

Supporting Information

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

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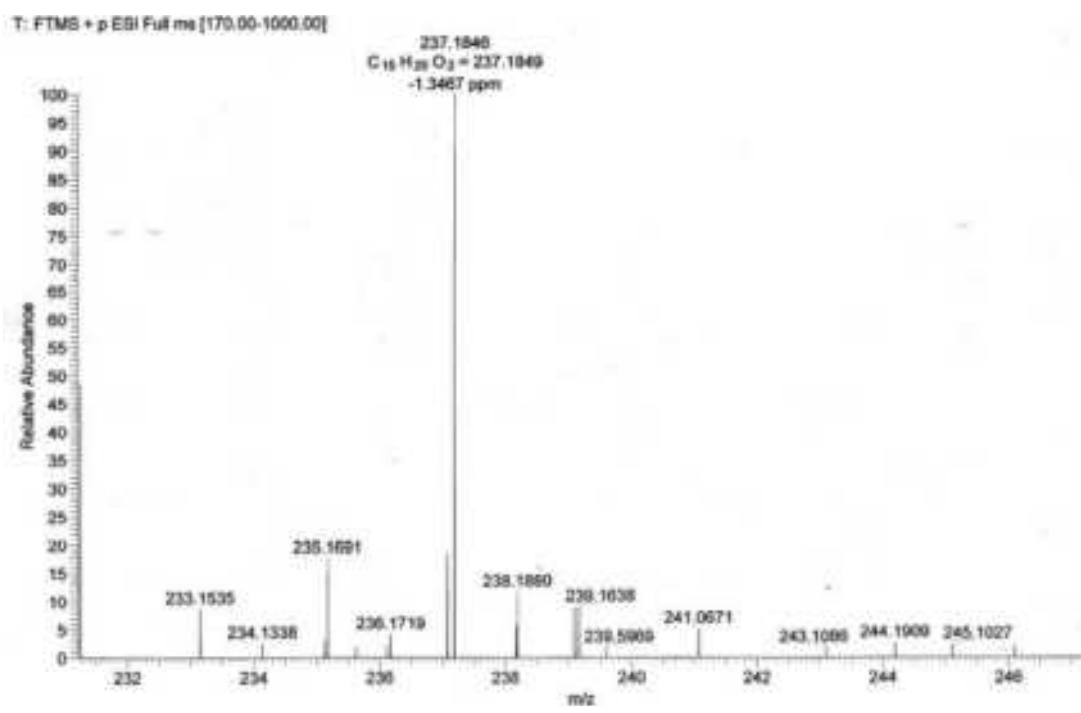


