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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 CD₃OH, at 298 K, at 400 MHz)

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

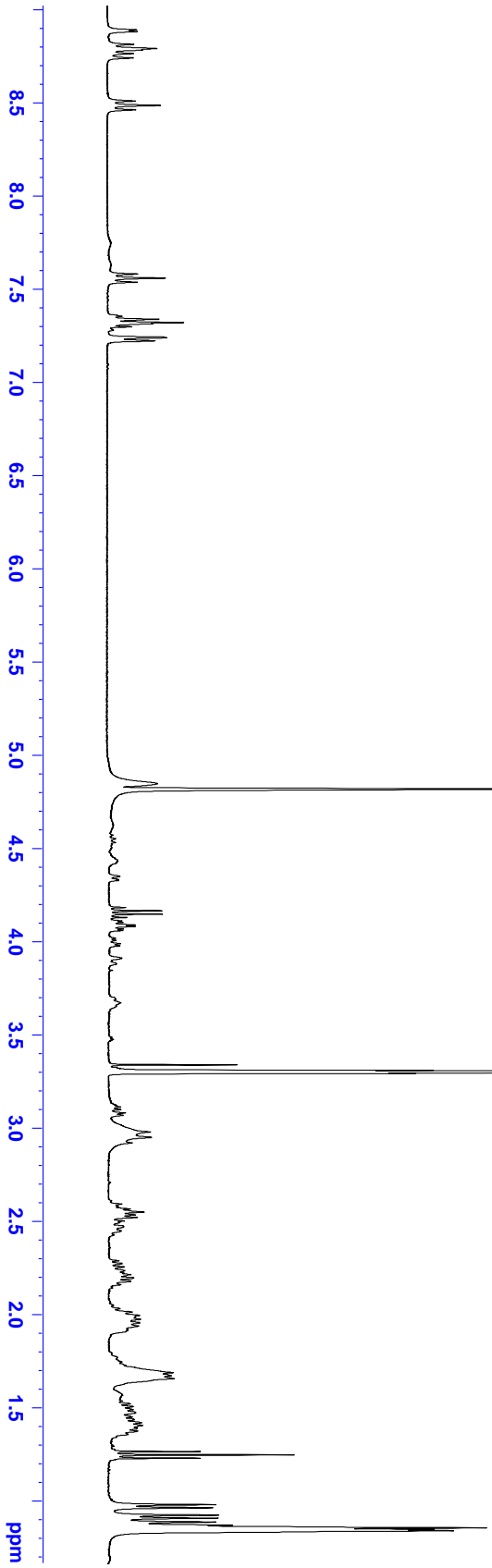
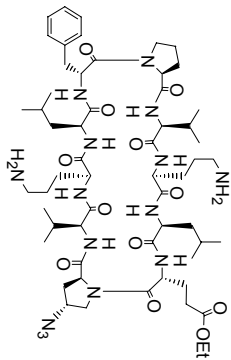
‡ Variation in the experimental conditions, such as the solvent system or temperature, could not resolve the severe overlap of resonances in the ¹H NMR spectra due to the high degree of symmetry present in the gramicidin S analogues and the dimers thereof.

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
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2.212
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2.175
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2.030
2.012
1.994
1.973
1.953
1.937



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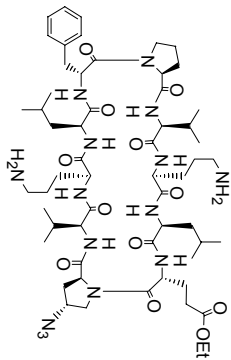
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PULPROG      zgpr
TD            19228
SOLVENT      MeOD
NS            64
DS            0
SWH           3720.238 Hz
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AQ           2.5842931 sec
RG            161.3
DW           134.400 usec
DE            8.50 usec
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d12           0.0002000 sec
d13           0.0000300 sec

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NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL2           52.29 dB
SFO1          400.1319405 MHz

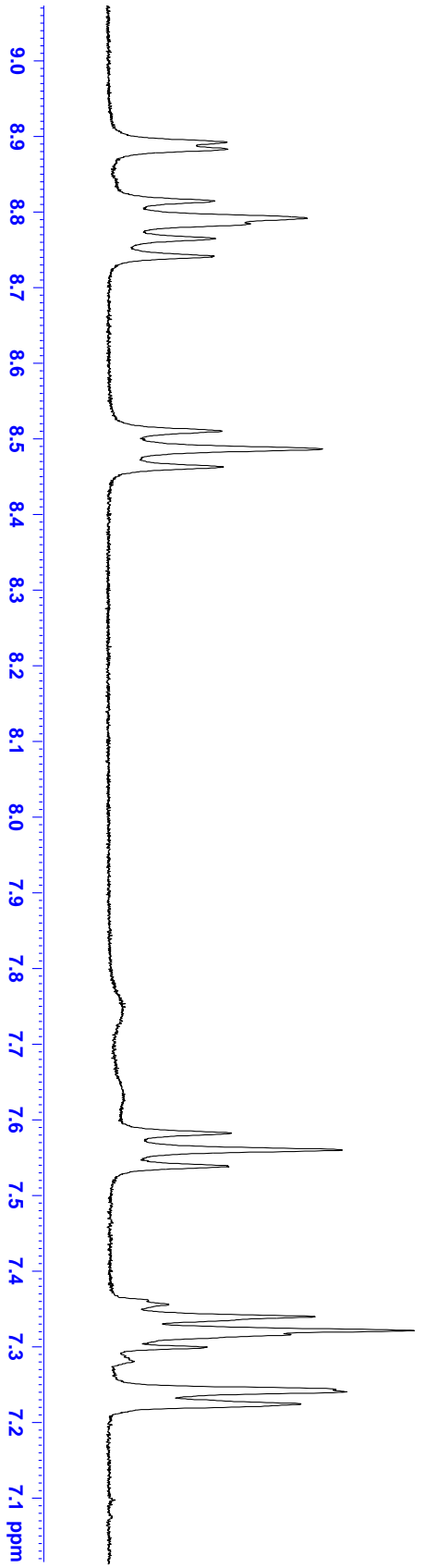
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SSB           0
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GB            0.4
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mwe1101 (epje 1) 298 K

- 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

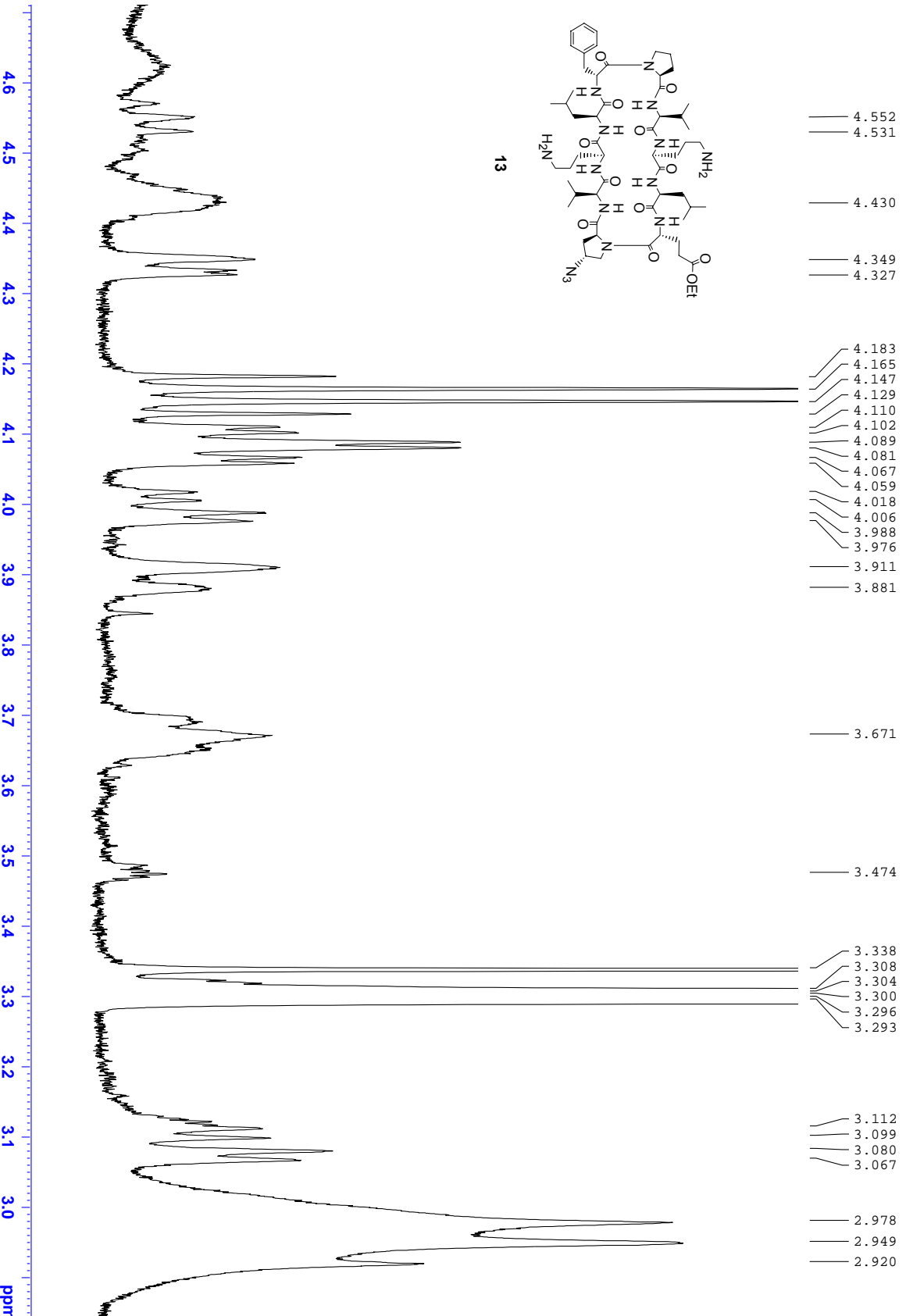


13



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Current Data Parameters
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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
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SF            400.1300114 MHz
WDW           GM
SSB           0
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GB            0.4
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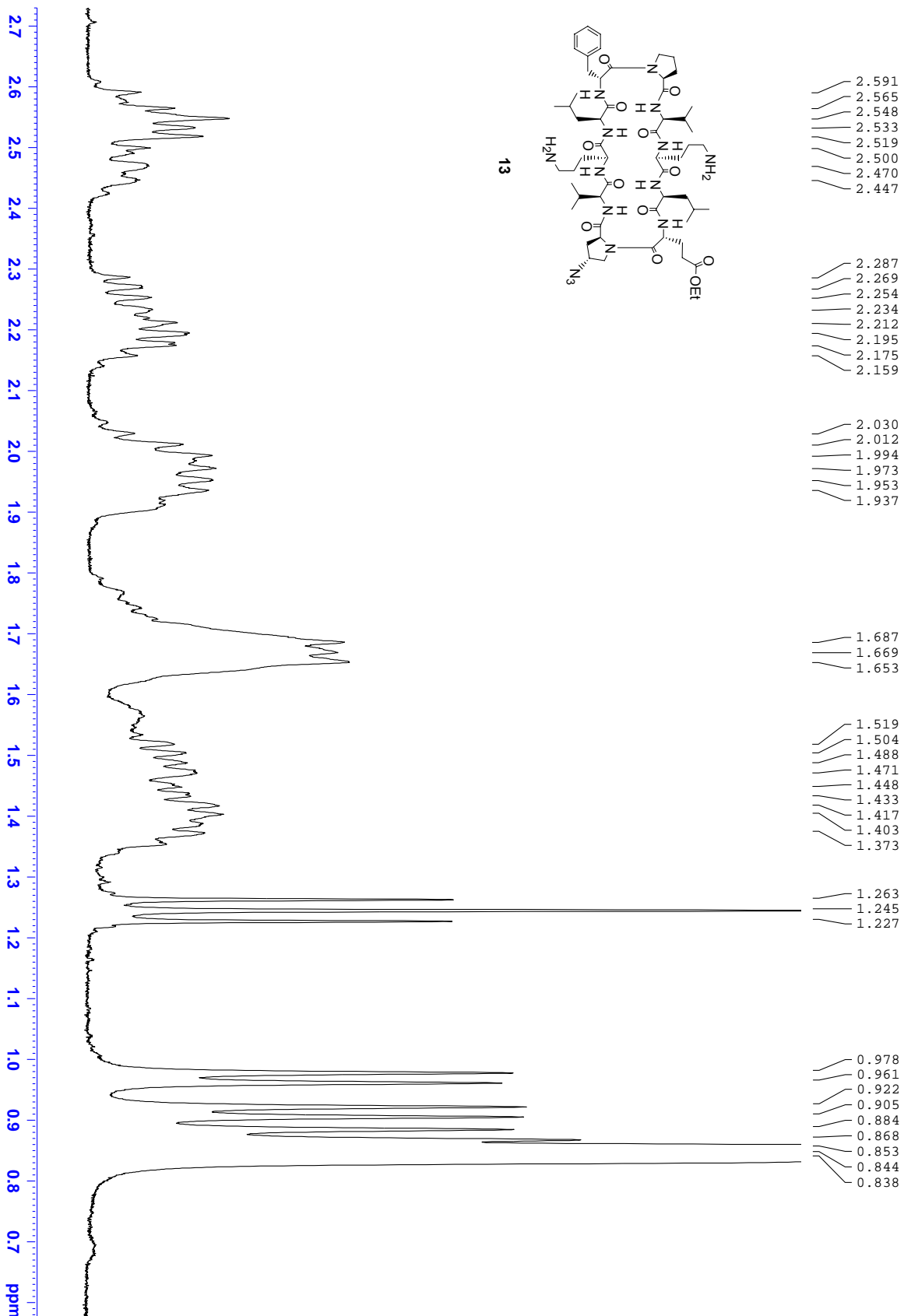
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 PROCNO 1

