

Supporting Information

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A New Cytotoxic Sesquiterpenoid from *Penicillium oxalicum* 2021CDF-3

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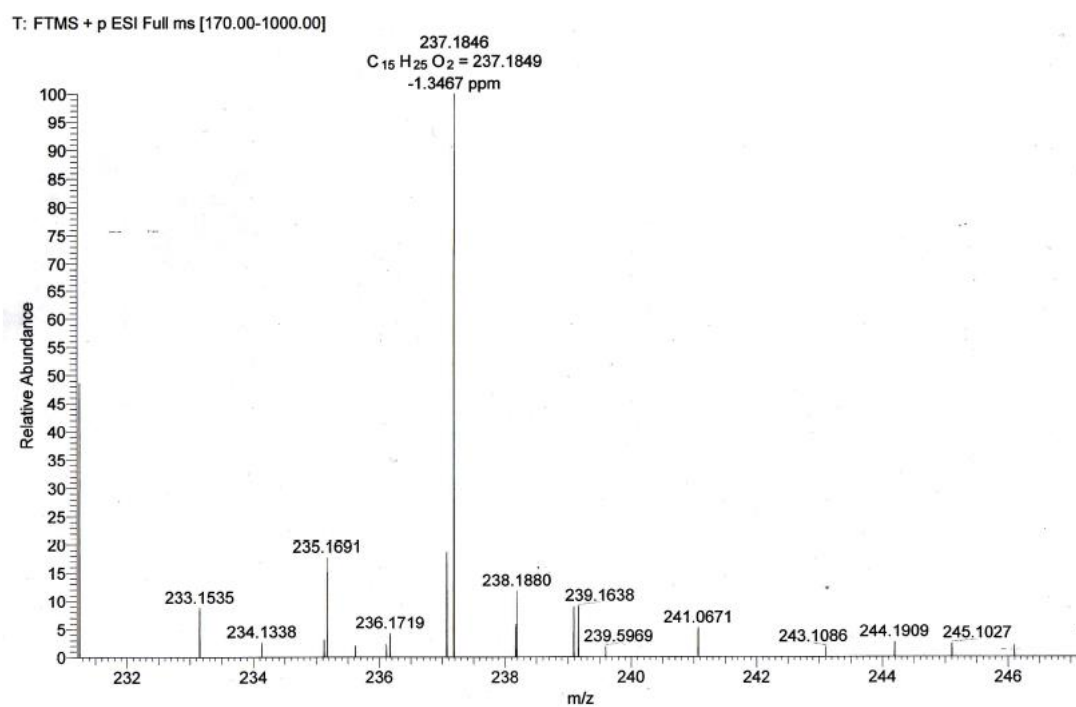


