

Supporting Information

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A new antifungal α -pyrone secondary metabolite isolated from the tobacco-derived fungus *Aspergillus aculeatus* Aa-1

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Figure S1: HRESIMS spectrum of **1**

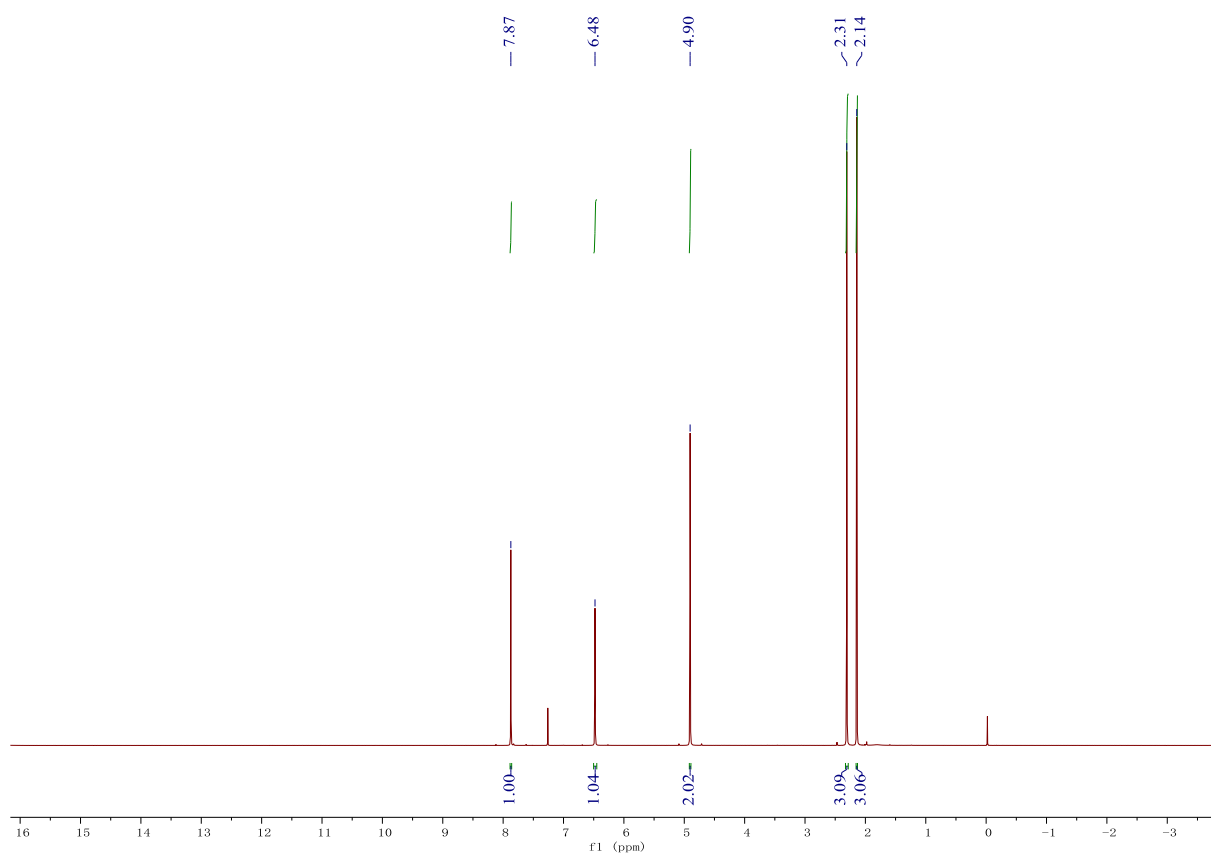


Figure S2: ^1H NMR (400 MHz, CDCl_3) spectrum of **1**

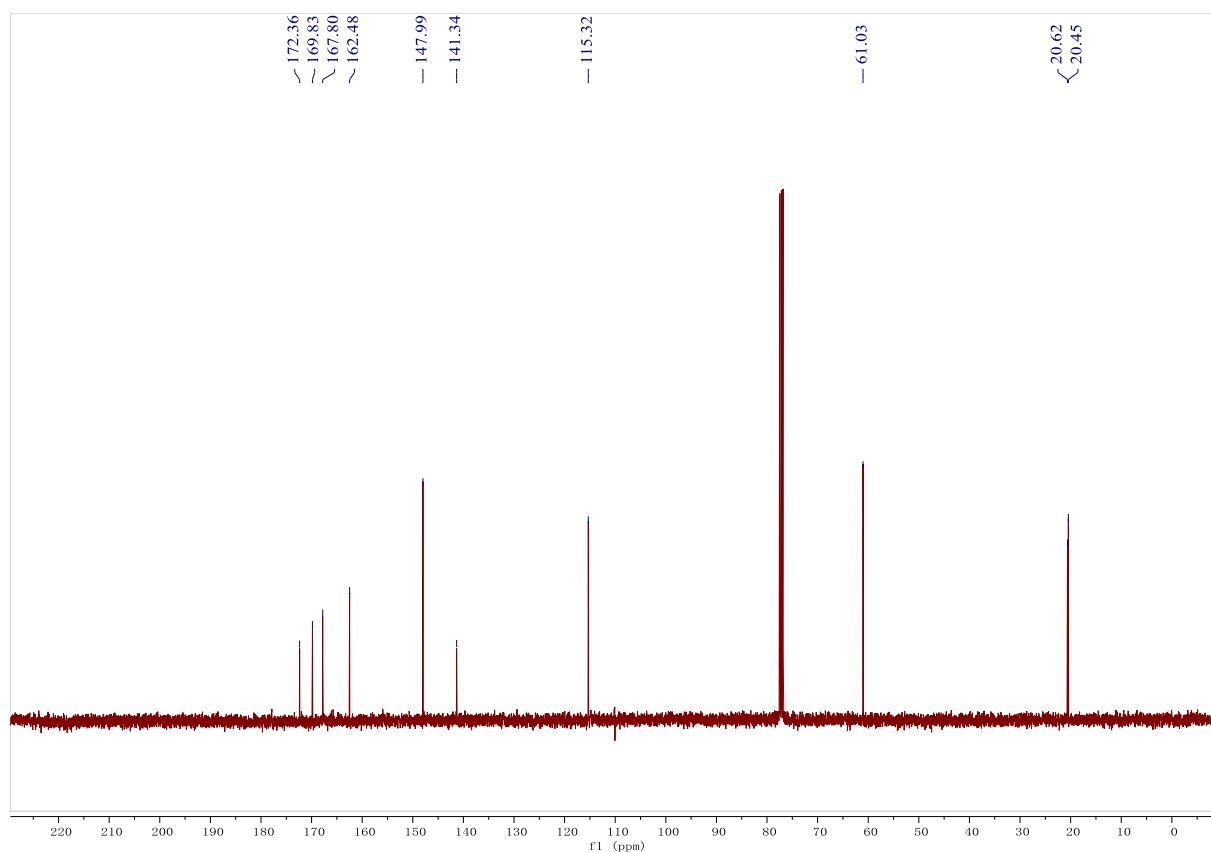


