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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)

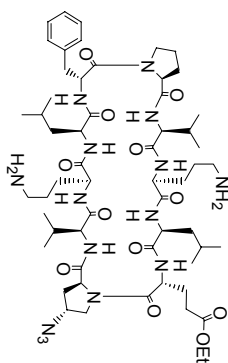
Compound <b>13</b>	<sup>1</sup> H	Page 2-5
Compound <b>13</b>	TOCSY	Page 6,7
Compound <b>14</b>	<sup>1</sup> H	Page 8-11
Compound <b>14</b>	TOCSY	Page 12,13
Compound <b>17</b>	<sup>1</sup> H	Page 14-17
Compound <b>18</b>	<sup>1</sup> H	Page 18-21
Compound <b>21</b>	<sup>1</sup> H	Page 22-25
Compound <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.

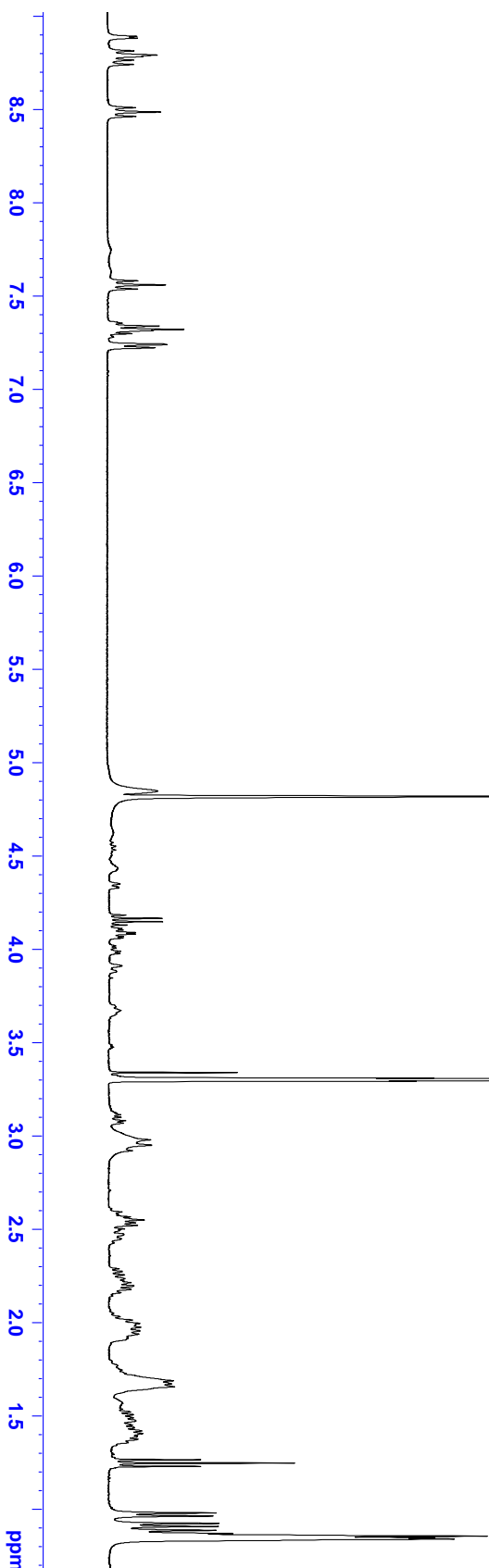
mwe1101 (epje 1) 298 K

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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PROCNO 1

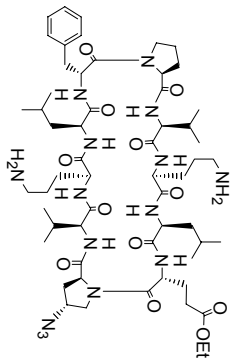
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TD 19228  
SOLVENT MeOD  
NS 64  
DS 0  
SWH 3720.238 Hz  
FIDRES 0.193480 Hz  
AQ 2.5842931 sec  
RG 161.3  
DW 134.400 usec  
DE 8.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
D12 0.00020000 sec  
D13 0.00000300 sec

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PL1 4.00 dB  
PL9 52.29 dB  
SFO1 400.1319405 MHz

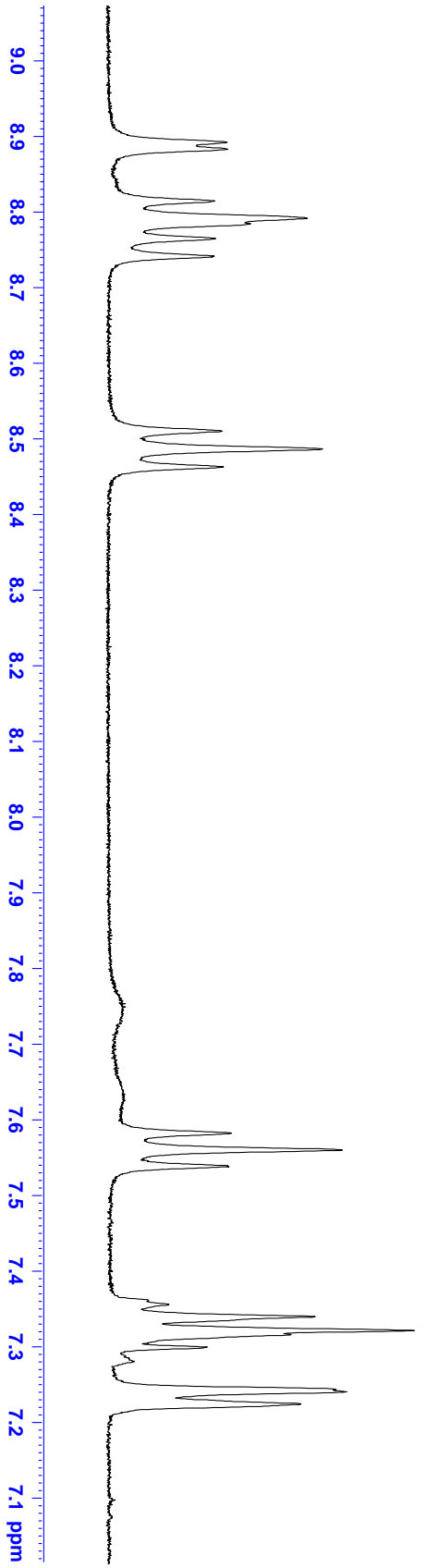
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SF 400.1300114 MHz  
WDW GM  
SSB 0  
LB -0.20 Hz  
GB 0.4  
PC 1.00

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



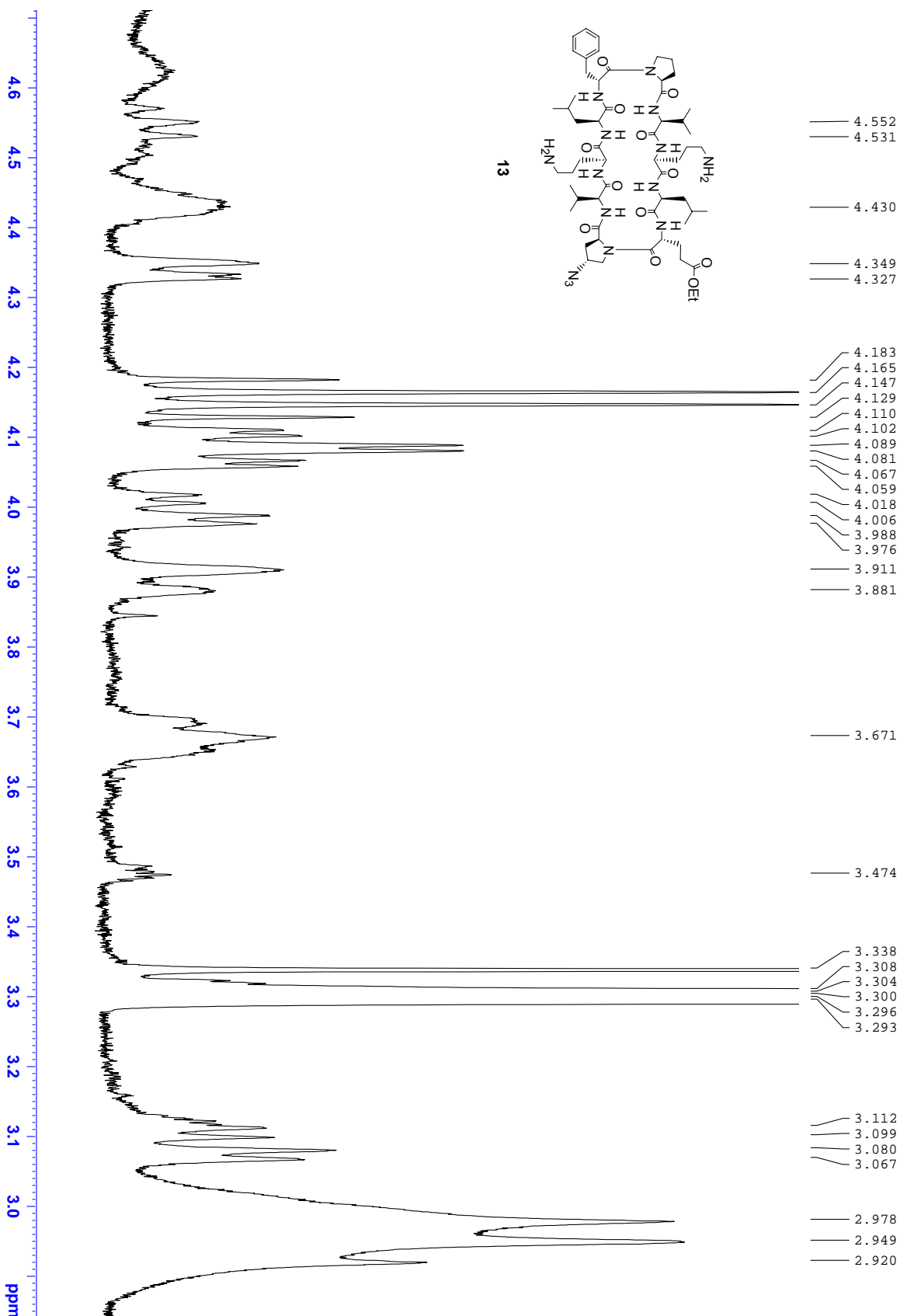
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Current Data Parameters
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PROCNO       1
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Time          18.03
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PROBHD       5 mm BBI 1H-BB
PULPROG      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
D1           8.50 usec
D12          1.00002000 sec
D13          0.00002300 sec
===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL9           52.29 dB
SFO1         400.1319405 MHz
F2 - Processing parameters
SI            32768
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WDW           GM
SSB           0
LB            -0.20 Hz
GB            0.4
PC            1.00
  
