

SUPPLEMENTARY MATERIAL

Biologically active new metabolites from a Florida collection of *Moorea producens*

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Abstract: A bioassay guided investigation (cancer cell cytotoxicity) of a *Moorea producens* collection from Key West, Florida, led to the discovery of two new bioactive natural products [(+)-malyngamide Y and a cyclic depsipeptide, (+)-floridamide]. Their planar structures were deduced through extensive analysis of 1D and 2D NMR spectroscopic data and supported by HRFAB mass spectrometry. The new cyclic depsipeptide contains four amino acids units, including N-methyl phenylalanine (N-MePhe), proline (Pro), valine (Val) and alanine (Ala), beside the unique unit, 2,2-dimethyl-3-hydroxy-octanoic acid (Dhoaa). In addition to the discovery of these two new compounds, two previously reported metabolites were also isolated and identified from this cyanobacterial collection; (-)-C-12 lyngbic acid and the antibacterial agent (-)-malyngolide.

S1 ¹H NMR spectrum of compound **1** in CDCl₃

S2 COSY spectrum of compound **1** in CDCl₃

S3 TOCSY spectrum of compound **1** in CDCl₃

S4 ¹³C NMR spectrum of compound **1** in CDCl₃

S5 HSQC spectrum of compound **1** in CDCl₃

S6 HMBC spectrum of compound **1** in CDCl₃

S7 COSY spectrum of compound **2** in CDCl₃

S8 TOCSY spectrum of compound **2** in CDCl₃

S9 ¹³C NMR spectrum of compound **2** in CDCl₃

S10 HSQC spectrum of compound **2** in CDCl₃

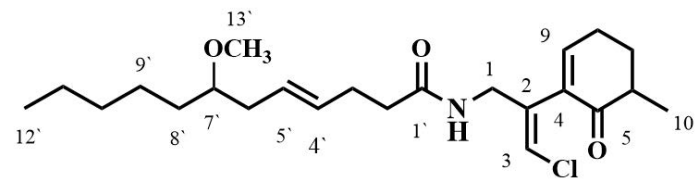
S11 CIMS fragmentation observed for Floridamide

S12 Partial structures of **2** connected by HMBC correlations

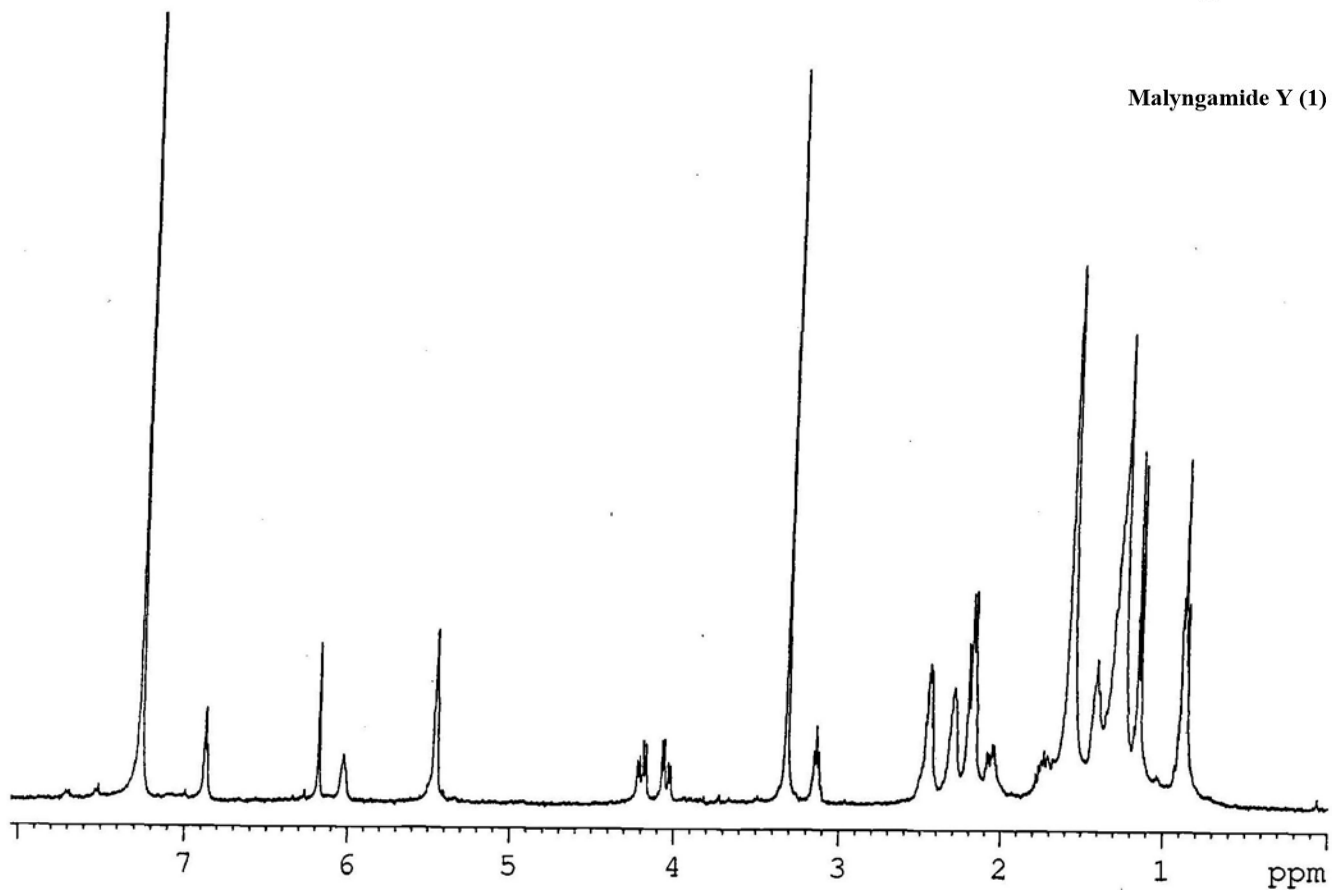
S13 Cytotoxic activity of malyngamide Y

S14 Table 1. ¹H and ¹³C NMR Data of Malyngamide Y (1) in CDCl₃

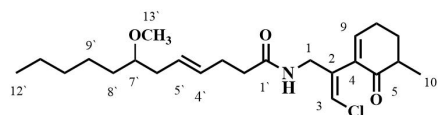
S15 Table 2. NMR spectroscopic data for Floridamide at 400 MHz (¹H) and 150 MHz (¹³C) in CDCl₃.



