

Supplementary Information for

# Phocoenamicins B and C, new antibacterial spirotetonates from the Marine Actinomycete *Micromonospora chiyaphumensis*

Mercedes Pérez-Bonilla\*, Daniel Oves-Costales, Mercedes de la Cruz, María Kokkini, Jesús Martín, Francisca Vicente, Olga Genilloud and Fernando Reyes\*

Fundación MEDINA, Centro de Excelencia en Investigación de Medicamentos Innovadores en Andalucía.

Parque Tecnológico Ciencias de la Salud. Avda. del Conocimiento 34, 18016, Armilla, Granada, Spain;

[daniel.oves@medinaandalucia.es](mailto:daniel.oves@medinaandalucia.es) (D.O.-C.); [mercedes.delacruz@medinaandalucia.es](mailto:mercedes.delacruz@medinaandalucia.es) (M.d.l.C.);

[maria.kokkini@medinaandalucia.es](mailto:maria.kokkini@medinaandalucia.es) (M.K.); [jesus.martin@medinaandalucia.es](mailto:jesus.martin@medinaandalucia.es) (J.M.);

[francisca.vicente@medinaandalucia.es](mailto:francisca.vicente@medinaandalucia.es) (F.V.); [olga.genilloud@medinaandalucia.es](mailto:olga.genilloud@medinaandalucia.es) (O.G.)

\* Correspondence: [mercedes.perez@medinaandalucia.es](mailto:mercedes.perez@medinaandalucia.es) (M.P.-B.); [fernando.reyes@medinaandalucia.es](mailto:fernando.reyes@medinaandalucia.es) (F.R.)  
Tel.: +34-958-993-965 (F.R.)

## Contents:

**Figure S1.**  $^1\text{H}$ - $^1\text{H}$  COSY and key HMBC correlations for **2**.

**Figure S2.** Conformation and configuration of the decalin, cyclohexene and sugars moieties of **2** determined by NOESY data and *J*-based analysis.

**Text S3.** 16S rRNA gene sequence from strain CA-214671.

**Table S4.** NMR spectroscopic data (500 Mz, CD<sub>3</sub>OD) for phocoenamicin (**3**).

**Figure S5.**  $^1\text{H}$ -NMR (500 MHz, methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).

**Figure S6.**  $^{13}\text{C}$ -NMR (125 MHz, methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).

**Figure S7.** HSQC (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).

**Figure S8.** HMBC (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).

**Figure S9.** COSY (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).

**Figure S10.** NOESY (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).

**Figure S11.** TOCSY (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).

**Figure S12.**  $^1\text{H}$ -NMR (500 MHz, methanol-*d*<sub>4</sub>) spectrum of phocoenamicin C (**2**).

**Figure S13.**  $^{13}\text{C}$ -NMR (125 MHz, methanol-*d*<sub>4</sub>) spectrum of phocoenamicin C (**2**).

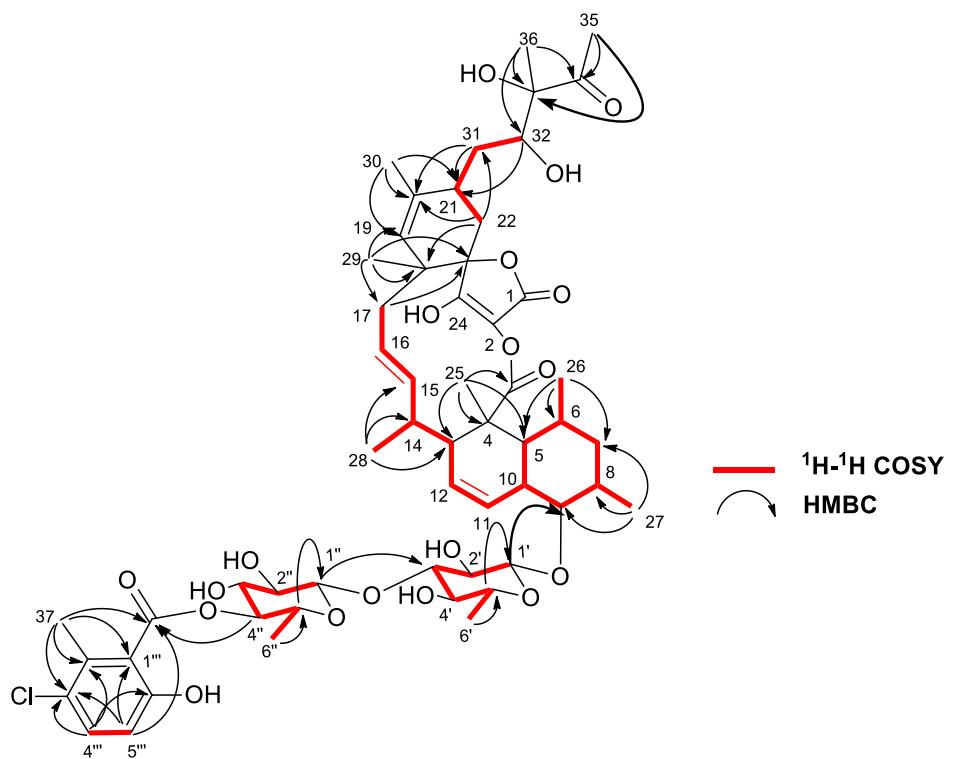
**Figure S14.** HSQC (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin C (**2**).

**Figure S15.** HMBC (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin C (**2**).

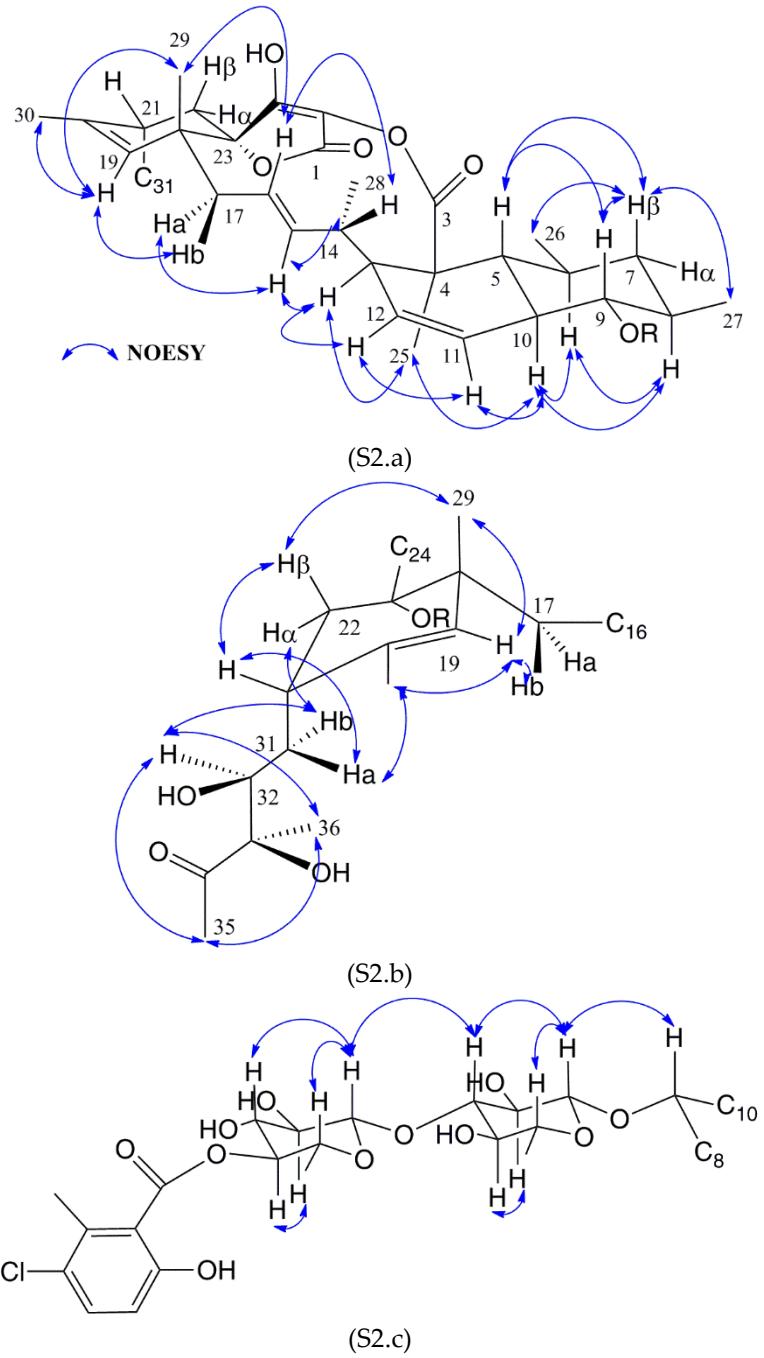
**Figure S16.** COSY (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin C (**2**).

