Supplementary Materials: 5-Hydroxycyclopenicillone, a New β-Amyloid Fibrillization Inhibitor from a Sponge-Derived Fungus *Trichoderma* sp. HPQJ-34

Fang Fang, Jiaying Zhao, Lijian Ding, Chunhui Huang, C. Benjamin Naman, Shan He, Bin Wu, Peng Zhu, Qijun Luo, William H. Gerwick, Xiaojun Yan, Qinwen Wang, Zaijun Zhang and Wei Cui

List of Supplementary Materials:

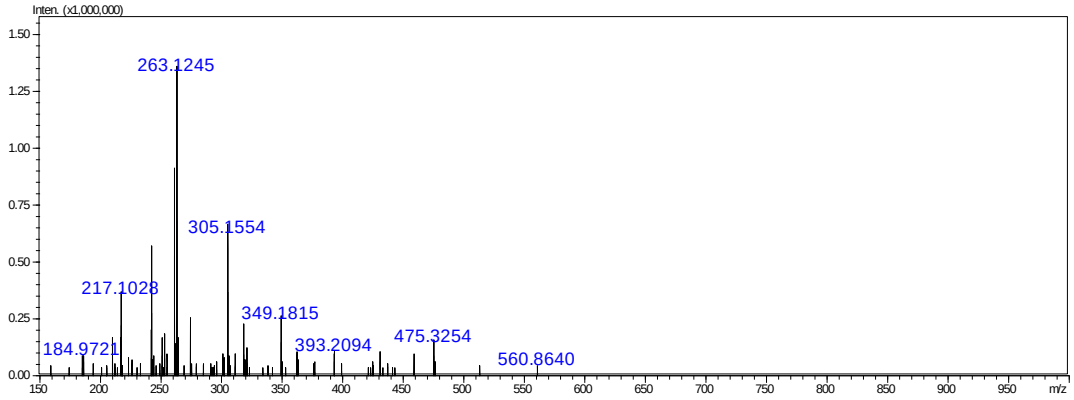

Figure S1. HRESIMS for compound **1**.