F2 - Acquisition Parameters
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 PROBHD 5 mm BBI 1H-5B
 PULPROG zgpr
 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 use
 DE 8.50 use
 TE 300.0 K
 D1 1.0000000 sec
 D12 0.0000000 sec
 D13 0.0000000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 7.30 use
 PL1 4.00 dB
 PL9 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
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 PC 1.00

mwe1101 (epje 1) 298 K

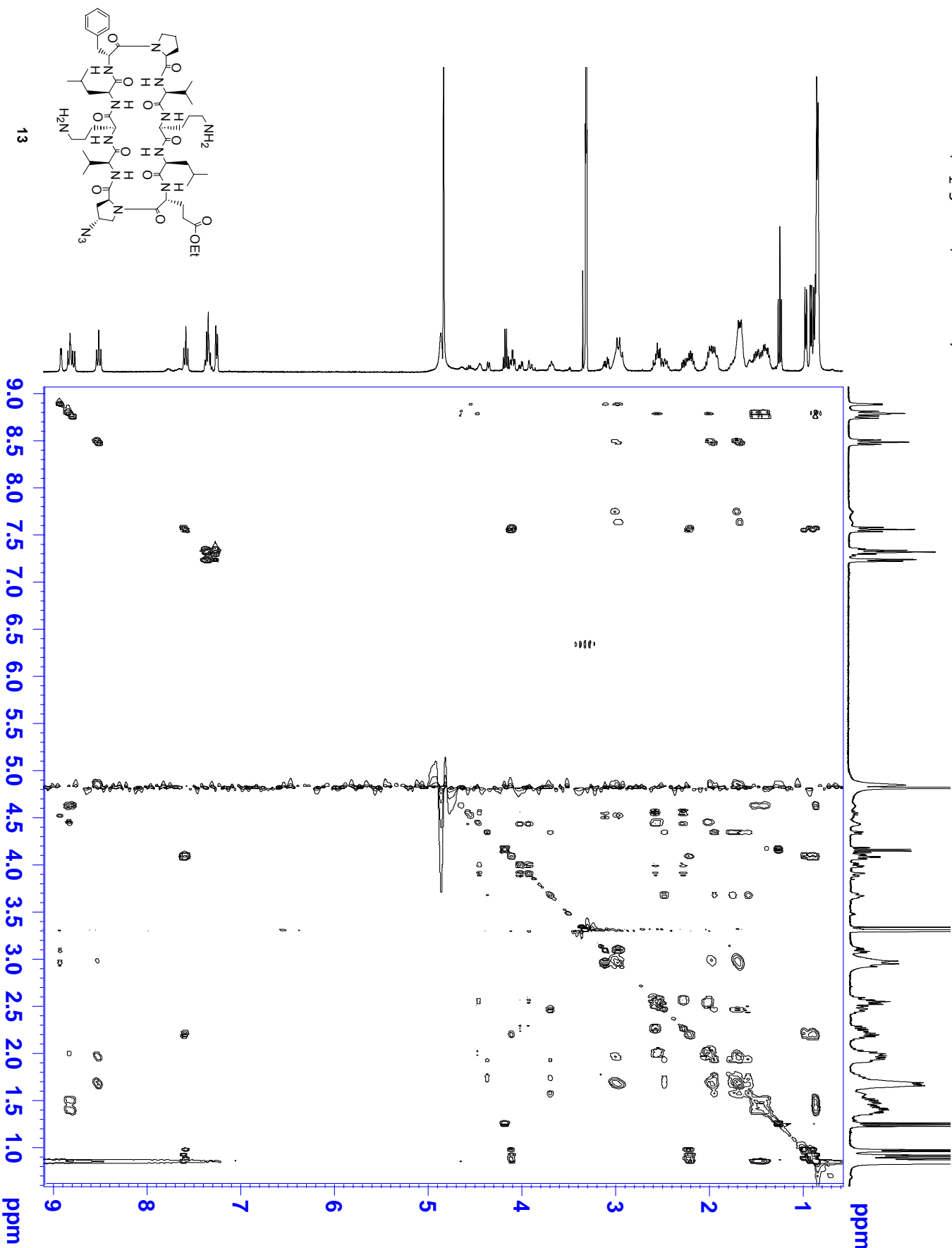


2.591	2.287	2.030	1.687	1.519	1.263	0.978
2.565	2.269	2.012	1.669	1.504	1.245	0.961
2.548	2.254	1.994	1.653	1.488	1.227	0.922
2.533	2.234	1.973		1.471		0.905
2.519	2.212	1.953		1.448		0.884
2.500	2.195	1.937		1.433		0.868
2.470	2.175			1.417		0.853
2.447	2.159			1.403		0.844
				1.373		0.838

```

Current Data Parameters
NAME          g1js042003
EXPNO         8
PROCNO       1
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Date_         20030405
Time_        18.03
INSTRUM      avance400
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
  
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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
 IL 18
 MCREST 0.0000000 sec
 MCWRR 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
 ENMODE States-TPPI

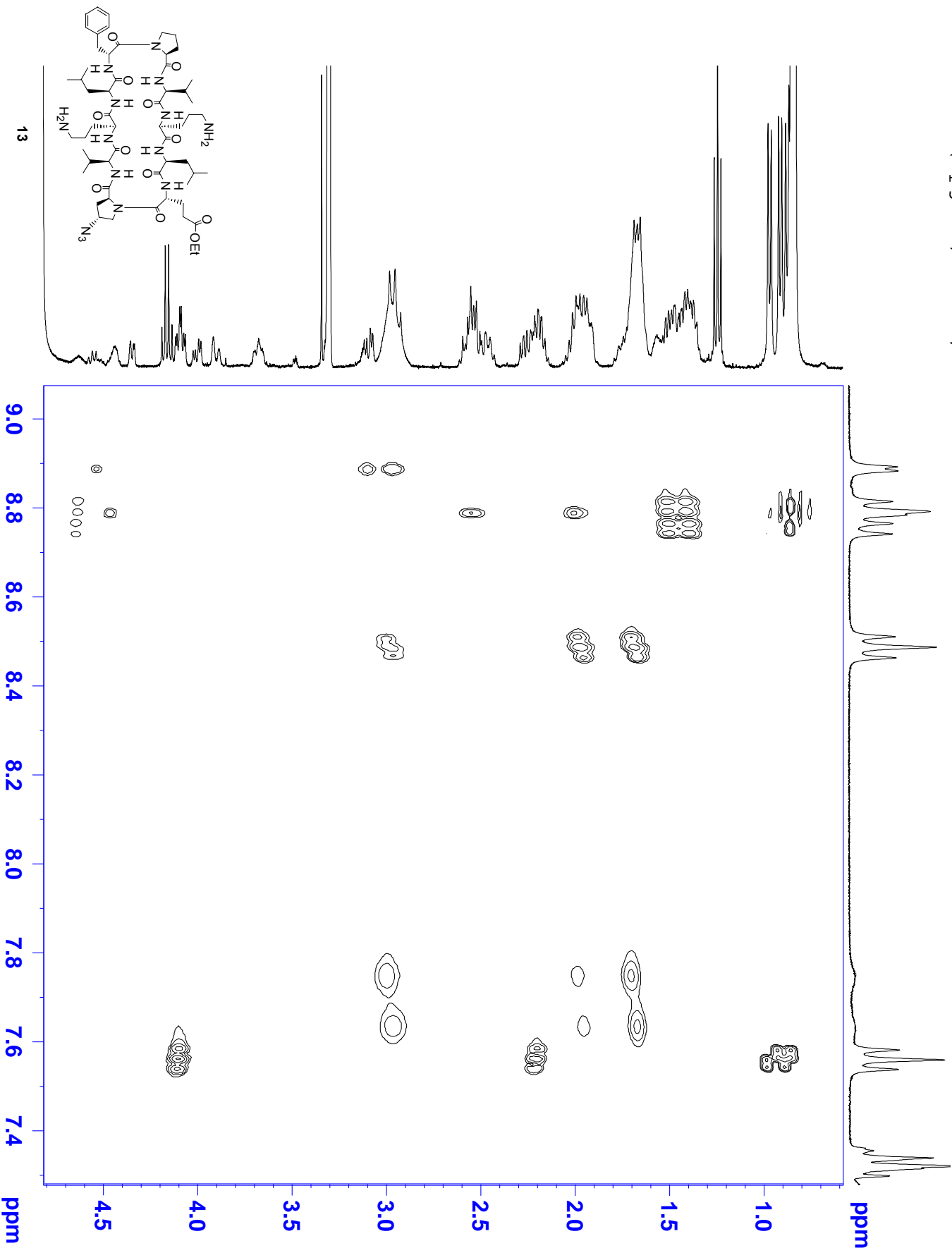
F2 - Processing Parameters

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 avance400
 PROBRD 5 mm BBI JH-25
 PULPROG zgpg30
 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 1.0000000 sec
 D1 0.0300000 sec
 d11 0.0000200 sec
 d12 0.0000400 sec
 d13 0.0000650 sec
 D20 0.00026880 sec
 INO 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

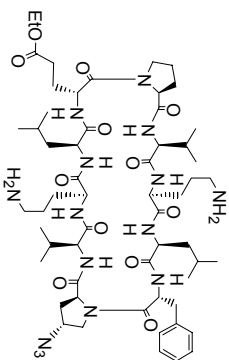
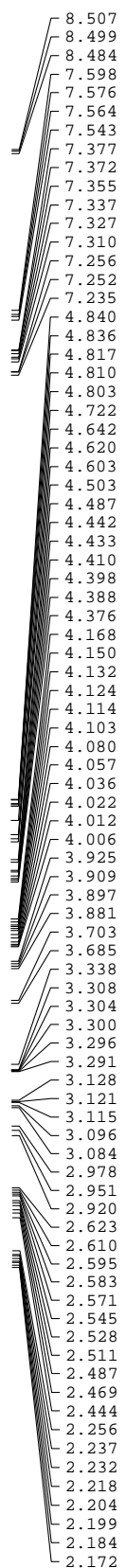
NUC2 1H
 SFO1 400.1319 MHz
 FIDRES 7.266090 Hz
 SW 9.298 ppm
 FMODE States-TPPI

F2 - Processing parameters

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

F1 - Processing parameters

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

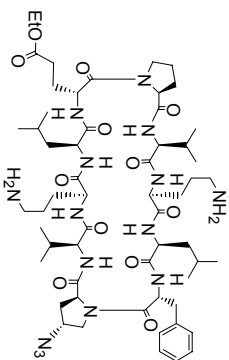


Current Data Parameters
 NAME g1j504203
 EXPRNO 6
 PROCNO 1
 P2 - Acquisition Parameters
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 Time 15 21
 INSTRUM avance400
 PROSHD 5 mm BBI 1H-BB
 PULPROG zgpr
 TD 19228
 SOLVENT MeOD
 NS 64
 DS 0
 SMH 4807.692 Hz
 FIDRES 0.250036 Hz
 AQ 1.9997621 sec
 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

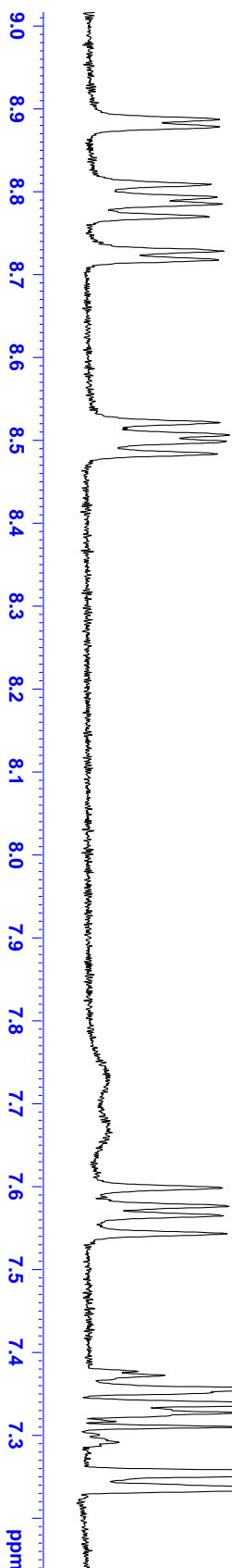
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8.879
8.809
8.793
8.785
8.770
8.728
8.718
8.522
8.507
8.499
8.484

7.598
7.576
7.564
7.543

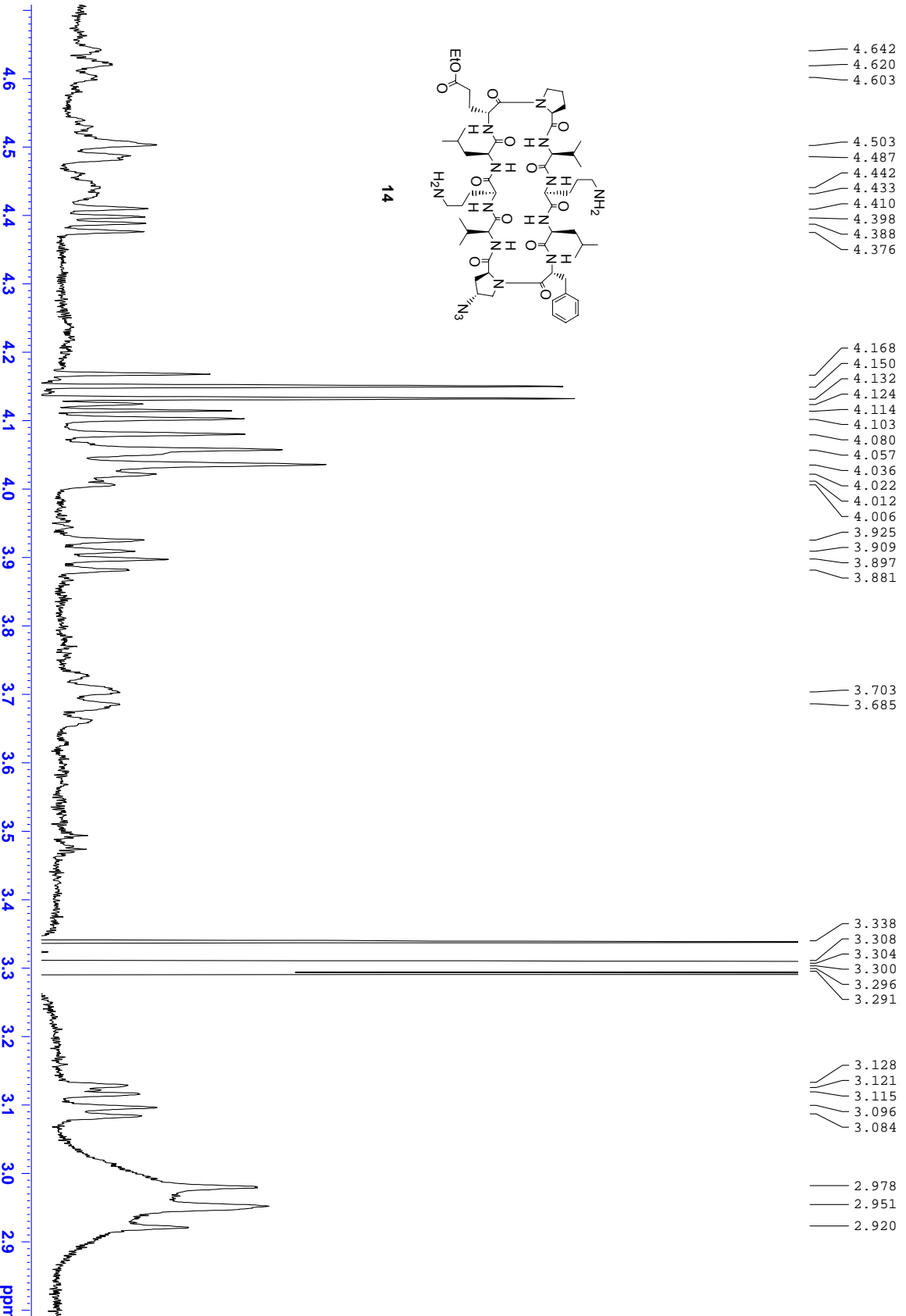
7.377
7.372
7.355
7.337
7.327
7.310
7.256
7.252
7.235



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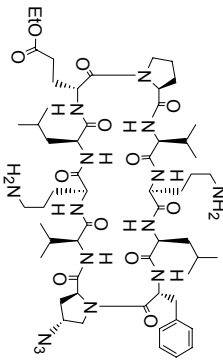
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 PROCNO 1
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 Date_ 20030405
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 PULPROG zgpg