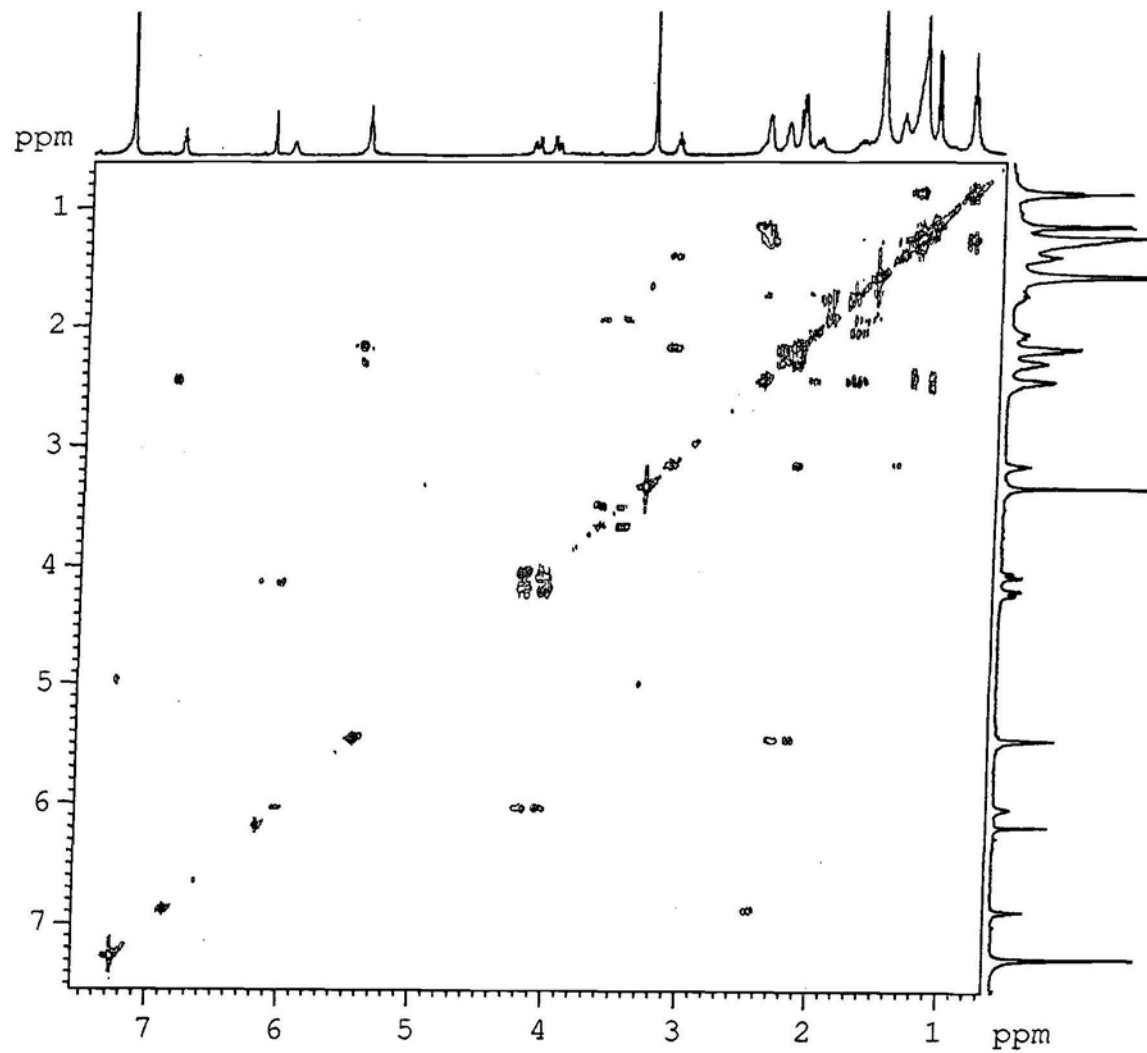
Malyngamide Y (1)



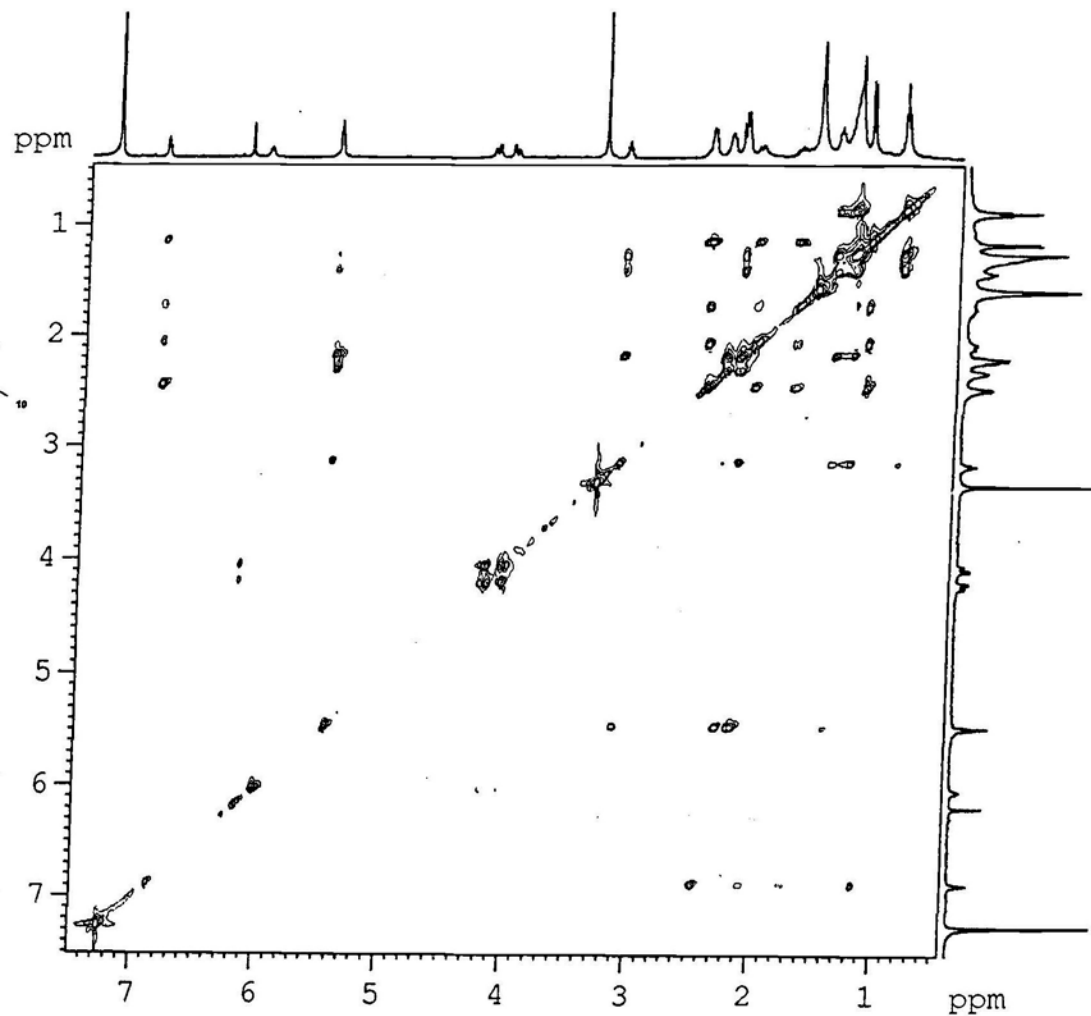
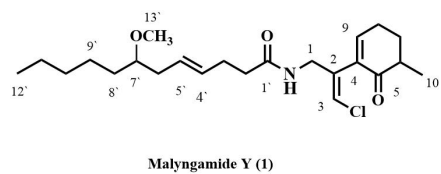
S1 ¹H NMR spectrum of compound 1 in CDCl₃



