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A NOVEL 6-BUTYL-3-HYDROXYFLAVANONE FROM HEARTWOOD OF *BAUHINIA PURPUREA*

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Key Word Index—*Bauhinia purpurea*; Leguminosae; heartwood; 6-butyl-3-hydroxyflavanone; 6-(3″-oxobutyl)taxifolin.

Abstract—Three glycerol derivatives and a novel 6-butyl-3-hydroxyflavanone derivative were isolated from the heartwood of *Bauhinia purpurea* L. The latter compound was elucidated as 6-(3″-oxobutyl)taxifolin on the basis of spectral evidence.

INTRODUCTION

Thirteen species of *Bauhinia* have been transplanted to Taiwan from different foreign locations. Only one species, *B. championii*, is indigenous to Taiwan. Chemical studies on this species reported flavones and cyanide compounds [1, 2]. *Bauhinia purpurea* is a popular ornamental plant in Taiwan. Chemical studies [3, 4] of the methanolic extract from seeds of this plant identified flavonoids and their glycosides. In previous work [5], we have isolated 22 compounds including flavonoids, phenols, chromones and sugars from the methanolic extract of heartwood of *B. purpurea*. In the present study, we reinvestigated in detail the same extract and three glycerol derivatives, 2,3-dihydroxypropyl oleate [6], 2,3-dihydroxypropyl linoleate [7], 2,3-dihydroxypropyl 16-hydroxyhexadecanoate [8], together with a novel 6-butyl-3-hydroxyflavanone, 6-(3″-oxobutyl)-taxifolin (**1**), were obtained.

RESULTS AND DISCUSSION

Compound **1**, pale yellow prisms, mp 125–126°, was formulated as $C_{19}H_{18}O_8$ on the basis of its HR mass spectrum. The IR absorption bands showed it contained hydroxyl (3393 cm^{-1}), carbonyl and conjugated carbonyl groups (1710 and 1686 cm^{-1}), and an aromatic group (1627 and 1581 cm^{-1}). It also gave a positive Mg–HCl test. The UV spectrum at λ_{max} (MeOH): 253 and 293 nm, as well as NMR signals of an AB-system at δ 4.58 (*d*, J = 11.4 Hz, H-3) and 5.0 (*d*, J = 11.4 Hz, H-2) indicated that **1** is a 3-hydroxyflavanone [9]. A chelated OH group at C-5 is responsible for a low-field signal at δ 12.01 (*s*) and a bathochromic shift upon addition of $AlCl_3$ which did not change in the presence of HCl. The addition of sodium acetate caused a bathochromic shift that suggests that the C-7 hydroxyl is free. Signals due to three aromatic protons were discernible at δ 6.82 (1H, *d*, J = 8.1 Hz), 6.88 (1H, *d*, J = 8.1, 1.9 Hz), and 7.05 (1H, *d*, J = 1.9 Hz) and these could be readily assigned to a 1,3,4-trisubstituted B ring with 1,2-oxygenation. A singlet at δ 5.99 (1H) and the signals at δ 2.62 and 2.72 (each 2H, *t*, J = 4.8 Hz) and 2.12 (3H, *s*) suggested a 3-oxobutyl group substituted at C-6 or C-8. By comparison of ^1H and ^{13}C NMR data (Table 1) of **1** and taxifolin **2** [5], compound **1** can be assigned as 6- or 8-(3″-oxobutyl)taxifolin. The HMBC correlation of **1** is shown in Fig. 1. This evidence confirmed the structure of **1** as 6-(3″-oxobutyl)taxifolin.

EXPERIMENTAL

General

Mps are uncorr. ^1H and ^{13}C, NOE and HMBC spectra were run on Bruker AM-300 spectrometer.

Plant material

The heartwood of *B. purpurea* L. was collected in September 1993 on the campus of the National Taiwan University. Plant material was identified by Mr Gun Muh-Tsuen, formerly a technician of the Department of Botany, National Taiwan University. A voucher specimen is deposited at the National Research Institute of Chinese Medicine, Taipei, Taiwan.