**Figure S17.** NOESY (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin C (**2**).

**Figure S18.** TOCSY (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin C (**2**).



**Figure S1.**  $^1\text{H}$ - $^1\text{H}$  COSY and key HMBC correlations for **2**.



**Figure S2.** Conformation and configuration of the decalin, cyclohexene and sugars moieties of **2** determined by NOESY data and *J*-based analysis.

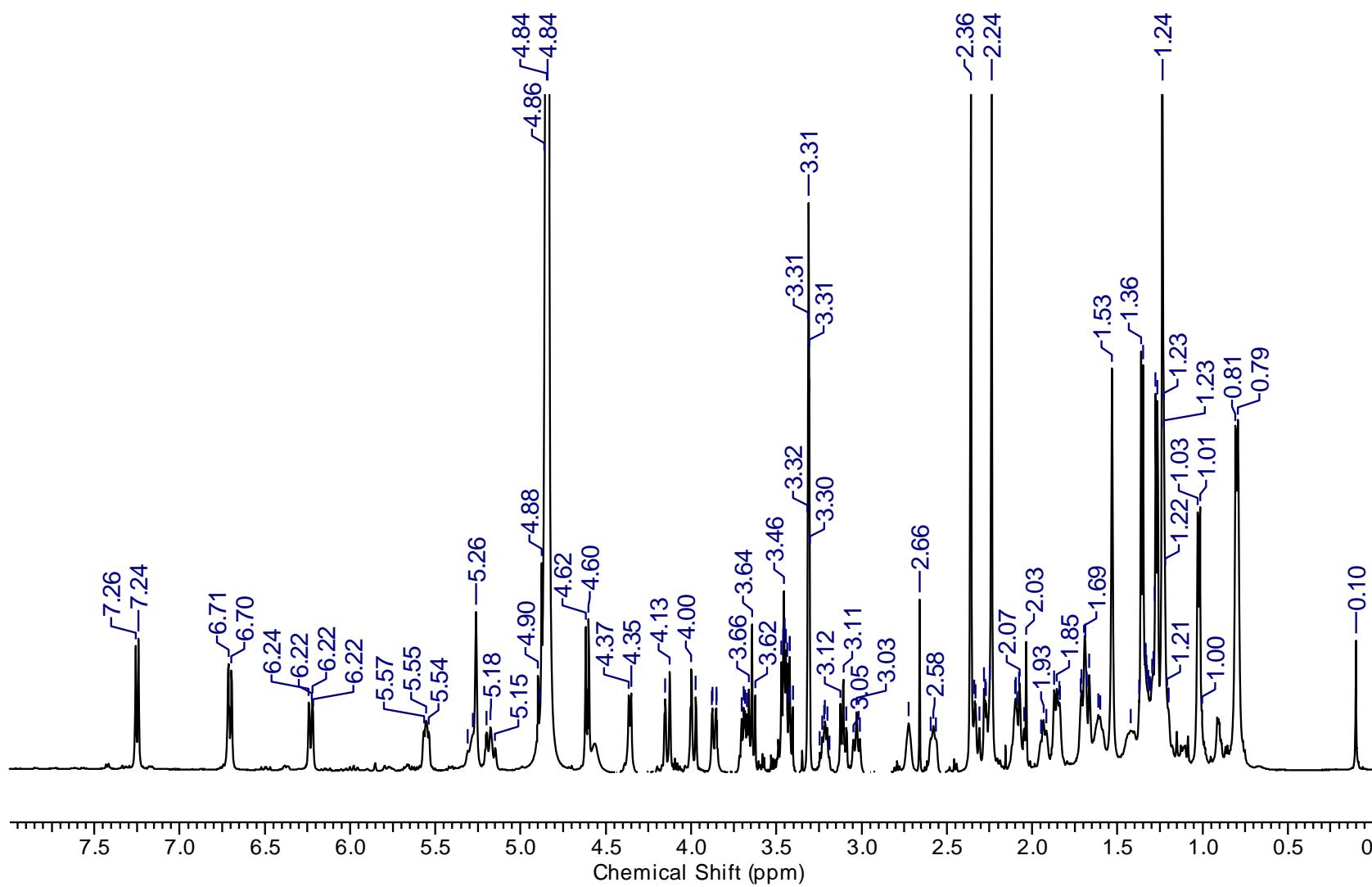
### **Text S3. 16S rRNA gene sequence from strain CA-214671.**

**Table S4.** NMR spectroscopic data (500 Mz, CD<sub>3</sub>OD) for phocoenamicin (3).

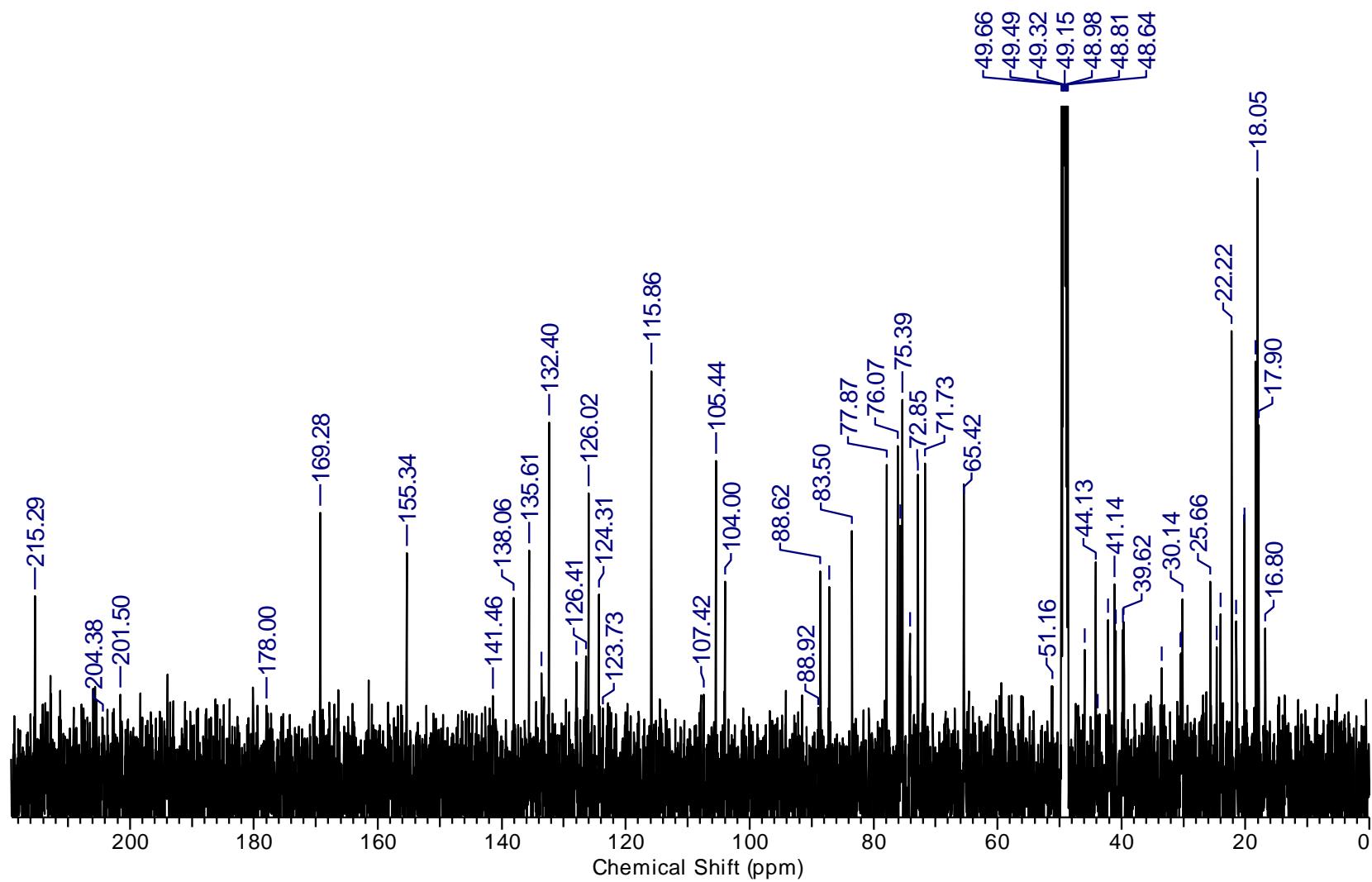
phocoenamicin (3)		
Position	$\delta_C$ , type	$\delta_H$ ( <i>J</i> in Hz)
1	177.8, C	
2	107.3, C	
3	200.1, C	
4	50.9, C	
5	43.6, CH	1.82, m
6	39.5, CH	1.49, m
7 $\alpha$	45.7, CH <sub>2</sub>	1.72, m
7 $\beta$		1.21, m
8	40.9, CH	1.64, m
9	88.6, CH	3.04, t (9.7)
10	48.4, CH	1.97, m
11	126.0, CH	6.29, d (10.0)
12	126.7, CH	5.57, dd (10.0, 6.2)
13	43.0, CH	2.67, *
14	40.0, CH	2.05, m
15	144.1, CH	5.36, dd (15.1, 9.1)
16	123.2, CH	5.14, dd (15.1, 10.4)
17a		2.31, m
17b	44.0, CH <sub>2</sub>	1.86, m
18	41.2, C	
19	132.1, CH	5.02, s
20	134.6, C	
21	34.3, CH	2.37, m
22 $\alpha$		2.28, m
22 $\beta$	30.3, CH <sub>2</sub>	1.71, m
23	87.5, C	
24	205.7, C	
25	17.0, CH <sub>3</sub>	1.59, s
26	23.7, CH <sub>3</sub>	0.82, brs
27	20.1, CH <sub>3</sub>	1.03, d (6.2)

