Chemistry of Natural Compounds, Vol. 42, No. 4, 2006

AN UNSATURATED ω-HYDROXY METHYL ESTER FROM A SPONGE *Sarcotragus* SPECIES

Yonghong Liu,[1] Jee H. Jung,[2] and Si Zhang[1]

UDC 547.314

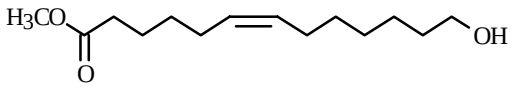
Marine sponges of the order Dictyoceratida have frequently provided a large number of linear furanoterpenoids [1, 2]. In the course of our study on the cytotoxic substances of the sponge *Sarcotragus* sp., 35 cytotoxic terpenoids, three cyclitol derivatives, and a macrolide were isolated [3–7]. In a continuing study of the same sponge, an unsaturated ω-hydroxymethyl ester was isolated.

The sponge was collected in July 1998 (15–25 m depth), off Cheju Island, Korea. The specimen has been described elsewhere [3].

Isolation was described in our previous report [3]. The compound (1.7 mg) was obtained by purification of fraction Fg4–7 by ODS HPLC.

The molecular formula was established as $C_{14}H_{26}O_3$ on the basis of HRFABMS. In the ^{1}H NMR spectrum, a singlet at δ_H 3.64 was attributed to methoxy group protons. A triplet at δ_H 3.52 was attributed to the H-13. In the HMBC spectrum, the methoxy proton (δ_H 3.61, s), H-2 (δ_H 2.29, t) and H-3 (δ_H 1.59, quint) were correlated with the carbonyl carbon (δ 174.1). The chemical shifts of the allylic carbons (d 27.8 and 27.6) indicated that the double bond geometry is *cis* [5]. The double bond position was clearly recognized from the FAB-CID tandem mass spectrum of the $[M+Na]^+$ ion. The location of the double bond was clear from the 54-mass gap between the major fragment ions of allylic cleavage at *m/z* 177 and 123 [5]. The structure of the compound was elucidated with the aid of COSY, HSQC, and HMBC experiments.

Thus, the structure was determined as an unsaturated ω-hydroxymethyl ester (**1**).



1

Compound 1. Colorless oil; $[\alpha]_D^{21}$ –23.1°, (*c* 0.04, $CHCl_3$); ^{1}H NMR (500 MHz, acetone-d_6, J/Hz): δ 3.61 (3H, s, OCH_3), 2.29 (2H, t, J = 7.5, H-2), 1.59 (2H, quint, J = 7.5, H-3), 2.05 (overlap with solvent peak, H-5 and H-8), 5.36 (2H, m, H-6 and H-7), 1.25–1.35 (8H, m, H-4, H-9-H-11), 1.51 (2H, quint, J = 7, H-12), 3.52 (2H, t, J = 6.5, H-13); ^{13}C NMR (50 MHz, δ, acetone-d_6) 174.1 (C-1), 34.3 (C-2), 25.5 (C-3), 27.8 (C-5), 130.6 (C-6), 130.4 (C-7), 27.6 (C-8), 28.9–30.5 (overlap with solvent peak C-4, C-9, and C-10), 26.3 (C-11), 33.6 (C-12), 62.4 (C-13), 51.4 (OCH_3); FABMS *m/z* 265 $[M+Na]^+$ (18), 243 $[M+H]^+$ (12), 219 (3). HRFABMS *m/z* 265.3433 (calc for $C_{14}H_{26}O_3Na$, 265.3442).

ACKNOWLEDGMENT

Our thanks are due to Dr. Chung Ja Sim of Hannam University for the identification of the sponge. This study was supported by a grant from the Ministry of Maritime Affairs and Fisheries (Korea Sea Grant Program) and Guangdong Key Laboratory of Marine Materia Medica Foundation.

1) Guangdong Key Laboratory of Marine Materia Medica, South China Sea Institute of Oceanology, Chinese Academy of Sciences, Guangzhou 510-301, China, fax: +86 20 89023103, e-mail: yhliu6@yahoo.com.cn; 2) College of Pharmacy, Pusan National University, Busan 609-735, Korea. Published in Khimiya Prirodnykh Soedinenii, No. 4, p. 392, July-August, 2006. Original article submitted August 5, 2005.

0009-3130/06/4204-0487

REFERENCES

1. D. J. Faulkner, *Nat. Prod. Rep*., 1, 1 (2002), and earlier reviews sited therein.
2. J. W. Blunt, B. R. Copp, M. H. G. Munro, P. T. Northcote, and M. R. Prinsep, *Nat. Prod. Rep*., 1, 15 (2005), and earlier reviews sited therein.
3. Y. Liu, B. K. Bae, N. Alam, J. Hong, C. J. Sim, C-O. Lee, K. S. Im, and J. H. Jung, *J. Nat. Prod.*, **64**, 1301 (2001).
4. Y. Liu, J. Hong, C-O. Lee, K. S. Im, N. D. Kim, J. S. Choi, and J. H. Jung, *J. Nat. Prod.*, **65**, 1307 (2002).
5. Y. Liu, C-O. Lee, J. Hong, and J. H. Jung, *Bull. Korean Chem. Soc*., **23**, 1467 (2002).
6. Y. Liu, T. A. Mansoor, J. Hong, C-O. Lee, C. J. Sim, K. S. Im, and J. H. Jung, *J. Nat. Prod.*, **11**, 1451 (2003).
7. Y. Liu, P. B. Shinde, J. Hong, C-O. Lee, K. S. Im, and J. H. Jung, *Nat. Prod. Sci.*, **11**, 50 (2005).