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A NEW PHENOLIC GLYCOSIDE FROM THE FRUITS OF *Capsicum annuum*

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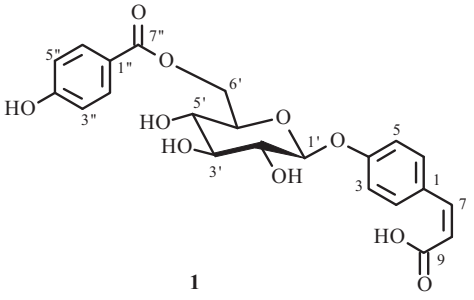
*A new compound, 4-*O*-(6′-*O*-p-hydroxybenzoyl-β-D-glucopyranosyl)-*cis*-p-coumaric acid, was isolated from the fruits of hot pepper (*Capsicum annuum *L.). The structure of the compound was established on the basis of NMR, FAB-MS, and IR spectroscopic data.*

Keywords: *Capsicum annuum* L., 4-*O*-(6′-*O*-*p*-hydroxybenzoyl-*β*-D-glucopyranosyl)-*cis*-*p*-coumaric acid.

Capsicum annuum L. (hot pepper), Solanaceae, is distributed mainly in tropical America, Korea, and India. Among the most commonlycultivated species, namely *C. frutescens*, *C. chinense*, *C. pubescens*, *C. baccatum*, and *C. annuum*, the latter is cultivated as a commercial crop in Korea and is therefore one of the most important vegetables for both farmers and consumers in Korea [1]. *C. annuum* has been reported to have several biological effects, including antioxidant [2], neurological [3], anti-inflammatory [4], and cancer chemoprevention effects [5]. More than 400 compounds have been isolated or analyzed from *Capsicum* species, including capsaicins [6], capsianosides [7], capsanthin [8], and phenolic compounds [9]. We therefore initiated this study to isolate and identify secondary metabolites of *C. annuum*. Dried and powdered hot peppers were extracted with 80% aqueous MeOH, and the concentrated extract was partitioned successively with EtOAc, *n*-BuOH, and H_2O. Repeated column chromatography of the EtOAc fraction using silica gel and octadecyl silica gel (ODS) led to the isolation of a new phenolic glycoside. Spectroscopic data, including FAB-MS, UV, IR, $[\alpha]_D^{22}$, ^1H and ^{13}C NMR, DEPT, and 2D NMR (COSY, HSQC, HMBC), revealed that the chemical structure of the new phenolic glycoside was 4-*O*-(6′-*O*-*p*-hydroxybenzoyl-*β*-D-glucopyranosyl)-*cis*-*p*-coumaric acid (**1**).



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EXPERIMENTAL

General Methods. The NMR spectra were measured on a Varian FT-NMR 400 MHz using deuterated methanol (CD_3OD) as a solvent and tetramethylsilane (TMS) as an internal standard. Two-dimensional (2D) NMR was performed with ^1H–^1H COSY, HSQC, and HMBC experiments. FAB-MS spectra were obtained using a JEOL JMS 700 mass spectrometer. Optical rotation was measured on a JASCO P-1010 digital polarimeter. The IR spectrum was obtained using a Perkin–Elmer Spectrum One FT-IR spectrometer. Thin-layer chromatography (TLC) was performed using silica gel 60 F254 and silica gel 60 RP-18 F254(ODS).

Plant Material. The fruits of *Capsicum annuum* L. were purchased at a market in EumSeong, Korea, in October 2006, and positively identified by Prof. Dae-Keun Kim, Woosuk University, Jeonju, Korea. A voucher specimen (KHU061027) was deposited at the Laboratory of Natural Products Chemistry, Kyung Hee University, Yongin, Korea.

Extraction and Isolation. The dried powder of the fruits of *C. annuum* (18 kg) was extracted with 80% aqueous MeOH (15 L × 3) at room temperature. The concentrated extracts were successively partitioned with water (2 L), EtOAc (2 L × 3), and *n*-BuOH (1.8 L × 3). The concentrated EtOAc fraction (132 g) was subjected to silica gel (SiO_2) column (9 × 16 cm) chromatography (c.c.) and eluted with *n*-hexane–EtOAc (10:1→9:1→7:1→5:1→3:1→1:1, v/v) and $CHCl_3$–MeOH (10:1→7:1, v/v). Each eluant was monitored by thin layer chromatography (TLC), and 25 fractions (CAE1 to CAE25) were obtained. Fraction CAE15 (10.7 g) was subjected to SiO_2 c.c. and was eluted with $CHCl_3$–MeOH–H_2O (30:3:1, v/v) to give 15 subfractions (CAE15-1 to CAE15-15). Subfraction CAE15-14 (1.64 g) was subjected to SiO_2 c.c. and eluted with $CHCl_3$–MeOH–H_2O (12:3:1, v/v) to give 18 subfractions (CAE15-14-1 to CAE15-14-18). Subfraction CAE15-14-14 (104 mg) was subjected to SiO_2 c.c. and eluted with $CHCl_3$–MeOH (5:2→1:1, v/v) to give seven subfractions (CAE15-14-14-1 to CAE15-14-14-7). Subfraction CAE15-14-14-2 (48 mg) was subjected to ODS c.c. and eluted with MeOH–H_2O (1:3, v/v) to ultimately produce a new compound [7.5 mg, R_f 0.5 on the TLC (RP-18 F254) in MeOH–H_2O (1:1)].

4-*O*-(6′-*O*-*p*-Hydroxybenzoyl-*β*-D-glucopyranosyl)-*cis*-*p*-coumaric Acid (1). Yellow oil (MeOH); $[\alpha]_D^{22}$ –5° (*c* 0.10, MeOH); UV (MeOH, λ_{max}, nm): 260; neg. FAB-MS *m*/*z*: 445 $[M - H]^-$; IR (CaF_2 window, ν, cm^{-1}): 3304, 2915, 1705, 1607; PMR (400 MHz, CD_3OD, δ, ppm, J/Hz): 7.89 (2H, dd, J = 6.4, 1.6, H-2″,6″), 7.46 (2H, br.d, J = 8.8, H-2,6), 7.00 (2H, br.d, J = 8.8, H-3,5), 6.89 (2H, dd, J = 6.4, 1.6, H-3″,5″), 6.24 (1H, d, J = 12.8, H-8), 5.95 (1H, d, J = 12.8, H-7), 4.90 (1H, d, J = 7.6, H-1′), 4.70 (1H, dd, J = 11.6, 1.6, H-6′a), 4.24 (1H, dd, J = 11.6, 8.0, H-6′b), 3.75–3.35 (4H, H-2′,3′,4′,5′); ^{13}C NMR (100 MHz, CD_3OD, δ): 176.8 (C-9), 167.8(C-7″), 163.8 (C-4″), 158.1 (C-4), 132.7 (C-2″,6″), 132.2 (C-1), 130.9 (C-2,6), 129.5 (C-8), 127.4 (C-7), 121.6 (C-1″), 117.1 (C-3,5), 116.4 (C-3″,5″), 102 (C-1′), 77.9 (C-3′), 75.6 (C-5′), 74.8 (C-2′), 72.1 (C-4′), 65.1 (C-6′).

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