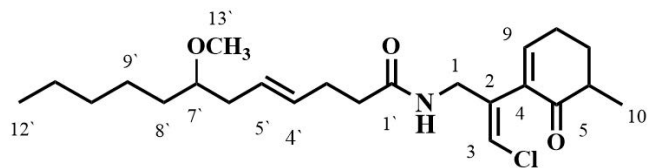
Malyngamide Y (1)



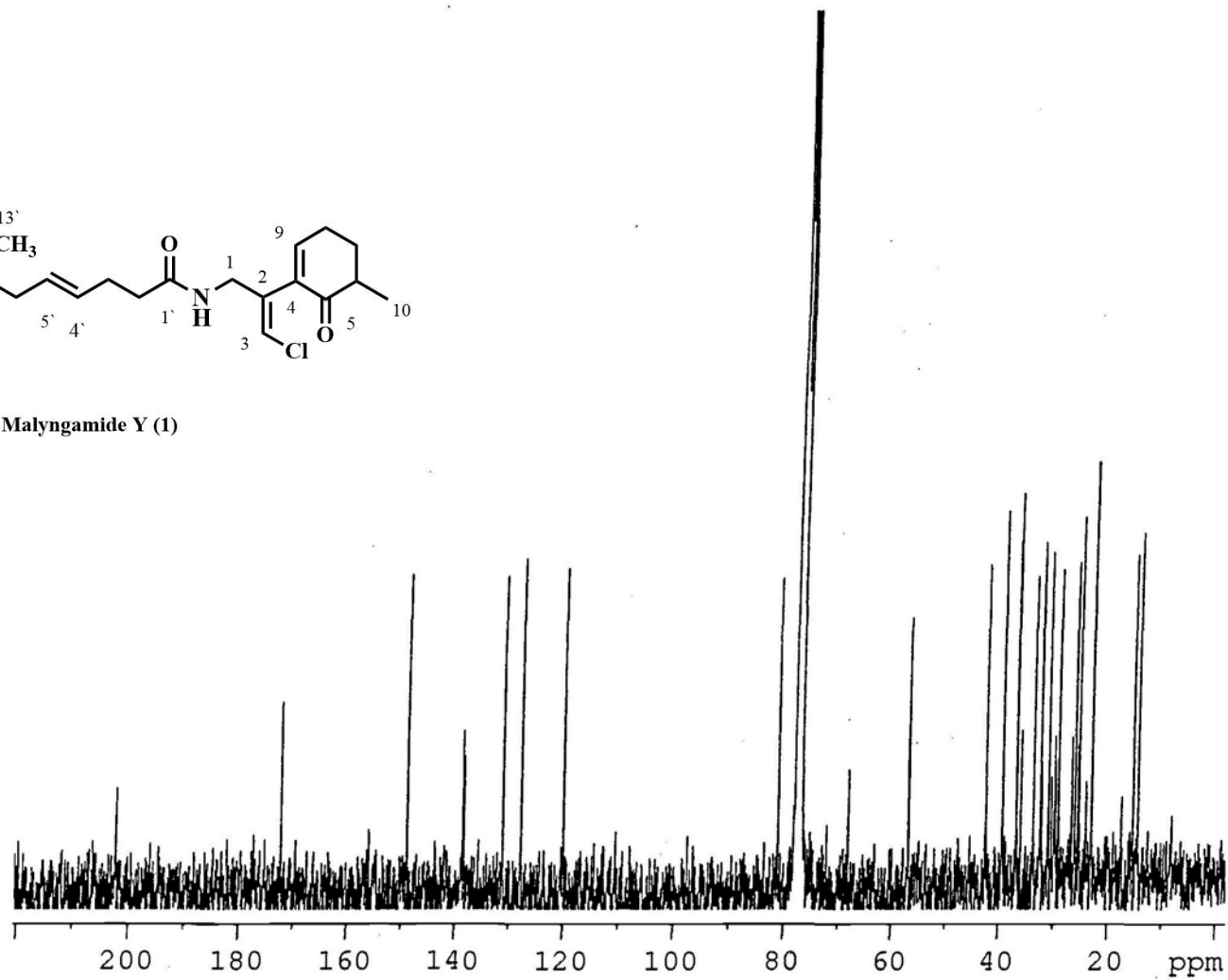
S2 COSY spectrum of compound 1 in CDCl_3



