

## FLAVONOIDS FROM THE ROOTS OF *Sophora flavescens*

Tran Hong Quang<sup>1</sup>, Nguyen Xuan Nhiem<sup>1</sup>, Do Thi Trang<sup>1</sup>, Hoang Le Tuan Anh<sup>1</sup>,  
Bui Huu Tai<sup>1</sup>, Chau Van Minh<sup>1</sup>, Young Ho Kim<sup>2</sup>, Phan Van Kiem<sup>1\*</sup>

<sup>1</sup>Institute of Marine Biochemistry, Vietnam Academy of Science and Technology

<sup>2</sup>College of Pharmacy, Chungnam National University, Daejeon 305-764, Korea

Received 23 January 2015; Accepted for Publication 18 March 2015

### Abstract

Phytochemical study on the roots of *Sophora flavescens* resulted in the isolation of eight compounds. Their structures were identified as isoxanthohumol (**1**), norkurarinone (**2**), kurarinone (**3**), 2'-methoxykurarinone (**4**), kushenol T (**5**), norkurarinol (**6**), kuraridin (**7**), and formononetin (**8**) by detailed analyses of 1D and 2D NMR, and MS in comparison with the data reported in the literature.

**Keywords.** *Sophora flavescens*, Leguminosae, flavonoid.

### 1. INTRODUCTION

The dried roots of *S. flavescens* (Leguminosae) are commonly used as the traditional Chinese medicine and possess various physiological properties such as anti-bacterial, anti-inflammatory, antipyretic, anti-asthmatic, anti-ulcerative, and anti-neoplastic effects [1]. A series of isoprenylated or lavandulylated flavonoids have been isolated from this plant [2-7]. Some of these compounds exhibited significant antibacterial activity against Gram-positive bacteria [2], antiviral activity against herpes simplex virus types I and II [3], as well as cytotoxic activity against human myeloid leukemia HL-60 cells [5, 7], and potent inhibitory activity against cGMP phosphodiesterase 5 [6]. The present study describes the isolation and structural elucidation of eight known flavonoids (**2-9**) from the methanol extract of the roots of *S. flavescens*.

### 2. MATERIAL AND METHODS

#### 2.1. Plant materials

The roots of *S. flavescens* were purchased from herbal market at Kumsan, Chungnam, Korea, in August 2010. The plant material was identified by one of us (Y. H. Kim). A voucher specimen (CNU10106) was deposited at herbarium, College of Pharmacy, Chungnam National University.

#### 2.2. General experimental procedures

Optical rotation was determined using a Jasco P-2000 digital polarimeter. Electron-impact mass spectra (EIMS) were obtained using a Hewlett-Packard MS 5988 mass spectrometer. The NMR spectra were recorded on a Jeol ECA 600 spectrometer using TMS as an internal standard. CD spectra were recorded with a Jasco J-720 spectropolarimeter. TLC was performed on Kieselgel 60 F254 (1.05715; Merck, Darmstadt, Germany) or RP-18 F254s (Merck) plates. Spots were visualized by spraying with 10 % aqueous H<sub>2</sub>SO<sub>4</sub> solution, followed by heating. Column chromatography (CC) was performed on silica gel (Kieselgel 60, 70-230 mesh and 230-400 mesh, Merck) and YMC RP-18 resins.

#### 2.3. Extraction and Isolation

The dried stem bark of *S. flavescens* (3.0 kg) was extracted with hot MeOH. After concentration, the MeOH extract (250 g) was suspended in water and then partitioned successively with CH<sub>2</sub>Cl<sub>2</sub> and EtOAc to give CH<sub>2</sub>Cl<sub>2</sub> (A), EtOAc (B) and water (C) fractions, respectively. Fraction B was subjected to silica gel column chromatography, eluted with acetone in CH<sub>2</sub>Cl<sub>2</sub> (0-100 %, stepwise) to yield five fractions (B1-5). Fraction B2 was then separated by column chromatography over C<sub>18</sub> reverse-phase, using MeOH-H<sub>2</sub>O (2:1) to afford **7** (30 mg) and **8**