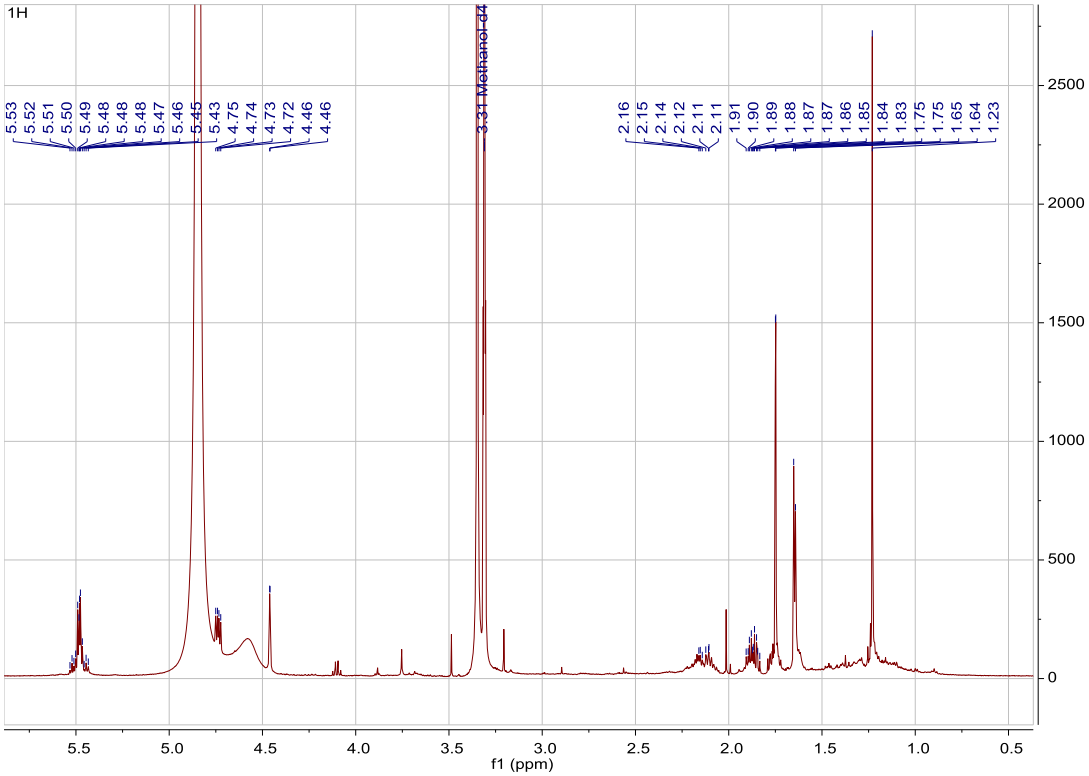

Figure S2. ^{1}H NMR spectrum (CD_3OD, 500 MHz) of compound **1**.

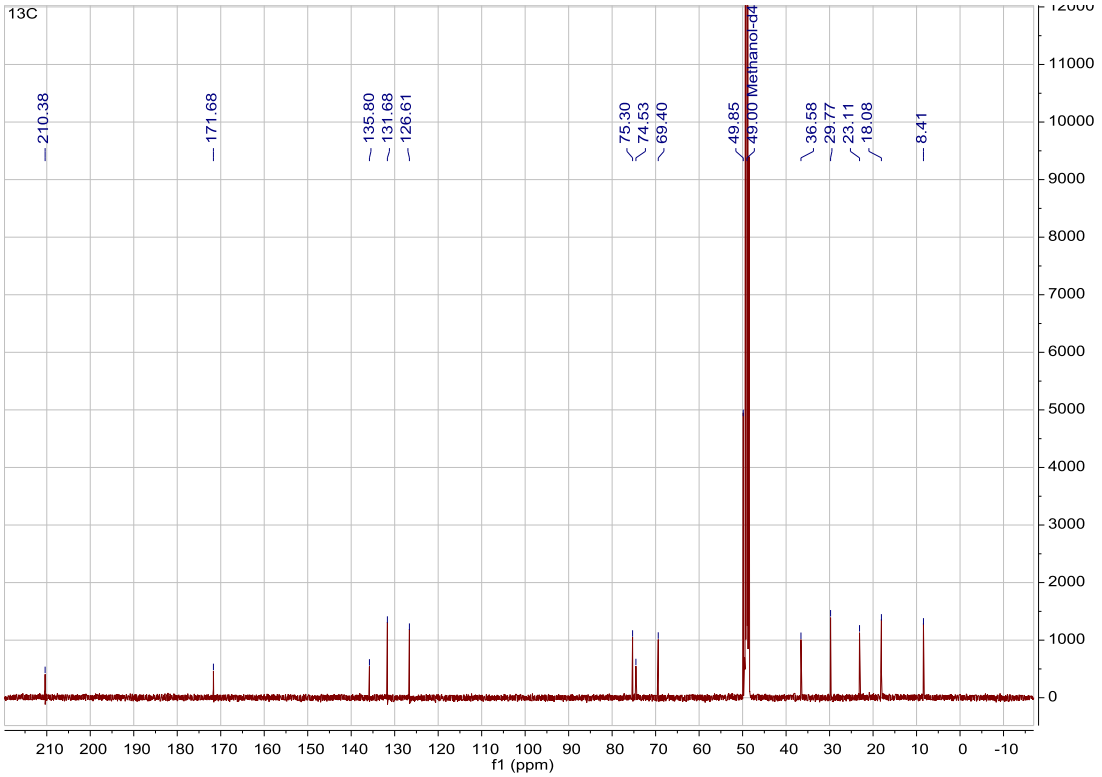

Figure S3. ^{13}C NMR spectrum (CD_3OD, 125 MHz) of compound **1**.

