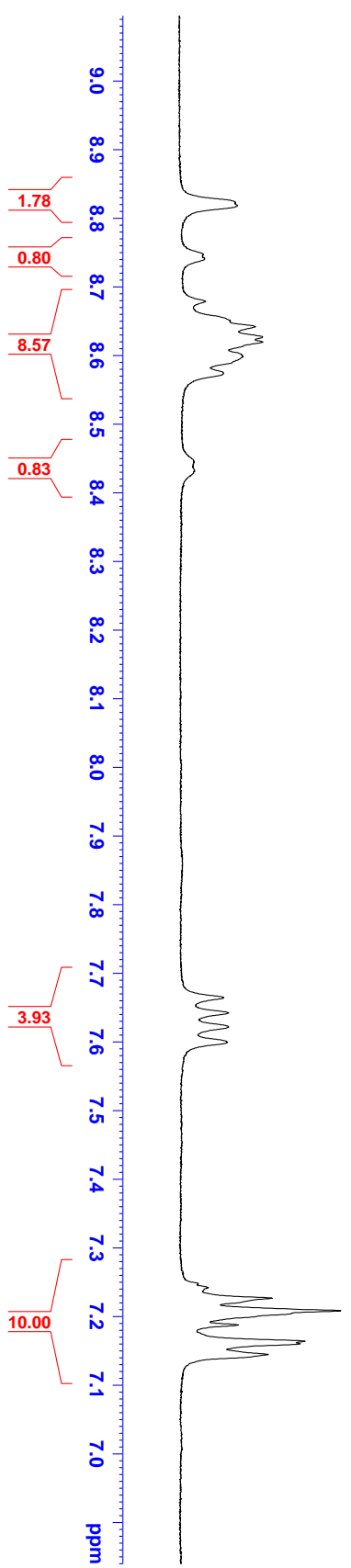
Current Data Parameters  
 NAME G13092004  
 EXPNO 3  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20040915  
 Time 11.43  
 INSTRUM avance400  
 PROBD 5 mm BBI 1H-BB  
 PULPROG zgpg  
 TD 19228  
 SOLVENT MeOD  
 NS 1024  
 DS 0  
 SWH 4807.692 Hz  
 FIDRES 0.250036 Hz  
 AQ 1.9997621 sec  
 RG 256  
 DW 104.000 usec  
 DE 8.50 usec  
 TE 298.0 K  
 D1 1.0000200 sec  
 d12 0.0000000 sec  
 MCREST 0.0000000 sec  
 MCWRRK 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  
 GB 0  
 DB 0  
 PC 1.00

mwe1501 - dimer NH2/COOH turn 1H, bbi-av400



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8.818	
8.747	
8.741	
8.679	
8.642	
8.626	
8.619	
8.598	
8.574	
8.445	
8.432	
7.665	
7.642	
7.621	
7.599	
7.247	
7.242	
7.226	
7.208	
7.187	
7.164	
7.160	
7.144	



```

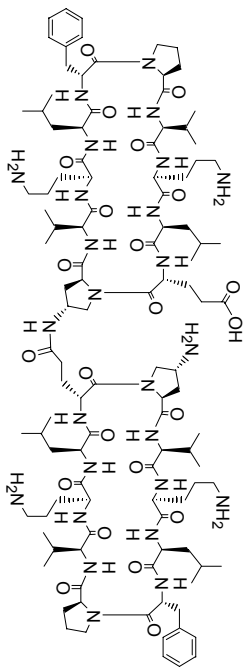
Current Data Parameters
NAME          G1J5092004
EXPNO         3
PROCNO       1
F2 - Acquisition Parameters
Date_         20040915
Time          11.43
INSTRUM      avance400
PROBHD       5 mm BBI 1H-BB
PULPROG      zgpr
TD            19228
SOLVENT      MeOD
NS            1024
DS            0
SWH           4807.692 Hz
FIDRES        0.250036 Hz
AQ            1.9997621 sec
RG            256
DE            104.000 usec
TE            298.0 K
DE            8.50 usec
D1            1.0000000 sec
d12           0.0000000 sec
MCPRST       0.0000000
MCRMK        0.01500000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL9           58.54 dB
SFO1         400.1319575 MHz

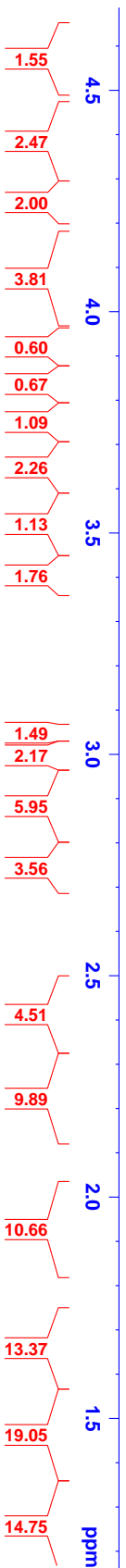
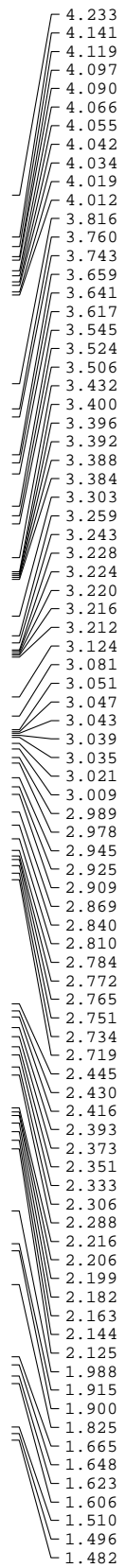
F2 - Processing parameters
SI            32768
SF            400.1300435 MHz
WDW           EM
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
  
```



mwe1501 - dimer NH2/COOH turn 1H, bbi-av400



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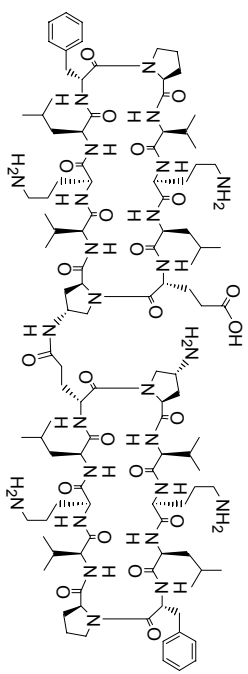
```

Current Data Parameters
NAME          G1J5092004
EXPNO         3
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time_        11.43
INSTRUM      advance400
PROBHD       5 mm BBI 1H-BB
PULPROG      zgpr
TD            19228
SOLVENT      MeOD
NS            1024
DS            0
SWH           4807.692 Hz
AQ            0.250036 Hz
RG            256
DE            104.000 usec
TE            28.50 K
D1            1.00002000 sec
d12           0.00002000 sec
MCWRES1      0.00000000 sec
MCWRES2      0.01500000 sec

===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL2           58.54 dB
SF01          400.1319575 MHz

F2 - Processing parameters
SI            32768
SF            400.1300435 MHz
WDW           EM
SSB           0
GB            0
CB            0
PC            1.00
  
```

mwe1501 - dimer NH2/COOH turn 1H, bbi-av400



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1.665	
1.648	
1.623	
1.606	
1.510	
1.496	
1.482	
1.468	
1.450	
1.437	
1.421	
1.404	
1.388	
1.373	
1.334	
1.321	
1.304	
1.286	
1.269	
1.262	
1.251	
1.232	
1.214	
1.208	
1.190	
1.160	
1.143	
1.131	
1.123	
1.098	
1.080	
1.063	
1.047	
1.002	
0.983	
0.941	
0.927	
0.912	
0.867	
0.850	
0.832	
0.814	
0.809	
0.795	
0.774	