28	21.5, CH <sub>3</sub>	0.82, brs
29	24.7, CH <sub>3</sub>	1.23, brs
30	22.3, CH <sub>3</sub>	1.74, s
31a	33.7, CH <sub>2</sub>	1.95, m
31b		1.74, m
32	74.0, CH	3.82, d (10.6)
33	83.4, C	
34	215.4, C	
35	25.7, CH <sub>3</sub>	2.24, s
36	22.2, CH <sub>3</sub>	1.22, s
1'	104.0, CH	4.35, d (6.2)
2'	75.3, CH	3.45, m
3'	88.6, CH	3.46, m
4'	75.6, CH	3.11, t (8.7)
5'	72.9, CH	3.22, m
6'	18.4, CH <sub>3</sub>	1.27, d (6.0)
1''	105.4, CH	4.61, d (7.8)
2''	76.0, CH	3.42, t (8.6)
3''	75.3, CH	3.65, t (9.7)
4''	77.9, CH	4.89, *
5''	71.7, CH	3.68, m
6''	18.0, CH <sub>3</sub>	1.36, d (6.2)
1'''	124.3, C	
2'''	135.6, C	
3'''	126.0, C	
4'''	132.4, CH	7.25, d (8.7)
5'''	115.8, CH	6.70, d (8.7)
6'''	155.3, C	
7'''	169.3, C	
37	17.9, CH <sub>3</sub>	2.36, s

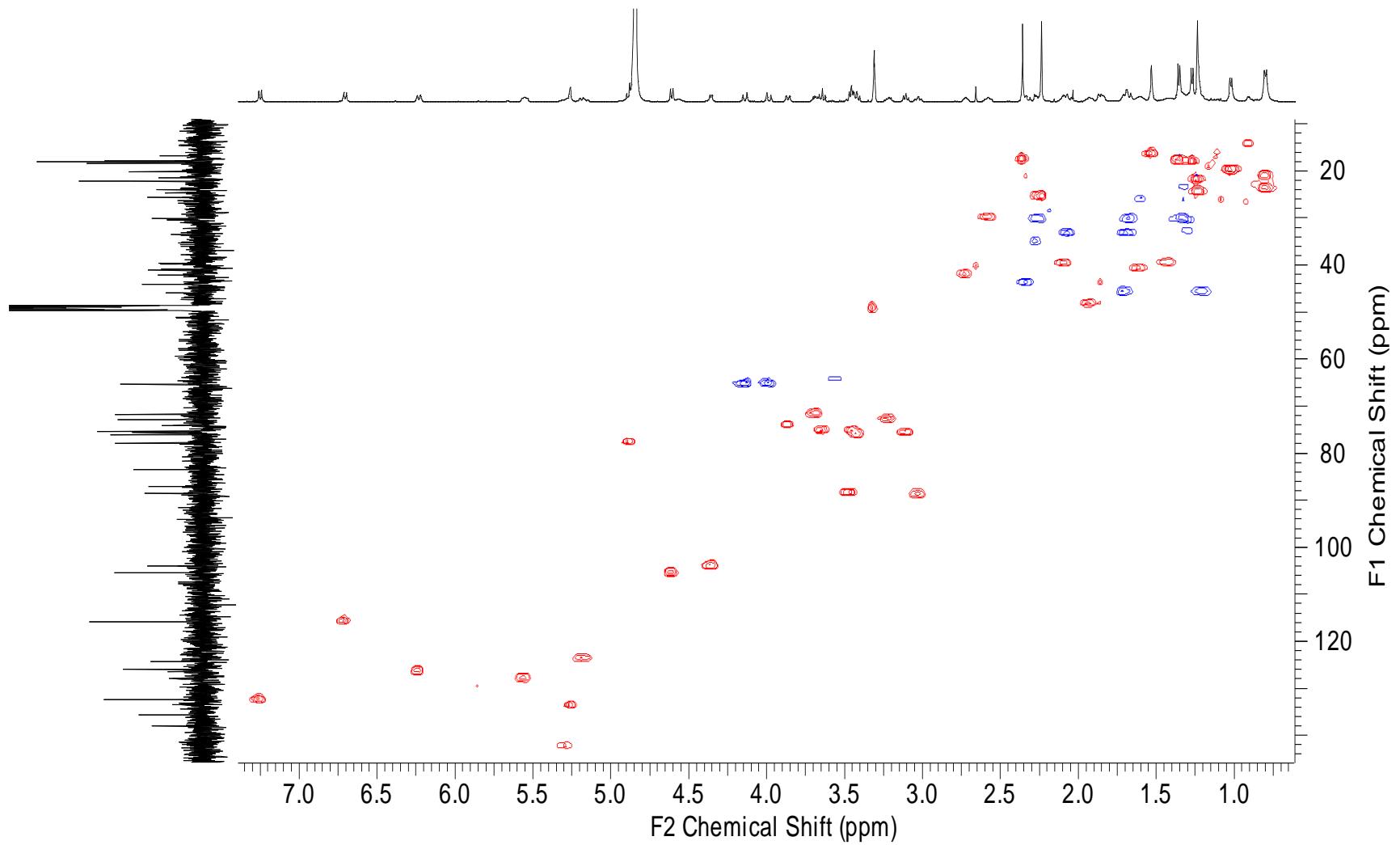
\*Multiplicity not clear, the signal is overlapped.



