Chinese Chemical Letters Vol. 17, No. 11, pp 1463-1465, 2006
http://www.imm.ac.cn/journal/ccl.html

A New Degraded Sesquiterpene from Marine Actinomycete *Streptomyces sp.* 0616208

Xiu Chao XIE[1], Wen Li MEI[1], You Xing ZHAO[2], Kui HONG[1]*, Hao Fu DAI[1]*

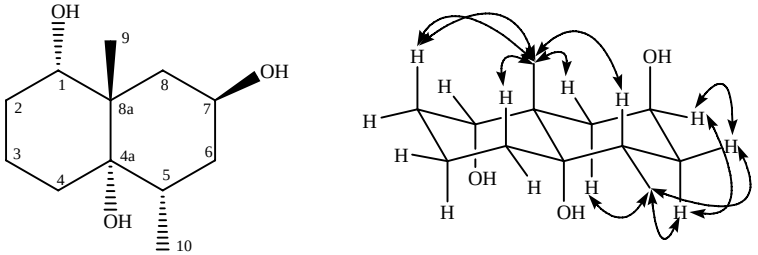
[1]State Key Laboratory of Tropical Crops Biotechnology, Institute of Tropical Bioscience and Biotechnology, Chinese Academy of Tropical Agriculture Sciences, Haikou 571101
[2]State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204

Abstract: A new degraded sesquiterpene was isolated from the marine actinomycete *Streptomyces sp.* 0616208. Its structure was elucidated as (1α, 4aα, 5α, 7β, 8aβ)-5, 8a-dimethyl-decahydronaphthalene-1, 4a, 7-triol on the basis of spectroscopic data.

Keywords: Marine actinomycete, *Streptomyces sp.*, degraded sesquiterpene, (1α, 4aα, 5α, 7β, 8aβ)-5, 8a-dimethyl-decahydronaphthalene-1,4a,7-triol.

Marine-derived microorganisms have recently come into the focus of research as one of the richest source of new and bioactive secondary metabolites in the marine environment[1,2]. In our screening for cytotoxic agents to human hepatoma SMMC-7721 cell line, methanol extract from the fermentation product of a marine actinomycete *Streptomyces sp.* 0616208 was found to be highly potent. The experimental material *Streptomyces sp.* 0616208 was isolated from mangrove sediment, collected in the South China Sea. Bioassay-guided fractionation led to the isolation of a new compound, the structure of which was characterized as (1α, 4aα, 5α, 7β, 8aβ)-5, 8a-dimethyldecahydronaphthalene-1, 4a, 7-triol **1** on the basis of spectroscopic evidences. Compound **1** showed moderate cytotoxicity against human hepatoma SMMC-7721 cell line *in vitro* with MTT method.

