Chemical compounds from *Chenopodium album* Linn.

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Abstract. Bioactive components from *Chenopodium album* Linn. were isolated and identified in this research. Light petroleum, dichloromethane and n-BuOH were firstly applied to partition the 75% EtOH extract of *Chenopodium album* Linn. which were then subjected to normal-phase silica, ODS silica gel column chromatography and semi-preparative HPLC chromatography. By the employment of NMR method in this study, chemical structures of the compounds were elucidated. Three known compounds were isolated from *Chenopodium album* Linn., and identified as Isolariciresinol 4-O-β-D-glucopyranoside (1), (7'S, 8R, 8'R)-Isolariciresinol (2) and (7'S, 8R, 8'S)-Isolariciresinol (3) by comparison of their spectral data with references. This is the first time that isolation of the compounds mentioned above from *Chenopodium album* Linn. was achieved.

1. Introduction

Chenopodium album Linn. is a native plant widely distributed around the world, which contains more than 250 species [1]. According to the reports, C. Album can be represented by 21 species in Indian. Some species are grown as edible vegetables, providing people vitamins, fibre, essential fatty acids and minerals. A few other species were cultivated for the grains gained from the plant [2]. In addition, it was also reported that C. Album naturally grow as weed in the fields of barley, wheat, gram, mustard and some other crops [3-4]. Compared with the weed of low growing, the cultivated plants are leafy and tall. The entire young plant is not only a sorts of nutritious food, but also a herbal medicine [5-6]. C. Album has been traditionally employed as a diuretic, blood purifier, hepatoprotective, sedative, antiscorbutic laxative. Pharmacological research reveals its containing anthelmintic, contraceptive and sperm immobilizing properties [7].

2. Material and Methods

2.1. Materials and Chemicals

The Chenopodium album Linn., leaves were purchased from Hebei Qixin Traditional Chinese Medicine Pellets Co., Ltd., P.R. China, and identified by Dr. Chen Ning, Research Center on Life Sciences and Environmental Sciences, Harbin University of Commerce. Organic solvents (analytical grade or HPLC grade) for the experiment were purchased from Kermel Chemical Co., (Tianjin, China).

2.2. General Experimental Procedures

In this research, tetramethylsilane was used as internal standard on a Bruck AVANCE 500 FT-NMR spectrometer to record the nuclear magnetic resonance (NMR) spectra. Silica gel (200-300 mesh)

(Marine Chemical Factory, Qingdao, China) and Octa Decylsilyl Silicion (ODS) (YMC C18, 40-70 μm) were adopted to perform column chromatography. The ODS column (YMC ODS-A, 5 μm, 250×10 mm) was applied to perform High Performance Liquid Chromatography (HPLC) separation.

2.3. Extraction and Isolation

Dried leaves of Chenopodium album Linn., (20 kg) were powdered and extracted twice times by using of 75% EtOH under reflux. A condensed extract (2.2 kg) was obtained via evaporation of the solvent under reduced pressure, and then subjected to macroporous resin and eluted with a gradient of EtOH-H2O (0%, 20%, 50%, 95%, v/v). 11 fractions were obtained after 50% fraction went through normal phase silica gel column chromatography and was eluted with a gradient of CH2Cl2-MeOH (100:0 → 0:100, v/v). Fraction 3 (CH2Cl2-MeOH, 30:1, v/v) was further separated using ODS silica gel column chromatography eluted with MeOH in water. Subfraction 3.2 and 3.4 were purified by semi-preparative HPLC to give compound 1 (14.1 mg), 2 (16.7 mg) and 3 (18.6 mg).

