

## Supplementary Materials

# Leptogorgins A-C, Humulane Sesquiterpenoids from the Vietnamese Gorgonian *Leptogorgia* sp.

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## List

- Figure S1.** HRESIMS of leptogorgin A (**1**).  
**Figure S2.**  $^1\text{H}$ -NMR spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .  
**Figure S3.**  $^{13}\text{C}$ -NMR spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .  
**Figure S4.**  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .  
**Figure S5.** HSQC spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .  
**Figure S6.** HMBC spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .  
**Figure S7.** ROESY spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .  
**Table S1.**  $^1\text{H}$  NMR Data ( $\text{CDCl}_3$ ) for compounds **1a** and **1b**.  
**Figure S8.** HRESIMS of leptogorgin B (**2**).  
**Figure S9.**  $^1\text{H}$ -NMR spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .  
**Figure S10.**  $^{13}\text{C}$ -NMR spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .  
**Figure S11.**  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .  
**Figure S12.** HSQC spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .  
**Figure S13.** HMBC spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .  
**Figure S14.** ROESY spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .  
**Figure S15.** HRESIMS of leptogorgin C (**3**).  
**Figure S17.**  $^{13}\text{C}$ -NMR spectrum of leptogorgin C (**3**) in  $\text{CDCl}_3$ .  
**Figure S18.**  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum of leptogorgin C (**3**) in  $\text{CDCl}_3$ .  
**Figure S19.** HSQC spectrum of leptogorgin C (**3**) in  $\text{CDCl}_3$ .  
**Figure S20.** HMBC spectrum of leptogorgin C (**3**) in  $\text{CDCl}_3$ .  
**Figure S21.** HRESIMS of leptogorgoid A (**4**).  
**Figure S22.**  $^1\text{H}$ -NMR spectrum of leptogorgoid A (**4**) in  $\text{CDCl}_3$ .  
**Figure S23.**  $^{13}\text{C}$ -NMR spectrum of leptogorgoid A (**4**) in  $\text{CDCl}_3$ .  
**Figure S24.**  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum of leptogorgoid A (**4**) in  $\text{CDCl}_3$ .  
**Figure S25.** HSQC spectrum of leptogorgoid A (**4**) in  $\text{CDCl}_3$ .  
**Figure S26.** HMBC spectrum of leptogorgoid A (**4**) in  $\text{CDCl}_3$ .  
**Figure S27.** ECD spectra of leptogorgin A (**1**) and leptogorgin B (**2**).



Foto of gorgonian *Leptogorgia* sp. (#038-011)

**Figure S1.** HRESIMS of leptogorgin A (**1**).

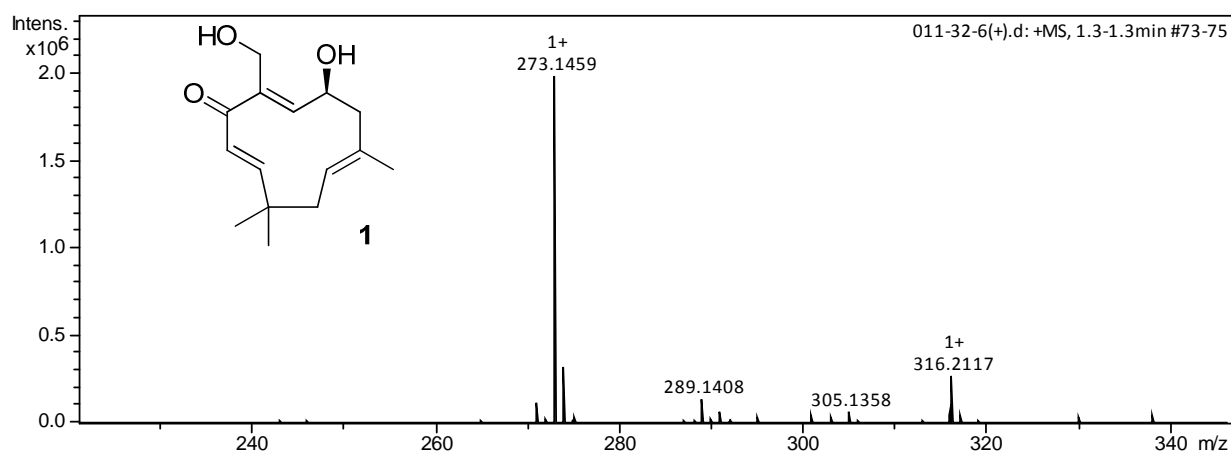
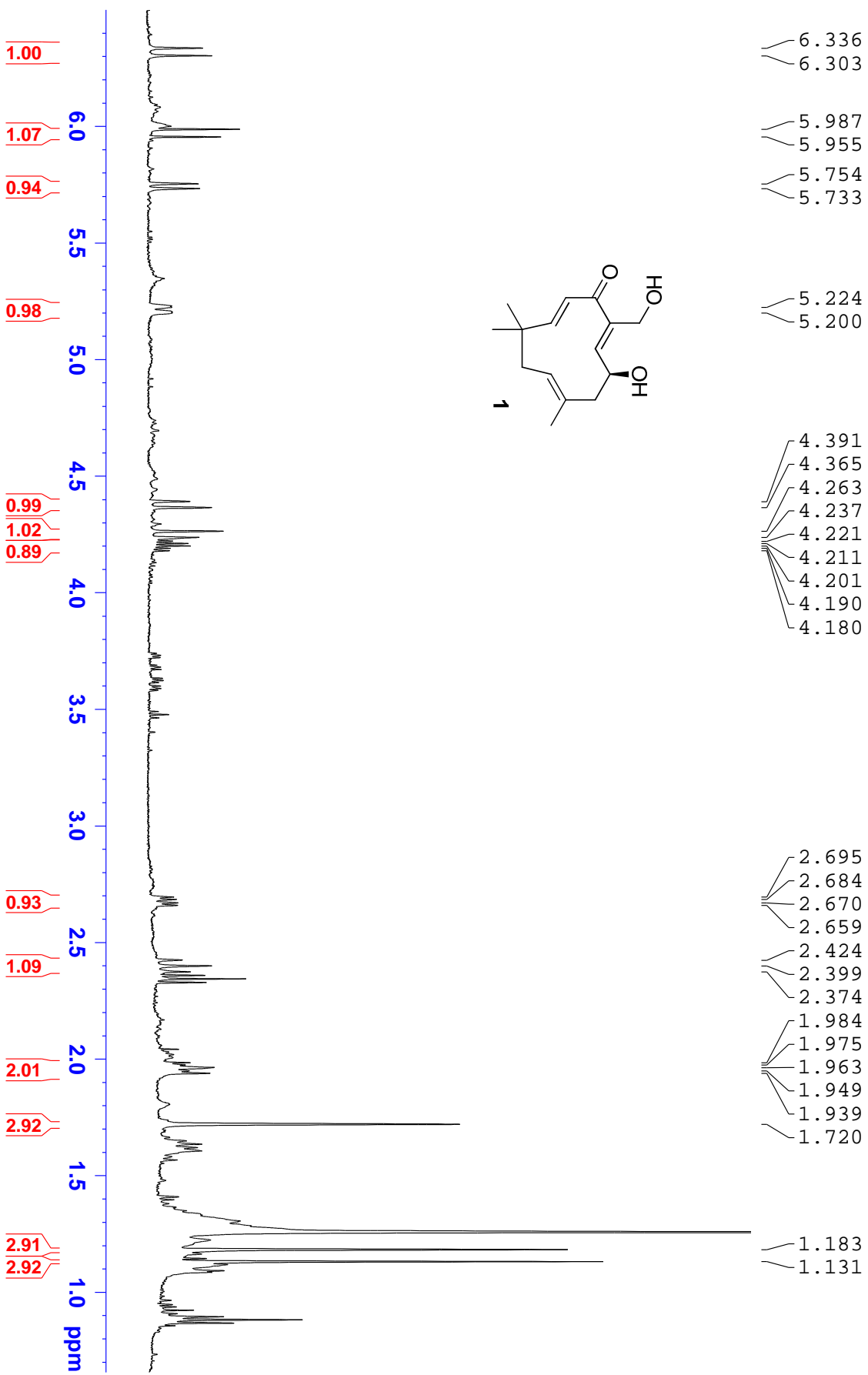
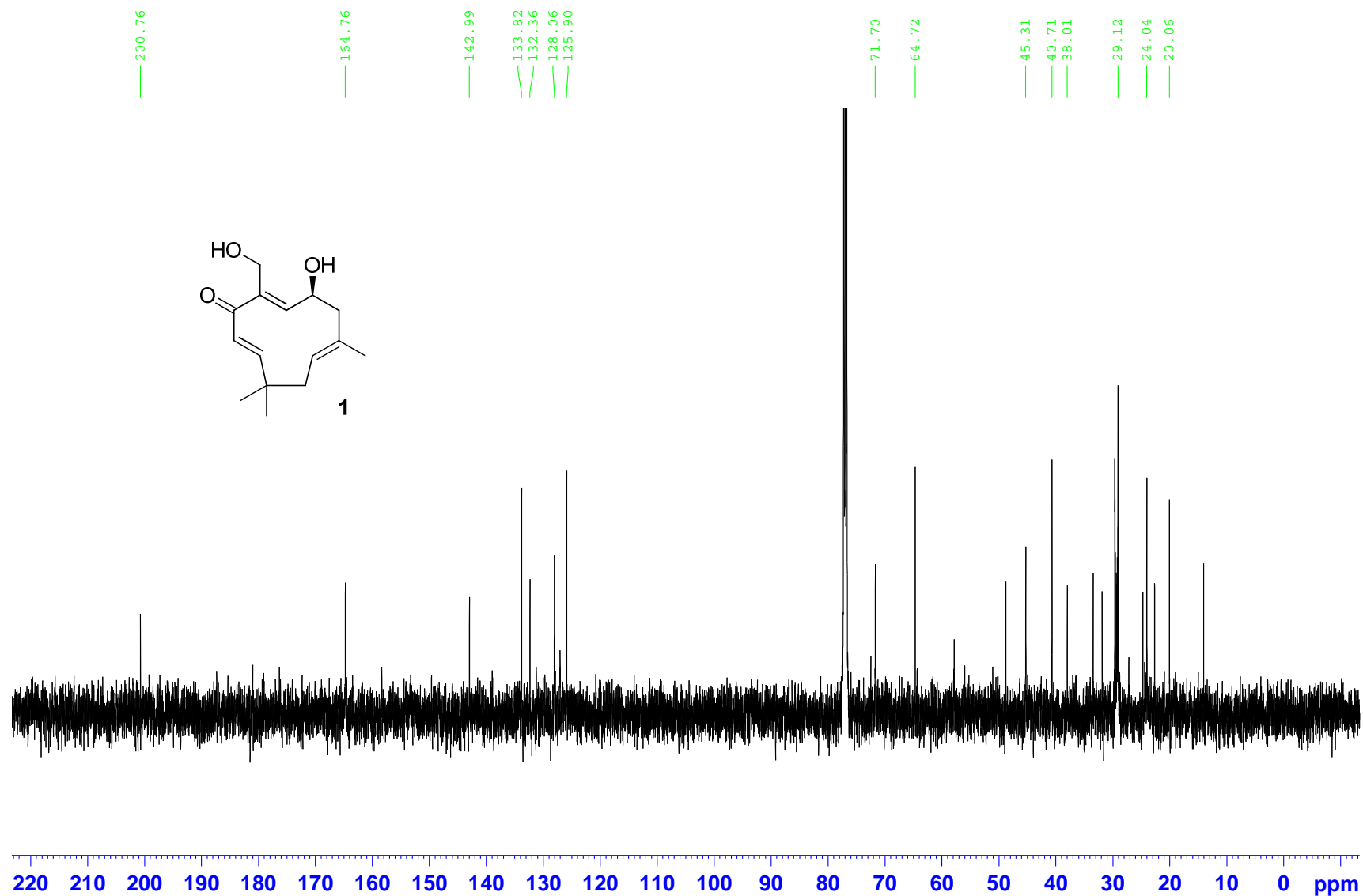


Figure S2.  $^1\text{H}$ -NMR spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .