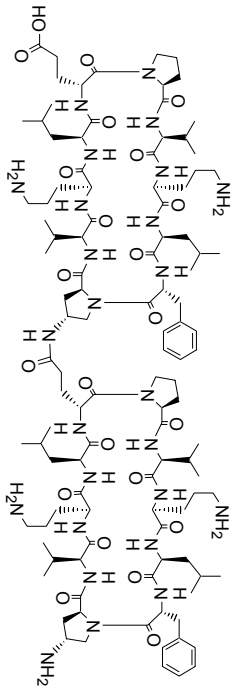
```

Current Data Parameters
NAME      G158092004
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        1.9997621 sec
RG        286
DW        104.000 usec
DE        38.50 usec
TE        298.0 K
D1        1.0000200 sec
d12       0.0000000 sec
MCOREST  0.0000000 sec
MCWRK    0.01500000 sec

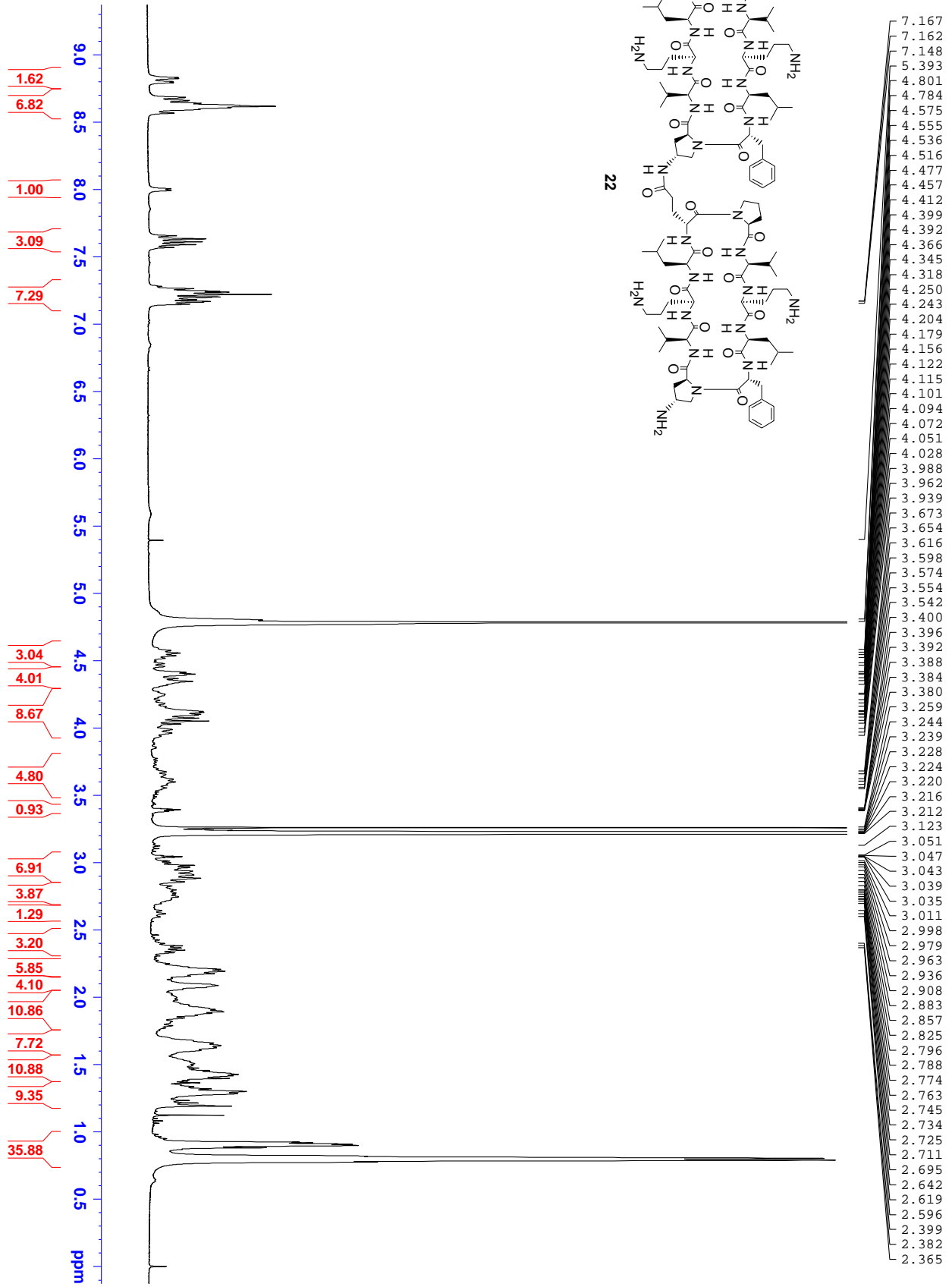
===== CHANNEL f1 =====
NUC1      1H
P1        7.30 usec
PL1       4.00 dB
PL2
PL3
PL4
PL5
SFO1      400.1319575 MHz

F2 - Processing parameters
SI        32768
SF        400.1300435 MHz
WDW       EM
SSB       0
LB        0
GB        0
PC        1.00
  
```

mwc1501 - dimer NH2/COOH sheet 1H, bbi-av400



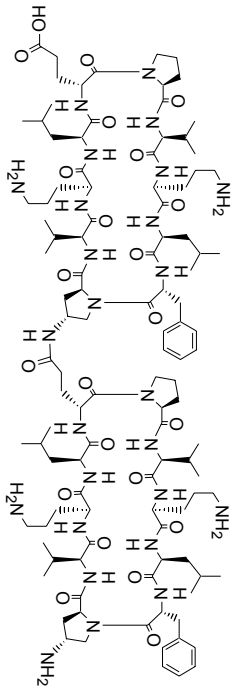
22



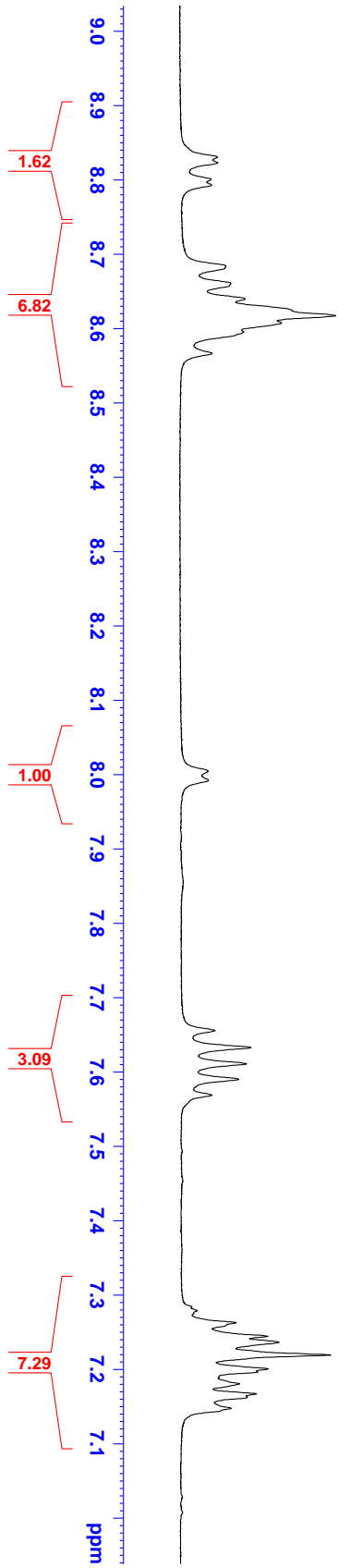
```

Current Data Parameters
NAME          G1J5092004
EXPNO         5
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time          14.09
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
DM             104.000 usec
DE             28.90 usec
TE             300.2 K
D1             1.00002000 sec
d12            0.00000000 sec
MCWRES        0.01500000 sec
===== CHANNEL f1 =====
NUC1           1H
P1             7.30 usec
PL1            4.00 dB
PL19           60.89 dB
SF01           400.1319579 MHz
F2 - Processing parameters
SI             32768
SF             400.1300433 MHz
WDW            EM
SSB            0
GB             0
CB             0.00 Hz
DB             0
PC             1.00
  