Figure S3: ¹³C NMR (100 MHz, CDCl₃) spectrum of **1**

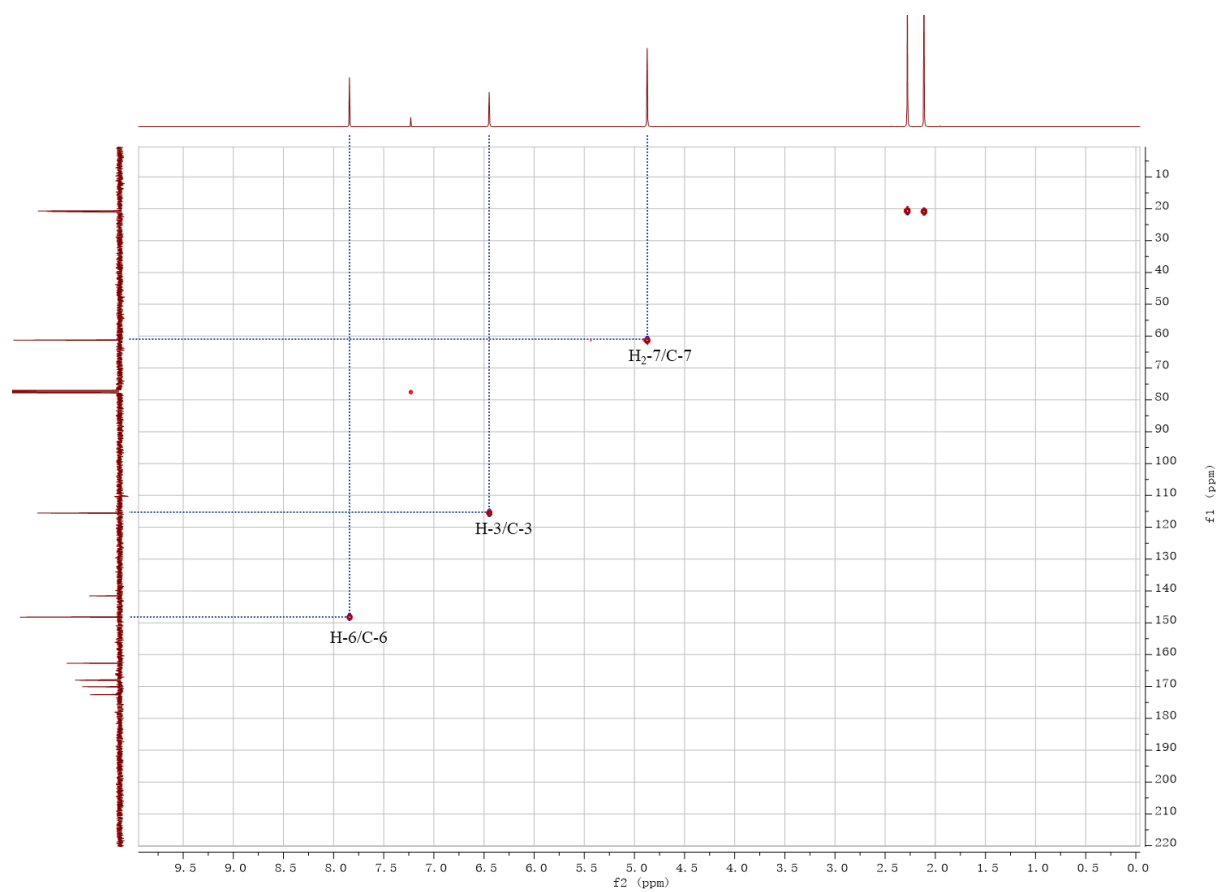


Figure S4: HSQC spectrum of **1**

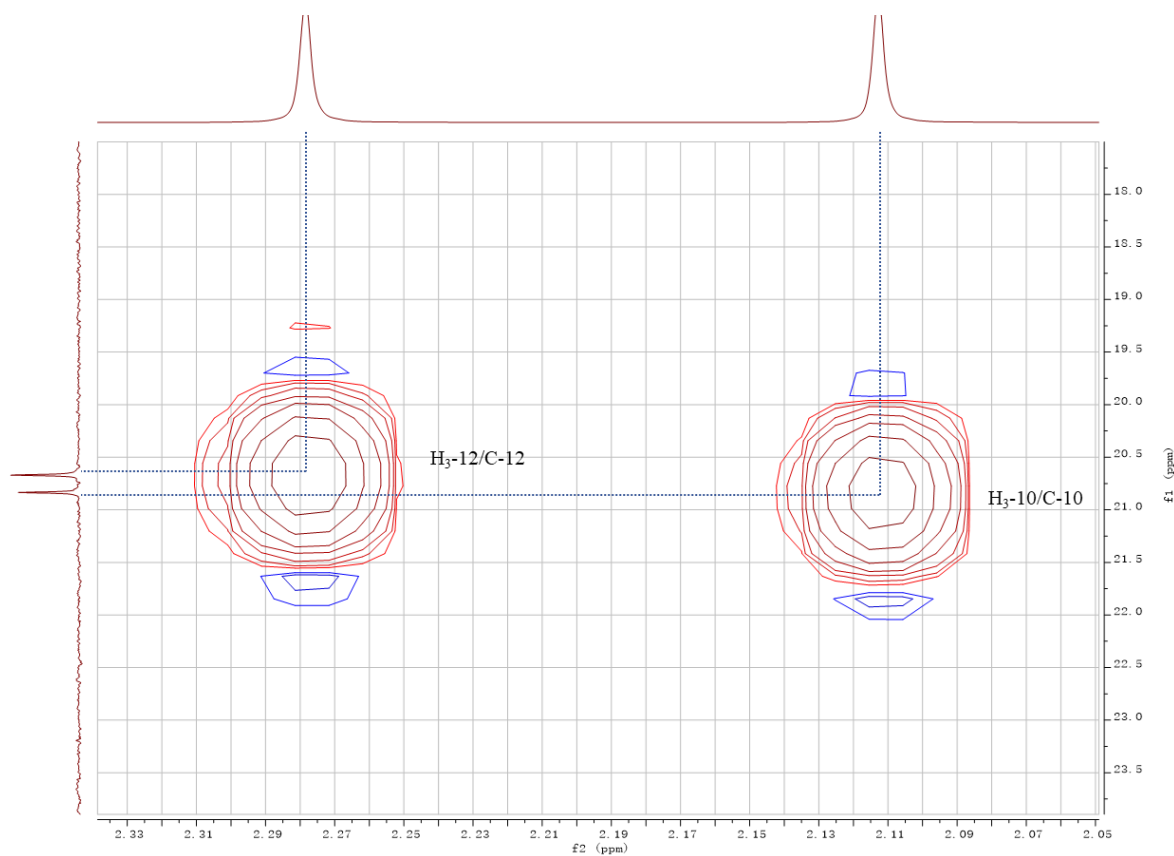


Figure S5: Enlarged HSQC spectrum of **1**

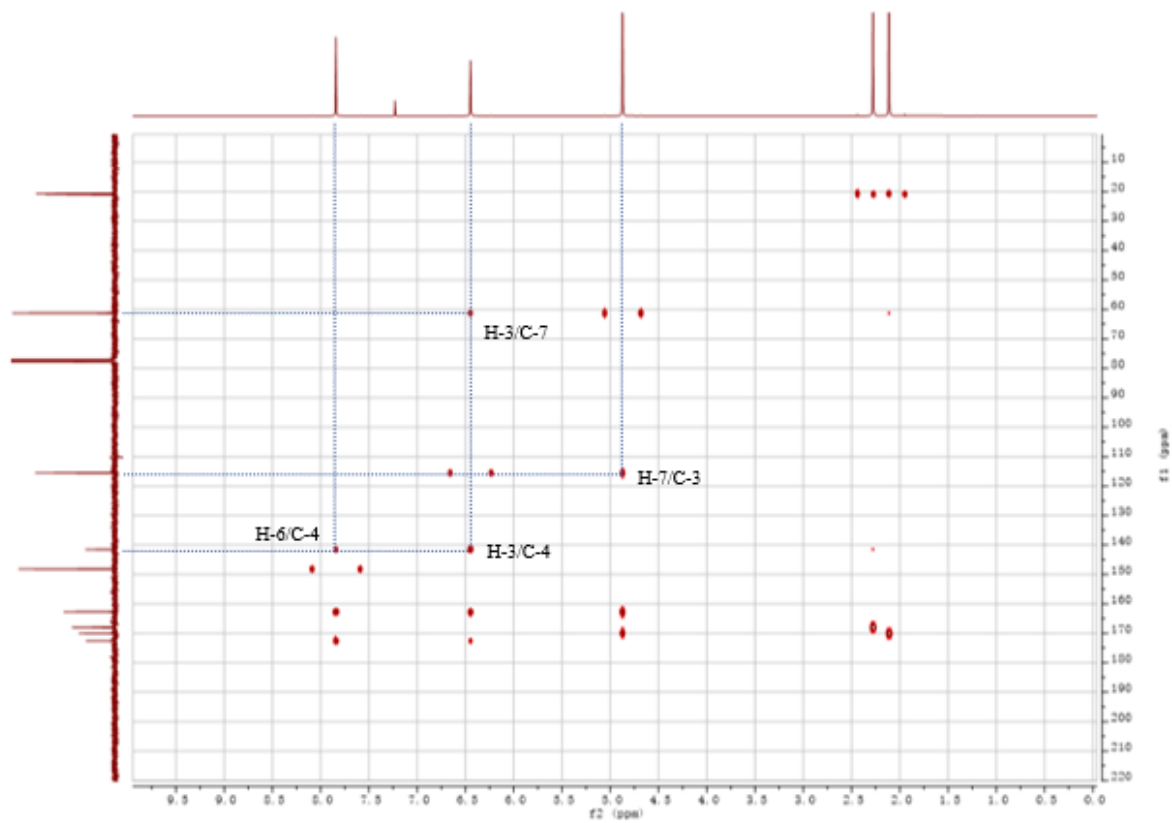


Figure S6: HMBC spectrum of **1**

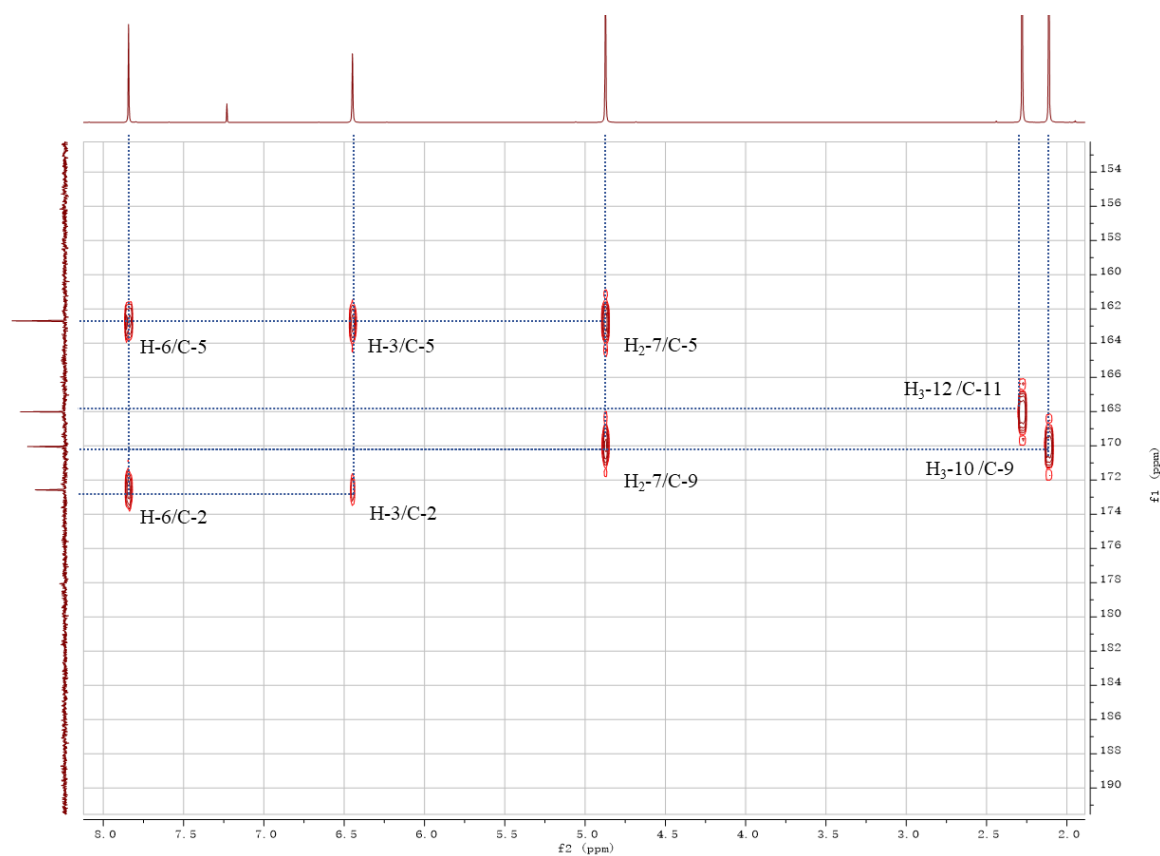


Figure S7: Enlarged HMBC spectrum of **1**

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[Substances](#)
[Reactions](#)
