Supplementary Files

Citrinin Monomer and Dimer Derivatives with Antibacterial and Cytotoxic Activities Isolated from the Deep Sea-Derived Fungus *Penicillium citrinum* NLG-S01-P1

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Content

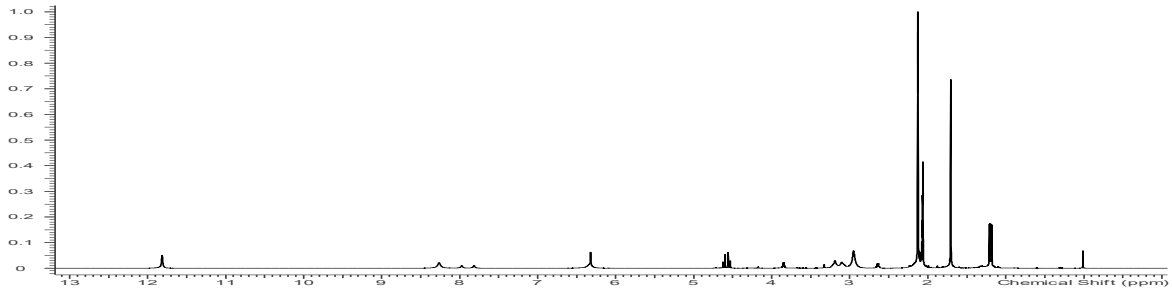