(15 mg). Fraction B3 was separated by column chromatography over silica gel, using  $\text{CH}_2\text{Cl}_2$ -EtOAc (4:1) as eluent to give three subfractions (B3A-C). Fraction B3A was chromatographed over silica gel column, eluting with  $\text{CH}_2\text{Cl}_2$ -acetone (5:1) to provide **2** (50 mg). Subfraction B3B was then chromatographed over  $\text{C}_{18}$  reverse-phase, using MeOH-H<sub>2</sub>O (3:1), and further purified by column chromatography over silica gel, eluting with  $\text{CH}_2\text{Cl}_2$ -MeOH (15:1) to obtain and **5** (7 mg). Subfraction B3C was separated by  $\text{C}_{18}$  reverse-phase chromatography, using MeOH-H<sub>2</sub>O (2:1) as eluent, and further purified by column chromatography over silica gel, eluting with  $\text{CH}_2\text{Cl}_2$ -MeOH (12:1) to obtain **1** (10 mg) and **6** (45 mg). Fraction B4 was separated by column chromatography over silica gel, eluted with  $\text{CH}_2\text{Cl}_2$ -Acetone (4:1) to provide three subfractions (B4A-C). Fraction B4B was then purified by column chromatography over  $\text{C}_{18}$  reverse-phase, using MeOH-H<sub>2</sub>O (2:1) to afford **3** (45 mg) and **4** (10 mg).

**Isoxanthohumol (1):** pale yellow, amorphous powder,  $[\alpha]_{\text{D}}^{25} -25$  ( $c = 0.5$ , MeOH). EIMS  $m/z$  354  $[\text{M}^+]$ . <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD)  $\delta$ : 5.23 (dd,  $J = 2.4$ , 13.2 Hz, H-2), 2.93 (dd,  $J = 13.2$ , 16.8 Hz, H-3a), 2.62 (dd,  $J = 3.6$ , 16.8 Hz, H-3b), 6.07 (br s, H-6), 7.27 (each d,  $J = 9.0$  Hz, H-2' and H-6'), 6.78 (each d,  $J = 9.0$  Hz, H-3' and H-5'), 3.16 (t,  $J = 6.0$  Hz, H<sub>2</sub>-1''), 5.10 (m, H-2''), 1.52 (s, H<sub>3</sub>-4''), 1.58 (s, H<sub>3</sub>-5''), 55.9 (5-OCH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD)  $\delta$ : 79.9 (C-2), 46.1 (C-3), 192.9 (C-4), 161.7 (C-5), 93.3 (C-6), 164.2 (C-7), 109.9 (C-8), 163.8 (C-9), 105.7 (C-10), 131.5 (C-1'), 128.8 (C-2'), 116.2 (C-3'), 158.7 (C-4'), 116.2 (C-5'), 128.8 (C-6'), 22.7 (C-1''), 123.9 (C-2''), 131.6 (C-3''), 17.9 (C-4''), 25.9 (C-5''), 55.9 (5-OCH<sub>3</sub>).

**Norkurarinone (2):** yellow, amorphous powder,  $[\alpha]_{\text{D}}^{25} +10.3$  ( $c = 0.7$ , MeOH). EIMS  $m/z$  424  $[\text{M}^+]$ . <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD)  $\delta$ : 5.52 (dd,  $J = 3.0$ , 13.8 Hz, H-2), 2.90 (dd,  $J = 13.2$ , 16.8 Hz, H-3a), 2.70 (dd,  $J = 3.0$ , 17.4 Hz, H-3b), 5.87 (br s, H-6), 6.32 (d,  $J = 1.8$  Hz, H-3'), 6.34 (dd,  $J = 1.8$ , 8.4 Hz, H-5'), 7.26 (d,  $J = 8.4$  Hz, H-6'), 2.52 (m, H<sub>2</sub>-1''), 2.41 (m, H-2''), 4.92 (t,  $J = 6.6$  Hz, H-4''), 1.49 (s, H<sub>3</sub>-6''), 1.41 (s, H<sub>3</sub>-7''), 4.53 (d,  $J = 1.2$  Hz, H-9''a), 4.47 (d,  $J = 1.2$  Hz, H-9''b), 1.57 (s, H<sub>3</sub>-10''). <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD)  $\delta$ : 74.9 (C-2), 42.3 (C-3), 198.2 (C-4), 162.1 (C-5), 95.5 (C-6), 165.6 (C-7), 107.9 (C-8), 161.7 (C-9), 102.5 (C-10), 117.6 (C-1'), 155.7 (C-2'), 102.6 (C-3'), 158.4 (C-4'), 106.9 (C-5'), 127.9 (C-6'), 27.1 (C-1''), 47.3 (C-2''), 31.5 (C-

3''), 123.9 (C-4''), 131.2 (C-5''), 25.1 (C-6''), 17.1 (C-7''), 148.8 (C-8''), 110.4 (C-9''), 18.4 (C-10'').