Figure S1: HRESIMS spectrum of **1**

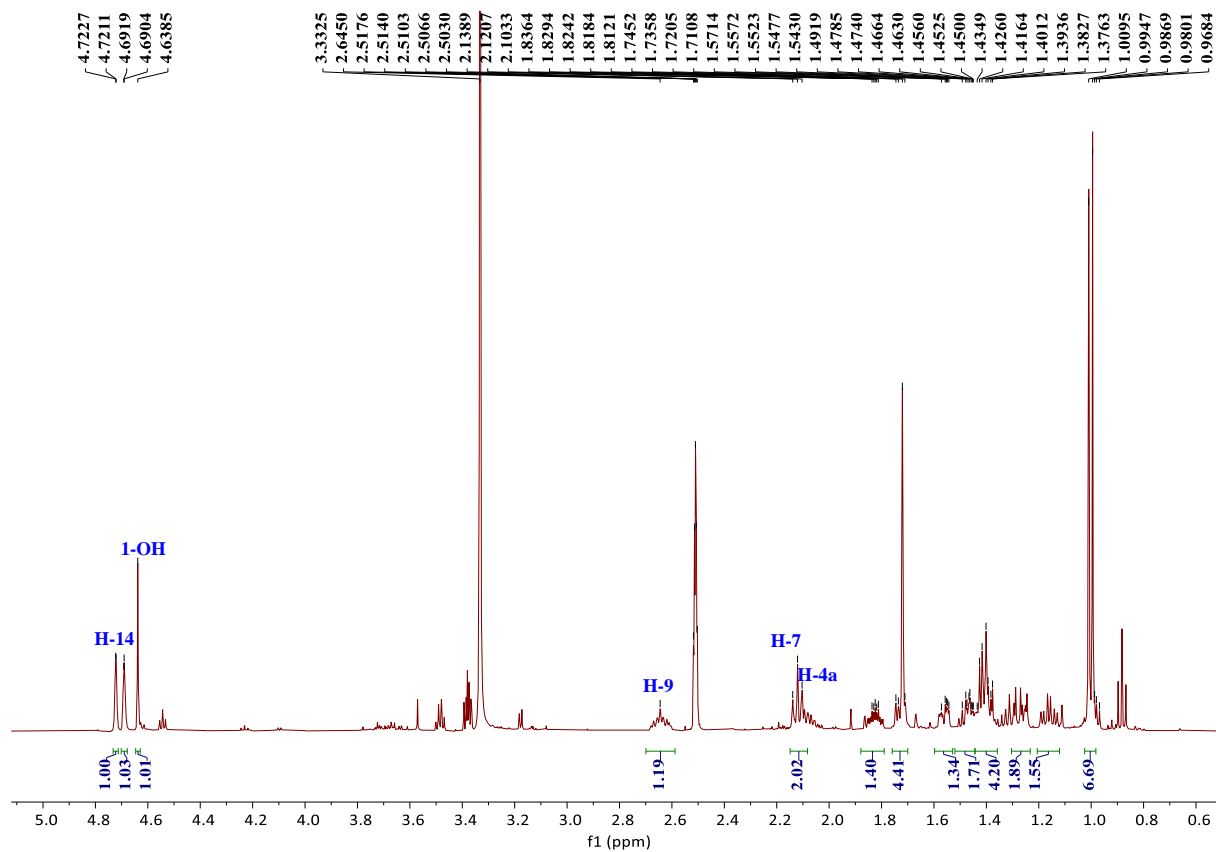


Figure S2: ^1H NMR (500 MHz, $\text{DMSO-}d_6$) spectrum of **1**

