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# Two new prenylflavonoids from *Morus nigra* L.

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**Abstract**

Two new prenylflavonoids, mornigrol E(**1**) and mornigrol F(**2**) were isolated from *Morus nigra* L. Their structures were elucidated on the basis of spectroscopic methods, especially 2D-NMR techniques.


*Keywords:* *Morus nigra*; Moraceae; Mornigrols E and F; Prenylflavonoid

Many plants of *Morus* genus are the well known traditional Chinese medicine, such as *Morus nigra* L., distributed in Xin Jiang Provence, has long been used for the treatment of diabetes, arthritis, rheumatism [1,2]. From the 95% EtOH extract of the barks of *M. nigra* L., two new isomeric prenylflavonoids **1** and **2** were isolated. In this paper, we reported the structural elucidation of them.

Compound **1** was obtained as yellow powder, mp 125–128 °C. The molecular formula $C_{25}H_{26}O_7$ was deduced from HRESIMS spectrum for $[M+H]^+$ at *m/z* 439.1752 (calcd. 439.1756). Absorption for hydroxyl (3270 $cm^{-1}$), carbonyl group (1653 $cm^{-1}$), and aromatic ring functionalities (1559 and 1447 $cm^{-1}$) were observed in IR. The UV spectrum showed absorption maxima at 278 and 376 nm which can be assigned to the cinnamoyl group and benzoyl group of the flavonoid skeleton. The $^1H$ NMR (see Table 1) showed the presence of a ABX group at $\delta_H$ 7.34 (d, 1H, $J$ = 8.4 Hz), 6.53 (dd, 1H, $J$ = 2.7, 8.4 Hz), 6.54 (d, 1H, $J$ = 2.7 Hz) and one singlet $\delta_H$ 6.34 (1H, s); the $^{13}C$ NMR (Table 1) showed one carbonyl resonance at $\delta$ 183.9 and six oxygenated aromatic carbon signals at $\delta$ 163.2, 162.6, 161.5, 160.6, 157.1, 156.6, which were similar to the NMR spectral data of kuwanon C [3,4]. In the HMBC experiment, H-6 at $\delta_H$ 6.34 (s, 1H) showed correlations with C-5 ($\delta_C$ 160.6) and C-7 ($\delta_C$ 162.6); H-3′ at $\delta_H$ 6.54 (d, 1H, $J$ = 2.7 Hz) with C-5′($\delta_C$ 108.2), C-2′($\delta_C$ 157.1), C-4′($\delta_C$ 161.5) and C-1′($\delta_C$ 113.2); H-5′ at $\delta_H$ 6.53 (dd, 1H, $J$ = 2.7, 8.4 Hz) with C-3′($\delta_C$ 104.2) and C-4′($\delta_C$ 161.5); H-6′ at $\delta_H$ 7.34 (d, 1H, $J$ = 8.4 Hz) with C-5′($\delta_C$ 108.2), C-4′($\delta_C$ 161.5) and C-2′($\delta_C$ 157.1). According to the above data and comparing to the data of kuwanon C suggested that 1 also was 5, 7, 2′, 4′-four hydroxyl flavonoid. The $^1H$ NMR (Table 1) revealed the presence of an isopentene group $\delta_H$ 3.41 (d, 2H, $J$ = 7.5 Hz), 5.21 (m, 1H), 1.56 (s, 6H) and a changed isopentene group $\delta_H$ 2.74 (dd, 1H, $J$ = 4.5, 13.8 Hz), 2.60 (dd, 1H, $J$ = 8.4, 13.8 Hz), 4.44 (1H, dd, $J$ = 8.4, 4.5 Hz), 4.84 (s, 1H), 4.65 (s, 1H), 1.57 (s, 3H). The HMBCs H-14/C-4, 2, 3, 15, 16; H-9/C-7, 8a, 8, 10; H-10/ C-8, 11, 12 suggested that the isopentene group located at C-8 in ring A and the changed isopentene group connected at C-3 in ring C. So, the structure of **1** was confirmed (Fig. 1) and named mornigrol E.

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Table 1
$^{1}$H NMR and $^{13}$C NMR chemical shift for mornigrol E(**1**) and mornigrol F(**2**).

