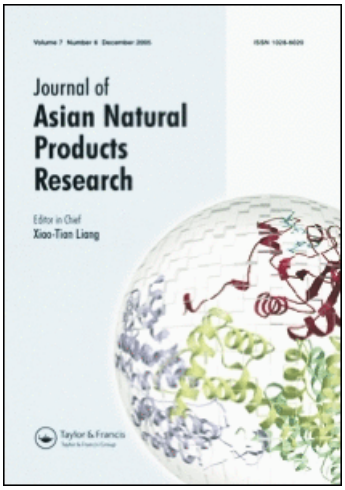

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A new flavonol from *Sophora tonkinensis*

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A new flavonol, tonkinensisol, was isolated from the roots of *Sophora tonkinensis*, together with three known compounds named as bayin, vitexin and lupeol. Their structures were elucidated on the basis of spectroscopic evidence. Additionally, tonkinensisol showed moderate cytotoxicity suppressing the proliferation of HL-60 cells *in vitro*.

Keywords: *Sophora tonkinensis*; Tonkinensisol; Vitexin; HL-60

1. Introduction

The roots of *Sophora tonkinensis* Gapnep ("Shan Dou Gen" in Chinese) have been used as an antipyretic, diuretic, stomachic and anti-tumour agent in traditional Chinese medicine. Phytochemical studies have yielded more than 80 compounds, including alkaloids, flavones and triterpenoid saponins, which exhibited anti-virus [1], anti-inflammatory [2] and cytotoxic activity [3,4]. In our investigation, a new compound, named tonkinensisol (**1**), has been isolated from this plant along with three known compounds called bayin (**2**), vitexin (**3**) and lupeol (**4**). Additionally, **3** was firstly reported in this plant and **1** exhibited moderate activity suppressing the proliferation of HL-60 cells *in vitro*.

2. Results and discussion

Compound **1** was obtained as yellow needles. The molecular formula was established as $C_{25}H_{24}O_6$ by HREI-MS (at *m/z* 420.1578 $[M]^+$). The UV spectrum was consistent with typical absorptions of flavone skeleton. The ^1H NMR spectrum exhibited a couple of

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doublets at δ 6.98 and 8.14 (each 2H, $J = 8.8$ Hz) assignable to H-3′, 5′ and H-2′, 6′ of the B-ring. The signals at δ 3.51 (2H, d, 7.2 Hz, H-1″), 5.22 (1H, t, 7.2 Hz, H-2″), 1.69 (3H, s, H-4″) and 1.83 (3H, s, H-5″) proved the presence of isoprenyl fragment. The carbon signals at δ 131.8, 122.1, 28.2, 25.8 and 18.1 were consistent with isoprenyl fragment. The HMBC spectrum indicated that H-1″ (δ 3.51) had long-range correlations with C-10 (δ 107.7). Two doublets at δ 6.74 and 5.65 (each 1H, $J = 10.0$ Hz) were assignable to H-6 and H-7. The carbon signals at δ 115.6, 128.2, 77.9, 28.2 and 21.5 were identical to 3,3-dimethyl-3-oxygen- propene. In the HMBC spectrum, H-6 (δ 6.74) was correlated with the carbon signals at C-5a (δ 104.9), C-5 (δ 153.0), C-9a (δ 157.0); H-1‴ and H-2‴ (δ 1.47) were correlated with C-9a (δ 157.0). The hydroxyl group at δ 6.62 was deduced as 3-OH due to the long-range correlation with C-4 (δ 175.4). The chelated hydroxyl group at δ 11.95 was 5-OH. Therefore, **1** was elucidated as 3,5-dihydroxy-8,8-dimethyl-10-(3-methyl-3-butenyl)-2-(4-hydroxy-phenyl)-4H,8H-Benzol[1,2-b:3,4-b′]dipyran-4-one, named as tonkinensisol (scheme 1).

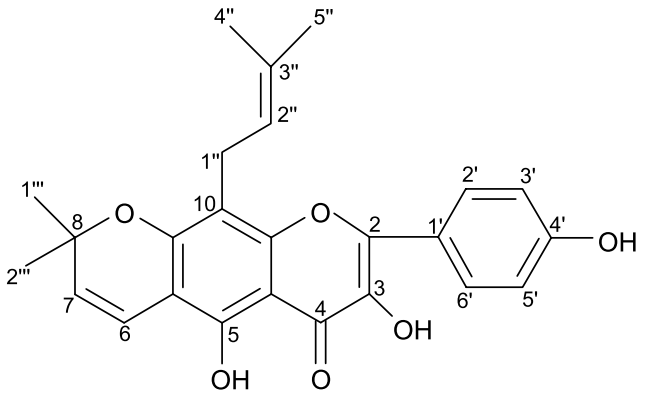
3. Experimental

3.1 General experimental procedures

Melting points were measured on Büchi-540 melting apparatus and are uncorrected; UV spectra were performed on a Shimadzu UV-2450 instrument (Japan); IR spectra were obtained on a Nicolet Avatar (USA) 360 FT-IR spectroscope; NMR spectra were recorded on a Varian (USA) INOVA-400NB spectrometer; MS spectra were measured on an LCQ-Advantage (USA) mass spectrometer; HRMS spectra were recorded on a Micromass Zabspec (UK) HRMS spectrometer.

3.2 Plant material

The roots of *Sophora tonkinensis* were collected in Jingxi county of Guangxi Province (China) in October 2001. The specimen was taxonomically identified as *S. tonkinensis* Gapnep by Professor Lin-han Liu of Hunan Normal University. A voucher specimen



Scheme 1. Structure of compound **1**.