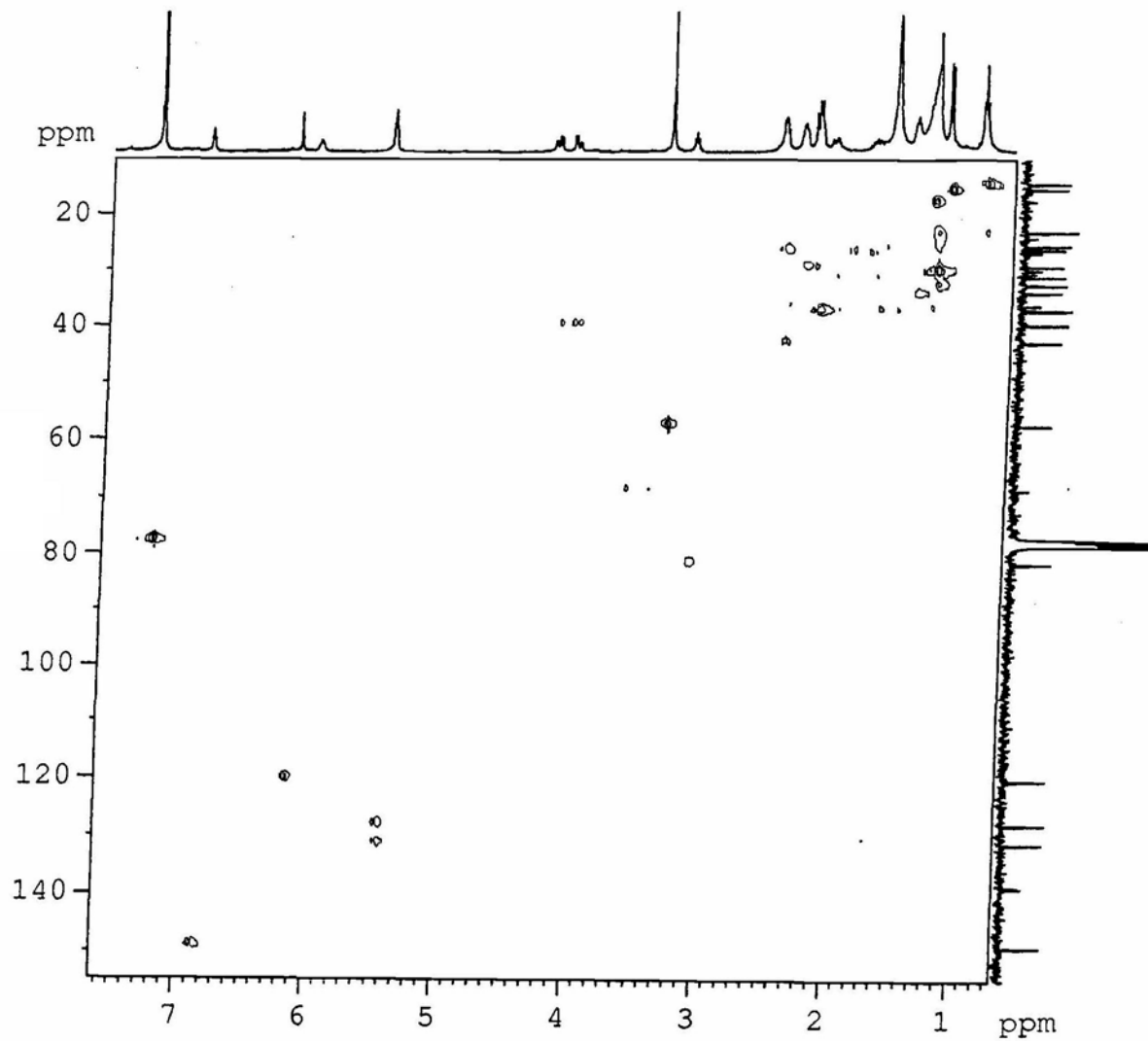
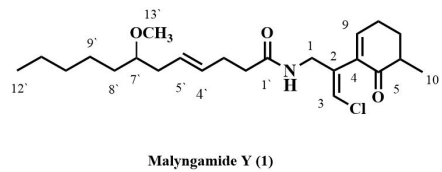
S3 TOCSY spectrum of compound **1** in CDCl₃



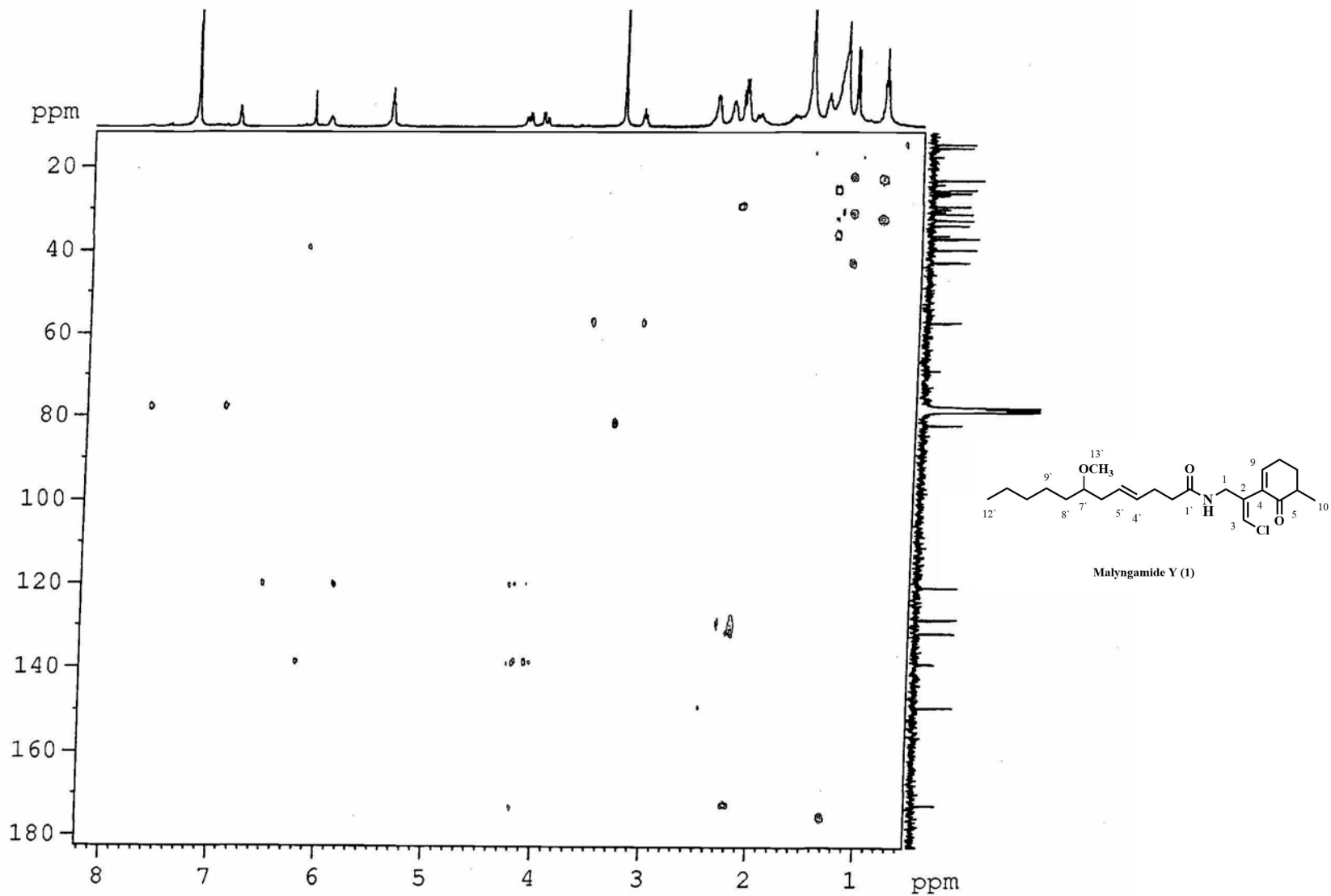
Malyngamide Y (1)



