SUPPLEMENTARY MATERIAL

A new sesquiterpene from the gorgonian coral Menella sp.

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A new sesquiterpene named menecubebane B (1) and a known analogue (2) were isolated from the gorgonian coral *Menella* sp.. Their structures were elucidated by the extensive analyses of spectroscopic data, and by the comparison with related literature. Cytotoxic effect against both Eca9706 and HeLa cell lines was evaluated, revealing 1 exhibited moderate cytotoxicity against the two cell lines involved with IC$_{50}$ values being 20.8 and 30.6 μM, respectively.

**Keywords:** Gorgonian coral; *Menella* sp.; sesquiterpene; cytotoxicity
Table S1: $^1$H (500 MHz), $^{13}$C (125 MHz) data of compound 1 in CD$_3$OD

| No. | $\delta$C (mult.) | $\delta$H (mult., $J$ in Hz) |
|-----|-------------------|-----------------------------|
| 1   | 160.5 (C)         |                             |
| 2   | 63.8 (CH)         | 4.94 (ddd, $J = 5.0, 4.5, 2.0$ Hz) |
| 3   | 46.2 (CH$_2$)     | 2.19 (dd, $J = 14.0, 4.5$ Hz) |
| 4   | 73.2 (C)          |                             |
| 5   | 204.1 (C)         |                             |
| 6   | 136.0 (C)         |                             |
| 7   | 39.0 (CH)         | 2.75 (m)                    |
| 8   | 19.5 (CH$_2$)     | 1.74 (m), 1.56 (m)          |
| 9   | 38.4 (CH$_2$)     | 1.82 (m), 1.58 (m)          |
| 10  | 72.2 (C)          |                             |
| 11  | 29.9 (CH)         | 2.06 (m)                    |
| 12  | 17.8 (CH$_3$)     | 0.75 (d, $J = 6.5$ Hz)      |
| 13  | 21.0 (CH$_3$)     | 0.89 (d, $J = 6.5$ Hz)      |
| 14  | 28.5 (CH$_3$)     | 1.50 (s)                    |
| 15  | 27.5 (CH$_3$)     | 1.46 (s)                    |
Figure legends

Figure S1. Key $^1$H-$^1$H COSY and HMBC correlations of 1

Figure S2. Key NOESY correlations of 1

Figure S3. $^1$H NMR (500 MHz, CD$_3$OD) of 1

Figure S4. $^{13}$C NMR (125 MHz, CD$_3$OD) of 1

Figure S5. COSY (500 MHz, CD$_3$OD) of 1

Figure S6. HSQC (500 MHz, CD$_3$OD) of 1

Figure S7. HMBC (500 MHz, CD$_3$OD) of 1

Figure S8. NOESY (500 MHz, CD$_3$OD) of 1

Figure S9. HRMS of 1
Figure S1. Key $^1$H-$^1$H COSY and HMBC correlations of 1
Figure S2. Key NOESY correlations of 1
Figure S3. $^1$H NMR (500 MHz, CD$_3$OD) of compound 1.
Figure S4. $^{13}$C NMR (125 MHz, CD$_3$OD) of compound 1.
Figure S5. $^1$H-$^1$H COSY (500 MHz, CD$_3$OD) of compound 1.
Figure S6. HSQC (500 MHz, CD$_3$OD) of compound 1.
Figure S7. HMBC (500 MHz, CD$_3$OD) of compound 1
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