Figure S1: HRESIMS spectrum of **1**

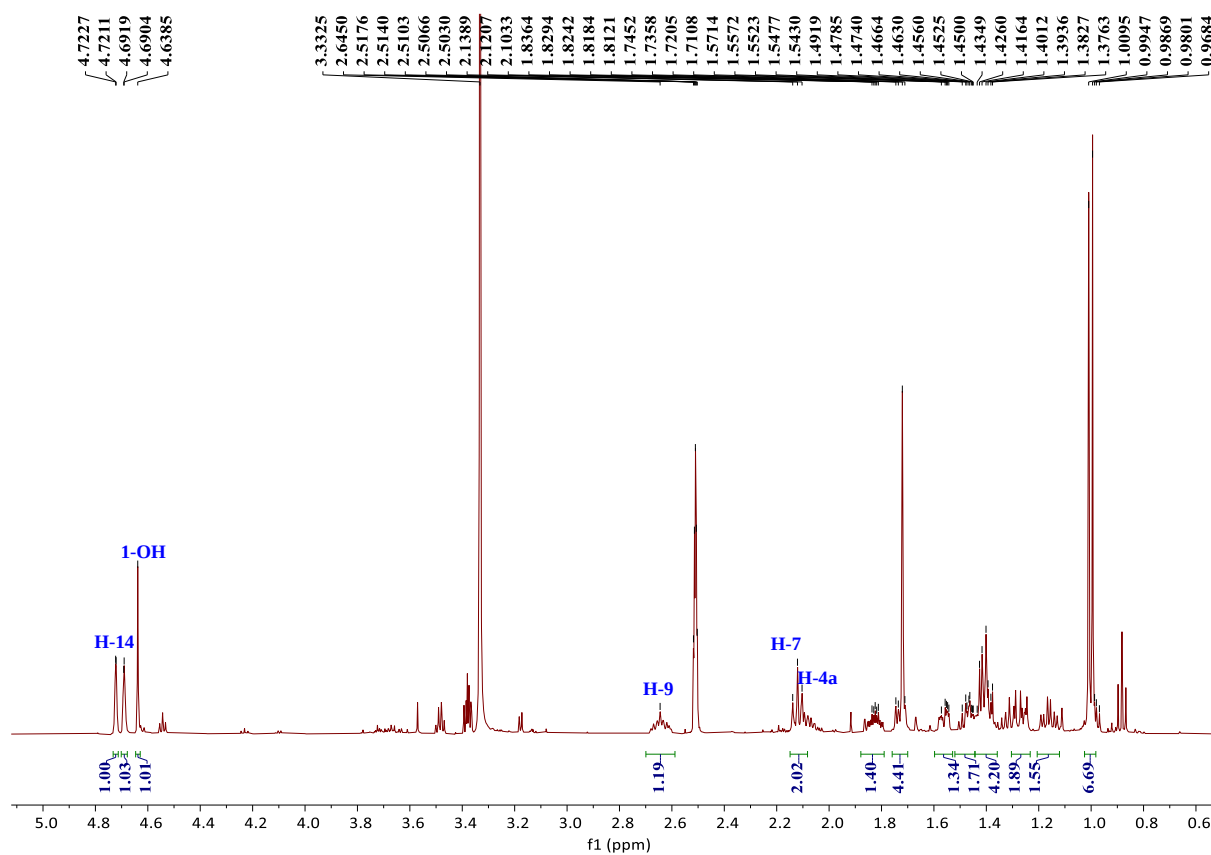


Figure S2: ^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of **1**

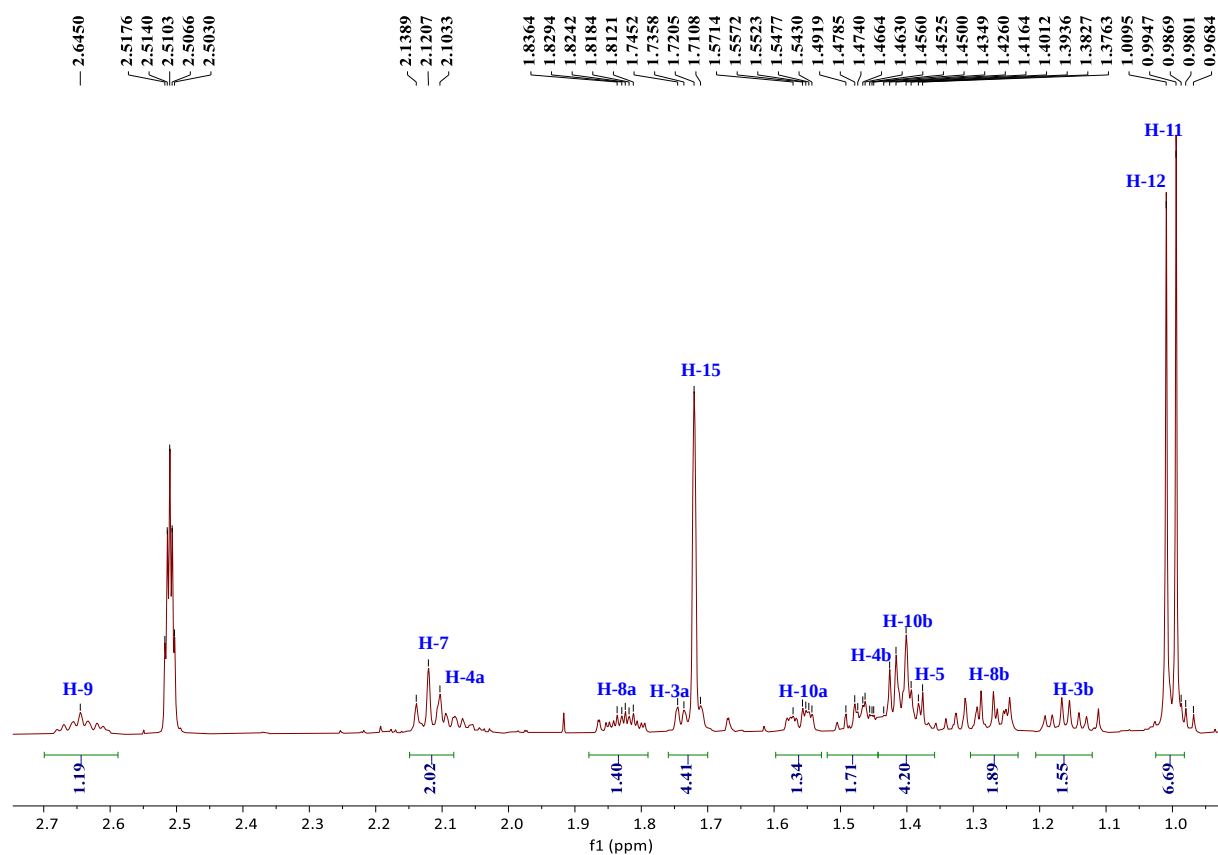


Figure S3: Enlarged ^1H NMR (500 MHz, $\text{DMSO-}d_6$) spectrum of **1**