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mwe1101 (epje 1) 298 K

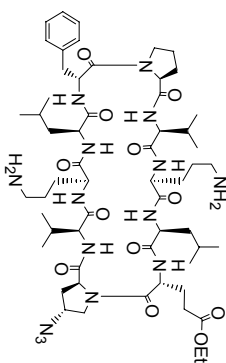


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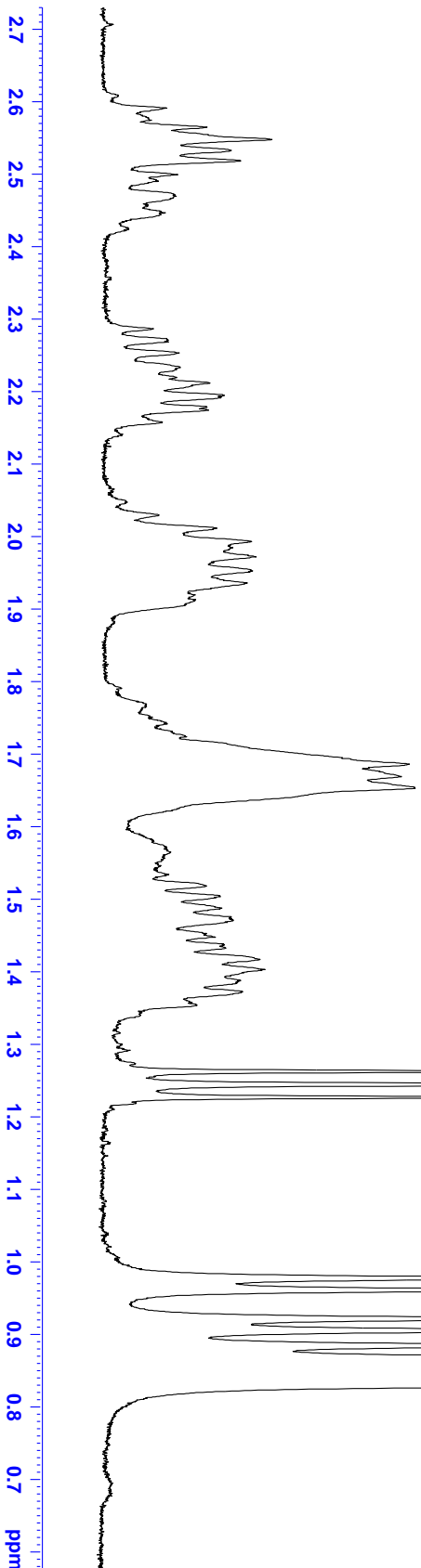
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EXPNO        9
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PULPROG     zgpg
TD           19228
SOLVENT     MeOD
NS           64
DS           0
SWH          3720.238 Hz
FIDRES       0.193480 Hz
AQ           2.5842931 sec
RG           161.3
DW           134.400 usec
DE           8.50 usec
TE           300.0 K
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
  
```

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	1.653	1.471	1.227	0.905
2.519	2.212	1.953	1.653	1.448	1.227	0.884
2.500	2.195	1.937	1.653	1.433	1.227	0.868
2.470	2.175	1.937	1.653	1.417	1.227	0.853
2.447	2.159	1.937	1.653	1.403	1.227	0.844
	2.159	1.937	1.653	1.373	1.227	0.838



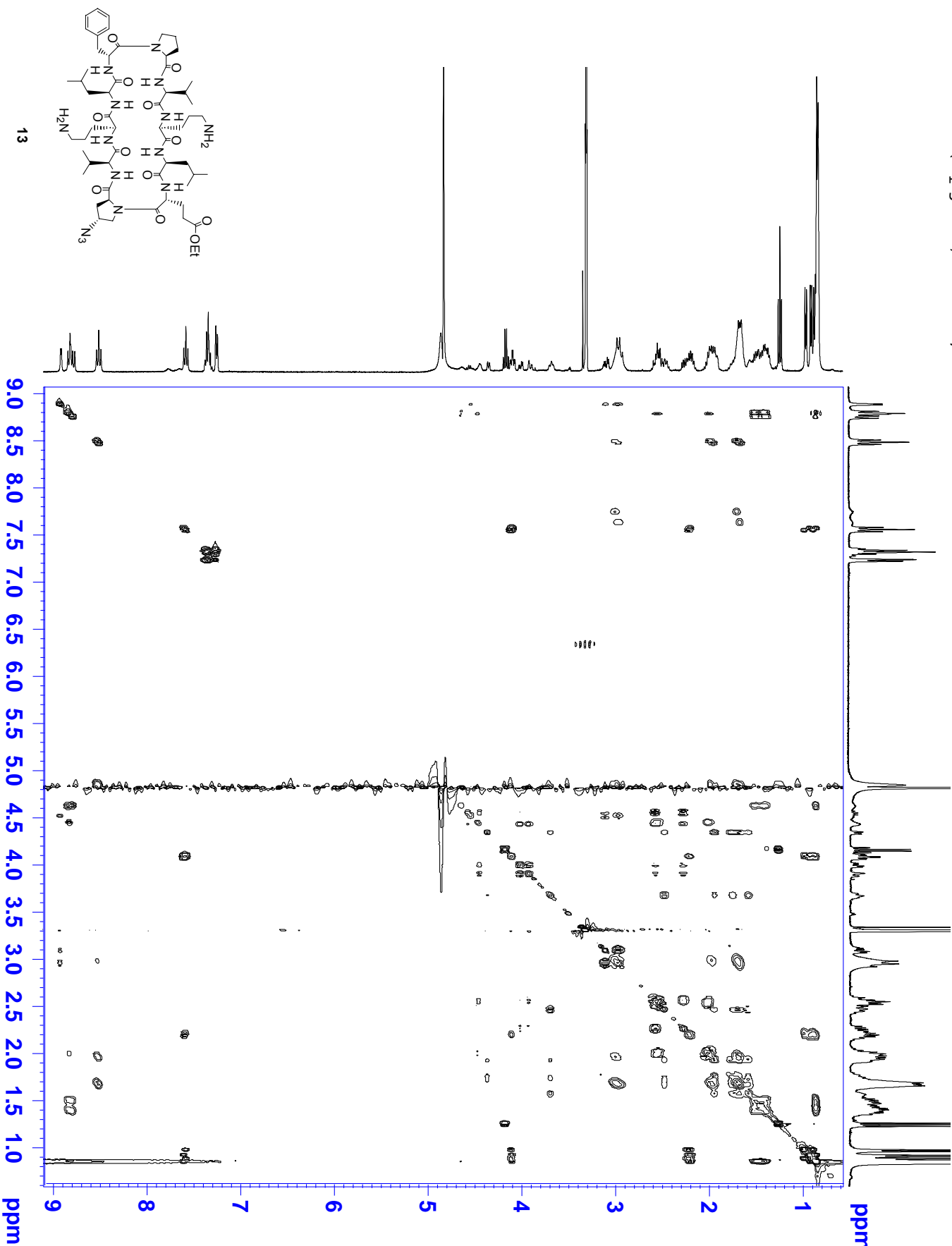
13



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Current Data 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  
 SFO2 400.1319 MHz  
 FIDRES 7.266090 Hz  
 SW 9.298 ppm  
 FMODE States-TPPI

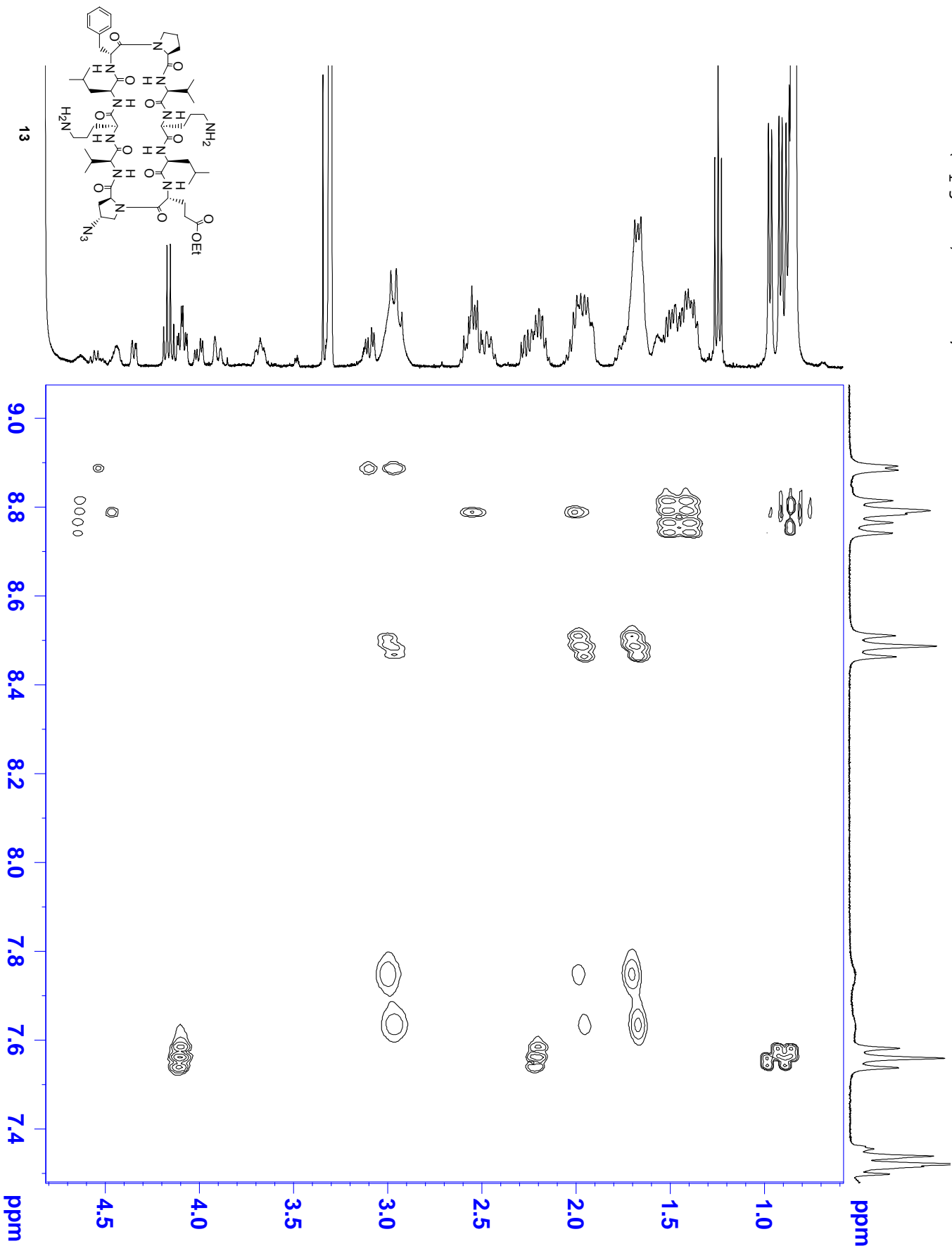
F2 - Processing Parameters

SI 2048  
 SF 400.1300114 MHz  
 WDW QSI  
 SSB 2.3 Hz  
 LB 0.00 Hz  
 GB 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 avance400  
 PROBRD 5 mm BBI JH-25  
 PULPROG zgpg30

TD 65536  
 SOLVENT CDCl3

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 1.0000000 sec  
 D0 1.0000000 sec  
 d11 0.0300000 sec

d12 0.0000200 sec  
 d13 0.0000400 sec  
 D20 0.0006500 sec

IN0 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 400.131988 MHz  
 F1 - Acquisition Parameters  
 MD 512  
 SFO1 400.1319 MHz

FIDRES 7.266090 Hz  
 SW 9.298 ppm  
 F2 - Processing Parameters  
 SI 2048  
 SF 400.1300114 MHz

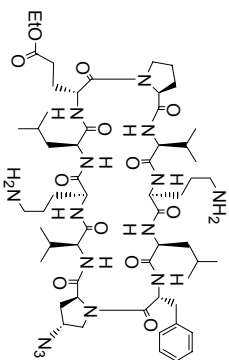
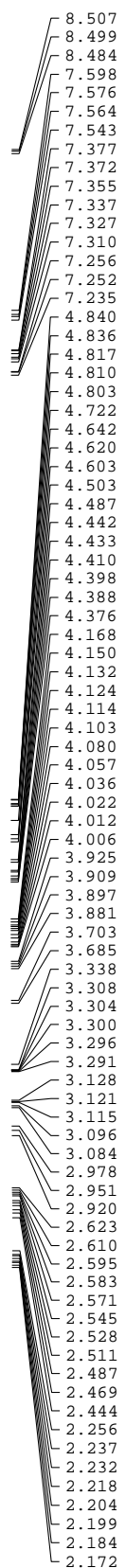
WDW QSINE  
 SSB 2.3 Hz  
 GB 0.00 Hz

PC 1.00  
 F1 - Processing Parameters  
 SI 1024  
 States-TPPI 1024

MC2 400.1300064 MHz  
 SF QSINE  
 MDW 2.1 Hz

SSB 0.00 Hz  
 LB 0  
 GB 0



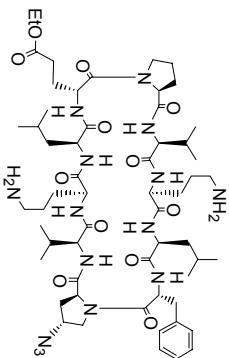


Current Data Parameters  
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 EXPRNO 6  
 PROCNO 1  
 P2 - Acquisition Parameters  
 Date\_ 20030405  
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 PROBRD 5 mm BBI 1H-BB  
 PULPROG zgpr  
 TD 19228  
 SOLVENT MeOD  
 NS 64  
 DS 0  
 SMH 4807.692 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 =====  
 NUCL 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

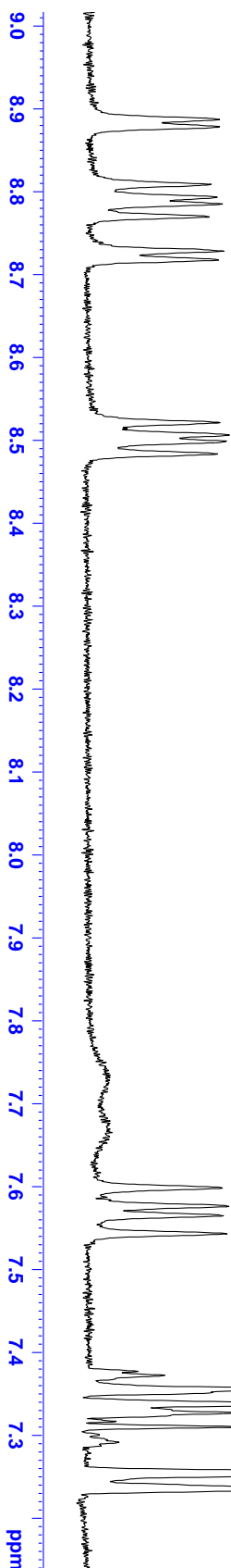
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8.879  
8.809  
8.793  
8.785  
8.770  
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8.522  
8.507  
8.499  
8.484

7.598  
7.576  
7.564  
7.543

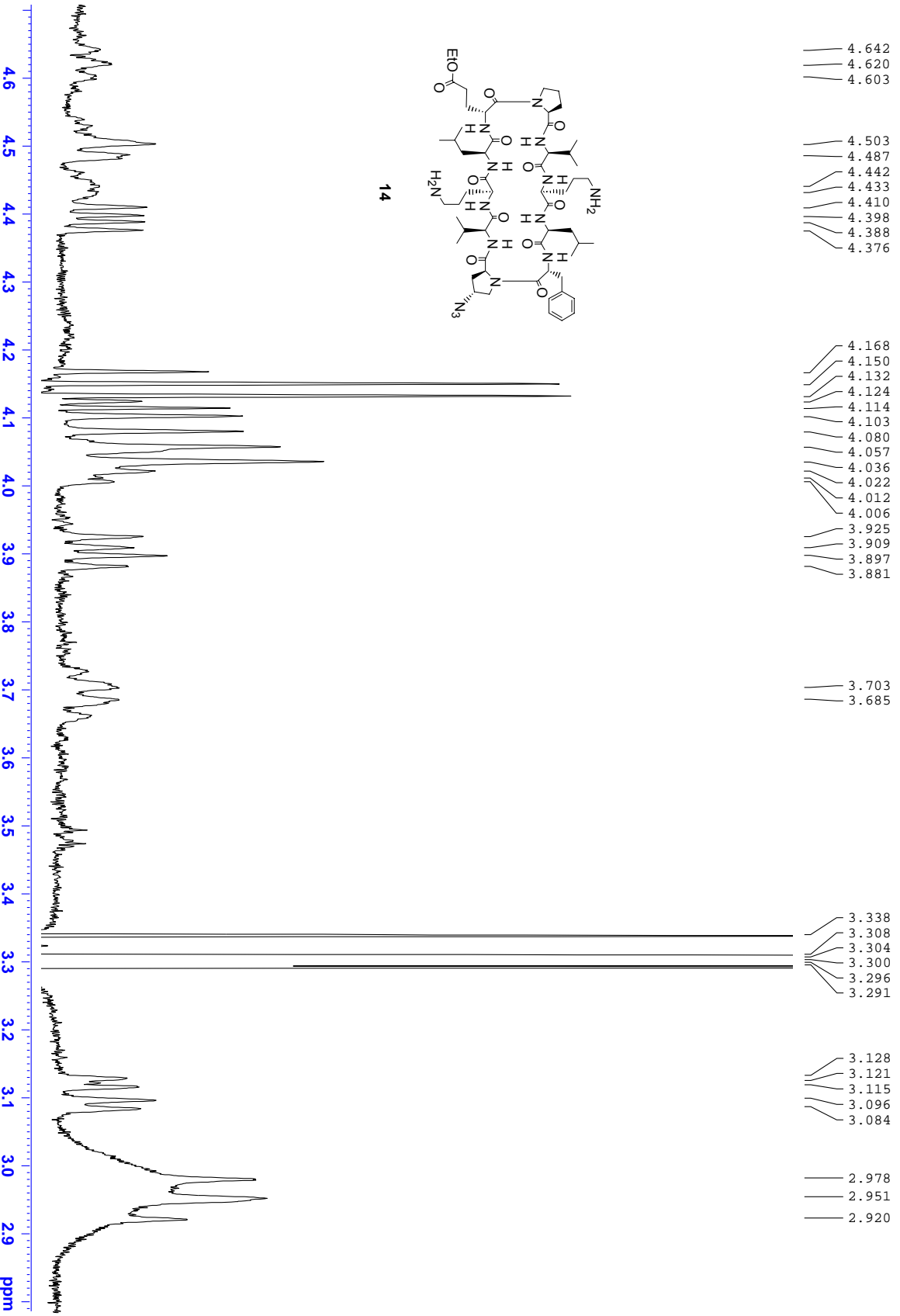
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7.355  
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7.327  
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7.256  
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7.235



14

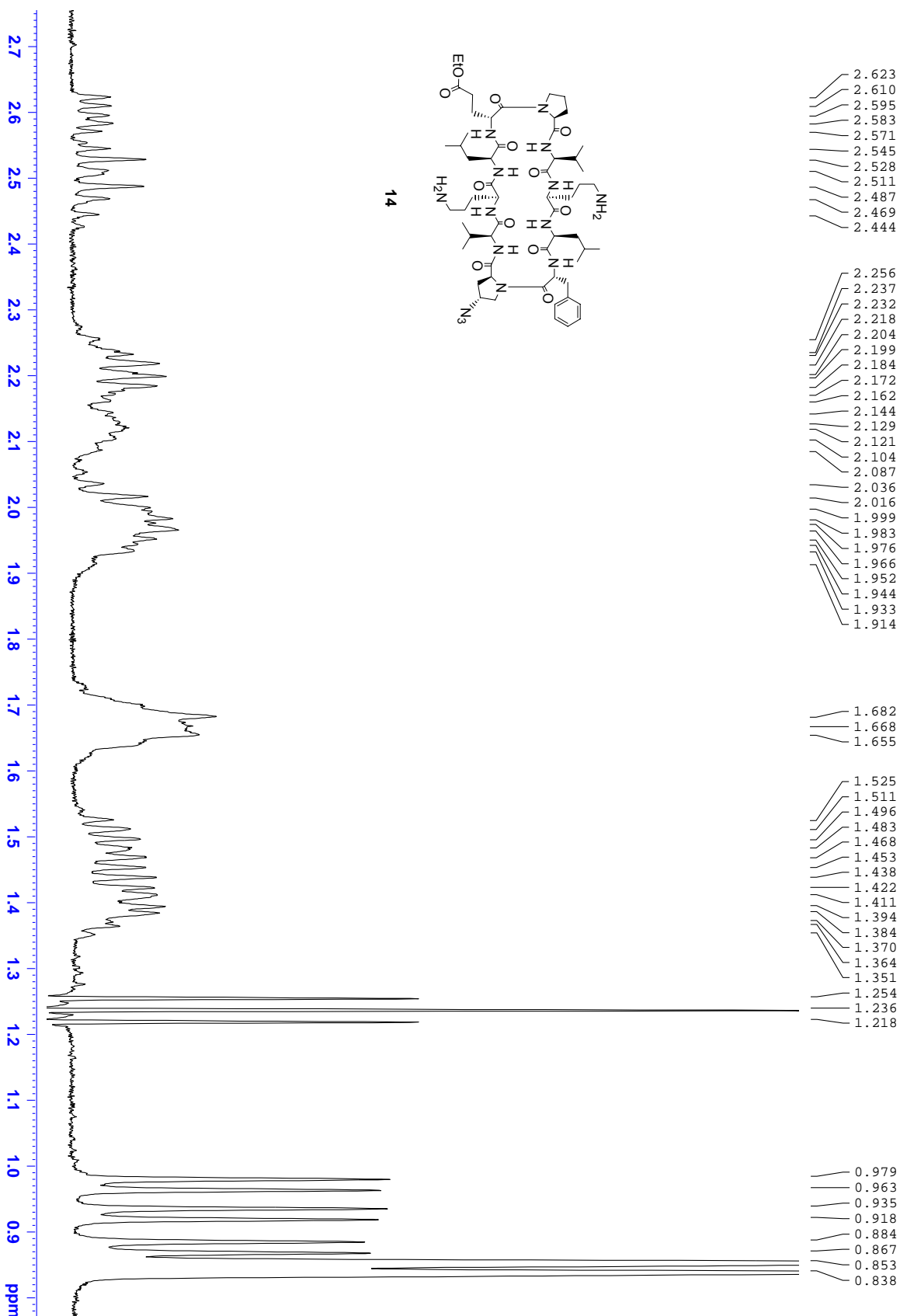


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 PULPROG zgpg  
 TD 19228  
 SOLVENT MeOD  
 NS 64  
 DS 0  
 SWH 4807.692 Hz  
 FIDRES 0.250036 Hz  
 AQ 1.9997621 sec  
 RG 456.1  
 DW 104.000 usec  
 DE 8.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 D12 0.0000000 sec  
