SUPPLEMENTARY MATERIAL

Cytotoxic pimarane-type diterpenes from the marine sediment-derived fungus *Eutypella* sp. FS46

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Abstract

Two new pimarane-type diterpenes, scoparanes H-I (1-2), along with five known ones (3-7) were isolated from the culture broth of a marine sediment-derived fungus *Eutypella* sp. FS46, which was obtained from the South China Sea. Their structures were established by extensive spectroscopic analysis. All of them were evaluated for their cytotoxic activities against MCF-7, NCI-H460, and SF-268 tumor cell lines. Scopararane I (2) showed moderate inhibitory activities.

**Keywords:** pimarane diterpenes; *Eutypella* sp. FS46; scopararane H; scopararane I; cytotoxic activity

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Figure S2. $^{13}$C NMR spectrum of 1
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Figure S4. $^1$H–$^1$H COSY spectrum of 1
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Figure S6. HMBC spectrum of 1
Figure S7. NOESY spectrum of 1

Elemental Composition Report

Single Mass Analysis
Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotopic peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
329 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-100  H: 0-1000  N: 0-5  O: 0-200  Na: 1-1

MS+
ES(+) 29 (1.67E) AM (C6, 60.00, Ar, 6500, 0.555, 0.70, 0.75, 0.75); 3m (Me, 2x3.00); 5b (1x4.00); Cm (4.33)
1: TDF MS ES+ 6.34e+004

Figure S8. HREIMS spectrum of 1
Figure S9. UV spectrum of 1

Figure S10. IR spectrum of 1
Figure S11. $^1$H NMR spectrum of 2

Figure S12. $^{13}$C NMR spectrum of 2
Figure S13. DEPT spectrum of 2

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Table S1. $^1$H (500 MHz) and $^{13}$C (125 MHz) NMR data of compounds 1 and 2 in CD$_3$OD ($J$ in Hz, $\delta$ in ppm).

| no. | $\delta$ | $\delta$ | no. | $\delta$ | $\delta$ |
|-----|---------|---------|-----|---------|---------|
| 1   | 7.11, d, 10.4 | 157.3, CH | 1 | 1.77, m | 13.2, CH |
| 2   | 5.93, d, 10.4 | 126.7, CH | 2a | 2.29, ddd, 3.0, 9.3, 16.0 | 25.8, CH$_2$ |
| 3   | 206.9, C | 45.8, C | 2b | 1.92, dd, 3.0, 6.3 | 43.5, CH |
| 4   | 2.63, d, 1.5 | 44.2, CH | 3 | 4.88, t, 3.0 | 71.7, CH |
| 5   | 4.29* | 71.6, CH | 4 | 2.44, d, 12.6 | 40.2, C |
| 6   | 7.1, d, 1.5 | 71.4, CH | 5 | 4.26, d, 12.6 | 77.4, CH |
| 7   | 4.29* | 136.8, C | 6 | 1.92, ddd, 3.0, 9.3, 16.0 | 201.4, C |
| 8   | 2.55, m | 75.5, C | 7 | 1.95, ddd, 3.0, 9.3, 16.0 | 131.8, C |
| 9   | 46.4, C | 10 | 1.88, m | 167.4, C |
| 10  | 25.2, CH$_2$ | 11a | 2.20, ddd, 3.0, 9.3, 16.0 | 23.8, CH$_2$ |
| 11a | 1.85, m | 28.1, C |
| 11b | 2.33, ddd, 3.0, 9.3, 16.0 | 11b | 1.88, m | 39.8, C |
| 12a | 1.56, m | 32.1, CH$_2$ | 12a | 1.95, ddd, 3.0, 9.3, 16.0 | 26.1, CH$_2$ |
| 12b | 1.78, m | 12b | 1.44, m | 112.6, CH$_2$ |
| 13  | 38.3, C | 13 | 4.18, s | 68.0, CH |
| 14  | 5.95, ddd, 3.0, 9.3, 16.0 | 14 | 6.06, m | 146.6, CH |
| 15  | 132.9, CH | 15 | 5.07, d, 1.3 | 112.6, CH$_2$ |
| 16a | 148.7, CH | 16a | 5.07, d, 1.3 | 70.5, CH$_2$ |
| 16b | 110.9, CH$_2$ | 16b | 5.45, d, 1.3 | 20.9, CH$_3$ |
| 17  | 23.3, CH$_3$ | 17 | 5.04, dd, 1.3, 5.1 | 20.9, CH$_3$ |
| 18  | 25.6, CH$_3$ | 18 | 0.76, s | 171.9, C |
| 19  | 24.5, CH$_3$ | 19 | 1.19, s | 21.0, CH$_3$ |
| 20  | 21.3, CH$_3$ | 20b | 0.69, dd, 5.2, 9.5 | 178.1, C |
|     | 2.12, t, 5.2 | 1" | 1.99, s | 35.2, CH |
|     | 0.69, dd, 5.2, 9.5 | 1" | 1.99, s | 19.2, CH$_3$ |
|     | 1.12, d, 7.0 | 1" | 1.99, s | 19.2, CH$_3$ |

*aoverlapped
Table S2. Cytotoxic activities of compounds 1–7.

| Compounds | IC\textsubscript{50} (μg mL\textsuperscript{-1}) |
|-----------|----------------------------------------------|
|           | MCF-7 | NCI-H460 | SF-268  |
| 1         | 80.63 | >100     | >100    |
| 2         | 13.59 | 83.91    | 25.31   |
| 3         | 5.18  | >100     | 62.34   |
| 4         | 5.18  | 34.29    | 13.27   |
| 5         | 10.03 | 53.91    | >100    |
| 6         | >100  | >100     | >100    |
| 7         | 0.84  | 10.74    | 1.37    |
| Cisplatin | 1.20  | 0.87     | 1.43    |