**Kurarinone (3):** yellow, amorphous powder,  $[\alpha]_{\text{D}}^{25} +13.5$  ( $c = 0.2$ , MeOH). EIMS  $m/z$  438  $[\text{M}^+]$ . <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD)  $\delta$ : 5.52 (dd,  $J = 3.0$ , 13.8 Hz, H-2), 2.84 (dd,  $J = 13.2$ , 16.8 Hz, H-3a), 2.68 (dd,  $J = 2.4$ , 16.2 Hz, H-3b), 6.05 (br s, H-6), 6.33 (br s, H-3'), 6.34 (dd,  $J = 2.4$ , 8.4 Hz, H-5'), 7.28 (d,  $J = 8.4$  Hz, H-6'), 2.58 (dd,  $J = 3.0$ , 7.2 Hz, H<sub>2</sub>-1''), 2.45 (m, H-2''), 1.94 (m, H<sub>2</sub>-3''), 4.91 (t,  $J = 6.6$  Hz, H-4''), 1.51 (s, H<sub>3</sub>-6''), 1.41 (s, H<sub>3</sub>-7''), 4.52 (d,  $J = 1.8$  Hz, H-9''a), 4.47 (d,  $J = 1.8$  Hz, H-9''b), 1.57 (s, H<sub>3</sub>-10''), 3.73 (5-OCH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD)  $\delta$ : 74.5 (C-2), 44.6 (C-3), 193.2 (C-4), 160.8 (C-5), 92.4 (C-6), 163.9 (C-7), 108.6 (C-8), 163.8 (C-9), 104.8 (C-10), 117.6 (C-1'), 155.6 (C-2'), 102.5 (C-3'), 158.4 (C-4'), 106.8 (C-5'), 127.6 (C-6'), 27.3 (C-1''), 47.2 (C-2''), 31.5 (C-3''), 123.9 (C-4''), 131.1 (C-5''), 25.0 (C-6''), 17.0 (C-7''), 148.8 (C-8''), 110.3 (C-9''), 18.3 (C-10''), 55.0 (5-OCH<sub>3</sub>).

**2'-Methoxykurarinone (4):** pale yellow, amorphous powder,  $[\alpha]_{\text{D}}^{25} -35.2$  ( $c = 0.1$ , MeOH). EIMS  $m/z$  452  $[\text{M}^+]$ . <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD)  $\delta$ : 5.50 (dd,  $J = 2.4$ , 13.2 Hz, H-2), 2.83 (dd,  $J = 13.2$ , 16.8 Hz, H-3a), 2.59 (dd,  $J = 2.4$ , 16.8 Hz, H-3b), 6.06 (br s, H-6), 6.43 (d,  $J = 2.4$  Hz, H-3'), 6.42 (dd,  $J = 2.4$ , 7.8 Hz, H-5'), 7.33 (d,  $J = 8.4$  Hz, H-6'), 2.56 (m, H<sub>2</sub>-1''), 2.45 (m, H-2''), 1.94 (m, H<sub>2</sub>-3''), 4.90 (t,  $J = 6.6$  Hz, H-4''), 1.51 (s, H<sub>3</sub>-6''), 1.42 (s, H<sub>3</sub>-7''), 4.53 (d,  $J = 1.8$  Hz, H-9''a), 4.46 (d,  $J = 1.8$  Hz, H-9''b), 1.59 (s, H<sub>3</sub>-10''), 3.76 (5-OCH<sub>3</sub>), 3.75 (2'-OCH<sub>3</sub>). <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD)  $\delta$ : 74.1 (C-2), 44.5 (C-3), 192.7 (C-4), 160.9 (C-5), 92.6 (C-6), 164.5 (C-7), 108.7 (C-8), 163.8 (C-9), 104.6 (C-10), 118.7 (C-1'), 158.0 (C-2'), 98.8 (C-3'), 159.1 (C-4'), 107.2 (C-5'), 127.6 (C-6'), 27.3 (C-1''), 47.2 (C-2''), 31.4 (C-3''), 123.9 (C-4''), 131.1 (C-5''), 25.0 (C-6''), 16.9 (C-7''), 148.8 (C-8''), 110.3 (C-9''), 18.2 (C-10''), 54.9 (5-OCH<sub>3</sub>), 55.0 (2'-OCH<sub>3</sub>).