Figure S1. ^{1}H NMR spectrum of compound **1**

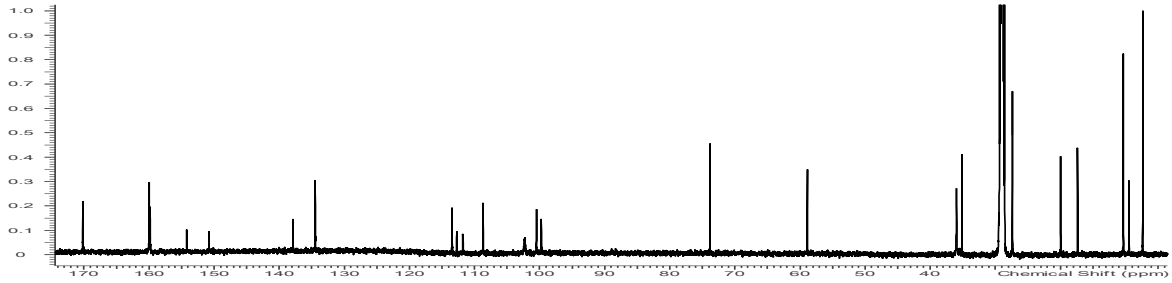


Figure S2. ^{13}C NMR spectrum of compound **1**

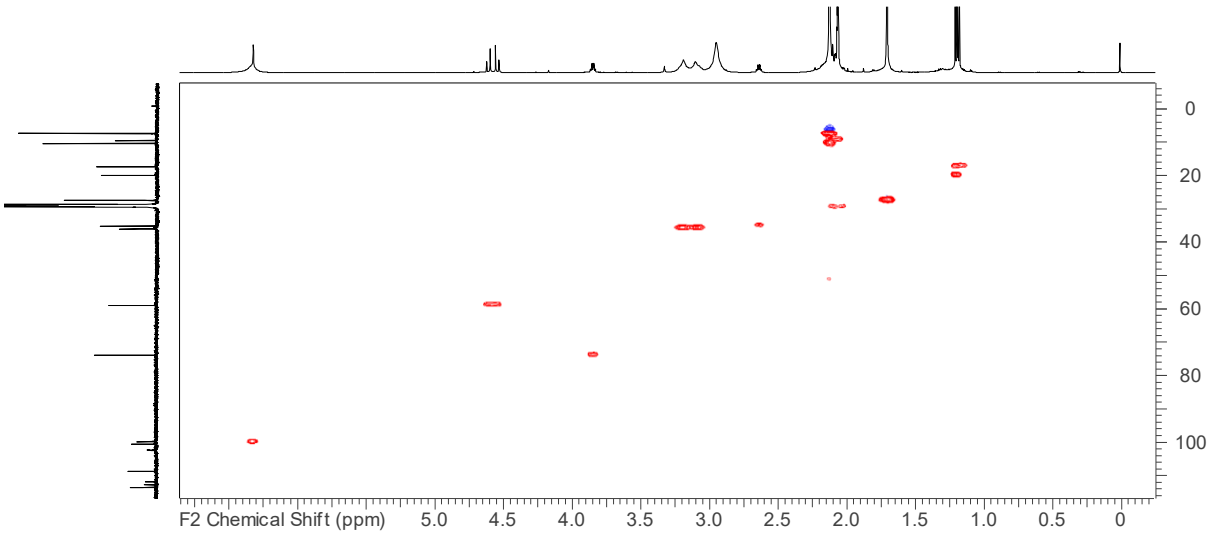


Figure S3. HSQC spectrum of compound **1**

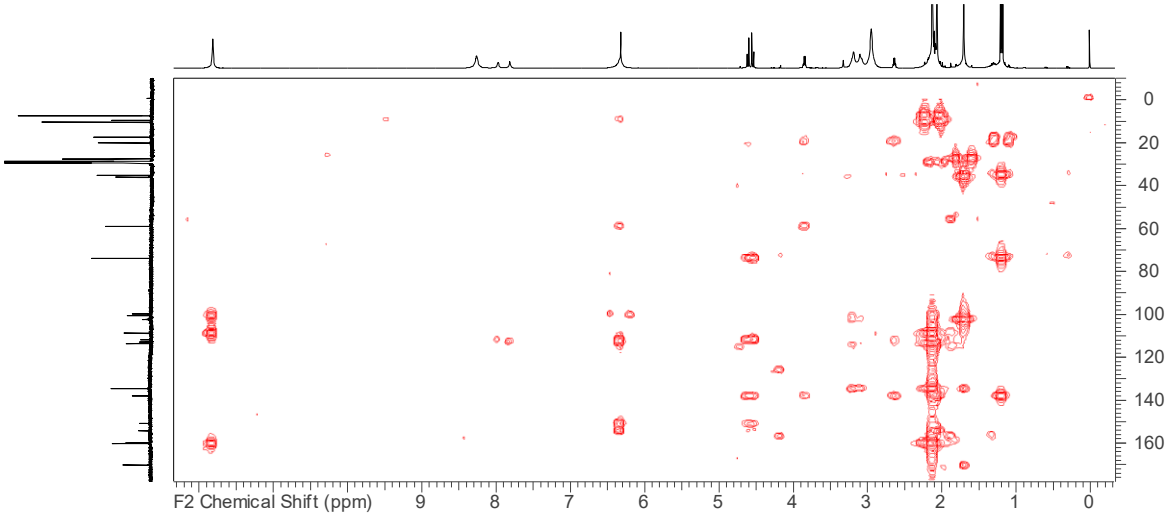
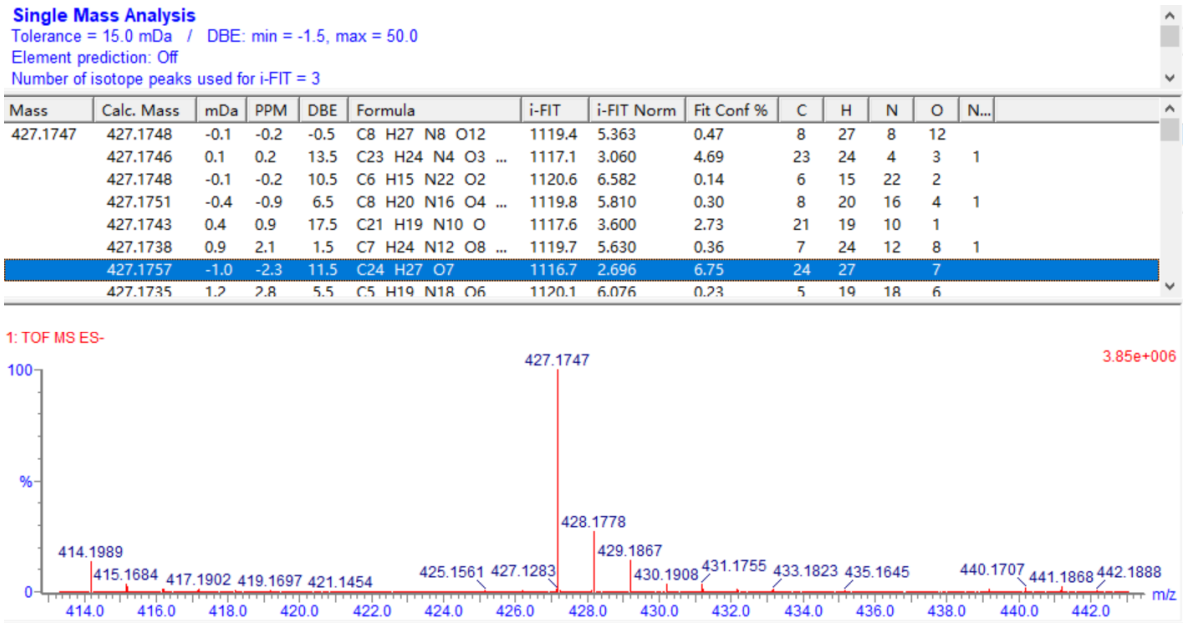