[References](#)
[Suppliers](#)
[Patent Markush](#)

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As Drawn (0)

Substructure (1)

Similarity (7,965)

Behavior

Filter by Exclude

Search Within Results

Similarity

☒ 85-89 (5)

☐ 80-84 (19)

☐ 75-79 (134)

☐ 70-74 (360)

☐ 65-69 (1,386)

☐ 60-64 (5,809)

Reaction Role

☐ Product (2)

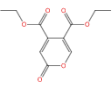
☐ Reactant (2)

5 Results

1

88 ***

101967-99-1



C11H12O6
4,5-Diethyl 2-oxo-2H-pyran-4,5-dicarboxylate

12 37 8

2

88 ***

1038917-84-8



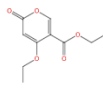
C8H8O5
4-[(Acetyloxy)methyl]-5-hydroxy-2H-pyran-2-one

6 0 0

3

88 ***

127351-39-7



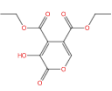
C10H12O5
Ethyl 4-ethoxy-2-oxo-2H-pyran-5-carboxylate

4 5 5

4

86 ***

854457-97-9



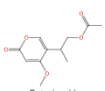
C11H12O7
4,5-Diethyl 3-hydroxy-2-oxo-2H-pyran-4,5-dicarboxylate

