

Supporting Information

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A New Polyketide Derivative from the *Nicotiana tabacum* Symbiotic Fungus *Aspergillus japonicus* TE-739D

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4-60-1-1 #50 RT: 0.40 AV: 1 NL: 3.23E7
T: FTMS + p ESI Full ms [150.00-2000.00]

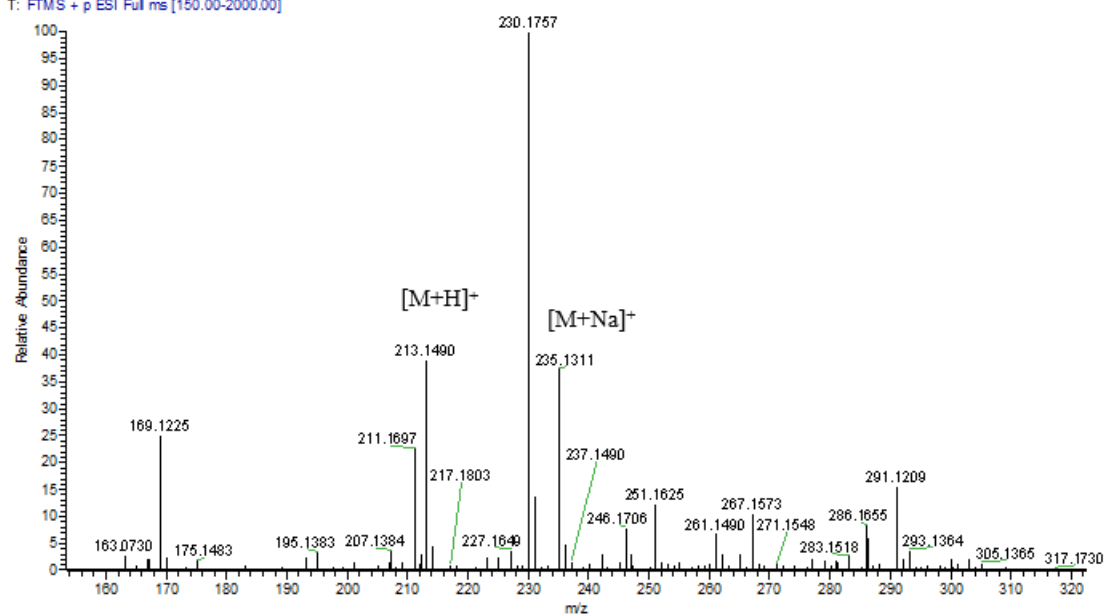


Figure S1: HRESIMS spectrum of **1**

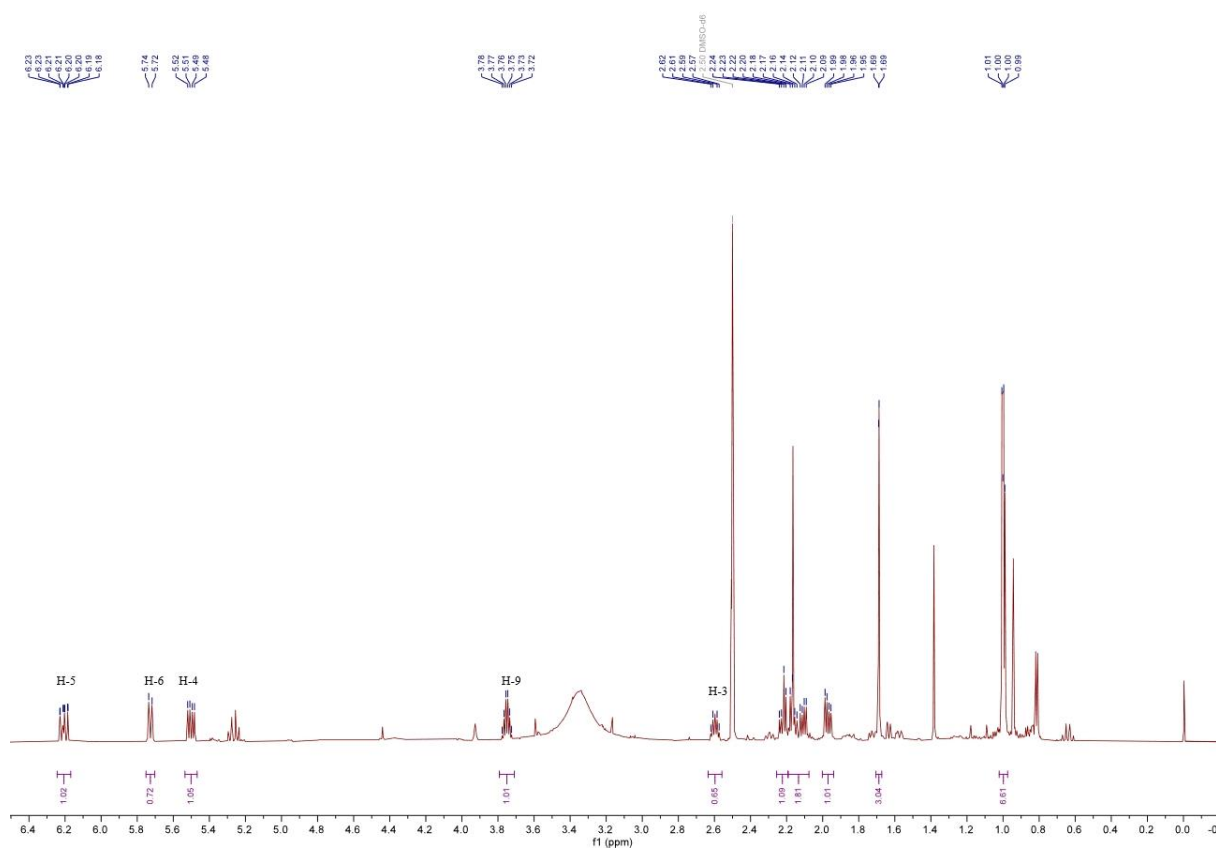


