SUPPLEMENTARY MATERIAL

A new sesquiterpene from the South China Sea gorgonian coral *Subergorgia suberosa*

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A new sesquiterpene from the South China Sea gorgonian coral

*Subergorgia suberosa*

A new sesquiterpene, namely suberosoid (1), was isolated from the South China Sea gorgonian coral *Subergorgia suberosa*. The chemical structure of 1 was established as an unusual sesquiterpene containing 4-methylenecyclohex-2-enone system, by extensive analyses of NMR spectroscopy and high-resolution mass spectrometry. Suberosoid (1) exhibited cytotoxic effect against HeLa cell lines with IC₅₀ value being 10.6 μM.

**Keywords:** Gorgonian coral; *Subergorgia suberosa*; 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   | 207.1 (C)         |                               |
| 2   | 125.8 (CH)        | 5.86 (d, $J = 10.0$ Hz)       |
| 3   | 149.3 (CH)        | 7.21 (d, $J = 10.0$ Hz)       |
| 4   | 144.1 (C)         |                               |
| 5   | 24.7 (CH$_2$)     | 2.19 (ddd, $J = 14.0, 2.0, 1.5$) |
| 6   | 43.7 (CH)         | 1.70 (ddd, $J = 14.0, 12.0, 1.5$) |
| 7   | 22.2 (CH$_2$)     | 1.61 (m)                      |
| 8   | 33.9 (CH$_2$)     | 1.52 (m), 1.34 (m)            |
| 9   | 47.0(C)           |                               |
| 10  | 44.0 (CH)         | 2.74 (dd, $J = 2.0, 1.5$)     |
| 11  | 122.9 (CH$_2$)    | 5.65 (s), 5.54 (s)            |
| 12  | 73.2 (C)          |                               |
| 13  | 27.2 (CH$_3$)     | 1.19 (s)                      |
| 14  | 26.8 (CH$_3$)     | 1.20 (s)                      |
| 15  | 20.0 (CH$_3$)     | 1.26 (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. HMBC (500 MHz, CD$_3$OD) of 1 (part 1)

Figure S9. HMBC (500 MHz, CD$_3$OD) of 1 (part 2)

Figure S10. HMBC (500 MHz, CD$_3$OD) of 1 (part 3)

Figure S11. NOESY (500 MHz, CD$_3$OD) of 1

Figure S12. NOESY (500 MHz, CD$_3$OD) of 1 (part 1)

Figure S13. NOESY (500 MHz, CD$_3$OD) of 1 (part 2)

Figure S14. 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 I.
Figure S4. $^{13}$C NMR (125 MHz, CD$_3$OD) of compound I.
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
Figure S8. HMBC (500 MHz, CD$_3$OD) of compound 1 (part 1)
Figure S9. HMBC (500 MHz, CD$_3$OD) of compound 1 (part 2)
Figure S10. HMBC (500 MHz, CD$_3$OD) of compound 1 (part 3)
Figure S11. NOESY (500 MHz, CD3OD) of compound 1
Figure S12. NOESY (500 MHz, CD$_3$OD) of compound 1 (part 1)
Figure S13. NOESY (500 MHz, CD$_3$OD) of compound 1 (part 2)
Figure S14. HRMS of compound 1.