 D13 0.0000000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.30 usec  
 PL1 4.00 dB  
 PL9 52.29 dB  
 SFO1 400.1319379 MHz  
 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 avanca400  
 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  
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 SF 400.1300115 MHz  
 WDW GM  
 SSB 0  
 LB -1.61 Hz  
 GB 0.4  
 PC 1.00

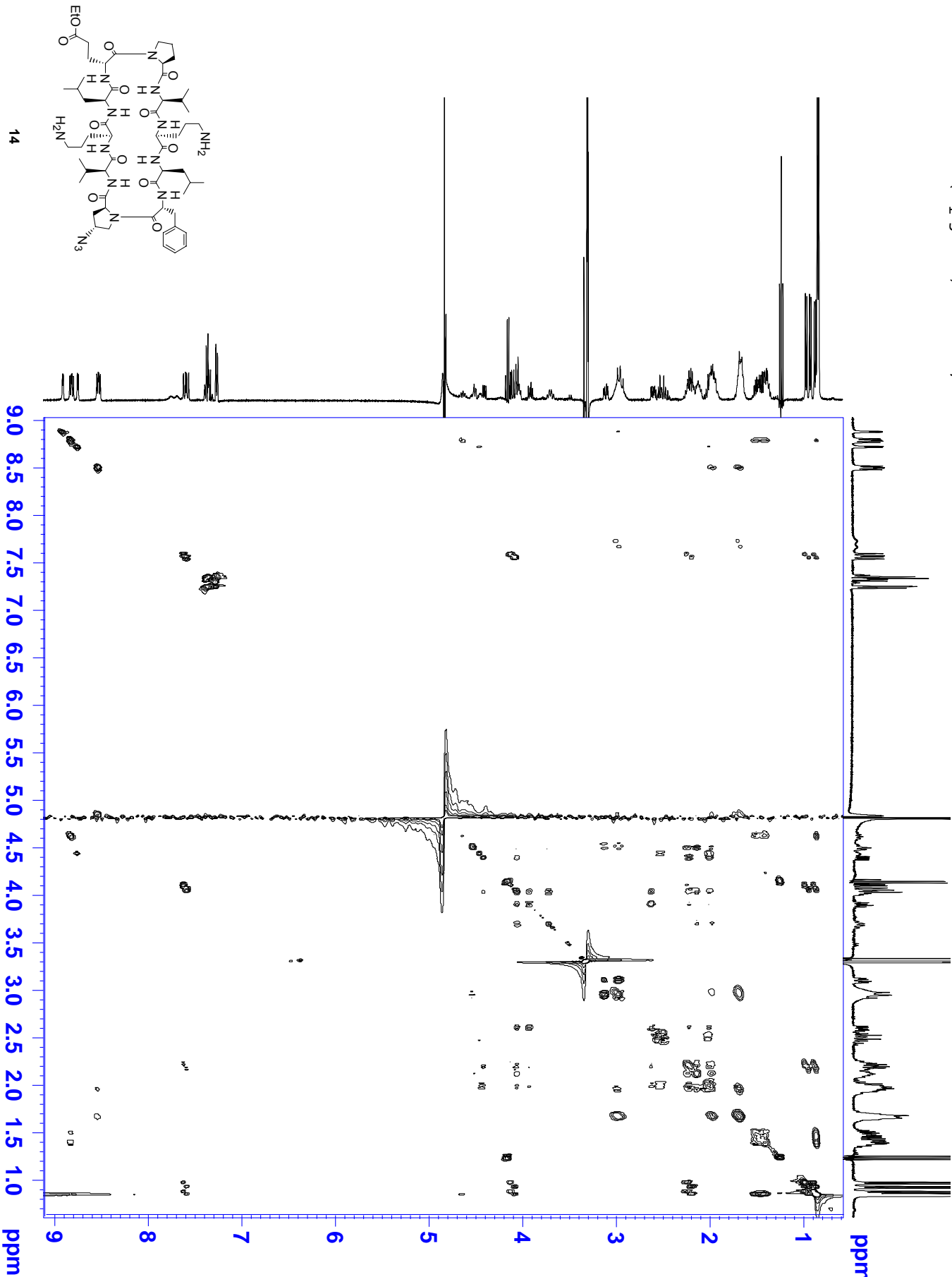
14



- 2.623
- 2.610
- 2.595
- 2.583
- 2.571
- 2.545
- 2.528
- 2.511
- 2.487
- 2.469
- 2.444
  
- 2.256
- 2.237
- 2.232
- 2.218
- 2.204
- 2.199
- 2.184
- 2.172
- 2.162
- 2.144
- 2.129
- 2.121
- 2.104
- 2.087
- 2.036
- 2.016
- 1.999
- 1.983
- 1.976
- 1.966
- 1.952
- 1.944
- 1.933
- 1.914
  
- 1.682
- 1.668
- 1.655
  
- 1.525
- 1.511
- 1.496
- 1.483
- 1.468
- 1.453
- 1.438
- 1.422
- 1.411
- 1.394
- 1.384
- 1.370
- 1.364
- 1.351
- 1.254
- 1.236
- 1.218
  
- 0.979
- 0.963
- 0.935
- 0.918
- 0.884
- 0.867
- 0.853
- 0.838

Current Data Parameters  
 NAME g1j5042003  
 EXPNO 6  
 PROCNO 1  
 F2 - Acquisition Parameters:  
 Date\_ 20030405  
 Time 15:21  
 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

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



Current Data Parameters  
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 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20030405  
 Time 15.39  
 INSTRUM advance400  
 PROBRD 5 mm BBI JH-25  
 PULPROG zgpg30  
 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  
 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 52.29 dB  
 PL10 16.50 dB  
 SFO1 400.131975 MHz

F1 - Acquisition Parameters

NUC0 1H  
 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 QSIGN  
 SSB 2.3 Hz  
 LB 0.00 Hz  
 GB 1.00

F1 - Processing parameters

SI 1024  
 States-TPPI  
 MC2 400.1300065 MHz  
 SF QSIGN  
 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 avance400  
PROBHD 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 1000000  
D1 1.0000000 sec  
d11 0.0300000 sec  
d12 0.0000200 sec  
d13 0.0000400 sec  
D20 0.0006500 sec  
D21 0.00026880 sec

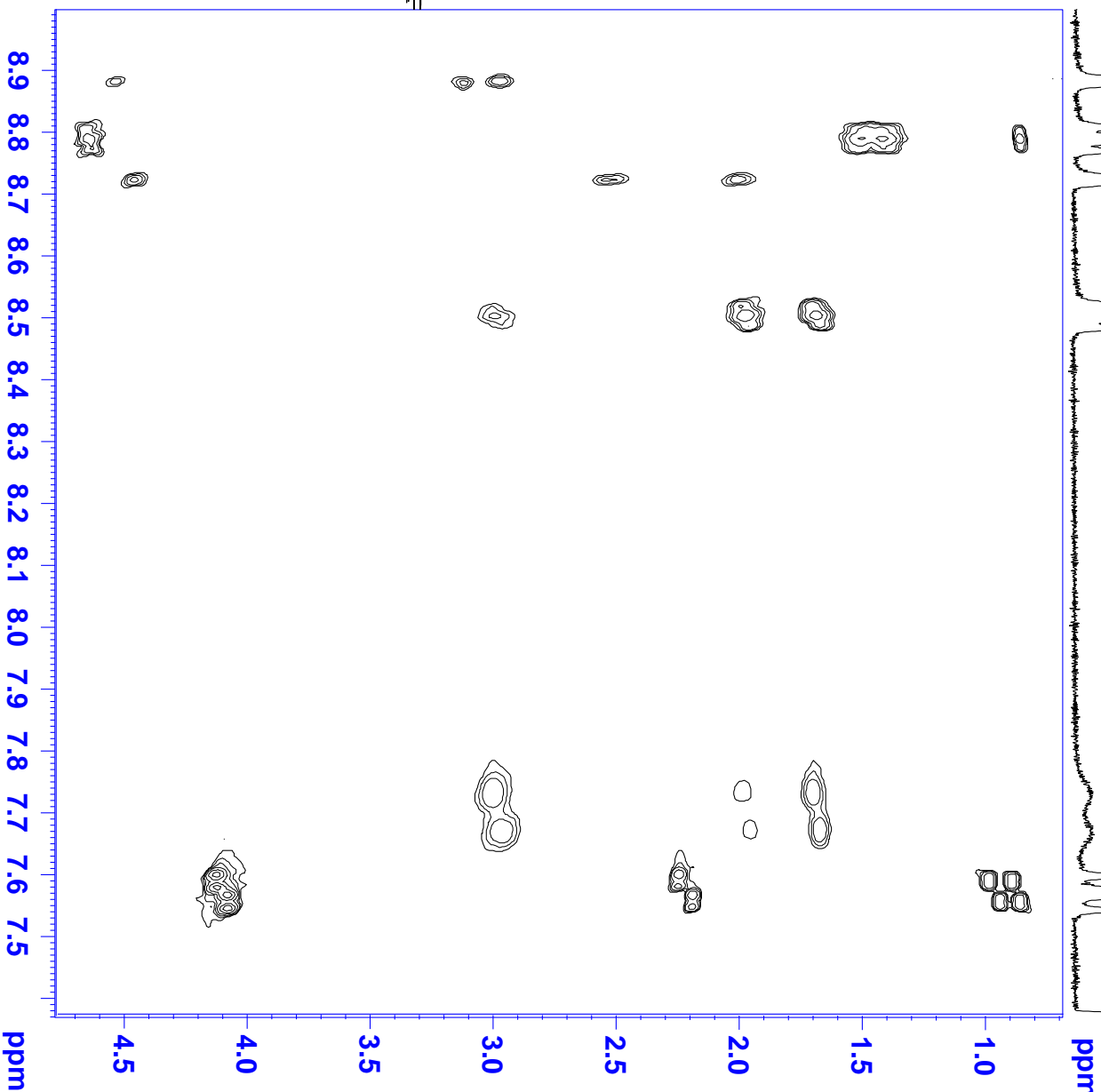
LL 18  
MCREST 0.0000000 sec  
MCWRK 0.00999999 sec  
STICNT 256

===== CHANNEL f1 =====  
NUC1 <sup>1</sup>H  
P 6.10 usec  
P5 16.67 usec  
P6 25.00 usec  
P7 50.00 usec  
P17 2500.00 usec  
P11 4.00 dB  
P19 52.29 dB  
P10 16.50 dB  
SFO1 400.131975 MHz

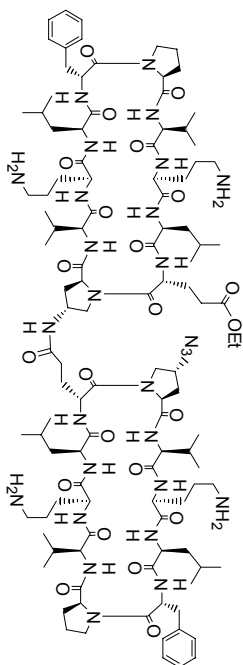
F1 - Acquisition Parameters  
NUC2 <sup>1</sup>H  
SFO1 400.1319 MHz  
FIDRES 7.266090 Hz  
SW 9.298 ppm  
FMODE States-TFPI

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

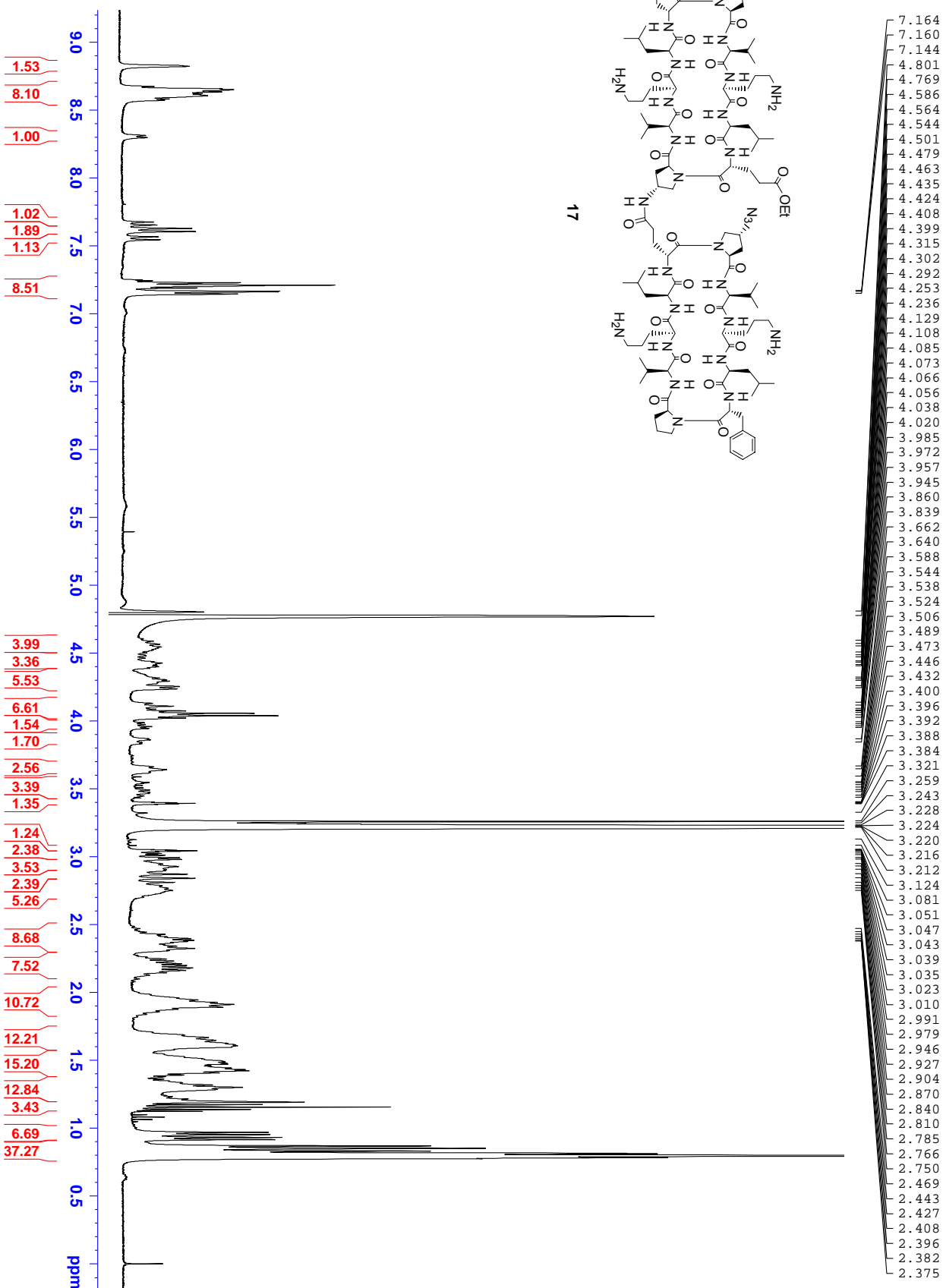
F1 - Processing parameters  
SI 1024  
MC2 States-TFPI  
SF 400.1300065 MHz  
WDW QSI  
SSB 2.1 Hz  
LB 0.00 Hz  
GB 0



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



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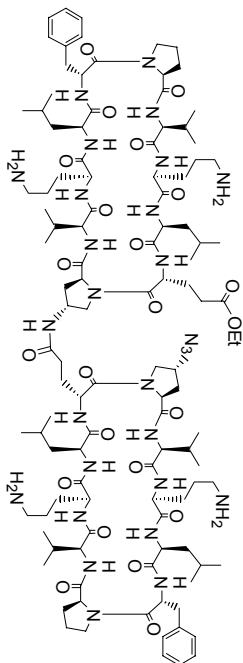
7.164
7.160
7.144
4.801
4.769
4.586
4.564
4.544
4.501
4.479
4.463
4.435
4.424
4.408
4.399
4.315
4.302
4.292
4.253
4.236
4.129
4.108
4.085
4.073
4.066
4.056
4.038
4.020
3.985
3.972
3.957
3.945
3.860
3.839
3.662
3.640
3.588
3.544
3.538
3.524
3.506
3.489
3.473
3.446
3.432
3.400
3.396
3.392
3.388
3.384
3.321
3.259
3.243
3.228
3.224
3.220
3.216
3.212
3.124
3.081
3.051
3.047
3.043
3.039
3.035
3.023
3.010
2.991
2.979
2.946
2.927
2.904
2.870
2.840
2.810
2.785
2.766
2.750
2.469
2.443
2.427
2.408
2.396
2.382
2.375