Figure S2: ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of **1**

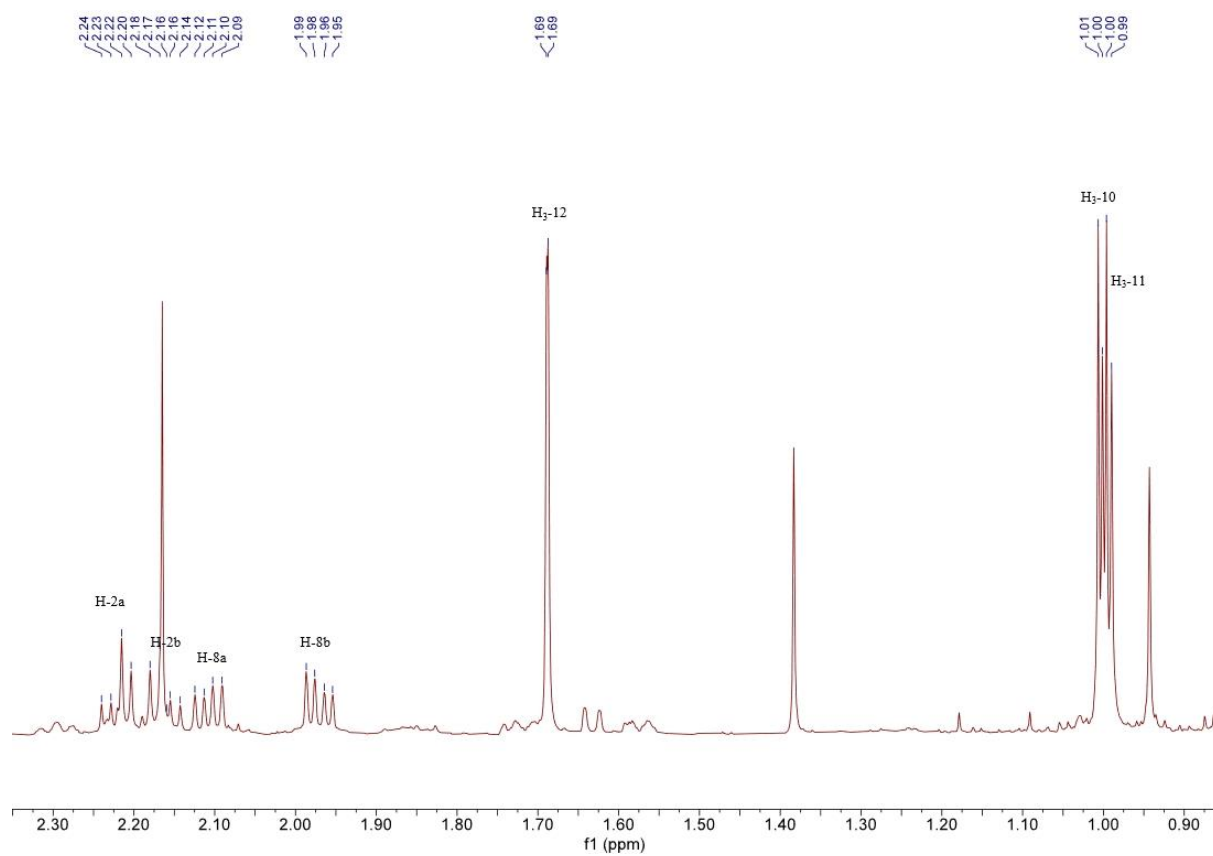


Figure S3: Enlarged ^1H NMR (600 MHz, $\text{DMSO}-d_6$) spectrum of **1**

