

Supporting Information

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Butenolide Derivatives from the Fungus *Aspergillus terreus* and Their α -Glucosidase Inhibitory Effects

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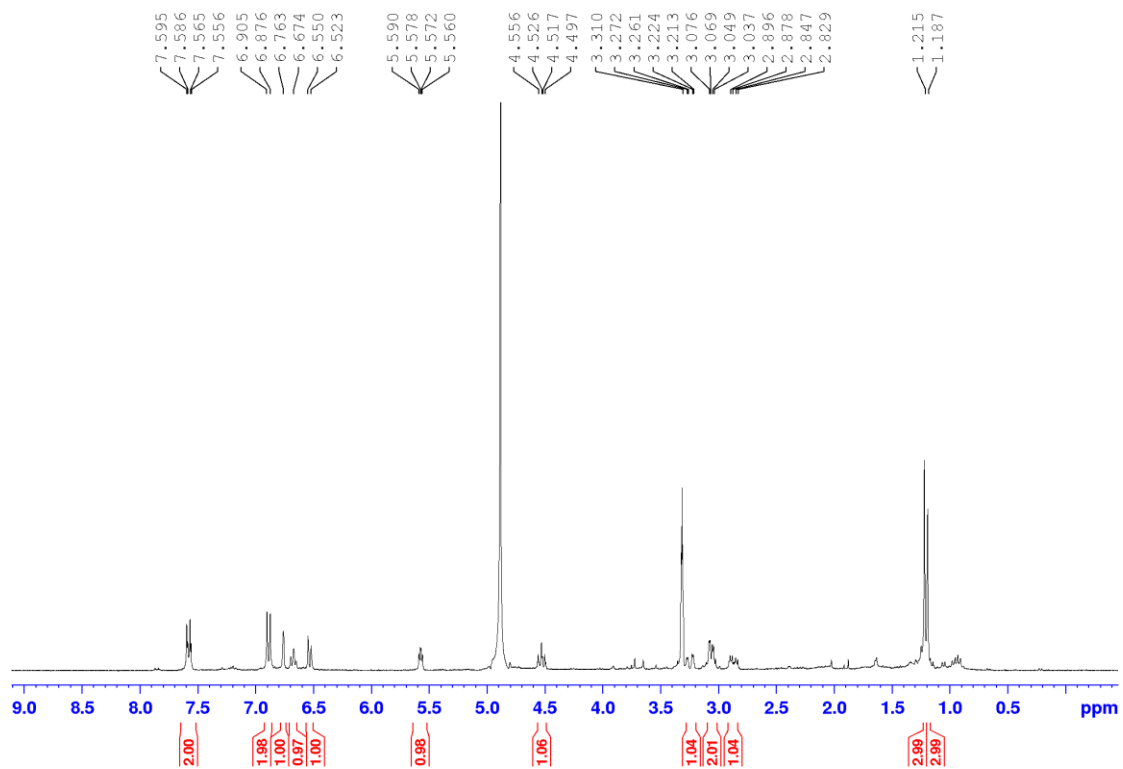


Figure S1: ^1H NMR Spectrum of **1** in CD_3OD (400 MHz)

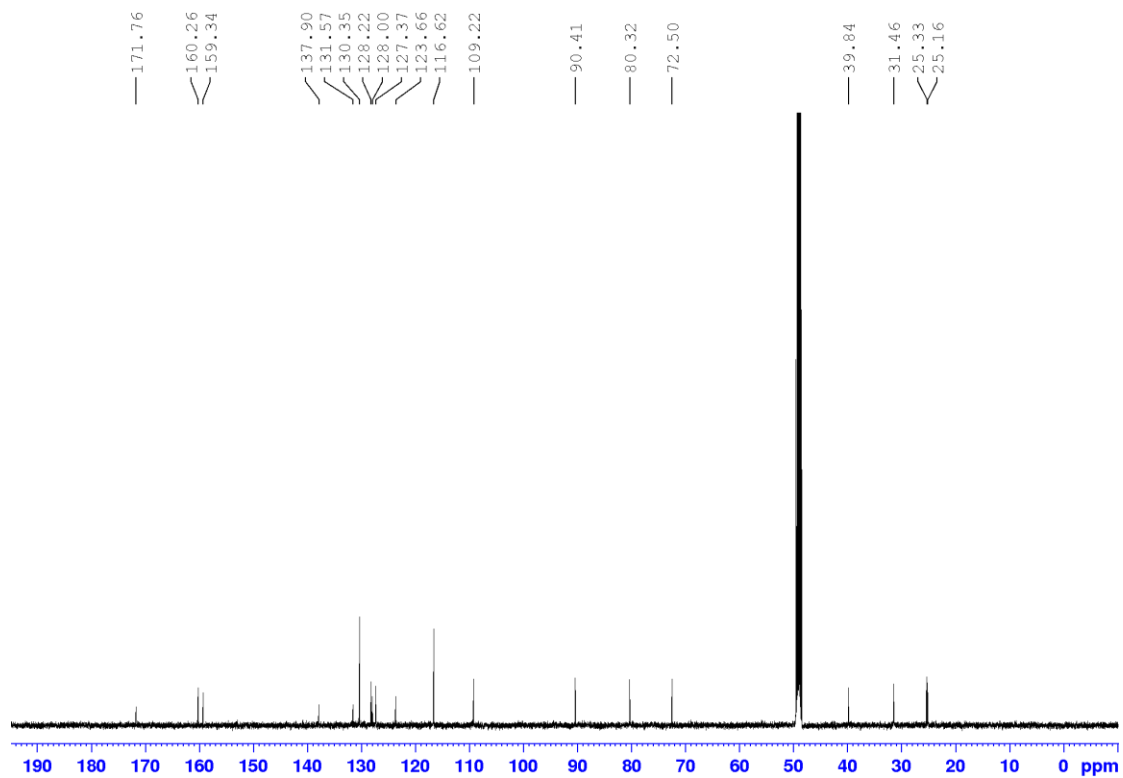


Figure S2: ^{13}C NMR Spectrum of **1** in CD_3OD (100 MHz)