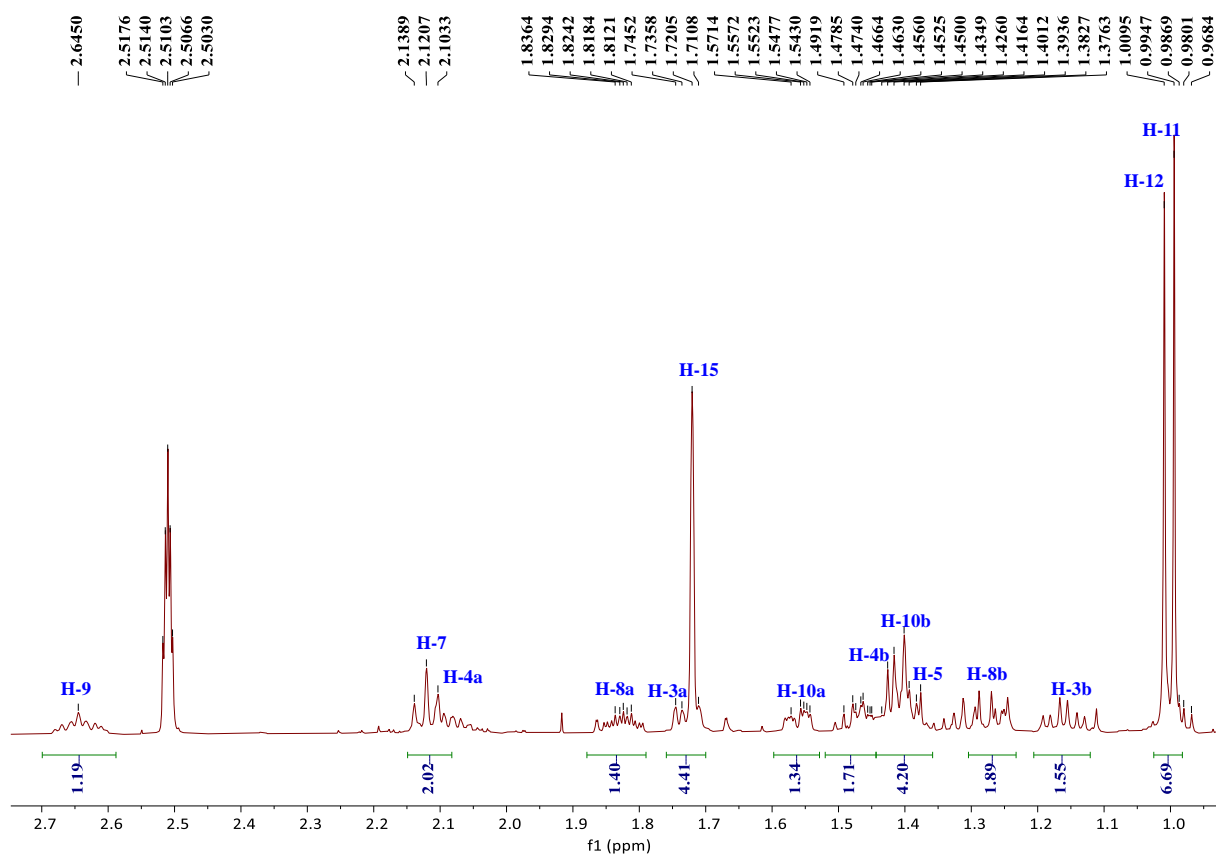


Figure S3: Enlarged ^1H NMR (500 MHz, $\text{DMSO-}d_6$) spectrum of **1**

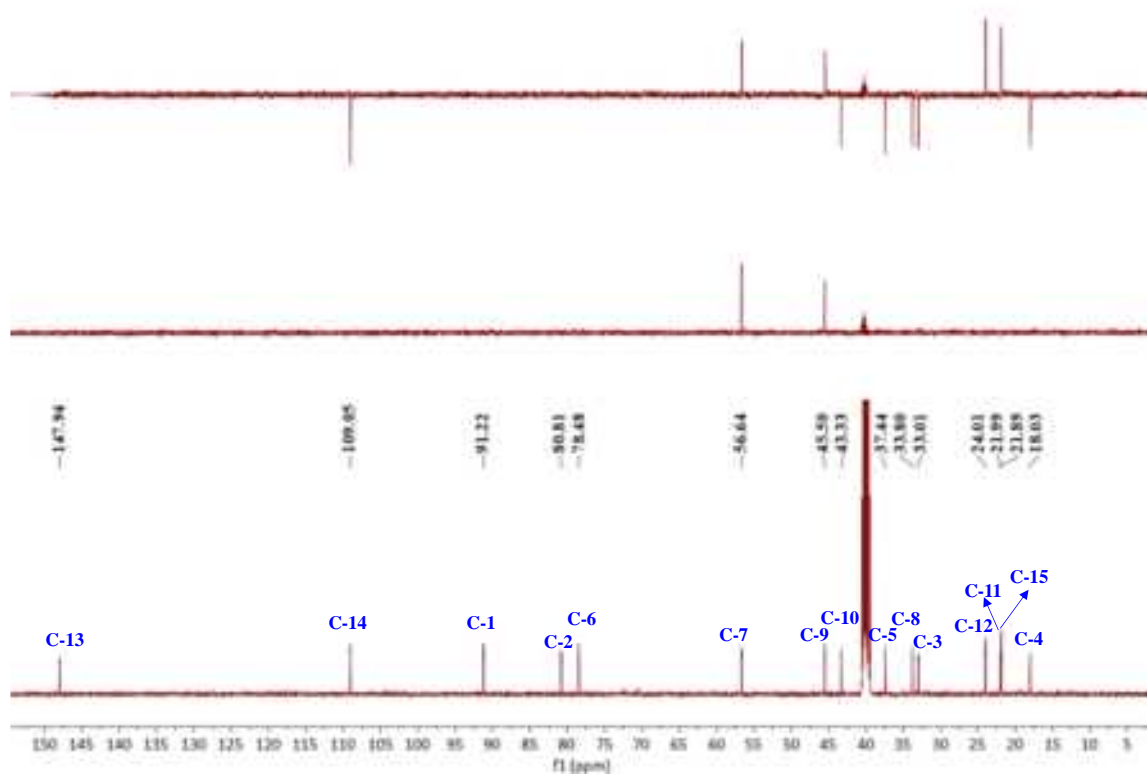


