

Supporting Information

Rec. Nat. Prod. 19:6 (2026) 717-721

Trichothecene Sesquiterpenes with Anti-osteosarcoma Cytotoxicity from the Fungus *Fusarium* sp. XPW68

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#These authors contributed equally to the study.



Figure S: ^1H -NMR (500 MHz, CDCl_3) spectrum of **1**



Figure S2: Enlarged ^1H -NMR (500 MHz, CDCl_3) spectrum of **1**

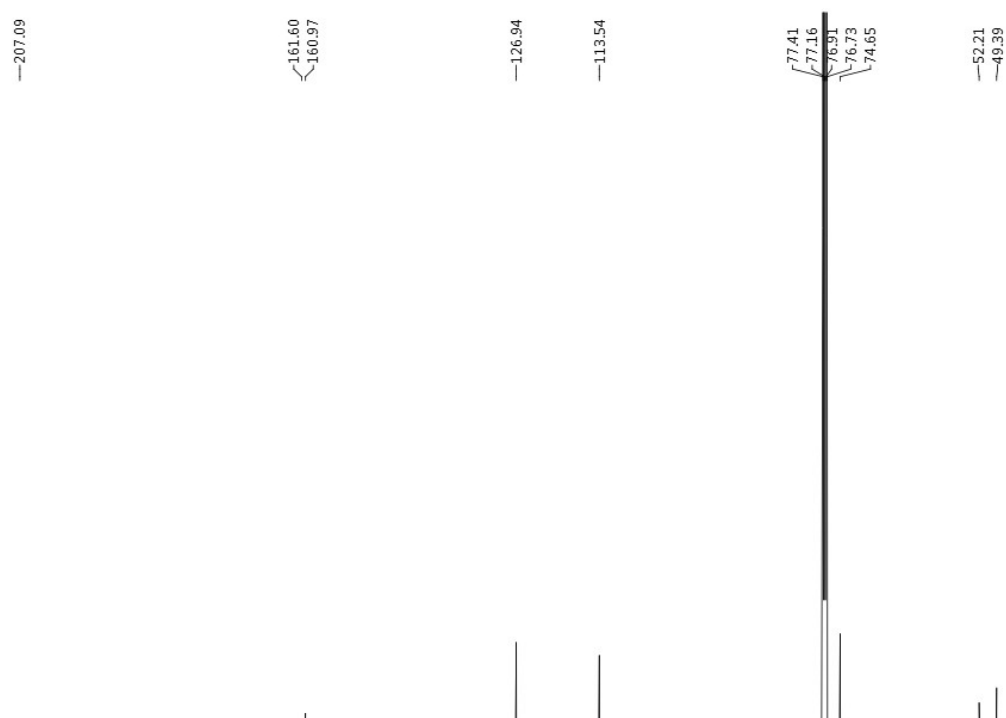


Figure S3: ^{13}C -NMR (125 MHz, CDCl_3) spectrum of **1**

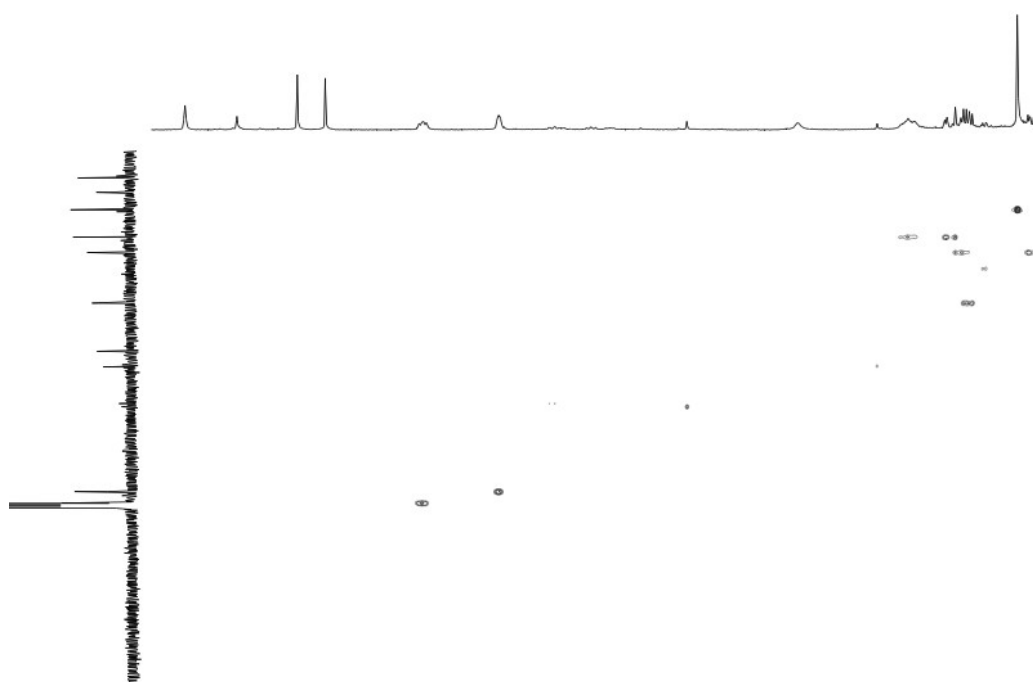


