

Supplementary data 1:

Components of aplysin structure analyzed by infrared radiation (IR), electron impact-mass spectrometry (EI-MS), ¹H-nuclear magnetic resonance (NMR) and ¹³C-NMR.

IR $\nu_{\text{max}}^{\text{KBr}}$ cm^{-1} : 2 952, 2 864, 1 577, 1 487, 1 460, 1 375, 1 308, 1 267, 1 234, 1 192, 1 007, 904, 881, 862.

EI-MS m/z (%): 296 [$\text{M} (^{81}\text{Br})^+$] (100), 294 [$\text{M} (^{79}\text{Br})^+$] (100), 281 [$\text{M} (^{81}\text{Br}) - \text{CH}_3$]⁺ (95), 279 [$\text{M} (^{79}\text{Br}) - \text{CH}_3$]⁺ (95), 239 (45), 237 (45), 200 [$\text{M}-\text{Br}$]⁺ (35), 160 (16), 115 (12), 109 (10), 69 (5).

¹H-NMR (CD_3COCD_3 , 500 MHz)W: 1.06 (3H, d, J = 6.5 Hz, H-9), 1.04~1.08 (1H, m, H-2a), 1.27 (3H, s, H-10), 1.33 (3H, s, H-12), 1.60~1.68 (2H, m, H-2b, 1a), 1.81~1.86 (2H, m, H-1b, 3), 2.26 (3H, s, H-11), 6.60 (1H, s, H-5), 7.2 (1H, s, H-8).

¹³C-NMR (CD_3COCD_3 , 125 MHz)W: 43.0 (C-1), 31.9 (C-2), 46.6 (C-3), 100.4 (C-3a), 159.4 (C-4a), 110.5 (C-5), 137.5 (C-6), 114.3 (C-7), 127.3 (C-8), 137.4 (C-8a), 55.1 (C-8b), 13.3 (C-9), 23.1 (C-10), 23.4 (C-11), 20.1 (C-12).

By comparing with corresponding literature data [1,2], this compound was identified as aplysin.

References

- [1] J. Y. Laronze, R. E. I. Boukili, D. Patigny, S. Dridi, D. Cartier and J. Lévy, "The rearrangement of some cyclopentanone-aryloximes: synthesis of (±)-aplysin, (±)-filiformin and of their debromo analogues," *Tetrahedron*, vol. 47, no. 48, pp. 10003-10014, 1991.
- [2] D. C. Harrowven, M. C. Lucas and P. D. Howes, "The synthesis of a natural product family: from debromoisolaurinterol to the aplysin," *Tetrahedron*, vol. 57, no. 2001, pp. 791-804, 2001.