**Bioactive α-pyrone meroterpenoids from mangrove endophytic fungus Penicillium sp.**

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Five α-pyrone meroterpenoids, including one new 3-epiarigsgacan E (1) and four known compounds, arisugacin D (2), arisugacin B (3), territrem C (4) and terreulactone C (5) were obtained from marine fungus Penicillium sp. SK5GW1L. Their structures were identified by MS and NMR experiments, and the absolute configuration of compound 1 was further confirmed by low temperature (150 K) single crystal X-ray diffraction with Cu Kα radiation. Compounds 3, 4 and 5 showed strong inhibitory activities against acetylcholinesterase (AchE) with IC50 values of 3.03 μM, 0.23 μM and 0.028 μM, respectively.
Support Information

Table S1. $^1$H NMR (500 MHz), $^{13}$C NMR (125M), and 2D- NMR data for compound 1 (ppm from TMS, $J$ = Hz, in CDCl$_3$).

Table S2. The single crystal parameters of compound 1

Figure S1. The single crystal structure of compound 1

Figure S2. $^1$H and $^{13}$C NMR, HSQC, and HMBC data for compound 1

Figure S3. UV of compound 1

Figure S4. IR of compound 1

Figure S5. ESIMS of compound 1

Figure S6. HRESIMS of compound 1

The single crystal cif file of compound 1
Table S1 $^1$H NMR (500 MHz), $^{13}$C NMR (125M), and 2D- NMR data for compound 1 (ppm from TMS, $J =$ Hz, in CDCl$_3$).

| No. | $\delta_C$ | $\delta_H$ | $^1$H-$^1$H COSY | HMBC(H→C) |
|-----|------------|------------|-----------------|-----------|
| 1   | 30.9       | 1.67-1.65, m | 2, 10, 19, 3, 5 |           |
|     |            | 1.45, dd (8.5, 2.3) |               |           |
| 2   | 27.4       | 1.79-1.76, m | H-3            | 1, 10, 4, 3 |
|     |            | 1.68-1.65, m |                 |           |
| 3   | 73.8       | 3.88, dd (11.0, 5.7) | H-2            | 17, 18    |
| 4   | 43.9       |             |                 |           |
| 5   | 78.1       |             |                 |           |
| 6   | 25.3       | 1.91-1.87, m | H-7            | 7, 5, 8   |
|     |            | 1.71-1.69, m |                 |           |
| 7   | 33.9       | 2.18-2.14, m | H-6            | 20, 6, 9, 8 |
|     |            | 1.89-1.86, m |                 |           |
| 8   | 80.2       |             |                 |           |
| 9   | 43.1       | 2.46, dd (13.1, 4.7) | H-11          | 20, 11, 1, 10, 8 |
| 10  | 40.6       |             |                 |           |
| 11  | 17.4       | 2.39, dd (16.7, 4.7) | H-9           | 9, 8, 12, 13 |
|     |            | 2.21-2.24, m |                 |           |
| 12  | 98.8       |             |                 |           |
| 13  | 163.7      |             |                 |           |
| 14  | 97.0       | 6.24, s     | 12, 1’, 15, 13 |           |
| 15  | 158.4      |             |                 |           |
| 16  | 164.8      |             |                 |           |
| 1’  | 124.2      |             |                 |           |
| 2’  | 127.1      | 7.73, d (8.8) | H-3’          | 15, 4’, 6’ |
| 3’  | 114.3      | 6.93, d (8.8) | H-2’          | 1’, 4’, 2’ |
| 4’  | 158.4      |             |                 |           |
| 5’  | 114.3      | 6.93, d (8.8) | H-6’          | 1’, 4’, 6’ |
| 6’  | 127.1      | 7.73, d (8.8) | H-5’          | 15, 2’, 4’ |
| 17  | 17.6       | 0.96, s     | 18, 4, 3, 5   |           |
| 18  | 22.8       | 1.09, s     | 17, 4, 3, 5   |           |
| 19  | 18.4       | 1.06, s     | 1, 10, 9, 5   |           |
| 4’-OCH$_3$ | 55.6     | 3.86, s     | 4’            |           |
| 20  | 21.2       | 1.28, s     | 8, 9, 7, 10, 6 |           |
**Table S2.** The single crystal parameters of compound 1