2 0 0

5

86 ***

120461-98-5



C11H14O5
(-)-5-[2-(Acetyloxy)-1-methylethyl]-4-methoxy-2H-pyran-2-one

1 0 1

Figure S8: Scifinder search results of **1**

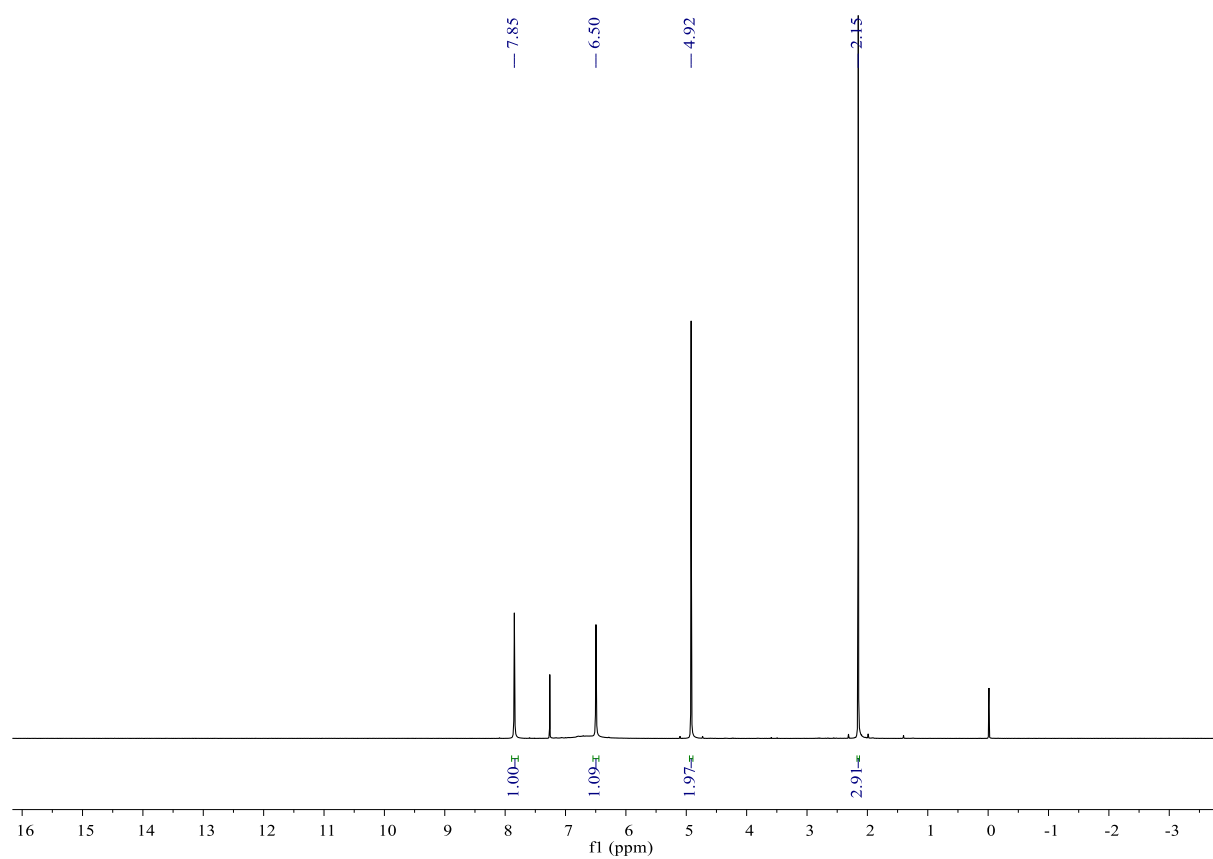


Figure S9: ¹H NMR (400 MHz, CDCl₃) spectrum of **2**

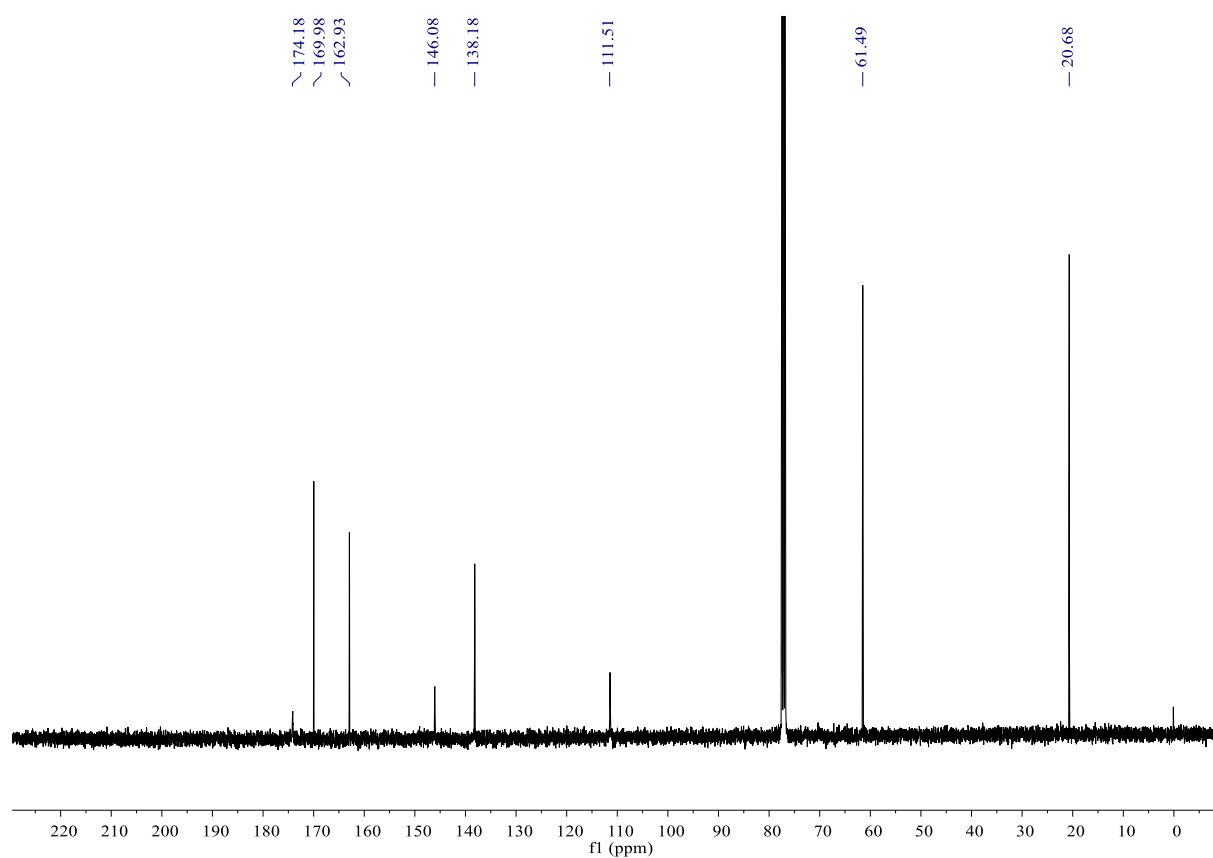


Figure S10: ¹³C NMR (100 MHz, CDCl₃) spectrum of **2**

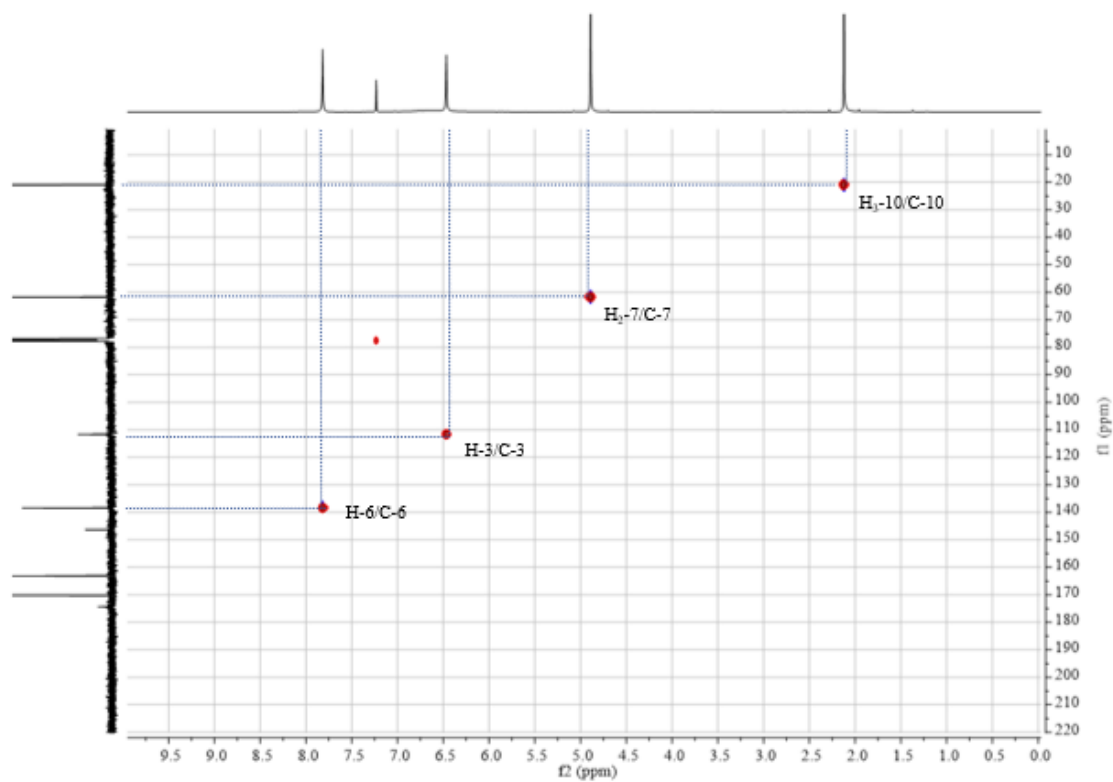


Figure S11: HSQC spectrum of **2**

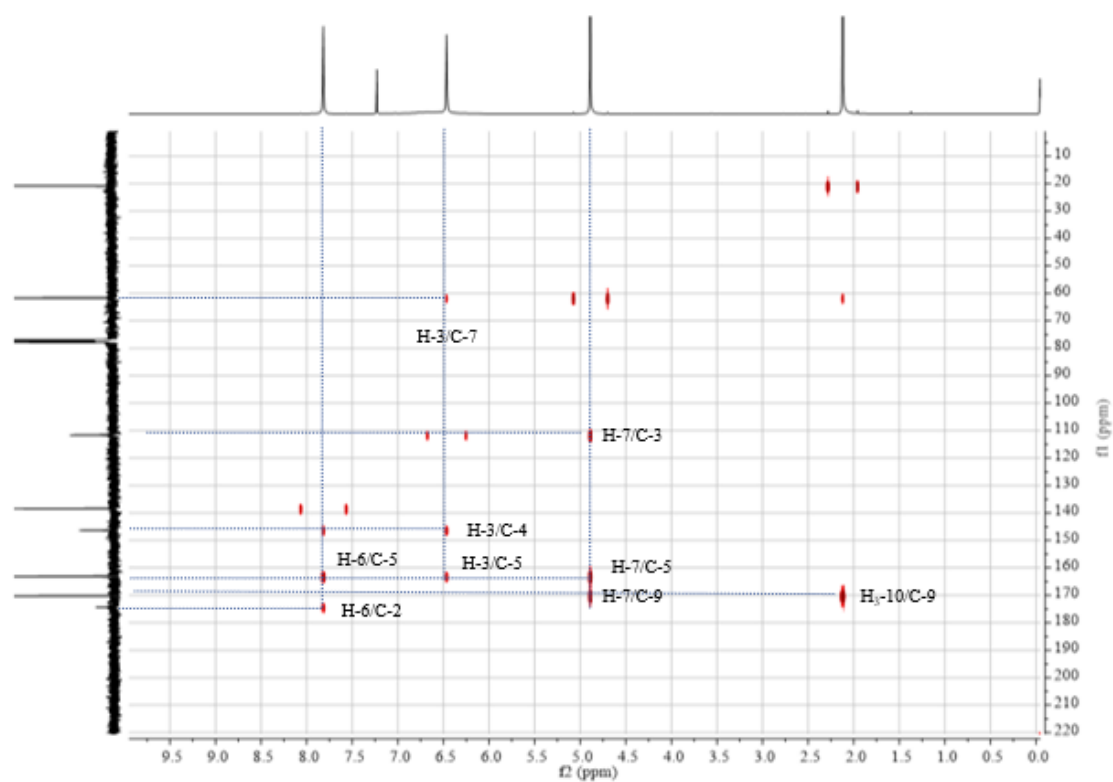