**Figure S5.**  $^1\text{H}$ -NMR (500 MHz, methanol- $d_4$ ) spectrum of phocoenamycin B (**1**).



**Figure S6.**  $^{13}\text{C}$ -NMR (125 MHz, methanol- $d_4$ ) spectrum of phocoenamicin B (1).



**Figure S7.** HSQC (methanol- $d_4$ ) spectrum of phocoenamicin B (**1**).

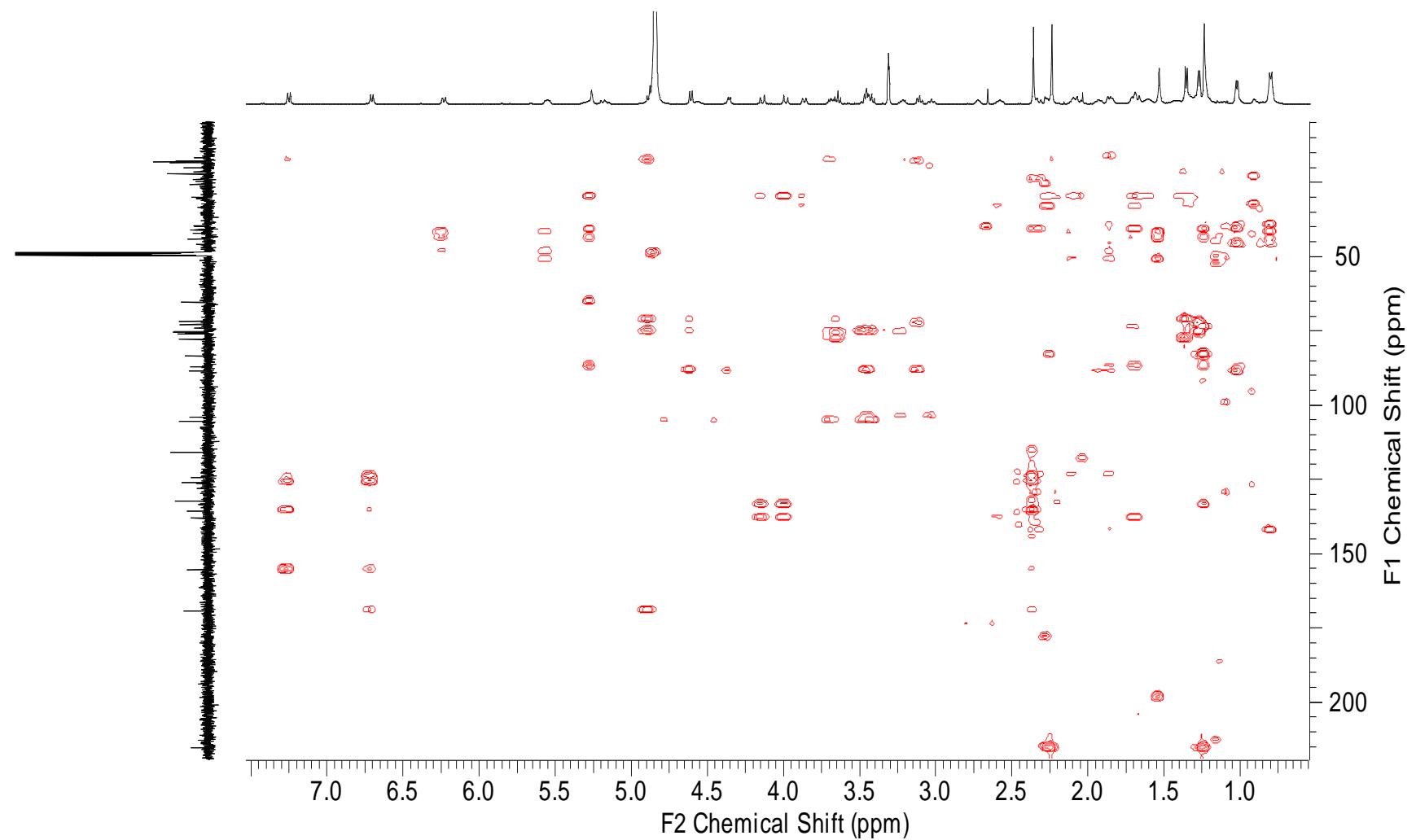


Figure S8. HMBC (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).

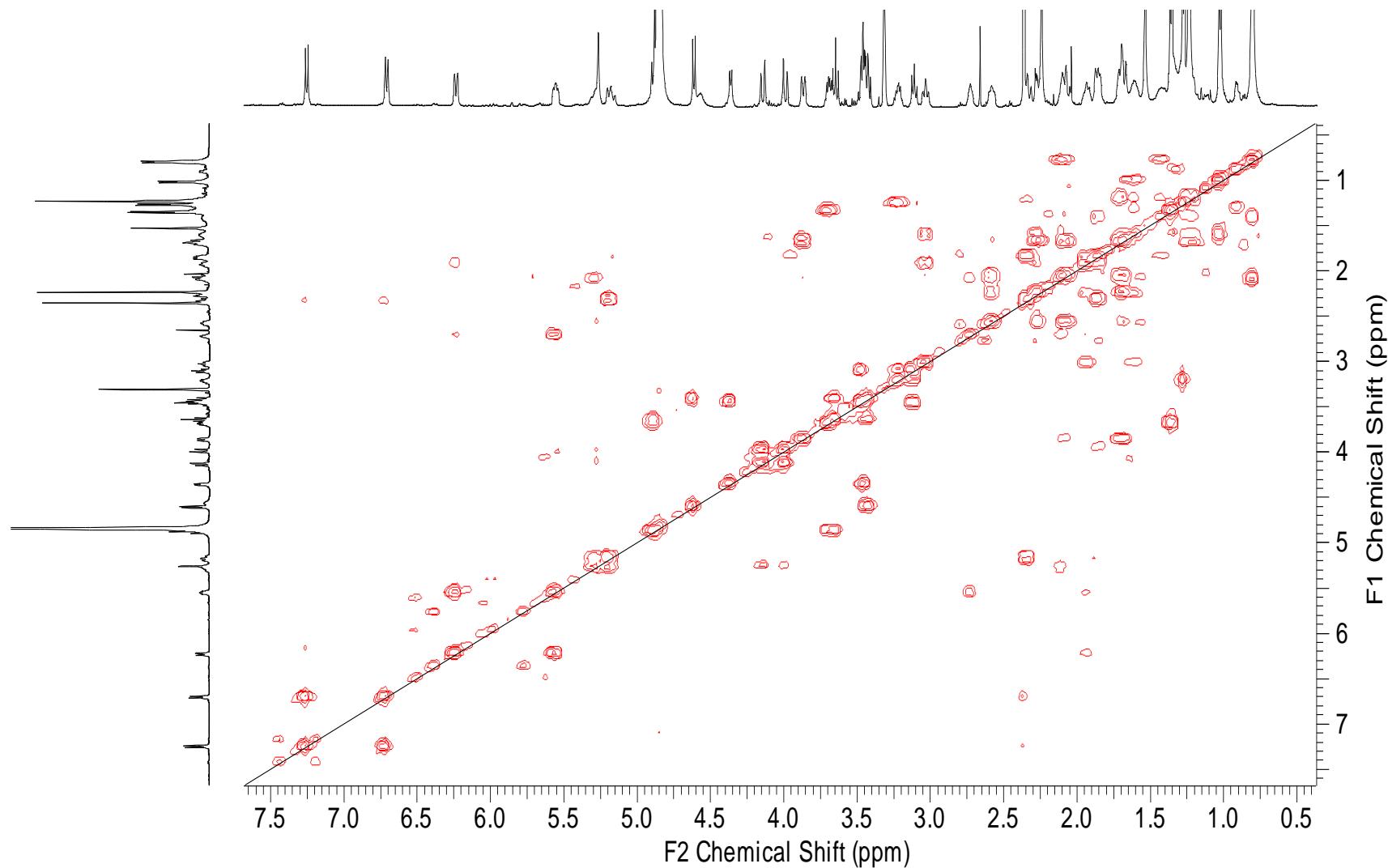
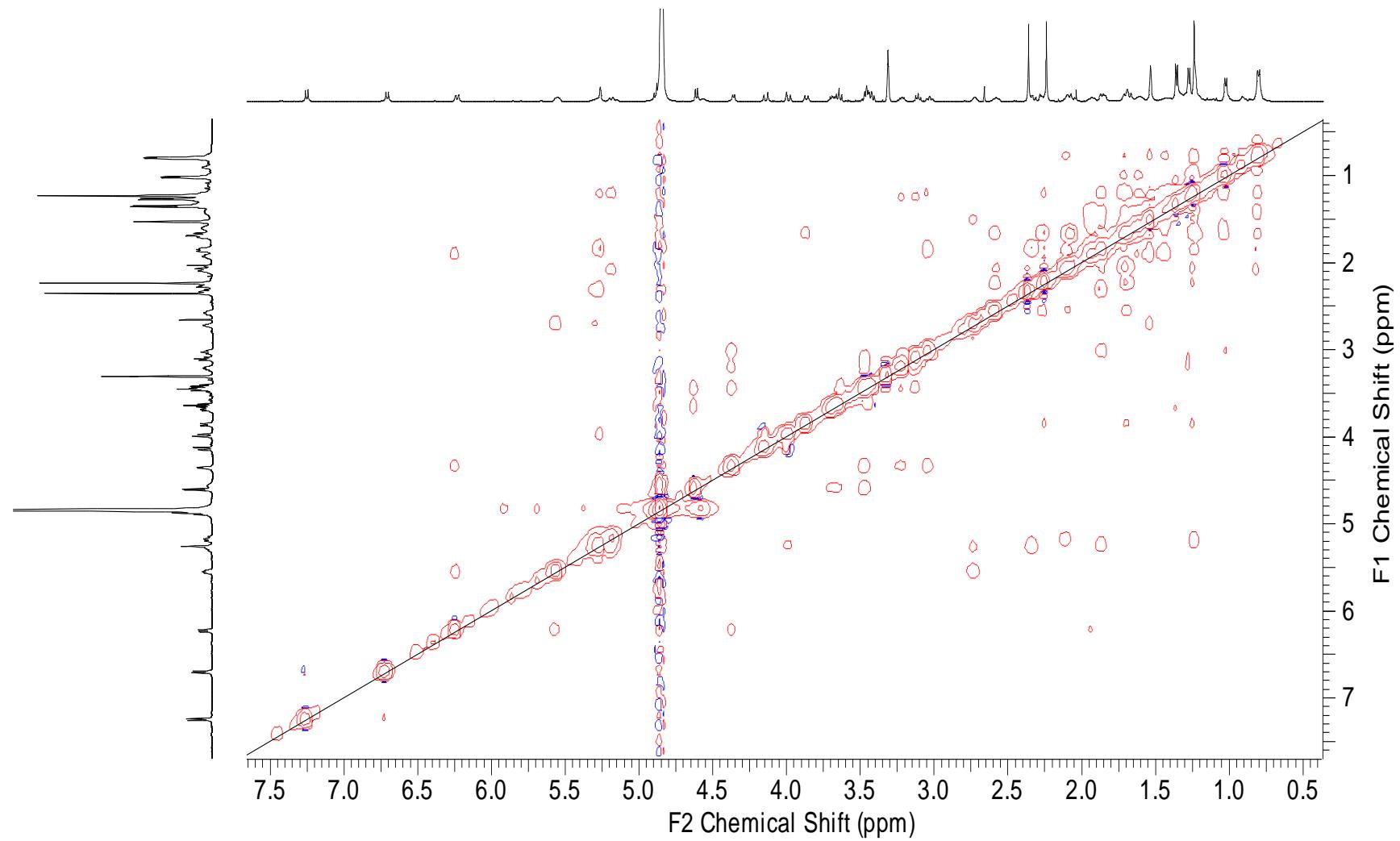
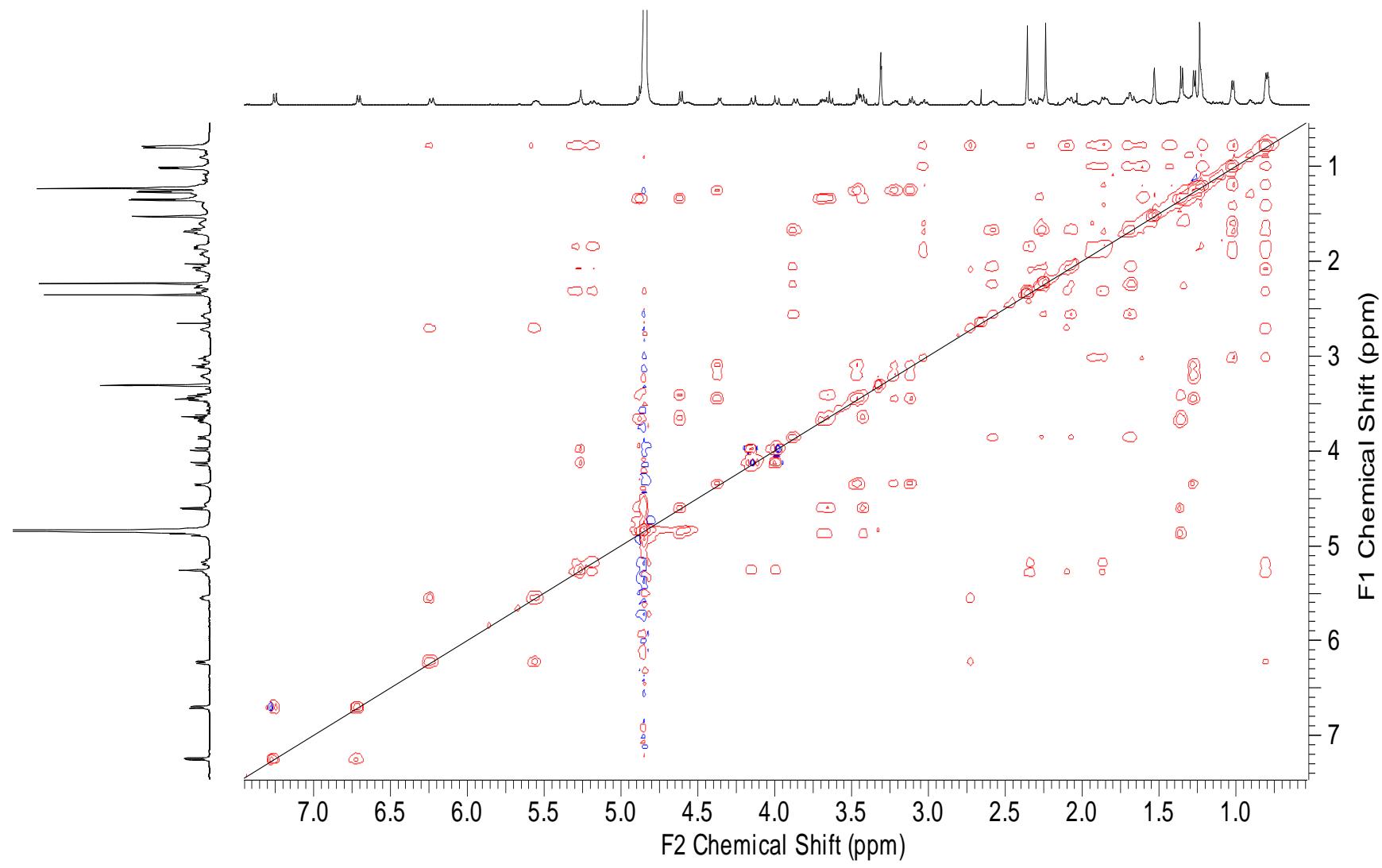