**Figure S3.**  $^{13}\text{C}$ -NMR spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .



**Figure S4.**  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum of leptogorgin A (**1**) in  $\text{CDCl}_3$ .

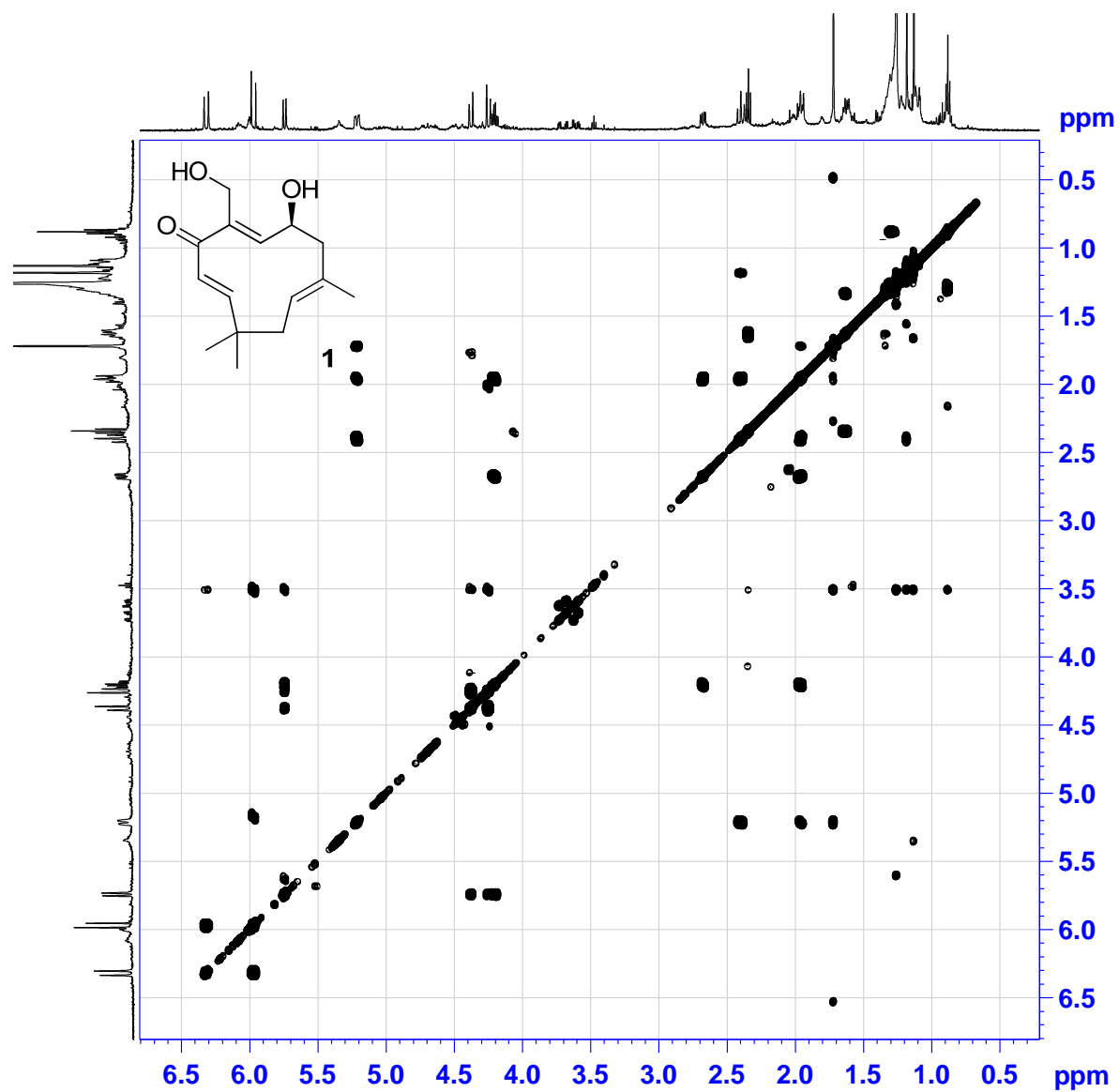


Figure S5. HSQC spectrum of leptogorgin A (1) in CDCl<sub>3</sub>.

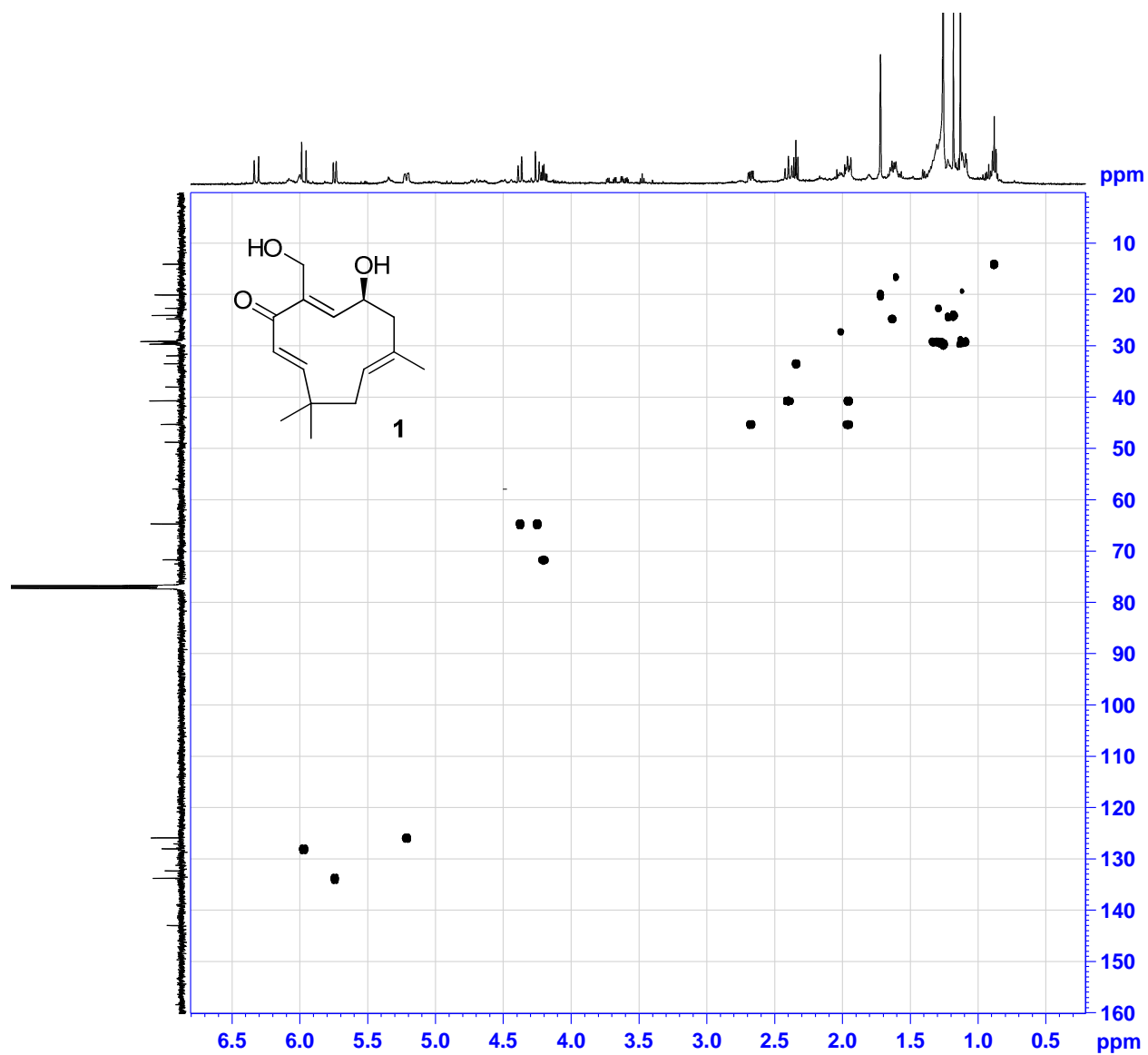
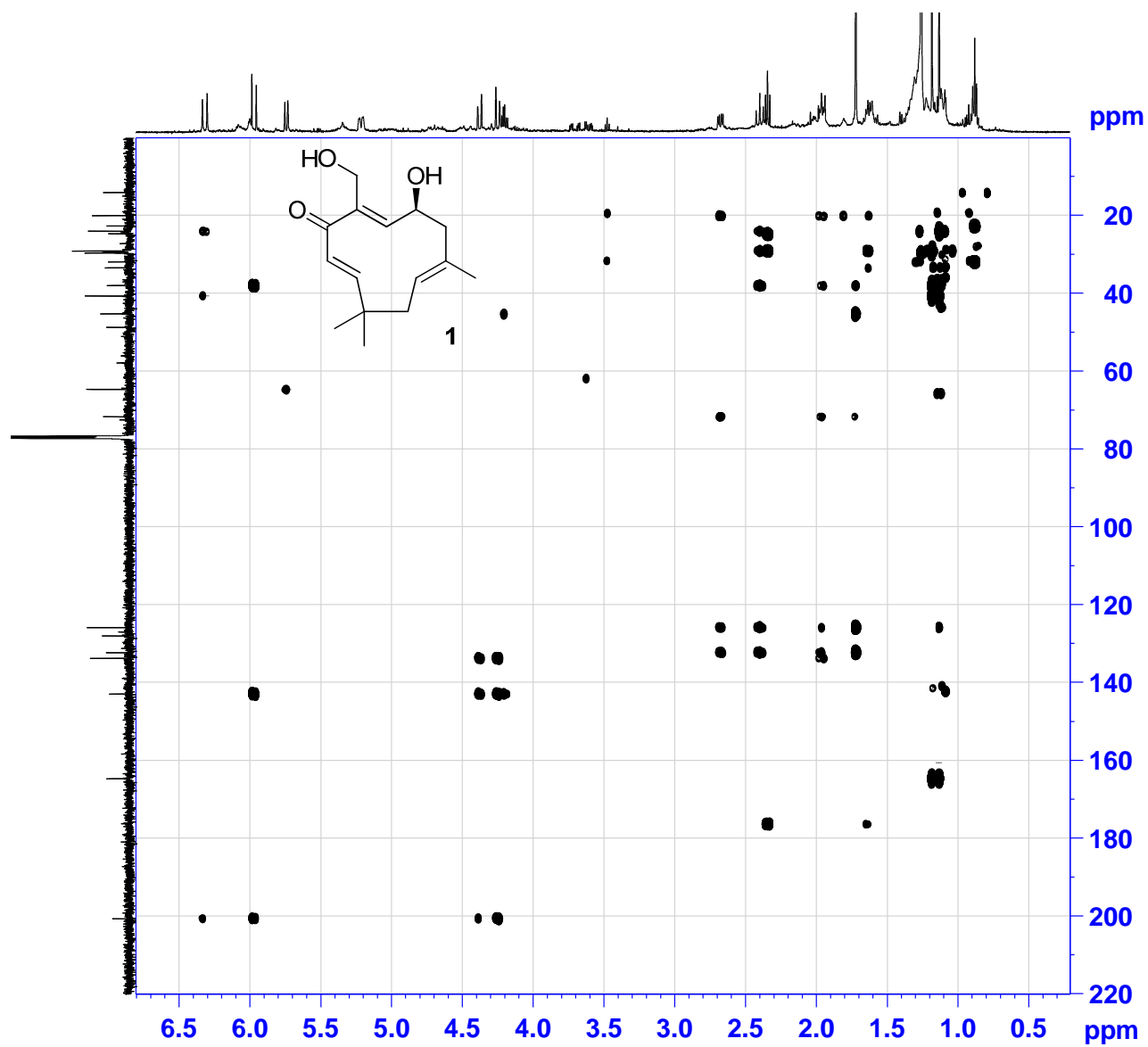
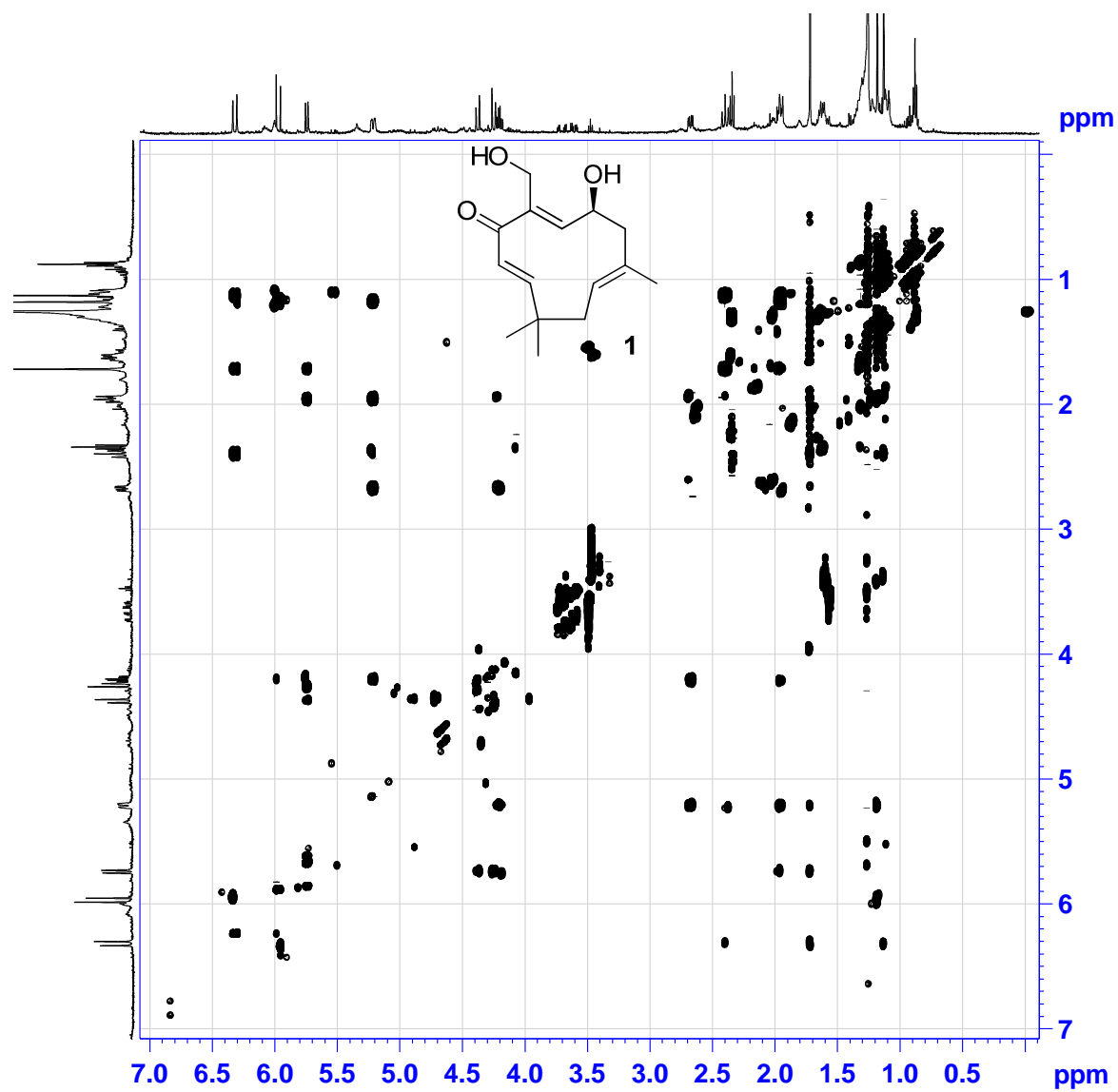


