

A Novel Sesquiterpene Isolated from *Stereum* sp. 8954

Guo Hong LI, Ke Qin ZHANG*

Laboratory for Conservation and Utilization of Bio-resource, Yunnan University, Kunming 650091

Abstract: Stereumone A, a novel sesquiterpene was isolated from the fermentation broth of *Stereum* sp. 8954. Its structure was determined to be 5-hydroxy-6,6,9-trimethyl-4,8a-epoxy-2,3,4a,5,6,7,8a,9-octahydro-4*H*-naphtho[2,3-*b*]furan-8-one on the basis of the spectral data.

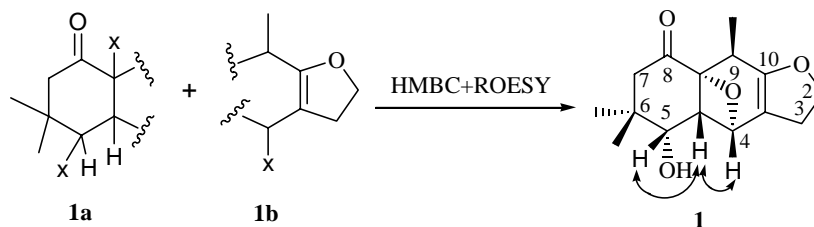
Keywords: Stereumone A, sesquiterpene, *Stereum* sp..

The basidiomycete *Stereum* sp. 8954 was collected in Xishuangbanna, Yunnan Province, and the mycelium of *Stereum* sp. 8954 was separated from fruit body and deposited in Laboratory for Conservation and Utilization of Bio-resources, Yunnan University. After fermentation, a novel sesquiterpene was isolated from the culture of the strain. The present paper deals with the structural elucidation of the new compound.

Experimental

Stereum sp. 8954 was fermented with PDA medium (10 L) at 26 °C for 10 days. After filtration, the fermentation broth was exhaustively extracted four times with *n*-butanol and 5.5 g residue (FB) was obtained from the filtrate. Fraction FB was chromatographed on a silica gel column eluting with petroleum ether and acetone (6:1, v/v) and further repeatedly purified on Sephadex LH-20 column eluting with acetone to yield compound **1** (5 mg).

Figure 1 The structure and significant ROESY correlation for **1**



* E-mail: Kqzhang111@yahoo.com.cn

Table 1 The NMR data of compound **1** in acetone- d_6^a (δ ppm, JHz)

Position	δ_C	δ_H	HMBC	1H - 1H COSY
2	59.0	4.34(dt, 2.35, 16.5)	C-3a, C-4(w), C-10	2.23
		4.27(dt, 2.05, 16.5)	C-3a, C-4(w), C-10	2.66
3	30.5	2.23(m, 2.66, m)	C-4(w), C-10, C-3a, C-10	4.34, 4.27
3a	129.0	\	\	\
4	90.6	5.04, br	\	\
4a	53.9	2.79, m	C-4, C-5, C-6, C-8a, C-8	3.85
5	81.6	3.85(t, 4.3)	C-8(w)	2.79
6	40.6	\	\	\
7	41.3	1.26, m	C-6 α -CH ₃ , C-6 β -CH ₃ , C-6, C-8(w)	\
8	195.9	\	\	\
8a	68.1	\	\	\
9	46.2	2.83, m	C-8a, C-8, C-10	1.27
10	151.0	\	\	\
6 α -CH ₃	21.1	0.99, s	C-5, C-6 β -CH ₃ , C-6, C-7	\
6 β -CH ₃	27.9	0.93, s	C-5, C-6 α -CH ₃ , C-6, C-7	\
9-CH ₃	23.0	1.27(d, 7.9)	C-8a, C-9, C-10	2.83

^aThe NMR data for compound **1** were recorded on Bruker ADX-500.

