黄果西番莲中的一个新内酯类成分

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摘要:从黄果西番莲 (*Passiflora edulis Sims*) 压榨果汁中分离得到一个新的内酯类成分,波谱技术鉴定其结构为西番莲内酯。该化合物未显示对 DPPH 自由基的清除活性。

关键词: 黄果西番莲; 西番莲内酯; DPPH

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A New Lactone from Passiflora edulis (Passifloraceae)

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Abstract: A new unsaturated hexalactone named passiflactone (1) has been isolated from the petroleum ether extract of crude juice of *Passiflora edulis* Sims. The structure was identified on the basis of extensive NMR and MS techniques. No antioxidative effect was observed for compound 1 against DPPH scavenging assay.

Key words: Passiflora edulis; Passiflactone; DPPH assay

The *Passiflora* is the largest genus in the family Passifloraceae, which includes about 500 species, distributing over temperate and tropical zones of the world. The plants of this genus are shrubs and herbs, some of them are grown in the tropics for their edible fruits, many others are grown outdoors in the warmer part of the world for their exotic flowers. Passiflora edulis Sims, known as passion fruit, is the most widely grown plant of the genus Passiflora, its leaves are used in the treatment of sedative, diuretic, tonic, hypertension, skin diseases, anthelmintic, anti-diarrheal, menopausal symptoms, colic of infants and dysentery (Dhawan et al. 2004; Jamir et al. 1999), while, the fruits are used as digestive stimulant and gastric carcinoma, in addition, fruits of Passiflora edulis is well known for its unique flavor as popular juice. To date, much investigations has been done on this plant. The

structure types covered glycosides, phenols, alkaloids, carotenoids, L-scorbic acid, ahocyanins, -lctones, favor components, volatile oil constituents, carbohydrates, minerals, enzyme cytoplasmic pyruvate kinase, ccloartane triterpenes (Dhawan *et al.* 2004). Pharmacological effects involved non specific CNS depressant effects of the aqueous extracts, mild anti-fungal activity against Microsporum gypseum, Chrysosporium tropicum and Trichophyton terrestre (Dhawan *et al.* 2004). During our phytochemical investigation on *Passiflora edulis* cultured in southwest China, a new compound, passiflactone, was readily isolated by liquild-liquild partition following by re-crystallization. Herein, we reported its isolation and structure elucidation.

Passiflactone (1) was purified from the petroleum ether extract of the crude juice of *Passiflora edulis* as colorless needles. The UV maximum absorption at 310

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nm indicated the presence of conjugated ketone group. The high-resolution EIMS implied a molecular formula of $C_8 H_8 O_4 [M + Na]^+$ at m/z 191.0325 (calcd. for C₈ H₈ O₄Na 191.0320). The ¹ H NMR displayed three singlets at 5.90, 2.62 and 2.23, respectively. Two methyls, one methine and five quarternary carbons were demonstrated in the 13 C NMR and DEPT spectra, thereinto, the signal resonated at 205.2 was assigned as ketone due to its chemical shift, the signals at 161.2, 169.0 and 181.0 were oxygen atom bearing carbons. Due to the scarcity of proton-proton spin system, the assembly of backbone was completely performed via HMBC interactions. The observation of HM-BC correlations of H-8 with C-7 and C-4, H-5 with C-3, C-4, C-6, C-7 and C-9, H-9 with C - 5 and C- 6 indicated the partial structure of C- 3 to C-9. Taking the chemical shifts of C-2, C-3, C-6 and the degrees of unsaturation into account, the remaining moiety should be a lactone functional group and C - 2 linked with C - 6 via oxygen atom. Thus, the structure of compound 1 was assigned as 4-acetyl-3hydroxy-6-methyl-pyran-2-one.

Passiflora species are very popular, not only because of their fruits, but also because the tea of their leaves has been largely used in America and European countries as a folk medicine. The phytochemical investigations of leaves extracts from *P. alata* and *P. edulis* has been extensively studied over the past decades, however, passiflactone as a new natural occurring product was the first isolation in the genus of Passiflora, which will add new facet for the structure profile of this plant. Considering the presence of ketone-enol functional group, antioxidant efficiency of 1 was evaluated against DPPH scavenging assay, only slight effect was observed even at a concentration of 300 µg/mL.

Experimental

General Experimental Procedures Melting point was determined on a XRC-1 micro-melting point apparatus and was uncorrected. UV spectrum was recorded on a Shimadzu UV-2401PC spectrophotometer. ¹H (400 MHz) and ¹³ C NMR (100.6 MHz) spectra were recorded at 300 K on a Brucker AM-400 spectrometer in CDCl₃ with TMS as an internal reference. HMBC spectrum were measured with a Bruker DRX-500 spectrometer. EFMS, including high resolution EFMS was carried out on a VG Auto Spec-3000 spectrometer.

Plant Material The fruits of *Passiflora edulis* Sims were collected at Jiangcheng County of Yunnan Province, China, in September 2004. The species was presented by Mrs. Jia Wang at the Xishuangbanna Green Ecological Food Corporation Limited, who was responsible for collection of cultured *P. edulis* around foregoing reagion.

Extraction and Purification The fresh fruits of P. edulis (1.25 kg) were coldly squeezed to afford the crude juice (450 g). The crude juice was diluted with water and followed by partition against petroleum ether, EtOAC and r-BuOH, respectively. Removal of part solvent from petroleum ether extracts under reduced pressure and placement at ambient temperature yielded colorless needles, which was recrystalized to afford 1 (80.0 mg).

4-acetyl-3-hydroxy-6-methyl-pyran-2-one (1): colorless needle; mp: 105- 107; UV max (CHCl₃) nm: 310 (log 4.08), 212 (log 3.57); 1 H NMR (400 MHz, CDCl₃): 5.90 (1H, s, H-5), 2.62 (3H, s, H-8), 2.23 (3H, s, H-9); 13 C NMR (100 MHz, CDCl₃): 205.2 (s, C-7), 181.0 (s, C-3), 169.0 (s, C-6), 161.2 (s, C-2), 101.4 (d, C-5), 99.8 (s, C-4), 30.1 (q, C-8), 20.7 (q, C-9); EMS m/z: 168 (100) [M] ${}^{+}$, 153 (85) [M-Me] ${}^{+}$, 125 (40) [M-Ac] ${}^{+}$, 85 (72). HREIMS m/z: 191.0325 (calcd. for $C_8H_8O_4Na$ 191.0320).

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