Figure S6. HMBC spectrum of leptogorgin A (**1**) in CDCl<sub>3</sub>.





**Figure S7.** ROESY spectrum of leptogorgin A (**1**) in CDCl<sub>3</sub>.



**Table S1.** <sup>1</sup>H NMR Data (CDCl<sub>3</sub>) for compounds **1a** and **1b**.

position	<i>S</i> -Ester ( <b>1a</b> )	<i>R</i> -Ester ( <b>1b</b> )
	$\delta_{\text{Hmult}}$ ( <i>J</i> in Hz)	$\delta_{\text{Hmult}}$ ( <i>J</i> in Hz)
2	6.18, d (16.3)	6.37, d (16.3)
3	6.07, d (16.3)	6.24, d (16.3)
6	5.75, d (10.6)	5.71, d (10.6)
7	5.47 td (10.6; 5.4)	5.90, td (10.6; 5.4)
8	1.96, m	2.54, m
	2.70, dd (12.2; 5.4)	2.71, dd (12.2; 5.4)
10	5.32, m	5.36, m
11	1.91, m	1.96, m
	2.28, t (12.5)	2.38, t (12.5)
12	4.76, d (13.3)	4.72, d (13.3)
	5.16, d (13.3)	5.15, d (13.3)
13	1.74, s	1.75, s
14	1.18, s	1.32, s
15	0.97, s	1.01, s

**Figure S8.** HRESIMS of leptogorgin B (**2**).

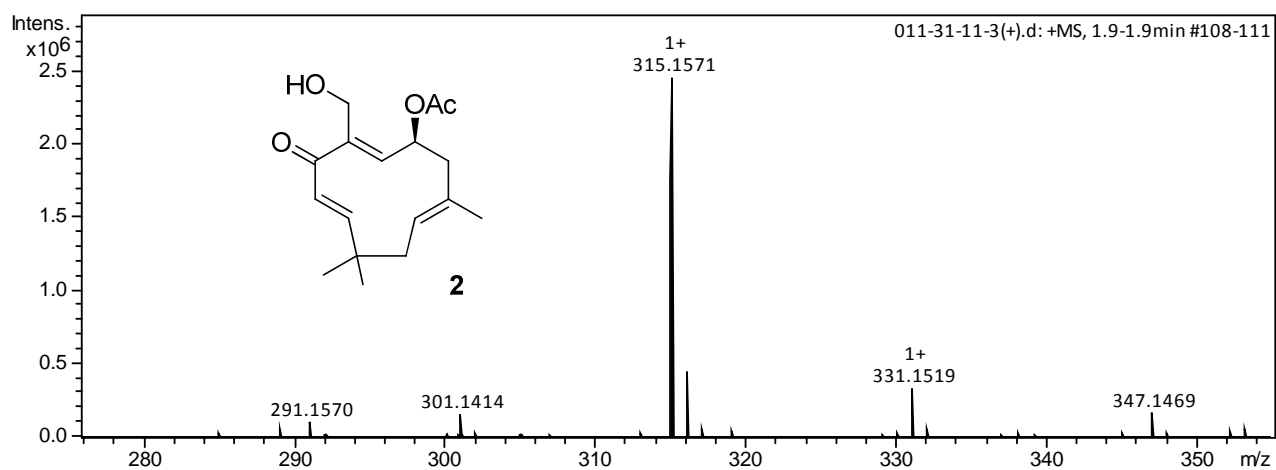
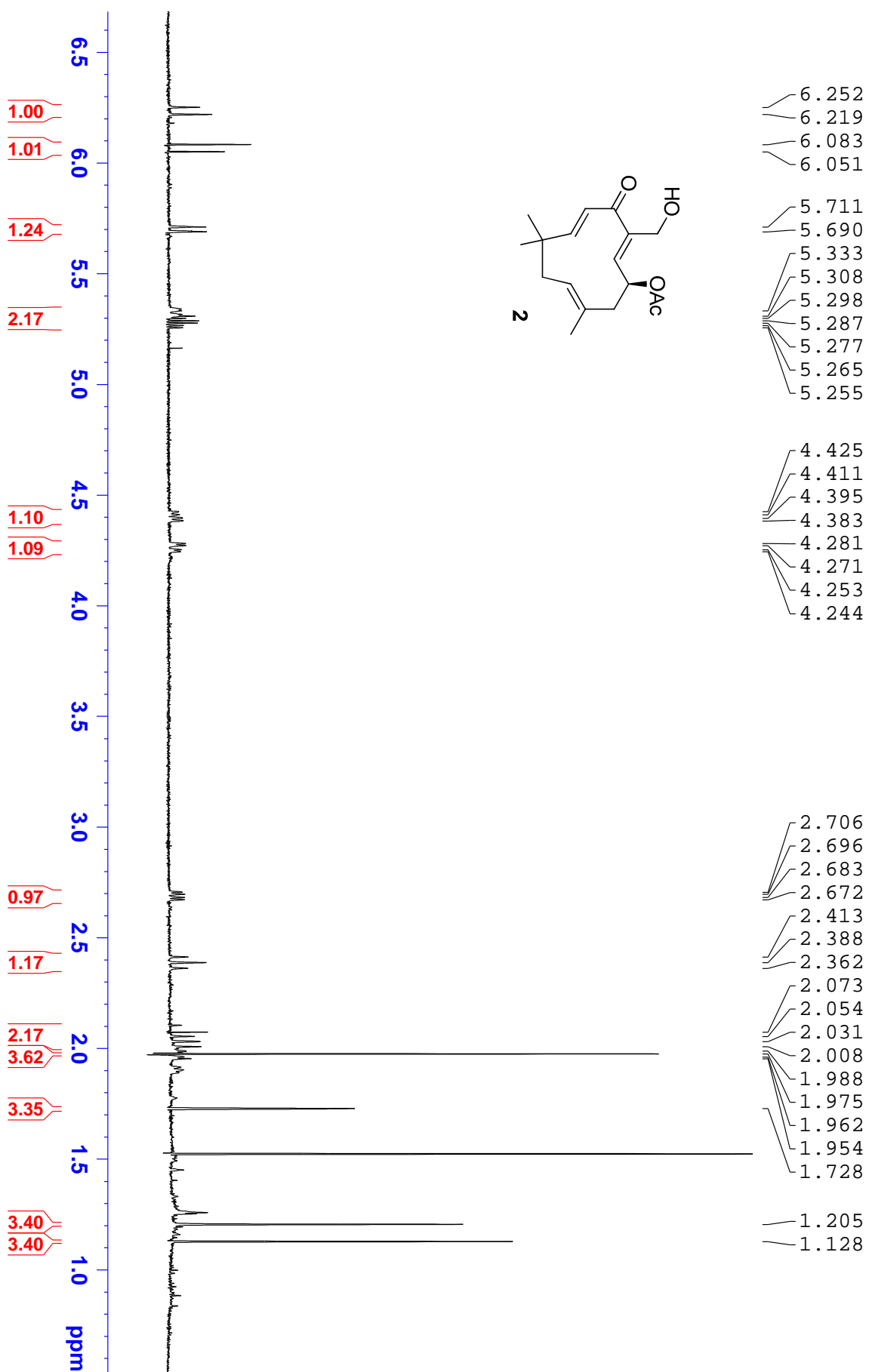
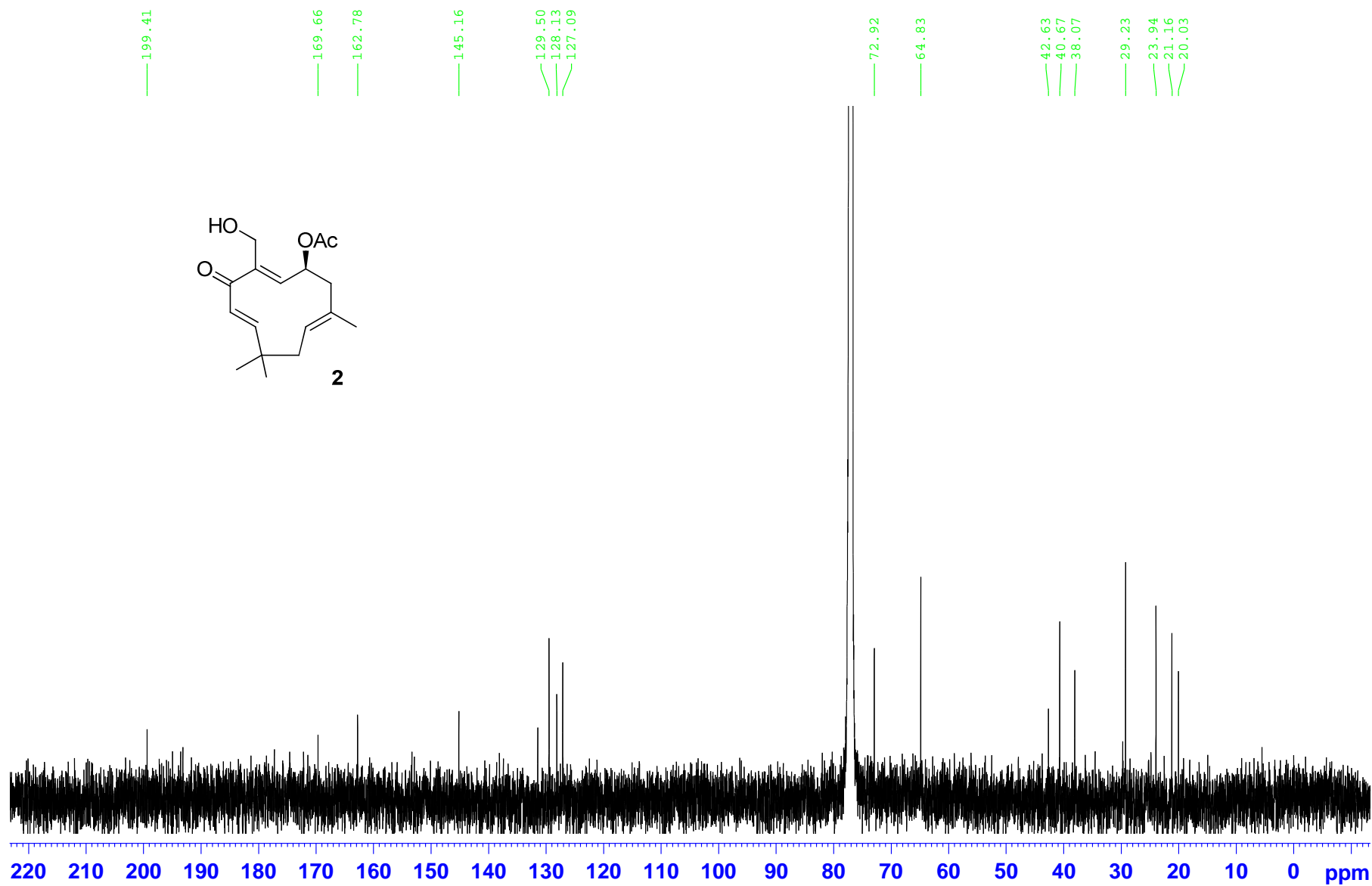


Figure S9.  $^1\text{H}$ -NMR spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .



**Figure S10.**  $^{13}\text{C}$ -NMR spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .



**Figure S11.**  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum of leptogorgin B (**2**) in  $\text{CDCl}_3$ .

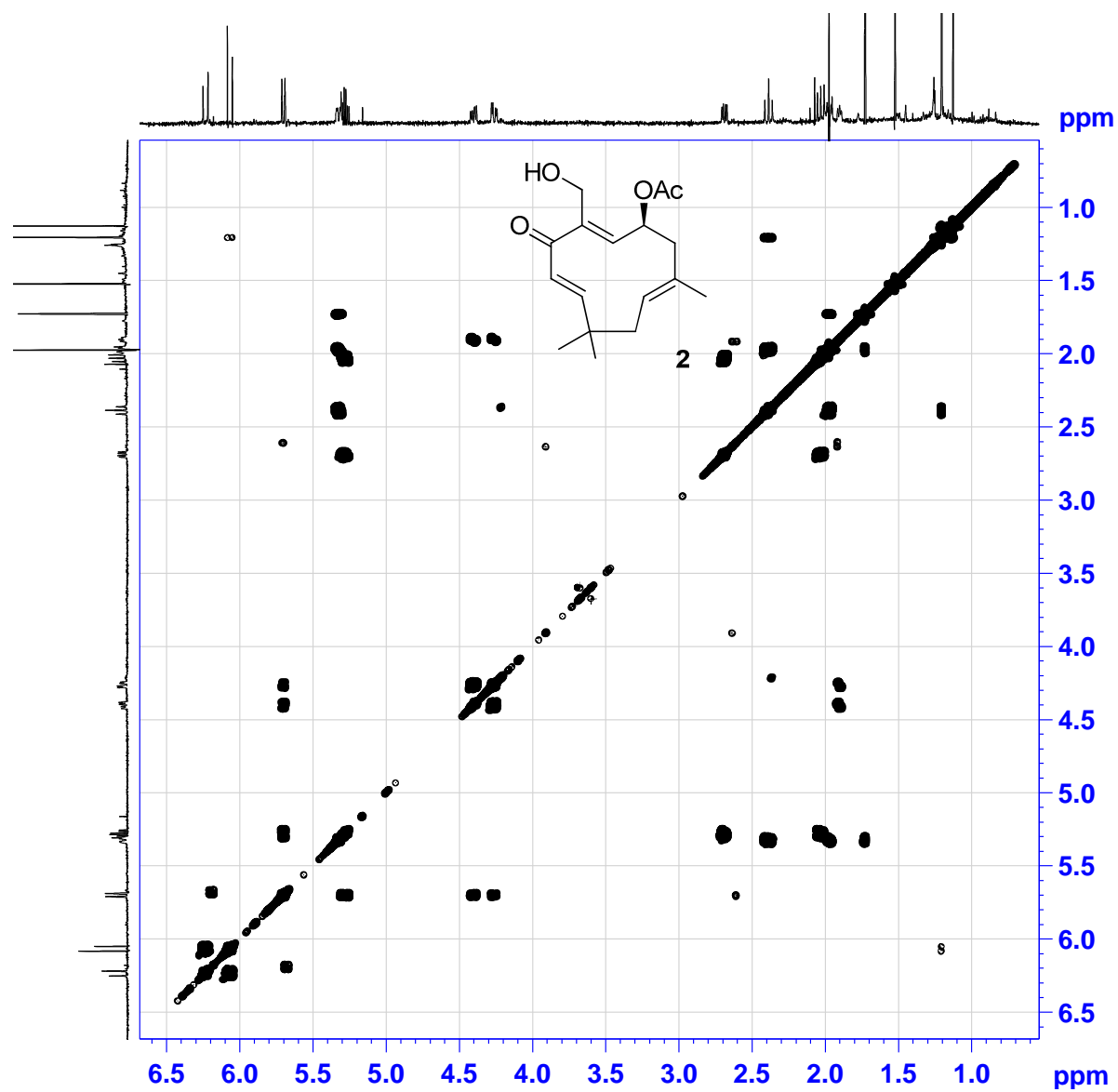


Figure S12. HSQC spectrum of leptogorin B (2) in CDCl<sub>3</sub>.

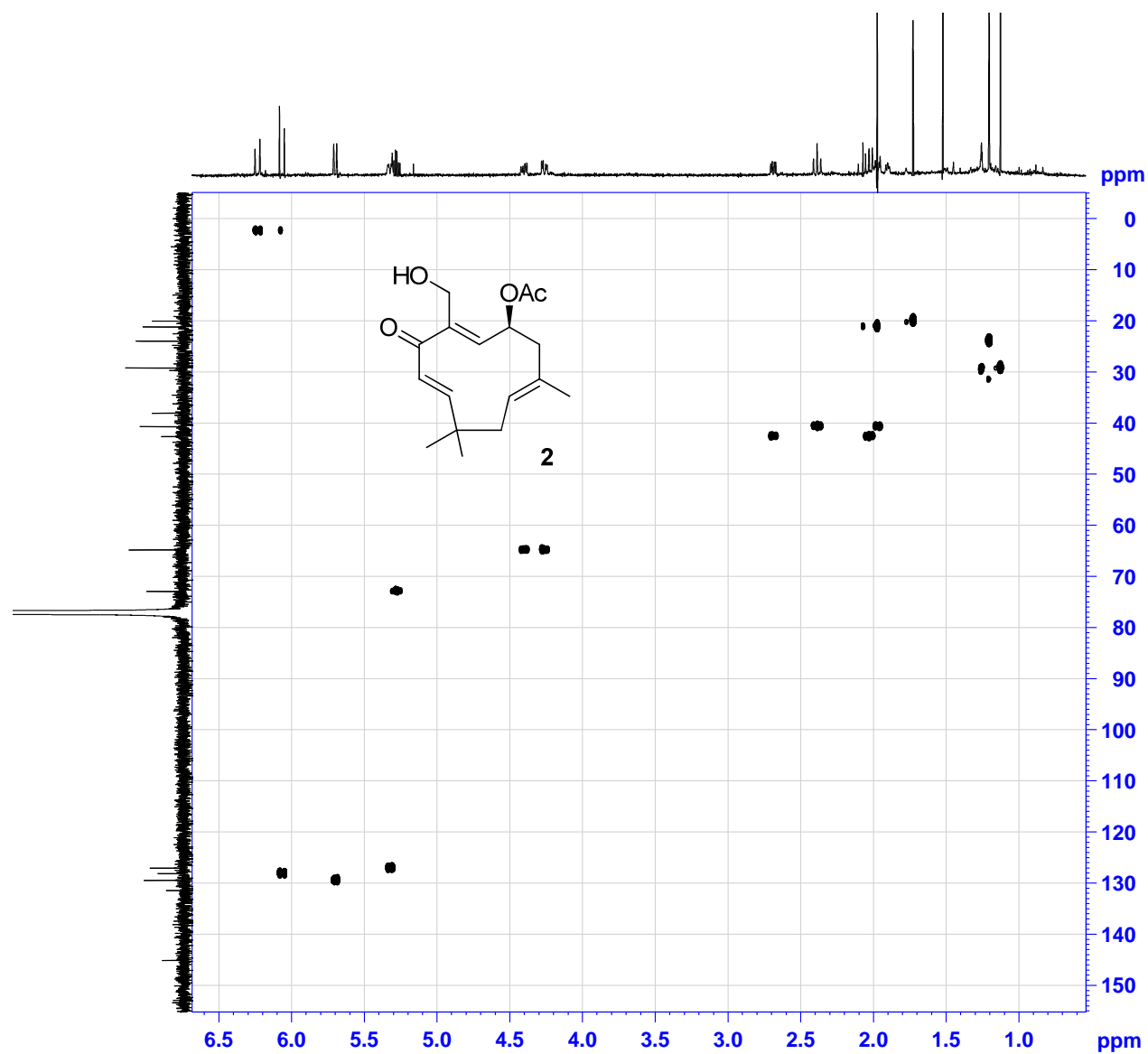


Figure S13. HMBC spectrum of leptogorgin B (2) in CDCl<sub>3</sub>.