Figure S4: HSQC spectrum of **1**

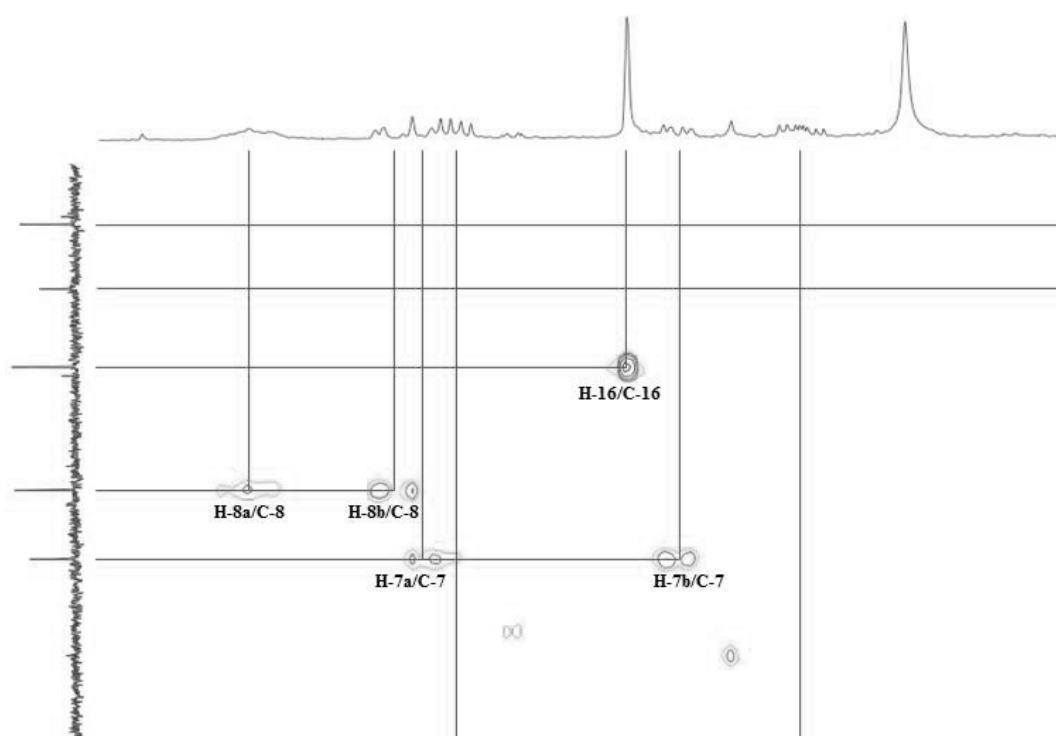


Figure S5: Enlarged HSQC spectrum of **1**

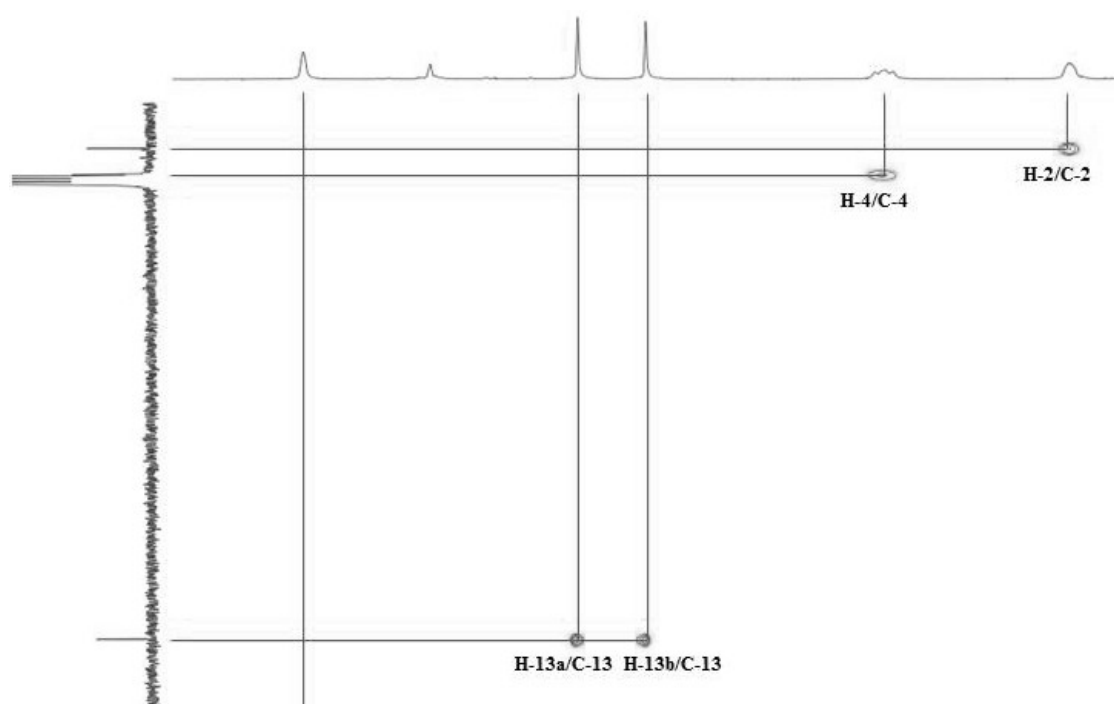


Figure S6: Enlarged HSQC spectrum of **1**

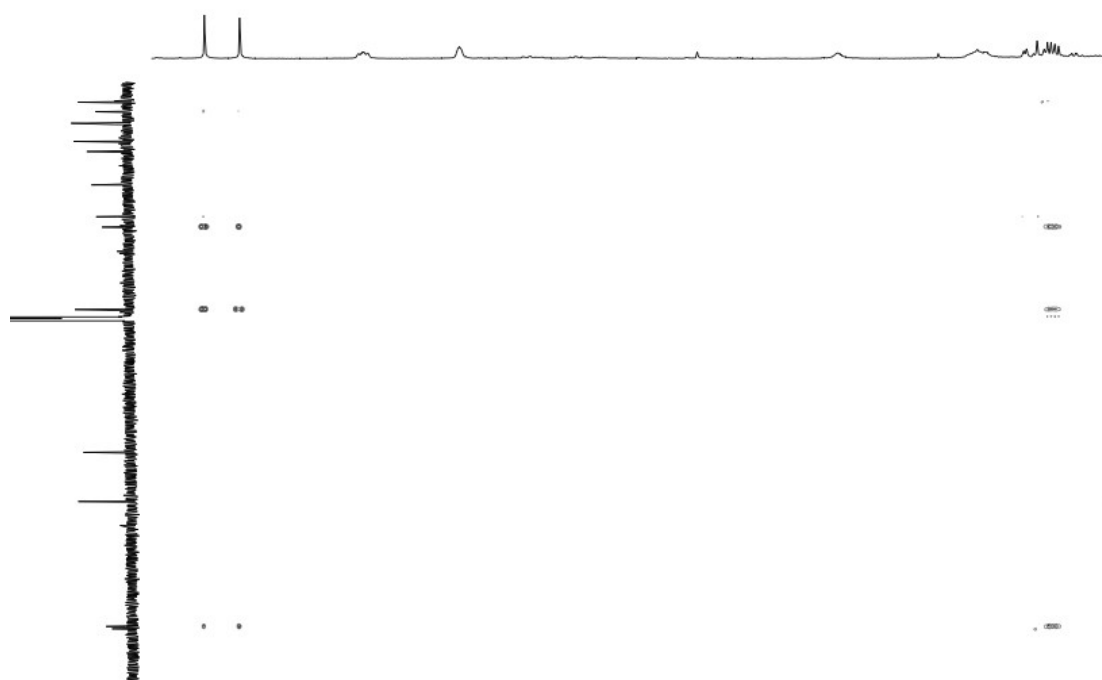