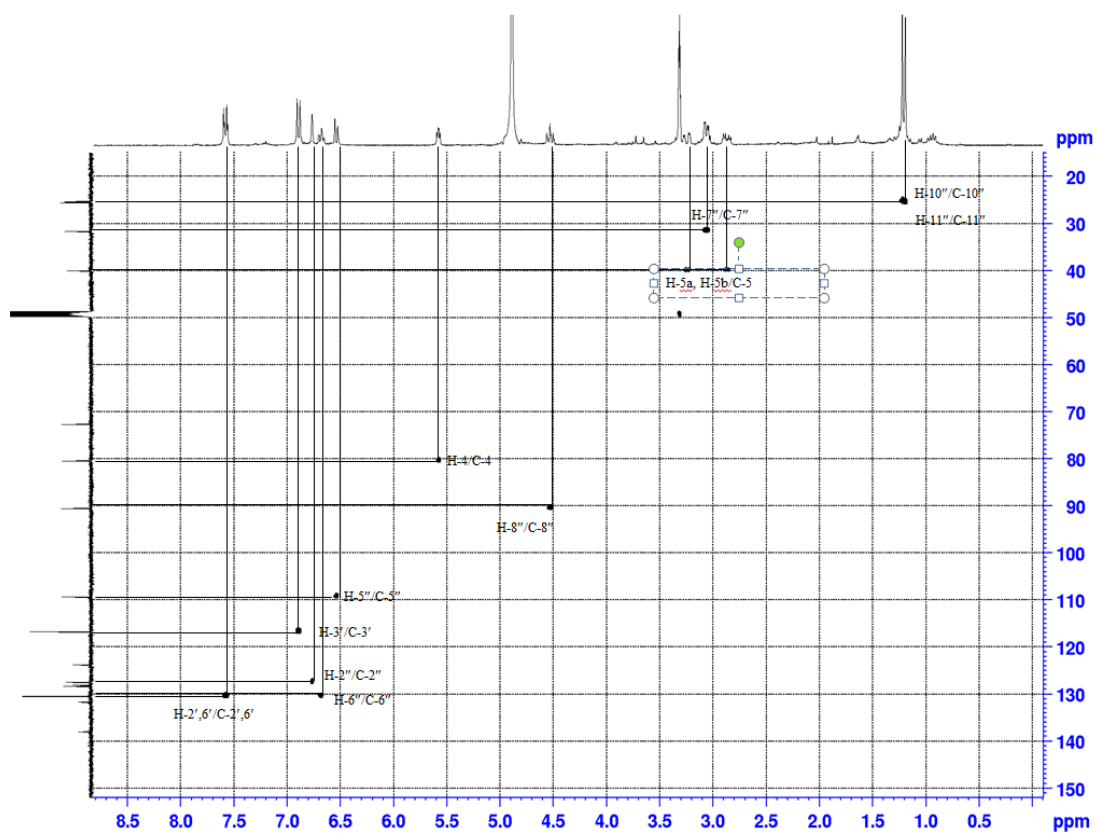


Figure S3:HSQC Spectrum of **1** in CD₃OD

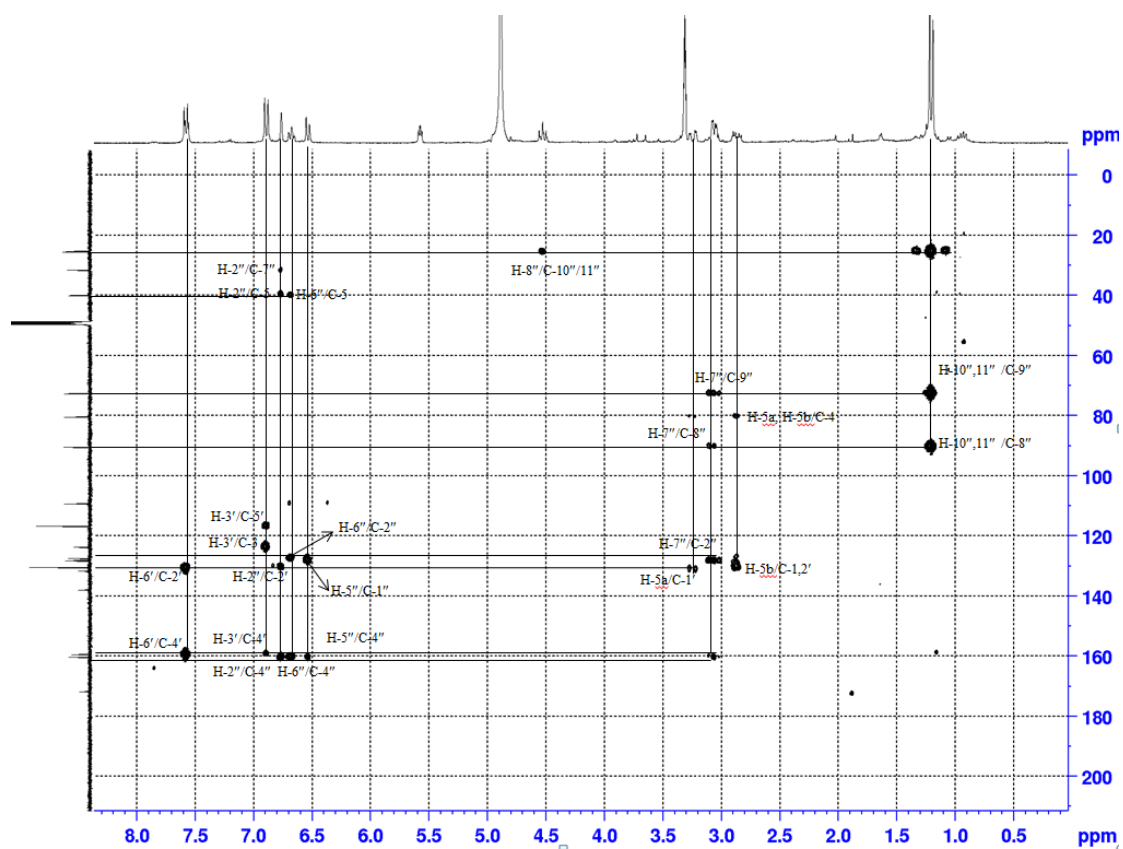


Figure S4:HMBC Spectrum of **1** in CD₃OD