| Position | **1** | | **2** | |
|---|---|---|---|---|
| | H[a] | C[b] | H[a] | C[b] |
| 2 | | 163.2 | | 162.1 |
| 3 | | 119.3 | | 120.9 |
| 4 | | 183.9 | | 183.4 |
| 4a | | 104.9 | | 105.0 |
| 5 | | 160.6 | | 161.2 |
| 6 | 6.34 (s, 1H) | 98.8 | 6.25 (s, 1H) | 98.8 |
| 7 | | 162.6 | | 164.1 |
| 8 | | 106.9 | | 104.7 |
| 8a | | 156.6 | | 156.8 |
| 9 | 3.41 (d, 2H, 7.5) | 22.1 | 2.90 (dd, 1H, 8.4, 14.4); 3.06 (dd, 1H, 3.6, 14.4) | 30.5 |
| 10 | 5.21 (m, 1H) | 123.2 | 4.35 (dd, 1H, 8.4, 3.6) | 76.4 |
| 11 | | 131.6 | | 148.5 |
| 12 | 1.56 (s, 3H) | 17.7 | 4.68 (s, 1H); 4.87 (s, 1H) | 110.2 |
| 13 | 1.56 (s, 3H) | 24.7 | 1.68 (s, 3H) | 18.4 |
| 14 | 2.60 (dd, 1H, 8.4, 13.8); 2.74 (dd, 1H, 4.5, 13.8) | 33.1 | 3.14 (d, 2H, 6.9) | 24.7 |
| 15 | 4.44 (dd, 1H, 8.4, 4.5) | 74.1 | 5.16 (m, 1H) | 122.9 |
| 16 | | 148.9 | | 132.0 |
| 17 | 4.85 (s, 1H); 4.65 (s, 1H) | 110.2 | 1.56 (s, 3H) | 25.7 |
| 18 | 1.57 (s, 3H) | 17.8 | 1.43 (s, 3H) | 17.6 |
| 1′ | | 113.2 | | 113.0 |
| 2′ | | 157.1 | | 157.4 |
| 3′ | 6.54 (d, 1H, 2.7) | 104.2 | 6.57 (d, 1H, 2.7) | 104.1 |
| 4′ | | 161.5 | | 161.5 |
| 5′ | 6.53 (dd, 1H, 8.4, 2.7) | 108.2 | 6.51 (dd,1H, 8.4, 2.7) | 108.1 |
| 6′ | 7.34 (d, 1H, 8.4) | 132.8 | 7.24 (d, 1H, 8.4) | 132.4 |
| 5-OH | 13.01 (s, 1H) | | 12.98 (s, 1H) | |

[a] Recorded at 500 MHz in $CD_3COCD_3$.
[b] Recorded at 125 MHz in $CD_3COCD_3$.

Compound **2** was isolated as yellow powder, mp 124–126 °C. $C_{25}H_{26}O_7$ as the molecular formula was determined by HRESIMS spectrum for $[M+H]^+$ at *m/z* 439.1761 (calcd. 439.1756). The IR spectrum for **2** displays absorption bands of hydroxyl group 3282 $cm^{-1}$ (broad), carbonyl group (1653 $cm^{-1}$), and aromatic ring functionalities (1558 and 1427 $cm^{-1}$). The UV spectrum showed absorption maxima at 264 and 316 nm. $^{1}$H and $^{13}$C NMR (Table 1) spectral data suggested that **2** had the same skeleton as **1** with difference in the location of the isopentene group [$\delta_H$ 3.14 (d, 2H, $J$ = 6.9 Hz), 5.16 (m, 1H), 1.43 (s, 3H), 1.56 (s, 3H)] and the changed isopentene group [$\delta_H$ 2.90 (dd, 1H, $J$ = 8.4, 14.4 Hz), 3.06 (dd, 1H, $J$ = 3.6, 14.4 Hz), 4.35 (dd, 1H, $J$ = 8.4, 3.6 Hz), 4.87 (s, 1H), 4.68 (s, 1H), 1.68 (s, 3H)]. In the

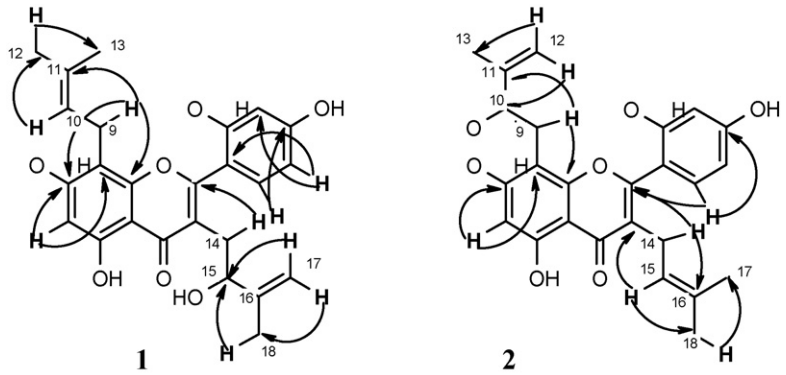


Fig. 1. Key long-range (HMBC) correlations of **1** and **2**.

HMBC experiment, H-14/C-4, 2, 3, 15, 16; H-9/C-7, 8a, 10, 8; H-10/C-8, 11, 12, suggested that the isopentene group located at C-3 in ring C and the changed isopentene group connected at C-8 in ring A. Thus, the structure of **2** was determined (Fig. 1) and named mornigrol F.

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