```

mwc1501 - dimer NH2/COOH sheet 1H, bbi-av400



- 8.830
- 8.823
- 8.800
- 8.792
- 8.684
- 8.660
- 8.639
- 8.617
- 8.607
- 8.595
- 8.566
- 8.005
- 7.992
- 7.655
- 7.632
- 7.611
- 7.590
- 7.568
- 7.279
- 7.263
- 7.245
- 7.237
- 7.219
- 7.201
- 7.197
- 7.181
- 7.167
- 7.162
- 7.148



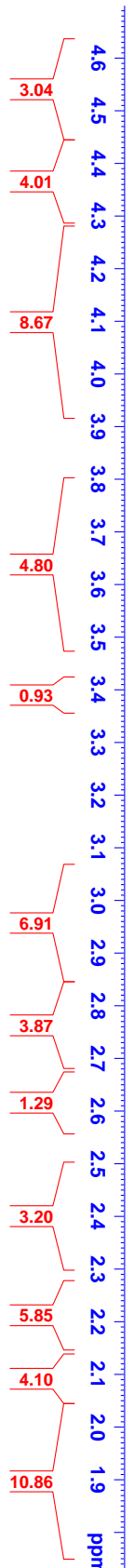
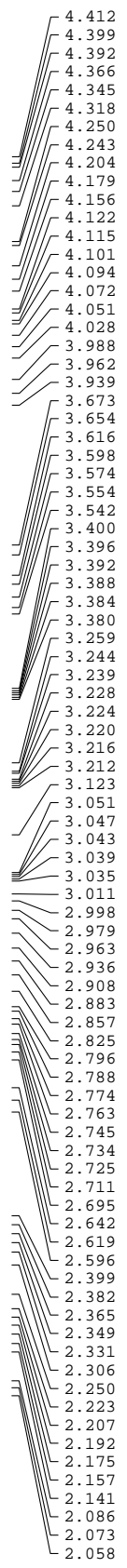
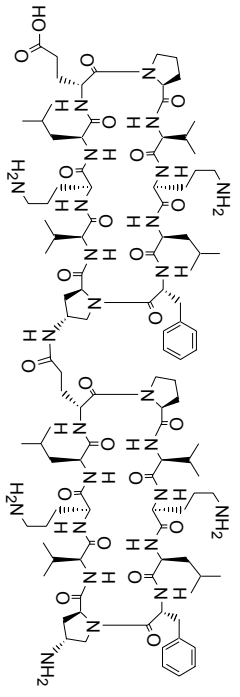
Current Data Parameters  
 NAME G1J5092004  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20040915  
 Time 14.09  
 INSTRUM advance400  
 PROBRD 5 mm BBI 1H-BB  
 PULPROG zgpr  
 TD 19228  
 MeOD  
 SOLVENT MeOD  
 NS 1024  
 DS 0  
 SWH 4807.692 Hz  
 FIDRES 0.250036 Hz  
 AQ 1.9997621 sec  
 RG 286  
 DE 104.000 use  
 DW 8.50 use  
 TE 298.0 K  
 D1 1.0000200 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 60.89 dB  
 SFO1 400.1319579 MHz

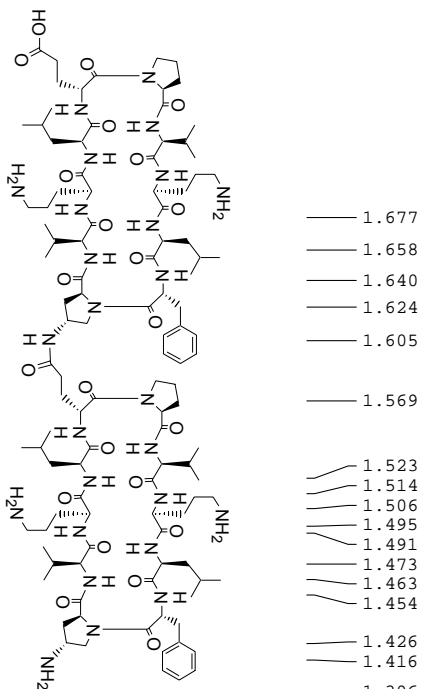
F2 - Processing parameters  
 SI 32768  
 SF 400.1300433 MHz  
 WDW EM  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

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



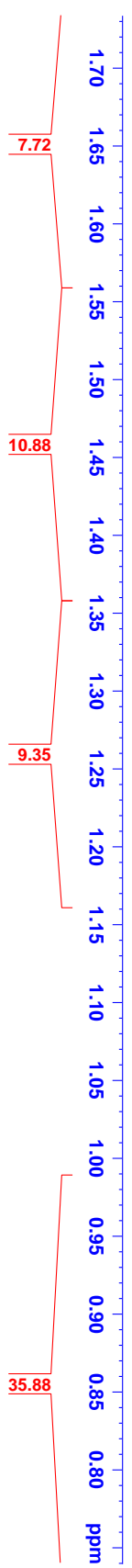
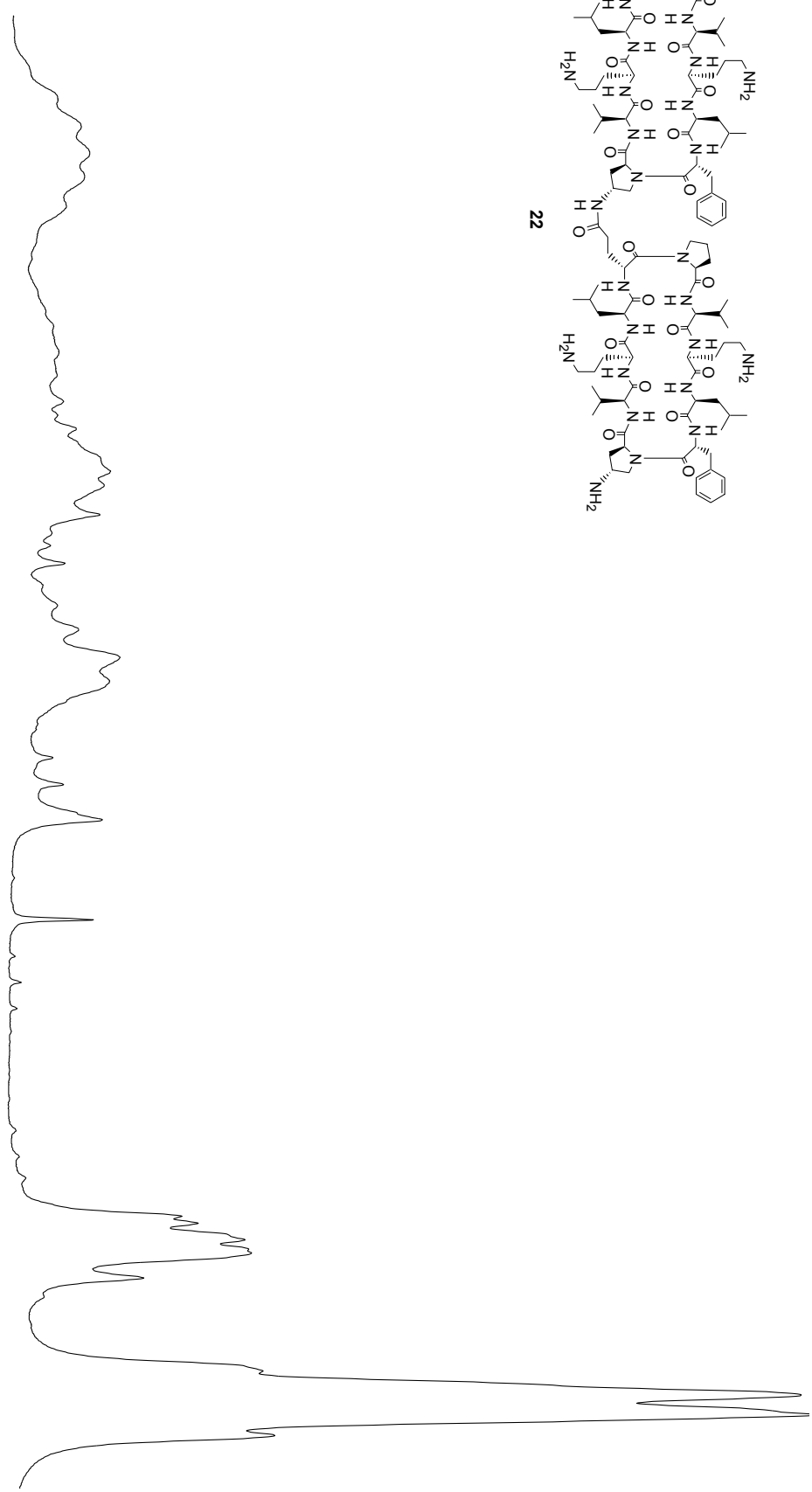
Current Data Parameters  
 NAME G1J5092004  
 EXNO 5  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20040915  
 Time\_ 14.09  
 INSTRUM advance400  
 PROBD 5 mm BBI 1H-BB  
 PULPROG zgpg  
 TD 19228  
 SOLVENT MeOD  
 NS 1024  
 DS 0  
 SWH 4807.692 Hz  
 FIDRES 0.250036 Hz  
 AQ 1.9997621 sec  
 RG 256  
 DW 104.000 usec  
 DE 28.90 usec  
 TE 283.0 K  
 D1 1.00002000 sec  
 d12 0.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRX 0.01500000 sec  
 ===== CHANNEL f1 =====  
 NUCL 1H  
 P1 7.30 usec  
 PL1 4.00 dB  
 PL9 60.89 dB  
 SF01 400.1319579 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 400.1300433 MHz  
 WDM EM  
 SSB 0  
 GB 0.00 Hz  
 CB 0  
 PC 1.00