| parameter                      | parameter values | parameter                      | parameter values |
|--------------------------------|------------------|--------------------------------|------------------|
| Empirical formula              | C₂₇H₃₄O₆         | Reflections                    | 15932/4078[R(int)=0.02] |
| Formula weight                 | 454.54           | collected/unique               | 48               |
| Temperature                    | 150(2) K         |                                |                  |
| Wavelength                     | 1.54178 Å        | Absorption correction          | Semi-empirical from Equivalents |
| Crystal system, space group    | Orthorhombic, P 21 21 21 |                              |                  |
| Unit cell dimensions           |                  |                                |                  |
| a                              | 10.70160(10) Å   | a=90°                          |                  |
| b                              | 10.75190(10) Å   | A, β=90°                        |                  |
| c                              | 20.1484(2) Å     | A, γ=90°                        |                  |
| Volume                         | 2318.33(4) Å³    |                                |                  |
| Z, calculated density          | 4.1.302 mg/m³    |                                |                  |
| Absorption coefficient        | 0.737 mm⁻¹       | Max./min.transmission          | 0.8726 / 0.7470  |
| F (000)                        | 976              | Refinement method              | Full-matrix      |
| Crystal size                   | 0.40x0.32x0.19 mm| Refinement method              | Full-matrix      |
| Theta range for data collection| 4.39-66.91°      | Data/restraints/parameters     | 4078 / 0 / 305   |
| Limiting indices               | -12≤h≤12, -12≤k≤12, -23≤l≤22 |                            |                  |
| completeness to theta=62.77    | 99.3%            | Largest diff. peak and         | 0.133 and -0.196 e. Å⁻³ |

**Figure S1.** The single crystal structure of compound 1
**Figure S2.** $^1$H and $^{13}$C NMR, COSY, HSQC, HMBC and NOE data for compound 1

$^1$H-NMR
HSQC

HMBC
Figure S3. UV of compound 1
Figure S4. IR of compound 1

Figure S5. ESIMS of compound 1
**Figure S6. HRESIMS of compound 1**

[SPECTRUM - simulation:

| m/z     | Theo. Mass | Delta (ppm) | RDB equiv. | Composition |
|---------|------------|-------------|------------|-------------|
| 455.24319 | 455.24282  | 0.82        | 10.5       | C27 H35 O6  |

**Limits:**

1. Charge: 1
2. Nitrogen-Rule: Do not use
3. Mass tolerance: 10.00 ppm
4. Elements in use: $^{12}$C (0~30), $^1$H (0~60), $^{16}$O (0~15);
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H11A C11 H11B 108.2 . . ?
C13 C12 C16 118.42(13) . . ?
C13 C12 C11 122.59(13) . . ?
C16 C12 C11 118.98(13) . . ?
O3 C13 C12 123.27(12) . . ?
O3 C13 C14 115.67(13) . . ?
C12 C13 C14 121.06(13) . . ?
O4 C16 O5 115.96(13) . . ?
O4 C16 C12 125.57(13) . . ?
O5 C16 C12 118.47(13) . . ?
C1 C10 C25 107.90(12) . . ?
C1 C10 C9 108.85(11) . . ?
C25 C10 C9 110.50(11) . . ?
C1 C10 C5 108.84(11) . . ?
C25 C10 C5 113.14(12) . . ?
C9 C10 C5 107.53(11) . . ?
C5 C6 C7 111.57(12) . . ?
C5 C6 H6A 109.3 . . ?
C7 C6 H6A 109.3 . . ?
C5 C6 H6B 109.3 . . ?
C7 C6 H6B 109.3 . . ?
H6A C6 H6B 108.0 . . ?
C8 C7 C6 112.97(12) . . ?
C8 C7 H7A 109.0 . . ?
C6 C7 H7A 109.0 . . ?
C8 C7 H7B 109.0 . . ?
C6 C7 H7B 109.0 . . ?
H7A C7 H7B 107.8 . . ?
O2 C5 C6 107.90(11) . . ?
O2 C5 C4 106.84(11) . . ?
C6 C5 C4 113.94(12) . . ?
O2 C5 C10 103.37(10) . . ?
C6 C5 C10 109.85(11) . . ?
C4 C5 C10 114.16(11) . . ?
C19 C18 C17 120.90(14) . . ?
C19 C18 H18 119.6 . . ?
C17 C18 H18 119.6 . . ?
O1 C3 C2 110.83(12) . . ?
O1 C3 C4 108.05(12) . . ?
C2 C3 C4 113.67(12) . . ?
O1 C3 H3 108.0 . . ?
C2 C3 H3 108.0 . . ?
C4 C3 H3 108.0 . . ?
C2 C1 C10 112.50(12) . . ?
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C2 C1 H1B 109.1 . . ?
C10 C1 H1B 109.1 . . ?
H1A C1 H1B 107.8 . . ?
C15 C14 C13 119.29(14) . . ?
C15 C14 C14 120.4 . . ?
C13 C14 H14 120.4 . . ?
C14 C15 O5 120.46(13) . . ?
C14 C15 C17 126.43(14) . . ?
O5 C15 C17 113.10(12) . . ?
C11 C9 C8 110.13(11) . . ?
C11 C9 C10 114.76(11) . . ?
C8 C9 C10 114.06(11) . . ?
C11 C9 H9 105.7 . . ?
C8 C9 H9 105.7 . . ?
C10 C9 H9 105.7 . . ?
O6 C20 C21 125.06(15) . . ?
O6 C20 C19 115.06(15) . . ?
C21 C20 C19 119.88(14) . . ?
C21 C22 C17 120.97(15) . . ?
C23 C4 C5 114.42(12) . . ?
C24 C4 C5 110.60(12) . . ?
C3 C4 C5 107.76(11) . . ?
C8 C32 H32A 109.5 . . ?
C8 C32 H32B 109.5 . . ?
H32A C32 H32B 109.5 . . ?
C8 C32 H32C 109.5 . . ?
H32A C32 H32C 109.5 . . ?
H32B C32 H32C 109.5 . . ?
O6 C26 H26A 109.5 . . ?
O6 C26 H26B 109.5 . . ?
H26A C26 H26B 109.5 . . ?
O6 C26 H26C 109.5 . . ?
H26A C26 H26C 109.5 . . ?
H26B C26 H26C 109.5 . . ?