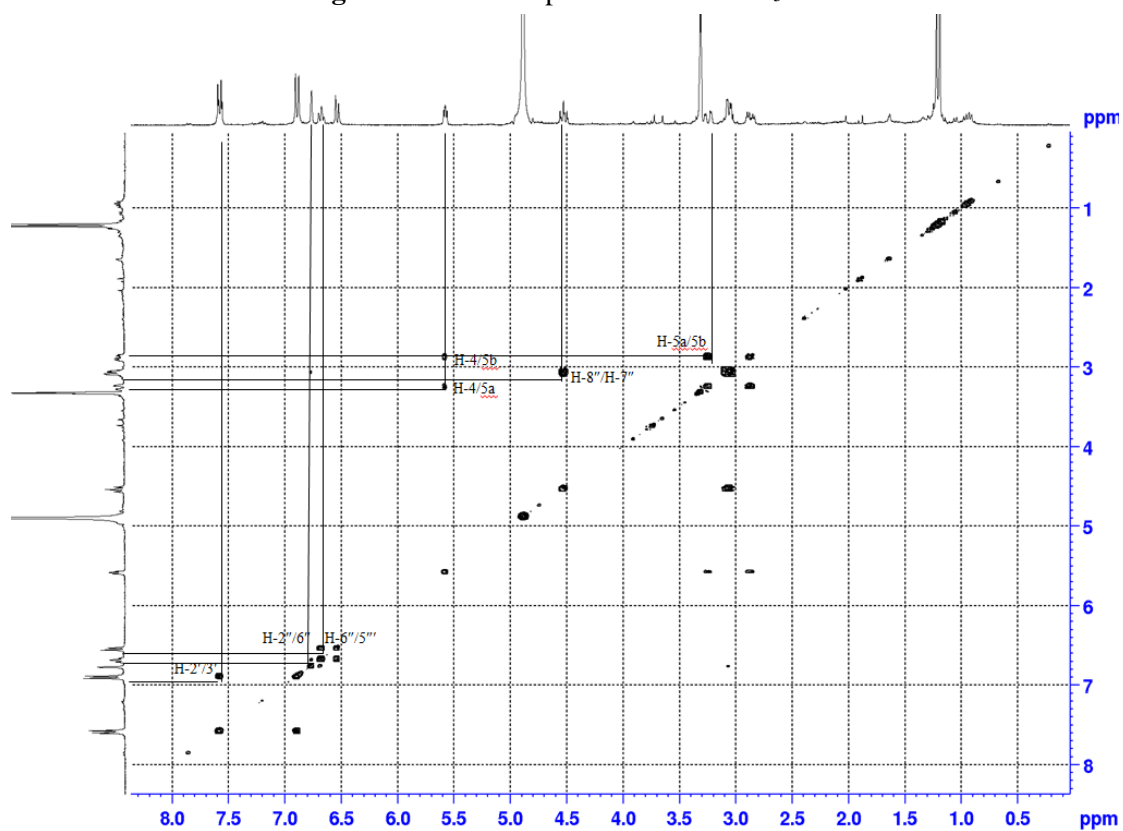


Figure S5:¹H-¹H COSY Spectrum of compound **1** in CD₃OD

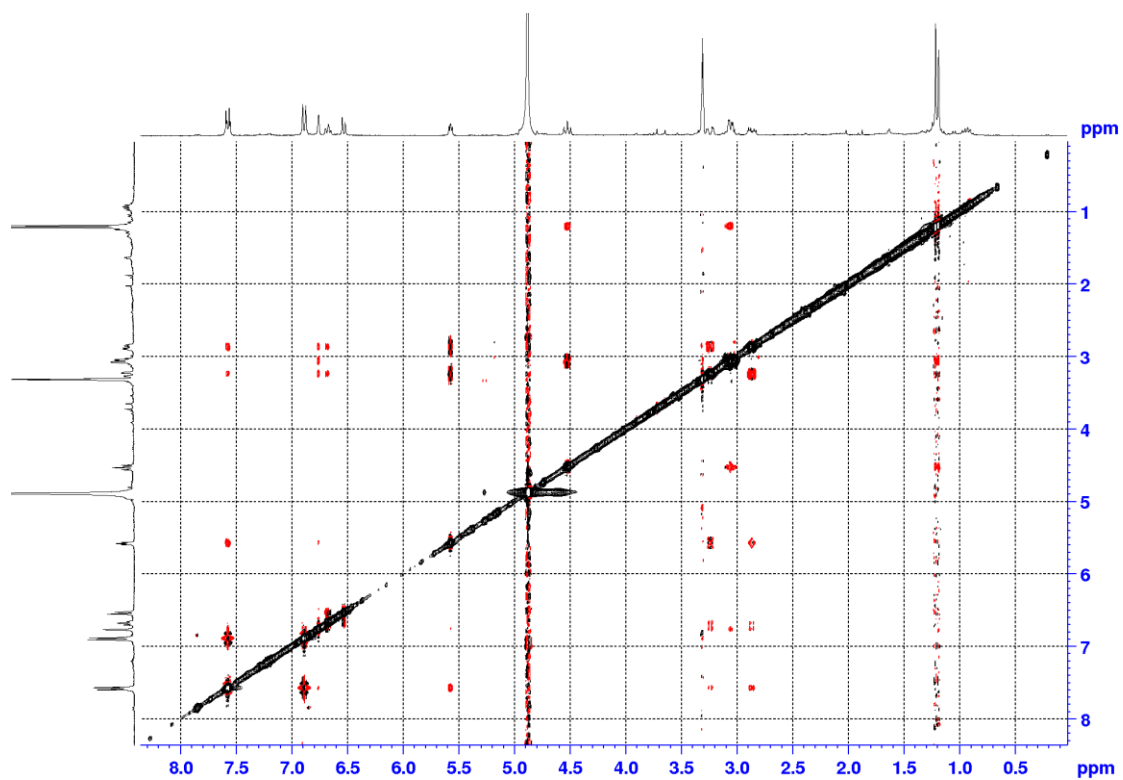


Figure S6:NOESY spectrum of compound **1** in CD₃OD