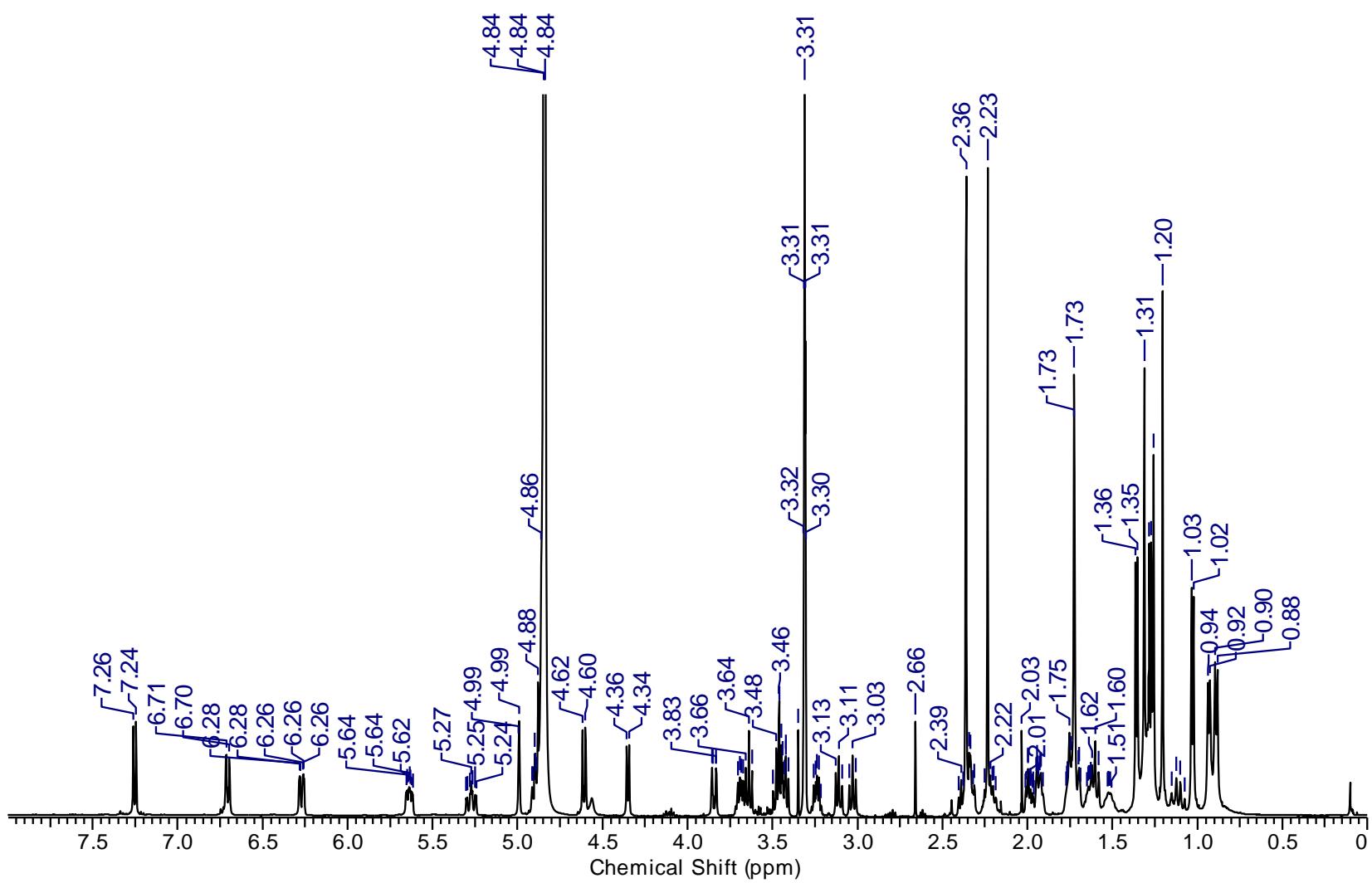
Figure S9. COSY (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).