 TD 19228
 SOLVENT MeOD
 NS 64
 DS 0
 SWH 4807.692 Hz
 FIDRES 0.250036 Hz
 AQ 1.9997621 sec
 RG 456.1
 DW 104.000 usec
 DE 8.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 D12 0.000200 sec
 D13 0.0000300 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



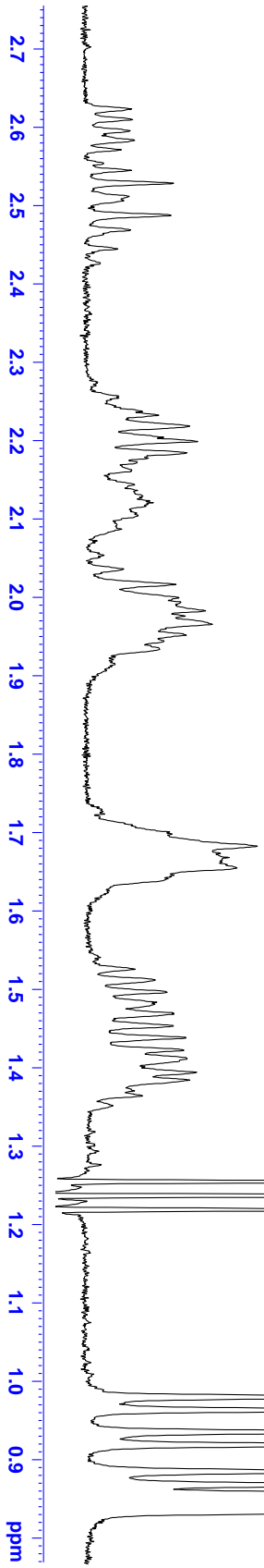
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PULPROG      zgpg
TD            13228
SOLVENT      MeOD
NS            64
DS            0
SWH           4807.692 Hz
FIDRES       0.250036 Hz
AQ           1.9997621 sec
RG            456.1
DW           104.000 usec
DE            8.50 usec
TE            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
PL2           52.29 dB
SFO1         400.131379 MHz
F2 - 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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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	
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	1.976			
	1.966			
	1.952			
	1.944			
	1.933			
	1.914			

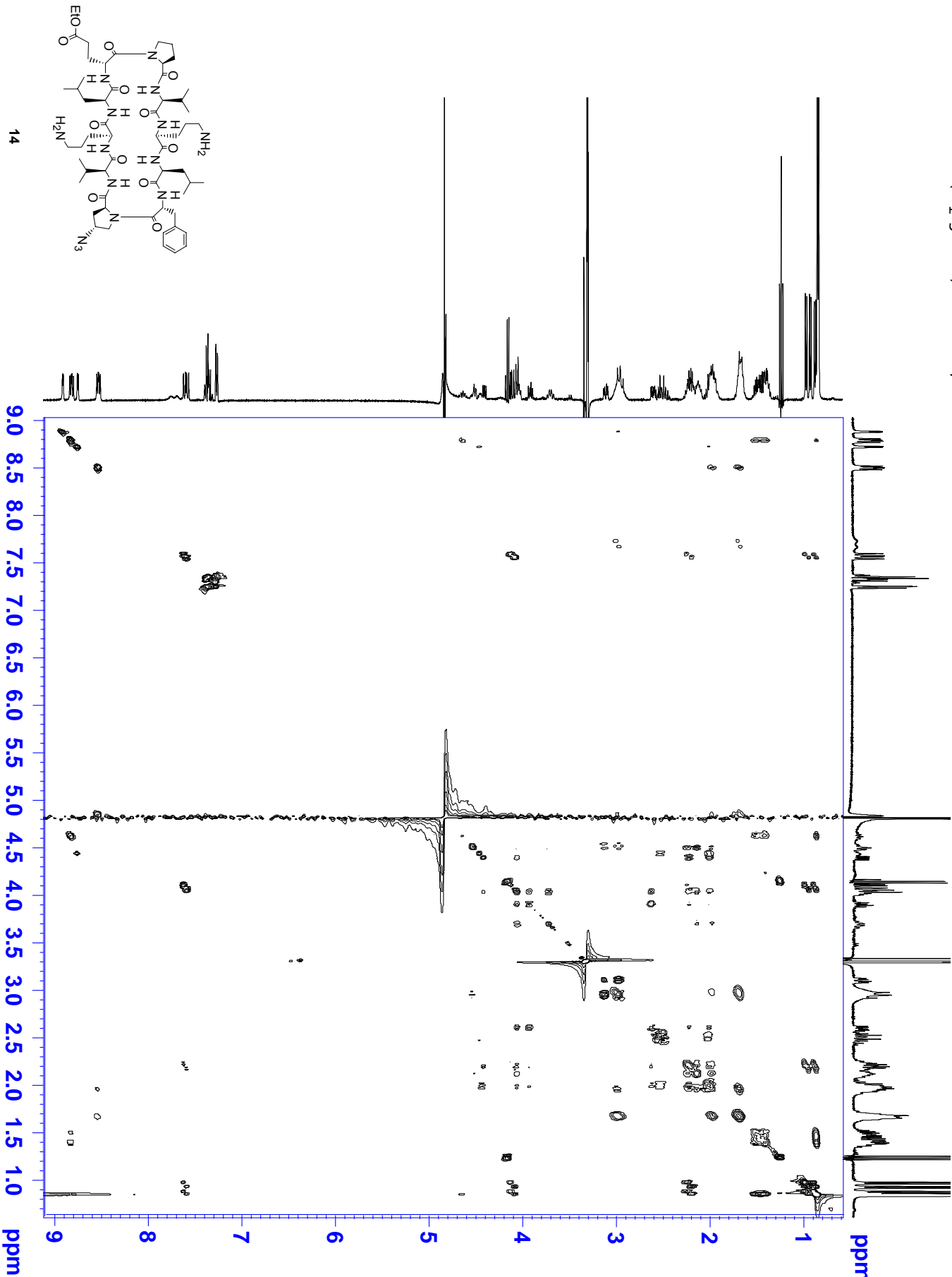


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Current Data Parameters
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 EXPNO 6
 PROCNO 1
 F2 - Acquisition Parameters:
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 Time 15:421
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 PULPROG zgpc
 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
 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 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 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

mw1101 (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
 PROBHD 5 mm BBI JH-385
 PULPROG zgpg30
 TD 24288
 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 0.0000000 sec
 D1 1.0000000 sec
 d11 0.0300000 sec
 d12 0.0000200 sec
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 D20 0.00006500 sec
 INO 0.00026880 sec

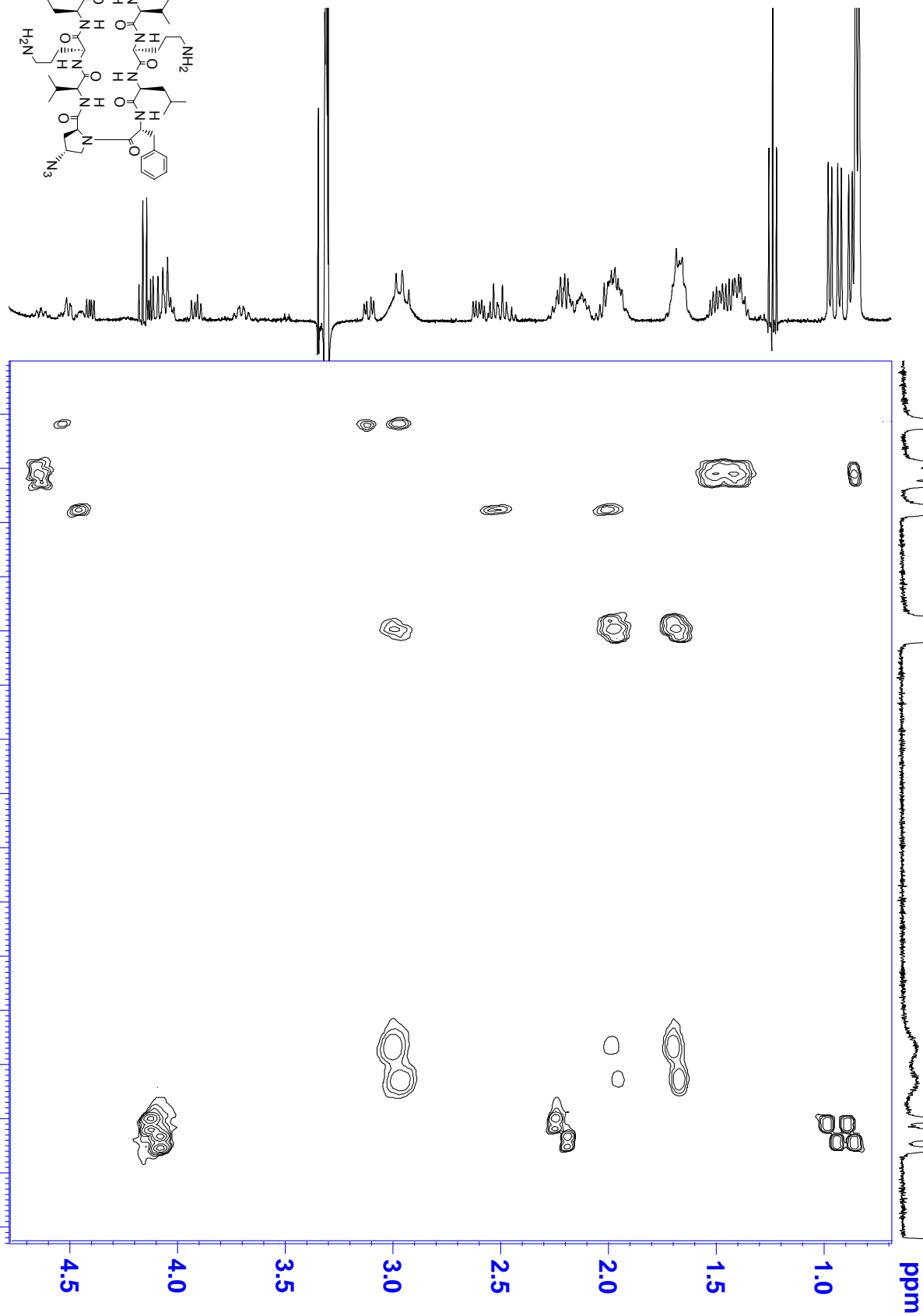
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===== CHANNEL f1 =====
 NUC1 1H
 P1 6.10 usec
 P5 16.67 usec
 P6 25.00 usec
 P7 50.00 usec
 P17 2500.00 usec
 PL1 4.00 dB
 PL9 52.29 dB
 PL10 16.50 dB
 SFO1 400.131975 MHz

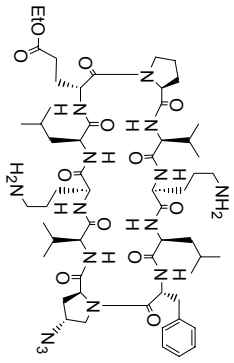
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 SFO2 512 MHz
 SFO1 400.1319 MHz
 FIDRES 7.266090 Hz
 SW 9.298 ppm
 FMODE States-TFPI

F2 - Processing Parameters
 SI 2048
 SF 400.1300115 MHz
 WDW QSI
 SSB 2.3 Hz
 LB 0.00 Hz
 GB 0

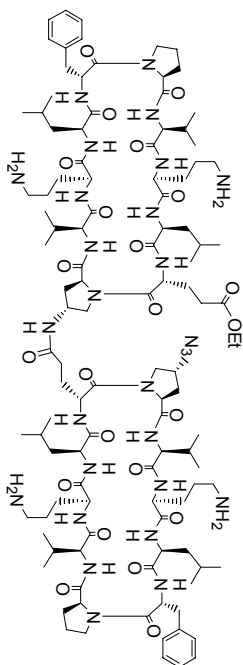
F1 - Processing Parameters
 SI 1024
 MC2 States-TFPI
 SF 400.1300065 MHz
 WDW QSI
 SSB 2.1 Hz
 LB 0.00 Hz
 GB 0



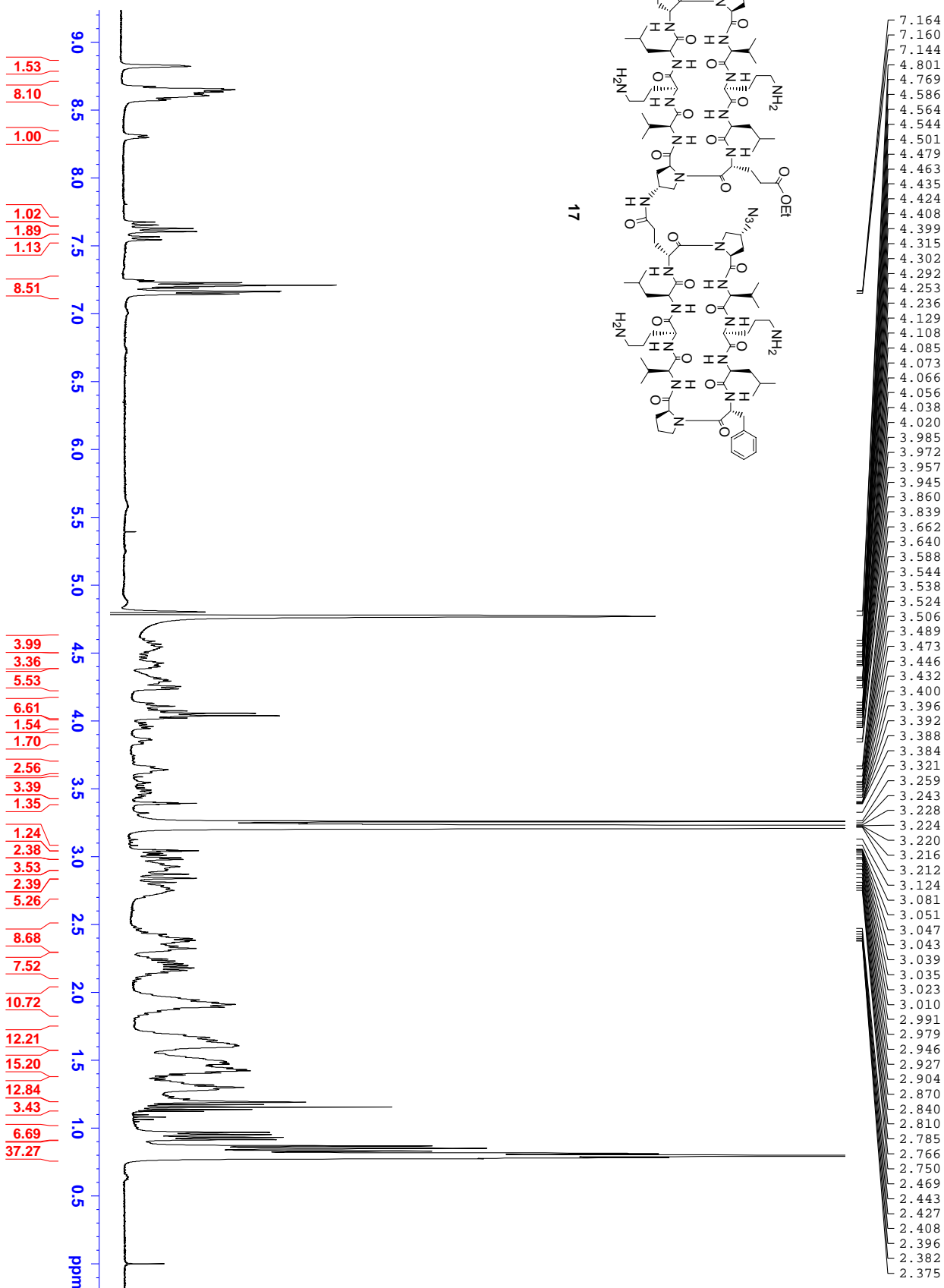
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mwe0806 - dimer N3/Et turn 1H, bbi-av400



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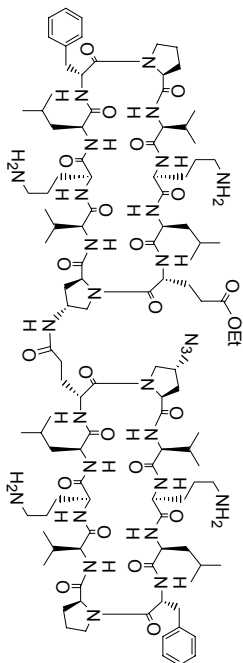
```

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           226.0
TE           300.2 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

