SUPPLEMENTARY MATERIAL

A new isoflavone from the roots of Ficus auriculata

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Abstract

A new isoflavone, 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1), together with three known

3'-formyl-5,4'-dihydroxy-7-methoxyisoflavone isoflavones,

(2),ficuisoflavone **(3)** and

alpinumisoflavone (4), were isolated from the roots of Ficus auriculata. Among them, 1 is a rare

isoflavone containing 16 carbon atoms on the carbon skeleton. The structure of 1 was elucidated by

extensive spectroscopic methods and the known compounds were identified by comparisons with data

reported in the literature. All compounds were evaluated for their antibacterial activities against five

terrestrial pathogenic bacteria in vitro. Compounds 1-4 showed significant antibacterial activities

against various terrestrial pathogenic bacteria with MIC values ranging from 1.30 to 39.93 µM.

Keywords:

Ficus auriculata; isoflavonoid;

5,7,4'-trihydroxy-3'-hydroxymethylisoflavone;

antibacterial activities.

1

Figure S1. Selected 2D NMR correlations for 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1).

Figure S2. ¹H-NMR spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_6 .

Figure S3. 13 C-NMR spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_{6} .

Figure S4. HSQC spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_6 .

Figure S5. HMBC spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_6 .

Figure S6. ${}^{1}\text{H-}{}^{1}\text{H COSY}$ spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_{6} .

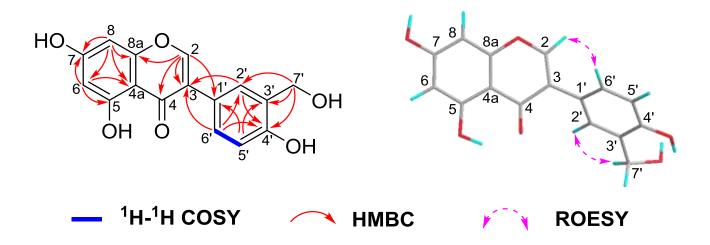


Figure S1. Selected 2D NMR correlations for 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1).

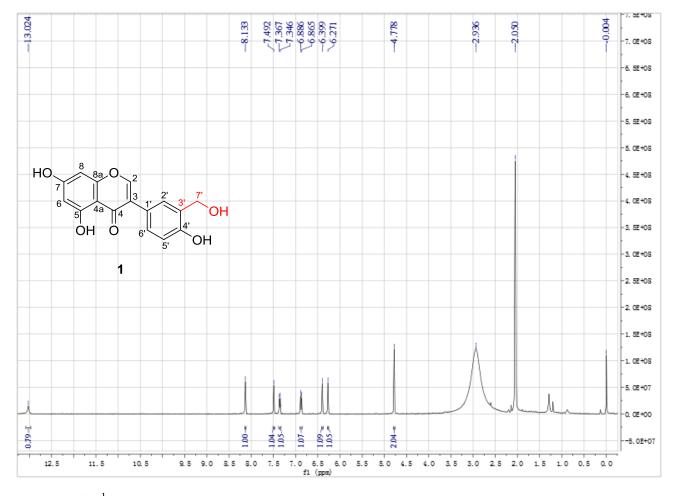


Figure S2. ¹H-NMR spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in DMSO- d_6 .

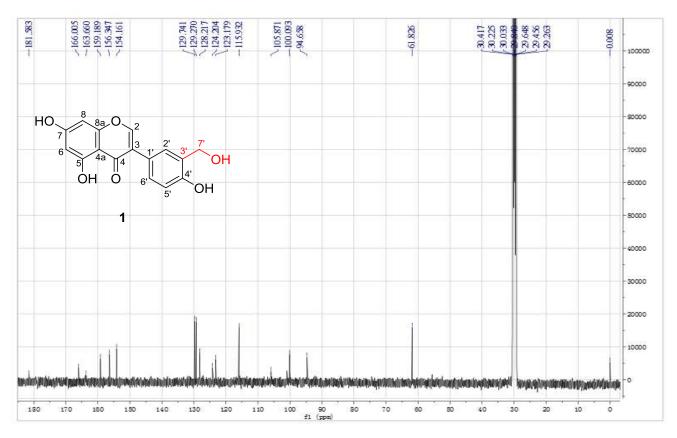


Figure S3. 13 C-NMR spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_6 .