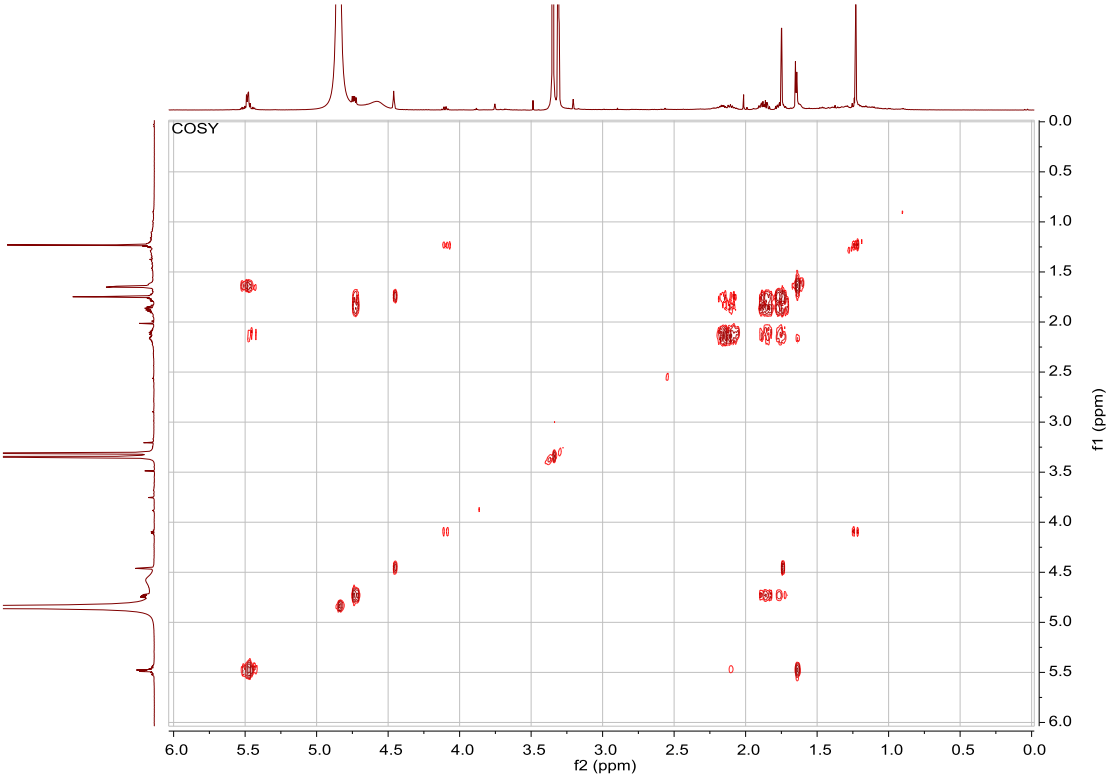

Figure S4. COSY spectrum (CD_3OD, 500 MHz) of compound **1**.

