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
List

Figure S1. The $^1$H-NMR Spectrum of Compound 1 in CDCl$_3$.

Figure S2. The $^{13}$C-NMR Spectrum of Compound 1 in CDCl$_3$.

Figure S3. The HSQC Spectrum of Compound 1 in CDCl$_3$.

Figure S4. The HMBC Spectrum of Compound 1 in CDCl$_3$.

Figure S5. The $^1$H-$^1$H COSY Spectrum of Compound 1 in CDCl$_3$.

Figure S6. The NOESY Spectrum of Compound 1 in CDCl$_3$.

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

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

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

Figure S10. Key NOESY correlations of compound 1.

Table S1. NMR spectroscopic data of compound 1 (in CDCl$_3$)
Figure S1. The $^1$H-NMR Spectrum of Compound 1 in CDCl$_3$. 
Figure S2. The $^{13}$C-NMR Spectrum of Compound 1 in CDCl$_3$. 
Figure S3. The HSQC Spectrum of Compound 1 in CDCl₃.
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Figure S6. The NOESY Spectrum of Compound 1 in CDCl$_3$. 
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 ± 9.00ppm
- Charge = -1

**Possible Elements:**

| Element | Exact Mass | Min | Max |
|---------|------------|-----|-----|
| C       | 12.0000000 | 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_{16}H_{15}O_{6}^{-1} |
| 371.07589 | 2.17            | 18.0 | C_{16}H_{17}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_{16}H_{11}N_{6}O_{6}^{-1} |
| 371.07992 | -8.67           | 22.0 | C_{21}H_{7}N_{6}^{-1}  |
Figure S9. Key HMBC and $^1\text{H}-^1\text{H}$ 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. (J Hz) | δ_C | HMBC | NOESY |
|----------|-----------------|-----|------|-------|
| 2        | 5.01 (1H, d, J = 12.3 Hz, H-2a) 5.08 (1H, d, J = 12.3 Hz, H-2b) | 72.0 (t) | C-3, C-4, C-5, C-8, C-11 | H-10a |
| 3        | 6.37 (1H, s)    | 131.9 (s) | C-2, C-5, C-6, C-8 | H-2b, 5-OCH₃ |
| 4        | 96.0 (d)        | C-3, C-4, C-5, C-7, C-8, C-10 | H-4 |
| 5        | 148.0 (s)       | 96.0 (d) | C-2, C-5, C-6, C-8 | H-2b, 5-OCH₃ |
| 6        | 131.6 (s)       | 139.7 (s) | C-2, C-5, C-6, C-8 | H-2b, 5-OCH₃ |
| 7        | 118.5 (s)       | 118.5 (s) | C-2, C-5, C-6, C-8 | H-2b, 5-OCH₃ |
| 8        | 4.99 (1H, d, J = 9.3 Hz) | 82.3 (d) | C-3, C-7, C-8, C-11, C-13, C-15 | H-10b |
| 9        | 3.10 (1H, d, J = 15.9 Hz, H-10a) 2.77 (1H, dd, J = 15.9, 9.3 Hz, H-10b) | 33.5 (t) | C-8, C-11, C-15 | H-2a, H-9, H-12 |
| 10       | 7.04 (1H, s)    | 138.3 (d) | C-16, C-17, C-20 | H-12 |
| 11       | 3.90 (1H, m)    | 88.8 (s) | C-10, C-11, C-13, C-16, C-19 | H-10b, H-19 |
| 12       | 168.8 (s)       | 168.8 (s) | C-10, C-11, C-13, C-16, C-19 | H-10b, H-19 |
| 13       | 189.9 (s)       | 189.9 (s) | C-10, C-11, C-13, C-16, C-19 | H-10b, H-19 |
| 14       | 117.2 (s)       | 117.2 (s) | C-10, C-11, C-13, C-16, C-19 | H-10b, H-19 |
| 15       | 161.9 (s)       | 161.9 (s) | C-10, C-11, C-13, C-16, C-19 | H-10b, H-19 |
| 16       | 117.4 (s)       | 117.4 (s) | C-10, C-11, C-13, C-16, C-19 | H-10b, H-19 |
| 17       | 3.88 (3H, s)    | 56.5 (q) | C-5 | H-4 |
| 18       | 7.04 (1H, s)    | 138.3 (d) | C-16, C-17, C-20 | H-12 |
| 19       | 3.96 (1H, s)    | 168.8 (s) | C-10, C-11, C-13, C-16, C-19 | H-10b, H-19 |
| 20       | 5.35 (1H, s)    | 117.2 (s) | C-10, C-11, C-13, C-16, C-19 | H-10b, H-19 |
| 5-OCH₃   | 56.5 (q)        | C-5 | H-4 |
| 6-OH     | 4.96 (1H, s)²   | 7.04 (1H, s) | 138.3 (d) | C-16, C-17 |
| 7-OH     | 5.35 (1H, s)²   | 14.3 (q) | C-16, C-17 |
| 17-CH₃   | 2.64 (3H, s)    | 14.3 (q) | C-16, C-17 |

Note: ² These chemical shifts are interchangeable.