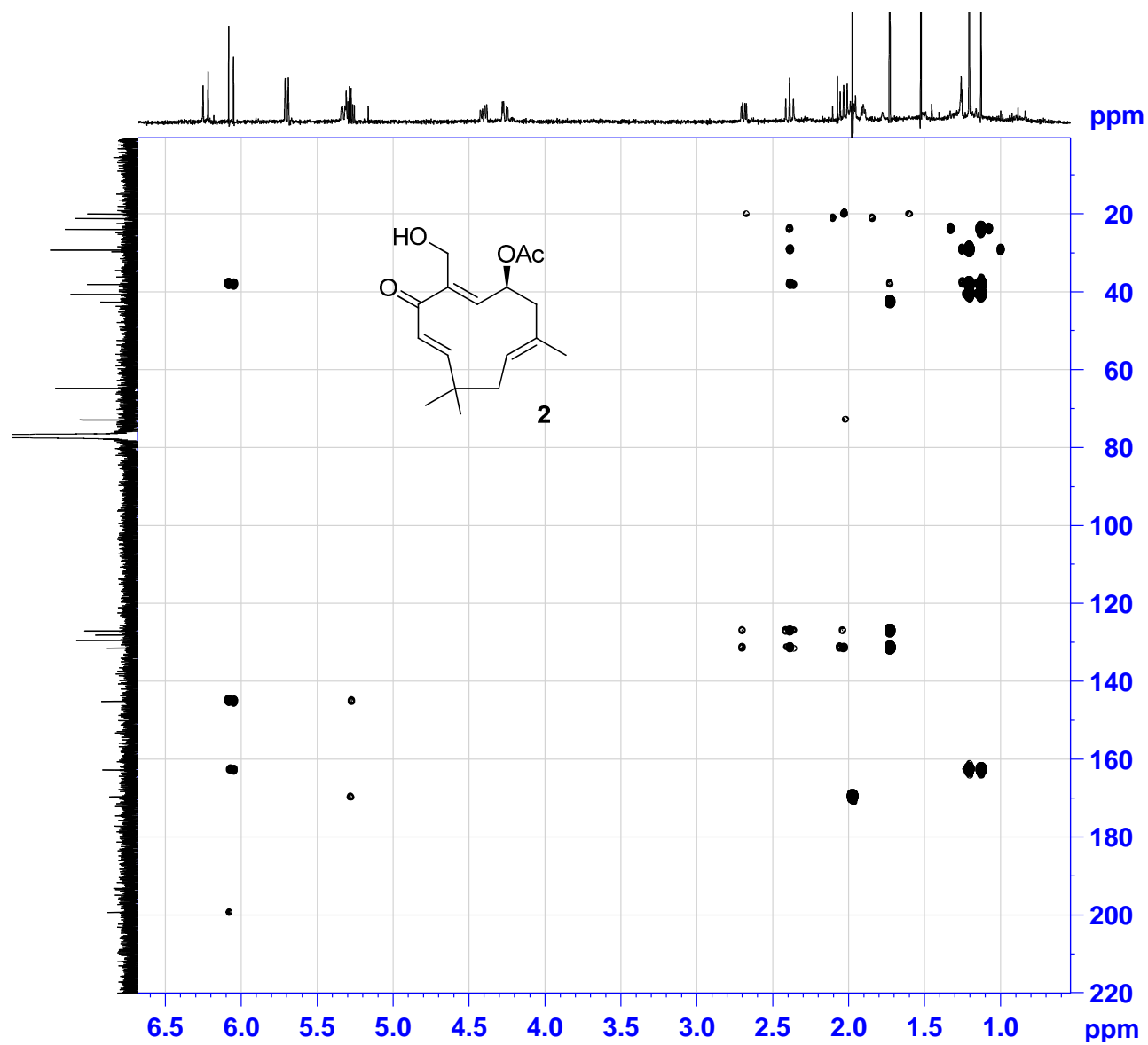
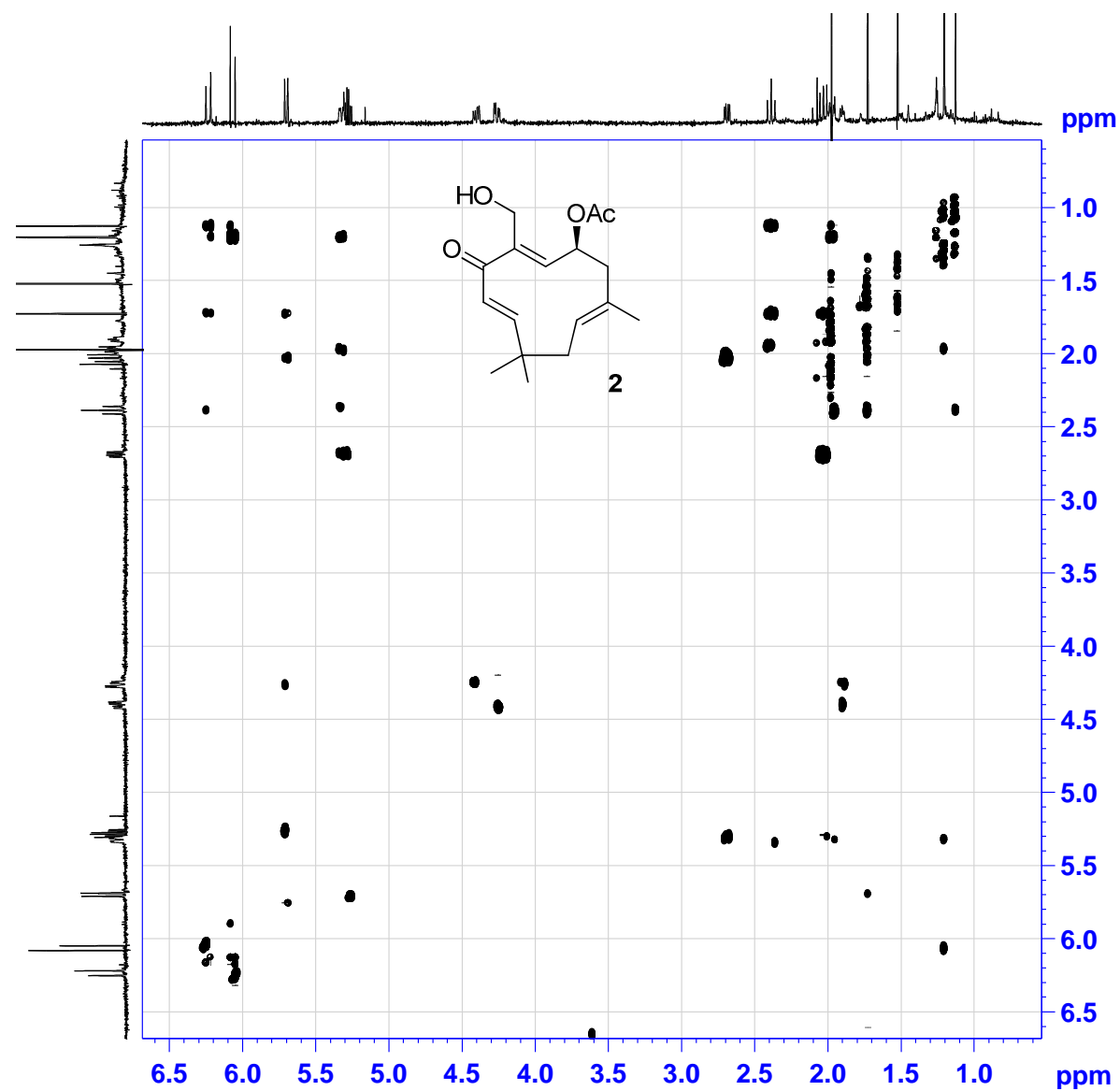




Figure S14. ROESY spectrum of leptogorgin B (2) in CDCl<sub>3</sub>.



**Figure S15.** HRESIMS of leptogorgin C (**3**).

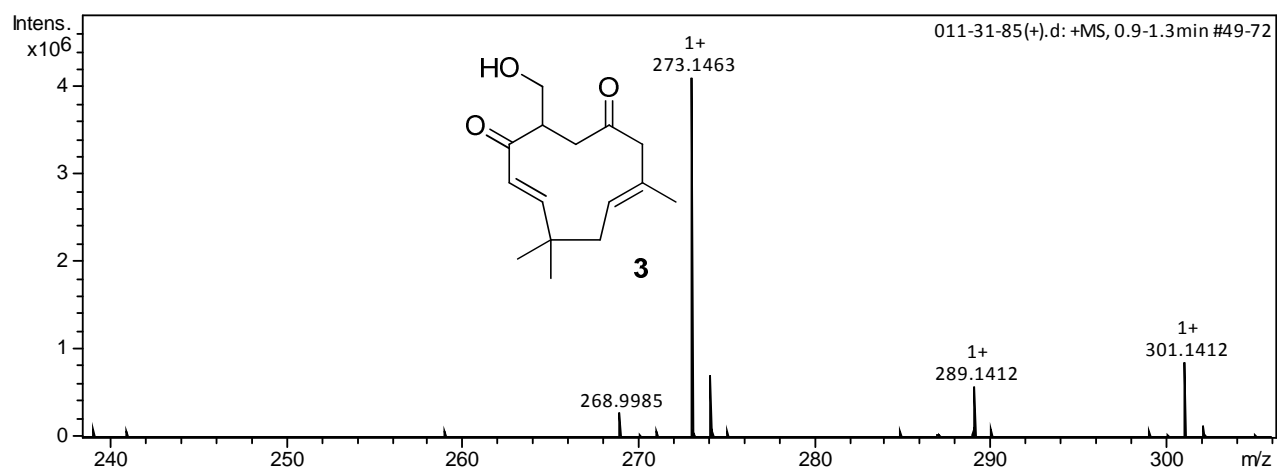
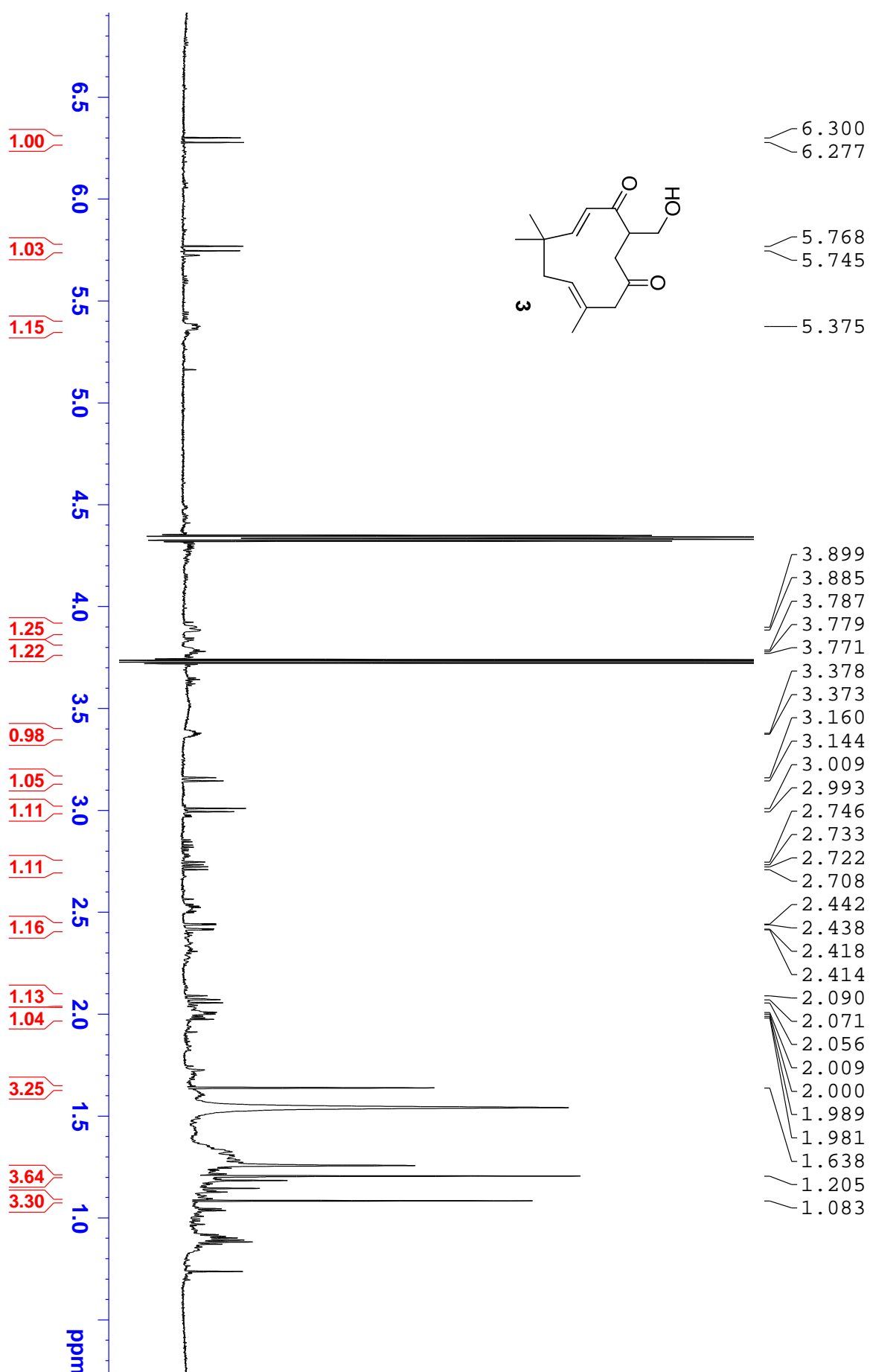


Figure S16.  $^1\text{H}$ -NMR spectrum of leptogorgin C (**3**) in  $\text{CDCl}_3$ .