**Figure S10.** NOESY (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin B (**1**).



**Figure S11.** TOCSY (methanol-*d*<sub>4</sub>) spectrum of phcoenamicin B (**1**).



**Figure S12.**  ${}^1\text{H}$ -NMR (500 MHz, methanol- $d_4$ ) spectrum of phocoenamicin C (2).

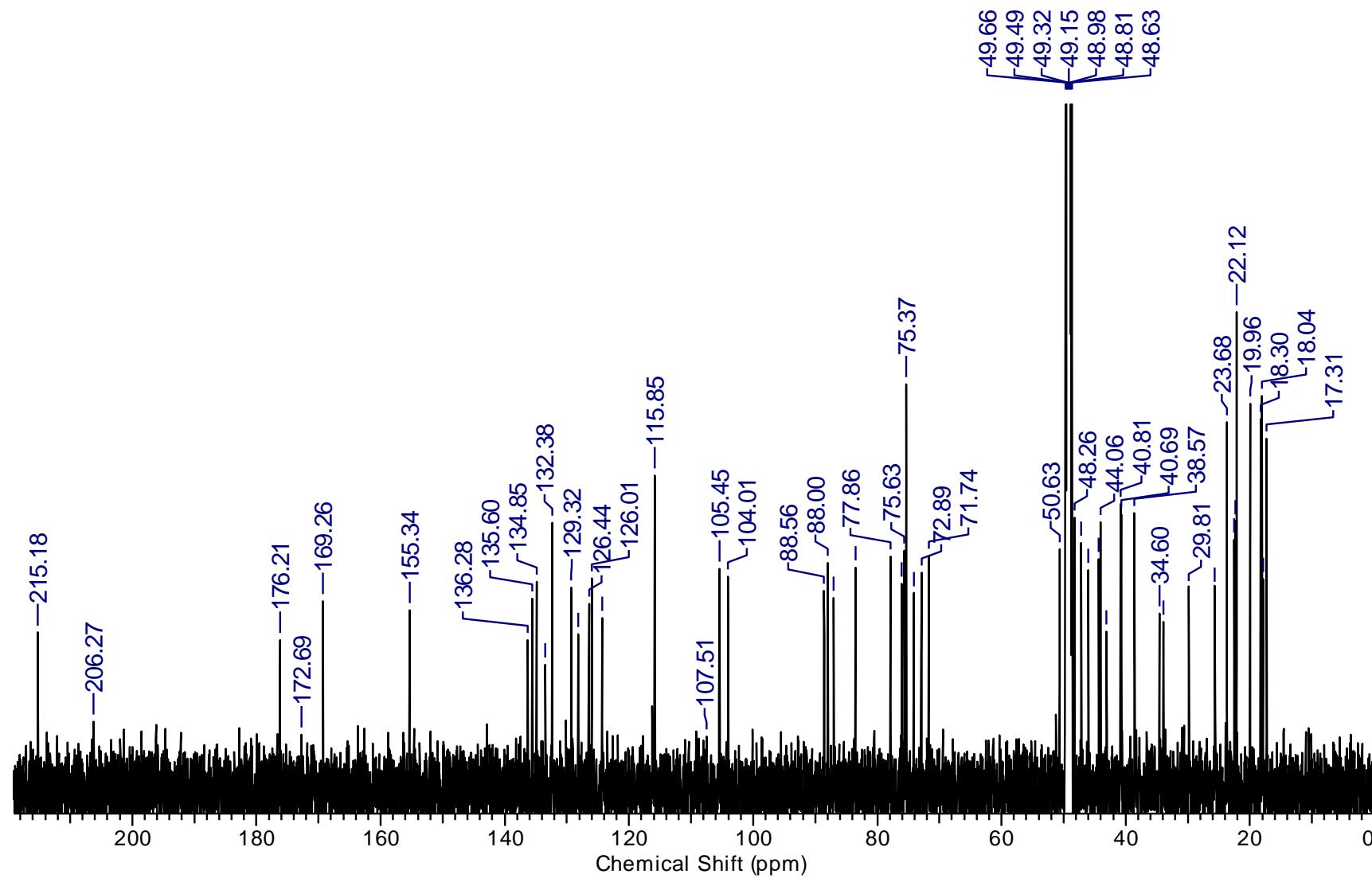


Figure S13.  $^{13}\text{C}$ -NMR (125 MHz, methanol- $d_4$ ) spectrum of phocoenamicin C (2).