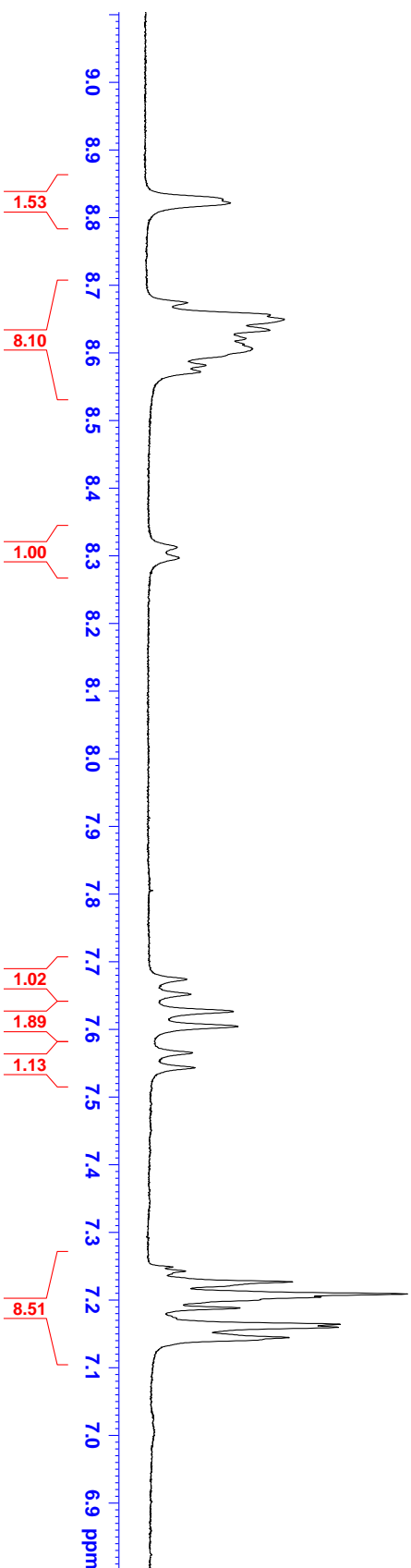
F2 - Processing parameters
SI           32768
SF           400.1300435 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
```

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



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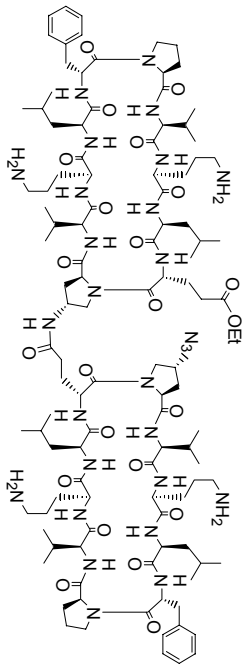
8.821	8.673	8.312	7.674	7.249
8.649	8.633	8.296	7.652	7.242
8.620	8.606		7.627	7.227
8.581			7.604	7.209
8.571			7.566	7.204
			7.543	7.188
				7.164
				7.160
				7.144



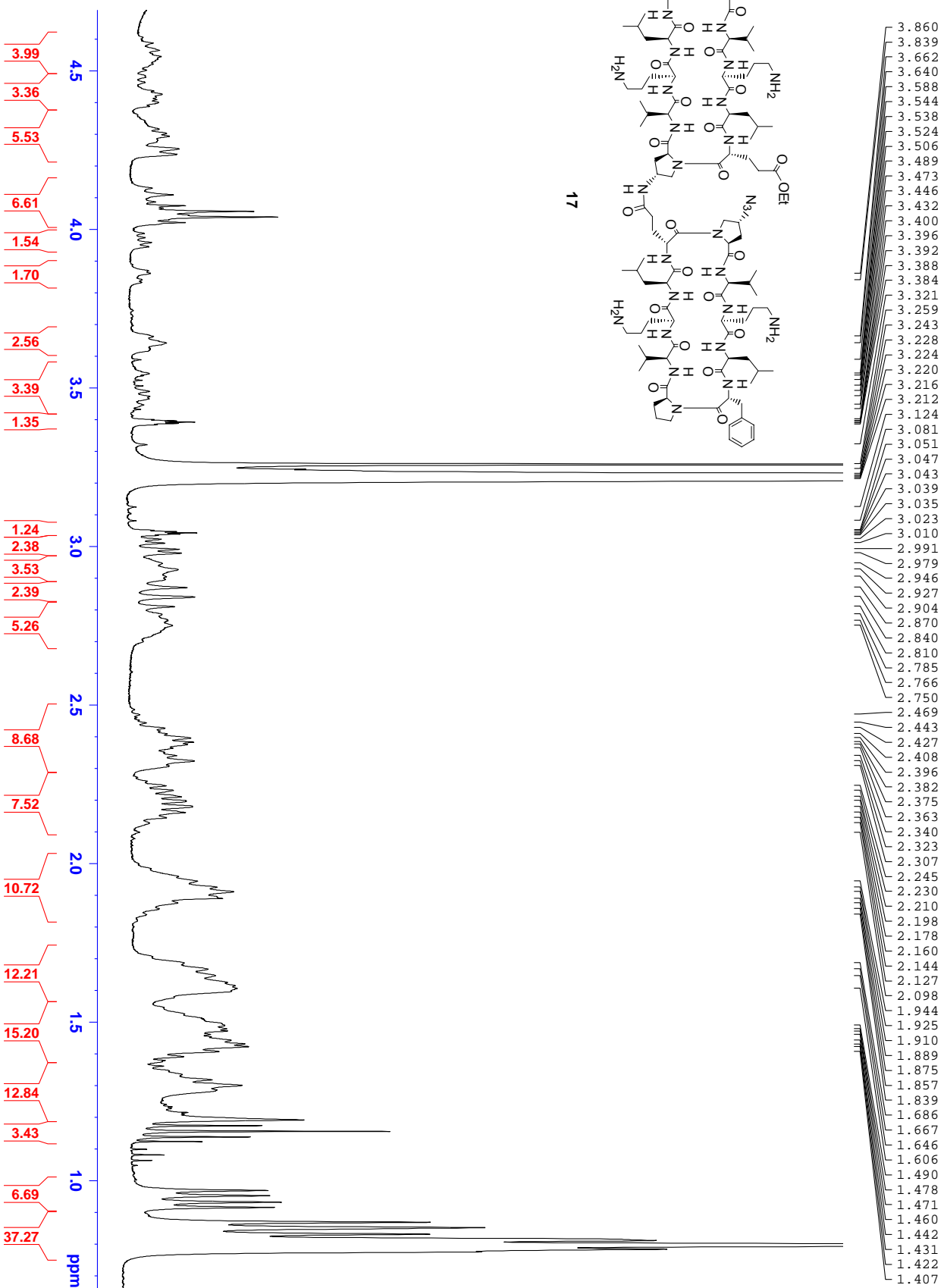
```

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         0
SOLVENT     H2O
NS           1024
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
MCMRFX      0.01500000 sec
===== CHANNEL f1 =====
NUC1         1H
P1           7.30 use
PL1          4.00 dB
PL2          58.54 dB
PL3          0
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



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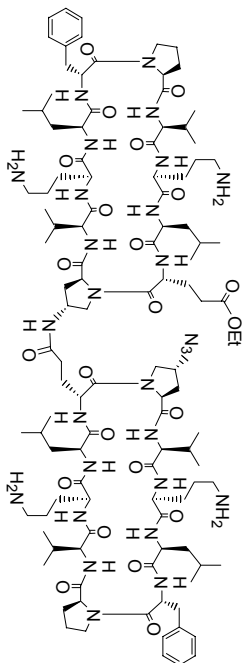
```

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
DDE          0.0002000 sec
MORSEST     0.00000000 sec
MCWRRK      0.01500000 sec

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

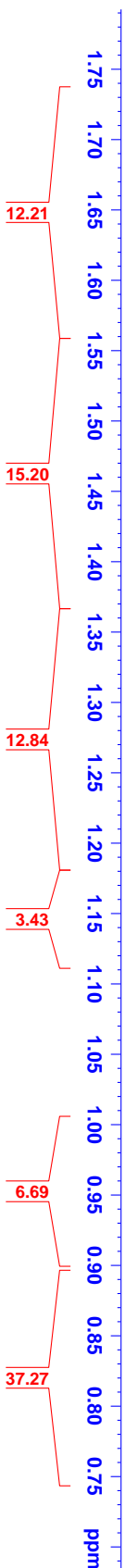
F2 - Processing parameters
SI           32768
SF           400.1300435 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
```

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	

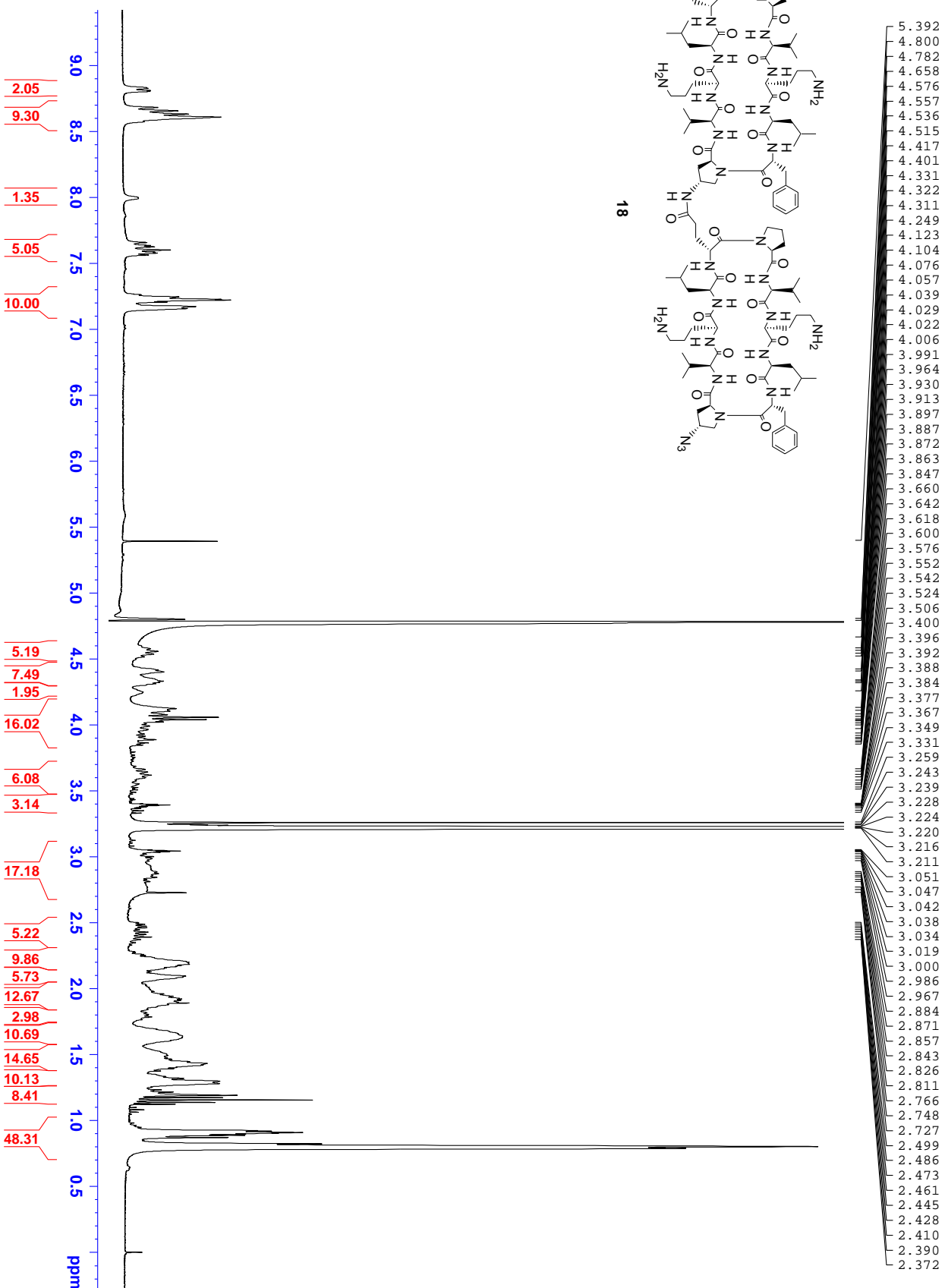
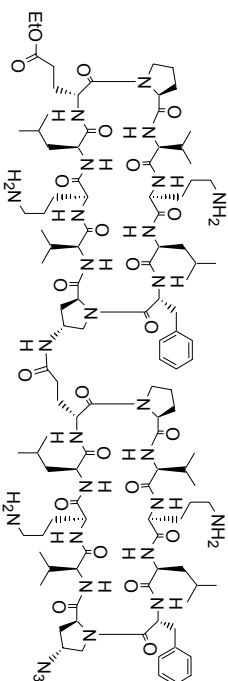


```

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     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           8.50 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          58.54 dB
PL3          400.1319575 MHz
SFO1         400.1319575 MHz

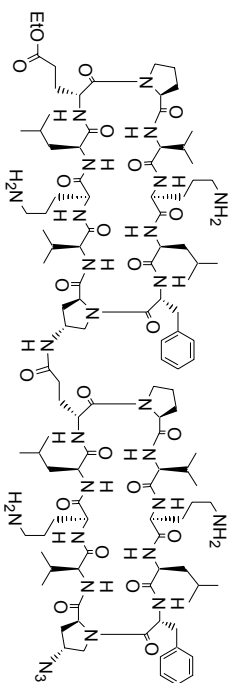
F2 - Processing parameters
SI           32768
SF           400.1300435 MHz
WDW          EM
SSB          0
LB           0.00 Hz
GB           0
PC           1.00
  
```



```

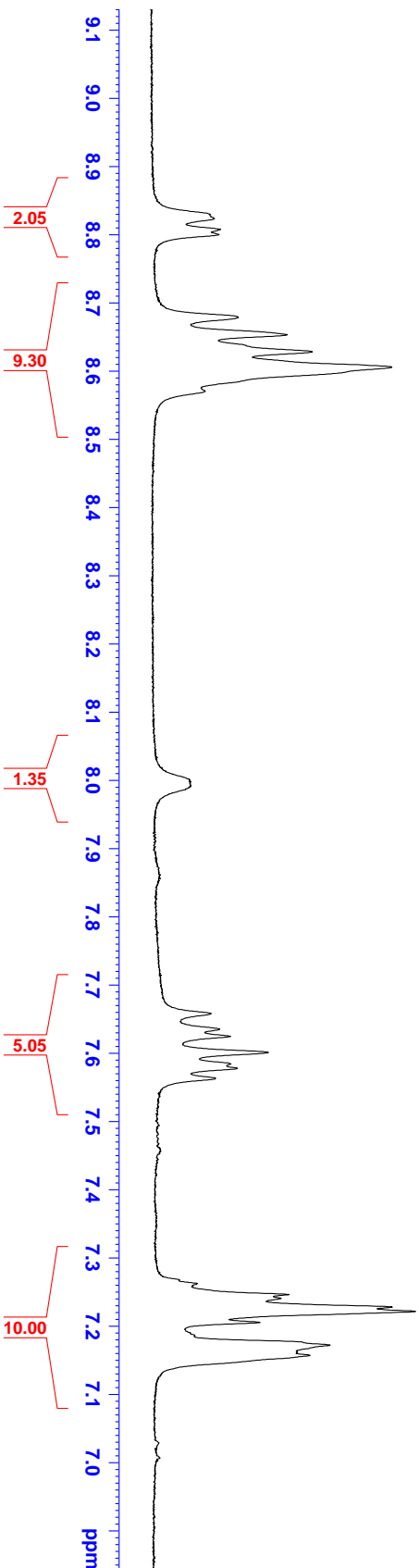
Current Data Parameters
NAME          G1J5092004
EXPNO         4
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time          13.00
INSTRUM       advanced400
PROBHD        5 mm BBI 1H-BB
PULPROG       zgpr
TD            19228
SOLVENT       MeOD
NS            1024
DS            0
SWH           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            1.0000200 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	



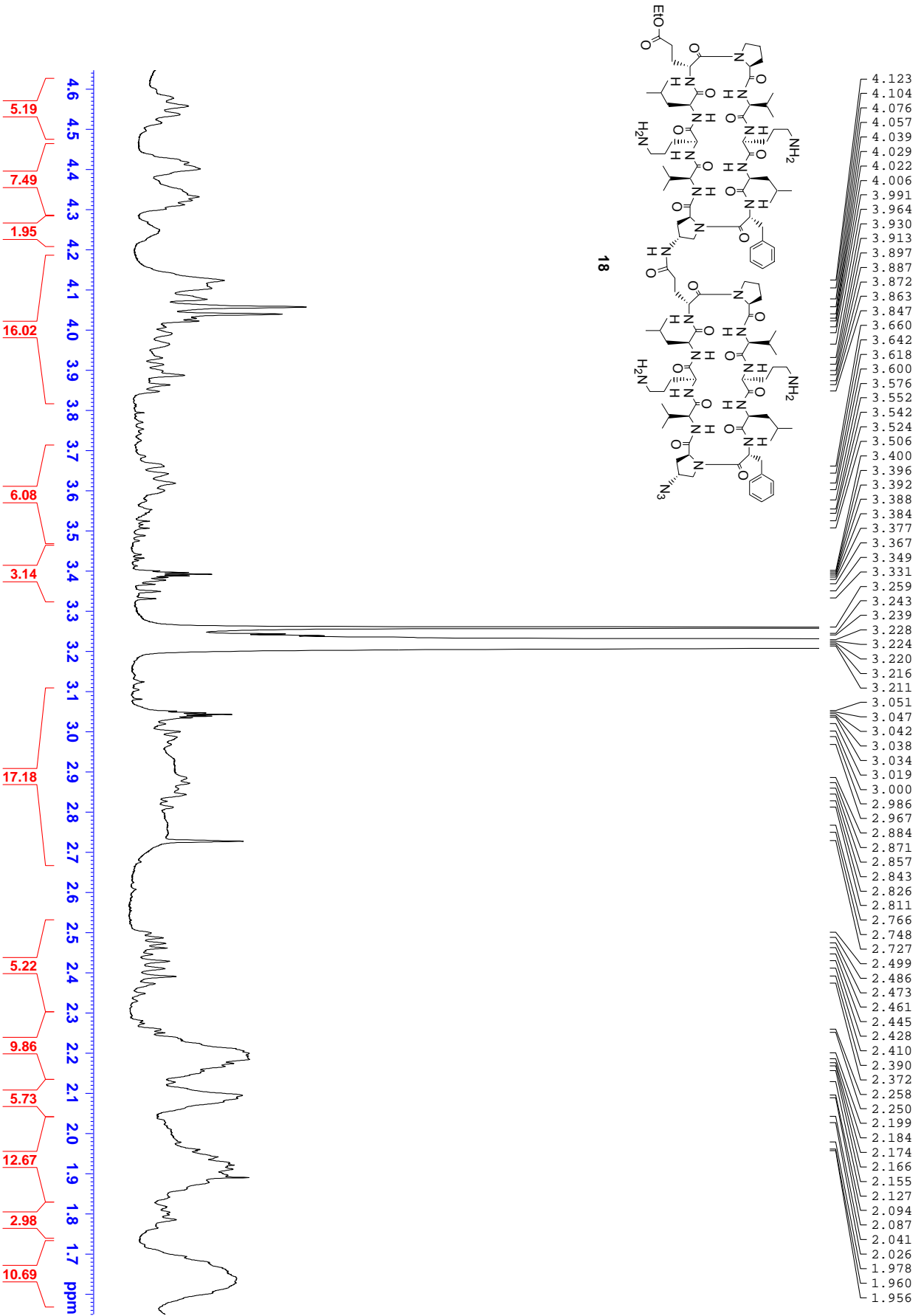
```