**Figure S17.**  $^{13}\text{C}$ -NMR spectrum of leptogorgin C (**3**) in  $\text{CDCl}_3$ .

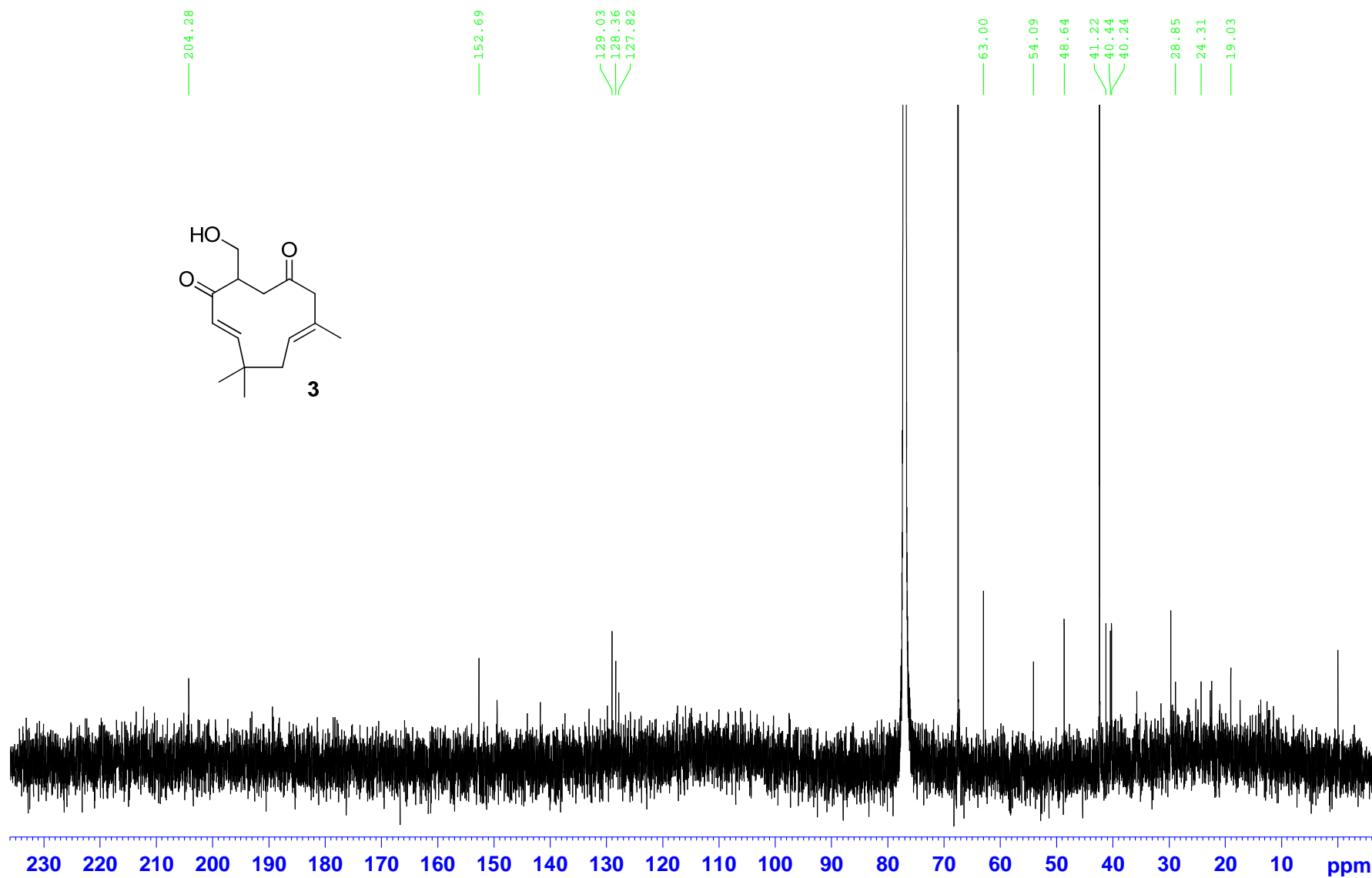


Figure S18.  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum of leptogorgin C (3) in  $\text{CDCl}_3$ .

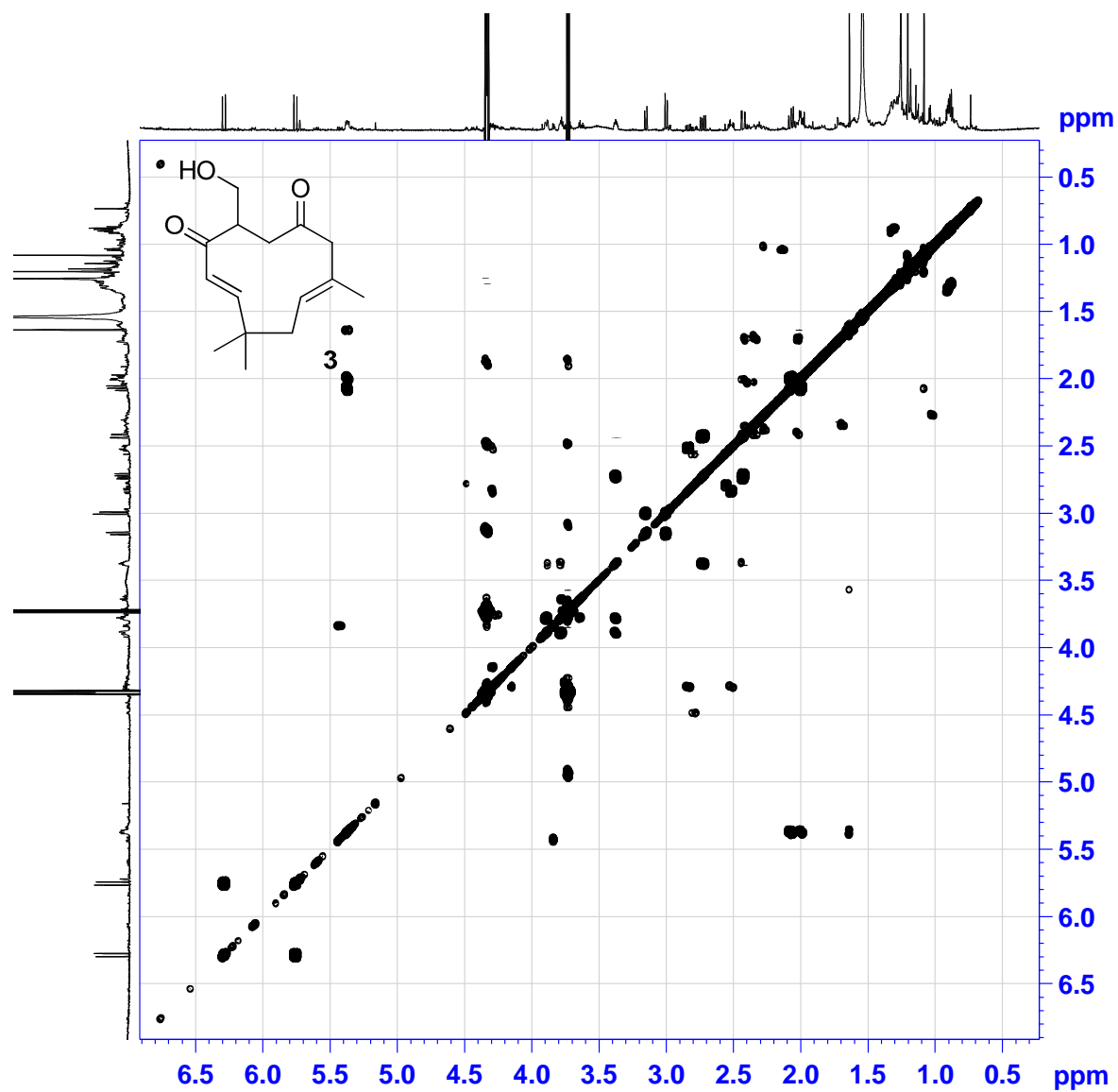


Figure S19. HSQC spectrum of leptogorgin C (3) in CDCl<sub>3</sub>.

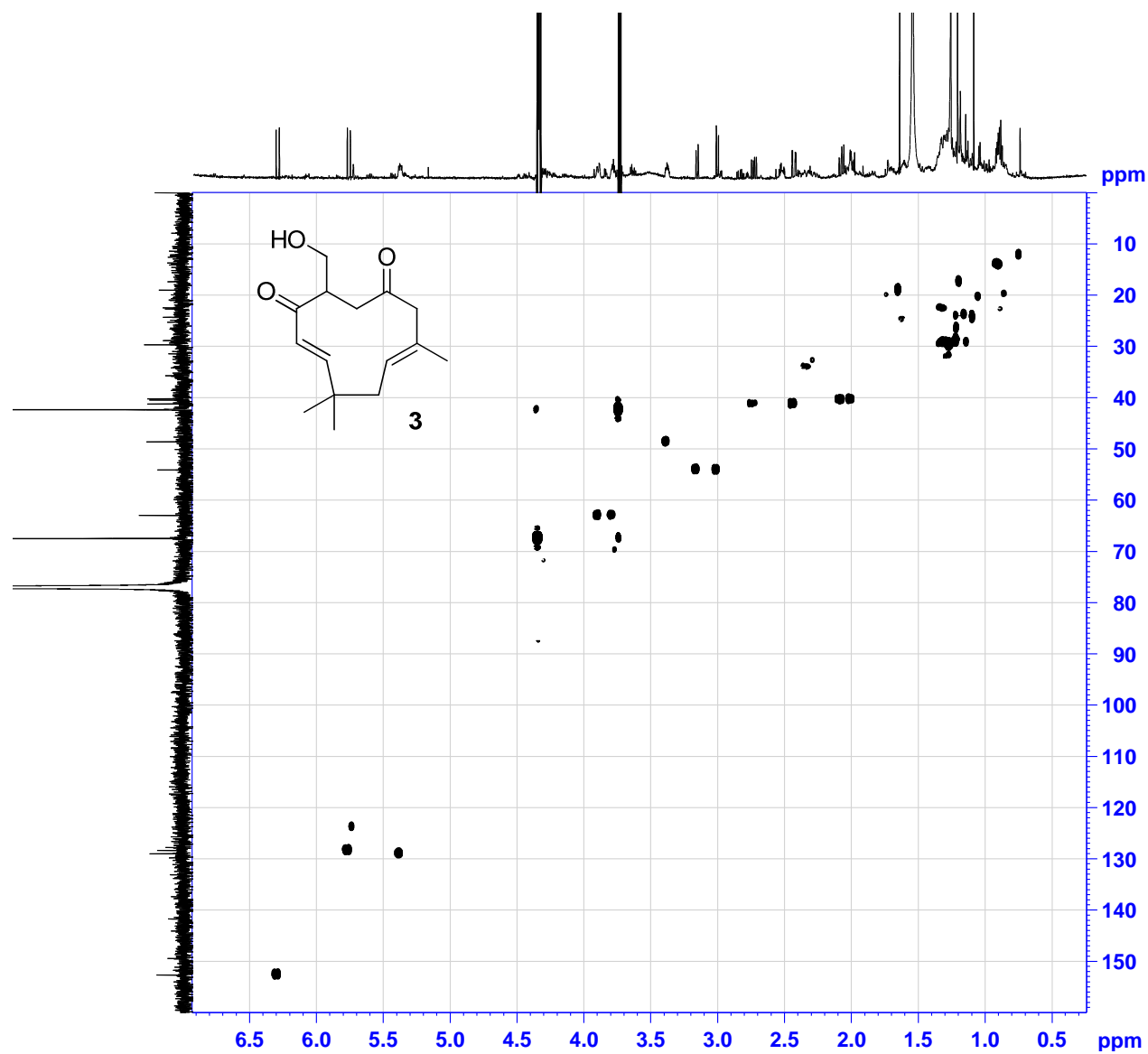
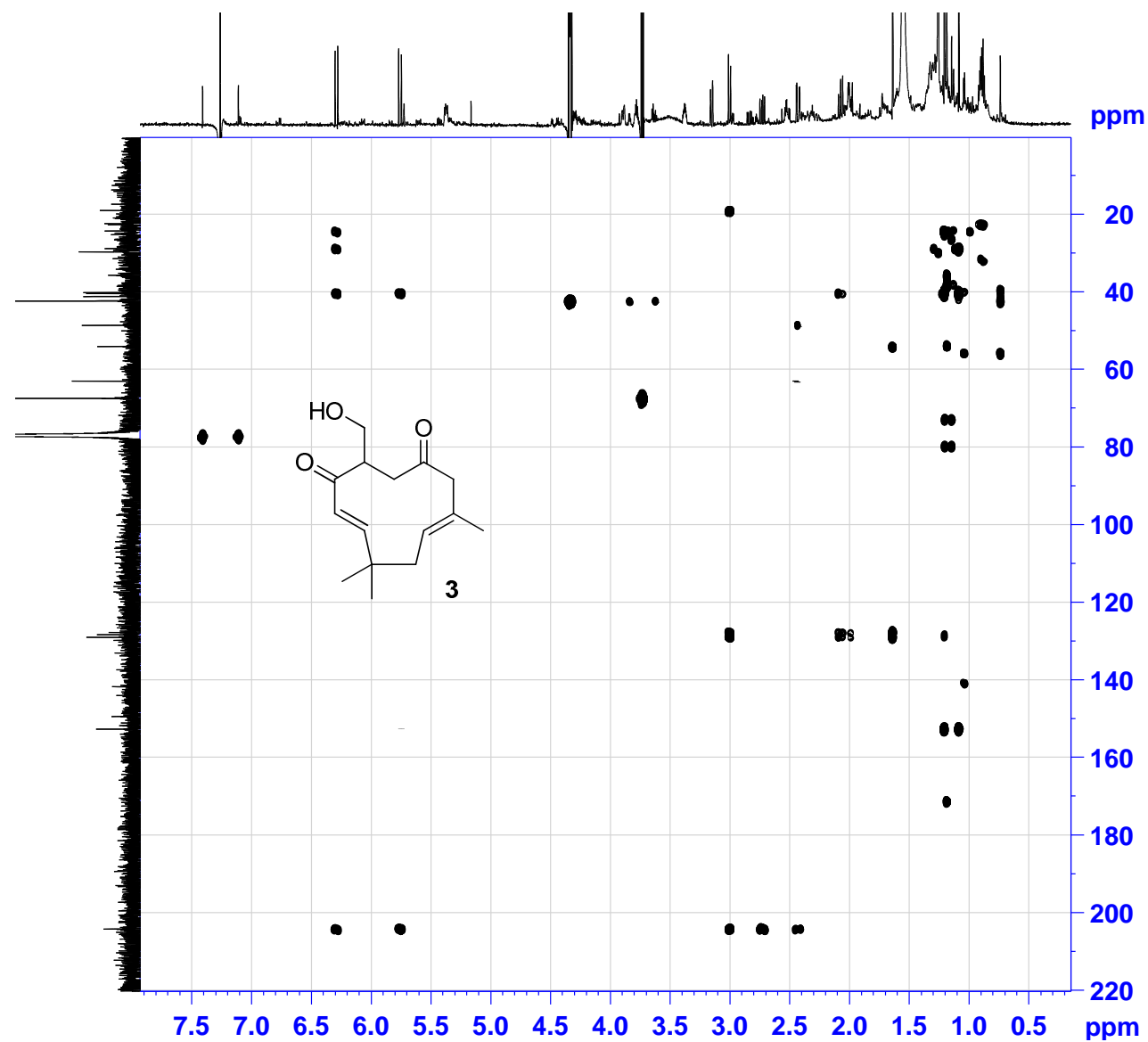
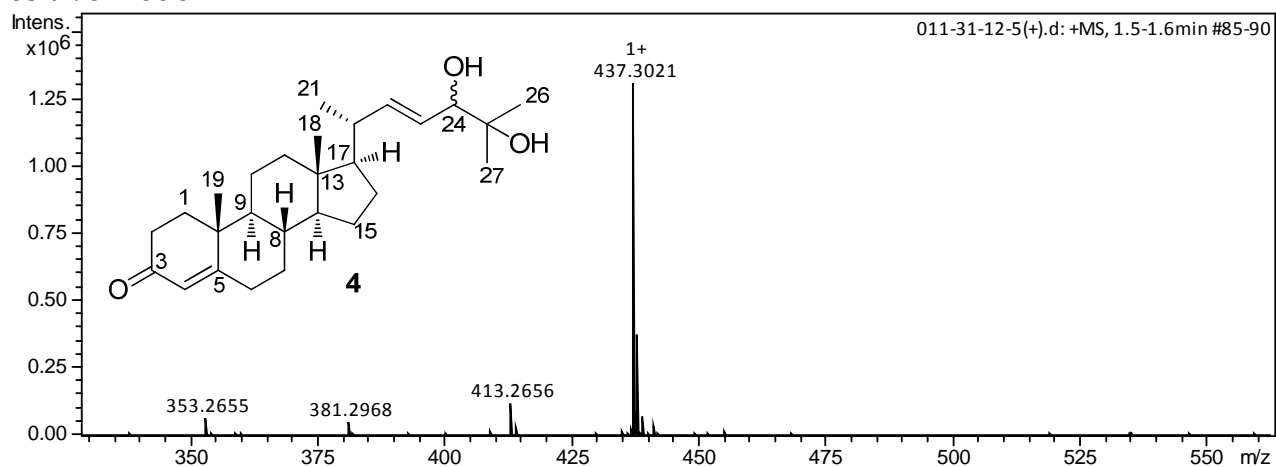