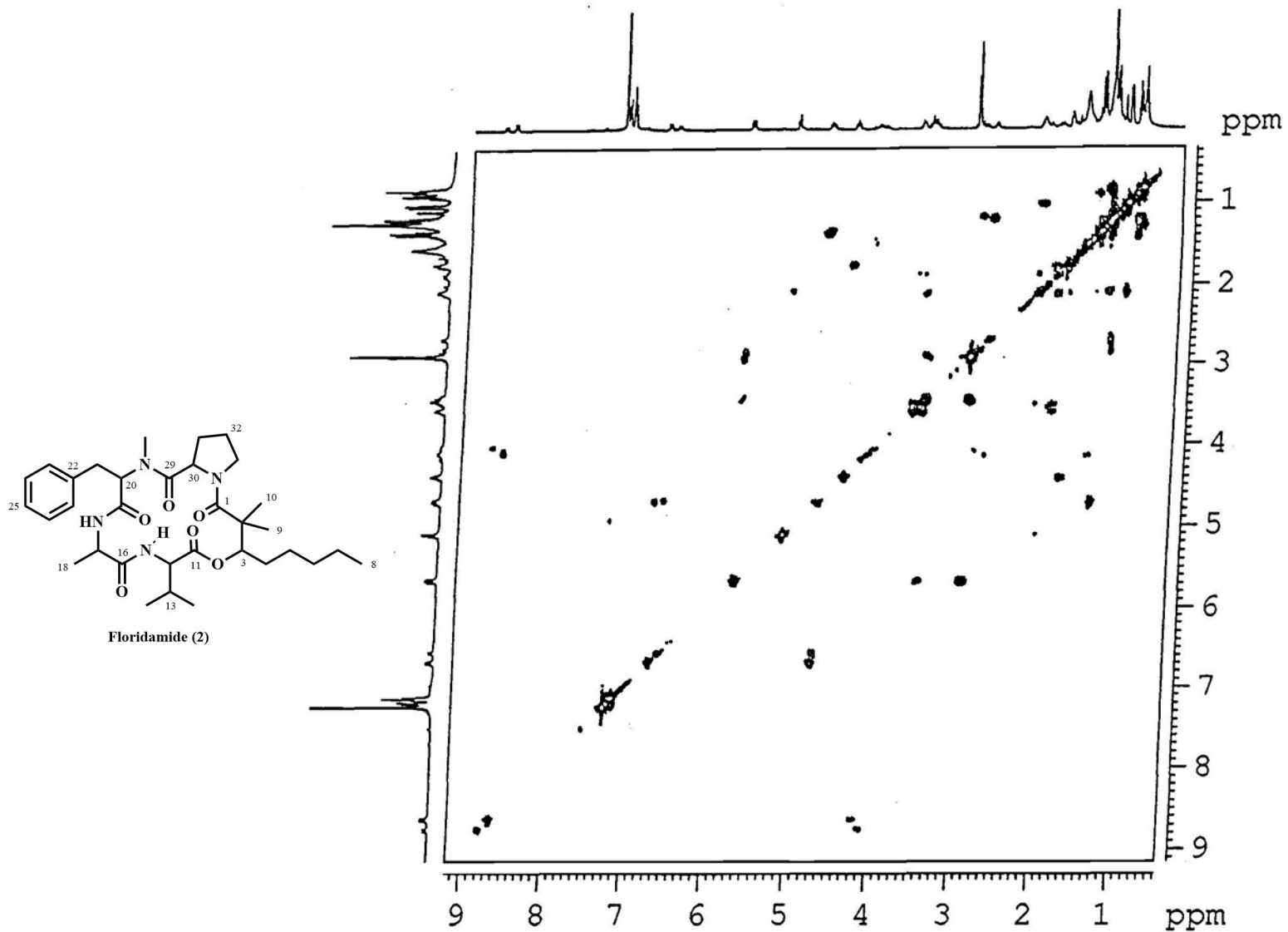
S4 ¹³C NMR spectrum of compound 1 in CDCl₃



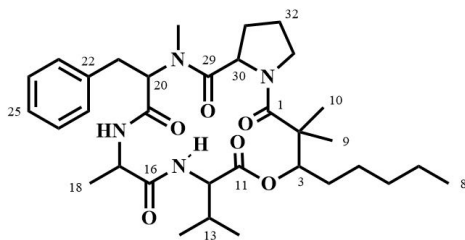
S5 HSQC spectrum of compound **1** in CDCl_3