mwc1501 - dimer NH2/COOH sheet 1H, bbi-av400



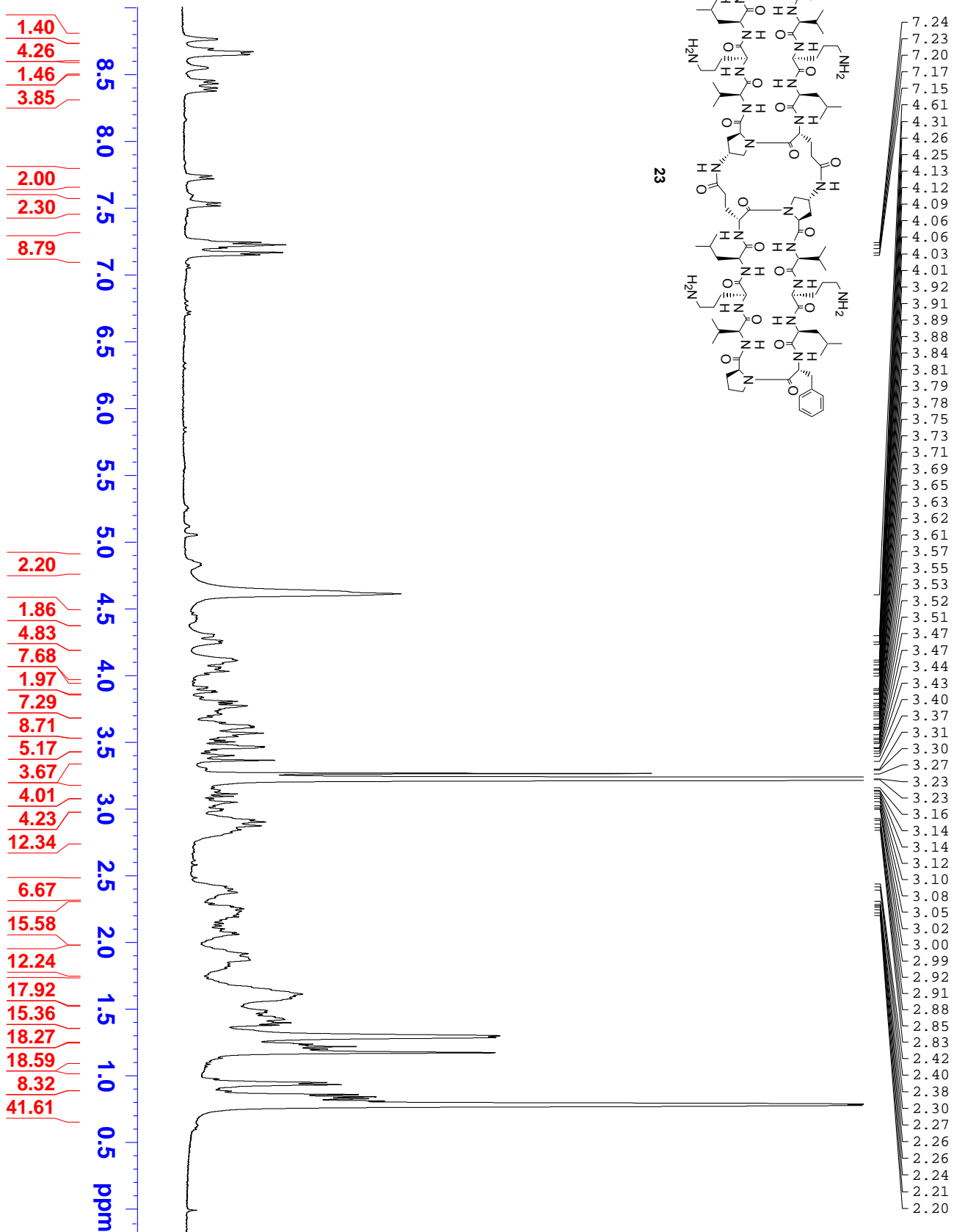
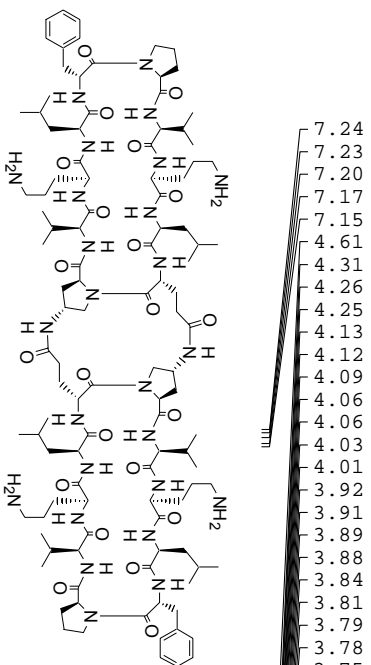
22

1.677	1.658	1.640	1.624	1.605	1.569	1.523	1.514	1.506	1.495	1.491	1.473	1.463	1.454	1.426	1.416	1.396	1.384	1.375	1.363	1.349	1.335	1.319	1.300	1.284	1.255	1.232	1.214	1.190	1.123	1.081	0.963	0.949	0.923	0.918	0.907	0.901	0.898	0.881	0.869	0.819	0.802	0.789	0.775
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------



