

Antimalarial Linear Lipopeptides from a Panamanian Strain of the Marine

Cyanobacterium Lyngbya majuscula

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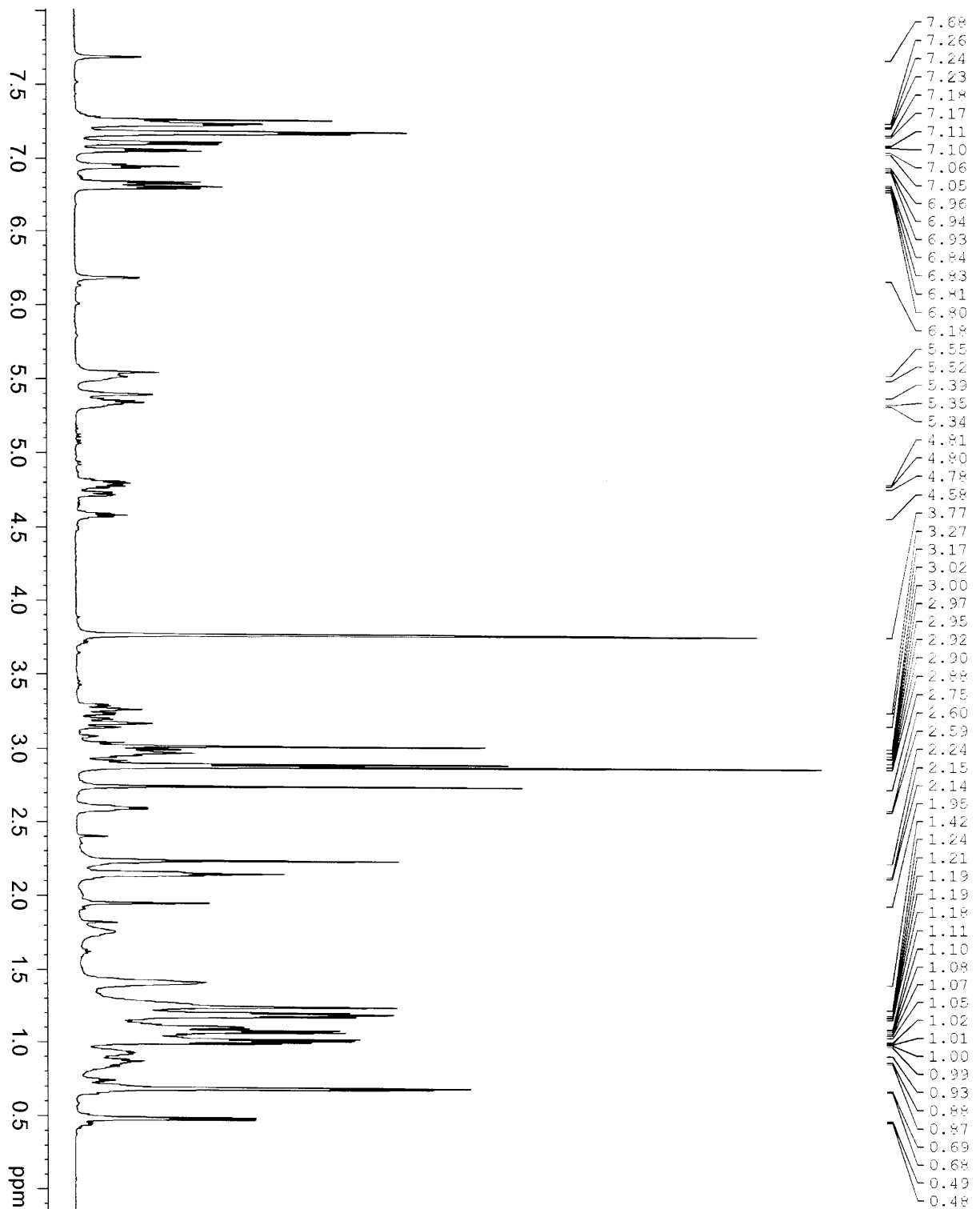
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7.68
7.26
7.24
7.23
7.18
7.17
7.11
7.10
7.06
7.05
6.96
6.94
6.93
6.84
6.83
6.81
6.80
6.18
5.55
5.52
5.39
5.35
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4.81
4.80
4.78
4.58
3.77
3.27
3.17
3.02
3.00
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2.95
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2.90
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1.18
1.11
1.10
1.08
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0.48