Figure S4: ^{13}C NMR and DEPT (125 MHz, $\text{DMSO-}d_6$) spectra of **1**

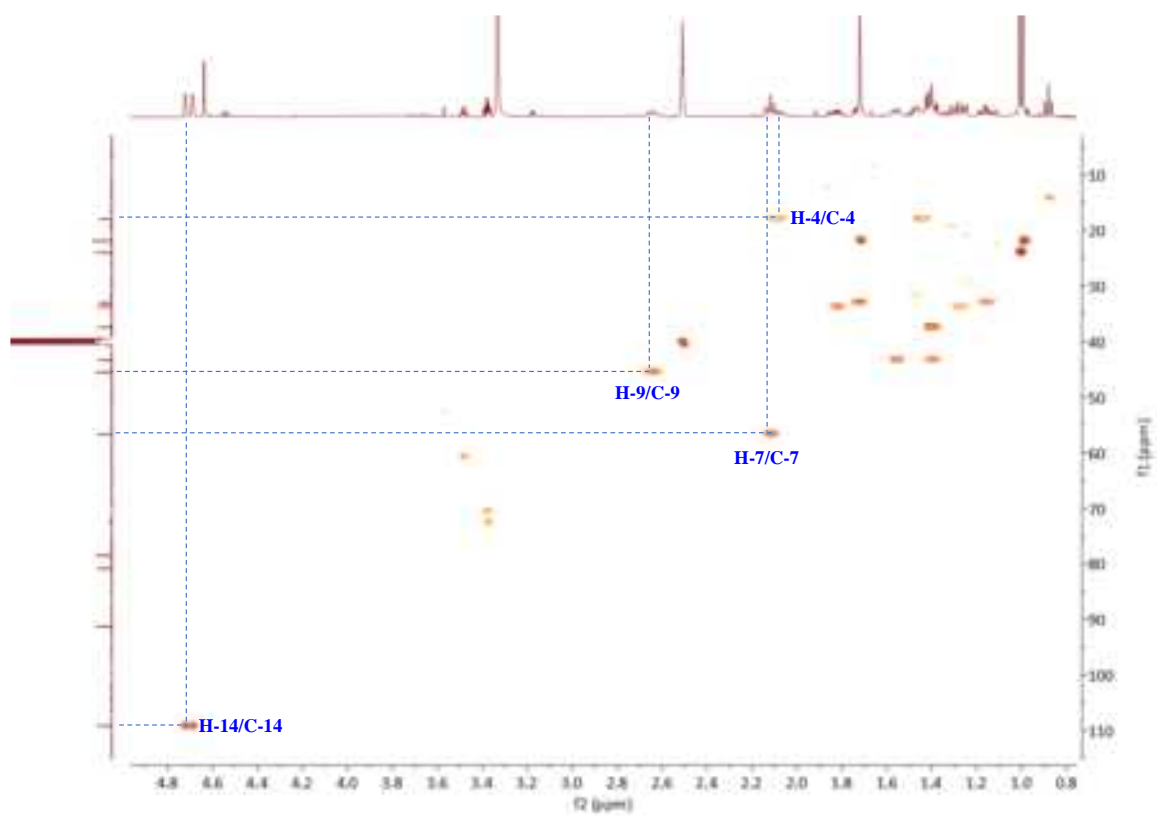


Figure S5: HSQC spectrum of **1**