Figure S4. HMBC spectrum of compound **1**



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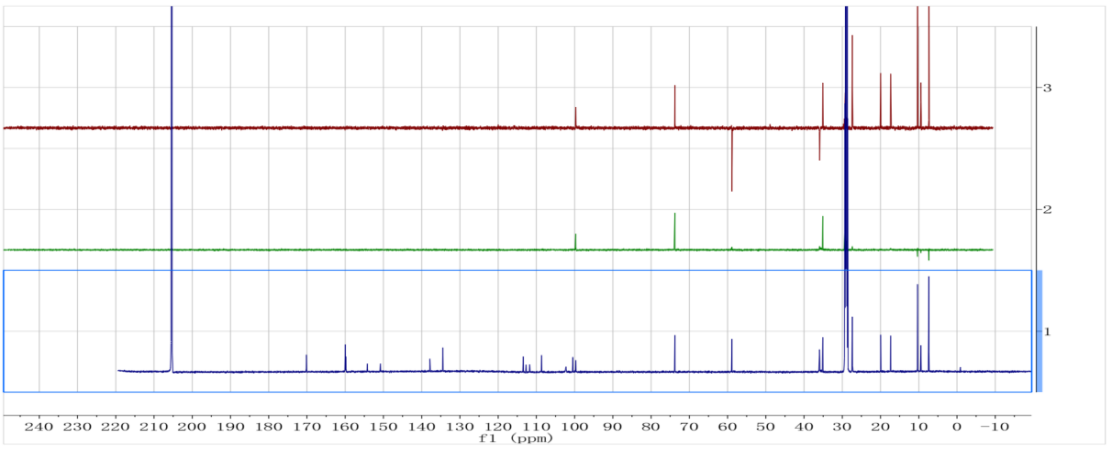