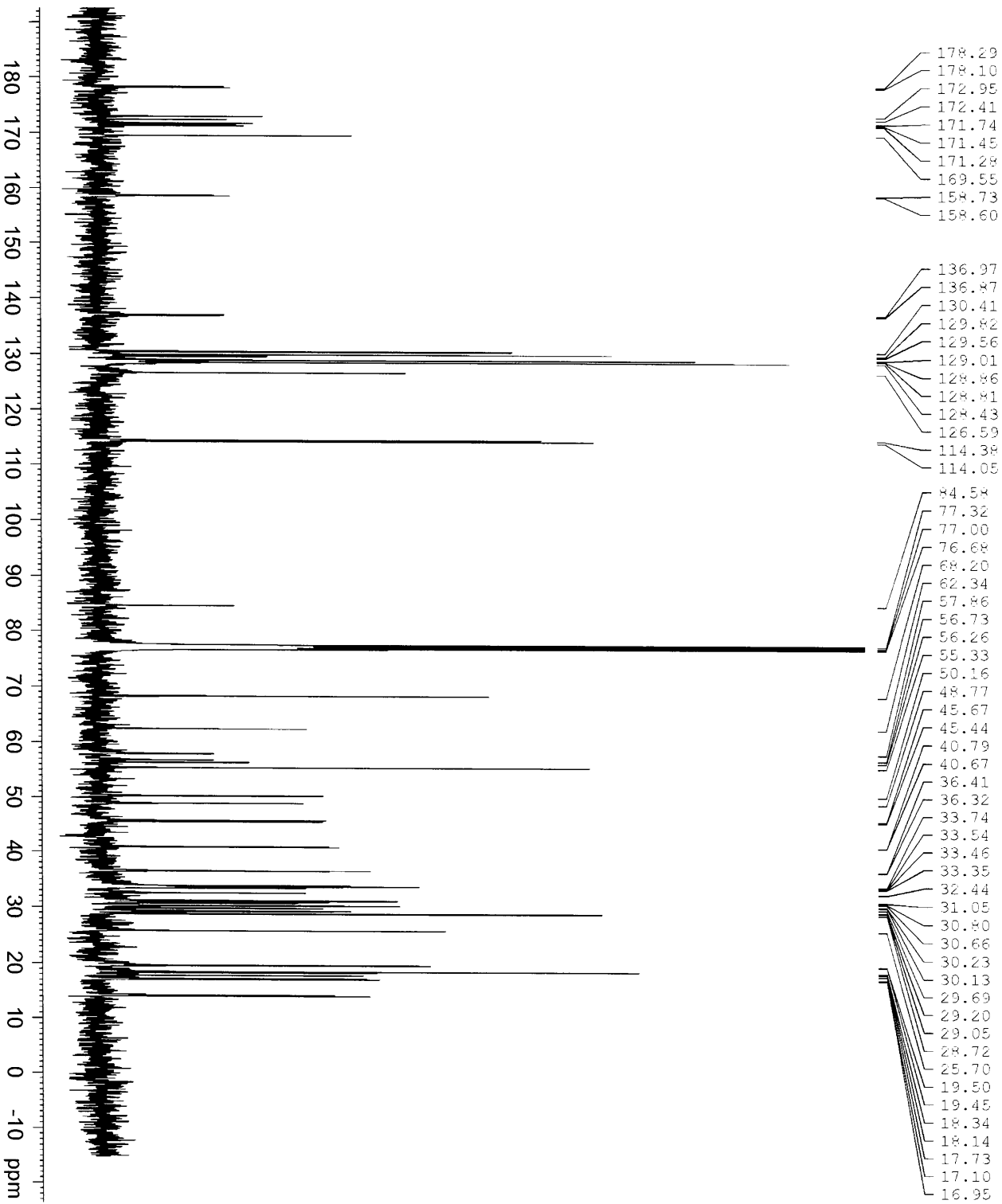
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S1. ¹H NMR Spectrum for Carmabin A (1) in CDCl₃ (600 MHz)



S2. ¹³C NMR Spectrum for Cammabin A (1) in CDCl₃ (100 MHz)