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
SOLVENT     MeOD
NS          1024
DS          0
SWH         4807.692 Hz
FIDRES     0.250036 Hz
AQ         1.9997621 sec
RG         256
DE         104.000 use
TE         8.50 use
D1         2.9810 K
d12        1.0000200 sec
MCREPST    0.0000000
MCWRRK     0.01500000 sec

===== CHANNEL f1 =====
NUC1        1H
P1          7.30 use
PL1         4.00 dB
PL2         60.89 dB
PL3         0
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



4.123
4.104
4.076
4.057
4.039
4.029
4.022
4.006
3.991
3.964
3.930
3.913
3.897
3.887
3.872
3.863
3.847
3.660
3.642
3.618
3.600
3.576
3.552
3.542
3.524
3.506
3.400
3.396
3.392
3.388
3.384
3.377
3.367
3.349
3.331
3.259
3.243
3.239
3.228
3.224
3.220
3.216
3.211
3.051
3.047
3.042
3.038
3.034
3.019
3.000
2.986
2.967
2.884
2.871
2.857
2.843
2.826
2.811
2.766
2.748
2.727
2.499
2.486
2.473
2.461
2.445
2.428
2.410
2.390
2.372
2.258
2.250
2.199
2.184
2.174
2.166
2.155
2.127
2.094
2.087
2.041
2.026
1.978
1.960
1.956

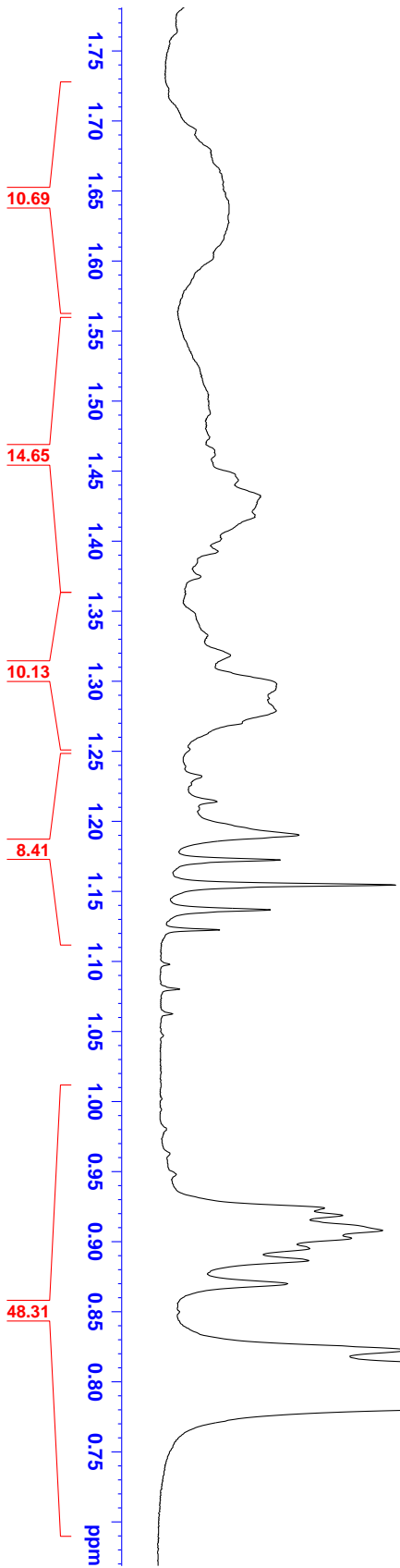
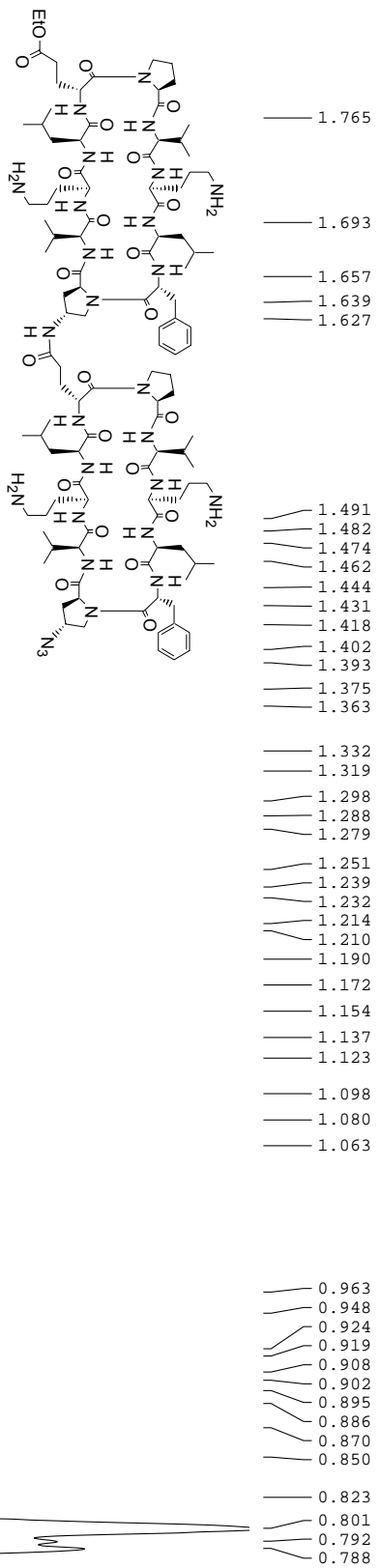
```

Current Data Parameters
NAME          G15052004
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
D1           1.00000000 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

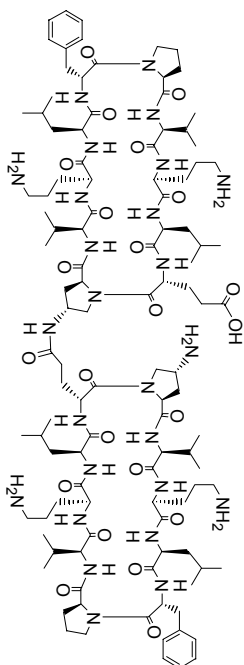
F2 - Processing parameters
SI           32768
SF           400.1300436 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
```

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

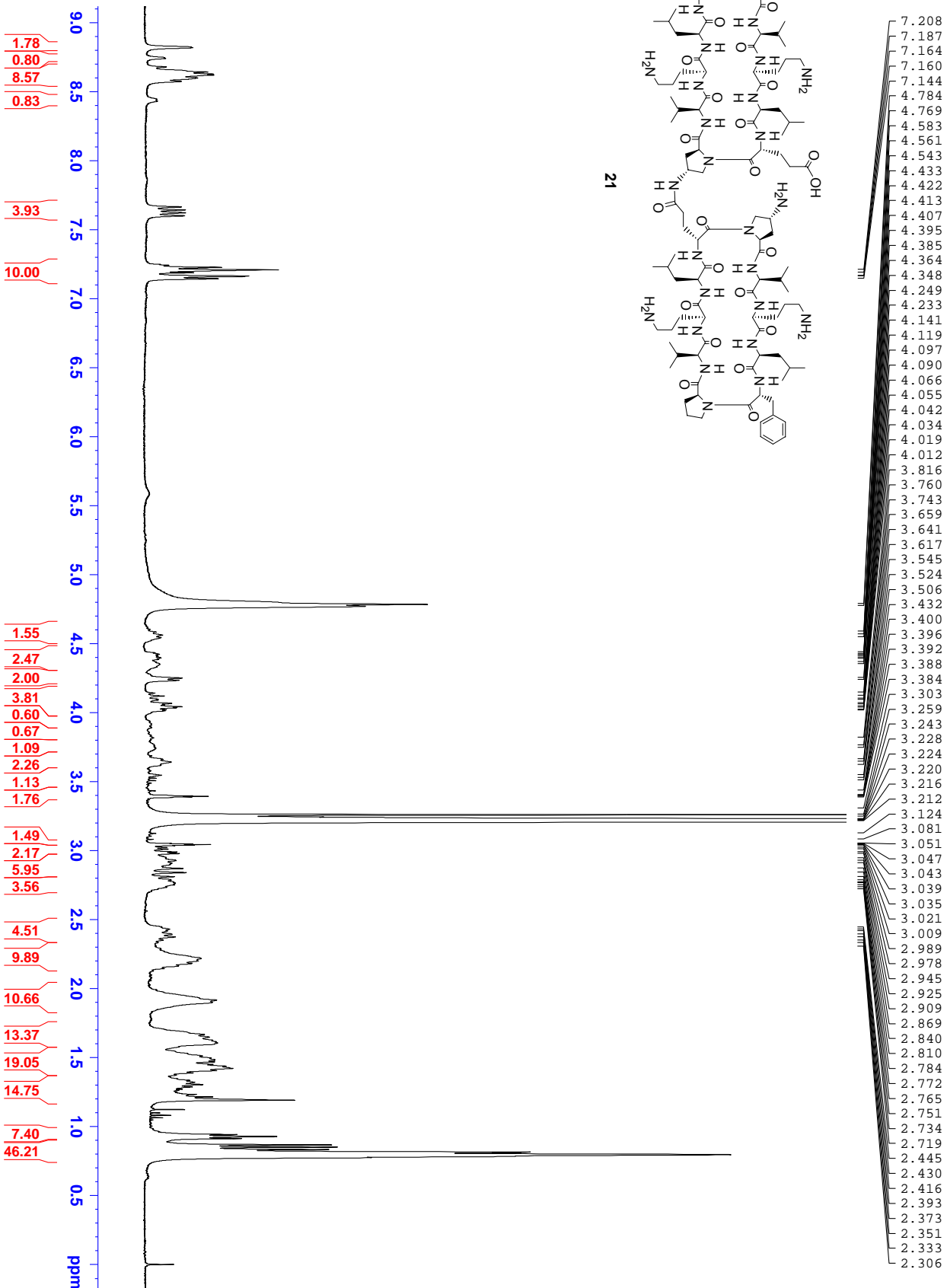


Current Data Parameters
NAME G158092004
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20040915
Time 13.00
INSTRUM avance400
PROBHD 5 mm BBI 1H-BB
PULPROG zgpg
TD 19228
SOLVENT MeOD
NS 1024
DS 0
SWH 4807.692 Hz
FIDRES 0.250036 Hz
AQ 1.9997621 sec
RG 256
DW 104.000 usec
DE 8.90 usec
TE 298.0 K
D1 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

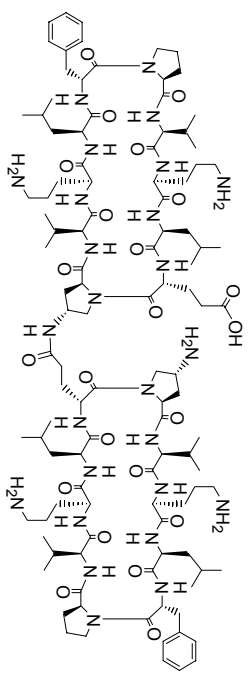


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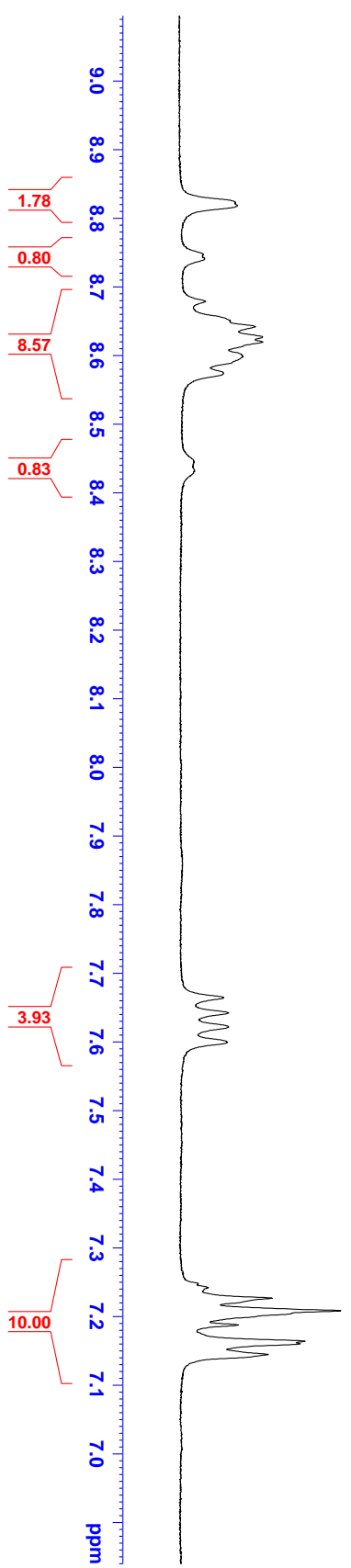
Current Data Parameters
 NAME G13092004
 EXPNO 3
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20040915
 Time 11.43
 INSTRUM avance400
 PROBD 5 mm BBI 1H-BB
 PULPROG zgpg
 TD 19228
 SOLVENT MeOD
 NS 1024
 DS 0
 SWH 4807.692 Hz
 FIDRES 0.250036 Hz
 AQ 1.9997621 sec
 RG 256
 DW 104.000 usec
 DE 8.50 usec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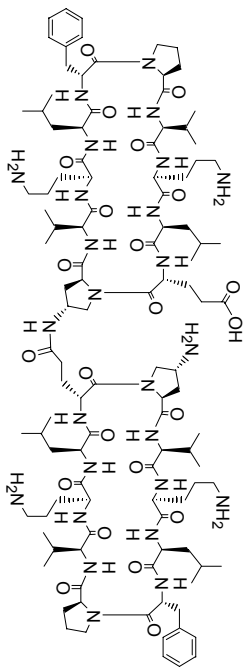
```

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
TE            28.50 usec
DE            28.50 K
D1            1.0000200 sec
d12           0.0000200 sec
MCPRST       0.0000000
MCRMK        0.01500000 sec

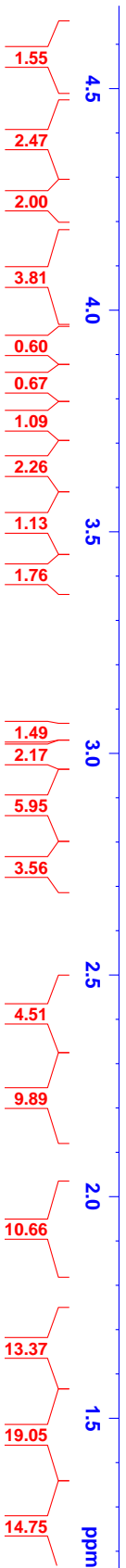
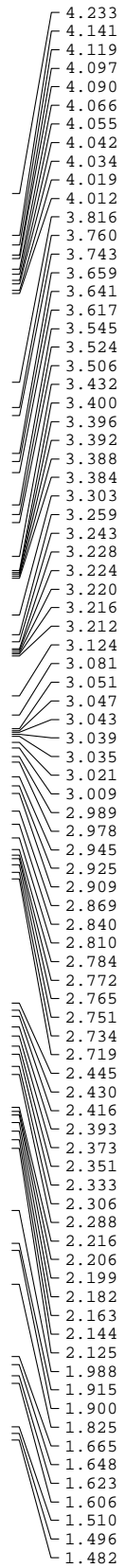
===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL9           58.54 dB
SFO1         400.1319575 MHz

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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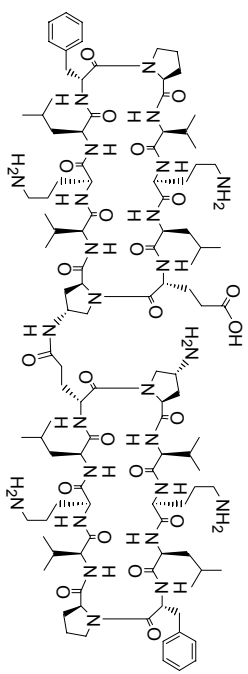
```

