Anthraquinone derivatives from a coral associated fungus

Stemphylium lycopersici

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**ABSTRACT:** Two new anthraquinone derivatives, alterporriol Y (1) and macrosporin 2-O-α-D-glucopyranoside (2), together with five known analogues (3-7) were isolated from the fungus *Stemphylium lycopersici* associated with the gorgonian coral *Dichotella gemmacea* collected from the South China Sea. Their structures were determined on the basis of detailed spectroscopic analysis and comparison with reported data. The absolute configurations were determined by the ECD method. In an *in vitro* cytotoxic assay, compound 3 and 4 showed potent effects against HCT-116 and MCF-7 cell lines. Compound 4 also exhibited cytotoxicity toward Huh7 stem cell-like cells.

**Keywords:** anthraquinone; *Stemphylium lycopersici*; cytotoxicity

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Table S1. $^1$H and $^{13}$C NMR Data for Compounds 1 and 2 (in DMSO-$d_6$).

| Position | $^1$H (J in Hz) | $^{13}$C | Type |
|----------|----------------|--------|------|
| 1 $\alpha$ | 36.1, CH$_2$ | 2.37, d (19.2) |  |
| 1 $\beta$ | 2.21, d (19.2) |  |
| 1a | 143.4, C |  |
| 2 | 69.2, C |  |
| 3 | 70.2, CH | 3.53, ov$^d$ |  |
| 4 $\alpha$ | 29.3, CH$_2$ | 2.49, ov$^d$ |  |
| 4 $\beta$ | 2.71, dd (19.2, 5.0) |  |
| 4a | 141.7, C |  |
| 5 | 163.9, C |  |
| 6 | 103.9, C | 6.87, s |  |
| 7 | 164.1, C |  |
| 8 | 122.6, C |  |
| 9 | 183.6, C |  |
| 9a | 129.2, C |  |
| 10 | 187.9, C |  |
| 10a | 108.8, C |  |
| 11 | 25.3, CH$_3$ | 1.07, s |  |
| 12 | 56.9, CH$_3$ | 3.66, s |  |
| OH-2 | 4.42, s |  |
| OH-3 | 4.80, d (5.2) |  |
| OH-5 | 13.1, s |  |

| Position | $^1$H (J in Hz) | $^{13}$C | Type |
|----------|----------------|--------|------|
| 1 | 110.2, CH | 8.00, s |  |
| 1a | 133.1, C |  |
| 2 | 160.0, C |  |
| 3 | 134.9, C |  |
| 4 | 129.6, CH | 7.87, s |  |
| 4a | 126.8, C |  |
| 5 | 107.3, CH | 7.19, s |  |
| 6 | 166.0, C |  |
| 7 | 105.9, CH | 6.86, s |  |
| 8 | 164.2, C |  |
| 9 | 186.2, C |  |
| 9a | 110.2, C |  |
| 10 | 180.8, C |  |
| 10a | 134.9, C |  |
| Me-3 | 16.3, CH$_3$ | 2.38, s |  |
| OMe-6 | 56.4, CH$_3$ | 3.93, s |  |
| OH-2 | 97.7, CH | 5.73, d (3.3) |  |
| OH-3 | 71.3, CH | 3.49, dd (9.5, 3.3) |  |
| OH-5 | 72.9, CH | 3.70, t (9.5) |  |
| 4’ | 69.4, CH | 3.28, t (9.7) |  |
| 5’ | 74.5, CH | 3.38, ddd (9.7, 4.6, 2.2) |  |
| 6’ | 60.2, CH$_2$ | 3.52, dd (12.5, 2.2) |  |
| OH-8 | 12.77, s |  |

$^a$150 MHz. $^b$600 MHz. $^c$100 MHz. $^d$ov = overlapped signal.
**Figure S1.** Key $^1$H-$^1$H COSY and HMBC correlations of compounds 1 and 2

**Figure S2.** Key NOE correlations of compound 1.

**Figure S3.** ECD spectrum of 1
Figure S4. HRESI-MS spectrum of 1

Figure S5. UV spectrum of 1
Figure S6. FTIR spectrum of 1

Figure S7. $^1$H NMR (600 MHz, DMSO-$d_6$) spectrum of compound 1
**Figure S8.** $^{13}$C-NMR and DEPT (150 MHz, DMSO-$d_6$) spectrum of compound 1

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Figure S17. HMBC spectrum of 1 in pyridine-$d_5$
Figure S18. NOESY spectrum of 1 in pyridine-$d_5$

Figure S19. HRESI-MS spectrum of 2
Figure S20. UV spectrum of 2

![UV spectrum of 2]

Table 1: UV data of 2

| No. | W/V | 谱长 (nm) | Abs. | 描述 |
|-----|-----|-----------|------|------|
| 1   | 1   | 372.00    | 0.477|      |
| 2   | 1   | 278.82    | 2.812|      |
| 3   | 1   | 224.80    | 1.949|      |
| 4   | 1   | 201.00    | 2.768|      |
| 5   | 1   | 348.20    | 0.450|      |
| 6   | 1   | 241.20    | 1.034|      |
| 7   | 1   | 218.80    | 1.872|      |

Figure S21. FTIR spectrum of 2

![FTIR spectrum of 2]
Figure S22. $^1$H NMR (600 MHz, DMSO-$d_6$) spectrum of compound 2

Figure S23. $^{13}$C-NMR and DEPT (100 MHz, DMSO-$d_6$) spectrum of compound 2
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