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PROCNO        1

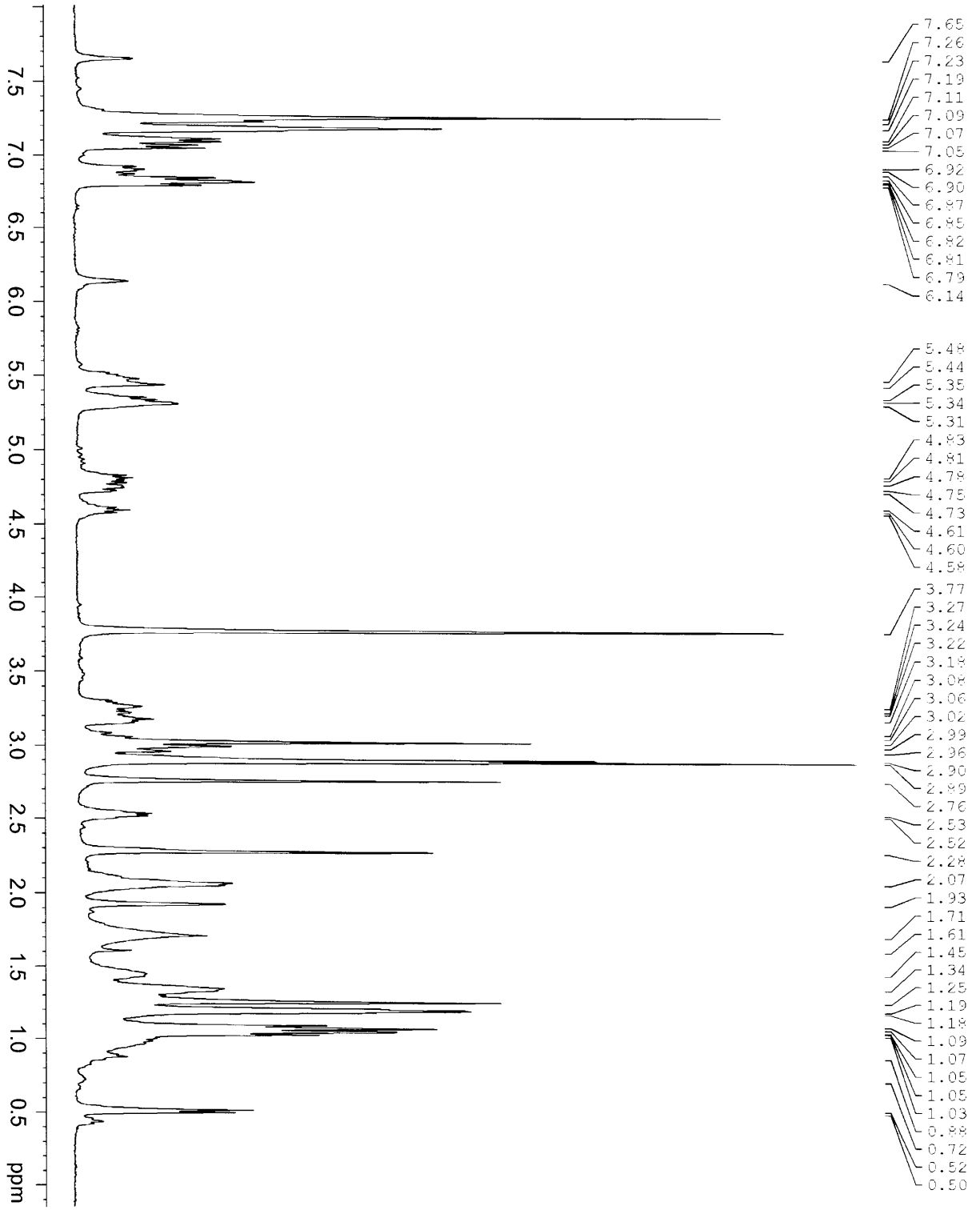
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FIDRES        0.383387 Hz
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D11           0.03000000 sec
D12           0.00002000 sec

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P1            7.50 usec
PL1           -3.00 dB
SFO1         100.5936186 MHz

===== CHANNEL f2 =====
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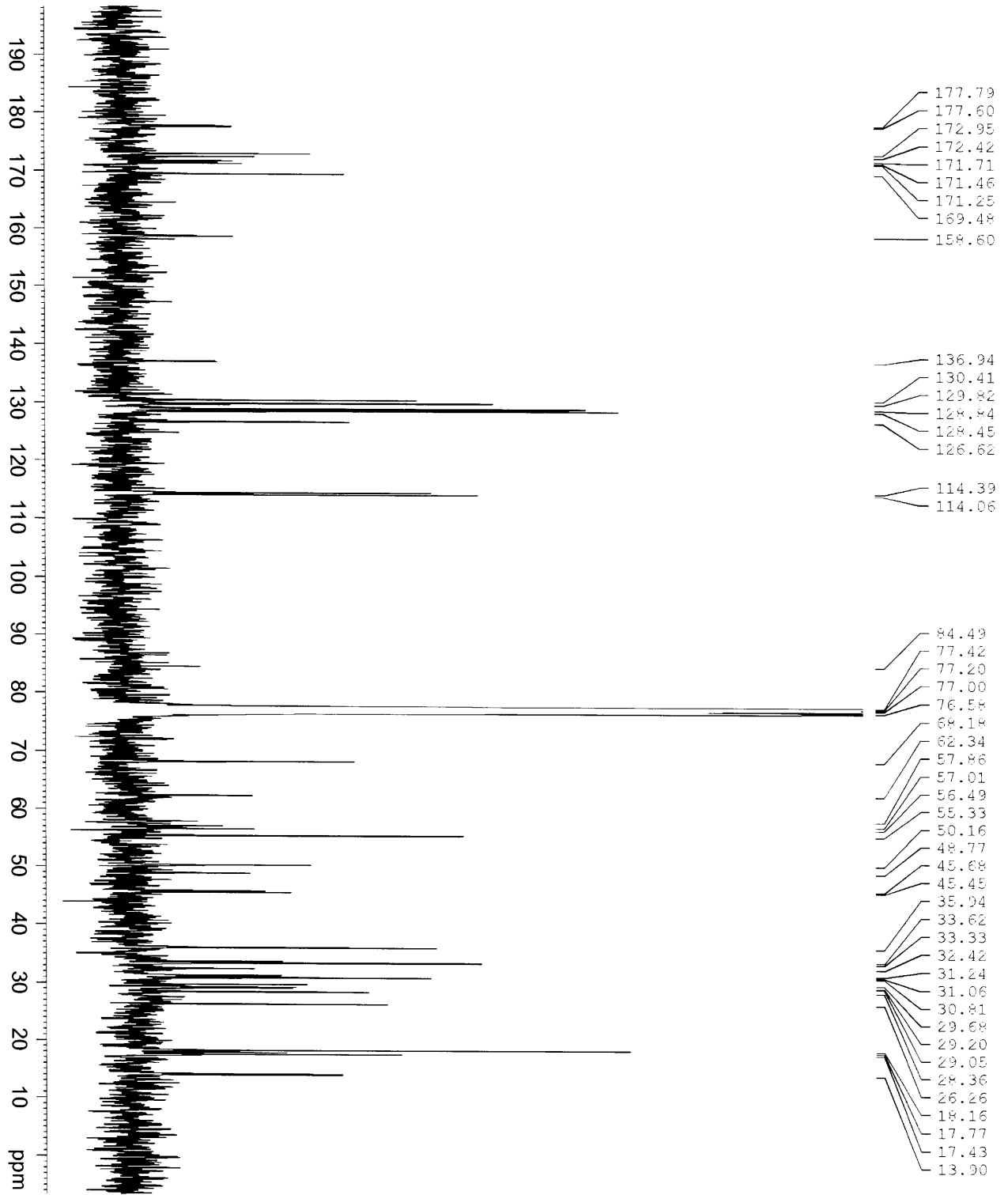
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 PULPROG zgpg30
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 574.7126 Hz
 FIDRES 0.4102661 Hz
 AQ 2.4102661 sec
 RG 456.1
 DW 87.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
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 NUC1 1H
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 SFO1 400.012601 MHz
 F2 - Processing parameters
 SI 65536
 SF 400.0100148 MHz
 HF 0
 SSF 0
 LB 0.70 Hz
 GB 0
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S3. ¹H NMR Spectrum for Dragomabin (2) in CDCl₃ (400 MHz)