**Kushenol T (5):** yellow, amorphous powder,  $[\alpha]_{\text{D}}^{25} -118.5$  ( $c = 0.2$ , MeOH). EIMS  $m/z$  426  $[\text{M}^+]$ . <sup>1</sup>H NMR (600 MHz, CD<sub>3</sub>OD)  $\delta$ : 5.63 (dd,  $J = 2.4$ , 13.2 Hz, H-2), 3.28 (H-3a), 2.86 (H-3b), 5.91 (br s, H-6), 6.81 (d,  $J = 7.8$  Hz, H-3'), 7.14 (t,  $J = 7.8$  Hz, H-4'), 6.87 (t,  $J = 7.8$  Hz, H-5'), 7.23 (d,  $J = 7.8$  Hz, H-6'), 2.84 (m, H-1''a), 2.36 (m, H-1''b), 1.02 (s, H<sub>3</sub>-6''), 1.01 (s, H<sub>3</sub>-7''), 4.61 (s, H-9''a), 4.54 (s, H-9''b), 1.62 (s, H<sub>3</sub>-10''). <sup>13</sup>C NMR (150 MHz, CD<sub>3</sub>OD)  $\delta$ : 75.0 (C-2), 42.2 (C-3), 197.7 (C-4), 161.4 (C-5), 95.5 (C-6), 162.3 (C-7), 107.7 (C-8), 165.6 (C-9),

102.4 (C-10), 126.1 (C-1'), 154.3 (C-2'), 115.2 (C-3'), 129.2 (C-4'), 119.7 (C-5'), 126.5 (C-6'), 27.6 (C-1''), 47.7 (C-2''), 27.0 (C-3''), 41.8 (C-4''), 70.6 (C-5''), 27.9 (C-6''), 28.3 (C-7''), 148.6 (C-8''), 110.7 (C-9''), 17.8 (C-10'').

**Norkurarinol (6):** yellow, amorphous powder,  $[\alpha]_D^{25} -25.5$  ( $c = 0.1$ , MeOH). EIMS  $m/z$  442  $[M^+]$ .  $^1H$  NMR (600 MHz,  $CD_3OD$ )  $\delta$ : 5.53 (dd,  $J = 2.4$ , 13.2 Hz, H-2), 2.92 (dd,  $J = 13.8$ , 17.4 Hz, H-3a), 2.70 (dd,  $J = 3.0$ , 17.4 Hz, H-3b), 5.88 (br s, H-6), 6.31 (d,  $J = 3.0$  Hz, H-3'), 6.33 (dd,  $J = 3.0$ , 8.4 Hz, H-5'), 7.27 (d,  $J = 8.4$  Hz, H-6'), 2.56 (m,  $H_2$ -1''), 2.34 (m, H-2''), 1.04 (s,  $H_3$ -6''), 1.03 (s,  $H_3$ -7''), 4.57 (br s, H-9''a), 4.51 (d,  $J = 1.8$  Hz, H-9''b), 1.59 (s,  $H_3$ -10'').  $^{13}C$  NMR (150 MHz,  $CD_3OD$ )  $\delta$ : 74.8 (C-2), 42.3 (C-3), 198.1 (C-4), 162.2 (C-5), 95.4 (C-6), 165.5 (C-7), 107.7 (C-8), 161.0 (C-9), 102.4 (C-10), 117.4 (C-1'), 155.7 (C-2'), 102.5 (C-3'), 158.5 (C-4'), 106.8 (C-5'), 127.7 (C-6'), 27.5 (C-1''), 47.6 (C-2''), 27.1 (C-3''), 41.8 (C-4''), 70.7 (C-5''), 28.3 (C-6''), 27.9 (C-7''), 148.5 (C-8''), 110.7 (C-9''), 17.8 (C-10'').

**Kurarinidin (7):** yellow, amorphous powder,  $[\alpha]_D^{25} -25.5$  ( $c = 0.1$ , MeOH). EIMS  $m/z$  438  $[M^+]$ .  $^1H$  NMR (600 MHz,  $CD_3OD$ )  $\delta$ : 7.98 (d,  $J = 15.6$  Hz, H-2), 7.91 (d,  $J = 15.6$  Hz, H-3), 5.95 (br s, H-

