Research Article ISSN 2689-1050

Chemical & Pharmaceutical Research

A New Homomonoterpenoid of Plectranthus Amboinicus

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Received: 02 Apr 2022; **Accepted:** 25 Apr 2022; **Published:** 01 May 2022

Citation: Zhang Jian YP, Kao CL, Tsai YS, et al. A New Homomonoterpenoid of Plectranthus Amboinicus. Chem Pharm Res. 2022; 4(2): 1-3.

ABSTRACT

*A novel homomonoterpenoid, amboinol (**1**) was isolated from the stems of Plectranthus amboinicus (Lamiaceae). The structure of the new compound was unambiguously elucidated on the basis of extensive spectroscopic-data analysis and comparison with literature data.*

Keywords

Plectranthus amboinicus, Lamiaceae, Homomonoterpenoid.

Introduction

Herbal medicines are very commonly used in Unani, Ayurveda, Sidda, folk and other traditional practices of healthcare management [1]. The Lamiaceae members of plant species belonging to commercially important genera, such as *Plectranthus*, *Salvia*, *Ocimum* and *Mentha*, are attributed with a rich diversity of ethnobotanical benefits [2]. In over 85% of the literature, documentation of *Plectranthus* is on the therapeutic values of this genus followed by its nutritional and horticultural properties attributed to its aromatic nature and essential oil producing capability [3]. *Plectranthus amboinicus* (Loureiro) Sprengel is one of the most documented species in the family Lamiaceae. *P. amboinicus*, also commonly known as Indian borage, and is a fleshy, succulent herb famous for its distinct oregano-like flavor and odor [4]. The literature survey has emphasized the occurrence of different classes of phytocompounds including 76 volatiles and 30 non-volatile compounds [5]. Many studies have cited numerous pharmacological properties including antimicrobial, anti-inflammatory, antitumor, wound healing, anti-epileptic, larvicidal, antioxidant and analgesic activities [5]. Previously, we isolated 12 compounds, including four flavonoids, three benzenoids, one lignan, one quinol, and three steroids from the leaves of this plant [6]. In the course of screening for biologically and chemically novel agents from Formosan plants in the family Lamiaceae, *P. amboinicus* was chosen for further phytochemical investigation. In this paper, we report the isolation and structural elucidation of this novel homomonoterpenoid.

Results and Discussion

Amboinol (**1**) was obtained as a colorless oil and had the molecular formula $C_{11}H_{20}O$, was determined on the basis of the positive HRESIMS at m/z 191.1409 $[M + Na]^+$ (calcd 191.1412) and supported by the ^1H, ^{13}C, and DEPT NMR data. The IR spectrum revealed the presence of hydroxyl group absorption at 3300 cm^{-1}. The ^1H-NMR spectrum showed three methyls [δ 0.84,

0.85, 0.86 (each 3H, s), two methines [δ 1.62 (1H, t, J = 6.8 Hz), 4.01 (1H, m)], one of which belongs to oxymethine, and four methylenes at δ 0.94/2.27, 1.25, 1.25/1.72 and 1.25/1.89. The ^{13}C NMR spectrum and a DEPT experiments indicated that compound **1** had a total of eleven carbons, with the skeleton consisting of eleven carbons, consistent with a homomonoterpenoid. The carbons of the homomonoterpene were assigned, from ^{13}C NMR and DEPT experiments, as three methyls at δ 13.3, 18.6 and 20.2; four methylenes at δ 25.9, 28.3, 29.7 and 39.0; two methines at δ 45.1 and 77.4 and two quaternary carbons at δ 48.0 and 49.5. The structure of **1** was also confirmed by 2D NMR experiments. Examination of the ^{1}H-^{1}H COSY and ^{1}H-^{13}C COSY spectra provided one continuous fragment as shown by bold lines in Figure 1. The long-range couplings in the HMBC spectrum established the connectivity of these fragment units, including methyl groups, methylenes, and oxymethine, as shown in Figure 1, to furnish a 5,8,8-trimethylbicyclo[3.2.1]octan-6-ol skeleton.

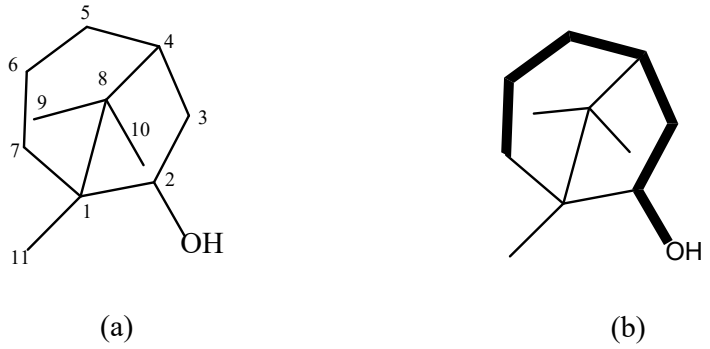

Figure 1: Chemical structure (a) and COSY (b) correlations of **1**.