S4. ¹³C NMR Spectrum for Dragomabin (2) in CDCl₃ (75 MHz)



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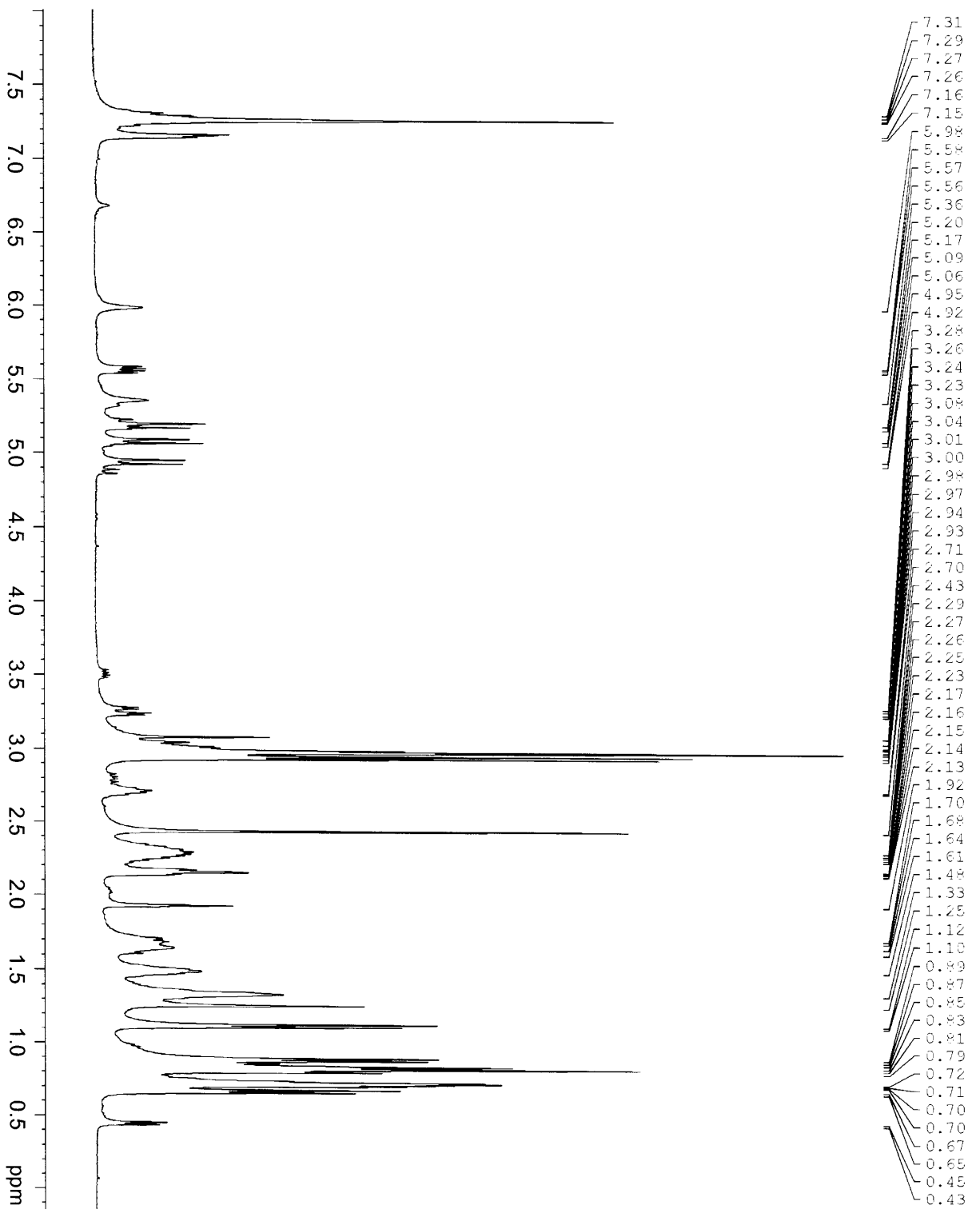
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D12        0.00020000 sec
I2         45