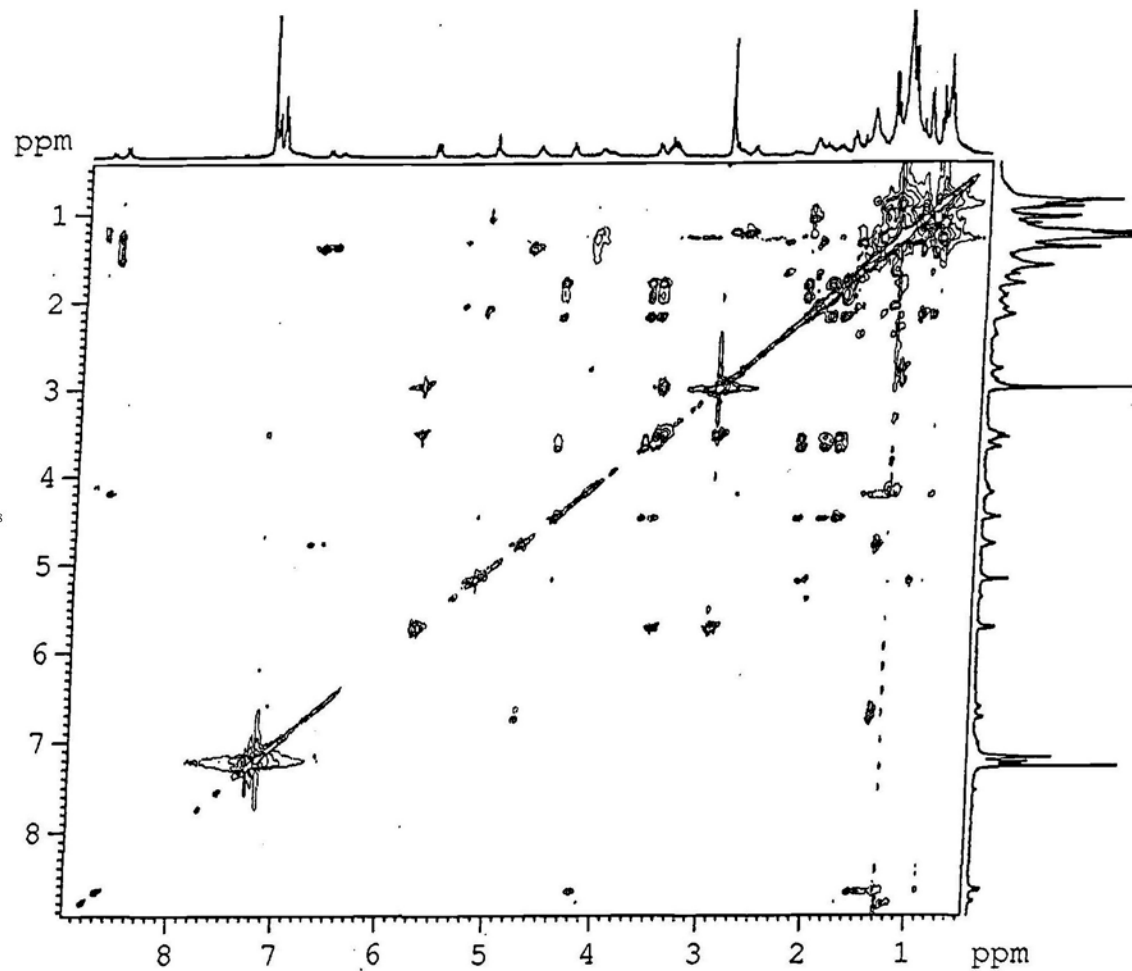
S6 HMBC spectrum of compound 1 in CDCl₃



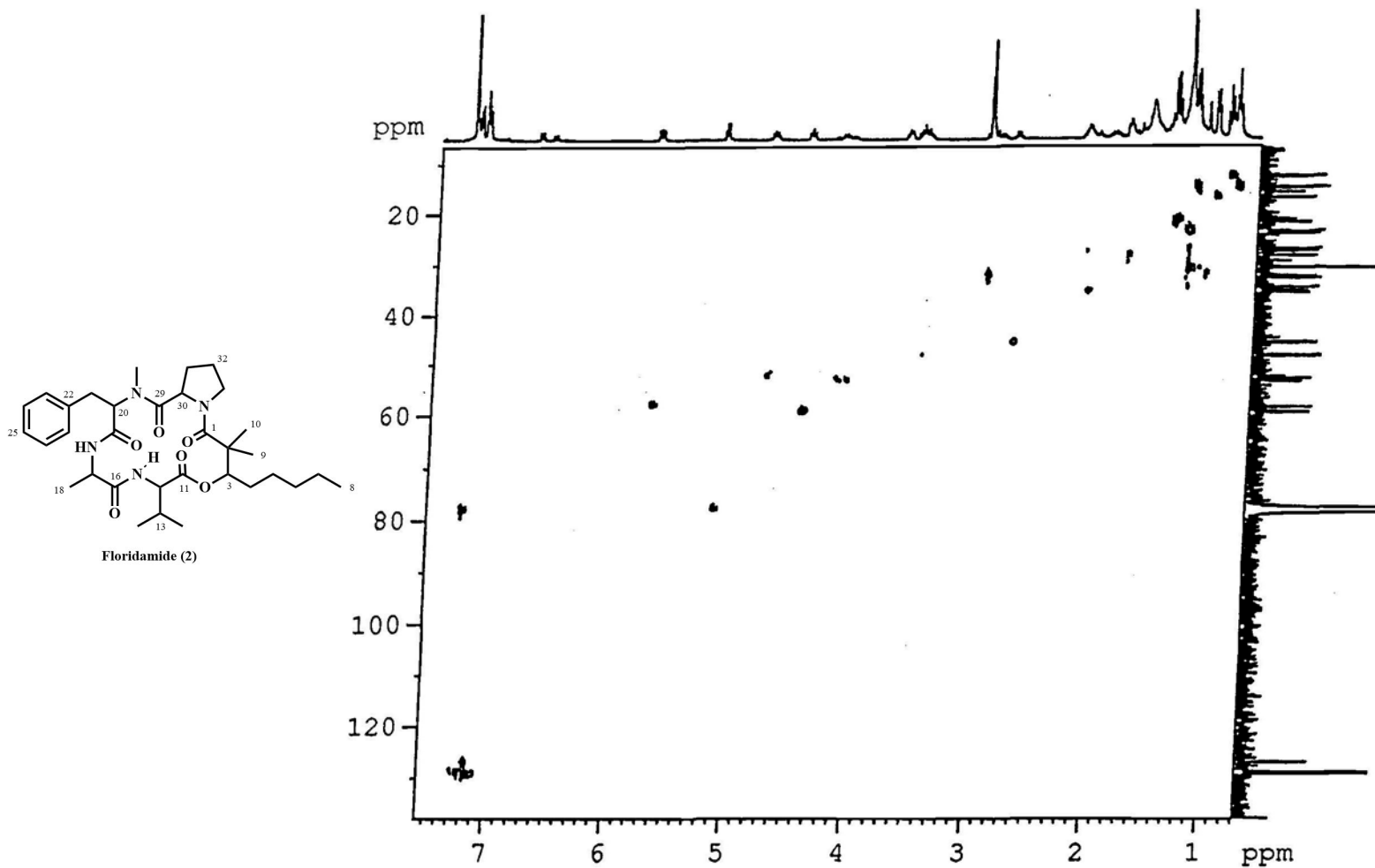
S7 COSY spectrum of compound 2 in CDCl₃