Current Data Parameters  
 NAME G1J5092004  
 EXPNO 5  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20040915  
 Time 14.09  
 INSTRUM avance400  
 PROBHD 5 mm BBI 1H-BB  
 PULPROG zgpr  
 TD 19228  
 MeOD  
 SOLVENT 1024  
 NS 0  
 DS 4807.692 Hz  
 SWH 0.250036 Hz  
 FIDRES 1.9997621 sec  
 AQ 286  
 RG 104.000 use  
 DW 8.90 use  
 DE 28.0 K  
 TE 300.2 K  
 D1 1.00002000 sec  
 d12 0.00002000 sec  
 MCRST 0.01500000 sec  
 MCWRK 0.01500000 sec  
 ===== CHANNEL f1 =====  
 NUCL 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  
 GB 0  
 PC 1.00

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



```

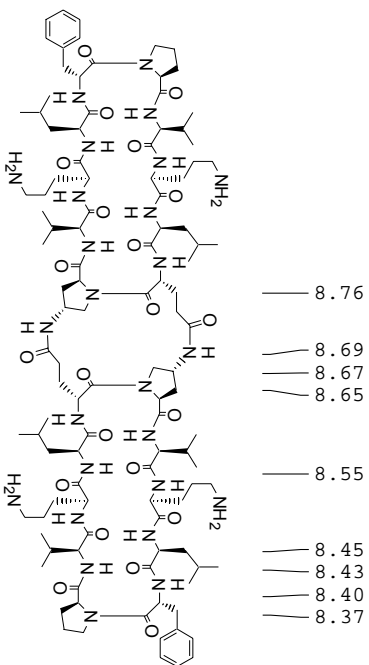
Current Data Parameters
NAME      G1Jsr72003
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20030723
Time      10.20
INSTRUM   avance400
PROBHD    5 mm BBI 1H-BB
PULPROG   zgpg2
TD         13228
SOLVENT   MeD2
NS         128
DS         2
SH         4807.692 Hz
FIDRES    0.250036 Hz
AQ         1.9997621 sec
RG         1.992281
DE         104.000 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       400.1318653 MHz

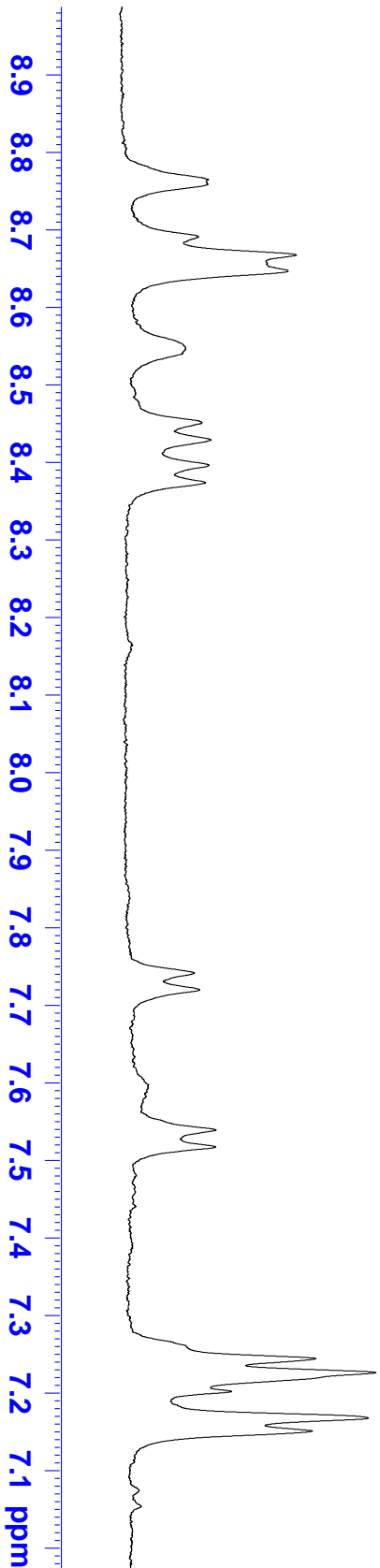
F2 - Processing parameters
SI         131072
SF         400.1300389 MHz
WDW        EM
SSB        0
LB         0.50 Hz
GB         0
PC         1.00
    
```

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



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8.76	
8.69	
8.67	
8.65	
8.55	
8.45	
8.43	
8.40	
8.37	
7.74	
7.72	
7.54	
7.52	
7.24	
7.23	
7.20	
7.17	
7.15	



```

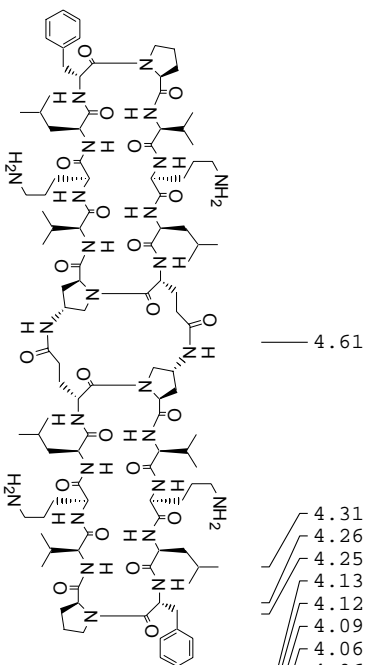
Current Data Parameters
NAME          GIJ5072003
EXPNO         1
PROCNO        1
F2 - Acquisition Parameters
Date_         20030723
Time          10.20
INSTRUM       avance400
PROBHD        5 mm BBI 1H-BB
PULPROG       zgpg
TD            13228
SOLVENT       MeOD
NS            128
DS            4
SFO1          400.131863 MHz
FIDRES        0.250036 Hz
AQ            1.9997621 sec
RG            328.1
DE            104.000 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
PL19          58.19 dB
SF01          400.131863 MHz

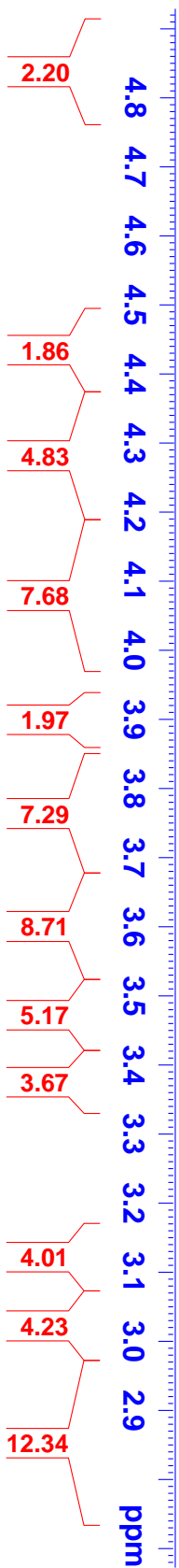
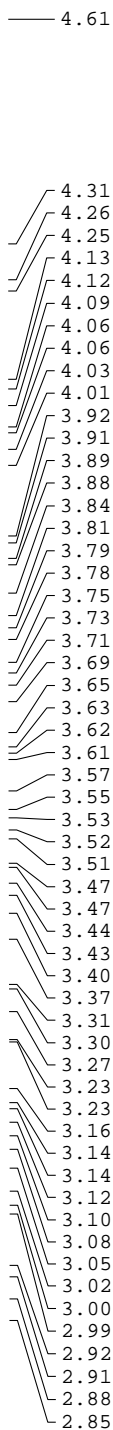
F2 - Processing Parameters
SI            131072
SF            400.1300389 MHz
WDW           EM
SSB           0
LB            0.50 Hz
GB            0
PC            1.00
  