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NUC1       13C
P1         7.60 usec
PL1        -3.00 dB
SFO1       75.4756431 MHz

=====
CHANNEL F2
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
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PL12       17.55 dB
PL13       19.00 dB
SFO2       300.1315007 MHz

F2 - Processing parameters
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WDW        EM
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```



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7.27
7.26
7.16
7.15
5.98
5.98
5.98
5.57
5.56
5.36
5.20
5.17
5.09
5.06
4.95
4.92
3.28
3.26
3.24
3.23
3.08
3.04
3.01
3.00
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2.97
2.94
2.93
2.71
2.70
2.43
2.29
2.27
2.26
2.25
2.23
2.17
2.16
2.15
2.14
2.13
1.92
1.70
1.68
1.64
1.61
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1.33
1.25
1.12
1.10
0.99
0.97
0.93
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0.79
0.72
0.71
0.70
0.67
0.65
0.47
0.4

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Current Data Parameters
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EXPNO         100
PROCNO        1

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PULPROG      zg30
TD           32768
SOLVENT      CDCl3
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DS           2
SWH          5995.204 Hz
FIDRES       0.182959 Hz
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RG           228.1
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TE           300.0 K
D1           1.00000000 sec

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SFO1         400.0126001 MHz

F2 - Processing parameters
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SF           400.0100142 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
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S5. ¹H NMR Spectrum for Dragonamide A (3) in CDCl₃ (400 MHz)

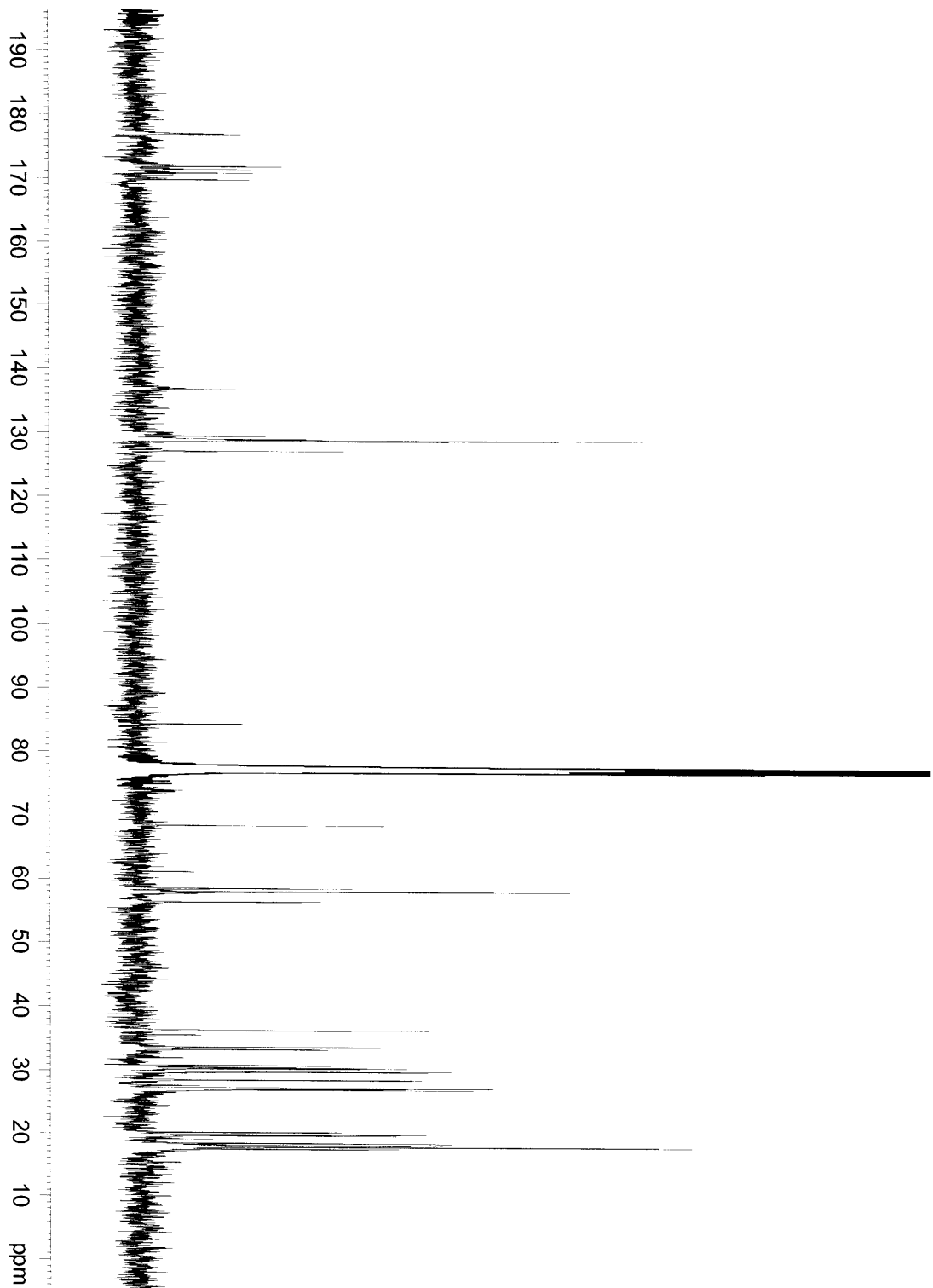
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 170.77
 169.69