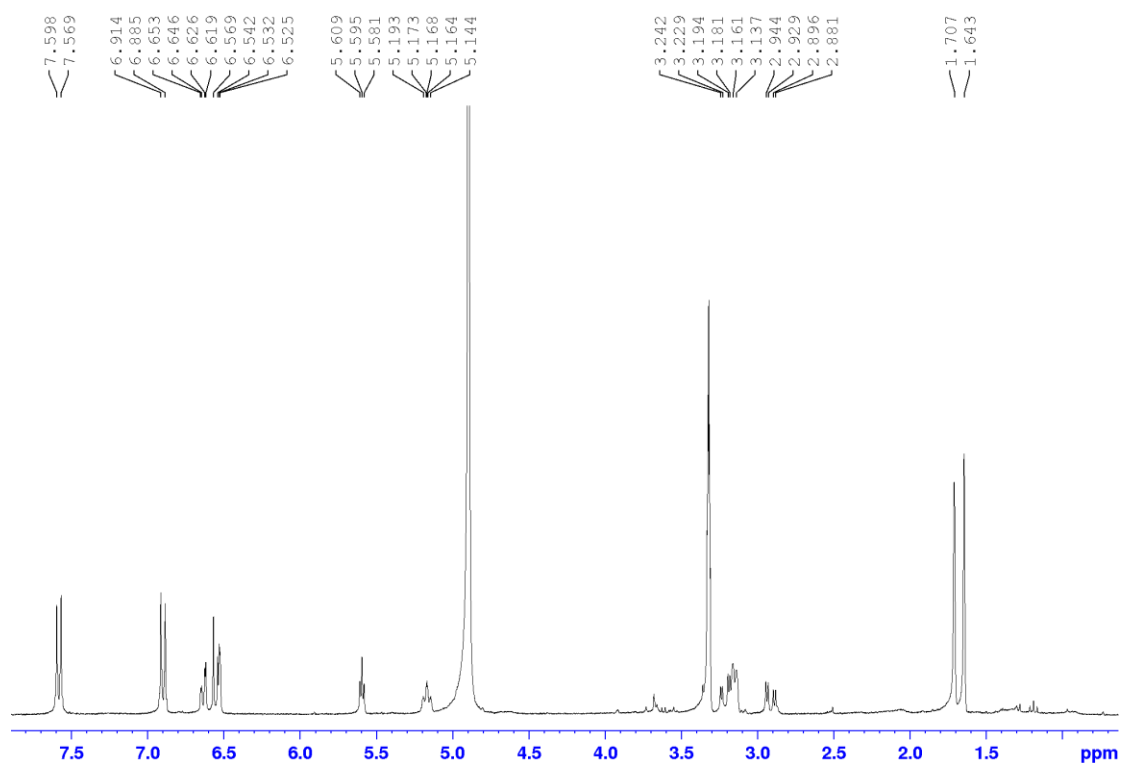


Figure S7:¹H NMR Spectrum of **2** in DMSO-*d*₄ (400 MHz)

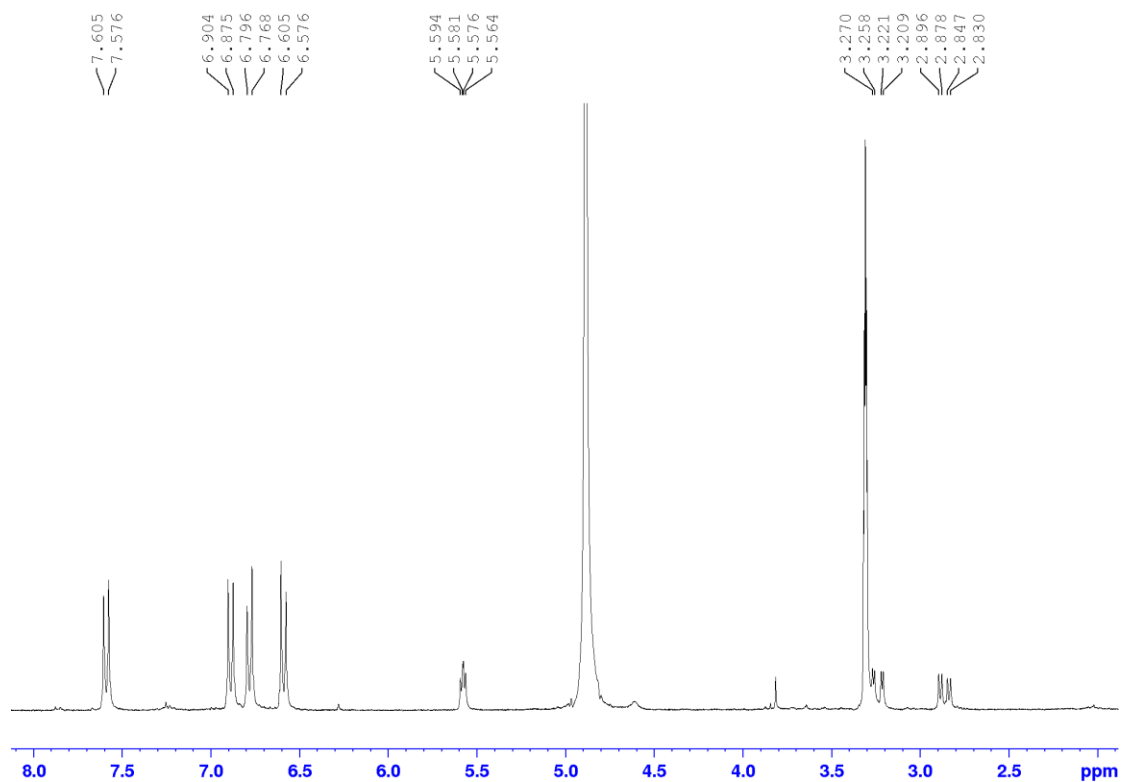


Figure S8: ^1H NMR Spectrum of **3** in CD_3OD (400 MHz)