Figure 1 Structure and ROESY correlations of Compound **1**



* E-mail: hfdai2001@yahoo.com.cn; k1022@163.net

Compound **1**, colorless needles, mp: 151-153°C, $[\alpha]_D^{24}$ 5.4 (*c* 0.5, MeOH), its molecular formula $C_{12}H_{22}O_3$ was established according to the high-resolution ESI-MS spectrometric data at *m/z* 237.1465 $(M+Na)^+$ (calcd. for $C_{12}H_{22}O_3Na$, 237.1466). This formula can also be validated through ^{13}C NMR, ^1H NMR, and DEPT spectra. The ^{13}C NMR and DEPT spectra of **1** presented twelve carbon signals for two methyls (δ 14.3, 23.4), five methylenes (δ 17.0, 28.3, 30.5, 37.0, 38.4), three methines (δ 31.9, 68.3, 77.8) including two oxygenated carbons, and two quaternary carbons (δ 40.6, 78.0) including an oxygenated carbon. Compound **1** was deduced to be degraded sesquiterpene with a eudesmane-type skeleton by inspection of 1Dand 2D-NMR spectra[3]. From the HMQC and ^1H-^1H COSY spectra, the chemical shifts of all the carbons and protons were assigned respectively (**Table 1**). The HMBC correlations (**Table 1**) between the signals of two methyl groups and those of neighbouring carbons were helpful to define the neighbouring functional groups, locating in the eudesmane framework. The long-range correlations of the methyl protons signals at δ_H 0.80 (H-10) with the quaternary carbon signal at δ_C 78.0 placed a hydroxyl group at C-4a. Similarly, the placement of the hydroxyl group at C-1 was supported by an observation of the long-range correlations of H-9 at δ_H 1.23 with the C-1 at δ_C 77.8, which was confirmed by the correlation from δ_H 3.40 (H-1) to δ_H 1.59, 1.99 (H-2) in the ^1H-^1H COSY spectrum of **1**. The last hydroxyl group was attached to C-7 for the obvious correlations from δ_H 1.95 (H-5) to δ_H 0.80 (H-10) and δ_H 1.48, 1.92 (H-6), δ_H 4.15 (H-7) to δ_H 1.48, 1.92 (H-6) and δ_H 1.18, 2.41 (H-8) in the ^1H-^1H COSY spectrum, which was supported by the correlations of δ_H 4.15 (H-7) with δ_C 40.6 (C-8a) and δ_C 31.9 (C-5) in the HMBC spectrum.

The relative stereochemistry at the chiral centers in compound **1** was established by the ROESY spectrum (**Figure 1**). The NOE interactions from δ_H 1.23 (H-9) to δ_H 3.40 (H-1), δ_H 1.58 (H-4b), and δ_H 1.95 (H-5) indicated that H-9, H-1, H-4b, and H-5 were at the same side. When they were in β-orientations, 1-OH, 4a-OH, and 5-Me should be in α-orientations. H-7 was assumed to be α-orientated because of the cross peaks from δ_H 4.15 (H-7) to δ_H 1.48, 1.92 (H-6) were observed while the cross peak from δ_H 1.23 (H-9) to δ_H 4.15 (H-7) was not observed.

Table 1 ^1H NMR (500 MHz) and ^{13}C NMR (125 MHz) data of **1** in CD_3OD (δ ppm, *J* Hz)

No.	δ_C	δ_H	HMBC
1	77.8	3.40 brs	C-3, 8, 8a, 9, 4a
2	28.3	1.59 m; 1.99 m	C-3, 4, 8a
3	17.0	1.51 m; 1.99 m	C-1, 2, 4a
4	30.5	1.58 m; 1.66 brd (14.0)	C-2, 3, 4a, 8a
4a	78.0		
5	31.9	1.95 m	C-6, 10
6	38.4	1.48 dd (1.8, 12.6); 1.92 brd (3.7)	C-4a, 5, 7, 8
7	68.3	4.15 brs	C-5, 8, 8a
8	37.0	1.18 d (14.5); 2.41 dd (4.1, 14.6)	C-1, 9, 8a
8a	40.6		
9	23.4	1.23 s	C-1, 4a 8, 8a
10	14.3	0.80 d (6.2)	C-4a, 5, 6

Accordingly, the structure of compound **1** was determined as (1α, 4aα, 5α, 7β, 8aβ)-5, 8a-dimethyl-decahydronaphthalene-1, 4a, 7-triol. Accordingly, the structure of compound **1** was determined as (1α, 4aα, 5α, 7β, 8aβ)-5, 8a-dimethyldecahydro-naphthalene-1, 4a, 7-triol.

Acknowledgment

This work was supported by the Social Commonweal Project of Chinese Ministry of Science and Technology (No.2004DIB3J072).

References

1. T. S. Bugni, C. M. Ireland, *Nat. Prod. Rep.*, **2004**, *21***,** 143.
2. S. B. Tim, M. I. Chris, *Nat. Prod. Rep.*, **2004**, *21***,** 163.
3. A. A. William, G. P. Michael, *Can. J. Chem.*, **1975**, *54,* 910.

Received 12 June, 2006