

CHEMICAL CONSTITUENTS OF *Edgeworthia chrysantha*

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UDC 547.972

Edgeworthia chrysantha Lindl. is a member of the Thymelaeaceae family, distributed mainly in Eastern Asia. The traditional usage of *E. chrysantha* is very extensive. It is used to make paper in Japan, while the flowers are used in the crude drug “Meng hua” as an anti-bacterial. Its barks and stems are also used as the folkloric medicine “Zhu shima” in South China because of its detumescence and acesodyne effects. The antibacterial properties of this plant have been extensively studied [1, 2]. Phytochemical studies revealed that *E. chrysantha* contains various constituents, such as coumarins [3, 4], triterpenes [5], and flavonoids [6]. In our studies of the chemical constituents of *E. chrysantha*, nine compounds were isolated and identified. All compounds were obtained from this plant for the first time.

Stems and barks of *E. chrysantha* were collected in Nancang, Jiangxi Province in China, in May, 2005. The plant material was identified by Prof. Huang Baokang and Zheng Hanchen, Department of Phytochemistry, Second Military Medical University. The air dried powdered aerial parts of *E. chrysantha* (4.5 kg) were extracted with 75% ethanol four times at room temperature. The solution was concentrated and partitioned with solvents starting with petroleum ether, chloroform, ethyl acetate, and *n*-butanol, yielding 102.5, 78.0, 146.5, and 200.0 g of extracts, respectively. Part of the chloroform fraction (50 g) was subjected to a series of chromatographic techniques, such as silica gel column (mesh 200–300) and Sephadex LH-20 and PTLC, yielding compounds 1–9.

The compounds were identified using UV, IR, mass, and NMR spectrum, and all these data were in good agreement with the literature data [7–14]. All these compounds were isolated from *E. chrysantha* for the first time.

2,6-Dimethoxyquinone (1): C₈H₈O₄, yellow crystal, ESI-MS *m/z*: 169.32 [M+H]⁺; ¹H NMR (DMSO-d₆, 500 Hz) δ: 3.80 (6H, s, 2×OCH₃), 5.85 (2H, s, 3,5-H); ¹³C NMR (DMSO-d₆, 125 MHz) δ: 56.46 (2×OCH₃), 107.43 (C-3, C-5), 157.37 (C-2, 6), 176.64 (C-1), 186.82 (C-4) [7].

Apigenin (2): C₁₅H₁₀O₅, yellow crystal, ESI-MS *m/z*: 271.15 [M+H]⁺; ¹H NMR spectral data were identical to those reported in the literature [8].

Rutamontine (3): C₁₉H₁₂O₇, colorless powder, ESI-MS *m/z*: 351.06 [M-H]⁻; ¹H NMR (CDCl₃, 500 MHz, J/Hz) δ: 3.90 (3H, s, OCH₃), 6.31 (1H, d, J = 9.5, H-3'), 6.86 (1H, s, H-5), 6.90 (1H, s, H-8), 6.93 (1H, d, J = 2.0, H-8'), 6.99 (1H, dd, J = 8.5, 2.0, H-6'), 7.48 (1H, d, J = 8.5, H-5'), 7.49 (1H, s, H-4), 7.74 (1H, d, J = 9.5, H-4'); ¹³C NMR (CDCl₃, 125 MHz) δ: 56.0 (OCH₃), 103.2 (C-8'), 104.4 (C-5), 107.7 (C-8), 110.1 (C-4a), 113.8 (C-6'), 114.1 (C-3'), 114.7 (C-4'a), 129.3 (C-5'), 130.3 (C-4), 136.3 (C-3), 143.6 (C-4'), 145.5 (C-6), 147.7 (C-8a), 150.7 (C-7), 155.1 (C-8'a), 158.0 (C-7'), 159.7 (C-2'), 161.0 (C-2) [9].