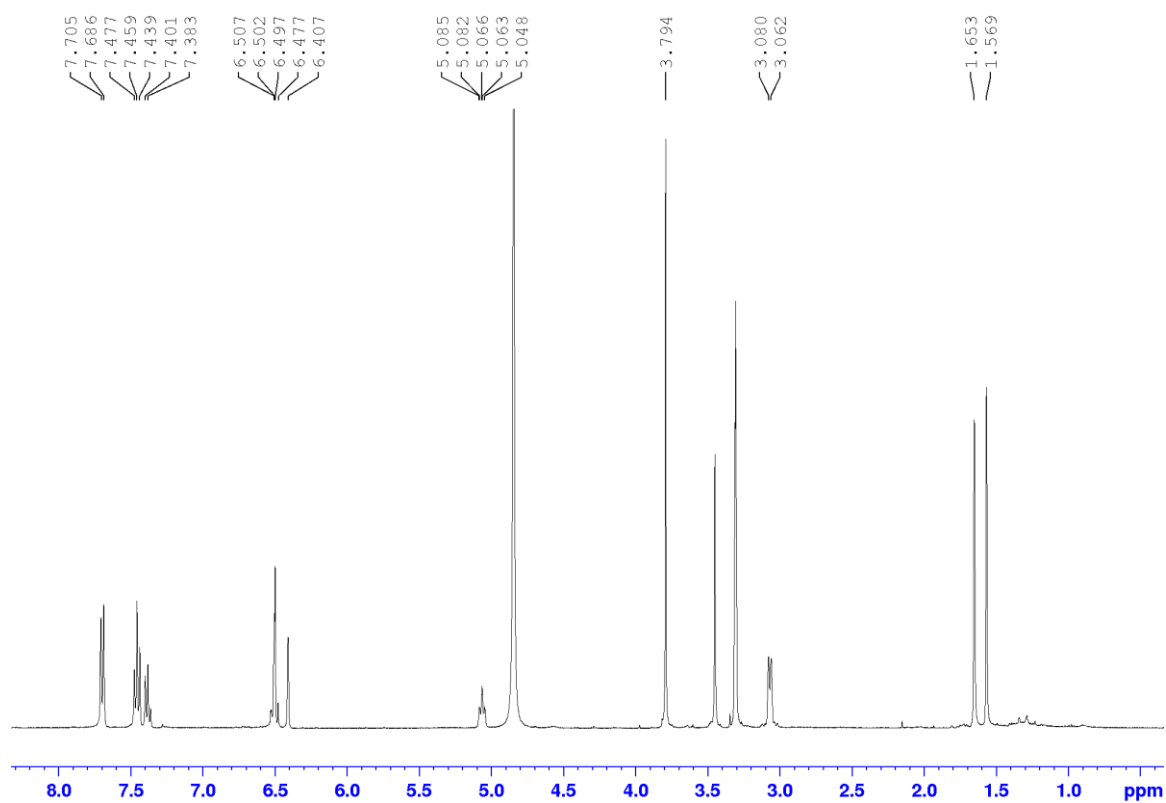


Figure S9: ^1H NMR Spectrum of **4** in CD_3OD (400 MHz)

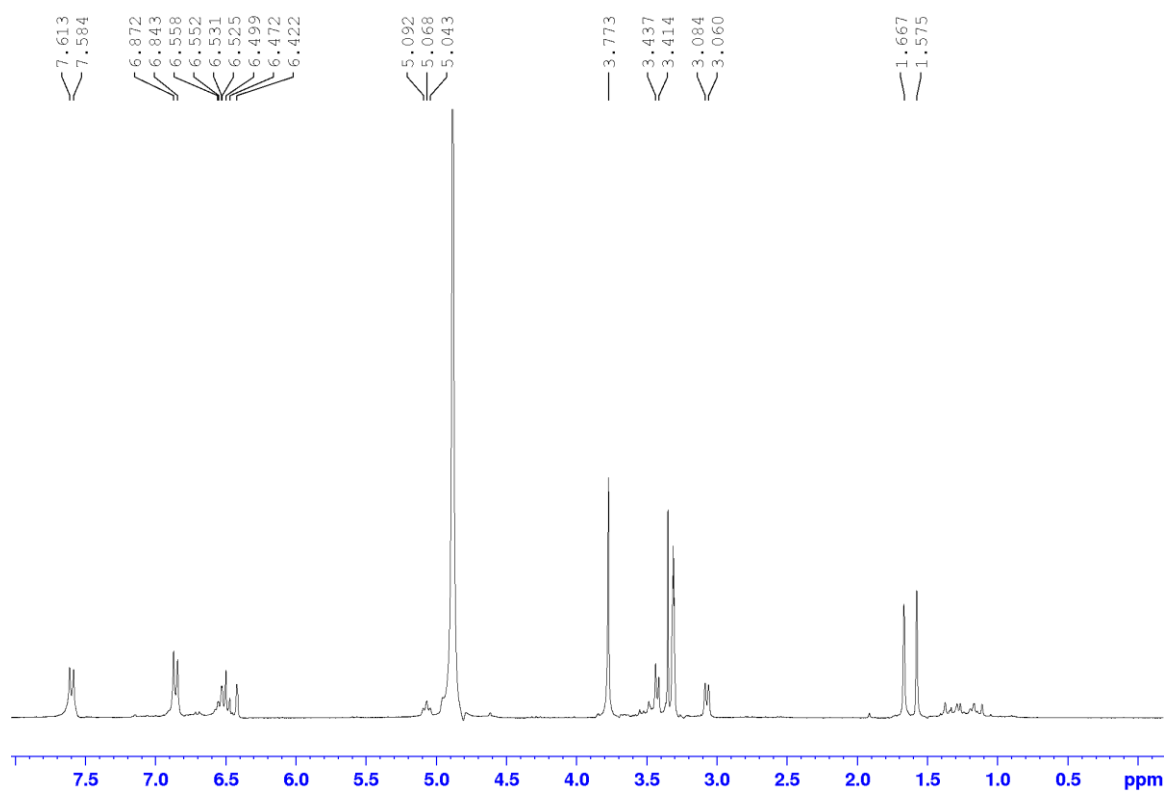


Figure S10: ^1H NMR Spectrum of **5** in in CD_3OD (400 MHz)