(No. 0015) is deposited in the Department of Chinese Traditional Medicines, Central South University.

3.3 Extraction and isolation

The crude powdered roots of *S. tonkinensis* (12 kg) were immersed with 75% EtOH three times at room temperature. After concentration under reduced pressure, the extraction (250 g) was subjected to column chromatography on silica gel eluting with $CHCl_3$/MeOH (in gradient) to obtain seven fractions. Fraction 1 (2.5 g) was re-chromatographed on silica gel column chromatography with PE/Me_2CO (10:0.5–10:2) as eluant to afford **1** (11 mg) and **4** (800 mg). Fraction 3 (13 g) was carried on silica gel column chromatography, $CHCl_3$/MeOH (10:1.5–10:3) as eluant, to obtain four sections. Among them, Section 3 (600 mg) was run repeatedly on Sephadex LH-20 with MeOH as eluant to obtain **2** (29 mg) and **3** (14 mg).

3.4 Identification

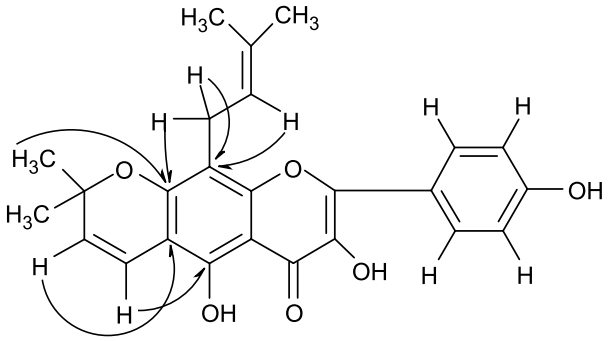
3.4.1 3.4.1 Compound 1. Yellow needles ($CHCl_3$); mp 154.9–156.0°C; UV λ_{max}^{MeOH} nm (log ϵ): 359 (3.81), 291 (4.39); IR (KBr) cm^{-1}: 3422, 2965, 2919, 1648, 1623, 1557, 1486, 1360, 1229; EI-MS *m/z*: 420.3 $[M]^+$, 405.2, 391.2, 377.2, 365.2; HREI-MS found *m/z*: 420.1578 $[M]^+$ (calcd for $C_{25}H_{24}O_6$, 420.1573); ^1H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (100 MHz, $CDCl_3$) data: see table 1. For the key HMBC correlations see scheme 2.

3.4.2 Compound 2. white powder (MeOH); mp 213.6–214.5°C; ^{13}C NMR (100 MHz, CD_3OD): 166.3 (C-2), 104.8 (C-3), 180.5 (C-4), 127.2 (C-5), 116.9 (C-6), 163.3 (C-7), 113.7 (C-8), 158.4 (C-9), 117.8 (C-10), 123.9 (C-1′), 130.0 (C-2′, 6′), 116.9 (C-3′, 5′), 162.6 (C-4′), 80.3 (C-1″), 75.6 (C-2″), 73.1 (C-3″), 72.3 (C-4″), 83.1 (C-5″), 63.1 (C-6″). These data were identical with bayin [5].

3.4.3 Compound 3. Yellow powder (MeOH); mp 251.6–252.7°C (dec.); ^{13}C NMR (100 MHz, DMSO-d_6): 163.9 (C-2), 102.4 (C-3), 182.0 (C-4), 160.3 (C-5), 98.0 (C-6), 162.4 (C-7), 104.5 (C-8), 155.9 (C-9), 104.0 (C-10), 121.5 (C-1′), 128.9 (C-2′, 6′), 115.7 (C-3′, 5′),

Table 1. NMR data of compound **1** in $CDCl_3$ (ppm).

No.	δ_C	δ_H *(Hz)*	*No.*	δ_C	δ_H *(Hz)*
2	145.2		2′	129.6	8.14 d (8.8)
3	135.4	6.62 s (OH)	3′	115.7	6.98 d (8.8)
4	175.4		4′	157.2	5.41 s (OH)
4a	103.5		5′	115.7	6.98 d (8.8)
5	153.0	11.95 s (OH)	6′	129.6	8.14 d (8.8)
5a	104.9		1″	28.2	3.51 d (7.2)
6	115.6	6.74 d (10.0)	2″	122.1	5.22 t (7.2)
7	128.2	5.65 d (10.0)	3″	131.8	
8	77.9		4″	25.8	1.69 s (CH_3)
9a	157.0		5″	18.1	1.83 s (CH_3)
10	107.7		1‴	21.5	1.47 s (CH_3)
10a	153.5		2‴	28.2	1.47 s (CH_3)
1′	123.8				



Scheme 2. The key HMBC correlations of compound **1**.

161.0 (C-4′), 78.6 (C-1″), 73.3 (C-2″), 70.7 (C-3″), 70.5 (C-4″), 81.7 (C-5″), 61.2 (C-6″). These data were identical with vitexin [6].

3.4.4 Compound 4. White needles ($CHCl_3$); mp 173.4–174.5°C. NMR data were identical with lupeol [7].

3.5 Cytotoxicity assays

Tonkinensisol was tested cytotoxicity to human acute promyelocytic leukemia-60 (HL-60) *in vitro* by MTT assay. As a result, tonkinensisol exhibited moderate cytotoxicity against HL-60 cells, with AN IC_{50} value of 36.48 μg/ml.

Acknowledgements

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