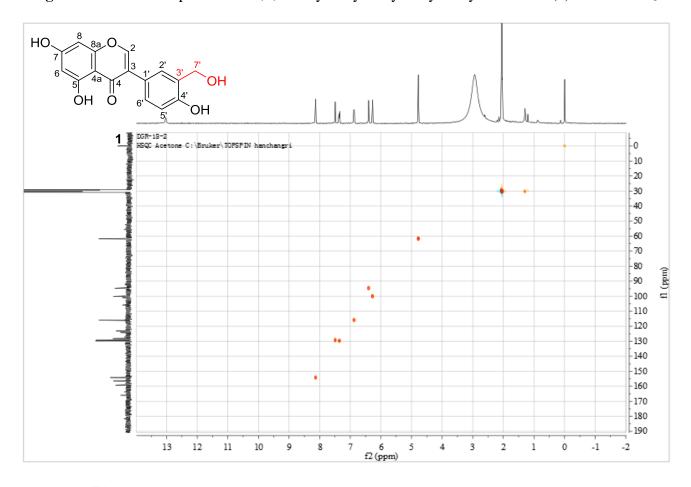


Figure S4. HSQC spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_6 .

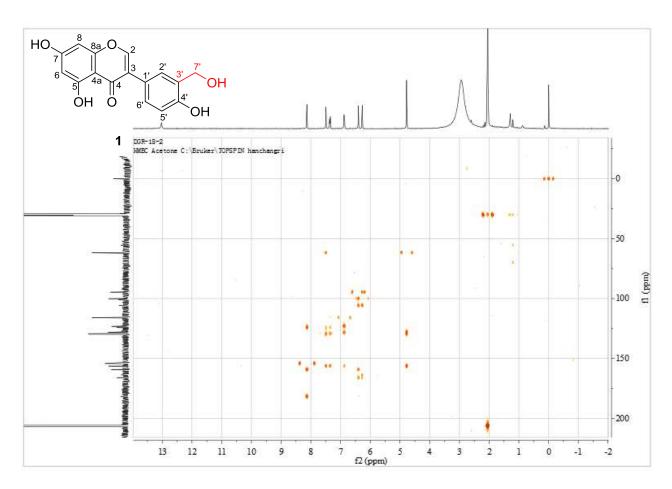


Figure S5. HMBC spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_6 .

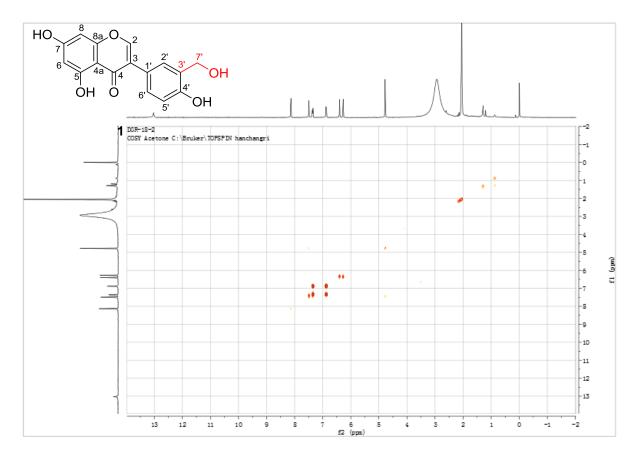


Figure S6. $^{1}\text{H-}^{1}\text{H COSY}$ spectrum of 5,7,4'-trihydroxy-3'-hydroxymethylisoflavone (1) in acetone- d_{6} .