Daphneticin (4): C₂₀H₁₈O₈, colorless crystal, ESI-MS *m/z*: 409.07 [M+Na]⁺; ¹H NMR (DMSO-d₆, 500 MHz, J/Hz) δ: 3.41 (1H, m, H-3'a), 3.67 (1H, m, H-3'b), 3.78 (6H, s, 2×OCH₃), 4.32 (1H, m, H-2'), 4.34 (1H, s, 3'-OH), 5.04 (1H, d, J = 8.0, H-1'), 6.33 (1H, d, J = 10.0, H-3), 6.76 (2H, s, H-2'', 6''), 6.98 (1H, d, J = 9.0, H-6), 7.21 (1H, d, J = 9.0, H-5), 8.00 (1H, d, J = 10.0, H-4), 8.53 (1H, s, 4''-OH); ¹³C NMR (DMSO-d₆, 125 MHz) δ: 56.3 (2×OCH₃), 60.5 (C-3'), 77.6 (C-1'), 79.8 (C-2'), 106.2 (C-2'', 6''), 112.9 (C-6), 113.5 (C-3), 113.6 (C-10), 119.7 (C-5), 126.3 (C-1''), 132.3 (C-4''), 138.2 (C-8), 144.1 (C-4), 147.8 (C-7), 149.4 (C-3'', 5''), 149.7 (C-9), 160.4 (C-2) [10].

[8,8'-Bi-2H-1-benzopyran]-2,2'-dione,7'-(α-D-glucopyranosyloxy)-7-hydroxy-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy] (5): C₃₃H₂₄O₁₄, white powder, ESI-MS *m/z*: 667.44 [M+Na]⁺; ¹H NMR (DMSO-d₆, 500 MHz, J/Hz) δ: 3.00–3.65 (5H, m, glu:

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H-2-6), 4.88 (1H, d, J = 5.0, glu: H-1), 6.34 (1H, d, J = 9.0, H-3), 6.37 (1H, d, J = 10.0, H-3''), 7.05 (1H, d, J = 9.0, H-6'), 7.13 (1H, dd, J = 9.0, 8.0, H-6), 7.19 (1H, d, J = 2.0, H-8), 7.34 (1H, d, J = 9.0, H-6''), 7.63 (1H, d, J = 9.0, H-5'), 7.71 (1H, d, J = 9.0, H-5), 7.79 (1H, d, J = 9.0, H-5''), 8.02 (1H, s, H-4'), 8.06 (1H, d, J = 9.0, H-4), 8.10 (1H, d, J = 10.0, H-4''); ¹³C NMR (DMSO-d₆, 125 MHz) δ: 60.6 (glu: C-6), 69.5 (glu: C-2), 73.3 (glu: C-3), 76.4 (glu: C-4), 77.1 (glu: C-5), 100.6 (glu: C-1), 104.3 (C-8), 106.7 (C-8'), 106.8 (C-8''), 109.8 (C-4''a), 111.0 (C-4'a), 112.3 (C-6''), 113.2 (C-3), 113.4 (C-6), 113.7 (C-6'), 114.0 (C-3''), 114.6 (C-4a), 129.2 (C-5'), 129.4 (C-5''), 130.0 (C-5), 131.2 (C-4), 135.3 (C-8'a), 144.1 (C-4'), 144.7 (C-4''), 151.1 (C-3'), 152.6 (C-8'a), 155.1 (C-8a), 156.9 (C-7'), 158.2 (C-7''), 158.5 (C-7), 159.5 (C-2), 160.0 (C-2'), 160.2 (C-2'') [11].