Figure S6. ^{13}C/DEPT spectrum of compound **1**

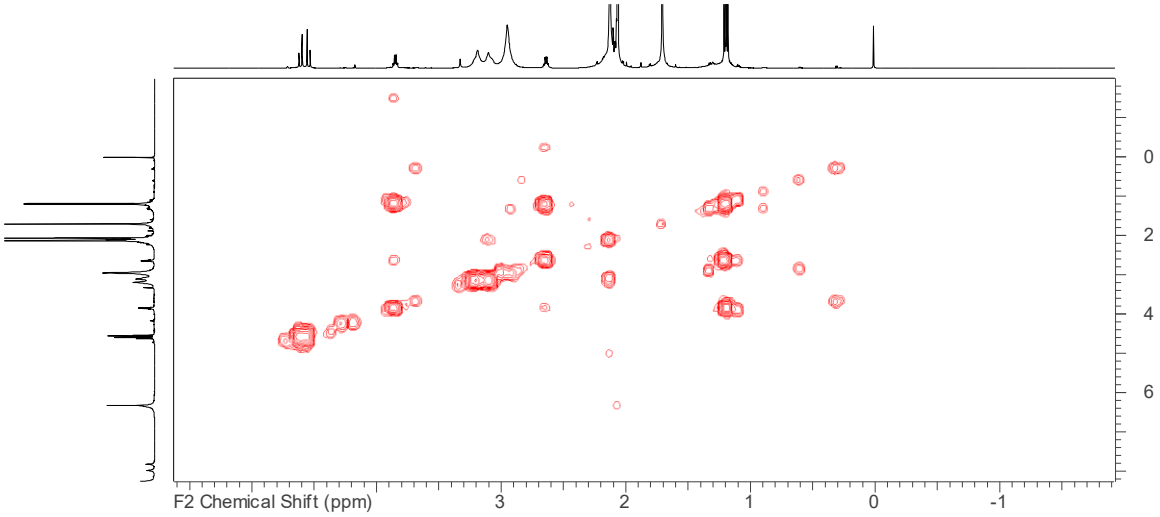


Figure S7. ^{1}H-^{1}H COSY spectrum of compound **1**

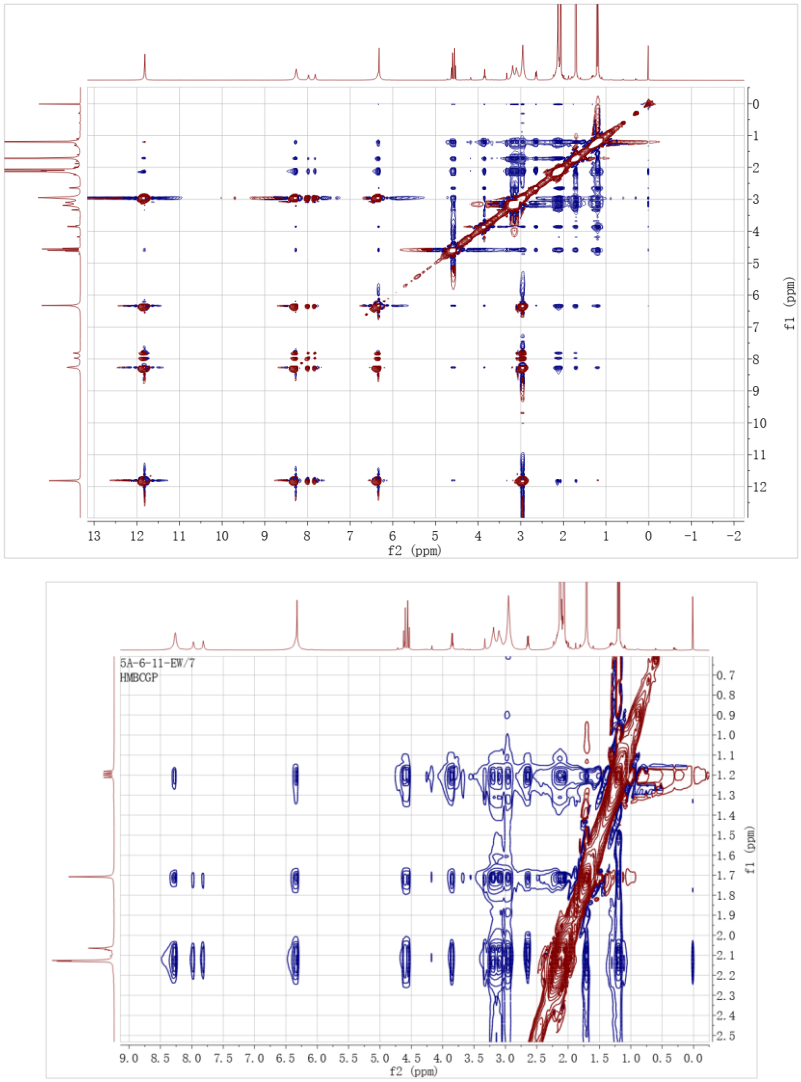


Figure S8. NOESY spectrum of compound **1**

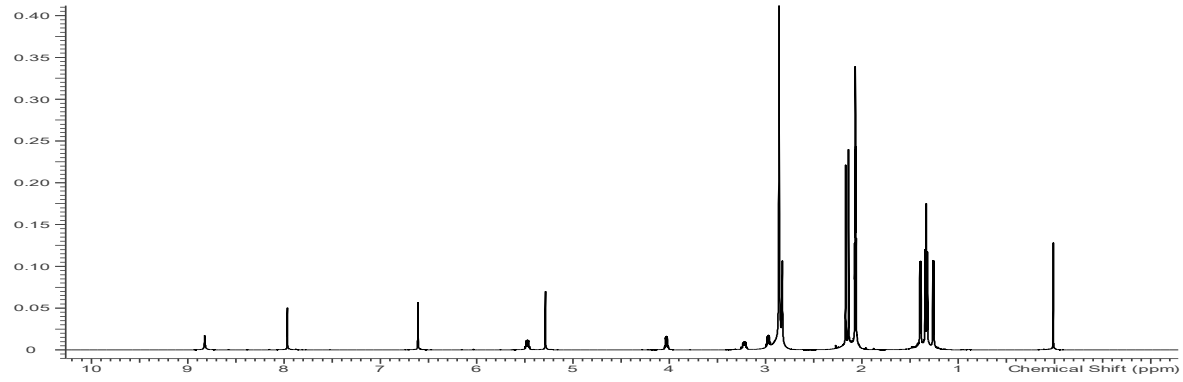
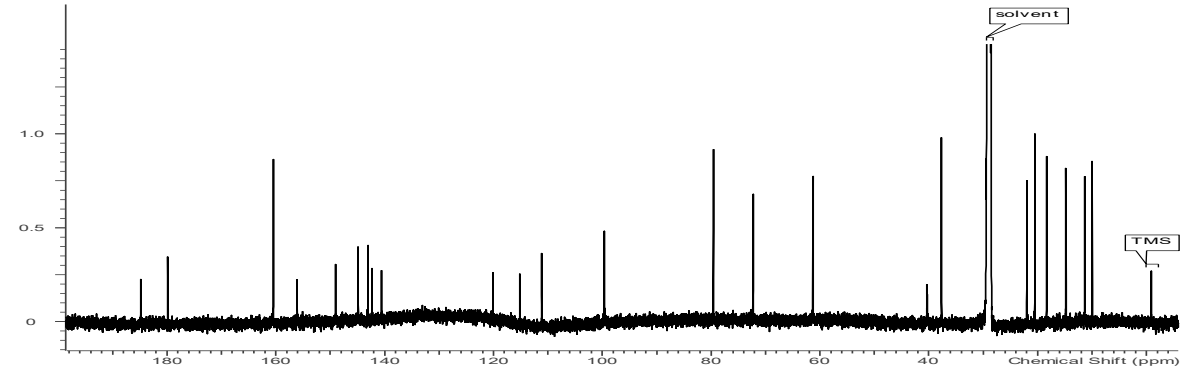


