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BRIEF COMMUNICATIONS

A NEW PROPANOL DERIVATIVE FROM MARINE *Pseudomonas* sp. M474

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Marine microorganisms have proved to be rich sources of bioactive secondary metabolites, and numerous compounds with potent biological activities and unique chemical structures have been isolated [1]. As terricolous microorganisms, marine microorganisms are new and important sources of bioactive compounds, including terpenes, polyketides, flavonoids, peptides, alkaloids, and many unidentified and uncharacterized structures [2]. Marine *Pseudomonas* is also a new and important resource, and propanol derivatives are reported from them for the first time.

In our screening program for bioactive principles from marine *Pseudomonas*, a new propanol derivative was isolated from the acetic ether extract of marine *Pseudomonas* sp. M474. In this paper, we report the isolation and structure elucidation of this new propanol derivative on the basis of analysis of the spectral data, including 1D and 2D NMR spectroscopic data.

The strain M474 has been derived from sediment of *Jiaozhou* Bay in China. It was isolated on Gause′s starch medium with incubation at 28°C. The pure culture was maintained on Gause′s starch agar medium with $K_2Cr_2O_7$ at 4°C. The strain forms a yellow soluble pigment. Due to its chemical and morphological features, as well as the 16S rRNA, the strain can be classified as a marine *Pseudomonas* species. The strain is deposited in the culture collection of marine microorganisms at the Institute of Oceanology, Chinese Academy of Sciences.

The marine strain *Pseudomonas* sp. isolate M474 was inoculated from its slant agar culture on M_2+ agar plates with 50% seawater. It formed yellow colonies with a gray aerial mycelium on incubation at 28°C. With fresh agar cultures of the strain, 100 1-L Erlenmeyer flasks each containing 250 mL of M_2+ medium (set to pH 7.8 before sterilization) were inoculated and grown for 4 days at 28°C with shaking at 120 rpm. The entire culture broth was mixed with ca. 1 kg of diatomaceous earth and pressed through a pressure filter, and both filtrate and residue were extracted with acetic ether. The combined extracts were evaporated to dryness to yield 12 g of the crude extract. The crude extract was subjected to middle-pressure LC with methanol–H_2O gradient to yield 32 fractions. Then the fraction (100 mg) was chromatographyed on a C_8 half-preparative column (Zorbax columns, R_X-C_8, 9.4 mm × 25 cm) using isocratic elution of CH_3CN–H_2O (30:70), yielding a novel propanol derivative (5 mg).

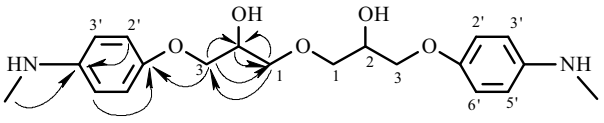

Fig. 1. Key HMBC correlations of compound **1**.

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TABLE 1. ^{1}H (600 MHz) and ^{13}C (125 MHz) NMR Spectral Data of Compound **1** in CD_3OD (δ, ppm, J/Hz)

C atom	δ_H	δ_C	HMBC	C atom	δ_H	δ_C	HMBC
3, 3	3.9 (4H, m)	70.39	C-1, C-2, C-1′	2′, 6′	6.82 (4H, d, J = 6.6)	115.02	C-2′, C-4′
2, 2	4.1 (2H, m)	71.86	C-1	3′, 5′	7.11 (4H, d, J = 7.2)	128.75	C-3′, C-1′
1, 1	3.5 (4H, m)	64.25	C-2, C-3	4′		144.66	
1′		158.22		N-CH_3	1.59 (6H, s)	31.53	C-4′

Compound **1** was determined to be $C_{20}H_{28}N_2O_5$ on the basis of high-resolution ESI–MS [$(M+Na)^+$, 399.1896 *m/z*] in combination with ^{1}H and ^{13}C NMR data. The ^{1}H and ^{13}C NMR data (Table 1) with DEPT and HMQC data suggested the presence of three methines (δ_C 128.75, 115.02, 71.86), including one oxygenated methine, two oxygenated methylenes (δ_C 70.39, 64.25), a methyl (δ_C 31.53), and two quaternary carbons (δ_C 158.22, 144.66). On the basis of the formula, the compound is highly symmetry. In the ^{1}H NMR spectrum, signals at δ 7.11 (2H, m, J = 7.2 Hz) and 6.82 (2H, m, J = 6.6 Hz) indicated the presence of an *ortho*-substituted aromatic ring. The ^{1}H–^{1}H COSY spectrum indicated the presence of one partial structure. The presence of this partial structure was confirmed by the HMBC spectrum (Table 1 and Fig. 1). The quaternary carbon δ_C 158.22 was long-range coupled to the δ_H 4.1, and the quaternary carbon δ_C 144.66 was long-range coupled to the δ_H 1.8. Because of its symmetry, the structure of **1** was elucidated as shown in Fig. 1 and named di-[2-hydroxy-3-(4′-(methylamino)phenoxy)]propyl ether.

This compound showed no antibacterial activity against *E. coli*, *S. aureus,* and *B. subtilis*. In the cytotoxicity experiment, it only showed quite weak activity towards HL-60 cell line.

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