```



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



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```

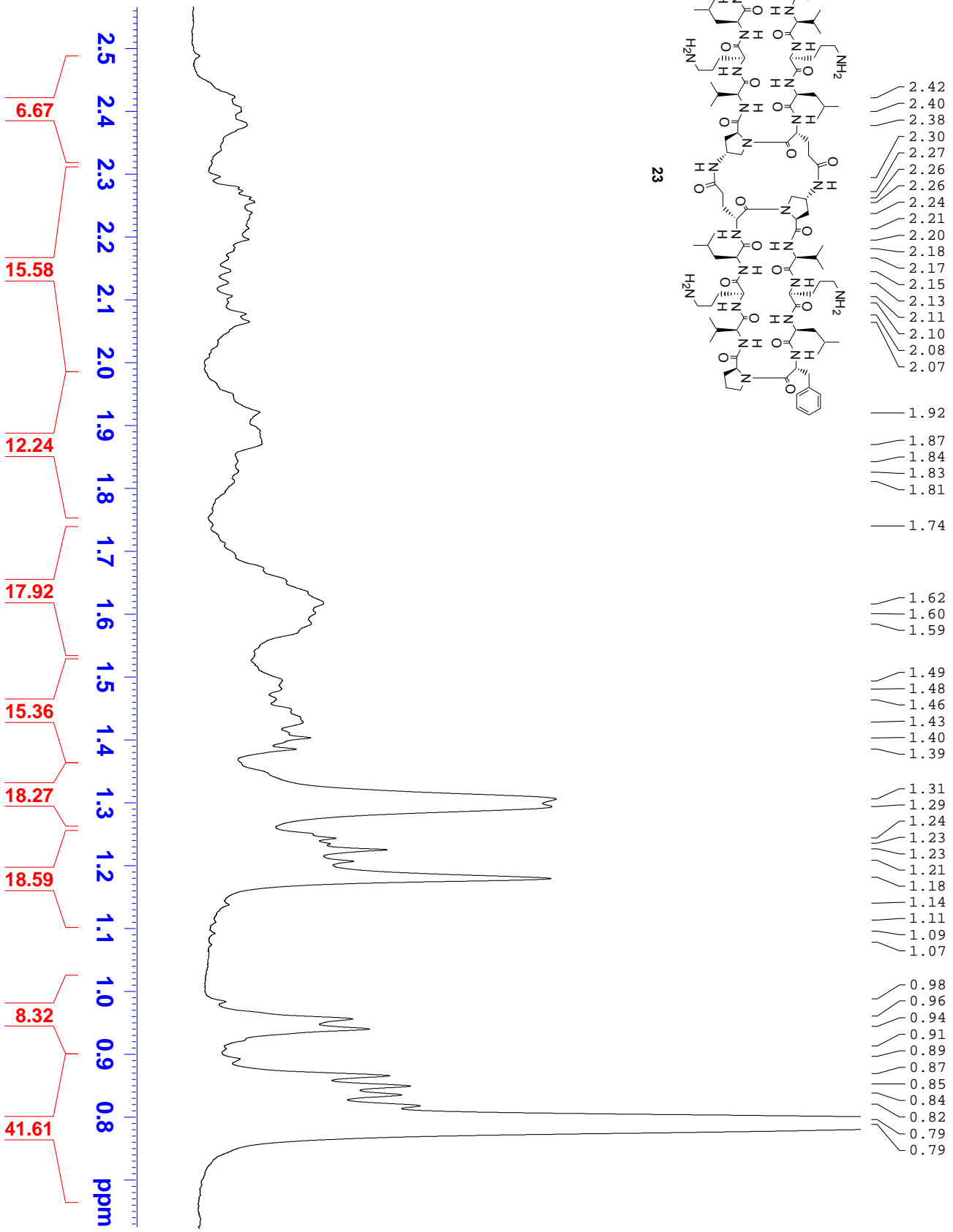
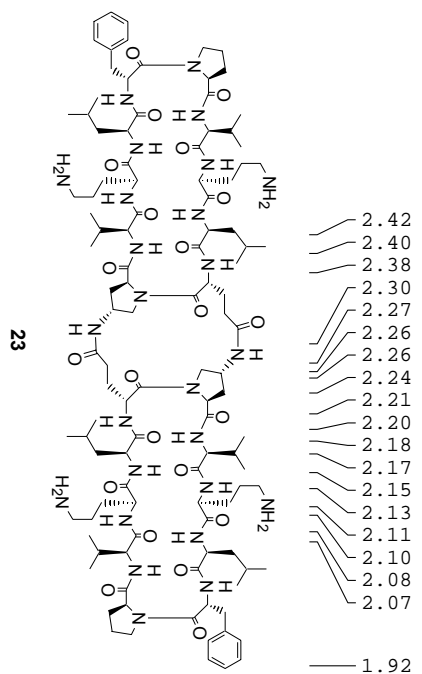
Current Data Parameters
NAME      G1js072003
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20030723
Time      10.20
INSTRUM   avance400
PROBHD    5 mm BBI 1H-BB
PULPROG   zgpg2
TD         13228
SOLVENT   MeD2O
NS         128
DS         2
SH         4807.692 Hz
FIDRES    0.2560036 Hz
AQ         1.9997621 sec
RG         1.992281
DE         104.000 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
PL2        58.19 dB
SFO1       400.1318853 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



```

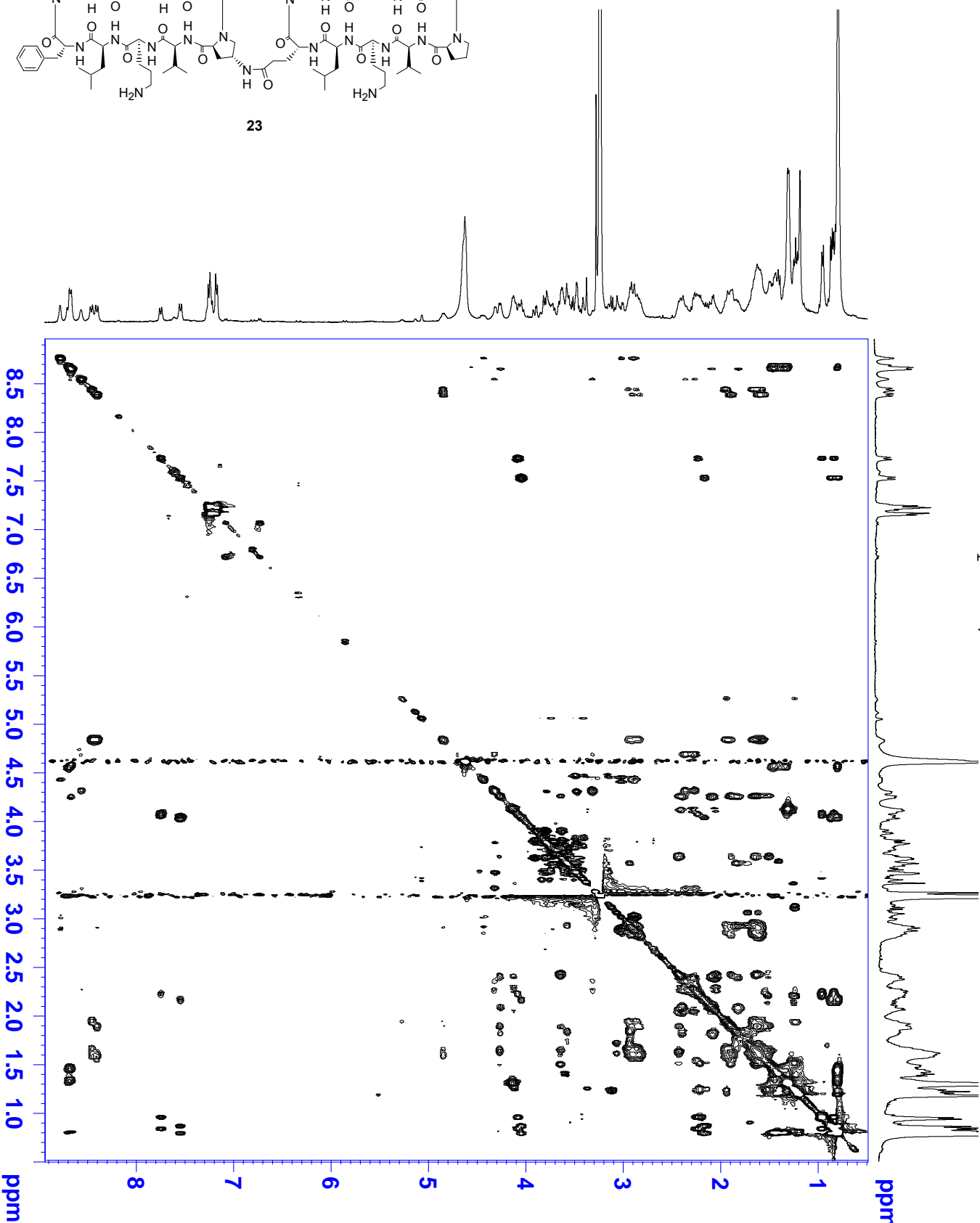
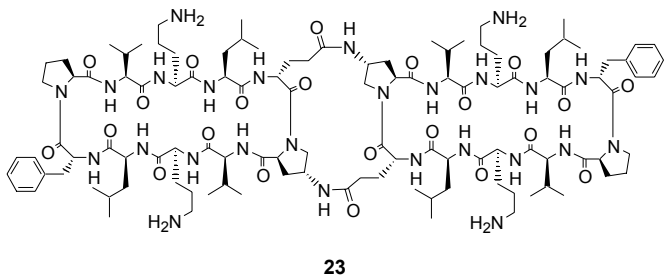
Current Data Parameters
NAME      G1js072003
EXPNO     1
PROCNO    2

F2 - Acquisition Parameters
Date_     20030723
Time      10.20
INSTRUM   avance400
PROBHD    5 mm BBI 1H-BB5
PULPROG   zgpg2
TD         13228
SOLVENT   MeOD
NS         128
DS         2
SWH        4807.692 Hz
FIDRES     0.250026 Hz
AQ         1.99297621 sec
RG         1.9722841
DE         104.000 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
PL2        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, cleanTOCSY Tmix=70msec



Current Data Parameters  
 NAME G13s072003  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20030723  
 Time 10.54

INSTRUM advance400  
 PROBRD 5 mm BBI 1H-2B  
 PULPROG cmladvpr2  
 TD 65536  
 SOLVENT CDCl3