136.67
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 128.69
 128.63
 126.98

84.19
 77.32
 77.00
 76.68

68.36

58.45
 57.89
 56.33
 36.18
 33.57
 33.20
 30.66
 30.36
 30.20
 29.69
 28.39
 27.12
 27.07
 26.99
 26.78
 20.04
 19.66
 19.49
 18.28
 17.95
 17.68
 17.38



S6. ¹³C NMR Spectrum for Dragonamide A (3) in CDCl₃ (100 MHz)

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Current Data Parameters
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PROCNO       1

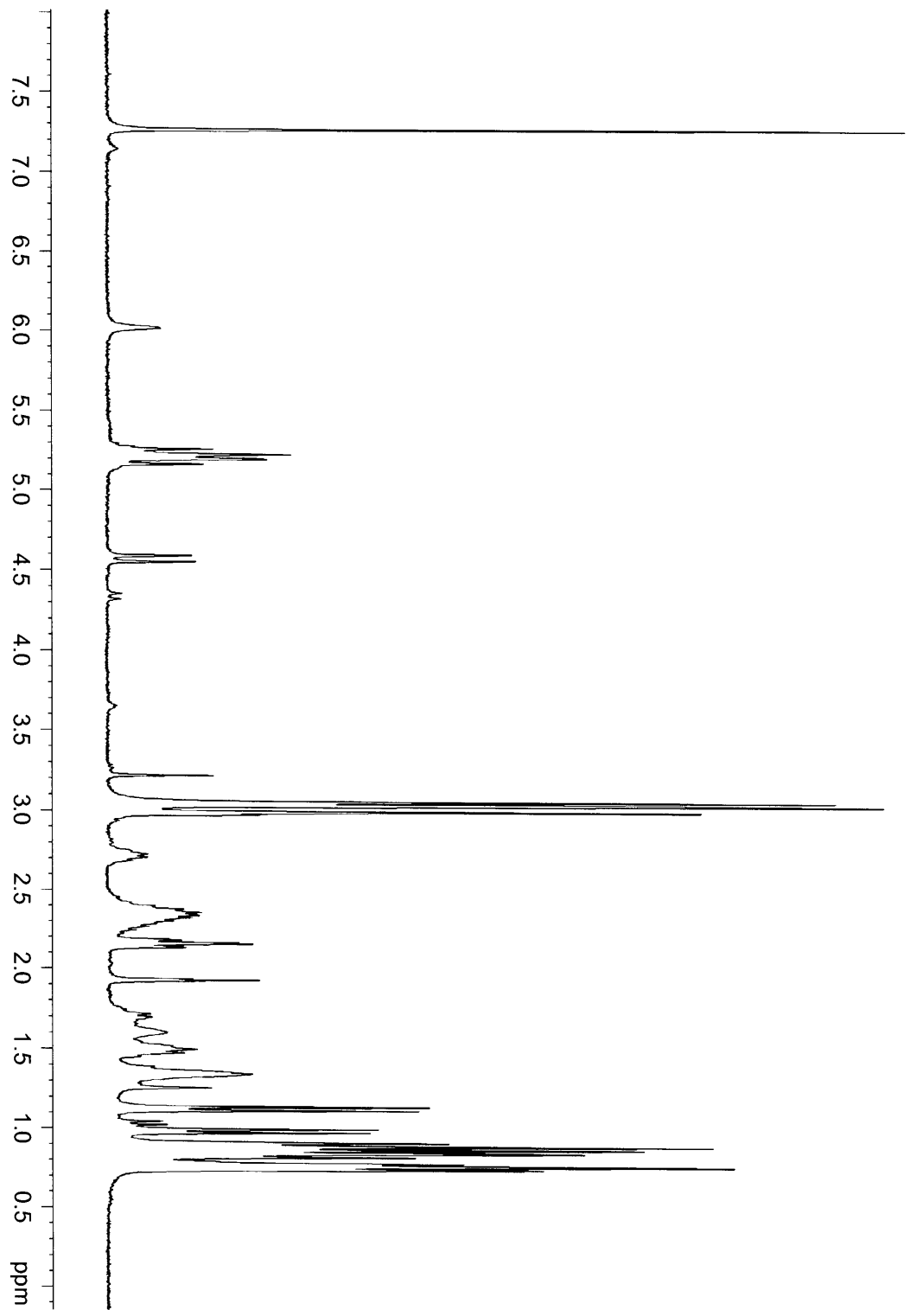
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PULPROG      zgpg30
ID           65536
SOLVENT      Pyr
NS           4520
DS           4
SWH          25125.629 Hz
FIDRES       0.383387 Hz
AQ           1.3042164 sec
RG           1024
DE           19.900 usec
TE           300.0 K
D1           0.00300000 sec
D11          0.03000000 sec
D12          0.00002000 sec