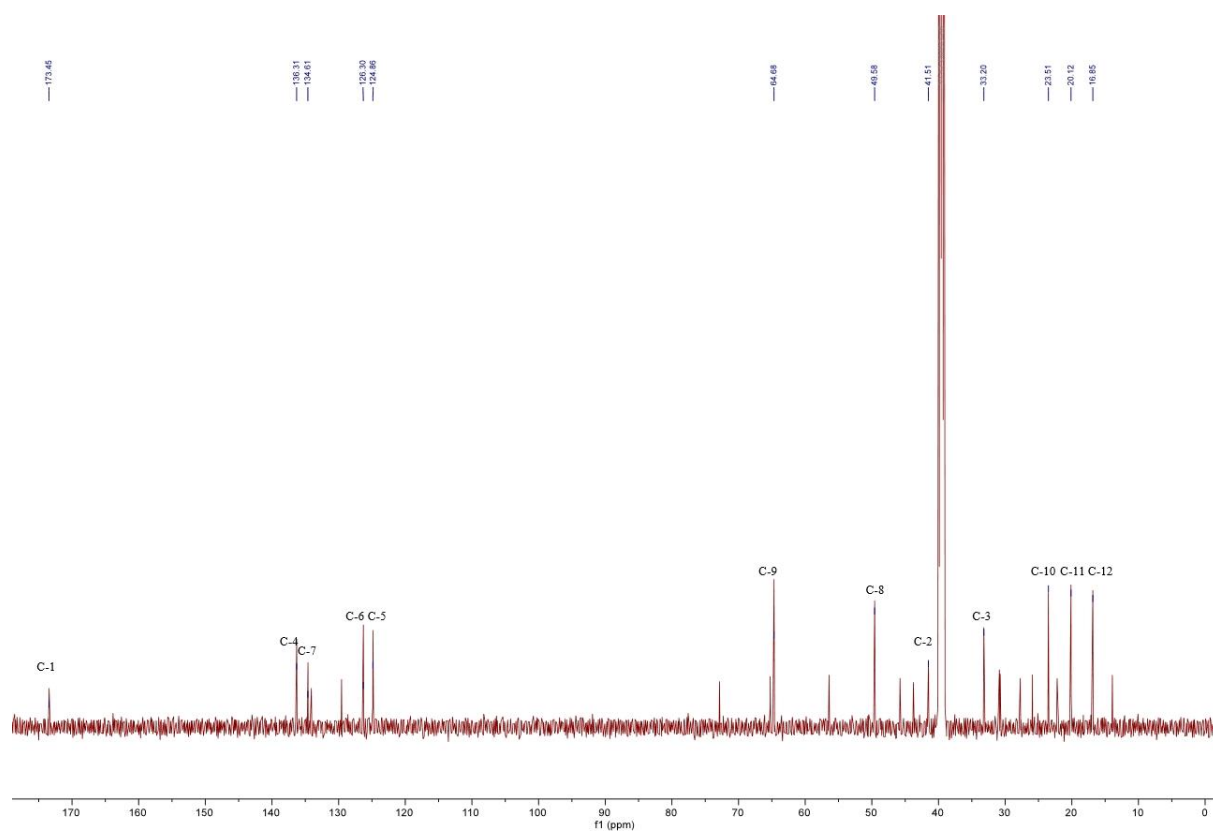


Figure S4: ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectra of **1**

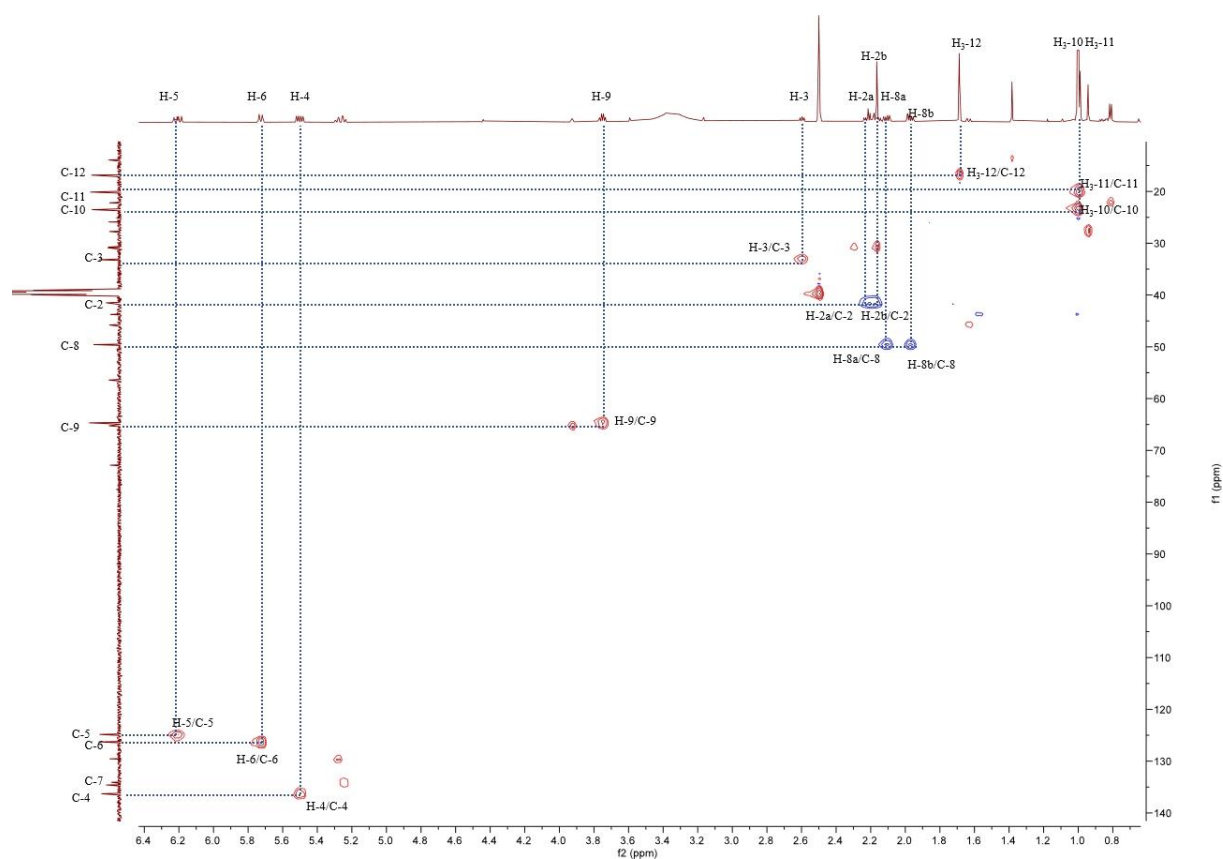


Figure S5: HSQC spectrum of **1**

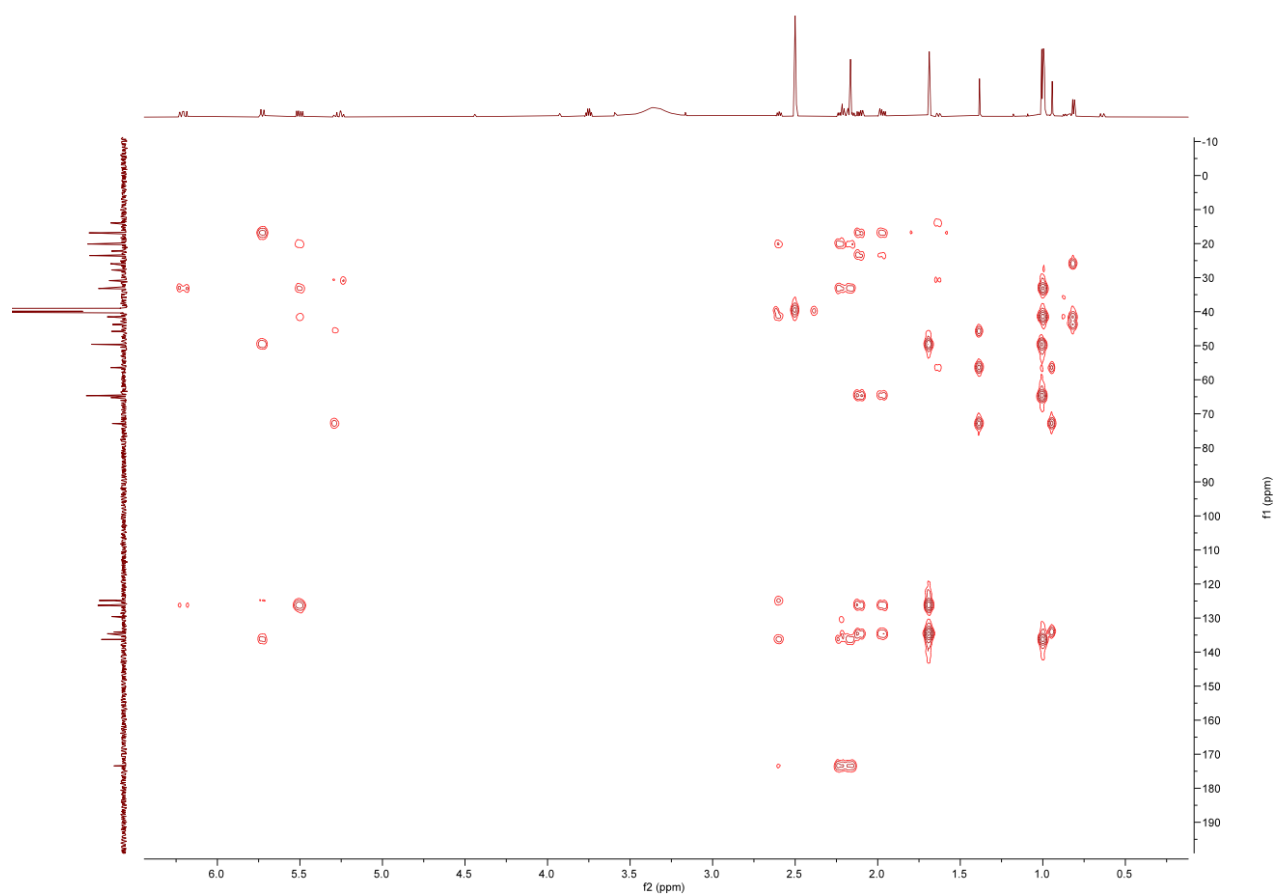