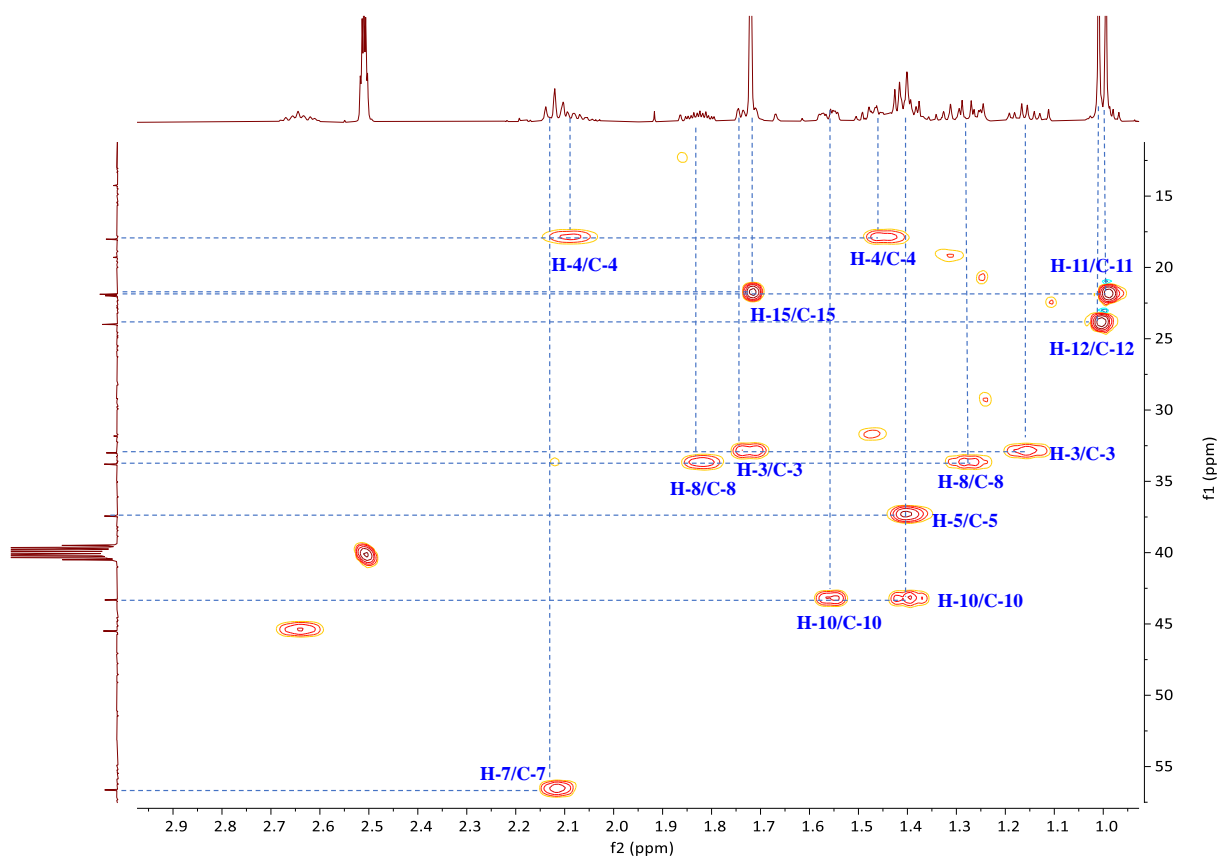


Figure S6: Enlarged HSQC spectrum of **1**

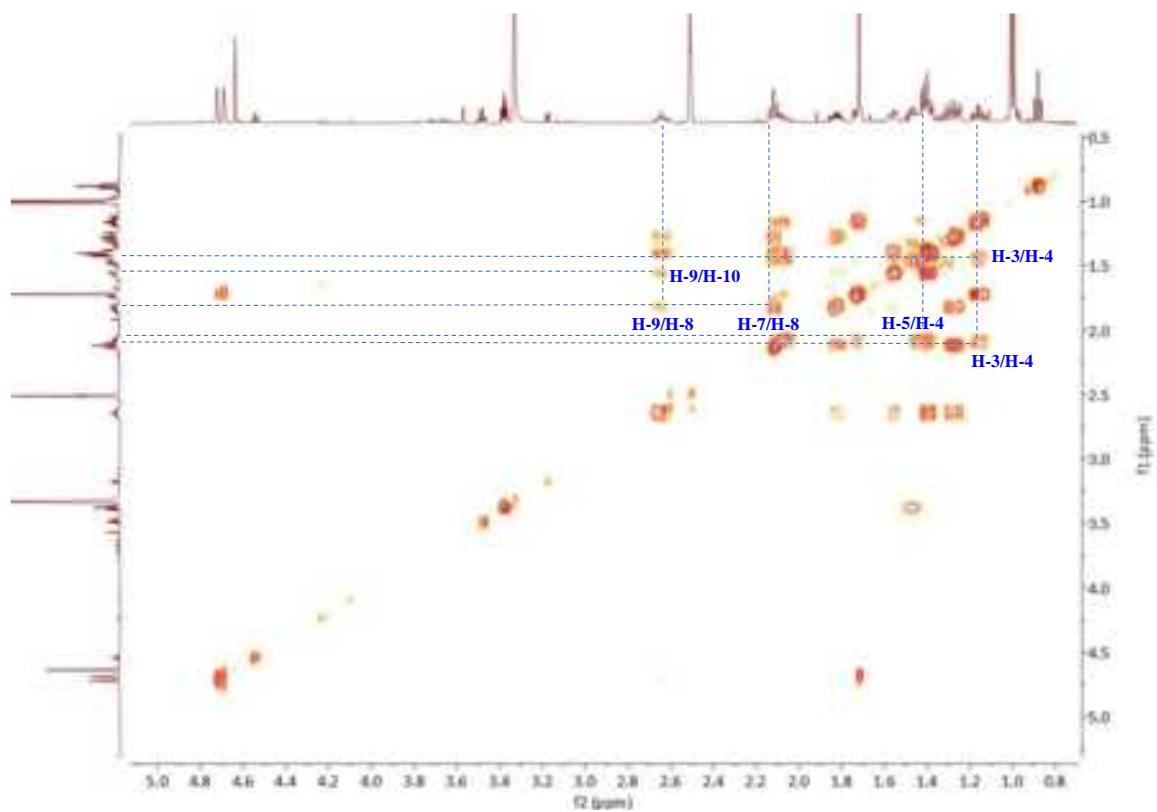