Triumbellin (6): C₃₃H₂₄O₁₃, white powder, ESI-MS *m/z*: 627.25 [M-H]⁻; ¹H NMR (DMSO-d₆, 500 MHz, J/Hz) δ: 1.15 (3H, d, J = 3.0, rha: CH₃), 3.03 (1H, m, rha: H-3), 3.20 (1H, m, rha: H-4), 3.29 (1H, m, rha: H-5), 3.51 (1H, m, rha: H-2), 5.50 (1H, d, J = 2.0, rha: H-1), 6.13 (1H, d, J = 10.0, H-3''), 6.30 (1H, d, J = 10.0, H-3'), 7.07 (1H, d, J = 9.0, H-6''), 7.09 (1H, d, J = 9.0, H-6'), 7.10 (1H, s, H-8'), 7.32 (1H, d, J = 9.0, H-6), 7.60 (1H, d, J = 9.0, H-5''), 7.70 (1H, d, J = 9.0, H-5'), 7.75 (1H, d, J = 9.0, H-5), 7.80 (1H, d, J = 10.0, H-4''), 7.85 (1H, s, H-4), 7.89 (1H, d, J = 10.0, H-4'), 10.53 (1H, s, OH); ¹³C NMR (DMSO-d₆, 125 MHz) δ: 17.8 (rha: C-6), 69.6 (rha: C-5), 70.0 (rha: C-2), 70.2 (rha: C-3), 71.4 (rha: C-4), 98.9 (rha: C-1), 104.2 (C-8'), 106.4 (C-8''), 110.4 (C-10), 110.5 (C-10''), 111.2 (C-6''), 112.0 (C-6), 112.9 (C-3''), 113.5 (C-8), 113.0 (C-6'), 113.9 (C-3'), 114.4 (C-10'), 129.0 (C-5'), 129.4 (C-5), 129.8 (C-4), 129.9 (C-5'), 137.0 (C-3), 143.9 (C-4'), 144.5 (C-4''), 150.9 (C-9), 153.6 (C-9''), 154.9 (C-9'), 156.4 (C-7'), 156.6 (C-7''), 159.4 (C-2''), 159.0 (C-2), 159.9 (C-2'), 160.0 (C-2) [12].

Skimming (7): C₁₅H₁₆O₈, white powder, ESI-MS *m/z*: 325.10 [M+H]⁺; ¹H NMR (DMSO-d₆, 500 MHz, H/Hz) δ: 3.16–3.70 (5H, m, glu: H-2-6), 5.11 (1H, d, J = 7.5, glu: H-1), 6.33 (1H, d, J = 9.5, H-3), 7.02 (1H, dd, J = 8.5, 2.5, H-6), 7.06 (1H, d, J = 2.5, H-8), 7.65 (1H, d, J = 8.5, H-5), 8.01 (1H, d, J = 9.5, H-4); ¹³C NMR (DMSO-d₆, 125 MHz) δ: 60.6 (glu: C-6), 69.9 (glu: C-4), 73.1 (glu: C-2), 76.5 (glu: C-3), 77.1 (glu: C-5), 100.0 (glu: C-1), 103.2 (C-8), 113.1 (C-10), 113.2 (C-3), 113.6 (C-6), 129.4 (C-5), 144.2 (C-4), 155.0 (C-9), 160.2 (C-7), 160.2 (C-2) [13].

Daphkoreanin (8): C₆H₁₂O₆, white powder, ESI-MS *m/z*: 393.15 [M+Na]⁺; ¹H NMR (DMSO-d₆, 500 MHz, J/Hz) δ: 3.00–3.70 (5H, m, glu: H-2-6), 3.81 (3H, s, OCH₃), 4.90 (1H, d, J = 7.5, glu: H-1), 6.11 (1H, d, J = 9.6, H-4), 6.45 (1H, s, H-6), 7.91 (1H, d, J = 9.6, H-4), 10.05 (1H, s, OH); ¹³C NMR (DMSO-d₆, 125 MHz) δ: 60.6 (glu: C-6), 69.2 (glu: C-2), 73.3 (glu: C-3), 76.2 (glu: C-4), 77.0 (glu: C-5), 100.2 (glu: C-1), 111.0 (C-4a), 112.1 (C-6), 113.4 (C-3), 135.8 (C-8), 143.5 (C-4), 144.5 (C-8a), 150.3 (C-7), 151.5 (C-5), 160.8 (C-2) [14].

Inositol (9): C₆H₁₂O₆, white crystal, ESI-MS *m/z*: 203.12 [M+Na]⁺; ¹H NMR (DMSO-d₆, 500 MHz, J/Hz) δ: 2.80–3.30 (5H, m), 3.78 (1H, t, J = 3.3) [15].

ACKNOWLEDGMENT

The work was supported by the program for Changjiang Scholars and Innovative Research Team in University (PCSIRT), NCET Foundation, NSFC (C03050201), National 863 Program (2006AA02Z338), and in part by the Scientific Foundation of Shanghai China (07DZ19728, 06DZ19717, 06DZ19005).

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