Figure S9. ^{1}H NMR spectrum of compound **2**



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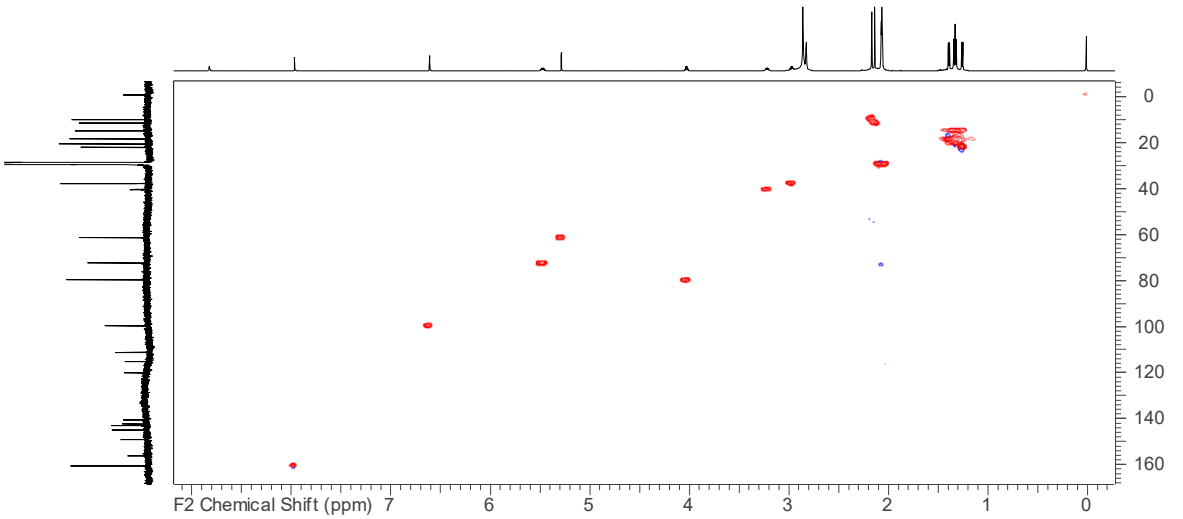