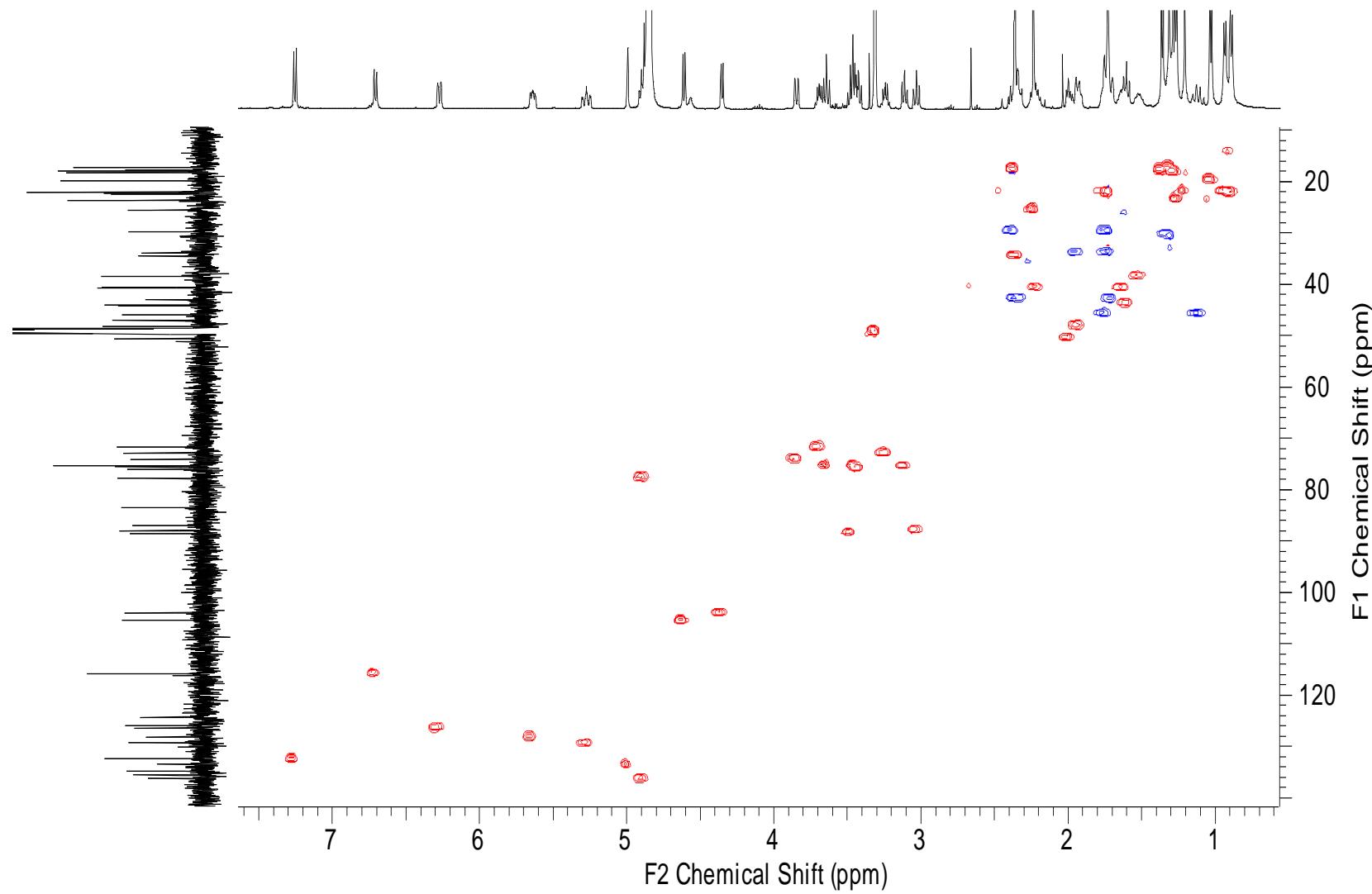
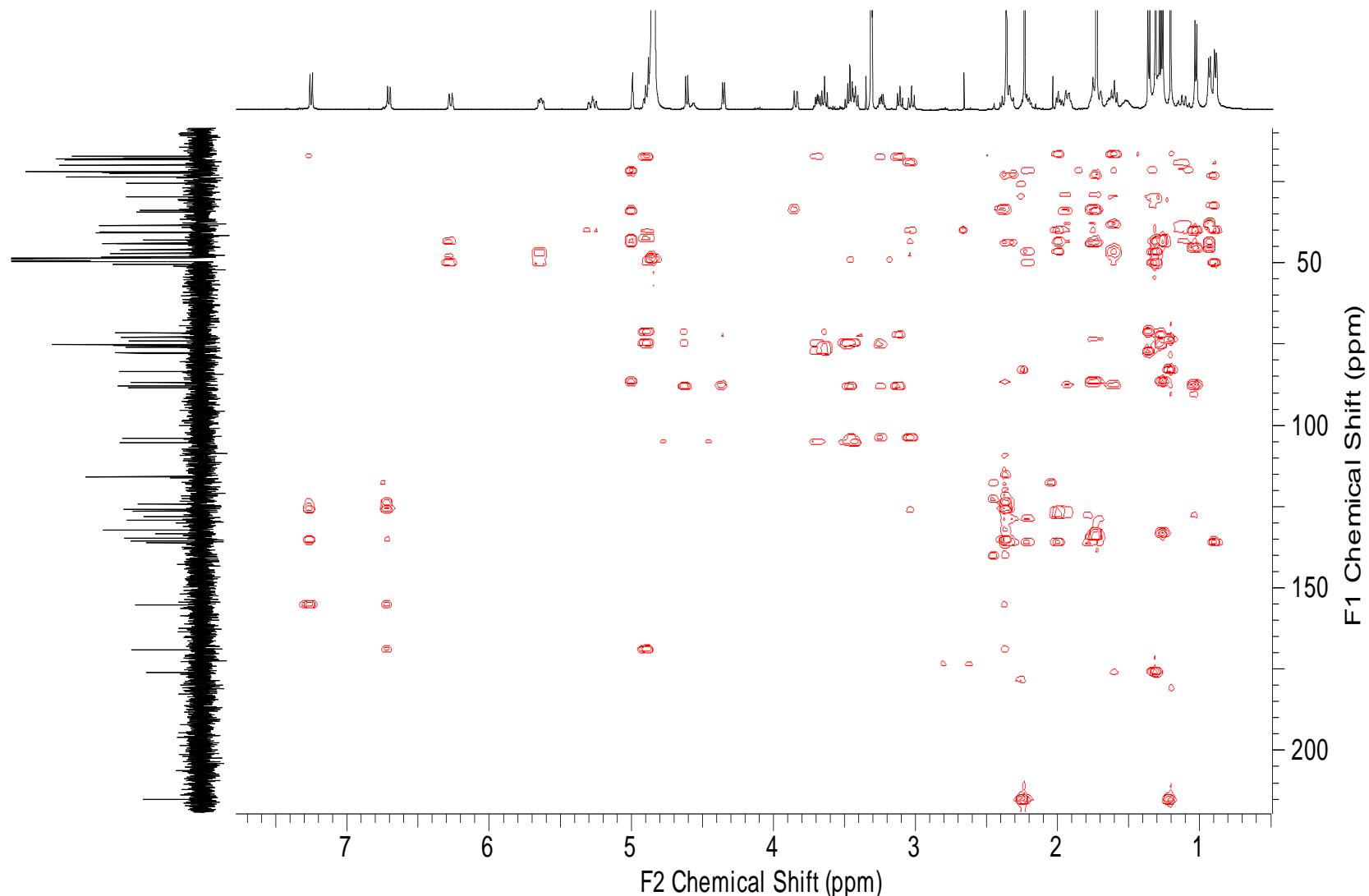
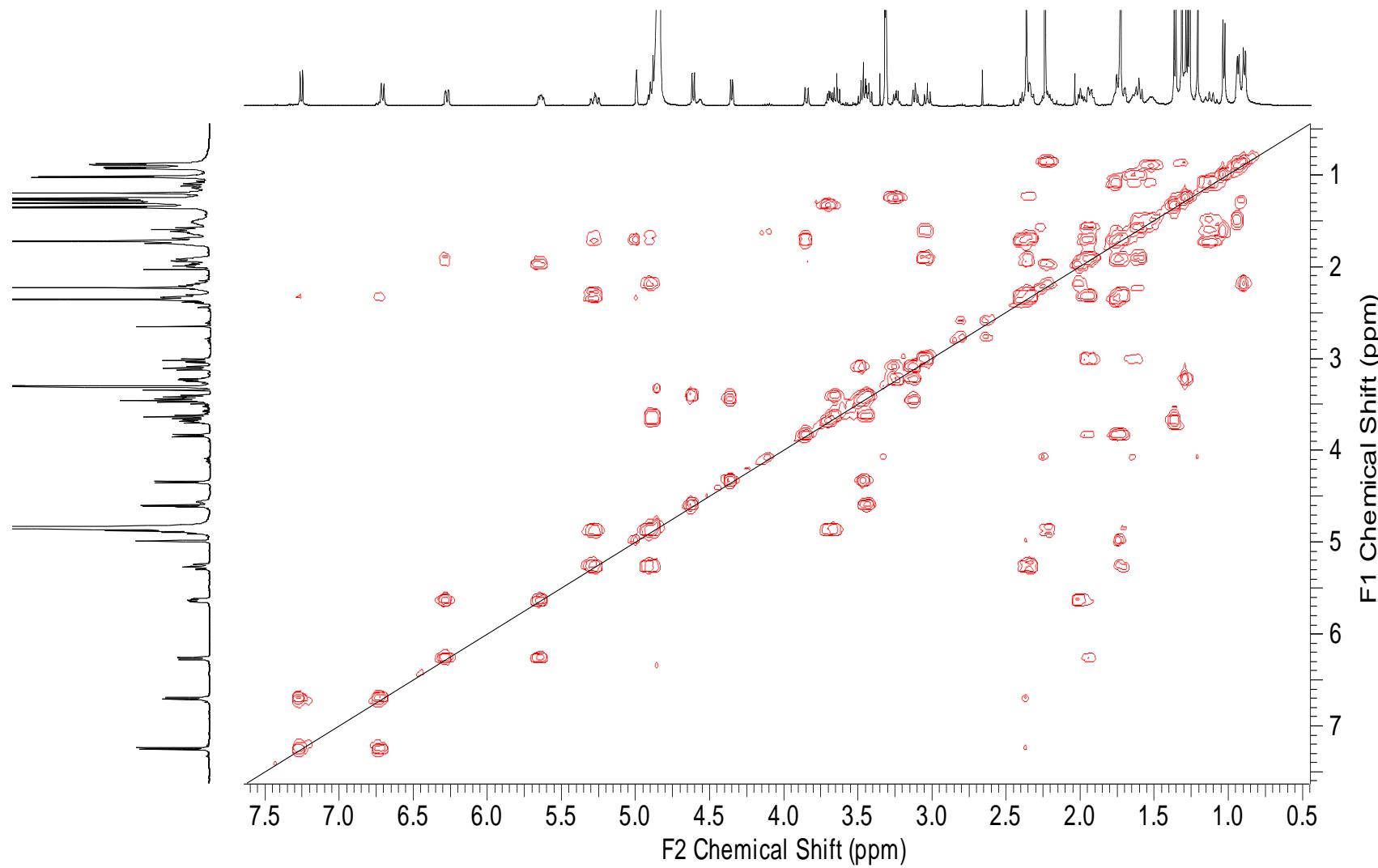


Figure S14. HSQC (methanol- $d_4$ ) spectrum of phocoenamicin C (2).