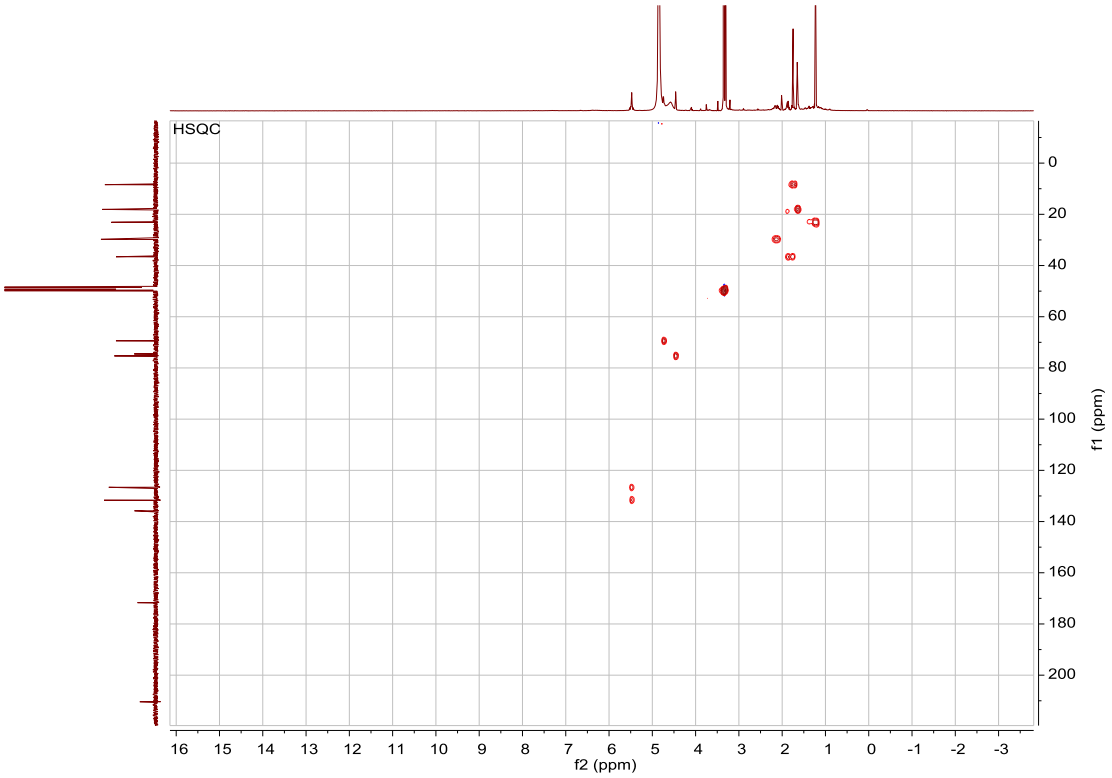

Figure S5. HSQC spectrum (CD_3OD, 500 MHz ^{1}H and 125 MHz ^{13}C) of compound **1**.