Figure S11. HSQC spectrum of compound **2**

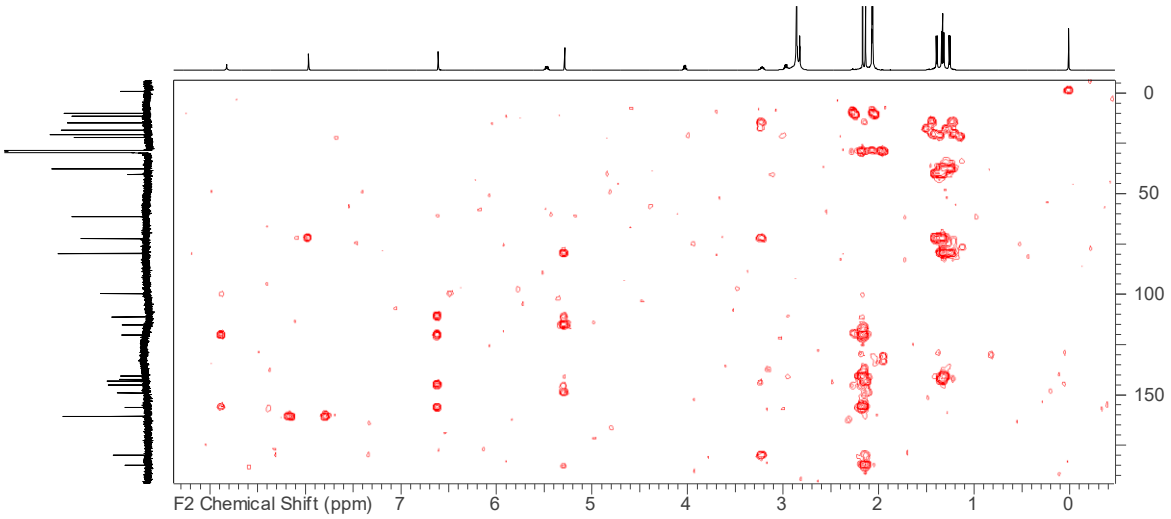


Figure S12. HMBC spectrum of compound **2**

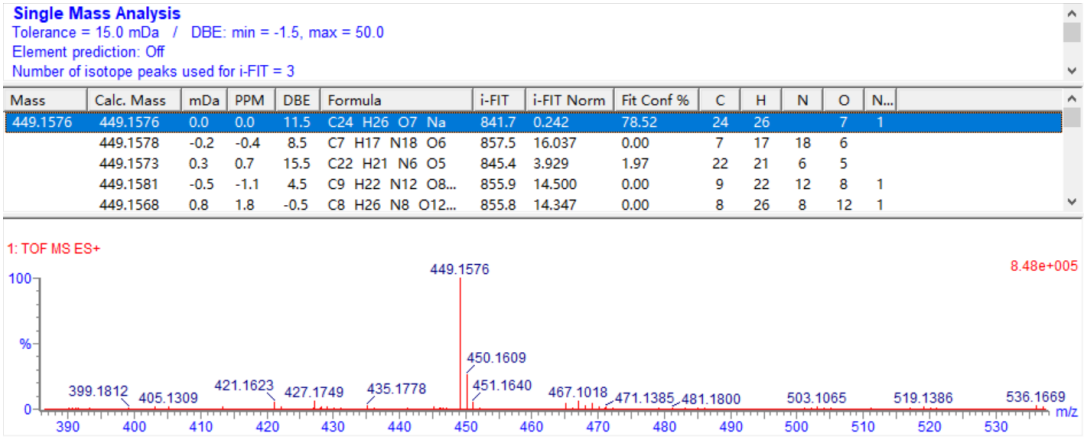


Figure S13. HRESIMS spectrum of compound **2**

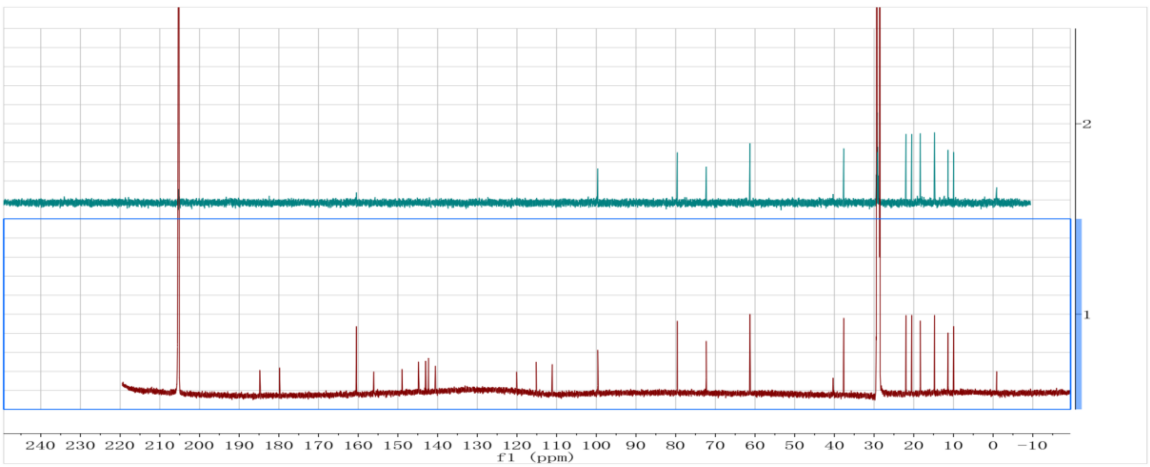


Figure S14. ^{13}C/DEPT spectrum of compound **2**

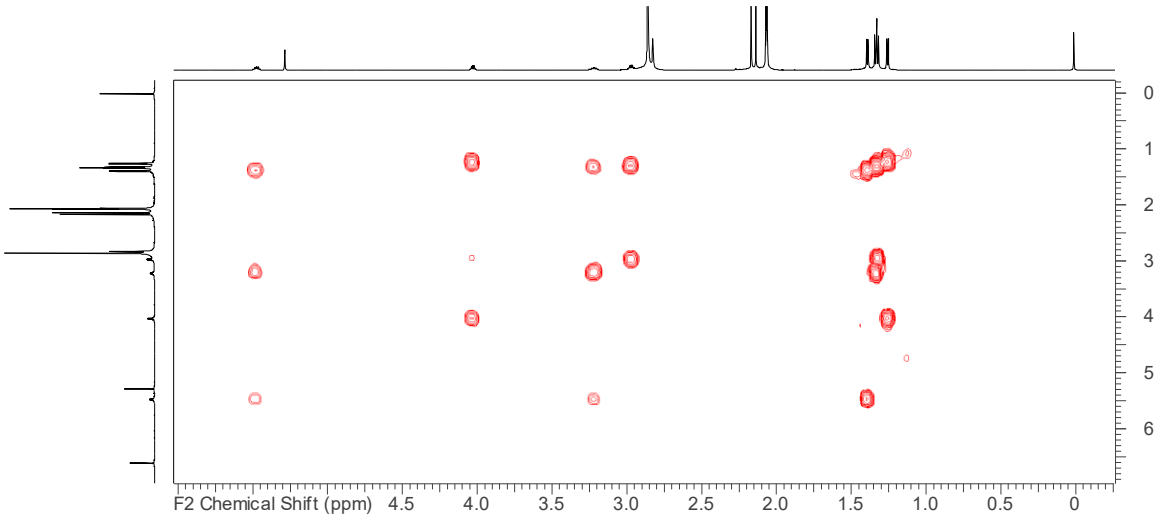


Figure S15. ^{1}H-^{1}H COSY spectrum of compound **2**

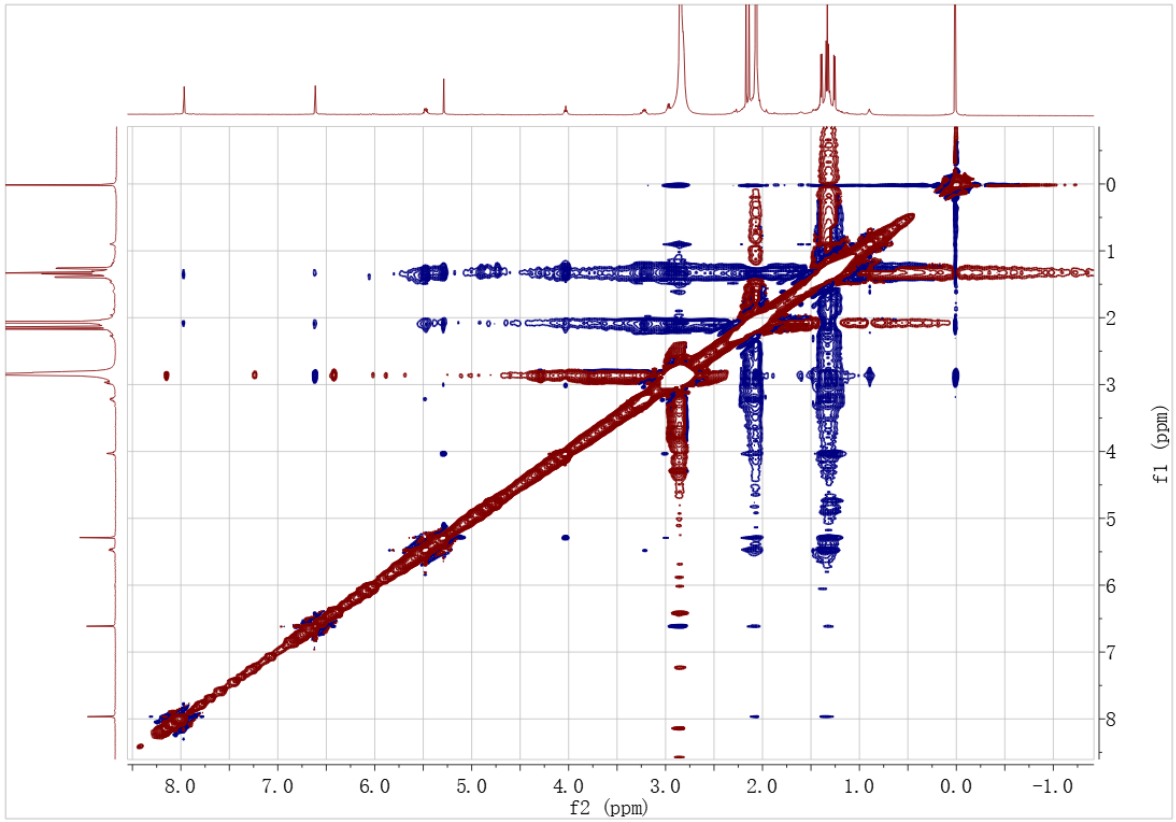
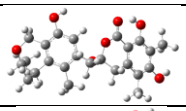
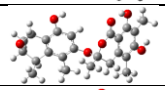
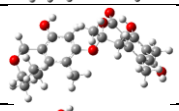
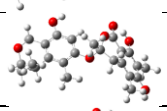
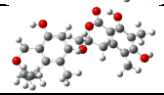


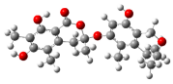
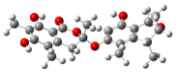