Figure S7: HMBC spectrum of **1**

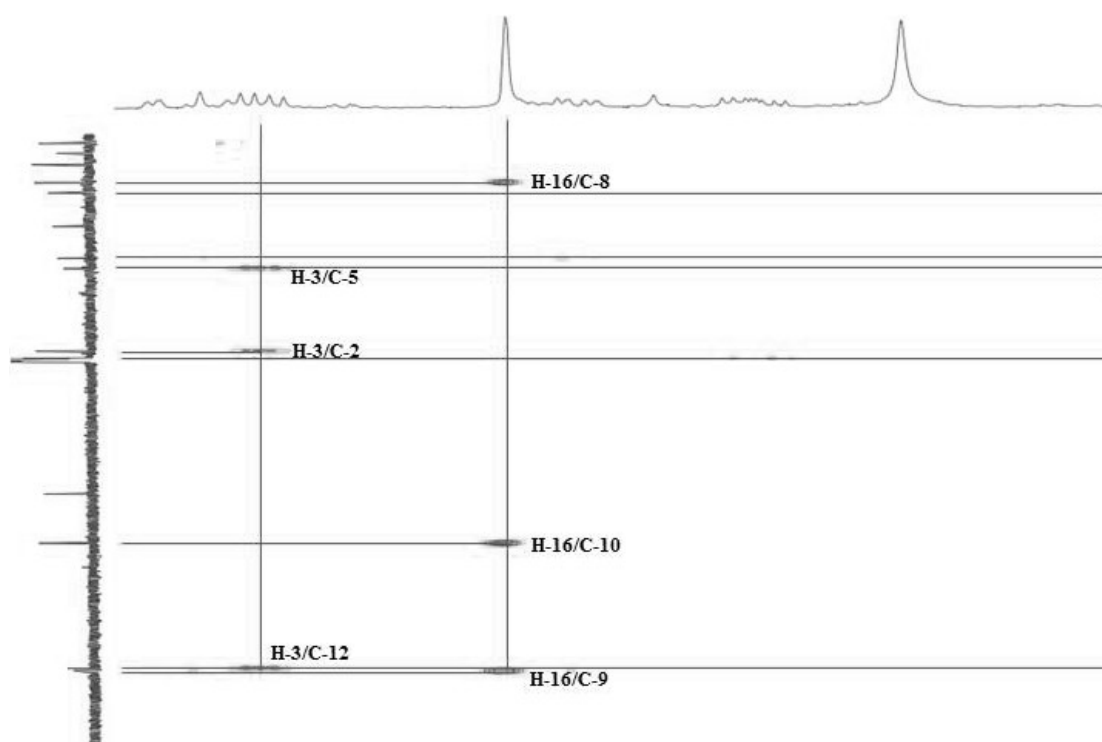


Figure S8: Enlarged HMBC spectrum of **1**

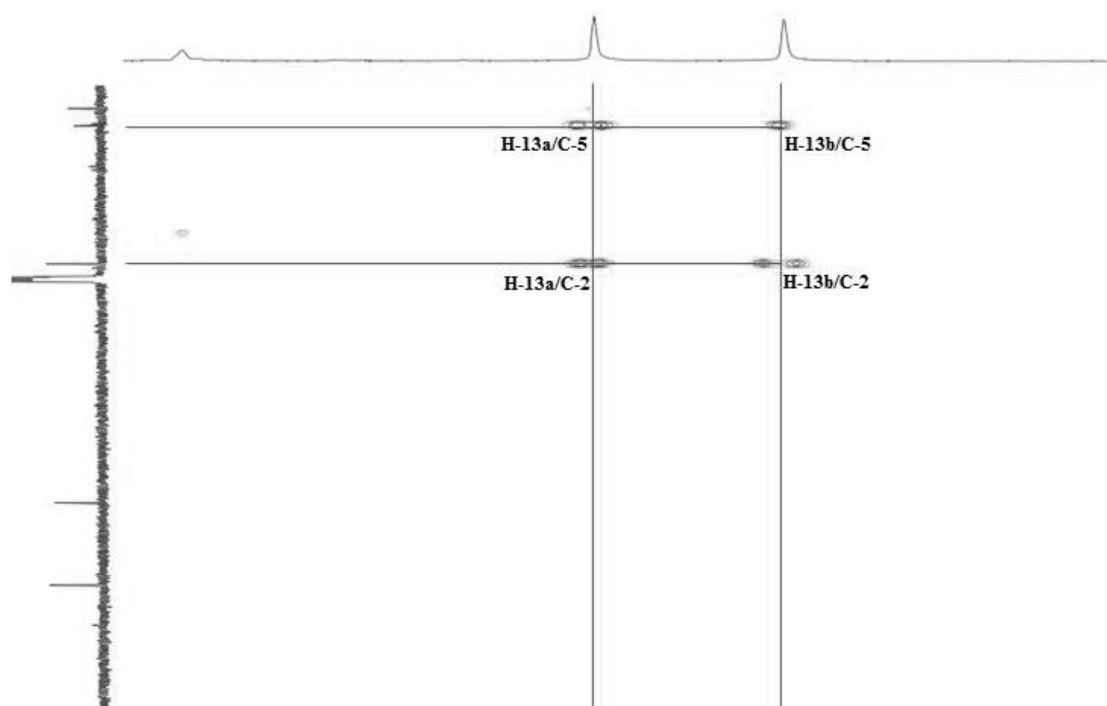


Figure S9: Enlarged HMBC spectrum of **1**

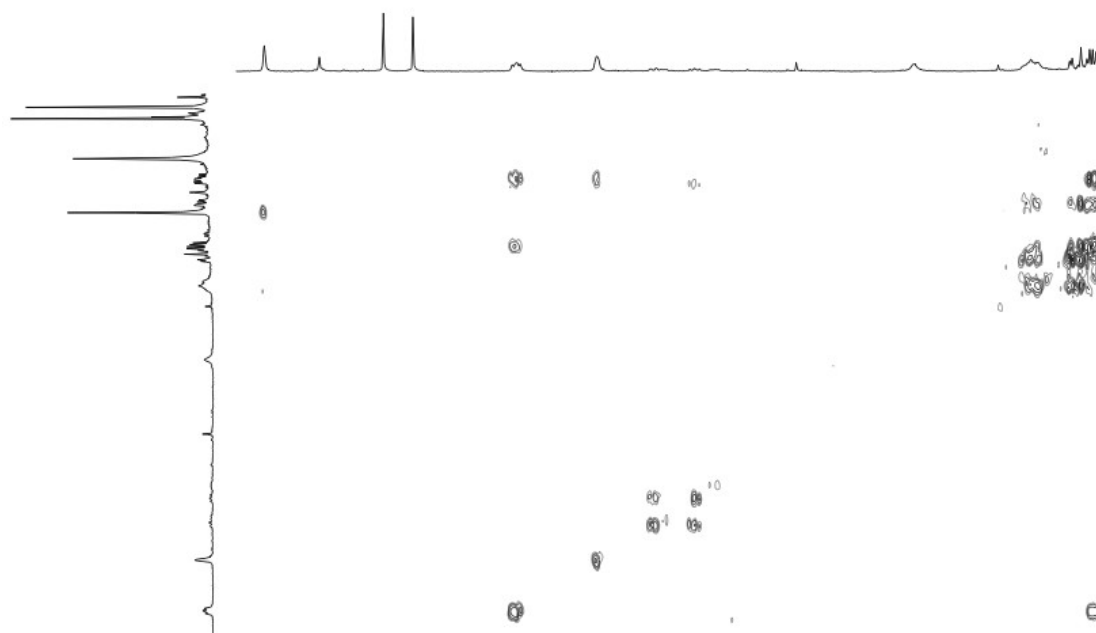