Current Data Parameters
NAME          G1J5092004
EXPNO         3
PROCNO        1
F2 - Acquisition Parameters
Date_         20040915
Time_         11.43
INSTRUM       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
MCWRES       0.00000000 sec
MCRX         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	



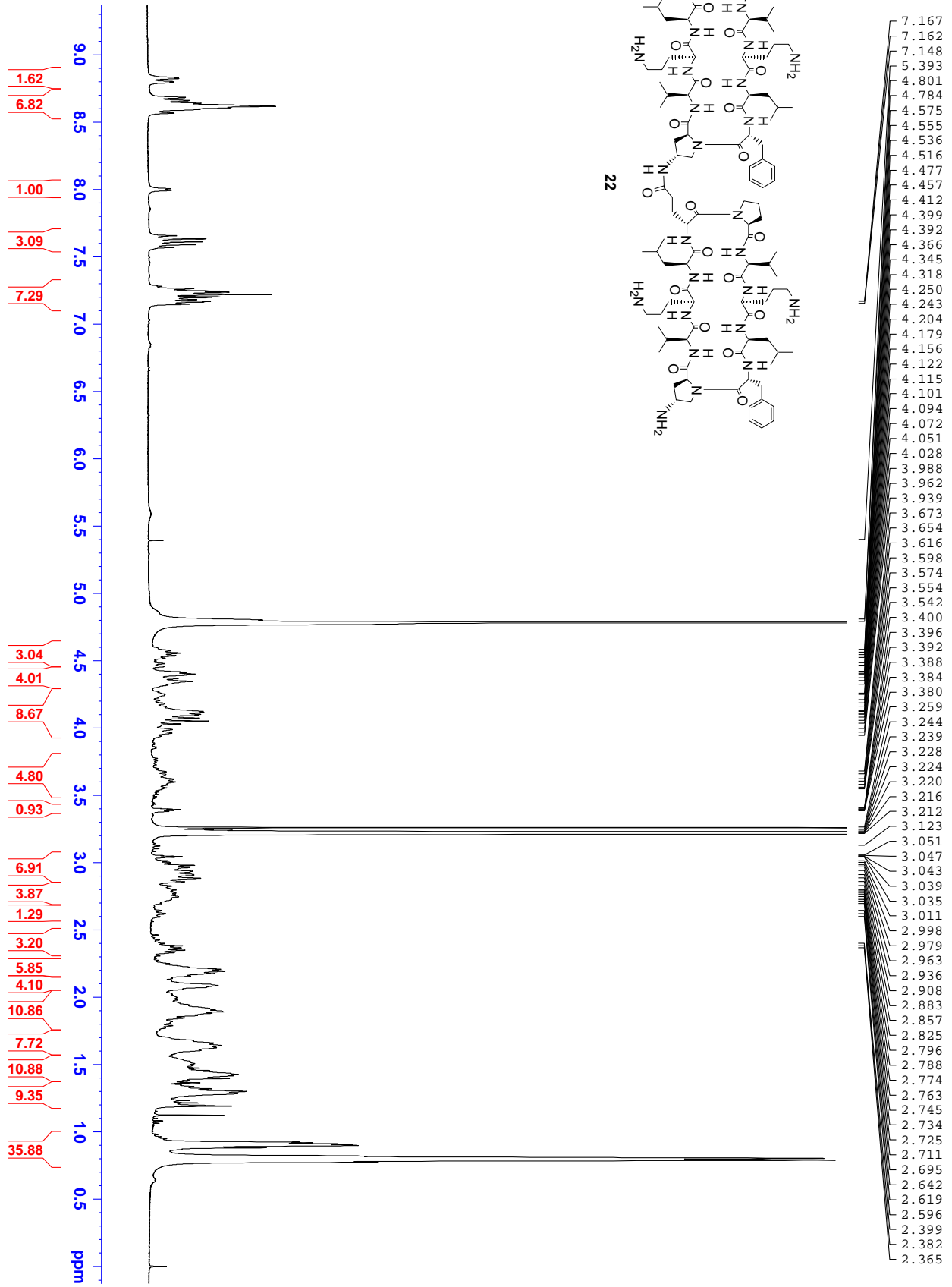
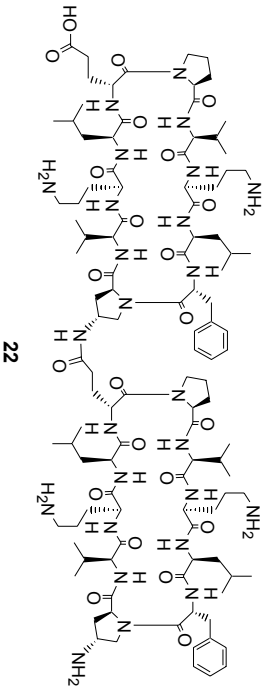
```

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           58.54 dB
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

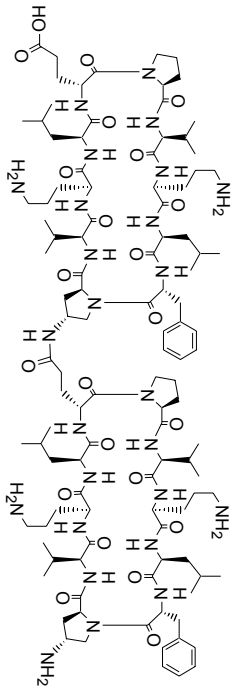


7.167
7.162
7.148
5.393
4.801
4.784
4.575
4.555
4.536
4.516
4.477
4.457
4.412
4.399
4.392
4.366
4.345
4.318
4.250
4.243
4.204
4.179
4.156
4.122
4.115
4.101
4.094
4.072
4.051
4.028
3.988
3.962
3.939
3.673
3.654
3.616
3.598
3.574
3.554
3.542
3.400
3.396
3.392
3.388
3.384
3.380
3.259
3.244
3.239
3.228
3.224
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

```

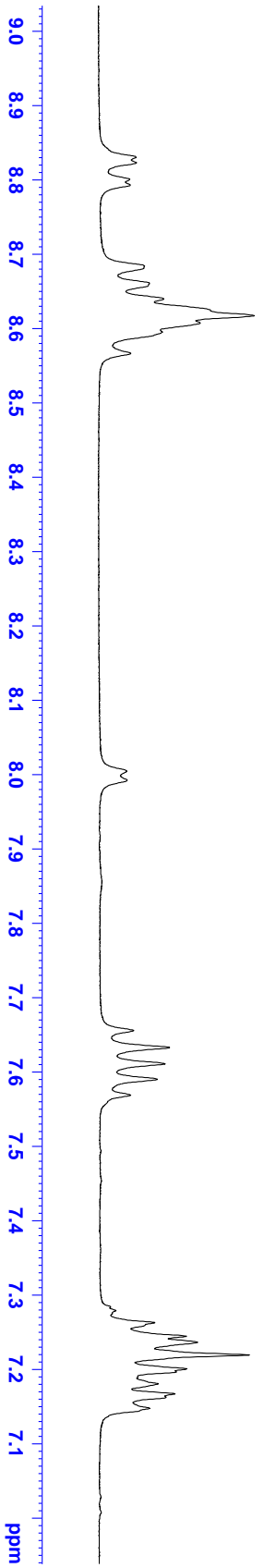
Current Data Parameters
NAME          G15092004
EXPNO         5
PROCNO       1
F2 - Acquisition Parameters
Date_         20040915
Time_        14.09
INSTRUM      avance400
PROBHD       5 mm BBI 1H-BB
PULPROG      zgpg
TD            19228
SOLVENT      MeOD
NS            1024
DS            0
SWH           4807.692 Hz
FIDRES       0.250036 Hz
AQ           1.9997621 sec
RG            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

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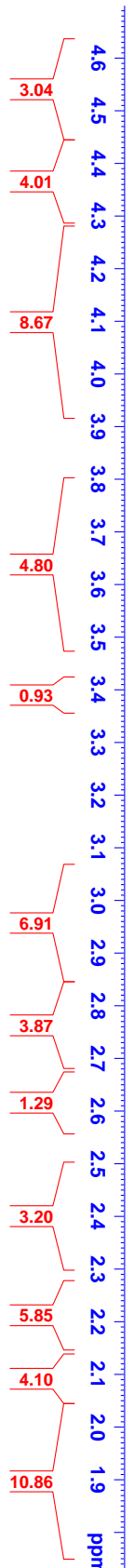
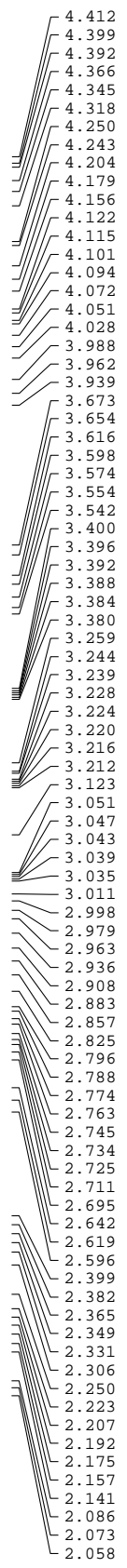
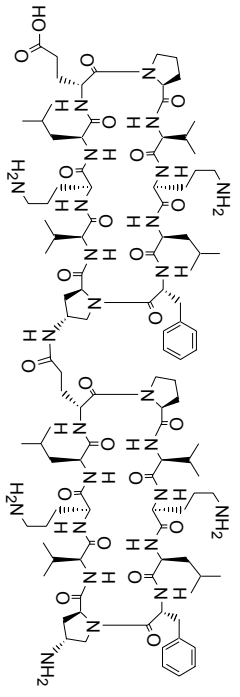
Current Data Parameters
 NAME G1J5092004
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040915
 Time 14.09
 INSTRUM advance400
 PROBHD 5 mm BBI 1H-BB
 PULPROG zgpr
 TD 19228
 MeOD
 SOLVENT MeOD
 NS 1024
 DS 0
 SWH 4807.692 Hz
 FIDRES 0.250036 Hz
 AQ 1.9997621 sec
 RG 286
 DE 104.000 use
 DM 8.50 use
 PE 28.0 K
 DI 1.0000200 sec
 d12 0.0000200 sec
 MCPRST 0.0000000 sec
 MCMRK 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



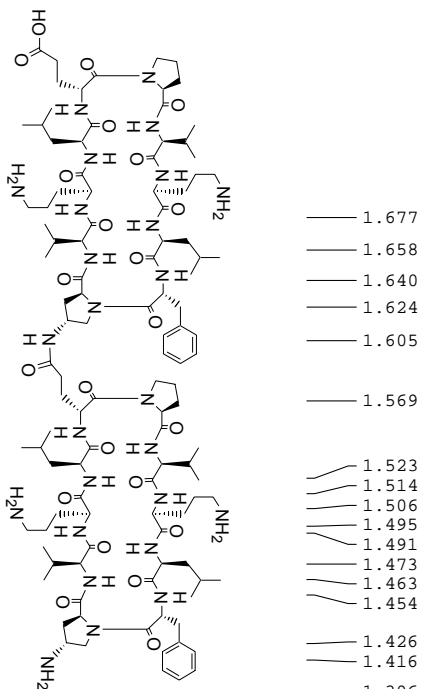
Current Data Parameters
 NAME G15012004
 EXNO 5
 PROCNO 1

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
 MCOREST 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

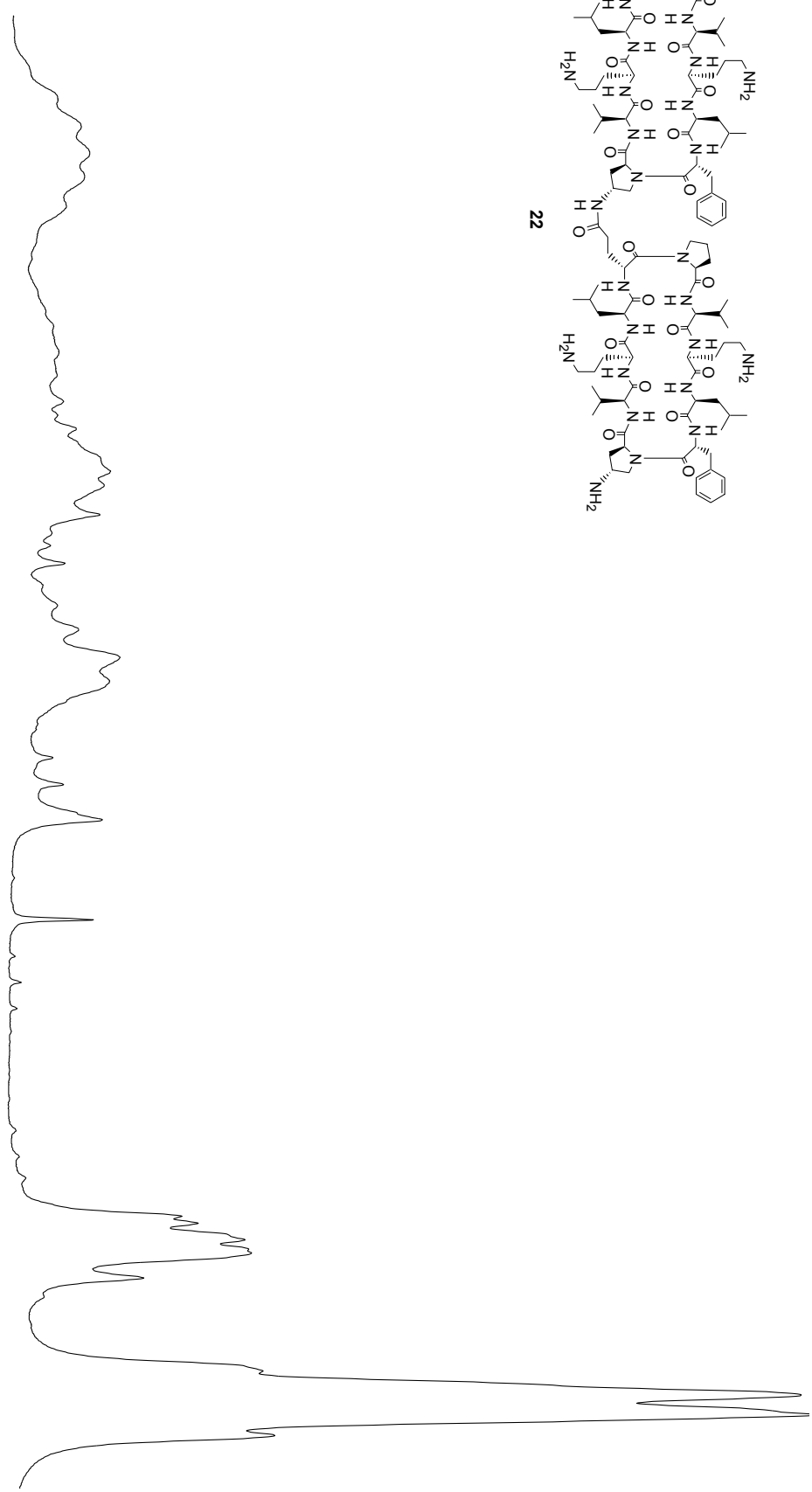
F2 - Processing parameters
 SI 32768
 SF 400.1300433 MHz
 WDM EM
 SSB 0
 GB 0.00 Hz
 CB 0
 PC 1.00