Figure S7: ^1H - ^1H COSY spectrum of **1**

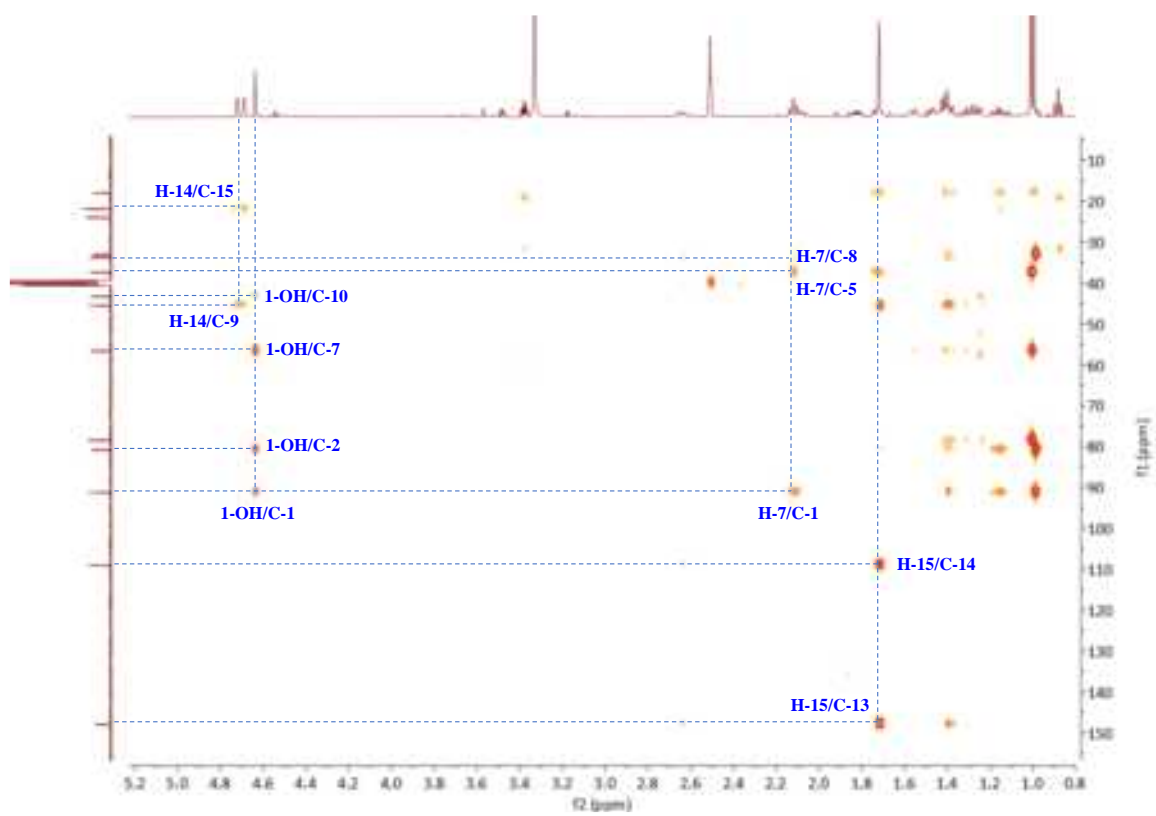


Figure S8: HMBC spectrum of **1**

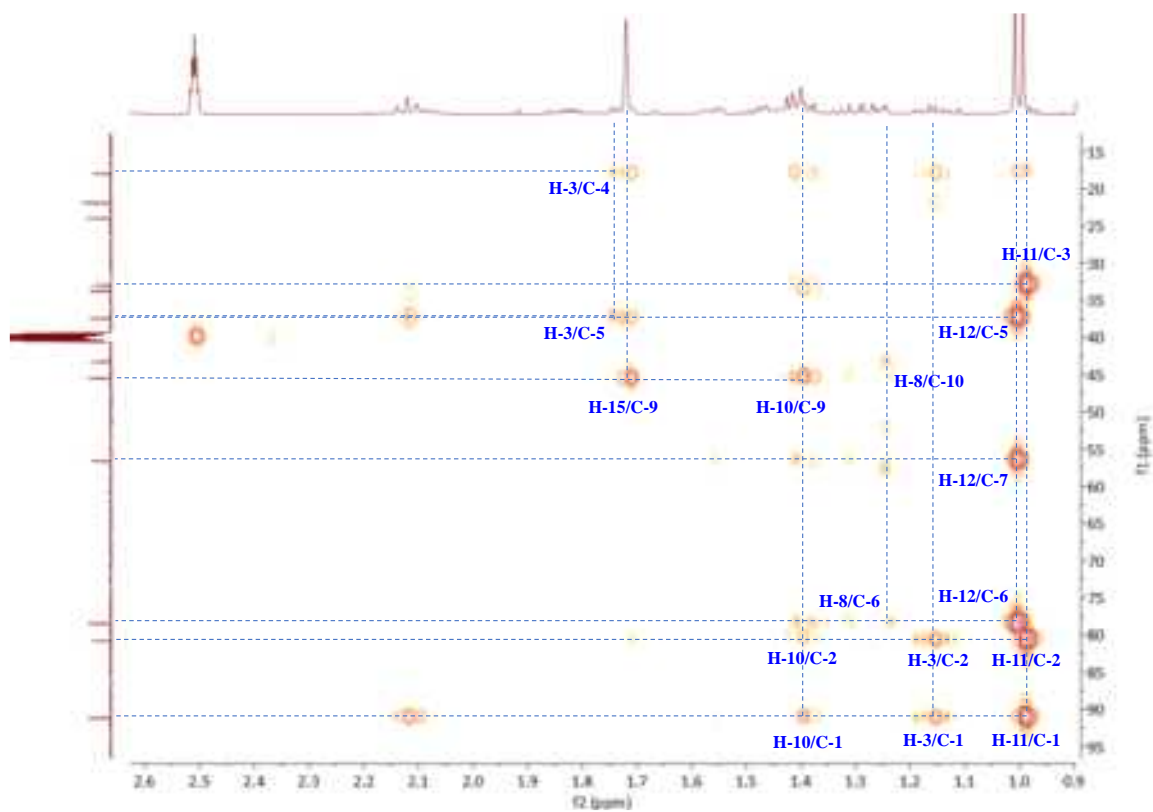


