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A New Flavone of *Passiflora Edulis*

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ABSTRACT

A new flavone, 5-hydroxy-7,2',3',5'-tetramethoxyflavone (1) was isolated from the leaves of Passiflora edulis. The structure of the new flavone was elucidated by chemical and physical evidence.

Keywords

Passiflora edulis, Flavone, Leaves.

Introduction

The genus *Passiflora* comprises approximately 450 species, but only a few are commercially exploited. *Passiflora edulis*, usually called passion fruit, is the best known among them. It originated in Brazil and is now being cultivated in many other countries for its edible fruits and pharmacologic properties [1]. In fact, *P. edulis* is very popular, not only because of its pleasant fruits but also because the infusion of their leaves has been largely used in American and European countries as sedative or tranquilizer, being much appreciated due to its agreeable taste [2]. Leaf extracts are also used in many pharmaceutical preparations and are widely employed as a flavor and as a juice by the food industries [3]. Besides the anxiolytic effects, *P. edulis* leaves are recognized for their anti- inflammatory activity [4-7]. In continuation of some studies of chemotaxonomy and biologically active metabolites from this plant, a methanol extraction of the leaves of *P. edulis* afforded 12 known compounds, including four flavonoids, two amides, three benzenoids, one lignan and one steroid [8]. In this paper, we report the isolation and structural elucidation of this new flavone.

Compound 1, $C_{19}H_{18}O_7$ $[M + Na]^+$ at *m/z* 381, yellow needle crystals from methanol, mp. 195-197 °C, was isolated first. In the IR spectrum, bands for hydroxyls (3600 cm^{-1}) and hydrogen-bonded carbonyl (1665 cm^{-1}) were observed. The UV spectrum disclosed an absorption maximum at 268 nm attributable to the benzoyl moiety in A-ring of a flavonoid among other bands [9]. Its ^1H NMR spectrum showed flavone-nucleus with two *meta*-coupled protons at δ 6.68 (H-8, J = 2.0 Hz) and 6.41 (H-6, J = 2.0 Hz). Its ^1H NMR spectrum showed flavone-nucleus protons with one singlet (1H each) at δ 6.59 for C-3 plus two doublets (1H each) with chemical shifts and coupling constants typical of *meta*-coupled protons at δ 7.17 (H-6′, J = 2.0 Hz) and 6.95 (H-4′, J = 2.0 Hz). Resonances between δ 3.91 and 4.00 due to four methoxyl groups were clearly observed when ^1H NMR spectrum was determined in $CDCl_3$. The presence of a hydrogen-bonded hydroxyl proton signal at δ 12.34 indicated that the hydroxyl group must be at C-5. A signal at δ 181.6 assignable to carbonyl carbon was discernible in the ^{13}C NMR spectrum. The sequential correlation of the NOESY spectrum were successfully established as shown in Figure 1. Thus, the structure of this compound was determined to be 5-hydroxy-7,2′,3,5′-tetramethoxyflavone (1), which was further confirmed by HMBC experiments (Table 1).

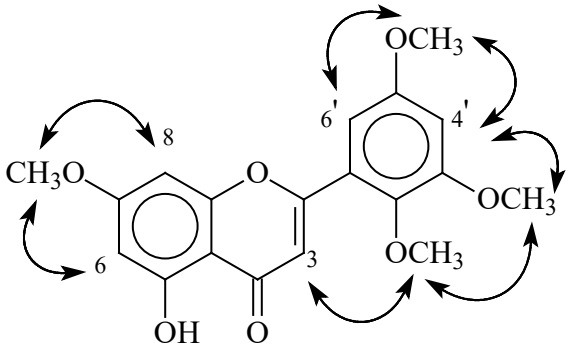

Figure 1. NOESY experiments of 5-hydroxy-7,2′,3′,5′-tetramethoxy-flavone (1).

Table 1: ^{13}C (100 MHz, $CDCl_3$) and ^{1}H HMR (400 MHz, $CDCl_3$) data of 5-hydroxy-7,2′,3,5′-tetramethoxyflavone (**1**).

C#	δ_C	δ_H	mult., *J* (Hz)	HMBC ($^{1}H \rightarrow {}^{13}C$)
2	161.7	-	-	-
3	110.1	6.59	s	C-2, C-4, C-4a, C-1′
4	181.6	-	-	-
4a	105.4	-	-	-
5	161.9	-	-	-
6	98.1	6.41	d, 2.0	C-4a, C-5, C-7, C-8
7	164.8	-	-	-
8	92.1	6.68	d, 2.0	C-6, C-7, C-4a, C-8a
8a	157.2	-	-	-
1′	120.1	-	-	-
2′	149.2	-	-	-
3′	146.3	-	-	-
4′	103.5	6.95	d, 2.0	C-3′, C-5′
5′	147.1	-	-	-
6′	105.8	7.17	d, 2.0	C-1′, C-5′
5-OH	-	12.34	br s	C-5
7-OCH_3	56.6	3.91	s	C-7
2′-OCH_3	61.3	4.00	s	C-2′
3′-OCH_3	61.4	3.97	s	C-3′
5′-OCH_3	61.4	3.99	s	C-5′

Experimental

General

IR spectra were measured on a Hitachi 260-30 spectrophotometer. ^{1}H NMR (400 MHz, C_5D_5N) 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. edulis* was collected from Daliao District, Kaohsiung City, Taiwan in April, 2010. 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 (2.4 kg) of *P. edulis* were airdried and extracted repeatedly with MeOH (4 L× 4) at room temperature. The combined MeOH extracts (42.6 g) were then evaporated and further separated into 8 fractions by column chromatography on silica gel (8.7 kg, 70-230 mesh) with gradients of *n*-hexane/CH_2Cl_2/acetone/ MeOH. Part of fraction 8 (7.3 g) was subjected to silica gel chromatography by eluting with *n*-hexane-acetone (35:1), enriched with acetone to furnish five further fractions (8-1−8-5). Part of fraction 8-2 (1.5 g) was subjected to silica gel chromatography by eluting with *n*-hexane-acetone (50:1) and enriched gradually with acetone to furnish five fractions (8-2-1−8-2-5). Fraction 8-2-3 (0.2 g) was separated by preparative TLC (*n*-hexane-acetone, 45:1) to afford 5-hydroxy-7,2′,3′,5- tetramethoxyflavone (1) (8 mg).

5-hydroxy-7,2′,3′,5′-tetramethoxyflavone (1)

Yellow needles (MeOH), mp 195-197 °C, UV λ_{max} 268, 297, 355 nm, IR ν_{max} 3600, 1665, 1590 cm^{-1}, ESI-MS *m/z* 381 $[M + Na]^+$; HR-ESI-MS *m/z* 381.0952 $[M + Na]^+$ (calcd for $C_{19}H_{18}O_7Na$, 381.0950). ^{1}H NMR (400 MHz, $CDCl_3$) : see Table 1; ^{13}C NMR (100 MHz, $CDCl_3$) (Table 1).

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