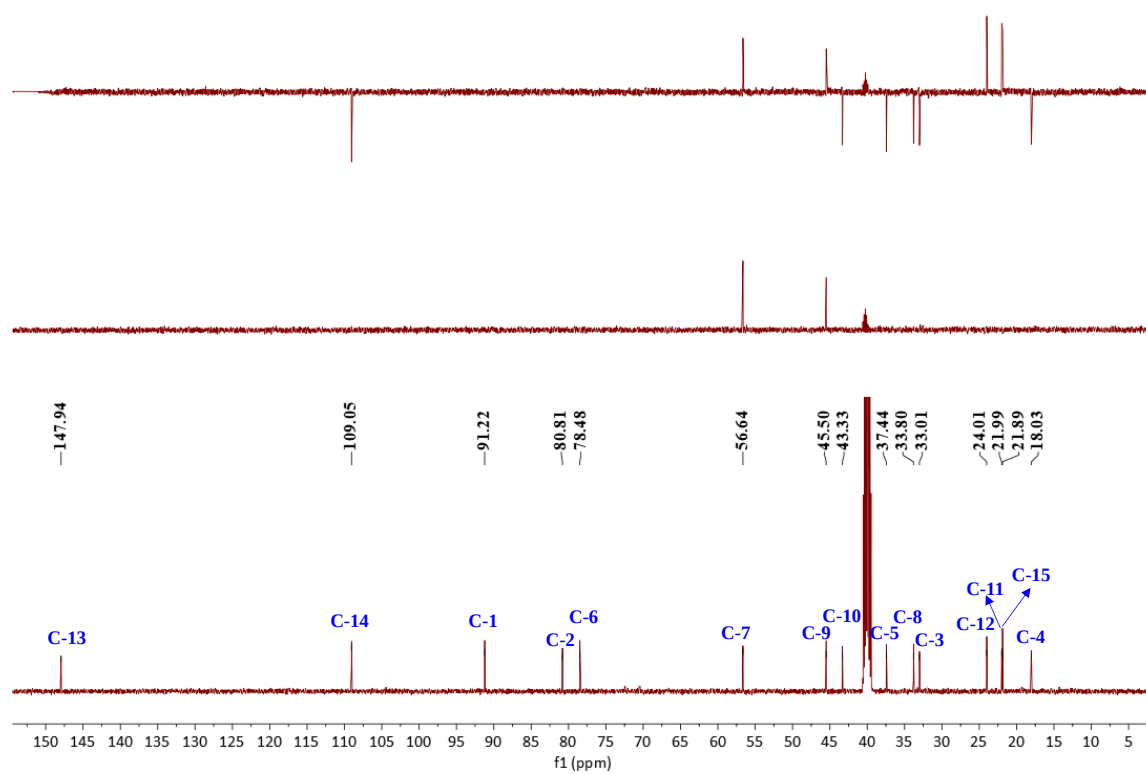


Figure S4: ^{13}C NMR and DEPT (125 MHz, $\text{DMSO}-d_6$) spectra of **1**

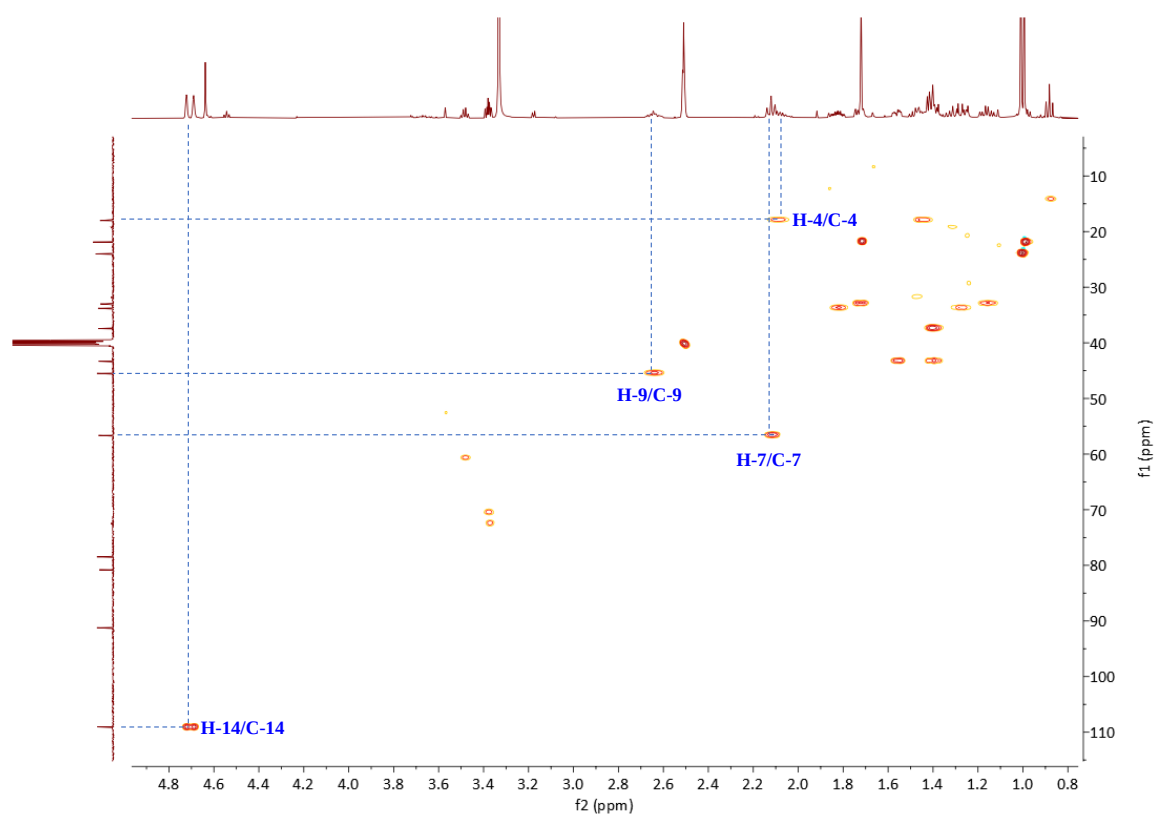


Figure S5: HSQC spectrum of **1**

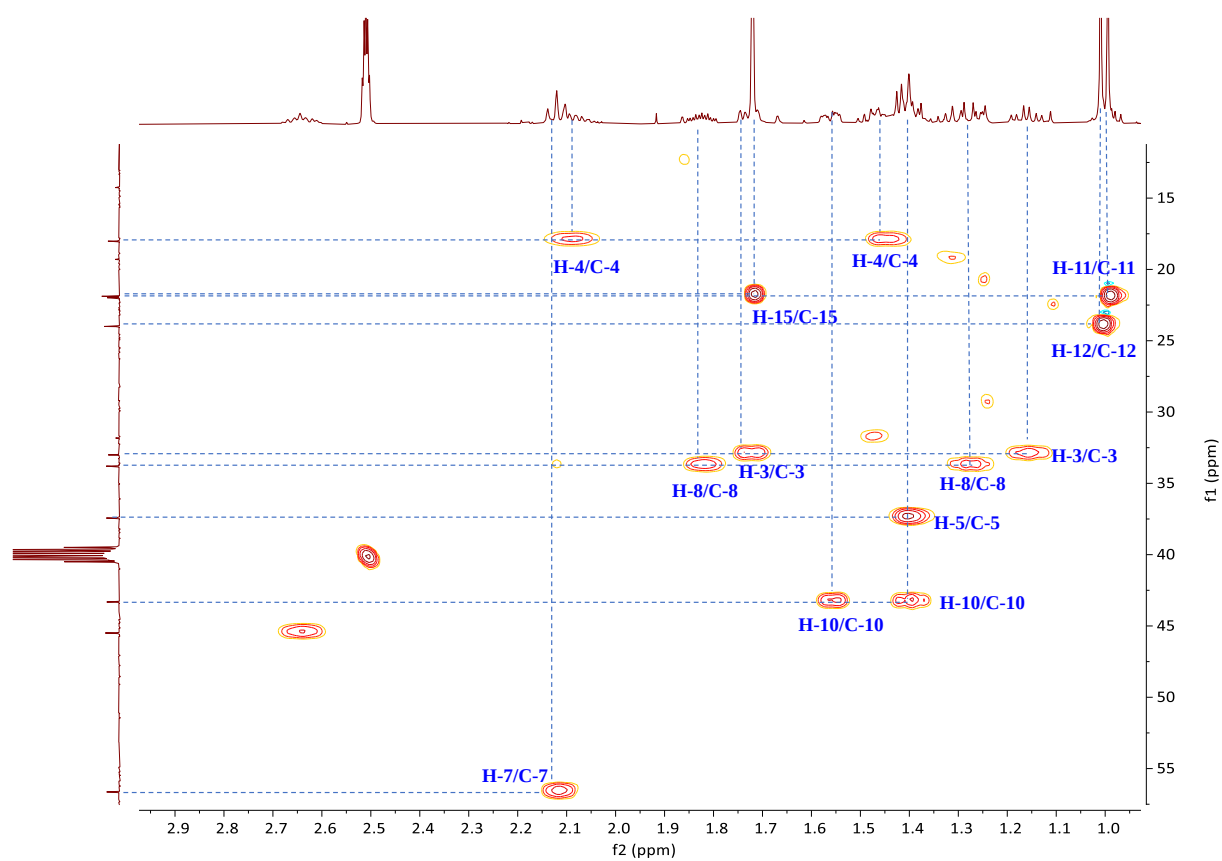


Figure S6: Enlarged HSQC spectrum of **1**