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



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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
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

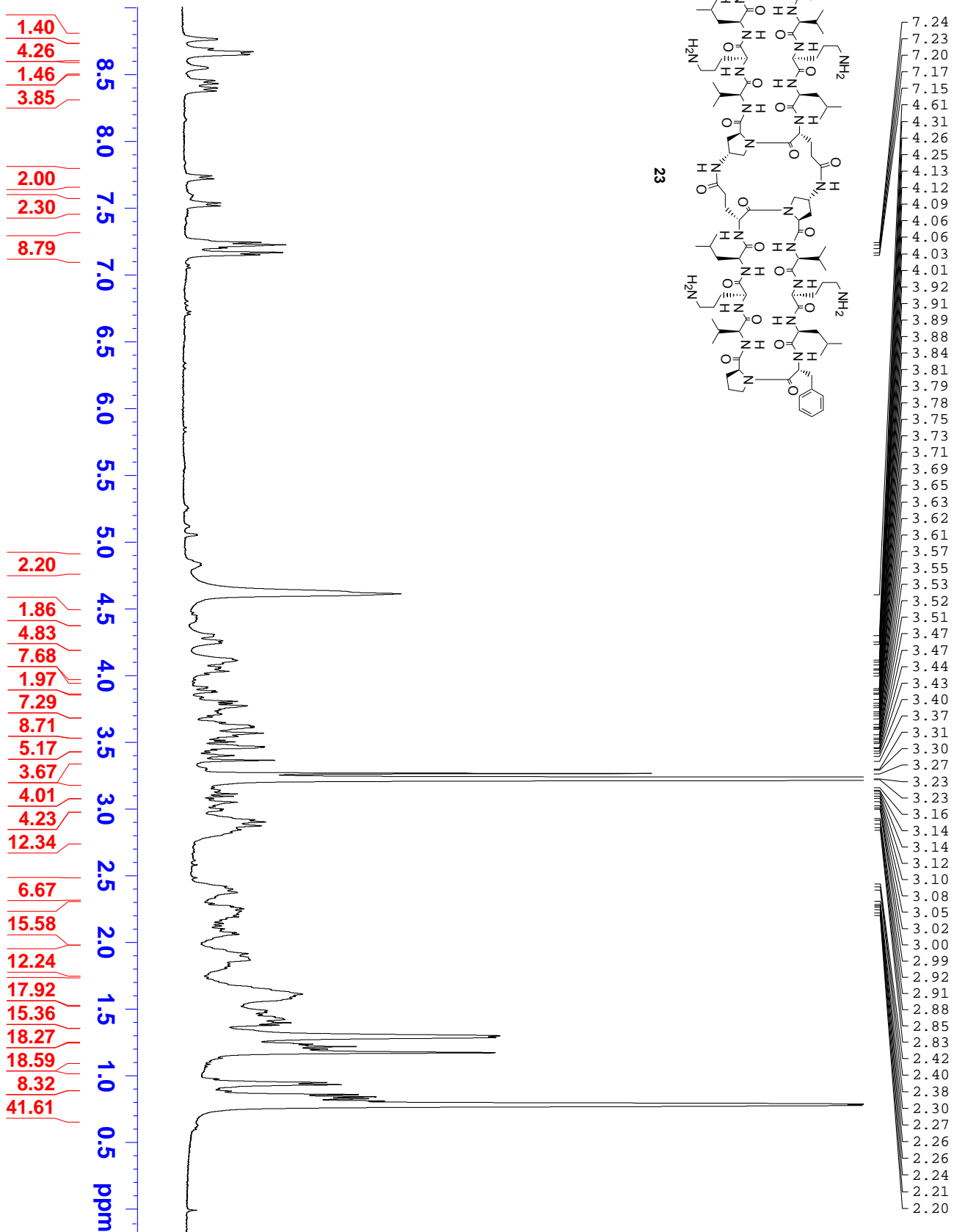
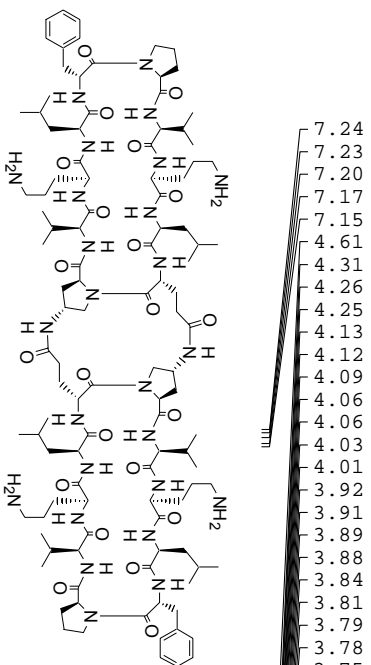


1.70 1.65 1.60 1.55 1.50 1.45 1.40 1.35 1.30 1.25 1.20 1.15 1.10 1.05 1.00 0.95 0.90 0.85 0.80 ppm

7.72 10.88 9.35 35.88

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 =====
 NUCL1 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



```

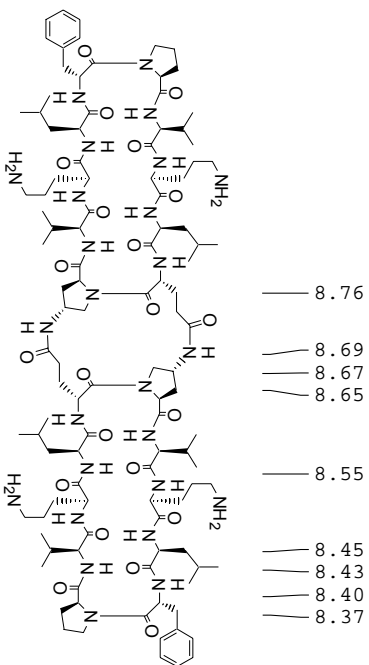
Current Data Parameters
NAME      G1Jsr72003
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20030723
Time      10.20
INSTRUM   avance400
PROBHD    5 mm BBI-BS
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

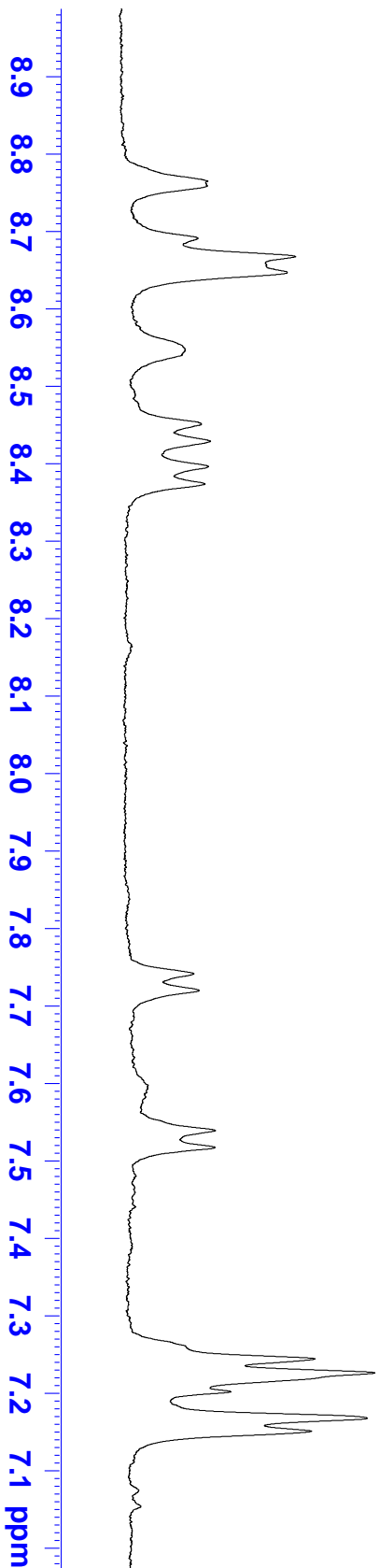
F2 - Processing parameters
SI         131072
SF         400.1300389 MHz
WDW        EM
SSB        0
LB         0.50 Hz
GB         0
PC         1.00
    
```

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	



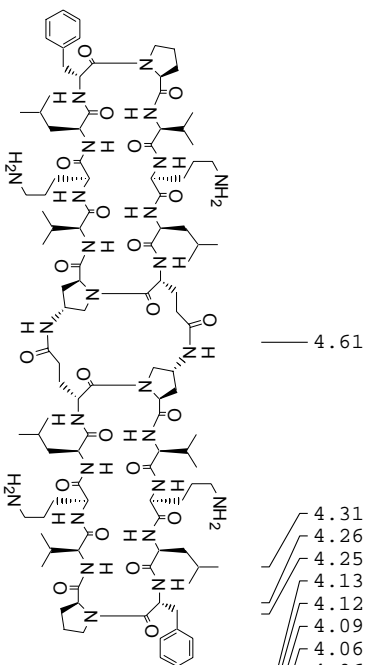
```

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            2
SFE          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

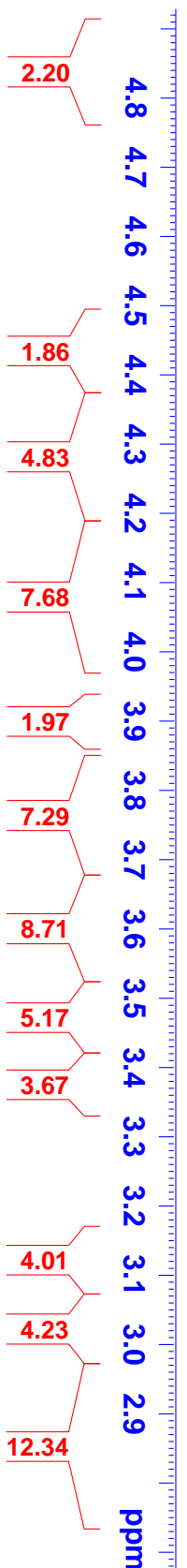
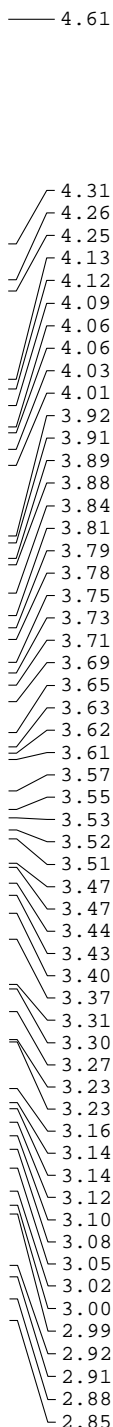
===== CHANNEL f1 =====
NUC1          1H
P1            7.30 usec
PL1           4.00 dB
PL19          58.19 dB
SF01          400.1318653 MHz

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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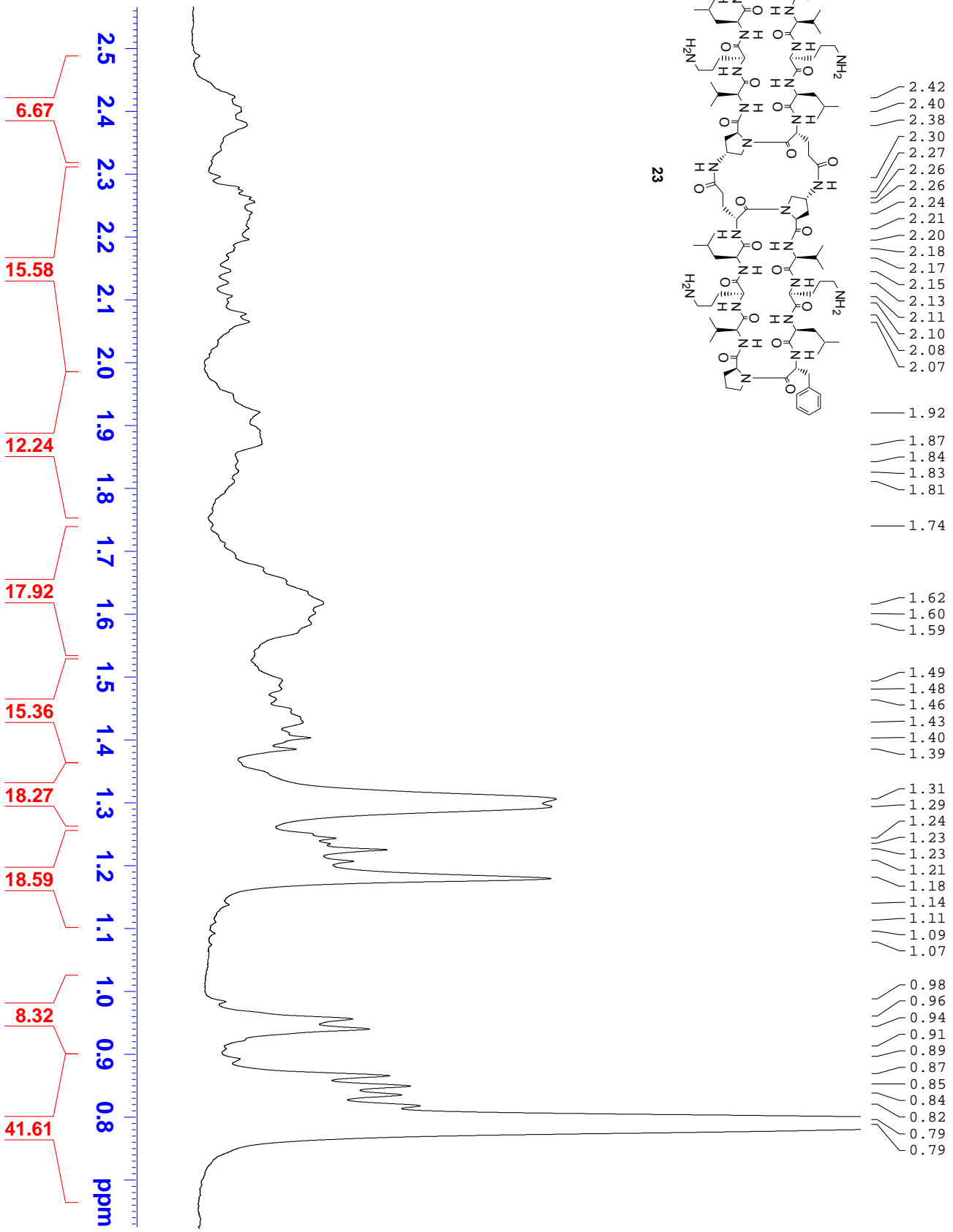
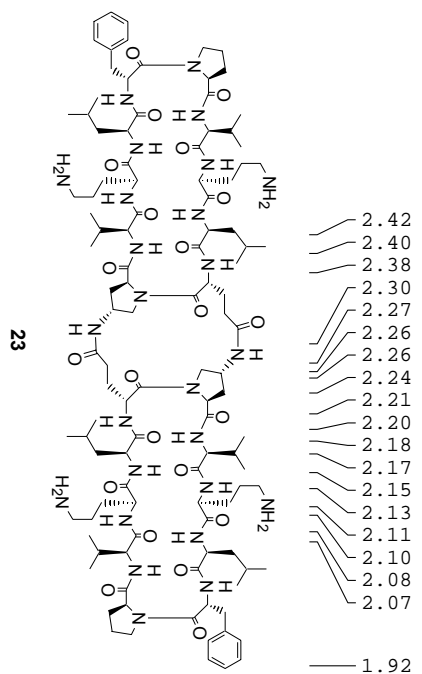
```