===== CHANNEL f1 =====
NUC1         13C
P1           7.50 usec
PL1         -3.00 dB
SFO1        100.5936186 MHz

===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2       80.00 usec
PL2         0.00 dB
PL12        17.40 dB
PL13        18.00 dB
SFO2        400.0116000 MHz

F2 - Processing parameters
SI           65536
SF           100.5825985 MHz
WDW          EM
SSB          0
LB           3.00 Hz
GB           0
PC           1.40
  
```


7.26
7.14
6.01
5.30
5.26
5.23
5.19
5.16
4.59
4.55
4.35
4.32
4.22
3.22
3.05
3.03
3.03
2.99
2.97
2.72
2.70
2.68
2.45
2.38
2.35
2.34
2.33
2.32
2.30
2.26
2.24
2.22
2.18
2.17
2.16
2.15
2.14
2.13
1.93
1.92
1.92
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1.71
1.69
1.65
1.60
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1.34
1.25
1.13
1.11
1.04
1.02
1.00
0.99
0.97
0.90
0.88
0.84
0.81
0.77
0.75
0.73



S7. ¹H NMR Spectrum for Dragonamide B (4) in CDCl₃ (300 MHz)

Current Data Parameters
NAME 1455G9
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
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Time 11.01

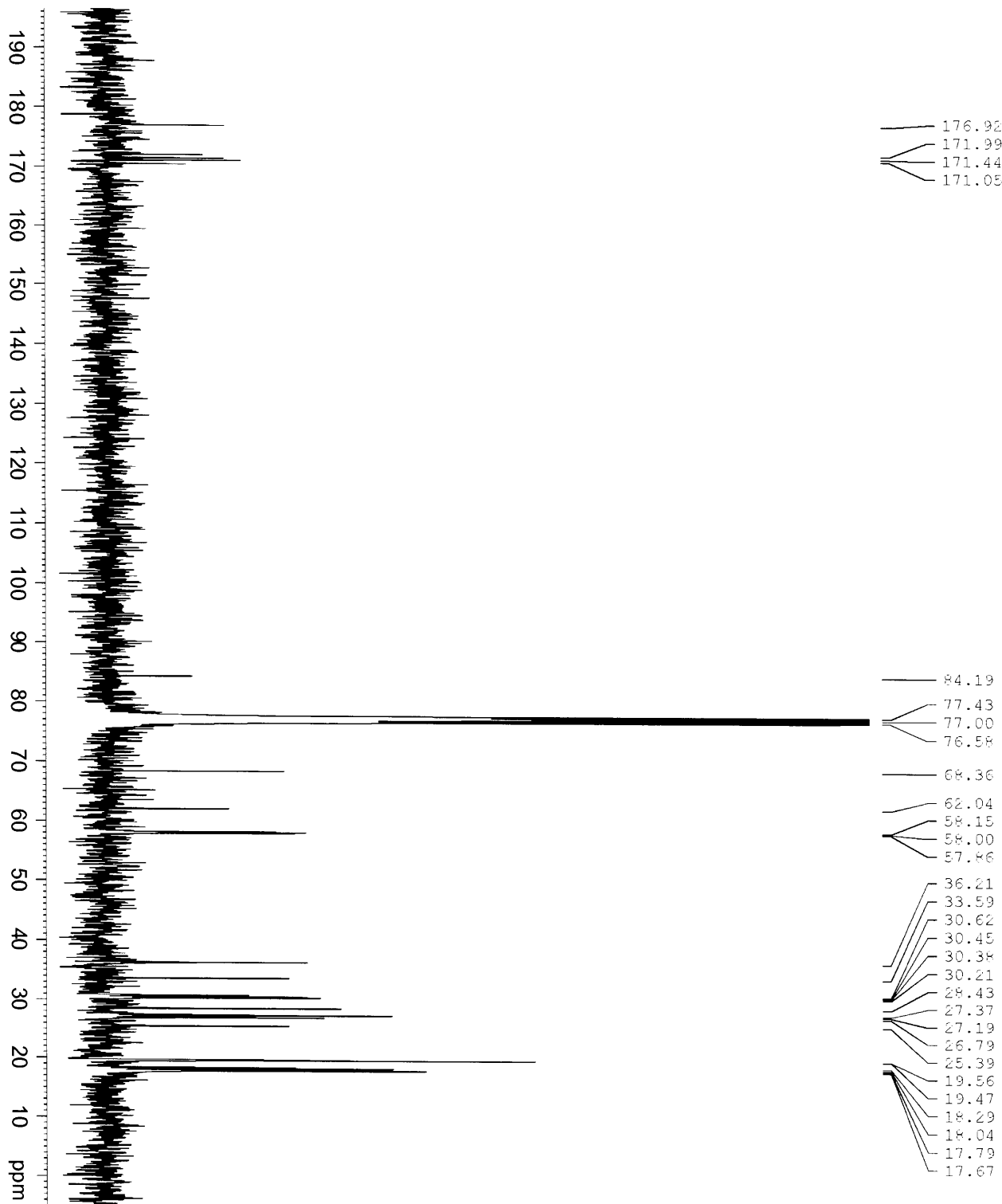
INSTRUM spect
PROBHD 5 mm BBO BB/2H
PULPROG zg30
TD 65536
SOLVENT CDCl3

NS 20
DS 4
SWH 4496.403 Hz
FIDRES 0.068610 Hz
AQ 7.2877645 sec
RG 1290.2
DM 111.200 usec
DE 158.64 usec
TE 300.0 K

D1 1.60000002 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SFO1 300.1319508 MHz

F2 - Processing parameters
SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



176.92
171.99
171.44
171.05

84.19
77.43
77.00
76.58
68.36
62.04
58.15
58.00
57.86
36.21
33.59
30.62
30.45
30.38
30.21
28.43
27.37
27.19
26.79
25.39
19.56
19.47
18.29
17.04
17.79
17.67

Current Data Parameters
NAME 1455G9
EXPNO 105
PROCNO 1

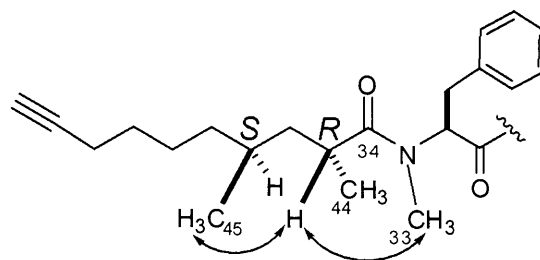
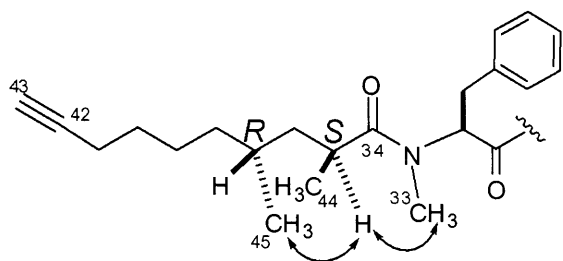
F2 - Acquisition Parameters
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Time 6.17