```

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         2.26
TE         298.0 K
D1        1.00002000 sec
d12       0.00000000 sec
MCOREST   0.00000000 sec
MCMARK    0.01500000 sec

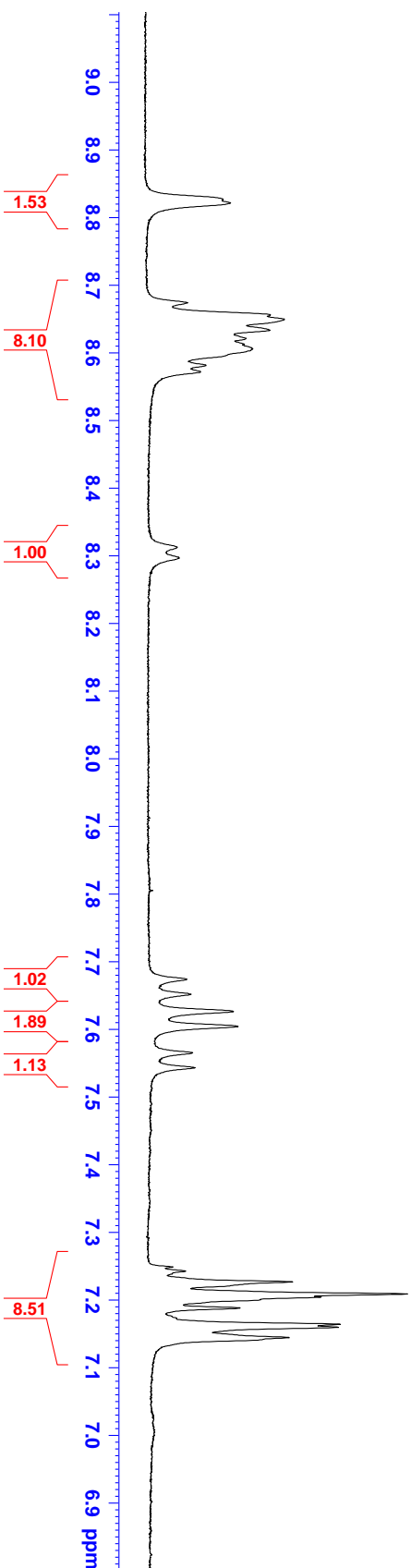
===== CHANNEL f1 =====
NUC1      1H
P1        7.30 usec
PL1       4.00 dB
PL19      58.54 dB
SFO1     400.1319575 MHz

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



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

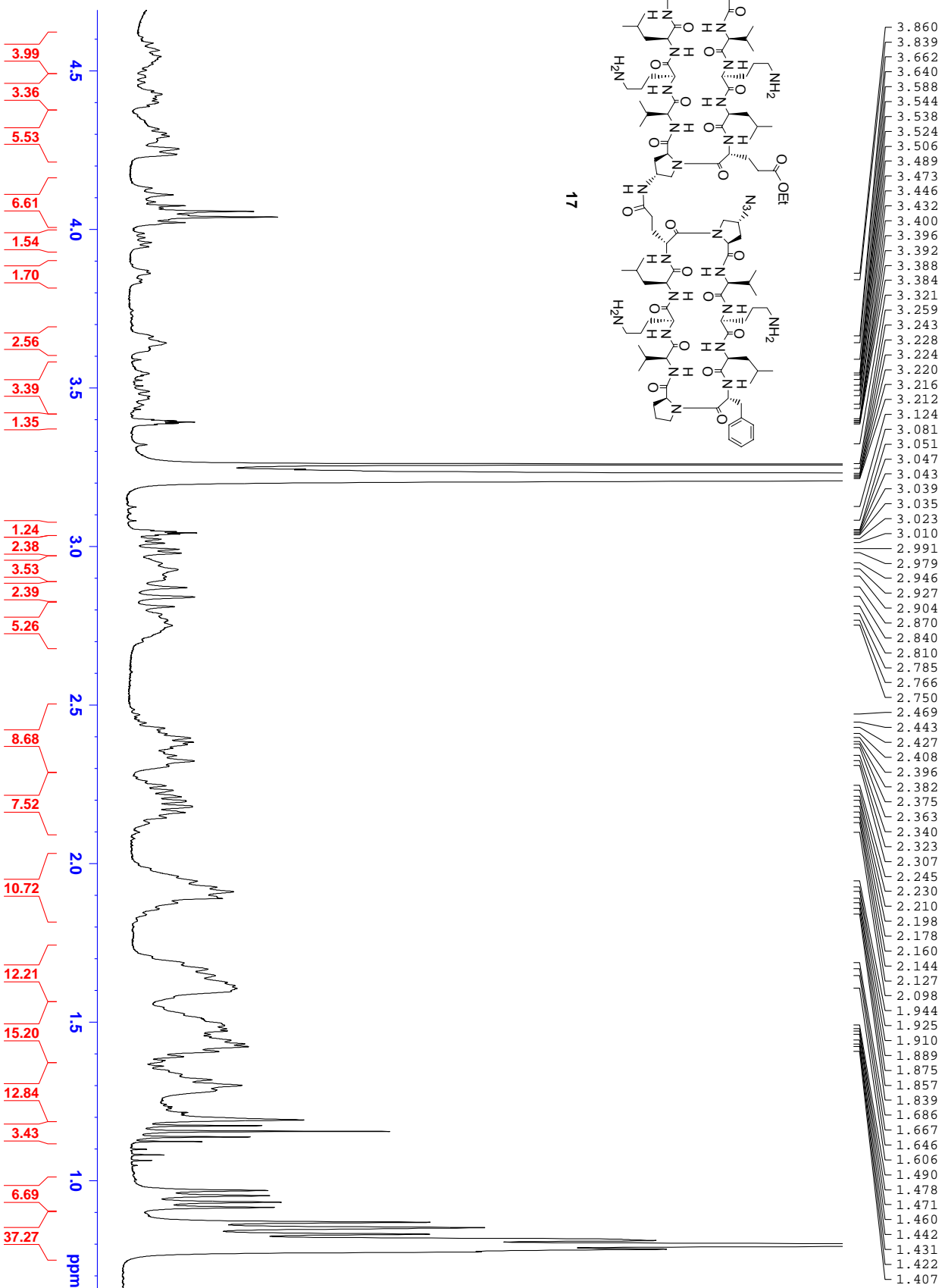
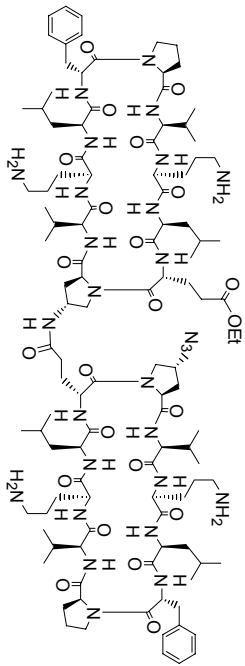


```

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            1024
DS            0
SWH           4807.692 Hz
AQ            0.250036 Hz
RG            1.9997621 sec
RG            104.000 usec
DE            8.50 usec
DE            28.00 K
DI            1.0000200 sec
d12           0.0000000 sec
MCPRST       0.00000000
MCMRFX       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
    
```



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



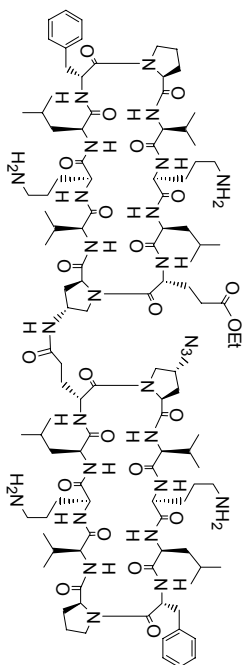
```

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 K
D1           1.00000000 sec
d12          0.00000000 sec
MCWRES1     0.00000000 sec
MCWRES2     0.01500000 sec

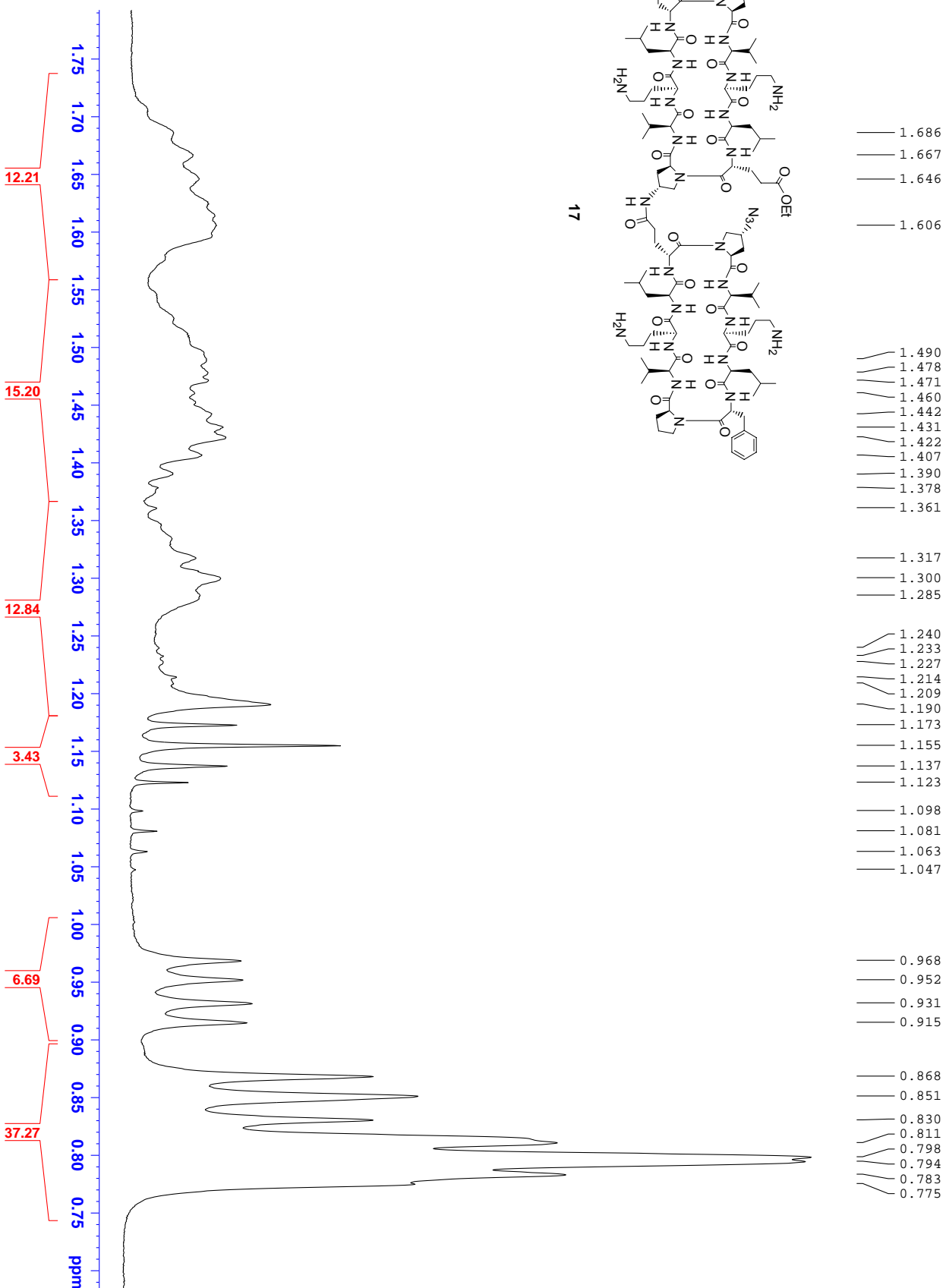
===== CHANNEL f1 =====
NUC1         1H
P1           7.30 usec
PL1         4.00 dB
PL2         58.54 dB
SF01        400.1319575 MHz

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

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



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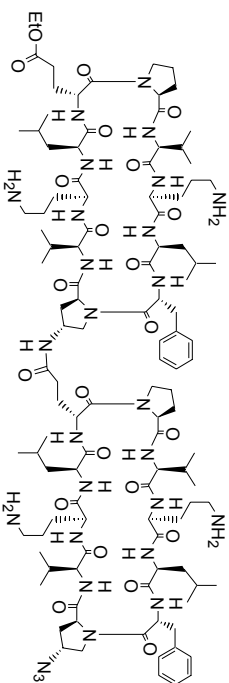


```

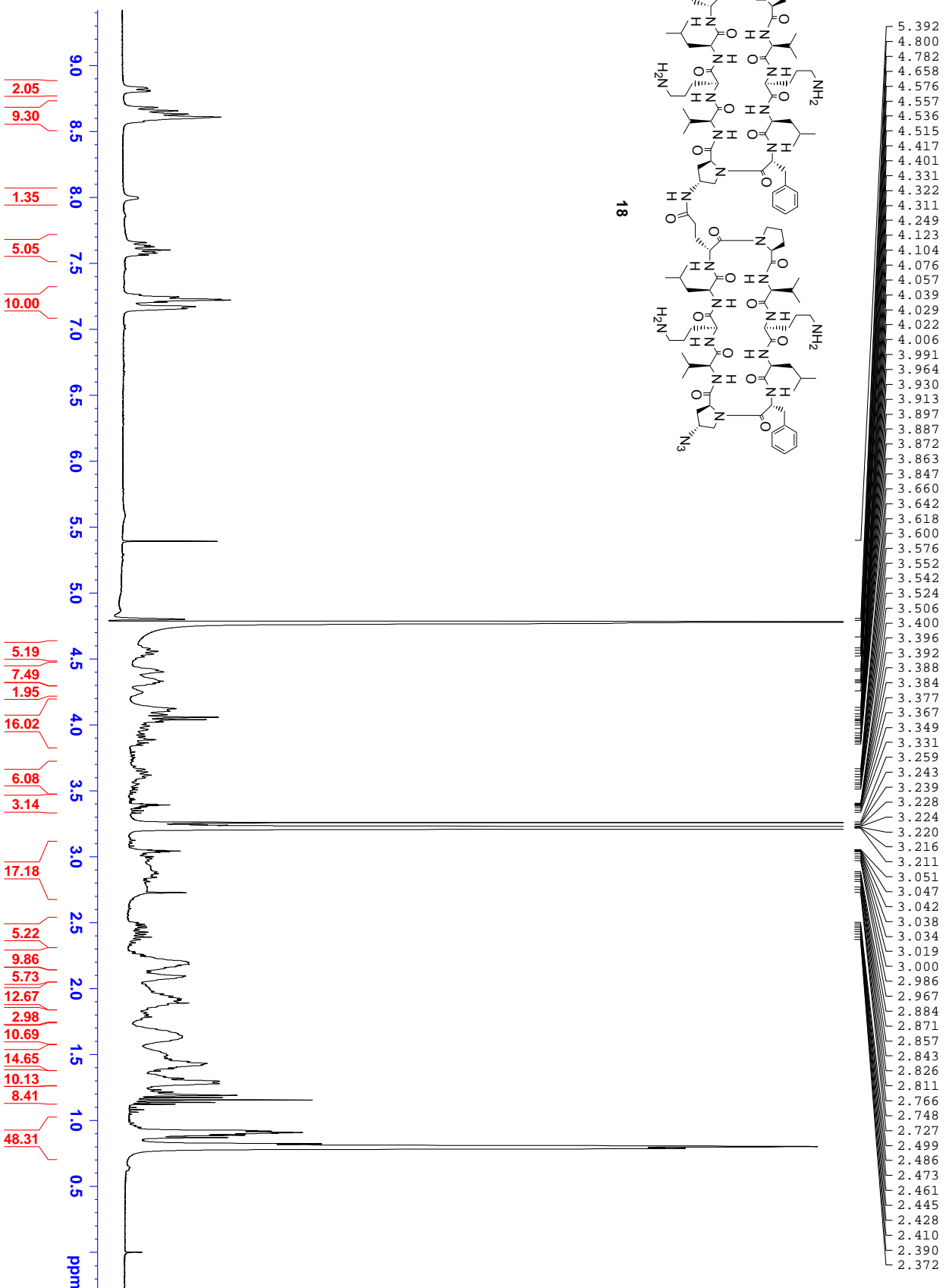
Current Data Parameters
NAME          G15092004
EXPNO        1
PROCNO       1
F2 - Acquisition Parameters
Date_        20040915
Time         10.01
INSTRUM      avance400
PROBHD       5 mm BBI 1H-BB
PULPROG      zgpg
TD           19228
SOLVENT      H2O
NS           1024
DS           0
SWH          4807.692 Hz
FIDRES       0.250036 Hz
AQ           1.9997621 sec
RG           256
DW           104.000 usec
DE           8.90 usec
TE           298.0 K
D1           1.00000000 sec
d12          0.00000000 sec
MCOREST     0.00000000 sec
MCURK       0.01500000 sec