6), 6.30 (br s, H-3'), 6.32 (dd,  $J = 2.4$ , 7.8 Hz, H-5'), 7.37 (d,  $J = 7.8$  Hz, H-6'), 2.59 (m,  $H_2$ -1''), 2.51 (m, H-2''), 2.04 (m,  $H_2$ -3''), 5.00 (t,  $J = 6.6$  Hz, H-4''), 1.58 (s,  $H_3$ -6''), 1.51 (s,  $H_3$ -7''), 4.55 (s, H-9''a), 4.50 (s, H-9''b), 1.66 (s,  $H_3$ -10''), 3.83 (s, 5-OCH<sub>3</sub>).  $^{13}C$  NMR (150 MHz,  $CD_3OD$ )  $\delta$ : 138.6 (C-2), 124.3 (C-3), 193.6 (C-4), 165.5 (C-5), 90.4 (C-6), 162.9 (C-7), 107.7 (C-8), 161.3 (C-9), 105.4 (C-10), 115.2 (C-1'), 159.1 (C-2'), 102.5 (C-3'), 161.0 (C-4'), 107.8 (C-5'), 130.5 (C-6'), 27.0 (C-1''), 46.9 (C-2''), 31.3 (C-3''), 123.9 (C-4''), 130.7 (C-5''), 24.9 (C-6''), 16.8 (C-7''), 148.7 (C-8''), 110.1 (C-9''), 18.0 (C-10''), 54.9 (5-OCH<sub>3</sub>).

**Formononetin (8):** pale yellow, amorphous powder. EIMS  $m/z$  268  $[M^+]$ .  $^1H$  NMR (600 MHz, DMSO- $d_6$ )  $\delta$ : 8.29 (d,  $J = 1.2$  Hz, H-2), 7.94 (d,  $J = 9.0$  Hz, H-5), 6.91 (dd,  $J = 1.2$ , 9.0 Hz, H-6), 6.83 (br s, H-8), 7.47 (each d,  $J = 8.4$  Hz, H-2' and H-6'), 6.95 (each d,  $J = 8.4$  Hz, H-3' and H-5'), 3.74 (s, 4'-OCH<sub>3</sub>).  $^{13}C$  NMR (150 MHz, DMSO- $d_6$ )  $\delta$ : 154.0 (C-2), 124.0 (C-3), 175.5 (C-4), 117.5 (C-4a), 128.2 (C-5), 116.0 (C-6), 163.4 (C-7), 103.0 (C-8), 158.3 (C-8a), 125.1 (C-1'), 130.9 (C-2'), 114.5 (C-3'), 159.8 (C-4'), 114.5 (C-5'), 130.9 (C-6'), 56.0 (4'-OCH<sub>3</sub>).

