

## A New Antimicrobial Flavonol Glycoside from *Alchornea davidii*

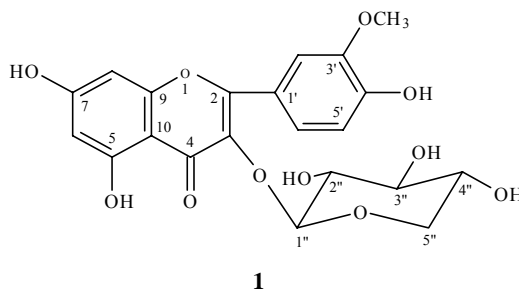
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**Abstract:** A new flavonol glycoside, isorhamnetin-3-*O*- $\beta$ -D-xyloside, was isolated from the extract of leaves and twigs of *Alchornea davidii* (Euphorbiaceae). Its structure was established on the basis of the spectral analysis and chemical degradation. Antimicrobial assay showed that it moderately inhibited the growth of test bacteria (*Staphylococcus aureus*, *Bacillus subtilis* and *Pseudomonas fluorescens*) and fungi (*Candida albicans*, *Aspergillus niger* and *Trichophyton rubrum*) with MICs at 50  $\mu$ g/mL.

**Keywords:** *Alchornea davidii*, Euphorbiaceae, flavonol glycoside, antimicrobial activity.

*Alchornea davidii* Franch. belonging to the family Euphorbiaceae is a shrub or small tree widely distributed in central and east China. Decoction of the leaves is being used for the treatment of inflammatory or infectious diseases. In this paper, we report the characterization of a new flavonol glycoside obtained from the title plant. Bioassay results showed that this constituent exhibited an antimicrobial activity.



Compound **1**, yellowish needles, was isolated from the EtOAc-soluble part of the MeOH extract of the leaves and twigs of the species. Its HRESI mass spectrum indicated the protonated molecular ion ( $[M + H]^+$ ) at  $m/z$  449.0985 corresponding to its molecular formula  $C_{21}H_{20}O_{11}$ . This formula was reinforced by its  $^{13}C$  NMR data containing in total 21 carbon signals. The UV spectrum of **1** showed absorption bands I and II at 351 and 255 nm, respectively, which were typical of a 3-*O*-flavonol and indicated the attachment of the sugar residue at C-3 position of the aglycone<sup>1</sup>. The  $^1H$

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and  $^{13}\text{C}$  NMR data of aglycone was similar to those of reported analogs such as isorhamnetin-3-*O*- $\beta$ -D-(6''-acetyl)-galactopyranoside<sup>2</sup> and isorhamnetin-3-*O*-glucoside<sup>3</sup>. The  $^1\text{H}$  NMR spectrum of glycoside **1** displayed an aromatic doublet ( $J = 2.4$  Hz) of H-2' at  $\delta$  7.67, a doublet ( $J = 8.1$  Hz) of H-5' at  $\delta$  6.90, and a double doublet ( $J = 2.4, 8.1$  Hz) of H-6' at  $\delta$  7.61, in addition to the characteristic 2H AX system ( $\delta$  6.42,  $J = 2.4$  Hz and  $\delta$  6.28,  $J = 2.4$  Hz) found in the A-ring of 5,7-dihydroxyflavonol. Furthermore, the one-proton doublet ( $J = 6.3$  Hz) at  $\delta$  5.01 was assigned to the anomeric proton of the  $\beta$ -D-xylose. This observation suggested that compound **1** was most likely isorhamnetin-3-*O*- $\beta$ -D-xyloside. This assumption was subsequently confirmed by its  $^{13}\text{C}$  NMR spectral data assigned unambiguously by comparing them with those of other isorhamnetin glycosides<sup>2,3</sup> (Table 1). As anticipated, treatment of **1** with 1 mol/L  $\text{H}_2\text{SO}_4$  liberated xylose identified by co-TLC with the authentic sample. In conclusion, the structure of compound **1** was isorhamnetin-3-*O*- $\beta$ -D-xyloside.

**Table 1**  $^1\text{H}$  (500 MHz) and  $^{13}\text{C}$  (125 MHz) NMR data for compound **1**\*

Proton	$\delta$ ppm	Carbon	$\delta$ ppm	Carbon	$\delta$ ppm
H-6	6.28 (1H, <i>d</i> , $J = 2.1$ Hz)	C-2	158.0	C-3'	149.6
H-8	6.42 (1H, <i>d</i> , $J = 2.1$ Hz)	C-3	135.0	C-4'	145.8
H-2'	7.67 (1H, <i>d</i> , $J = 2.4$ Hz)	C-4	178.9	C-5'	117.2
H-5'	6.90 (1H, <i>d</i> , $J = 8.1$ Hz)	C-5	162.6	C-6'	123.0
H-6'	7.61 (1H, <i>dd</i> , $J = 2.4$ and 8.1 Hz)	C-6	99.8	C-1''	104.0
H-1''	5.01 (1H, <i>d</i> , $J = 6.3$ Hz)	C-7	165.6	C-2''	73.8
H-2'', 3'', 4'', 5'' <i>a</i>	3.08-3.63 (4H, <i>m</i> )	C-8	94.7	C-3''	75.1
H-5'' <i>b</i>	3.83 (1H, <i>dd</i> , $J = 4.8$ and 11.2 Hz)	C-9	158.2	C-4''	70.9
OCH <sub>3</sub>	3.85 (3H, <i>s</i> )	C-10	105.4	C-5''	67.2
		C-1'	122.8	OMe	55.1
		C-2'	111.6		

\* In  $\text{CD}_3\text{OD}+\text{DMSO}-d_6$  (30:1)

The minimal inhibitory concentrations (MICs) of antimicrobial assay were measured by the serial 2-fold dilution method as reported<sup>4</sup>. As a result, compound **1** was inhibitory to the fungi (*C. albicans*, *A. niger* and *T. rubrum*) as well as Gram positive (*S. aureus* and *B. subtilis*) and negative bacteria (*P. fluorescens*) with MICs of 50  $\mu\text{g}/\text{mL}$ .

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