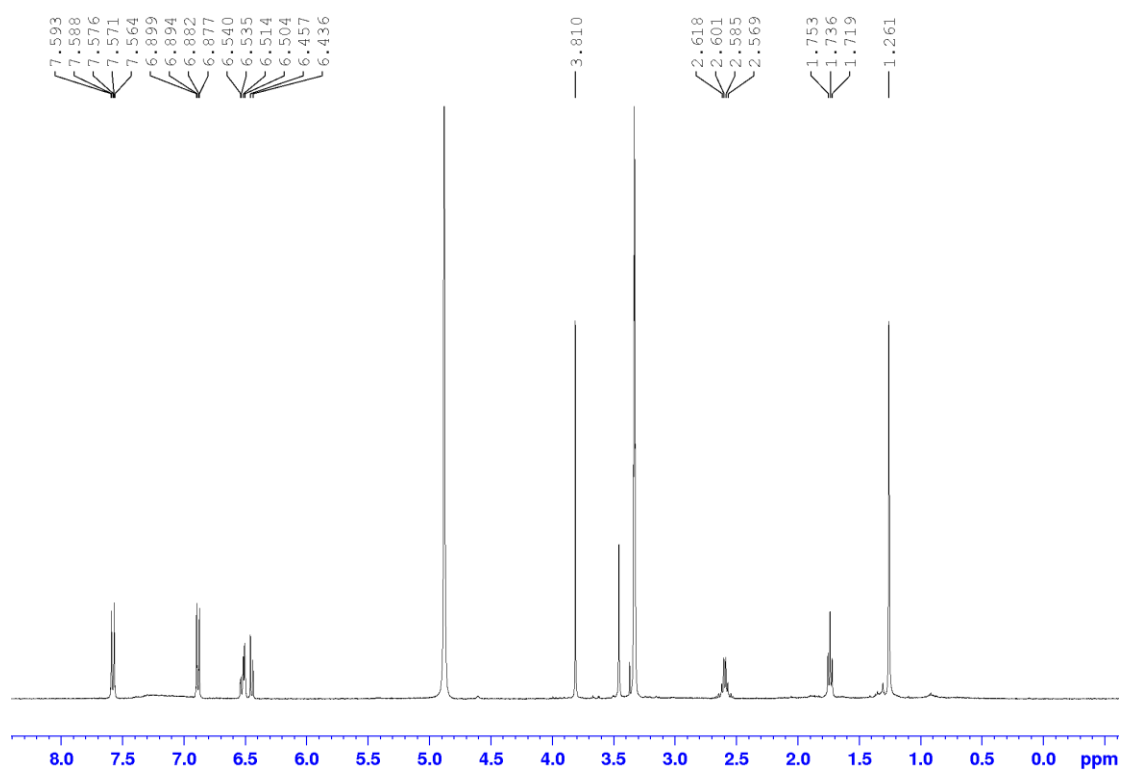


Figure S11: ^1H NMR Spectrum of **6** in CD_3OD (400 MHz)

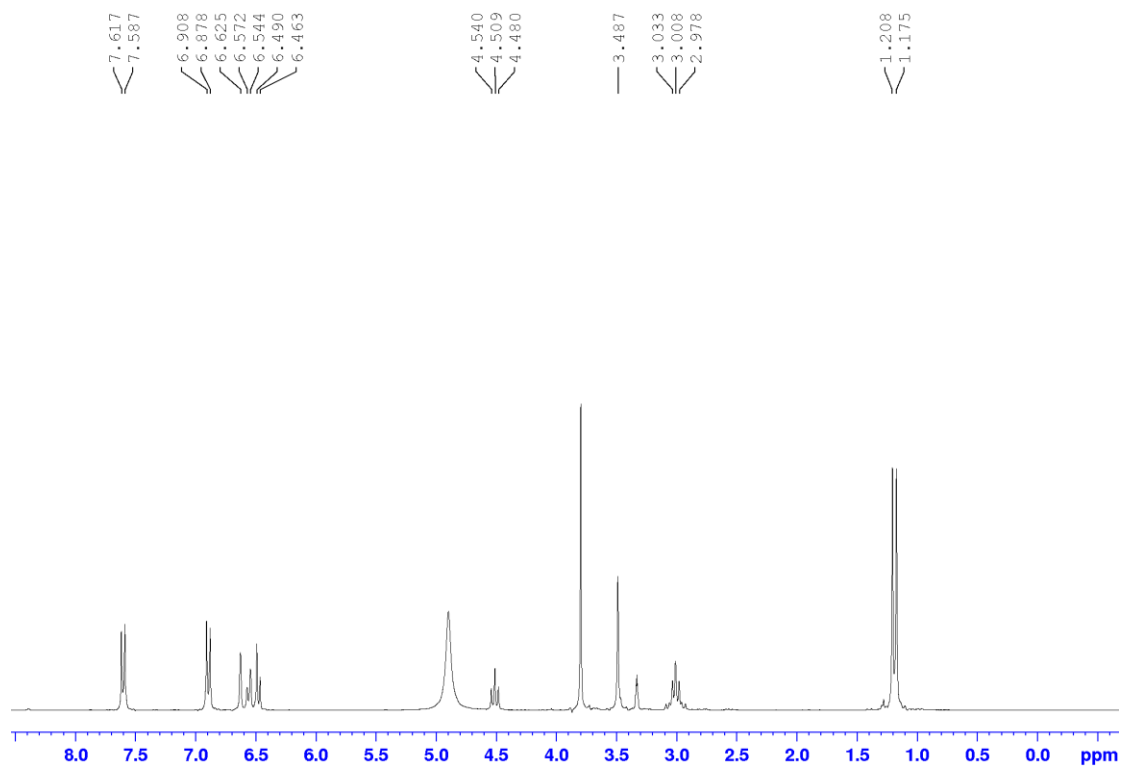


Figure S12: ^1H NMR Spectrum of **7** in CD_3OD (400 MHz).