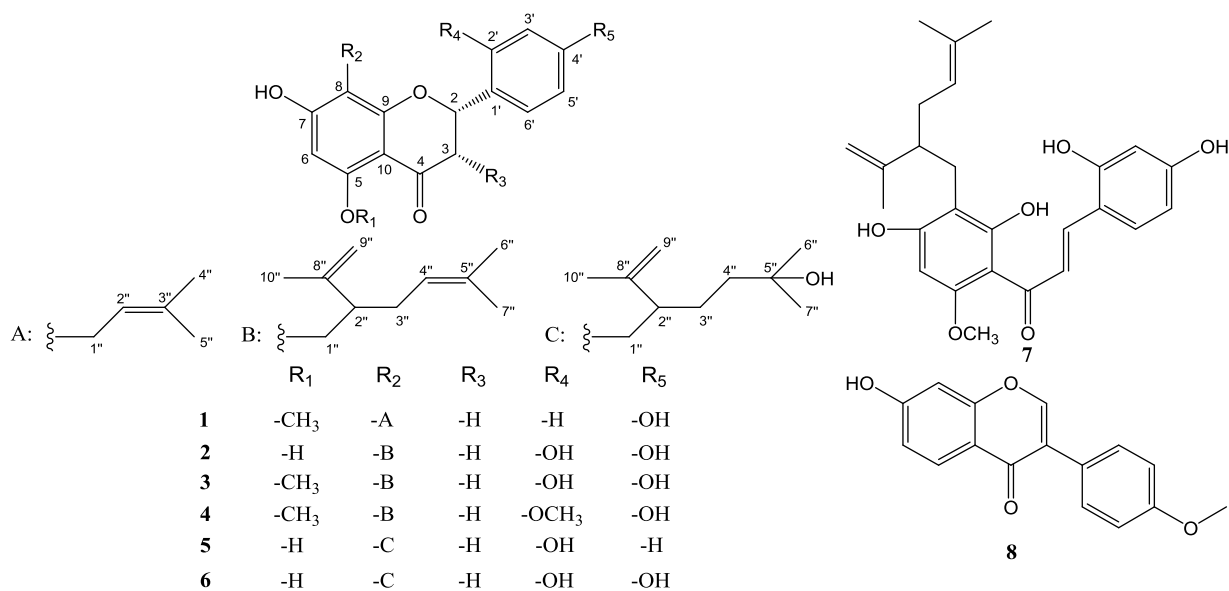


Figure 1: Chemical structures of compounds 1-8

### 3. RESULTS AND DISCUSSION

Compound 1 was isolated as a pale yellow, amorphous powder and its molecular formula was established to be C<sub>21</sub>H<sub>22</sub>O<sub>5</sub> by  $^1H$  and  $^{13}C$  NMR spectroscopic analysis and EIMS at  $m/z$  354  $[M^+]$ . The  $^1H$  NMR spectrum of 1 showed an aromatic

proton singlet at  $\delta_H$  6.07 (H-6), and a typical A<sub>2</sub>B<sub>2</sub> system at  $\delta_H$  7.27 (d,  $J = 9.0$  Hz, H-2' and H-6') and 6.78 (d,  $J = 9.0$  Hz, H-3' and H-5'). The  $^1H$  NMR of 1 further showed signals for a 3,3-dimethylallyl group at  $\delta_H$  3.16 (t,  $J = 6.0$  Hz,  $H_2$ -1''), 5.10 (m, H-2''), 1.52 (s,  $H_3$ -4''), and 1.58 (s,  $H_3$ -5''). The

position of 3,3-dimethylallyl group was assigned to C-8 by the HMBC correlations from 3.16 (H<sub>2</sub>-1'') to  $\delta_C$  164.2 (C-7), 109.9 (C-8), and 163.8 (C-9). The signals of a methoxyl group at 3.75 (s), an oxymethine group at 5.23 (dd,  $J = 2.4, 13.2$  Hz, H-2), and a methylene group at 2.93 (dd,  $J = 13.2, 16.8$  Hz, H-3a) and 2.62 (dd,  $J = 3.6, 16.8$  Hz, H-3b) were also observed in the <sup>1</sup>H NMR spectrum of **1**. The <sup>13</sup>C NMR spectrum showed signals of a carbonyl carbon at 192.9 (C-4) and a methylene carbon at  $\delta_C$  46.1 (C-3) implying that **1** belongs to the flavanone skeleton. The methoxyl group was located at C-5 based on the HMBC correlation of  $\delta_H$  3.75 with  $\delta_C$  161.7 (C-5). Based on the above analysis and comparison of the NMR data of **1** with those of reported compound, the structure of **1** was identified as isoxanthohumol [8].

Compound **2** was obtained as yellow, amorphous powder. Its molecular formula was determined to be C<sub>25</sub>H<sub>28</sub>O<sub>6</sub> by an ion  $m/z$  424 [M<sup>+</sup>] in the EIMS. The <sup>1</sup>H NMR spectrum contained signals for an ABX aromatic ring system [ $\delta_H$  6.32 (d,  $J = 1.8$  Hz, H-3'), 6.34 (dd,  $J = 1.8, 8.4$  Hz, H-5'), and 7.26 (d,  $J = 8.4$  Hz, H-6')], a singlet at 5.87 (H-6), an oxymethine group at 5.52 (dd,  $J = 3.0, 13.8$  Hz, H-2), and a methylene group at 2.90 (dd,  $J = 13.2, 16.8$  Hz, H-3a) and 2.70 (dd,  $J = 3.0, 17.4$  Hz, H-3b). The <sup>1</sup>H NMR spectrum further showed the signals of three olefinic protons at  $\delta_H$  4.92 (1H, t,  $J = 6.6$  Hz, H-4''), 4.53 (d,  $J = 1.2$  Hz, H-9''a), 4.47 (d,  $J = 1.2$  Hz, H-9''b), three tertiary methyl groups at  $\delta_H$  1.49 (s, H-6''), 1.41 (s, H-7''), and 1.57 (3H, s, H-10''), two methylene groups at  $\delta_H$  2.52 (m, H<sub>2</sub>-1'') and 1.94 (m, H<sub>2</sub>-3''), and one methine group at  $\delta_H$  2.41 (m, H-2'') suggesting the presence of a lavandulyl group. The <sup>13</sup>C NMR and DEPT spectra displayed 25 carbons, including signals for a flavanone and a lavandulyl group. The <sup>13</sup>C NMR signals at  $\delta_C$  117.6 (C-1'), 155.7 (C-2'), 102.6 (C-3'), 158.4 (C-4'), 106.9 (C-5'), and 127.9 (C-6') characterized for a 1,2,4-trisubstituted aromatic ring of the flavanone. The lavandulyl group was located at C-8 by the HMBC correlations from  $\delta_H$  7.26 (H-1'') to 165.6 (C-7), 107.9 (C-8), and 161.7 (C-9). Finally, the structure of **2** was established as norkurarinone [9].

