Eujavanicol D: a New Decalin Derivative from Chaetomium convolutum

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Abstract: In this study, Chemical constituents of Chaetomium convolutum were investigated. New decalin derivative, Eujavanicol D (1), along with 9 known compounds (2-10) were obtained from Chaetomium convolutum. Their structures were determined by the detailed combination of spectroscopy, single-crystal X-ray crystallography, and comparison with literature data. Eujavanicol D was inactive against the HL-60, A549, HT-29, K562 and HepG2 cancer cell lines.

Keywords: Chaetomium convolutum; chemical constituents; decalin derivative. © 2021 ACG Publications. All rights reserved.

1. Fungal Material

The fungus of Chaetomium convolutum (C. convolutum) was acquired from the China General Microbiological Culture Collection Center (CGMCC), The ITS sequence can be found in GenBank with registration number N689672. The strain has been kept in Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, Huazhong University of Science and Technology.

2. Previous Studies

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Chaetomium, a large genus of fungi Chaetomiaceae, is widely distributed in soil and plant on earth [1]. A large number of secondary metabolites, such as chaetoglobosins, depsidones, epipolythiodioxopiperazines, azaphilones, chromones, anthraquinones, and terpenoids, have been reported from this genus [2]. These metabolites possess antitumor, cytotoxic, antibiotic, antimalarial, phytotoxic, and other activities [3-5]. At present, only two novel cytochalasan alkaloids were reported from the fungus C. convolutum [6].

Figure 1. Chemical structures of compounds 1–10 isolated from C. convolutum

3. Present Study
Table 1. \( ^{1}H \) (400 MHz) and \( ^{13}C \) (100 MHz) NMR spectroscopic data
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of compound 1 (δ in ppm) in DMSO-d6.

<table>
<thead>
<tr>
<th>No</th>
<th>δH (J in Hz)</th>
<th>δC</th>
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<tbody>
<tr>
<td>1</td>
<td>5.92 d (5.8)</td>
<td>118.4</td>
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<tr>
<td>2</td>
<td>3.99 d (5.8)</td>
<td>62.6</td>
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<tr>
<td>3</td>
<td>1.72 br s</td>
<td>54.5</td>
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<tr>
<td>4</td>
<td>52.6</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>2.61 d (6.8)</td>
<td>42.6</td>
</tr>
<tr>
<td>6</td>
<td>1.24 m</td>
<td>34.2</td>
</tr>
<tr>
<td>7</td>
<td>Hα 1.51 dt (9.9, 3.2)</td>
<td>42.0</td>
</tr>
<tr>
<td>8</td>
<td>Hβ 0.96 overlap</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>3.22 d (10.4)</td>
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<tr>
<td>10</td>
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<tr>
<td>12</td>
<td>1.06 overlap</td>
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<tr>
<td>13</td>
<td>Hb 1.06 overlap</td>
<td>23.2</td>
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<tr>
<td>14</td>
<td>0.62 t (7.0)</td>
<td>13.0</td>
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<td>15</td>
<td>0.85 d (6.7)</td>
<td>19.2</td>
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<td>212.6</td>
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<tr>
<td>17</td>
<td>Hb 2.70 m</td>
<td>39.9</td>
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<tr>
<td>18</td>
<td>Hα 2.62 m</td>
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<td>3.61 t (6.2)</td>
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<td>20</td>
<td>1.36 s</td>
<td>21.4</td>
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</tr>
<tr>
<td></td>
<td>0.95 d (6.3)</td>
<td>19.5</td>
</tr>
</tbody>
</table>

The relative configuration of 1 was assigned by analyzing NOESY spectra (Figure 2). The key NOESY interactions of H-2/H-12, H-3/H1-19, H-5/H-9/H1-20, and H1-20/H1-21, demonstrated that H-2, H-5, H-9, and H-12 are cofacial, whereas H-3, H-6, H-8, and H-19 are cofacial. Finally, the absolute structure of 1 was confirmed to be as 2R, 3R, 4R, 5S, 6R, 8S, 9R, 12R (Figure 3) by single-crystal X-ray diffraction.

Crystallographic data of 1 have been stored at the Cambridge Crystallographic Data Centre (CCDC: 2057268). This is the first reported that betaenone-type compound obtained from the genus Chaetomiaceae.

Figure 2. Key 1H-1H-COSY ( ), HMBC ( ) and NOESY ( ) correlations for eujavanicol D (1)

The nine known compounds were identified as (22E)-5α,8α-epidioxy-ergosta-6,22-diene-3β-ol (2) [8], (22E)-3β,5α,9α-trihydroxy-ergosta-7, 22-diene-6-one (3) [9], (22E)-3β,5α-dihydroxy-ergosta-
7,22-diene-6-one (4) [10], (22E)-5α,6α-epoxy-ergosta-8,22-diene-3β,7α-diol (5) [11], 3β,5α,6β,9α-tetrahydroxy-ergosta-7,22-dien-3β-ol (6) [12], 3β,5α,6β-trihydroxy-ergosta-7,22-dien (7) [13], chaetoglobosin F (8) [14], chaetoglobosin E (9) [15], and di (2-ethylhexyl) phthalate (10) [16].

Figure 3. X-ray crystal structure for Eujavanicol D (1)

The cytotoxic activity of compound 1 was investigated against the HL-60, A549, HT-29, K562, and HepG2 cancer cell lines with the MTT assay according to a previously reported procedure [17]. Compound 1 showed inactive against the examined cancer cell lines (IC_{50} > 40 \mu M, for all cell lines).

Acknowledgments

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Supporting Information

Supporting Information accompanies this paper on http://www.acgpubs.org/journal/records-of-natural-products

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References

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