===== CHANNEL f1 =====
NUC1          1H
P1           7.30 usec
PL1          4.00 dB
PL2
PL3
PL4
PL5
PL6
PL7
PL8
PL9
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
  
```



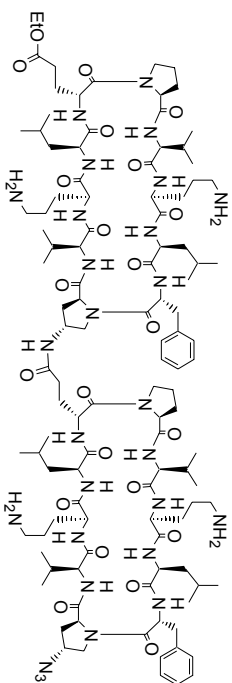
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```

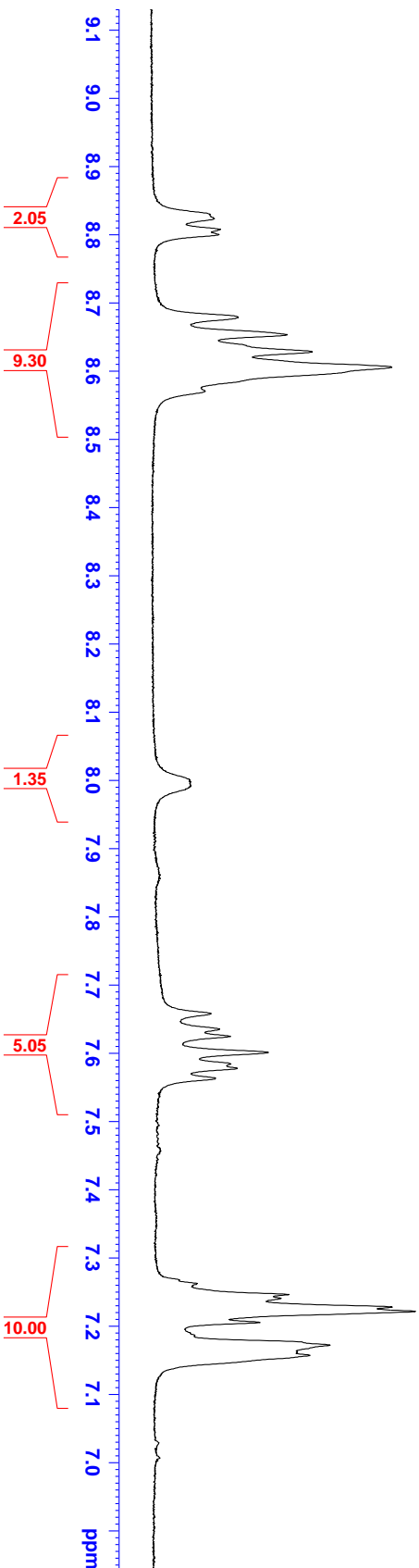
Current Data Parameters
NAME          G1J5092004
EXPNO         4
PROCNO       1
F2 - Acquisition Parameters
Date_         20040915
Time_        13.00
INSTRUM      advanced400
PROBHD       5 mm BBI 1H-BB
PULPROG      zgpr
TD           19228
SOLVENT      MeOD
NS           1024
DS           0
SWH          4807.692 Hz
FIDRES       0.250036 Hz
AQ           1.9997621 sec
RG           256
DE           104.000 usec
TE           28.50 usec
DE           28.50 usec
D1           1.00002000 sec
d12          0.00002000 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	



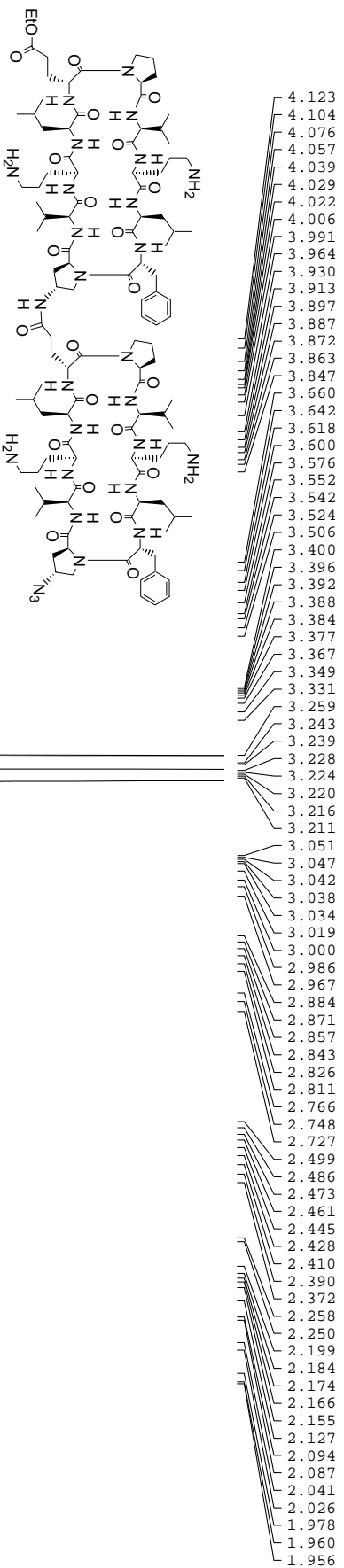
```

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
FIDRES     0.250036 Hz
AQ         1.9997621 sec
RG         286
DE         104.000 use
TE         8.50 use
DE         288.0 K
D1         1.0000000 sec
d12        0.0000000 sec
MCPRST     0.0000000
MCMRST     0.01500000 sec

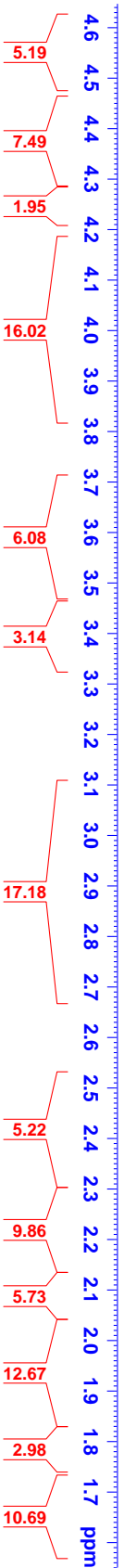
===== CHANNEL f1 =====
NUC1        1H
P1          7.30 use
PL1         4.00 dB
PL2         60.89 dB
PL9
SF01        400.1319575 MHz

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



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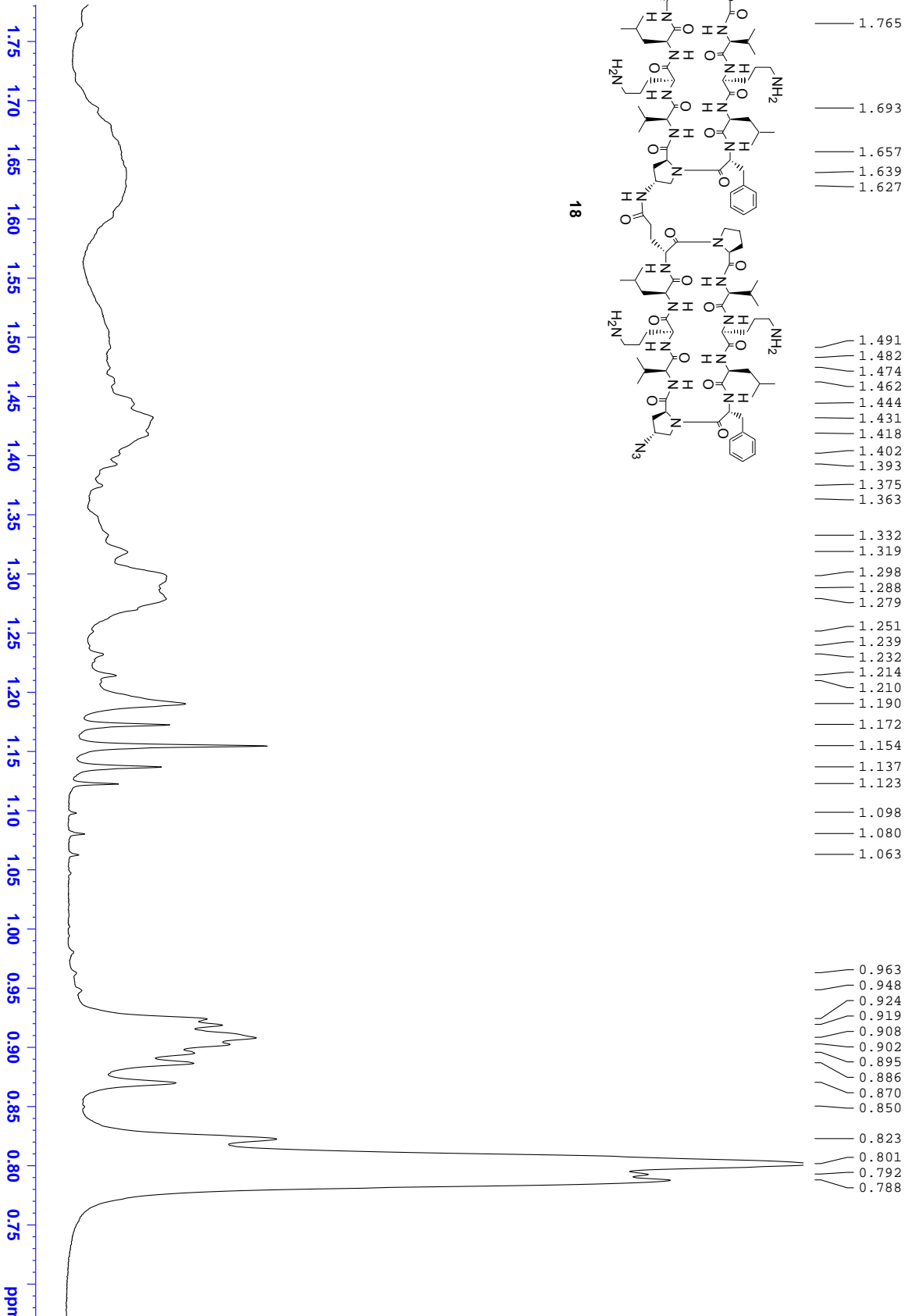
```

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
AQ            0.250036 Hz
RG            256
DE            104.000 usec
TE            28.90 K
D1            1.00002000 sec
d12           0.00002000 sec
MCWRESR      0.00000000 sec
MCWRESR      0.01500000 sec

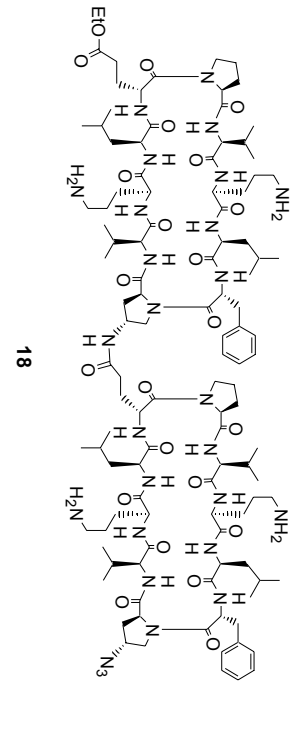
===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL2           60.89 dB
SF01          400.1319575 MHz

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	1.693	1.657	1.639	1.627	1.491	1.482	1.474	1.462	1.444	1.431	1.418	1.402	1.393	1.375	1.363	1.332	1.319	1.298	1.288	1.279	1.251	1.239	1.232	1.214	1.210	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
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------



Current Data Parameters

NAME	GIJ5092004
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20040915
Time	13.00
INSTRUM	avance400
PROBHD	5 mm BBI 1H-5B
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
DE	1.0000200 sec
d12	0.0000200 sec
MCOREST	0.0000000 sec
MCWRK	0.01500000 sec

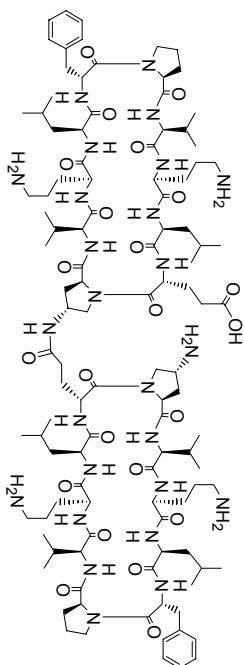
==== CHANNEL f1 =====

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

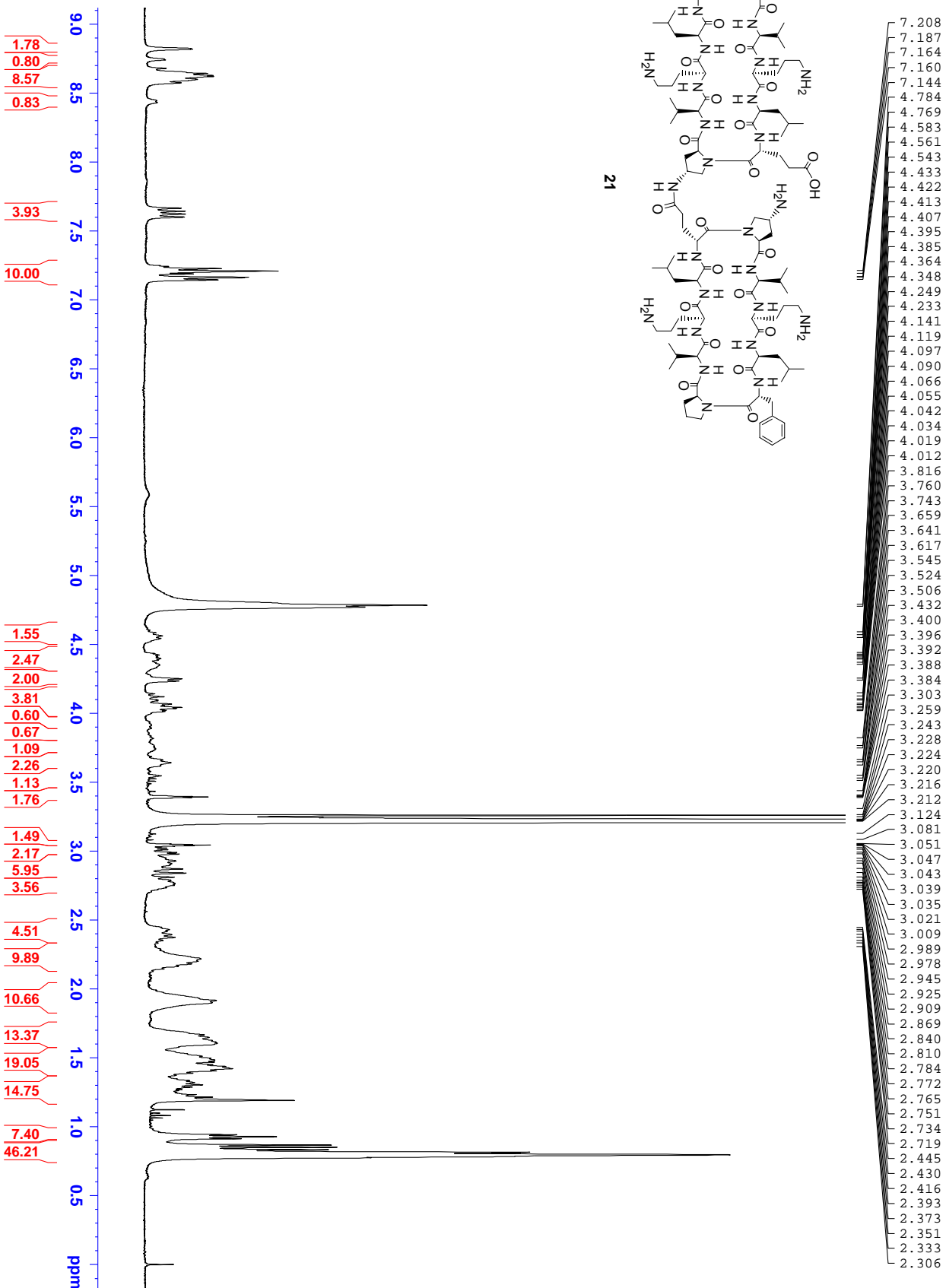
F2 - Processing parameters

SI	32768
SF	400.1300436 MHz
WDW	EM
SSB	0
L8	0.00 Hz
L9	0
PC	1.00

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

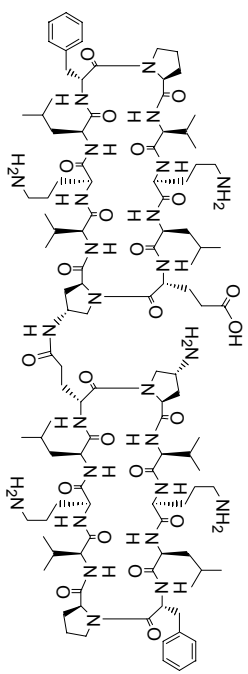


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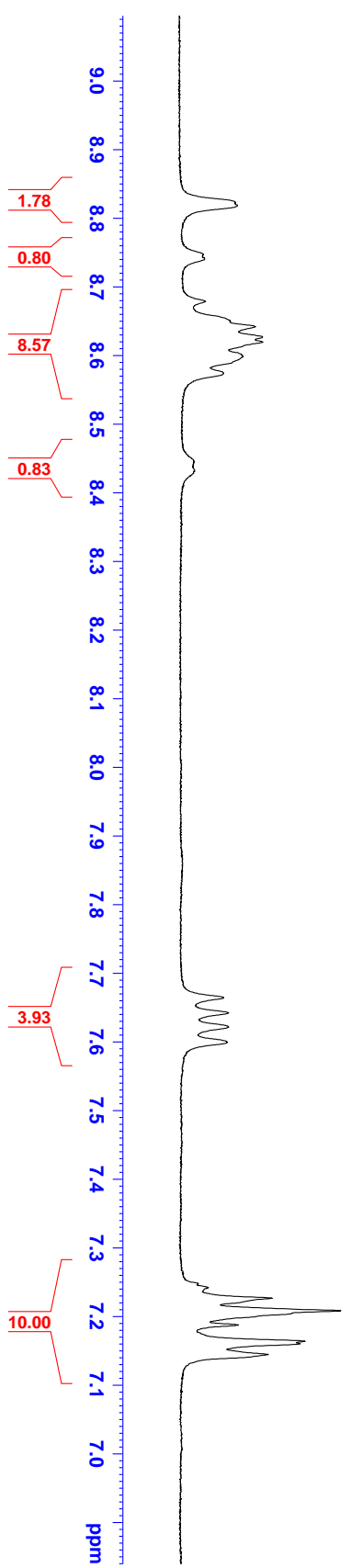
Current Data Parameters  
 NAME G13692004  
 EXPNO 3  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20040915  
 Time 11.43  
 INSTRUM avance400  
 PROBD 5 mm BBI 1H-BB  
 PULPROG zgpg  
 TD 19228  
 SOLVENT MeOD  
 NS 1024  
 DS 0  
 SWH 4807.692 Hz  
 FIDRES 0.250036 Hz  
 AQ 1.9997621 sec  
 RG 256  
 DW 104.000 usec  
 DE 8.50 usec  
 TE 298.0 K  
 DI 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  
 PC 1.00

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



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	

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```

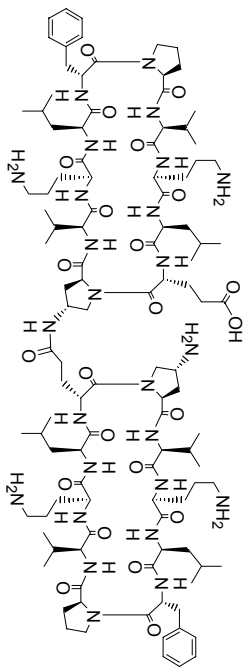
Current Data Parameters
NAME          G1J5092004
EXPNO         3
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time          11.43
INSTRUM       avance400
PROBHD        5 mm BBI 1H-BB
PULPROG       zgpr
TD            19228
SOLVENT       MeOD
NS            1024
DS            0
SWH           4807.692 Hz
FIDRES       0.250036 Hz
AQ           1.9997621 sec
RG           286
DE           104.000 usec
DM           8.50 usec
PE           28.10
DE           1.0000200 sec
d12          0.0000200 sec
MCPRST       0.00000000
MCMRK        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
  