Figure S6: HMBC spectrum of **1**

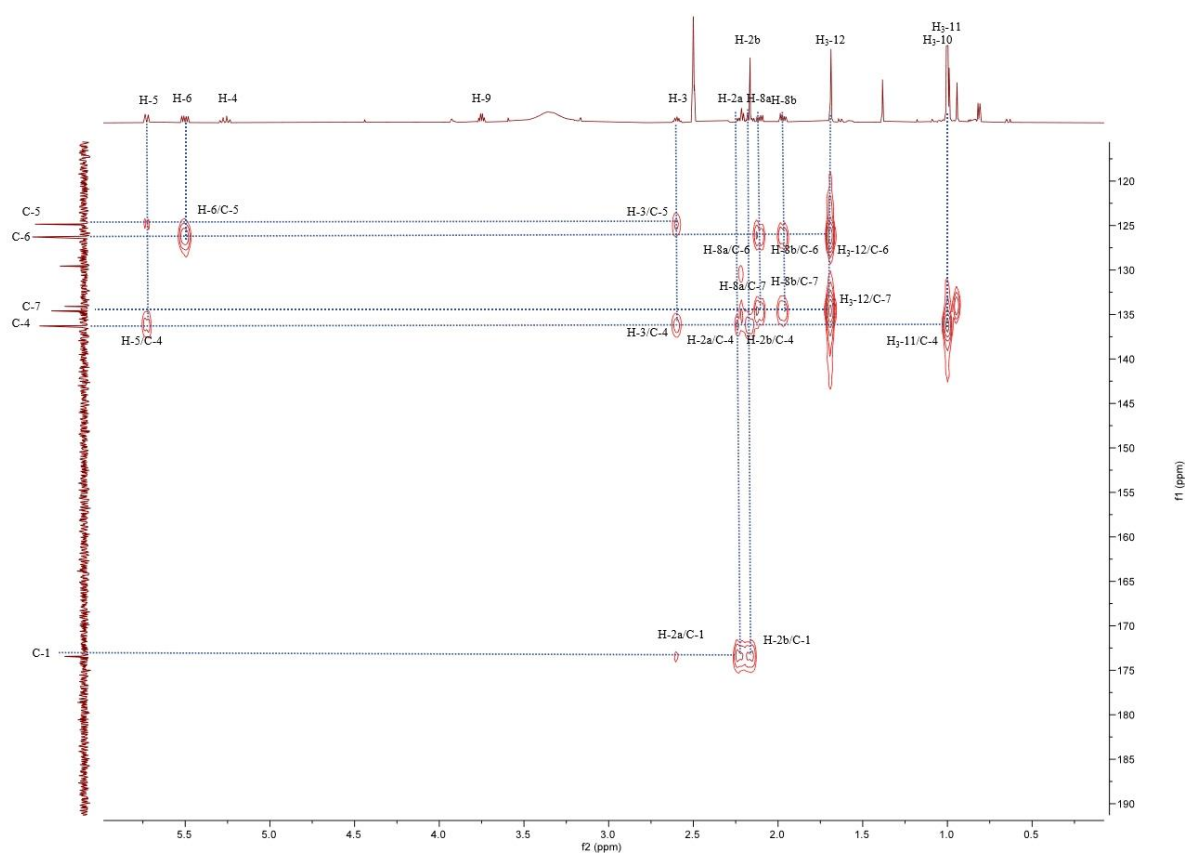


Figure S7: Enlarged HMBC spectrum of **1**

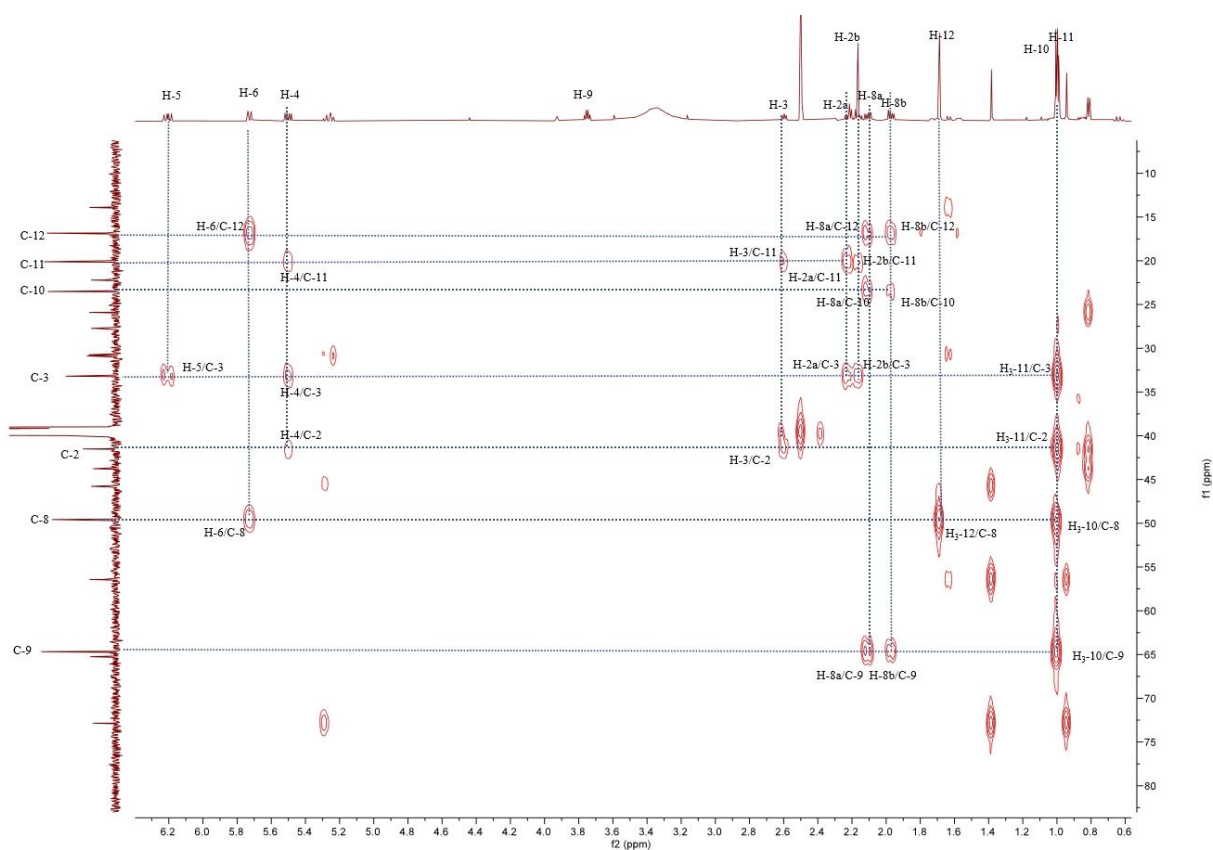


Figure S8: Enlarged HMBC spectrum of **1**

Substances search for drawn structure

References Reactions Suppliers

Structure Match

As Drawn (0)

Substructure (3,896)

Similarity (100K)

Chemscape Analysis

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Filter Behavior

Filter by Exclude

Search Within Results

Similarity

90-94 (23)

85-89 (115)

80-84 (766)

75-79 (3,548)

Filtering: Similarity: 2 Selected X Number of Components: 1 X [Clear All Filters](#)

