A NEW C-GLUCOSIDE FROM *Commelina communis*

Qin Yang and Guan Ye*

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*A new C-glucoside, 3,4-epoxy-5-hydroxymethyl benzoate 2-C-β-glucoside (**1**), together with a known alkaloid, 1H-indole-3-carbaldehyde (**2**), were isolated from the whole plant of* Commelina communis *L. The structures of these compounds were determined by 1D, 2D NMR and MS techniques.*

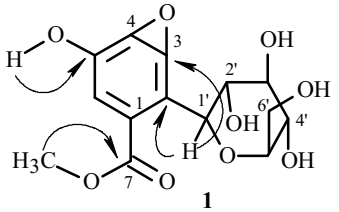
Key words: *Commelina communis* L., C-glucoside, indole alkaloid.

Plants of the genus *Commelina* (Commelinaceae) contain mainly flavonoids, alkaloids, terpenoids, lignans, and sterols [1–6]. Some of them are used in traditional Chinese medicine for the treatment of wind-heat type common cold, fever, sore throat, and dropsy [4, 5, 7].

Commelina communis L., a species of the *Commelina* genus, is widespread in the world, especially in the tropics and subtropics. It has long been used in folk medicine in China, and modern pharmaceutical investigations had revealed its anti-inflammatory, antiviral, and antihyperglycemia [1, 8–11] effects. In our continution of a phytochemical study on the subject, we herein reported two compounds isolated from the title plant.

The whole plant of *Commelina communis* L. was collected in Cixi County, Zhejiang Province of People's Republic of China, in July 2004 and authenticated by Prof. Jin-Gui Shen of Shanghai Institute of Medica Materia. Dried whole plant materials (21 kg) were extracted exhaustively with cold 95% EtOH. The solution was concentrated, suspended in 15% EtOH (4.5 L), and filtrated. The filtrate after concentration was partitioned sequentially with petroleum ether, EtOAc, and *n*-BuOH and afforded the PE, EA, and Bu extracts. The Bu extract was chromatographed on the silica gel (200~300 mesh) column using $CHCl_3$–MeOH as eluent. The fractions obtained were monitored by TLC, and those with similar TLC behavior were collected to give two fractions, A and B. When further purified by silica gel column ($CHCl_3$–MeOH as eluent) and repeated Sephadex LH-20 (eluated with MeOH) chromatography, fraction A afforded compound **1**, and B gave compound **2**.

Compound **1** was isolated as a white amorphous powder and was assigned the molecular formula $C_{14}H_{16}O_9$ by its HR-ESI-MS (329.0877 $[M+H]^+$, calcd 329.0873 $[M+H]^+$). It had a neat ^1H NMR spectrum with a singlet at δ 6.98 (1H, s), a doublet at δ 4.95 (1H, d, J = 10.8 Hz), a singlet integrated as 3H at δ 3.75 (3H, s), and a number of protons with chemical shifts between δ 3.42–4.09. The downfield signal in the ^1H NMR spectrum and the singlet at δ 7.08 (1H, s) implied a penta-substituted benzene structure. The doublet at δ 4.95 (10.8 Hz) together with proton signals between δ 3.42–4.09 suggested that compound **1** may contain a glycose. The ^{13}C NMR spectrum showed 14 signals: six were characteristic of aromatic carbons, six were glucosyl carbons, one was a methoxy carbon, and one was a carbonyl carbon as evidenced by a chemical shift of δ 165.8. The above information on compound **1** indicated a benzoate glucoside structure.



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Shanghai Institute of Materia Medica, Shanghai Institute of Biological Sciences, Chinese Academy of Sciences, 555 Zuchongzhi Road, Zhangjiang Hi-tech Park, Shanghai, P. R. China, 201203, fax: +86 21 50806623, e-mail: yg4847@yahoo.com.cn. Published in Khimiya Prirodnykh Soedinenii, No. 1, pp. 51-52, January-February, 2009. Original article submitted July 24, 2007.

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^{1}H NMR and ^{13}C NMR data of the aglycon of compound **1** resembled those of the methyl gallate [12]. Besides, its HMBC spectrum displayed an interaction peak between δ 3.75 (3H, s, OMe) and δ 165.9 (CO), which further confirmed the occurrence of the carbomethoxy in the molecule. Since **1** possessed seven degrees of unsaturation and the already elucidated moieties of the molecule contributed only six degrees of unsaturation, compound **1** should bear a new cyclic group. All substituents on the benzyl ring were thereby revealed, and they were a free hydroxyl, an epoxy, a carbomethoxy, and a glucosyl.

In terms of the glucose moiety of **1**, it was determined to be a C-glucoside as its anomeric proton had a larger coupling constant of 10.8 Hz, which was characteristic of a C-glucoside. The location of the glucose was further confirmed with the aid of 2D NMR spectra. In the HMBC spectrum, the anomeric proton δ 4.95 (10.8 Hz) interacted with δ 117.0 (C-2) and δ 149.0 (C-3). In the NOESY spectrum, correlation between the hydroxyl proton δ 8.43(s) and the aromatic proton δ 6.98 (1H, s) was observed. Both of the NOESY and HMBC correlations listed above demonstrated that the glucose should be located at C-2 of the aglycon, which was next to the epoxy and away from the free hydroxyl. Thus compound **1** was elucidated as 3,4-epoxy-5-hydroxymethyl benzoate 2-C-*β*-glucoside.

EXPERIMENTAL

3,4-Epoxy-5-hydroxymethyl benzoate 2-C-*β*-glucoside (1): $C_{14}H_{16}O_9$, white amorphous powder; IR (ν, cm^{-1}): 3590, 3028, 1713, 1589, 1409, 1065, 1054, 1018, 887; HR-ESI-MS: *m/z* 329.0877 $[M+H]^+$ (calcd 329.0873 $[M+H]^+$); ^{1}H NMR (300 MHz, DMSO-d_6, J/Hz): δ 8.43 (5-OH), 6.98 (1H, s, H-6), 4.95 (1H, d, J = 10.8, H-1′), 3.75 (3H, s, OMe), 3.12–4.05 (6H, m, sugar-H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 165.8 (CO), 151.2 (C-5), 149.0 (C-3), 141.4 (C-4), 119.1 (C-1), 117.0 (C-2), 110.2 (C-6), 81.8 (C-5′), 78.8 (C-3′), 74.4 (C-1′), 71.9 (C-2′), 70.5 (C-4′), 61.5 (C-6′), 60.2 (OMe).

1H-Indole-3-carbaldehyde (2): C_9H_7NO, white amorphous powder; ESI-MS: *m/z* 168.0 $[M+Na]^+$, 146.2 $[M+H]^+$; EI-MS: *m/z* 145 $[M]^+$; ^{1}H NMR (300 MHz, CD_3OD, J/Hz): δ 9.87 (1H, s, -CHO), 8.14 (1H, dd, J = 7.0, 2.0, H-4), 8.10 (1H, s, H-2), 7.48 (1H, dd, J = 7.3, 1.5, H-7), 7.19–7.29 (2H, m, H-5, H-6); ^{13}C NMR (100 MHz, CD_3OD): δ 188.0 (CHO), 140.2 (C-2), 139.4 (C-7′), 126.2 (C-3′), 125.5 (C-6), 124.1 (C-4), 122.9 (C-5), 120.6 (C-3), 113.6 (C-7) [13].

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