SUPPLEMENTARY DATA

Highly oxygenated ent-atisane and podocarpane diterpenoids from Excoecaria agallocha

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ABSTRACT

A new highly oxygenated ent-atisane diterpenoid, namely excagallonoid A (1), together with five known analogues (2–6) were isolated from the leaves and twigs of Excoecaria agallocha. Their structures were elucidated on the basis of extensive spectroscopic analyses (HRESIMS, UV, IR, 1D and 2D NMR), and the absolute
configurations of 1 and 5 were determined by single-crystal X-ray diffraction. Compound 1 represents the first example of an ent-atisane diterpenoid featuring a vicinal 2,3-diol moiety. Compounds 1 and 4 exhibited weak cytotoxicities in vitro against RKO colon cancer cells with IC$_{50}$ values of 28.7 ± 1.98 and 32.6 ± 2.81 µM, respectively.

**Keywords:** *Excoecaria agallocha*; ent-atisane diterpenoid; podocarpane diterpenoid; cytotoxicity

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| No. | $\delta_\text{H}$ (J in Hz) | $\delta_\text{C}$ | $\delta_\text{H}$ (J in Hz) | $\delta_\text{C}$ |
|-----|-----------------------------|-------------------|-----------------------------|-------------------|
| 1a  | 1.98, dd (14.7, 3.0)        | 42.1              | a 2.40, m                  | 32.6              |
| 1b  | 1.12, dd (14.7, 3.5)        |                   | b 2.07, m                  |                   |
| 2   | 4.06, dddd (3.7, 3.5, 3.0)  | 70.7              | a 2.81, m                  | 33.0              |
|     |                             |                   | b 2.73, m                  |                   |
| 3   | 3.18, d (3.7)               | 78.3              |                            | 215.0             |
| 4   |                             | 38.0              |                            | 48.5              |
| 5   | 0.89, m                     | 54.6              |                            | 137.3             |
| 6a  | 1.59, m                     | 18.6              |                            | 142.3             |
| 6b  | 1.54, m                     |                   |                            |                   |
| 7a  | 2.33, m                     | 31.4              |                            | 179.5             |
| 7b  | 0.87, m                     |                   |                            |                   |
| 8   |                             | 47.6              |                            | 120.8             |
| 9   | 1.51, dd (10.9, 6.7)$^a$    | 53.3              |                            | 151.1             |
| 10  |                             | 37.2              |                            | 39.4              |
| 11a | 1.84, m                     | 27.8              | 6.92, s                    | 111.7             |
| 11b | 1.72, dddd (13.5, 6.7, 2.4)|                   |                            |                   |
| 12  | 2.69, m                     | 38.4              |                            | 159.2             |
| 13  | 2.29, m                     | 44.5              |                            | 124.5             |
| 14  |                             | 216.9             | 8.00, s                    | 129.9             |
| 15a | 2.21, m                     | 42.9              | 2.31, s                    | 15.4              |
| 15b | 2.16, m                     |                   |                            |                   |
| 16  |                             |                   |                            | 147.4             |
| 17a | 4.86, br s                  | 106.8             |                            |                   |
| 17b | 4.64, br s                  |                   |                            |                   |
| 18  | 0.96, s                     | 17.1              | 1.58, s                    | 20.9              |
| 19  | 0.99, s                     | 29.9              | 1.54, s                    | 24.4              |
| 20  | 0.96, s                     | 14.5              | 1.27, s                    | 26.2              |
| 6-OH|                             | 7.13, s           |                            |                   |

$^a$ Overlapped signals in the same vertical column.
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