In the ^{1}H NMR spectrum of **1**, the small coupling constants of H-4 and 2 indicated that the A/B ring is in an envelope conformation. NOE between H-7 and H-5ax, H-6ax and H-4, and H-3ax and H-2 together with long-range ^{1}H-^{1}H coupling between H-5 and H-4 (W arrangement), indicated a *cis* ring fusion in AB The chemical shift (δ 0.84) for the C-11 methyl group was also consistent with a *cis* ring fusion. From the observations described above, the structure of amboinol was concluded to be represented by formula **1**. However, because the small sample size precluded further examination, the absolute configurations of C-4/2 are still not clear. Thus, the structure of this compound was determined to be a new homomonoterpenoid, which was further confirmed by HMBC experiments (Table 1). The structure of **1** was determined to be 5,8,8-trimethylbicyclo[3.2.1]octan-6-ol and named amboinol (**1**).

Table 1: NMR data of **1** in $CDCl_3$ (δ in ppm, J in Hz, 400 MHz for ^{1}H NMR, and 100 MHz for ^{13}C NMR).

Position	δ_C	δ_H	mult., J (Hz)	HMBC (^{1}H → ^{13}C)
1	49.5	–	–	–
2	77.4	4.01	m	C-1, C-3
3	39.0	2.27 0.94	m m	C-2, C-4 C-2, C-4
4	45.1	1.62	t, 6.8	C-3, C-5, C-8
5	25.9	1.72 1.25	m m	C-4, C-6 C-4, C-6
6	28.3	1.25	m	C-5, C-7
7	29.7	1.89 1.25	m m	C-1, C-6 C-1, C-6
8	48.0	–	–	–
9-Me	20.2	0.85	s	C-1, C-4, C-8, C-10
10-Me	18.6	0.86	s	C-1, C-4, C-8, C-9
11-Me 2-OH	13.3 –	0.84 1.70	s br d	C-1, C-2, C-7, C-8 C-1, C-2, C-3

Materials and Methods

General

UV spectra were obtained in MeCN, IR spectra were measured on Hitachi 260-30 spectrophotometer. ^{1}H NMR (400 MHz), ^{13}C NMR (100 MHz), HETCOR, HMBC, COSY and NOESY spectra were obtained on a Varian (Unity Plus) NMR spectrometer. Low-resolution ESI-MS spectra were obtained on an API 3000 (Applied Biosystems) and high-resolution ESI-MS spectra on a Bruker Daltonics APEX II 30e spectrometer. Silica gel 60 (Merck, 70~230 mesh, 230~400 mesh) was used for column chromatography. Precoated Silica gel plates (Merck, Kieselgel 60 F-254), 0.20 mm and 0.50 mm, were used for analytical TLC and preparative TLC, respectively, visualized with 50% H_2SO_4.

Plant material

The specimen of *P. amboinicus* was collected from Kaohsiung City, Taiwan in May, 2015. A voucher specimen was identified by Professor Fu-Yuan Lu (Department of Forestry and Natural Resources College of Agriculture, National Chiayi University) and was deposited in the School of Medical and Health Sciences, Fooyin University, Kaohsiung, Taiwan.

Extraction and isolation

The leaves (1.2 kg) of *P. amboinicus* were chipped and airdried and extracted repeatedly with MeOH (2 L × 4) at room temperature. The combined MeOH extracts (26.3 g) were then evaporated and further separated into 8 fractions by column chromatography on silica gel (4.5 kg, 70-230 mesh) with gradients of *n*-hexane/CH_2Cl_2/acetone/MeOH. Part of fraction 1 (4.2 g) was subjected to silica gel chromatography by eluting with *n*-hexane-acetone (100:1), enriched with acetone to furnish five further fractions (1-1−1-5). Fraction 1-2 (1.1 g) was further purified on a silica gel column using *n*-hexane/acetone mixtures to obtain amboinol (**1**) (7.2 mg).

Amboinol (1). Colourless oil. $[\alpha]^{25}_{D}$ +24.4 (*c* 0.45, $CHCl_3$). IR (ν_{max}, cm^{-1}): 3400 (OH). ESI-MS *m/z* 191 $[M+Na]^+$; HR-ESI-MS *m/z* 191.1409 $[M+Na]^+$ (calcd for $C_{11}H_{20}ONa$, 191.1412). For ^{1}H and ^{13}C NMR, see Table 1.

Acknowledgments

This investigation was supported by a grant from the Fooyin University Hospital (FY-HR-108-14) awarded to C. Y. Chen and Y. S. Tsai.

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