```

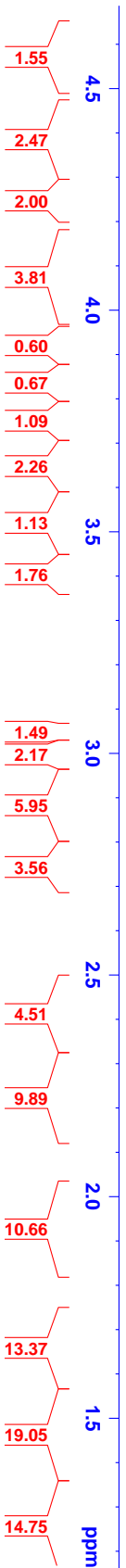


mwe1501 - dimer NH2/COOH turn 1H, bbi-av400



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4.233
4.141
4.119
4.097
4.090
4.066
4.055
4.042
4.034
4.019
4.012
3.816
3.760
3.743
3.659
3.641
3.617
3.545
3.524
3.506
3.432
3.400
3.396
3.392
3.388
3.384
3.303
3.259
3.243
3.228
3.224
3.220
3.216
3.212
3.124
3.081
3.051
3.047
3.043
3.039
3.035
3.021
3.009
2.989
2.978
2.945
2.925
2.909
2.869
2.840
2.810
2.784
2.772
2.765
2.751
2.734
2.719
2.445
2.430
2.416
2.393
2.373
2.351
2.333
2.306
2.288
2.216
2.206
2.199
2.182
2.163
2.144
2.125
1.988
1.915
1.900
1.825
1.665
1.648
1.623
1.606
1.510
1.496
1.482



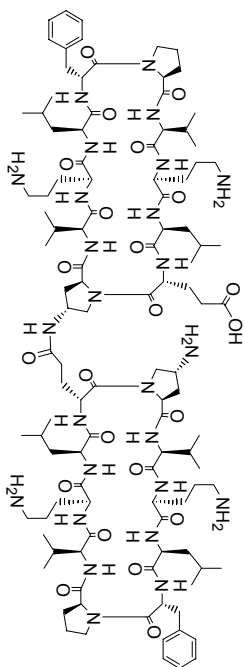
```

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
AQ            0.250036 Hz
RG            256
DE            104.000 usec
TE            283.0 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



21

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	



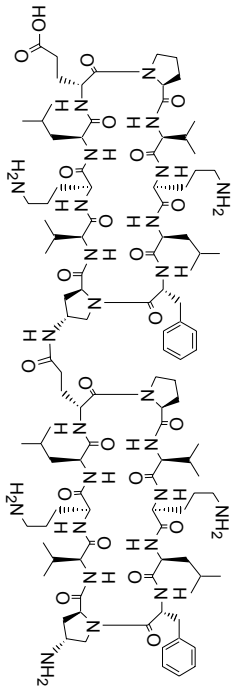
```

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         256
DW         104.000 usec
DE         38.50 usec
TE         298.0 K
D1         1.0000000 sec
d12        0.0000000 sec
MCOREST    0.0000000 sec
MCWRK      0.01500000 sec

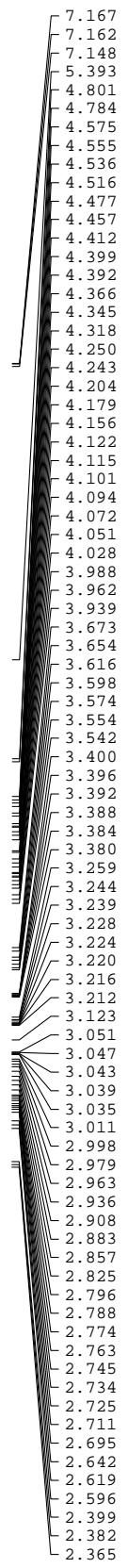
===== CHANNEL f1 =====
NUC1        1H
P1          7.30 usec
PL1         4.00 dB
PL2
PL3
PL4
PL5
PL6
PL7
PL8
PL9
SFO1        400.1319575 MHz

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



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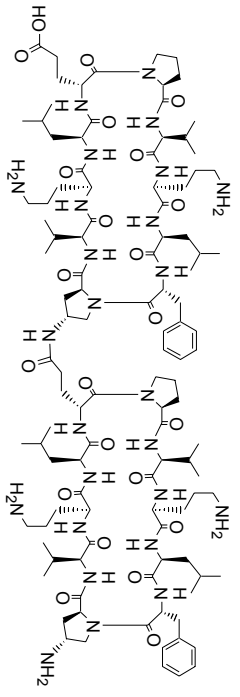
Current Data Parameters  
 NAME G15092004  
 EXNO 5  
 PROCNO 1

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 1.0000200 sec  
 d12 0.0000200 sec  
 MCWRES 0.0000000 sec  
 MCWRX 0.0150000 sec

===== CHANNEL f1 =====  
 NUCL 1H  
 P1 7.30 usec  
 PL1 4.00 dB  
 PL9 60.89 dB  
 SF01 400.1319579 MHz

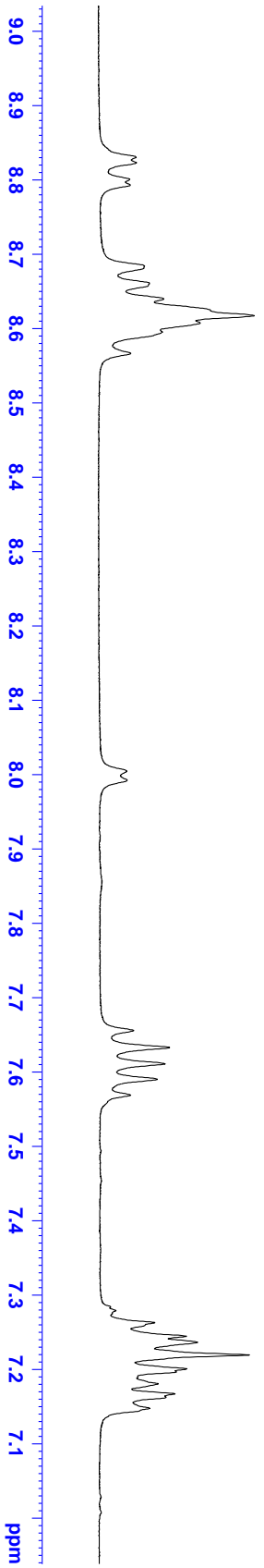
F2 - Processing parameters  
 SI 32768  
 SF 400.1300433 MHz  
 WDM 0  
 SSB 0  
 GB 0.00 Hz  
 DB 0  
 PC 1.00

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

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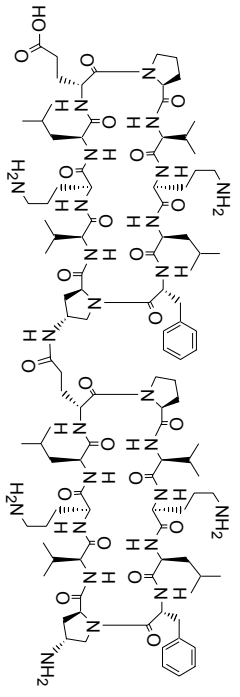
Current Data Parameters  
 NAME G1J5092004  
 EXPNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20040915  
 Time 14.09  
 INSTRUM advance400  
 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 8.50 use  
 DE 28.0 K  
 DI 1.0000200 sec  
 d12 0.0000000 sec  
 MCPRST 0.0000000 sec  
 MCWRK 0.01500000 sec

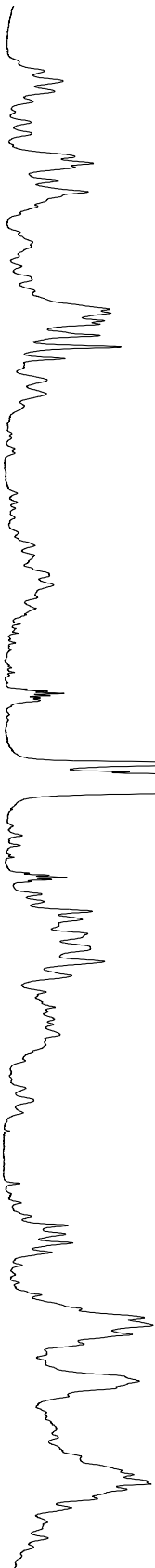
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.30 use  
 PL1 4.00 dB  
 PL9 60.89 dB  
 SFO1 400.1319579 MHz

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

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



4.412	
4.399	
4.392	
4.366	
4.345	
4.318	
4.250	
4.243	
4.204	
4.179	
4.156	
4.122	
4.115	
4.101	
4.094	
4.072	
4.051	
4.028	
3.988	
3.962	
3.939	
3.673	
3.654	
3.616	
3.598	
3.574	
3.554	
3.542	
3.400	
3.396	
3.392	
3.388	
3.384	
3.380	
3.259	
3.244	
3.239	
3.228	
3.224	
3.220	
3.216	
3.212	
3.123	
3.051	
3.047	
3.043	
3.039	
3.035	
3.011	
2.998	
2.979	
2.963	
2.936	
2.908	
2.883	
2.857	
2.825	
2.796	
2.788	
2.774	
2.763	
2.745	
2.734	
2.725	
2.711	
2.695	
2.642	
2.619	
2.596	
2.399	
2.382	
2.365	
2.349	
2.331	
2.306	
2.250	
2.223	
2.207	
2.192	
2.175	
2.157	
2.141	
2.086	
2.073	
2.058	

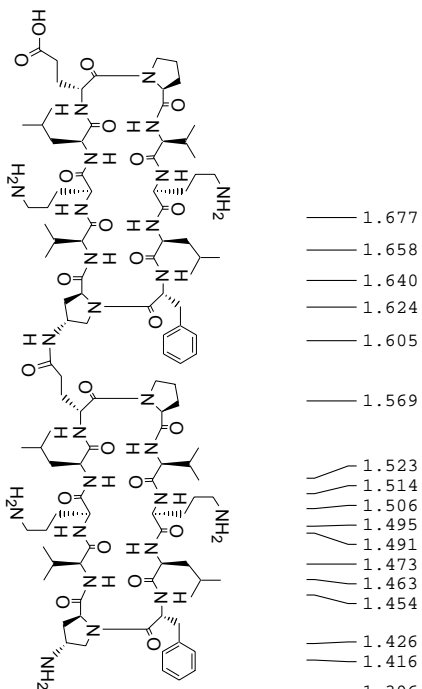


4.6	3.04
4.5	
4.4	4.01
4.3	
4.2	
4.1	8.67
4.0	
3.9	
3.8	
3.7	
3.6	4.80
3.5	
3.4	0.93
3.3	
3.2	
3.1	
3.0	6.91
2.9	
2.8	3.87
2.7	
2.6	1.29
2.5	
2.4	3.20
2.3	
2.2	5.85
2.1	4.10
2.0	
1.9	10.86

```

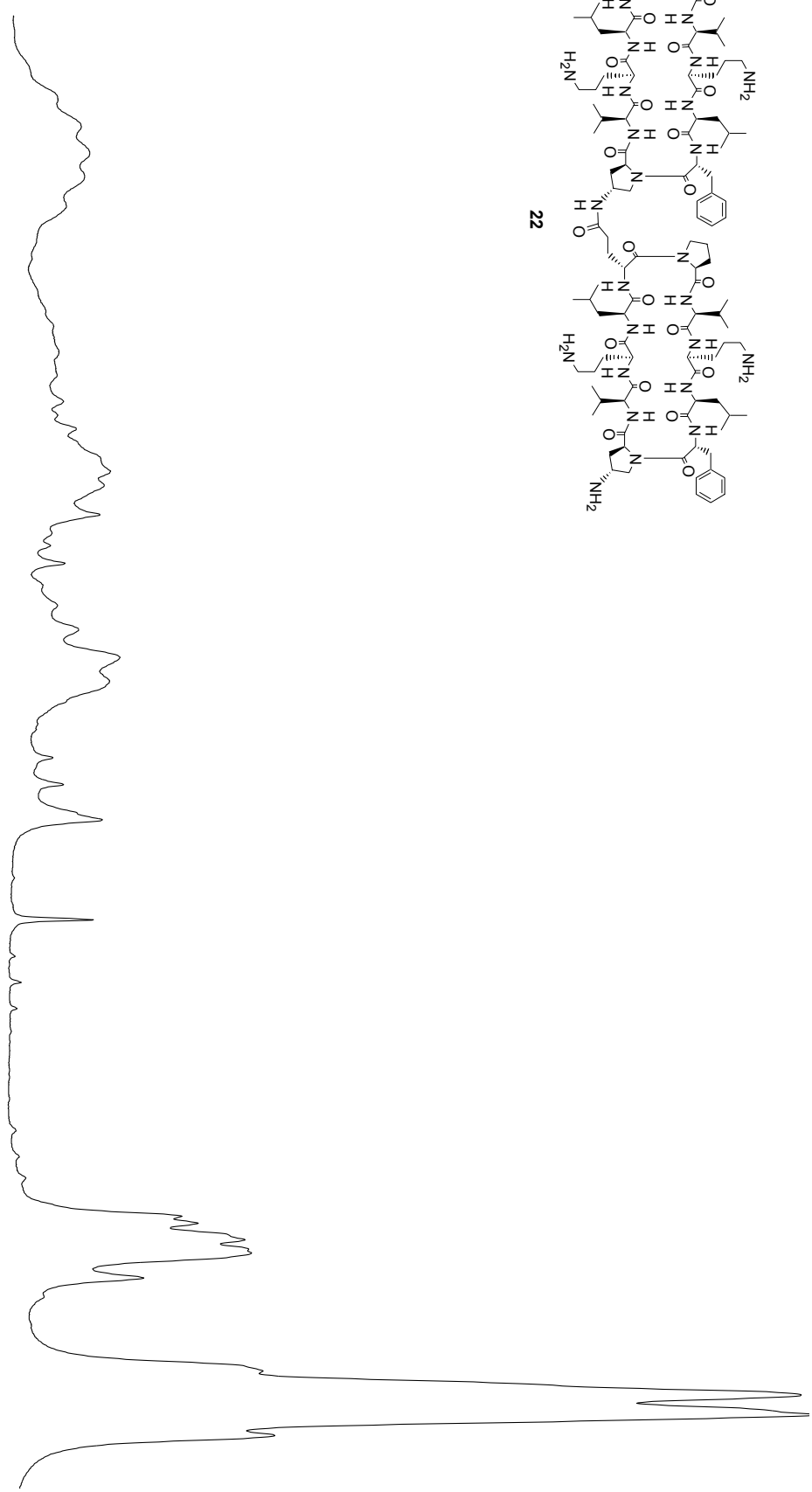
Current Data Parameters
NAME          G1J5092004
EXPNO         5
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time          14.09
INSTRUM       avance400
PROBHD        5 mm BBI 1H-BB
PULPROG       zgpr
TD            19228
SOLVENT       MeOD
NS            1024
DS            0
SWH           4807.692 Hz
AQ            0.250036 Hz
RG            1.9997621 sec
DE           256
DM           104.000 usec
DE           28.90 usec
TE           300.2 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          60.89 dB
SF01         400.1319579 MHz
F2 - Processing parameters
SI           32768
SF           400.1300433 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
```

