Cytotoxic sesquiterpenoids from soft coral Capnella imbricata

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Supplementary Information

Table S1. \textsuperscript{1}H and \textsuperscript{13}C NMR data (600 and 150 MHz) of 1 in C\textsubscript{6}D\textsubscript{6} (\textdelta in ppm).

Figure S1. Structures of compounds 2-8.
Figure S2. \textsuperscript{1}H NMR spectrum of cap germacrene H (1) in CDCl\textsubscript{3} (600 MHz).
Figure S3. \textsuperscript{13}C NMR spectrum of cap germacrene H (1) in CDCl\textsubscript{3} (150 MHz).
Figure S4. HSQC spectrum of cap germacrene H (1) in CDCl\textsubscript{3}.
Figure S5. \textsuperscript{1}H-\textsuperscript{1}H COSY spectrum of cap germacrene H (1) in CDCl\textsubscript{3}.
Figure S6. HMBC spectrum of cap germacrene H (1) in CDCl\textsubscript{3}.
Figure S7. NOESY spectrum of cap germacrene H (1) in CDCl\textsubscript{3}.
Figure S8. \textsuperscript{1}H NMR spectrum of cap germacrene H (1) in C\textsubscript{6}D\textsubscript{6} (600 MHz).
Figure S9. Expended \textsuperscript{1}H NMR spectrum of cap germacrene H (1) in C\textsubscript{6}D\textsubscript{6} (600 MHz).
Figure S10. \textsuperscript{13}C NMR spectrum of cap germacrene H (1) in C\textsubscript{6}D\textsubscript{6} (150 MHz).
Figure S11. HSQC spectrum of cap germacrene H (1) in C\textsubscript{6}D\textsubscript{6}.
Figure S12. HMBC spectrum of cap germacrene H (1) in C\textsubscript{6}D\textsubscript{6}.
Figure S13. NOESY spectrum of cap germacrene H (1) in C\textsubscript{6}D\textsubscript{6}.
Figure S14. HRESIMS spectrum of cap germacrene H (1).
Table S1: $^1$H and $^{13}$C NMR data (600 and 150 MHz) of 1 in CD$_6$(δ in ppm).

| Position | $\delta$ C | $\delta$ H (mult., J in Hz) |
|----------|-------------|----------------------------|
| 1        | 136.4       | 5.08 dd (10.3, 4.8)         |
| 2        | 24.1        | 2.61 m                      |
|          |             | 1.94 m                      |
| 3        | 42.1        | 1.49 dd (14.4, 8.9)         |
|          |             | 1.16 dd (14.4, 11.0)        |
| 4        | 73.4        |                            |
| 5        | 139.7       | 5.05 d (15.1)               |
| 6        | 124.5       | 5.55 dd (15.1, 10.3)        |
| 7        | 47.8        | 2.94 m                      |
| 8        | 44.7        | 2.69 dd (12.4, 5.5)         |
|          |             | 2.51 t (12.4)               |
| 9        | 205.0       |                            |
| 10       | 138.2       |                            |
| 11       | 146.3       |                            |
| 12       | 20.9        | 1.69 s                      |
| 13       | 110.2       | 4.89 s                      |
|          |             | 4.85 s                      |
| 14       | 19.9        | 1.65 s                      |
| 15       | 29.3        | 1.12 s                      |

Figure S1: Structures of compounds 2-8.
Figure S2. $^1$H NMR spectrum of capgermacrene H (1) in CDCl$_3$ (600 MHz).
Figure S3. $^{13}$C NMR spectrum of capgermacrene H (1) in CDCl$_3$ (150 MHz).
Figure S4. HSQC spectrum of capgermacrene H (1) in CDCl₃.
Figure S5. $^1$$^1$H-COSY spectrum of capgermacrene H (1) in CDCl$_3$. 
Figure S6. HMBC spectrum of capgermacrene H (1) in CDCl₃.
Figure S7. NOESY spectrum of capgermacrene H (1) in CDCl₃.
Figure S8. $^1$H NMR spectrum of capgermacrene H (1) in C$_6$D$_6$ (600 MHz).
**Figure S9.** Expanded $^1$H NMR spectrum of capgermacrene $H$ (1) in CD$_6$D$_6$ (600 MHz).

Proton signal of H-5 with d ($J = 15.1$ Hz)

Proton signal of H-6 with dd ($J = 15.1, 10.3$ Hz)

Note: $^1$H NMR spectrum of 1 in CDCl$_3$ do not provided a good resolution for proton signals of H-5 and H-6. This limitation was solved by exploiting different shift-inducing power CD$_6$D$_6$ to run the NMR experiments.
Figure S10. $^{13}$C NMR spectrum of capgermacrene H (1) in C$_6$D$_6$ (150 MHz).
Figure S11. HSQC spectrum of capgermacrene H (1) in C₆D₆.
Figure S12. HMBC spectrum of capgermacrene H (1) in CD$_6$. 
Figure S13. NOESY spectrum of capgermacrene H (1) in C$_6$D$_6$. 
Figure S14. HRESIMS spectrum of capgermacrene H (1).
Measured region for 217.1981 m/z

217.1981
217.1995
218.1621
218.1625

Calculated region for 217.0887 m/z

217.0887
218.1621

| Rank | Score | Formula (DS) | Ion  | Meas m/z  | Pred m/z | Diff (ppm) | Diff (ppm) | Ion Score | DRE |
|------|-------|--------------|------|-----------|----------|------------|------------|-----------|------|
| 1    | 0.897 | C8H24NO       | [M+H]+ | 217.0887  | 217.0887 | 0          | 0          | 1.0000    | 2.0 |

Error Margin: 33 ppm
Mass Range: 2.0 - 5000.0
Electron Ion: Both configurations
HC Ratio: Limit 0.0 - 3.0
Apply Nitrogen Rule: Yes
Search Results:
Advanced Settings...