Compound **1**, obtained as yellowish amorphous solid. The HRESIMS determined the molecular formula to be C₁₅H₁₉O₄ (m/z 263.1281 [M - H]⁻, calcd. 263.1283). The IR (KBr) spectrum of **1** revealed the presence of the hydroxyl (3438 cm⁻¹), ketone (1718 cm⁻¹) (s), double bond (1654 cm⁻¹), ether (1138 cm⁻¹) groups. The ¹³C-NMR and DEPT experiments (**Table 1**) showed fifteen carbon signals for three methyls, three methylenes, four methines and five quaternary carbons including one ketone (δ 195.9) and a carbon-carbon double bond (δ 129.0 and δ 151.0). Fragments **1a** and **1b** (**Figure 1**) were determined based on the experiments of HMQC, HMBC and ¹H-¹H COSY (**Table 1**). The HMBC experiments showed the ¹H-¹³C NMR long-rang correlation between the protons of methyl group at δ_H 0.93 and the C-atoms at δ_C 21.1 q, 40.6 s, 41.3 t, 81.6 d, and between the protons of methyl group at δ_H 0.99 and the C-atoms at δ_C 27.9 q, 40.6 s, 41.3 t, 81.6 d, and between the protons of methylene at δ_H 1.26 and the C-atoms at δ_C 21.1 q, 27.9 q, 40.6 s and 195.9 s, and the proton of methine at δ_H 2.79 and the C-atoms at δ_C 40.6 s, 68.1 s, 81.6 d, 195.9 s. Moreover, the ¹H-¹H COSY spectrum showed that the proton of methine at δ_H 2.79 correlated with the proton of methine at δ_H 3.85 afforded the fragment **1a** (**Figure 1**). Besides, analysis of ¹H-¹H COSY plots revealed that the protons of methylene at δ_H 4.34 and 4.27 correlated with the protons of methylene at δ_H 2.23 and 2.66, and between the protons of methyl group at δ_H 1.27 and the proton at δ_H 2.83, which together with the HMBC data led to the fragment **1b** (**Figure 1**). Fragment **1a** and **1b** can be connected based on the correlation between the proton of δ_H 2.83 and the C-atoms at δ_C 68.1 s and 195.5 s, and between the δ_H 2.79 and the C-atom at δ_C 90.6 d. The demand of the number of unsaturated degrees and a relative downfield methine at δ_C 90.6 d displayed in ¹³C-NMR spectrum implied that except for the naphthaline ring and furan ring, there should be an extra ring in the molecular skeleton, linking with C-4

and C-8a through an oxygen bridge. The relative configuration was deduced from ROESY experiment, H-4 correlation with H-4a, and between H-4a and H-5 and the methyl (9-CH₃) δ_{H} 1.27, and between H-5 and the methyl (6 β) δ_{H} 0.93 (**Figure 1**). The spectroscopic data established the structure of **1** to be 5-hydroxy-6,6,9-trimethyl-4,8a-epoxy-2,3,4a,5,6,7,8a,9-octahydro-4*H*-naphtho[2,3-*b*]furan-8-one¹ (**Figure 1**), namely stereumone A.

Compound **1**: Yellowish amorphous solid, $[\alpha]_{\text{D}}^{22} +112$ (*c* 0.25, acetone), ESIMS⁻ m/z 263 [M - H]⁻; IR (KBr) ν 3438, 2958, 1718 (s), 1654, 1138, 1089 cm⁻¹. The ¹H- and ¹³C-NMR spectral data see **Table 1**.

Acknowledgments

The authors gratefully acknowledge support for this work from the Natural Science Foundation of Yunnan Province (2004C00032), the Key Applied Foundation Program of Yunnan Province (1999C0001Z) and the Ministry of Science and Technology of P. R. China (2002BA901A21).

Reference

1. S. R. Peraza-Sanchez, D. Chavez, H. B. Chai *et al.*, *J. Nat. Prod.*, **2000**, 63(4), 492.

Received 11 April, 2005