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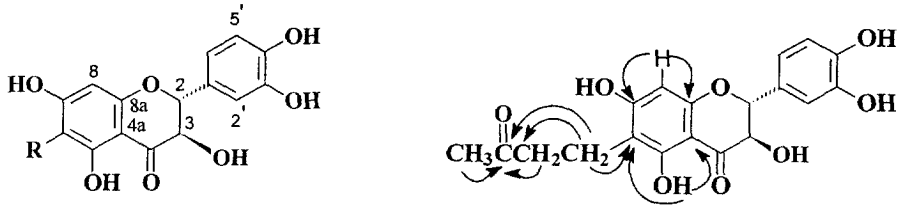
Table 1. ^1H (300 MHz) and ^{13}C NMR (75 MHz) spectral data of compounds **1** and **2**

H	2	1	C	2	1
2	5.03 *d* (11.4)	5.00 *d* (11.4)	2	84.3	84.2
3	4.63 *d* (11.4)	4.58 *d* (11.4)	3	73.0	72.9
6	5.94 *d* (0.8)		4	198.0	198.1
8	5.98 *d* (0.8)	5.99 *s*	5	164.8	161.8
2′	7.06 *d* (1.9)	7.05 *d* (1.9)	6	96.9	108.3
5′	6.82 *d* (8.1)	6.82 *d* (8.1)	7	167.6	165.1
6′	6.89 *dd* (8.1, 1.9)	6.88 *dd* (8.1, 1.9)	8	95.8	95.5
5-OH	11.69 *s*	12.01 *s*	8a	164.0	161.7
1″		2.72 *t* (4.8)	4a	101.4	101.1
2″		2.62 *t* (4.8)	1′	129.3	129.5
4″		2.12 *s*	2′	115.7	115.6
			3′	145.5	145.4
			4′	146.4	146.3
			5′	115.6	115.5
			6′	120.7	120.5
			1″		30.6
			2″		42.8
			3″		208.9
			4″		27.9



1 R=$CH_2CH_2C(=O)CH_3$ (1″ 2″ 4″)

2 R=H

Fig. 1. The HMBC correlation of **1**.

Extraction and isolation

Pieces of heartwood (10 kg) were extracted ×3 with MeOH (30 l) at 60° (6 d for each time). The crude extract was evapd *in vacuo* to leave a black syrup (390 g), to which H_2O (1 l) was added. The aq. layer was partitioned ×5 with *n*-BuOH (1 l). The upper layer was evapd *in vacuo* to yield residue (85 g) which was subjected to chromatography on silica gel and HPLC, repeatedly. 2,3-Dihydroxypropyl oleate (20 mg), 2,3-dihydroxypropyl linoleate (41 mg), and 2,3-dihydroxypropyl 16-hydroxyhexadecanoate (78 mg) were eluted using 40% EtOAc in hexane, and compound **1** (23 mg) was purified using 90% EtOAc in hexane.

6-(3″-Oxobutyl)taxifolin **1**

Mp 125–126°, $[\alpha]_D^{21}$ +17.5° (*c* 1.5, Me_2CO). UV (MeOH) λ_{max} (log ϵ) 253 (3.57), 293 (4.29); +$AlCl_3$ 272 (3.45), 304 (4.87); +NaOAc 268 (3.27), 332 (4.36). IR ν_{max}^{KBr} cm^{-1}: 3393, 3030, 1710, 1686, 1627, 1581, 1270, 1160 and 1084 cm^{-1}. EIMS (70 eV) *m/z* (rel. int.): 374 (50), 356 (60), 345 (20), 150 (100), 123 (65), 69 (35). HRMS calcd for $C_{19}H_{18}O_8$: 374.3464; found: 374.3456. ^1H and ^{13}C NMR: Table 1.

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