Figure S9: Enlarged HMBC spectrum of **1**

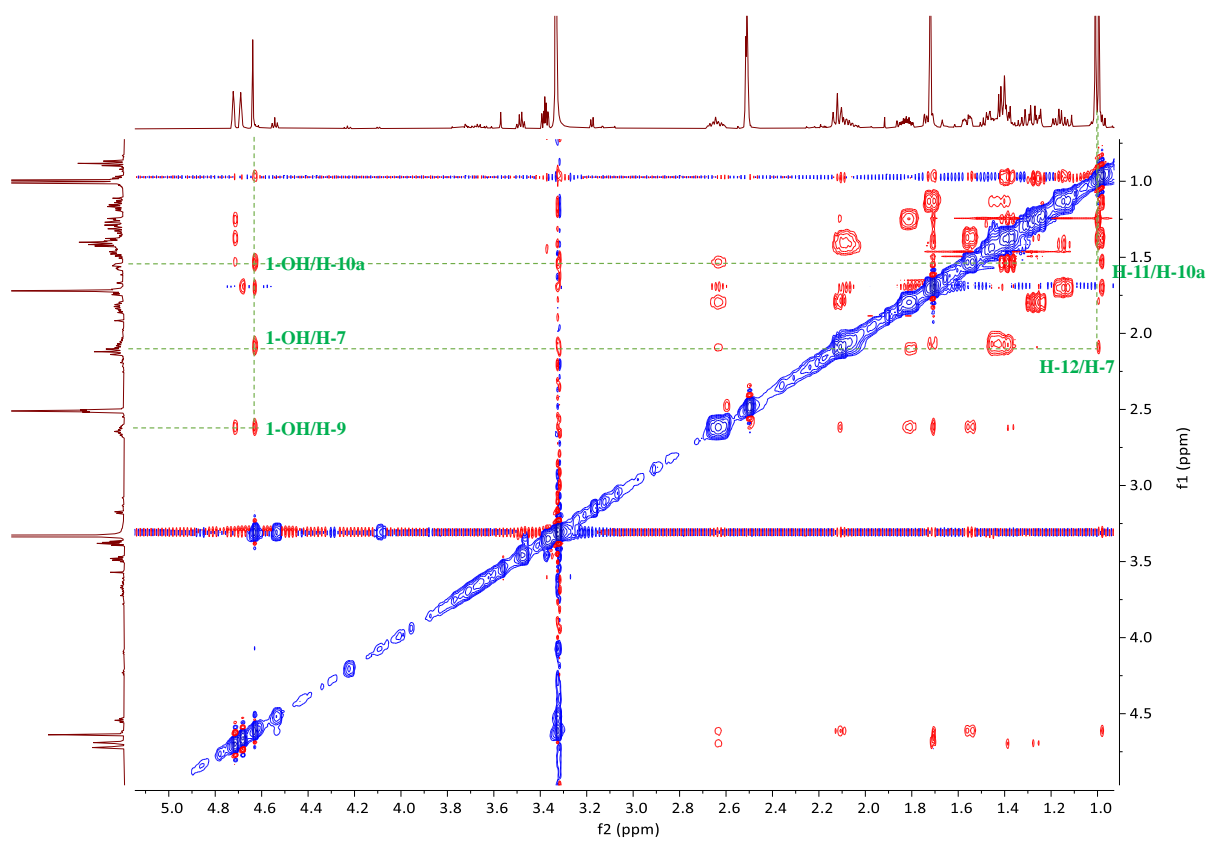


Figure S10: NOESY spectrum of **1**

Structure Match

All Drawn (0)

