SUPPLEMENTARY MATERIAL

A new polyketide, penicillolide from the marine-derived fungus *Penicillium sacculum*

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A new polyketide, penicillolide (**1**) was isolated from the fermentation broth of the marine-derived fungus *Penicillium sacculum* GT-308. Compound **1** is a polyketide with a unique carbon skeleton. The structure of this compound was established via extensive spectroscopic analyses including 1D-, 2D-NMR, and HRESI-MS.

Keywords: marine-derived fungus; *Penicillium sacculum*; polyketide; penicillolide

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Figure S1. The ^1H -NMR Spectrum of Compound **1** in CDCl_3 .

Figure S2. The ^{13}C -NMR Spectrum of Compound **1** in CDCl_3 .

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Figure S4. The HMBC Spectrum of Compound **1** in CDCl_3 .

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Figure S9. Key HMBC and ^1H - ^1H COSY correlations of compound **1**.

Figure S10. Key NOESY correlations of compound **1**.

Table S1. NMR spectroscopic data of compound **1** (in CDCl_3)

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Figure S7. The ESI-MS Spectrum of Compound 1.

Figure S8. The HRESI-MS Spectrum of Compound 1.

Elemental Composition Search Report:

Target Mass:

Target m/z = 371.0767 $\pm$ 9.00ppm

Charge = -1

Possible Elements:

Element:	Exact Mass:	Min:	Max:
C	12.000000	0	100
H	1.007825	0	100
N	14.003074	0	100
O	15.994915	0	100

Additional Search Restrictions:

Seven Golden Rules

Nitrogen Rule

DBE Limit Mode = Both Integer and Half-Integer

-Minimum DBE = 0

-Maximum DBE = 100

Search Results:

Number of Hits = 5

m/z	Delta m/z (ppm)	DBE	Formula
371.07724	-1.46	12.0	C ₁₉ H ₁₅ O ₈ ⁻¹
371.07589	2.17	18.0	C ₁₆ H ₇ N ₁₀ O ₂ ⁻¹
371.07858	-5.07	17.0	C ₂₀ H ₁₁ N ₄ O ₄ ⁻¹
371.07456	5.77	13.0	C ₁₅ H ₁₁ N ₆ O ₆ ⁻¹
371.07992	-8.67	22.0	C ₂₁ H ₇ N ₈ ⁻¹

Varian QFT-ESI
File: GT-308-9_ESI.trans

Mode: Negative
Scans: 1

Date: 05-AUG-2010
Time: 15:24:26
Scale: 22.8650

Figure S9. Key HMBC and ^1H - ^1H COSY correlations of compound **1**.

Figure S10. Key NOESY correlations of compound **1**.

Table S1. NMR spectroscopic data of compound **1** (in CDCl₃)

position	δ_{H} mult. (<i>J</i> Hz)	δ_{C}	HMBC	NOESY
2	5.01 (1H, d, <i>J</i> = 12.3 Hz, H-2a)	72.0 (t)	C-3, C-4, C-5, C-8, C-11	H-10a
	5.08 (1H, d, <i>J</i> = 12.3 Hz , H-2b)		C-3, C-4, C-5, C-7, C-8, C-10	H-4
3		131.9 (s)		
4	6.37 (1H, s)	96.0 (d)	C-2, C-5, C-6, C-8	H-2b, 5-OCH ₃
5		148.0 (s)		
6		131.6 (s)		
7		139.7 (s)		
8		118.5 (s)		
9	4.99 (1H, d, <i>J</i> = 9.3 Hz)	82.3 (d)	C-3, C-7, C-8, C-11, C-13, C-15	H-10b
10	3.10 (1H, d, <i>J</i> = 15.9 Hz, H-10a)	33.5 (t)	C-8, C-11, C-15	H-2a,
	2.77 (1H, dd, <i>J</i> = 15.9, 9.3 Hz, H-10b)		C-9, C-11, C-15	H-9, H-12
11		88.8 (s)		
12	3.90 (1H, m)	50.5 (d)	C-10, C-11, C-13, C-16, C-19	H-10b, H-19
13		168.8 (s)		
15		189.9 (s)		
16		117.2 (s)		
17		161.9 (s)		
19	7.04 (1H, s)	138.3 (d)	C-16, C-17, C-20	H-12
20		117.4 (s)		
5-OCH ₃	3.88 (3H, s)	56.5 (q)	C-5	H-4
6-OH	4.96 (1H, s) ^a			7-OH
7-OH	5.35 (1H, s) ^b			6-OH
17-CH ₃	2.64 (3H, s)	14.3 (q)	C-16, C-17	

Note: ^{a,b} These chemical shifts are interchangeable.