Figure S12: HMBC spectrum of **2**

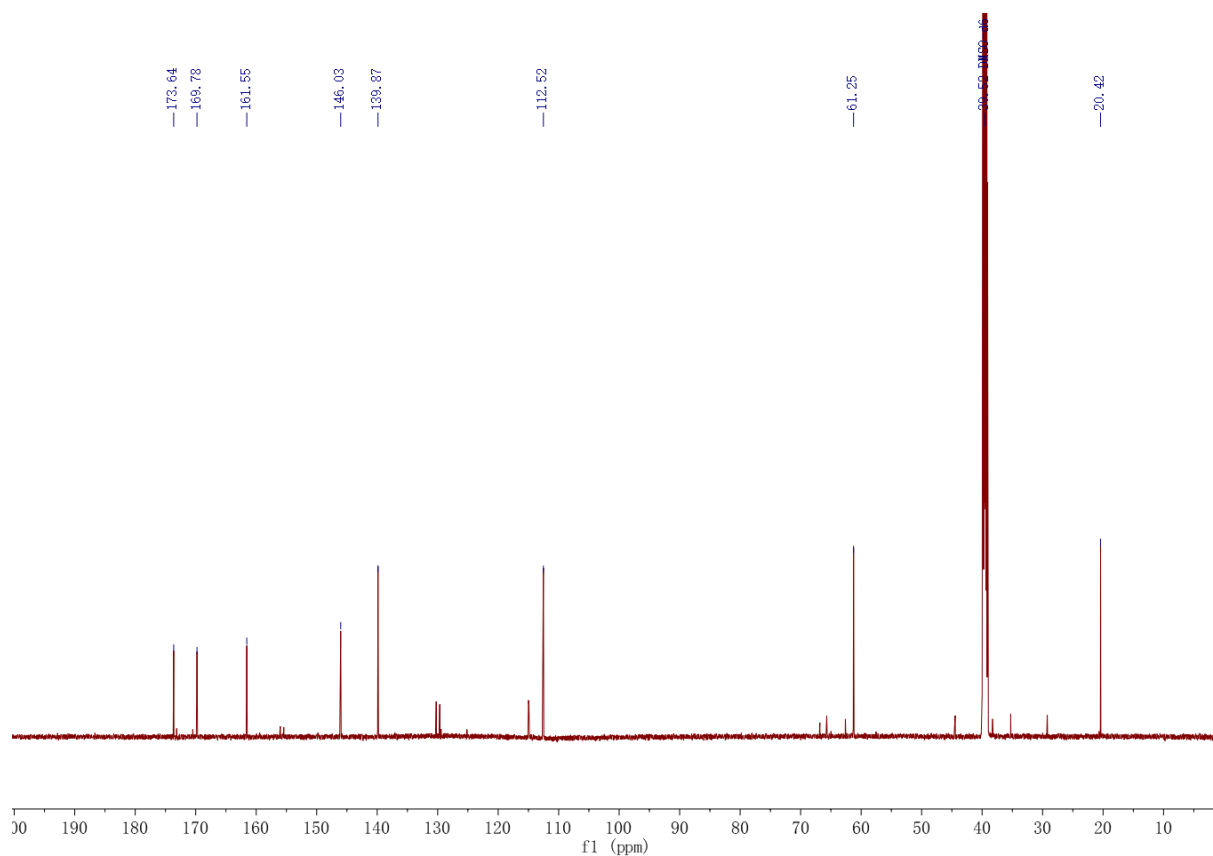


Figure S13: ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of **2**

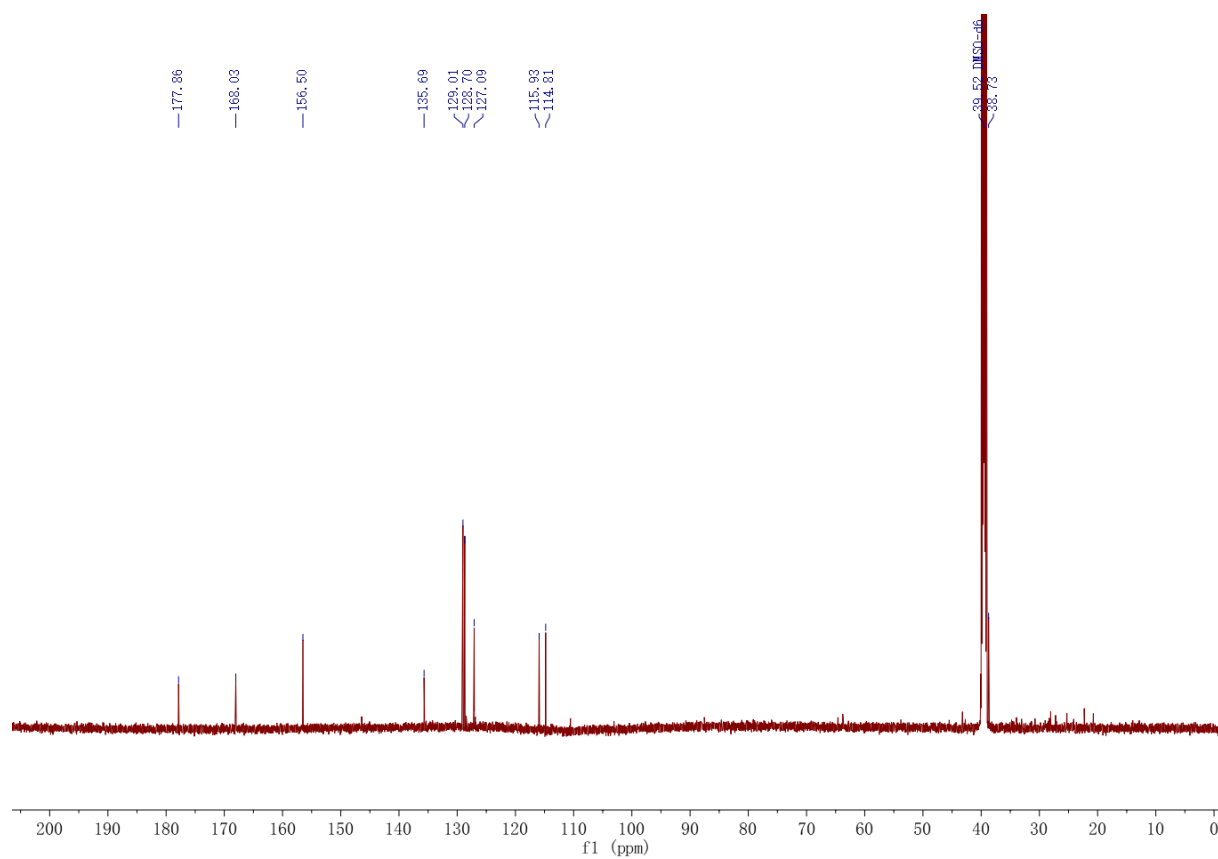


Figure S14: ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) spectrum of **3**

Table S1. Antifungal activities of the isolated compounds **1–3** (µg/mL)

Compound	F.O. ^a	F.E. ^a	R.C. ^a	A.A. ^a	V.M. ^a	C.G. ^a
1	— ^b	—	—	8	—	—