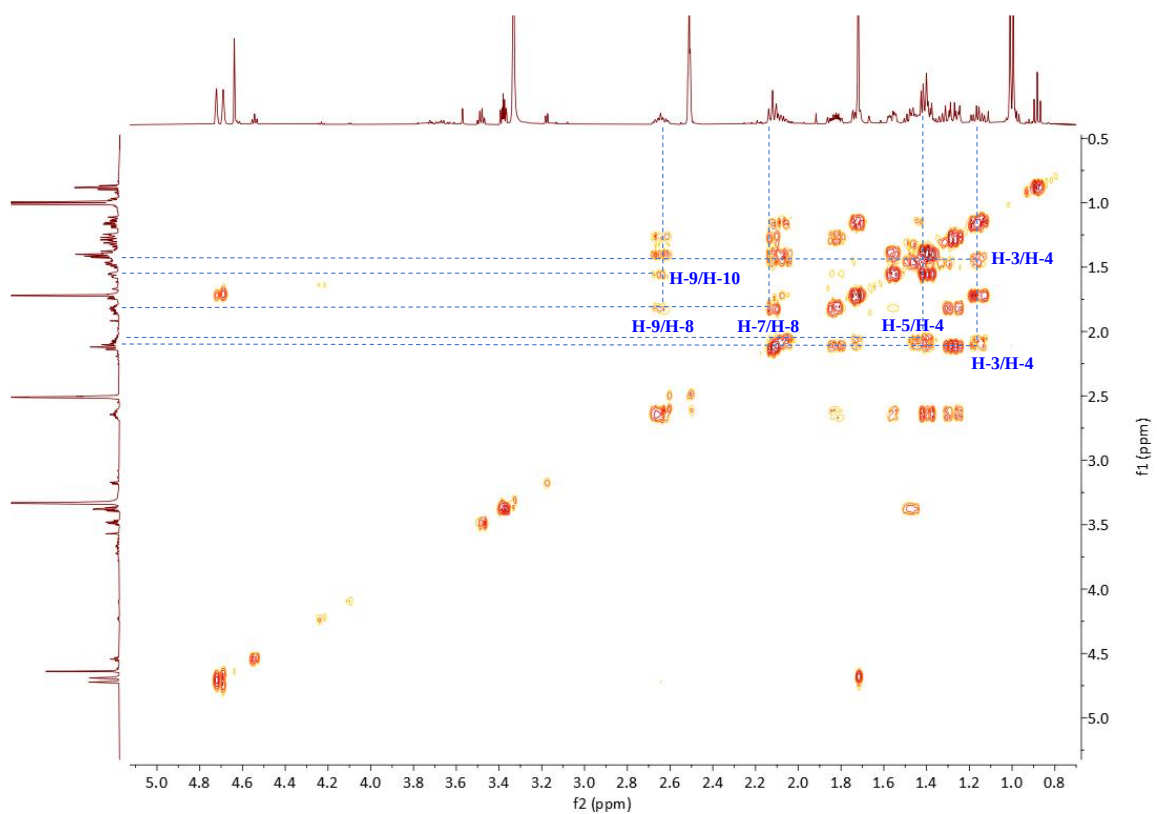


Figure S7: ^1H - ^1H COSY spectrum of **1**

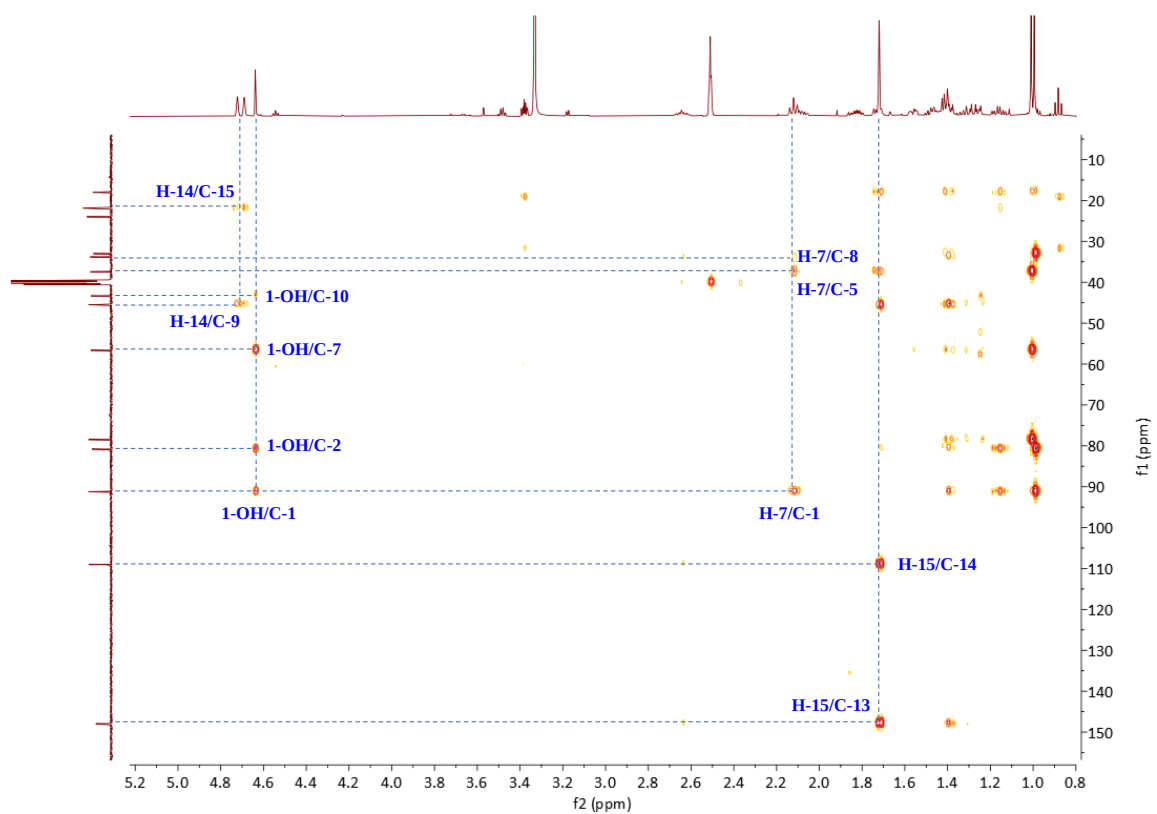


Figure S8: HMBC spectrum of **1**

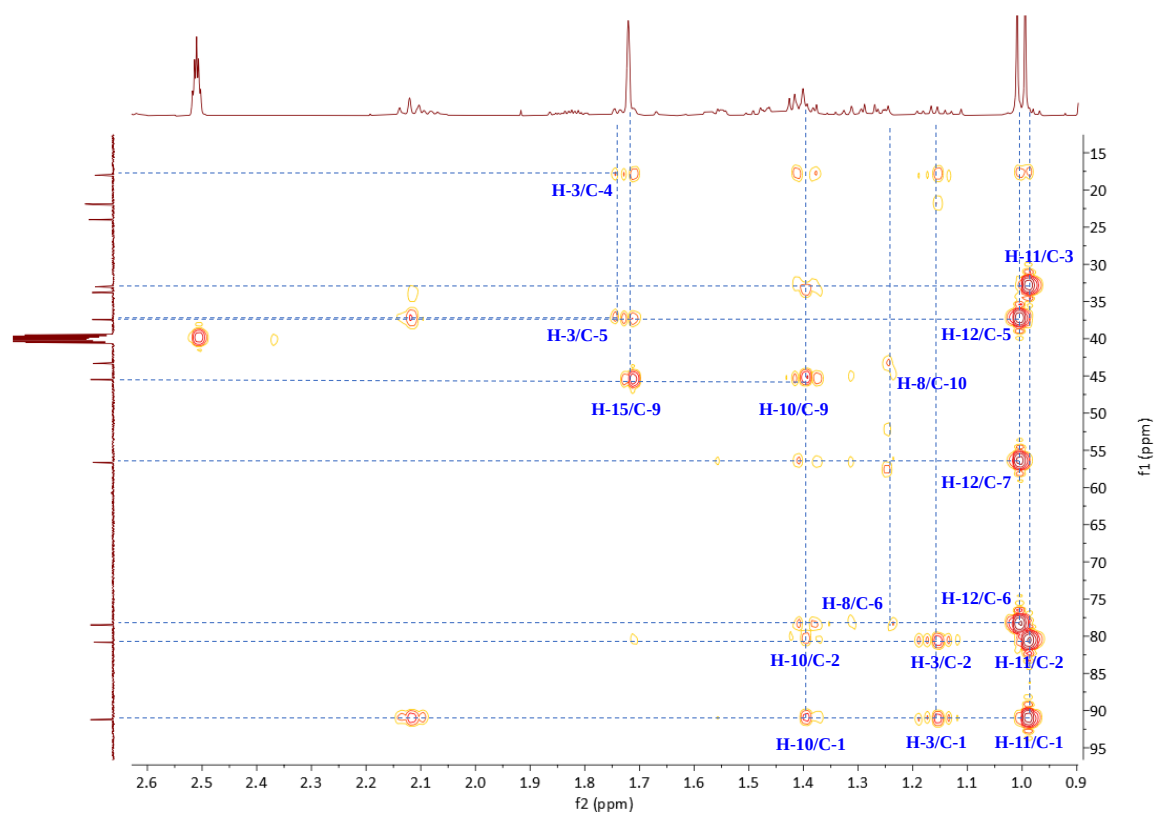


Figure S9: Enlarged HMBC spectrum of **1**

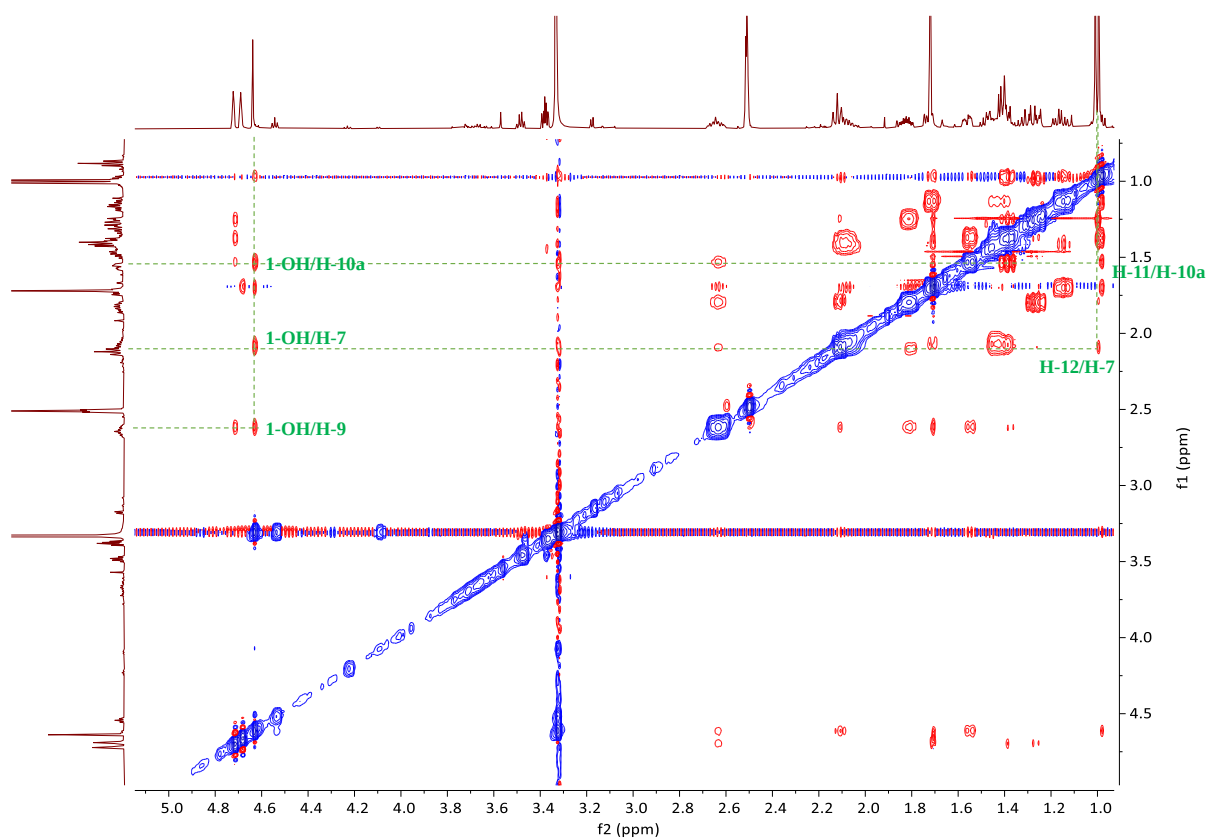


Figure S10: NOESY spectrum of **1**

Structure Match

As Drawn (0)

Substructure (0)

Similarity (17K)

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Similarity

☒ 85-89 (2)
☒ 80-84 (41)
☐ 75-79 (196)
☐ 70-74 (691)
☐ 65-69 (3,090)
☐ 60-64 (13K)

Reaction Role

☐ Product (14)
☐ Reactant (5)

Reference Role

☐ Preparation (31)
☐ Biological Study (20)
☐ Synthetic Preparation (15)
☐ Biological Study, Unclassified (14)
☐ Properties (14)

View All

Life Science Data

Commercial Availability

☐ Available (4)
☐ Not Available (39)

Filtering:

Similarity:2 Selected

Number of Components: 1

Clear All Filters

43 Results

Sort: Number of References: Descending View: Partial

1 85

259875-21-3

Available stereochemistry shown

$C_{15}H_{26}O_2$
rel-(1*R*,3*aS*,4*R*,7*R*,8*S*,8*aR*)-Decahydro-1,4-dimethyl-7-(1-methylethyl)-1,4-epoxyazul...