Substructure (0)

Similarity (170)

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Similarity

85-99 (2)

80-84 (61)

75-79 (195)

70-74 (691)

65-69 (3,090)

60-64 (130)

Reaction Role

Product (14)

Reactant (5)

Reference Role

Preparation (31)

Biological Study (29)

Synthetic Preparation (13)

Biological Study, Unclassified (14)

Properties (14)

View All

Life Science Data

Commercial Availability

Available (4)

Not Available (37)

Filtering: Similarity: 2 Selected Number of Components: 1 Clear All Filters

43 Results Sort: Number of References: Descending View: Partial

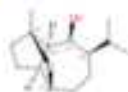


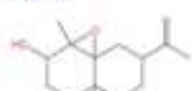


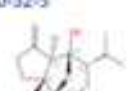


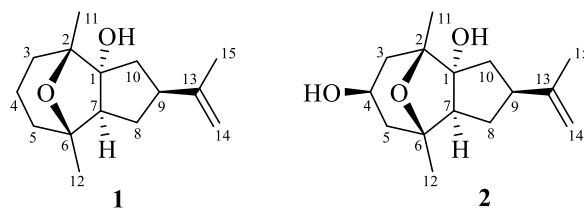
<p>1</p> <p>259875-21-3</p>  <p>Absolute stereochemistry shown</p> <p>$C_{15}H_{24}O_2$ (1R,3aS,4aE,7R,8E,9aP)-Decahydro-1,4-dimethyl-7-(1-methylethyl)-1,4-epoxynaphthalene</p> <p>2 References</p>	<p>2</p> <p>911714-01-5</p>  <p>Absolute stereochemistry shown, Rotation (1)</p> <p>$C_{15}H_{24}O_2$ (1R,3aE,4E,7R,8E,9aD)-Decahydro-1,4-dimethyl-7-(1-methylethyl)-4,8-epoxynaphthalene</p> <p>5 References 4 Reactions 27 Suppliers</p>	<p>3</p> <p>142569-89-0</p>  <p>Absolute stereochemistry unknown, Rotation (1)</p> <p>$C_{15}H_{24}O_2$ (1R,3aE,4E,7R,8E,9aD)-Decahydro-5,8a-dimethyl-3-(1-methylethyl)-4,8-epoxynaphthalene</p> <p>3 References 1 Supplier</p>
<p>4</p> <p>13741-35-0</p>  <p>$C_{15}H_{24}O_2$ 3H-naphtho[1,8a-f]piperin-2-ol, octahydro-1a,4a-dimethyl-7-(1-methylethyl)-, (1a)-</p> <p>2 References 4 Reactions 3 Suppliers</p>	<p>5</p> <p>109717-27-3</p>  <p>$C_{15}H_{24}O_2$ Octahydro-1,4-dimethyl-5-(1-methylethyl)-6H-3a,7-epoxypiperin-3-ol</p> <p>3 References 2 Reactions 1 Supplier</p>	<p>6</p> <p>861929-06-8</p>  <p>Relative stereochemistry shown</p> <p>$C_{15}H_{24}O_2$ (1aE,4E,7aE,7bE,8aE)-Octahydro-1a,4a-dimethyl-7-(1-methylethyl)-3H-naphthalene</p> <p>3 References 10 Reactions 1 Supplier</p>
<p>7</p> <p>1393370-32-5</p>  <p>Absolute stereochemistry shown, Rotation (1)</p> <p>$C_{15}H_{24}O_2$ (3aE,4E,5E,7E,8E,9aE)-Octahydro-4-methyl-1-methylsine-7-(1-methylethyl)-4,8-epoxynaphthalene</p> <p>2 References</p>	<p>8</p> <p>61248-42-8</p>  <p>$C_{15}H_{24}O_2$ 3H-naphtho[1,8a-f]piperin-2-ol, octahydro-1a,4a-dimethyl-7-(1-methylethyl)-, (1a)-</p> <p>2 References 1 Supplier</p>	<p>9</p> <p>146276-38-2</p>  <p>Absolute stereochemistry shown</p> <p>$C_{15}H_{24}O_2$ 3H-Azulen[3a-f]piperin-8-ol, octahydro-1a,6-dimethyl-4-(1-methylethyl)-, (1a)-</p> <p>2 References 3 Reactions 1 Supplier</p>

Figure S11: Scifinder search results of 1

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

No	1		2	
	δ_{H} (<i>J</i> in Hz)	δ_{C} , type	δ_{H} (<i>J</i> 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			