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A New Carbohydrate of *Aquilaria Agallocha*

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ABSTRACT

*A new carbohydrate, agalloside ((2R,3S,4R,5R,6S)-2-(hydroxymethyl)-6- methoxytetrahydro-2H-pyran-3,4,5-triol) (**1**) was isolated from the flowers of Aquilaria agallocha. The structure was elucidated on the basis of physical and spectral analysis.*

Keywords

Aquilaria agallocha, Carbohydrate, Agalloside, Flowers.

Introduction

The genus *Aquilaria* (Thymelaeaceae) is widely distributed in Asia. *Aquilaria sinensis* (Lour.) Gilg. is of particular interest economically because it is the principal source of agarwood, one of the most highly valuable forest products currently traded internationally. The flowers of *A. sinensis* (Lour.) Gilg., which widely cultivated in Guangdong, Hainan and Taiwan provinces in China are orally reported to be used locally in trauma-related diseases such as fracture, bruise, etc [1]. Previous phytochemical investigation on Chinese eaglewood revealed characteristic sesquiterpenes and chromone derivatives [2-15]. Previously, we have isolated flavonoids, benzenoids, and steroids from this plant [16-26]. To further understand the chemotaxonomy and to continue searching for novel agents from Thymelaeaceous plants, the flower of *A. agallocha* were chosen for phytochemical investigation. In this paper, we report the isolation and structural elucidation of this new carbohydrate (agalloside (**1**)).

Agalloside (**1**) was obtained as pale yellow crystals from CH_3OH. Its molecular formula was deduced as $C_7H_{14}O_6Na$ by HR-ESI-MS (*m/z* 217.0684 ([M+Na]$^+$; calc. 217.0688)). The IR spectrum show absorption for hydroxyl group (3400 cm^{-1}). The ^{1}H NMR spectrum of **1** was closely identical to that of methyl-α-D-glucopyranoside [27] indicating the same sugar structure (Figure 1).

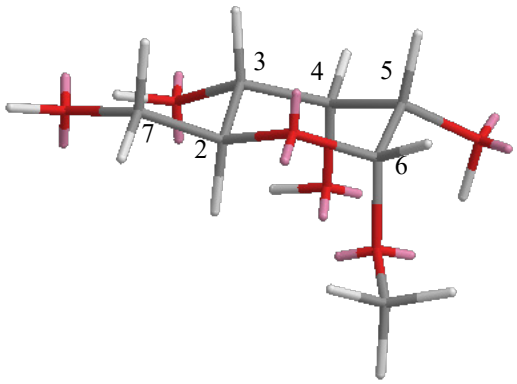

Figure 1: Structure of agalloside (**1**).

The full assignment of the carbon resonances based on HSQC and HMBC techniques are shown in Table 1. NOESY plot (Figure 2) showed correlations of both H–C(5) and H–C(7) to H–C(3), H–C(4) to H–C(2), and H–C(6) to H–C(5). In conclusion, **1** had the different relative configuration as the similar compound methyl-α-D-glucopyranoside [23]. The attachment of one oxymethylene group at C-2 was confirmed by the correlation between H-7/H-2

in NOESY spectrum. The full assignment of **1** was further confirmed by COSY, HSQC, and HMBC spectra. The ^{1}H- and ^{13}C-NMR (Table 1), COSY, NOESY, HSQC and HMBC (Table 1) experiments confirmed the structure as (2*R**,3*S**,4*R**,5*R**,6*S**)-2-(hydroxymethyl)-6-methoxytetrahydro-2*H*-pyran-3,4,5-triol, named as agalloside (**1**).

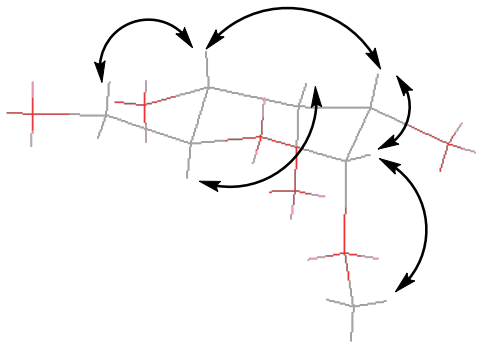

Figure 2: Key NOESY (↔) correlations of **1**.

Table 1: ^{13}C and ^{1}H NMR (Py-d_5 and CD_3OD) data of agalloside (**1**).

C#	δ_C	δ_H	mult., *J* (Hz)	HMBC (^{1}H → ^{13}C)
2	77.9	3.85	ddd, 9.6, 5.6, 2.4	C-3, C-4, C-6, C-7
3	71.2	4.10	t, 9.0	C-2, C-4, C-5, C-7
4	78.0	4.18	t, 9.0	C-2, C-3, C-5, C-6
5	74.6	3.93	dd, 9.0, 8.0	C-3, C-4, C-6
6	105.1	4.64	d, 8.0	C-4, C-5, OCH_3
7a 7b	62.3	4.25 4.45	dd, 12.0, 5.6 dd, 12.0, 2.2	C-2, C-3 C-2, C-3
OCH_3	56.5	3.56	s	C-6

Experimental

General

IR spectra were measured on a Hitachi 260-30 spectrophotometer. ^{1}H NMR (400 MHz) and 2D spectra were obtained on Varian-Mercury-400 spectrometers. 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. The anion-exchange resin, di-ethyl-amino-ethyl (DEAE) sephacel™ (GE healthcare, USA) was used for column chromatography.

Plant Material

The specimen of *A. agallocha* was collected from Shanshang District, Tainan City, Taiwan in May, 2011. 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 flowers (853 g) of *A. agallocha* were air dried and extracted repeatedly with MeOH (2 L × 5) at room temperature. The combined MeOH extracts (83.6 g) were then evaporated and further separated into 5 fractions by column chromatography on silica gel (5.5 kg, 70-230 mesh) with gradients of *n*-hexane/CH_2Cl_2/MeOH. Part of fraction 5 (14.8 g) was subjected to silica gel chromatography by eluting with EtOAc-MeOH (1:8), enriched with MeOH to furnish three further fractions (5-1−5-3). Fraction 5-3 (5.2 g) was further purified on a silica gel column using EtOAc/MeOH mixtures to obtain agalloside (**1**) (33.6 mg).

Agallooside (**1**): Pale yellow crystals. mp 177-179 °C. $[\alpha]^{25}_{D}$ + 33.6° (c 0.23, MeOH). IR (KBr, $_{max}$, cm^{-1}) ν_{max}: 3400 (OH) cm^{-1}. HR-EI-MS: *m/z* $[M+Na]^+$ calcd for $C_7H_{14}O_6Na$: 217.0688; found: 217.0684. ^{1}H and ^{13}C NMR (400 MHz, Py-d_5 and CD_3OD, δ, ppm, J/Hz): see Table 1.

Acknowledgment

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