Figure S10: ^1H - ^1H COSY spectrum of **1**

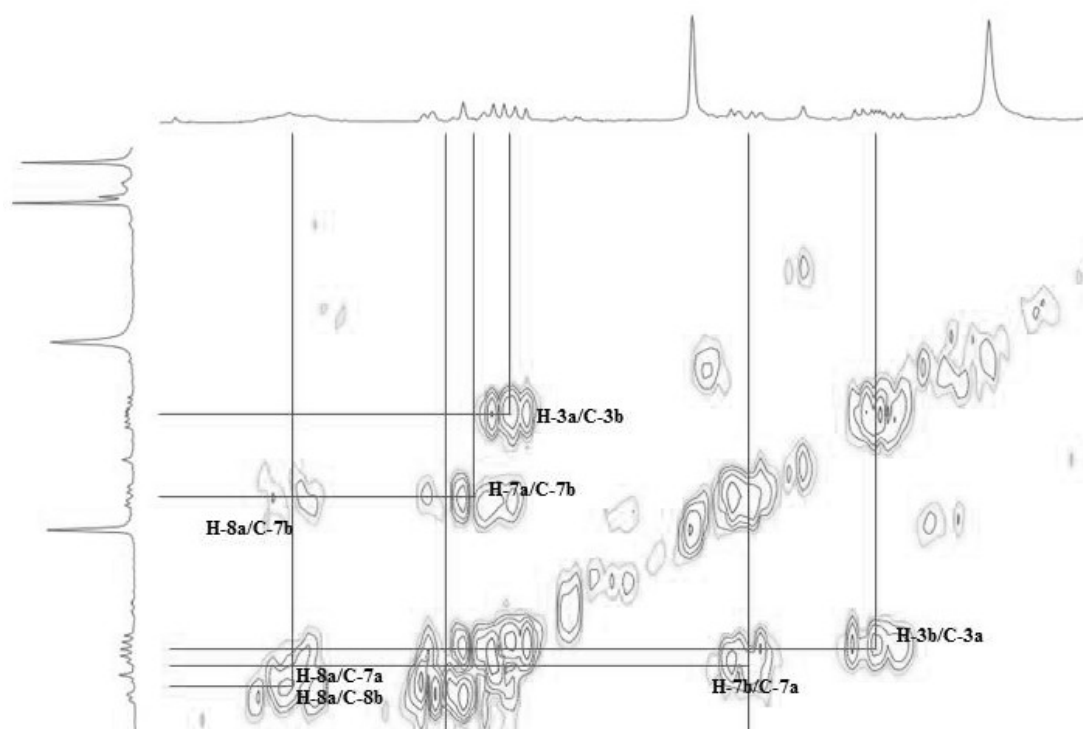


Figure S11: Enlarged ^1H - ^1H COSY spectrum of **1**

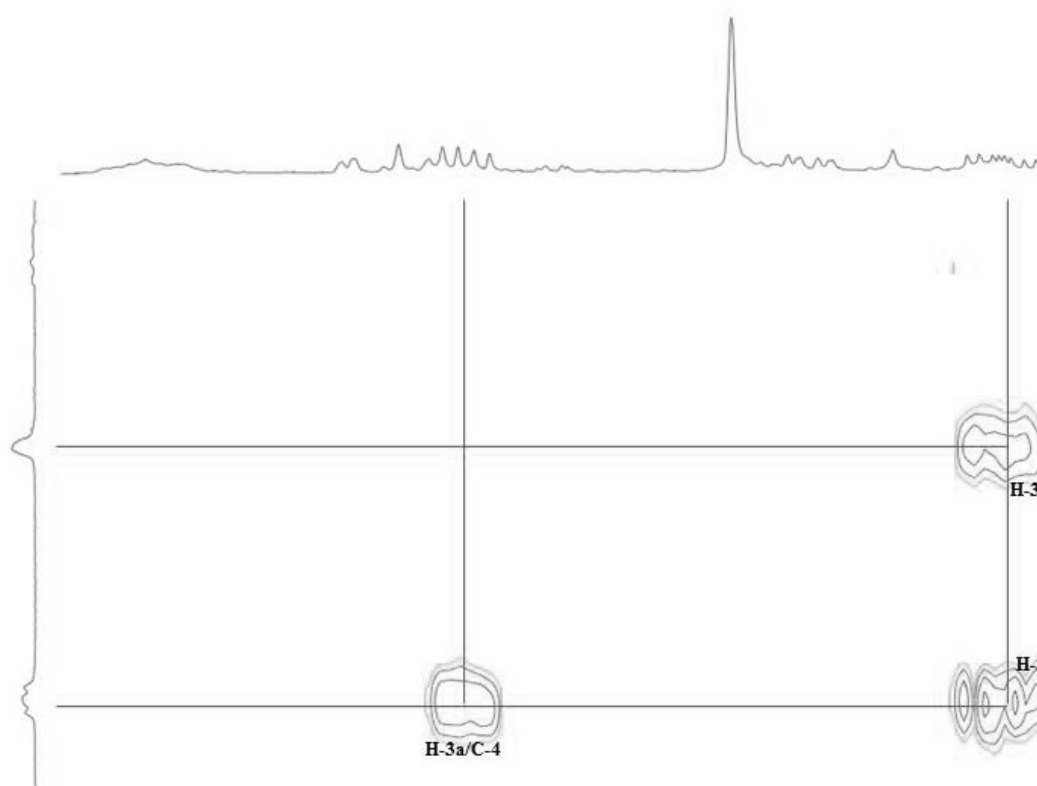


Figure S12: Enlarged ^1H - ^1H COSY spectrum of **1**

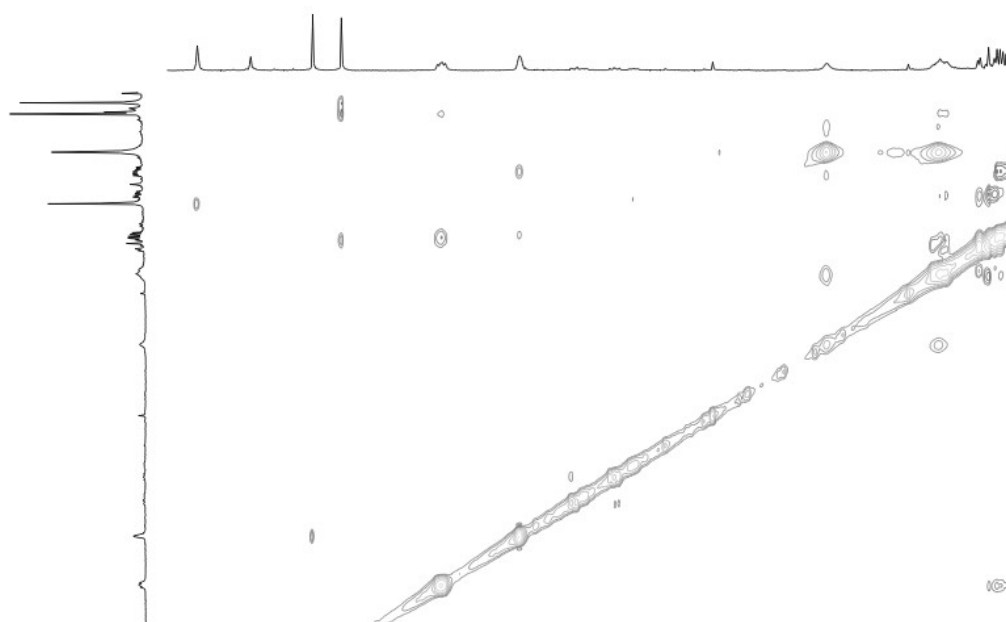