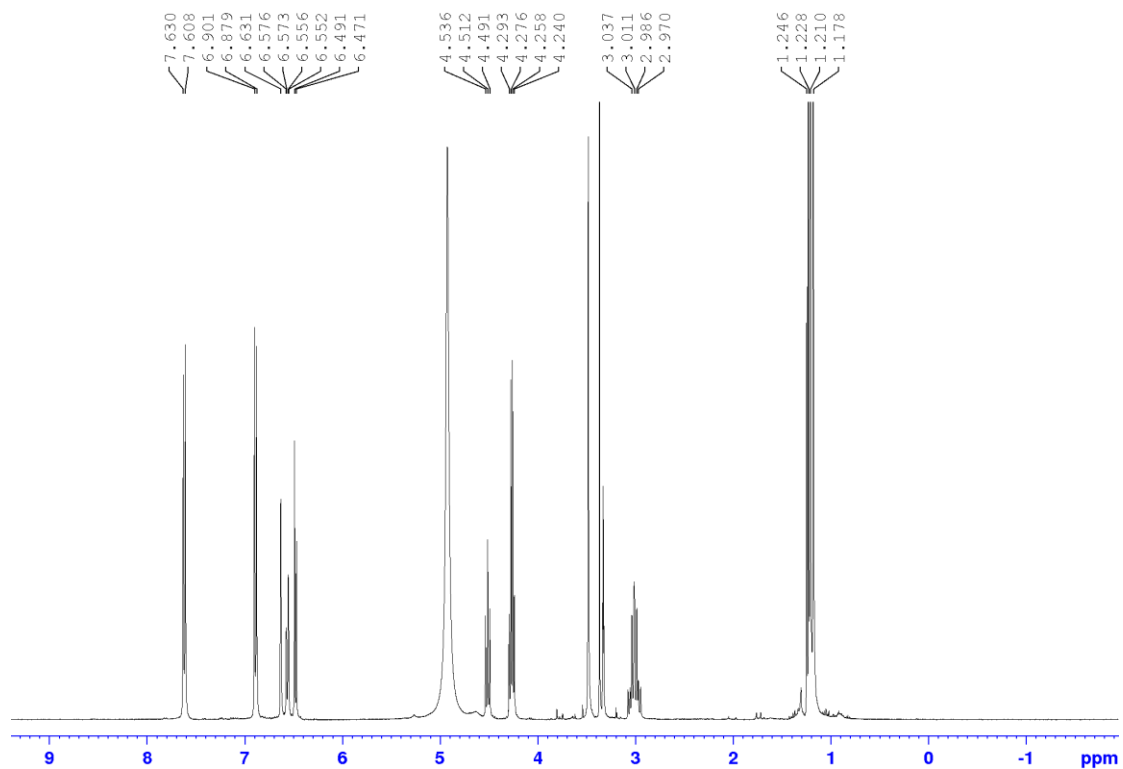


Figure S13: ^1H NMR Spectrum of **8** in CD_3OD (400 MHz).

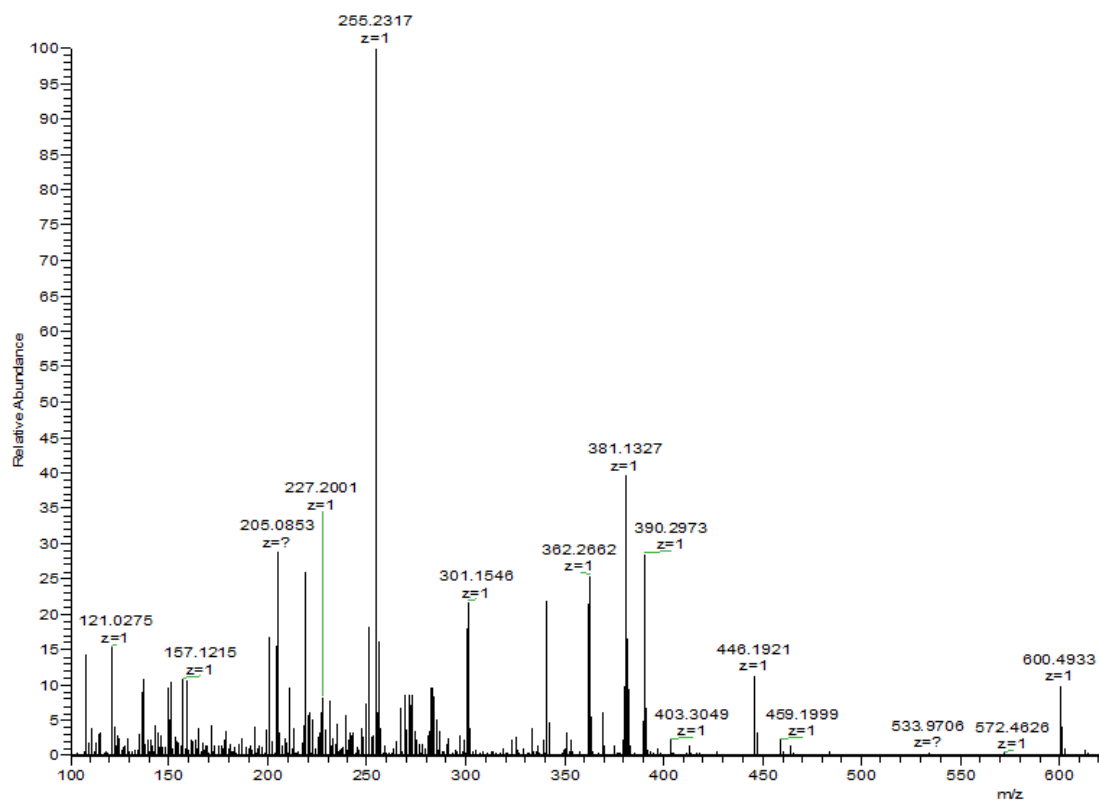


Figure S14: HRESIMS Spectrum of 1

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Analyze by: Substance Role

Biological Study 1

Occurrence 1

Reactant or Reagent 1

Uses 1

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Score: ≥ 99

1. 2376800-14-3

~2 ~1

Absolute stereochemistry, Currently available stereo shown.