138 Results

Sort: Number of References: Descending View: Partial

1 86

38609-44-8

Double bond geometry shown

$C_{12}H_{20}O_3$
(4E,8E)-10-Hydroxy-4,8-dimethyl-4,8-decadienoic acid

12 References 20 Reactions 1 Supplier

2 87

1312925-57-7

Absolute stereochemistry shown
Double bond geometry shown

$C_{12}H_{20}O_4$
leodomycin C

7 References 38 Reactions 1 Supplier

3 90

945997-09-1

Absolute stereochemistry shown
Double bond geometry shown

$C_{15}H_{26}O_3$
(3R,4E,6E)-3-Hydroxy-4-methyl-4,6-tetradecadienoic acid

5 References 38 Reactions 0 Suppliers

4 86

137592-09-7

Double bond geometry shown

$C_{12}H_{20}O_2$
(E,E)-4,8-dimethyl-4,8-decadienoic acid

12 References 20 Reactions 1 Supplier

5 90

945997-12-6

Absolute stereochemistry shown
Double bond geometry shown

$C_{15}H_{26}O_3$
(3R,4E,6E)-3-Hydroxy-4-methyl-4,6-tetradecadienoic acid

5 References 38 Reactions 0 Suppliers

6 89

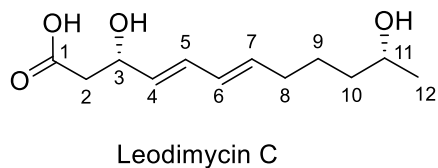
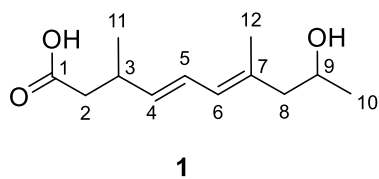
1060673-80-4

Double bond geometry shown

$C_{12}H_{20}O_2$
(E,E)-4,8-dimethyl-4,8-decadienoic acid

12 References 20 Reactions 1 Supplier

Figure S9: Scifinder search results of **1**

Table S1: Structural and NMR comparative analysis of **1** and ieodomycin C [1]

Compound 1 ^a			Ieodomycin C ^b	
No	δ_{H} (J in Hz)	δ_{C} , type	δ_{H} (J in Hz)	δ_{C} , type
1		173.5 C		175.6 C
2	2.21 dd (15.0, 7.0)	41.5 CH ₂	2.45 d (6.0)	43.7 CH ₂
	2.17 m			
3	2.60 m	33.2 CH	4.50 m	70.2 CH
4	5.50 dd (15.2, 7.3)	136.3 CH	5.60 dd (15.3, 6.5)	133.6 CH
5	6.21 ddd (15.2, 11.1, 1.2)	124.9 CH	6.22 dd (15.3, 10.5)	132.1 CH
6	5.73 d (11.1)	126.3 CH	6.03 dd (15.3, 10.5)	131.0 CH
7		134.6 C	5.70 dt (15.3, 7.0)	136.1 CH
8	2.11 dd (13.3, 6.9)	49.6 CH ₂	2.10 m	33.7 CH ₂
	1.97 dd (13.3, 6.2)			
9	3.75 p (6.3)	64.7 CH	1.50 m	26.7 CH ₂
			1.38 m	
10	1.00 d (6.8)	23.5 CH ₃	1.42 m	39.8 CH ₂
11	0.96 d (6.1)	20.1 CH ₃	3.70 m	68.5 CH
12	1.69 s	16.9 CH ₃	1.13 d (6.0)	23.6 CH ₃

^a In DMSO-*d*₆; ^b In CD₃OD**Reference:**

1. M. A. M. Mondol, J. H. Kim, M. A. Lee, F. S. Tareq, H. S. Lee, Y. J. Lee and H. J. Shin (2011). Ieodomycins A-D, Antimicrobial Fatty Acids from a Marine *Bacillus* sp. *J. Nat. Prod.* **74**, 1606–1612.