2	8	—	4	16	8	16
3	—	—	—	—	—	—
azoxystrobin ^c	8	16	2	16	4	4
carbendazim ^c	8	4	1	8	8	2

^a F.O.: *Fusarium oxysporum*; F.E.: *Fusarium equiseti*; R.C.: *Rhizoctonia cerealis*; A.A.: *Alternaria alternata*; V.M.: *Valsa mali*; C.G.: *Colletotrichum gloeosporioides*; ^b MIC > 64 µg/mL; ^c Positive control

CTTCGGGGGCCAACCTCCCACCCGTGCTTACCGTACCCTGTTGCTTCGGCGGGGCCCGCCTT
CGGGCGGGCCCGGGGCCTGCCCCGGGACCGCGCCCGCCGGAGACCCAATGGAACACTG
TCTGAAAGCGTGCAGTCTGAGTTGATTGATACCAATCAGTTAAACTTTCAACAATGGAT
CTCTTGTTCCGGCATCGATGAAGAACGCAGCGAAATGCGATAACTAATGTGAATTGCAG
AATTCAGTGAATCATCGAGTCTTTGAACGCACATTGCGCCCCCTGGTATTCCGGGGGGCA
TGCCTGTCCGAGCGTCATTTCTCCCCTCCAGCCCCGCTGGTTGTTGGGCCGCGCCCCCGG
GGGGCGGGCCTCGAGAGAAACGGCGGCACCGTCCGGTCCTCGAGCGTATGGGGCTCTGT
CACCCGCTCTATGGGCCCCGGCCGGGGCTTGCCTCGACCCCAATCTTCTCAGATTGACCTC
GGATCAGGTAGGGATACCCGCTGAACTTAAGCATATCAAAAACCCGGAAGGAAGG

The ITS1-5.8S-ITS2 partial sequences of *Aspergillus aculeatus* Aa-1.