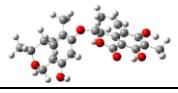
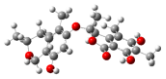
Figure S16. NOESY spectrum of compound **2**

Table S1. Gibbs free energies [a] and equilibrium populations [b] of low-energy conformers of (3*S*, 4*R*, 3′*R*)-**1**

configuration	conformer	structure	△G (kcal/mol)	Percent
(3*S*, 4*R*, 3′*R*)-**1**	a		0.00000	29.29%
	b		0.00188	29.20%
	c		0.24221	19.46%
	d		0.24472	19.38%
	e		1.41815	2.67%

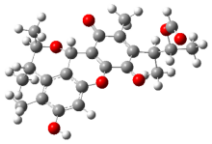
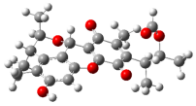
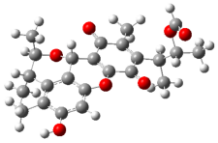
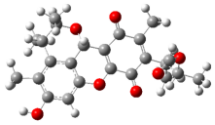
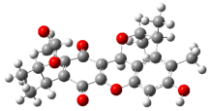
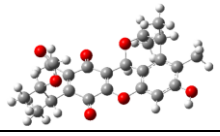
[a] B3LYP/6-31G(d), in kcal/mol. [b] From ΔG values at 298.15 K.

