Chinese Chemical Letters Vol. 16, No. 5, pp 613-615, 2005
http://www.imm.ac.cn/journal/ccl.html

A New Compound Isolated from a Bioactive Streptomycete

Yi Qing LI[1], Xue Shi HUANG[2], Ming Gang LI[1], Isabel SATTLER[2],
Meng Liang WEN[1]*, Susanne GRABLEY[2]

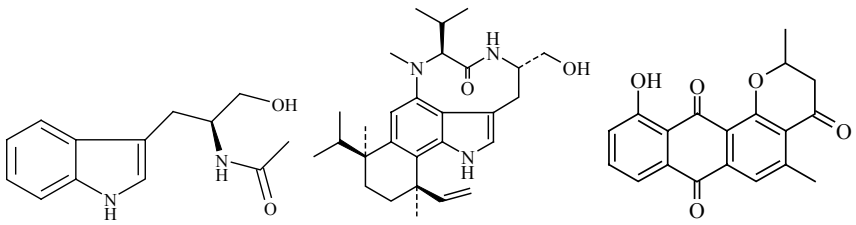
[1] The Key Laboratory for Microbial Resources of the Ministry of Education, Yunnan Institute of Microbiology, Yunnan University, Kunming 650091
[2] Hans-Knöll-Institute for Natural Product Research Beutenbergstraße 11a, D-07745 Jena, Germany

Abstract: A new compound, named (*S*)-α-acetylamino-β-(3-indole)propanol (**1**) was isolated, along with two known compounds teleocidin B1 and emycin B from culture broth of a streptomycete strain YIM33176 (*streptomyces pleomorphus*). The structure of **1** was determined by detailed spectroscopic investigation.

Keywords: Streptomycete, (*S*)-α-acetylamino-β-(3-indole)propanol , teleocidin B1, emycin B.

Strain YIM33176 (*streptomyces pleomorphus*) is a streptomycete isolated from the soil sample collected from Dali, Yunnan province, China. In previous studies on the actinomycetes resources, we found the metabolites of this strain had the potential antitumor activity. With the application of a chemical screening[1], a new compound, named (*S*)-α-acetylamino-β-(3-indole)propanol **1**, and two known compounds teleocidin B1 and emycin B were isolated from the culture broth of this strain. In this paper, we present the structural elucidation of the new compound.

Compounds **2** and **3** were identified as teleocidin B1 **2** and emycin B **3**, respectively by comparing their spectra data (^{1}H NMR, ^{13}C NMR, DEPT and ESIMS) with literatures[2, 3].



1 **2** **3**

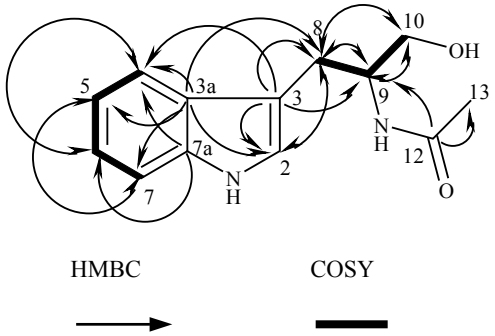
* E-mail: mlwen@ynu.edu.cn

Compound **1**, white amorphous powder, $[\alpha]_D^{25}$ + 27 (*c* 1.2, $CHCl_3$), has a molecular formula $C_{13}H_{16}N_2O_2$ determined by the quasi-molecular weight at *m/z* 233.2 $[M+H]^+$, 255.2 $[M+Na]^+$, 487.3 $[2M+Na]^+$ and 231.2 [M-H] (calcd. for $C_{13}H_{16}N_2O_2$, 232.1212) as well as NMR data. The UV absorption at 221 (logε 4.49), 281 (logε 3.77) nm were similar to those of indol skeleton. The IR spectrum suggested the presence of hydroxyl group (3285 cm^{-1}) and carbonyl group (1650 cm^{-1}). The ^1H NMR spectrum of **1** showed one acetate signal at δ 1.89 (s, 3H), a methylene at δ 2.89 (dd, 1H, J=6.85, 14.6 Hz) and 3.01 (dd, 1H, J=6.85, 14.6 Hz), an oxymethylene at δ 3.52 (dd, 1H, J=5.65, 11.4 Hz) and 3.58 (dd, 1H, J=5.65, 11.4 Hz), a methine at δ 4.20 (m, 1H) as well as five aromatic protons at δ 7.06 (s, 1H, H-2), 7.31 (br. d, 1H, *J* = 7.85 Hz, H-7), 7.08 (m, 1H, H-6), 7.00 (m, 1H, H-5) and 7.60 (br. d, 1H, *J* = 7.85 Hz, H-4), which were similar to those of Na-Ac-tryptophan[4]. The ^{13}C NMR and DEPT spectra (see **Table 1**) of **1** showed 13 carbons, including three aromatic quaternary carbons and a carbonyl carbon. The spin systems (see **Figure 1**) of COSY spectrum indicated the fragment: CH_2CH (NR) CH_2OH in **1**. HMBC experiment (see **Figure 1**) showed the attachment sites of the fragments. According to the optical rotation of **1** showing the similar positive value as that of (S)-N_a-Ac-tryptophan[4], the absolute configuration of C-9 in **1** is the same as (S)-N_a-Ac-tryptophan. Thus, the structure of **1** is determined as (S)-α-acetylamino-β-(3-indole)propanol.

Table 1 The data of ^1H NMR (300 MHz, $CDCl_3$), ^{13}C NMR (75 MHz, $CDCl_3$ δ ppm) of **1**

Position	δ_H	δ_C	DEPT
2	7.06 s, 1H	124.2	CH
3		112.3	C
3a		129.1	C
4	7.60 br. d, 1H, *J* = 7.85 Hz	119.6	CH
5	7.00 m, 1H	119.8	CH
6	7.08 m, 1H	22.3	CH
7	7.31 br. d, 1H, *J* = 7.85 Hz	112.2	CH
7a		138.0	C
8	2.89 dd, 1H, *J* = 6.85, 14.6 Hz	27.6	CH_2
	3.01 dd, 1H, *J* = 6.85, 14.6 Hz		
9	4.20 m, 1H	53.6	CH
10	3.52 dd, 1H, *J* = 5.65, 11.4 Hz	64.2	CH_2
	3.58 dd, 1H, *J* = 5.65, 11.4 Hz		
12		173.2	C
13	1.89 s, 3H	22.8	CH_3

Figure 1 The correlation of HMBC and COSY of compound **1**



Acknowledgments

We thank Dr. Gollmick, Dr. Berg and colleagues in HKI for recording spectral data, large-scale fermentation and initial workup procedures. This work was performed in the course of a collaboration project between the Hans-Knöll-Institute for Natural Product Research (HKI) and Yunnan Institute of Microbiology (YIM), Yunnan University. Funded granted by the German Federal Ministry for Education and Research (Grant No. CHN 01/328) and Yunnan Provincial Science and Technology Department (Grant No. 2002GH02).

References

1. S. Grabley, R. Thiericke, A. Zeeck, *Drug Discovery from Nature* (Eds.: S. Grabley, R. Thiericke), Springer Verlag, Berlin, **1999**, 124.
2. Y. Hitotsuyanagi, *et al*., *Chem. Pharm. Bull.*, **1984**, *32*, 4233.
3. J. Rohr, *J. Org. Chem.*, **1992**, *57*, 5217.
4. P. B. Holst, *et al*., *Acta Chem. Scand.,* **1998**, *52*, 683.

Received 22 April, 2004