3. Structural Identification

Isolariciresinol 4-O-β-D-glucopyranoside (1): yellow oil. 1H-NMR (600 MHz, DMSO-d6) δH: 6.94 (1H, brs, H-2), 6.63(1H, d, J = 1.6 Hz, H-2'), 6.53 (1H, d, J = 8.1 Hz, H-5'), 6.50(1H, brs, H-5), 6.49 (1H, dd, J = 8.1, 1.6 Hz, H-6'), 4.51 (1H, d, J = 7.8 Hz, H-1''), 3.75 (1H, d, J = 8.4 Hz, H-7'), 3.70 (3H, s, 3-OMe), 3.69 (3H, s, H-3'-OMe), 3.61 (1H, m, H-6''b), 3.56 (2H, m, H-9), 3.41 (2H, m, H-9'), 3.32 (1H, m, H-6''a), 3.26 (1H, m, H-5''), 3.25 (1H, m, H-3''), 3.23 (1H, m, H-2''), 3.11 (2H, m, H-4''), 2.75 (2H, d, J = 9.6 Hz, H-7), 1.83 (1H, m, H-8'), 1.65 (1H, t, J = 9.8 Hz, H-8); 13C-NMR (125 MHz, DMSO-d6) δC: 147.2 (C-3), 146.7 (C-3'), 144.7 (C-4'), 144.1 (C-4), 136.4 (C-1'), 132.6 (C-6), 130.1 (C-1), 121.4 (C-6'), 116.5 (C-5), 115.2 (C-5'), 113.3 (C-2'), 112.1 (C-2), 100.1 (C-1''), 76.9 (C-5''), 76.6 (C-3''), 73.0 (C-2''), 68.5 (C-4''), 63.5 (C-9), 59.9 (C-6''), 59.3 (C-9'), 55.7 (C-3'-OMe), 55.6 (C-3-OMe), 45.9 (C-7'), 45.3 (C-8'), 38.0 (C-8), 32.2 (C-7).

(7'S, 8R, 8'R)-Isolariciresinol (2): yellow oil. 1H-NMR (600 MHz, DMSO-d6) δH: 6.96 (1H, brs, H-2), 6.70 (1H, d, J = 8.1 Hz, H-5'), 6.65 (1H, d, J = 1.7 Hz, H-2'), 6.50 (1H, dd, J = 8.1, 1.7 Hz, H-6'), 6.11 (1H, brs, H-5), 3.74 (1H, d, J = 10.1 Hz, H-7'), 3.73 (6H, s, H-3-OMe, -3'-OMe), 3.59(2H, dd, J = 10.6, 4.0 Hz, H-9), 3.46 (2H, m, H-9'), 2.68 (2H, dd, J= 12.7, 7.4 Hz, H-7), 1.86 (1H, m, H-8'), 1.64 (1H, t, J = 10.1 Hz, H-8); 13C-NMR (125 MHz, DMSO-d6) δC: 147.5 (C-3), 145.6 (C-3'), 144.8 (C-4'), 144.2 (C-4), 137.2 (C-1'), 132.8 (C-1), 126.8 (C-6'), 122.5 (C-6), 116.4 (C-5), 115.4 (C-5'), 113.4 (C-2'), 111.9 (C-2), 63.8 (C-9), 60.0 (C-9'), 55.8 (C-3'-OMe), 55.6 (C-3-OMe), 46.1 (C-7', -8'), 38.3 (C-8), 32.4 (C-7).

(7'S, 8R, 8'S)-Isolariciresinol (3):yellow oil. 1H-NMR (600 MHz, DMSO-d6) δH: 6.69 (1H, d, J = 1.6 Hz, H-2'), 6.61 (1H, brs, H-2), 6.55 (1H, d, J = 8.1 Hz, H-5'), 6.21 (1H, brs, H-5), 6.20 (1H, dd, J = 8.1, 1.6 Hz, H-6'), 4.08 (1H, d, J = 3.9 Hz, H-7'), 3.69 (3H, s, H-3-OMe), 3.64 (3H, s, H-3'-OMe), 3.30 (2H, m, H-9'), 3.13 (2H, m, H-9), 2.78 (2H, dd, J = 16.9, 5.5 Hz, H-7), 1.98 (1H, m, H-8'), 1.79 (1H, t, J = 10.1 Hz, H-8); 13C-NMR (125 MHz, DMSO-d6) δC: 146.5 (C-3), 146.2 (C-3'), 144.5 (C-4), 144.2 (C-4'), 134.1 (C-1'), 131.5 (C-1), 126.8 (C-6'), 122.5 (C-6), 116.1 (C-5), 114.7 (C-5'), 114.6 (C-2'), 111.7 (C-2), 63.3 (C-9), 60.6 (C-9'), 55.6 (C-3'-OMe), 55.4 (C-3-OMe), 44.1 (C-7'), 43.1 (C-8'), 38.5 (C-8), 31.8 (C-7).

4. Conclusion

In this study, Isolariciresinol 4-O-β-D-glucopyranoside (1), (7'S, 8R, 8'R)-Isolariciresinol (2) and (7'S, 8R, 8'S)-Isolariciresinol (3) from Chenopodium album Linn. were successfully isolated and identified by comparison of their spectral data with the reported reference [8-10].

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