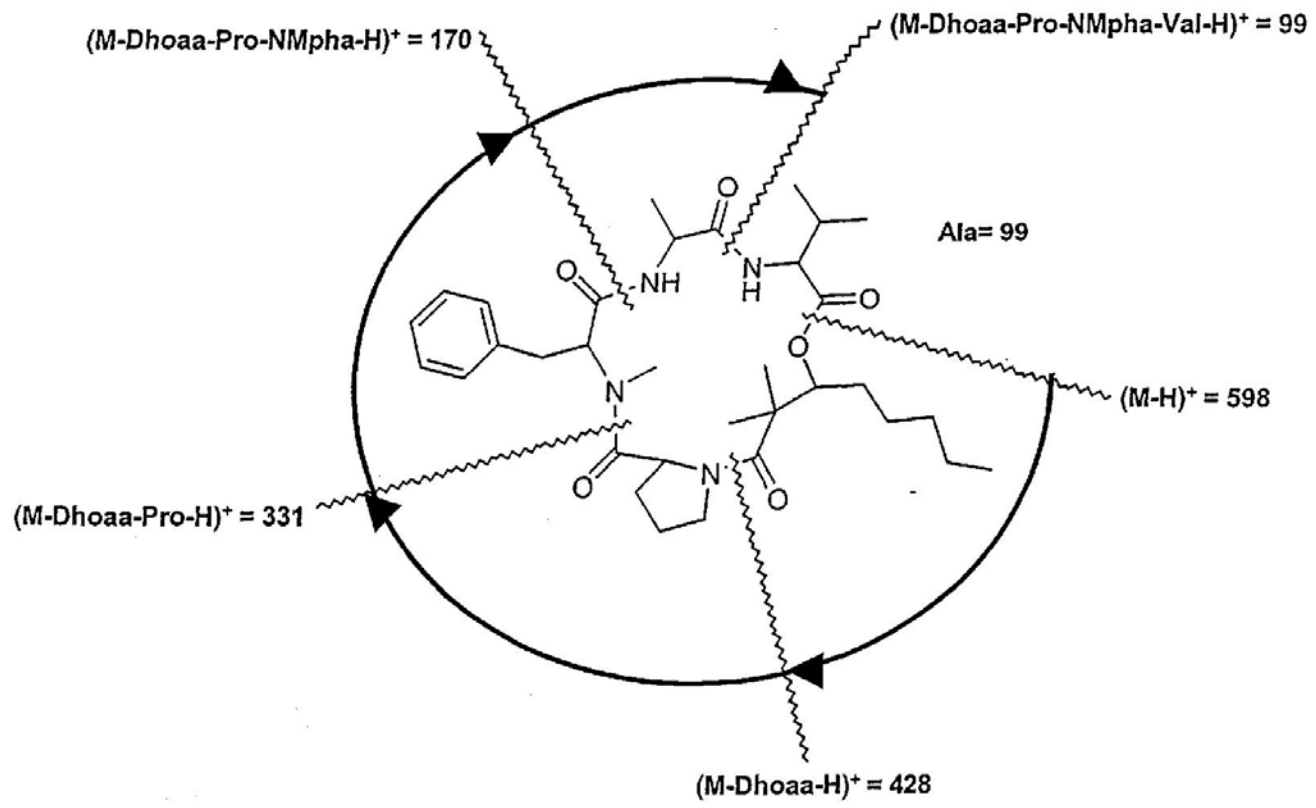
Floridamide (2)



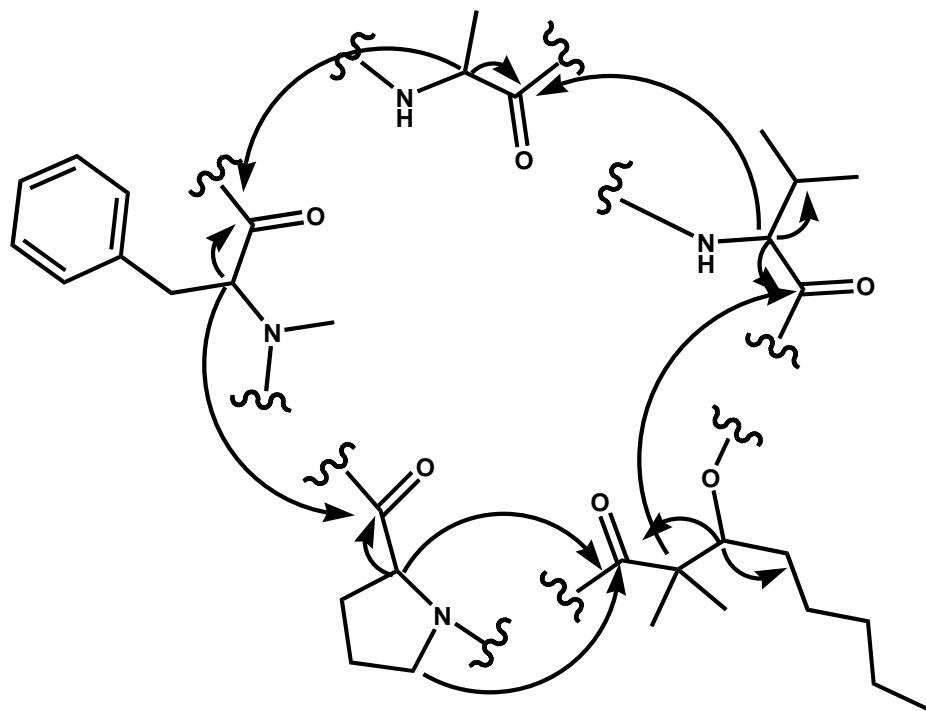
S8 TOCSY spectrum of compound **2** in CDCl_3