Figure S13: NOESY spectrum of **1**

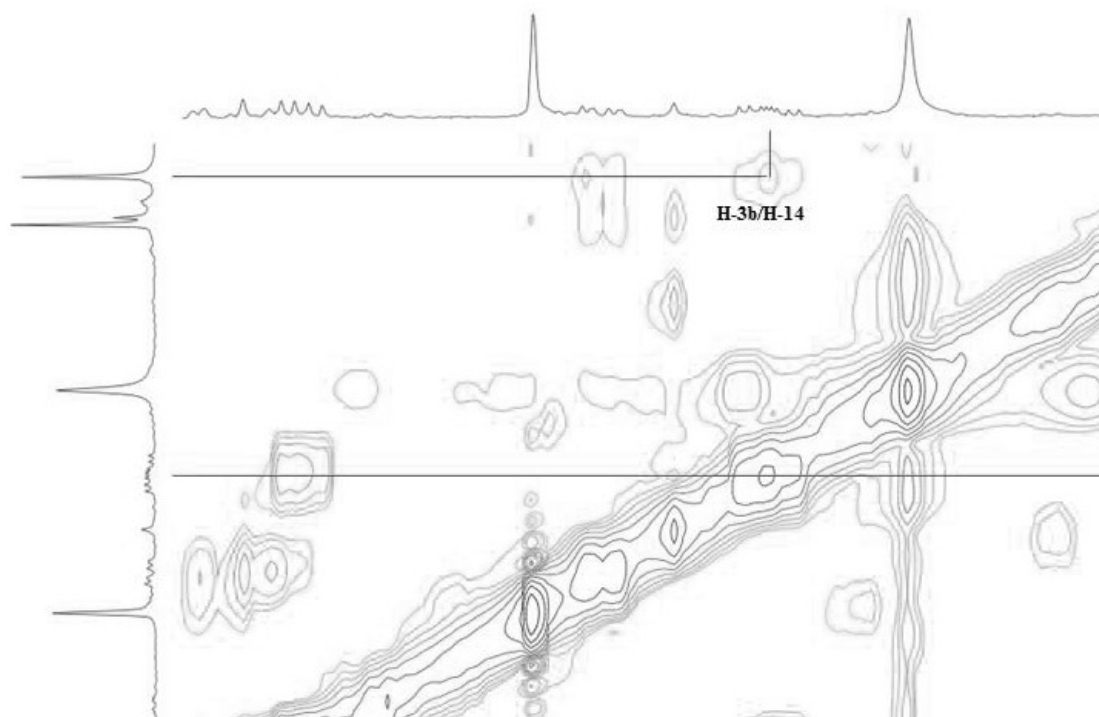


Figure S14: Enlarged NOESY spectrum of **1**

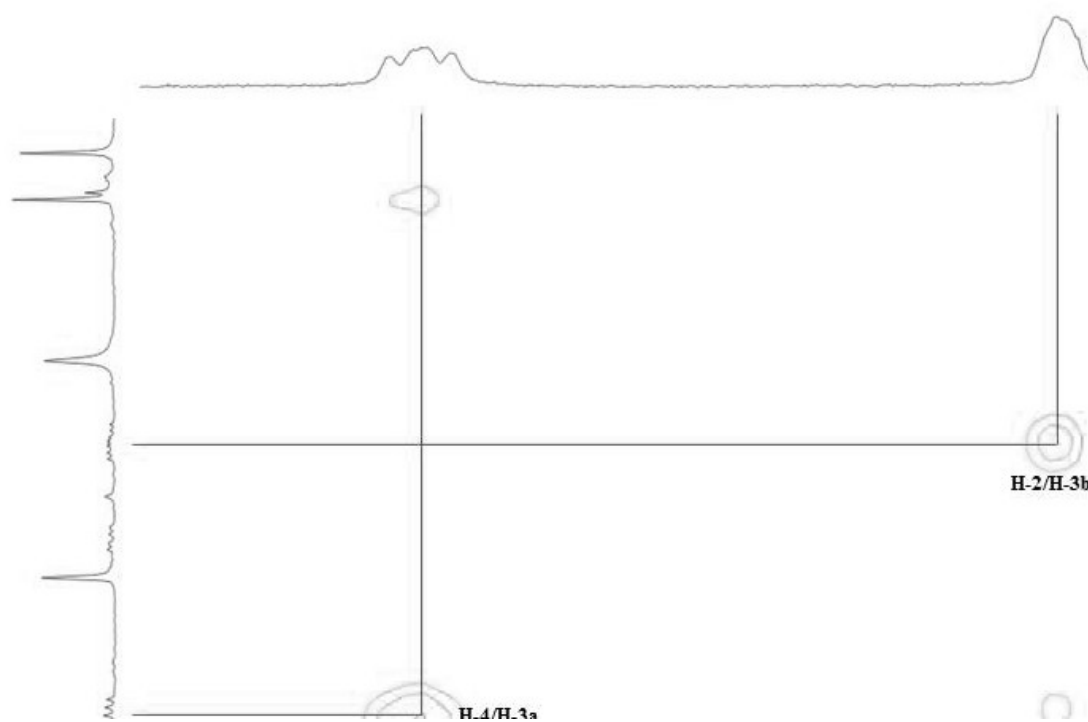


Figure S15: Enlarged NOESY spectrum of **1**

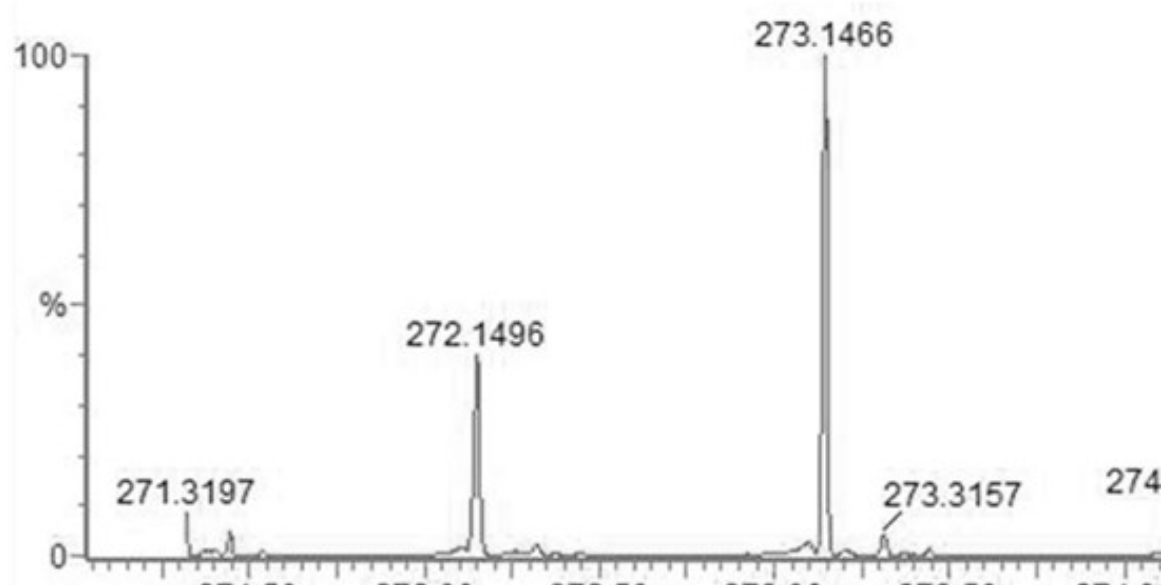


Figure S16: HRESIMS spectrum of **1**

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80-84 (57)

75-79 (249)

70-74 (1,239)

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17 Results

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1 94 ...