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



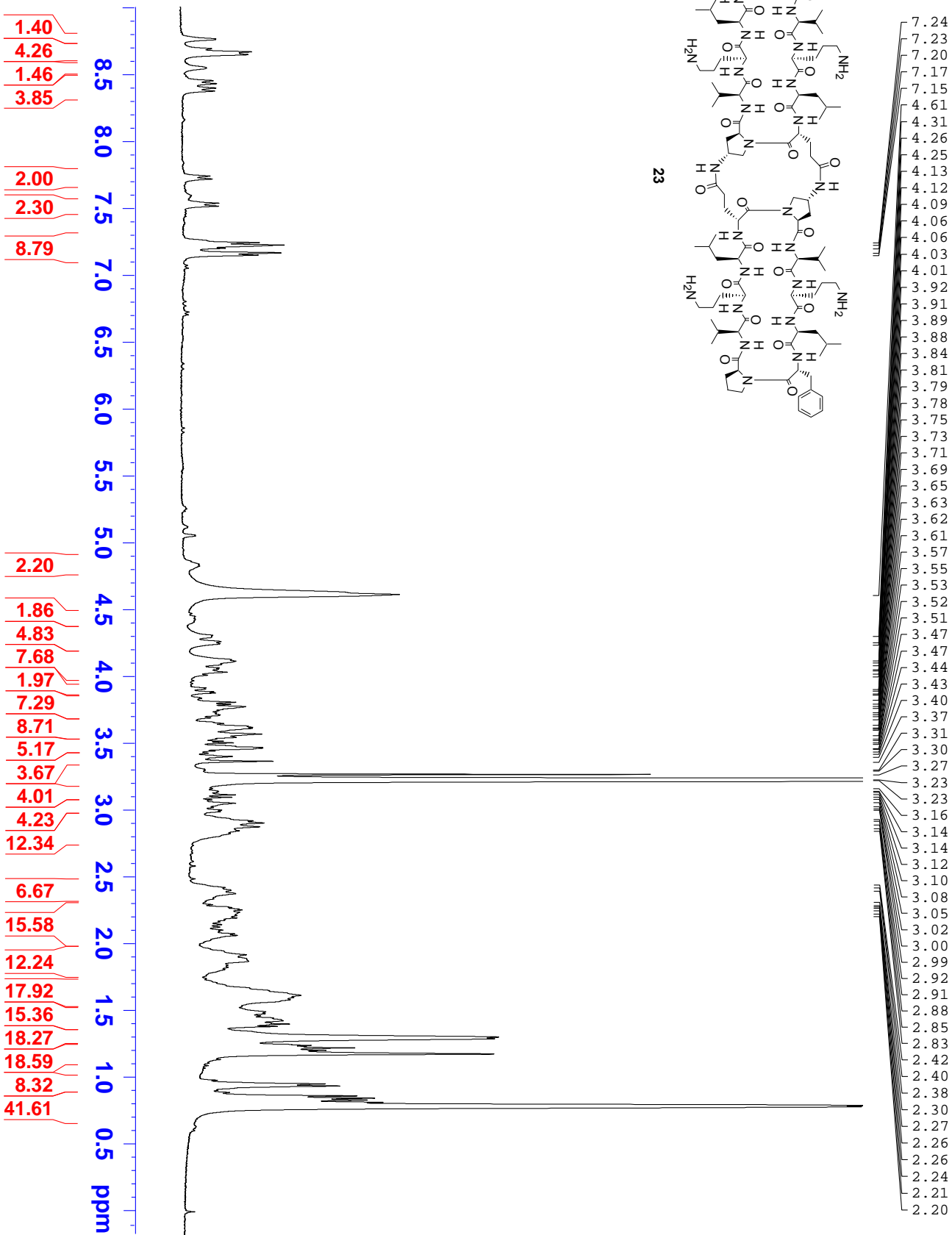
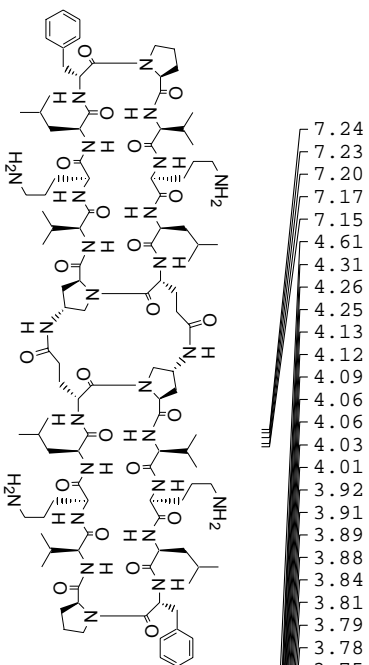
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1.677	1.658	1.640	1.624	1.605	1.569	1.523	1.514	1.506	1.495	1.491	1.473	1.463	1.454	1.426	1.416	1.396	1.384	1.375	1.363	1.349	1.335	1.319	1.300	1.284	1.255	1.232	1.214	1.190	1.123	1.081	0.963	0.949	0.923	0.918	0.907	0.901	0.898	0.881	0.869	0.819	0.802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



Current Data Parameters  
 NAME G1J5092004  
 EXPNO 5  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20040915  
 Time 14.09  
 INSTRUM avance400  
 PROBDI 1H-BB  
 PULPROG 5 mm BBI 1H-BB  
 zppr  
 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 84.90 use  
 DE 28.0  
 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



```

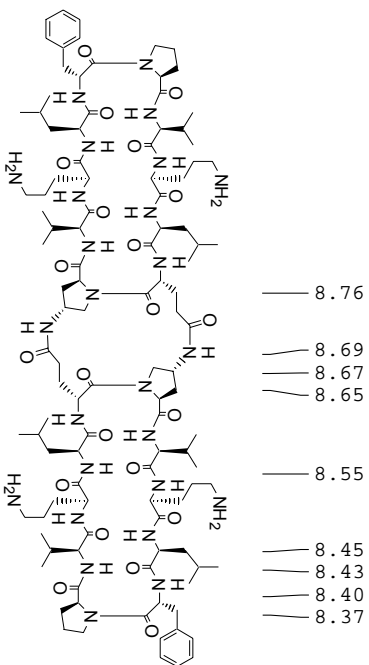
Current Data Parameters
NAME      G1Jsr72003
EXPNO     2
PROCNO    1

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         1.9922841
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

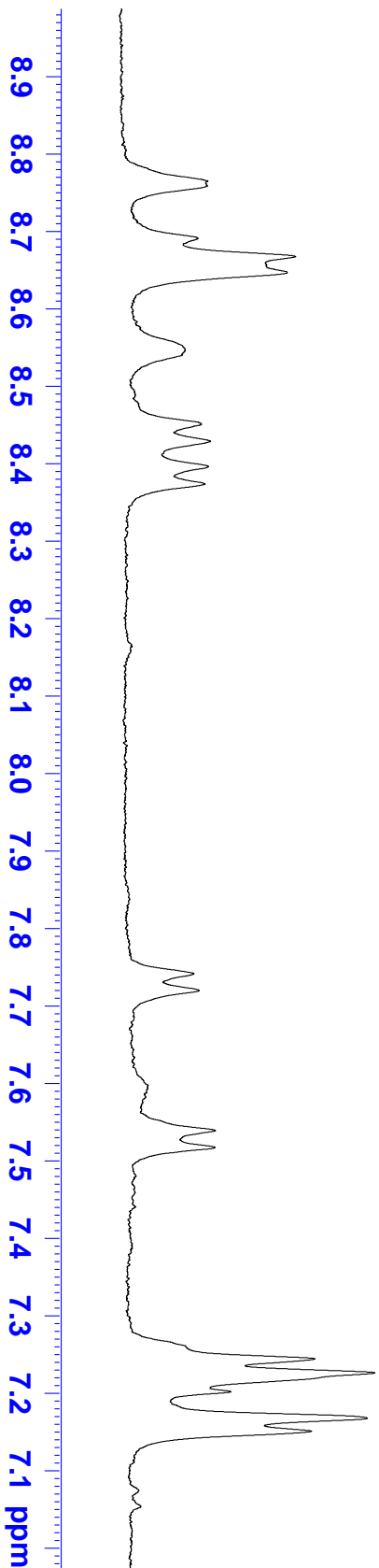
F2 - Processing parameters
SI         131072
SF         400.1300389 MHz
WDW        EM
SSB        0
LB         0.50 Hz
GB         0
PC         1.00
    
```

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



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8.76	
8.69	
8.65	
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	