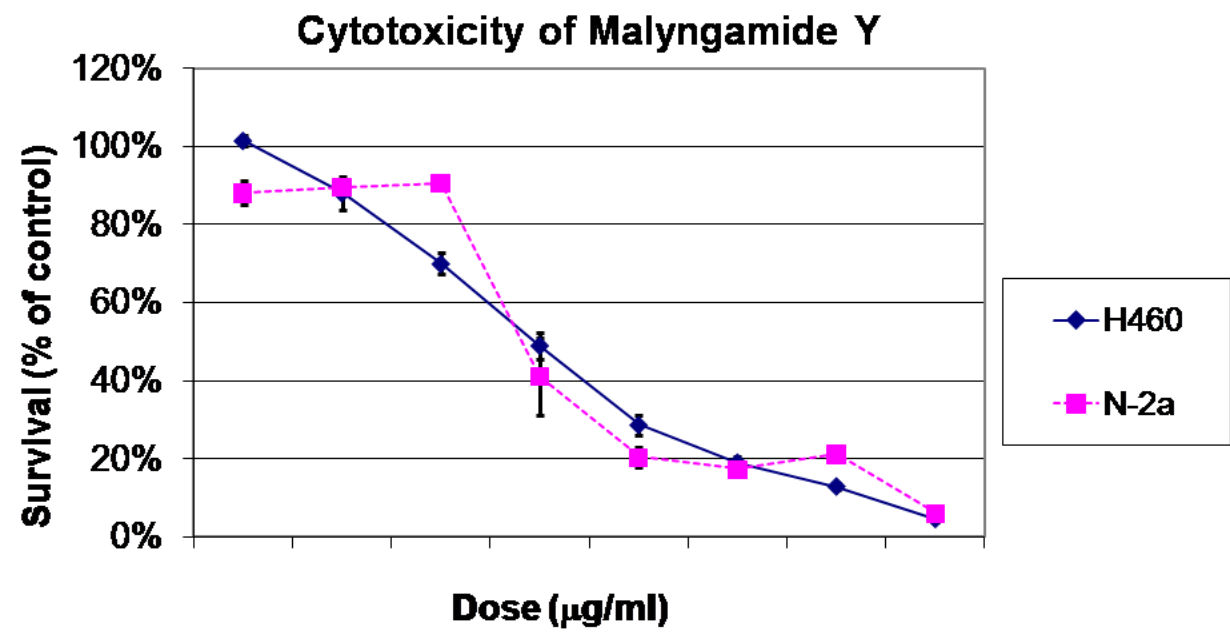
S10 HSQC spectrum of compound **2** in CDCl₃



S11 CIMS fragmentation observed for Floridamide



S12 Partial structures of **2** connected by HMBC correlations.



S13 Cytotoxic activity of malyngamide Y

Table 1. ^1H and ^{13}C NMR Data of Malyngamide **Y** (**1**) in CDCl_3 ^a

Position	^1H mult J (Hz)	^{13}C	COSY	HMBC ^b
1 _a	4.2 (dd, 4.9, 6.0)	39.4 CH ₂	H-3, N-H	C-2, C-3, C-4, C-1'
1 _b	4.0 (dd, 4.9, 6.0)		H-3, N-H	
2		138.7 C		
3	6.1 (s)	120.1 CH	H-1	C-1, C-2, C-4
4		138.4 C		
5		32.4 C		
6	2.4 (m)	42.5 CH	H-7	C-7, C-5
7 _a	2.0	31.0 CH ₂	H-6, H-8	C-6, C-8
7 _b	1.7		H-6, H-8	
8 _a	2.4 (m)	26.1 CH ₂	H-7, H-9	C-6, C-7, C-9, C-10
8 _b	1.8 (m)		H-7, H-9	
9	6.8 (m)	130.9 CH	H-8	C-5, C-8, C-4
10	1.12	14.6 CH ₃		C-5, C-6, C-7, C-8
N-H	6.02 (brt, 6.0)			
1'		172.4 C		
2'	1.6 (m)	25.4 CH ₂		C-1'
3'	2.2 (m)	29.1 CH ₂	H-4'	
4'	5.4 (m)	127.0 CH	H-3', H-5'	C-5', C-3'
5'	5.4 (m)	12.0 CH	H-4', H-6'	C-6', C-4'
6'	2.15 (m)	36.9 CH ₂	H-5', H-7'	C-5', C-7'
7'	3.12 (m)	81.1 CH	H-6', H-8'	C-6', C-8', C-12'
8'	1.60 (m)	36.8 CH ₂	H-7'	C-9', C-10
9'	1.35 (m)	33.7 CH ₂		C-8, C-10
10'	1.23 (m)	32.4 CH ₂		C-9
11'	1.22 (m)	23.9 CH ₂	H-12'	C-9, C12
12'	0.88 (t, 6.8)	14.5 CH ₃	H-11'	C-11
13'	3.4 (s)	56.9 CH ₃		C-7'

^a Spectral data reported in ppm.^b Optimized for 6 Hz.

Table 2. NMR spectroscopic data for Floridamide (**2**) at 400 MHz (^1H) and 150 MHz (^{13}C) in CDCl_3 .^a

Position	^1H	mult	J (Hz)	^{13}C	HMBC ^b
2,2-dimethyl-3-hydroxy-octanoic acid (Dhoaa)					
1				169.3 C	
2				44.7 C	
3	5.13	dd	7.0, 5.5	77.2 CH	1, 4, 11
4	2.13	m		4.0 CH_2	3, 5
5	1.77	m		27.0 CH_2	4, 6
6	1.38	m		23.4 CH_2	5, 7
7	1.00	m		22.9 CH_2	8
8	0.88	t	7.0	14.3 CH_3	7
9	0.92	s		16.4 CH_3	2, 3, 11
10	1.26	s		20.8 CH_3	2, 3, 11
Val					
11				173.3 C	
12	4.14	d	11.0	52.5 CH	11, 13, 16
13	2.7	m		35.1 CH	12, 14, 15
14	1.26	d	6.7	14.5 CH_3	13
15	1.44	d	6.4	12.3 CH_3	13
(N-H)	8.60	s			12, 16
Ala					
16				172.0 C	
17	4.76	m		51.8 CH	16, 18, 19
18	1.36	d	7.2	23.4 CH_3	17
NH	6.7	d	brd 5.0		17, 19
N-MePhe					
19				172.9 C	
3	5.7	dd	12.1, 4.8	57.5 CH	19, 21, 4
21	3.45	dd	15.0, 5.0	33.8 CH_2	20, 22
	2.95	m			
22				137.0 CH	
23/27	7.15	m		128.6 CH	
24/26	7.21	m		129.0 CH	
25	7.16	m		126.7 CH	
28 (N- CH_3)	2.95	s		31.7 CH_3	20, 29
Pro					
4				169.0 C	
1	4.40	m		58.5 CH	29, 31, 1
2	2.10	m		30.1 CH_2	30, 32
	1.87	m			
32	1.3	m		22.9 CH_2	31, 33
	1.04	m			
33	3.60	m		47.0 CH_2	32, 1
	3.50	m			

^a Spectral data reported in ppm.

^b Optimized for 6 Hz.