FLAVONOIDS FROM *Dracocephalum moldavica*

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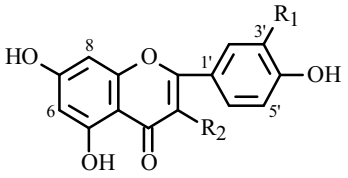
UDC 547.972

The annual plant *Dracocephalum moldavica* L., height 30-100 cm, is widely distributed in northern, northeastern, and northwestern Xinjiang Autonomous Region of the PRC. It flowers in July and sets fruit in August and contains flavones, terpenes, proteins, amino acids, polypeptides, and 16 amino acids, of which 8 are essential. It also contains 1.03% required microelements such as Fe, Cu, Mn, and Sr. Tincture of the dry herb has been used for ages in Uyghur folk medicine to treat heart disease, blood pressure, angina, tracheitis, atherosclerosis, neuralgia, migraine, and headache and toothache. Extracts of *Dracocephalum* possess sedative, analgesic, wound-healing, and anticramping activity [1-4].

Ground air-dried raw material (280 g) that was collected during flowering was extracted exhaustively with ethanol (70%) at room temperature. The combined extract was distilled in vacuo. The condensed residue was diluted with water and treated successively with petroleum ether, $CHCl_3$, ethylacetate, and *n*-butanol. The ethylacetate fraction was chromatographed over a column of silica gel using petroleum ether:ethylacetate (50:1-1:20). Elution by 45:1-40:1, 20:1-15:1, and 1:5-1:15 isolated **1-3**.



1 - 3

1: R_1 = H, R_2 = OH; **2:** R_1 = OCH_3, R_2 = H

3: R_1 = OH, R_2 = α-L-Rha*p*(1→6)-β-D-Glc*p*-*O*-

We used UV (with added NaOAc, $AlCl_3$/HCl, CH_3ONa, and CH_3COONa/H_3BO_3), PMR, IR, and mass spectra in addition to comparison with literature data to identify the isolated compounds.

Compound 1, yellow crystals, $C_{15}H_{10}O_6$, mp 277-279°C. UV spectrum (MeOH, λ_{max}, nm): 294, 367; +NaOAc/H_3BO_3: 297, 372; +$AlCl_3$/HCl: 384, 424. PMR spectrum (500 MHz, DMSO-d_6, δ, ppm, J/Hz): 6.20 (1H, d, J = 2.0, H-6), 6.46 (1H, d, J = 2.0, H-8), 6.98 (2H, d, J = 8.5, H-3′,5′), 8.10 (2H, d, J = 8.5, H-2′,6′), 9.40 (1H, s, 4′-OH), 10.9 (1H, s, 3-OH). The aglycon was characterized as 3,5,7,4′-tetrahydroxyflavone (kaempferol) [5-7].

Compound 2, yellow crystals, $C_{16}H_{12}O_6$, mp 312-314°C. UV spectrum (MeOH, λ_{max}, nm): 257, 268, 370. The IR spectrum contained absorption bands for hydroxyls (3484 cm^{-1}) γ-pyrone carbonyl (1660 cm^{-1}), and aromatic C=C (1605, 1583, 1501 cm^{-1}).

Mass spectrum (*m*/*z*): 302 $[M]^+$, 273, 262, 153, 141 ,137, 128, 110, 95, 69, 57.

PMR spectrum (500 MHz, DMSO-d_6 + CCl_4, δ, ppm, J/Hz): 3.80 (3H, s, 3′-OCH_3), 6.8 (1H, d, J = 7.9, H-5′), 6.12 (1H, dd, J = 2.0, 7.9, H-6′), 7.76 (1H, d, J = 2.0, H-2′), 8.87 (1H, br.s, 4′-OH), 9.08 (1H, br.s, 7-OH), 10.35 (1H, s, 5-OH). The compound was identified as 5,7,4′-trihydroxy-3′-methoxyflavone (chrysoeriol) [8, 9].

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 0009-3130/08/4403-0366

Compound 3, yellow crystals, $C_{27}H_{30}O_{16}$, mp 193-195°C. UV spectrum (MeOH, λ_{max}, nm): 255, 265, 360; +CH_3COONa: 271, 390; +CH_3COONa/H_3BO_3: 260, 383; +$AlCl_3$: 273, 430; +$AlCl_3$/HCl: 270, 401; +CH_3ONa: 272, 411.

The IR spectrum contained absorption bands for hydroxyl (3369 cm^{-1}), γ-pyrone carbonyl (1656 cm^{-1}), and aromatic C=C (1605, 1498 cm^{-1}).

PMR spectrum (500 MHz, DMSO-d_6 + CCl_4, δ, ppm, J/Hz): 1.12 (3H, d, J = 6.0, CH_3), 3.00-4.20 (sugar protons), 5.03 (1H, d, J = 7.0, H-1″), 5.23 (1H, d, J = 7.0, H-1‴), 6.16 (1H, d, J = 2.0, H-6), 6.36 (1H, d, J = 2.0, H-8), 6.38 (1H, d, J = 8.0, H-5′), 7.53 (2H, m, H-6′,2′), 9.15 (2H, br.s, 3′-OH,4′-OH), 12.46 (1H, s, 5-OH). The compound was characterized as quercetin 3-*O*-[α-L-rhamnopyranosyl(1→6)]-β-D-glucopyranoside [10, 11].

These compounds were isolated from *D. moldavica* for the first time.

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