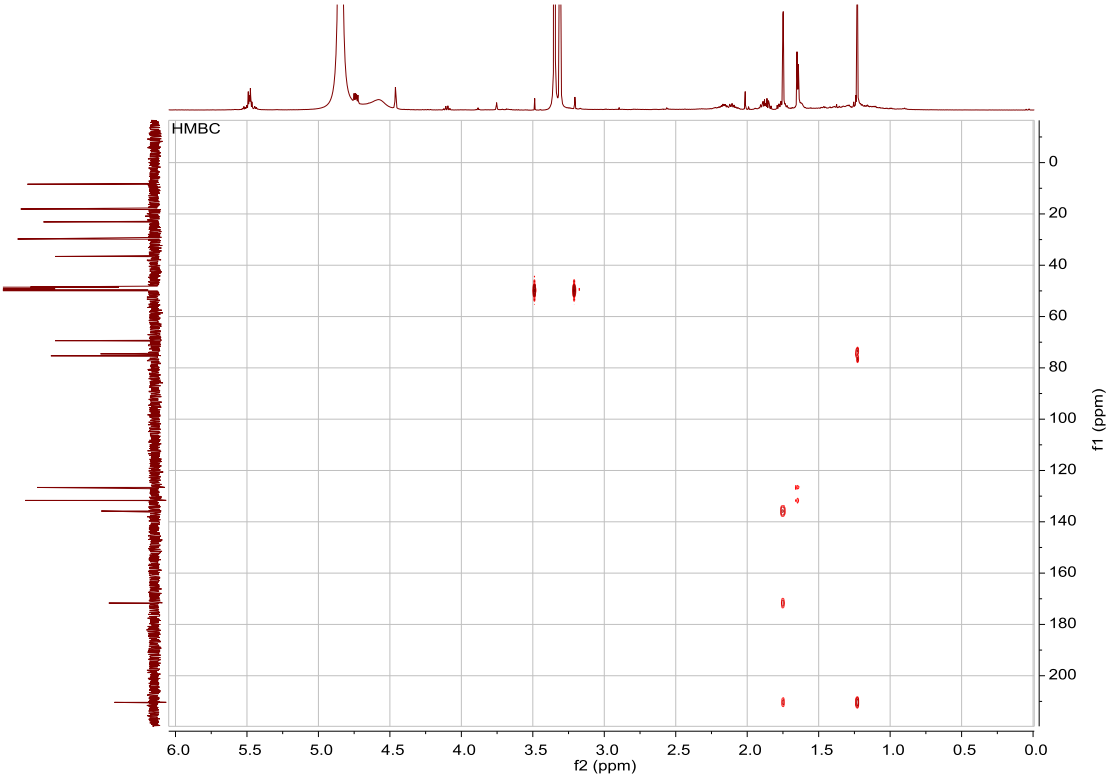

Figure S6. HMBC spectrum (CD_3OD, 500 MHz ^{1}H and 125 MHz ^{13}C) of compound **1**.

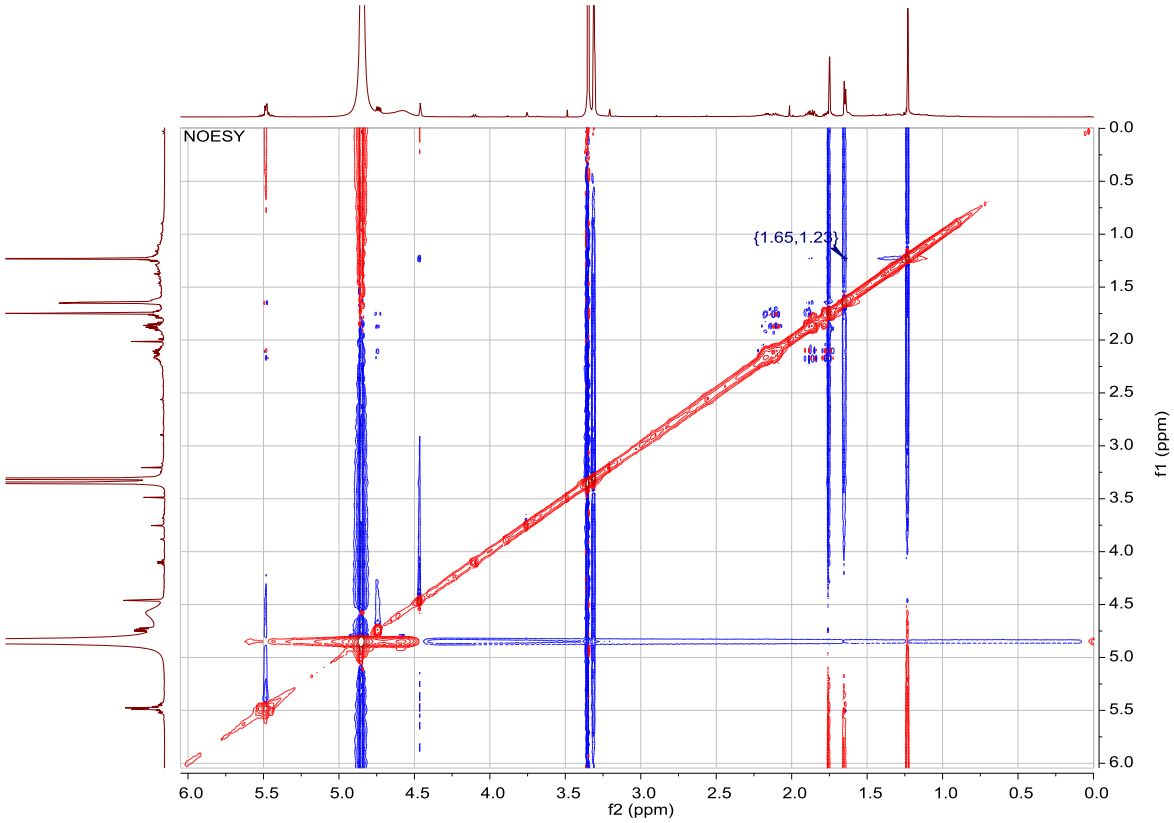

Figure S7. NOESY spectrum (CD_3OD, 500 MHz) of compound **1**.