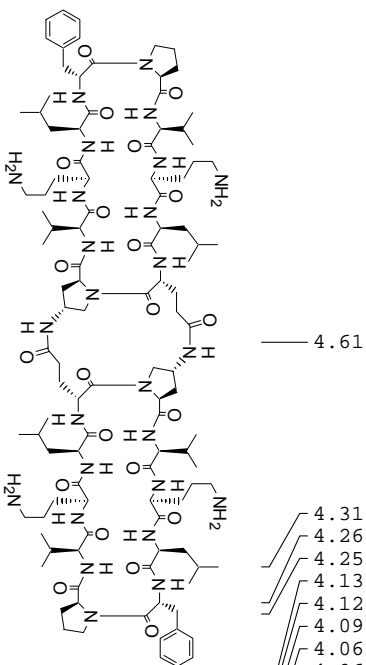


```

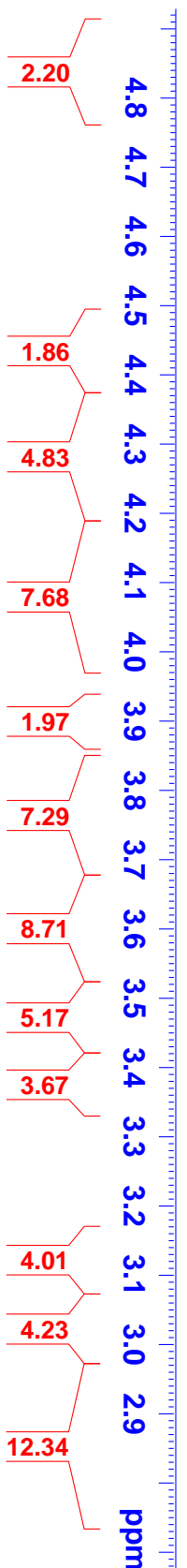
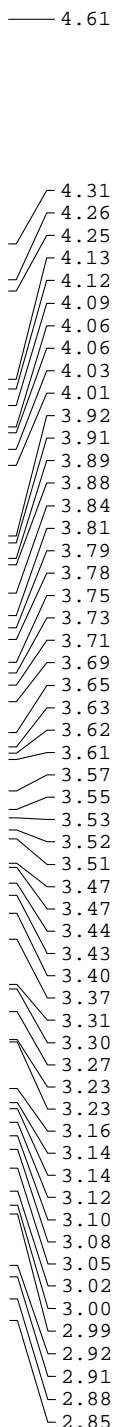
Current Data Parameters
NAME          GIJ5072003
EXPNO         2
PROCNO        1
F2 - Acquisition Parameters
Date_         20030723
Time          10.20
INSTRUM      avance400
PROBHD       5 mm BBI 1H-BB
PULPROG      zgpg
TD           13228
SOLVENT      MeOD
NS           128
DS           2
SFO1         4807.692 Hz
FIDRES       0.250036 Hz
AQ           1.9997621 sec
RG           228.1
DE           104.000 usec
DM           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
PL19         58.19 dB
SF01         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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```

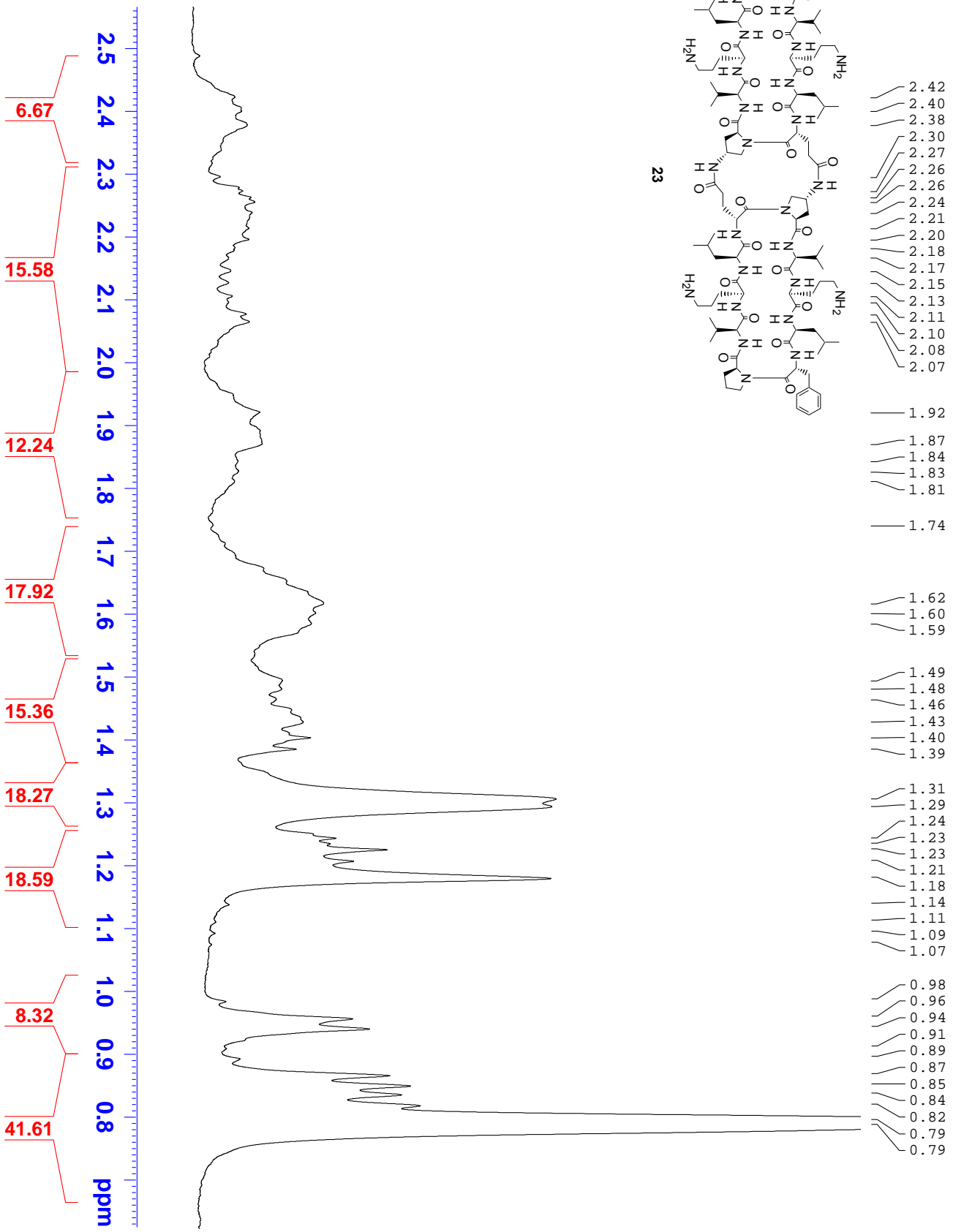
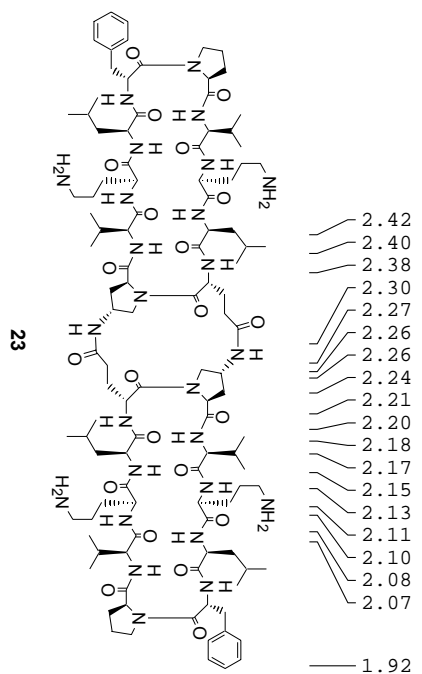
Current Data Parameters
NAME      G1js072003
EXPNO     2
PROCNO    1

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       400.1318653 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-bbigs probe



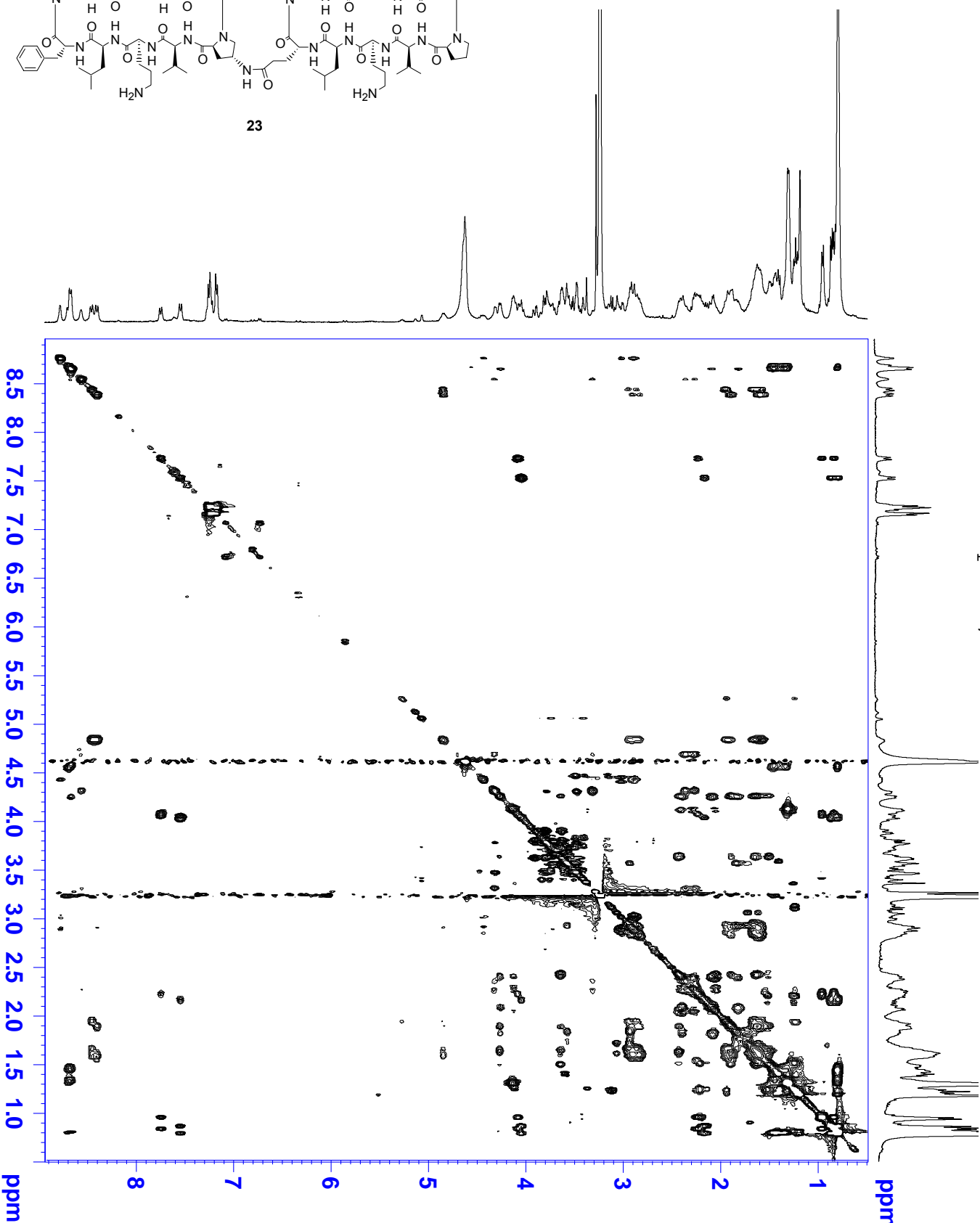
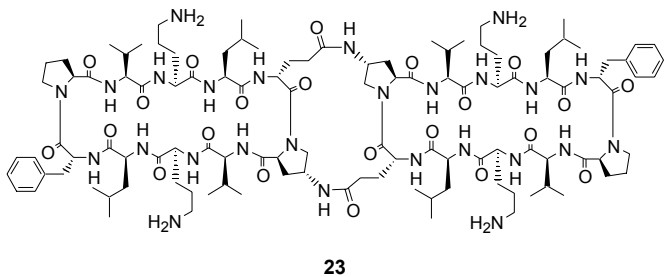
```

Current Data Parameters
NAME      G4js072003
EXPNO     1
PROCNO    2

F2 - Acquisition Parameters
Date_     20030723
Time      10.20
INSTRUM   avance400
PROBHD    5 mm BBI-5B5
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         8.50 usec
D1         300.0 K
D12        1.00000000 sec
D13        0.00002000 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-bbig5 probe, cleanTOCSY Tmix=70msec



Current Data Parameters  
 NAME G13s072003  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20030723  
 Time 10.54

INSTRUM advance400  
 PROBED 5 mm BBI 1H-2B  
 PULPROG cmllepr2  
 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

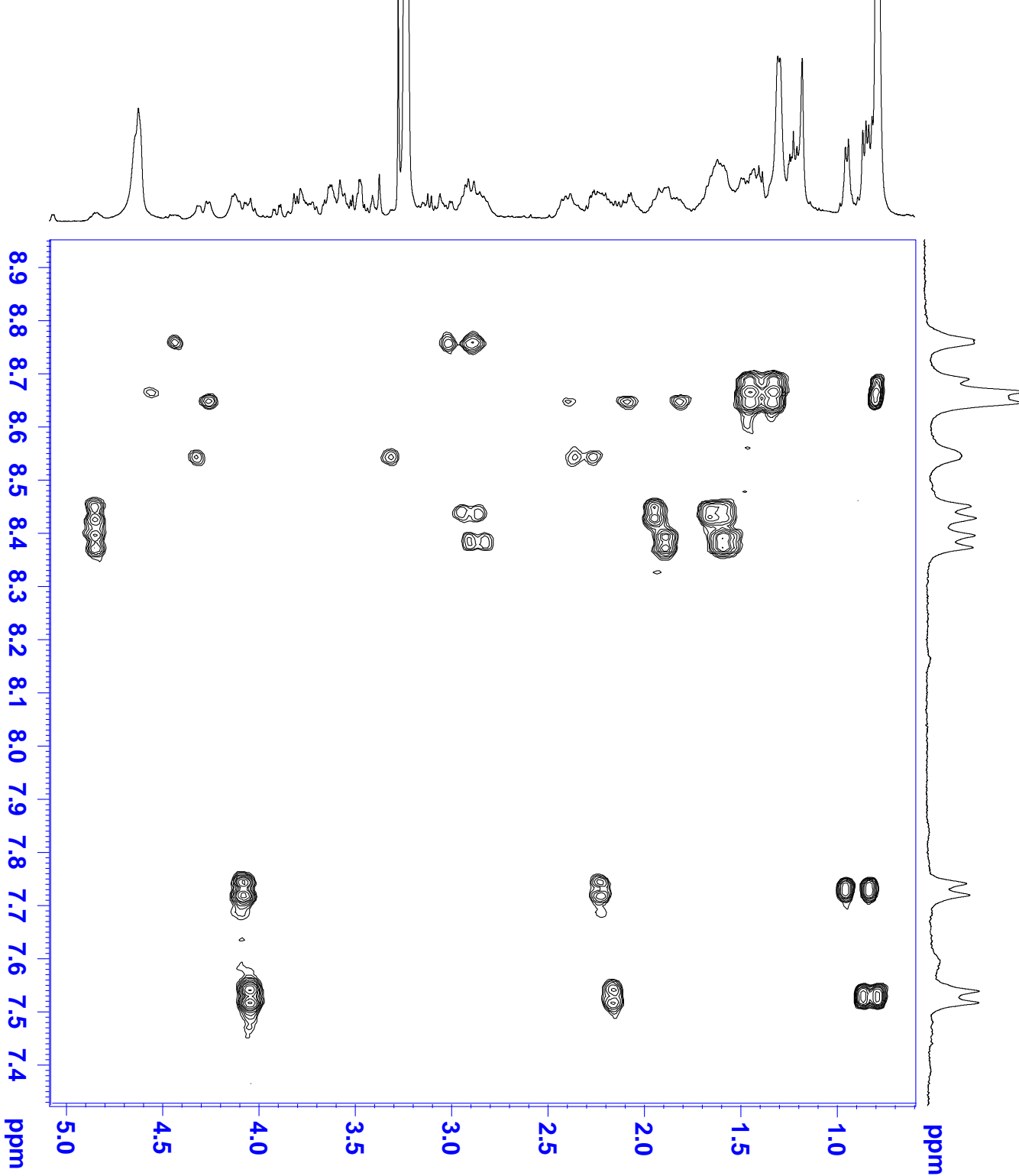
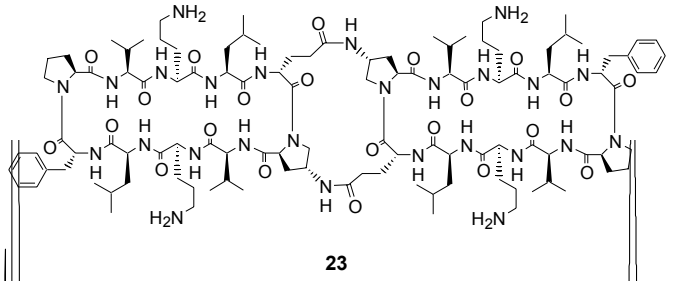
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 6.10 usec  
 P5 16.67 usec  
 P6 25.00 usec  
 P7 50.00 usec  
 P17 2500.00 usec  
 PL1 4.00 dB  
 PL9 58.51 dB  
 PL10 16.50 dB  
 SFO1 400.1318941 MHz

F1 - Acquisition Parameters  
 FID 512  
 SFO1 400.1318 MHz  
 FIDRES 9.390024 Hz  
 SW 12.015 ppm  
 ENMODE States-TPPI

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

F1 - Processing parameters  
 SI 1024  
 M2 States-TPPI  
 SF 400.1300389 MHz  
 MDW QSIIMS  
 SSB 2.1 Hz  
 LB 0.00 Hz  
 GB 0

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



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 cmlpevpr2

TD 242  
 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  
 D0 0.0000000 sec  
 D1 1.0000000 sec

d11 0.0300000 sec  
 d12 0.0000200 sec  
 d13 0.0000400 sec

D20 0.00006500 sec  
 D20 0.00006500 sec  
 INO 0.00020800 sec

LL 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

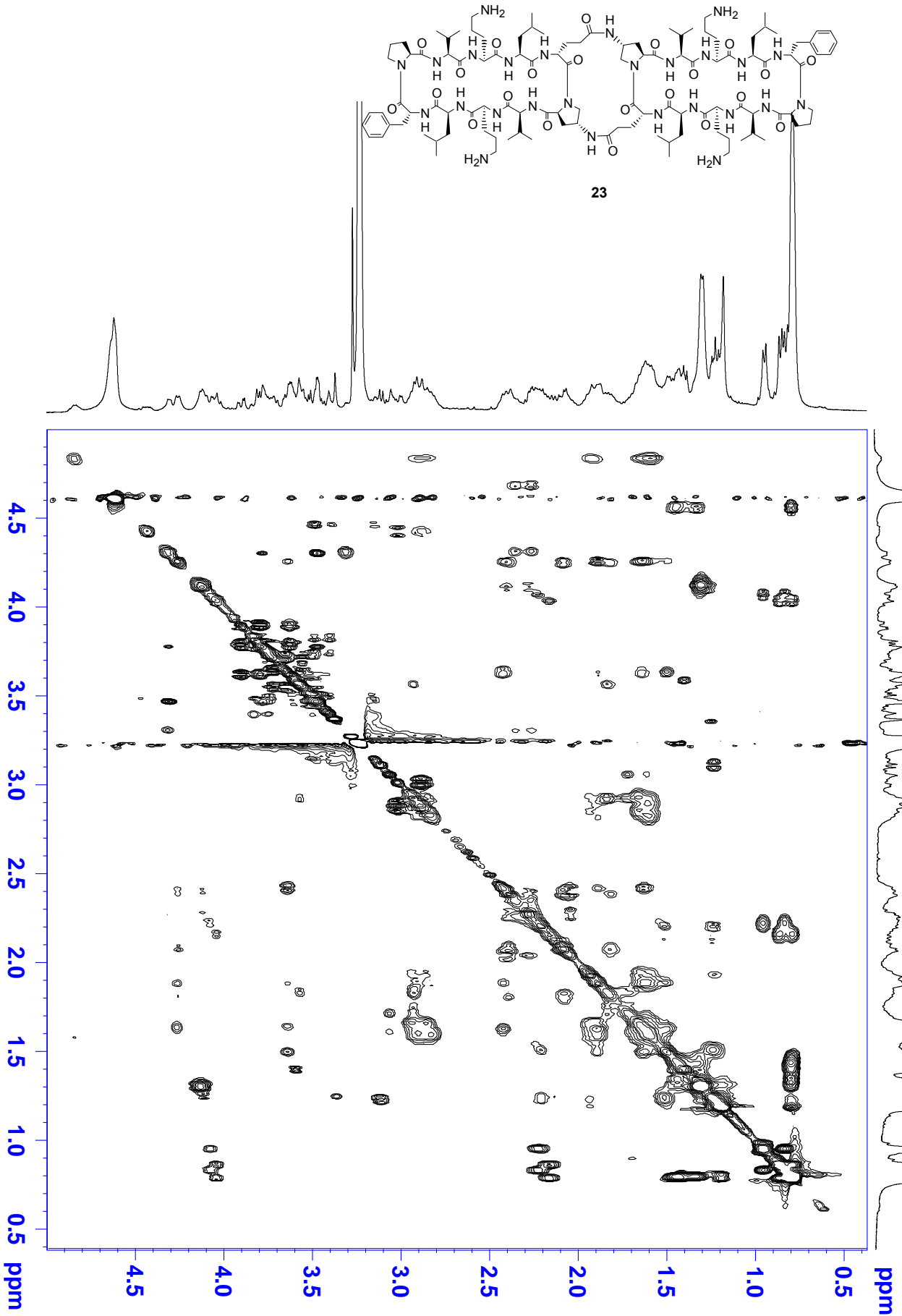
FMODE States-TPPI  
 F2 - Processing parameters  
 SI 2048  
 SF 400.1300389 MHz

WDW QSINE  
 SSB 2.3 Hz  
 GB 0.00 Hz  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 States-TPPI 1024  
 MC2 400.1300389 MHz

SF 400.1300389 MHz  
 QSINE 2.1 Hz  
 SSB 0.00 Hz  
 GB 0

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-2BS  
 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  
 T0 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  
 IL 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  
 FIDRES 400.1319 MHz  
 FIDRES 9.390024 Hz  
 SW 12.015 ppm  
 FMODE States-TPPI

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

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