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

TD 0.0000000 sec  
 D0 1.0000000 sec  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 d13 0.0000400 sec  
 D20 0.00006500 sec  
 INO 0.00020800 sec  
 L1 18  
 MCREST 0.00000000 sec  
 MCWRK 0.00999999 sec  
 STCNT 256

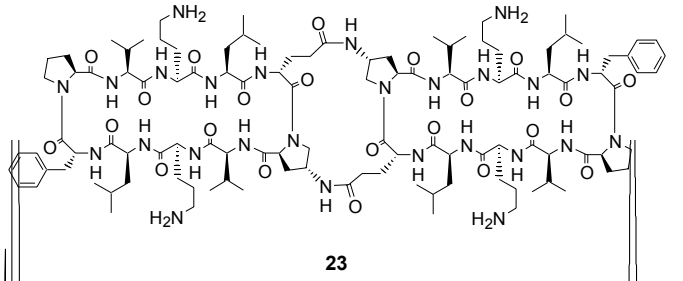
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 6.10 usec  
 P5 16.67 usec  
 P6 25.00 usec  
 P7 50.00 usec  
 P17 2500.00 usec  
 PL1 4.00 dB  
 PL9 58.51 dB  
 PL10 16.50 dB  
 SFO1 400.1318941 MHz

F1 - Acquisition Parameters  
 FIDRES 400.1319 MHz  
 FIDRES 9.390024 Hz  
 SW 12.015 ppm  
 ENMODE States-TPPI

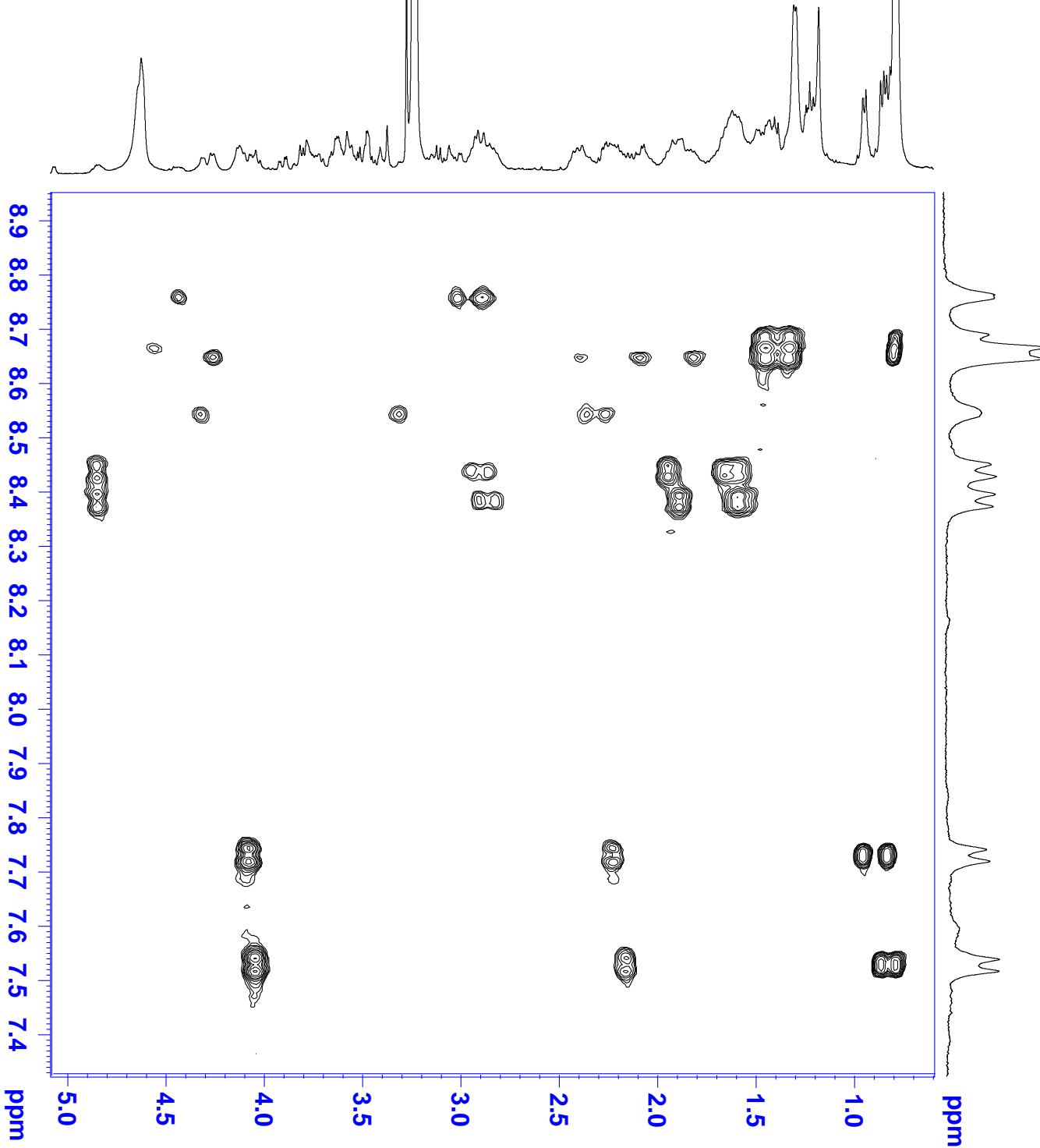
F2 - Processing parameters  
 SI 2048  
 SF 400.1300389 MHz  
 MDW QSIGN2  
 SSB 2.3 Hz  
 LB 0.00 Hz  
 GB 1.40  
 PC

F1 - Processing parameters  
 SI 1024  
 States-TPPI  
 SF 400.1300389 MHz  
 MDW QSIGN2  
 SSB 2.1 Hz  
 LB 0.00 Hz  
 GB

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



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Current Data Parameters  
 NAME G1j3072003  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20030723  
 Time 10.54

INSTRUM advance400  
 PROBRD 5 mm BBI 1H-2B  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3

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

TD 1.0000000 sec  
 D0 1.0000000 sec  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 d13 0.0000400 sec  
 D20 0.00006500 sec  
 INO 0.00020800 sec  
 L1 18  
 MCREST 0.0000000 sec  
 MCWRK 0.00999999 sec  
 STCNT 256

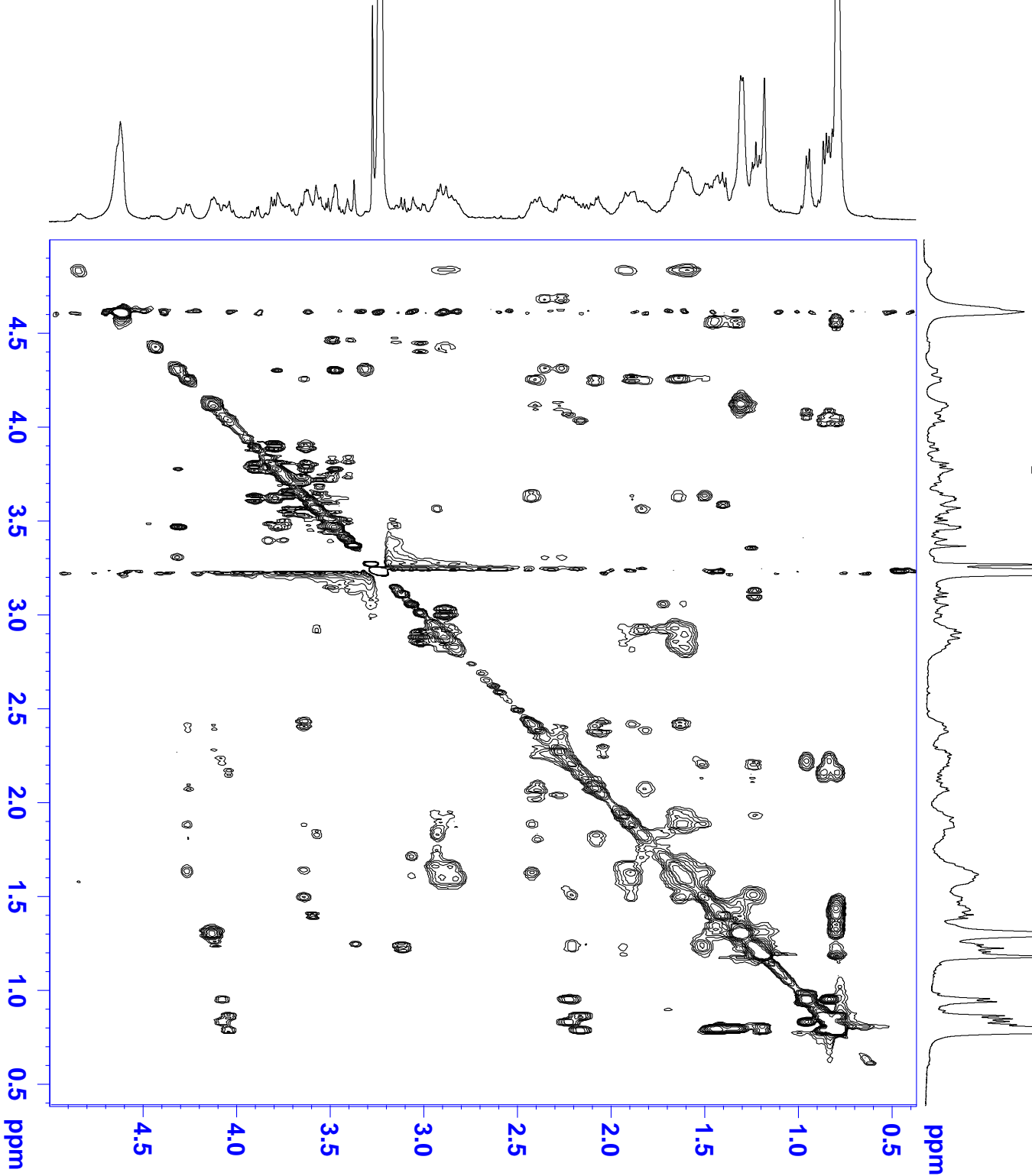