Figure S20. HMBC spectrum of leptogorgin C (3) in CDCl<sub>3</sub>.



**Figure S21.** HRESIMS of leptogorgoid A (**4**).

Positive mode



Negative mode

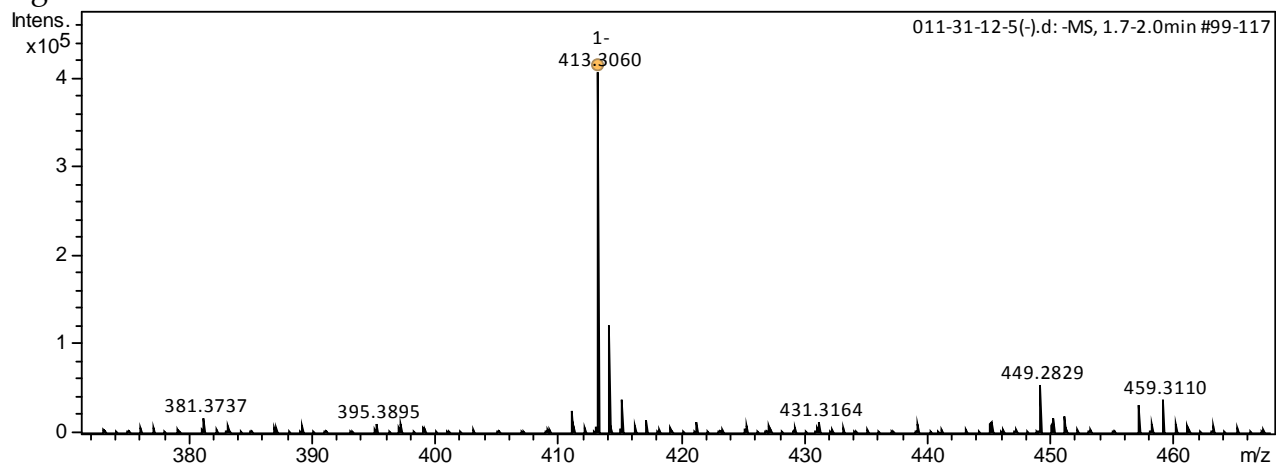




Figure S22.  $^1\text{H}$ -NMR spectrum of leptogorgoid A (4) in  $\text{CDCl}_3$ .

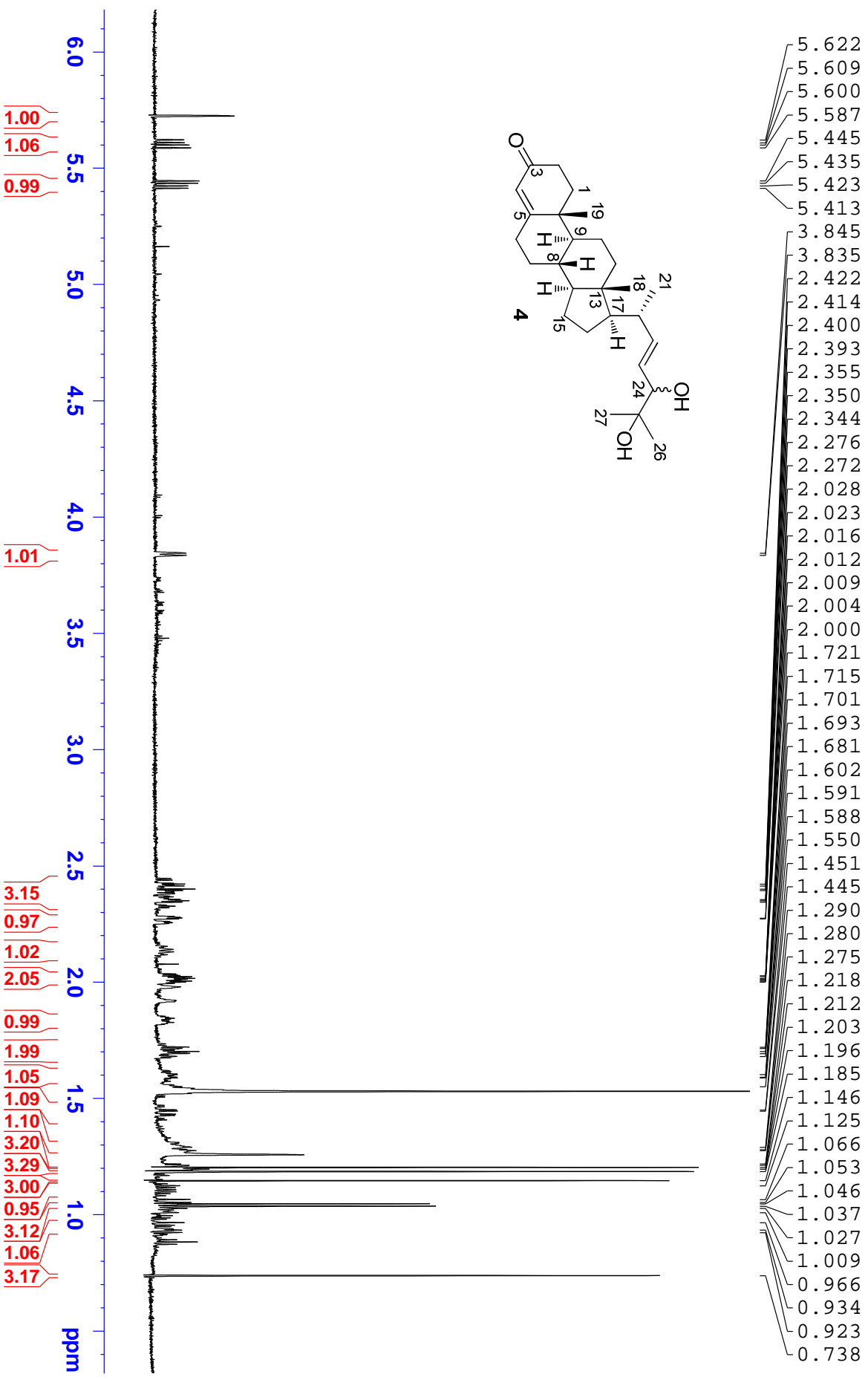
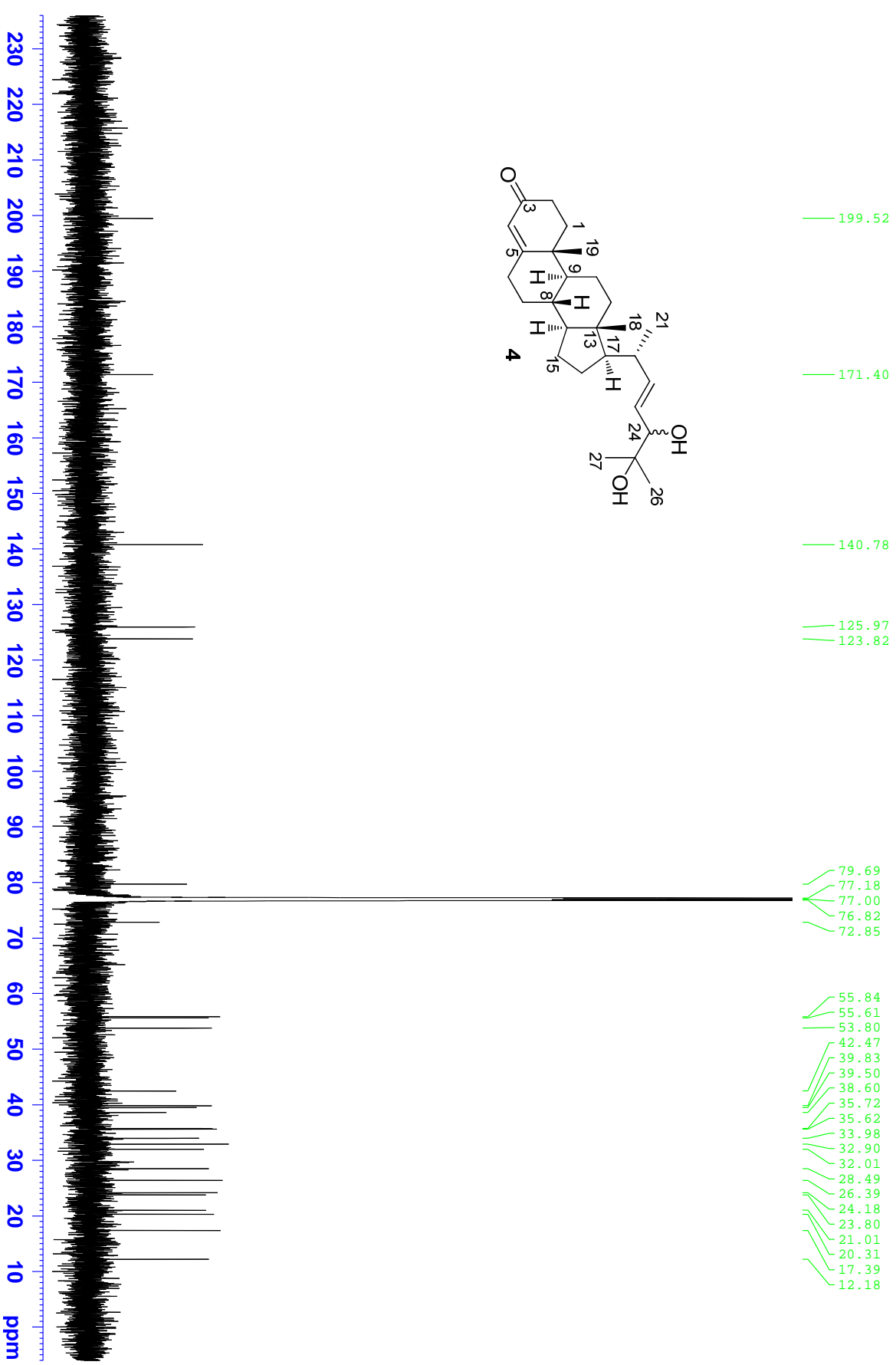


Figure S23.  $^{13}\text{C}$ -NMR spectrum of leptogorgoid A (**4**) in  $\text{CDCl}_3$ .