**Figure S15.** HMBC (methanol-*d*<sub>4</sub>) spectrum of phocoenamicin C (2).



**Figure S16.** COSY ( $\text{methanol-}d_4$ ) spectrum of phocoenamicin C (2).

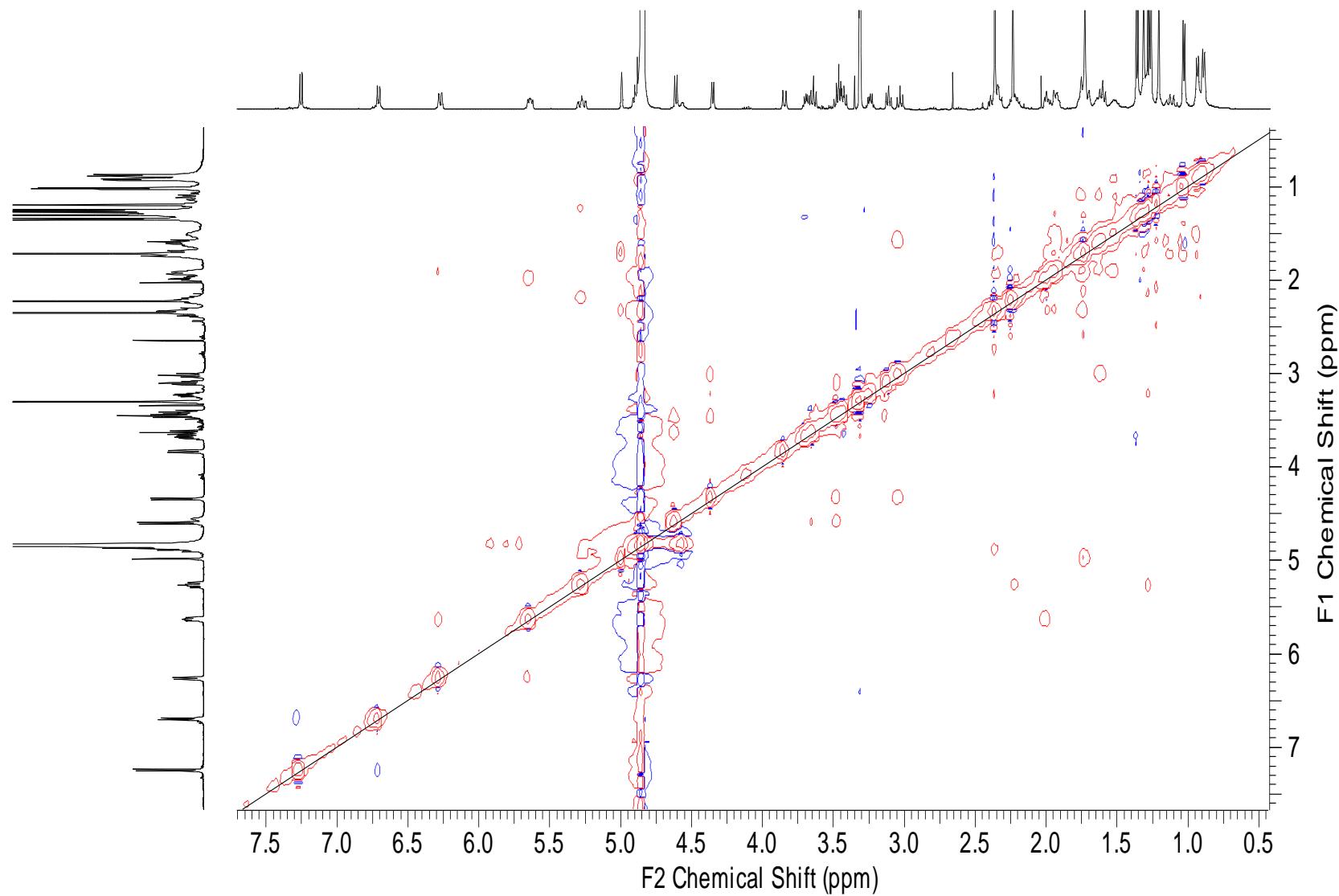


Figure S17. NOESY ( $\text{methanol-}d_4$ ) spectrum of phocoenamicin C (2).

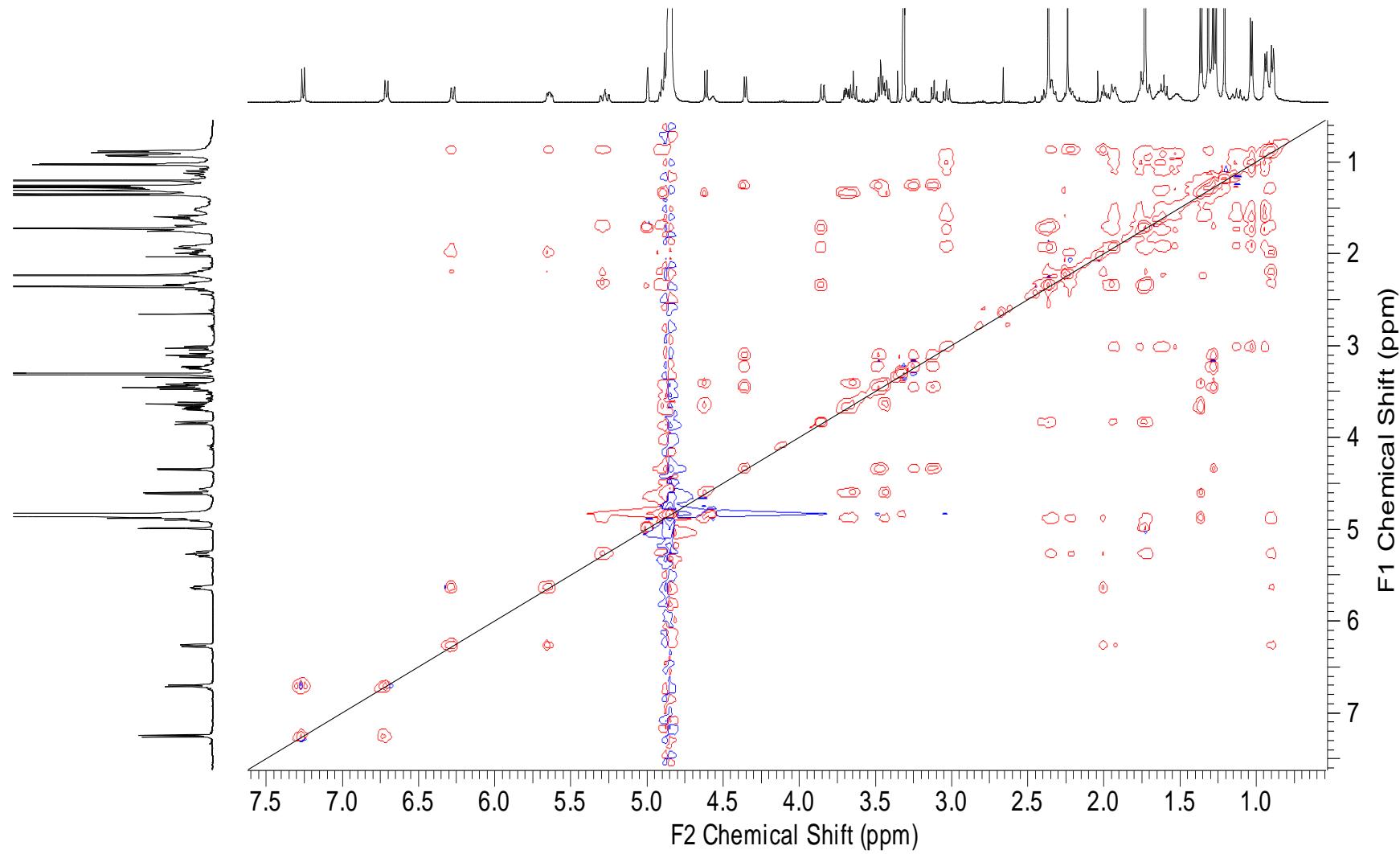


Figure S18. TOCSY ( $\text{methanol-}d_4$ ) spectrum of phocoenamicin C (2).