Text S8. ITS rDNA gene sequence from strain HPQJ-34.

TCCGTAGGTGGAACCTGCGGAGGGATCATTACCGAGTTTACAACTCCCAAACCC
CAATGTGAACGTTACCAATCTGTTGCCTCGGCGGGATTCTCTTGCCCCGGGCGC
GTCGCAGCCCCGGATCCCATGGCGCCCGCCGGAGGACCAACTCCAAACTCTTTT
TTCTCTCCGTCGCGGCTCCCGTCGCGGCTCTGTTTTATTTTTGCTCTGAGCCTTTC
TCGGCGACCCTAGCGGGCGTCTCGAAAATGAATCAAAACTTTCAACAACGGATC
TCTTGGTTCTGGCATCGATGAAGAACGCAGCGAAATGCGATAAGTAATGTGAAT
TGCAGAATTCAGTGAATCATCGAATCTTTGAACGCACATTGCGCCCGCCAGTAT
TCTGGCGGGCATGCCTGTCCGAGCGTCATTTCAACCCTCGAACCCCTCCGGGGG
GTCGGCGTTGGGGATCGGCCCCTCACCGGGCCGCCCCCGAAATACAGTGGCGGT
CTCGCCGCAGCCTCTCATGCGCAGTAGTTTGCACACTCGCACCGGGAGCGCGGC
GCGGCCACAGCCGTAAAACACCCCAAATTTTCTGAAATGTTGACCTCGGATCAG
GTAGGAATACCCGCTGAACTTAAGCATATCAATAAGCGGAAGAA

Text S9. Computational molecular model coordinates for an energy minimized conformer of compound **1**.

HEADER
REMARK Spartan '10 exported M0001

HETATM	1	C	UNK	0001	-1.637	-1.053	0.131
HETATM	2	C	UNK	0001	-0.687	-0.037	-0.488
HETATM	3	C	UNK	0001	-1.230	1.170	-0.597
HETATM	4	C	UNK	0001	-2.600	1.142	-0.015
HETATM	5	C	UNK	0001	-2.773	-0.191	0.725
HETATM	6	O	UNK	0001	-3.403	2.017	-0.086
HETATM	7	C	UNK	0001	-0.694	2.436	-1.193
HETATM	8	O	UNK	0001	-2.193	-1.884	-0.854
HETATM	9	C	UNK	0001	-2.587	0.056	2.220
HETATM	10	C	UNK	0001	0.690	-0.465	-0.926
HETATM	11	C	UNK	0001	1.707	-0.333	0.213
HETATM	12	C	UNK	0001	3.132	-0.750	-0.181
HETATM	13	C	UNK	0001	4.099	-0.585	0.962
HETATM	14	O	UNK	0001	0.571	-1.806	-1.366
HETATM	15	C	UNK	0001	5.146	0.218	1.041
HETATM	16	C	UNK	0001	5.667	1.184	0.012
HETATM	17	H	UNK	0001	-1.148	-1.658	0.887
HETATM	18	H	UNK	0001	0.229	2.281	-1.740
HETATM	19	H	UNK	0001	-1.429	2.863	-1.866
HETATM	20	H	UNK	0001	-0.509	3.173	-0.418
HETATM	21	H	UNK	0001	-1.484	-2.303	-1.327
HETATM	22	H	UNK	0001	-3.353	0.738	2.567
HETATM	23	H	UNK	0001	-2.690	-0.881	2.754
HETATM	24	H	UNK	0001	-1.614	0.483	2.439
HETATM	25	H	UNK	0001	1.009	0.153	-1.760
HETATM	26	H	UNK	0001	1.718	0.702	0.541
HETATM	27	H	UNK	0001	1.371	-0.931	1.055
HETATM	28	H	UNK	0001	3.133	-1.798	-0.475
HETATM	29	H	UNK	0001	3.451	-0.179	-1.047
HETATM	30	H	UNK	0001	3.886	-1.208	1.818
HETATM	31	H	UNK	0001	1.364	-2.080	-1.806
HETATM	32	H	UNK	0001	5.716	0.192	1.956
HETATM	33	H	UNK	0001	6.685	0.927	-0.268
HETATM	34	H	UNK	0001	5.070	1.210	-0.890
HETATM	35	H	UNK	0001	5.696	2.191	0.421
HETATM	36	O	UNK	0001	-4.031	-0.751	0.557

```
HETATM   37  H    UNK  0001       -4.044  -1.232  -0.261
CONECT    1   17    2    5    8
CONECT    2    1    3   10
CONECT    3    2    4    7
CONECT    4    3    5    6
CONECT    5    4    1    9   36
CONECT    6    4
CONECT    7    3   18   19   20
CONECT    8    1   21
CONECT    9    5   22   23   24
CONECT   10    2   11   14   25
CONECT   11   10   12   26   27
CONECT   12   11   13   28   29
CONECT   13   12   15   30
CONECT   14   10   31
CONECT   15   13   16   32
CONECT   16   15   33   34   35
CONECT   17    1
CONECT   18    7
CONECT   19    7
CONECT   20    7
CONECT   21    8
CONECT   22    9
CONECT   23    9
CONECT   24    9
CONECT   25   10
CONECT   26   11
CONECT   27   11
CONECT   28   12
CONECT   29   12
CONECT   30   13
CONECT   31   14
CONECT   32   15
CONECT   33   16
CONECT   34   16
CONECT   35   16
CONECT   36   37    5
CONECT   37   36
END
```