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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5120
DS 8
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418640 sec
RG 1625.5
DM 22.000 usec
DE 6.00 usec
TE 300.0 K

==== CHANNEL f1 =====
NUC1 13C
P1 8.95 usec
PL1 0.00 dB
SFO1 75.4783145 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S8. ¹³C NMR Spectrum for Dragonamide B (4) in CDCl₃ (75 MHz)



S9. Two potential diastereomers for the 2,4-dimethyldecynoic acid units in carmabin A (**1**). The ROESY correlations observed (represented by double-headed arrows) are consistent with either structure.

S10. Table. ^{13}C and ^1H NMR Data in CDCl_3 for Dragonamide A (3).^a

dragonamide A (3)			
unit ^b	position	δ_{C} , mult.	δ_{H} (J in Hz)
NH ₂	1	-	5.99, br s
N-MePhe	2	171.8, qC	-
	3	56.3, CH	5.56, dd (11, 5)
	4	N	-
	5	33.2, CH ₂	3.00, dd (ob) 3.25, dd (15, 5)
	6	136.7, qC	-
	7	128.6, CH	7.16, m
	8	128.7, CH	7.29, m
	9	127.03 / 126.97, CH	7.25, m
	10	128.7, CH	7.29, m
	11	128.6, CH	7.16, m
	12	30.7, CH ₃	2.93, m
N-Me Val-1	13	171.3, qC	-
	14	58.4 / 58.3, CH	5.08, d (11)
	15	N	-
	16	27.1, CH	2.29, m
	17	20.0, CH ₃	0.88, d (6)
	18	17.4, CH ₃	0.66, d (7)
	19	29.7, CH ₃	2.43, s
N-Me Val-2	20	169.7, qC	-
	21	57.9, CH	4.94, d (11)
	22	N	-
	23	27.1, CH	2.25, m
	24	19.7, CH ₃	0.71, d (7)
	25	17.6, CH ₃	0.70, d (6)
	26	30.4, CH ₃	2.94, s
N-Me Val-3	27	170.8, qC	-
	28	57.9, CH	5.18, d (11)
	29	N	-
	30	27.0, qCH	2.33, m
	31	19.5, CH ₃	0.82, d (ob)
	32	17.6, CH ₃	0.80, d (ob)
	33	30.2, CH ₃	2.97, s
Moya	34	176.9 / 176.8, qC	-
	35	36.2, CH	2.70, m
	36	33.6, CH ₂	1.69, m
	37	26.8, CH ₂	1.33, m
	38	28.4, CH ₂	1.49, m
	39	18.3, CH ₂	2.16, dt (7, 2)
	40	84.2, qC	-
	41	68.4, CH	1.93, t (2)
	42	17.95, CH ₃	1.11, d (7)

^aMeasured at 100 MHz (^{13}C) and 400 MHz (^1H).^bMoya = 2-methyloct-7-ynoic acid. ob = obscured.