Table S2. Gibbs free energies [a] and equilibrium populations [b] of low-energy conformers of (3*S*, 4*R*, 3′*S*)-**1**

configuration	conformer	structure	△G (kcal/mol)	Percent
(3*S*, 4*R*, 3′*S*)-**1**	a		0.00000	68.58%
	b		0.72037	20.31%
	c		1.28449	7.83%
	d		1.80155	3.27%

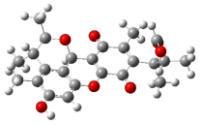
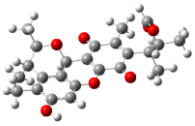
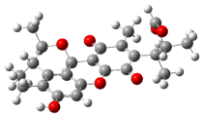
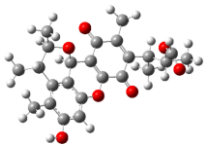
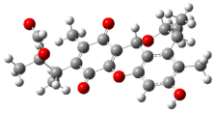
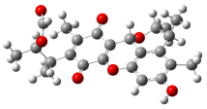
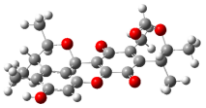
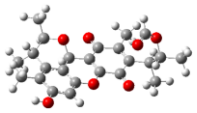
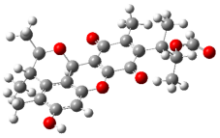
[a] B3LYP/6-31G(d), in kcal/mol. [b] From ΔG values at 298.15 K.

Table S3. Gibbs free energies [a] and equilibrium populations [b] of low-energy conformers of (1*S*, 3*R*, 4*S*, 7′*S*, 8′*R*)-**2**

configuration	conformer	structure	ΔG (kcal/mol)	Percent
(1*S*, 3*R*, 4*S*, 7′*S*, 8′*R*)-2	a		0.00000	58.25%
	b		0.72727	17.06%
	c		0.86783	13.45%
	d		1.50851	4.56%
	e		1.69174	3.35%
	f		1.69362	3.33%

[a] B3LYP/6-31G(d), in kcal/mol. [b] From ΔG values at 298.15 K.

Table S4. Gibbs free energies [a] and equilibrium populations [b] of low-energy conformers of (1*R*, 3*R*, 4*S*, 7′*S*, 8′*R*)-**3**

configuration	conformer	structure	ΔG (kcal/mol)	Percent
(1*R*, 3*R*, 4*S*, 7′*S*, 8′*R*)-3	a		0.00000	48.79%
	b		0.78312	13.00%
	c		0.80696	12.49%
	d		0.80885	12.45%
	e		1.54930	3.56%
	f		1.55494	3.53%
	g		1.85740	2.12%
	h		1.85928	2.11%
	i		1.90572	1.95%

[a] B3LYP/6-31G(d), in kcal/mol. [b] From ΔG values at 298.15 K.

Text S1. ITS1-5.8S-ITS2 rDNA sequence of strain NLG-S01-P1

LOCUS Seq1 487 bp DNA linear PLN 05-DEC-2018
DEFINITION Penicillium citrinum NLG-S01-P1 18S ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence.
ACCESSION Seq1
VERSION
KEYWORDS .
SOURCE Penicillium citrinum
ORGANISM Penicillium citrinum
Eukaryota; Fungi; Dikarya; Ascomycota; Pezizomycotina; Eurotiomycetes; Eurotiomycetidae; Eurotiales; Aspergillaceae; Penicillium.
REFERENCE 1 (bases 1 to 487)
AUTHORS Wang,W.
TITLE Citrinin Monomer and Dimer Derivatives with Antibacterial and Cytotoxic Activities Isolated from the Deep Sea Derived Fungus Penicillium citrinum NLG-S01-P1
JOURNAL unpublished
REFERENCE 2 (bases 1 to 487)
AUTHORS Wang,W.
TITLE Direct Submission
JOURNAL Submitted (05-DEC-2018) Key Laboratory of Marine Biogenetic Resources, Third Institute of Oceanography, State Oceanic Administration, 178 Daxue Road, Xiamen, Fujian 361005, China
COMMENT Bankit Comment: ALT EMAIL:wywang_cas@163.com
Bankit Comment: TOTAL # OF SEQS:1

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Sequencing Technology :: Sanger dideoxy sequencing
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