Compound **3**, a yellow, amorphous powder, had a molecular formula of C<sub>26</sub>H<sub>30</sub>O<sub>6</sub> as indicated by the ion  $m/z$  438 [M<sup>+</sup>] in the EIMS. The <sup>1</sup>H and <sup>13</sup>C NMR spectra of **3** were found nearly similar with those of **2**, except for the additional presence of a methoxyl group at  $\delta_H$  3.73/ $\delta_C$  55.0. By HMBC correlation of  $\delta_H$  3.73 with  $\delta_C$  160.8 (C-5), the methoxyl group was located at C-5. Thus, **3** was established as kurarinone [10].

Compound **4**, a pale yellow, amorphous powder, showed a molecular formula of C<sub>27</sub>H<sub>32</sub>O<sub>6</sub> as deduced by the ion  $m/z$  452 [M<sup>+</sup>] in the EIMS. Comparison of the <sup>1</sup>H and <sup>13</sup>C NMR spectra of **4** with those of **3** suggested the structures of these two compounds are nearly identical, except for the additional presence of a methoxyl signal at  $\delta_H$  3.75/ $\delta_C$  55.0. This methoxyl group was connected to C-2' based on the HMBC correlation of  $\delta_H$  3.75 with  $\delta_C$  158.0 (C-2'). Therefore the structure of **4** was identified as 2'-methoxykurarinone [5].

Compound **5** was separated as a yellow, amorphous powder, with the molecular formula of C<sub>25</sub>H<sub>30</sub>O<sub>6</sub> as determined by <sup>1</sup>H and <sup>13</sup>C NMR spectroscopic analyses and EIMS. The <sup>1</sup>H NMR spectrum showed a singlet at  $\delta_H$  5.91 (H-6), an oxymethine group at  $\delta_H$  5.63 (dd,  $J = 2.4, 13.2$ , H-2), two olefinic protons [ $\delta_H$  4.61 (s, H-9''a) and 4.54 (s, H-9''b)], three tertiary methyl groups [ $\delta_H$  1.02 (C-6''), 1.01 (C-7''), and 1.62 (C-10'')], and signals characterized for a 1,2-disubstituted aromatic ring [ $\delta_H$  6.81 (d,  $J = 7.8$  Hz, H-3'), 7.14 (t,  $J = 7.8$  Hz, H-4'), 6.87 (t,  $J = 7.8$  Hz, H-5'), and 7.23 (d,  $J = 7.8$  Hz, H-6')]. The <sup>13</sup>C NMR and DEPT spectra displayed 25 signals, including three tertiary methyl, five methylene, and seven methine groups, and 10 quaternary carbons. The <sup>13</sup>C NMR contained signals of one olefinic methylene group ( $\delta_C$  110.7, C-9''), one quaternary carbon ( $\delta_C$  70.6, C-5''), one methine group ( $\delta_C$  47.7, C-2''), three methylene groups [ $\delta_C$  27.6 (C-1''), 27.0 (C-3''), and 41.8 (C-4'')], and three tertiary methyl groups [ $\delta_C$  27.9 (C-6''), 28.3 (C-7''), and 17.8 (C-10'')] suggesting the presence of a 5-hydroxy-2-isopropenyl-5-methylhexyl group. The HMBC correlations of  $\delta_H$  2.84 and 2.36 (H<sub>2</sub>-1'') with  $\delta_C$  162.3 (C-7), 107.7 (C-8), and 165.6 (C-9) indicated that the 5-hydroxy-2-isopropenyl-5-methylhexyl group was connected to C-8. Based on the aforementioned analysis, along with comparison of the NMR data of **5** with those of reported data, the structure of **5** was established as kushenol T [2].