C₂₂H₂₂O₆
 2(5H)-furanone, 5-[[2,3-dihydro-2-(1-hydroxy-1-methylethyl)-5-benzofuranyl]methyl]-3-hydroxy-4-(4-hydroxyphenyl)-, (5R)-
 ▶ Key Physical Properties

Chemical Structure similarity > substances (4) > get references (2)

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He Fei	1
Hu Zhengxi	1
Lai Yongji	1
Li Xiu Xiu	1
Liu Mengting	1
Qi Changxing	1

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0 of 2 References Selected

- Bioactive aromatic butenolides from a mangrove sediment originated fungal species, *Aspergillus terreus* SCAU011**

By Bao, Jie; Li, Xiu-Xiu; Zhu, Kongkai; He, Fei; Wang, Yin-Yin; Yu, Jin-Hai; Zheng, Xiaoyong; Zheng, Hua
 From *Phytochemistry* (2021), 155, 104895. | Language: English, Database: CAPLUS

Seven new comps. including five arom. butenolide analogs (1-5), one quinazolinone alkaloid (6) and one benzoic acid deriv. (7), along with eleven known co-metabolites (8-18), were isolated from *Aspergillus terreus* SCAU011, a fungus from the rhizosphere sediment of a mangrove plant *Rhizophora stylosa*. The structures of these isolates were established by a combination of MS, NMR and ECD data analyses, as well as chem. method. Compd. 3 is a rare ring-open arom. butenolide, while 6 represents the first natural ring-open benzoxalvin-type quinazolinone alkaloid. Also, the previously reported str...
- Butenolides from a marine-derived fungus *Aspergillus terreus* with antitumor activities against pancreatic ductal adenocarcinoma cells**

By Qi, Changxing; Gao, Wei; Guan, Danyingzi; Wang, Jiang; Liu, Mengting; Chen, Chunmei; Zhu, Hucheng; Zhou, Yuan; Lai, Yongji; Hu, Zhengxi; et al
 From *Biorganic & Medicinal Chemistry* (2018), 26(22), 5903-5910. | Language: English, Database: CAPLUS

Chem. study on the ext. of a marine-derived fungus *Aspergillus terreus* yielded twelve butenolide derivs., including three new comps., namely asperides A-C (1-3) and nine known butenolides (4-12). The structures of 1-3 were confirmed by comprehensive spectroscopic anal., including HRESIMS, NMR spectroscopy, and calcd. electronic CD (ECD). The cytotoxicity of the comps. was evaluated using PANC-1, HCC1806, HepG2, BEAS-2B and HT-29 cancer cells. The results showed that (+)-3',3''-di-(dimethylallyl)-butyrolactone II (4) and versicolactone B (6) exhibited the most potent cytotoxin of PANC-1 ce...

Chemical Structure similarity

SUBSTANCES Select All Deselect All

0 of 8 Similarity Candidates Selected

Similarity Range	Substances
≥ 99 (most similar)	1
95-98	0
90-94	3
85-89	2

Figure S15: Scifinder similarity report for compound 1.

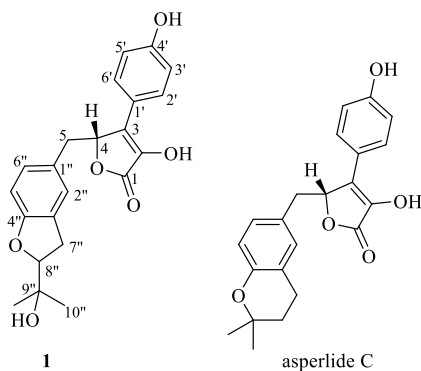


Table S1: The NMR data of **1** and the most similar analogue.

No.	1		asperlide C (1)	
	δ_{H}	δ_{C}	δ_{H}	δ_{C}
1		171.8		170.5
2		137.9		136.6
3		123.7		126.5
4	5.57, dd (3.6, 5.3)	80.3	5.52 m	78.9
5	3.24, dd (14.6, 3.6) 2.87, dd (14.6, 5.3)	39.8	3.16 m 2.79 m	38.3
1'		131.6		122.3
2'	7.58, d (8.7)	130.4	7.52 d (8.6)	128.9
3'	6.89, d (8.7)	116.6	6.85 d (8.7)	115.2
4'		159.3		157.9
5'	6.89, d (8.7)	116.6	6.85 d (8.7)	128.9
6'	7.58, d (8.7)	130.4	7.52 d (8.6)	126.5
1''		128.2		128.5
2''	6.76, d (1.6)	127.4	6.60 m	130.8
3''		128.0		119.3
4''		160.3		151.8
5''	6.54, d (8.0)	109.2	6.51 m	116.0
6''	6.69, d (8.0, 1.6)	130.4	6.66 m	128.5
7''	3.06, m	31.5	2.82 dd (5.1, 16.3) 2.57 dd (5.7, 16.7)	30.7
8''	4.52, dd (9.2, 8.7)	90.4	3.66 t (5.2)	69.1
9''		72.5		76.6
10''	1.19, s	25.3	1.25 s	24.5
11''	1.21, s	25.2	1.16 s	19.5