loop_

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C9 C11 C12 C13 -8.07(19) . . ?
C9 C11 C12 C16 172.89(12) . . . . ?
C8 O3 C13 C12 -17.84(18) . . . . ?
C8 O3 C13 C14 162.46(11) . . . . ?
C16 C12 C13 O3 173.57(13) . . . . ?
C11 C12 C13 O3 -5.5(2) . . . . ?
C16 C12 C13 C14 -6.7(2) . . . . ?
C11 C12 C13 C14 174.20(13) . . . . ?
C15 O5 C16 O4 178.27(12) . . . . ?
C15 O5 C16 C12 -0.96(19) . . . . ?
C13 C12 C16 O4 -174.02(14) . . . . ?
C11 C12 C16 O4 5.1(2) . . . . ?
C13 C12 C16 O5 5.1(2) . . . . ?
C11 C12 C16 O5 -175.79(12) . . . . ?
C5 C6 C7 C8 55.66(17) . . . . ?
C7 C6 C5 O2 53.23(15) . . . . ?
C7 C6 C5 C4 171.69(11) . . . . ?
C19 C18 C17 C22 0.0(2) . . . . ?
C19 C18 C17 C15 -178.16(14) . . . . ?
C21 C22 C17 C18 -1.0(2) . . . . ?
C21 C22 C17 C15 177.23(15) . . . . ?
C14 C15 C17 C18 29.1(2) . . . . ?
O5 C15 C17 C18 -152.53(14) . . . . ?
C14 C15 C17 C22 -149.08(16) . . . . ?
O5 C15 C17 C22 29.3(2) . . . . ?
C17 C18 C19 C20 0.6(2) . . . . ?
O6 C20 C19 C18 179.90(14) . . . . ?
C21 C20 C19 C18 -0.3(2) . . . . ?
O6 C20 C21 C22 179.15(15) . . . . ?
C19 C20 C21 C22 -0.6(3) . . . . ?
C17 C22 C21 C20 1.2(3) . . . . ?
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C2 C3 C4 C23 71.85(16) . . . . ?
O1 C3 C4 C24 63.45(15) . . . . ?
C2 C3 C4 C24 -173.11(12) . . . . ?
O1 C3 C4 C5 -177.44(11) . . . . ?
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O2 C5 C4 C23 177.18(12) . . . . ?
C6 C5 C4 C23 58.11(16) . . . . ?
C10 C5 C4 C23 -69.21(16) . . . . ?
O2 C5 C4 C24 57.79(15) . . . . ?
C6 C5 C4 C24 -61.27(16) . . . . ?
C10 C5 C4 C24 171.40(12) . . . . ?
O2 C5 C4 C3 -59.19(14) . . . . ?
C6 C5 C4 C3 -178.26(11) . . . . ?
C10 C5 C4 C3 54.42(15) . . . . ?

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