1111174-85-6

Absolute stereochemistry shown

C₁₅H₂₂O₂
(6R)-6-[(1S,3R)-3-Hydroxy-1-methyl-2-methylenecyclopentyl]-3,6-dimethyl-2-cyclohexen-1-one...

1 Reference 0 Reactions 0 Suppliers

2 89 ...

66389-07-9

Absolute stereochemistry shown

C₁₅H₂₄O₂
(4R,5R)-4-Hydroxy-2-methyl-5-[(1S)-1,2,2-trimethylcyclopentyl]-2-cyclohexen-1-one...

6 References 0 Reactions 1 Supplier

3 89 ...

244092-78-2

Absolute stereochemistry shown, Rotation (+)

C₁₅H₂₄O₂
(4S,5R)-4-Hydroxy-2-methyl-5-[(1S)-1,2,2-trimethylcyclopentyl]-2-cyclohexen-1-one...

1 Reference 0 Reactions 0 Suppliers

4 88 ...

1362114-50-8

Absolute stereochemistry shown, Rotation (-)

C₁₅H₂₄O₃
(6S)-6-Hydroxy-3-[(1S,4S)-4-hydroxy-1,2,2-trimethylcyclopentyl]-2-cyclohexen-1-one...

1 Reference 0 Reactions 0 Suppliers

5 88 ...

1362114-49-5

Absolute stereochemistry shown, Rotation (-)

C₁₅H₂₄O₃
(6S)-6-Hydroxy-3-[(1S,4R)-4-hydroxy-1,2,2-trimethylcyclopentyl]-2-cyclohexen-1-one...

1 Reference 0 Reactions 0 Suppliers

6 87 ...

1362114-47-3

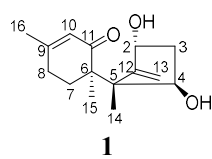
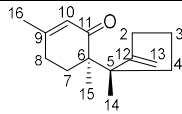
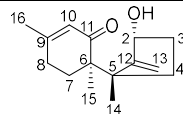
Absolute stereochemistry shown, Rotation (-)

C₁₅H₂₂O₄
(4S,6S)-4,6-Dihydroxy-6-methyl-3-[(1R)-1,2,2-trimethylcyclopentyl]-2-cyclohexen-1-one...

1 Reference 0 Reactions 0 Suppliers

Figure S17: Scifinder search result of 1

Table S1: NMR data of compounds **1**, 3,6 α -dimethyl-2 β -(1 β -methyl-2-methylenecyclopentyl)cyclohex-2-enone, and 2 α -hydroxytrichodiene-11-one

Position	 1	 3,6α-dimethyl-2β-(1β-methyl-2-methylenecyclopentyl)cyclohex-2-enone [11]	 2α-hydroxytrichodiene-11-one [15]	
	δ_{H}	δ_{C}	δ_{C}	δ_{H}
2	4.32, d (4.3)	74.7, CH	38.4, CH ₂	4.33, dd (8.3, 4.5)
3a	2.16, dd (13.5, 6.6)	40.7, CH ₂	23.4, CH ₂	1.78, dd (13.8, 6.9)
3b	1.70, ddd (13.5, 10.9, 5.1)			1.71, dddd (13.8, 13.1, 6.9, 4.5)
4a	4.67, dd (10.6, 6.8)	76.6, CH	39.0, CH ₂	2.60, ddd (13.1, 13.1, 6.9)
4b				1.48, dd (13.1, 6.9)
5		52.2, C	48.5, C	
6		49.4, C	49.4, C	
7a	2.20, m	31.6, CH ₂	30.3, CH ₂	2.31, ddd (13.1, 11.7, 5.1)
7b	1.87, ddd (13.6, 5.2, 1.7)			1.97, ddd (13.1, 5.2, 2.1)
8a	2.43, m	28.9, CH ₂	28.4, CH ₂	2.43, m
8b	2.24, m			2.23, ddd (18.6, 5.1, 2.1)
9		161.6, C	160.7, C	
10	5.76, s	126.9, CH	127.2, CH	5.73, s
11		207.1, C	204.2, C	
12		161.0, C	159.0, C	
13a	5.24, s	113.5, CH ₂	106.2, CH ₂	5.22, s
13b	5.11, s			5.12, s
14	1.21, s	20.8, CH ₃	26.1, CH ₃	1.10, d (0.7)
15	1.29, s	18.2, CH ₃	17.4, CH ₃	1.22, s
16	1.93, s	23.9, CH ₃	23.8, CH ₃	1.92, s

- [15] T. Tokai, H. Koshino, T. Kawasaki, T. Igawa, Y. Suzuki, M. Sato, M. Fujimura, T. Eizuka, H. Watanabe, T. Kitahara, K. Ohta, T. Shibata, T. Kudo, H. Inoue, I. Yamaguchi and M. Kimura (2005). Screening of putative oxygenase genes in the *Fusarium graminearum* genome sequence database for their role in trichothecene biosynthesis, *FEMS Microbiol. Lett.* **251**, 193-201.