Compound **6** was isolated as a yellow, amorphous powder and its molecular formula was identified as C<sub>25</sub>H<sub>30</sub>O<sub>7</sub> by EIMS. The <sup>1</sup>H and <sup>13</sup>C NMR spectra of **6** were found nearly identical with those of **2**, the difference is that the lavandulyl group in **2** was replaced by a 5-hydroxy-2-isopropenyl-5-methylhexyl group in **6**. Thus the structure of **6** was identified as norkurarinol [10].

Compound **7**, showed the molecular formula of C<sub>26</sub>H<sub>30</sub>O<sub>6</sub> by analysis of the <sup>1</sup>H and <sup>13</sup>C NMR data and EIMS. The <sup>1</sup>H NMR spectrum contained signals for an ABX aromatic ring system [ $\delta_H$  6.30 (br s, H-

3'), 6.32 (dd,  $J = 2.4, 7.8$  Hz, H-5'), and 7.37 (d,  $J = 7.8$  Hz, H-6')], a singlet at 5.95 (H-6), a methoxyl group at  $\delta_{\text{H}}$  3.83 (s), and signals for a lavandulyl moiety [ $\delta_{\text{H}}$  5.00 (t,  $J = 6.6$  Hz, H-4''), 4.55 (s, H-9''a), 4.50 (s, H-9''b), 2.59 (m, H<sub>2</sub>-1''), 2.51 (m, H-2''), 2.04 (m, H<sub>2</sub>-3''), 1.58 (s, H<sub>3</sub>-6''), 1.51 (s, H-7''), and 1.66 (s, H<sub>3</sub>-10'')]. The <sup>1</sup>H NMR spectrum further showed signals for two olefinic protons at  $\delta_{\text{H}}$  7.98 (d,  $J = 15.6$  Hz, H-2) and 7.91 (d,  $J = 15.6$  Hz, H-3). The large coupling constant (15.6 Hz) between these olefinic protons implied *trans*-configured double bond. The <sup>13</sup>C NMR and DEPT spectra exhibited one carbonyl carbon at  $\delta_{\text{C}}$  193.6 (C-4) and two olefinic methine carbon at  $\delta_{\text{C}}$  138.6 (C-2) and 124.3 (C-3) suggesting that the structure of **7** belongs to a chalcone skeleton. By HMBC correlation of  $\delta_{\text{H}}$  2.59 (H<sub>2</sub>-1'') with  $\delta_{\text{C}}$  162.9 (C-7), 107.7 (C-8), and 161.3 (C-9), the lavandulyl moiety was located at C-8. The methoxyl group was connected to C-5 based on HMBC correlation from  $\delta_{\text{H}}$  3.83 to  $\delta_{\text{C}}$  165.5 (C-5). Based the above spectroscopy analysis and comparison with the reported data, the structure of **7** was established as kuraridin [10].

Compound **8** was given as a pale yellow, amorphous powder and its molecular formula was deduced from EIMS. The <sup>1</sup>H NMR spectrum exhibited signals for an ABX spin aromatic ring [ $\delta_{\text{H}}$  7.94 (d,  $J = 9.0$  Hz, H-5), 6.91 (dd,  $J = 1.2, 9.0$  Hz, H-6), and 6.83 (br s, H-8)] and an A<sub>2</sub>B<sub>2</sub> system at  $\delta_{\text{H}}$  7.47 (d,  $J = 8.4$  Hz, H-2', 6') and 6.95 (d,  $J = 8.4$  Hz, H-3', 5'). The <sup>1</sup>H NMR spectrum further showed signals of an olefinic proton at  $\delta_{\text{H}}$  8.29 (d, 1.2, H-2) and a methoxyl group at  $\delta_{\text{H}}$  3.74 (s). The <sup>13</sup>C NMR and DEPT presented 16 carbons, including one carbonyl carbon ( $\delta_{\text{C}}$  175.5, C-4), one olefin [ $\delta_{\text{C}}$  154.0 (C-2) and 124.0 (C-3)] suggesting that **8** belongs to the isoflavone skeleton. The methoxyl group was located at C-4' based on the HMBC correlation of  $\delta_{\text{H}}$  3.74 with  $\delta_{\text{C}}$  159.8 (C-4'). Finally the structure of **8** was identified as formononetin [11].

**Acknowledgements.** This work was financially supported by the Priority Research Center Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2009-0093815), Republic of Korea.

Corresponding author: **Phan Van Kiem**

Institute of Marine Biochemistry, Vietnam Academy of Science and Technology  
18, Hoang Quoc Viet, Cau Giay, Hanoi, Vietnam  
E-mail: phankiem@yahoo.com.

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