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       400.1318853 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



2.42	2.40	2.38	2.30	2.27	2.26	2.24	2.21	2.20	2.18	2.17	2.15	2.13	2.11	2.10	2.08	2.07	1.92	1.87	1.84	1.83	1.81	1.74	1.62	1.60	1.59	1.49	1.48	1.46	1.43	1.40	1.39	1.31	1.29	1.24	1.23	1.23	1.21	1.18	1.14	1.11	1.09	1.07	0.98	0.96	0.94	0.91	0.89	0.87	0.85	0.84	0.82	0.79
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

```

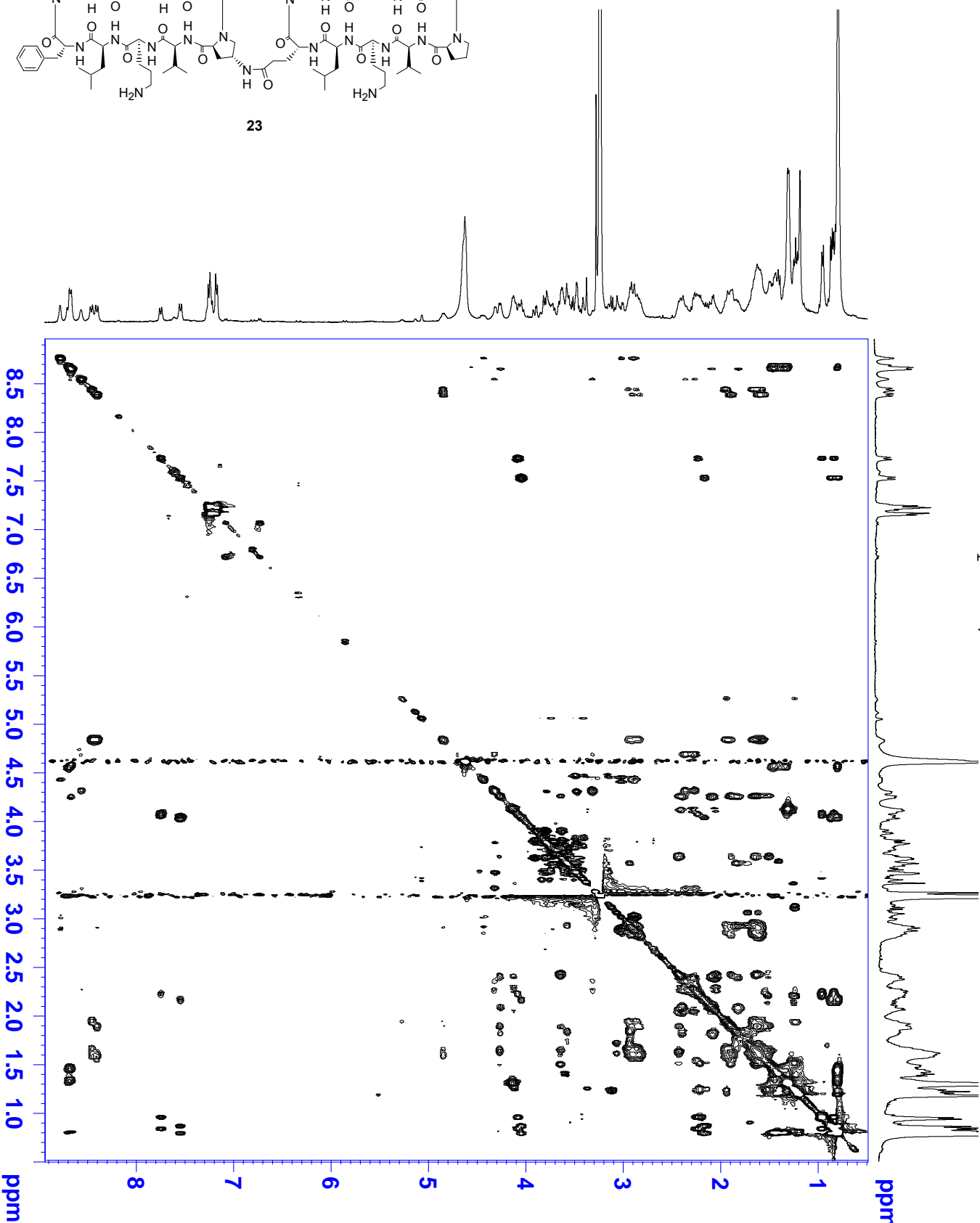
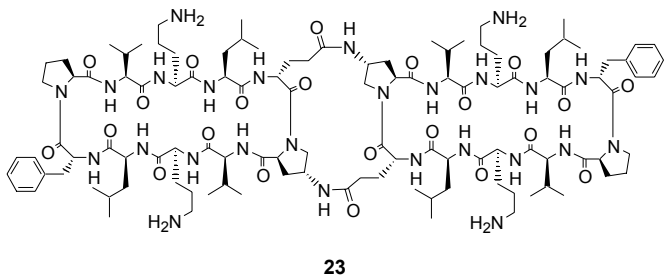
Current Data Parameters
NAME      G4js072003
EXPNO     1
PROCNO    2

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         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 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

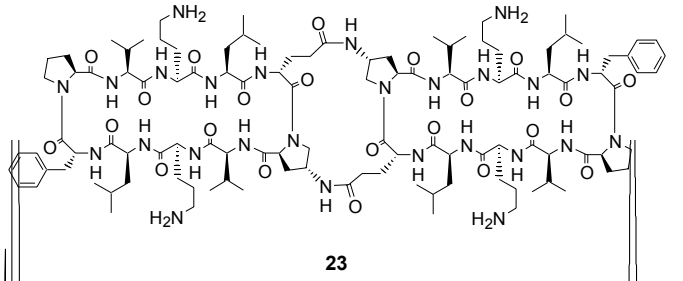
===== CHANNEL f1 =====
 NUC1 1H
 P1 6.10 usec
 P5 16.67 usec
 P6 25.00 usec
 P7 50.00 usec
 P17 2500.00 usec
 PL1 4.00 dB
 PL9 58.51 dB
 PL10 16.50 dB
 SFO1 400.1318941 MHz

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

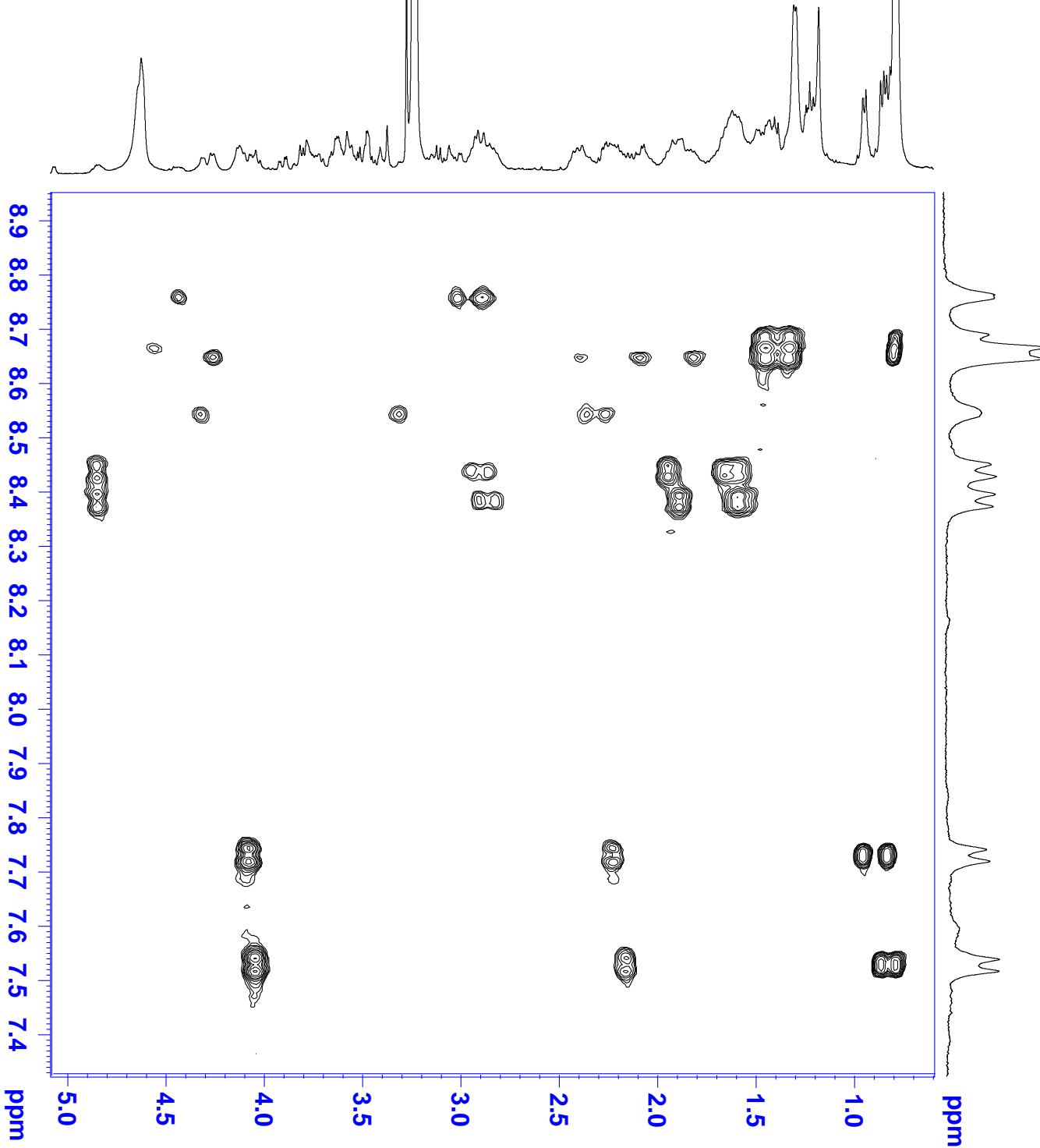
F2 - Processing parameters
 SI 2048
 SF 400.1300389 MHz
 MDW QSIGN2
 SSB 2.3 Hz
 LB 0.00 Hz
 GB 1.40
 PC

F1 - Processing parameters
 SI 1024
 M2 States-TPPI
 SF 400.1300389 MHz
 MDW QSIGN2
 SSB 2.1 Hz
 LB 0.00 Hz
 GB 0

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 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

TD 1.0000000 sec
 D0 0.0300000 sec
 d11 0.0000200 sec
 d12 0.0000400 sec
 d13 0.0000600 sec
 D20 0.00020800 sec
 INO 18
 MCREST 0.0000000 sec
 MCWRK 0.00999999 sec
 STCNT 256

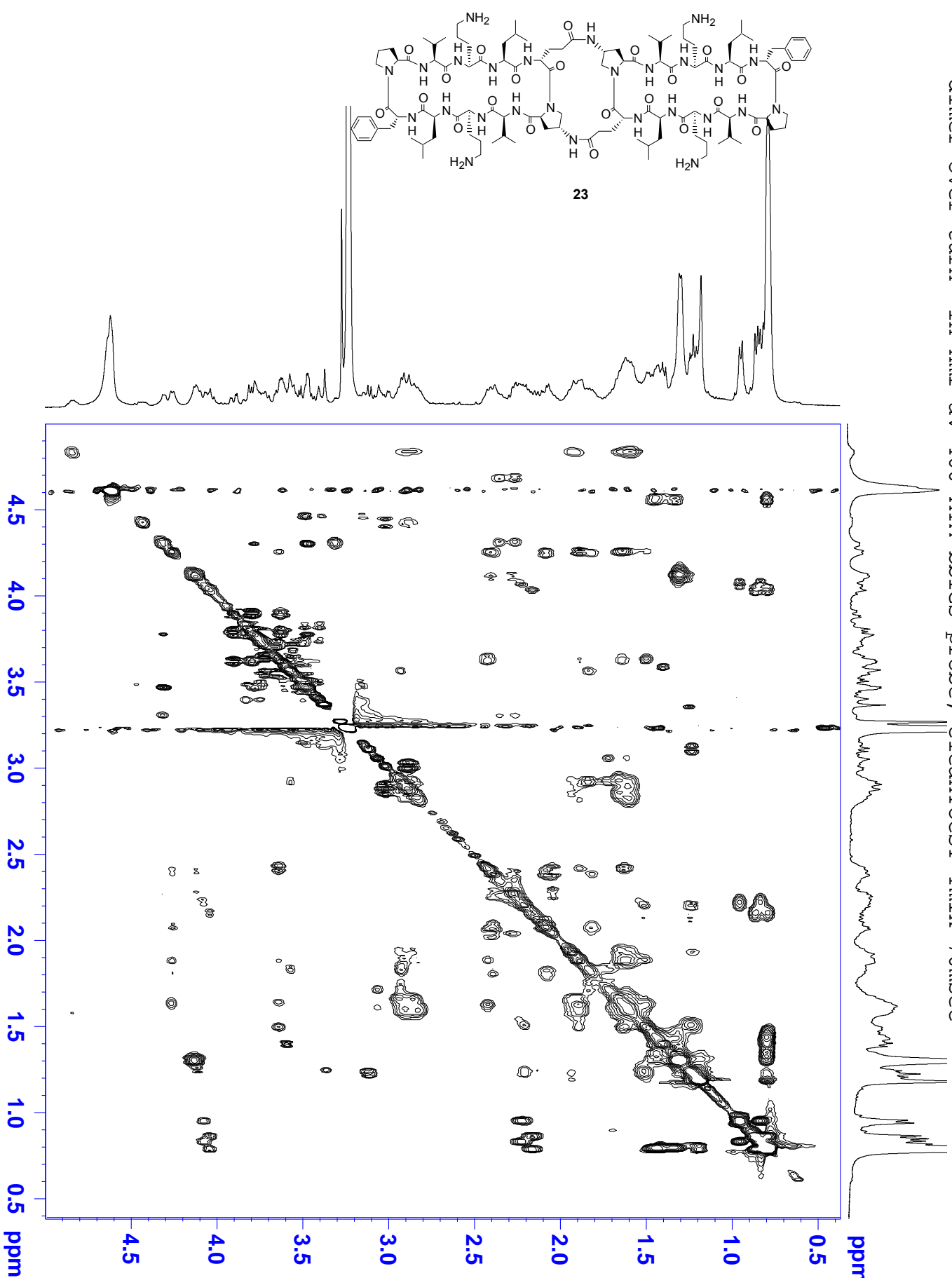
===== CHANNEL f1 =====
 NUC1 1H
 P1 6.10 usec
 P5 16.67 usec
 P6 25.00 usec
 P7 50.00 usec
 P17 2500.00 usec
 PL1 4.00 dB
 PL9 58.51 dB
 PL10 16.50 dB
 SFO1 400.1318941 MHz

F1 - Acquisition Parameters
 FID 512
 SFO1 400.1319 MHz
 FIDRES 9.390024 Hz
 SW 12.015 ppm
 ENMODE 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



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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
 TUPROG ctmlePFG2
 PULPROG zgpg30

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

TD 0
 D1 1.0000000 sec
 d11 0.0300000 sec
 d12 0.0000200 sec
 d13 0.0000400 sec
 D20 0.0000650 sec
 INO 0.00020800 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 400.1318941 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
 WDW QSI
 SSB 2.3 Hz
 LB 0.70 Hz
 GB 1.40

PC 1.40
 F1 - Processing parameters
 SI 1024
 MCF2 States-TPPI
 SF 400.1300389 MHz
 WDW QSI
 SSB 2.1 Hz
 LB 0.70 Hz
 GB 0