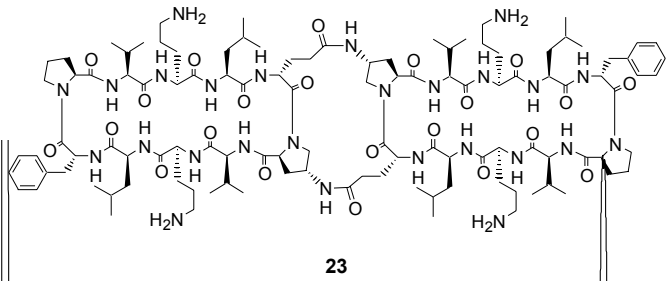
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 6.10 usec  
 P5 16.67 usec  
 P6 25.00 usec  
 P7 50.00 usec  
 P17 2500.00 usec  
 PL1 4.00 dB  
 PL9 58.51 dB  
 PL10 16.50 dB  
 SFO1 400.1318941 MHz

F1 - Acquisition Parameters  
 FID 512  
 SFO1 400.1319 MHz  
 FIDRES 9.390024 Hz  
 SW 12.015 ppm  
 FMODE States-TPPI

F2 - Processing parameters  
 SI 2048  
 SF 400.1300389 MHz  
 MDW QSIGN  
 SSB 2.3 Hz  
 GB 0.00 Hz  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 MC2 States-TPPI  
 SF 400.1300389 MHz  
 MDW QSIGN  
 SSB 2.1 Hz  
 GB 0.00 Hz

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



Current Data Parameters  
 NAME G13s072003  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20030723  
 Time 10.54  
 INSTRUM advance400  
 PROBRD 5 mm BBI 1H-2HS  
 PULPROG cmllepr2  
 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  
 TO 0.0000000 sec  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 d13 0.0000040 sec  
 D20 0.0000650 sec  
 INO 0.0002080 sec  
 I1 18  
 MCREST 0.0000000 sec  
 MCWRK 0.0099999 sec  
 SFLCNT 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  
 SP01 400.1318841 MHz

F1 - Acquisition Parameters  
 MD 512  
 SFO1 400.1319 MHz  
 FIDRES 9.390024 Hz  
 SW 12.015 ppm  
 FMODE States-TPPI

F2 - Processing parameters  
 SI 2048  
 SF 400.1300389 MHz  
 MDW QSIGN2  
 SSB 2.3 Hz  
 LB 0.00 Hz  
 GB 1.40

F1 - Processing parameters  
 SI 1024  
 MC2 States-TPPI  
 SF 400.1300389 MHz  
 MDW QSIGN  
 SSB 2.1 Hz  
 LB 0.00 Hz  
 GB 0