7 References

0 Reactions

0 Suppliers

2 83

911714-91-5

Absolute stereochemistry shown, Rotation (+)

$C_{15}H_{26}O_2$
(1*R*,3*aS*,4*S*,7*R*,8*R*,8*aS*)-Decahydro-1,4-dimethyl-7-(1-methylethyl)-4,8-epoxyazulen-1...

5 References

4 Reactions

21 Suppliers

3 80

142569-89-9

Absolute stereochemistry unknown, Rotation (-)

$C_{15}H_{26}O_2$
rel-(1*R*,3*aR*,4*S*,5*S*,8*S*,8*aS*)-Decahydro-5,8a-dimethyl-7-(1-methylethyl)-4,8-epox...

5 References

0 Reactions

1 Supplier

4 85

13741-35-0

$C_{15}H_{24}O_2$
3*H*-Naphth[1,8*a-b*]oxiren-2-ol, octahydro-1*a*,4*a*-dimethyl-7-(1-methylethenyl)-, [1*a*...

3 References

4 Reactions

0 Suppliers

5 82

109717-27-3

$C_{15}H_{26}O_2$
Octahydro-1,4-dimethyl-7-(1-methylethyl)-1*H*-3*a*,7-epoxyazulen-3-ol

3 References

0 Reactions

0 Suppliers

6 81

861929-06-8

Relative stereochemistry shown

$C_{15}H_{24}O_3$
rel-(1*aR*,4*S*,4*aR*,7*R*,8*S*,8*aR*)-Octahydro-1*a*,4*a*-dimethyl-7-(1-methylethenyl)-3*H*-naph...

3 References

10 Reactions

0 Suppliers

7 80

1393370-32-5

Absolute stereochemistry shown, Rotation (+)

$C_{15}H_{24}O_4$
(3*aS*,4*R*,5*S*,7*S*,8*S*,8*aR*)-Octahydro-4-methyl-1-methylene-7-(1-methylethyl)-4,8-epoxy...

3 References

0 Reactions

0 Suppliers

8 85

61248-42-8

$C_{15}H_{24}O_2$
3*H*-Naphth[1,8*a-b*]oxiren-2-ol, octahydro-1*a*,4*a*-dimethyl-7-(1-methylethenyl)-, [1*a*...

2 References

0 Reactions

1 Supplier

9 83

146276-38-2

Absolute stereochemistry shown

$C_{15}H_{24}O_2$
3*H*-Azuleno[3*a*,4-*b*]oxiren-8-ol, octahydro-1*a*,6-dimethyl-4-(1-methylethenyl)-, [1*a*...

2 References

3 Reactions

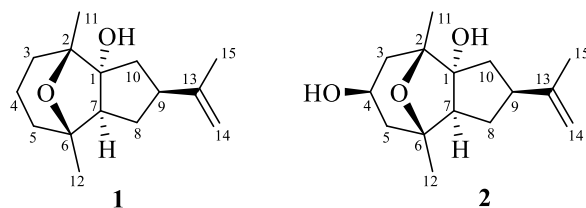
0 Suppliers

Figure S11: Scifinder search results of 1

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Table S1: The comparison of NMR data of compounds **1** and **2**



No	1		2	
	δ_{H} (J in Hz)	δ_{C} , type	δ_{H} (J in Hz)	δ_{C} , type
1		91.2, C		91.2, C
2		80.8, C		81.0, C
3	1.73, m; 1.16, td (12.8, 5.5)	33.0, CH ₂	2.03, dd (12.4, 5.8); 0.95, m	43.7, CH ₂
4	2.09, m; 1.46, m	18.0, CH ₂	4.14, ddd (16.5, 10.8, 5.8)	62.1, CH
5	1.38, m	37.4, CH ₂	1.76, m (overlap); 1.14, m	47.8, CH ₂
6		78.5, C		78.5, C
7	2.12, t (8.9)	56.6, CH	1.97, t (9.0)	57.3, CH
8	1.82, m; 1.27, m	33.8, CH ₂	1.76, m (overlap); 1.20, m	33.8, CH ₂
9	2.64, tq (8.8, 4.9)	45.5, CH	2.56, m	45.4, CH
10	1.56, ddd (11.9, 4.9, 2.5); 1.38, m	43.3, CH ₂	1.52, ddd (12.0, 4.4, 2.4); 1.36 t (12.0)	43.2, CH ₂
11	0.99, s	22.0, CH ₃	1.01, s (overlap)	21.9, CH ₃
12	1.00, s	24.0, CH ₃	1.01, s (overlap)	23.5, CH ₃
13		147.9, C		147.8, C
14	4.72, br s; 4.69, br s	109.1, CH ₂	4.67, br d (12.5)	109.1, CH ₂
15	1.72, s	21.9, CH ₃	1.68, s	21.7, CH ₃
1-OH	4.64, s			