Text S10. Computational molecular model coordinates for an energy minimized conformer of compound **5**.

HEADER
REMARK Spartan '10 exported M0001

HETATM	1	C	UNK	0001	-1.879	-1.202	0.182
HETATM	2	C	UNK	0001	-0.933	-0.161	-0.408
HETATM	3	C	UNK	0001	-1.443	1.067	-0.395
HETATM	4	C	UNK	0001	-2.783	1.036	0.240
HETATM	5	C	UNK	0001	-3.124	-0.403	0.589
HETATM	6	O	UNK	0001	-3.467	1.989	0.459
HETATM	7	C	UNK	0001	-0.868	2.370	-0.866
HETATM	8	O	UNK	0001	-2.252	-2.186	-0.741
HETATM	9	C	UNK	0001	-3.551	-0.554	2.049
HETATM	10	C	UNK	0001	0.456	-0.536	-0.868
HETATM	11	C	UNK	0001	1.495	-0.240	0.222
HETATM	12	C	UNK	0001	2.935	-0.575	-0.192
HETATM	13	C	UNK	0001	3.920	-0.255	0.902
HETATM	14	O	UNK	0001	0.446	-1.912	-1.198
HETATM	15	C	UNK	0001	4.901	0.632	0.889
HETATM	16	C	UNK	0001	5.310	1.561	-0.221
HETATM	17	H	UNK	0001	-1.413	-1.669	1.048
HETATM	18	H	UNK	0001	-3.938	-0.713	-0.058
HETATM	19	H	UNK	0001	0.037	2.238	-1.448
HETATM	20	H	UNK	0001	-1.595	2.896	-1.473
HETATM	21	H	UNK	0001	-0.638	3.012	-0.021
HETATM	22	H	UNK	0001	-1.463	-2.594	-1.074
HETATM	23	H	UNK	0001	-4.402	0.082	2.258
HETATM	24	H	UNK	0001	-3.826	-1.581	2.261
HETATM	25	H	UNK	0001	-2.749	-0.272	2.725
HETATM	26	H	UNK	0001	0.701	0.038	-1.757
HETATM	27	H	UNK	0001	1.436	0.812	0.480
HETATM	28	H	UNK	0001	1.230	-0.801	1.114
HETATM	29	H	UNK	0001	3.011	-1.639	-0.412
HETATM	30	H	UNK	0001	3.183	-0.046	-1.106
HETATM	31	H	UNK	0001	3.784	-0.829	1.805
HETATM	32	H	UNK	0001	1.235	-2.141	-1.668
HETATM	33	H	UNK	0001	5.498	0.715	1.783
HETATM	34	H	UNK	0001	6.337	1.367	-0.519
HETATM	35	H	UNK	0001	4.687	1.475	-1.102
HETATM	36	H	UNK	0001	5.269	2.593	0.116

```
CONECT    1   17    2    5    8
CONECT    2    1    3   10
CONECT    3    2    4    7
CONECT    4    3    5    6
CONECT    5    4    1    9   18
CONECT    6    4
CONECT    7    3   19   20   21
CONECT    8    1   22
CONECT    9    5   23   24   25
CONECT   10    2   11   14   26
CONECT   11   10   12   27   28
CONECT   12   11   13   29   30
CONECT   13   12   15   31
CONECT   14   10   32
CONECT   15   13   16   33
CONECT   16   15   34   35   36
CONECT   17    1
CONECT   18    5
CONECT   19    7
CONECT   20    7
CONECT   21    7
CONECT   22    8
CONECT   23    9
CONECT   24    9
CONECT   25    9
CONECT   26   10
CONECT   27   11
CONECT   28   11
CONECT   29   12
CONECT   30   12
CONECT   31   13
CONECT   32   14
CONECT   33   15
CONECT   34   16
CONECT   35   16
CONECT   36   16
END
```