**Figure S24.**  $^1\text{H}$ - $^1\text{H}$ -COSY spectrum of leptogorgoid A (**4**) in  $\text{CDCl}_3$ .

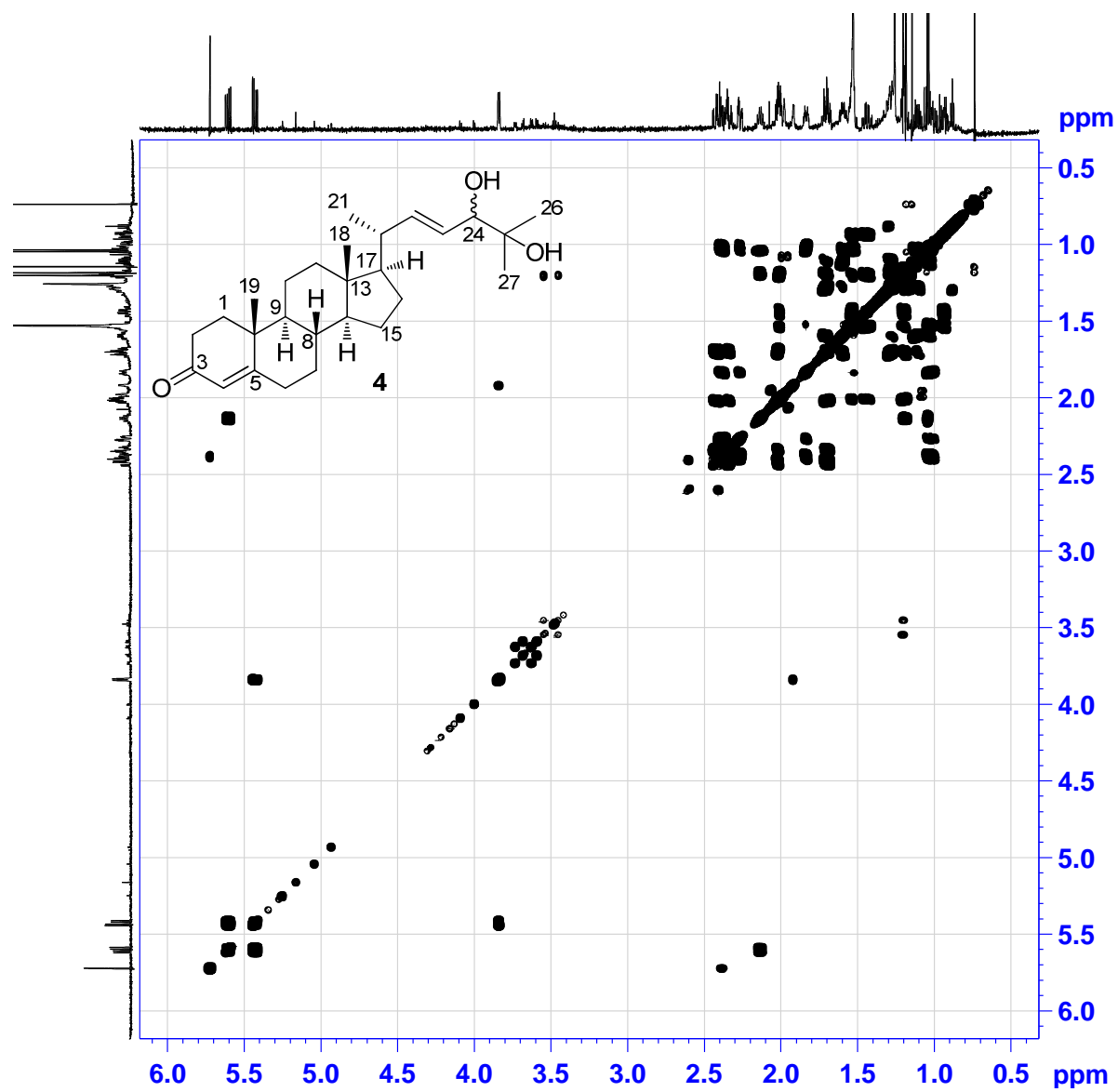


Figure S25. HSQC spectrum of leptogorgoid A (4) in CDCl<sub>3</sub>.

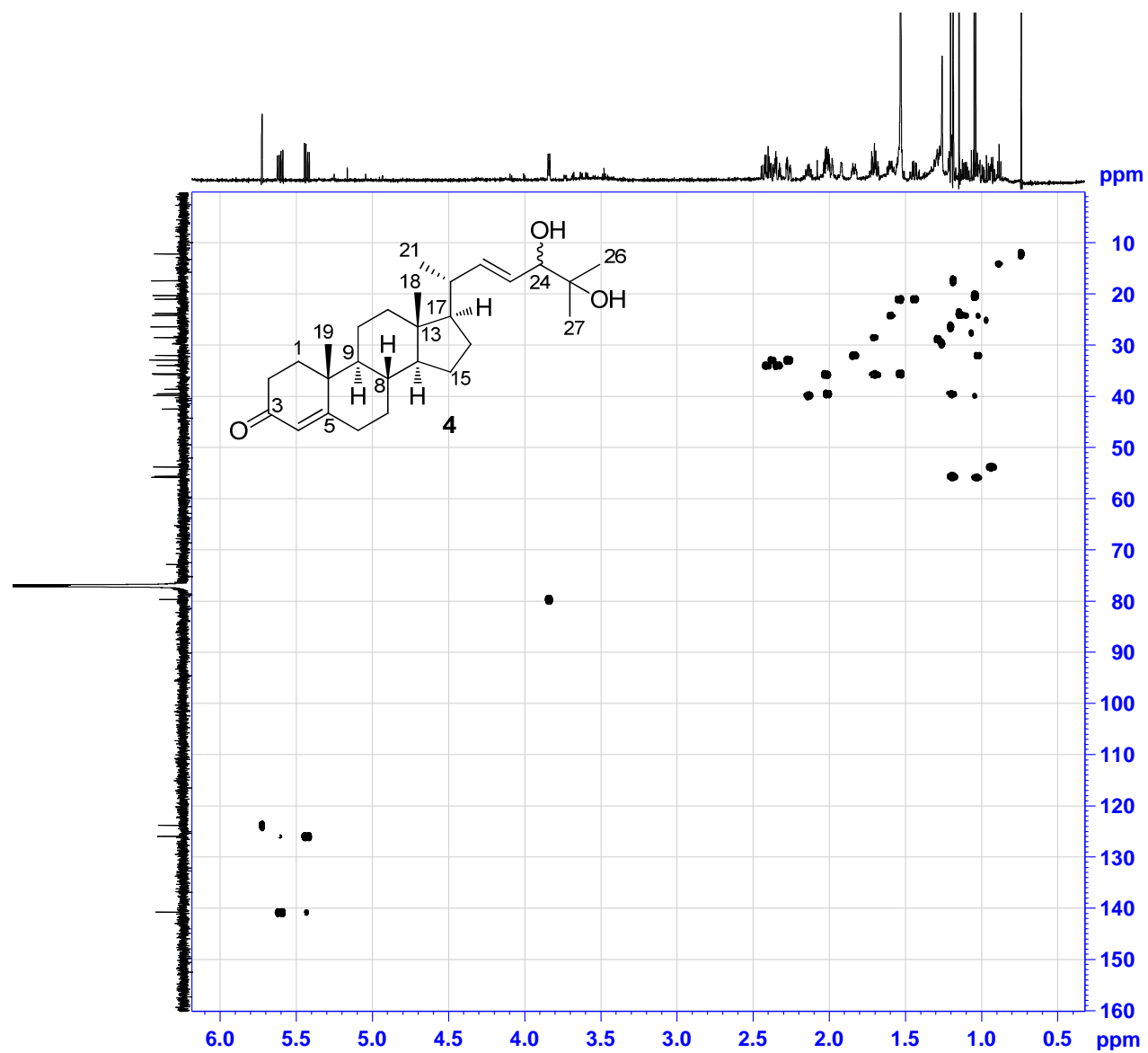
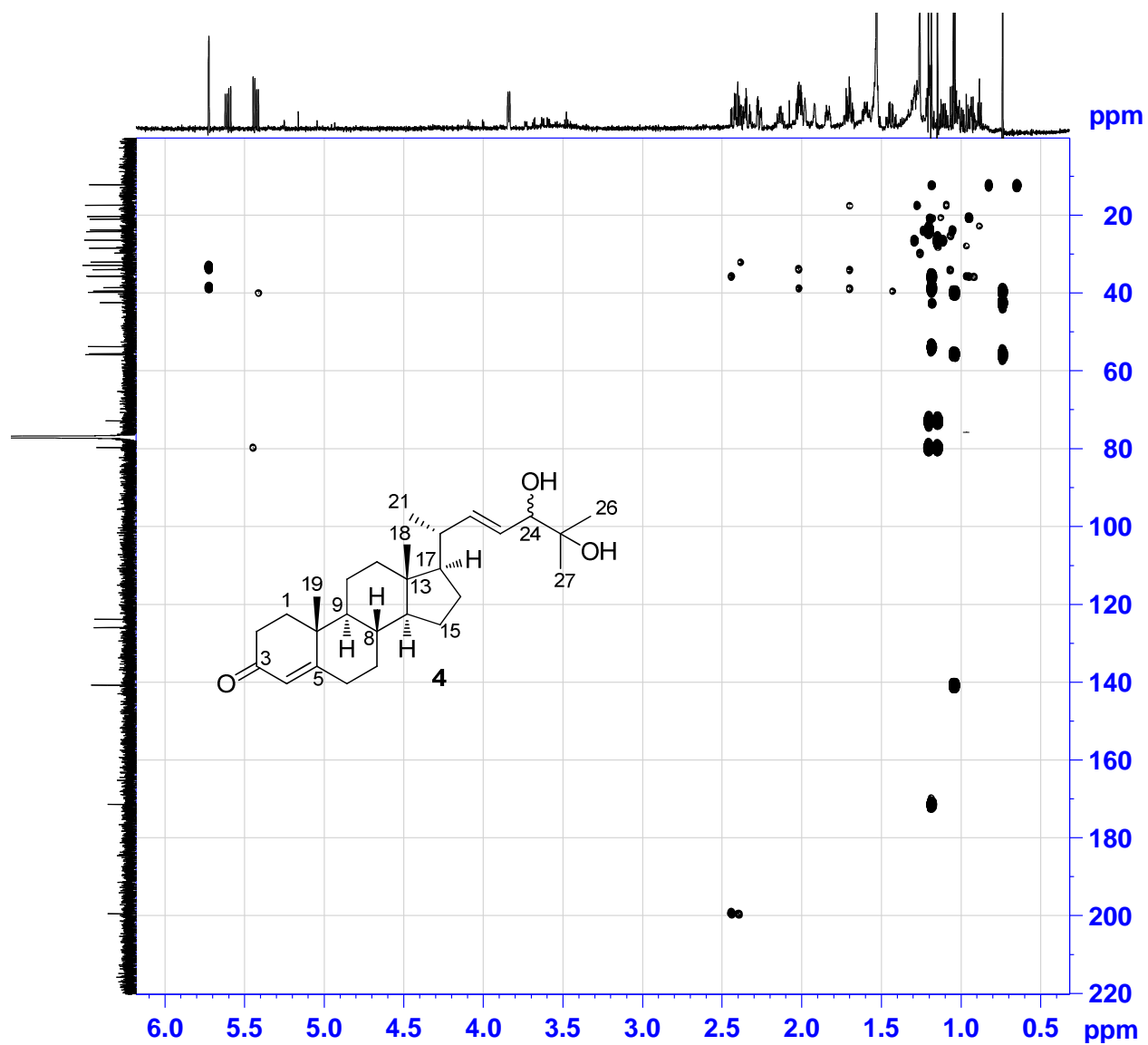


Figure S26. HMBC spectrum of leptogorgoid A (**4**) in CDCl<sub>3</sub>.



**Figure S27.** ECD spectra of leptogorgin A (**1**) and leptogorgin B (**2**).