Table S11. Comparison of the NMR data of compound **1**[a] and **5**[b]

Position	δ_C, type.	δ_H, mult. (*J* in Hz)	δ_C, type.	δ_H, mult. (*J* in Hz)
	1		**5**	
1	210.4, C		210.3, C	
2	135.8, C		136.4, C	
3	171.7, C		173.5, C	
4	75.3, CH	4.49, d (1.0)	77.6, CH	4.46, br s
5	74.5, C		50.9, CH	2.18, q (7.8)
6	8.4, CH_3	1.75, d (1.0)	8.3, CH_3	1.73, br s
7	23.1, CH_3	1.23, s	13.8, CH_3	1.16, d (7.8)
1′	69.4, CH	4.72, dd (8.6, 4.8)	69.7, CH	4.75, dd (8.4, 4.2)
2′	36.6, CH_2	1.86, dtd (14.2, 8.6, 5.5), 1.76, m	36.9, CH_2	1.85, m, 1.64, m
3′	29.8, CH_2	2.12, m	29.8, CH_2	2.18, m, 2.10 m
4′	131.6, CH	5.49, m	131.7, CH	5.49, m
5′	126.7, CH	5.48, m	126.6, CH	5.48, m
6′	18.1, CH_3	1.64, d (4.8)	18.1, CH_3	1.63, d (6.6)

[a] Isolated in this study; "NMR spectra were obtained at 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR on a Bruker AVANCE-500 spectrometer. Chemical shifts (δ) are referenced to the residual solvent peaks of CD_3OD (δ_H 3.31 and δ_C 49.0) and given in ppm".

[b] Not isolated in this study; "… in CD_3OD. Data were recorded on a Bruker Avance 600 spectrometer; chemical shifts (δ) are given in parts per million with references to the center peak of CD_3OD with δ 3.30 for ^1H and δ 49.0 for ^{13}C." from manuscript reference 19 [Lin, S.; Shi, T.; Chen, K. Y.; Zhang, Z. X.; Shan, L.; Shen, Y. H.; Zhang, W. D. Cyclopenicillone, a unique cyclopentenone from the cultures of *Penicillium decumbens*. *Chem. Commun.* **2011**, *47*, 10413–10418.].